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## Deoxyuridine -- Introduction

SYNONYM: 2'-Deoxyuridine; dU; 1-(2-Deoxy-beta-D-erythro-pentofuranosyl)-2,4(1H,3H)-pyrimidinedione; 1-(2-Deoxy-beta-D-ribofuranosyl)-2,4(1H,3H)-pyrimidinedione; 1-(2-Deoxy-beta-delta-erythro-pentofuranosyl)-2,4(1H,3H)-pyrimidinedione; 1-(2-Deoxy-beta-delta-ribofuranosyl)-2,4(1H,3H)-pyrimidinedione; 1-(2-Deoxy-D-erythro-pentofuranosyl)uracil; 1-(2-Deoxy-delta-erythro-pentofuranosyl)uracil; 2'-Deoxyuridine; 2'-Desoxyuridine; Deoxyribose uracil; Desoxyuridine; Uracil deoxyriboside; Uracil desoxyuridine; (beta 1-(2-Deoxyribopyranosyl))thymidine

HMDB: HMDB0000012; HMDB00012

CAS: 951-78-0

2'-Deoxyuridine is a naturally occurring nucleoside. It is similar in chemical structure to uridine, but without the 2'-hydroxyl group. It is considered to be an antimetabolite that is converted to deoxyuridine triphosphate during DNA synthesis. Laboratory suppression of deoxyuridine is used to diagnose megaloblastic anemia due to vitamin B12 and folate deficiencies.

This compound belongs to the class of organic compounds known as pyrimidine 2'-deoxyribonucleosides. These are compounds consisting of a pyrimidine linked to a ribose which lacks a hydroxyl group at position 2.

## Deoxyuridine -- Colorectal cancer

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### Deoxyuridine -- Ulcerative colitis

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## Adenine -- Introduction

SYNONYM: 6-Aminopurine; A; Ade; Adenin; 1,6-dihydro-6-Iminopurine; 1H-Purin-6-amine; 1H-Purine-6-amine; 3,6-dihydro-6-Iminopurine; 6-amino-1H-Purine; 6-amino-3H-Purine; 6-amino-7H-Purine; 6-amino-9H-Purine; 6-amino-Purine; 9H-Purin-6-amine; 9H-Purin-6-ylamin; 9H-Purin-6-ylamine; 9H-Purine-6-amine; Adeninimine; Vitamin b4; Vitamin b 4; 4, Vitamin b; b 4, Vitamin

HMDB: HMDB0000034; HMDB00034

CAS: 73-24-5

Adenine is a purine base. Adenine is found in both DNA and RNA. Adenine is a fundamental component of adenine nucleotides. Adenine forms adenosine, a nucleoside, when attached to ribose, and deoxyadenosine when attached to deoxyribose; it forms adenosine triphosphate (ATP), a nucleotide, when three phosphate groups are added to adenosine. Adenosine triphosphate is used in cellular metabolism as one of the basic methods of transferring chemical energy between chemical reactions. Purine inborn errors of metabolism (IEM) are serious hereditary disorders, which should be suspected in any case of neonatal fitting, failure to thrive, recurrent infections, neurological deficit, renal disease, self-mutilation and other manifestations. Investigation usually starts with uric acid (UA) determination in urine and plasma. (OMIM 300322, 229600, 603027, 232400, 232600, 232800, 201450, 220150, 232200, 162000, 164050, 278300). (PMID: 17052198, 17520339).

This compound belongs to the class of organic compounds known as 6-aminopurines. These are purines that carry an amino group at position 6. Purine is a bicyclic aromatic compound made up of a pyrimidine ring fused to an imidazole ring.

## Adenine -- Alzheimer's disease

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## Adenine -- Crohn's disease



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## Adenine -- Lewy body disease

Tsuruoka M, Hara J, Hirayama A, Sugimoto M, Soga T, Shankle WR, Tomita M: Capillary electrophoresis-mass spectrometry-based metabolome analysis of serum and saliva from neurodegenerative dementia patients. *Electrophoresis.* 2013 Oct;34(19):2865-72. doi: 10.1002/elps.201300019. Epub 2013 Sep 6. PMID: 23857558

## Ascorbic acid -- Introduction

SYNONYM: Acide ascorbique; acido Ascorbico; Acidum ascorbicum; Acidum ascorbinicum; Ascoltin; Ascorbicap; Ascorbinsaeure; e 300; e-300; e300; L-(+)-Ascorbic acid; L-Ascorbate; Vitamin C; Ascorbate; L-(+)-Ascorbate; L-Ascorbic acid; (+)-Ascorbate; (+)-Ascorbic acid; (+)-Sodium L-ascorbate; 3-keto-L-Gulofuranolactone; 3-oxo-L-Gulofuranolactone; Adenex; Allercorb; Antiscorbie vitamin; Antiscorbutic vitamin; arco-Cee; Ascor-b.i.d.; Ascorb; Ascorbajen; Ascorbicab; Ascorbicin; Ascorbin; Ascorbutina; Ascorin; Ascorteal; Ascorvit; C-Level; C-Long; C-Quin; C-

Span; C-Vimin; Cantan; Cantaxin; Catavin C; Ce lent; Ce-mi-lin; Ce-vi-sol; Cebicure; Cebid; Cebion; Cebione; Cecon; Cee-caps TD; Cee-vite; Cegiolan; Ceglion; Ceklin; Celaskon; Celin; Cell C; Cemagyl; Cemill; Cenetone; Cenolate; Cereon; Cergona; Cescorbat; Cetamid; Cetane; Cetane-caps TC; Cetane-caps TD; Cetebe; Cetemican; Cevalin; Cevatine; Cevex; Cevi-bid; Cevimin; Cevital; Cevitamate; Cevitamic acid; Cevitamin; Cevitan; Cevitex; Cewin; Chewcee; Ciamin; Cipca; Citriscorb; Citrovit; Colascor; Concemin; Davitamon C; Dora-C-500; Duoscorb; Ferrous ascorbate; gamma-Lactone L-threo-hex-2-enonate; gamma-Lactone L-threo-hex-2-enonic acid; HiCee; Hybrin; ido-C; Juvamine; Kangbingfeng; Kyselina askorbova; L(+)-Ascorbate; L(+)-Ascorbic acid; L-3-Ketothrohexuronic acid lactone; L-Lyxoascorbate; L-Lyxoascorbic acid; L-threo-Ascorbic acid; L-Xyloascorbate; L-Xyloascorbic acid; Laroscorbine; Lemascorb; Liqui-cee; Meri-c; Natrascorb; Natrascorb injectable; Planavit C; Proscorbin; Redoxon; Ribena; Ronotec 100; Rontex 100; Roscorbic; Rovimix C; Scorbacid; Scorbuc C; Scorbuc-C; Secorbate; Sodascorbate; Suncoat VC 40; Testascorbic; VASC; Vicelat; Vicin; Vicomin C; Viforce; Viscorin; Viscorin 100m; Vitace; Vitacee; Vitacimin; Vitacin; Vitamins; Vitascorbol; Xitix; L Ascorbic acid; Acid, ascorbic; Ascorbate, ferrous; Ascorbate, sodium; Magnesium ascorbate; Magnesium ascorbic acid; Magnesium di-L-ascorbate; Di-L-ascorbate, magnesium; Ascorbic acid, monosodium salt; Magnesium di L ascorbate; Magnorbin; Sodium ascorbate; Acid, L-ascorbic; Ascorbate, magnesium

HMDB: HMDB0000044; HMDB00044; HMDB0014273; HMDB0029945; HMDB14273; HMDB29945

CAS: 50-81-7

Ascorbic acid is found naturally in citrus fruits and many vegetables and is an essential nutrient in human diets. It is necessary to maintain connective tissue and bone. The biologically active form of ascorbic acid is vitamin C. Vitamin C is a water soluble vitamin. Primates (including humans) and a few other species in all divisions of the animal kingdom, notably the guinea pig, have lost the ability to synthesize ascorbic acid and must obtain it in their food. Vitamin C functions as a reducing agent and coenzyme in several metabolic pathways. Vitamin C is considered an antioxidant (PubChem). Ascorbic acid is an electron donor for enzymes involved in collagen hydroxylation, biosynthesis of carnitine and norepinephrine, tyrosine metabolism, and amidation of peptide hormones. Ascorbic acid (vitamin C) deficiency causes scurvy. The amount of vitamin C necessary to prevent scurvy may not be adequate to maintain optimal health. The ability of vitamin C to donate electrons also makes it a potent water-soluble antioxidant that readily scavenges free radicals such as molecular oxygen, superoxide, hydroxyl radical, and hypochlorous acid. In this setting, several mechanisms could account for a link between vitamin C and heart disease. One is the relation between LDL oxidation and vitamins C and E. Vitamin C in vitro can recycle vitamin E, which can donate electrons to prevent LDL oxidation in vitro. As the lipid-phase vitamin E is oxidized, it can be regenerated by aqueous vitamin C. Other possibilities are that vitamin C could decrease cholesterol by mechanisms not well characterized, or could improve vasodilatation and vascular reactivity, perhaps by decreasing the interactions of nitric oxide with oxidants (PMID: 10799361). Moreover, ascorbic acid is found to be associated with hyperoxalemia, which is an inborn error of metabolism.

This compound belongs to the class of organic compounds known as butenolides. These are dihydrofurans with a carbonyl group at the C2 carbon atom.

### Ascorbic acid -- Traumatic brain injury

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## Adenosine -- Introduction

SYNONYM: (2R,3R,4S,5R)-2-(6-Aminopurin-9-yl)-5-(hydroxymethyl)oxolane-3,4-diol; 6-amino-9-beta-D-Ribofuranosyl-9H-purine; 9-beta-D-Ribofuranosidoadenine; 9-beta-D-Ribofuranosyl-9H-purin-6-amine; Ade-rib; Adenine deoxyribonucleoside; Adenocard; Adenocor; Adenoscan; Adenosin; Adenyldeoxyriboside; Ado; beta-D-Adenosine; Deoxyadenosine; Desoxyadenosine; 6-amino-9-b-D-Ribofuranosyl-9H-purine; 6-amino-9- $\hat{1}^2$ -D-ribofuranosyl-9H-purine; 9-b-D-Ribofuranosidoadenine; 9- $\hat{1}^2$ -D-ribofuranosidoadenine; 9-b-D-Ribofuranosyl-9H-purin-6-amine; 9- $\hat{1}^2$ -D-ribofuranosyl-9H-purin-6-amine; b-D-Adenosine;  $\hat{1}^2$ -D-adenosine; 1-(6-amino-9H-Purin-9-yl)-1-deoxy-beta-D-ribofuranose; 1-(6-amino-9H-Purin-9-yl)-1-deoxy-beta-delta-ribofuranose; 6-amino-9beta-D-Ribofuranosyl-9H-purine; 6-amino-9beta-delta-Ribofuranosyl-9H-purine; 9-beta-D-Arabinofuranosyladenine; 9-beta-D-Ribofuranosyladenine; 9-beta-delta-Arabinofuranosyladenine; 9-beta-delta-Ribofuranosidoadenine; 9-beta-delta-Ribofuranosyl-9H-purin-6-amine; 9-beta-delta-Ribofuranosyladenine; 9beta-D-Ribofuranosyl-9H-purin-6-amine; 9beta-D-Ribofuranosyladenine; 9beta-delta-Ribofuranosyl-9H-purin-6-amine; 9beta-delta-Ribofuranosyladenine; Adenine nucleoside; Adenine riboside; Adenine-9beta-D-ribofuranoside; Adenine-9beta-delta-ribofuranoside; beta-Adenosine; beta-delta-Adenosine; Boniton; Myocol; Nucleocardyl; Sandesin

HMDB: HMDB0000050; HMDB0004401; HMDB0004402; HMDB0004421; HMDB00050; HMDB04401; HMDB04402; HMDB04421

CAS: 58-61-7

Adenosine is a nucleoside that is composed of adenine and D-ribose. Adenosine or adenosine derivatives play many important biological roles in addition to being components of DNA and RNA. For instance, adenosine plays an important role in energy transfer as adenosine triphosphate (ATP) and adenosine diphosphate (ADP). It also plays a role in signal transduction as cyclic adenosine monophosphate (cAMP). Adenosine itself is both a neurotransmitter and potent vasodilator. When administered intravenously adenosine causes transient heart block in the AV node. Due to the effects of adenosine on AV node-dependent supraventricular tachycardia, adenosine is considered a class V antiarrhythmic agent. Overdoses of adenosine intake (as a drug) can lead to several side effects including chest pain, feeling faint, shortness of breath, and tingling of the senses. Serious side effects include a worsening dysrhythmia and low blood pressure. When present in sufficiently high levels, adenosine can act as an immunotoxin and a metabotoxin. An immunotoxin disrupts, limits the function, or destroys immune cells. A metabotoxin is an endogenous metabolite that causes adverse health effects at chronically high levels. Chronically high levels of adenosine are associated with adenosine deaminase deficiency. Adenosine is a precursor to deoxyadenosine, which is a precursor to dATP. A buildup of dATP in cells inhibits ribonucleotide reductase and prevents DNA synthesis, so cells are unable to divide. Since developing T cells and B cells are some of the most mitotically active cells, they are unable to divide and propagate to respond to immune challenges. High levels of deoxyadenosine also lead to an increase in S-adenosylhomocysteine, which is toxic to immature lymphocytes.

This compound belongs to the class of organic compounds known as purine nucleosides. These are compounds comprising a purine base attached to a ribosyl or deoxyribosyl moiety.

## Adenosine -- Adenylosuccinate lyase deficiency

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## Adenosine -- Adenosine kinase deficiency

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## Adenosine -- Lewy body disease



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## L-Carnitine -- Introduction

SYNONYM: (-)-Carnitine; (-)-L-Carnitine; 3-Carboxy-2-hydroxy-N,N,N-trimethyl-1-propanaminium hydroxide, inner salt; Carnicor; Carnitene; Carnitine; Carnitor; Karnitin; Levocarnitine; Vitamin BT; (-)-(R)-3-Hydroxy-4-(trimethylammonio)butyrate; (R)-(3-Carboxy-2-hydroxypropyl)trimethylammonium hydroxide; (R)-Carnitine; (S)-Carnitine; 1-Carnitine; 3-Carboxy-2-hydroxy-N,N,N-trimethyl-1-propanaminium; 3-Hydroxy-4-trimethylammoniobutanoate; 3-Hydroxy-4-trimethylammoniobutanoic acid; Bicarnesine; Carniking; Carniking 50; Carnilean; Carnipass; Carnipass 20; D-Carnitine; delta-Carnitine; DL-Carnitine; gamma-Trimethyl-ammonium-beta-hydroxybutyrate; gamma-Trimethyl-beta-hydroxybutyrobetaine; gamma-Trimethyl-hydroxybutyrobetaine; L-(-)-Carnitine; L-gamma-Trimethyl-beta-hydroxybutyrobetaine; Levocarnitina; Levocarnitium; R-(-)-3-Hydroxy-4-trimethylaminobutyrate; L Carnitine

HMDB: HMDB0000062; HMDB0001467; HMDB00062; HMDB01467

CAS: 541-15-1

Carnitine is not an essential amino acid; it can be synthesized in the body. However, it is so important in providing energy to muscles (including the heart) that some researchers are now recommending carnitine supplements in the diet, particularly for people who do not consume much red meat (the main food source for carnitine). Carnitine has been described as a vitamin, an amino acid, or a metabimin (i.e. an essential metabolite). Like the B vitamins, carnitine contains nitrogen and is very soluble in water, and to some researchers carnitine is a vitamin (Liebovitz 1984). It was found that an animal (yellow mealworm) could not grow without carnitine in its diet. However, as it turned out, almost all other animals, including humans, do make their own carnitine; thus, it is no longer considered a vitamin. Nevertheless, in certain circumstances, such as deficiencies of methionine, lysine, or vitamin C or kidney dialysis, carnitine shortages develop. Under these conditions, carnitine must be absorbed from food, and for this reason, it is sometimes referred to as a "metabimin" or a conditionally essential metabolite. Like the other amino acids used or manufactured by the body, carnitine is an amine. But like choline, which is sometimes considered to be a B vitamin, carnitine is also an alcohol (specifically, a trimethylated carboxy-alcohol). Thus, carnitine is an unusual amino acid and has different functions than most other amino acids, which are usually employed by the body in the construction of protein. Carnitine is an essential factor in fatty acid metabolism in mammals. Its most important known metabolic function is to transport fat into the mitochondria of muscle cells, including those in the heart, for oxidation. This is how the heart gets most of its energy. In humans, about 25% of carnitine is synthesized in the liver, kidney, and brain from the amino acids lysine and methionine. Most of the carnitine in the body comes from dietary sources such as red meat and dairy products. Inborn errors of carnitine metabolism can lead to brain deterioration like that of Reye's syndrome, gradually worsening muscle weakness, Duchenne-like muscular dystrophy, and extreme muscle weakness with fat accumulation in muscles. Borum et al. (1979) describe carnitine as an essential nutrient for pre-term babies and individuals who are unable to eat a normal diet (e.g. non-ketotic hypoglycemics, kidney dialysis patients) (PMID: 115309). In conditions such as kwashiorkor, cirrhosis, and heart muscle disease (cardiomyopathy) as well as in inborn errors of metabolism such as type IV hyperlipidemia and propionic or organic aciduria (acid urine resulting from genetic or other anomalies), carnitine is essential to life and carnitine supplements are valuable. Carnitine therapy may also be useful in a wide variety of clinical conditions. Carnitine supplementation has improved some patients who have angina secondary to coronary artery disease. It may also be worth a trial for patients with any form of hyperlipidemia or muscle weakness. Carnitine supplements may also be useful in many forms of toxic or metabolic liver disease and in cases of heart muscle disease. Hearts undergoing severe arrhythmia quickly deplete their stores of carnitine. Athletes, particularly in Europe, have used carnitine supplements for improved endurance. Carnitine may improve muscle building by improving fat utilization and may even be useful in treating obesity. Carnitine joins a long list of nutrients which may be of value in treating pregnant women, hypothyroid individuals, and male infertility due to the low motility of sperm. Carnitine deficiency is noted in abnormal liver function, renal dialysis patients, and severe to moderate muscular weakness with associated anorexia (<http://www.dcnutrition.com>). Carnitine is a biomarker for the consumption of meat.

This compound belongs to the class of organic compounds known as carnitines. These are organic compounds containing the quaternary ammonium compound carnitine.

## L-Carnitine -- 3-Hydroxy-3-methylglutaryl-CoA lyase deficiency

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### L-Carnitine -- 2,4-dienoyl-CoA reductase deficiency

Houten SM, Denis S, Te Brinke H, Jongejan A, van Kampen AH, Bradley EJ, Baas F, Hennekam RC, Millington DS, Young SP, Frazier DM, Gucavas-Calikoglu M, Wanders RJ: Mitochondrial NADP(H) deficiency due to a mutation in NADK2 causes dienoyl-CoA reductase deficiency with hyperlysinemia. *Hum Mol Genet.* 2014 Sep 15;23(18):5009-16. doi: 10.1093/hmg/ddu218. Epub 2014 May 8. PMID: 24847004

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### L-Carnitine -- Carnitine transporter defect; primary systemic carnitine deficiency

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## L-Carnitine -- Methylmalonic aciduria mitochondrial encephalopathy Leigh-like

Carrozzo R, Dionisi-Vici C, Steuerwald U, Lucioli S, Deodato F, Di Giandomenico S, Bertini E, Franke B, Kluijtmans LA, Meschini MC, Rizzo C, Piemonte F, Rodenburg R, Santer R, Santorelli FM, van Rooij A, Vermunt-de Koning D, Morava E, Wevers RA: SUCLA2 mutations are associated with mild methylmalonic aciduria, Leigh-like encephalomyopathy, dystonia and deafness. *Brain*. 2007 Mar;130(Pt 3):862-74. Epub 2007 Feb 14. PMID: 17301081

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## L-Carnitine -- Early preeclampsia

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## Creatine -- Introduction

**SYNONYM:** ((amino(imino)Methyl)(methyl)amino)acetic acid; (alpha-methylguanido)Acetic acid; (N-methylcarbamimidamido)Acetic acid; alpha-methylguanidino Acetic acid; Creatin; Kreatin; Methylglycocyamine; N-(Aminoiminomethyl)-N-methylglycine; N-[e-amino(imino)METHYL]-N-methylglycine; N-Amidinosarcosine; N-Carbamimidoyl-N-methylglycine; N-Methyl-N-guanylglycine; ((amino(imino)Methyl)(methyl)amino)acetate; (a-methylguanido)Acetate; (a-methylguanido)Acetic acid; (alpha-methylguanido)Acetate; ( $\hat{L}$ -methylguanido)acetate; ( $\hat{L}$ -methylguanido)acetic acid; (N-methylcarbamimidamido)Acetate; a-methylguanidino Acetate; a-methylguanidino Acetic acid; alpha-methylguanidino Acetate;  $\hat{L}$ -methylguanidino acetate;  $\hat{L}$ -methylguanidino acetic acid; Cosmoair C 100; Creatine hydrate; Krebiozon; Methylguanidoacetate; Methylguanidoacetic acid; N-(Aminoiminomethyl)-N-methyl-glycine; Phosphagen; [[amino(imino)Methyl](methyl)amino]acetate; [[amino(imino)Methyl](methyl)amino]acetic acid

**HMDB:** HMDB0000064; HMDB00064

**CAS:** 57-00-1

Creatine is an amino acid that occurs in vertebrate tissues and in urine. In muscle tissue, creatine generally occurs as phosphocreatine. Creatine is excreted as creatinine in the urine. Creatine functions as part of the cell's energy shuttle. The high energy phosphate group of ATP is transferred to creatine to form phosphocreatine in the following reaction: Cr + ATP  $\leftrightarrow$  PCr + ADP. This reaction is reversibly catalyzed by creatine kinase. In the human body, creatine is synthesized mainly in the liver by the use of parts from three different amino acids: arginine, glycine, and methionine. 95% of it is later stored in the skeletal muscles and the rest is stored in the brain, heart, and testes.

This compound belongs to the class of organic compounds known as alpha amino acids and derivatives. These are amino acids in which the amino group is attached to the carbon atom immediately adjacent to the carboxylate group (alpha



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carbon), or a derivative thereof.

### Creatine -- Alzheimer's disease

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## Deoxyinosine -- Introduction

SYNONYM: 9-(2-Deoxy-beta-D-erythro-pentofuranosyl)-9H-purin-6-ol; 9-(2-Deoxy-b-D-erythro-pentofuranosyl)-9H-purin-6-ol; 9-(2-Deoxy- $\beta$ -D-erythro-pentofuranosyl)-9H-purin-6-ol; 2'-Deoxyinosine; 2-Deoxy-inosine; 9-(2-Deoxy-b-D-erythro-pentofuranosyl)-1,9-dihydro-6H-purin-6-one; 9-(2-Deoxy-b-D-erythro-pentofuranosyl)-hypoxanthine; 9-(2-Deoxy-beta-D-erythro-pentofuranosyl)-hypoxanthine; 9-(2-Deoxy-beta-delta-erythro-pentofuranosyl)-1,9-dihydro-6H-purin-6-one; 9-(2-Deoxy-beta-delta-erythro-pentofuranosyl)-hypoxanthine; D-Ino; delta-Ino; DIinosine; Deoxyribose-inosine

HMDB: HMDB0000071; HMDB00071

CAS: 890-38-0

Deoxyinosine is a nucleoside that is formed when hypoxanthine is attached to a deoxyribose ring (also known as a ribofuranose) via a beta-N9-glycosidic bond. Deoxyinosine is found in DNA while inosine is found in RNA. Inosine is a nucleic acid important for RNA editing. Adenosine deaminase (ADA) catalyzes the conversion of adenosine and deoxyadenosine to inosine and deoxyinosine, respectively. ADA-deficient individuals suffer from severe combined immunodeficiency (SCID) and are unable to produce significant numbers of mature T or B lymphocytes. This occurs as a



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consequence of the accumulation of ADA substrates or their metabolites. Inosine is also an intermediate in a chain of purine nucleotides reactions required for muscle movements. Moreover, deoxyinosine is found to be associated with purine nucleoside phosphorylase (PNP) deficiency, which is an inborn error of metabolism.

This compound belongs to the class of organic compounds known as purine 2'-deoxyribonucleosides. These are compounds consisting of a purine linked to a ribose which lacks a hydroxyl group at position 2.

## Deoxyinosine -- Colorectal cancer

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### **cis-Aconitic acid -- Introduction**

SYNONYM: (Z)-1-Propene-1,2,3-tricarboxylic acid; cis-1-Propene-1,2,3-tricarboxylic acid; (Z)-1-Propene-1,2,3-tricarboxylate; cis-Aconitate; cis-1-Propene-1,2,3-tricarboxylate; (1Z)-1-Propene-1,2,3-tricarboxylate; (1Z)-1-Propene-1,2,3-tricarboxylic acid; (Z)-Aconitate; (Z)-Aconitic acid; 1-cis-2,3-Propenetricarboxylate; 1-cis-2,3-Propenetricarboxylic acid; 1-Propene-1,2,3-tricarboxylate; 1-Propene-1,2,3-tricarboxylic acid; cis-Aconate; cis-Aconic acid; cis-Oxaloacetate; cis-Oxaloacetic acid; Acid, citridic; Acid, citridinic; Aconitic acid; Aconitic acid; Adonic acid; Achilleic acid; Acid, aconitic; Acid, equisetic; Citridinic acid; Acid, achilleic; Aconitate; Citridic acid; Pyrocitric acid; Acid, aconitic; Acid, adonic; Acid, carboxyglutaconic; Acid, pyrocitric; Carboxyglutaconic acid; Equisetic acid

HMDB: HMDB0000072; HMDB0000461; HMDB00072; HMDB00461

CAS: 585-84-2

cis-Aconitic acid is an intermediate in the tricarboxylic acid cycle produced by the dehydration of citric acid. The enzyme aconitase (aconitate hydratase; EC 4.2.1.3) catalyses the stereo-specific isomerization of citrate to isocitrate via cis-aconitate in the tricarboxylic acid cycle.

This compound belongs to the class of organic compounds known as tricarboxylic acids and derivatives. These are carboxylic acids containing exactly three carboxyl groups.

### **cis-Aconitic acid -- Alzheimer's disease**

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### **cis-Aconitic acid – Frontotemporal dementia**

Tsuruoka M, Hara J, Hirayama A, Sugimoto M, Soga T, Shankle WR, Tomita M: Capillary electrophoresis-mass spectrometry-based metabolome analysis of serum and saliva from neurodegenerative dementia patients. *Electrophoresis*. 2013 Oct;34(19):2865-72. doi: 10.1002/elps.201300019. Epub 2013 Sep 6. PMID: 23857558

### **cis-Aconitic acid – Lung Cancer**

Wishart DS, Knox C, Guo AC, Eisner R, Young N, Gautam B, Hau DD, Psychogios N, Dong E, Bouatra S, Mandal R, Sinelnikov I, Xia J, Jia L, Cruz JA, Lim E, Sobsey CA, Srivastava S, Huang P, Liu P, Fang L, Peng J, Fradette R, Cheng D, Tzur D, Clements M, Lewis A, De Souza A, Zuniga A, Dawe M, Xiong Y, Clive D, Greiner R, Nazirova A, Shaykhutdinov R, Li L, Vogel HJ, Forsythe I: HMDB: a knowledgebase for the human metabolome. *Nucleic Acids Res*. 2009 Jan;37(Database issue):D603-10. doi: 10.1093/nar/gkn810. Epub 2008 Oct 25. PMID: 18953024

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### **cis-Aconitic acid – Amish lethal microcephaly**

Kelley RI, Robinson D, Puffenberger EG, Strauss KA, Morton DH: Amish lethal microcephaly: a new metabolic disorder with severe congenital microcephaly and 2-ketoglutaric aciduria. *Am J Med Genet*. 2002 Nov 1;112(4):318-26. doi: 10.1002/ajmg.10529. PMID: 12376931

### **cis-Aconitic acid – Lewy body disease**

Tsuruoka M, Hara J, Hirayama A, Sugimoto M, Soga T, Shankle WR, Tomita M: Capillary electrophoresis-mass spectrometry-based metabolome analysis of serum and saliva from neurodegenerative dementia patients. *Electrophoresis*. 2013 Oct;34(19):2865-72. doi: 10.1002/elps.201300019. Epub 2013 Sep 6. PMID: 23857558

### **Dihydouracil -- Introduction**

SYNONYM: 2,4-Dioxotetrahydropyrimidine; 5,6-dihydro-2,4-Dihydroxypyrimidine; dihydro-2,4(1H,3H)-Pyrimidinedione; DIHYDROPYRIMIDINE-2,4(1H,3H)-dione; Dihydouracile; Hydouracil; 5,6-dihydro-2,4(1H,3H)-Pyrimidinedione; 5,6-Dihydouracil; dihydro-Pyrimidine-2,4-dione

HMDB: HMDB0000076; HMDB00076

CAS: 504-07-4

Dihydouracil is an intermediate breakdown product of uracil. Dihydropyrimidine dehydrogenase (DHP) catalyzes the



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reduction of uracil into 5,6-dihydrouracil then dihydrourimidinase hydrolyzes 5,6-dihydrouracil into N-carbamyl-beta-alanine. Finally, beta-ureidopropionase catalyzes the conversion of N-carbamyl-beta-alanine into beta-alanine. When present at abnormally high levels, dihydrouracil can be toxic although the mechanism of toxicity is not clear. In particular, patients with dihydrourimidinase deficiency exhibit highly increased concentrations of 5,6-dihydrouracil and 5,6-dihydrothymine, and moderately increased concentrations of uracil and thymine can be detected in urine. Dihydrourimidinase deficiency is a disorder that can cause neurological and gastrointestinal problems in some affected individuals (OMIM: 222748). The neurological abnormalities that occur most often in people with dihydrourimidinase deficiency are intellectual disability, seizures, weak muscle tone (hypotonia), an abnormally small head size (microcephaly), and autistic behaviours that affect communication and social interaction. Gastrointestinal problems that occur in dihydrourimidinase deficiency include backflow of acidic stomach contents into the esophagus (gastroesophageal reflux) and recurrent episodes of vomiting. The direct measurement of the activity of DHP in patients has been hampered by the fact that the enzyme is expressed almost exclusively in liver tissue.

This compound belongs to the class of organic compounds known as pyrimidones. These are compounds that contain a pyrimidine ring, which bears a ketone. Pyrimidine is a 6-membered ring consisting of four carbon atoms and two nitrogen centers at the 1- and 3- ring positions.

## Dihydrouracil -- Colorectal cancer

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### Dihydrouracil -- Dihydropyrimidine dehydrogenase deficiency

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### Dihydrouracil -- Liver disease

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### Dihydouracil -- Cerebral infarction

Hayashi K, Kidouchi K, Sumi S, Mizokami M, Orito E, Kumada K, Ueda R, Wada Y: Possible prediction of adverse reactions to pyrimidine chemotherapy from urinary pyrimidine levels and a case of asymptomatic adult dihydropyrimidinuria. Clin Cancer Res. 1996 Dec;2(12):1937-41. PMID: 9816152

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### Glycerophosphocholine -- Introduction

SYNONYM: 2-[[(2,3-Dihydroxypropoxy)hydroxyphosphinyl]oxy]-N,N,N-trimethyl-ethanaminium inner salt; a-Glycerophosphorylcholine; a-Glycerylphosphorylcholine; alpha-Glycerophosphorylcholine; alpha-Glycerylphosphorylcholine; Choline alfoscerate; Choline glycerophosphate; Glycerol 3-phosphocholine; Glycerol phosphorylcholine; Glycerol-3-phosphatidylcholine; Glycerophosphatidylcholine; Glycerophosphorylcholine; GPC; GPCho; Hydrogen glycerophosphate choline; L-alpha-Glycerophosphocholine; L-alpha-Glycerophosphorylcholine; L-alpha-Glycerylphosphorylcholine; L-Choline hydroxide 2,3-dihydroxypropyl hydrogen phosphate inner salt; sn-glycero-3-Phosphocholine; Alfoscerate, choline; Choline alfoscerate; Glycerophosphate, choline; Alfoscerate, choline; L alpha Glycerylphosphorylcholine; 3-Phosphocholine, glycerol; Glycerol 3 phosphocholine; Glycerylphosphorylcholine

HMDB: HMDB0000086; HMDB0000049; HMDB00049; HMDB00086

CAS: 28319-77-9

Glycerophosphorylcholine (GPC) is a choline derivative and one of the two major forms of choline storage (along with phosphocholine) in the cytosol. Glycerophosphorylcholine is also one of the four major organic osmolytes in renal medullary cells, changing their intracellular osmolyte concentration in parallel with extracellular tonicity during cellular osmoadaptation. As an osmolyte, Glycerophosphorylcholine counteracts the effects of urea on enzymes and other macromolecules. Kidneys (especially medullar cells), which are exposed under normal physiological conditions to widely fluctuating extracellular solute concentrations, respond to hypertonic stress by accumulating the organic osmolytes glycerophosphorylcholine (GPC), betaine, myo-inositol, sorbitol and free amino acids. Increased intracellular contents of these osmolytes are achieved by a combination of increased uptake (myo-inositol and betaine) and synthesis (sorbitol, GPC), decreased degradation (GPC) and reduced osmolyte release. GPC is formed in the breakdown of phosphatidylcholine (PtC). This pathway is active in many body tissues, including mammary tissue.

This compound belongs to the class of organic compounds known as glycerophosphocholines. These are lipids containing a glycerol moiety carrying a phosphocholine at the 3-position.

### Glycerophosphocholine -- Alzheimer's disease

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### Glycerophosphocholine -- Perillyl alcohol administration for cancer treatment

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### Glycerophosphocholine -- Kidney cancer

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## Glycerophosphocholine -- Periodontal disease

Sugimoto M, Wong DT, Hirayama A, Soga T, Tomita M: Capillary electrophoresis mass spectrometry-based saliva metabolomics identified oral, breast and pancreatic cancer-specific profiles. *Metabolomics*. 2010 Mar;6(1):78-95. Epub 2009 Sep 10. PMID: 20300169

## Glycerophosphocholine -- Multi-infarct dementia

Walter A, Korth U, Hilgert M, Hartmann J, Weichel O, Hilgert M, Fassbender K, Schmitt A, Klein J: Glycerophosphocholine is elevated in cerebrospinal fluid of Alzheimer patients. *Neurobiol Aging*. 2004 Nov-Dec;25(10):1299-303. PMID: 15465626

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Bar KJ, Franke S, Wenda B, Muller S, Kientsch-Engel R, Stein G, Sauer H: Pentosidine and N(epsilon)-(carboxymethyl)-lysine in Alzheimer's disease and vascular dementia. *Neurobiol Aging*. 2003 Mar-Apr;24(2):333-8. PMID: 12498967

Jia JP, Jia JM, Zhou WD, Xu M, Chu CB, Yan X, Sun YX: Differential acetylcholine and choline concentrations in the cerebrospinal fluid of patients with Alzheimer's disease and vascular dementia. *Chin Med J (Engl)*. 2004 Aug;117(8):1161-4. PMID: 15361288

## Glycerophosphocholine -- Pancreatic cancer

Loser C, Folsch UR, Paprotny C, Creutzfeldt W: Polyamine concentrations in pancreatic tissue, serum, and urine of patients with pancreatic cancer. *Pancreas*. 1990 Mar;5(2):119-27. PMID: 2315288

Sugimoto M, Wong DT, Hirayama A, Soga T, Tomita M: Capillary electrophoresis mass spectrometry-based saliva metabolomics identified oral, breast and pancreatic cancer-specific profiles. *Metabolomics*. 2010 Mar;6(1):78-95. Epub 2009 Sep 10. PMID: 20300169

Zhang L, Jin H, Guo X, Yang Z, Zhao L, Tang S, Mo P, Wu K, Nie Y, Pan Y, Fan D: Distinguishing pancreatic cancer from chronic pancreatitis and healthy individuals by <sup>1</sup>H nuclear magnetic resonance-based metabonomic profiles. *Clin Biochem*. 2012 Sep;45(13-14):1064-9. doi: 10.1016/j.clinbiochem.2012.05.012. Epub 2012 May 19. PMID: 22613268

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## Dimethylglycine -- Introduction

SYNONYM: (dimethylamino)Acetic acid; 2-(dimethylamino)Acetic acid; N,N-Dimethylaminoacetic acid; N-Methylsarcosine; (dimethylamino)Acetate; 2-(dimethylamino)Acetate; N,N-Dimethylaminoacetate; N,N-Dimethylglycine; N-Methylsarcosine N,N-dimethyl-glycine; Dimethylglycine, monopotassium salt; Dimethylglycine, sodium salt; Dimethylglycine, calcium salt; Dimethylglycine monohydrochloride

HMDB: HMDB0000092; HMDB00092

CAS: 1118-68-9

Dimethylglycine (DMG) is an amino acid derivative found in the cells of all plants and animals and can be obtained in the diet in small amounts from grains and meat. The human body produces DMG when metabolizing choline into Glycine. Dimethylglycine that is not metabolized in the liver is transported by the circulatory system to body tissue. Dimethylglycine was popular with Russian athletes and cosmonauts owing to its reputed ability to increase endurance and reduce fatigue. DMG is also a byproduct of homocysteine metabolism. Homocysteine and betaine are converted to methionine and N, N-dimethylglycine by betaine-homocysteine methyltransferase. Dimethylglycine in the urine is a biomarker for the consumption of



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legumes.

This compound belongs to the class of organic compounds known as alpha amino acids. These are amino acids in which the amino group is attached to the carbon atom immediately adjacent to the carboxylate group (alpha carbon).

### Dimethylglycine -- Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. *Tohoku J Exp Med.* 1995 May;176(1):61-8. PMID: 7482520

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### Cytidine monophosphate -- Introduction



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SYNONYM: Cytidine 5'-monophosphate; Cytidine-5'-monophosphate; Cytidylate; Cytidylic acid; pC; Cytidine 5'-monophosphoric acid; Cytidine monophosphoric acid; Cytidine-5'-monophosphoric acid; 5'-CMP; 5-Cytidylate; 5-Cytidylic acid; CMP; Cytidine 5'-monophosphorate; Cytidine 5'-phosphate; Cytidine 5'-phosphorate; Cytidine 5'-phosphoric acid; Cytidine mono(dihydrogen phosphate); Acid, cytidylic; Monophosphate, cytidine; 2' CMP; 2'-CMP; 3' CMP; Acids, cytidylic; Cytidylic acids; 3'-CMP

HMDB: HMDB0000095; HMDB00095

CAS: 63-37-6

Cytidine monophosphate, also known as 5'-cytidylic acid and abbreviated CMP, is a nucleotide. It is an ester of phosphoric acid with the nucleoside cytidine. CMP consists of the phosphate group, the pentose sugar ribose, and the nucleobase cytosine. Cytidine monophosphate (CMP) is derived from cytidine triphosphate (CTP) with subsequent loss of two phosphates. The synthesis of the pyrimidines CTP and UTP occurs in the cytoplasm and starts with the formation of carbamoyl phosphate from glutamine and CO<sub>2</sub>. Next, aspartate undergoes a condensation reaction with carbamoyl-phosphate to form orotic acid. In a subsequent cyclization reaction, the enzyme Aspartate carbamoyltransferase forms N-carbamoyl-aspartate which is converted into dihydroorotic acid by Dihydroorotase. The latter is converted to orotate by Dihydroorotate oxidase. Orotate is covalently linked with a phosphorylated ribosyl unit with Orotate phosphoribosyltransferase (aka "PRPP transferase") catalyzing reaction, yielding orotidine monophosphate (OMP). Orotidine-5-phosphate is decarboxylated by Orotidine-5'-phosphate decarboxylase to form uridine monophosphate (UMP). UMP is phosphorylated by two kinases to uridine triphosphate (UTP) via two sequential reactions with ATP. CTP is subsequently formed by amination of UTP by the catalytic activity of CTP synthetase. Cytidine monophosphate (CMP) and uridine monophosphate (UMP) have been prescribed for the treatment of neuromuscular afflictions in humans. Patients treated with CMP/UMP recover from altered neurological functions. Additionally, the administration of CMP/UMP appears to favour the entry of glucose in the muscle and CMP/UMP may be important in maintaining the level of hepatic glycogen constant during exercise. [PMID:18663991].

This compound belongs to the class of organic compounds known as pyrimidine ribonucleoside monophosphates. These are pyrimidine ribonucleotides with monophosphate group linked to the ribose moiety.

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## Cytidine monophosphate -- Frontotemporal dementia

Tsuruoka M, Hara J, Hirayama A, Sugimoto M, Soga T, Shankle WR, Tomita M: Capillary electrophoresis-mass spectrometry-based metabolome analysis of serum and saliva from neurodegenerative dementia patients. *Electrophoresis.*



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### Cytidine monophosphate -- Lewy body disease

Tsuruoka M, Hara J, Hirayama A, Sugimoto M, Soga T, Shankle WR, Tomita M: Capillary electrophoresis-mass spectrometry-based metabolome analysis of serum and saliva from neurodegenerative dementia patients. Electrophoresis. 2013 Oct;34(19):2865-72. doi: 10.1002/elps.201300019. Epub 2013 Sep 6. PMID: 23857558

### Choline -- Introduction

SYNONYM: Bilineurine; CHOLINE ion; N,N,N-Trimethylethanol-ammonium; N-Trimethylethanolamine; Trimethylethanolamine; (2-Hydroxyethyl)trimethyl ammonium; (2-Hydroxyethyl)trimethylammonium; (beta-Hydroxyethyl)trimethylammonium; 2-Hydroxy-N,N,N-trimethyl-ethanaminium; 2-Hydroxy-N,N,N-trimethylethanaminium; Biocolina; Biocoline; Choline cation; Cholinum; Hepacholine; Hormocline; Lipotril; N,N,N-Trimethylethanolammonium; Neocolina; Paresan; Choline O-sulfate; Citrate, choline; Fagine; Hydroxide, choline; Vidine; Bursine; Chloride, choline; Choline chloride; Choline citrate; Bitartrate, choline; Choline bitartrate; Choline hydroxide; Choline O sulfate; O-Sulfate, choline

HMDB: HMDB0000097; HMDB00097

CAS: 62-49-7

Choline is a basic constituent of lecithin that is found in many plants and animal organs. It is important as a precursor of acetylcholine, as a methyl donor in various metabolic processes, and in lipid metabolism. Choline is now considered to be an essential vitamin. While humans can synthesize small amounts (by converting phosphatidylethanolamine to phosphatidylcholine), it must be consumed in the diet to maintain health. Required levels are between 425 mg/day (female) and 550 mg/day (male). Milk, eggs, liver, and peanuts are especially rich in choline. Most choline is found in phospholipids, namely phosphatidylcholine or lecithin. Choline can be oxidized to form betaine, which is a methyl source for many reactions (i.e. conversion of homocysteine into methionine). Lack of sufficient amounts of choline in the diet can lead to a fatty liver condition and general liver damage. This arises from the lack of VLDL, which is necessary to transport fats away from the liver. Choline deficiency also leads to elevated serum levels of alanine amino transferase and is associated with increased incidence of liver cancer.

This compound belongs to the class of organic compounds known as cholines. These are organic compounds containing a N,N,N-trimethylethanolammonium cation.

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## Choline – Perillyl alcohol administration for cancer treatment



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## Choline -- Colorectal cancer

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## L-Cystathionine -- Introduction

SYNONYM: (R)-S-(2-amino-2-Carboxyethyl)-L-homocysteine; L-(+)-Cystathionine; S-(beta-amino-beta-Carboxyethyl)homocysteine; S-(b-amino-b-Carboxyethyl)homocysteine; S-(Î²-amino-Î²-carboxyethyl)homocysteine; Cystathionine; S-[(2R)-2-amino-2-Carboxyethyl]-L-homocysteine; [R-(R\*,s\*)]-2-amino-4-[(2-amino-2-carboxyethyl)thio]-butanoate; [R-(R\*,s\*)]-2-amino-4-[(2-amino-2-carboxyethyl)thio]-butanoic acid

HMDB: HMDB0000099; HMDB0003614; HMDB00099; HMDB03614

CAS: 56-88-2

Cystathionine is a dipeptide formed by serine and homocysteine. Cystathioninuria is a prominent manifestation of vitamin-B6 deficiency. The transsulfuration of methionine yields homocysteine, which combines with serine to form



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cystathione, the proximate precursor of cysteine through the enzymatic activity of cystathionase. In conditions in which cystathione gamma-synthase or cystathionase is deficient, for example, there is cystathioninuria. Although cystathione has not been detected in normal human serum or plasma by most conventional methods, gas chromatographic/mass spectrometric methodology detected a mean concentration of cystathione in normal human serum of 140 nM, with a range of 65 to 301 nM. Cystathione concentrations in CSF have been 10, 1, and 0.5 uM, and "not detected". Only traces (i.e., <1 uM) of cystathione are present in normal CSF.<sup>587</sup> Gamma-cystathionase deficiency (also known as Cystathioninuria), which is an autosomal recessive disorder (NIH: 2428), provided the first instance in which, in a human, the major biochemical abnormality due to a defined enzyme defect was clearly shown to be alleviated by administration of large doses of pyridoxine. The response in gamma-cystathionase-deficient patients is not attributable to correction of a preexisting deficiency of this vitamin (OMMBID, Chap. 88).

This compound belongs to the class of organic compounds known as l-cysteine-s-conjugates. These are compounds containing L-cysteine where the thio-group is conjugated.

## L-Cystathionine -- Alzheimer's disease

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## Glycerylphosphorylethanolamine -- Introduction

SYNONYM: 2-Aminoethyl ester 1-glycerophosphoric acid; a-Glycerophosphorylethanolamine; alpha-Glycerophosphorylethanolamine; Glycerol 3-phosphoethanolamine; Glycerol 3-phosphorylethanolamine; Glycerophosphoethanolamine; Glycerophosphorylethanolamine; Glyceryl-3-phosphorylethanolamine; GPEA

HMDB: HMDB0000114; HMDB00114

CAS: 1190-00-7

Glycerylphosphorylethanolamine is a membrane breakdown product resulting from the cleavage of the lipid group from glycerophosphoethanolamine fatty acids (i.e. phosphatidylethanolamine). It acts as a growth stimulant for hepatocytes.

This compound belongs to the class of organic compounds known as organic phosphoramides. These are organic compounds containing the phosphoric acid amide functional group.

## Glycolic acid -- Introduction

SYNONYM: 2-Hydroxyacetic acid; 2-Hydroxyethanoic acid; alpha-Hydroxyacetic acid; Glycollic acid; HOCH<sub>2</sub>COOH; Hydroxyacetic acid; Hydroxyethanoic acid; 2-Hydroxyacetate; Glycolate; 2-Hydroxyethanoate; a-Hydroxyacetate; a-Hydroxyacetic acid; alpha-Hydroxyacetate; l- hydroxyacetate; l-hydroxyacetic acid; Glycollate; Hydroxyacetate; Hydroxyethanoate; Glycocide; GlyPure; GlyPure 70; Sodium glycolate; Glycolic acid, 2-(14)C-labeled; Glycolic acid, 1-



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(14)C-labeled; Glycolic acid, potassium salt; Glycolic acid, monopotassium salt; Glycolic acid, calcium salt; Glycolic acid, monoammonium salt; Glycolic acid, monolithium salt; Glycolic acid, monosodium salt

HMDB: HMDB0000115; HMDB0003035; HMDB00115; HMDB03035

CAS: 79-14-1

Glycolic acid (or hydroxyacetic acid) is the smallest alpha-hydroxy acid (AHA). This colourless, odourless, and hygroscopic crystalline solid is highly soluble in water. Due to its excellent capability to penetrate skin, glycolic acid is often used in skin care products, most often as a chemical peel. It may reduce wrinkles, acne scarring, and hyperpigmentation and improve many other skin conditions, including actinic keratosis, hyperkeratosis, and seborrheic keratosis. Once applied, glycolic acid reacts with the upper layer of the epidermis, weakening the binding properties of the lipids that hold the dead skin cells together. This allows the outer skin to dissolve, revealing the underlying skin. It is thought that this is due to the reduction of calcium ion concentrations in the epidermis and the removal of calcium ions from cell adhesions, leading to desquamation. Glycolic acid is a known inhibitor of tyrosinase. This can suppress melanin formation and lead to a lightening of skin colour. Acute doses of glycolic acid on skin or eyes leads to local effects that are typical of a strong acid (e.g. dermal and eye irritation). Glycolate is a nephrotoxin if consumed orally. A nephrotoxin is a compound that causes damage to the kidney and kidney tissues. Glycolic acid's renal toxicity is due to its metabolism to oxalic acid. Glycolic and oxalic acid, along with excess lactic acid, are responsible for the anion gap metabolic acidosis. Oxalic acid readily precipitates with calcium to form insoluble calcium oxalate crystals. Renal tissue injury is caused by widespread deposition of oxalate crystals and the toxic effects of glycolic acid. Glycolic acid does exhibit some inhalation toxicity and can cause respiratory, thymus, and liver damage if present in very high levels over long periods of time.

This compound belongs to the class of organic compounds known as alpha hydroxy acids and derivatives. These are organic compounds containing a carboxylic acid substituted with a hydroxyl group on the adjacent carbon.

### Glycolic acid -- Biliary atresia

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### Glycine -- Introduction

SYNONYM: Aminoacetic acid; Aminoessigsaeure; Aminoethanoic acid; G; Gly; Glycin; Glycocol; Glykokoll; Glyzin; H2N-CH2-COOH; Hgly; Leimzucker; Aminoacetate; Aminoethanoate; 2-Aminoacetate; 2-Aminoacetic acid; Aciport; amino-



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Acetate; amino-Acetic acid; Glicoamin; Glycolixir; Glycosthene; Gyn-hydralin; Padil; Glycine carbonate (1:1), monosodium salt; Glycine carbonate (2:1), monopotassium salt; Glycine sulfate (3:1); Glycine, monoammonium salt; Glycine, monosodium salt; Glycine, sodium hydrogen carbonate; Monoammonium salt glycine; Calcium salt glycine; Glycine hydrochloride (2:1); Glycine phosphate (1:1); Glycine, monopotassium salt; Monopotassium salt glycine; Monosodium salt glycine; Glycine carbonate (2:1), monolithium salt; Glycine carbonate (2:1), monosodium salt; Glycine hydrochloride; Glycine, copper salt; Hydrochloride, glycine; Salt glycine, monoammonium; Acid, aminoacetic; Cobalt salt glycine; Copper salt glycine; Glycine phosphate; Glycine, calcium salt; Glycine, calcium salt (2:1); Glycine, cobalt salt; Phosphate, glycine; Salt glycine, monosodium

HMDB: HMDB0000123; HMDB00123

CAS: 56-40-6

Glycine is a simple, nonessential amino acid, although experimental animals show reduced growth on low-glycine diets. The average adult ingests 3 to 5 grams of glycine daily. Glycine is involved in the body's production of DNA, phospholipids and collagen, and in release of energy. Glycine levels are effectively measured in plasma in both normal patients and those with inborn errors of glycine metabolism (<http://www.dcnutrition.com/AminoAcids/>). Nonketotic hyperglycinemia (OMIM 606899) is an autosomal recessive condition caused by deficient enzyme activity of the glycine cleavage enzyme system (EC 2.1.1.10). The glycine cleavage enzyme system comprises four proteins: P-, T-, H- and L-proteins (EC 1.4.4.2, EC 2.1.2.10 and EC 1.8.1.4 for P-, T- and L-proteins). Mutations have been described in the GLDC (OMIM 238300), AMT (OMIM 238310), and GCSH (OMIM 238330) genes encoding the P-, T-, and H-proteins respectively. The glycine cleavage system catalyses the oxidative conversion of glycine into carbon dioxide and ammonia, with the remaining one-carbon unit transferred to folate as methylenetetrahydrofolate. It is the main catabolic pathway for glycine and it also contributes to one-carbon metabolism. Patients with a deficiency of this enzyme system have increased glycine in plasma, urine and cerebrospinal fluid (CSF) with an increased CSF: plasma glycine ratio (PMID 16151895). Glycine is also found to be associated with carbamoyl phosphate synthetase deficiency, iminoglycinuria, maple syrup urine disease, phenylketonuria, propionic acidemia, sarcosinemia, and tyrosinemia I, which are inborn errors of metabolism.

This compound belongs to the class of organic compounds known as alpha amino acids. These are amino acids in which the amino group is attached to the carbon atom immediately adjacent to the carboxylate group (alpha carbon).

### Glycine -- 3-Phosphoglycerate dehydrogenase deficiency

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## Glycine -- Early preeclampsia

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## Guanidoacetic acid -- Introduction

SYNONYM: Glycocyamine; Guanidinoacetate; N-(Carbamimidoyl)glycine; N-[amino(imino)Methyl]glycine; N-Amidinoglycine; Guanidoacetate; Guanidinoacetic acid; (Carboxymethyl)-guanidine; 2-[[amino(imino)Methyl]amino]acetate; 2-[[amino(imino)Methyl]amino]acetic acid; a-Guanidinoacetate; a-Guanidinoacetic acid; alpha-Guanidinoacetate; alpha-Guanidinoacetic acid; b-Guanidinoacetate; b-Guanidinoacetic acid; beta-Guanidinoacetate; beta-Guanidinoacetic acid; Betacyamine; Betasyamine; Guanidineacetate; Guanidineacetic acid; Guanidylacetate; Guanidylacetic acid; Guanyl glycine; N-amidino-Glycine; [(Aminoiminomethyl)amino]-acetate; [(Aminoiminomethyl)amino]-acetic acid; Glycocyamine, 2-(14)C-



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labeled; Glycocyamine, ion (1-); Glycocyamine monohydrochloride

HMDB: HMDB0000128; HMDB00128

CAS: 352-97-6

Guanidoacetic acid is a metabolite in the Urea cycle and metabolism of amino groups, and in the metabolic pathways of several amino acids. This includes glycine, serine, threonine, arginine and proline metabolism. Guanidinoacetic acid is also a precursor of creatine, an essential substrate for muscle energy metabolism.

This compound belongs to the class of organic compounds known as alpha amino acids and derivatives. These are amino acids in which the amino group is attached to the carbon atom immediately adjacent to the carboxylate group (alpha carbon), or a derivative thereof.

### Guanidoacetic acid -- Chronic renal failure

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## Guanosine -- Introduction

SYNONYM: 2(3H)-imino-9-beta-D-Ribofuranosyl-9H-purin-6(1H)-one; 2-amino-1,9-dihydro-9-beta-D-Ribofuranosyl-6H-purin-6-one; 2-amino-9-beta-D-Ribofuranosyl-1,9-dihydro-6H-purin-6-one; 9-beta-D-Ribofuranosyl-guanine; G; Guanine riboside; Guanine-9-beta-D-ribofuranoside; Guanosin; Guo; 2(3H)-imino-9-b-D-Ribofuranosyl-9H-purin-6(1H)-one; 2(3H)-imino-9- $\beta$ -D-ribofuranosyl-9H-purin-6(1H)-one; 2-amino-1,9-dihydro-9-b-D-Ribofuranosyl-6H-purin-6-one; 2-amino-1,9-dihydro-9- $\beta$ -D-ribofuranosyl-6H-purin-6-one; 2-amino-9- $\beta$ -D-ribofuranosyl-1,9-dihydro-6H-purin-6-one; 9-b-D-Ribofuranosyl-guanine; 9- $\beta$ -D-ribofuranosyl-guanine; Guanine-9-b-D-ribofuranoside; Guanine-9- $\beta$ -D-ribofuranoside; 2-amino-1,9-dihydro-9-beta-D-Ribofuranosyl-6H-purin-6-one; 2-amino-Inosine; 9-beta-D-Ribofuranosyl-guanine; b-D-Ribofuranoside guanine-9; beta-D-Ribofuranoside guanine-9; Ribonucleoside; Vernine

HMDB: HMDB0000133; HMDB00133

CAS: 118-00-3

Guanosine is a nucleoside comprising guanine attached to a ribose (ribofuranose) ring via a beta-N9-glycosidic bond. Guanosine can be phosphorylated to become GMP (guanosine monophosphate), cGMP (cyclic guanosine monophosphate), GDP (guanosine diphosphate), and GTP (guanosine triphosphate) (Wikipedia). This nucleoside exerts important neuroprotective and neuromodulator roles in the central nervous system, which may be related to inhibition of the glutamatergic neurotransmission activity. Guanosine is the specific extracellular guanine-based purines effector and its conversion occurs not only in the central nervous system but also peripherally (PMID: 16325434). Guanosine is found to be associated with purine nucleoside phosphorylase (PNP) deficiency, which is an inborn error of metabolism.



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This compound belongs to the class of organic compounds known as purine nucleosides. These are compounds comprising a purine base attached to a ribosyl or deoxyribosyl moiety.

## Guanosine -- Colorectal cancer

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### Fumaric acid -- Introduction



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SYNONYM: (2E)-2-Butenedioic acid; (e)-2-Butenedioic acid; e297; Fumarsaeure; trans-1,2-Ethylenedcarboxylic acid; trans-But-2-enedioic acid; trans-Butenedioic acid; (2E)-2-Butenedioate; Fumarate; (e)-2-Butenedioate; trans-1,2-Ethylenedcarboxylate; trans-But-2-enedioate; trans-Butenedioate; (2E)-But-2-enedioate; (2E)-But-2-enedioic acid; 2-(e)-Butenedioate; 2-(e)-Butenedioic acid; Allomaleate; Allomaleic acid; Boletate; Boletic acid; FC 33; Lichenate; Lichenic acid; Sodium fumarate; trans-2-Butenedioate; trans-2-Butenedioic acid; Furamag; Ammonium fumarate; Magnesium fumarate

HMDB: HMDB0000134; HMDB00134

CAS: 110-17-8

Fumaric acid is a dicarboxylic acid. It is a precursor to L-malate in the Krebs tricarboxylic acid (TCA) cycle. It is formed by the oxidation of succinic acid by succinate dehydrogenase. Fumarate is converted by the enzyme fumarase to malate. Fumaric acid has recently been identified as an oncometabolite or an endogenous, cancer causing metabolite. High levels of this organic acid can be found in tumors or biofluids surrounding tumors. Its oncogenic action appears to due to its ability to inhibit prolyl hydroxylase-containing enzymes. In many tumours, oxygen availability becomes limited (hypoxia) very quickly due to rapid cell proliferation and limited blood vessel growth. The major regulator of the response to hypoxia is the HIF transcription factor (HIF-alpha). Under normal oxygen levels, protein levels of HIF-alpha are very low due to constant degradation, mediated by a series of post-translational modification events catalyzed by the prolyl hydroxylase domain-containing enzymes PHD1, 2 and 3, (also known as EglN2, 1 and 3) that hydroxylate HIF-alpha and lead to its degradation. All three of the PHD enzymes are inhibited by fumarate. Fumaric acid is found to be associated with fumarase deficiency, which is an inborn error of metabolism.

This compound belongs to the class of organic compounds known as dicarboxylic acids and derivatives. These are organic compounds containing exactly two carboxylic acid groups.

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### Glycocholic acid -- Introduction



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SYNONYM: 3a,7a,12a-Trihydroxy-5b-cholan-24-oylglycine; 3a,7a,12a-Trihydroxy-5b-cholanic acid-24-glycine; 3a,7a,12a-Trihydroxy-N-(carboxymethyl)-5b-cholan-24-amide; Cholylglycine; Glycine cholate; Glycocholate; Glycoreductodehydrocholic acid; Glycylcholate; Glycylcholic acid; N-(Carboxymethyl)-3a,7a,12a-trihydroxy-5b-cholan-24-amide; N-Choloyl-glycine; N-Choloylglycine; Glycocholic acid, sodium salt; Glycocholate sodium

HMDB: HMDB0000138; HMDB00138

CAS: 475-31-0

Glycocholic acid is an acyl glycine and a bile acid-glycine conjugate. It is a secondary bile acid produced by the action of enzymes existing in the microbial flora of the colonic environment. In hepatocytes, both primary and secondary bile acids undergo amino acid conjugation at the C-24 carboxylic acid on the side chain, and almost all bile acids in the bile duct therefore exist in a glycine conjugated form (PMID:16949895). More specifically, glycocholic acid or cholylglycine, is a crystalline bile acid involved in the emulsification of fats. It occurs as a sodium salt in the bile of mammals. Its anion is called glycocholate. As the glycine conjugate of cholic acid, this compound acts as a detergent to solubilize fats for absorption and is itself absorbed (PubChem). Bile acids are steroid acids found predominantly in bile of mammals. The distinction between different bile acids is minute, depends only on presence or absence of hydroxyl groups on positions 3, 7, and 12. Bile acids are physiological detergents that facilitate excretion, absorption, and transport of fats and sterols in the intestine and liver. Bile acids are also steroid amphipathic molecules derived from the catabolism of cholesterol. They modulate bile flow and lipid secretion, are essential for the absorption of dietary fats and vitamins, and have been implicated in the regulation of all the key enzymes involved in cholesterol homeostasis. Bile acids recirculate through the liver, bile ducts, small intestine and portal vein to form an enterohepatic circuit. They exist as anions at physiological pH and, consequently, require a carrier for transport across the membranes of the enterohepatic tissues. The unique detergent properties of bile acids are essential for the digestion and intestinal absorption of hydrophobic nutrients. Bile acids have potent toxic properties (e.g., membrane disruption) and there are a plethora of mechanisms to limit their accumulation in blood and tissues (PMID: 11316487 , 16037564 , 12576301 , 11907135 ). Glycocholic acid is found to be associated with alpha-1-antitrypsin deficiency, which is an inborn error of metabolism.

This compound belongs to the class of organic compounds known as glycinated bile acids and derivatives. These are compounds with a structure characterized by the presence of a glycine linked to a bile acid skeleton.

### Glycocholic acid -- Alpha-1-antitrypsin deficiency

Matsui A, Psacharopoulos HT, Mowat AP, Portmann B, Murphy GM: Radioimmunoassay of serum glycocholic acid, standard laboratory tests of liver function and liver biopsy findings: comparative study of children with liver disease. J Clin Pathol. 1982 Sep;35(9):1011-7. PMID: 7119120

### Glycocholic acid -- Biliary atresia

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### Glycocholic acid -- Acute liver failure

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## Glycocholic acid -- Glycogen storage disease

Matsui A, Psacharopoulos HT, Mowat AP, Portmann B, Murphy GM: Radioimmunoassay of serum glycocholic acid, standard laboratory tests of liver function and liver biopsy findings: comparative study of children with liver disease. *J Clin Pathol.* 1982 Sep;35(9):1011-7. PMID: 7119120

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## Glycocholic acid -- Intrahepatic biliary hypoplasia

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## Glycocholic acid -- Portal vein obstruction

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## Glycocholic acid -- Neonatal hepatitis

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## Glycocholic acid -- Wilson's disease

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## Hypoxanthine -- Introduction

SYNONYM: 6(1H)-Purinone; 6-Oxopurine; 9H-Purin-6(1H)-one; Hyp; Purin-6(1H)-one; Purine-6-ol; 1,7-dihydro-6H-Purin-6-one; 1,7-dihydro-6H-Purine-6-one; 1H,7H-Hypoxanthine; 3H-Purin-6-ol; 4-Hydroxy-1H-purine; 6-Hydroxy-1H-purine; 6-Hydroxypurine; 7H-Purin-6-ol; 9H-Purin-6-ol; Hypoxanthine enol; Purin-6(3H)-one; Purin-6-ol; Sarcine; Sarkine

HMDB: HMDB0000157; HMDB00157

CAS: 68-94-0

Hypoxanthine is a naturally occurring purine derivative and a reaction intermediate in the metabolism of adenosine and in the formation of nucleic acids by the salvage pathway. Hypoxanthine is also a spontaneous deamination product of adenine. Lesch-Nyhan disease, an inborn error of metabolism, is caused by deficiency of the purine salvage enzyme hypoxanthine-guanine phosphoribosyltransferase (OMIM 308000). Hypoxanthine is also found to be associated with xanthinuria type 1, which is an inborn error of metabolism.

This compound belongs to the class of organic compounds known as hypoxanthines. These are compounds containing the purine derivative 1H-purin-6(9H)-one. Purine is a bicyclic aromatic compound made up of a pyrimidine ring fused to an imidazole ring.

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### Hypoxanthine -- Lewy body disease



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## L-Tyrosine -- Introduction

**SYNONYM:** (-)-alpha-amino-P-Hydroxyhydrocinnamic acid; (2S)-2-amino-3-(4-Hydroxyphenyl)propanoic acid; (S)-(-)-Tyrosine; (S)-2-amino-3-(P-Hydroxyphenyl)propionic acid; (S)-3-(P-Hydroxyphenyl)alanine; (S)-alpha-amino-4-Hydroxybenzenepropanoic acid; (S)-Tyrosine; 4-Hydroxy-L-phenylalanine; L-Tyrosin; Tyr; TYROSINE; Y; (-)-a-amino-P-Hydroxyhydrocinnamate; (-)-a-amino-P-Hydroxyhydrocinnamic acid; (-)-alpha-amino-P-Hydroxyhydrocinnamate; (-)-l±-amino-P-hydroxyhydrocinnamate; (-)-l±-amino-P-hydroxyhydrocinnamic acid; (2S)-2-amino-3-(4-Hydroxyphenyl)propanoate; (S)-2-amino-3-(P-Hydroxyphenyl)propionate; (S)-a-amino-4-Hydroxybenzenepropanoate; (S)-a-amino-4-Hydroxybenzenepropanoic acid; (S)-alpha-amino-4-Hydroxybenzenepropanoate; (S)-l±-amino-4-hydroxybenzenepropanoate; (S)-l±-amino-4-hydroxybenzenepropanoic acid; (S)-a-amino-4-Hydroxy-benzenepropanoate; (S)-a-amino-4-Hydroxy-benzenepropanoic acid; (S)-alpha-amino-4-Hydroxy-benzenepropanoate; (S)-alpha-amino-4-Hydroxy-benzenepropanoic acid; 2-amino-3-(4-Hydroxyphenyl)-2-amino-3-(4-hydroxyphenyl)-propanoate; 2-amino-3-(4-Hydroxyphenyl)-2-amino-3-(4-hydroxyphenyl)-propanoic acid; 3-(4-Hydroxyphenyl)-L-alanine; Benzenepropanoate; Benzenepropanoic acid; L-P-Tyrosine; P-Tyrosine; L Tyrosine; Tyrosine, L-isomer; Tyrosine, L isomer; Para tyrosine; Para-tyrosine

**HMDB:** HMDB0000158; HMDB0000647; HMDB00158; HMDB00647

**CAS:** 60-18-4

Tyrosine is an essential amino acid that readily passes the blood-brain barrier. Once in the brain, it is a precursor for the neurotransmitters dopamine, norepinephrine and epinephrine, better known as adrenalin. These neurotransmitters are an important part of the body's sympathetic nervous system, and their concentrations in the body and brain are directly dependent upon dietary tyrosine. Tyrosine is not found in large concentrations throughout the body, probably because it is rapidly metabolized. Folic acid, copper and vitamin C are cofactor nutrients of these reactions. Tyrosine is also the precursor for hormones, thyroid, catecholestrogens and the major human pigment, melanin. Tyrosine is an important amino acid in many proteins, peptides and even enkephalins, the body's natural pain reliever. Valine and other branched amino acids, and possibly tryptophan and phenylalanine may reduce tyrosine absorption. A number of genetic errors of tyrosine metabolism occur, such as hawkinsuria and tyrosinemia I. Most common is the increased amount of tyrosine in the blood of premature infants, which is marked by decreased motor activity, lethargy and poor feeding. Infection and intellectual deficits may occur. Vitamin C supplements reverse the disease. Some adults also develop elevated tyrosine in their blood. This indicates a need for more vitamin C. More tyrosine is needed under stress, and tyrosine supplements prevent the stress-induced depletion of norepinephrine and can cure biochemical depression. However, tyrosine may not be good for psychosis. Many antipsychotic medications apparently function by inhibiting tyrosine metabolism. L-dopa, which is directly used in Parkinson's, is made from tyrosine. Tyrosine, the nutrient, can be used as an adjunct in the treatment of Parkinson's. Peripheral metabolism of tyrosine necessitates large doses of tyrosine, however, compared to L-dopa (<http://www.denutrition.com>).

This compound belongs to the class of organic compounds known as tyrosine and derivatives. These are compounds containing tyrosine or a derivative thereof resulting from reaction of tyrosine at the amino group or the carboxy group, or from the replacement of any hydrogen of glycine by a heteroatom.

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## L-Tyrosine -- Late-onset preeclampsia

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## L-Tyrosine -- Lewy body disease

Tsuruoka M, Hara J, Hirayama A, Sugimoto M, Soga T, Shankle WR, Tomita M: Capillary electrophoresis-mass spectrometry-based metabolome analysis of serum and saliva from neurodegenerative dementia patients. Electrophoresis. 2013 Oct;34(19):2865-72. doi: 10.1002/elps.201300019. Epub 2013 Sep 6. PMID: 23857558

## L-Phenylalanine -- Introduction

SYNONYM: (S)-2-amino-3-Phenylpropionic acid; (S)-alpha-amino-beta-Phenylpropionic acid; 3-Phenyl-L-alanine; beta-Phenyl-L-alanine; F; Phe; PHENYLALANINE; (S)-2-amino-3-Phenylpropionate; (S)-a-amino-b-Phenylpropionate; (S)-a-amino-b-Phenylpropionic acid; (S)-alpha-amino-beta-Phenylpropionate; (S)-l-amino-l-phenylpropionate; (S)-l-amino-l-phenylpropionic acid; b-Phenyl-L-alanine; l-phenyl-L-alanine; (-)-beta-Phenylalanine; (L)-Phenylalanine; (S)-(-)-Phenylalanine; (S)-2-amino-3-Phenylpropanoate; (S)-2-amino-3-Phenylpropanoic acid; (S)-alpha-amino-Benzenepropanoate; (S)-alpha-amino-Benzenepropanoic acid; (S)-alpha-Aminobenzenepropanoate; (S)-alpha-Aminobenzenepropanoic acid; (S)-alpha-Aminohydrocinnamate; (S)-alpha-Aminohydrocinnamic acid; (S)-Phenylalanine; alpha-Aminohydrocinnamate; alpha-Aminohydrocinnamic acid; beta-Phenyl-alpha-alanine; beta-Phenylalanine; L-2-amino-3-Phenylpropionate; L-2-amino-3-Phenylpropionic acid; Phenyl-alanine; Phenylalanine; L-Isomer phenylalanine; Phenylalanine, L isomer; Phenylalanine, L-isomer; Endorphin

HMDB: HMDB0000159; HMDB0000612; HMDB00159; HMDB00612

CAS: 63-91-2

Phenylalanine is an essential amino acid and the precursor of the amino acid tyrosine. Like tyrosine, phenylalanine is also a precursor for catecholamines including tyramine, dopamine, epinephrine, and norepinephrine. Catecholamines are neurotransmitters that act as adrenalin-like substances. Interestingly, several psychotropic drugs (mescaline, morphine, codeine, and papaverine) also have phenylalanine as a constituent. Phenylalanine is highly concentrated in the human brain and plasma. Normal metabolism of phenylalanine requires biotin, iron, niacin, vitamin B6, copper, and vitamin C. An average adult ingests 5 g of phenylalanine per day and may optimally need up to 8 g daily. Phenylalanine is highly concentrated in a number of high protein foods, such as meat, cottage cheese, and wheat germ. An additional dietary source of phenylalanine is artificial sweeteners containing aspartame. As a general rule, aspartame should be avoided by phenylketonurics and pregnant women. When present in sufficiently high levels, phenylalanine can act as a neurotoxin and a metabotoxin. A neurotoxin is a compound that disrupts or attacks neural cells and neural tissue. A metabotoxin is an endogenously produced metabolite that causes adverse health effects at chronically high levels. Chronically high levels of phenylalanine are associated with at least five inborn errors of metabolism, including Hartnup disorder, hyperphenylalaninemia due to guanosine triphosphate cyclohydrolase deficiency, phenylketonuria (PKU), tyrosinemia type 2 (or Richner-Hanhart syndrome), and tyrosinemia type III (TYRO3). Phenylketonurics have elevated serum plasma levels of phenylalanine up to 400 times normal. High plasma concentrations of phenylalanine influence the blood-brain barrier transport of large neutral amino acids. The high plasma phenylalanine concentrations increase phenylalanine entry into the brain and restrict the entry of other large neutral amino acids (PMID: 19191004). Phenylalanine has been found to interfere with different cerebral enzyme systems. Untreated phenylketonuria (PKU) can lead to intellectual disability, seizures, behavioural problems, and mental disorders. It may also result in a musty smell and lighter skin. Classic PKU dramatically affects myelination and white matter tracts in untreated infants; this may be one major cause of neurological disorders associated with phenylketonuria. Mild phenylketonuria can act as an unsuspected cause of hyperactivity, learning problems, and other developmental problems in children. It has been recently suggested that PKU may resemble amyloid diseases, such as Alzheimer's disease and Parkinson's disease, due to the formation of toxic amyloid-like assemblies of phenylalanine (PMID: 22706200). Phenylalanine also has some potential benefits. Phenylalanine can act as an effective pain reliever. Its use in premenstrual syndrome and Parkinson's may enhance the effects of acupuncture and electric transcutaneous nerve stimulation (TENS). Phenylalanine and tyrosine, like L-DOPA, produce a catecholamine-like effect. Phenylalanine is better absorbed than tyrosine and may cause fewer headaches. Low phenylalanine diets have been prescribed for certain cancers with mixed results. For instance, some tumours use more phenylalanine than others (particularly melatonin-producing tumours called melanomas).

This compound belongs to the class of organic compounds known as phenylalanine and derivatives. These are



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compounds containing phenylalanine or a derivative thereof resulting from reaction of phenylalanine at the amino group or the carboxy group, or from the replacement of any hydrogen of glycine by a heteroatom.

### L-Phenylalanine -- 6-Pyruvyltetrahydropterin synthase deficiency

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## L-Phenylalanine -- Pregnancy

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## L-Phenylalanine -- Early preeclampsia

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## L-Phenylalanine -- Late-onset preeclampsia

Bahado-Singh RO, Akolekar R, Mandal R, Dong E, Xia J, Kruger M, Wishart DS, Nicolaides K: First-trimester metabolomic detection of late-onset preeclampsia. Am J Obstet Gynecol. 2013 Jan;208(1):58.e1-7. doi: 10.1016/j.ajog.2012.11.003. Epub 2012 Nov 13. PMID: 23159745



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## L-Phenylalanine -- Lewy body disease

Tsuruoka M, Hara J, Hirayama A, Sugimoto M, Soga T, Shankle WR, Tomita M: Capillary electrophoresis-mass spectrometry-based metabolome analysis of serum and saliva from neurodegenerative dementia patients. *Electrophoresis*. 2013 Oct;34(19):2865-72. doi: 10.1002/elps.201300019. Epub 2013 Sep 6. PMID: 23857558

## L-Proline -- Introduction

SYNONYM: (-)-(S)-Proline; (-)-2-Pyrrolidinecarboxylic acid; (-)-Proline; (2S)-Pyrrolidine-2-carboxylic acid; (S)-2-Carboxypyrrolidine; (S)-2-Pyrrolidinecarboxylic acid; (S)-Pyrrolidine-2-carboxylic acid; 2-Pyrrolidinecarboxylic acid; L-(-)-Proline; L-alpha-Pyrrolidinecarboxylic acid; L-Prolin; L-Pyrrolidine-2-carboxylic acid; P; Prolina; PROLINE; Prolinum; (-)-2-Pyrrolidinecarboxylate; (2S)-Pyrrolidine-2-carboxylate; (S)-2-Pyrrolidinecarboxylate; (S)-Pyrrolidine-2-carboxylate; 2-Pyrrolidinecarboxylate; L-a-Pyrrolidinecarboxylate; L-a-Pyrrolidinecarboxylic acid; L-alpha-Pyrrolidinecarboxylate; L- $\dot{\mu}$ -pyrrolidinecarboxylate; L- $\dot{\mu}$ -pyrrolidinecarboxylic acid; L-Pyrrolidine-2-carboxylate; (S)-(-)-Proline; (S)-(-)-Pyrrolidine-2-carboxylate; (S)-(-)-Pyrrolidine-2-carboxylic acid; (S)-2-Pyrrolidinecarboxylate; (S)-2-Pyrrolidinecarboxylic acid; (S)-Proline; L Proline

HMDB: HMDB0000162; HMDB00162

CAS: 147-85-3

L-proline is one of the twenty amino acids used in living organisms as the building blocks of proteins. Proline is sometimes called an imino acid, although the IUPAC definition of an imine requires a carbon-nitrogen double bond. Proline is a non-essential amino acid that is synthesized from glutamic acid. It is an essential component of collagen and is important for proper functioning of joints and tendons. Proline is derived from the amino acid L-glutamate in which glutamate-5-semialdehyde is first formed by glutamate 5-kinase and glutamate-5-semialdehyde dehydrogenase (which requires NADH or NADPH). This semialdehyde can then either spontaneously cyclize to form 1-pyrroline-5-carboxylic acid, which is reduced to proline by pyrroline-5-carboxylate reductase, or turned into ornithine by ornithine aminotransferase, followed by cyclization by ornithine cyclodeaminase to form proline. L-Proline has been found to act as a weak agonist of the glycine receptor and of both NMDA and non-NMDA ionotropic glutamate receptors. It has been proposed to be a potential endogenous excitotoxin/neurotoxin. Studies in rats have shown that when injected into the brain, proline non-selectively destroys pyramidal and granule cells (PMID: 3409032). Therefore, under certain conditions proline can act as a neurotoxin and a metabotoxin. A neurotoxin causes damage to nerve cells and nerve tissues. A metabotoxin is an endogenously produced metabolite that causes adverse health effects at chronically high levels. Chronically high levels of proline are associated with at least five inborn errors of metabolism, including hyperprolinemia type I, hyperprolinemia type II, iminoglycinuria, prolinemia type II, and pyruvate carboxylase deficiency. People with hyperprolinemia type I often do not show any symptoms even though they have proline levels in their blood between 3 and 10 times the normal level. Some individuals with hyperprolinemia type I exhibit seizures, intellectual disability, or other neurological or psychiatric problems. Hyperprolinemia type II results in proline levels in the blood between 10 and 15 times higher than normal, and high levels of a related compound called pyrroline-5-carboxylate. Hyperprolinemia type II has signs and symptoms that vary in severity, and is more likely than type I to involve seizures or intellectual disability.

This compound belongs to the class of organic compounds known as proline and derivatives. These are compounds containing proline or a derivative thereof resulting from reaction of proline at the amino group or the carboxy group, or from the replacement of any hydrogen of glycine by a heteroatom.

## L-Proline -- Alzheimer's disease

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## L-Proline -- Pregnancy

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## L-Proline -- Early preeclampsia

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## L-Proline -- Lewy body disease

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## L-Threonine -- Introduction

SYNONYM: (2S)-Threonine; (2S,3R)-(-)-Threonine; (2S,3R)-2-amino-3-Hydroxybutanoic acid; 2-amino-3-Hydroxybutyric acid; L-(-)-Threonine; L-2-amino-3-Hydroxybutyric acid; L-alpha-amino-beta-Hydroxybutyric acid; L-Threonine; T; Thr; THREONINE; (2S,3R)-2-amino-3-Hydroxybutanoate; 2-amino-3-Hydroxybutyrate; L-2-amino-3-Hydroxybutyrate; L-a-amino-b-Hydroxybutyrate; L-a-amino-b-Hydroxybutyric acid; L-alpha-amino-beta-Hydroxybutyrate; L- $\dot{\text{I}}$ -amino- $\dot{\text{I}}$ -hydroxybutyrate; L- $\dot{\text{I}}$ -amino- $\dot{\text{I}}$ -hydroxybutyric acid; (2S,3R)-2-amino-3-Hydroxybutyrate; (2S,3R)-2-amino-3-Hydroxybutyric acid; (R-(R\*,s\*))-2-amino-3-hydroxybutanoate; (R-(R\*,s\*))-2-amino-3-hydroxybutanoic acid; (S)-Threonine; 2-amino-3-Hydroxybutanoate; 2-amino-3-Hydroxybutanoic acid; Threonin; [R-(R\*,s\*)]-2-amino-3-hydroxybutanoate; [R-(R\*,s\*)]-2-amino-3-hydroxybutanoic acid; [R-(R\*,s\*)]-2-amino-3-hydroxybutanoate; [R-(R\*,s\*)]-2-amino-3-hydroxybutanoic acid; L Threonine



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HMDB: HMDB0000167; HMDB00167

CAS: 72-19-5

Threonine is an essential amino acid in humans. It is abundant in human plasma, particularly in newborns. Severe deficiency of threonine causes neurological dysfunction and lameness in experimental animals. Threonine is an immunostimulant which promotes the growth of thymus gland. It also can probably promote cell immune defense function. This amino acid has been useful in the treatment of genetic spasticity disorders and multiple sclerosis at a dose of 1 gram daily. It is highly concentrated in meat products, cottage cheese and wheat germ. (<http://www.dcnutrition.com/AminoAcids/>) The threonine content of most of the infant formulas currently on the market is approximately 20% higher than the threonine concentration in human milk. Due to this high threonine content the plasma threonine concentrations are up to twice as high in premature infants fed these formulas than in infants fed human milk. The whey proteins which are used for infant formulas are sweet whey proteins. Sweet whey results from cheese production. Threonine catabolism in mammals appears to be due primarily (70-80%) to the activity of threonine dehydrogenase (EC 1.1.1.103) that oxidizes threonine to 2-amino-3-oxobutyrate, which forms glycine and acetyl CoA, whereas threonine dehydratase (EC 4.2.1.16) that catabolizes threonine into 2-oxobutyrate and ammonia, is significantly less active. Increasing the threonine plasma concentrations leads to accumulation of threonine and glycine in the brain. Such accumulation affects the neurotransmitter balance which may have consequences for the brain development during early postnatal life. Thus, excessive threonine intake during infant feeding should be avoided. (PMID 9853925).

This compound belongs to the class of organic compounds known as L-alpha-amino acids. These are alpha amino acids which have the L-configuration of the alpha-carbon atom.

## L-Threonine -- Alzheimer's disease

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### L-Threonine -- Lewy body disease

Tsuruoka M, Hara J, Hirayama A, Sugimoto M, Soga T, Shankle WR, Tomita M: Capillary electrophoresis-mass spectrometry-based metabolome analysis of serum and saliva from neurodegenerative dementia patients. *Electrophoresis*. 2013 Oct;34(19):2865-72. doi: 10.1002/elps.201300019. Epub 2013 Sep 6. PMID: 23857558

### L-Asparagine -- Introduction

SYNONYM: (2S)-2,4-diamino-4-Oxobutanoic acid; (2S)-2-amino-3-Carbamoylpropanoic acid; (S)-2-amino-3-Carbamoylpropanoic acid; (S)-Asparagine; 2-Aminosuccinamic acid; alpha-Aminosuccinamic acid; Asn; ASPARAGINE; Aspartamic acid; L-2-Aminosuccinamic acid; L-Asparagin; L-Aspartic acid beta-amide; N; (2S)-2,4-diamino-4-Oxobutanoate; (2S)-2-amino-3-Carbamoylpropanoate; (S)-2-amino-3-Carbamoylpropanoate; 2-Aminosuccinamate; a-Aminosuccinamate; a-Aminosuccinamic acid; alpha-Aminosuccinamate;  $\hat{\text{I}}\pm$ -aminosuccinamate;  $\hat{\text{I}}\pm$ -aminosuccinamic acid; Aspartamate; L-2-Aminosuccinamate; L-Aspartate b-amide; L-Aspartate beta-amide; L-Aspartate  $\hat{\text{I}}^2$ -amide; L-Aspartic acid b-amide; L-Aspartic acid  $\hat{\text{I}}^2$ -amide; (-)-Asparagine; (S)-2,4-diamino-4-Oxobutanoate; (S)-2,4-diamino-4-Oxobutanoic acid; Agedoite; alpha Amminosuccinamate; alpha Amminosuccinamic acid; Altheine; Asparagine acid; Asparamide; Aspartic acid amide; Aspartic acid b-amide; Aspartic acid beta amide; b2,4-(S)-diamino-4-oxo-Utanoate; b2,4-(S)-diamino-4-oxo-Utanoic acid; Crystal VI; L-2,4-diamino-4-Oxobutanoate; L-2,4-diamino-4-Oxobutanoic acid; L-Aspartamine; L-b-Asparagine; L-beta-Asparagine

HMDB: HMDB0000168; HMDB00168

CAS: 70-47-3

Asparagine (Asn) is one of the 20 most common natural amino acids on Earth. It has carboxamide as the side chain's functional group. Asparagine is not an essential amino acid, which means that it can be synthesized from central metabolic pathway intermediates in humans and is not required in the diet. The precursor to asparagine is oxaloacetate. Oxaloacetate is converted to aspartate using a transaminase enzyme. The enzyme transfers the amino group from glutamate to oxaloacetate producing alpha-ketoglutarate and aspartate. The enzyme asparagine synthetase produces asparagine, AMP, glutamate, and pyrophosphate from aspartate, glutamine, and ATP. In the asparagine synthetase reaction, ATP is used to activate aspartate, forming beta-aspartyl-AMP. Glutamine donates an ammonium group which reacts with beta-aspartyl-AMP to form asparagine and free AMP. Since the asparagine side chain can make efficient hydrogen bond interactions with the peptide backbone, asparagines are often found near the beginning and end of alpha-helices, and in turn motifs in beta sheets. Its role can be thought as "capping" the hydrogen bond interactions which would otherwise need to be satisfied by the polypeptide backbone. Glutamines have an extra methylene group and have more conformational entropy, and thus are less useful in this regard. Asparagine also provides key sites for N-linked glycosylation, modification of the protein chain with the addition of carbohydrate chains. A reaction between asparagine and reducing sugars or reactive carbonyls produces acrylamide (acrylic amide) in food when heated to sufficient temperature (i.e. baking). These occur primarily in baked goods such as french fries, potato chips, and roasted coffee. Asparagine was first isolated in 1806 from asparagus juice, in which it is abundant--hence its name--becoming the first amino acid to be isolated. The smell observed in the urine of some individuals after their consumption of asparagus is attributed to a byproduct of the metabolic breakdown of asparagine, asparagine-amino-succinic-acid monoamide. However, some scientists disagree and implicate other substances in the smell, especially methanethiol (Wikipedia).

This compound belongs to the class of organic compounds known as asparagine and derivatives. These are compounds containing asparagine or a derivative thereof resulting from reaction of asparagine at the amino group or the carboxy group, or from the replacement of any hydrogen of glycine by a heteroatom.

### L-Asparagine -- Alzheimer's disease

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## L-Asparagine -- Pregnancy

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### L-Asparagine -- Lewy body disease

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### L-Isoleucine -- Introduction

SYNONYM: (2S,3S)-2-amino-3-Methylpentanoic acid; 2-amino-3-Methylvaleric acid; alpha-amino-beta-Methylvaleric acid; I; Ile; ISOLEUCINE; (2S,3S)-2-amino-3-Methylpentanoate; 2-amino-3-Methylvalerate; a-amino-b-Methylvalerate; a-amino-b-Methylvaleric acid; alpha-amino-beta-Methylvalerate;  $\hat{I}$ -amino- $\hat{I}$ -methylvalerate;  $\hat{I}$ -amino- $\hat{I}$ -methylvaleric acid; (2S,3S)-2-amino-3-Methyl-pentanoate; (2S,3S)-2-amino-3-Methyl-pentanoic acid; (2S,3S)-a-amino-b-Methyl-N-valerate; (2S,3S)-a-amino-b-Methyl-N-valeric acid; (2S,3S)-a-amino-b-Methylvalerate; (2S,3S)-a-amino-b-Methylvaleric acid; (2S,3S)-Alph-amino-beta-methylvalerate; (2S,3S)-Alph-amino-beta-methylvaleric acid; (2S,3S)-alpha-amino-beta-Methyl-N-valerate; (2S,3S)-alpha-amino-beta-Methyl-N-valeric acid; (2S,3S)-alpha-amino-beta-Methylvalerate; (2S,3S)-alpha-amino-beta-Methylvaleric acid; (2S,3S)-alpha-amino-beta-Methyl-N-valerate; (2S,3S)-alpha-amino-beta-Methylvaleric acid; (S)-Isoleucine; (S,S)-Isoleucine; 2-amino-3-Methylpentanoate; 2-amino-3-Methylpentanoic acid; 2S,3S-Isoleucine; erythro-L-Isoleucine; iso-Leucine; L-(+)-Isoleucine; L-Ile; [S-(R\*,r\*)]-2-amino-3-methylpentanoate; [S-(R\*,r\*)]-2-amino-3-methylpentanoic acid; Isoleucine, L-isomer; Alloisoleucine; Isoleucine, L isomer; L-Isomer isoleucine

HMDB: HMDB0000172; HMDB00172

CAS: 73-32-5

Branched chain amino acids (BCAA) are essential amino acids whose carbon structure is marked by a branch point.



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These three amino acids are critical to human life and are particularly involved in stress, energy and muscle metabolism. BCAA supplementation as therapy, both oral and intravenous, in human health and disease holds great promise. "BCAA" denotes valine, isoleucine and leucine which are branched chain essential amino acids. Despite their structural similarities, the branched amino acids have different metabolic routes, with valine going solely to carbohydrates, leucine solely to fats and isoleucine to both. The different metabolism accounts for different requirements for these essential amino acids in humans: 12 mg/kg, 14 mg/kg and 16 mg/kg of valine, leucine and isoleucine respectively. Furthermore, these amino acids have different deficiency symptoms. Valine deficiency is marked by neurological defects in the brain, while isoleucine deficiency is marked by muscle tremors. BCAA are decreased in patients with liver disease, such as hepatitis, hepatic coma, cirrhosis, extrahepatic biliary atresia or portacaval shunt; aromatic amino acids (AAA)-tyrosine, tryptophan and phenylalanine, as well as methionine-are increased in these conditions. Valine, in particular, has been established as a useful supplemental therapy to the ailing liver. All the BCAA probably compete with AAA for absorption into the brain. Supplemental BCAA with vitamin B6 and zinc help normalize the BCAA:AAA ratio. The BCAA are not without side effects. Leucine alone, for example, exacerbates pellagra and can cause psychosis in pellagra patients by increasing excretion of niacin in the urine. Leucine may lower brain serotonin and dopamine. A dose of 3 g of isoleucine added to the niacin regime has cleared leucine-aggravated psychosis in schizophrenic patients. Isoleucine may have potential as an antipsychotic treatment. Leucine is more highly concentrated in foods than other amino acids. A cup of milk contains 800 mg of leucine and only 500 mg of isoleucine and valine. A cup of wheat germ has about 1.6 g of leucine and 1 g of isoleucine and valine. The ratio evens out in eggs and cheese. One egg and an ounce of most cheeses each contain about 400 mg of leucine and 400 mg of valine and isoleucine. The ratio of leucine to other BCAA is greatest in pork, where leucine is 7 to 8 g and the other BCAA together are only 3 to 4 g (<http://www.dcnutrition.com>). Moreover, L-isoleucine is found to be associated with maple syrup urine disease, which is an inborn error of metabolism.

This compound belongs to the class of organic compounds known as isoleucine and derivatives. These are compounds containing isoleucine or a derivative thereof resulting from reaction of isoleucine at the amino group or the carboxy group, or from the replacement of any hydrogen of glycine by a heteroatom.

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### L-Lysine -- Introduction

SYNONYM: (S)-2,6-Diaminohexanoic acid; (S)-alpha,epsilon-Diaminocaproic acid; (S)-Lysine; 6-ammonio-L-Norleucine; K; L-2,6-Diaminocaproic acid; L-Lysin; Lys; Lysina; Lysine; Lysine acid; Lysinum; (S)-2,6-Diaminohexanoate; (S)-a,epsilon-Diaminocaproate; (S)-a,epsilon-Diaminocaproic acid; (S)-alpha,epsilon-Diaminocaproate; (S)-l±,epsilon-Diaminocaproate; (S)-l±,epsilon-Diaminocaproic acid; L-2,6-Diaminocaproate; (+)-S-Lysine; (S)-2,6-diamino-Hexanoate; (S)-2,6-diamino-Hexanoic acid; (S)-a,e-Diaminocaproate; (S)-a,e-Diaminocaproic acid; 2,6-Diaminohexanoate; 2,6-Diaminohexanoic acid; 6-amino-Aminutrin; 6-amino-L-Norleucine; a-Lysine; alpha-Lysine; Aminutrin; H-Lys-OH; L-(+)-Lysine; L-2,6-Diainohexanoate; L-2,6-Diainohexanoic acid; L-Lys; Acetate, lysine; Enisyl; Lysine hydrochloride; L Lysine; Lysine acetate

HMDB: HMDB0000182; HMDB00182

CAS: 56-87-1

L-lysine is an essential amino acid. Normal requirements for lysine have been found to be about 8 g per day or 12 mg/kg in adults. Children and infants need more, 44 mg/kg per day for an eleven to-twelve-year old, and 97 mg/kg per day for three-to six-month old. Lysine is highly concentrated in muscle compared to most other amino acids. Lysine is high in foods such as wheat germ, cottage cheese and chicken. Of meat products, wild game and pork have the highest concentration of lysine. Fruits and vegetables contain little lysine, except avocados. Normal lysine metabolism is dependent upon many nutrients including niacin, vitamin B6, riboflavin, vitamin C, glutamic acid and iron. Excess arginine antagonizes lysine. Several inborn errors of lysine metabolism are known, such as cystinuria, hyperdibasic aminoaciduria I, lysinuric protein intolerance, propionic acidemia, and tyrosinemia I. Most are marked by mental retardation with occasional diverse symptoms such as absence of secondary sex characteristics, undescended testes, abnormal facial structure, anemia, obesity, enlarged liver and spleen, and eye muscle imbalance. Lysine also may be a useful adjunct in the treatment of osteoporosis. Although high protein diets result in loss of large amounts of calcium in urine, so does lysine deficiency. Lysine may be an adjunct therapy because it reduces calcium losses in urine. Lysine deficiency also may result in immunodeficiency. Requirements for this amino acid are probably increased by stress. Lysine toxicity has not occurred with oral doses in humans. Lysine dosages are presently too small and may fail to reach the concentrations necessary to prove potential therapeutic applications. Lysine metabolites, amino caproic acid and carnitine have already shown their therapeutic potential.



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Thirty grams daily of amino caproic acid has been used as an initial daily dose in treating blood clotting disorders, indicating that the proper doses of lysine, its precursor, have yet to be used in medicine. Low lysine levels have been found in patients with Parkinson's, hypothyroidism, kidney disease, asthma and depression. The exact significance of these levels is unclear, yet lysine therapy can normalize the level and has been associated with improvement of some patients with these conditions.

Abnormally elevated hydroxylysines have been found in virtually all chronic degenerative diseases and coumadin therapy. The levels of this stress marker may be improved by high doses of vitamin C. Lysine is particularly useful in therapy for marasmus (wasting) and herpes simplex. It stops the growth of herpes simplex in culture, and has helped to reduce the number and occurrence of cold sores in clinical studies. Dosing has not been adequately studied, but beneficial clinical effects occur in doses ranging from 100 mg to 4 g a day. Higher doses may also be useful, and toxicity has not been reported in doses as high as 8 g per day. Diets high in lysine and low in arginine can be useful in the prevention and treatment of herpes. Some researchers think herpes simplex virus is involved in many other diseases related to cranial nerves such as migraines, Bell's palsy and Meniere's disease. Herpes blister fluid will produce fatal encephalitis in the rabbit (<http://www.dcnutrition.com>).

This compound belongs to the class of organic compounds known as l-alpha-amino acids. These are alpha amino acids which have the L-configuration of the alpha-carbon atom.

## L-Lysine -- Alzheimer's disease

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## L-Serine -- Introduction

SYNONYM: (2S)-2-amino-3-Hydroxypropanoic acid; (S)-(-)-Serine; (S)-2-amino-3-Hydroxypropanoic acid; (S)-alpha-amino-beta-Hydroxypropionic acid; (S)-Serine; beta-Hydroxy-L-alanine; beta-Hydroxyalanine; L-(-)-Serine; L-2-amino-3-Hydroxypropionic acid; L-3-Hydroxy-2-aminopropionic acid; L-3-Hydroxy-alanine; L-Ser; L-Serin; S; Ser; SERINE; (2S)-2-amino-3-Hydroxypropanoate; (S)-2-amino-3-Hydroxypropanoate; (S)-a-amino-b-Hydroxypropionate; (S)-a-amino-b-Hydroxypropionic acid; (S)-alpha-amino-beta-Hydroxypropionate; (S)-l±-amino-l̂-hydroxypropionate; (S)-l±-amino-l̂-hydroxypropionic acid; b-Hydroxy-L-alanine; l̂-hydroxy-L-alanine; b-Hydroxyalanine; l̂-hydroxyalanine; L-2-amino-3-Hydroxypropionate; L-3-Hydroxy-2-aminopropionate; (-)-Serine; (S)-2-amino-3-Hydroxy-propanoate; (S)-2-amino-3-Hydroxy-propanoic acid; (S)-b-amino-3-Hydroxypropionate; (S)-b-amino-3-Hydroxypropionic acid; (S)-beta-amino-3-Hydroxypropionate; (S)-beta-amino-3-Hydroxypropionic acid; 2-amino-3-Hydroxypropanoate; 2-amino-3-Hydroxypropanoic acid; 3-Hydroxy-L-alanine; L Serine

HMDB: HMDB0000187; HMDB0000589; HMDB00187; HMDB00589

CAS: 56-45-1

Serine is a nonessential amino acid derived from glycine. Like all the amino acid building blocks of protein and peptides, serine can become essential under certain conditions, and is thus important in maintaining health and preventing disease. Low-average concentration of serine compared to other amino acids is found in muscle. Serine is highly concentrated in all cell membranes. (<http://www.dcnutrition.com/AminoAcids/>) L-Serine may be derived from four possible sources: dietary intake; biosynthesis from the glycolytic intermediate 3-phosphoglycerate; from glycine ; and by protein and phospholipid degradation. Little data is available on the relative contributions of each of these four sources of l-serine to serine homoeostasis. It is very likely that the predominant source of l-serine will be very different in different tissues and during different stages of human development. In the biosynthetic pathway, the glycolytic intermediate 3-phosphoglycerate is converted into phosphohydroxypyruvate, in a reaction catalyzed by 3-phosphoglycerate dehydrogenase (3-PGDH; EC 1.1.1.95). Phosphohydroxypyruvate is metabolized to phosphoserine by phosphohydroxypyruvate aminotransferase (EC 2.6.1.52) and, finally, phosphoserine is converted into l-serine by phosphoserine phosphatase (PSP; EC 3.1.3.3). In liver tissue, the serine biosynthetic pathway is regulated in response to dietary and hormonal changes. Of the three synthetic enzymes, the properties of 3-PGDH and PSP are the best documented. Hormonal factors such as glucagon and corticosteroids also influence 3-PGDH and PSP activities in interactions dependent upon the diet. L-serine plays a central role in cellular proliferation. L-Serine is the predominant source of one-carbon groups for the de novo synthesis of purine nucleotides and deoxythymidine monophosphate. It has long been recognized that, in cell cultures, L-serine is a conditional essential amino acid, because it cannot be synthesized in sufficient quantities to meet the cellular demands for its utilization. In recent years, L-serine and the products of its metabolism have been recognized not only to be essential for cell proliferation, but also to be necessary for specific functions in the central nervous system. The findings of altered levels of serine and glycine in patients with psychiatric disorders and the severe neurological abnormalities in patients with defects of L-serine synthesis underscore the importance of L-serine in brain development and function. (PMID 12534373).

This compound belongs to the class of organic compounds known as serine and derivatives. These are compounds containing serine or a derivative thereof resulting from reaction of serine at the amino group or the carboxy group, or from the replacement of any hydrogen of glycine by a heteroatom.

## L-Serine -- 3-Phosphoglycerate dehydrogenase deficiency



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## L-Aspartic acid -- Introduction

SYNONYM: (S)-2-Aminobutanedioic acid; (S)-2-Aminosuccinic acid; 2-Aminosuccinic acid; Asp; ASPARTIC ACID; D; L-Asparaginsaeure; (S)-2-Aminobutanedioate; L-Aspartate; (S)-2-Aminosuccinate; 2-Aminosuccinate; ASPARTate; (+)-Aspartate; (+)-Aspartic acid; (2S)-Asparte; (2S)-Aspartic acid; (L)-Aspartate; (L)-Aspartic acid; (R)-2-Aminosuccinate; (S)-(+)-Asparte; (S)-(+)-Aspartic acid; (S)-amino-Butanedioate; (S)-amino-Butanedioic acid; (S)-Aminobutanedioate; (S)-Aminobutanedioic acid; (S)-Aspartate; (S)-Aspartic acid; 2-amino-3-Methylsuccinate; 2-amino-3-Methylsuccinic acid; alpha-Aminosuccinate; alpha-Aminosuccinic acid; Aminosuccinate; Asparagine; Asparagine acid; Asparagine; Asparagine acid; Asparatate; H-Asp-OH; L-(+)-Aspartate; L-(+)-Aspartic acid; L-Aminosuccinate; L-Aminosuccinic acid; L-Asparagine; L-Asparagine acid; L-Asparagine; L-Asparagine acid; (+)-Aspartic acid; (R,S)-Aspartic acid; Aspartate, disodium; Aspartate, magnesium; Aspartate, monopotassium; Aspartic acid, dipotassium salt; Aspartic acid, hydrobromide; Aspartic acid, monopotassium salt; Aspartic acid, monosodium salt; Aspartic acid, potassium salt; L Aspartate; MG5Longoral; Potassium aspartate; Polysuccinimide; Ammonium aspartate; Aspartate, ammonium; Aspartate, calcium; Aspartate, monosodium; Aspartic acid, calcium salt; Aspartic acid, disodium salt; Aspartic acid, magnesium (1:1) salt, hydrochloride, trihydrate; Dipotassium aspartate; Disodium aspartate; Hydrochloride, aspartate magnesium; Monopotassium aspartate; Sodium aspartate; Aspartate, dipotassium; Aspartic acid, magnesium (2:1) salt; Aspartic acid, sodium salt; Hydrobromide aspartic acid; Magnesium aspartate; MG 5 Longoral; Monosodium aspartate; Aspartate magnesium



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hydrochloride; Aspartate, potassium; Aspartate, sodium; Aspartic acid, ammonium salt; Aspartic acid, hydrochloride; Aspartic acid, magnesium-potassium (2:1:2) salt; Calcium aspartate; Hydrochloride aspartic acid; L Aspartic acid; Magnesiocard; MG-5-Longoral; Poly-DL-succinimide

HMDB: HMDB0000191; HMDB00191

CAS: 56-84-8

Aspartic acid (Asp, D), also known as aspartate, the name of its anion, is one of the 20 natural proteinogenic amino acids which are the building blocks of proteins. As its name indicates, aspartic acid is the carboxylic acid analog of asparagine. As a neurotransmitter, aspartic acid may provide resistance to fatigue and thus lead to endurance, although the evidence to support this idea is not strong (Wikipedia). Aspartic acid is a nonessential amino acid that is made from glutamic acid by enzymes using vitamin B6. The amino acid has important roles in the urea cycle and DNA metabolism. Aspartic acid is a major excitatory neurotransmitter, which is sometimes found to be increased in epileptic and stroke patients. It is decreased in depressed patients and in patients with brain atrophy. Aspartic acid supplements are being evaluated. Five grams can raise blood levels. Magnesium and zinc may be natural inhibitors of some of the actions of aspartic acid. Aspartic acid, with the amino acid phenylalanine, is a part of a new natural sweetener, aspartame. This sweetener is an advance in artificial sweeteners, and is probably safe in normal doses to all except phenylketonurics. The jury is still out on the long-term effects it has on many brain neurohormones. Aspartic acid may be a significant immunostimulant of the thymus and can protect against some of the damaging effects of radiation. Many claims have been made for the special value of administering aspartic acid in the form of potassium and magnesium salts. Since aspartic acid is relatively nontoxic, studies are now in progress to elucidate its pharmacological and therapeutic roles (<http://www.dcnutrition.com/AminoAcids>).

This compound belongs to the class of organic compounds known as aspartic acid and derivatives. These are compounds containing an aspartic acid or a derivative thereof resulting from reaction of aspartic acid at the amino group or the carboxy group, or from the replacement of any hydrogen of glycine by a heteroatom.

## L-Aspartic acid -- Alzheimer's disease

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## Inosine -- Introduction

SYNONYM: 9-beta-D-Ribofuranosyl-9H-purin-6-ol; 9-beta-D-Ribofuranosylhypoxanthine; Hypoxanthine D-riboside; Hypoxanthosine; i; Inosin; Inosina; Inosinum; 9-b-D-Ribofuranosyl-9H-purin-6-ol; 9- $\beta$ -D-ribofuranosyl-9H-purin-6-ol; 9-b-D-Ribofuranosylhypoxanthine; 9- $\beta$ -D-ribofuranosylhypoxanthine; (-)-Inosine; 1,9-dihydro-9-b-D-Ribofuranosyl-6H-purin-6-one; 1,9-dihydro-9-beta-D-Ribofuranosyl-6H-purin-6-one; 1,9-dihydro-9-beta-D-Ribofuranosyl-6H-purin-6-one; 9-b-D-Ribofuranosyl-hypoxanthine; 9-beta-D-Ribofuranosyl-hypoxanthine; 9-beta-Delta-Ribofuranosyl-hypoxanthine; 9-beta-Delta-Ribofuranosylhypoxanthine; 9beta-D-Ribofuranosylhypoxanthine; 9beta-Delta-Ribofuranosylhypoxanthine; Atorel; beta-D-Ribofuranoside hypoxanthine-9; beta-Delta-Ribofuranoside hypoxanthine-9; beta-Inosine; HXR; Hypoxanthine 9-beta-D-ribofuranoside; Hypoxanthine 9-beta-Delta-ribofuranoside; Hypoxanthine nucleoside; Hypoxanthine ribonucleoside; Hypoxanthine riboside; Hypoxanthine-9 beta-D-ribofuranoside; Hypoxanthine-9 beta-Delta-ribofuranoside;



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Hypoxanthine-9-beta-D-ribofuranoside; Hypoxanthine-9-beta-delta-ribofuranoside; Hypoxanthine-9-D-ribofuranoside; Hypoxanthine-9-delta-ribofuranoside; Hypoxanthine-ribose; Indole-3-carboxaldehyde; Ino; Inosie; iso-Prinosine; Oxiamin; Panholic-L; Pantholic-L; Ribenosine; Selfer; Trophicardyl

HMDB: HMDB0000195; HMDB00195

CAS: 58-63-9

Inosine is a purine nucleoside that has hypoxanthine linked by the N9 nitrogen to the C1 carbon of ribose. It is an intermediate in the degradation of purines and purine nucleosides to uric acid and in pathways of purine salvage. It also occurs in the anticodon of certain transfer RNA molecules (Dorland, 28th ed). Inosine is found to be associated with purine nucleoside phosphorylase deficiency and xanthinuria type I, which are inborn errors of metabolism.

This compound belongs to the class of organic compounds known as purine nucleosides. These are compounds comprising a purine base attached to a ribosyl or deoxyribosyl moiety.

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### Indoleacetic acid -- Introduction

SYNONYM: (indol-3-yl)Acetate; (indol-3-yl)Acetic acid; 2-(indol-3-yl)Ethanoic acid; 3-Indolylessigsaeure; Heteroauxin; IAA; IES; Indoleacetate; 2-(indol-3-yl)Ethanoate; (1H-indol-3-yl)-Acetate; (1H-indol-3-yl)-Acetic acid; 1H-indol-3-Ylacetate; 1H-indol-3-Ylacetic acid; 1H-Indole-3-acetate; 1H-Indole-3-acetic acid; 2-(1H-indol-3-yl)Acetate; 2-(1H-indol-3-yl)Acetic acid; 2-(3-Indolyl)acetate; 2-(3-Indolyl)acetic acid; 3-(Carboxymethyl)indole; 3-IAA; 3-Indole-acetic acid; 3-Indoleacetate; 3-Indoleacetic acid; 3-Indolylacetate; 3-Indolylacetic acid; alpha-indol-3-yl-Acetic acid; b-Indoleacetate; b-Indoleacetic acid; b-Indolylacetate; b-Indolylacetic acid; beta-Indole-3-acetic acid; beta-Indoleacetate; beta-Indoleacetic acid; beta-Indolylacetate; beta-Indolylacetic acid; indol-3-Ylacetate; indol-3-Ylacetic acid; Indole-3-acetate; Indole-3-acetic acid; Indolyl-3-acetate; Indolyl-3-acetic acid; Indolylacetate; Indolylacetic acid; Kyselina 3-indolyloctova; Rhizopin; Rhizopon a; Skatole carboxylate; Skatole carboxylic acid; Indoleacetic acid, calcium salt; Indoleacetic acid, monopotassium salt; Indoleacetic acid, monosodium salt; IES CPD; Indole acetic acid; Indoleacetic acid, alpha-(14)C-labeled

HMDB: HMDB0000197; HMDB00197

CAS: 87-51-4

Indoleacetic acid (IAA) is a breakdown product of tryptophan metabolism and is often produced by the action of bacteria in the mammalian gut. Some endogenous production of IAA in mammalian tissues also occurs. It may be produced by the decarboxylation of tryptamine or the oxidative deamination of tryptophan. IAA frequently occurs at low levels in urine and has been found in elevated levels in the urine of patients with phenylketonuria ((PMID: 13610897). Using material extracted from human urine, it was discovered by Kogl in 1933 that Indoleacetic acid is also an important plant hormone (PMID: 13610897). Specifically IAA is a member of the group of phytohormones called auxins. IAA is generally considered to be the most important native auxin. Plant cells synthesize IAA from tryptophan. (wikipedia) IAA and some derivatives can be oxidised by horseradish peroxidase (HRP) to cytotoxic species. IAA is only toxic after oxidative decarboxylation; the effect of IAA/HRP is thought to be due in part to the formation of methylene-oxindole, which may conjugate with DNA bases and protein thiols. IAA/HRP could be used as the basis for targeted cancer, a potential new role for plant auxins in cancer therapy. (PMID: 11163327).

This compound belongs to the class of organic compounds known as indole-3-acetic acid derivatives. These are compounds containing an acetic acid (or a derivative) linked to the C3 carbon atom of an indole.

### Indoleacetic acid -- Appendicitis

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### L-Acetylcarnitine -- Introduction

SYNONYM: (-)-Acetylcarnitine; (R)-Acetylcarnitine; Acetyl-L-(-)-carnitine; Acetyl-L-carnitine; L-Acetylcarnitine; L-Carnitine acetyl ester; L-O-Acetylcarnitine; O-Acetyl-(R)-carnitine; R-Acetylcarnitine; Branigen; Levocarnitine acetyl; Acetyl carnitine; Carnitine, acetyl; Alcar; Acetyl L carnitine; Acetylcarnitine, (R)-isomer; Medosan; ALC; 3-(Acetoxy)-4-(trimethylammonio)butanoate; Acetyl-DL-carnitine; Acetylcarnitine; DL-O-Acetylcarnitine; 3-(Acetoxy)-4-(trimethylammonio)butanoic acid; (+)-Acetylcarnitine; Acetyl-carnitine; Nicetile; O-Acetyl-L-carnitine; O-Acetylcarnitine

HMDB: HMDB0000201; HMDB0000456; HMDB0000515; HMDB00201; HMDB00456; HMDB00515

CAS: 3040-38-8

L-Acetylcarnitine (ALCAR or ALC) is an acetic acid ester of carnitine that facilitates movement of acetyl-CoA into the matrices of mammalian mitochondria during the oxidation of fatty acids. In addition to its metabolic role, acetyl-L-carnitine possesses unique neuroprotective, neuromodulatory, and neurotrophic properties this may play an important role in counteracting various disease processes (PMID ID: 15363640).

This compound belongs to the class of organic compounds known as acyl carnitines. These are organic compounds containing a fatty acid with the carboxylic acid attached to carnitine through an ester bond.

### L-Acetylcarnitine -- Very Long Chain Acyl-CoA Dehydrogenase Deficiency

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## Oleic acid -- Introduction



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SYNONYM: (9Z)-Octadecenoic acid; (Z)-Octadec-9-enoic acid; 18:1 N-9; 18:1DElta9cis; C18:1 N-9; cis-9-Octadecenoic acid; cis-Delta(9)-Octadecenoic acid; cis-Oleic acid; Octadec-9-enoic acid; Oelsaeure; Oleate; (9Z)-Octadecenoate; (Z)-Octadec-9-enoate; cis-9-Octadecenoate; cis-delta(9)-Octadecenoate; cis-Î'(9)-octadecenoate; cis-Î'(9)-octadecenoic acid; cis-Oleate; Octadec-9-enoate; (9Z)-9-Octadecenoate; (9Z)-9-Octadecenoic acid; (Z)-9-Octadecanoate; (Z)-9-Octadecanoic acid; 9,10-Octadecenoate; 9,10-Octadecenoic acid; 9-(Z)-Octadecenoate; 9-(Z)-Octadecenoic acid; 9-Octadecenoate; 9-Octadecenoic acid; Century CD fatty acid; cis-Octadec-9-enoate; cis-Octadec-9-enoic acid; Distoline; Emersol 210; Emersol 211; Emersol 213; Emersol 220 white oleate; Emersol 220 white oleic acid; Emersol 221 low titer white oleate; Emersol 221 low titer white oleic acid; Emersol 233LL; Emersol 6321; Emersol 6333 NF; Emersol 7021; Glycon ro; Glycon wo; groco 2; groco 4; groco 5; groco 6; Industrene 104; Industrene 105; Industrene 205; Industrene 206; L'acide oleique; Metaupon; Oelsauere; Oleic acid extra pure; Oleinate; Oleinic acid; Pamolyn; Pamolyn 100; Pamolyn 100 FG; Pamolyn 100 FGK; Pamolyn 125; Priolene 6900; Red oil; tego-Oleic 130; Vopcolene 27; Wecoline oo; Z-9-Octadecenoate; Z-9-Octadecenoic acid; Acid, 9-octadecenoic; Acid, oleic; 9 Octadecenoic acid; Acid, cis-9-octadecenoic; cis 9 Octadecenoic acid

HMDB: HMDB0000207; HMDB0002066; HMDB00207; HMDB02066

CAS: 112-80-1

Oleic acid is an unsaturated fatty acid that is the most widely distributed and abundant fatty acid in nature. It is used commercially in the preparation of oleates and lotions, and as a pharmaceutical solvent (Stedman, 26th ed). Biological source: Major constituent of plant oils e.g. olive oil (about 80%), almond oil (about 80%) and many others, mainly as glyceride. Constituent of tall oil and present in fruits Use/Importance: Food additive. Oleic acid is used in manufacturing of surfactants, soaps, plasticizers. Emulsifying agent in foods and pharmaceuticals. Biological Use/Importance: Skin penetrant. Herbicide, insecticide, fungicide (Dictionary of Organic Compounds). Oleic acid is a fatty acid that occurs naturally in various animal and vegetable fats and oils. It is an odourless, colourless oil, although commercial samples may be yellowish. In chemical terms, oleic acid is classified as a monounsaturated omega-9 fatty acid. It has the formula CH<sub>3</sub>(CH<sub>2</sub>)<sub>7</sub>CH=CH(CH<sub>2</sub>)<sub>7</sub>COOH. The term "oleic" means related to, or derived from, oil or olive, the oil that is predominantly composed of oleic acid (Wikipedia). Oleic acid is found to be associated with isovaleric acidemia, which is an inborn error of metabolism.

This compound belongs to the class of organic compounds known as long-chain fatty acids. These are fatty acids with an aliphatic tail that contains between 13 and 21 carbon atoms.

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## Pantothenic acid -- Introduction

SYNONYM: (+)-Pantothenic acid; (R)-N-(2,4-Dihydroxy-3,3-dimethyl-1-oxobutyl)-beta-alanine; Chick antidermatitis factor; D(+)-N-(2,4-Dihydroxy-3,3-dimethylbutyryl)-beta-alanine; D-(+)-Pantothenic acid; D-Pantothenic acid; N-[(2R)-2,4-Dihydroxy-3,3-dimethylbutanoyl]-beta-alanine; PANTOTHENOIC ACID; Vitamin b5

HMDB: HMDB0000210; HMDB00210; HMDB0062717; HMDB62717

CAS: 79-83-4

Pantothenic acid, also called vitamin B5, is a water-soluble vitamin required to sustain life. Pantothenic acid is needed to form coenzyme-A (CoA), and is thus critical in the metabolism and synthesis of carbohydrates, proteins, and fats. Its name is derived from the Greek pantothen meaning "from everywhere" and small quantities of pantothenic acid are found in nearly every food, with high amounts in whole grain cereals, legumes, eggs, meat, and royal jelly. Pantothenic acid is classified as a member of the secondary alcohols. Secondary alcohols are compounds containing a secondary alcohol functional group, with the general structure  $\text{HOC(R)(R') (R,R'=alkyl, aryl)}$ . Pantothenic acid is considered to be soluble (in water) and acidic.

This compound belongs to the class of organic compounds known as polyols. These are organic compounds containing more than one hydroxyl groups.

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## myo-Inositol -- Introduction

SYNONYM: (1R,2R,3S,4S,5R,6S)-Cyclohexane-1,2,3,4,5,6-hexol; 1,2,3,4,5,6-HEXAHYDROXY-cyclohexane; 1,2,3,5/4,6-cyclohexanhexol; 1D-myoinositol; 1L-myoinositol; Bios I; cis-1,2,3,5-trans-4,6-Cyclohexanhexol; Cyclohexitol; D-myoinositol; Dambose; L-inositol; Inosite; Inositol; Ins; L-myoinositol; Meat sugar; meso-Inositol; iso-Inositol; MI; myoinositol; Myoinosite; Phaseomannite; Rat antispectacled eye factor; Myoinositol; Myo inositol; Vitamin B8

HMDB: HMDB0000211; HMDB0002256; HMDB00211; HMDB02256

CAS: 87-89-8

myo-Inositol is an inositol isoform. Inositol is a derivative of cyclohexane with six hydroxyl groups, making it a polyol. It also is known as a sugar alcohol, having exactly the same molecular formula as glucose or other hexoses. Inositol exists in nine possible stereoisomers, of which cis-1,2,3,5-trans-4,6-cyclohexanhexol, or myo-inositol is the most widely occurring form in nature. The other known inositols include scyllo-inositol, muco-inositol, D-chiro-inositol, L-chiro-inositol, neo-inositol, allo-inositol, epi-inositol and cis-inositol. myo-Inositol is found naturally in many foods (particularly in cereals with high bran content) and can be used as a sweetner as it has half the sweetness of sucrose (table sugar). myo-Inositol was once considered a member of the vitamin B complex and given the name: vitamin B8. However, because it is produced by the human body from glucose, it is not an essential nutrient, and therefore cannot be called a vitamin. myo-Inositol is a precursor molecule for a number of secondary messengers including various inositol phosphates. In addition, inositol/myo-inositol is an important component of the lipids known as phosphatidylinositol (PI) phosphatidylinositol phosphate (PIP). myo-Inositol is synthesized from glucose, via glucose-6-phosphate (G-6-P) in two steps. First, G-6-P is isomerised by an inositol-3-phosphate synthase enzyme to myo-inositol 1-phosphate, which is then dephosphorylated by an inositol monophosphatase enzyme to give free myo-inositol. In humans, myo-inositol is primarily synthesized in the kidneys at a rate of a few grams per day. myo-Inositol can be used in the management of preterm babies who have or are at a risk of infant respiratory distress syndrome. It is also used as a treatment for polycystic ovary syndrome (PCOS). It works by increasing insulin sensitivity, which helps to improve ovarian function and reduce hyperandrogenism. Reduced levels of myo-inositol have been found in the spinal fluid of depressed patients and levels are significantly reduced in brain samples of suicide victims.

This compound belongs to the class of organic compounds known as cyclohexanols. These are compounds containing an alcohol group attached to a cyclohexane ring.

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### Norepinephrine -- Introduction

SYNONYM: (-)-Arterenol; (-)-Noradrenaline; (-)-Norepinephrine; (R)-(-)-Norepinephrine; (R)-4-(2-amino-1-Hydroxyethyl)-1,2-benzenediol; (R)-Norepinephrine; 4-[(1R)-2-amino-1-Hydroxyethyl]-1,2-benzenediol; Arterenol; L-Noradrenaline; L-NOREPINEPHRINE; Noradrenaline; Norepinefrina; Norepinephrinum; (-)-(R)-Norepinephrine; (-)-alpha-(Aminomethyl)protocatechual alcohol; (R)-Noradrenaline; 4-(2-amino-1-Hydroxyethyl)-1,2-benzenediol; Adrenor; Aktamin; L-2-amino-1-(3,4-Dihydroxyphenyl)ethanol; L-3,4-Dihydroxyphenylethanolamine; L-alpha-(Aminomethyl)-3,4-dihydroxybenzyl alcohol; L-Arterenol; Levarterenol; Levoarterenol; Levonor; Levonoradrenaline; Levonorepinephrine; Levophed; Nor-epirenan; Noradrenalin; Norartrinal; Norepirenamine; Sympathin e; Hydrochloride, norepinephrine; Levophed bitartrate; Noradr $\ddot{\text{a}}$ naline tartrate reaudin; Norepinephrine hydrochloride, (+)-isomer; Norepinephrine hydrochloride, (+,-)-isomer; Norepinephrine L-tartrate (1:1), monohydrate; Norepinephrine, (+,-)-isomer; Renaudin brand OF norepinephrine bitartrate; Bitartrate, noradrenaline; Noradrenaline bitartrate; Norepinephrine L-tartrate (1:1); Norepinephrine L-tartrate (1:1), (+,-)-isomer; Norepinephrine L-tartrate (1:1), monohydrate, (+)-isomer; Abbott brand OF levophed bitartrate; Aventis brand OF norepinephrine hydrochloride; Bitartrate, norepinephrine; Norepinephrin D-tartrate (1:1); Norepinephrine bitartrate; Norepinephrine hydrochloride; Norepinephrine D-tartrate (1:1); Norepinephrine L-tartrate, (+)-isomer; Tartrate reaudin, noradr $\ddot{\text{a}}$ naline; Bitartrate, levophed; Norepinephrine L-tartrate (1:2); Norepinephrine, (+)-isomer; Renaudin, noradr $\ddot{\text{a}}$ naline tartrate

HMDB: HMDB0000216; HMDB00216

CAS: 51-41-2

Precursor of epinephrine that is secreted by the adrenal medulla and is a widespread central and autonomic neurotransmitter. Norepinephrine is the principal transmitter of most postganglionic sympathetic fibers and of the diffuse projection system in the brain arising from the locus ceruleus. It is also found in plants and is used pharmacologically as a sympathomimetic. Norepinephrine is elevated in the urine of people who consume bananas.

This compound belongs to the class of organic compounds known as catechols. These are compounds containing a 1,2-



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benzenediol moiety.

### Norepinephrine -- Subarachnoid hemorrhage

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## Norepinephrine -- Dopamine-serotonin Vesicular Transport Defect

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## L-Palmitoylcarnitine -- Introduction

SYNONYM: (3R)-3-(Hexadecanoyloxy)-4-(trimethylazaniumyl)butanoate; (3R)-3-Palmitoyloxy-4-(trimethylammonio)butanoate; Hexadecanoyl-L-carnitine; Hexadecanoylcarnitine; Hexadecenoyl carnitine; L-Carnitine palmitoyl ester; O-Hexadecanoyl-(R)-carnitine; O-Hexadecanoyl-R-carnitine; Palmitoyl-L-carnitine; Palmitoylcarnitine; (3R)-3-(Hexadecanoyloxy)-4-(trimethylazaniumyl)butanoic acid; (3R)-3-Palmitoyloxy-4-(trimethylammonio)butanoic acid; (+)-Palmitoylcarnitine; (3S)-3-Hexadecanoyloxy-4-(trimethylammonio)butanoate; (3S)-3-Hexadecanoyloxy-4-(trimethylammonio)butanoic acid; (3S)-3-Palmitoyloxy-4-(trimethylammonio)butanoate; (3S)-3-Palmitoyloxy-4-(trimethylammonio)butanoic acid; 3-Carboxy-N,N,N-trimethyl-2-[(1-oxohexadecyl)oxy]-1-propanaminium; D-Palmitoylcarnitine; L(-)-Palmitoylcarnitine; L-Palmitoyl-L-carnitine; Palmitoyl D-carnitine; Palmitoyl(-)-carnitine; Palmitoyl-L-carnitine; Palmitoylcarnitine

HMDB: HMDB0000222; HMDB0000846; HMDB00222; HMDB00846

CAS: 2364-67-2

L-palmitoylcarnitine is a long-chain acyl fatty acid derivative ester of carnitine which facilitates the transfer of long-chain fatty acids from cytoplasm into mitochondria during the oxidation of fatty acids. L-palmitoylcarnitine, due to its amphipathic character is, like detergents, a surface-active molecule and by changing the membrane fluidity and surface charge can change activity of several enzymes and transporters localized in the membrane. L-palmitoylcarnitine has been also reported to change the activity of certain proteins. On the contrary to carnitine, palmitoylcarnitine was shown to stimulate the activity of caspases 3, 7 and 8 and the level of this long-chain acylcarnitine increased during apoptosis. Palmitoylcarnitine was also reported to diminish completely binding of phorbol esters, the protein kinase C activators and to decrease the autophosphorylation of the enzyme. Apart from these isoform nonspecific phenomena, palmitoylcarnitine was also shown to be responsible for retardation in cytoplasm of protein kinase C isoforms  $\beta$  and  $\delta$  and, in the case of the latter one, to decrease its interaction with GAP-43. Some of the physico-chemical properties of palmitoylcarnitine may help to explain the need for coenzyme A-carnitine-coenzyme A acyl exchange during mitochondrial fatty acid import. The amphiphilic character of palmitoylcarnitine may also explain its proposed involvement in the pathogenesis of myocardial ischemia. L-palmitoylcarnitine accumulates in ischemic myocardium and potentially contribute to myocardial damage through alterations in membrane molecular dynamics, one mechanism through which could play an important role in ischemic injury. Palmitoylcarnitine is characteristically elevated in carnitine palmitoyltransferase II deficiency, late-onset (OMIM 255110 PMID 2540838, 15363641, 8706815). Moreover, L-palmitoylcarnitine is found to be associated with celiac disease, which is an inborn error of metabolism.

This compound belongs to the class of organic compounds known as acyl carnitines. These are organic compounds containing a fatty acid with the carboxylic acid attached to carnitine through an ester bond.



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## L-Palmitoylcarnitine -- Very Long Chain Acyl-CoA Dehydrogenase Deficiency

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## L-Palmitoylcarnitine -- Colorectal cancer

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## O-Phosphoethanolamine -- Introduction

SYNONYM: 2-amino-Ethanol dihydrogen phosphate; 2-amino-Ethanol phosphate; Colamine phosphate; Colamine phosphoric acid; Colaminophosphoric acid; EAP; Ethanolamine acid phosphate; Ethanolamine O-phosphate; Ethanolamine phosphate; mono(2-Aminoethyl) phosphate; Monoaminoethyl phosphate; O-Phosphocolamine; O-Phosphylethanolamine; OPE; PE; PEA; PETN; Phosphoethanolamine; Phosphonoethanolamine; Phosphoric acid 2-aminoethyl phenyl ester; Phosphoryl-ethanolamine; 2-amino-Ethanol dihydrogen phosphoric acid; 2-amino-Ethanol phosphoric acid; Colaminophosphate; Ethanolamine acid phosphoric acid; Ethanolamine O-phosphoric acid; Ethanolamine phosphoric acid; mono(2-Aminoethyl) phosphoric acid; Monoaminoethyl phosphoric acid; Phosphate 2-aminoethyl phenyl ester; 2-amino-Ethanol dihydrogen phosphate (ester); 2-Aminoethanol O-phosphate; 2-Aminoethyl dihydrogen phosphate; 2-Aminoethyl dihydrogen phosphate (acd/name 4.0); 2-Aminoethyl phosphate; Colamine acid phosphate; Colaminephosphoric acid; Ethamp; O-Phosphonatoethanaminium; Phosphoryethanolamine; Phosphorylethanolamine; Phosphorylethanolamine, 3H-labeled CPD; Phosphorylethanolamine magnesium (1:1) salt; Phosphorylethanolamine zinc salt; Phosphorylethanolamine, cobalt (2+) (1:1) salt; Calcium 2-aminoethanol phosphate; Phosphorylethanolamine ca (1:1) salt

HMDB: HMDB0000224; HMDB0012279; HMDB00224; HMDB0060151; HMDB0060152; HMDB12279; HMDB60151; HMDB60152

CAS: 1071-23-4

Phosphoethanolamine (PE) is a phosphomonoester metabolite of the phospholipid metabolism. PE is a precursor of phospholipid synthesis and a product of phospholipid breakdown. Phosphomonoesters are present at much higher levels in



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brain than in other organs. In developing brain, phosphomonoesters are normally elevated during the period of neuritic proliferation. This also coincides with the occurrence of normal programmed cell death and synaptic pruning in developing brain. These findings are consistent with the role of phosphomonoesters in membrane biosynthesis. PE shows a strong structural similarity to the inhibitory neurotransmitter, GABA, and the GABAB receptor partial agonist, 3-amino-propylphosphonic acid. PE is a phosphomonoester which is decreased in post-mortem Alzheimer's disease (AD) brain. (PMID: 7791524, 8588821, 11566853).

This compound belongs to the class of organic compounds known as phosphoethanolamines. These are compounds containing a phosphate linked to the second carbon of an ethanolamine.

### O-Phosphoethanolamine -- Traumatic brain injury

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### O-Phosphoethanolamine -- Colorectal cancer

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## Pyrophosphate -- Introduction

**SYNONYM:** [(ho)2P(O)OP(O)(OH)2]; Acide diphosphorique; Diphosphorsaeure; H4P2O7; PYROphosphATE; Pyrophosphoric acid; Pyrophosphorsaeure; Diphosphoric acid

**HMDB:** HMDB0000250; HMDB00250

**CAS:** 14000-31-8

The anion, the salts, and the esters of pyrophosphoric acid are called pyrophosphates. The pyrophosphate anion is abbreviated PP<sub>i</sub> and is formed by the hydrolysis of ATP into AMP in cells. This hydrolysis is called pyrophosphorolysis. The pyrophosphate anion has the structure P<sub>2</sub>O<sub>7</sub><sup>4-</sup>, and is an acid anhydride of phosphate. It is unstable in aqueous solution and rapidly hydrolyzes into inorganic phosphate. Pyrophosphate is an osteotoxin (arrests bone development) and an arthritogen (promotes arthritis). It is also a metabotoxin (an endogenously produced metabolite that causes adverse health affects at chronically high levels). Chronically high levels of pyrophosphate are associated with hypophosphatasia. Hypophosphatasia (also called deficiency of alkaline phosphatase or phosphoethanolaminuria) is a rare, and sometimes fatal, metabolic bone disease. Hypophosphatasia is associated with a molecular defect in the gene encoding tissue non-specific alkaline phosphatase (TNSALP). TNSALP is an enzyme that is tethered to the outer surface of osteoblasts and chondrocytes. TNSALP hydrolyzes several substances, including inorganic pyrophosphate (PP<sub>i</sub>) and pyridoxal 5'-phosphate (PLP), a major form of vitamin B6. When TNSALP is low, inorganic pyrophosphate (PP<sub>i</sub>) accumulates outside of cells and inhibits the formation of hydroxyapatite, one of the main components of bone, causing rickets in infants and children and osteomalacia (soft bones) in adults. Vitamin B6 must be dephosphorylated by TNSALP before it can cross the cell membrane. Vitamin B6 deficiency in the brain impairs synthesis of neurotransmitters which can cause seizures. In some cases, a build-up of calcium pyrophosphate dihydrate crystals in the joints can cause pseudogout.

This compound belongs to the class of inorganic compounds known as non-metal pyrophosphates. These are inorganic non-metallic compounds containing a pyrophosphate as its largest oxoanion.

## Taurine -- Introduction

**SYNONYM:** 2-Aminoethanesulfonic acid; 2-Aminoethyl sulfonate; Aminoethylsulfonic acid; beta-Aminoethylsulfonic acid; 2-Aminoethanesulfonate; 2-Aminoethanesulphonate; 2-Aminoethanesulphonic acid; 2-Aminoethyl sulfonic acid; 2-Aminoethyl sulphonate; 2-Aminoethyl sulphonic acid; Aminoethylsulfonate; Aminoethylsulphonate; Aminoethylsulphonic acid; b-Aminoethylsulfonate; b-Aminoethylsulfonic acid; b-Aminoethylsulphonate; b-Aminoethylsulphonic acid; beta-Aminoethylsulfonate; beta-Aminoethylsulphonate; beta-Aminoethylsulphonic acid;  $\hat{\beta}$ -aminoethylsulfonate;  $\hat{\beta}$ -aminoethylsulfonic acid;  $\hat{\beta}$ -aminoethylsulphonate;  $\hat{\beta}$ -aminoethylsulphonic acid; 1-Aminoethane-2-sulfonate; 1-Aminoethane-2-sulfonic acid; 2-Aminoethylsulfonate; 2-Aminoethylsulfonic acid; 2-Sulfoethylamine; Taurine hydrochloride; Taurine zinc salt (2:1); Taurine, monopotassium salt; Taufon; Taupon

**HMDB:** HMDB0000251; HMDB00251

**CAS:** 107-35-7

Taurine is a sulfur amino acid like methionine, cystine, cysteine and homocysteine. It is a lesser-known amino acid because it is not incorporated into the structural building blocks of protein. Yet taurine is an essential amino acid in pre-term



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and newborn infants of humans and many other species. Adults can synthesize their own taurine, yet are probably dependent in part on dietary taurine. Taurine is abundant in the brain, heart, breast, gallbladder and kidney and has important roles in health and disease in these organs. Taurine has many diverse biological functions serving as a neurotransmitter in the brain, a stabilizer of cell membranes and a facilitator in the transport of ions such as sodium, potassium, calcium and magnesium. Taurine is highly concentrated in animal and fish protein, which are good sources of dietary taurine. It can be synthesized by the body from cysteine when vitamin B6 is present. Deficiency of taurine occurs in premature infants and neonates fed formula milk, and in various disease states. Inborn errors of taurine metabolism have been described. OMIM 168605, an unusual neuropsychiatric disorder inherited in an autosomal dominant fashion through 3 generations of a family. Symptoms began late in the fifth decade in 6 affected persons and death occurred after 4 to 6 years. The earliest and most prominent symptom was mental depression not responsive to antidepressant drugs or electroconvulsive therapy. Sleep disturbances, exhaustion and marked weight loss were features. Parkinsonism developed later, and respiratory failure occurred terminally. OMIM 145350 describes congestive cardiomyopathy and markedly elevated urinary taurine levels (about 5 times normal). Other family members had late or holosystolic mitral valve prolapse and elevated urinary taurine values (about 2.5 times normal). In 2 with mitral valve prolapse, congestive cardiomyopathy eventually developed while the amounts of urinary taurine doubled. Taurine, after GABA, is the second most important inhibitory neurotransmitter in the brain. Its inhibitory effect is one source of taurine's anticonvulsant and antianxiety properties. It also lowers glutamic acid in the brain, and preliminary clinical trials suggest taurine may be useful in some forms of epilepsy. Taurine in the brain is usually associated with zinc or manganese. The amino acids alanine and glutamic acid, as well as pantothenic acid, inhibit taurine metabolism while vitamins A and B6, zinc and manganese help build taurine. Cysteine and B6 are the nutrients most directly involved in taurine synthesis. Taurine levels have been found to decrease significantly in many depressed patients. One reason that the findings are not entirely clear is because taurine is often elevated in the blood of epileptics who need it. It is often difficult to distinguish compensatory changes in human biochemistry from true metabolic or deficiency disease. Low levels of taurine are found in retinitis pigmentosa. Taurine deficiency in experimental animals produces degeneration of light-sensitive cells. Therapeutic applications of taurine to eye disease are likely to be forthcoming. Taurine has many important metabolic roles. Supplements can stimulate prolactin and insulin release. The parathyroid gland makes a peptide hormone called glutataurine (glutamic acid-taurine), which further demonstrates taurine's role in endocrinology. Taurine increases bilirubin and cholesterol excretion in bile, critical to normal gallbladder function. It seems to inhibit the effect of morphine and potentiates the effects of opiate antagonists. Low plasma taurine levels have been found in a variety of conditions, i.e., depression, hypertension, hypothyroidism, gout, institutionalized patients, infertility, obesity, kidney failure and others (<http://www.dcnutrition.com/AminoAcids/>). Moreover, taurine is found to be associated with maple syrup urine disease, which is an inborn error of metabolism.

This compound belongs to the class of organic compounds known as organosulfonic acids. These are compounds containing the sulfonic acid group, which has the general structure RS(=O)2OH (R is not a hydrogen atom).

### Taurine -- Autosomal dominant polycystic kidney disease

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### Succinic acid -- Introduction

SYNONYM: 1,2-Ethanedicarboxylic acid; Acide butanedioique; Acide succinique; Acidum succinicum; Amber acid; Asuccin; Bernsteinsaeure; Butanedisaeure; Butanedionic acid; Dihydrofumaric acid; e363; Ethylenesuccinic acid; HOOC-CH<sub>2</sub>-CH<sub>2</sub>-COOH; Spirit OF amber; 1,2-Ethanedicarboxylate; Succinate; Butanedionate; Dihydrofumarate; Ethylenesuccinate; 1,4-Butanedioate; 1,4-Butanedioic acid; Katasuccin; Wormwood acid; 1,2 Ethanedicarboxylic acid; 1,4-Butanedioic acid; Potassium succinate; Succinate, ammonium; Butanedioic acid; Succinate, potassium; Ammonium succinate



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HMDB: HMDB0000254; HMDB00254

CAS: 110-15-6

Succinic acid is a dicarboxylic acid. The anion, succinate, is a component of the citric acid or TCA cycle and is capable of donating electrons to the electron transfer chain. Succinate dehydrogenase (SDH) plays an important role in mitochondrial function, being both part of the respiratory chain and the Krebs cycle. SDH with a covalently attached FAD prosthetic group, is able to bind several different enzyme substrates (succinate and fumarate) and physiological regulators (oxaloacetate and ATP). Oxidizing succinate links SDH to the fast-cycling Krebs cycle portion where it participates in the breakdown of acetyl-CoA throughout the entire Krebs cycle. Succinate can readily be imported into the mitochondrial matrix by the n-butylmalonate- (or phenylsuccinate-) sensitive dicarboxylate carrier in exchange with inorganic phosphate or another organic acid, e. g. malate (PMID 16143825). Mutations in the four genes encoding the subunits of the mitochondrial succinate dehydrogenase are associated with a wide spectrum of clinical presentations, i.e.: Huntington's disease (PMID 11803021). Moreover, succinic acid is found to be associated with D-2-hydroxyglutaric aciduria, which is an inborn error of metabolism. Succinic acid has recently been identified as an oncometabolite or an endogenous, cancer causing metabolite. High levels of this organic acid can be found in tumors or biofluids surrounding tumors. Its oncogenic action appears to due to its ability to inhibit prolyl hydroxylase-containing enzymes. In many tumours, oxygen availability becomes limited (hypoxia) very quickly due to rapid cell proliferation and limited blood vessel growth. The major regulator of the response to hypoxia is the HIF transcription factor (HIF-alpha). Under normal oxygen levels, protein levels of HIF-alpha are very low due to constant degradation, mediated by a series of post-translational modification events catalyzed by the prolyl hydroxylase domain-containing enzymes PHD1, 2 and 3, (also known as EglN2, 1 and 3) that hydroxylate HIF-alpha and lead to its degradation. All three of the PHD enzymes are inhibited by succinate. Succinic acid is found to be associated with D-2-hydroxyglutaric aciduria, which is an inborn error of metabolism.

This compound belongs to the class of organic compounds known as dicarboxylic acids and derivatives. These are organic compounds containing exactly two carboxylic acid groups.

### Succinic acid -- 2-Ketoglutarate dehydrogenase complex deficiency

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## Pyroglutamic acid -- Introduction

**SYNONYM:** (-)-2-Pyrrolidone-5-carboxylic acid; (S)-(-)-2-Pyrrolidone-5-carboxylic acid; (S)-Pyroglutamic acid; 5-Pyrrolidone-2-carboxylic acid; L-5-Pyrrolidone-2-carboxylic acid; L-Pyroglutamic acid; Pidolic acid; Pyroglutamate; (-)-2-Pyrrolidone-5-carboxylate; (S)-(-)-2-Pyrrolidone-5-carboxylate; (S)-Pyroglutamate; 5-Pyrrolidone-2-carboxylate; L-5-Pyrrolidone-2-carboxylate; L-Pyroglutamate; Pidolate; (-)-Pyroglutamate; (-)-Pyroglutamic acid; (5S)-2-Oxopyrrolidine-5-carboxylate; (5S)-2-Oxopyrrolidine-5-carboxylic acid; (S)-(-)-g-Butyrolactam-g-carboxylate; (S)-(-)-g-Butyrolactam-g-carboxylic acid; (S)-(-)-gamma-Butyrolactam-gamma-carboxylate; (S)-(-)-gamma-Butyrolactam-gamma-carboxylic acid; (S)-2-Pyrrolidone-5-carboxylate; (S)-2-Pyrrolidone-5-carboxylic acid; (S)-5-oxo-2-Pyrrolidinecarboxylate; (S)-5-oxo-2-Pyrrolidinecarboxylic acid; 2-L-Pyrrolidone-5-carboxylate; 2-L-Pyrrolidone-5-carboxylic acid; 2-Oxopyrrolidine-5(S)-carboxylate; 2-Oxopyrrolidine-5(S)-carboxylic acid; 2-Pyrrolidinone-5-carboxylate; 2-Pyrrolidinone-5-carboxylic acid; 5-Carboxy-2-pyrrolidinone; 5-L-Oxoproline; 5-oxo-L-Proline; 5-Oxoproline; 5-Pyrrolidinone-2-carboxylate; 5-Pyrrolidinone-2-carboxylic acid; Ajidew a 100; Glutimate; Glutimic acid; Glutiminate; Glutiminic acid; L-2-Pyrrolidone-5-carboxylate; L-2-Pyrrolidone-5-carboxylic acid; L-5-Carboxy-2-pyrrolidinone; L-5-oxo-2-Pyrrolidinecarboxylate; L-5-oxo-2-Pyrrolidinecarboxylic acid; L-5-Oxoproline; L-Glutamic acid g-lactam; L-Glutimate; L-Glutimic acid; L-Glutiminate; L-Glutiminic acid; L-Pyrrolidinonecarboxylate; L-Pyrrolidinonecarboxylic acid; L-Pyrrolidonecarboxylate; L-Pyrrolidonecarboxylic acid; Oxoproline; Oxopyrrolidinonecarboxylate; Oxopyrrolidinecarboxylic acid; Pidolidone; Pyrrolidinonecarboxylate; Pyrrolidinonecarboxylic acid; Pyrrolidone-5-carboxylate; Pyrrolidone-5-carboxylic acid; Pyrrolidonecarboxylic acid; 5-Ketoproline; Pidolate, magnesium; 5-Oxopyrrolidine-2-carboxylic acid; Magnesium pidolate

HMDB: HMDB0000267; HMDB00267

CAS: 98-79-3

Pyroglutamic acid (5-oxoproline) is a cyclized derivative of L-glutamic acid. It is an uncommon amino acid derivative in which the free amino group of glutamic acid cyclizes to form a lactam. It is formed nonenzymatically from glutamate, glutamine, and gamma-glutamylated peptides, but it can also be produced by the action of gamma-glutamylcyclotransferase on an L-amino acid. Elevated blood levels may be associated with problems of glutamine or glutathione metabolism. This compound is found in substantial amounts in brain tissue and other tissues in bound form, especially skin. It is also present in plant tissues. It is sold, over the counter, as a "smart drug" for improving blood circulation in the brain. Pyroglutamate in the urine is a biomarker for the consumption of cheese. When present in sufficiently high levels, pyroglutamic acid can act as an acidogen and a metabotoxin. An acidogen is an acidic compound that induces acidosis, which has multiple adverse effects on many organ systems. A metabotoxin is an endogenously produced metabolite that causes adverse health effects at chronically high levels. Chronically high levels of pyroglutamic acid are associated with at least five inborn errors of metabolism including 5-oxoprolinuria, 5-oxoprolinase deficiency, glutathione synthetase deficiency, hawkinsinuria, and propionic acidemia. Pyroglutamic acid is an organic acid. Abnormally high levels of organic acids in the blood (organic acidemia), urine (organic aciduria), the brain, and other tissues lead to general metabolic acidosis. Acidosis typically occurs when arterial pH falls below 7.35. In infants with acidosis the initial symptoms include poor feeding, vomiting, loss of appetite, weak muscle tone (hypotonia), and lack of energy (lethargy). These can progress to heart, liver, and kidney abnormalities, seizures, coma, and possibly death. These are also the characteristic symptoms of the untreated IEMs mentioned above. Many affected children with organic acidemias experience intellectual disability or delayed development. In adults, acidosis or acidemia is characterized by headaches, confusion, feeling tired, tremors, sleepiness, and seizures.

This compound belongs to the class of organic compounds known as alpha amino acids and derivatives. These are amino acids in which the amino group is attached to the carbon atom immediately adjacent to the carboxylate group (alpha carbon), or a derivative thereof.



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### Pyroglutamic acid -- 5-oxoprolinase deficiency



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### Sphinganine -- Introduction



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SYNONYM: (2S,3R)-2-amino-1,3-Octadecanediol; (2S,3R)-2-Amino-octadecane-1,3-diol; (R-(R\*,S\*))-2-amino-octadecane-1,3-diol; 2-amino-1,3-Dihydroxyoctadecane; C18-Dihydrosphingosine; C18-Sphinganine; D-erythro-1,3-Dihydroxy-2-amino-octadecane; D-erythro-2-amino-1,3-Octadecanediol; D-erythro-C18-Dihydrosphingosine; D18:0; Dihydrosphingosine; Octadecaspinganine; Safingol; 2-amino-D-erythro-1,3-Octadecanediol; C18-dihydro-Sphingosine; D-erythro-Sphinganine; dihydro-C18-Sphingosine; erythro-Sphinganine; [R-(R\*,S\*)]-2-amino-1,3-octadecanediol; Safingol, (R-(r\*,r\*))-isomer; Safingol, ((r\*,s\*)-(+))-isomer; erythro-D-Sphinganine; Safingol, (S-(r\*,s\*))-isomer; 2-Amino-octadecane-1,3-diol; Safingol hydrochloride; Saginfol; threo-Dihydrosphingosine

HMDB: HMDB0000269; HMDB00269

CAS: 764-22-7

Sphinganine is a blocker postlysosomal cholesterol transport by inhibition of low-density lipoprotein-induced esterification of cholesterol and cause unesterified cholesterol to accumulate in perinuclear vesicles. It has been suggested the possibility that endogenous sphinganine may inhibit cholesterol transport in Niemann-Pick Type C (NPC) disease. (PMID 1817037).

This compound belongs to the class of organic compounds known as 1,2-aminoalcohols. These are organic compounds containing an alkyl chain with an amine group bound to the C1 atom and an alcohol group bound to the C2 atom.

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## Thymidine -- Introduction

**SYNONYM:** 1-(2-Deoxy-beta-D-erythro-pentofuranosyl)-5-methylpyrimidine-2,4(1H,3H)-dione; 2'-Deoxy-5-methyluridine; 2'-Deoxythymidine; 2'-Thymidine; 5-Methyl-2'-deoxyuridine; Deoxythymidine; DTHD; T; Thymine 2'-deoxyriboside; 1-(2-Deoxy-b-D-erythro-pentofuranosyl)-5-methylpyrimidine-2,4(1H,3H)-dione; 1-(2-Deoxy- $\beta$ -D-erythro-pentofuranosyl)-5-methylpyrimidine-2,4(1H,3H)-dione; 1-(2-Deoxy-b-D-erythro-pentofuranosyl)-5-methyl-2,4(1H,3H)-pyrimidinedione; 1-(2-Deoxy-beta-delta-erythro-pentofuranosyl)-5-methyl-2,4(1H,3H)-pyrimidinedione; 1-[4-Hydroxy-5-(hydroxymethyl)oxolan-2-yl]-5-methyl-pyrimidine-2,4-dione; 2'-Deoxy-5-methyl-uridine; 5-Methyldeoxyuridine; Deoxyribothymidine; DT; DThyd; Thymidin; Thymine 2'-desoxyriboside; Thymine deoxyriboside; Thymine-1 2-deoxy-b-D-ribofuranoside; Thymine-1 2-deoxy-beta-delta-ribofuranoside; 2' Deoxythymidine

**HMDB:** HMDB0000273; HMDB00273

**CAS:** 50-89-5

Thymidine is non-toxic and is a naturally occurring compound that exists in all living organisms and DNA viruses. 25% of DNA is composed of thymidine. RNA does not have thymidine and has uridine instead. Thymidine is a chemical compound which is a pyrimidine nucleoside. Thymidine is the DNA base T, which pairs with adenine in double stranded DNA.

This compound belongs to the class of organic compounds known as pyrimidine 2'-deoxyribonucleosides. These are compounds consisting of a pyrimidine linked to a ribose which lacks a hydroxyl group at position 2.

## Thymidine -- Canavan disease

Wevers RA, Engelke U, Wendel U, de Jong JG, Gabreels FJ, Heerschap A: Standardized method for high-resolution 1H-NMR of cerebrospinal fluid. *Clin Chem.* 1995 May;41(5):744-51. PMID: 7729054

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## Thymidine -- Colorectal cancer

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Silke Matysik, Caroline Ivonne Le Roy, Gerhard Liebisch, Sandrine Paule Claus. Metabolomics of fecal samples: A practical consideration. Trends in Food Science & Technology. Vol. 57, Part B, Nov. 2016, p.244-255:  
<http://www.sciencedirect.com/science/article/pii/S0924224416301984> PMID: 7482520

### Thymidine -- Degenerative disc disease

Eells JT, Spector R: Purine and pyrimidine base and nucleoside concentrations in human cerebrospinal fluid and plasma. Neurochem Res. 1983 Nov;8(11):1451-7. PMID: 6656991

### Thymidine -- Thymidine phosphorylase deficiency

Bakker JA, Schlessner P, Smeets HJ, Francois B, Bierau J: Biochemical abnormalities in a patient with thymidine phosphorylase deficiency with fatal outcome. J Inherit Metab Dis. 2010 Dec;33 Suppl 3:S139-43. doi: 10.1007/s10545-010-9049-y. Epub 2010 Feb 12. PMID: 20151198

### Xanthine -- Introduction

SYNONYM: 2,6-Dihydroxypurine; 2,6-dioxo-1,2,3,6-Tetrahydropurine; 9H-Purine-2,6-(1H,3H)-dione; Purine-2(3H),6(1H)-dione; Xan; 1H-Purine-2,6-diol; 2,6(1,3)-Purinedion; 2,6-Dioxopurine; 3,7-dihydro-1H-Purine-2,6-dione; 3,7-Dihydropurine-2,6-dione; 9H-Purine-2,6(1H,3H)-dione; 9H-Purine-2,6-diol; Dioxopurine; Isoxanthine; Pseudoxanthine; Purine-2,6(1H,3H)-dione; Purine-2,6-diol; Xanthic oxide; Xanthin

HMDB: HMDB0000292; HMDB00292

CAS: 69-89-6

Xanthine is a purine base found in most body tissues and fluids, certain plants, and some urinary calculi. It is an intermediate in the degradation of adenosine monophosphate to uric acid, being formed by oxidation of hypoxanthine. The methylated xanthine compounds caffeine, theobromine, and theophylline and their derivatives are used in medicine for their bronchodilator effects (Dorland, 28th ed.). Xanthine is found to be associated with Lesch-Nyhan syndrome and xanthinuria type I, which are inborn errors of metabolism.

This compound belongs to the class of organic compounds known as xanthines. These are purine derivatives with a ketone group conjugated at carbons 2 and 6 of the purine moiety.

### Xanthine -- 3-Methylcrotonyl-glycinuria

Koeberl DD, Millington DS, Smith WE, Weavil SD, Muenzer J, McCandless SE, Kishnani PS, McDonald MT, Chaing S, Boney A, Moore E, Frazier DM: Evaluation of 3-methylcrotonyl-CoA carboxylase deficiency detected by tandem mass spectrometry newborn screening. J Inherit Metab Dis. 2003;26(1):25-35. PMID: 12872837

Rutledge SL, Berry GT, Stanley CA, van Hove JL, Millington D: Glycine and L-carnitine therapy in 3-methylcrotonyl-CoA carboxylase deficiency. J Inherit Metab Dis. 1995;18(3):299-305. PMID: 7474896

Thomsen JA, Lund AM, Olesen JH, Mohr M, Rasmussen J: Is L-Carnitine Supplementation Beneficial in 3-Methylcrotonyl-CoA Carboxylase Deficiency? JIMD Rep. 2015;21:79-88. doi: 10.1007/8904\_2014\_393. Epub 2015 Mar 3. PMID: 25732994

de Kremer RD, Latini A, Suormala T, Baumgartner ER, Larovere L, Civallero G, Guelbert N, Paschini-Capra A, Depetris-Boldini C, Mayor CQ: Leukodystrophy and CSF purine abnormalities associated with isolated 3-methylcrotonyl-CoA carboxylase deficiency. Metab Brain Dis. 2002 Mar;17(1):13-8. PMID: 11893004

### Xanthine -- Canavan disease

Wevers RA, Engelke U, Wendel U, de Jong JG, Gabreels FJ, Heerschap A: Standardized method for high-resolution 1H-NMR of cerebrospinal fluid. Clin Chem. 1995 May;41(5):744-51. PMID: 7729054

Rothstein JD, Tsai G, Kuncl RW, Clawson L, Cornblath DR, Drachman DB, Pestronk A, Stauch BL, Coyle JT: Abnormal excitatory amino acid metabolism in amyotrophic lateral sclerosis. Ann Neurol. 1990 Jul;28(1):18-25. PMID: 2375630



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Burlina AP, Ferrari V, Burlina AB, Ermani M, Boespflug-Tanguy O, Bertini E: N-acetylaspartyglutamate (NAAG) in Pelizaeus-Merzbacher disease. *Adv Exp Med Biol*. 2006;576:353-9; discussion 361-3. doi: 10.1007/0-387-30172-0\_26. PMID: 16802726

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## Xanthine – Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. *Tohoku J Exp Med*. 1995 May;176(1):61-8. PMID: 7482520

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Phua LC, Chue XP, Koh PK, Cheah PY, Ho HK, Chan EC: Non-invasive fecal metabonomic detection of colorectal cancer. *Cancer Biol Ther*. 2014 Apr;15(4):389-97. doi: 10.4161/cbt.27625. Epub 2014 Jan 14. PMID: 24424155

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Goedert JJ, Sampson JN, Moore SC, Xiao Q, Xiong X, Hayes RB, Ahn J, Shi J, Sinha R: Fecal metabolomics: assay performance and association with colorectal cancer. *Carcinogenesis*. 2014 Sep;35(9):2089-96. doi: 10.1093/carcin/bgu131. Epub 2014 Jul 18. PMID: 25037050

Sinha R, Ahn J, Sampson JN, Shi J, Yu G, Xiong X, Hayes RB, Goedert JJ: Fecal Microbiota, Fecal Metabolome, and



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## Xanthine – Crohn's disease

Lapidus A, Akerlund JE, Einarsson C: Gallbladder bile composition in patients with Crohn's disease. World J Gastroenterol. 2006 Jan 7;12(1):70-4. PMID: 16440420

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Walton C, Fowler DP, Turner C, Jia W, Whitehead RN, Griffiths L, Dawson C, Waring RH, Ramsden DB, Cole JA, Cauchi M, Bessant C, Hunter JO: Analysis of volatile organic compounds of bacterial origin in chronic gastrointestinal diseases. Inflamm Bowel Dis. 2013 Sep;19(10):2069-78. doi: 10.1097/MIB.0b013e31829a91f6. PMID: 23867873

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### Xanthine -- Cystic fibrosis

Matsui A, Psacharopoulos HT, Mowat AP, Portmann B, Murphy GM: Radioimmunoassay of serum glycocholic acid, standard laboratory tests of liver function and liver biopsy findings: comparative study of children with liver disease. J Clin Pathol. 1982 Sep;35(9):1011-7. PMID: 7119120

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### Xanthine -- Degenerative disc disease

Eells JT, Spector R: Purine and pyrimidine base and nucleoside concentrations in human cerebrospinal fluid and plasma. Neurochem Res. 1983 Nov;8(11):1451-7. PMID: 6656991

### Xanthine -- Hydrocephalus

Castro-Gago M, Rodriguez IN, Rodriguez-Nunez A, Guitian JP, Rocamonde SL, Rodriguez-Segade S: Therapeutic criteria in hydrocephalic children. Childs Nerv Syst. 1989 Dec;5(6):361-3. PMID: 2611770

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Westcott JY, Murphy RC, Stenmark K: Eicosanoids in human ventricular cerebrospinal fluid following severe brain injury. Prostaglandins. 1987 Dec;34(6):877-87. PMID: 2835791

### Xanthine -- Lesch-Nyhan syndrome

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## Xanthine -- Sulfite oxidase deficiency, ISOLATED

Touati G, Rusthoven E, Depondt E, Dorche C, Duran M, Heron B, Rabier D, Russo M, Saudubray JM: Dietary therapy in two patients with a mild form of sulphite oxidase deficiency. Evidence for clinical and biological improvement. *J Inherit Metab Dis.* 2000 Feb;23(1):45-53. PMID: 10682307

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Rocha S, Ferreira AC, Dias AI, Vieira JP, Sequeira S: Sulfite oxidase deficiency--an unusual late and mild presentation. *Brain Dev.* 2014 Feb;36(2):176-9. doi: 10.1016/j.braindev.2013.01.013. Epub 2013 Feb 27. PMID: 23452914

## Xanthine -- Xanthinuria type 1

Mateos FA, Puig JG, Jimenez ML, Fox IH: Hereditary xanthinuria. Evidence for enhanced hypoxanthine salvage. *J Clin Invest.* 1987 Mar;79(3):847-52. PMID: 3818951

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Eggermann T, Spengler S, Denecke B, Zerres K, Mache CJ: Multi-exon deletion in the XDH gene as a cause of classical xanthinuria. *Clin Nephrol.* 2013 Jan;79(1):78-80. PMID: 23249873

## Xanthine -- Molybdenum cofactor deficiency

Wevers RA, Engelke UF, Moolenaar SH, Brautigam C, de Jong JG, Duran R, de Abreu RA, van Gennip AH: 1H-NMR spectroscopy of body fluids: inborn errors of purine and pyrimidine metabolism. *Clin Chem.* 1999 Apr;45(4):539-48. PMID: 10102915

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## Xanthine -- Xanthinuria type II

Zannolli R, Micheli V, Mazzei MA, Sacco P, Piomboni P, Bruni E, Miracco C, de Santi MM, Terrosi Vagnoli P, Volterrani L, Pellegrini L, Livi W, Lucani B, Gonnelli S, Burlina AB, Jacomelli G, Macucci F, Pucci L, Fimiani M, Swift JA, Zappella M, Morgese G: Hereditary xanthinuria type II associated with mental delay, autism, cortical renal cysts, nephrocalcinosis, osteopenia, and hair and teeth defects. *J Med Genet.* 2003 Nov;40(11):e121. PMID: 14627688

## Xanthine -- Adenosine kinase deficiency

Bjursell MK, Blom HJ, Cayuela JA, Engvall ML, Lesko N, Balasubramaniam S, Brandberg G, Halldin M, Falkenberg M, Jakobs C, Smith D, Struys E, von Dobeln U, Gustafsson CM, Lundeberg J, Wedell A: Adenosine kinase deficiency disrupts the methionine cycle and causes hypermethioninemia, encephalopathy, and abnormal liver function. *Am J Hum Genet.* 2011 Oct 7;89(4):507-15. doi: 10.1016/j.ajhg.2011.09.004. Epub 2011 Sep 28. PMID: 21963049

## Xanthine -- Molybdenum co-factor deficiency



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### Xanthine -- Phosphoribosylpyrophosphate Synthetase Superactivity

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## Uridine -- Introduction

SYNONYM: 1-beta-D-Ribofuranosylpyrimidine-2,4(1H,3H)-dione; 1-beta-D-Ribofuranosyluracil; beta-Uridine; u; Urd; Uridin; 1-b-D-Ribofuranosylpyrimidine-2,4(1H,3H)-dione; 1- $\hat{D}$ -ribofuranosylpyrimidine-2,4(1H,3H)-dione; 1-b-D-Ribofuranosyluracil; 1- $\hat{D}$ -ribofuranosyluracil; b-Uridine;  $\hat{D}$ -uridine; 1-b-D-Ribofuranosyl-2,4(1H,3H)-pyrimidinedione; 1-beta-delta-Ribofuranosyl-2,4(1H,3H)-pyrimidinedione; 1-beta-delta-Ribofuranosyluracil; b-D-Ribofuranoside 2,4(1H,3H)-pyrimidinedione-1; beta-delta-Ribofuranoside 2,4(1H,3H)-pyrimidinedione-1; allo Uridine; allo-Uridine; Allouridine

HMDB: HMDB0000296; HMDB00296

CAS: 58-96-8

Uridine, also known as beta-uridine or 1-beta-D-ribofuranosylpyrimidine-2,4(1H,3H)-dione, is a member of the class of compounds known as pyrimidine nucleosides. Pyrimidine nucleosides are compounds comprising a pyrimidine base attached to a ribosyl or deoxyribosyl moiety. More specifically, uridine is a nucleoside consisting of uracil and D-ribose and a component of RNA. Uridine is soluble (in water) and a very weakly acidic compound (based on its pKa). Uridine can be synthesized from uracil. It is one of the five standard nucleosides which make up nucleic acids, the others being adenosine, thymidine, cytidine and guanosine. The five nucleosides are commonly abbreviated to their one-letter codes U, A, T, C and G respectively. Uridine is also a parent compound for other transformation products, including but not limited to, nikkomycin Z, 3'-(enolpyruvyl)uridine 5'-monophosphate, and 5-aminomethyl-2-thiouridine. Uridine can be found in most biofluids, including urine, breast milk, cerebrospinal fluid (CSF), and blood. Within the cell, uridine is primarily located in the mitochondria, in the nucleus and the lysosome. It can also be found in the extracellular space. As an essential nucleoside, uridine exists in all living species, ranging from bacteria to humans. In humans, uridine is involved in several metabolic disorders, some of which include dhydroxyuridylate deficiency, MNGIE (mitochondrial neurogastrointestinal encephalopathy), and beta-ureidopropionase deficiency. Moreover, uridine is found to be associated with Lesch-Nyhan syndrome, which is an inborn error of metabolism. Uridine is a nucleoside consisting of uracil and D-ribose and a component of RNA. Uridine plays a role in the glycolysis pathway of galactose. In humans there is no catabolic process to metabolize galactose. Therefore, galactose is converted to glucose and metabolized via the normal glucose metabolism pathways. More specifically, consumed galactose is converted into galactose 1-phosphate (Gal-1-P). This molecule is a substrate for the enzyme galactose-1-phosphate uridylyl transferase which transfers a UDP molecule to the galactose molecule. The end result is UDP-galactose and glucose-1-phosphate. This process is continued to allow the proper glycolysis of galactose. Uridine is found in many foods (anything containing RNA) but is destroyed in the liver and gastrointestinal tract, and so no food, when consumed, has ever been reliably shown to elevate blood uridine levels. On the other hand, consumption of RNA-rich foods may lead to high levels of purines (adenine and guanosine) in blood. High levels of purines are known to increase uric acid production and may aggravate or lead to conditions such as gout.

This compound belongs to the class of organic compounds known as pyrimidine nucleosides. These are compounds comprising a pyrimidine base attached to a ribosyl or deoxyribosyl moiety.

## Uridine -- Argininemia

Michels VV, Beaudet AL: Arginase deficiency in multiple tissues in argininemia. Clin Genet. 1978 Jan;13(1):61-7. PMID: 624188

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## Uracil -- Introduction

**SYNONYM:** 2,4(1H,3H)-Pyrimidinedione; 2,4-Dioxopyrimidine; 2,4-Pyrimidinedione; U; Ura; Urazil; 2,4-Dihydroxypyrimidine; 2,4-Pyrimidinediol; Hybar X; Pirod; Pyrod

**HMDB:** HMDB0000300; HMDB00300

**CAS:** 66-22-8

Uracil is a common naturally occurring pyrimidine found in RNA, it base pairs with adenine and is replaced by thymine in DNA. Methylation of uracil produces thymine. Uracil's use in the body is to help carry out the synthesis of many enzymes necessary for cell function through bonding with riboses and phosphates. Uracil serves as allosteric regulator and coenzyme for many important biochemical reactions. UDP and UTP regulate CPSase II activity in animals. UDP-glucose regulates the conversion of glucose to galactose in the liver and other tissues in the process of carbohydrate metabolism. Uracil is also involved in the biosynthesis of polysaccharides and the transportation of sugars containing aldehydes. Uracil is found to be associated with argininemia and carbamoyl phosphate synthetase deficiency, which are inborn errors of metabolism.

This compound belongs to the class of organic compounds known as pyrimidones. These are compounds that contain a pyrimidine ring, which bears a ketone. Pyrimidine is a 6-membered ring consisting of four carbon atoms and two nitrogen centers at the 1- and 3- ring positions.

## Uracil -- Argininemia

Michels VV, Beaudet AL: Arginase deficiency in multiple tissues in argininemia. *Clin Genet.* 1978 Jan;13(1):61-7. PMID: 624188

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## Uracil -- Carbamoyl Phosphate Synthetase Deficiency

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### Uracil -- Cerebral infarction

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## Urocanic acid -- Introduction

SYNONYM: (2E)-3-(1H-Imidazol-4-yl)acrylic acid; (e)-3-(1H-Imidazol-4-yl)-2-propenoic acid; (2E)-3-(1H-Imidazol-4-yl)acrylate; Urocanate; (e)-3-(1H-Imidazol-4-yl)-2-propenoate; 3-(1H-Imidazol-4-yl)-2-propenoate; 3-(1H-Imidazol-4-yl)-2-propenoic acid; 3-(1H-Imidazol-4-yl)acrylate; 3-(1H-Imidazol-4-yl)acrylic acid; 3-(4-Imidazolyl)acrylate; 3-(4-Imidazolyl)acrylic acid; 5-Imidazoleacrylate; 5-Imidazoleacrylic acid; Imidazole-4-acrylate; Imidazole-4-acrylic acid; Imidazoleacrylic acid; Acid, glyoxalinyacrylic; Acid, urocanic; Glyoxalinyacrylic acid

HMDB: HMDB0000301; HMDB0002280; HMDB00301; HMDB02280

CAS: 104-98-3

Urocanic acid is a breakdown (deamination) product of histidine. In the liver, urocanic acid is an intermediate in the conversion of histidine to glutamic acid, whereas in the epidermis, it accumulates and may be both a UV protectant and an immunoregulator. Urocanic acid (UA) exists as a trans isomer (t-UA, approximately 30 mg/cm<sup>2</sup>) in the uppermost layer of the skin (stratum corneum). t-UA is formed as the cells of the second layer of skin become metabolically inactive. During this process, proteins and membranes degrade, histidine is released, and histidase (histidine ammonia lyase) catalyzes the deamination of histidine to form t-UA. t-UA accumulates in the epidermis until removal by either the monthly skin renewal cycle or sweat. Upon absorption of UV light, the naturally occurring t-UA isomerizes to its cis form, c-UA. Because DNA lesions (e.g., pyrimidine dimers) in the lower epidermis can result from UV-B absorption, initial research proposed that t-UA acted as a natural sunscreen absorbing UV-B in the stratum corneum before the damaging rays could penetrate into lower epidermal zones. Researchers have found that c-UA also suppresses contact hypersensitivity and delayed hypersensitivity, reduces the Langerhans cell count in the epidermis, prolongs skin-graft survival time, and affects natural killer cell activity.



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This compound belongs to the class of organic compounds known as imidazolyl carboxylic acids and derivatives. These are organic compounds containing a carboxylic acid chain (of at least 2 carbon atoms) linked to an imidazole ring.

## Urocanic acid -- Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. *Tohoku J Exp Med.* 1995 May;176(1):61-8. PMID: 7482520

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## Citramalic acid -- Introduction

SYNONYM: (+)-2-Hydroxy-2-methylsuccinic acid; 2-Hydroxy-2-methylbutanedioic acid; 2-Hydroxy-2-methylsuccinic acid; 2-Methylmalic acid; alpha-Hydroxypyrotartaric acid; Citramalic acids; (+)-2-Hydroxy-2-methylsuccinate; Citramalate; 2-Hydroxy-2-methylbutanedioate; 2-Hydroxy-2-methylsuccinate; 2-Methylmalate; a-Hydroxypyrotartarate; a-Hydroxypyrotartaric acid; alpha-Hydroxypyrotartarate; l(+)-hydroxypyrotartarate; l(+)-hydroxypyrotartaric acid; (b)-2-Methylmalate; (b)-2-Methylmalic acid; (b)-Citramalate; (b)-Citramalic acid; (R,S)-(b)-Citramalate; (R,S)-(b)-Citramalic acid; (R,S)-b-Methylmalate; (R,S)-b-Methylmalic acid; (R,S)-beta-Methylmalate; (R,S)-beta-Methylmalic acid; 2-Deoxy-3-C-methyltetraurate; 2-Deoxy-3-C-methyltetric acid; 2-Hydroxy-2-methyl-(b)-butanedioate; 2-Hydroxy-2-methyl-(b)-butanedioic acid; 2-Hydroxy-2-methyl-butanedioate; 2-Hydroxy-2-methyl-butanedioic acid; 2-Methyl-(b)-malate; 2-Methyl-(b)-malic acid; DL-Citramalate; DL-Citramalic acid; Citramalate, (+)-isomer; Citramalate, (R)-isomer; Citramalate, (S)-isomer; alpha-Methylmalate

HMDB: HMDB0000426; HMDB00426

CAS: 597-44-4

Citramalic acid is an analog of malic acid. The structure of citramalic acid is similar to the structure of malic acid except it has an extra CH<sub>3</sub> group on it. It can inhibit the production of malic acid.

This compound belongs to the class of organic compounds known as hydroxy fatty acids. These are fatty acids in which the chain bears a hydroxyl group.

## Citramalic acid -- Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. Tohoku J Exp Med. 1995 May;176(1):61-8. PMID: 7482520

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## Allantoin -- Introduction

SYNONYM: (2,5-dioxo-4-Imidazolidinyl)urea; 2,5-dioxo-4-Imidazolidinyl-urea; 4-ureido-2,5-Imidazolidinedione; 5-ureido-2,4-Imidazolidindione; 5-Ureidohydantoin; Glyoxyldiureide; N-(2,5-dioxo-4-Imidazolidinyl)urea; (S)-Allantoin; 5-ureido-Hydantoin; 5-Ureidohydrantoin; Alantan; Allantol; Alloxantin; AVC/Dienestrolcream; Cordianine; D00121; Fancol toin; Glyoxyldiureid; Glyoxylic diureide; Psoralon; Sebical; Septalan; Sween brand OF allantoin; Herpecin-L; HerpecinL; Reed and carnrick brand OF allantoin; Woun'dres; Allantoin sween brand; Campbell brand OF allantoin; Allantoin campbell brand; Herpecin L

HMDB: HMDB0000462; HMDB00462

CAS: 97-59-6

Allantoin is a diureide of glyoxylic acid with the chemical formula C<sub>4</sub>H<sub>6</sub>N<sub>4</sub>O<sub>3</sub>. It is also called 5-ureidohydantoin or glyoxyldiureide. It is a product of the oxidation of uric acid. It is also a product of purine metabolism in most mammals except for higher apes, and it is present in their urine. In humans, uric acid is excreted instead of allantoin. The presence of allantoin in the urine can be an indication of microbial overgrowth or it can be created via non-enzymatic means through high levels of reactive oxygen species. In this regard, allantoin is sometimes used as a marker of oxidative stress. Allantoin can be isolated from cow urine or as a botanical extract of the comfrey plant. It has long been used for its healing, soothing, and anti-irritating properties. Allantoin helps to heal wounds and skin irritations and stimulates the growth of healthy tissue. Allantoin can be found in anti-acne products, sun care products, and clarifying lotions because of its ability to help heal minor wounds and promote healthy skin. Allantoin is frequently present in toothpaste, mouthwash, and other oral hygiene products as well as in shampoos, lipsticks, various cosmetic lotions and creams, and other cosmetic and pharmaceutical products.

This compound belongs to the class of organic compounds known as imidazoles. These are compounds containing an imidazole ring, which is an aromatic five-member ring with two nitrogen atoms at positions 1 and 3, and three carbon atoms.



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## Allantoin -- Chronic renal failure

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### 3-Methylhistidine -- Introduction

SYNONYM: (2S)-2-amino-3-(1-Methyl-1H-imidazol-5-yl)propanoic acid; 3-Methyl-L-histidine; N(Pai)-methyl-L-histidine; N-pros-Methyl-L-histidine; Tau-methylhistidine; (2S)-2-amino-3-(1-Methyl-1H-imidazol-5-yl)propanoate; 3-N-Methyl-L-histidine; L-3-Methylhistidine; N(Pi)-methyl-L-histidine; N(pros)-Methyl-L-histidine; N3-Methyl-L-histidine; Pi-methyl-L-histidine; Tau-methyl-L-histidine; 3-Methylhistidine hydride; N(Tau)-methylhistidine; 3-Methylhistidine dihydrochloride

HMDB: HMDB0000479; HMDB00479

CAS: 368-16-1

3-Methylhistidine is a product of peptide bond synthesis and methylation of actin and myosin. The measurement of 3-methylhistidine provides an index of the rate of muscle protein breakdown. 3-Methylhistidine is a biomarker for meat consumption, especially chicken. It is also a biomarker for the consumption of soy products.

This compound belongs to the class of organic compounds known as histidine and derivatives. These are compounds containing cysteine or a derivative thereof resulting from reaction of cysteine at the amino group or the carboxy group, or from



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the replacement of any hydrogen of glycine by a heteroatom.

### 3-Methylhistidine -- Alzheimer's disease

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### L-Arginine -- Introduction

SYNONYM: (2S)-2-amino-5-(carbamimidamido)Pentanoic acid; (2S)-2-amino-5-Guanidinopentanoic acid; (S)-2-amino-5-Guanidinopentanoic acid; (S)-2-amino-5-Guanidinovaleric acid; Arg; Arginine; L-(+)-Arginine; L-Arg; L-Arginin; R; (2S)-2-amino-5-(carbamimidamido)Pentanoate; (2S)-2-amino-5-Guanidinopentanoate; (S)-2-amino-5-Guanidinopentanoate; (S)-2-amino-5-Guanidinovalerate; (S)-2-amino-5-[(Aminoiminomethyl)amino]-pentanoate; (S)-2-amino-5-[(Aminoiminomethyl)amino]-pentanoic acid; (S)-2-amino-5-[(Aminoiminomethyl)amino]pentanoate; (S)-2-amino-5-[(Aminoiminomethyl)amino]pentanoic acid; 2-amino-5-Guanidinovalerate; 2-amino-5-Guanidinovaleric acid; 5-[(Aminoiminomethyl)amino]-L-norvaline; L-a-amino-D-Guanidinovalerate; L-a-amino-D-Guanidinovaleric acid; L-alpha-amino-delta-Guanidinovalerate; L-alpha-amino-delta-Guanidinovaleric acid; N5-(Aminoiminomethyl)-L-ornithine; DL-Arginine acetate, monohydrate; L-Isomer arginine; Monohydrate DL-arginine acetate; L Arginine; Arginine, L isomer; Arginine, L-isomer; Hydrochloride, arginine; Arginine hydrochloride; DL Arginine acetate, monohydrate

HMDB: HMDB0000517; HMDB00517

CAS: 74-79-3

Arginine is an essential amino acid that is physiologically active in the L-form. In mammals, arginine is formally classified as a semi-essential or conditionally essential amino acid, depending on the developmental stage and health status of the individual. Infants are unable to effectively synthesize arginine, making it nutritionally essential for infants. Adults, however, are able to synthesize arginine in the urea cycle. Arginine can be considered to be a basic amino acid as the part of the side chain nearest to the backbone is long, carbon-containing, and hydrophobic, whereas the end of the side chain is a complex guanidinium group. With a pKa of 12.48, the guanidinium group is positively charged in neutral, acidic, and even most basic environments. Because of the conjugation between the double bond and the nitrogen lone pairs, the positive charge is delocalized. This group is able to form multiple H-bonds. L-Arginine is an amino acid that has numerous functions in the body. It helps dispose of ammonia, is used to make compounds such as nitric oxide, creatine, L-glutamate, and L-proline, and it can be converted into glucose and glycogen if needed. In large doses, L-arginine also stimulates the release of the hormones growth hormone and prolactin. Arginine is a known inducer of mTOR (mammalian target of rapamycin) and is responsible for inducing protein synthesis through the mTOR pathway. mTOR inhibition by rapamycin partially reduces arginine-induced protein synthesis (PMID: 20841502). Catabolic disease states such as sepsis, injury, and cancer cause an increase in arginine utilization, which can exceed normal body production, leading to arginine depletion. Arginine also activates AMP kinase (AMPK) which then stimulates skeletal muscle fatty acid oxidation and muscle glucose uptake, thereby increasing insulin secretion by pancreatic beta-cells (PMID: 21311355). Arginine is found in plant and animal proteins, such as dairy products, meat, poultry, fish, and nuts. The ratio of L-arginine to lysine is also important: soy and other plant proteins have more L-arginine than animal sources of protein.

This compound belongs to the class of organic compounds known as l-alpha-amino acids. These are alpha amino acids which have the L-configuration of the alpha-carbon atom.



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## L-Arginine – Alzheimer's disease

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## L-Arginine -- Early preeclampsia

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## L-Arginine -- Late-onset preeclampsia

Bahado-Singh RO, Akolekar R, Mandal R, Dong E, Xia J, Kruger M, Wishart DS, Nicolaides K: First-trimester metabolomic detection of late-onset preeclampsia. *Am J Obstet Gynecol.* 2013 Jan;208(1):58.e1-7. doi: 10.1016/j.ajog.2012.11.003. Epub 2012 Nov 13. PMID: 23159745

## L-Arginine -- Lewy body disease

Tsuruoka M, Hara J, Hirayama A, Sugimoto M, Soga T, Shankle WR, Tomita M: Capillary electrophoresis-mass spectrometry-based metabolome analysis of serum and saliva from neurodegenerative dementia patients. *Electrophoresis.* 2013 Oct;34(19):2865-72. doi: 10.1002/elps.201300019. Epub 2013 Sep 6. PMID: 23857558



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## Chenodeoxycholic acid -- Introduction

SYNONYM: 3alpha,7alpha-Dihydroxy-5beta-cholanic acid; 7alpha-Hydroxylithocholic acid; Anthropodeoxycholic acid; Anthropodesoxycholic acid; CDCA; Chenic acid; Chenix; Chenodiol; Gallodesoxycholic acid; 3a,7a-Dihydroxy-5b-cholanate; 3a,7a-Dihydroxy-5b-cholanic acid; 3alpha,7alpha-Dihydroxy-5beta-cholanate; 3 $\beta$  $\pm$ ,7 $\beta$  $\pm$ -dihydroxy-5 $\beta$ -cholanate; 3 $\beta$  $\pm$ ,7 $\beta$  $\pm$ -dihydroxy-5 $\beta$ -cholic acid; Chenodeoxycholate; 7a-Hydroxylithocholate; 7a-Hydroxylithocholic acid; 7alpha-Hydroxylithocholate; 7 $\beta$  $\pm$ -hydroxylithocholate; 7 $\beta$  $\pm$ -hydroxylithocholic acid; Anthropodeoxycholate; Anthropodesoxycholate; Chenate; Gallodesoxycholate; (+)-Chenodeoxycholate; (+)-Chenodeoxycholic acid; (3a,5b,7a)-3,7-Dihydroxy-cholan-24-Oate; (3a,5b,7a)-3,7-Dihydroxy-cholan-24-Oic acid; 3a,7a-Dihydroxy-5b,14a,17b-cholanate; 3a,7a-Dihydroxy-5b,14a,17b-cholanic acid; 3a,7a-Dihydroxy-5b-cholan-24-Oate; 3a,7a-Dihydroxy-5b-cholan-24-Oic acid; 7a-Hydroxydesoxycholsaeure; Chenodesoxycholsaeure; Acid, chenique; Chenofalk; Chenophalk; Acid, chenodeoxycholic; Chenodeoxycholate, sodium; Quenocol; Solvay brand OF chenodeoxycholic acid; Antigen brand OF chenodeoxycholic acid; Falk brand OF chenodeoxycholic acid; Quenobilan; Sodium chenodeoxycholate; tramedico Brand OF chenodeoxycholic acid; Zambon brand OF chenodeoxycholic acid; Acid, chenic; Acid, gallodesoxycholic; Chenique acid; Estedi brand OF chenodeoxycholic acid; Henohol

HMDB: HMDB0000518; HMDB00518

CAS: 474-25-9

Chenodeoxycholic acid is a bile acid. Bile acids are steroid acids found predominantly in bile of mammals. The distinction between different bile acids is minute, depends only on presence or absence of hydroxyl groups on positions 3, 7, and 12. Bile acids are physiological detergents that facilitate excretion, absorption, and transport of fats and sterols in the intestine and liver. Bile acids are also steroid amphipathic molecules derived from the catabolism of cholesterol. They modulate bile flow and lipid secretion, are essential for the absorption of dietary fats and vitamins, and have been implicated in the regulation of all the key enzymes involved in cholesterol homeostasis. Bile acids recirculate through the liver, bile ducts, small intestine and portal vein to form an enterohepatic circuit. They exist as anions at physiological pH and, consequently, require a carrier for transport across the membranes of the enterohepatic tissues. The unique detergent properties of bile acids are essential for the digestion and intestinal absorption of hydrophobic nutrients. Bile acids have potent toxic properties (e.g., membrane disruption) and there are a plethora of mechanisms to limit their accumulation in blood and tissues. (PMID: 11316487, 16037564, 12576301, 11907135). Usually conjugated with either glycine or taurine. It acts as a detergent to solubilize fats for intestinal absorption and is reabsorbed by the small intestine. It is used as cholagogue, a choleretic laxative, and to prevent or dissolve gallstones.

This compound belongs to the class of organic compounds known as dihydroxy bile acids, alcohols and derivatives. These are compounds containing or derived from a bile acid or alcohol, and which bears exactly two carboxylic acid groups.

## Chenodeoxycholic acid -- Biliary atresia

Matsui A, Psacharopoulos HT, Mowat AP, Portmann B, Murphy GM: Radioimmunoassay of serum glycocholic acid, standard laboratory tests of liver function and liver biopsy findings: comparative study of children with liver disease. J Clin Pathol. 1982 Sep;35(9):1011-7. PMID: 7119120

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## Chenodeoxycholic acid -- Cirrhosis

Cynober LA: Plasma amino acid levels with a note on membrane transport: characteristics, regulation, and metabolic significance. Nutrition. 2002 Sep;18(9):761-6. PMID: 12297216



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### Chenodeoxycholic acid -- Cystic fibrosis

Matsui A, Psacharopoulos HT, Mowat AP, Portmann B, Murphy GM: Radioimmunoassay of serum glycocholic acid, standard laboratory tests of liver function and liver biopsy findings: comparative study of children with liver disease. *J Clin Pathol.* 1982 Sep;35(9):1011-7. PMID: 7119120

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### Chenodeoxycholic acid -- Hepatocellular carcinoma

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. *Tohoku J Exp Med.* 1995 May;176(1):61-8. PMID: 7482520

Matsumata T, Yamamoto K, Shirabe K, Shimada M, Sugimachi K, Takesue F, Muto Y, Ikeda T: Urinary excretion of prostaglandins and renal function after hepatic resection. *Hepatogastroenterology.* 1997 May-Jun;44(15):774-8. PMID: 9222688

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### Chenodeoxycholic acid -- Primary biliary cirrhosis

Nikkila K, Hockerstedt K, Miettinen TA: High cholestanol and low campesterol-to-sitosterol ratio in serum of patients with primary biliary cirrhosis before liver transplantation. *Hepatology.* 1991 Apr;13(4):663-9. PMID: 2010161

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Braganza JM, Day JP: Serum octadeca-9-11 dienoic acid concentrations in primary biliary cirrhosis. *Lancet.* 1987 Apr 25;1(8539):987. PMID: 2882386

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ME: Comparative metabolism and structure of BCKD-E2 in primary biliary cirrhosis. J Autoimmun. 1993 Aug;6(4):459-66.  
PMID: 8216688

### 3-Methoxy-4-hydroxyphenylethyleneglycol sulfate -- Introduction

SYNONYM: (3-Methoxy-4-hydroxyphenyl)ethylene glycol sulfate; (3-Methoxy-4-hydroxyphenyl)ethylene glycol sulphate; (3-Methoxy-4-hydroxyphenyl)glycol O-sulfate; (3-Methoxy-4-hydroxyphenyl)glycol O-sulphate; (3-Methoxy-4-hydroxyphenyl)glycol sulfate ester; (3-Methoxy-4-hydroxyphenyl)glycol sulphate ester; 3-Methoxy-4-hydroxyphenylethyleneglycol sulphate; 3-Methoxy-4-hydroxyphenylglycol 4-sulfate; 3-Methoxy-4-hydroxyphenylglycol 4-sulphate; MOPEG sulfate; MOPEG sulphate

HMDB: HMDB0000559; HMDB00559

CAS: 3415-67-6

3-methoxy-4-hydroxyphenylethyleneglycol sulfate (MHPG-SO<sub>4</sub>) is the major metabolite of noradrenaline in serum. Chronic schizophrenics have lower serum levels than healthy individuals. Treatment of both groups with 7 daily 3-mg doses of Haloperidol caused similar decreases in MHPG-SO<sub>4</sub> concentration. (PMID 7343757). In human urine, constitutes 44% of the total 3-methoxy-4-hydroxyphenylethyleneglycol. (PMID 7379456).

This compound belongs to the class of organic compounds known as phenylsulfates. These are compounds containing a sulfuric acid group conjugated to a phenyl group.

### Creatinine -- Introduction

SYNONYM: 1-Methylglycocyamidine; 1-Methylhydantoin-2-imide; 2-amino-1,5-dihydro-1-Methyl-4H-imidazol-4-one; 2-amino-1-Methylimidazolin-4-one; Creatine anhydride; Creatinina; Kreatinin; 2-amino-1-Methyl-1,5-dihydroimidazol-4-one; Krebiozen; Sulfate salt, creatinine; Creatinine sulfate salt; Salt, creatinine sulfate

HMDB: HMDB0000562; HMDB00562

CAS: 60-27-5

Creatinine, or creatine anhydride, is a breakdown product of creatine phosphate in muscle. The loss of a water molecule from creatine results in the formation of creatinine. Creatinine is transferred to the kidneys by blood plasma, whereupon it is eliminated from the body by glomerular filtration and partial tubular excretion. Creatinine is usually produced at a fairly constant rate by the body. Measuring serum creatinine is a simple test and it is the most commonly used indicator of renal function. A rise in blood creatinine levels is observed only with marked damage to functioning nephrons. Therefore, this test is not suitable for detecting early kidney disease. The typical reference range for women is considered about 45-90  $\mu\text{mol/L}$ ; for men 60-110  $\mu\text{mol/L}$ . Creatine and creatinine are metabolized in the kidneys, muscle, liver, and pancreas.

This compound belongs to the class of organic compounds known as alpha amino acids and derivatives. These are amino acids in which the amino group is attached to the carbon atom immediately adjacent to the carboxylate group (alpha carbon), or a derivative thereof.

### Creatinine -- 21-Hydroxylase deficiency

Tonetto-Fernandes V, Lemos-Marini SH, Kuperman H, Ribeiro-Neto LM, Verreschi IT, Kater CE: Serum 21-Deoxycortisol, 17-Hydroxyprogesterone, and 11-deoxycortisol in classic congenital adrenal hyperplasia: clinical and hormonal correlations and identification of patients with 11beta-hydroxylase deficiency among a large group with alleged 21-hydroxylase deficiency. J Clin Endocrinol Metab. 2006 Jun;91(6):2179-84. Epub 2006 Mar 21. PMID: 16551734

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## Creatinine -- Late-onset preeclampsia

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## Creatinine -- Lewy body disease

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## PC(16:0/16:0) -- Introduction

SYNONYM: 1,2-Bis(hexadecanoyl)-sn-glycero-3-phosphocholine; 1,2-Dipalmitoyl-L-lecithin; 1,2-Dipalmitoyl-sn-glycero-3-phosphatidylcholine; 1,2-Dipalmitoyl-sn-glycero-3-phosphocholine; 1,2-Dipalmitoylphosphatidylcholine; 1-16:0-2-16:0-Phosphatidylcholine; 16:0-16:0-PC; Colfosceril palmitate; Colfoscerili palmitas; Dipalmitoyl phosphatidylcholine; Dipalmitoyl-GPC; Dipalmitoylphosphatidylcholine; GPC(16:0/16:0); gpcho 16:0/16:0; gpcho(16:0/16:0); Palmitate de colfosceril; palmitato De colfoscerilo; PC 16:0/16:0; PC(32:0); Phosphatidylcholine 16:0/16:0; Phosphatidylcholine(16:0/16:0); Phosphatidylcholine(32:0); Colfosceril palmitic acid; Palmitic acid de colfosceril; (R)-4-Hydroxy-N,N,N-trimethyl-10-oxo-7-[(1-oxohexadecyl)oxy]-3,5,9-trioxa-4-phosphapentacosan-1-aminium 4-oxide hydroxide inner salt; (R)-4-Hydroxy-N,N,N-trimethyl-10-oxo-7-[(1-oxohexadecyl)oxy]-3,5,9-trioxa-4-phosphapentacosan-1-aminium 4-oxide inner salt; 1,2-Bis(palmitoyl)-sn-glycero-3-phosphocholine; 1,2-Dihexadecanoyl-sn-glycerol-3-phosphorylcholine; 1,2-Dipalmitoyl-3-sn-phosphatidylcholine; 1,2-Dipalmitoyl-L-3-phosphatidylcholine; 1,2-Dipalmitoyl-L-a-lecithin; 1,2-Dipalmitoyl-L-a-phosphatidylcholine; 1,2-Dipalmitoyl-L-alpha-lecithin; 1,2-Dipalmitoyl-L-alpha-phosphatidylcholine; 1,2-Dipalmitoyl-L-phosphatidylcholine; 1,2-Dipalmitoyl-rac-glycero-3-phosphocholine; 1,2-Dipalmitoyl-sn-3-glycerophosphocholine; 1,2-Dipalmitoyl-sn-glycero-3-phosphorylcholine; 1,2-Dipalmitoyl-sn-glycerol-3-phosphocholine; 1,2-Dipalmitoyl-sn-glycerophosphocholine; 1,2-Dipalmitoyl-sn-glycerophosphorylcholine; 1,2-Dipalmitoyl-sn-glyceryl-3-phosphocholine; 1,2-Dipalmitoyl-sn-phosphatidylcholine; 1,2-dipalmitoylglycero-3-Phosphocholine; 1,2-L-a-Dipalmitoylphosphatidylcholine; 1,2-L-alpha-Dipalmitoylphosphatidylcholine; b,g-Dipalmitoyl L-a-phosphatidylcholine; b,g-Dipalmitoyl L-alpha-phosphatidylcholine; b,g-Dipalmitoyl-L-(a)-lecithin; b,g-Dipalmitoyl-L-phosphatidylcholine; Dihexadecanoyl-sn-glycero-3-phosphocholine; Dipalmitoyl L-a-phosphatidylcholine; Dipalmitoyl L-alpha-phosphatidylcholine; Dipalmitoyl-L-3-glycerylphosphorylcholine; Dipalmitoyl-L-a-lecithin; Dipalmitoyl-L-a-phosphatidylcholine; Dipalmitoyl-L-alpha-lecithin; Dipalmitoyl-L-alpha-phosphatidylcholine; Dipalmitoyl-sn-3-phosphatidylcholine; DPPC; gpcho(32:0); L-1,2-Dipalmitoyl-a-lecithin; L-1,2-Dipalmitoyl-alpha-lecithin; L-1,2-Dipalmitoylphosphatidylcholine; L-a-1,2-Dipalmitoyl lecithin; L-a-Dipalmitoylecithin; L-a-Dipalmitoyllecithin; L-a-Dipalmitoylphosphatidylcholine; L-a-DPPC; L-alpha-1,2-Dipalmitoyl lecithin; L-alpha-Dipalmitoylecithin; L-alpha-Dipalmitoyllecithin; L-alpha-Dipalmitoylphosphatidylcholine; L-alpha-DPPC; L-b,g-Dipalmitoyl-a-lecithin; L-b,g-Dipalmitoyl-a-phosphatidylcholine; L-b,g-Dipalmitoyl-alpha-lecithin; L-b,g-Dipalmitoyl-alpha-phosphatidylcholine; L-b,g-Dipalmitoylphosphatidylcholine; L-Dipalmitoyl lecithin; L-DPPC; Lecithin; PC Aa C32:0; sn-3-Dipalmitoyllecithin; PC(16:0/16:0); 1,2-dihexadecanoyl-rac-glycero-3-phosphocholine

HMDB: HMDB0000564; HMDB0000804; HMDB0005250; HMDB0007968; HMDB00564; HMDB00804; HMDB05250; HMDB07968

CAS: 63-89-8

PC(16:0/16:0) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(16:0/16:0), in particular, consists of two chains of palmitic acid at the C-1 and C-2 positions. The palmitic acid moieties are derived from fish oils, milk fats, vegetable oils and animal fats. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. Dipalmitoylphosphatidylcholine (DPPC) is the major constituent of pulmonary surfactant. It is also used for research purposes in studying liposomes, lipid bilayers, and model biological membranes. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

## PC(16:0/16:0) -- Pregnancy



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## PC(16:0/16:0) -- Obesity

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## DL-Dopa -- Introduction

SYNONYM: (+)-3-(3,4-Dihydroxyphenyl)alanine; (+)-Dopa; (R,S)-Dopa; 3',4'-Dihydroxyphenylalanine; 3-Hydroxy-DL-tyrosine; 3-Hydroxytyrosine; beta-(3,4-Dihydroxyphenyl)-DL-alpha-alanine; DL-3,4-Dopa; DL-beta-(3,4-Dihydroxyphenyl)-alpha-alanine; DL-beta-(3,4-Dihydroxyphenyl)alanine; DL-Dihydroxyphenylalanine; DL-Dioxophenylalanine; b-(3,4-Dihydroxyphenyl)-DL-a-alanine; l<sup>2</sup>-(3,4-dihydroxyphenyl)-DL-l±-alanine; DL-b-(3,4-Dihydroxyphenyl)-a-alanine; DL-l<sup>2</sup>-(3,4-dihydroxyphenyl)-l±-alanine; DL-b-(3,4-Dihydroxyphenyl)alanine; DL-l<sup>2</sup>-(3,4-dihydroxyphenyl)alanine; (+/-) 3-(3,4-dihydroxyphenyl)alanine; 2-amino-3-(3,4-Dihydroxyphenyl)propanoate; 2-amino-3-(3,4-Dihydroxyphenyl)propanoic acid; 3,4-Dihydroxy-DL-phenylalanine; 3,4-Dihydroxyphenylalanine; 3-(3,4-Dihydroxyphenyl)-DL-alanine; a-amino-3,4-Dihydroxy-benzenepropanoate; a-amino-3,4-Dihydroxy-benzenepropanoic acid; alpha-amino-3,4-Dihydroxy-benzenepropanoate; alpha-amino-3,4-Dihydroxy-benzenepropanoic acid; alpha-amino-Hydrocaffic acid; b-(3,4-Dihydroxyphenyl)-a-alanine; beta-(3,4-Dihydroxyphenyl)-alpha-alanine; DL-3',4'-Dihydroxyphenylalanine; DL-3,4-Dihydroxyphenylalanine; DL-3-Hydroxytyrosine; DL-4,5-Dihydroxyphenylalanine; Dopa; 3 Hydroxy DL tyrosine; 3,4 Dihydroxyphenylalanine; beta-Hydroxytyrosine; Dihydroxyphenylalanine hydrochloride, (2:1); beta Hydroxytyrosine

HMDB: HMDB0000609; HMDB00609

CAS: 63-84-3

The naturally occurring form of DIHYDROXYPHENYLALANINE and the immediate precursor of DOPAMINE. Unlike dopamine itself, it can be taken orally and crosses the blood-brain barrier. It is rapidly taken up by dopaminergic neurons and converted to DOPAMINE. It is used for the treatment of PARKINSONIAN DISORDERS and is usually given



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with agents that inhibit its conversion to dopamine outside of the central nervous system.

This compound belongs to the class of organic compounds known as tyrosine and derivatives. These are compounds containing tyrosine or a derivative thereof resulting from reaction of tyrosine at the amino group or the carboxy group, or from the replacement of any hydrogen of glycine by a heteroatom.

### DL-Dopa -- Alzheimer's disease

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## Deoxycholic acid -- Introduction

SYNONYM: (3ALPHA,5ALPHA,12ALPHA)-3,12-DIHYDROXYCHOLAN-24-OIC ACID; (3alpha,5beta,12alpha)-3,12-Dihydroxycholan-24-Oic acid; 3alpha,12alpha-Dihydroxy-5beta-cholanic acid; 7alpha-Deoxycholic acid; Desoxycholic acid; Desoxocholsaeure; (3a,5a,12a)-3,12-DIHYDROXYCHOLAN-24-Oate; (3a,5a,12a)-3,12-DIHYDROXYCHOLAN-24-Oic acid; (3alpha,5alpha,12alpha)-3,12-DIHYDROXYCHOLAN-24-Oate; (3 $\bar{\beta}$ ,5 $\bar{\beta}$ ,12 $\bar{\beta}$ )-3,12-dihydroxycholan-24-Oate; (3 $\bar{\beta}$ ,5 $\bar{\beta}$ ,12 $\bar{\beta}$ )-3,12-dihydroxycholan-24-Oic acid; Deoxycholate; (3a,5b,12a)-3,12-Dihydroxycholan-24-Oate; (3a,5b,12a)-3,12-Dihydroxycholan-24-Oic acid; (3alpha,5beta,12alpha)-3,12-Dihydroxycholan-24-Oate; (3 $\bar{\beta}$ ,5 $\bar{\beta}$ ,12 $\bar{\beta}$ )-3,12-dihydroxycholan-24-Oate; (3 $\bar{\beta}$ ,5 $\bar{\beta}$ ,12 $\bar{\beta}$ )-3,12-dihydroxycholan-24-Oic acid; 3a,12a-Dihydroxy-5b-cholanate; 3a,12a-Dihydroxy-5b-cholanic acid; 3alpha,12alpha-Dihydroxy-5beta-cholanate; 3 $\bar{\beta}$ ,12 $\bar{\beta}$ -dihydroxy-5 $\bar{\beta}$ -cholanate; 3 $\bar{\beta}$ ,12 $\bar{\beta}$ -dihydroxy-5 $\bar{\beta}$ -cholanic acid; 7a-Deoxycholate; 7a-Deoxycholic acid; 7alpha-Deoxycholate; 7 $\bar{\beta}$ -deoxycholate; 7 $\bar{\beta}$ -deoxycholic acid; Desoxycholate; 5b-Cholanic acid-3a,12a-diol; 5b-Deoxycholate; 5b-Deoxycholic acid; 7-Deoxycholate; 7-Deoxycholic acid; Cholericbic; Cholorebic; Degalol; Deoxy-cholate; Deoxy-cholic acid; Deoxycholatate; Deoxycholatic acid; Acid, lagodeoxycholic; Deoxycholic acid, 5alpha isomer; Deoxycholic acid, sodium salt, 12beta-isomer; Lagodeoxycholic acid; Acid, choleic; Deoxycholic acid, 12beta isomer; Deoxycholic acid, 3beta-isomer; Deoxycholic acid, monoammonium salt; 12beta-Isomer deoxycholic acid; 3beta-Isomer deoxycholic acid; Acid, 5alpha-isomer deoxycholic; Acid, deoxycholic; Acid, desoxycholic; Deoxycholate, sodium; Deoxycholic acid, 12beta-isomer; Deoxycholic acid, 5alpha-isomer; Deoxycholic acid, monopotassium salt; Deoxycholic acid, monosodium salt; 5alpha-Isomer deoxycholic acid; Acid, dihydroxycholanoic; Choleic acid; Deoxycholic acid, 3beta isomer; Deoxycholic acid, disodium salt; Deoxycholic acid, magnesium (2:1) salt; Dihydroxycholanoic acid; Sodium deoxycholate

HMDB: HMDB0000626; HMDB00626

CAS: 83-44-3

Deoxycholic acid is a secondary bile acid produced in the liver and is usually conjugated with glycine or taurine. It



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facilitates fat absorption and cholesterol excretion. Bile acids are steroid acids found predominantly in the bile of mammals. The distinction between different bile acids is minute, and depends only on the presence or absence of hydroxyl groups on positions 3, 7, and 12. Bile acids are physiological detergents that facilitate excretion, absorption, and transport of fats and sterols in the intestine and liver. Bile acids are also steroid amphiphatic molecules derived from the catabolism of cholesterol. They modulate bile flow and lipid secretion, are essential for the absorption of dietary fats and vitamins, and have been implicated in the regulation of all the key enzymes involved in cholesterol homeostasis. Bile acids recirculate through the liver, bile ducts, small intestine, and portal vein to form an enterohepatic circuit. They exist as anions at physiological pH, and consequently require a carrier for transport across the membranes of the enterohepatic tissues. The unique detergent properties of bile acids are essential for the digestion and intestinal absorption of hydrophobic nutrients. Bile acids have potent toxic properties (e.g. membrane disruption) and there are a plethora of mechanisms to limit their accumulation in blood and tissues (PMID: 11316487, 16037564, 12576301, 11907135). When present in sufficiently high levels, deoxycholic acid can act as a hepatotoxin, a metabotxin, and an oncometabolite. A hepatotoxin causes damage to the liver or liver cells. A metabotxin is an endogenously produced metabolite that causes adverse health effects at chronically high levels. An oncometabolite is a compound, when present at chronically high levels, that promotes tumour growth and survival. Among the primary bile acids, cholic acid is considered to be the least hepatotoxic while deoxycholic acid is the most hepatotoxic (PMID: 1641875). The liver toxicity of bile acids appears to be due to their ability to peroxidate lipids and to lyse liver cells. High bile acid levels lead to the generation of reactive oxygen species and reactive nitrogen species, disruption of the cell membrane and mitochondria, induction of DNA damage, mutation and apoptosis, and the development of reduced apoptosis capability upon chronic exposure (PMID: 24884764). Chronically high levels of deoxycholic acid are associated with familial hypercholesterolemia. In hypercholesterolemia, bile acids, including deoxycholic acid, are elevated in the blood. This disease causes liver damage, extensive itching, poor fat absorption, and can lead to rickets due to lack of calcium in bones. The deficiency of normal bile acids in the intestines results in a deficiency of vitamin K, which also adversely affects clotting of the blood. The bile acid ursodiol (ursodeoxycholic acid) can improve symptoms associated with familial hypercholesterolemia. Chronically high levels of deoxycholic acid are also associated with several forms of cancer including colon cancer, pancreatic cancer, esophageal cancer, and many other GI cancers.

This compound belongs to the class of organic compounds known as dihydroxy bile acids, alcohols and derivatives. These are compounds containing or derived from a bile acid or alcohol, and which bears exactly two carboxylic acid groups.

### Deoxycholic acid -- Colorectal cancer

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## Deoxycholic acid -- Cystic fibrosis

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## Deoxycholic acid -- Irritable bowel syndrome

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Metabolomics of fecal extracts detects altered metabolic activity of gut microbiota in ulcerative colitis and irritable bowel syndrome. *J Proteome Res.* 2011 Sep 2;10(9):4208-18. doi: 10.1021/pr2003598. Epub 2011 Aug 8. PMID: 21761941

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### Deoxycholic acid -- Primary biliary cirrhosis

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### Deoxycholic acid -- Ulcerative colitis

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## Cytosine -- Introduction

SYNONYM: 4-amino-2(1H)-Pyrimidinone; 4-amino-2-Hydroxypyrimidine; C; Cyt; Cytosin; Zytosin; 4-amino-2-oxo-1,2-Dihydropyrimidine; 4-Aminouracil; Cytosinimine

HMDB: HMDB0000630; HMDB00630

CAS: 71-30-7

Cytosine is a pyrimidine base that is a fundamental unit of nucleic acids. The deamination of cytosine alone is apparent and the nucleotide of cytosine is the prime mutagenic nucleotide in leukaemia and cancer.

This compound belongs to the class of organic compounds known as pyrimidones. These are compounds that contain a pyrimidine ring, which bears a ketone. Pyrimidine is a 6-membered ring consisting of four carbon atoms and two nitrogen centers at the 1- and 3- ring positions.

## Cytosine -- Colorectal cancer

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## Cytosine -- Ulcerative colitis

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## Citraconic acid -- Introduction

SYNONYM: (Z)-2-Methyl-2-butenedioic acid; 2-Methyl-2-butenedioic acid; 2-Methylmaleic acid; alpha-Methylmaleic acid; cis-2-Methylbutenedioic acid; cis-Methylbutenedioic acid; Citraconsaeure; Methyl-maleinsaeure; Methylmaleic acid; (Z)-2-Methyl-2-butenedioate; Citraconate; 2-Methyl-2-butenedioate; 2-Methylmaleate; a-Methylmaleate; a-Methylmaleic acid; alpha-Methylmaleate;  $\pm$ -methylmaleate;  $\pm$ -methylmaleic acid; cis-2-Methylbutenedioate; cis-Methylbutenedioate; Methylmaleate; Citraconic acid, ammonium salt; Citraconic acid, calcium salt; Citraconic acid, sodium salt; Methylfumaric acid; (e)-2-Methyl-2-butenedioic acid; Citraconic acid, (e)-isomer; Mesaconic acid; Monomethylfumarate

HMDB: HMDB0000634; HMDB00634

CAS: 498-23-7

Mesaconic acid is one of several isomeric carboxylic acids obtained from citric acid. Is used as a fire retardant, recent studies revealed this acid is a competitive inhibitor of fumarate reduction.

This compound belongs to the class of organic compounds known as methyl-branched fatty acids. These are fatty acids with an acyl chain that has a methyl branch. Usually, they are saturated and contain only one or more methyl group. However, branches other than methyl may be present.

## Citraconic acid -- Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. *Tohoku J Exp Med*. 1995 May;176(1):61-8. PMID: 7482520

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## L-Glutamine -- Introduction

SYNONYM: (2S)-2,5-diamino-5-Oxopentanoic acid; (2S)-2-amino-4-Carbamoylbutanoic acid; (S)-2,5-diamino-5-Oxopentanoic acid; Glutamic acid 5-amide; Glutamic acid amide; GLUTAMINE; L-(+)-Glutamine; L-2-Aminoglutaramic acid; L-Glutamic acid gamma-amide; L-Glutamin; L-Glutaminsaeure-5-amid; Levoglutamide; Q; (2S)-2,5-diamino-5-Oxopentanoate; (2S)-2-amino-4-Carbamoylbutanoate; (S)-2,5-diamino-5-Oxopentanoate; Glutamate 5-amide; Glutamate amide; L-2-Aminoglutaramate; L-Glutamate g-amide; L-Glutamate gamma-amide; L-Glutamate  $\beta$ -amide; L-Glutamic acid g-amide; L-Glutamic acid  $\beta$ -amide; 2-Aminoglutaramic acid; Cebrogen; gamma-Glutamine; Glavamin; Glumin; L-2-Aminoglutaramic acid; L-Glutamic acid 5-amide; L-Glutamid; L-Glutamide; Levoglutamid; Levoglutamida; Levoglutamidum; Levoglutamina; Polyglutamine; Stimulina; D-Glutamine; D Glutamine; L Glutamine

HMDB: HMDB0000641; HMDB00641

CAS: 56-85-9

Glutamine (Gln) is one of the 20 amino acids encoded by the standard genetic code. In humans it is considered a non-essential amino acid. Structurally, glutamine is similar to the amino acid glutamic acid. However, instead of having a terminal carboxylic acid, it has an amide. Enzymatically, glutamine is formed by replacing a side-chain hydroxyl of glutamic acid with an amine functional group. Glutamine is found in foods high in proteins, such as fish, red meat, beans, and dairy products. Glutamine is often used as a supplement in weightlifting, bodybuilding, endurance and other sports, as well as by those who



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suffer from muscular cramps or pain, particularly elderly people. The main use of glutamine within the diet of either group is as a means of replenishing the body's stores of amino acids that have been used during exercise or everyday activities. Studies which have looked into problems with excessive consumption of glutamine thus far have proved inconclusive. However, normal supplementation is healthy mainly because glutamine is supposed to be supplemented after prolonged periods of exercise (for example, a workout or exercise in which amino acids are required for use) and replenishes amino acid stores. This is one of the main reasons glutamine is recommended during fasting or for people who suffer from physical trauma, immune deficiencies, or cancer. There is a significant body of evidence that links glutamine-enriched diets with positive intestinal effects. These include maintenance of gut barrier function, aiding intestinal cell proliferation and differentiation, as well as generally reducing septic morbidity and the symptoms of Irritable Bowel Syndrome (IBS). The reason for such "cleansing" properties is thought to stem from the fact that the intestinal extraction rate of glutamine is higher than that for other amino acids, and is therefore thought to be the most viable option when attempting to alleviate conditions relating to the gastrointestinal tract. These conditions were discovered after comparing plasma concentration within the gut between glutamine-enriched and non glutamine-enriched diets. However, even though glutamine is thought to have "cleansing" properties and effects, it is unknown to what extent glutamine has clinical benefits, due to the varied concentrations of glutamine in varieties of food. It is also known that glutamine has positive effects in reducing healing time after operations. Hospital waiting times after abdominal surgery are reduced by providing parenteral nutrition regimens containing amounts of glutamine to patients. Clinical trials have revealed that patients on supplementation regimes containing glutamine have improved nitrogen balances, generation of cysteinyl-leukotrienes from polymorphonuclear neutrophil granulocytes and improved lymphocyte recovery and intestinal permeability (in postoperative patients) - in comparison to those who had no glutamine within their dietary regime; all without any side-effects (<http://en.wikipedia.org/wiki/glutamine>). L-Glutamine is found to be associated with carbamoyl phosphate synthetase deficiency, which is an inborn error of metabolism.

This compound belongs to the class of organic compounds known as l-alpha-amino acids. These are alpha amino acids which have the L-configuration of the alpha-carbon atom.

### L-Glutamine -- Alzheimer's disease

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### L-Glutamine -- Early preeclampsia

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### Decanoylcarnitine -- Introduction

SYNONYM: Decanoyl-L-carnitine; Decanoylcarnitine, (+)-isomer; Decanoylcarnitine, (R)-isomer; Decanoylcarnitine, (S)-isomer

HMDB: HMDB0000651; HMDB00651

CAS: 1492-27-9

Decanoylcarnitine is a member of the class of compounds known as acylcarnitines. Acylcarnitines are organic compounds containing a fatty acid with the carboxylic acid attached to carnitine through an ester bond. Thus, decanoylcarnitine is considered to be a fatty ester lipid molecule. Decanoylcarnitine is practically insoluble (in water) and a weakly acidic compound (based on its pKa). Decanoylcarnitine can be found in blood, feces, and urine. Within the cell, decanoylcarnitine is primarily located in the membrane. It can also be found in the extracellular space. Acylcarnitines are useful in the diagnosis of genetic disorders such as fatty acid oxidation disorders and differentiation between biochemical phenotypes of medium-chain acyl-CoA dehydrogenase (MCAD) deficiency disorders (PMID: 12385891). Moreover, decanoylcarnitine is found to be associated with very long chain acyl-CoA dehydrogenase (VLAD) deficiency, glutaric aciduria II, and celiac disease, which are inborn errors of metabolism.

This compound belongs to the class of organic compounds known as acyl carnitines. These are organic compounds containing a fatty acid with the carboxylic acid attached to carnitine through an ester bond.

### Decanoylcarnitine -- Very Long Chain Acyl-CoA Dehydrogenase Deficiency

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## Indoxyl sulfate -- Introduction

SYNONYM: 3-Indolyl hydrogen sulfate; 3-Indolyl sulfate; 3-Indoxyl sulfate; 3-Indoxylsulfuric acid; Indican; indol-3-yl Hydrogen sulfate; indol-3-yl Sulfate; indol-3-yl Sulphate; Indoxyl sulfic acid; Indoxyl sulphate; Indoxylsulfuric acid; 3-Indolyl hydrogen sulfuric acid; 3-Indolyl hydrogen sulphate; 3-Indolyl hydrogen sulphuric acid; Indoxyl sulfuric acid; Indoxyl sulphuric acid; 3-Indolyl sulfuric acid; 3-Indolyl sulphate; 3-Indolyl sulphuric acid; 3-Indoxyl sulphuric acid; 3-Indoxyl sulphate; 3-Indoxylsulfate; 3-Indoxylsulphate; 3-Indoxylsulphuric acid; indol-3-yl Hydrogen sulfuric acid; indol-3-yl Hydrogen sulphate; indol-3-yl Hydrogen sulphuric acid; indol-3-yl Sulfuric acid; indol-3-yl Sulphuric acid; Indoxylsulfate; Indoxylsulphate; Indoxylsulphuric acid; 1H-indol-3-yl Hydrogen sulfate; 1H-indol-3-yl Hydrogen sulphate; indol-3-Ol; Indican monosodium salt; Monopotassium salt, indican; Monosodium salt, indican; Sulfate, indoxyl; Indican monopotassium salt; 1H-indol-3-Ol hydrogen sulfate ester

HMDB: HMDB0000682; HMDB0003309; HMDB00682; HMDB03309

CAS: 487-94-5

Indoxyl sulfate is a dietary protein metabolite and also a metabolite of the common amino acid tryptophan. Indoxyl sulfate is a circulating uremic toxin stimulating glomerular sclerosis and interstitial fibrosis. Indoxyl sulfate is one of the well-known substances of a group of protein-bound uremic retention solutes. Indoxyl sulfate increases the rate of progression of renal failure. In plasma, indoxyl sulfate is a protein-bound uremic solute that induces endothelial dysfunction by inhibiting endothelial proliferation and migration in vitro. Some studies suggest that indoxyl sulfate is also involved in oxidative stress. In hemodialyzed patients, serum levels of indoxyl sulfate are associated with levels of pentosidine, a marker of carbonyl and oxidative stress. In vitro, indoxyl sulfate increases reactive oxygen species (ROS) production in tubular cells and increases NAD(P)H oxidase activity in endothelial cells. Indoxyl sulfate impairs osteoblast function and induces abnormalities of bone turnover. Indoxyl sulfate strongly decreases the levels of glutathione, one of the most active antioxidant systems of the cell (PMID: 10681668, 14681860, 17471003, 17403109).

This compound belongs to the class of organic compounds known as arylsulfates. These are organic compounds containing a sulfate group that carries an aryl group through an ether group.

## Indoxyl sulfate – Colorectal cancer

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## Malonic acid -- Introduction

SYNONYM: H<sub>2</sub>Malo; HOOC-CH<sub>2</sub>-COOH; Propanedioic acid; Malonate; Propanedioate; alpha,Omega-dicarboxylic acid; Carboxyacetic acid; Dicarboxylate; Dicarboxylic acid; Dicarboxymethane; Kyselina malonova; Malonate dicarboxylic acid; Metahmedicarboxylic acid; Methanedicarbonic acid; Methanedicarboxylic acid; Propanedioic acid dithallium salt; Propanediolic acid; Thallium malonate; Malonic acid, 2-(14)C-labeled; Malonic acid, monocalcium salt; Malonic acid, 1,3-(14)C2-labeled; Malonic acid, diammonium salt; Malonic acid, disodium salt; Malonic acid, dithallium salt; Malonic acid, dipotassium salt; Malonic acid, disodium salt, 1-(14)C-labeled; Malonic acid, monosodium salt; Malonic acid, potassium salt; Malonic acid, sodium salt; Thallous malonate

HMDB: HMDB0000691; HMDB00691

CAS: 141-82-2

Malonic acid (IUPAC systematic name: propanedioic acid) is a dicarboxylic acid with structure CH<sub>2</sub>(COOH)<sub>2</sub>. The ionised form of malonic acid, as well as its esters and salts, are known as malonates. For example, diethyl malonate is malonic acid's ethyl ester. The name originates from Latin malum, meaning apple. Malonic acid is the archetypal example of a competitive inhibitor: it acts against succinate dehydrogenase (complex II) in the respiratory electron transport chain. Malonic acid is found to be associated with malonyl-CoA decarboxylase deficiency, which is an inborn error of metabolism.

This compound belongs to the class of organic compounds known as dicarboxylic acids and derivatives. These are organic compounds containing exactly two carboxylic acid groups.

## Malonic acid -- Pregnancy

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## Malonic acid -- Colorectal cancer

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### Malonic acid -- Malonyl-CoA decarboxylase deficiency

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### Malonic acid -- Combined malonic and methylmalonic aciduria

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### Hydroxyoctanoic acid -- Introduction

SYNONYM: 2-Hydroxycaprylic acid; alpha-Hydroxyoctanoic acid; 2-Hydroxycaprylate; Hydroxyoctanoate; a-Hydroxyoctanoate; a-Hydroxyoctanoic acid; alpha-Hydroxyoctanoate;  $\hat{L}\pm$ -hydroxyoctanoate;  $\hat{L}\pm$ -hydroxyoctanoic acid; 2-Hydroxyoctanoate; 2-Hydroxyoctanoic acid; a-Hydroxy-N-caprylate; a-Hydroxy-N-caprylic acid; a-Hydroxycaprylate; a-Hydroxycaprylic acid; alpha-Hydroxy-N-caprylate; alpha-Hydroxy-N-caprylic acid; alpha-Hydroxycaprylate; alpha-Hydroxycaprylic acid; DL-2-Hydroxycaprylate; DL-2-Hydroxycaprylic acid; DL-2-Hydroxyoctanoate; DL-2-Hydroxyoctanoic acid; alpha-HCA acid

HMDB: HMDB0000711; HMDB00711

CAS: 617-73-2

Hydroxyoctanoic acid medium chain substrate of the 2-hydroxy acid oxidases associated with the 3 distinct human 2-hydroxy acid oxidase genes, HAOX1, HAOX2, and HAOX3. (PMID: 10777549).

This compound belongs to the class of organic compounds known as medium-chain fatty acids. These are fatty acids with an aliphatic tail that contains between 4 and 12 carbon atoms.

### Hydroxyoctanoic acid -- Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. *Tohoku J Exp Med.* 1995 May;176(1):61-8. PMID: 7482520

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<http://www.sciencedirect.com/science/article/pii/S0924224416301984> PMID: 7482520

## Hippuric acid -- Introduction

SYNONYM: Benzamidoacetic acid; Benzamidoessigsaeure; Benzoyleminoacetic acid; Benzoyleminoessigsaeure; Hippurate; Hippursaeure; Phenylcarbonylaminooacetic acid; Benzamidoacetate; Hippate; Hippic acid; Benzoyleminoacetate; Phenylcarbonylaminooacetate; (benzoylamo)-Acetate; (benzoylamo)-Acetic acid; 2-Benzamidoacetate; 2-Benzamidoacetic acid; Benzoylglycine; N-Benzoylglycine; Hippuric acid, monosodium salt; Hippuric acid, (14)C-labeled; Hippuric acid, monoammonium salt; Hippuric acid, monopotassium salt

HMDB: HMDB0000714; HMDB00714

CAS: 495-69-2

Hippuric acid is an acyl glycine formed by the conjugation of benzoic acid with glycine. Acyl glycines are produced through the action of glycine N-acetyltransferase (EC 2.3.1.13) which is an enzyme that catalyzes the chemical reaction: acyl-CoA + glycine <--> CoA + N-acetylglycine. Hippuric acid is a normal component of urine and is typically increased with increased consumption of phenolic compounds (tea, wine, fruit juices). These phenols are converted to benzoic acid which is then converted to hippuric acid and excreted in the urine. Hippuric acid is the most frequently used biomarker in the biological monitoring of occupational exposure to toluene. This product of solvent biotransformation may be also found in the urine of individuals who have not been exposed to the solvent. A smaller fraction of the absorbed toluene is oxidized to aromatic compounds including ortho-cresol, which is not found significantly in the urine of nonexposed individuals. The concentration of hippuric acid in the urine of individuals exposed to a low toluene concentration does not differ from that of individuals not exposed to the solvent. This has led to the conclusion that hippuric acid should not be utilized in the biological monitoring of occupational exposure to low levels of toluene in the air. Protein-bound organic acids such as hippuric acid are markedly



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accumulated in uremic plasma and produce defective protein binding of drugs (PMID: 9120876, 8734460). Hippuric acid is found to be associated with phenylketonuria, propionic acidemia, and tyrosinemia I, which are inborn errors of metabolism.

This compound belongs to the class of organic compounds known as hippuric acids. These are compounds containing hippuric acid, which consists of a benzoyl group linked to the N-terminal of a glycine.

### Hippuric acid -- Argininosuccinic aciduria

Kleijer WJ, Garritsen VH, Linnebank M, Mooyer P, Huijmans JG, Mustonen A, Simola KO, Arslan-Kirchner M, Battini R, Briones P, Cardo E, Mandel H, Tschiedel E, Wanders RJ, Koch HG: Clinical, enzymatic, and molecular genetic characterization of a biochemical variant type of argininosuccinic aciduria: prenatal and postnatal diagnosis in five unrelated families. *J Inherit Metab Dis.* 2002 Sep;25(5):399-410. PMID: 12408190

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## Hippuric acid -- Schizophrenia

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## Kynurenic acid -- Introduction

**SYNONYM:** 4-Hydroxy-2-chinolincarbonsaeure; 4-Hydroxy-2-quinolinecarboxylic acid; 4-Hydroxyquinaldic acid; 4-Hydroxyquinaldinic acid; Kynurenate; Kynurensaeure; 4-Hydroxy-2-quinolinecarboxylate; 4-Hydroxyquinaldate; 4-Hydroxyquinaldinate; 2-Carboxy-4-hydroxyquinoline; 4-Hydroxy-quinaldate; 4-Hydroxy-quinaldic acid; 4-Hydroxyquino-line-2-carboxylate; 4-Hydroxyquino-line-2-carboxylic acid; Quinurenic acid; Acid, kynurenic

**HMDB:** HMDB0000715; HMDB00715

**CAS:** 492-27-3

Kynurenic acid (KYNA) is a well-known endogenous antagonist of the glutamate ionotropic excitatory amino acid receptors N-methyl-D-aspartate (NMDA), alphaamino-3-hydroxy-5-methylisoxazole-4-propionic acid and kainate receptors and of the nicotine cholinergic subtype alpha 7 receptors. KYNA neuroprotective and anticonvulsive activities have been demonstrated in animal models of neurodegenerative diseases. Because of KYNA's neuromodulatory character, its involvement has been speculatively linked to the pathogenesis of a number of neurological conditions including those in the ageing process. Different patterns of abnormalities in various stages of KYNA metabolism in the CNS have been reported in Alzheimer's disease, Parkinson's disease and Huntington's disease. In HIV-1-infected patients and in patients with Lyme neuroborreliosis a marked rise of KYNA metabolism was seen. In the ageing process KYNA metabolism in the CNS of rats shows a characteristic pattern of changes throughout the life span. A marked increase of the KYNA content in the CNS occurs before the birth, followed by a dramatic decline on the day of birth. A low activity was seen during ontogenesis, and a slow and progressive enhancement occurs during maturation and ageing. This remarkable profile of KYNA metabolism alterations in the mammalian brain has been suggested to result from the development of the organisation of neuronal connections and synaptic plasticity, development of receptor recognition sites, maturation and ageing. There is significant evidence that KYNA can improve cognition and memory, but it has also been demonstrated that it interferes with working memory. Impairment of cognitive function in various neurodegenerative disorders is accompanied by profound reduction and/or elevation of KYNA metabolism. The view that enhancement of CNS KYNA levels could underlie cognitive decline is supported by the increased KYNA metabolism in Alzheimer's disease, by the increased KYNA metabolism in down's syndrome and the enhancement of KYNA function during the early stage of Huntington's disease. Kynurenic acid is the only endogenous N-methyl-D-aspartate (NMDA) receptor antagonist identified up to now, that mediates glutamatergic hypofunction. Schizophrenia is a disorder of dopaminergic neurotransmission, but modulation of the dopaminergic system by glutamatergic neurotransmission seems to play a key role. Despite the NMDA receptor antagonism, kynurenic acid also blocks, in lower doses, the nicotinic acetylcholine receptor, i.e., increased kynurenic acid levels can explain psychotic symptoms and cognitive deterioration. Kynurenic acid levels are described to be higher in the cerebrospinal fluid (CSF) and in critical central nervous system (CNS) regions of schizophrenics as compared to controls. (PMID: 17062375, 16088227).

This compound belongs to the class of organic compounds known as quinoline carboxylic acids. These are quinolines in which the quinoline ring system is substituted by a carboxyl group at one or more positions.

## Kynurenic acid -- Anemia

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## 4-Hydroxyproline -- Introduction

SYNONYM: (2S,4R)-4-Hydroxy-2-pyrrolidinecarboxylic acid; (2S,4R)-trans-4-Hydroxyproline; delta-Hydroxyproline; Hydroxy-L-proline; Hydroxyproline; Hyp; Hypro; L-4-Hydroxyproline; L-threo-4-Hydroxyproline; trans-Hydroxyproline; trans-L-Hydroxyproline; (2S,4R)-4-Hydroxy-2-pyrrolidinecarboxylate; l'-hydroxyproline; (2S,4R)-4-Hydroxypyrrolidine-2-carboxylic acid; (4R)-4-Hydroxy-L-proline; 4-Hydroxy-2-pyrrolidinecarboxylic acid; 4-Hydroxy-L-proline; 4-L-Hydroxyproline; Hydroxiproline; Hydroxy-proline; L-Hydroxyproline; LS-Hydroxyproline; Oxaceprol; trans-4-Hydroxy-L-proline; trans-4-Hydroxyproline; 4 Hydroxyproline; Oxyproline; (-)-4-Hydroxy-2-pyrrolidinecarboxylic acid; (2S,4R)-(-)-4-Hydroxyproline; (2S,4R)-4-Hydroxyproline; (R)-4-Hydroxy-(S)-proline; (R)-4-Hydroxy-L-proline; (S)-Hydroxyproline; 4(R)-Hydroxy-2(S)-pyrrolidinecarboxylic acid; 4(R)-Hydroxyproline; 4-Hydroxy-(S)-proline; 4-Hydroxyproline; 4-trans-Hydroxy-L-proline; L-Hypro; L-trans-4-Hydroxyproline; NSC 46704; trans-L-4-Hydroxyproline

HMDB: HMDB0000725; HMDB0006055; HMDB00725; HMDB06055

CAS: 51-35-4

4-Hydroxyproline (hydroxyproline or Hyp) is a major component of the protein collagen. Hydroxyproline is produced by hydroxylation of the amino acid proline and is, therefore, a post-translationally modified amino acid. Hydroxyproline and proline play key roles for collagen stability. In particular, they permit the sharp twisting of the collagen helix. Hydroxyproline is found in few proteins other than collagen. The only other mammalian protein which includes hydroxyproline is elastin. For this reason, hydroxyproline content has been used as an indicator to determine collagen and/or gelatin amount in tissue or biological samples. Increased serum and urine levels of hydroxyproline have been found in Paget's disease (PMID: 436278). Hydroxyproline (Hyp) content in biological fluids is used as a parameter of collagen catabolism, especially bone resorption or tissue degradation. Bedridden and elderly individuals show significantly elevated serum levels of hydroxyproline in comparison to normal, active individuals (PMID: 10706420). Elevated levels of urinary hydroxyproline are also indicative of muscle damage (PMID: 21988268). Increased reactive oxygen species (ROS) are also known to accelerate collagen degradation. Hydroxyproline levels increase in cases of depression and stress (PMID: 21483218). 4-Hydroxyproline is found to be associated with Alzheimer's disease, and also hydroxyprolinemia and iminoglycinuria which are both inborn errors of metabolism. 4-Hydroxyproline is also involved in metabolic disorders such as hyperprolinemia type I, hyperornithinemia with gyrate atrophy (HOGA), L-arginine:glycine amidinotransferase deficiency, creatine deficiency, and guanidinoacetate methyltransferase deficiency. A deficiency in ascorbic acid can result in impaired hydroxyproline formation (PubChem). trans-4-Hydroxy-L-proline is a biomarker for the consumption of processed meat.

This compound belongs to the class of organic compounds known as proline and derivatives. These are compounds containing proline or a derivative thereof resulting from reaction of proline at the amino group or the carboxy group, or from the replacement of any hydrogen of glycine by a heteroatom.

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017-09958-9. PMID: 28842642

## Mesaconic acid -- Introduction

SYNONYM: (Z)-2-Methyl-2-butenedioic acid; 2-Methyl-2-butenedioic acid; 2-Methylmaleic acid; alpha-Methylmaleic acid; cis-2-Methylbutenedioic acid; cis-Methylbutenedioic acid; Citraconsaeure; Methyl-maleinsaeure; Methylmaleic acid; (Z)-2-Methyl-2-butenedioate; Citraconate; 2-Methyl-2-butenedioate; 2-Methylmaleate; a-Methylmaleate; a-Methylmaleic acid; alpha-Methylmaleate;  $\hat{L}$ -methylmaleate;  $\hat{L}$ -methylmaleic acid; cis-2-Methylbutenedioate; cis-Methylbutenedioate; Methylmaleate; Citraconic acid, ammonium salt; Citraconic acid, calcium salt; Citraconic acid, sodium salt; Methylfumaric acid; (e)-2-Methyl-2-butenedioic acid; Citraconic acid, (e)-isomer; Mesaconic acid; Monomethylfumarate

HMDB: HMDB0000749; HMDB00749

CAS: 498-24-8

Mesaconic acid is one of several isomeric carboxylic acids obtained from citric acid. Is used as a fire retardant, recent studies revealed this acid is a competitive inhibitor of fumarate reduction.

This compound belongs to the class of organic compounds known as methyl-branched fatty acids. These are fatty acids with an acyl chain that has a methyl branch. Usually, they are saturated and contain only one or more methyl group. However, branches other than methyl may be present.

## Hydroxyphenyllactic acid -- Introduction

SYNONYM: 2-Hydroxy-3-(4-hydroxyphenyl)propanoate; 2-Hydroxy-3-(P-hydroxyphenyl)propionic acid; 4-Hydroxyphenyllactic acid; beta-(4-Hydroxyphenyl)lactic acid; beta-(P-Hydroxyphenyl)lactic acid; DL-P-Hydroxyphenyllactic acid; P-Hydroxyphenyl lactic acid; 2-Hydroxy-3-(4-hydroxyphenyl)propanoic acid; Hydroxyphenyllactate; 2-Hydroxy-3-(P-hydroxyphenyl)propionate; 4-Hydroxyphenyllactate; b-(4-Hydroxyphenyl)lactate; b-(4-Hydroxyphenyl)lactic acid; beta-(4-Hydroxyphenyl)lactate;  $\hat{L}$ -(4-hydroxyphenyl)lactate;  $\hat{L}$ -(4-hydroxyphenyl)lactic acid; b-(P-Hydroxyphenyl)lactate; b-(P-Hydroxyphenyl)lactic acid; beta-(P-Hydroxyphenyl)lactate;  $\hat{L}$ -(P-hydroxyphenyl)lactate;  $\hat{L}$ -(P-hydroxyphenyl)lactic acid; DL-P-Hydroxyphenyllactate; P-Hydroxyphenyl lactate; (RS)-3-(4-Hydroxyphenyl)lactate; (RS)-3-(4-Hydroxyphenyl)lactic acid; 3-(4-Hydroxyphenyl)-DL-lactate; 3-(4-Hydroxyphenyl)-DL-lactic acid; 3-(4-Hydroxyphenyl)lactate; 3-(4-Hydroxyphenyl)lactic acid; 3-(P-Hydroxyphenyl)-lactate; 3-(P-Hydroxyphenyl)-lactic acid; a,4-Dihydroxybenzenepropanoate; a,4-Dihydroxybenzenepropanoic acid; b-(P-Hydroxyphenyl)-DL-lactate; b-(P-Hydroxyphenyl)-DL-lactic acid; beta-(P-Hydroxyphenyl)-DL-lactate; beta-(P-Hydroxyphenyl)-DL-lactic acid; DL-3-(4-Hydroxyphenyl)lactate; DL-3-(4-Hydroxyphenyl)lactic acid; HPLA; 4-Hydroxyphenyllactic acid, (DL)-isomer; Para-hydroxyphenyllactic acid; P-Hydroxyphenyllactate

HMDB: HMDB0000755; HMDB00755

CAS: 306-23-0

Hydroxyphenyllactic acid or 4-hydroxyphenyllactate (the L-form) is a tyrosine metabolite. The level of L-hydroxyphenyllactic acid is elevated in patients with a deficiency of the enzyme p-hydroxyphenylpyruvate oxidase (EC 1.14.2.2) (PMID: 4720815). L-hydroxyphenyllactate is present in relatively higher concentrations in the cerebrospinal fluid and urine of patients with phenylketonuria (PKU) and tyrosinemia (PMID: 3126358). However, the D-form of hydroxyphenyllactate is of bacterial origin and is also found in individuals with bacterial overgrowth or unusual gut microflora (PMID: 3126358). Microbial hydroxyphenyllactate is likely derived from phenolic or polyphenolic compounds in the diet. Bifidobacteria and lactobacilli produce considerable amounts of phenyllactic and p-hydroxyphenyllactic acids (PMID: 23061754). It has also been shown that hydroxyphenyllactate decreases ROS (reactive oxygen species) production in both mitochondria and neutrophils and so hydroxyphenyllactate may function as a natural anti-oxidant (PMID: 23061754).

This compound belongs to the class of organic compounds known as phenylpropanoic acids. These are compounds with a structure containing a benzene ring conjugated to a propanoic acid.

## Hydroxyphenyllactic acid – Colorectal cancer

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## Hydroxyphenyllactic acid -- Supradiaphragmatic malignancy

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## Azelaic acid -- Introduction

SYNONYM: 1,7-Dicarboxyheptane; 1,7-Heptanedicarboxylic acid; 1,9-Nonanedioic acid; Acide azelaïque; Acidum azelaicum; Anchoic acid; Azelainsaeure; Azelex; Finacea; Lepargyllic acid; N-Nonanedioic acid; Nonandisaeure; Nonanedioic acid; Skinoren; Azelaate; 1,7-Heptanedicarboxylate; 1,9-Nonanedioate; Anchoate; Lepargylate; N-Nonanedioate; Nonanedioate; Azalaic acid; Azelaicacidtech; Azelainic acid; Azelate; Emerox 1110; Emerox 1144; Emery'S L-110; Finevin; Heptanedicarboxylic acid; Nonanedioic acid azelaic acid; Nonanedioic acid homopolymer; Poly(azelaic anhydride); Polyazelaic anhydride; Skinorem; Azelaic acid, dilithium salt; Azelaic acid, dipotassium salt; Azelaic acid, disodium salt; Azelaic acid, monosodium salt; Azelaic acid, potassium salt; Azelaic acid, sodium salt

HMDB: HMDB0000784; HMDB00784

CAS: 123-99-9

Azelaic acid (AZA) is a naturally occurring saturated nine-carbon dicarboxylic acid ( $\text{COOH}(\text{CH}_2)_7\text{COOH}$ ). It possesses a variety of biological actions both in vitro and in vivo. Interest in the biological activity of AZA arose originally out of studies of skin surface lipids and the pathogenesis of hypochromia in pityriasis versicolor infection. Later, it was shown that *Pityrosporum* can oxidize unsaturated fatty acids to C8-C12 dicarboxylic acids that are competitive inhibitors of tyrosinase in vitro. Azelaic acid was chosen for further investigation and development of a new topical drug for treating hyperpigmentary disorders for the following reasons: it possesses a middle-range of antityrosinase activity, is inexpensive, and more soluble to



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be incorporated into a base cream than other dicarboxylic acids. Azelaic acid is another option for the topical treatment of mild to moderate inflammatory acne vulgaris. It offers effectiveness similar to that of other agents without the systemic side effects of oral antibiotics or the allergic sensitization of topical benzoyl peroxide and with less irritation than tretinoin. Azelaic acid is less expensive than certain other prescription acne preparations, but it is much more expensive than nonprescription benzoyl peroxide preparations. Whether it is safe and effective when used in combination with other agents is not known. (PMID: 7737781, 8961845).

This compound belongs to the class of organic compounds known as medium-chain fatty acids. These are fatty acids with an aliphatic tail that contains between 4 and 12 carbon atoms.

### Azelaic acid -- Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. *Tohoku J Exp Med.* 1995 May;176(1):61-8. PMID: 7482520

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Ritchie SA, Ahiahou PW, Jayasinghe D, Heath D, Liu J, Lu Y, Jin W, Kavianpour A, Yamazaki Y, Khan AM, Hossain M, Su-Myat KK, Wood PL, Krenitsky K, Takemasa I, Miyake M, Sekimoto M, Monden M, Matsubara H, Nomura F, Goodenow DB: Reduced levels of hydroxylated, polyunsaturated ultra long-chain fatty acids in the serum of colorectal cancer patients: implications for early screening and detection. *BMC Med.* 2010 Feb 15;8:13. doi: 10.1186/1741-7015-8-13. PMID: 20156336

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Ikeda A, Nishiumi S, Shinohara M, Yoshie T, Hatano N, Okuno T, Bamba T, Fukusaki E, Takenawa T, Azuma T, Yoshida M: Serum metabolomics as a novel diagnostic approach for gastrointestinal cancer. *Biomed Chromatogr.* 2012 May;26(5):548-58. doi: 10.1002/bmc.1671. Epub 2011 Jul 20. PMID: 21773981

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Lin Y, Ma C, Liu C, Wang Z, Yang J, Liu X, Shen Z, Wu R: NMR-based fecal metabolomics fingerprinting as predictors of earlier diagnosis in patients with colorectal cancer. *Oncotarget.* 2016 May 17;7(20):29454-64. doi: 10.18633/oncotarget.8762. PMID: 27107423

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### Azelaic acid -- Stomach cancer

Higashijima H, Ichimiya H, Nakano T, Yamashita H, Kuroki S, Satoh H, Chijiwa K, Tanaka M: Deconjugation of bilirubin accelerates coprecipitation of cholesterol, fatty acids, and mucin in human bile--in vitro study. *J Gastroenterol.* 1996 Dec;31(6):828-35. PMID: 9027647

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### Myristic acid -- Introduction

SYNONYM: 1-Tetradecanecarboxylic acid; 14; 14:0; 14:00; Acide tetradecanoïque; C14; CH<sub>3</sub>-[CH<sub>2</sub>]12-COOH; Myristinsaeure; N-Tetradecan-1-Oic acid; N-Tetradecanoic acid; N-Tetradecoic acid; Tetradecoic acid; 1-Tetradecanecarboxylate; Myristate; N-Tetradecan-1-Oate; N-Tetradecanoate; N-Tetradecocoate; Tetradecocoate; 1-Tridecanecarboxylate; 1-Tridecanecarboxylic acid; Crodacid; Myristic acid pure; Myristoate; Myristoic acid; Tetradecanoate; Tetradecanoic (myristic) acid; Tetradecanoic acid; Acid, tetradecanoic; Acid, myristic

HMDB: HMDB0000806; HMDB00806

CAS: 544-63-8

Myristic acid is a saturated 14-carbon fatty acid occurring in most animal and vegetable fats, particularly butterfat and coconut, palm, and nutmeg oils. It is used to synthesize flavor and as an ingredient in soaps and cosmetics. (From Dorland, 28th ed). Myristic acid is also commonly added to a penultimate nitrogen terminus glycine in receptor-associated kinases to confer the membrane localisation of the enzyme. This is achieved by the myristic acid having a high enough hydrophobicity to become incorporated into the fatty acyl core of the phospholipid bilayer of the plasma membrane of the eukaryotic cell. (wikipedia).

This compound belongs to the class of organic compounds known as long-chain fatty acids. These are fatty acids with an aliphatic tail that contains between 13 and 21 carbon atoms.

### Myristic acid -- Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. *Tohoku J Exp Med.* 1995 May;176(1):61-8. PMID: 7482520



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Monleon D, Morales JM, Barrasa A, Lopez JA, Vazquez C, Celda B: Metabolite profiling of fecal water extracts from human colorectal cancer. *NMR Biomed.* 2009 Apr;22(3):342-8. doi: 10.1002/nbm.1345. PMID: 19006102

Weir TL, Manter DK, Sheflin AM, Barnett BA, Heuberger AL, Ryan EP: Stool microbiome and metabolome differences between colorectal cancer patients and healthy adults. *PLoS One.* 2013 Aug 6;8(8):e70803. doi: 10.1371/journal.pone.0070803. Print 2013. PMID: 23940645

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Ikeda A, Nishiumi S, Shinohara M, Yoshie T, Hatano N, Okuno T, Bamba T, Fukusaki E, Takenawa T, Azuma T, Yoshida M: Serum metabolomics as a novel diagnostic approach for gastrointestinal cancer. *Biomed Chromatogr.* 2012 May;26(5):548-58. doi: 10.1002/bmc.1671. Epub 2011 Jul 20. PMID: 21773981

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Sinha R, Ahn J, Sampson JN, Shi J, Yu G, Xiong X, Hayes RB, Goedert JJ: Fecal Microbiota, Fecal Metabolome, and Colorectal Cancer Interrelations. *PLoS One.* 2016 Mar 25;11(3):e0152126. doi: 10.1371/journal.pone.0152126. eCollection 2016. PMID: 27015276

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## Myristic acid -- Schizophrenia

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10.1186/gm300. PMID: 22257447

## N-Acetyl-L-aspartic acid -- Introduction

SYNONYM: (S)-2-(acetylamino)Butanedioic acid; (S)-2-(acetylamino)Succinic acid; Acetyl-L-aspartic acid; Acetylaspartic acid; L-N-Acetylaspartic acid; N-Acetylaspartic acid; NAA; (S)-2-(acetylamino)Butanedioate; N-Acetyl-L-aspartate; (S)-2-(acetylamino)Succinate; Acetyl-L-aspartate; Acetylaspartate; L-N-Acetylaspartate; N-Acetylaspartate; (2S)-2-Acetamidobutanedioate; (2S)-2-Acetamidobutanedioic acid; N-Acetyl-S-aspartate; N-Acetyl-S-aspartic acid; N-Acetyl aspartate; N-Acetylaspartate, monopotassium salt

HMDB: HMDB0000812; HMDB00812

CAS: 997-55-7

N-Acetylaspartic acid is a derivative of aspartic acid. It is the second most concentrated molecule in the brain after the amino acid glutamate. It is synthesized in neurons from the amino acid aspartate and acetyl coenzyme A (acetyl CoA). The various functions served by N-acetylaspartic acid are still under investigation, but the primary proposed functions include (1) acting as a neuronal osmolyte that is involved in fluid balance in the brain, (2) serving as a source of acetate for lipid and myelin synthesis in oligodendrocytes (the glial cells that myelinate neuronal axons), (3) serving as a precursor for the synthesis of the important dipeptide neurotransmitter N-acetylaspartylglutamate (NAAG), and (4) playing a potential role in energy production from the amino acid glutamate in neuronal mitochondria. High neurotransmitter levels can lead to abnormal neural signaling, delayed or arrested intellectual development, and difficulties with general motor skills. When present in sufficiently high levels, N-acetylaspartic acid can be a neurotoxin, an acidogen, and a metabotoxin. A neurotoxin is a compound that disrupts or attacks neural tissue. An acidogen is an acidic compound that induces acidosis, which has multiple adverse effects on many organ systems. A metabotoxin is an endogenously produced metabolite that causes adverse health effects at chronically high levels. Chronically high levels of N-acetylaspartic acid are associated with Canavan disease. N-acetylaspartic acid is an organic acid. Abnormally high levels of organic acids in the blood (organic acidemia), urine (organic aciduria), the brain, and other tissues lead to general metabolic acidosis. Acidosis typically occurs when arterial pH falls below 7.35. Infants with acidosis have symptoms that include poor feeding, vomiting, loss of appetite, weak muscle tone (hypotonia), and lack of energy (lethargy). These can progress to heart abnormalities, seizures, coma, and possibly death. Many affected children with organic acidemias experience intellectual disability or delayed development. In adults, acidosis or acidemia is characterized by headaches, confusion, feeling tired, tremors, sleepiness, and flapping tremors.

This compound belongs to the class of organic compounds known as aspartic acid and derivatives. These are compounds containing an aspartic acid or a derivative thereof resulting from reaction of aspartic acid at the amino group or the carboxy group, or from the replacement of any hydrogen of glycine by a heteroatom.

## N-Acetyl-L-aspartic acid -- Canavan disease

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### N-Acetyl-L-aspartic acid -- Obesity

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### Phenylacetylglycine -- Introduction

SYNONYM: N-Phenacyl glycine; N-Phenylacetyl glycine; Phenaceturic acid; Phenacyl glycine; Phenacetate; Phenacetic acid; ((Phenylacetyl)amino)acetic acid; N-(Phenylacetyl)-glycine; N-(Phenylacetyl)glycine; PAA; PAG; Phenaceturate; Phenylacetyl glycine; [(Phenylacetyl)amino]acetate; [(Phenylacetyl)amino]acetic acid

HMDB: HMDB0000821; HMDB00821



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CAS: 500-98-1

Phenylacetylglycine is an acyl glycine. Acyl glycines are normally minor metabolites of fatty acids. However, the excretion of certain acyl glycines is increased in several inborn errors of metabolism. In certain cases the measurement of these metabolites in body fluids can be used to diagnose disorders associated with mitochondrial fatty acid beta-oxidation. Acyl glycines are produced through the action of glycine N-acetyltransferase (EC 2.3.1.13) which is an enzyme that catalyzes the chemical reaction: acyl-CoA + glycine  $\rightleftharpoons$  CoA + N-acetylglycine. Phenylacetylglycine or PAG is a glycine conjugate of phenylacetic acid. Phenylacetic acid may arise from exposure to styrene (plastic) or through the consumption of fruits and vegetables. Phenylacetic acid is used in some perfumes, possessing a honey-like odour in low concentrations, and is also used in penicillin G production. PAG is a putative biomarker of phospholipidosis. Urinary PAG is elevated in animals exhibiting abnormal phospholipid accumulation in many tissues and may thus be useful as a surrogate biomarker for phospholipidosis. (PMID: 15764292) The presence of phenylacetylglycine in urine has been confirmed for dogs, rats and mice. However, the presence of this compound in human urine is controversial. GC-MS studies have not found this compound (PMID: 7492634) while NMR studies claimed to have identified it (PMID: 21167146). It appears that phenylacetylglycine may sometimes be mistaken for phenylacetylglutamine via NMR.

This compound belongs to the class of organic compounds known as n-acyl-alpha amino acids. These are compounds containing an alpha amino acid which bears an acyl group at its terminal nitrogen atom.

### Phenylacetylglycine -- Heart failure

Norrelund H, Wiggers H, Halbirk M, Frystyk J, Flyvbjerg A, Botker HE, Schmitz O, Jorgensen JO, Christiansen JS, Moller N: Abnormalities of whole body protein turnover, muscle metabolism and levels of metabolic hormones in patients with chronic heart failure. *J Intern Med.* 2006 Jul;260(1):11-21. PMID: 16789974

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### Propionylcarnitine -- Introduction

SYNONYM: 3-Carboxy-N,N,N-trimethyl-2-(1-oxoproxy)-1-propanaminium inner salt; O-Propionylcarnitine; Propionyl carnitine; (+/-)-propionylcarnitine chloride; (3-Carboxy-2-hydroxypropyl)trimethyl-hydroxide ammonium inner salt; L-Propionylcarnitine; O-Propanoylcarnitine; Propionyl-carnitine; Propionyl-L-carnitine; Propionylcarnitine, (+)-isomer; Propionylcarnitine, (R)-isomer

HMDB: HMDB0000824; HMDB00824

CAS: 17298-37-2

Propionylcarnitine is present in high abundance in the urine of patients with Methylmalonyl-CoA mutase (MUT) deficiency, (together with Methylmalonic acid). MUT is a mitochondrial enzyme that catalyzes the isomerization of methylmalonyl-CoA to succinyl-CoA (OMIM 609058). Propionylcarnitine is found to be associated with propionic aciduria, which is an inborn error of metabolism.

This compound belongs to the class of organic compounds known as acyl carnitines. These are organic compounds containing a fatty acid with the carboxylic acid attached to carnitine through an ester bond.

### Propionylcarnitine -- Celiac disease

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## Propionylcarnitine -- Propionic acidemia



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## Pentadecanoic acid -- Introduction

SYNONYM: 15:00; C15; C15:0; N-Pentadecanoic acid; Pentadecyllic acid; Pentadecanoate; N-Pentadecanoate; Pentadecylate; N-Pentadecylate; N-Pentadecyllic acid; Pentadecylate; Pentadecyclic acid

HMDB: HMDB0000826; HMDB00826

CAS: 1002-84-2

Pentadecanoic acid is a fatty acid of exogenous (primarily ruminant) origin. Many "odd" length long chain amino acids are derived from the consumption of dairy fats (milk and meat). Pentadecanoic acid constitutes 1.05% of milk fat and 0.43% of ruminant meat fat. The content of heptadecanoic acid in the subcutaneous adipose tissue of humans appears to be a good biological marker of long-term milk fat intake in free-living individuals in populations with high consumption of dairy products. (PMID 9701185; PMID 11238766).

This compound belongs to the class of organic compounds known as long-chain fatty acids. These are fatty acids with an aliphatic tail that contains between 13 and 21 carbon atoms.

## Pentadecanoic acid -- Colorectal cancer

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### Pentadecanoic acid -- Schizophrenia

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## Stearic acid -- Introduction

**SYNONYM:** 18:0; Acide octadecanoïque; Acide stearique; C18:0; CH<sub>3</sub>-[CH<sub>2</sub>]16-COOH; N-Octadecanoic acid; Octadecanoic acid; Octadecansaeure; Octadecocic acid; Oktadekansaeure; Stearate; Stearinsaeure; N-Octadecanoate; Octadecanoate; Octadecante; 1-Heptadecanecarboxylate; 1-Heptadecanecarboxylic acid; Stearex beads; Stearic acid cherry; Stearophanate; Stearophanic acid; Calcium stearate; Aluminum tristearate; Ammonium stearate; Zinc stearate; Magnesium stearate; Sodium stearate; Aluminum monostearate

**HMDB:** HMDB0000827; HMDB00827

**CAS:** 57-11-4

Stearic acid, also called octadecanoic acid, is one of the useful types of saturated fatty acids that comes from many animal and vegetable fats and oils. It is a waxy solid, and its chemical formula is CH<sub>3</sub>(CH<sub>2</sub>)<sub>16</sub>COOH. Its name comes from the Greek word stear, which means tallow. Its IUPAC name is octadecanoic acid. -- Wikipedia.

This compound belongs to the class of organic compounds known as long-chain fatty acids. These are fatty acids with an aliphatic tail that contains between 13 and 21 carbon atoms.

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## Pelargonic acid -- Introduction

SYNONYM: 1-Nonanoic acid; 1-Octanecarboxylic acid; CH<sub>3</sub>-[CH<sub>2</sub>]7-COOH; N-Nonanoic acid; Nonanoate; Nonansaeure; Nonoic acid; Nonylic acid; Pelargic acid; Pelargon; Pelargonsaeure; Pergonic acid; 1-Nonanoate; Pelargonate; 1-Octanecarboxylate; N-Nonanoate; Nonanoic acid; Nonoate; Nonylate; Pelargate; Pergonate; Cirrasol 185a; Emery 1202; Emery'S L-114; Emfac 1202; Hexacid C-9; N-Nonoate; N-Nonanoic acid; N-Nonylate; N-Nonylic acid; N-Pelargonate; N-Pelargonic acid; Pelargonic acid, calcium salt; Potassium nonanoate; Pelargonic acid, cadmium salt; Pelargonic acid, sodium salt; Pelargonic acid, zinc salt; Pelargonic acid, aluminum salt; Pelargonic acid, potassium salt

HMDB: HMDB0000847; HMDB00847

CAS: 112-05-0

Pelargonic acid, or nonanoic acid, is a fatty acid which occurs naturally as esters in the oil of pelargonium. Synthetic esters, such as methyl nonanoate, are used as flavorings. Pelargonic acid is an organic compound composed of a nine-carbon chain terminating in a carboxylic acid. It is an oily liquid with an unpleasant, rancid odor. It is nearly insoluble in water, but well soluble in chloroform and ether. The derivative 4-nonanoylmorpholine is an ingredient in some pepper sprays.

This compound belongs to the class of organic compounds known as medium-chain fatty acids. These are fatty acids with an aliphatic tail that contains between 4 and 12 carbon atoms.

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## L-Valine -- Introduction

SYNONYM: (2S)-2-amino-3-Methylbutanoic acid; (S)-Valine; 2-amino-3-Methylbutyric acid; L-(+)-alpha-Aminoisovaleric acid; L-alpha-amino-beta-Methylbutyric acid; L-Valin; V; Val; VALINE; (2S)-2-amino-3-Methylbutanoate; 2-amino-3-Methylbutyrate; L-(+)-a-Aminoisovalerate; L-(+)-a-Aminoisovaleric acid; L-(+)-alpha-Aminoisovalerate; L-(+)-l-aminoisovalerate; L-(+)-l-aminoisovaleric acid; L-a-amino-b-Methylbutyrate; L-a-amino-b-Methylbutyric acid; L-alpha-amino-beta-Methylbutyrate; L-l-amin-l-methylbutyrate; L-l-amin-l-methylbutyric acid; (S)-2-amino-3-Methyl-butanoate; (S)-2-amino-3-Methyl-butanoic acid; (S)-2-amino-3-Methylbutanoate; (S)-2-amino-3-Methylbutanoic acid; (S)-2-amino-3-Methylbutyrate; (S)-2-amino-3-Methylbutyric acid; (S)-a-amino-b-Methylbutyrate; (S)-a-amino-b-Methylbutyric acid; (S)-alpha-amino-beta-Methylbutyrate; (S)-alpha-amino-beta-Methylbutyric acid; 2-amino-3-Methylbutanoate; 2-amino-3-Methylbutanoic acid; L Valine

HMDB: HMDB0000883; HMDB0034366; HMDB00883; HMDB34366

CAS: 72-18-4

Valine (abbreviated as Val or V) is an -amino acid with the chemical formula HO<sub>2</sub>CCH(NH<sub>2</sub>)CH(CH<sub>3</sub>)<sub>2</sub>. It is named after the plant valerian. L-Valine is one of 20 proteinogenic amino acids. Its codons are GUU, GUC, GUA, and GUG. This essential amino acid is classified as nonpolar. Along with leucine and isoleucine, valine is a branched-chain amino acid. Branched chain amino acids (BCAA) are essential amino acids whose carbon structure is marked by a branch point. These



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three amino acids are critical to human life and are particularly involved in stress, energy and muscle metabolism. BCAA supplementation as therapy, both oral and intravenous, in human health and disease holds great promise. "BCAA" denotes valine, isoleucine and leucine which are branched chain essential amino acids. Despite their structural similarities, the branched amino acids have different metabolic routes, with valine going solely to carbohydrates, leucine solely to fats and isoleucine to both. The different metabolism accounts for different requirements for these essential amino acids in humans: 12 mg/kg, 14 mg/kg and 16 mg/kg of valine, leucine and isoleucine respectively. Furthermore, these amino acids have different deficiency symptoms. Valine deficiency is marked by neurological defects in the brain, while isoleucine deficiency is marked by muscle tremors. Many types of inborn errors of BCAA metabolism exist, and are marked by various abnormalities. The most common form is the maple syrup urine disease, marked by a characteristic urinary odor. Other abnormalities are associated with a wide range of symptoms, such as mental retardation, ataxia, hypoglycemia, spinal muscle atrophy, rash, vomiting and excessive muscle movement. Most forms of BCAA metabolism errors are corrected by dietary restriction of BCAA and at least one form is correctable by supplementation with 10 mg of biotin daily. BCAA are decreased in patients with liver disease, such as hepatitis, hepatic coma, cirrhosis, extrahepatic biliary atresia or portacaval shunt; aromatic amino acids (AAA) — tyrosine, tryptophan and phenylalanine, as well as methionine — are increased in these conditions. Valine in particular, has been established as a useful supplemental therapy to the ailing liver. All the BCAA probably compete with AAA for absorption into the brain. Supplemental BCAA with vitamin B6 and zinc help normalize the BCAA:AAA ratio (<http://www.dcnutrition.com>). In sickle-cell disease, valine substitutes for the hydrophilic amino acid glutamic acid in hemoglobin. Because valine is hydrophobic, the hemoglobin does not fold correctly. Hypervalinemia is another example of an inborn error of metabolism involving Valine. Valine is an essential amino acid, hence it must be ingested, usually as a component of proteins.

This compound belongs to the class of organic compounds known as valine and derivatives. These are compounds containing valine or a derivative thereof resulting from reaction of valine at the amino group or the carboxy group, or from the replacement of any hydrogen of glycine by a heteroatom.

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## L-Valine -- Cachexia

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## L-Valine -- Lewy body disease

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## Ribothymidine -- Introduction

SYNONYM: 1-(beta-D-Ribofuranosyl)thymine; Ribosylthymidine; t; Thymine riboside; 1-(b-D-Ribofuranosyl)thymine; 1-( $\beta$ -D-ribofuranosyl)thymine; 1-b-D-Ribofuranosylthymine; 1-beta-delta-Ribofuranosylthymine; 5-Methyl-1-beta-D-ribofuranosyl-2,4(1H,3H)-pyrimidinedione; 5-Methyl-1-beta-delta-ribofuranosyl-2,4(1H,3H)-pyrimidinedione; 5-Methyluridine; 5-Methyluridine; b-D-Ribofuranoside thymine-1; beta-D-Ribofuranoside; beta-delta-Ribofuranoside; beta-delta-Ribofuranoside thymine-1; Ribosylthymine; Thymine ribofuranoside; Thymine ribonucleoside; Thymine-1 beta-D-ribofuranosylthymine; Thymine-1 beta-delta-ribofuranosylthymine

HMDB: HMDB0000884; HMDB00884

CAS: 1463-10-1

Ribothymidine is an endogenous methylated nucleoside found in human fluids; methylated purine bases are present in higher amounts in tumor-bearing patients compared to healthy controls. DNA hypermethylation is a common finding in malignant cells and has been explored as a therapeutic target for hypomethylating agents. When chemical bonds to DNA, the DNA becomes damaged and proper and complete replication cannot occur to make the normal intended cell. A DNA adduct is an abnormal piece of DNA covalently-bonded to a cancer-causing chemical. This has shown to be the start of a cancerous cell, or carcinogenesis. DNA adducts in scientific experiments are used as bio-markers and as such are themselves measured to reflect quantitatively, for comparison, the amount of cancer in the subject. (PMID: 3506820, 17044778, 17264127, 16799933).

This compound belongs to the class of organic compounds known as pyrimidine nucleosides. These are compounds comprising a pyrimidine base attached to a ribosyl or deoxyribosyl moiety.

## Ribothymidine -- Perillyl alcohol administration for cancer treatment

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## Citrulline -- Introduction

SYNONYM: (S)-2-amino-5-Ureidopentanoic acid; 2-amino-5-Ureidovaleric acid; alpha-amino-delta-Ureidovaleric acid; Cit; delta-Ureidonorvaline; L-2-amino-5-Ureidovaleric acid; N(5)-(Aminocarbonyl)-L-ornithine; N5-(Aminocarbonyl)ornithine; N5-Carbamoylornithine; N(delta)-Carbamylornithine; (S)-2-amino-5-Ureidopentanoate; 2-amino-5-Ureidovalerate; a-amino-delta-Ureidovalerate; a-amino-delta-Ureidovaleric acid; alpha-amino-delta-Ureidovalerate;  $\text{I}^{\pm}$ -amino- $\text{I}'$ -ureidovalerate;  $\text{I}^{\pm}$ -amino- $\text{I}'$ -ureidovaleric acid;  $\text{I}'$ -ureidonorvaline; L-2-amino-5-Ureidovalerate; N( $\text{I}'$ )-carbamylornithine; a-amino- $\text{I}'$ -ureidovalerate; a-amino- $\text{I}'$ -ureidovaleric acid; (2S)-2-amino-5-(carbamoylamino)Pentanoate; (2S)-2-amino-5-(Aminocarbonyl)aminopentanoic acid; 2-amino-5-Ureidovalerate; 2-amino-5-Ureidovaleric acid; a-amino-D-Ureidovalerate; a-amino-D-Ureidovaleric acid; alpha-amino-gamma-Ureidovalerate; alpha-amino-gamma-Ureidovaleric acid; amino-Ureidovalerate; amino-Ureidovaleric acid; CIR; Citrulline; D-Ureidonorvaline; DL-Citrulline; Gammaureidonorvaline; H-Cit-OH; L(+)-2-amino-5-Ureidovalerate; L(+)-2-amino-5-Ureidovaleric acid; L(+)-Citrulline; L-2-amino-5-ureido-Valerate; L-2-amino-5-ureido-Valeric acid; L-Citrulline; L-Citrulline; L-N5-Carbamoyl-ornithine; N()-Carbamylornithine; N(5)-(Aminocarbonyl)-DL-ornithine; N-Carbamylornithine; N5-(Aminocarbonyl)-L-ornithine; N5-(Aminocarbonyl)-ornithine; N5-Carbamoyl-L-ornithine; N5-Carbamylornithine; ND-Carbamylornithine; Ndelta-carbamyl-ornithine; Ndelta-carbamylornithine; Ngamma-carbamylornithine; Sitrulline; Ureidonorvaline; Ureidovalerate; Ureidovaleric acid

HMDB: HMDB0000904; HMDB00904

CAS: 372-75-8

Citrulline is an amino acid made from ornithine and carbamoyl phosphate in one of the central reactions in the urea cycle. It is also produced from arginine as a by-product of the reaction catalyzed by NOS family (NOS). In this reaction, arginine is first oxidized into N(omega)-hydroxyarginine, which is then further oxidized to citrulline concomitant with the release of nitric oxide (EC 1.14.13.39). Citrulline's name is derived from *citrullus*, the Latin word for watermelon, from which it was first isolated.

This compound belongs to the class of organic compounds known as l-alpha-amino acids. These are alpha amino acids which have the L-configuration of the alpha-carbon atom.

## Citrulline -- Alzheimer's disease

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## Citrulline -- Phosphoenolpyruvate Carboxykinase Deficiency 1, Cytosolic

Vieira P, Cameron J, Rahikkala E, Keski-Filppula R, Zhang LH, Santra S, Matthews A, Myllynen P, Nuutinen M, Moilanen JS, Rodenburg RJ, Rolfs A, Uusimaa J, van Karnebeek CDM: Novel homozygous PCK1 mutation causing cytosolic phosphoenolpyruvate carboxykinase deficiency presenting as childhood hypoglycemia, an abnormal pattern of urine metabolites and liver dysfunction. *Mol Genet Metab.* 2017 Apr;120(4):337-341. doi: 10.1016/j.ymgme.2017.02.003. Epub 2017 Feb 6. PMID: 28216384

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## Citrulline -- Ulcerative colitis

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## Deoxyadenosine monophosphate -- Introduction

SYNONYM: 2'-dAMP; 2'-Deoxy-5'-adenosine monophosphate; 2'-Deoxy-AMP; 2'-Deoxyadenosine 5'-(dihydrogen phosphate); 2'-Deoxyadenosine 5'-monophosphate; 2'-Deoxyadenosine 5'-phosphate; 2'-Deoxyadenosine monophosphate; 2'-DEOXYADENOSINE-5'-monophosphATE; 2'-Deoxyadenylic acid; Deoxy-5'-adenylic acid; Deoxy-AMP; Deoxyadenosine 5'-monophosphate; Deoxyadenosine 5'-phosphate; Deoxyadenylic acid; Deoxyadenosine monophosphoric acid; 2'-Deoxy-5'-adenosine monophosphoric acid; 2'-Deoxyadenosine 5'-(dihydrogen phosphoric acid); 2'-Deoxyadenosine 5'-monophosphoric acid; 2'-Deoxyadenosine 5'-phosphoric acid; 2'-Deoxyadenosine monophosphoric acid; 2'-DEOXYADENOSINE-5'-monophosphoric acid; 2'-Deoxyadenylate; Deoxy-5'-adenylate; Deoxyadenosine 5'-monophosphoric acid; Deoxyadenosine 5'-phosphoric acid; Deoxyadenylate; 2'-Deoxy-5'-adenylate; 2'-Deoxy-5'-adenylic acid; 2'-Deoxy-adenosine 5'-phosphorate; 2'-Deoxy-adenosine 5'-phosphoric acid; 2'-Deoxyadenosine-5'-phosphate; dAMP; Deoxyadenosine-phosphate; PdA; 2'-Deoxy-5'-adenosine monophosphate, ammonium salt; 2'-Deoxy-5'-adenosine monophosphate, disodium salt; 2'Deoxy-5'-AMP; dAMP CPD

HMDB: HMDB0000905; HMDB00905

CAS: 653-63-4

Adenosine is a nucleoside comprised of adenine attached to a ribose (ribofuranose) moiety via a -N9-glycosidic bond. Deoxyadenosine monophosphate is a derivative of the common nucleic acid ATP, or adenosine triphosphate, in which the -OH (hydroxyl) group on the 2' carbon on the nucleotide's pentose has been removed (hence the deoxy- part of the name). Additionally, the monophosphate of the name indicates that two of the phosphoryl groups of GTP have been removed, most likely by hydrolysis. Deoxyadenosine monophosphate is abbreviated dAMP. (Wikipedia).

This compound belongs to the class of organic compounds known as purine 2'-deoxyribonucleoside monophosphates. These are purine nucleotides with monophosphate group linked to the ribose moiety lacking a hydroxyl group at position 2.

## Trimethylamine N-oxide -- Introduction

SYNONYM: (CH<sub>3</sub>)<sub>3</sub>NO; Me<sub>3</sub>n(+)-O(-); Me<sub>3</sub>n(O); N(CH<sub>3</sub>)<sub>3</sub>O; TMAO; Trimethylamine oxide; Trimethylaminoxid; Trimethyloxamine; N,N-Dimethylmethanamine N-oxide; TMA-oxide; Trimethylamine-N-oxide; Triox; Trimethylammonium oxide

HMDB: HMDB0000925; HMDB00925

CAS: 1184-78-7

Trimethylamine N-oxide (TMAO) is an oxidation product of trimethylamine and a common metabolite in animals and humans. In particular, trimethylamine-N-oxide is biosynthesized endogenously from trimethylamine, which is derived from choline, which can be derived from dietary lecithin (phosphatidylcholines) or dietary carnitine. TMAO decomposes to trimethylamine (TMA), which is the main odorant that is characteristic of degrading seafood. TMAO is an osmolyte that the body will use to counteract the effects of increased concentrations of urea (due to kidney failure) and high levels can be used as a biomarker for kidney problems. Fish odor syndrome or trimethylaminuria is a defect in the production of the enzyme flavin containing monooxygenase 3 (FMO3) causing incomplete breakdown of trimethylamine from choline-containing food into trimethylamine oxide. Trimethylamine then builds up and is released in the person's sweat, urine, and breath, giving off a strong fishy odor. The concentration of TMAO in the blood increases after consuming foods containing carnitine or lecithin (phosphatidylcholines), if the bacteria that convert those substances to TMAO are present in the gut (PMID: 23614584). High concentrations of carnitine are found in red meat, some energy drinks, and certain dietary supplements; lecithin is found in eggs and is commonly used as an ingredient in processed food. High levels of TMAO are found in many seafoods. Some types of normal gut bacteria (e.g. species of *Acinetobacter*) in the human gut convert dietary carnitine and dietary lecithin to



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TMAO (PMID: 21475195). TMAO alters cholesterol metabolism in the intestines, in the liver and in arterial wall. When TMAO is present, cholesterol metabolism is altered and there is an increased deposition of cholesterol within, and decreased removal of cholesterol from, peripheral cells such as those in the artery wall (PMID: 23563705). Urinary TMAO is a biomarker for the consumption of fish, especially cold-water fish. Trimethylamine N-oxide is found to be associated with maple syrup urine disease and propionic acidemia, which are inborn errors of metabolism.

This compound belongs to the class of organic compounds known as trialkyl amine oxides. These are hydrocarbyl derivatives of the aminoxide anion, with the general formula R<sub>3</sub>N+[O-] or R<sub>3</sub>N=O, where R is an alkyl group.

### Trimethylamine N-oxide -- Argininosuccinic aciduria

Kleijer WJ, Garritsen VH, Linnebank M, Mooyer P, Huijmans JG, Mustonen A, Simola KO, Arslan-Kirchner M, Battini R, Briones P, Cardo E, Mandel H, Tschiedel E, Wanders RJ, Koch HG: Clinical, enzymatic, and molecular genetic characterization of a biochemical variant type of argininosuccinic aciduria: prenatal and postnatal diagnosis in five unrelated families. *J Inherit Metab Dis.* 2002 Sep;25(5):399-410. PMID: 12408190

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### Trimethylamine N-oxide -- Dimethylglycine Dehydrogenase Deficiency

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### **Trimethylamine N-oxide -- Ulcerative colitis**

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## S-Adenosylhomocysteine -- Introduction

**SYNONYM:** (2S)-2-amino-4-((2S,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxytetrahydrofuran-2-yl)methyl)sulfanylbutanoic acid; 2-S-Adenosyl-L-homocysteine; Adenosyl-L-homocysteine; Adenosylhomocysteine; AdoHcy; S-(5'-Adenosyl)-L-homocysteine; S-[1-(Adenin-9-yl)-1,5-dideoxy-beta-D-ribofuranos-5-yl]-L-homocysteine; SAH; (2S)-2-amino-4-((2S,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxytetrahydrofuran-2-yl)methyl)sulfanylbutanoate; (2S)-2-amino-4-((2S,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxytetrahydrofuran-2-yl)methyl)sulphanylbutoanoate; (2S)-2-amino-4-((2S,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-

dihydroxytetrahydrofuran-2-yl]methyl} sulphanyl)butanoic acid; S-[1-(Adenin-9-yl)-1,5-dideoxy-b-D-ribofuranos-5-yl]-L-homocysteine; S-[1-(Adenin-9-yl)-1,5-dideoxy- $\beta$ -D-ribofuranos-5-yl]-L-homocysteine; (S)-5'-(S)-(3-amino-3-Carboxypropyl)-5'-thioadenosine; 5'-Deoxy-S-adenosyl-L-homocysteine; 5'-S-(3-amino-3-Carboxypropyl)-5'-thio-L-adenosine; Adenosyl-homo-cys; adenosylhomo-CYS; Formycinylhomocysteine; L-5'-S-(3-amino-3-Carboxypropyl)-5'-thior-adenosine; L-S-Adenosyl-homocysteine; L-S-Adenosylhomocysteine; S-(5'-Deoxyadenosin-5'-yl)-L-homocysteine; S-(5'-Deoxyadenosine-5')-L-homocysteine; S-Adenosyl-homocysteine; S-Adenosyl-L-homocysteine; Adenosylhomocysteine, S; S Adenosylhomocysteine

HMDB: HMDB0000939; HMDB00939

CAS: 979-92-0

S-Adenosyl-L-homocysteine (SAH) is formed by the demethylation of S-adenosyl-L-methionine. S-Adenosylhomocysteine (AdoHcy or SAH) is also the immediate precursor of all of the homocysteine produced in the body. The reaction is catalyzed by S-adenosylhomocysteine hydrolase and is reversible with the equilibrium favoring formation of SAH. In vivo, the reaction is driven in the direction of homocysteine formation by the action of the enzyme adenosine deaminase which converts the second product of the S-adenosylhomocysteine hydrolase reaction, adenosine, to inosine. Except for methyl transfer from betaine and from methylcobalamin in the methionine synthase reaction, SAH is the product of all methylation reactions that involve S-adenosylmethionine (SAM) as the methyl donor. Methylation is significant in epigenetic regulation of protein expression via DNA and histone methylation. The inhibition of these SAM-mediated processes by SAH is a proven mechanism for metabolic alteration. Because the conversion of SAH to homocysteine is reversible, with the equilibrium favoring the formation of SAH, increases in plasma homocysteine are accompanied by an elevation of SAH in most cases. Disturbances in the transmethylation pathway indicated by abnormal SAH, SAM, or their ratio have been reported in many neurodegenerative diseases, such as dementia, depression, and Parkinson's disease (PMID: 18065573, 17892439). Therefore, when present in sufficiently high levels, S-adenosylhomocysteine can act as an immunotoxin and a metabotoxin. An immunotoxin disrupts, limits the function, or destroys immune cells. A metabotoxin is an endogenous metabolite that causes adverse health effects at chronically high levels. Chronically high levels of S-adenosylhomocysteine are associated with S-adenosylhomocysteine (SAH) hydrolase deficiency and adenosine deaminase deficiency. S-Adenosylhomocysteine forms when there are elevated levels of homocysteine and adenosine. S-Adenosyl-L-homocysteine is a potent inhibitor of S-adenosyl-L-methionine-dependent methylation reactions. It is toxic to immature lymphocytes and can lead to immunosuppression (PMID: 221926).

This compound belongs to the class of organic compounds known as 5'-deoxy-5'-thionucleosides. These are 5'-deoxyribonucleosides in which the ribose is thio-substituted at the 5'position by a S-alkyl group.

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## S-Adenosylhomocysteine -- Adenosine kinase deficiency

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## gamma-Glutamylcysteine -- Introduction

SYNONYM: 5-L-Glutamyl-L-cysteine; gamma-Glu-cys; gamma-L-Glutamyl-L-cysteine; GammaGluCys; Glu(-cys); L-gamma-Glutamylcysteine; g-Glutamylcysteine;  $\hat{\beta}$ -glutamylcysteine; g-Glu-cys;  $\hat{\beta}$ -glu-cys; g-L-Glutamyl-L-cysteine;  $\hat{\beta}$ -L-glutamyl-L-cysteine; L-g-Glutamylcysteine; L- $\hat{\beta}$ -glutamylcysteine; (Des-gly)-glutathione; 3GC; 5-L-Glutamylcysteine; H-gamma-Glu-cys-OH; H-Glu(cys-OH)-OH; L-g-Glutamyl-L-cysteine; L-gamma-Glutamyl-L-cysteine; N-(1-Carboxy-2-mercaptoethyl)-L-glutamine; N-L-gamma-Glutamyl-L-cysteine; XN-L-g-Glutamyl-glutamine; XN-L-gamma-Glutamyl-glutamine;  $\hat{\beta}$ -L-Glu-L-Cys; L- $\hat{\beta}$ -Glutamyl-L-cysteine; N- $\hat{\beta}$ -Glutamylcysteine; N-L- $\hat{\beta}$ -Glutamylcysteine; N-L- $\hat{\beta}$ -Glutamyl-L-cysteine; gamma-L-Glu-L-Cys; N-gamma-Glutamylcysteine; N-L-gamma-Glutamylcysteine; gamma-Glutamylcysteine; N- $\hat{\beta}$ -L-Glutamyl-L-cysteine

HMDB: HMDB0001049; HMDB0029146; HMDB01049; HMDB29146

CAS: 636-58-8

gamma-Glutamylcysteine is a dipeptide composed of gamma-glutamate and cysteine, and is a proteolytic breakdown product of larger proteins. It belongs to the family of N-acyl-alpha amino acids and derivatives. These are compounds containing an alpha amino acid which bears an acyl group at its terminal nitrogen atom. gamma-Glutamylcysteine is an incomplete breakdown product of protein digestion or protein catabolism. Some dipeptides are known to have physiological or cell-signaling effects although most are simply short-lived intermediates on their way to specific amino acid degradation pathways following further proteolysis. gamma-Glutamylcysteine is a product of enzyme glutamate-cysteine ligase [EC 6.3.2.2] and a substrate of enzyme glutathione synthase [EC 6.3.2.3] in the glutamate metabolism pathway (KEGG).

This compound belongs to the class of organic compounds known as n-acyl-alpha amino acids. These are compounds containing an alpha amino acid which bears an acyl group at its terminal nitrogen atom.

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## Glyceraldehyde -- Introduction

SYNONYM: (+)-Glyceraldehyde; 2,3-Dihydroxypropanal; 2,3-Dihydroxypropionaldehyde; Aldotriose; alpha,beta-Dihydroxypropionaldehyde; DL-Glyceraldehyde; Gliceraldeido; Glyceraldehyd; Glyceric aldehyde; Glycerinaldehyd; Glycerinaldehyde; Glycerinformal; Glycerose; Glyzerinaldehyd; a,b-Dihydroxypropionaldehyde;  $\hat{1}\pm,\hat{1}^2$ -dihydroxypropionaldehyde; (+/-)-2,3-dihydroxy-propanal; (+/-)-glyceraldehyde; D-(+)-Glyceraldehyde; D-2,3-Dihydroxypropanal; D-2,3-Dihydroxypropionaldehyde; D-Aldotriose; D-Glyceraldehyde; D-Glycerose; delta-(+)-Glyceraldehyde; delta-2,3-Dihydroxypropanal; delta-2,3-Dihydroxypropionaldehyde; delta-Aldotriose; delta-Glyceraldehyde; delta-Glycerose; Dihydroxypropionaldehyde

HMDB: HMDB0001051; HMDB01051

CAS: 56-82-6

Glyceraldehyde is a triose monosaccharide with chemical formula C<sub>3</sub>H<sub>6</sub>O<sub>3</sub>. It is the simplest of all common aldoses. It is a sweet, colourless crystalline solid that is an intermediate compound in carbohydrate metabolism. The word "glyceraldehyde" comes from combining glycerine and aldehyde, as glyceraldehyde is merely glycerine with one hydroxide changed to an aldehyde. Glyceraldehyde is produced from the action of the enzyme glyceraldehyde dehydrogenase, which converts glycerol to glyceraldehyde using NADP as a cofactor. When present at sufficiently high levels, glyceraldehyde can be a cytotoxin and a mutagen. A cytotoxin is a compound that kills cells. A mutagen is a compound that causes mutations in



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DNA. Glyceraldehyde is a highly reactive compound that can modify and cross-link proteins. Glyceraldehyde-modified proteins appear to be cytotoxic, depress intracellular glutathione levels, and induce reactive oxygen species (ROS) production (PMID: 14981296). Glyceraldehyde has been shown to cause chromosome damage to human cells in culture and is mutagenic in the Ames bacterial test.

This compound belongs to the class of organic compounds known as monosaccharides. These are compounds containing one carbohydrate unit not glycosidically linked to another such unit, and no set of two or more glycosidically linked carbohydrate units. Monosaccharides have the general formula C<sub>n</sub>H<sub>2n</sub>O<sub>n</sub>.

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Kolho KL, Pessia A, Jaakkola T, de Vos WM, Velagapudi V: Faecal and Serum Metabolomics in Paediatric Inflammatory Bowel Disease. J Crohns Colitis. 2017 Mar 1;11(3):321-334. doi: 10.1093/ecco-jcc/jjw158. PMID: 27609529

Azario I, Pievani A, Del Priore F, Antolini L, Santi L, Corsi A, Cardinale L, Sawamoto K, Kubaski F, Gentner B, Bernardo ME, Valsecchi MG, Riminucci M, Tomatsu S, Aiuti A, Biondi A, Serafini M: Neonatal umbilical cord blood transplantation halts skeletal disease progression in the murine model of MPS-I. Sci Rep. 2017 Aug 25;7(1):9473. doi: 10.1038/s41598-017-09958-9. PMID: 28842642

## Leukotriene B4 -- Introduction

SYNONYM: (5S,6E,8E,10E,12R,14Z)-5,12-Dihydroxyeicosanoic acid; (6E,5S,12R)-Leukotriene b4; 5(S),12(R)-Dihydroxy-6,8,10,14-(trans,trans,trans,cis)-eicosatetraenoic acid; 5S,12R-Dihydroxy-6E,8E,10E,14Z-eicosatetraenoic acid; 5S,12R-Dihydroxy-6E,8E,10E,14Z-eicosatetraenoic acid; 6-trans-LTB4; Delta(6)-trans-Leukotriene b4; Delta(6)-trans-LT b4; (5S,6E,8E,10E,12R,14Z)-5,12-Dihydroxyeicosanoic acid; 5(S),12(R)-Dihydroxy-6,8,10,14-(trans,trans,trans,cis)-eicosatetraenoate; 5S,12R-Dihydroxy-6E,8E,10E,14Z-eicosatetraenoate; 5S,12R-Dihydroxy-6E,8E,10E,14Z-eicosatetraenoate;  $\hat{1}'$ (6)-trans-leukotriene b4;  $\hat{1}'$ (6)-trans-LT b4; D6-trans-Leukotriene b4; D6-trans-LTB4; [S-[R\*,s\*(e,e,e,Z)]]-5,12-dihydroxy-6,8,10,14-eicosatetraenoate; [S-[R\*,s\*(e,e,e,Z)]]-5,12-dihydroxy-6,8,10,14-eicosatetraenoic acid

HMDB: HMDB0001085; HMDB0005072; HMDB01085; HMDB05072

CAS: 71160-24-2

Leukotriene B4 is the major metabolite in neutrophil polymorphonuclear leukocytes. Leukotrienes are metabolites of arachidonic acid derived from the action of 5-LO (5-lipoxygenase). The immediate product of 5-LO is LTA4 (leukotriene A4), which is enzymatically converted into either LTB4 (leukotriene B4) by LTA4 hydrolase or LTC4 (leukotriene C4) by LTC4 synthase. The regulation of leukotriene production occurs at various levels, including expression of 5-LO, translocation of 5-LO to the perinuclear region and phosphorylation to either enhance or inhibit the activity of 5-LO. Biologically active LTB4 is metabolized by  $\omega$ -oxidation carried out by specific cytochrome P450s (CYP4F) followed by  $\beta$ -oxidation from the  $\omega$ -carboxy position and after CoA ester formation. Other specific pathways of leukotriene metabolism include the 12-hydroxydehydrogenase/ 15-oxo-prostaglandin-13-reductase that form a series of conjugated diene metabolites that have been observed to be excreted into human urine. Metabolism of LTC4 occurs by sequential peptide cleavage reactions involving a gamma-glutamyl transpeptidase that forms LTD4 (leukotriene D4) and a membrane-bound dipeptidase that converts LTD4 into LTE4 (leukotriene E4) before  $\omega$ -oxidation. These metabolic transformations of the primary leukotrienes are critical for termination of their biological activity, and defects in expression of participating enzymes may be involved in specific genetic disease. The term leukotriene was coined to indicate the presence of three conjugated double bonds within the 20-carbon structure of arachidonic acid as well as the fact that these compounds were derived from leucocytes such as PMNNs or transformed mast cells. Interestingly, most of the cells known to express 5-LO are of myeloid origin, which includes neutrophils, eosinophils, mast cells, macrophages, basophils and monocytes. Leukotriene biosynthesis begins with the specific oxidation of arachidonic acid by a free radical mechanism as a consequence of interaction with 5-LO. The first enzymatic step involves the abstraction of a hydrogen atom from C-7 of arachidonate followed by the addition of molecular oxygen to form 5-HpETE (5-hydroperoxyeicosatetraenoic acid). A second enzymatic step is also catalysed by 5-LO and involves removal of a hydrogen atom from C-10, resulting in formation of the conjugated triene epoxide LTA4. LTA4 must then be released by 5-LO and encounter either LTA4-H (LTA4 hydrolase) or LTC4-S [LTC4 (leukotriene C4) synthase]. LTA4-H can stereospecifically add water to C-12 while retaining a specific double-bond geometry, leading to LTB4 [leukotriene B4, 5(S),12(R)-dihydroxy-6,8,10,14-(Z,E,E,Z)-eicosatetraenoic acid]. If LTA4 encounters LTC4-S, then the reactive epoxide is opened at C-6 by the thiol anion of glutathione to form the product LTC4 [5(S)-hydroxy-6(R)-S-glutathionyl-7,9,11,14-(E,E,Z,Z)-eicosatetraenoic acid], essentially a glutathionyl adduct of oxidized arachidonic acid. Both of these terminal leukotrienes are biologically active in that specific GPCRs recognize these chemical structures and receptor recognition initiates complex intracellular signalling cascades. In order for these molecules to serve as lipid mediators, however, they must be released from the biosynthetic cell into the extracellular milieu so that they can encounter the corresponding GPCRs. Surprising features of this cascade include the recognition of the assembly of critical enzymes at the perinuclear region of the cell and even localization of 5-LO within the nucleus of some cells. Under some situations, the budding phagosome has been found to assemble these proteins. Non-enzymatic proteins such as FLAP are now known as critical partners of this protein-machine assembly. An unexpected pathway of leukotriene biosynthesis involves the transfer of the chemically reactive intermediate, LTA4, from the biosynthetic cell followed by conversion into LTB4 or LTC4 by other cells that do not express 5-LO. (PMID 17623009). Leukotrienes are eicosanoids. The eicosanoids consist of the



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prostaglandins (PGs), thromboxanes (TXs), leukotrienes (LTs) and lipoxins (LXs). The PGs and TXs are collectively identified as prostanoids. Prostaglandins were originally shown to be synthesized in the prostate gland, thromboxanes from platelets (thrombocytes) and leukotrienes from leukocytes, hence the derivation of their names. All mammalian cells except erythrocytes synthesize eicosanoids. These molecules are extremely potent, able to cause profound physiological effects at very dilute concentrations. All eicosanoids function locally at the site of synthesis, through receptor-mediated G-protein linked signaling pathways.

This compound belongs to the class of organic compounds known as leukotrienes. These are eicosanoids containing a hydroxyl group attached to the aliphatic chain of an arachidonic acid. Leukotrienes have four double bonds, three (and only three) of which are conjugated.

### Leukotriene B4 -- Aseptic meningitis

Matsuo M, Hamasaki Y, Masuyama T, Ohta M, Miyazaki S: Leukotriene B4 and C4 in cerebrospinal fluid from children with meningitis and febrile seizures. *Pediatr Neurol*. 1996 Feb;14(2):121-4. PMID: 8703223

### Leukotriene B4 -- Cardiopulmonary bypass

Pearl JM, Manning PB, McNamara JL, Saucier MM, Thomas DW: Effect of modified ultrafiltration on plasma thromboxane B2, leukotriene B4, and endothelin-1 in infants undergoing cardiopulmonary bypass. *Ann Thorac Surg*. 1999 Oct;68(4):1369-75. PMID: 10543508

### Leukotriene B4 -- Glutathione synthetase deficiency

Mayatepek E, Meissner T, Grobe H: Acute metabolic crisis with extreme deficiency of glutathione in combination with decreased levels of leukotriene C4 in a patient with glutathione synthetase deficiency. *J Inher Metab Dis*. 2004;27(2):297-9. PMID: 15243994

Li X, Ding Y, Liu Y, Ma Y, Song J, Wang Q, Yang Y: Five Chinese patients with 5-oxoprolinuria due to glutathione synthetase and 5-oxoprolinase deficiencies. *Brain Dev*. 2015 Nov;37(10):952-9. doi: 10.1016/j.braindev.2015.03.005. Epub 2015 Apr 4. PMID: 25851806

### Leukotriene B4 -- Hydrocephalus

Castro-Gago M, Rodriguez IN, Rodriguez-Nunez A, Guitian JP, Rocamonde SL, Rodriguez-Segade S: Therapeutic criteria in hydrocephalic children. *Childs Nerv Syst*. 1989 Dec;5(6):361-3. PMID: 2611770

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Westcott JY, Murphy RC, Stenmark K: Eicosanoids in human ventricular cerebrospinal fluid following severe brain injury. *Prostaglandins*. 1987 Dec;34(6):877-87. PMID: 2835791

### Leukotriene B4 -- Meningitis

Subramanian A, Gupta A, Saxena S, Gupta A, Kumar R, Nigam A, Kumar R, Mandal SK, Roy R: Proton MR CSF analysis and a new software as predictors for the differentiation of meningitis in children. *NMR Biomed*. 2005 Jun;18(4):213-25. PMID: 15627241

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Lerche A, Svenson M, Wiik A: Cerebrospinal fluid levels of cyclic nucleotides in meningitis and idiopathic polyneuritis. *Acta Neurol Scand*. 1984 Mar;69(3):168-75. PMID: 6326460

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Leoni V, Masterman T, Mousavi FS, Wretlind B, Wahlund LO, Diczfalusy U, Hillert J, Bjorkhem I: Diagnostic use of cerebral and extracerebral oxysterols. *Clin Chem Lab Med.* 2004 Feb;42(2):186-91. PMID: 15061359

Westcott JY, Murphy RC, Stenmark K: Eicosanoids in human ventricular cerebrospinal fluid following severe brain injury. *Prostaglandins.* 1987 Dec;34(6):877-87. PMID: 2835791

Silva SO, Ximenes VF, Livramento JA, Catalani LH, Campa A: High concentrations of the melatonin metabolite, N1-acetyl-N2-formyl-5-methoxykynuramine, in cerebrospinal fluid of patients with meningitis: a possible immunomodulatory mechanism. *J Pineal Res.* 2005 Oct;39(3):302-6. PMID: 16150112

Rodriguez-Nunez A, Cid E, Rodriguez-Garcia J, Camina F, Rodriguez-Segade S, Castro-Gago M: Neuron-specific enolase, nucleotides, nucleosides, purine bases, oxypurines and uric acid concentrations in cerebrospinal fluid of children with meningitis. *Brain Dev.* 2003 Mar;25(2):102-6. PMID: 12581805

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Laurent UB, Laurent TC, Hellsing LK, Persson L, Hartman M, Lilja K: Hyaluronan in human cerebrospinal fluid. *Acta Neurol Scand.* 1996 Sep;94(3):194-206. PMID: 8899053

## Leukotriene B4 -- Sjögren-Larsson syndrome

Willemse MA, Rotteveel JJ, de Jong JG, Wanders RJ, IJlst L, Hoffmann GF, Mayatepek E: Defective metabolism of leukotriene B4 in the Sjögren-Larsson syndrome. *J Neurol Sci.* 2001 Jan 15;183(1):61-7. PMID: 11166796

## Leukotriene B4 -- Leukotriene C4-Synthesis Deficiency

Mayatepek E, Flock B: Leukotriene C4-synthesis deficiency: a new inborn error of metabolism linked to a fatal developmental syndrome. *Lancet.* 1998 Nov 7;352(9139):1514-7. PMID: 9820300

## Inositol 1,3,4-trisphosphate -- Introduction

SYNONYM: (1S,3S,4S)-1,3,4-triphospho-myo-INOSITOL; D-myo-Inositol 1,3,4-trisphosphate; Inositol 1,3,4-trisphosphoric acid; D-myo-Inositol 1,3,4-trisphosphoric acid; 1,3,4-Itp; 1D-myo-Inositol 1,3,4-trisphosphate; I3S; Inositol 1,3,4-trisphosphate; myo-Inositol 1,3,4-trisphosphate; Inositol 1,3,4-trisphosphate, (D)-isomer

HMDB: HMDB0001143; HMDB01143

CAS: 98102-63-7

Inositol 1,3,4-trisphosphate is a specific regulator of cellular signaling.

This compound belongs to the class of organic compounds known as inositol phosphates. These are compounds containing a phosphate group attached to an inositol (or cyclohexanehexol) moiety.

## 5'-Methylthioadenosine -- Introduction

SYNONYM: 5'-Deoxy-5'-(methylthio)adenosine; 5-Methylthioadenosine; 9-(5-S-Methyl-5-thio-beta-D-ribofuranosyl)-9H-purin-6-amine; Methylthioadenosine; MTA; S-Methyl-5'-thioadenosine; Thiomethyladenosine; 9-(5-S-Methyl-5-thio-beta-D-ribofuranosyl)-9H-purin-6-amine; 9-(5-S-Methyl-5-thio- $\beta$ -D-ribofuranosyl)-9H-purin-6-amine; 1-(6-amino-9H-Purin-9-yl)-1-deoxy-5-S-methyl-5-thio-beta-D-ribofuranose; 1-(6-amino-9H-Purin-9-yl)-1-deoxy-5-S-methyl-5-thio-beta-D-ribofuranose; 5'-(methylthio)-5'-Deoxyadenosine; 5'-(methylthio)Adenosine; 5'-S-Methyl-5'-thio-adenosine; 5'-S-Methyl-5'-thioadenosine; S-Methyl-5-thioadenosine; Adenine(5'-deoxy-5'-methylthio)9-beta-D-furanoriboside; 5-MTDA; 5'-methylthio-5'-Deoxyadenosine; 5'-Deoxy-5'-methylthioadenosine; 5'-Methylthioadenosine, methyl-(14)C-labeled

HMDB: HMDB0001173; HMDB01173

CAS: 2457-80-9

5'-Methylthioadenosine (MTA) is a naturally occurring sulfur-containing nucleoside present in all mammalian tissues. It is produced from S-adenosylmethionine mainly through the polyamine biosynthetic pathway, where it behaves as a powerful



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inhibitory product. MTA is metabolized solely by MTA-phosphorylase, to yield 5-methylthioribose-1-phosphate and adenine, a crucial step in the methionine and purine salvage pathways, respectively. Evidence suggests that MTA can affect cellular processes in many ways. For instance, MTA has been shown to influence the regulation of gene expression, proliferation, differentiation, and apoptosis (PMID: 15313459). 5-Methylthioadenosine can be found in human urine. Elevated excretion appears in children with severe combined immunodeficiency syndrome (SCID) (PMID: 3987052).

This compound belongs to the class of organic compounds known as 5'-deoxy-5'-thionucleosides. These are 5'-deoxyribonucleosides in which the ribose is thio-substituted at the 5'position by a S-alkyl group.

## 5'-Methylthioadenosine – Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. *Tohoku J Exp Med.* 1995 May;176(1):61-8. PMID: 7482520

Cheng Y, Xie G, Chen T, Qiu Y, Zou X, Zheng M, Tan B, Feng B, Dong T, He P, Zhao L, Zhao A, Xu LX, Zhang Y, Jia W: Distinct urinary metabolic profile of human colorectal cancer. *J Proteome Res.* 2012 Feb 3;11(2):1354-63. doi: 10.1021/pr201001a. Epub 2011 Dec 28. PMID: 22148915

Monleon D, Morales JM, Barrasa A, Lopez JA, Vazquez C, Celda B: Metabolite profiling of fecal water extracts from human colorectal cancer. *NMR Biomed.* 2009 Apr;22(3):342-8. doi: 10.1002/nbm.1345. PMID: 19006102

Weir TL, Manter DK, Sheflin AM, Barnett BA, Heuberger AL, Ryan EP: Stool microbiome and metabolome differences between colorectal cancer patients and healthy adults. *PLoS One.* 2013 Aug 6;8(8):e70803. doi: 10.1371/journal.pone.0070803. Print 2013. PMID: 23940645

Phua LC, Chue XP, Koh PK, Cheah PY, Ho HK, Chan EC: Non-invasive fecal metabonomic detection of colorectal cancer. *Cancer Biol Ther.* 2014 Apr;15(4):389-97. doi: 10.4161/cbt.27625. Epub 2014 Jan 14. PMID: 24424155

Ritchie SA, Ahiahonu PW, Jayasinghe D, Heath D, Liu J, Lu Y, Jin W, Kavianpour A, Yamazaki Y, Khan AM, Hossain M, Su-Myat KK, Wood PL, Krenitsky K, Takemasa I, Miyake M, Sekimoto M, Monden M, Matsubara H, Nomura F, Goodenow DB: Reduced levels of hydroxylated, polyunsaturated ultra long-chain fatty acids in the serum of colorectal cancer patients: implications for early screening and detection. *BMC Med.* 2010 Feb 15;8:13. doi: 10.1186/1741-7015-8-13. PMID: 20156336

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Ni Y, Xie G, Jia W: Metabonomics of human colorectal cancer: new approaches for early diagnosis and biomarker discovery. *J Proteome Res.* 2014 Sep 5;13(9):3857-70. doi: 10.1021/pr500443c. Epub 2014 Aug 14. PMID: 25105552

Ikeda A, Nishiumi S, Shinohara M, Yoshie T, Hatano N, Okuno T, Bamba T, Fukusaki E, Takenawa T, Azuma T, Yoshida M: Serum metabolomics as a novel diagnostic approach for gastrointestinal cancer. *Biomed Chromatogr.* 2012 May;26(5):548-58. doi: 10.1002/bmc.1671. Epub 2011 Jul 20. PMID: 21773981

Goedert JJ, Sampson JN, Moore SC, Xiao Q, Xiong X, Hayes RB, Ahn J, Shi J, Sinha R: Fecal metabolomics: assay performance and association with colorectal cancer. *Carcinogenesis.* 2014 Sep;35(9):2089-96. doi: 10.1093/carcin/bgul131. Epub 2014 Jul 18. PMID: 25037050

Sinha R, Ahn J, Sampson JN, Shi J, Yu G, Xiong X, Hayes RB, Goedert JJ: Fecal Microbiota, Fecal Metabolome, and Colorectal Cancer Interrelations. *PLoS One.* 2016 Mar 25;11(3):e0152126. doi: 10.1371/journal.pone.0152126. eCollection 2016. PMID: 27015276

Lin Y, Ma C, Liu C, Wang Z, Yang J, Liu X, Shen Z, Wu R: NMR-based fecal metabolomics fingerprinting as predictors of earlier diagnosis in patients with colorectal cancer. *Oncotarget.* 2016 May 17;7(20):29454-64. doi: 10.18632/oncotarget.8762. PMID: 27107423

Brown DG, Rao S, Weir TL, O'Malia J, Bazan M, Brown RJ, Ryan EP: Metabolomics and metabolic pathway networks from human colorectal cancers, adjacent mucosa, and stool. *Cancer Metab.* 2016 Jun 6;4:11. doi: 10.1186/s40170-016-0151-y. eCollection 2016. PMID: 27275383



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Wang X, Wang J, Rao B, Deng L: Gut flora profiling and fecal metabolite composition of colorectal cancer patients and healthy individuals. *Exp Ther Med.* 2017 Jun;13(6):2848-2854. doi: 10.3892/etm.2017.4367. Epub 2017 Apr 20. PMID: 28587349

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<http://www.sciencedirect.com/science/article/pii/S0924224416301984> PMID: 7482520

## Indoleacetaldehyde -- Introduction

SYNONYM: 1H-Indole-3-acetaldehyde; 2-(indol-3-yl)Acetaldehyde; Indole-3-acetaldehyde; 1H-indol-3-Ylacetaldehyde; 2-(3-Indolyl)acetaldehyde; indol-3-Ylacetaldehyde; Tryptaldehyde; Indoleacetaldehyde sulfite

HMDB: HMDB0001190; HMDB01190

CAS: 2591-98-2

Indoleacetaldehyde is a substrate for Retina-specific copper amine oxidase, Aldehyde dehydrogenase X (mitochondrial), Amine oxidase B, Amiloride-sensitive amine oxidase, Aldehyde dehydrogenase (mitochondrial), Fatty aldehyde dehydrogenase, 4-trimethylaminobutyraldehyde dehydrogenase, Aldehyde dehydrogenase (dimeric NADP-preferring), Aldehyde dehydrogenase family 7 member A1, Amine oxidase A, Aldehyde dehydrogenase 1A3 and Membrane copper amine oxidase.

This compound belongs to the class of organic compounds known as 3-alkylindoles. These are compounds containing an indole moiety that carries an alkyl chain at the 3-position.

## 5-Aminoimidazole ribonucleotide -- Introduction

SYNONYM: AIR; 1-(5'-Phosphoribosyl)-5-aminoimidazole; 5'-Phosphoribosyl-5-aminoimidazole; 1-(5-phospho-D-Ribosyl)-5-aminoimidazole; 5-amino-1-(5-phospho-D-Ribosyl)imidazole; 5-Aminoimidazole ribotide; Aminoimidazole ribotide; Aminoimidazole ribotide, (beta-D-ribofuranosyl)-isomer; 5-amino-1-Ribofuranosylimidazole 5'-phosphate; Aminoimidazole ribotide, (alpha-D-ribofuranosyl)-isomer; Aminoimidazole ribotide, phosphonoribofuranosyl-isomer

HMDB: HMDB0001235; HMDB0002316; HMDB0011609; HMDB01235; HMDB02316; HMDB11609

CAS: 25635-88-5

5-aminoimidazole ribonucleotide (AIR), is an intermediate of purine nucleotide biosynthesis. It is also the precursor to 4-amino-2-methyl-5-hydroxymethylpyrimidine (HMP), the first product of pyrimidine biosynthesis. This reaction is mediated by the enzyme HMP-P kinase (ThiD). HMP is a precursor of thiamine phosphate (TMP), and subsequently to thiamine pyrophosphate (TPP). TPP is an essential cofactor in all living systems that plays a central role in metabolism. (PMID: 15326535). 5-Aminoimidazole ribonucleotide is a substrate for a number of proteins including: Scaffold attachment factor B2, Multifunctional protein ADE2, Pulmonary surfactant-associated protein B, Tumor necrosis factor receptor superfamily member 25, Pulmonary surfactant-associated protein C, Serine/threonine-protein kinase Chk1, Vinexin, Trifunctional purine biosynthetic protein adenosine-3, Antileukoproteinase 1 and Scaffold attachment factor B.

This compound belongs to the class of organic compounds known as pentose phosphates. These are carbohydrate derivatives containing a pentose substituted by one or more phosphate groups.

## 1-Pyrroline-5-carboxylic acid -- Introduction

SYNONYM: 3,4-dihydro-2H-Pyrrole-2-carboxylate; Delta(1)-Pyrroline-5-carboxylic acid; 3,4-dihydro-2H-Pyrrole-2-carboxylic acid; 1-Pyrroline-5-carboxylate; delta(1)-Pyrroline-5-carboxylate;  $\hat{\iota}$ (1)-pyrroline-5-carboxylate;  $\hat{\iota}$ (1)-pyrroline-5-carboxylic acid; (S)-1-Pyrroline-5-carboxylate; D1-Pyrroline-5-carboxylate; D1-Pyrroline-5-carboxylic acid; delta(1)Pyrroline-5-carboxylate; delta-1-Pyrroline-5-carboxylate; delta-1-Pyrroline-5-carboxylic acid; DL-1-Pyrroline-5-carboxylate; DL-1-Pyrroline-5-carboxylic acid; L-1-Pyrroline-5-carboxylate; L-delta 1-Pyrroline-5-carboxylate; Pyrroline 5-carboxylate; Pyrroline-5-carboxylate; delta-1-Pyrroline-5-carboxylate, (+)-isomer; delta-1-Pyrroline-5-carboxylate, 14C-labeled, (+)-isomer

HMDB: HMDB0001301; HMDB0002240; HMDB01301; HMDB02240



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CAS:2906-39-0

1-Pyrroline-5-carboxylic acid is an enamine or an imino acid that forms upon the spontaneous dehydration of L-glutamate gamma-semialdehyde in aqueous solutions. The stereoisomer (S)-1-pyrroline-5-carboxylate is an intermediate in glutamate metabolism, arginine degradation, and proline biosynthesis and degradation. It can also be converted into or be formed from three amino acids: L-glutamate, L-ornithine, and L-proline. In particular, it is synthesized via the oxidation of proline by pyrroline-5-carboxylate reductase 1 (PYCR1) (EC 1.5.1.2) or by proline dehydrogenase (PRODH) (EC 1.5.99.8). It is hydrolyzed to L-glutamate by delta-1-pyrroline-5-carboxylate dehydrogenase (ALDH4A1) (EC 1.5.1.12). It is also one of the few metabolites that can act as a precursor to other metabolites of both the urea cycle and the tricarboxylic acid (TCA) cycle. Under certain conditions, pyrroline-5-carboxylate can act as a neurotoxin and a metabotoxin. A neurotoxin causes damage to nerve cells and nerve tissues. A metabotoxin is an endogenously produced metabolite that causes adverse health effects at chronically high levels. Chronically high levels of pyrroline-5-carboxylate are associated with at least five inborn errors of metabolism, including hyperprolinemia type I, hyperprolinemia type II, iminoglycinuria, prolinemia type II, and pyruvate carboxylase deficiency. Hyperprolinemia type II results in high levels of pyrroline-5-carboxylate. People with hyperprolinemia type II have signs and symptoms that vary in severity, but they are more likely than type I to have seizures or intellectual disability. Pyrroline-5-carboxylate is highly reactive and excess quantities have been shown to cause cell death and apoptosis (PMID: 15548746).

This compound belongs to the class of organic compounds known as alpha amino acids and derivatives. These are amino acids in which the amino group is attached to the carbon atom immediately adjacent to the carboxylate group (alpha carbon), or a derivative thereof.

## D-Alanine -- Introduction

SYNONYM: (2R)-2-Aminopropanoic acid; (R)-2-Aminopropanoic acid; (R)-Alanine; D-2-Aminopropionic acid; D-Ala; D-Alanin; D-alpha-Alanine; D-alpha-Aminopropionic acid; DAL; (2R)-2-Aminopropanoate; (R)-2-Aminopropanoate; D-2-Aminopropionate; D-a-Alanine; D- $\dot{\text{I}}$ -alanine; D-a-Aminopropionate; D-a-Aminopropionic acid; D-alpha-Aminopropionate; D- $\dot{\text{I}}$ -aminopropionate; D- $\dot{\text{I}}$ -aminopropionic acid; Alanine; D(-)-a -Alanine; D(-)-alpha-Alanine; D(-)-Alanine; delta-(-)-Alanine; delta-2-Aminopropionic acid; delta-Alanine; delta-alpha-Alanine; DL-Alanine; Alanine, L isomer; L-Isomer alanine; Doms adrian brand OF alanine; Doms-adrian brand OF alanine; L Alanine; Abuf $\ddot{\text{A}}$ ne; Alanine doms-adrian brand; Alanine, L-isomer; L-Alanine

HMDB: HMDB0001310; HMDB01310

CAS: 338-69-2

Alanine is a nonessential amino acid made in the body from the conversion of the carbohydrate pyruvate or the breakdown of DNA and the dipeptides carnosine and anserine. It is highly concentrated in muscle and is one of the most important amino acids released by muscle, functioning as a major energy source. Plasma alanine is often decreased when the BCAA (Branched Chain Amino Acids) are deficient. This finding may relate to muscle metabolism. Alanine is highly concentrated in meat products and other high-protein foods like wheat germ and cottage cheese. Alanine is an important participant as well as regulator in glucose metabolism. Alanine levels parallel blood sugar levels in both diabetes and hypoglycemia, and alanine reduces both severe hypoglycemia and the ketosis of diabetes. It is an important amino acid for lymphocyte reproduction and immunity. Alanine therapy has helped dissolve kidney stones in experimental animals. Normal alanine metabolism, like that of other amino acids, is highly dependent upon enzymes that contain vitamin B6. Alanine, like GABA, taurine and glycine, is an inhibitory neurotransmitter in the brain. <http://www.dcnutrition.com/AminoAcids/>.

This compound belongs to the class of organic compounds known as alanine and derivatives. These are compounds containing alanine or a derivative thereof resulting from reaction of alanine at the amino group or the carboxy group, or from the replacement of any hydrogen of glycine by a heteroatom.

## D-Alanine -- Pregnancy

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### D-Alanine -- Early preeclampsia

Bahado-Singh RO, Akolekar R, Mandal R, Dong E, Xia J, Kruger M, Wishart DS, Nicolaides K: Metabolomics and first-trimester prediction of early-onset preeclampsia. J Matern Fetal Neonatal Med. 2012 Oct;25(10):1840-7. doi: 10.3109/14767058.2012.680254. Epub 2012 Apr 28. PMID: 22494326

### D-Alanine -- Late-onset preeclampsia

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### Purine -- Introduction

**SYNONYM:** Purine base; 1H-Purine; 6H-imidazo[4,5-D]Pyrimidine; 7-Methyltheophylline; 7H-imidazo(4,5-D)Pyrimidine; 7H-Purine; 9H-Purine; beta-Purine; Caffedrine; Caffein; Cafipel; Coffeine; Dasin; Dexitac; Diurex; Durvitan; imidazo(4,5-D)Pyrimidine; Isopurine; Koffein; Mateina; Methyltheobromine; Phensal; Propoxyphene compound 65; {6h-imidazo[4,5-D]pyrimidine}; {7h-imidazo[4,5-D]pyrimidine}; {Imidazo[4,5-D]pyrimidine}

HMDB: HMDB0001366; HMDB01366

CAS: 120-73-0

Purine is a heterocyclic aromatic organic compound, consisting of a pyrimidine ring fused to an imidazole ring. Two of the bases in nucleic acids, adenine and guanine, are purines. Purines from food (or from tissue turnover) are metabolised by several enzymes, including xanthine oxidase, into uric acid. High levels of uric acid can predispose to gout when the acid crystallises in joints; this phenomenon only happens in humans and some animal species (e.g. dogs) that lack an intrinsic uricase enzyme that can further degrade uric acid.

This compound belongs to the class of organic compounds known as purines and purine derivatives. These are aromatic heterocyclic compounds containing a purine moiety, which is formed a pyrimidine-ring fused to an imidazole ring.

### Niacinamide -- Introduction

**SYNONYM:** 3-Pyridinecarboxamide; beta-Pyridinecarboxamide; Niacin; Nicotinamid; Nicotinic acid amide; Nicotinsaeureamid; Nikotinamid; Nikotinsaeureamid; Vitamin b3; Vitamin PP; b-Pyridinecarboxamide; 3-pyridinecarboxamide; Nicotinate amide; 3-Carbamoylpyridine; 3-Pyridinecarboxylic acid amide; Acid amide; Amid kyseliny nikotinove; Amide PP; Aminicotin; Amixicotin; Amnicotin; Austrovit PP; Benicot; Delonin amide; Dipegyl; Dipigyl; Endobion; Factor PP; Hansamid; Inovitan PP; m-(Aminocarbonyl)pyridine; Mediatriac; NAM; Nandervit-N; Niacevit; Niamide; Niavit PP; Nicamide; Nicamina; Nicamindon; Nicasir; Nicobion; Nicoftor; Nicogen; Nicomidol; Nicosan 2; Nicosylamide; Nicota; Nicotamide; Nicotilamide; Nicotilamido; Nicotinamida; Nicotinamide; Nicotinamidum; Nicotine acid amide; Nicotine amide; Nicotinic amide; Nicotinsaureamid; Nicotol; Nicotylamide; Nicotylamidum; Nicovel; Nicovit; Nicovitina; Nicovitol; Nicozymin; Nictoamide; niko-Tamin; Niocinamide; Niozymin; Papulex; Pelmin; Pelmine; Pelomin amide; PP-Faktor; Propamine a; Pyridine-3-carboxylic acid amide; Savacotyl; Vi-nicotyl; Vi-noctyl; Witamina PP; 3 Pyridinecarboxamide; Astra brand OF niacinamide; b3, Vitamin; Niacinamide merck brand; Pharmagenix brand OF niacinamide; b3, Vitamin; Enduramide; Jenapharm, nicotinsaureamid; Niacinamide jenapharm brand; Niacinamide pharmagenix brand; Jenapharm brand OF niacinamide; Nicotinsaureamid jenapharm; Vitamin b3; Merck brand OF niacinamide; Niacinamide astra brand

HMDB: HMDB0001406; HMDB01406

CAS: 98-92-0

Niacinamide or vitamin B3 is an important compound functioning as a component of the coenzyme NAD. Its primary significance is in the prevention and/or cure of blacktongue and pellagra. Most animals cannot manufacture this compound in



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amounts sufficient to prevent nutritional deficiency and it therefore must be supplemented through dietary intake. Niacinamide is used to increase the effect of radiation therapy on tumor cells. Niacin (nicotinic acid) and niacinamide, while both labeled as vitamin B3 also have different applications. Niacinamide is useful in arthritis and early-onset type I diabetes while niacin is an effective reducer of high cholesterol levels.

This compound belongs to the class of organic compounds known as nicotinamides. These are heterocyclic aromatic compounds containing a pyridine ring substituted at position 3 by a carboxamide group.

### Niacinamide -- Colorectal cancer

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## Niacinamide -- Uremia



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## 3-Dehydroosphinganine -- Introduction

SYNONYM: 3-dehydro-D-Sphinganine; 3-Ketodihydroosphingosine; 3-Ketosphinganine; (2S)-2-amino-1-Hydroxyoctadecan-3-one; 1-Hydroxy-2-amino-3-oxo-octadecane; 2-amino-1-Hydroxy-3-octadecanone; KDHS; Ketodihydroosphingosine; (+)-Isomer OF ketodihydroosphingosine; (S)-Isomer OF ketodihydroosphingosine

HMDB: HMDB0001480; HMDB01480

CAS: 16105-69-4



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3-Dehydrosphinganine is an intermediate in the metabolism of Glycosphingolipids. It is a substrate for Serine palmitoyltransferase 1 and Serine palmitoyltransferase 2.

This compound belongs to the class of organic compounds known as beta-hydroxy ketones. These are ketones containing a hydroxyl group attached to the beta-carbon atom, relative to the C=O group.

## 20-Hydroxy-leukotriene B4 -- Introduction

SYNONYM: (6Z,8E,10E,14Z)-(5S,12R)-5,12,20-Trihydroxyeicosanoate; (6Z,8E,10E,14Z)-(5S,12R)-5,12,20-Trihydroxyicosanoate-6,8,10,14-tetraenoate; 20-Hydroxy-LTB4; 20-OH-Leukotriene b4; 20-OH-LTB4; (6Z,8E,10E,14Z)-(5S,12R)-5,12,20-Trihydroxyeicosanoate-6,8,10,14-tetraenoic acid; (6Z,8E,10E,14Z)-(5S,12R)-5,12,20-Trihydroxyicosanoate-6,8,10,14-tetraenoic acid; (5S,12R)-5,12,20-Trihydroxy-(6Z,8E,10E,14Z)-eicosatetraenoate; (5S,12R)-5,12,20-Trihydroxy-(6Z,8E,10E,14Z)-eicosatetraenoic acid; (5S,6Z,8E,10E,12R,14Z)-5,12,20-Trihydroxyicosanoate-6,8,10,14-tetraenoate; (5S,6Z,8E,10E,12R,14Z)-5,12,20-Trihydroxyicosanoate-6,8,10,14-tetraenoic acid; 20-Hydroxy LTB4; 20-Hydroxyleukotriene b4; 20-OH-5S,12S-Dihydroxy-6,10-trans-8,14-cis-eicosatetraenoate; 20-OH-5S,12S-Dihydroxy-6,10-trans-8,14-cis-eicosatetraenoic acid; 5,12,20-THETE; 5,12,20-TriHETE; 5S,12R,20-Trihydroxy-6Z,8E,10E,14Z-eicosatetraenoate; 5S,12R,20-Trihydroxy-6Z,8E,10E,14Z-eicosatetraenoic acid; Omega-hydroxy-LTB4; W-Hydroxy-LTB4; [S-[R\*,s\*-(e,Z,e,Z)]]-5,12,20-trihydroxy-6,8,10,14-eicosatetraenoate; [S-[R\*,s\*-(e,Z,e,Z)]]-5,12,20-trihydroxy-6,8,10,14-eicosatetraenoic acid; 20-Hydroxy-leukotriene b; 5,12,20-Trihydroxy-6,8,10,14-eicosatetraenoic acid; 5,12,20-Trihydroxy-6,8,10,14-eicosatetraenoic acid, (S-(r\*,s\*-(e,Z,e,Z)))-isomer

HMDB: HMDB0001509; HMDB0005092; HMDB01509; HMDB05092

CAS: 79516-82-8

20-hydroxy- Leukotriene B4 (20-OH-LTB4) is an omega-hydroxylated metabolite of leukotriene B4 in human neutrophils. Elevated urinary concentrations of 20-OH-LTB4 and LTB4 are found in patients with Sjogren-Larsson syndrome (SLS, OMIM 270220), an autosomal recessively inherited neurocutaneous disorder caused by a deficiency of the microsomal enzyme fatty aldehyde dehydrogenase (FALDH), which as an essential role in LTB4 metabolism. Preterm birth seems to be one of the features of the syndrome. The reason for the preterm birth is unclear. It is hypothesized that it relates to the defective LTB4 degradation in SLS. The pathological urinary excretion of LTB4 and 20-OH-LTB4 is a biochemical marker for SLS. Surprisingly, 20-OH-LTB4 concentrations are normal in CSF. Leukotriene B4 is the major metabolite in neutrophil polymorphonuclear leukocytes. Leukotrienes are metabolites of arachidonic acid derived from the action of 5-LO (5-lipoxygenase). The immediate product of 5-LO is LTA4 (leukotriene A4), which is enzymatically converted into either LTB4 (leukotriene B4) by LTA4 hydrolase or LTC4 (leukotriene C4) by LTC4 synthase. The regulation of leukotriene production occurs at various levels, including expression of 5-LO, translocation of 5-LO to the perinuclear region and phosphorylation to either enhance or inhibit the activity of 5-LO. Biologically active LTB4 is metabolized by w-oxidation carried out by specific cytochrome P450s (CYP4F) followed by beta-oxidation from the w-carboxy position and after CoA ester formation. Other specific pathways of leukotriene metabolism include the 12-hydroxydehydrogenase/ 15-oxo-prostaglandin-13-reductase that form a series of conjugated diene metabolites that have been observed to be excreted into human urine. Metabolism of LTC4 occurs by sequential peptide cleavage reactions involving a gamma-glutamyl transpeptidase that forms LTD4 (leukotriene D4) and a membrane-bound dipeptidase that converts LTD4 into LTE4 (leukotriene E4) before w-oxidation. These metabolic transformations of the primary leukotrienes are critical for termination of their biological activity, and defects in expression of participating enzymes may be involved in specific genetic disease. (PMID: 12709426, 9799565, 11408337, 17623009). Leukotrienes are eicosanoids. The eicosanoids consist of the prostaglandins (PGs), thromboxanes (TXs), leukotrienes (LTs) and lipoxins (LXs). The PGs and TXs are collectively identified as prostanoids. Prostaglandins were originally shown to be synthesized in the prostate gland, thromboxanes from platelets (thrombocytes) and leukotrienes from leukocytes, hence the derivation of their names. All mammalian cells except erythrocytes synthesize eicosanoids. These molecules are extremely potent, able to cause profound physiological effects at very dilute concentrations. All eicosanoids function locally at the site of synthesis, through receptor-mediated G-protein linked signaling pathways.

This compound belongs to the class of organic compounds known as leukotrienes. These are eicosanoids containing a hydroxyl group attached to the aliphatic chain of an arachidonic acid. Leukotrienes have four double bonds, three (and only three) of which are conjugated.

## 20-Hydroxy-leukotriene B4 -- Sjögren-Larsson syndrome

Willemse MA, Rotteveel JJ, de Jong JG, Wanders RJ, IJlst L, Hoffmann GF, Mayatepek E: Defective metabolism of



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leukotriene B4 in the Sjogren-Larsson syndrome. J Neurol Sci. 2001 Jan 15;183(1):61-7. PMID: 11166796

### Asymmetric dimethylarginine -- Introduction

SYNONYM: ADMA; guanidino-N,N-Dimethylarginine; N,N-Dimethylarginine; N(5)-((dimethylamino)Iminomethyl)-L-ornithine; NG,NG-Dimethyl-L-arginine; N(g),N(g)-Dimethylarginine; N(g)-Dimethylarginine; N(g1),N(g1)-Dimethylarginine; 2-amino-5-(amino-dimethylamino-Methylidene)amino-pentanoate; 2-amino-5-(amino-dimethylamino-Methylidene)amino-pentanoic acid; Dimethyl-L-arginine; N(Omega),N(omega)-dimethyl-L-arginine; NG,NG-Dimethylarginine; NG-Dimethylarginine; Nomega,nomega'-dimethyl-L-arginine

HMDB: HMDB0001539; HMDB01539

CAS: 30315-93-6

Asymmetric dimethylarginine (ADMA) is a naturally occurring chemical found in blood plasma. It is a metabolic by-product of continual protein modification processes in the cytoplasm of all human cells. It is closely related to L-arginine, a conditionally-essential amino acid. ADMA interferes with L-arginine in the production of nitric oxide, a key chemical to endothelial and hence cardiovascular health. Asymmetric dimethylarginine is created in protein methylation, a common mechanism of post-translational protein modification. This reaction is catalyzed by an enzyme set called S-adenosylmethionine protein N-methyltransferases (protein methylases I and II). The methyl groups transferred to create ADMA are derived from the methyl group donor S-adenosylmethionine, an intermediate in the metabolism of homocysteine. (Homocysteine is an important blood chemical, because it is also a marker of cardiovascular disease). After synthesis, ADMA migrates into the extracellular space and thence into blood plasma. Asymmetric dimethylarginine is measured using high performance liquid chromatography.

This compound belongs to the class of organic compounds known as arginine and derivatives. These are compounds containing arginine or a derivative thereof resulting from reaction of arginine at the amino group or the carboxy group, or from the replacement of any hydrogen of glycine by a heteroatom.

### Asymmetric dimethylarginine -- Autosomal dominant polycystic kidney disease

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### Asymmetric dimethylarginine -- Colorectal cancer

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### Asymmetric dimethylarginine -- Essential hypertension

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### Asymmetric dimethylarginine -- Duchenne Muscular Dystrophy

Nakagawa T, Takeuchi A, Kakiuchi R, Lee T, Yagi M, Awano H, Iijima K, Takeshima Y, Urade Y, Matsuo M: A prostaglandin D2 metabolite is elevated in the urine of Duchenne muscular dystrophy patients and increases further from 8 years old. *Clin Chim Acta.* 2013 Aug 23;423:10-4. doi: 10.1016/j.cca.2013.03.031. Epub 2013 Apr 19. PMID: 23603101

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### 3-Methylguanine -- Introduction

SYNONYM: N(3)-Methylguanine; 3-Methyl-guanine; 7-dihydro-3-Methyl-2-amino-3-6H-purin-6-one; 7-dihydro-3-Methyl-2-amino-3-6H-purin-6-one (9ci); N3-Methylguanine

HMDB: HMDB0001566; HMDB01566

CAS: 2958-98-7

3-Methylguanine is a methylated purine base. Methylated purine bases are known to be present in normal urine and to change under pathological conditions, in particular in the development of leukemia, tumors and immunodeficiency, by the altered turnover of nucleic acids typical of these diseases. (PMID 9069642).

This compound belongs to the class of organic compounds known as purines and purine derivatives. These are aromatic heterocyclic compounds containing a purine moiety, which is formed a pyrimidine-ring ring fused to an imidazole ring.

### N-Acryloylglycine -- Introduction

SYNONYM: 1-Aminopropenal acetic acid; N-(1-oxo-2-Propenyl)-glycine; N-Acryloyl-glycine; APAA

HMDB: HMDB0001843; HMDB01843

CAS: 24599-25-5

N-Acryloylglycine is an acyl glycine. Acyl glycines are normally minor metabolites of fatty acids. However, the excretion of certain acyl glycines is increased in several inborn errors of metabolism. In certain cases the measurement of these metabolites in body fluids can be used to diagnose disorders associated with mitochondrial fatty acid beta-oxidation. Acyl glycines are produced through the action of glycine N-acetyltransferase (EC 2.3.1.13) which is an enzyme that catalyzes the chemical reaction: acyl-CoA + glycine <--> CoA + N-acetylglycine. N-Acryloylglycine is an acylglycines found in normal human biofluids (PMID 7364920; 912020; 7438429).

This compound belongs to the class of organic compounds known as n-acyl-alpha amino acids. These are compounds containing an alpha amino acid which bears an acyl group at its terminal nitrogen atom.

### Methylsuccinic acid -- Introduction

SYNONYM: (S)-2-Hydroxy-2-methylsuccinate; (S)-2-Hydroxy-2-methylsuccinic acid; (S)-Citramalate; (S)-Citramalic acid; 2-Methylbutanedioate; 2-Methylbutanedioic acid; 2-Methylsuccinate; 2-Methylsuccinic acid; Methyl succinate; Methyl succinic acid; Methylbutanedioate; Methylbutanedioic acid; Methylsuccinate; MEZ; Pyrotartarate; Pyrotartaric acid; Methylsuccinic acid, (+)-isomer

HMDB: HMDB0001844; HMDB01844

CAS: 498-21-5

Methylsuccinic acid is a normal metabolite found in human fluids. Increased urinary levels of Methylsuccinic acid (together with ethylmalonic acid) are the main biochemical measurable features in ethylmalonic encephalopathy (OMIM 602473), a rare metabolic disorder with an autosomal recessive mode of inheritance that is clinically characterized by neuromotor delay, hyperlactic acidemia, recurrent petechiae, orthostatic acrocyanosis, and chronic diarrhea (PMID 12382164). The underlying biochemical defect involves isoleucine catabolism (PMID 9667231). It has been found decreases in the urine of animals under D-serine-induced nephrotoxicity (D-Serine causes selective necrosis of the proximal straight tubules in the rat kidney) (PMID 15596249). Moreover, Methylsuccinic acid is found to be associated with ethylmalonic encephalopathy, isovaleric acidemia, and medium chain acyl-CoA dehydrogenase deficiency, which are also inborn errors of metabolism.

This compound belongs to the class of organic compounds known as methyl-branched fatty acids. These are fatty acids



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with an acyl chain that has a methyl branch. Usually, they are saturated and contain only one or more methyl group. However, branches other than methyl may be present.

### Methylsuccinic acid -- Medium Chain Acyl-CoA Dehydrogenase Deficiency

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Bhala A, Willi SM, Rinaldo P, Bennett MJ, Schmidt-Sommerfeld E, Hale DE: Clinical and biochemical characterization of short-chain acyl-coenzyme A dehydrogenase deficiency. *J Pediatr.* 1995 Jun;126(6):910-5. PMID: 7776094

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### Methylsuccinic acid -- Refsum's disease

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## Methylsuccinic acid -- Irritable bowel syndrome

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### Methylsuccinic acid -- Isovaleric acidemia

Korman SH, Andresen BS, Zeharia A, Gutman A, Boneh A, Pitt JJ: 2-ethylhydracrylic aciduria in short-branched-chain acyl-CoA dehydrogenase deficiency: application to diagnosis and implications for the R-pathway of isoleucine oxidation. Clin Chem. 2005 Mar;51(3):610-7. Epub 2004 Dec 22. PMID: 15615815

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### Methylsuccinic acid -- Ethylmalonic encephalopathy

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## Methylsuccinic acid -- Ulcerative colitis

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## Acetaminophen -- Introduction

SYNONYM: 4'-Hydroxyacetanilide; 4-(acetylamino)Phenol; 4-Acetamidophenol; Acenol; Acetaminofen; Acetaminophene; APAP; N-Acetyl-P-aminophenol; P-Acetamidophenol; P-Acetaminophenol; P-Acetylaminophenol; P-Hydroxyacetanilide; P-Hydroxyphenolacetamide; Panadol; Paracetamolum; Tylenol; 4-Acetaminophenol; 4-Hydroxyacetanilide; 4-Hydroxyanilid kyseliny octove; a-Per; A.F. anacin; Abenol; Abensanil; Abrol; Abrolet; Acamol; Accu-tap; Acephen; Acertol; Aceta elixir; Aceta tablets; Acetagesic; Acetalgin; Acetaminophen uniserts; Acetamol; Acetofen; Actamin; Actamin extra; Actamin super;



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Actifed plus; Actimol chewable tablets; Actimol children's suspension; Actimol infants' suspension; Actimol junior strength caplets; Actron; Afébrin; Afébryl; Aferadol; Algesidal; Algina; Algommol; Algotropyl; Allay; alpha-Per; Alpiny; Alpinyin; Alvedon; Amadil; Aminofen; Aminofen max; Anacin-3; Anacin-3 extra strength; Anadin dla dzieci; Anaflon; Analter; Anapap; Andox; Anelix; Anexsia; Anexsia 10/660; Anexsia 5/325; Anexsia 7.5/325; Anexsia 7.5/650; Anhiba; Anoquan; Anti-algos; Antidol; Apacet; Apacet capsules; Apacet elixir; Apacet extra strength caplets; Apacet extra strength tablets; Apacet regular strength tablets; Apadon; Apamid; Apamide; Apitrelal; apo-Acetaminophen; Arfen; Asetam; Asomal; Aspac; Aspirin free anacin maximum strength caplets; Aspirin free anacin maximum strength gel caplets; Aspirin free anacin maximum strength tablets; Aspirin-free anacin; Aspirin-free excedrin caplets; Asplin; Atasol caplets; Atasol drops; Atasol forte caplets; Atasol forte tablets; Atasol oral solution; Atasol tablets; Atralidon; Babikan; Bacetamol; Bancap; Bancap HC; Banesin; Bayer select allergy-sinus; Bayer select head cold; Bayer select headache pain; Bayer select maximum strength headache pain relief formula; Bayer select menstrual multi-symptom; Bayer select sinus pain relief; Ben-u-ron; Benmyo; Bickie-mol; Biocetamol; Bucet; Butalbital; Butapap; Cadafen; Calapol; Calmanticold; Calpol; Capital with codeine; Captin; Causalon; Cefalex; Cetadol; Children'S acetaminophen elixir drops; Children'S acetaminophen oral solution; Children'S tylenol chewable; Claradol codeine; Clixodyne; CO-Gesic; COD-Acamol forte; Codabrol; Codalgan; Codapane; Codicet; Codisal; Codisal forte; Codoliprane; Codral pain relief; Cofamol; Conacetol; Contac cough & sore throat formula; Contra-schmerz P; Coricidin; Coricidin D; Coricidin sinus; Cosutone; Croix blanche; Cuponol; Curadon; Curpol; Custodial; Dapa X-S; Darocet; Darvocet; Darvocet-N 50; Datri; Datri extra-strength; Daygrip; Demilets; Deminofen; Democyl; Demogripal; Desfèbre; Dhamol; DHC Plus; Dial-a-gesic; Dial-alpha-gesic; Dimindol; Dirox; Disprol; Dol-stop; Dolcor; Dolefin; Dolegrippin; Dolene ap-65; Dolgesic; Doliprane; Dolko; Dolofugin; Doloreduct; Dolorfug; Dolorol forte; Dolorstop; Dolotec; Dolprone; Dorocoff; Dresan; Dristan cold no drowsiness; Dristancito; Duracetamol; Duradyne DHC; Durapan; Dymadon; Dymadon co; Dymadon forte; Dypap; Ecosetol; Elixodyne; Empracet; Endecon; Enelfa; Eneril; Esgic; Esgic-plus; Eu-med; Excedrin; Excedrin caplets; Excedrin extra strength caplets; Excipain; Exdol; Exdol strong; Fanalgic; Farmadol; Febranine; Febrectal; Febrectol; Febrex; Febricet; Febridol; Febrilix; Febrin; Febrinol; febro-Gesic; Febrolin; Femejet; Fendon; Fensum; Fepanil; Feverall junior strength; Feverall sprinkle caps junior strength; Fevor; Finimal; Finiweh; Fioricet; Fluparmol; Fortalidon P; Freka-cetamol; Gattaphen T; Gelocatil; Geluprane; Genapap children's elixir; Genapap children's tablets; Genapap extra strength caplets; Genapap extra strength tablets; Genapap regular strength tablets; Genebs extra strength caplets; Genebs regular strength tablets; Genebs X-tra; Geralgine-P; Gripin bebe; Grippostad; Gynospasmine; Hedex; Helon N; Homoolan; Hy-phen; Hycomine compound; Hydrocet; Ildamol; Inalgex; Infadrops; Infants' feverall; Influbene N; Injectapap; Intensin; Janupap; Junior disprop; Kataprin; Kinder finimal; Korum; Kratofin simplex; Labamol; Lekadol; Lemgrip; Lemspip; Lestemp; Liquagesic; Liquigesic co; Liquiprin; Liquiprin children's elixir; Liquiprin infants" drops; Lonarid; Lonarid mono; Loracet-HD; Lortab; Lupocet; Lyteca; Lyteca syrup; Magnidol; Malex N; Malgis; Malidens; Maxadol; Medigesic plus; Medinol paediatric; Medocodene; Melabon infantil; Mexalen; Midol maximum strength; Midol PM night time formula; Midol regular strength; Midol teen formula; Migraleve yellow; Minafen; Minoset; Miralgin; Momentum; mono Praecimed; Multin; N-(4-Hydroxyphenyl)acetamide; N-Acetyl-4-aminophenol; Naldegesic; NAPA; Napafen; Napap; Naprinol; Neagyl; Nebs; neo-Fepramol; NeoCitan; Neodol; Neodolito; Neopap; Neotrend; Neuridon; New cortal for children; NilnOcen; Nina; NO-Febril; Nobedon; Nodolex; Noral; Norcet; Norco; O-Acetaminophenol; Oltyl; Oralgan; Oraphen-PD; Ortensan; Oxycet; Oxycocet; Oxycodone 2.5/apap 500; Oxycodone 5/apap 500; P-(acetylamino)Phenol; Paceco; Pacemo; Pacemol; Pacet; Pacimol; Paedialgon; Paedol; Painex; Paldesic; Pamol; Panacete; Panadeine co; Panadiene; panado-Co; panado-co Caplets; Panadol extra strength; Panadol junior strength caplets; Panadol maximum strength caplets; Panadol maximum strength tablets; Panaleve; Panamax; Panasorb; Panasorbe; Panets; Panex; Panodil; Panofen; Pantalgin; Papa-deine #3; Papa-deine #4; Para-suppo; Para-tabs; Paracemol; Paraceno; Paracet; Paracetamol; Paracetamol al; Paracetamol antiparin P; Paracetamol basics; Paracetamol BC; Paracetamol DC; Paracetamol dr. schmidgall; Paracetamol fecofar; Paracetamol genericon; Paracetamol hanseler; Paracetamol harkley; Paracetamol heumann; Paracetamol hexal; Paracetamol italfarmaco; Paracetamol nycomed; Paracetamol PB; Paracetamol raffo; Paracetamol ratiopharm; Paracetamol rosch; Paracetamol saar; Paracetamol smithkline beecham; Paracetamol stada; Paracetamol von CT; Paracetamol winthrop; Paracetamole; Paracetamolo; Paracetanol; Paracetol; Paracin; Paracod; Paracodol; Parador; Paradrops; Parakaption; Parake; Paralen; Paralief; Paralink; Paralyoc; Paramol; Paramolan; Paranox; Parapan; Parasadol; Parasin; Paraspes; Paracetol; Parelan; Parmol; Parogal; Paroma; Pasolind; Pasolind N; PCM Paracetamol lichtenstein; Pettam; Pediapirin; Pedatrix; Pedric; Percocet; Percocet-5; Percocet-demi; Percogesic with codeine; Perdolan mono; Phenaphen; Phenaphen caplets; Phenaphen w/codeine; Phendom; Phenipirin; Phogoland; Phrenilin; Phrenilin forte; Pinex; Piramin; Pirinasol; Plicet; Polmofen; Predimol; Predualito; Prestwick\_13; Prodol; Prompt; Prontina; Propacet; Propacet 100; Proval #3; Puernal; Pulmofen; Pyregesic-C; Pyrigesic; Pyrinazine; Pyromed; Quiet world; Redutemp; Reliv; Remedol; Rhinex D-lay tablets; Rivalgyl; Robigesic; Robitussin night relief; Rockamol plus; Rounox; Roxicet; Roxicet 5/500; Roxilox; RubieMol; Rubophen; Rupemol; Salzone; Sanicet; Sanicopyrine; Scanol; Scentalgy; Scherzatabletten rezeptur 534; Schmerzex; Sedalito; Sedapap; Semolacin; Servigesic; Seskamol; Setakop; Setamol; Setol; Sifenol; Sinaspril; Sine-OFF sinus medicine caplets; Sinedol; Simmol; Sinubid; SK-Apap; Snaplets-FR; Spalt für die nacht; Spalt N; ST Joseph aspirin-free; ST Joseph aspirin-free for children; St. joseph cold tablets for children; St. joseph fever reducer; Stanback; Stopain; Sudafed severe cold formula; Sudafed sinus; Sunetheton; Supac; Supadol mono; Supofen; Suppap; Suppap-120; Suppap-



325; Suppap-650; Supramol-m; Synalgos-DC-a; Tabalgin; Tachiprina; Talacen; Tapanol extra strength caplets; Tapanol extra strength tablets; Tapar; Tavist allergy/sinus/headache; Tazamol; Temlo; Tempanal; Tempra; Tempra caplets; Tempra chewable tablets; Tempra d.s.; Tempra drops; Tempra syrup; Tencon; Termacet; Termalgin; Termalgine; Termofren; TheraFlu; Tibinide; Tibizide; Tiffy; Tisin; Tisiodrazida; Titralgan; Tizide; Tocris-1706; Toximer P; Tralgon; Treupel mon; Treupel N; Treuphadol; Triad; Triaminic sore throat formula; Triaprin; Tricoton; Tussapap; Tycolet; TYL; Tylenol allergy sinus; Tylenol arthritis extended relief; Tylenol caplets; Tylenol children's chewable tablets; Tylenol children's elixir; Tylenol children's suspension liquid; Tylenol drops; Tylenol elixir; Tylenol extra strength adult liquid pain reliever; Tylenol extra strength caplets; Tylenol extra strength gels; Tylenol extra strength tablets; Tylenol gelcaps; Tylenol infants drops; Tylenol infants' suspension drops; Tylenol junior strength caplets; Tylenol junior strength chewable tablets; Tylenol regular strength caplets; Tylenol regular strength tablets; Tylenol tablets; Tylex; Tylex CD; Tylo; Tylox; Tylox-325; Tymol; Ultracet; Upsanol; Utradin; Valadol; Valgesic; Valorin; Valorin extra; Vanquish; Veralgina; Vermidon; Verpol; Viclor richet; Vicodin; Vicodin es; Vicodin HP; Vips; Viruflu; Vivimed; Volpan; Wygesic; Zatinol; Zolben

HMDB: HMDB0001859; HMDB01859

CAS: 103-90-2

The excellent tolerability of therapeutic doses of paracetamol (acetaminophen) is a major factor in the very wide use of the drug. The major problem in the use of paracetamol is its hepatotoxicity after an overdose. Hepatotoxicity has also been reported after therapeutic doses, but critical analysis indicates that most patients with alleged toxicity from therapeutic doses have taken overdoses. Importantly, prospective studies indicate that therapeutic doses of paracetamol are an unlikely cause of hepatotoxicity in patients who ingest moderate to large amounts of alcohol (PMID: 15733027). Single doses of paracetamol are effective analgesics for acute postoperative pain and give rise to few adverse effects (PMID: 14974073). Acetaminophen (AAP) overdose and the resulting hepatotoxicity is an important clinical problem. In addition, AAP is widely used as a prototype hepatotoxin to study mechanisms of chemical-induced cell injury and to test the hepatoprotective potential of new drugs and herbal medicines. Because of its importance, the mechanisms of AAP-induced liver cell injury have been extensively investigated and controversially discussed for many years (PMID: 16863451).

This compound belongs to the class of organic compounds known as 1-hydroxy-2-unsubstituted benzenoids. These are phenols that are unsubstituted at the 2-position.

### Acetaminophen -- Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. *Tohoku J Exp Med.* 1995 May;176(1):61-8. PMID: 7482520

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Monleon D, Morales JM, Barrasa A, Lopez JA, Vazquez C, Celda B: Metabolite profiling of fecal water extracts from human colorectal cancer. *NMR Biomed.* 2009 Apr;22(3):342-8. doi: 10.1002/nbm.1345. PMID: 19006102

Weir TL, Manter DK, Sheflin AM, Barnett BA, Heuberger AL, Ryan EP: Stool microbiome and metabolome differences between colorectal cancer patients and healthy adults. *PLoS One.* 2013 Aug 6;8(8):e70803. doi: 10.1371/journal.pone.0070803. Print 2013. PMID: 23940645

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Ni Y, Xie G, Jia W: Metabonomics of human colorectal cancer: new approaches for early diagnosis and biomarker discovery. *J Proteome Res.* 2014 Sep 5;13(9):3857-70. doi: 10.1021/pr500443c. Epub 2014 Aug 14. PMID: 25105552

Ikeda A, Nishiumi S, Shinohara M, Yoshie T, Hatano N, Okuno T, Bamba T, Fukusaki E, Takenawa T, Azuma T, Yoshida M: Serum metabolomics as a novel diagnostic approach for gastrointestinal cancer. *Biomed Chromatogr.* 2012 May;26(5):548-58. doi: 10.1002/bmc.1671. Epub 2011 Jul 20. PMID: 21773981

Goedert JJ, Sampson JN, Moore SC, Xiao Q, Xiong X, Hayes RB, Ahn J, Shi J, Sinha R: Fecal metabolomics: assay performance and association with colorectal cancer. *Carcinogenesis.* 2014 Sep;35(9):2089-96. doi: 10.1093/carcin/bgu131. Epub 2014 Jul 18. PMID: 25037050

Sinha R, Ahn J, Sampson JN, Shi J, Yu G, Xiong X, Hayes RB, Goedert JJ: Fecal Microbiota, Fecal Metabolome, and Colorectal Cancer Interrelations. *PLoS One.* 2016 Mar 25;11(3):e0152126. doi: 10.1371/journal.pone.0152126. eCollection 2016. PMID: 27015276

Lin Y, Ma C, Liu C, Wang Z, Yang J, Liu X, Shen Z, Wu R: NMR-based fecal metabolomics fingerprinting as predictors of earlier diagnosis in patients with colorectal cancer. *Oncotarget.* 2016 May 17;7(20):29454-64. doi: 10.18632/oncotarget.8762. PMID: 27107423

Brown DG, Rao S, Weir TL, O'Malia J, Bazan M, Brown RJ, Ryan EP: Metabolomics and metabolic pathway networks from human colorectal cancers, adjacent mucosa, and stool. *Cancer Metab.* 2016 Jun 6;4:11. doi: 10.1186/s40170-016-0151-y. eCollection 2016. PMID: 27275383

Wang X, Wang J, Rao B, Deng L: Gut flora profiling and fecal metabolite composition of colorectal cancer patients and healthy individuals. *Exp Ther Med.* 2017 Jun;13(6):2848-2854. doi: 10.3892/etm.2017.4367. Epub 2017 Apr 20. PMID: 28587349

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## m-Aminobenzoic acid -- Introduction

SYNONYM: 3-Aminobenzoësaeure; 3-Carboxyaniline; m-Aminobenzoësaeure; m-Carboxyaniline; MABA; m-Aminobenzoate; Aniline-3-carboxylate; 3-Aminobenzoate; 3-Aminobenzoic acid; Aniline-3-carboxylic acid; m-Amonibenzoate; m-Amonibenzoic acid; 3-Aminobenzoic acid, monosodium salt; Meta-aminobenzoic acid

HMDB: HMDB0001891; HMDB0002129; HMDB01891; HMDB02129

CAS: 99-05-8

m-Aminobenzoic acid is an inactive analog of 3-aminobenzamide, a known modulator of PARP activity, inhibitor of poly ADP-ribose and of the PARP-specific protease (interleukin-1 beta converting enzyme (ICE)-like protease). (PMID 8657188). 3-Aminobenzoic acid is used as an intermediate for dyes, pesticides and other organic synthesis.

This compound belongs to the class of organic compounds known as aminobenzoic acids. These are benzoic acids containing an amine group attached to the benzene moiety.

## 1,7-Dimethylguanosine -- Introduction

SYNONYM:

HMDB: HMDB0001961; HMDB01961

CAS: 69453-64-1

1,7-dimethylguanosine is a modified ribonucleoside. 1,7-dimethylguanosine is formed in tRNA enzymatic methylation. 1,7-Dimethylguanosine was found to be formed in high amounts in the tRNA methylation reaction at high concentrations of methylating agents. 1,7-dimethylguanosine has a possible connection to chemical cancerogenesis and to the aberrant increase of tRNA methylases activity in tumor tissues. The amount of 1,7-dimethylguanosine produced by the kidney is higher than that produced by the liver. The immediate precursor in the formation of 1,7-dimethylguanosine in tRNA appears to be 1-



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methylguanosine. An accumulation of modified ribonucleosides appears in the serum of uremic patients. (PMID: 7046770, 6164398, 7259877, 7159514, 9607216).

This compound belongs to the class of organic compounds known as purine nucleosides. These are compounds comprising a purine base attached to a ribosyl or deoxyribosyl moiety.

## 5'-Deoxyadenosine -- Introduction

SYNONYM: 5'-Deoxy-adenosine

HMDB: HMDB0001983; HMDB01983

CAS: 4754-39-6

5'-Deoxyadenosine is an oxidized nucleoside found in the urine of normal subjects. Oxidized nucleosides represent excellent biomarkers for determining the extent of damage in genetic material, which has long been of interest in understanding the mechanism of aging, neurodegenerative diseases, and carcinogenesis. (PMID 15116424). The normal form of deoxyadenosine used in DNA synthesis and repair is 2'-deoxyadenosine where the hydroxyl group (-OH) is at the 2' position of its ribose sugar moiety. 5'-deoxyadenosine has its hydroxyl group at the 5' position of the ribose sugar.

This compound belongs to the class of organic compounds known as 5'-deoxyribonucleosides. These are nucleosides in which the oxygen atom at the 5'position of the ribose moiety has been replaced by another atom. The nucleobases here are limited to purine, pyrimidine, and pyridine derivatives.

## Myristoleic acid -- Introduction

SYNONYM: (9Z)-Tetradecenoic acid; (Z)-Tetradec-9-enoic acid; 9-Tetradecenoic acid; 9Z-Tetradecenoic acid; cis-9-Tetradecenoic acid; cis-Delta(9)-Tetradecenoic acid; cis-Tetradec-9-enoic acid; (9Z)-Tetradecenoate; Myristoleate; (Z)-Tetradec-9-enoate; 9-Tetradecenoate; 9Z-Tetradecenoate; cis-9-Tetradecenoate; cis-delta(9)-Tetradecenoate; cis-Î'(9)-tetradecenoate; cis-Î'(9)-tetradecenoic acid; cis-Tetradec-9-enoate; (9Z)-Tetradec-9-enoate; (9Z)-Tetradec-9-enoic acid

HMDB: HMDB0002000; HMDB02000

CAS: 544-64-9

Myristoleic acid is a monounsaturated fatty acid that represent approximately 0.3 - 0.7% of the total fatty acid composition of adipose tissue triacylglycerol in human. (PMID 10393134). It has been suggested that his cytotoxic and effective cell death inducer activity could be used for the treatment of prostate cancer. (PMID 11304730).

This compound belongs to the class of organic compounds known as long-chain fatty acids. These are fatty acids with an aliphatic tail that contains between 13 and 21 carbon atoms.

## Myristoleic acid -- Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. Tohoku J Exp Med. 1995 May;176(1):61-8. PMID: 7482520

Cheng Y, Xie G, Chen T, Qiu Y, Zou X, Zheng M, Tan B, Feng B, Dong T, He P, Zhao L, Zhao A, Xu LX, Zhang Y, Jia W: Distinct urinary metabolic profile of human colorectal cancer. J Proteome Res. 2012 Feb 3;11(2):1354-63. doi: 10.1021/pr201001a. Epub 2011 Dec 28. PMID: 22148915

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Phua LC, Chue XP, Koh PK, Cheah PY, Ho HK, Chan EC: Non-invasive fecal metabonomic detection of colorectal cancer. Cancer Biol Ther. 2014 Apr;15(4):389-97. doi: 10.4161/cbt.27625. Epub 2014 Jan 14. PMID: 24424155



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Ni Y, Xie G, Jia W: Metabonomics of human colorectal cancer: new approaches for early diagnosis and biomarker discovery. *J Proteome Res.* 2014 Sep 5;13(9):3857-70. doi: 10.1021/pr500443c. Epub 2014 Aug 14. PMID: 25105552

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Goedert JJ, Sampson JN, Moore SC, Xiao Q, Xiong X, Hayes RB, Ahn J, Shi J, Sinha R: Fecal metabolomics: assay performance and association with colorectal cancer. *Carcinogenesis.* 2014 Sep;35(9):2089-96. doi: 10.1093/carcin/bgu131. Epub 2014 Jul 18. PMID: 25037050

Sinha R, Ahn J, Sampson JN, Shi J, Yu G, Xiong X, Hayes RB, Goedert JJ: Fecal Microbiota, Fecal Metabolome, and Colorectal Cancer Interrelations. *PLoS One.* 2016 Mar 25;11(3):e0152126. doi: 10.1371/journal.pone.0152126. eCollection 2016. PMID: 27015276

Lin Y, Ma C, Liu C, Wang Z, Yang J, Liu X, Shen Z, Wu R: NMR-based fecal metabolomics fingerprinting as predictors of earlier diagnosis in patients with colorectal cancer. *Oncotarget.* 2016 May 17;7(20):29454-64. doi: 10.18632/oncotarget.8762. PMID: 27107423

Brown DG, Rao S, Weir TL, O'Malia J, Bazan M, Brown RJ, Ryan EP: Metabolomics and metabolic pathway networks from human colorectal cancers, adjacent mucosa, and stool. *Cancer Metab.* 2016 Jun 6;4:11. doi: 10.1186/s40170-016-0151-y. eCollection 2016. PMID: 27275383

Wang X, Wang J, Rao B, Deng L: Gut flora profiling and fecal metabolite composition of colorectal cancer patients and healthy individuals. *Exp Ther Med.* 2017 Jun;13(6):2848-2854. doi: 10.3892/etm.2017.4367. Epub 2017 Apr 20. PMID: 28587349

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<http://www.sciencedirect.com/science/article/pii/S0924224416301984> PMID: 7482520

## Tetracosahexaenoic acid -- Introduction

SYNONYM: 6Z,9Z,12Z,15Z,18Z,21Z-Tetracosahexaenoic acid; all-cis-6,9,12,15,18,21-Tetracosahexaenoic acid; all-cis-Tetracosa-6,9,12,15,18,21-hexaenoic acid; C24:6N-3; C24:6Omega-3; Nisinic acid; THA; 6Z,9Z,12Z,15Z,18Z,21Z-Tetracosahexaenoate; Tetracosahexaenoate; all-cis-6,9,12,15,18,21-Tetracosahexaenoate; all-cis-Tetracosa-6,9,12,15,18,21-hexaenoate; Nisinate

HMDB: HMDB0002007; HMDB02007

CAS: 81247-23-6

The formation of docosahexaenoic acid(DHA) involves the production of tetracosahexaenoic acid C24:6n-3) from dietary linolenic acid (C18:3n-3) via a series of elongation and desaturation reactions, followed by beta-oxidation of C24:6n-3 to C22:6n-3. DHA is deficient in patients lacking peroxisomes.(PMID: 11734571).

This compound belongs to the class of organic compounds known as very long-chain fatty acids. These are fatty acids with an aliphatic tail that contains at least 22 carbon atoms.

## Butyrylcarnitine -- Introduction



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SYNONYM: (3R)-3-(Butyryloxy)-4-(trimethylammonio)butanoate; Butyryl-L-carnitine; Butyrylcarnitine; L-Carnitine butyryl ester; N-Butyryl-L(-)-carnitin; O-Butanoyl-(R)-carnitine; (3R)-3-(Butyryloxy)-4-(trimethylammonio)butanoic acid; Butylcarnitine; O-Butanoyl-carnitine; O-Butanoylcarnitine

HMDB: HMDB0002013; HMDB0062510; HMDB02013; HMDB62510

CAS: 25576-40-3

Butyrylcarnitine, also known as (3R)-3-(butyryloxy)-4-(trimethylammonio)butanoate or L-carnitine butyryl ester, is classified as a member of the acylcarnitines. Acylcarnitines are organic compounds containing a fatty acid with the carboxylic acid attached to carnitine through an ester bond. Butyrylcarnitine is considered to be practically insoluble (in water) and acidic. Butyrylcarnitine is elevated in patients with short-chain acyl-CoA dehydrogenase (SCAD) deficiency, in infants with acute acidosis and generalized muscle weakness, and in middle-aged patients with chronic myopathy localized in muscle (OMIM: 201470).

belongs to the class of organic compounds known as acyl carnitines. These are organic compounds containing a fatty acid with the carboxylic acid attached to carnitine through an ester bond.

### Butyrylcarnitine -- Very Long Chain Acyl-CoA Dehydrogenase Deficiency

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### Butyrylcarnitine -- Short Chain Acyl-CoA Dehydrogenase Deficiency

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## Butyrylcarnitine -- Glutaric aciduria II

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## Imidazoleacetic acid -- Introduction

SYNONYM: 1H-Imidazole-4-acetic acid; 4(5)-Imidazoleacetate; 4-Imidazoleacetate; Imidazole-4-acetate; 1H-Imidazole-4-acetate; Imidazoleacetate; 4(5)-Imidazoleacetic acid; 4-Imidazoleacetic acid; Imidazole-4-acetic acid; 1H-Imidazol-4-ylacetic acid; IAA; IMAC; Imidazol-4-ylacetate; Imidazol-4-ylacetic acid; Imidazole acetate; Imidazolyl-4-acetic acid; IZC; Lopac-I-0375; Imidazole-4-acetic acid, sodium salt; Imidazole-4-acetic acid hydrochloride

HMDB: HMDB0002024; HMDB0060261; HMDB02024; HMDB60261

CAS: 645-65-8

Imidazoleacetic acid is a metabolite product of Histamine metabolism. It is present in normal urine and increased in histidinemic patients. (PMID 6530403).

This compound belongs to the class of organic compounds known as imidazolyl carboxylic acids and derivatives. These are organic compounds containing a carboxylic acid chain (of at least 2 carbon atoms) linked to an imidazole ring.

## 2-Pyrrolidinone -- Introduction

SYNONYM: 1-Azacyclopentan-2-one; 2-Ketopyrrolidine; 2-Oxopyrrolidine; 2-Pyrrolidone; 4-Aminobutyric acid lactam; alpha-Pyrrolidinone; alpha-Pyrrolidone; Butyrolactam; gamma-Aminobutyric acid lactam; gamma-Aminobutyric lactam; gamma-Butyrolactam; Pyrrolidone; Pyrrolidone; 4-Aminobutyrate lactam; a-Pyrrolidinone;  $\beta$ -pyrrolidinone; a-Pyrrolidone;  $\beta$ -pyrrolidone; g-Aminobutyrate lactam; g-Aminobutyric acid lactam; gamma-Aminobutyrate lactam;  $\beta$ -aminobutyrate lactam;  $\beta$ -aminobutyric acid lactam; g-Aminobutyric lactam;  $\beta$ -aminobutyric lactam; g-Butyrolactam;  $\beta$ -butyrolactam; 1-Methyl-2-pyrrolidinone; 2-Pyrol4-aminobutyric acid lactam; 2-Pyrrolidone for synthesis; 2-Pyrrolidone-butyrolactam; Aminobutyric acid lactam; Aminobutyric lactam; Aminobutyrolactam; N-Methyl-2-pyrrolidinone; Pyrrolidin-2-one; Pyrrolidon; Pyrrolidone-2; Tetrahydropyrrolone; 2-Pyrrolidone, (18)O-labeled; 2-Pyrrolidone, 5-(14)C-labeled; 2-Pyrrolidone, hydrotribromide; 2-Pyrrolidone, rubidium salt; 2-Pyrrolidone, aluminum salt; 2-Pyrrolidone, lithium salt; 2-Pyrrolidone, potassium salt; 2-Pyrrolidone, sodium salt; 2-Pyrrolidone, cerium salt; 2-Pyrrolidone, hydrobromide; 2-Pyrrolidone, hydrochloride

HMDB: HMDB0002039; HMDB02039

CAS: 616-45-5

2-Pyrrolidinone is a lactam cyclization product of gamma-aminobutyric acid (GABA). (PMID 10332870). Vigabatrin (VGB, an antiepileptic drug) increases human brain gamma-aminobutyric acid (GABA) and the related metabolites, including 2-pyrrolidinone. Patients taking VGB are expected to have an increase of these metabolites. (PMID 10403220, 10840398). 2-Pyrrolidone is an organic compound consisting of a five-membered lactam. It is a colorless liquid which is used in industrial settings as a high-boiling non-corrosive polar solvent for a wide variety of applications. It is miscible with a wide variety of other solvents including water, ethanol, diethyl ether, chloroform, benzene, ethyl acetate and carbon disulfide. -- Wikipedia.

This compound belongs to the class of organic compounds known as pyrrolidine-2-ones. These are pyrrolidines which bear a C=O group at position 2 of the pyrrolidine ring.

## 2-Pyrrolidinone -- Bladder infections

Tricker AR, Pfundstein B, Kalble T, Preussmann R: Secondary amine precursors to nitrosamines in human saliva, gastric juice, blood, urine and faeces. *Carcinogenesis.* 1992 Apr;13(4):563-8. PMID: 1576707

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## 12-Hydroxydodecanoic acid -- Introduction

SYNONYM: 12-Hydroxy lauric acid; 2-Hydroxy-dodecanoic acid; Omega-hydroxy lauric acid; Omega-hydroxydodecanoic acid; Omega-OH dodecanoic acid; Omega-OH lauric acid; 12-Hydroxy lae; 12-Hydroxy laic acid; 12-Hydroxydodecanoate; 2-Hydroxy-dodecanoate; Omega-hydroxy laate; Omega-hydroxy laic acid; Omega-hydroxydodecanoate; Omega-OH dodecanoate; Omega-OH laate; Omega-OH laic acid; 12-Hydroxylaurate; 12-Hydroxylauric acid; Omega hydroxy dodecanoate; Omega hydroxy dodecanoic acid; Omega-hydroxylauric acid

HMDB: HMDB0002059; HMDB02059

CAS: 505-95-3

12-hydroxydodecanoic acid is the substrate of the human glutathione-dependent formaldehyde dehydrogenase (EC1.1.1.1). The enzyme that catalyzes the conversion of alcohols to aldehydes is a zinc-containing dimeric enzyme responsible for the oxidation of long-chain alcohols and omega-hydroxy fatty acids. (OMIM). The human glutathione-dependent formaldehyde dehydrogenase is unique among the structurally studied members of the alcohol dehydrogenase family in that it follows a random bi kinetic mechanism forming a binary complex, and a ternary complex with NAD+. (PMID 12196016).

This compound belongs to the class of organic compounds known as medium-chain hydroxy acids and derivatives. These are hydroxy acids with a 6 to 12 carbon atoms long side chain.

## N-Acetylputrescine -- Introduction

SYNONYM: Acetylputrescine; Monoacetylputrescine; N-(4-Aminobutyl)acetamide; N-Acetylputrescine monohydrochloride

HMDB: HMDB0002064; HMDB02064

CAS: 18233-70-0

N-Acetylputrescine is a polyamine commonly occurring excreted in normal human urine (PMID 7775374). N-Acetylputrescine is the most abundant of all polyamines both in normal individuals and in patients with leukemia (PMID 9464484). N-Acetylputrescine is the N-acetylated form of the naturally occurring polyamine called putrescine. The N-acetylation is mediated by the enzyme diamine N-acetyltransferase. Putrescine is related to cadaverine (another polyamine). Both are produced by the breakdown of amino acids in living and dead organisms and both are toxic in large doses. Putrescine and cadaverine are largely responsible for the foul odor of putrefying flesh, but also contribute to the odor of such processes as bad breath and bacterial vaginosis. Putrescine is also found in semen. Putrescine attacks s-adenosyl methionine and converts it to spermidine. Spermidine in turn attacks another s-adenosyl methionine and converts it to spermine. Putrescine is synthesized in small quantities by healthy living cells by the action of ornithine decarboxylase.

This compound belongs to the class of organic compounds known as carboximidic acids. These are organic acids with the general formula  $\text{RC}(\text{=N})\text{-OH}$  ( $\text{R}=\text{H}$ , organic group).

## N-Acetylputrescine -- Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. Tohoku J Exp Med. 1995 May;176(1):61-8. PMID: 7482520

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Goedert JJ, Sampson JN, Moore SC, Xiao Q, Xiong X, Hayes RB, Ahn J, Shi J, Sinha R: Fecal metabolomics: assay performance and association with colorectal cancer. *Carcinogenesis.* 2014 Sep;35(9):2089-96. doi: 10.1093/carcin/bgu131. Epub 2014 Jul 18. PMID: 25037050

Sinha R, Ahn J, Sampson JN, Shi J, Yu G, Xiong X, Hayes RB, Goedert JJ: Fecal Microbiota, Fecal Metabolome, and Colorectal Cancer Interrelations. *PLoS One.* 2016 Mar 25;11(3):e0152126. doi: 10.1371/journal.pone.0152126. eCollection 2016. PMID: 27015276

Lin Y, Ma C, Liu C, Wang Z, Yang J, Liu X, Shen Z, Wu R: NMR-based fecal metabolomics fingerprinting as predictors of earlier diagnosis in patients with colorectal cancer. *Oncotarget.* 2016 May 17;7(20):29454-64. doi: 10.18632/oncotarget.8762. PMID: 27107423

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## N-Acetylputrescine -- Leukemia

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Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. *Tohoku J Exp Med.* 1995 May;176(1):61-8. PMID: 7482520

## Palmitoylethanolamide -- Introduction

**SYNONYM:** Anandamide (16:0); Hexadecanoyl ethanolamide; Hydroxyethylpalmitamide; Monoethanolamine palmitic acid amide; N-(2-Hydroxyethyl)palmitamide; N-Hexadecanoyl ethanolamine; N-Palmitoylethanolamine; Palmidrol; Palmidrolum; Palmitamide mea; Palmitic acid monoethanolamide; Palmitinsaeure-beta-hydroxyethylamid; Palmitoyl-ea; PEA; Monoethanolamine palmitate amide; Palmitate monoethanolamide; Palmitinsaeure-b-hydroxyethylamid; Palmitinsaeure- $\tilde{\text{I}}^2$ -hydroxyethylamid; Loramine P 256; N-(2-Hydroxyethyl)hexadecanamide; N-Hexadecyl-ethanolamine; Palmitoyl ethanolamide; Impulsin; Palmitoylethanolamide; MimyX; N-(2-Hydroxyethyl)palmitate

**HMDB:** HMDB0002100; HMDB02100

**CAS:** 544-31-0

N-Palmitoylethanolamide (PEA) is present in the tissues of most mammals. It was initially described as an agonist of the type 2 cannabinoid receptor (CB2), although it is now universally recognized that PEA is in fact incapable of binding to cannabinoid receptors, or at least not to the known receptors. In addition to its anti-inflammatory activity, PEA also produces analgesia, neuroprotection, and possesses anti-epileptic properties. It also reduces gastrointestinal motility and cancer cell proliferation, as well as protecting the vascular endothelium in the ischemic heart. The physiological stimuli that regulate PEA levels in mammalian tissues are largely unknown, however, multiple studies indicate that this lipid accumulates during cellular stress, particularly following tissue injury. For example, PEA increases post-mortem in the pig brain. Similar elevations in PEA levels have been observed in the ischemic brain and PEA is also up-regulated in response to ultraviolet-B irradiation in mouse epidermal cells. Adipose tissue is highly implicated in the systemic secretion of IL-6 and leptin, and human mature adipocytes are able to secrete large quantity of PEA. Human adipose tissue can be subjected to modulation of its inflammatory state by lipopolysaccharide (LPS). LPS strongly inhibits adipose cell leptin release, with PEA acting as a potentiator of this inhibitory effect. These actions are not linked to a reduction in leptin gene transcription. Thus, PEA does not have an anti-inflammatory role in the secretion of IL-6 via NFkappaB at the adipocyte level, but instead seems to act at the heart of the LPS-stimulated pathway, which, independently of NFkappaB, inhibits the secretion of leptin. (PMID: 16884908).

This compound belongs to the class of organic compounds known as carboximidic acids. These are organic acids with the general formula  $\text{RC}(\text{=N})\text{-OH}$  ( $\text{R}=\text{H}$ , organic group).

## Palmitoylethanolamide -- Colorectal cancer

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Monleon D, Morales JM, Barrasa A, Lopez JA, Vazquez C, Celda B: Metabolite profiling of fecal water extracts from human colorectal cancer. *NMR Biomed.* 2009 Apr;22(3):342-8. doi: 10.1002/nbm.1345. PMID: 19006102

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Phua LC, Chue XP, Koh PK, Cheah PY, Ho HK, Chan EC: Non-invasive fecal metabonomic detection of colorectal cancer. *Cancer Biol Ther.* 2014 Apr;15(4):389-97. doi: 10.4161/cbt.27625. Epub 2014 Jan 14. PMID: 24424155

Ritchie SA, Ahiahou PW, Jayasinghe D, Heath D, Liu J, Lu Y, Jin W, Kavianpour A, Yamazaki Y, Khan AM, Hossain M, Su-Myat KK, Wood PL, Krenitsky K, Takemasa I, Miyake M, Sekimoto M, Monden M, Matsubara H, Nomura F, Goodenow DB: Reduced levels of hydroxylated, polyunsaturated ultra long-chain fatty acids in the serum of colorectal cancer patients: implications for early screening and detection. *BMC Med.* 2010 Feb 15;8:13. doi: 10.1186/1741-7015-8-13. PMID: 20156336



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Ikeda A, Nishiumi S, Shinohara M, Yoshie T, Hatano N, Okuno T, Bamba T, Fukusaki E, Takenawa T, Azuma T, Yoshida M: Serum metabolomics as a novel diagnostic approach for gastrointestinal cancer. *Biomed Chromatogr.* 2012 May;26(5):548-58. doi: 10.1002/bmc.1671. Epub 2011 Jul 20. PMID: 21773981

Goedert JJ, Sampson JN, Moore SC, Xiao Q, Xiong X, Hayes RB, Ahn J, Shi J, Sinha R: Fecal metabolomics: assay performance and association with colorectal cancer. *Carcinogenesis.* 2014 Sep;35(9):2089-96. doi: 10.1093/carcin/bgu131. Epub 2014 Jul 18. PMID: 25037050

Sinha R, Ahn J, Sampson JN, Shi J, Yu G, Xiong X, Hayes RB, Goedert JJ: Fecal Microbiota, Fecal Metabolome, and Colorectal Cancer Interrelations. *PLoS One.* 2016 Mar 25;11(3):e0152126. doi: 10.1371/journal.pone.0152126. eCollection 2016. PMID: 27015276

Lin Y, Ma C, Liu C, Wang Z, Yang J, Liu X, Shen Z, Wu R: NMR-based fecal metabolomics fingerprinting as predictors of earlier diagnosis in patients with colorectal cancer. *Oncotarget.* 2016 May 17;7(20):29454-64. doi: 10.18632/oncotarget.8762. PMID: 27107423

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## Oleamide -- Introduction

SYNONYM: (9Z)-9-Octadecenamide; (Z)-9-Octadecenamide; (Z)-Octadec-9-enoic acid amide; 9-Octadecenamide; 9Z-Octadecenamide; cis-9,10-Octadecenoamide; Oleic acid amide; Oleyl amide; Oleylamide; (Z)-Octadec-9-enoate amide; Oleate amide; (9Z)-Octadec-9-enamide; (cis)-9-Octadecenoate; (cis)-9-Octadecenoic acid; (cis)-9-Octadecenoic acid amide; 14C-Labeled oleamide; 9,10-Octadecenamide; Adogen 73; Aliphatic amide; Amide O; Armid O; Armoslip CP; Crodamide O; Crodamide or; Diamide O 200; Diamit O 200; Elaidoylamide; ELD; Kermamide O; Octadecene amide; Petrac slip-eze; Polydis TR 121; Slip-eze; Tocris-0878; trans-9,10-Octadecenoamide; Unislip 1759; Oleylamide, (e)-isomer

HMDB: HMDB0002117; HMDB02117

CAS: 301-02-0

Oleamide is an amide of the fatty acid oleic acid. It is an endogenous substance: it occurs naturally in the body of animals. It accumulates in the cerebrospinal fluid during sleep deprivation and induces sleep in animals. It is being studied as a potential medical treatment for mood and sleep disorders, and cannabinoid-regulated depression. The mechanism of action of oleamide's sleep inducing effects is an area of current research. It is likely that oleamide interacts with multiple neurotransmitter systems. Oleamide is structurally related to the endogenous cannabinoid anandamide, and has the ability to bind to the CB1 receptor as a full agonist.

This compound belongs to the class of organic compounds known as fatty amides. These are carboxylic acid amide derivatives of fatty acids, that are formed from a fatty acid and an amine.

## Oleamide -- Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-

methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. *Tohoku J Exp Med.* 1995 May;176(1):61-8. PMID: 7482520

Cheng Y, Xie G, Chen T, Qiu Y, Zou X, Zheng M, Tan B, Feng B, Dong T, He P, Zhao L, Zhao A, Xu LX, Zhang Y, Jia W: Distinct urinary metabolic profile of human colorectal cancer. *J Proteome Res.* 2012 Feb 3;11(2):1354-63. doi: 10.1021/pr201001a. Epub 2011 Dec 28. PMID: 22148915

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Phua LC, Chue XP, Koh PK, Cheah PY, Ho HK, Chan EC: Non-invasive fecal metabonomic detection of colorectal cancer. *Cancer Biol Ther.* 2014 Apr;15(4):389-97. doi: 10.4161/cbt.27625. Epub 2014 Jan 14. PMID: 24424155

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Ikeda A, Nishiumi S, Shinohara M, Yoshie T, Hatano N, Okuno T, Bamba T, Fukusaki E, Takenawa T, Azuma T, Yoshida M: Serum metabolomics as a novel diagnostic approach for gastrointestinal cancer. *Biomed Chromatogr.* 2012 May;26(5):548-58. doi: 10.1002/bmc.1671. Epub 2011 Jul 20. PMID: 21773981

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Wang X, Wang J, Rao B, Deng L: Gut flora profiling and fecal metabolite composition of colorectal cancer patients and healthy individuals. *Exp Ther Med.* 2017 Jun;13(6):2848-2854. doi: 10.3892/etm.2017.4367. Epub 2017 Apr 20. PMID: 28587349

Silke Matysik, Caroline Ivonne Le Roy, Gerhard Liebisch, Sandrine Paule Claus. Metabolomics of fecal samples: A practical consideration. *Trends in Food Science & Technology.* Vol. 57, Part B, Nov. 2016, p.244-255: <http://www.sciencedirect.com/science/article/pii/S0924224416301984> PMID: 7482520

## Docosahexaenoic acid -- Introduction

SYNONYM: (4Z,7Z,10Z,13Z,16Z,19Z)-Docosahexaenoic acid; 22:6(N-3); 22:6-4, 7,10,13,16,19; 4,7,10,13,16,19-

Docosahexaenoic acid; all-cis-4,7,10,13,16,19-Docosahexaenoic acid; all-cis-DHA; Cervonic acid; DHA; Doconexent; DOCOSA-4,7,10,13,16,19-hexaenoIC ACID; (4Z,7Z,10Z,13Z,16Z,19Z)-Docosahexaenoate; Docosahexaenoate; 4,7,10,13,16,19-Docosahexaenoate; all-cis-4,7,10,13,16,19-Docosahexaenoate; Cervonate; DOCOSA-4,7,10,13,16,19-hexaenoate; all-Z-Docosahexaenoate; all-Z-Docosahexaenoic acid; cis-4,7,10,13,16,19-Docosahexanoate; cis-4,7,10,13,16,19-Docosahexanoic acid; Doconexento; Doconexentum; Doxonexent; Acids, docosahexaenoic; Acids, docosahexenoic; Docosahexaenoic acid, 3,6,9,12,15,18-isomer; Docosahexaenoic acid, 4,7,10,13,16,19-(all-Z-isomer); Docosahexaenoic acid, 4,7,10,13,16,19-(all-Z-isomer), cerium salt; Docosahexaenoic acid, 4,7,10,13,16,19-isomer, sodium salt; Docosahexaenoic acid, sodium salt; Docosahexaenoic acid (all-Z isomer); Docosahexaenoic acid dimer (all-Z isomer); Docosahexaenoic acid, 4,7,10,13,16,19-(all-Z-isomer), cesium salt; Docosahexaenoic acid, 4,7,10,13,16,19-(all-Z-isomer), potassium salt; Docosahexaenoic acids; Docosahexaenoic acid, 4,7,10,13,16,19-(Z,Z,Z,Z,Z,e-isomer); Docosahexaenoic acid, 4,7,10,13,16,19-isomer; Docosahexenoic acids

HMDB: HMDB0002183; HMDB02183

CAS: 6217-54-5

Docosahexaenoic acid (DHA) is an omega-3 essential fatty acid. Chemically, DHA is a carboxylic acid with a 22-carbon chain and six cis double bonds with the first double bond located at the third carbon from the omega end. DHA is most often found in fish oil. It is a major fatty acid in sperm and brain phospholipids, especially in the retina. Dietary DHA can reduce the level of blood triglycerides in humans, which may reduce the risk of heart disease (Wikipedia). Docosahexaenoic acid is found to be associated with isovaleric acidemia, which is an inborn error of metabolism.

This compound belongs to the class of organic compounds known as very long-chain fatty acids. These are fatty acids with an aliphatic tail that contains at least 22 carbon atoms.

### Docosahexaenoic acid – Thyroid cancer

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### Docosahexaenoic acid – Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. *Tohoku J Exp Med*. 1995 May;176(1):61-8. PMID: 7482520

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## Docosahexaenoic acid -- Major depressive disorder

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### Docosahexaenoic acid -- Essential hypertension

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### Docosahexaenoic acid -- Isovaleric acidemia

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### Docosahexaenoic acid -- Rhizomelic chondrodysplasia punctata

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### Docosahexaenoic acid -- Stroke

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### 3-Hydroxycapric acid -- Introduction

SYNONYM: 3-Hydroxy-decanoic acid; beta-Hydroxycapric acid; beta-Hydroxydecanoic acid; Myrmicacin; 3-Hydroxy-decanoate; 3-Hydroxycaprate; b-Hydroxycaprate; b-Hydroxycapric acid; beta-Hydroxycaprate;  $\tilde{\beta}$ -hydroxycaprate;  $\tilde{\beta}$ -hydroxycapric acid; b-Hydroxydecanoate; b-Hydroxydecanoic acid; beta-Hydroxydecanoate;  $\tilde{\beta}$ -hydroxydecanoate;  $\tilde{\beta}$ -hydroxydecanoic acid; (+/-)3-hydroxy-decanoate; (+/-)3-hydroxy-decanoic acid; 10:0(3-OH); 3-HDA; 3-Hydroxydecanoate; 3-Hydroxydecanoic acid; Myrmicacin, (R)-isomer; Myrmicacin monosodium (+)-isomer; Myrmicacin, (-)-isomer

HMDB: HMDB0002203; HMDB02203

CAS: 14292-26-3

3-Hydroxycapric acid is a normally occurring carboxylic acid in human blood plasma. Medium- and long-chain 3-hydroxymonocarboxylic acids represent intermediates in the beta-oxidation of fatty acids. They accumulate in the plasma of patients with an inherited deficiency of long-chain 3-hydroxyacyl-CoA dehydrogenase (EC 1.1.1.35) (PMID: 1912723). 3-Hydroxyacyl-CoA dehydrogenase (HADH) deficiency has been described in diverse clinical cases: juvenile-onset recurrent myoglobinuria, hypoketotic hypoglycemic encephalopathy, hypertrophic/dilatative cardiomyopathy, sudden infant death, and fulminant hepatic failure (OMIM: 231530). 3-Hydroxycapric acid has some shape-transforming action on the membrane of intact human erythrocytes (PMID: 7318031).

This compound belongs to the class of organic compounds known as medium-chain hydroxy acids and derivatives. These are hydroxy acids with a 6 to 12 carbon atoms long side chain.



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### 3-Hydroxycapric acid – Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. *Tohoku J Exp Med.* 1995 May;176(1):61-8. PMID: 7482520

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### 3-Hydroxycapric acid -- 3-Hydroxy-3-Methylglutaryl-CoA Synthase Deficiency

Thompson GN, Hsu BY, Pitt JJ, Treacy E, Stanley CA: Fasting hypoketotic coma in a child with deficiency of mitochondrial 3-hydroxy-3-methylglutaryl-CoA synthase. *N Engl J Med.* 1997 Oct 23;337(17):1203-7. doi: 10.1056/NEJM199710233371704. PMID: 9337379

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### 3-Hydroxycapric acid -- 3-Hydroxydicarboxylic aciduria

Tserng KY, Jin SJ, Kerr DS, Hoppel CL: Urinary 3-hydroxydicarboxylic acids in pathophysiology of metabolic disorders with dicarboxylic aciduria. *Metabolism.* 1991 Jul;40(7):676-82. PMID: 1870421

Hagenfeldt L, von Dobeln U, Holme E, Alm J, Brandberg G, Enocksson E, Lindeberg L: 3-Hydroxydicarboxylic aciduria--a fatty acid oxidation defect with severe prognosis. *J Pediatr.* 1990 Mar;116(3):387-92. PMID: 2308028

### Dodecanoylecarnitine -- Introduction

SYNONYM: (-)-Lauroylcarnitine; (3R)-3-(Dodecanoxy)-4-(trimethylammonio)butanoate; (R)-Dodecanoylecarnitine; Dodecanoyle-L-carnitine; L-Carnitine dodecanoyl ester; Lauroyl-L(-)-carnitin; Lauroyl-L-carnitine; Lauroylcarnitine; Laurylcarnitine; O-C12:0-L-Carnitine; O-Dodecanoyle-R-carnitine; (3R)-3-(Dodecanoxy)-4-(trimethylammonio)butanoic acid; C12 Carnitine; L-Lauroylcarnitine; Lauroyl-L(-)-carnitine; Dodecanoylecarnitine; O-Dodecanoylecarnitine; O-Lauroylcarnitine; O-Lauroyl-L-carnitine

HMDB: HMDB0002250; HMDB0062713; HMDB02250; HMDB62713

CAS: 25518-54-1

Dodecanoylecarnitine is an acylcarnitine present in fatty acid oxidation disorders such as long-chain acyl CoA dehydrogenase deficiency, carnitine palmitoyltransferase I deficiency, and carnitine palmitoyltransferase II deficiency (PMID 12828998). Moreover, dodecanoylecarnitine is found to be associated with celiac disease, which is also an inborn error of metabolism.

This compound belongs to the class of organic compounds known as acyl carnitines. These are organic compounds containing a fatty acid with the carboxylic acid attached to carnitine through an ester bond.

### Dodecanoylecarnitine -- Very Long Chain Acyl-CoA Dehydrogenase Deficiency

Onkenhout W, Venizelos V, van der Poel PF, van den Heuvel MP, Poorthuis BJ: Identification and quantification of intermediates of unsaturated fatty acid metabolism in plasma of patients with fatty acid oxidation disorders. *Clin Chem.* 1995 Oct;41(10):1467-74. PMID: 7586519

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### Dodecanoylecarnitine -- Pregnancy



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## Dodecanoylearnitine -- Celiac disease

Spiller RC, Frost PF, Stewart JS, Bloom SR, Silk DB: Delayed postprandial plasma bile acid response in coeliac patients with slow mouth-caecum transit. Clin Sci (Lond). 1987 Feb;72(2):217-23. PMID: 3816078

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## Dodecanoylcarnitine -- Obesity

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Reinehr T, Wolters B, Knop C, Lass N, Hellmuth C, Harder U, Peissner W, Wahl S, Grallert H, Adamski J, Illig T, Prehn C, Yu Z, Wang-Sattler R, Koletzko B: Changes in the serum metabolite profile in obese children with weight loss. *Eur J Nutr.* 2015 Mar;54(2):173-81. doi: 10.1007/s00394-014-0698-8. Epub 2014 Apr 17. PMID: 24740590

Wahl S, Yu Z, Kleber M, Singmann P, Holzapfel C, He Y, Mittelstrass K, Polonikov A, Prehn C, Romisch-Margl W, Adamski J, Suhre K, Grallert H, Illig T, Wang-Sattler R, Reinehr T: Childhood obesity is associated with changes in the serum metabolite profile. *Obes Facts.* 2012;5(5):660-70. doi: 10.1159/000343204. Epub 2012 Oct 4. PMID: 23108202



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Cho K, Moon JS, Kang JH, Jang HB, Lee HJ, Park SI, Yu KS, Cho JY: Combined untargeted and targeted metabolomic profiling reveals urinary biomarkers for discriminating obese from normal-weight adolescents. *Pediatr Obes.* 2017 Apr;12(2):93-101. doi: 10.1111/jopo.12114. Epub 2016 Feb 22. PMID: 26910390

## Heptadecanoic acid -- Introduction

SYNONYM: 17:0; C17:0; CH<sub>3</sub>-[CH<sub>2</sub>]15-COOH; Heptadecanoic acid; Heptadecylic acid; Margaric acid; Margarinic acid; Margarinsaeure; N-Heptadecanoic acid; N-Heptadecoic acid; N-Heptadecylic acid; Heptadecanoate; Heptadecooate; Heptadecylate; Margarate; Margarinate; N-Heptadecanoate; N-Heptadecylic acid; Margaroate; Margaroic acid; Normal-heptadecanoate; Normal-heptadecanoic acid; Margaric acid, 1-(11)C-labeled; Margaric acid, nickel (2+) salt; Omega I-123 heptadecanoic acid; Margaric acid, potassium salt; Margaric acid, sodium salt

HMDB: HMDB0002259; HMDB02259

CAS: 506-12-7

Heptadecanoic acid is a fatty acid of exogenous (primarily ruminant) origin. Many "odd" length long chain amino acids are derived from the consumption of dairy fats (milk and meat). Heptadecanoic acid constitutes 0.61% of milk fat and 0.83% of ruminant meat fat. The content of heptadecanoic acid in the subcutaneous adipose tissue of humans appears to be a good biological marker of long-term milk fat intake in free-living individuals in populations with high consumption of dairy products. (PMID 9701185).

This compound belongs to the class of organic compounds known as long-chain fatty acids. These are fatty acids with an aliphatic tail that contains between 13 and 21 carbon atoms.

## Heptadecanoic acid -- Colorectal cancer

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## 5,6-DHET -- Introduction

SYNONYM: (+/-)5,6-dihetre; (8Z,11Z,14Z)-5,6-Dihydroxyeicosa-8,11,14-trienoic acid; (8Z,11Z,14Z)-5,6-Dihydroxyicosa-8,11,14-trienoic acid; 5,6-DiHETrE; 5,6-Dihydroxy-8Z,11Z,14Z-eicosatrienoic acid; 5,6-Dihydroxy-8Z,11Z,14Z-icosatrienoic acid; (8Z,11Z,14Z)-5,6-Dihydroxyeicosa-8,11,14-trienoate; (8Z,11Z,14Z)-5,6-Dihydroxyicosa-8,11,14-trienoate; 5,6-Dihydroxy-8Z,11Z,14Z-eicosatrienoate; 5,6-Dihydroxy-8Z,11Z,14Z-icosatrienoate

HMDB: HMDB0002343; HMDB0004675; HMDB02343; HMDB04675

CAS: 213382-49-1

5,6-DHET is an epoxide intermediate in the oxygenation of arachidonic acid by hepatic monooxygenases pathway. 5,6-DHET is the hydrolysis metabolite of cis-5(6)Epoxy-cis-8,11,14-eicosatrienoic acid by epoxide hydrolases. Many drugs, chemicals, and endogenous compounds are oxygenated in mammalian tissues and in some instances reactive and potentially toxic or carcinogenic epoxides are formed. Naturally occurring olefins may also be oxygenated by mammalian enzymes. The most well known are lipoxygenases and microsomal cytochrome P-450-linked monooxygenases. The epoxides may be chemically labile or may be enzymatically hydrolyzed. When arene or olefinic epoxides are formed by microsomal P-450-linked monooxygenases, they are often rapidly converted to less reactive trans-diols through the action of microsomal epoxide hydrolases. (PMID: 6801052, 6548162).

This compound belongs to the class of organic compounds known as hydroxyeicosatrienoic acids. These are eicosanoic acids with an attached hydroxyl group and three CC double bonds.

## Nervonic acid -- Introduction

SYNONYM: (Z)-15-Tetracosenoic acid; (Z)-Tetracos-15-enoic acid; 15cis-Tetracosenoic acid; cis-15-Tetracosenoic acid; cis-Delta(15)-Tetracosenoic acid; Nervonsaeure; Selacholeic acid; (Z)-15-Tetracosenoate; Nervonate; (Z)-Tetracos-15-enoate; 15cis-Tetracosenoate; cis-15-Tetracosenoate; cis-delta(15)-Tetracosenoate; cis-Î'(15)-tetracosenoate; cis-Î



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'(15)-tetracosenoic acid; Selacholeate; (15Z)-Tetracos-15-enoate; (15Z)-Tetracos-15-enoic acid; (15Z)-Tetracosenoate; (15Z)-Tetracosenoic acid; 15-Tetracosenoate; 15-Tetracosenoic acid; 15Z-Tetracosenoate; 15Z-Tetracosenoic acid; cis-15-Teracosenoate; cis-15-Teracosenoic acid; cis-15-Tetracosenate; cis-15-Tetracosenic acid; cis-Selacholeate; cis-Selacholeic acid; trans-Tetracos-15-enoic acid; Nervonic acid, potassium salt(Z)-isomer; Nervonic acid, sodium salt, (Z)-isomer

HMDB: HMDB0002368; HMDB02368

CAS: 506-37-6

Nervonic acid is a long chain unsaturated fatty acid that is enriched in sphingomyelin. It consists of choline, sphingosine, phosphoric acid, and fatty acid. Nervonic acid may enhance the brain functions and prevent demyelination (Chemical Land21). Research shows that there is negative relationship between nervonic acid and obesity-related risk factors (PMID: 16394593). Demyelination in adrenoleukodystrophy (ALD) is associated with an accumulation of very long chain saturated fatty acids stemming from a genetic defect in the peroxisomal beta oxidation system responsible for the chain shortening of these fatty acids. Sphingolipids from post mortem ALD brain have decreased levels of nervonic acid, 24:1(n-9), and increased levels of stearic acid, 18:0. (PMID: 8072429).

This compound belongs to the class of organic compounds known as very long-chain fatty acids. These are fatty acids with an aliphatic tail that contains at least 22 carbon atoms.

### Nervonic acid -- Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. *Tohoku J Exp Med.* 1995 May;176(1):61-8. PMID: 7482520

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## Nervonic acid -- Isovaleric acidemia

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Krieger I, Tanaka K: Therapeutic effects of glycine in isovaleric acidemia. *Pediatr Res.* 1976 Jan;10(1):25-9. PMID: 1246461

## Cholesta-4,6-dien-3-one -- Introduction

SYNONYM: 4,6-Cholestadien-3-one; 4,6-Cholestadiene-3-one; Cholest-4,6-dien-3-one; Cholesta-4,6-diene-3-one

HMDB: HMDB0002394; HMDB02394

CAS: 566-93-8

Cholesta-4,6-dien-3-one is a product of the oxidation of cholesterol. It may be metabolized to 4-cholest-3-one and cholestanol by liver, adrenals and brain. An accumulation of cholesta-4,6-dien-3-one is found in serum of patients with cerebrotendinous xanthomatosis, and it is possible that accumulation of cholesterol in these patients is secondary to accumulation of cholesta-4,6-dien-3-one (PMID: 3557306; 16757819; 3676336).

This compound belongs to the class of organic compounds known as cholesterols and derivatives. These are



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compounds containing a 3-hydroxylated cholestane core.

## Galacturonic acid -- Introduction

SYNONYM: (2S,3R,4S,5R)-2,3,4,5-Tetrahydroxy-6-oxohexanoic acid; D-Galacturonic acid; (2S,3R,4S,5R)-2,3,4,5-Tetrahydroxy-6-oxohexanoate; Galacturonate; D-Galacturonate; DL-Galacturonic acid; D-Galactopyranuronic acid; Galacturonic acid, (D)-isomer; Galacturonic acid, (alpha-D)-isomer; Galacturonic acid, calcium, sodium salt, (D)-isomer; Galacturonic acid, monosodium salt, (D)-isomer

HMDB: HMDB0002545; HMDB0003348; HMDB02545; HMDB03348

CAS: 14982-50-4

D-Galacturonic acid is a sugar acid, the oxidized form of D-galactose. It is the main component of pectin, in which it exists as the polymer polygalacturonic acid. -- Wikipedia.

This compound belongs to the class of organic compounds known as glucuronic acid derivatives. These are compounds containing a glucuronic acid moiety (or a derivative), which consists of a glucose moiety with the C6 carbon oxidized to a carboxylic acid.

## Galacturonic acid -- Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. *Tohoku J Exp Med.* 1995 May;176(1):61-8. PMID: 7482520

Cheng Y, Xie G, Chen T, Qiu Y, Zou X, Zheng M, Tan B, Feng B, Dong T, He P, Zhao L, Zhao A, Xu LX, Zhang Y, Jia W: Distinct urinary metabolic profile of human colorectal cancer. *J Proteome Res.* 2012 Feb 3;11(2):1354-63. doi: 10.1021/pr201001a. Epub 2011 Dec 28. PMID: 22148915

Monleon D, Morales JM, Barrasa A, Lopez JA, Vazquez C, Celda B: Metabolite profiling of fecal water extracts from human colorectal cancer. *NMR Biomed.* 2009 Apr;22(3):342-8. doi: 10.1002/nbm.1345. PMID: 19006102

Weir TL, Manter DK, Sheflin AM, Barnett BA, Heuberger AL, Ryan EP: Stool microbiome and metabolome differences between colorectal cancer patients and healthy adults. *PLoS One.* 2013 Aug 6;8(8):e70803. doi: 10.1371/journal.pone.0070803. Print 2013. PMID: 23940645

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Ritchie SA, Ahiahou PW, Jayasinghe D, Heath D, Liu J, Lu Y, Jin W, Kavianpour A, Yamazaki Y, Khan AM, Hossain M, Su-Myat KK, Wood PL, Krenitsky K, Takemasa I, Miyake M, Sekimoto M, Monden M, Matsubara H, Nomura F, Goodenow DB: Reduced levels of hydroxylated, polyunsaturated ultra long-chain fatty acids in the serum of colorectal cancer patients: implications for early screening and detection. *BMC Med.* 2010 Feb 15;8:13. doi: 10.1186/1741-7015-8-13. PMID: 20156336

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Goedert JJ, Sampson JN, Moore SC, Xiao Q, Xiong X, Hayes RB, Ahn J, Shi J, Sinha R: Fecal metabolomics: assay performance and association with colorectal cancer. *Carcinogenesis.* 2014 Sep;35(9):2089-96. doi: 10.1093/carcin/bgu131. Epub 2014 Jul 18. PMID: 25037050



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Sinha R, Ahn J, Sampson JN, Shi J, Yu G, Xiong X, Hayes RB, Goedert JJ: Fecal Microbiota, Fecal Metabolome, and Colorectal Cancer Interrelations. *PLoS One*. 2016 Mar 25;11(3):e0152126. doi: 10.1371/journal.pone.0152126. eCollection 2016. PMID: 27015276

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Wang X, Wang J, Rao B, Deng L: Gut flora profiling and fecal metabolite composition of colorectal cancer patients and healthy individuals. *Exp Ther Med*. 2017 Jun;13(6):2848-2854. doi: 10.3892/etm.2017.4367. Epub 2017 Apr 20. PMID: 28587349

Silke Matysik, Caroline Ivonne Le Roy, Gerhard Liebisch, Sandrine Paule Claus. Metabolomics of fecal samples: A practical consideration. *Trends in Food Science & Technology*. Vol. 57, Part B, Nov. 2016, p.244-255: <http://www.sciencedirect.com/science/article/pii/S0924224416301984> PMID: 7482520

## N-Acetylserine -- Introduction

SYNONYM: Acetylserine; N-Acetyl-L-serine

HMDB: HMDB0002931; HMDB02931

CAS: 16354-58-8

Acetylation of the N-terminal amino acid (-NH<sub>2</sub> acetylation) is a common protein modification in eukaryotes but is rarely encountered in prokaryotes. In mammals, 80 to 90 percent of the cytosolic proteins are subjected to an irreversible, cotranslational amino acid acetylation at their N-terminus. Acetylation of the N-terminal amino acid (-NH<sub>2</sub> acetylation) is a common protein modification in eukaryotes but is rarely encountered in prokaryotes. In mammals, 80 to 90 percent of the cytosolic proteins are subjected to an irreversible, cotranslational amino acid acetylation at their N-terminus. N-acetylated proteins are catabolized in the cytosol by the ATP-ubiquitin-dependent proteasomal pathway. Several types of aminoacylases can be distinguished on the basis of substrate specificity. Aminoacylase I (ACY1; EC 3.5.1.14), the most abundant type, is a soluble homodimeric zinc binding enzyme that catalyzes the formation of free aliphatic amino acids from N-acetylated precursors. It is encoded by the aminoacylase 1 gene (ACY1) on chromosome 3p21 that comprises 15 exons (OMIM 609924). Preferred substrates of ACY1 are aliphatic amino acids with a short-chain acyl moiety, especially N-acetyl-methionine. However, ACY1 can also catalyze the reverse reaction, the synthesis of acetylated amino acids. Functional aminoacylase I is crucial in the last step in this degradation as it catalyzes the hydrolysis of N-acetylated amino acids into acetate and the free amino acid. Although N-acetylation occurs in many metabolic pathways and N-acetylated metabolites are known to accumulate in several inborn errors, such as aminoacylase I deficiency. There are only a few reports on N-acetylated amino acids detected in urine. Identification of N-acetylated amino acids by routine GC-MS may be problematic for several reasons. The major problem is linked to the identification strategy itself. Identification of an unknown compound in mass spectrometry is usually based on comparison of its spectrum against a library of reference spectra (PMID: 16465618, 16274666, 17723438).

This compound belongs to the class of organic compounds known as n-acyl-l-alpha-amino acids. These are n-acylated alpha amino acids which have the L-configuration of the alpha-carbon atom.

## N-Acetylserine -- Aminoacylase I deficiency

Van Coster RN, Gerlo EA, Giardina TG, Engelke UF, Smet JE, De Praeter CM, Meerschaut VA, De Meirlier LJ, Seneca SH, Devreese B, Leroy JG, Herga S, Perrier JP, Wevers RA, Lissens W: Aminoacylase I deficiency: a novel inborn error of metabolism. *Biochem Biophys Res Commun*. 2005 Dec 23;338(3):1322-6. Epub 2005 Nov 2. PMID: 16274666

Sass JO, Mohr V, Olbrich H, Engelke U, Horvath J, Fliegauf M, Loges NT, Schweitzer-Krantz S, Moebus R, Weiler P, Kispert A, Superti-Furga A, Wevers RA, Omran H: Mutations in ACY1, the gene encoding aminoacylase 1, cause a novel inborn error of metabolism. *Am J Hum Genet*. 2006 Mar;78(3):401-9. Epub 2006 Jan 18. PMID: 16465618



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A J, Trygg J, Gullberg J, Johansson AI, Jonsson P, Antti H, Marklund SL, Moritz T: Extraction and GC/MS analysis of the human blood plasma metabolome. *Anal Chem*. 2005 Dec 15;77(24):8086-94. PMID: 16351159

## Palmitoleic acid -- Introduction

SYNONYM: (9Z)-Hexadecenoic acid; (Z)-9-Hexadecenoic acid; (Z)-Hexadec-9-enoic acid; 16:1DEta9; 9-cis-Hexadecenoic acid; cis-9-Hexadecenoic acid; cis-Delta(9)-Hexadecenoic acid; Palmitolinoleic acid; Zoomaric acid; (9Z)-Hexadecenoate; Palmitoleate; (Z)-9-Hexadecenoate; (Z)-Hexadec-9-enoate; 9-cis-Hexadecenoate; cis-9-Hexadecenoate; cis-delta(9)-Hexadecenoate; cis- $\hat{\imath}^{\prime}$ (9)-hexadecenoate; cis- $\hat{\imath}^{\prime}$ (9)-hexadecenoic acid; Palmitolinoleate; Zoomarate; 9-Hexadecenoate; 9-Hexadecenoic acid; cis-9-Palmitoleic acid; cis-delta-9-Hexadecenoate; cis-delta-9-Hexadecenoic acid; cis-Palmitoleate; cis-Palmitoleic acid; Hexadecenoate; Hexadecenoate (N-C16:1); Hexadecenoic acid; Oleopalmitate; Oleopalmitic acid; Zoomerate; Zoomeric acid; Palmitoleic acid, (Z)-isomer; Palmitoleic acid, sodium salt, (Z)-isomer; Palmitoleic acid, (e)-isomer; Palmitoleic acid, potassium salt, (Z)-isomer; C16:1 trans-9; Palmelaidic acid

HMDB: HMDB0003229; HMDB0060082; HMDB03229; HMDB60082

CAS: 373-49-9

Palmitoleic acid, or 9-hexadecenoic acid, is an unsaturated fatty acid that is a common constituent of the glycerides of human adipose tissue. Present in all tissues, generally found in higher concentrations in the liver. Macadamia oil (*Macadamia integrifolia*) and Sea Buckthorn oil (*Hippophae rhamnoides*) are botanical sources of palmitoleic acid, containing 22 and 40% respectively (Wikipedia). Palmitoleic acid is found to be associated with isovaleric acidemia, which is an inborn error of metabolism.

This compound belongs to the class of organic compounds known as long-chain fatty acids. These are fatty acids with an aliphatic tail that contains between 13 and 21 carbon atoms.

## Palmitoleic acid -- Cirrhosis

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Halperin G, Elisaf M, Leitersdorf E, Harats D: A new method for determination of serum cholestanol by high-performance liquid chromatography with ultraviolet detection. *J Chromatogr B Biomed Sci Appl*. 2000 Jun 9;742(2):345-52. PMID: 10901139

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Kobayashi N, Katsumata H, Uto Y, Goto J, Niwa T, Kobayashi K, Mizuuchi Y: A monoclonal antibody-based enzyme-linked immunosorbent assay of glycolithocholic acid sulfate in human urine for liver function test. *Steroids*. 2002 Sep;67(10):827-33. PMID: 12231118

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## Palmitoleic acid -- Colorectal cancer

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## Palmitoleic acid -- Isovaleric acidemia

Korman SH, Andresen BS, Zeharia A, Gutman A, Boneh A, Pitt JJ: 2-ethylhydrylic aciduria in short/branched-chain acyl-CoA dehydrogenase deficiency: application to diagnosis and implications for the R-pathway of isoleucine oxidation. *Clin Chem.* 2005 Mar;51(3):610-7. Epub 2004 Dec 22. PMID: 15615815

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Dercksen M, Kulik W, Mienie LJ, Reinecke CJ, Wanders RJ, Duran M: Polyunsaturated fatty acid status in treated isovaleric acidemia patients. *Eur J Clin Nutr.* 2016 Oct;70(10):1123-1126. doi: 10.1038/ejcn.2016.100. Epub 2016 Jun 22.



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PMID: 27329611

Krieger I, Tanaka K: Therapeutic effects of glycine in isovaleric acidemia. *Pediatr Res.* 1976 Jan;10(1):25-9. PMID: 1246461

## 1-Methylguanine -- Introduction

SYNONYM: N1-Methylguanine; 1-Methyl-(8ci)-guanine; 1-Methyl-guanine; RNA containing N1-methylguanine

HMDB: HMDB0003282; HMDB03282

CAS: 938-85-2

1-Methylguanine is a naturally occurring modified purine derived from tRNA, found in elevated levels in the serum and urine of cancer patients. (PMID: 2413515). Increase of 1-methylguanine in the urine of colorectal tumor bearing patients, has been justified either by a more rapid turnover of nucleic acids in tumor tissue or by an increase in the extent of their methylation. (PMID: 9069642).

This compound belongs to the class of organic compounds known as 6-oxopurines. These are purines that carry a C=O group at position 6. Purine is a bicyclic aromatic compound made up of a pyrimidine ring fused to an imidazole ring.

## Indole-3-carboxylic acid -- Introduction

SYNONYM: 1H-Indole-3-carboxylate; 1H-Indole-3-carboxylic acid; 3-Indole carboxylic acid; 3-Indolecarboxylate; 3-Indolecarboxylic acid; 3-Indoleformate; 3-Indoleformic acid; 3-Indolylcarboxylate; 3-Indolylcarboxylic acid; Indole - 3 carboxylate; Indole - 3 carboxylic acid; Indole-3-carboxylate; Indole-3-carboxylicacid

HMDB: HMDB0003320; HMDB03320

CAS: 771-50-6

Indole-3-carboxylic acid is a normal urinary indolic tryptophan metabolite (PMID 4844607) and has been found elevated in patients with liver diseases (PMID 13905029).

This compound belongs to the class of organic compounds known as indolecarboxylic acids and derivatives. These are compounds containing a carboxylic acid group (or a derivative thereof) linked to an indole.

## Indole-3-carboxylic acid -- Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. *Tohoku J Exp Med.* 1995 May;176(1):61-8. PMID: 7482520

Cheng Y, Xie G, Chen T, Qiu Y, Zou X, Zheng M, Tan B, Feng B, Dong T, He P, Zhao L, Zhao A, Xu LX, Zhang Y, Jia W: Distinct urinary metabolic profile of human colorectal cancer. *J Proteome Res.* 2012 Feb 3;11(2):1354-63. doi: 10.1021/pr201001a. Epub 2011 Dec 28. PMID: 22148915

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### Indole-3-carboxylic acid -- Metastatic melanoma

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### 1-Methyladenosine -- Introduction

SYNONYM: m1a; N1-Methyladenosine; N(1)-Methyladenosine

HMDB: HMDB0003331; HMDB03331

CAS: 15763-06-1

1-Methyladenosine is one of the modified nucleosides, the levels of which are elevated in the urine of patients with malignant tumours. Examination of the expression of 1-methyladenosine is expected to be useful for the histological diagnosis of intraocular tumours (PMID: 8434538).

This compound belongs to the class of organic compounds known as purine nucleosides. These are compounds comprising a purine base attached to a ribosyl or deoxyribosyl moiety.

### 1-Methyladenosine -- Cervical cancer



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### 1-Methyladenosine – Cholangiocarcinoma

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## N-Acetylornithine -- Introduction

SYNONYM: N2-Acetyl-L-ornithine; (2S)-2-acetamido-5-Aminopentanoate; (2S)-2-acetamido-5-Aminopentanoic acid; Acetyl-ornithine; AOR; N(2)-Acetyl-L-ornithine; N(delta)-Acetylornithine; N(delta)-Acetylornithine, (DL)-isomer; delta-N-Acetylornithine

HMDB: HMDB0003357; HMDB0006489; HMDB03357; HMDB06489

CAS: 6205-08-9

N-Acetylornithine is a minor component of deproteinized blood plasma of human blood. Human blood plasma contains a variable amount of acetylornithine, averaging 1.1 +/- 0.4 μmol/L (range 0.8--0.2 μmol/L). Urine contains a very small amount of acetylornithine, approximately 1 nmol/mg creatinine (1 μmol/day) (PMID: 508804).

This compound belongs to the class of organic compounds known as n-acyl-l-alpha-amino acids. These are n-acylated alpha amino acids which have the L-configuration of the alpha-carbon atom.

## D-Ornithine -- Introduction

SYNONYM: (R)-Ornithine; (2R)-2,5-Diaminopentanoate; (2R)-2,5-Diaminopentanoic acid; Ornithine

HMDB: HMDB0003374; HMDB03374

CAS: 348-66-3



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D-Ornithine is an amino acid produced in the urea cycle by the splitting off of urea from arginine. Ornithine is one of the products of the action of the enzyme arginase on L-arginine, creating urea. Therefore, ornithine is a central part of the urea cycle, which allows for the disposal of excess nitrogen.

This compound belongs to the class of organic compounds known as d-alpha-amino acids. These are alpha amino acids which have the D-configuration of the alpha-carbon atom.

## D-Ornithine – Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. *Tohoku J Exp Med.* 1995 May;176(1):61-8. PMID: 7482520

Cheng Y, Xie G, Chen T, Qiu Y, Zou X, Zheng M, Tan B, Feng B, Dong T, He P, Zhao L, Zhao A, Xu LX, Zhang Y, Jia W: Distinct urinary metabolic profile of human colorectal cancer. *J Proteome Res.* 2012 Feb 3;11(2):1354-63. doi: 10.1021/pr201001a. Epub 2011 Dec 28. PMID: 22148915

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Phua LC, Chue XP, Koh PK, Cheah PY, Ho HK, Chan EC: Non-invasive fecal metabonomic detection of colorectal cancer. *Cancer Biol Ther.* 2014 Apr;15(4):389-97. doi: 10.4161/cbt.27625. Epub 2014 Jan 14. PMID: 24424155

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Goedert JJ, Sampson JN, Moore SC, Xiao Q, Xiong X, Hayes RB, Ahn J, Shi J, Sinha R: Fecal metabolomics: assay performance and association with colorectal cancer. *Carcinogenesis.* 2014 Sep;35(9):2089-96. doi: 10.1093/carcin/bgu131. Epub 2014 Jul 18. PMID: 25037050

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Lin Y, Ma C, Liu C, Wang Z, Yang J, Liu X, Shen Z, Wu R: NMR-based fecal metabolomics fingerprinting as predictors of earlier diagnosis in patients with colorectal cancer. *Oncotarget.* 2016 May 17;7(20):29454-64. doi: 10.18632/oncotarget.8762. PMID: 27107423

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Wang X, Wang J, Rao B, Deng L: Gut flora profiling and fecal metabolite composition of colorectal cancer patients and



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Silke Matysik, Caroline Ivonne Le Roy, Gerhard Liebsch, Sandrine Paule Claus. Metabolomics of fecal samples: A practical consideration. *Trends in Food Science & Technology.* Vol. 57, Part B, Nov. 2016, p.244-255:  
<http://www.sciencedirect.com/science/article/pii/S0924224416301984> PMID: 7482520

## D-Ornithine -- Short bowel syndrome

Pita AM, Wakabayashi Y, Fernandez-Bustos MA, Virgili N, Riudor E, Soler J, Farriol M: Plasma urea-cycle-related amino acids, ammonium levels, and urinary orotic acid excretion in short-bowel patients managed with an oral diet. *Clin Nutr.* 2003 Feb;22(1):93-8. PMID: 12553956

Ellegard L, Sunesson A, Bosaeus I: High serum phytosterol levels in short bowel patients on parenteral nutrition support. *Clin Nutr.* 2005 Jun;24(3):415-20. PMID: 15896428

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## D-Proline -- Introduction

SYNONYM: (2R)-Pyrrolidine-2-carboxylic acid; (R)-2-Carboxypyrrolidine; (R)-Pyrrolidine-2-carboxylic acid; D-Proline; DPR; (2R)-Pyrrolidine-2-carboxylate; (R)-Pyrrolidine-2-carboxylate; R-2-Carboxypyrrolidine; R-Proline; Proline

HMDB: HMDB0003411; HMDB03411

CAS: 344-25-2

D-proline is an isomer of the naturally occurring amino acid, L-Proline. D-amino acids have been found in relatively high abundance in human plasma and saliva (PMID: 16480744). These amino acids may be of bacterial origin, but there is also evidence that they are endogenously produced through amino acid racemase activity (PMID: 1426150).

This compound belongs to the class of organic compounds known as proline and derivatives. These are compounds containing proline or a derivative thereof resulting from reaction of proline at the amino group or the carboxy group, or from the replacement of any hydrogen of glycine by a heteroatom.

## D-Proline -- Autosomal dominant polycystic kidney disease

Wang D, Strandgaard S, Borresen ML, Luo Z, Connors SG, Yan Q, Wilcox CS: Asymmetric dimethylarginine and lipid peroxidation products in early autosomal dominant polycystic kidney disease. *Am J Kidney Dis.* 2008 Feb;51(2):184-91. doi: 10.1053/j.ajkd.2007.09.020. PMID: 18215696

Gronwald W, Klein MS, Zeltner R, Schulze BD, Reinhold SW, Deutschmann M, Immervoll AK, Boger CA, Banas B, Eckardt KU, Oefner PJ: Detection of autosomal dominant polycystic kidney disease by NMR spectroscopic fingerprinting of urine. *Kidney Int.* 2011 Jun;79(11):1244-53. doi: 10.1038/ki.2011.30. Epub 2011 Mar 9. PMID: 21389975

## D-Glutamine -- Introduction

SYNONYM: (2R)-2,5-diamino-5-Oxopentanoic acid; (2R)-2-amino-4-Carbamoylbutanoic acid; (R)-2,5-diamino-5-Oxopentanoic acid; D-2-Aminoglutaramic acid; D-Glutamin; D-Glutaminsaeure-5-amid; DGN; (2R)-2,5-diamino-5-Oxopentanoate; (2R)-2-amino-4-Carbamoylbutanoate; (R)-2,5-diamino-5-Oxopentanoate; D-2-Aminoglutaramate; Nutrestore; L-Glutamine; D Glutamine; L Glutamine; Glutamine

HMDB: HMDB0003423; HMDB03423

CAS: 5959-95-5

D-Glutamine is a non-essential amino acid present abundantly throughout the body and is involved in many metabolic processes. It is synthesized from glutamic acid and ammonia. It is the principal carrier of nitrogen in the body and is an important energy source for many cells.



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This compound belongs to the class of organic compounds known as d-alpha-amino acids. These are alpha amino acids which have the D-configuration of the alpha-carbon atom.

## Beta-D-Galactose -- Introduction

SYNONYM: beta-D-Gal; Gal-beta; b-D-Gal;  $\hat{1}^2$ -D-gal; b-D-Galactose;  $\hat{1}^2$ -D-galactose; Gal-b; Gal- $\hat{1}^2$ ; b-Galactose; beta D-Galactose; beta-D-Galactopyranose; beta-D-Galactoside; beta-D-Galactosides; beta-delta-Galactoside; beta-delta-Galactosides; beta-Galactose; delta-Galactose

HMDB: HMDB0003449; HMDB03449

CAS: 7296-64-2

Galactose is an optical isomer of glucose. An aldohexose that occurs naturally in the D-form in lactose, cerebrosides, gangliosides, and mucoproteins. Deficiency of galactosyl-1-phosphate uridylyltransferase (Galactose-1-phosphate uridyl-transferase deficiency disease) causes an error in galactose metabolism called galactosemia, resulting in elevations of galactose in the blood. Galactose (Gal) (also called brain sugar) is a type of sugar found in dairy products, in sugar beets and other gums and mucilages. It is also synthesized by the body, where it forms part of glycolipids and glycoproteins in several tissues. It is considered a nutritive sweetener because it has food energy. Galactose is less sweet than glucose and not very water-soluble. Galactose is a monosaccharide constituent, together with glucose, of the disaccharide lactose. The hydrolysis of lactose to glucose and galactose is catalyzed by the enzyme beta-galactosidase, a lactase. In the human body, glucose is changed into galactose in order to enable the mammary glands to secrete lactose. Galactan is a polymer of the sugar galactose. It is found in hemicellulose and can be converted to galactose by hydrolysis.

This compound belongs to the class of organic compounds known as hexoses. These are monosaccharides in which the sugar unit is a six-carbon containing moiety.

## 4-Guanidinobutanoic acid -- Introduction

SYNONYM: 4-Guanidinobutanoate; 4-Guanidinobutyric acid; gamma-Guanidinobutyrate; gamma-Guanidinobutyric acid; 4-Guanidinobutyrate; g-Guanidinobutyrate; g-Guanidinobutyric acid;  $\hat{1}^3$ -guanidinobutyrate;  $\hat{1}^3$ -guanidinobutyric acid; 4-(carbamimidamido)Butanoate; 4-(carbamimidamido)Butanoic acid; gamma-Guanidinobutyrate, monosodium salt

HMDB: HMDB0003464; HMDB0005991; HMDB03464; HMDB05991

CAS: 463-00-3

4-Guanidinobutanoate is a normal metabolite present in low concentrations. Patients with hyperargininemia have an arginase deficiency which leads to blockade of the urea cycle in the last step with several clinical symptoms. Owing to the arginase deficiency this patients accumulate arginine which leads eventually to epileptogenic guanidino compounds (PMID 7752905).

This compound belongs to the class of organic compounds known as gamma amino acids and derivatives. These are amino acids having a (-NH<sub>2</sub>) group attached to the gamma carbon atom.

## 4-Guanidinobutanoic acid – Cirrhosis

Cynober LA: Plasma amino acid levels with a note on membrane transport: characteristics, regulation, and metabolic significance. Nutrition. 2002 Sep;18(9):761-6. PMID: 12297216

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Batta AK, Arora R, Salen G, Tint GS, Eskreis D, Katz S: Characterization of serum and urinary bile acids in patients with primary biliary cirrhosis by gas-liquid chromatography-mass spectrometry: effect of ursodeoxycholic acid treatment. *J Lipid Res.* 1989 Dec;30(12):1953-62. PMID: 2621422

Yonekura T, Kamata S, Wasa M, Okada A, Yamatodani A, Watanabe T, Wada H: Simultaneous determination of plasma phenethylamine, phenylethanolamine, tyramine and octopamine by high-performance liquid chromatography using derivatization with fluorescamine. *J Chromatogr.* 1988 Jun 3;427(2):320-5. PMID: 3137238

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Thornton JR, Losowsky MS: Plasma leucine enkephalin is increased in liver disease. *Gut.* 1989 Oct;30(10):1392-5. PMID: 2583565

Hahn C, Reichel C, von Bergmann K: Serum concentration of 7 alpha-hydroxycholesterol as an indicator of bile acid synthesis in humans. *J Lipid Res.* 1995 Sep;36(9):2059-66. PMID: 8558093

Tamasawa N, Tamasawa A, Takebe K: Higher levels of plasma cholesterol sulfate in patients with liver cirrhosis and hypercholesterolemia. *Lipids.* 1993 Sep;28(9):833-6. PMID: 8231659

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#### 4-Guanidinobutanoic acid – Colorectal cancer

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Ritchie SA, Ahiahonu PW, Jayasinghe D, Heath D, Liu J, Lu Y, Jin W, Kavianpour A, Yamazaki Y, Khan AM, Hossain M, Su-Myat KK, Wood PL, Krenitsky K, Takemasa I, Miyake M, Sekimoto M, Monden M, Matsubara H, Nomura F, Goodenow DB: Reduced levels of hydroxylated, polyunsaturated ultra long-chain fatty acids in the serum of colorectal cancer patients: implications for early screening and detection. *BMC Med.* 2010 Feb 15;8:13. doi: 10.1186/1741-7015-8-13. PMID: 20156336

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Lin Y, Ma C, Liu C, Wang Z, Yang J, Liu X, Shen Z, Wu R: NMR-based fecal metabolomics fingerprinting as predictors of earlier diagnosis in patients with colorectal cancer. *Oncotarget.* 2016 May 17;7(20):29454-64. doi: 10.18632/oncotarget.8762. PMID: 27107423

Brown DG, Rao S, Weir TL, O'Malia J, Bazan M, Brown RJ, Ryan EP: Metabolomics and metabolic pathway networks from human colorectal cancers, adjacent mucosa, and stool. *Cancer Metab.* 2016 Jun 6;4:11. doi: 10.1186/s40170-016-0151-y. eCollection 2016. PMID: 27275383

Wang X, Wang J, Rao B, Deng L: Gut flora profiling and fecal metabolite composition of colorectal cancer patients and healthy individuals. *Exp Ther Med.* 2017 Jun;13(6):2848-2854. doi: 10.3892/etm.2017.4367. Epub 2017 Apr 20. PMID: 28587349

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<http://www.sciencedirect.com/science/article/pii/S0924224416301984> PMID: 7482520

### 3'-AMP -- Introduction

SYNONYM: 3'-Adenosine monophosphate; 3'-Adenylic acid; Adenosine 3'-monophosphate; Adenosine 3'-phosphate; Adenosine-3'-monophosphate; AMP 3'-Phosphate; Synadenylic acid; 3'-Adenosine monophosphoric acid; 3'-Adenylate;



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Adenosine 3'-monophosphoric acid; Adenosine 3'-phosphoric acid; Adenosine-3'-monophosphoric acid; AMP 3'-Phosphoric acid; Synadenylate; Adenosine-3'-phosphate; Yeast adenylic acid; 2' Adenylic acid; 5' Adenylic acid; Phosphate dipotassium, adenosine; 5'-Adenylic acid; Adenylic acid; 5'-Phosphate, adenosine; Adenosine 2'-phosphate; Dipotassium, adenosine phosphate; Phosphate disodium, adenosine; Monophosphate, 2'-adenosine; 2'-AMP; 2'-Adenosine monophosphate; Adenosine 2' phosphate; Adenosine phosphate dipotassium; Adenosine 3' phosphate; Disodium, adenosine phosphate; Phosphaden; 2'-Adenylic acid; AMP; Adenosine monophosphate; Adenosine phosphate disodium; 2' Adenosine monophosphate; Acid, 2'-adenylic; Acid, 5'-adenylic; Adenosine 5' phosphate; Adenosine 5'-phosphate

HMDB: HMDB0003540; HMDB0006550; HMDB03540; HMDB06550

CAS: 84-21-9

Adenylic acid. Adenine nucleotide containing one phosphate group esterified to the sugar moiety in the 2'-, 3'-, or 5'-position.

This compound belongs to the class of organic compounds known as ribonucleoside 3'-phosphates. These are ribonucleosides that contain a phosphate group attached to the C-3 carbon of the ribose or deoxyribose moiety. The nucleobases here are limited to purine, pyrimidine, and pyridine derivatives.

## 7-Methylinosine -- Introduction

SYNONYM:

HMDB: HMDB0003950; HMDB03950

CAS: 20245-33-4

7-Methylinosine is an endogenous methylated nucleoside found in human fluids; methylated purine bases are present in higher amounts in tumor-bearing patients compared to healthy controls. DNA hypermethylation is a common finding in malignant cells and has been explored as a therapeutic target for hypomethylating agents. When a chemical bonds to DNA, the DNA becomes damaged, and proper and complete replication cannot occur to make the normal intended cell. A DNA adduct is an abnormal piece of DNA covalently-bonded to a cancer-causing chemical. This has shown to be the start of a cancerous cell, or carcinogenesis. DNA adducts in scientific experiments are used as bio-markers and as such are themselves measured to reflect quantitatively, for comparison, the amount of cancer in the subject. 7-Methylguanosine has been identified in human urine and serum. (PMID: 3506820, 17044778, 17264127, 16799933, 15906010).

This compound belongs to the class of organic compounds known as purine nucleosides. These are compounds comprising a purine base attached to a ribosyl or deoxyribosyl moiety.

## Beta-Aminopropionitrile -- Introduction

SYNONYM: 2-Cyanoethylamine; 3-Aminopropionitrile; 3-Aminopropiononitrile; Aminopropionitrile; BAPN; beta-Alaninenitrile; beta-Aminoethyl cyanide; beta-Cyanoethylamine; H<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>CN; b-Aminopropionitrile;  $\hat{I}^2$ -aminopropionitrile; b-Alaninenitrile;  $\hat{I}^2$ -alaninenitrile; b-Aminoethyl cyanide;  $\hat{I}^2$ -aminoethyl cyanide; b-Cyanoethylamine;  $\hat{I}^2$ -cyanoethylamine; 3-Aminopropanenitrile; b-Alaminenitrile; beta-Alaminenitrile; beta Aminopropionitrile

HMDB: HMDB0004101; HMDB04101

CAS: 151-18-8

beta-Aminopropionitrile is a toxic amino-acid derivative. On an unusual case of the Cantrell-sequence in a premature infant with associated dysmelia, aplasia of the right kidney, cerebellar hypoplasia and circumscribed aplasia of the cutis, maternal history suggested an occupational exposure to aminopropionitriles prior to pregnancy. The characteristic features of the Cantrell-sequence--anterior thoraco-abdominal wall defect with ectopia cordis and diaphragm, sternum, pericardium, and heart defects--have been observed in animals following maternal administration of beta-aminopropionitrile. Some species of lathyrus (chickling pea, Lathyrus sativus- related), notably Lathyrus odoratus, are unable to induce human lathyrism but contain beta-aminopropionitrile, that induces pathological changes in bone ("osteolathyrism") and blood vessels ("angiolathyrism") of experimental animals without damaging the nervous system. The administration of beta-aminopropionitrile has been proposed for pharmacological control of unwanted scar tissue in human beings. beta-Aminopropionitrile is a reagent used as an intermediate in the manufacture of beta-alanine and pantothenic acid. (PMID:



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367235 , 6422318, 9394169, Am J Perinatol. 1997 Oct;14(9):567-71.).

This compound belongs to the class of organic compounds known as nitriles. These are compounds having the structure RC#N; thus C-substituted derivatives of hydrocyanic acid, HC#N.

## Diethanolamine -- Introduction

SYNONYM: Bis-(2-hydroxy-ethyl)-amine; Diolamine; H2dEa; N,N-Di(hydroxyethyl)amine; 2,2'-Dihydroxydiethylamine; 2,2'-Iminobis; 2,2'-Iminobisethanol; 2,2'-Iminodi-1-ethanol; 2,2'-Iminodiethanol; 2,2'Iminobisethanol; 2-(2-hydroxyethylamino)Ethanol; 2-[2-Hydroxyethyl]amino]ethanol; Aliphatic amine; Bis(2-hydroxyethyl)amine; Bis(2-hydroxyethyl)tallow amine oxide; Bis(hydroxyethyl)amine; Bis-2-hydroxyethylamine; DEA; Di(2-hydroxyethyl)amine; Di(beta-hydroxyethyl)amine; Diaethanolamin; Diethanolamin; Diethyloamine; Dihydroxyethyl tallowamine oxide; Iminodiethanol; N,N'-iminodiethanol; N,N-Bis(2-hydroxyethyl)amine; N,N-Diethanolamine; Niax deoa-LF; Diethanolamine fumarate; Diethanolamine maleate; Diethanolamine sulfate (1:1); Diethanolamine sulfite; Diethanolamine hydrochloride; Diethanolamine acetate; Diethanolamine maleate (1:1); Diethanolamine phosphate; Diethanolamine sulfate (2:1); Diethanolamine sulfite (1:1)

HMDB: HMDB0004437; HMDB0003091; HMDB03091; HMDB04437

CAS: 111-42-2

Diethanolamine, often abbreviated as DEA, is an organic chemical compound which is both a secondary amine and a dialcohol. A dialcohol has two hydroxyl groups in its molecule. Like other amines, diethanolamine acts as a weak base. Diethanolamine is widely used in the preparation of diethanolamides and diethanolamine salts of long-chain fatty acids that are formulated into soaps and surfactants used in liquid laundry and dishwashing detergents, cosmetics, shampoos, and hair conditioners. Diethanolamine is also used in textile processing, in industrial gas purification to remove acid gases, as an anticorrosion agent in metalworking fluids, and in preparations of agricultural chemicals. Aqueous diethanolamine solutions are used as solvents for numerous drugs that are administered intravenously.

This compound belongs to the class of organic compounds known as 1,2-aminoalcohols. These are organic compounds containing an alkyl chain with an amine group bound to the C1 atom and an alcohol group bound to the C2 atom.

## Phytosphingosine -- Introduction

SYNONYM: 4-D-Hydroxysphinganine; 4-R-Hydroxyoctadecasphinganine; (+)-D-ribo-Phytosphingosine; 4-D-Hydroxy-sphinganine; 4D-Hydroxysphinganine; C18-Phytosphingosine; D-ribo-1,3,4-Trihydroxy-2-aminoctadecane; D-ribo-2-amino-1,3,4-Octadecanetriol; [2S-(2R\*,3R\*,4S\*)]-2-amino-1,3,4-octadecanetriol; 8-(Z-e)-C18-Phytosphingenine

HMDB: HMDB0004610; HMDB04610

CAS: 554-62-1

Phytosphingosine is a phospholipid. Phospholipids are a class of lipids and a major component of all biological membranes; sphingolipid metabolites, such as sphingosine and ceramide, are highly bioactive compounds and are involved in diverse cell processes, including cell-cell interaction, cell proliferation, differentiation, and apoptosis. Phytosphingosine is also one of the most widely distributed natural sphingoid bases, which is abundant in fungi and plants, and also found in animals including humans. Phytosphingosine is structurally similar to sphingosine; phytosphingosine possesses a hydroxyl group at C-4 of the sphingoid long-chain base. The physiological roles of phytosphingosine are largely unknown. Phytosphingosine induces apoptosis in human T-cell lymphoma and non-small cell lung cancer cells, and induces caspase-independent cytochrome c release from mitochondria. In the presence of caspase inhibitors, phytosphingosine-induced apoptosis is almost completely suppressed, suggesting that phytosphingosine-induced apoptosis is largely dependent on caspase activities. (PMID: 12576463, 12531554, 8046331, 8048941, 8706124).

This compound belongs to the class of organic compounds known as 1,3-aminoalcohols. These are organic compounds containing an alkyl chain with an amine group bound to the C1 atom and an alcohol group bound to the C3 atom.

## Phytosphingosine -- Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. Tohoku J Exp Med. 1995



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Cheng Y, Xie G, Chen T, Qiu Y, Zou X, Zheng M, Tan B, Feng B, Dong T, He P, Zhao L, Zhao A, Xu LX, Zhang Y, Jia W: Distinct urinary metabolic profile of human colorectal cancer. *J Proteome Res.* 2012 Feb 3;11(2):1354-63. doi: 10.1021/pr201001a. Epub 2011 Dec 28. PMID: 22148915

Monleon D, Morales JM, Barrasa A, Lopez JA, Vazquez C, Celda B: Metabolite profiling of fecal water extracts from human colorectal cancer. *NMR Biomed.* 2009 Apr;22(3):342-8. doi: 10.1002/nbm.1345. PMID: 19006102

Weir TL, Manter DK, Sheflin AM, Barnett BA, Heuberger AL, Ryan EP: Stool microbiome and metabolome differences between colorectal cancer patients and healthy adults. *PLoS One.* 2013 Aug 6;8(8):e70803. doi: 10.1371/journal.pone.0070803. Print 2013. PMID: 23940645

Phua LC, Chue XP, Koh PK, Cheah PY, Ho HK, Chan EC: Non-invasive fecal metabonomic detection of colorectal cancer. *Cancer Biol Ther.* 2014 Apr;15(4):389-97. doi: 10.4161/cbt.27625. Epub 2014 Jan 14. PMID: 24424155

Ritchie SA, Ahiahonu PW, Jayasinghe D, Heath D, Liu J, Lu Y, Jin W, Kavianpour A, Yamazaki Y, Khan AM, Hossain M, Su-Myat KK, Wood PL, Krenitsky K, Takemasa I, Miyake M, Sekimoto M, Monden M, Matsubara H, Nomura F, Goodenow DB: Reduced levels of hydroxylated, polyunsaturated ultra long-chain fatty acids in the serum of colorectal cancer patients: implications for early screening and detection. *BMC Med.* 2010 Feb 15;8:13. doi: 10.1186/1741-7015-8-13. PMID: 20156336

Qiu Y, Cai G, Su M, Chen T, Zheng X, Xu Y, Ni Y, Zhao A, Xu LX, Cai S, Jia W: Serum metabolite profiling of human colorectal cancer using GC-TOFMS and UPLC-QTOFMS. *J Proteome Res.* 2009 Oct;8(10):4844-50. doi: 10.1021/pr9004162. PMID: 19678709

Ni Y, Xie G, Jia W: Metabonomics of human colorectal cancer: new approaches for early diagnosis and biomarker discovery. *J Proteome Res.* 2014 Sep 5;13(9):3857-70. doi: 10.1021/pr500443c. Epub 2014 Aug 14. PMID: 25105552

Ikeda A, Nishiumi S, Shinohara M, Yoshie T, Hatano N, Okuno T, Bamba T, Fukusaki E, Takenawa T, Azuma T, Yoshida M: Serum metabolomics as a novel diagnostic approach for gastrointestinal cancer. *Biomed Chromatogr.* 2012 May;26(5):548-58. doi: 10.1002/bmc.1671. Epub 2011 Jul 20. PMID: 21773981

Goedert JJ, Sampson JN, Moore SC, Xiao Q, Xiong X, Hayes RB, Ahn J, Shi J, Sinha R: Fecal metabolomics: assay performance and association with colorectal cancer. *Carcinogenesis.* 2014 Sep;35(9):2089-96. doi: 10.1093/carcin/bgu131. Epub 2014 Jul 18. PMID: 25037050

Sinha R, Ahn J, Sampson JN, Shi J, Yu G, Xiong X, Hayes RB, Goedert JJ: Fecal Microbiota, Fecal Metabolome, and Colorectal Cancer Interrelations. *PLoS One.* 2016 Mar 25;11(3):e0152126. doi: 10.1371/journal.pone.0152126. eCollection 2016. PMID: 27015276

Lin Y, Ma C, Liu C, Wang Z, Yang J, Liu X, Shen Z, Wu R: NMR-based fecal metabolomics fingerprinting as predictors of earlier diagnosis in patients with colorectal cancer. *Oncotarget.* 2016 May 17;7(20):29454-64. doi: 10.18632/oncotarget.8762. PMID: 27107423

Brown DG, Rao S, Weir TL, O'Malia J, Bazan M, Brown RJ, Ryan EP: Metabolomics and metabolic pathway networks from human colorectal cancers, adjacent mucosa, and stool. *Cancer Metab.* 2016 Jun 6;4:11. doi: 10.1186/s40170-016-0151-y. eCollection 2016. PMID: 27275383

Wang X, Wang J, Rao B, Deng L: Gut flora profiling and fecal metabolite composition of colorectal cancer patients and healthy individuals. *Exp Ther Med.* 2017 Jun;13(6):2848-2854. doi: 10.3892/etm.2017.4367. Epub 2017 Apr 20. PMID: 28587349

Silke Matysik, Caroline Ivonne Le Roy, Gerhard Liebisch, Sandrine Paule Claus. Metabolomics of fecal samples: A practical consideration. *Trends in Food Science & Technology.* Vol. 57, Part B, Nov. 2016, p.244-255: <http://www.sciencedirect.com/science/article/pii/S0924224416301984> PMID: 7482520

## 13S-hydroxyoctadecadienoic acid -- Introduction

SYNONYM: (13S)-Hydroxyoctadecadienoic acid; (9Z, 11E)-(13S)-13-Hydroxyoctadeca-9,11-dienoic acid; (9Z,11E)-(13S)-13-Hydroxyoctadeca-9,11-dienoic acid; (13S)-Hydroxyoctadecadienoate; 13S-Hydroxyoctadecadienoate; (9Z,



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11E)-(13S)-13-Hydroxyoctadeca-9,11-dienoate; (9Z,11E)-(13S)-13-Hydroxyoctadeca-9,11-dienoate; 13(S) HODE; 13-HODE; 13-Hydroxyoctadecadienoate; 13-Hydroxyoctadecadienoic acid; 13-Hydroxy-9,11-octadecadienoic acid, (Z,e)-isomer; 13-Hydroxy-9,11-octadecadienoic acid; 13-Hydroxy-9,11-octadecadienoic acid, (e,e)-isomer; 13-Hydroxy-9,11-octadecadienoic acid, (S)-(e,Z)-isomer; 13-Hydroxy-9,11-octadecadienoic acid, (e,Z)-isomer; 13-Hydroxy-9,11-octadecadienoic acid, (R)-(e,Z)-isomer; 13-HODD; 13-LOX

HMDB: HMDB0004667; HMDB0006939; HMDB04667; HMDB06939

CAS: 5204-88-6

13-hydroxyoctadecadienoic acid (13-HODE) is synthesized in the body from linoleic acid. 13-HODE prevents cell adhesion to endothelial cells and can inhibit cancer metastasis. 13-HODE synthesis is enhanced by cyclic AMP. Gamma-linolenic acid, a desaturated metabolite of linoleic acid, causes substantial stimulation of 13-HODE synthesis. A fall in gamma-linolenic acid synthesis with age may be related to the age-related fall in 13-HODE formation. (PMID 9561154) 13-HODE is considered an intermediate in Linoleic acid metabolism(KEGG ID C14762). It is generated from 13(S)-HPODE via the enzyme lipoxygenase [EC:1.13.11.12].

This compound belongs to the class of organic compounds known as lineolic acids and derivatives. These are derivatives of lineolic acid. Lineolic acid is a polyunsaturated omega-6 18 carbon long fatty acid, with two CC double bonds at the 9- and 12-positions.

### 13S-hydroxyoctadecadienoic acid -- Autosomal dominant polycystic kidney disease

Wang D, Strandgaard S, Borresen ML, Luo Z, Connors SG, Yan Q, Wilcox CS: Asymmetric dimethylarginine and lipid peroxidation products in early autosomal dominant polycystic kidney disease. Am J Kidney Dis. 2008 Feb;51(2):184-91. doi: 10.1053/j.ajkd.2007.09.020. PMID: 18215696

Gronwald W, Klein MS, Zeltner R, Schulze BD, Reinhold SW, Deutschmann M, Immervoll AK, Boger CA, Banas B, Eckardt KU, Oefner PJ: Detection of autosomal dominant polycystic kidney disease by NMR spectroscopic fingerprinting of urine. Kidney Int. 2011 Jun;79(11):1244-53. doi: 10.1038/ki.2011.30. Epub 2011 Mar 9. PMID: 21389975

### Proline betaine -- Introduction

SYNONYM: (S)-2-carboxylato-1,1-Dimethylpyrrolidinium; N,N-Dimethyl-L-proline; Stachydrine; (2S)-2-Carboxy-1,1-dimethylpyrrolidinium; (S)-2-Carboxy-1,1-dimethylpyrrolidinium; Homostachydrine; L-Proline betaine; Prestwick-08g03; Dimethylproline; Stachydrine chloride; Stachydrine chloride, (S)-isomer; Stachydrine, (+)-isomer

HMDB: HMDB0004827; HMDB04827

CAS: 471-87-4

Proline betaine is an osmoprotective compound found in urine. It is thought to serve an osmoprotective role for the kidney. Proline betaine is a glycine betaine analogue found in many citrus foods. Elevated levels of proline betaine in human urine are found after the consumption of citrus fruits and juices (PMID: 18060588). Proline betaine is a biomarker for the consumption of citrus fruits.

This compound belongs to the class of organic compounds known as proline and derivatives. These are compounds containing proline or a derivative thereof resulting from reaction of proline at the amino group or the carboxy group, or from the replacement of any hydrogen of glycine by a heteroatom.

### Proline betaine -- Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. Tohoku J Exp Med. 1995 May;176(1):61-8. PMID: 7482520

Cheng Y, Xie G, Chen T, Qiu Y, Zou X, Zheng M, Tan B, Feng B, Dong T, He P, Zhao L, Zhao A, Xu LX, Zhang Y, Jia W: Distinct urinary metabolic profile of human colorectal cancer. J Proteome Res. 2012 Feb 3;11(2):1354-63. doi: 10.1021/pr201001a. Epub 2011 Dec 28. PMID: 22148915



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Monleon D, Morales JM, Barrasa A, Lopez JA, Vazquez C, Celda B: Metabolite profiling of fecal water extracts from human colorectal cancer. *NMR Biomed.* 2009 Apr;22(3):342-8. doi: 10.1002/nbm.1345. PMID: 19006102

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Phua LC, Chue XP, Koh PK, Cheah PY, Ho HK, Chan EC: Non-invasive fecal metabonomic detection of colorectal cancer. *Cancer Biol Ther.* 2014 Apr;15(4):389-97. doi: 10.4161/cbt.27625. Epub 2014 Jan 14. PMID: 24424155

Ritchie SA, Ahiahou PW, Jayasinghe D, Heath D, Liu J, Lu Y, Jin W, Kavianpour A, Yamazaki Y, Khan AM, Hossain M, Su-Myat KK, Wood PL, Krenitsky K, Takemasa I, Miyake M, Sekimoto M, Monden M, Matsubara H, Nomura F, Goodenow DB: Reduced levels of hydroxylated, polyunsaturated ultra long-chain fatty acids in the serum of colorectal cancer patients: implications for early screening and detection. *BMC Med.* 2010 Feb 15;8:13. doi: 10.1186/1741-7015-8-13. PMID: 20156336

Qiu Y, Cai G, Su M, Chen T, Zheng X, Xu Y, Ni Y, Zhao A, Xu LX, Cai S, Jia W: Serum metabolite profiling of human colorectal cancer using GC-TOFMS and UPLC-QTOFMS. *J Proteome Res.* 2009 Oct;8(10):4844-50. doi: 10.1021/pr9004162. PMID: 19678709

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Ikeda A, Nishiumi S, Shinohara M, Yoshie T, Hatano N, Okuno T, Bamba T, Fukusaki E, Takenawa T, Azuma T, Yoshida M: Serum metabolomics as a novel diagnostic approach for gastrointestinal cancer. *Biomed Chromatogr.* 2012 May;26(5):548-58. doi: 10.1002/bmc.1671. Epub 2011 Jul 20. PMID: 21773981

Goedert JJ, Sampson JN, Moore SC, Xiao Q, Xiong X, Hayes RB, Ahn J, Shi J, Sinha R: Fecal metabolomics: assay performance and association with colorectal cancer. *Carcinogenesis.* 2014 Sep;35(9):2089-96. doi: 10.1093/carcin/bgu131. Epub 2014 Jul 18. PMID: 25037050

Sinha R, Ahn J, Sampson JN, Shi J, Yu G, Xiong X, Hayes RB, Goedert JJ: Fecal Microbiota, Fecal Metabolome, and Colorectal Cancer Interrelations. *PLoS One.* 2016 Mar 25;11(3):e0152126. doi: 10.1371/journal.pone.0152126. eCollection 2016. PMID: 27015276

Lin Y, Ma C, Liu C, Wang Z, Yang J, Liu X, Shen Z, Wu R: NMR-based fecal metabolomics fingerprinting as predictors of earlier diagnosis in patients with colorectal cancer. *Oncotarget.* 2016 May 17;7(20):29454-64. doi: 10.18632/oncotarget.8762. PMID: 27107423

Brown DG, Rao S, Weir TL, O'Malia J, Bazan M, Brown RJ, Ryan EP: Metabolomics and metabolic pathway networks from human colorectal cancers, adjacent mucosa, and stool. *Cancer Metab.* 2016 Jun 6;4:11. doi: 10.1186/s40170-016-0151-y. eCollection 2016. PMID: 27275383

Wang X, Wang J, Rao B, Deng L: Gut flora profiling and fecal metabolite composition of colorectal cancer patients and healthy individuals. *Exp Ther Med.* 2017 Jun;13(6):2848-2854. doi: 10.3892/etm.2017.4367. Epub 2017 Apr 20. PMID: 28587349

Silke Matysik, Caroline Ivonne Le Roy, Gerhard Liebsch, Sandrine Paule Claus. Metabolomics of fecal samples: A practical consideration. *Trends in Food Science & Technology.* Vol. 57, Part B, Nov. 2016, p.244-255: <http://www.sciencedirect.com/science/article/pii/S0924224416301984> PMID: 7482520

## Pi-Methylimidazoleacetic acid -- Introduction

SYNONYM: 1-Methyl-imidazole-5-acetic acid; pros-Methylimidazoleacetic acid; 1-Methyl-imidazole-5-acetate; Pi-methylimidazoleacetate; pros-Methylimidazoleacetate; 1-Methyl-5-imidazoleacetic acid; P-MIAA

HMDB: HMDB0004988; HMDB04988

CAS: 4200-48-0

Although pi-Methylimidazoleacetic acid's isomer (1,4-Methylimidazoleacetic acid) is a known metabolite of Histamine,



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the origin of N pi-methylimidazoleacetic acid is not certain (PMID 7130180).

This compound belongs to the class of organic compounds known as imidazolyl carboxylic acids and derivatives. These are organic compounds containing a carboxylic acid chain (of at least 2 carbon atoms) linked to an imidazole ring.

## Gingerol -- Introduction

SYNONYM: 6g [6]-Gingerol; 5-Hydroxy-1-(4-hydroxy-3-methoxyphenyl)-3-decanone; 5-Hydroxy-1-(4-hydroxy-3-methoxycyclohexyl)decan-3-one; 6-Gingerol; [6]-Gingerol; (6)-Gingerol; 10-Gingerol

HMDB: HMDB0005783; HMDB05783

CAS: 58253-27-3

Gingerol, a plant polyphenol, is the active constituent of fresh ginger. Chemically, gingerol is a relative of capsaicin, the compound that gives chile peppers their spiciness. It is normally found as a pungent yellow oil, but also can form a low-melting crystalline solid.

This compound belongs to the class of organic compounds known as gingerols. These are compounds containing a gingerol moiety, which is structurally characterized by a 4-hydroxy-3-methoxyphenyl group substituted at the C6 carbon atom by a 5-hydroxy-alkane-3-one.

## Sorbitol-6-phosphate -- Introduction

SYNONYM: Hexitol 1-phosphate; Hexitol 1-phosphoric acid; Sorbitol-6-phosphoric acid; Alditol 6-phosphate; D-Mannitol, 1-(dihydrogenphosphate); D-Mannitol-6-phosphate; D-Sorbitol 6-phosphate; Glucitol-6-phosphate; Sorbitol 6-phosphate

HMDB: HMDB0005831; HMDB05831

CAS: 20479-58-7

Sorbitol 6-phosphate (Sor6P) is an intermediate in sorbitol biosynthesis. It is a competitive inhibitor for both cytosolic and chloroplastic PGIs with a K(i) of 61 and 40muM, respectively. PMID: 18242768.

This compound belongs to the class of organic compounds known as monosaccharide phosphates. These are monosaccharides comprising a phosphated group linked to the carbohydrate unit.

## Sorbitol-6-phosphate -- Prostate cancer

Sreekumar A, Poisson LM, Rajendiran TM, Khan AP, Cao Q, Yu J, Laxman B, Mehra R, Lonigro RJ, Li Y, Nyati MK, Ahsan A, Kalyana-Sundaram S, Han B, Cao X, Byun J, Omenn GS, Ghosh D, Pennathur S, Alexander DC, Berger A, Shuster JR, Wei JT, Varambally S, Beecher C, Chinaiyan AM: Metabolomic profiles delineate potential role for sarcosine in prostate cancer progression. *Nature*. 2009 Feb 12;457(7231):910-4. doi: 10.1038/nature07762. PMID: 19212411

Nyman DW, Suzanne Stratton M, Kopplin MJ, Dalkin BL, Nagle RB, Jay Gandolfi A: Selenium and selenomethionine levels in prostate cancer patients. *Cancer Detect Prev*. 2004;28(1):8-16. PMID: 15041072

Key TJ, Appleby PN, Allen NE, Travis RC, Roddam AW, Jenab M, Egevad L, Tjonneland A, Johnsen NF, Overvad K, Linseisen J, Rohrmann S, Boeing H, Pischon T, Psaltopoulou T, Trichopoulou A, Trichopoulos D, Palli D, Vineis P, Tumino R, Berrino F, Kiemeney L, Bueno-de-Mesquita HB, Quiros JR, Gonzalez CA, Martinez C, Larranaga N, Chirlaque MD, Ardanaz E, Stattin P, Hallmans G, Khaw KT, Bingham S, Slimani N, Ferrari P, Rinaldi S, Riboli E: Plasma carotenoids, retinol, and tocopherols and the risk of prostate cancer in the European Prospective Investigation into Cancer and Nutrition study. *Am J Clin Nutr*. 2007 Sep;86(3):672-81. PMID: 17823432

Puah CM, Williams G, Ghanadian R: Urinary unconjugated 5 alpha-androstane-3 alpha, 17 beta-diol in patients with prostatic tumours. *Urol Res*. 1982;10(2):81-4. PMID: 6180540

Thysell E, Surowiec I, Hornberg E, Crnalic S, Widmark A, Johansson AI, Stattin P, Bergh A, Moritz T, Antti H, Wikstrom P: Metabolomic characterization of human prostate cancer bone metastases reveals increased levels of cholesterol. *PLoS One*. 2010 Dec 3;5(12):e14175. doi: 10.1371/journal.pone.0014175. PMID: 21151972



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Soliman LC, Hui Y, Hewavitharana AK, Chen DD: Monitoring potential prostate cancer biomarkers in urine by capillary electrophoresis-tandem mass spectrometry. *J Chromatogr A.* 2012 Dec 7;1267:162-9. doi: 10.1016/j.chroma.2012.07.021. Epub 2012 Jul 14. PMID: 22824219

Madu CO, Lu Y: Novel diagnostic biomarkers for prostate cancer. *J Cancer.* 2010 Oct 6;1:150-77. PMID: 20975847

## 8-isoprostaglandin E2 -- Introduction

SYNONYM: (5Z,8b,11a,13E,15S)-11,15-Dihydroxy-9-oxo-prosta-5,13-dien-1-Oate; (5Z,8b,11a,13E,15S)-11,15-Dihydroxy-9-oxo-prosta-5,13-dien-1-Oic acid; 7-[3-Hydroxy-2-(3-hydroxy-1-octenyl)-5-oxocyclopentyl]-5-heptenoate; 7-[3-Hydroxy-2-(3-hydroxy-1-octenyl)-5-oxocyclopentyl]-5-heptenoic acid; 8-iso-PGE2

HMDB: HMDB0005844; HMDB05844

CAS: 27415-25-4

8-isoprostaglandin E2 is an isoprostane generated from the endoperoxide intermediate 8-iso-PGH2. Isoprostanes (IsoPs) are formed in vivo from the free radical-catalyzed peroxidation of arachidonate independent of cyclooxygenase (COX). Although the structures of these compounds are very similar to COX-derived prostaglandins (PGs), an important distinction between IsoPs and PGs is that IsoP bicycloendoperoxide intermediates contain side chains that are predominantly (>90%) oriented cis in relation to the prostane ring because the generation of these intermediates is favored kinetically. In contrast to other types of prostanoids, E2/D2-IsoPs are beta-hydroxyketone-containing compounds that can undergo reversible keto-enol tautomerization under both acidic and basic conditions, allowing rearrangement of the side chains that are initially cis to the more stable trans-configuration (PMID: 12746435). Dinoprostone is a naturally occurring prostaglandin E2 (PGE2) and the most common and most biologically active of the mammalian prostaglandins. It has important effects in labour and also stimulates osteoblasts to release factors which stimulate bone resorption by osteoclasts (a type of bone cell that removes bone tissue by removing the bone's mineralized matrix). PGE2 has been shown to increase vasodilation and cAMP production, to enhance the effects of bradykinin and histamine, to induce uterine contractions and to activate platelet aggregation. PGE2 is also responsible for maintaining the open passageway of the fetal ductus arteriosus; decreasing T-cell proliferation and lymphocyte migration and activating the secretion of IL-1alpha and IL-2. PGE2 exhibits both pro- and anti-inflammatory effects, particularly on dendritic cells (DC). Depending on the nature of maturation signals, PGE2 has different and sometimes opposite effects on DC biology. PGE2 exerts an inhibitory action, reducing the maturation of DC and their ability to present antigen. PGE2 has also been shown to stimulate DC and promote IL-12 production when given in combination with TNF-alpha. PGE2 is an environmentally bioactive substance. Its action is prolonged and sustained by other factors especially IL-10. It modulates the activities of professional DC by acting on their differentiation, maturation and their ability to secrete cytokines. PGE2 is a potent inducer of IL-10 in bone marrow-derived DC (BM-DC), and PGE2-induced IL-10 is a key regulator of the BM-DC pro-inflammatory phenotype. (PMID: 16978535) Prostaglandins are eicosanoids. The eicosanoids consist of the prostaglandins (PGs), thromboxanes (TXs), leukotrienes (LTs) and lipoxins (LXs). The PGs and TXs are collectively identified as prostanoids. Prostaglandins were originally shown to be synthesized in the prostate gland, thromboxanes from platelets (thrombocytes) and leukotrienes from leukocytes, hence the derivation of their names. All mammalian cells except erythrocytes synthesize eicosanoids. These molecules are extremely potent, able to cause profound physiological effects at very dilute concentrations. All eicosanoids function locally at the site of synthesis, through receptor-mediated G-protein linked signaling pathways.

This compound belongs to the class of organic compounds known as prostaglandins and related compounds. These are unsaturated carboxylic acids consisting of a 20 carbon skeleton that also contains a five member ring, and are based upon the fatty acid arachidonic acid.

## O-Phosphotyrosine -- Introduction

SYNONYM: O-phospho-L-Tyrosine; O-phosphono-L-Tyrosine; Phosphonotyrosine; Phosphotyrosine; Tyrosine phosphate; Tyrosine phosphoric acid; L-Phosphotyrosine; L-3-(4-Hydroxyphenyl)alanine 4'-phosphate; L-Tyrosine-O-phosphate; phospho-L-Tyrosine; Phosphotyrosine (py); Tyrosine O-phosphate; Tyrosine O phosphate; Tyrosine-O-phosphate

HMDB: HMDB0006049; HMDB06049

CAS:

O-Phosphotyrosine is a phosphorylated amino acid that occurs in a number of proteins. Tyrosine phosphorylation and



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dephosphorylation plays a role in cellular signal transduction and possibly in cell growth control and carcinogenesis. Small amounts of free phosphotyrosine can be found in urine (PMID: 7693088). Levels of this amino acid appear to be elevated in mammalian urine during liver regeneration (PMID: 7516161). Phosphotyrosine is also able to induce platelet aggregation in vitro and it has been suggested that free phosphotyrosine in blood could be meaningful for in vivo platelet activation (PMID: 1282059).

This compound belongs to the class of organic compounds known as phenylalanine and derivatives. These are compounds containing phenylalanine or a derivative thereof resulting from reaction of phenylalanine at the amino group or the carboxy group, or from the replacement of any hydrogen of glycine by a heteroatom.

### trans-Hexadec-2-enoyl carnitine -- Introduction

SYNONYM: trans-2-Hexadecenoyl-carnitine; (2E)-Hexadecenoyl-carnitine

HMDB: HMDB0006317; HMDB06317

CAS:

trans-Hexadec-2-enoyl carnitine is an acylcarnitine. Numerous disorders have been described that lead to disturbances in energy production and in intermediary metabolism in the organism which are characterized by the production and excretion of unusual acylcarnitines. A mutation in the gene coding for carnitine-acylcarnitine translocase or the OCTN2 transporter aetiologically causes a carnitine deficiency that results in poor intestinal absorption of dietary L-carnitine, its impaired reabsorption by the kidney and, consequently, in increased urinary loss of L-carnitine. Determination of the qualitative pattern of acylcarnitines can be of diagnostic and therapeutic importance. The betaine structure of carnitine requires special analytical procedures for recording. The ionic nature of L-carnitine causes a high water solubility which decreases with increasing chain length of the ester group in the acylcarnitines. Therefore, the distribution of L-carnitine and acylcarnitines in various organs is defined by their function and their physico-chemical properties as well. High performance liquid chromatography (HPLC) permits screening for free and total carnitine, as well as complete quantitative acylcarnitine determination, including the long-chain acylcarnitine profile. (PMID: 17508264, Monatshefte fuer Chemie (2005), 136(8), 1279-1291., Int J Mass Spectrom. 1999;188:39-52.).

This compound belongs to the class of organic compounds known as acyl carnitines. These are organic compounds containing a fatty acid with the carboxylic acid attached to carnitine through an ester bond.

### trans-Hexadec-2-enoyl carnitine -- Very Long Chain Acyl-CoA Dehydrogenase Deficiency

Onkenhout W, Venizelos V, van der Poel PF, van den Heuvel MP, Poorthuis BJ: Identification and quantification of intermediates of unsaturated fatty acid metabolism in plasma of patients with fatty acid oxidation disorders. Clin Chem. 1995 Oct;41(10):1467-74. PMID: 7586519

Kumps A, Duez P, Mardens Y: Metabolic, nutritional, iatrogenic, and artifactual sources of urinary organic acids: a comprehensive table. Clin Chem. 2002 May;48(5):708-17. PMID: 11978597

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Costa CG, Struys EA, Bootsma A, ten Brink HJ, Dorland L, Tavares de Almeida I, Duran M, Jakobs C: Quantitative analysis of plasma acylcarnitines using gas chromatography chemical ionization mass fragmentography. J Lipid Res. 1997 Jan;38(1):173-82. PMID: 9034211

### Arachidyl carnitine -- Introduction

SYNONYM: 3-(Icosanoyloxy)-4-(trimethylammonio)butanoate; Arachidoylcarnitine; Eicosanoylcarnitine; Icosanoylcarnitine; O-Eicosanoylcarnitine; O-Icosanoylcarnitine; 3-(Icosanoyloxy)-4-(trimethylammonio)butanoic acid

HMDB: HMDB0006460; HMDB06460

CAS:

Arachidyl carnitine is an acylcarnitine. Numerous disorders have been described that lead to disturbances in energy



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production and in intermediary metabolism in the organism which are characterized by the production and excretion of unusual acylcarnitines. A mutation in the gene coding for carnitine-acylcarnitine translocase or the OCTN2 transporter aetiologically causes a carnitine deficiency that results in poor intestinal absorption of dietary L-carnitine, its impaired reabsorption by the kidney and, consequently, in increased urinary loss of L-carnitine. Determination of the qualitative pattern of acylcarnitines can be of diagnostic and therapeutic importance. The betaine structure of carnitine requires special analytical procedures for recording. The ionic nature of L-carnitine causes a high water solubility which decreases with increasing chain length of the ester group in the acylcarnitines. Therefore, the distribution of L-carnitine and acylcarnitines in various organs is defined by their function and their physico-chemical properties as well. High performance liquid chromatography (HPLC) permits screening for free and total carnitine, as well as complete quantitative acylcarnitine determination, including the long-chain acylcarnitine profile. (PMID: 17508264, Monatshefte fuer Chemie (2005), 136(8), 1279-1291., Int J Mass Spectrom. 1999;188:39-52.).

This compound belongs to the class of organic compounds known as acyl carnitines. These are organic compounds containing a fatty acid with the carboxylic acid attached to carnitine through an ester bond.

## Linoelaidyl carnitine -- Introduction

SYNONYM: 3-[(9E,12E)-Octadeca-9,12-dienoyloxy]-4-(trimethylammonio)butanoate; Acylcarnitine C18:2; 3-[(9E,12E)-Octadeca-9,12-dienoyloxy]-4-(trimethylammonio)butanoic acid

HMDB: HMDB0006461; HMDB06461

CAS:

Linoelaidyl carnitine is an acylcarnitine. Numerous disorders have been described that lead to disturbances in energy production and in intermediary metabolism in the organism which are characterized by the production and excretion of unusual acylcarnitines. A mutation in the gene coding for carnitine-acylcarnitine translocase or the OCTN2 transporter aetiologically causes a carnitine deficiency that results in poor intestinal absorption of dietary L-carnitine, its impaired reabsorption by the kidney and, consequently, in increased urinary loss of L-carnitine. Determination of the qualitative pattern of acylcarnitines can be of diagnostic and therapeutic importance. The betaine structure of carnitine requires special analytical procedures for recording. The ionic nature of L-carnitine causes a high water solubility which decreases with increasing chain length of the ester group in the acylcarnitines. Therefore, the distribution of L-carnitine and acylcarnitines in various organs is defined by their function and their physico-chemical properties as well. High performance liquid chromatography (HPLC) permits screening for free and total carnitine, as well as complete quantitative acylcarnitine determination, including the long-chain acylcarnitine profile. (PMID: 17508264, Monatshefte fuer Chemie (2005), 136(8), 1279-1291., Int J Mass Spectrom. 1999;188:39-52.).

This compound belongs to the class of organic compounds known as acyl carnitines. These are organic compounds containing a fatty acid with the carboxylic acid attached to carnitine through an ester bond.

## Linoelaidyl carnitine -- Obesity

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Modulate Gut Microbial Community Improving Insulin Sensitivity in a Human Obese Population. *J Clin Endocrinol Metab.* 2016 Jan;101(1):233-42. doi: 10.1210/jc.2015-3351. Epub 2015 Oct 27. PMID: 26505825

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## D-Aspartic acid -- Introduction

SYNONYM: (R)-2-Aminobutanedioic acid; (R)-2-Aminosuccinic acid; Aspartic acid D-form; D-Asparaginsaeure; DAS; (R)-2-Aminobutanedioate; D-Aspartate; (R)-2-Aminosuccinate; Aspartate D-form; (-)-Aspartic acid; (2R)-2-Aminobutanedioate; (2R)-2-Aminobutanedioic acid; (R)-Aspartic acid; 1-amino-1,2-Carboxyethane; Aspartic acid; D-(-)-Aspartic acid; delta-(-)-Aspartic acid; delta-Asparaginsaeure; delta-Aspartate; delta-Aspartic acid; Lopac-alpha-9256; Tocris-0213; D Aspartic acid; D Aspartate

HMDB: HMDB0006483; HMDB06483

CAS: 1783-96-6

D-Aspartic acid is the D-isomer of aspartic acid. Since its discovery in invertebrates, free D-aspartate (D-Asp) has been identified in a variety of organisms, including microorganisms, plants, and lower animals, mammals and humans. D-Asp in mammalian tissues is present in specific cells, indicating the existence of specific molecular components that regulate D-Asp levels and localization in tissues. In the rat adrenal medulla, D-Asp is closely associated with adrenaline-cells (A-cells), which account for approximately 80% of the total number of chromaffin cells in the tissue, and which make and store adrenaline. D-Asp appears to be absent from noradrenaline-cells (NA-cells), which comprise approximately 20% of the total number of chromaffin cells in the adrenal medulla, and which make and store noradrenaline. D-aspartate oxidase (EC 1.4.3.1, D-AspO), which catalyzes oxidative deamination of D-Asp, appears to be present only in NA-cells, suggesting that the lack of D-Asp in these cells is due to D-Asp oxidase-mediated metabolism of D-Asp. In the rat adrenal cortex, the distribution of D-Asp changes during development. It has been suggested that developmental changes in the localization of D-Asp reflects the participation of D-Asp in the development and maturation of steroidogenesis in rat adrenal cortical cells. D-Asp is involved in steroid hormone synthesis and secretion in mammals as well. D-Asp is synthesized intracellularly, most likely by Asp racemase (EC 5.1.1.13). Endogenous D-Asp apparently has two different intracellular localization patterns: cytoplasmic and vesicular. D-Asp release can occur through three distinct pathways: 1) spontaneous, continuous release of cytoplasmic D-Asp, which is not associated with a specific stimulus; 2) release of cytoplasmic D-Asp via a volume-sensitive organic anion channel that connects the cytoplasm and extracellular space; 3) exocytotic discharge of vesicular D-Asp. D-Asp can be released via a mechanism that involves the L-Glu transporter. D-Asp is thus apparently in dynamic flux at the cellular level to carry out its physiological function(s) in mammals. (PMID: 16755369).

This compound belongs to the class of organic compounds known as aspartic acid and derivatives. These are compounds containing an aspartic acid or a derivative thereof resulting from reaction of aspartic acid at the amino group or the carboxy group, or from the replacement of any hydrogen of glycine by a heteroatom.

## D-Aspartic acid -- Autism



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## D-Aspartic acid -- Colorectal cancer

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## D-Aspartic acid -- Crohn's disease

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## Coenzyme Q9 -- Introduction

SYNONYM: (all-e)-2,3-Dimethoxy-5-methyl-6-(3,7,11,15,19,23,27,31,35-nonamethyl-2,6,10,14,18,22,26,30,34-hexatriacontanonaenyl)-2,5-cyclohexadiene-1,4-dione; 2,3-Dimethoxy-5-methyl-6-[(2E,6E,10E,14E,18E,22E,26E,30E)-3,7,11,15,19,23,27,31,35-nonamethylhexatriaconta-2,6,10,14,18,22,26,30,34-nonaen-1-yl]-1,4-benzoquinone; CoQ9; Ubiquinone-45; 2-Methyl-3-nonaprenyl-5,6-dimethoxy-1,4-benzoquinone; Coenzyme Q(9); Coenzyme Q(sub 9); CoQ(sub 9); Ubiquinone 45; Ubiquinone 9; Ubiquinone Q(sub 9); Ubiquinone Q9; Ubiquinone-9; Ubiquinone 9, (Z,Z,Z,Z,e,e,e)



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isomer; Ubiquinone Q-9

HMDB: HMDB0006707; HMDB06707

CAS: 303-97-9

Coenzyme Q9 (CoQ9) is a normal constituent of human plasma. CoQ9 in human plasma may originate as a product of incomplete CoQ10 biosynthesis or from the diet. The estimated dietary CoQ9 intake is 0 to 1.3 umol/day, primarily from cereals and fats, but this is unreliable because many food items contain levels below the detection limit. Plasma CoQ9 increases after supplementation with CoQ10, and CoQ9 and CoQ10 are significantly correlated. (PMID: 17405953).

This compound belongs to the class of organic compounds known as ubiquinones. These are coenzyme Q derivatives containing a 5, 6-dimethoxy-3-methyl(1,4-benzoquinone) moiety to which an isoprenyl group is attached at ring position 2(or 6).

## 1-Phosphatidyl-D-myo-inositol -- Introduction

SYNONYM: (3-Phosphatidyl)-1-D-inositol; 1,2-Diacyl-sn-glycero-3-phosphoinositol; 1-Phosphatidyl-1D-myo-inositol; 1-Phosphatidyl-myo-inositol; Phosphatidyl-1D-myo-inositol; Phosphatidylinositol; Phosphoinositides; Inositol phospholipids; Phosphatidylinositol; Phospholipids, inositiide; PtdIns; Inositiide phospholipids; Inositol, phosphatidyl; Phosphoglycerides, inositol; Phospholipids, inositol; Inositol phosphoglycerides; Phosphatidyl inositol

HMDB: HMDB0006953; HMDB06953

CAS:

1-Phosphatidyl-D-myo-inositol is an intermediate in inositol phosphate metabolism (KEGG ID C04637). It is generated from 1-phosphatidyl-1D-myo-inositol-5P via the enzyme 1-phosphatidylinositol-5-phosphate 4-kinase [EC:2.7.1.149] and then converted to 1D-myo-inositol-1,4,5P3 via the enzyme 1-phosphatidylinositol-4,5-bisphosphate phosphodiesterase [EC:3.1.4.11].

This compound belongs to the class of organic compounds known as phosphatidylinositols. These are glycerophosphoinositols where the glycerol is esterified with two fatty acids.

## LyoPA(16:0/0:0) -- Introduction

SYNONYM: 1-Hexadecanoyl-sn-glycero-3-phosphate; 1-Hexadecanoyl-sn-glycero-3-phosphoric acid; 1-Palmitoylglycerol 3-phosphoric acid; 1-Palmitoyl-sn-glycerol 3-phosphate; PLPA; 1-Palmitoyl-lysophosphatidic acid; 1-Palmitoyl-lysophosphatidic acid, (R)-isomer; 1-Palmitoyl-rac-glycerol 3-phosphate; 1-Palmitoyl-lysophosphatidic acid, sodium salt, (R)-isomer; Lysophosphatidic Acid(16:0); 1-palmitoyl-glycero-3-phosphate; 1-hexadecanoyl-phosphatidic acid; LPA(16:0); LPA(16:0/0:0); 1-hexadecanoyl-glycero-3-phosphate; Lysophosphatidic Acid(16:0/0:0)

HMDB: HMDB0007853; HMDB0000327; HMDB00327; HMDB07853

CAS:

LyoPA(16:0/0:0) is a lysophosphatidic acid. It is a glycerophospholipid in which a phosphate moiety occupies a glycerol substitution site. Lysophosphatidic acids can have different combinations of fatty acids of varying lengths and saturation attached at the C-1 (sn-1) or C-2 (sn-2) position. Fatty acids containing 16 and 18 carbons are the most common. Lysophosphatidic acid is the simplest possible glycerophospholipid. It is the biosynthetic precursor of phosphatidic acid. Although it is present at very low levels only in animal tissues, it is extremely important biologically, influencing many biochemical processes. In particular, lysophosphatidic acid is an intercellular lipid mediator with growth factor-like activities, and is rapidly produced and released from activated platelets to influence target cells. 1-Palmitoyl lysophosphatidic acid is the major component of lysophosphatidic acid (LPA) in plasma, and is in a reduced ratio in individuals with gynecological cancers (PMID 11585410). LPA is a pluripotent lipid mediator controlling growth, motility, and differentiation, that has a strong influence on the chemotaxis and ultrastructure of human neutrophils (PMID 7416233). In serum and plasma, LPA is mainly converted from lysophospholipids, whereas in platelets and some cancer cells it is converted from phosphatidic acid. In each pathway, at least two phospholipase activities are required: phospholipase A1 (PLA1)/PLA2 plus lysophospholipase D (lysoPLD) activities are involved in the first pathway and phospholipase D (PLD) plus PLA1/PLA2 activities are involved in the second pathway. (PMID 15271293).



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This compound belongs to the class of organic compounds known as 1-acylglycerol-3-phosphates. These are lysophosphatidic acids where the glycerol is esterified with a fatty acid at O-1 position.

## PC(14:0/14:0) -- Introduction

**SYNONYM:** 1,2-Di-O-tetradecanoyl-sn-glycero-3-phosphocholine; 1,2-Dimyristoyl-GPC; 1,2-Dimyristoyl-L-3-phosphatidylcholine; 1,2-Dimyristoyl-sn-glycero-3-phosphocholine; 1,2-Dimyristoylphosphatidylcholine; 1,2-Ditetradecanoyl-sn-glycero-3-phosphocholine; Dimyristoyl lecithin; Dimyristoyl phosphatidylcholine; Dimyristoylphosphatidylcholine; DMPC; GPC(14:0/14:0); GPC(28:0); PC(28:0); Phosphatidylcholine(14:0/14:0); Phosphatidylcholine(28:0); 1,2 Ditetradecanoyl glycero 3 phosphocholine; 1,2-Ditetradecanoyl-glycero-3-phosphocholine; 1,2-Ditetradecyl-glycero-3-phosphocholine; DMCP; Dimyristoyllecithin; 1,2 Dimyristoyl glycero 3 phosphorylcholine; 1,2 Ditetradecyl glycero 3 phosphocholine; 1,2-Dimyristoyl-glycero-3-phosphorylcholine; Lecithin; 1,2-dimyristoyl-rac-glycero-3-phosphocholine; GPCho(28:0); PC(14:0/14:0); GPCho(14:0/14:0); 1,2-ditetradecanoyl-rac-glycero-3-phosphocholine

**HMDB:** HMDB0007866; HMDB07866

**CAS:**

PC(14:0/14:0) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(14:0/14:0), in particular, consists of two chains of myristic acid at the C-1 and C-2 positions. The myristic acid moieties are derived from nutmeg and butter. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

## PC(15:0/15:0) -- Introduction

**SYNONYM:** gpcho(15:0/15:0); gpcho(30:0); Phosphatidylcholine(15:0/15:0); DiC15-PC; Dipentadecanoylphosphatidylcholine; PC(15:0/15:0); PC(30:0); Lecithin; Phosphatidylcholine(30:0); 1,2-dipentadecanoyl-rac-glycero-3-phosphocholine

**HMDB:** HMDB0007934; HMDB07934

**CAS:**

PC(15:0/15:0) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(15:0/15:0), in particular, consists of two chains of pentadecanoic acid at the C-1 and C-2 positions. The pentadecanoic acid moieties are derived from dairy products and milk fat. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.



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## PC(15:0/15:0) -- Pregnancy

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## PC(16:0/15:0) -- Introduction

SYNONYM: 1-Palmitoyl-2-pentadecanoyl-sn-glycero-3-phosphocholine; gpcho(16:0/15:0); gpcho(31:0); Lecithin; PC(31:0); Phosphatidylcholine(16:0/15:0); Phosphatidylcholine(31:0); PC(16:0/15:0); 1-hexadecanoyl-2-pentadecanoyl-sn-glycero-3-phosphocholine

HMDB: HMDB0007967; HMDB07967

CAS:

PC(16:0/15:0) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(16:0/15:0), in particular, consists of one chain of palmitic acid at the C-1 position and one chain of pentadecanoic acid at the C-2 position. The palmitic acid moiety is derived from fish oils, milk fats, vegetable oils and animal fats, while the pentadecanoic acid moiety is derived from dairy products and milk fat. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the



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addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

## PC(16:0/P-16:0) -- Introduction

SYNONYM: Glycerophosphocholine; 1-Hexadecanoyl-2-(1Z-hexadecenyl)-sn-glycero-3-phosphocholine; Glycerophosphocholine(16:0/p-16:0); PC(16:0); gpcho(16:0); Phosphatidylcholine(16:0); gpcho(16:0/P-16:0); Phosphatidylcholine(16:0/p-16:0)

HMDB: HMDB0007994; HMDB07994

CAS:

PC(16:0/P-16:0) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(16:0/P-16:0), in particular, consists of one chain of palmitic acid at the C-1 position and one chain of plasmalogen 16:0 at the C-2 position. The palmitic acid moiety is derived from fish oils, milk fats, vegetable oils and animal fats, while the plasmalogen 16:0 moiety is derived from animal fats, liver and kidney. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC. Plasmalogens are glycerol ether phospholipids. They are of two types, alkyl ether (-O-CH<sub>2</sub>-) and alkenyl ether (-O-CH=CH-). Dihydroxyacetone phosphate (DHAP) serves as the glycerol precursor for the synthesis of plasmalogens. Three major classes of plasmalogens have been identified: choline, ethanolamine and serine derivatives. Ethanolamine plasmalogen is prevalent in myelin. Choline plasmalogen is abundant in cardiac tissue. Usually, the highest proportion of the plasmalogen form is in the ethanolamine class with rather less in choline, and commonly little or none in other phospholipids such as phosphatidylinositol. In choline plasmalogens of most tissues, a higher proportion is often of the O-alkyl rather than the O-alkenyl form, but the reverse tends to be true in heart lipids. In animal tissues, the alkyl and alkenyl moieties in both non-polar and phospholipids tend to be rather simple in composition with 16:0, 18:0 and 18:1 (double bond in position 9) predominating. Ether analogues of triacylglycerols, i.e. 1-alkyldiacyl-sn-glycerols, are present at trace levels only if at all in most animal tissues, but they can be major components of some marine lipids.

This compound belongs to the class of organic compounds known as 1-acyl,2-(1z-alkenyl)-glycerophosphocholines. These are glycerophosphocholines that carry exactly one acyl chain attached to the glycerol moiety through an ester linkage at the O1-position, and one 1Z-alkenyl chain attached through an ether linkage at the O2-position.

## PC(16:0/P-16:0) -- Pregnancy

Andreolini F, Borra C, Caccamo F, Di Corcia A, Nicoletti I, Samperi R, Improta F: Estriol and its conjugates in late pregnancy determined by extraction with Carbopack B and liquid chromatography with fluorometric detection. Clin Chem. 1985 Oct;31(10):1698-702. PMID: 2994907

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Ribar S, Mesaric M, Sedic M: Sphingoid bases as possible diagnostic parameters. Croat Med J. 2003 Apr;44(2):165-70. PMID: 12698507

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Cho K, Moon JS, Kang JH, Jang HB, Lee HJ, Park SI, Yu KS, Cho JY: Combined untargeted and targeted metabolomic profiling reveals urinary biomarkers for discriminating obese from normal-weight adolescents. *Pediatr Obes.* 2017 Apr;12(2):93-101. doi: 10.1111/ijpo.12114. Epub 2016 Feb 22. PMID: 26910390

## PC(16:1(9Z)/14:0) -- Introduction

SYNONYM: PC(16:1/14:0); GPCho(30:1); Phosphatidylcholine(16:1/14:0); PC(30:1); GPCho(16:1/14:0); Lecithin; Phosphatidylcholine(30:1); 1-palmitoleoyl-2-myristoyl-sn-glycero-3-phosphocholine; 1-(9Z-hexadecenoyl)-2-tetradecanoyl-sn-glycero-3-phosphocholine; PC(16:1(9Z)/14:0)

HMDB: HMDB0007998; HMDB07998

CAS:

PC(16:1(9Z)/14:0) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(16:1(9Z)/14:0), in particular, consists of one chain of palmitoleic acid at the C-1 position and one chain of myristic acid at the C-2 position. The palmitoleic acid moiety is derived from animal fats and vegetable oils, while the myristic acid moiety is derived from nutmeg and butter. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

## PC(16:1(9Z)/14:1(9Z)) -- Introduction

SYNONYM: 1-Palmitoleoyl-2-myristoleoyl-sn-glycero-3-phosphocholine; gpcho(16:1n7/14:1n5); gpcho(16:1W7/14:1W5); PC(16:1n7/14:1n5); PC(16:1W7/14:1W5); Phosphatidylcholine(16:1n7/14:1n5); Phosphatidylcholine(16:1W7/14:1W5); Phosphatidylcholine(16:1/14:1); Lecithin; GPCho(30:2); PC(16:1/14:1); PC(16:1(9Z)/14:1(9Z)); Phosphatidylcholine(30:2); GPCho(16:1/14:1); 1-(9Z-hexadecenoyl)-2-(9Z-tetradecenoyl)-sn-glycero-3-phosphocholine; PC(30:2)

HMDB: HMDB0007999; HMDB07999



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CAS:

PC(16:1(9Z)/14:1(9Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(16:1(9Z)/14:1(9Z)), in particular, consists of one chain of palmitoleic acid at the C-1 position and one chain of myristoleic acid at the C-2 position. The palmitoleic acid moiety is derived from animal fats and vegetable oils, while the myristoleic acid moiety is derived from milk fats. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

### PC(16:1(9Z)/14:1(9Z)) – Pregnancy

Andreolini F, Borra C, Caccamo F, Di Corcia A, Nicoletti I, Samperi R, Improta F: Estriol and its conjugates in late pregnancy determined by extraction with Carbopack B and liquid chromatography with fluorometric detection. Clin Chem. 1985 Oct;31(10):1698-702. PMID: 2994907

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Ribar S, Mesaric M, Sedic M: Sphingoid bases as possible diagnostic parameters. Croat Med J. 2003 Apr;44(2):165-70. PMID: 12698507

Khan HA, Sobki SH, Alhomida AS: Fluctuations in fasting blood glucose and serum fructosamine in pregnant women monitored on successive antenatal visits. Clin Exp Med. 2006 Oct;6(3):134-7. PMID: 17061063

Yang XL, Wu XR: The dynamic changes of several reproductive hormones during termination of early pregnancy by RU486 in combination with PG-05 in Chinese women. Adv Contracept. 1988 Dec;4(4):319-26. PMID: 3252730

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Burrows TL, Warren JM, Colyvas K, Garg ML, Collins CE: Validation of overweight children's fruit and vegetable intake using plasma carotenoids. *Obesity (Silver Spring).* 2009 Jan;17(1):162-8. doi: 10.1038/oby.2008.495. Epub 2008 Nov 6. PMID: 18997681

Reinehr T, Wolters B, Knop C, Lass N, Hellmuth C, Harder U, Peissner W, Wahl S, Grallert H, Adamski J, Illig T, Prehn C, Yu Z, Wang-Sattler R, Koletzko B: Changes in the serum metabolite profile in obese children with weight loss. *Eur J Nutr.* 2015 Mar;54(2):173-81. doi: 10.1007/s00394-014-0698-8. Epub 2014 Apr 17. PMID: 24740590

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### PC(16:1(9Z)/16:1(9Z)) -- Introduction

SYNONYM: 1,2-Di-(9Z-hexadecenoyl)-sn-glycero-3-phosphocholine; 1,2-Dipalmitoleoyl-sn-glycero-3-phosphorylcholine; Dipalmitoleoyl-L-alpha-glycerophosphorylcholine; gpcho(16:1/16:1); gpcho(16:1n7/16:1n7); gpcho(16:1W7/16:1W7); gpcho(32:2); L-Dipalmitoleyllecithin; PC 16:1(9Z)/16:1(9Z); PC(16:1/16:1); PC(16:1n7/16:1n7); PC(16:1W7/16:1W7); PC(32:2); Phosphatidylcholine(16:1/16:1); Phosphatidylcholine(16:1n7/16:1n7);

Phosphatidylcholine(16:1W7/16:1W7); Phosphatidylcholine(32:2); Dipalmitoleoyl-L-a-glycerophosphorylcholine; Dipalmitoleoyl-L-Î±-glycerophosphorylcholine; 1,2-Dipalmitoleoyl-rac-glycero-3-phosphocholine; Lecithin; PC Aa C32:2; PC(16:1(9Z)/16:1(9Z)); 1,2-di(9Z-hexadecenoyl)-rac-glycero-3-phosphocholine

HMDB: HMDB0008002; HMDB08002

CAS:

PC(16:1(9Z)/16:1(9Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(16:1(9Z)/16:1(9Z)), in particular, consists of two chains of palmitoleic acid at the C-1 and C-2 positions. The palmitoleic acid moieties are derived from animal fats and vegetable oils. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

### PC(16:1(9Z)/16:1(9Z)) – Pregnancy

Andreolini F, Borra C, Caccamo F, Di Corcia A, Nicoletti I, Samperi R, Improta F: Estriol and its conjugates in late pregnancy determined by extraction with Carbopack B and liquid chromatography with fluorometric detection. Clin Chem. 1985 Oct;31(10):1698-702. PMID: 2994907

Ball P, Emons G, Haupt O, Hoppen HO, Knuppen R: Radioimmunoassay of 2-hydroxyestrone. Steroids. 1978 Feb;31(2):249-58. PMID: 663967

Ribar S, Mesaric M, Sedic M: Sphingoid bases as possible diagnostic parameters. Croat Med J. 2003 Apr;44(2):165-70. PMID: 12698507

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Yang XL, Wu XR: The dynamic changes of several reproductive hormones during termination of early pregnancy by RU486 in combination with PG-05 in Chinese women. Adv Contracept. 1988 Dec;4(4):319-26. PMID: 3252730

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Huang PC, Kuo PL, Guo YL, Liao PC, Lee CC: Associations between urinary phthalate monoesters and thyroid hormones in pregnant women. Hum Reprod. 2007 Oct;22(10):2715-22. Epub 2007 Aug 17. PMID: 17704099

Mikkelsen TB, Osler M, Olsen SF: Validity of protein, retinol, folic acid and n-3 fatty acid intakes estimated from the food-frequency questionnaire used in the Danish National Birth Cohort. Public Health Nutr. 2006 Sep;9(6):771-8. PMID: 16925883

Shiraishi M, Haruna M, Matsuzaki M, Murayama R, Sasaki S, Murashima S: Validity and reproducibility of folate and vitamin B(12) intakes estimated from a self-administered diet history questionnaire in Japanese pregnant women. Nutr J. 2012 Mar 15;11:15. doi: 10.1186/1475-2891-11-15. PMID: 22420377

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## PC(16:1(9Z)/16:1(9Z)) -- Obesity

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Burrows TL, Warren JM, Colyvas K, Garg ML, Collins CE: Validation of overweight children's fruit and vegetable intake using plasma carotenoids. *Obesity (Silver Spring).* 2009 Jan;17(1):162-8. doi: 10.1038/oby.2008.495. Epub 2008 Nov 6. PMID: 18997681

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Wahl S, Yu Z, Kleber M, Singmann P, Holzapfel C, He Y, Mittelstrass K, Polonikov A, Prehn C, Romisch-Margl W, Adamski J, Suhre K, Grallert H, Illig T, Wang-Sattler R, Reinehr T: Childhood obesity is associated with changes in the serum metabolite profile. *Obes Facts.* 2012;5(5):660-70. doi: 10.1159/000343204. Epub 2012 Oct 4. PMID: 23108202

Cho K, Moon JS, Kang JH, Jang HB, Lee HJ, Park SI, Yu KS, Cho JY: Combined untargeted and targeted metabolomic profiling reveals urinary biomarkers for discriminating obese from normal-weight adolescents. *Pediatr Obes.* 2017



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Apr;12(2):93-101. doi: 10.1111/jpo.12114. Epub 2016 Feb 22. PMID: 26910390

## PC(16:1(9Z)/18:2(9Z,12Z)) -- Introduction

SYNONYM: 1-(9Z-Hexadecenoyl)-2-(9Z,12Z-octadecadienoyl)-sn-glycero-3-phosphocholine; gpcho(16:1/18:2); gpcho(16:1n7/18:2n6); gpcho(16:1W7/18:2W6); PC(16:1/18:2); PC(16:1n7/18:2n6); PC(16:1W7/18:2W6); Phosphatidylcholine(16:1/18:2); Phosphatidylcholine(16:1n7/18:2n6); Phosphatidylcholine(16:1W7/18:2W6); 1-palmitoleoyl-2-linoleoyl-sn-glycero-3-phosphocholine; PC(16:1(9Z)/18:2(9Z,12Z)); Lecithin; Phosphatidylcholine(34:3); GPCho(34:3); PC(34:3)

HMDB: HMDB0008006; HMDB08006

CAS:

PC(16:1(9Z)/18:2(9Z,12Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(16:1(9Z)/18:2(9Z,12Z)), in particular, consists of one chain of palmitoleic acid at the C-1 position and one chain of linoleic acid at the C-2 position. The palmitoleic acid moiety is derived from animal fats and vegetable oils, while the linoleic acid moiety is derived from seed oils. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

## PC(16:1(9Z)/18:2(9Z,12Z)) -- Pregnancy

Andreolini F, Borra C, Caccamo F, Di Corcia A, Nicoletti I, Samperi R, Improta F: Estriol and its conjugates in late pregnancy determined by extraction with Carbopack B and liquid chromatography with fluorometric detection. Clin Chem. 1985 Oct;31(10):1698-702. PMID: 2994907

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Cho K, Moon JS, Kang JH, Jang HB, Lee HJ, Park SI, Yu KS, Cho JY: Combined untargeted and targeted metabolomic profiling reveals urinary biomarkers for discriminating obese from normal-weight adolescents. *Pediatr Obes.* 2017 Apr;12(2):93-101. doi: 10.1111/jpo.12114. Epub 2016 Feb 22. PMID: 26910390

## PC(16:1(9Z)/P-18:0) -- Introduction

SYNONYM: 1-Palmitoleoyl-2-(1-enyl-stearoyl)-sn-glycero-3-phosphocholine; gpcho(16:1/18:0); gpcho(16:1n7/18:0); gpcho(16:1W7/18:0); gpcho(34:1); Lecithin; PC Aa C34:1; PC(16:1/18:0); PC(16:1n7/18:0); PC(16:1W7/18:0); PC(34:1); Phosphatidylcholine(16:1/18:0); Phosphatidylcholine(16:1n7/18:0); Phosphatidylcholine(16:1W7/18:0); Phosphatidylcholine(34:1)

HMDB: HMDB0008028; HMDB08028

CAS:

PC(16:1(9Z)/P-18:0) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(16:1(9Z)/P-18:0), in particular, consists of one chain of palmitoleic acid at the C-1 position and one chain of plasmalogen 18:0 at the C-2 position. The palmitoleic acid moiety is derived from animal fats and vegetable oils, while the plasmalogen 18:0 moiety is derived from animal fats, liver and kidney. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC. Plasmalogens are glycerol ether phospholipids. They are of two types, alkyl ether (-O-CH<sub>2</sub>-) and alkenyl ether (-O-CH=CH-). Dihydroxyacetone phosphate (DHAP) serves as the glycerol precursor for the synthesis of plasmalogens. Three major classes of plasmalogens have been identified: choline, ethanolamine and serine derivatives. Ethanolamine plasmalogen is prevalent in myelin. Choline plasmalogen is abundant in cardiac tissue. Usually, the highest proportion of the plasmalogen form is in the ethanolamine class with rather less in choline, and commonly little or none in other phospholipids such as phosphatidylinositol. In choline plasmalogens of most tissues, a higher proportion is often of the O-alkyl rather than the O-alkenyl form, but the reverse tends to be true in heart lipids. In animal tissues, the alkyl and alkenyl moieties in both non-polar and phospholipids tend to be rather simple in composition with 16:0, 18:0 and 18:1 (double bond in position 9) predominating. Ether analogues of triacylglycerols, i.e. 1-alkyldiacyl-sn-glycerols, are present at trace levels only if at all in most animal tissues, but they can be major components of some marine lipids.

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Andreolini F, Borra C, Caccamo F, Di Corcia A, Nicoletti I, Samperi R, Improta F: Estriol and its conjugates in late pregnancy determined by extraction with Carbopack B and liquid chromatography with fluorometric detection. *Clin Chem.* 1985 Oct;31(10):1698-702. PMID: 2994907

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## PC(16:1(9Z)/P-18:0) -- Obesity

Tuma P, Samcova E, Balinova P: Determination of 3-methylhistidine and 1-methylhistidine in untreated urine samples by capillary electrophoresis. *J Chromatogr B Analyt Technol Biomed Life Sci.* 2005 Jul 5;821(1):53-9. PMID: 15899597

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Vice E, Privette JD, Hickner RC, Barakat HA: Ketone body metabolism in lean and obese women. *Metabolism.* 2005 Nov;54(11):1542-5. PMID: 16253646

Brind J, Strain G, Miller L, Zumoff B, Vogelman J, Orentreich N: Obese men have elevated plasma levels of estrone sulfate. *Int J Obes.* 1990 Jun;14(6):483-6. PMID: 2401584

Driskell JA, Chrisley BM, Reynolds LK, Moak SW: Plasma B6 vitamer and plasma and urinary 4-pyridoxic acid concentrations of middle-aged obese black women. *J Chromatogr.* 1991 Aug 23;568(2):333-40. PMID: 1783639

Haro C, Montes-Borrego M, Rangel-Zuniga OA, Alcala-Diaz JF, Gomez-Delgado F, Perez-Martinez P, Delgado-Lista J, Quintana-Navarro GM, Tinahones FJ, Landa BB, Lopez-Miranda J, Camargo A, Perez-Jimenez F: Two Healthy Diets Modulate Gut Microbial Community Improving Insulin Sensitivity in a Human Obese Population. *J Clin Endocrinol Metab.* 2016 Jan;101(1):233-42. doi: 10.1210/jc.2015-3351. Epub 2015 Oct 27. PMID: 26505825



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Vioque J, Weinbrenner T, Asensio L, Castello A, Young IS, Fletcher A: Plasma concentrations of carotenoids and vitamin C are better correlated with dietary intake in normal weight than overweight and obese elderly subjects. *Br J Nutr.* 2007 May;97(5):977-86. PMID: 17408529

Burrows TL, Warren JM, Colyvas K, Garg ML, Collins CE: Validation of overweight children's fruit and vegetable intake using plasma carotenoids. *Obesity (Silver Spring).* 2009 Jan;17(1):162-8. doi: 10.1038/oby.2008.495. Epub 2008 Nov 6. PMID: 18997681

Reinehr T, Wolters B, Knop C, Lass N, Hellmuth C, Harder U, Peissner W, Wahl S, Grallert H, Adamski J, Illig T, Prehn C, Yu Z, Wang-Sattler R, Koletzko B: Changes in the serum metabolite profile in obese children with weight loss. *Eur J Nutr.* 2015 Mar;54(2):173-81. doi: 10.1007/s00394-014-0698-8. Epub 2014 Apr 17. PMID: 24740590

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Cho K, Moon JS, Kang JH, Jang HB, Lee HJ, Park SI, Yu KS, Cho JY: Combined untargeted and targeted metabolomic profiling reveals urinary biomarkers for discriminating obese from normal-weight adolescents. *Pediatr Obes.* 2017 Apr;12(2):93-101. doi: 10.1111/jpo.12114. Epub 2016 Feb 22. PMID: 26910390

## PC(18:1(9Z)/14:1(9Z)) -- Introduction

SYNONYM: PC(32:2); PC(18:1(9Z)/14:1(9Z)); Lecithin; Phosphatidylcholine(32:2); GPCho(18:1/14:1); PC(18:1/14:1); GPCho(32:2); 1-oleoyl-2-myristoleoyl-sn-glycero-3-phosphocholine; 1-(9Z-octadecenoyl)-2-(9Z-tetradecenoyl)-sn-glycero-3-phosphocholine; Phosphatidylcholine(18:1/14:1)

HMDB: HMDB0008098; HMDB08098

CAS:

PC(18:1(9Z)/14:1(9Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(18:1(9Z)/14:1(9Z)), in particular, consists of one chain of oleic acid at the C-1 position and one chain of myristoleic acid at the C-2 position. The oleic acid moiety is derived from vegetable oils, especially olive and canola oil, while the myristoleic acid moiety is derived from milk fats. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

## PC(18:1(9Z)/14:1(9Z)) -- Pregnancy

Andreolini F, Borra C, Caccamo F, Di Corcia A, Nicoletti I, Samperi R, Improta F: Estriol and its conjugates in late pregnancy determined by extraction with Carbopack B and liquid chromatography with fluorometric detection. *Clin Chem.* 1985 Oct;31(10):1698-702. PMID: 2994907

Ball P, Emons G, Haupt O, Hoppen HO, Knuppen R: Radioimmunoassay of 2-hydroxyestrone. *Steroids.* 1978 Feb;31(2):249-58. PMID: 663967

Ribar S, Mesarić M, Sedić M: Sphingoid bases as possible diagnostic parameters. *Croat Med J.* 2003 Apr;44(2):165-70. PMID: 12698507

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Yang YJ, Lee J, Choi MH, Chung BC: Direct determination of estriol 3- and 16-glucuronides in pregnancy urine by column-switching liquid chromatography with electrospray tandem mass spectrometry. *Biomed Chromatogr.* 2003 Jun;17(4):219-25. PMID: 12833386

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Mikkelsen TB, Osler M, Olsen SF: Validity of protein, retinol, folic acid and n-3 fatty acid intakes estimated from the food-frequency questionnaire used in the Danish National Birth Cohort. *Public Health Nutr.* 2006 Sep;9(6):771-8. PMID: 16925883

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Bahado-Singh RO, Akolekar R, Chelliah A, Mandal R, Dong E, Kruger M, Wishart DS, Nicolaides K: Metabolomic analysis for first-trimester trisomy 18 detection. *Am J Obstet Gynecol.* 2013 Jul;209(1):65.e1-9. doi: 10.1016/j.ajog.2013.03.028. Epub 2013 Mar 25. PMID: 23535240

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## PC(18:1(9Z)/14:1(9Z)) -- Obesity

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Serlie MJ, Meijer AJ, Groener JE, Duran M, Endert E, Fliers E, Aerts JM, Sauerwein HP: Short-term manipulation of plasma free fatty acids does not change skeletal muscle concentrations of ceramide and glucosylceramide in lean and overweight subjects. *J Clin Endocrinol Metab.* 2007 Apr;92(4):1524-9. Epub 2007 Jan 30. PMID: 17264178

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Driskell JA, Chrisley BM, Reynolds LK, Moak SW: Plasma B6 vitamer and plasma and urinary 4-pyridoxic acid concentrations of middle-aged obese black women. *J Chromatogr.* 1991 Aug 23;568(2):333-40. PMID: 1783639

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Vioque J, Weinbrenner T, Asensio L, Castello A, Young IS, Fletcher A: Plasma concentrations of carotenoids and vitamin C are better correlated with dietary intake in normal weight than overweight and obese elderly subjects. *Br J Nutr.* 2007 May;97(5):977-86. PMID: 17408529

Burrows TL, Warren JM, Colyvas K, Garg ML, Collins CE: Validation of overweight children's fruit and vegetable intake using plasma carotenoids. *Obesity (Silver Spring).* 2009 Jan;17(1):162-8. doi: 10.1038/oby.2008.495. Epub 2008 Nov 6. PMID: 18997681

Reinehr T, Wolters B, Knop C, Lass N, Hellmuth C, Harder U, Peissner W, Wahl S, Grallert H, Adamski J, Illig T, Prehn C, Yu Z, Wang-Sattler R, Koletzko B: Changes in the serum metabolite profile in obese children with weight loss. *Eur J Nutr.* 2015 Mar;54(2):173-81. doi: 10.1007/s00394-014-0698-8. Epub 2014 Apr 17. PMID: 24740590

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Cho K, Moon JS, Kang JH, Jang HB, Lee HJ, Park SI, Yu KS, Cho JY: Combined untargeted and targeted metabolomic profiling reveals urinary biomarkers for discriminating obese from normal-weight adolescents. *Pediatr Obes.* 2017 Apr;12(2):93-101. doi: 10.1111/jopo.12114. Epub 2016 Feb 22. PMID: 26910390

## PC(18:1(9Z)/18:1(11Z)) -- Introduction

**SYNONYM:** GPCho(36:2); PC(36:2); Phosphatidylcholine(36:2); GPCho(18:1/18:1); PC(18:1(9Z)/18:1(11Z)); Lecithin; 1-oleoyl-2-vaccenoyl-sn-glycero-3-phosphocholine; Phosphatidylcholine(18:1/18:1); 1-(9Z-octadecenoyl)-2-(11Z-octadecenoyl)-sn-glycero-3-phosphocholine; PC(18:1/18:1)

**HMDB:** HMDB0008103; HMDB08103

**CAS:**

PC(18:1(9Z)/18:1(11Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(18:1(9Z)/18:1(11Z)), in particular, consists of one chain of oleic acid at the C-1 position and one chain of vaccenic acid at the C-2 position. The oleic acid moiety is derived from vegetable oils, especially olive and canola oil, while the vaccenic acid moiety is derived from butter fat and animal fat. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

## PC(18:1(9Z)/18:1(11Z)) – Pregnancy

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Driskell JA, Chrisley BM, Reynolds LK, Moak SW: Plasma B6 vitamer and plasma and urinary 4-pyridoxic acid concentrations of middle-aged obese black women. J Chromatogr. 1991 Aug 23;568(2):333-40. PMID: 1783639

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## PC(18:1(9Z)/P-16:0) -- Introduction

SYNONYM: 1-Oleoyl-2-(1-enyl-palmitoyl)-sn-glycero-3-phosphocholine; gpcho(18:1/16:0); gpcho(18:1n9/16:0); gpcho(18:1W9/16:0); gpcho(34:1); Lecithin; PC Aa C34:1; PC(18:1/16:0); PC(18:1n9/16:0); PC(18:1W9/16:0); PC(34:1); Phosphatidylcholine(18:1/16:0); Phosphatidylcholine(18:1n9/16:0); Phosphatidylcholine(18:1W9/16:0); Phosphatidylcholine(34:1)

HMDB: HMDB0008126; HMDB08126

CAS:

PC(18:1(9Z)/P-16:0) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(18:1(9Z)/P-16:0), in particular, consists of one chain of oleic acid at the C-1 position and one chain of plasmalogen 16:0 at the C-2 position. The oleic acid moiety is derived from vegetable oils, especially olive and canola oil, while the plasmalogen 16:0 moiety is derived from animal fats, liver and kidney. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC. Plasmalogens are glycerol ether phospholipids. They are of two types, alkyl ether (-O-CH<sub>2</sub>-) and alkenyl ether (-O-CH=CH-). Dihydroxyacetone phosphate (DHAP) serves as the glycerol precursor for the synthesis of plasmalogens. Three major classes of plasmalogens have been identified: choline, ethanolamine and serine derivatives. Ethanolamine plasmalogen is prevalent in myelin. Choline plasmalogen is abundant in cardiac tissue. Usually, the highest proportion of the plasmalogen form is in the ethanolamine class with rather less in choline, and commonly little or none in other phospholipids



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such as phosphatidylinositol. In choline plasmalogens of most tissues, a higher proportion is often of the O-alkyl rather than the O-alkenyl form, but the reverse tends to be true in heart lipids. In animal tissues, the alkyl and alkenyl moieties in both non-polar and phospholipids tend to be rather simple in composition with 16:0, 18:0 and 18:1 (double bond in position 9) predominating. Ether analogues of triacylglycerols, i.e. 1-alkyldiacyl-sn-glycerols, are present at trace levels only if at all in most animal tissues, but they can be major components of some marine lipids.

This compound belongs to the class of organic compounds known as 1-acyl,2-(1z-alkenyl)-glycerophosphocholines. These are glycerophosphocholines that carry exactly one acyl chain attached to the glycerol moiety through an ester linkage at the O1-position, and one 1Z-alkenyl chain attached through an ether linkage at the O2-position.

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Cho K, Moon JS, Kang JH, Jang HB, Lee HJ, Park SI, Yu KS, Cho JY: Combined untargeted and targeted metabolomic profiling reveals urinary biomarkers for discriminating obese from normal-weight adolescents. Pediatr Obes. 2017 Apr;12(2):93-101. doi: 10.1111/jopo.12114. Epub 2016 Feb 22. PMID: 26910390

### PC(18:1(9Z)/P-18:1(11Z)) -- Introduction

SYNONYM: Glycerophosphocholine; 1-(9Z-Octadecenoyl)-2-(1Z,11Z-octadecadienyl)-sn-glycero-3-phosphocholine; Glycerophosphocholine(18:1(9Z)/p-18:1(11Z)); PC(18:2); gpcho(18:2); Phosphatidylcholine(18:2); PC(18:1/P-18:1); gpcho(18:1/P-18:1); Phosphatidylcholine(18:1/p-18:1)

HMDB: HMDB0008128; HMDB08128

CAS:

PC(18:1(9Z)/P-18:1(11Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines



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can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(18:1(9Z)/P-18:1(11Z)), in particular, consists of one chain of oleic acid at the C-1 position and one chain of plasmalogen 18:1n7 at the C-2 position. The oleic acid moiety is derived from vegetable oils, especially olive and canola oil, while the plasmalogen 18:1n7 moiety is derived from animal fats, liver and kidney. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC. Plasmalogens are glycerol ether phospholipids. They are of two types, alkyl ether (-O-CH<sub>2</sub>-) and alkenyl ether (-O-CH=CH-). Dihydroxyacetone phosphate (DHAP) serves as the glycerol precursor for the synthesis of plasmalogens. Three major classes of plasmalogens have been identified: choline, ethanolamine and serine derivatives. Ethanolamine plasmalogen is prevalent in myelin. Choline plasmalogen is abundant in cardiac tissue. Usually, the highest proportion of the plasmalogen form is in the ethanolamine class with rather less in choline, and commonly little or none in other phospholipids such as phosphatidylinositol. In choline plasmalogens of most tissues, a higher proportion is often of the O-alkyl rather than the O-alkenyl form, but the reverse tends to be true in heart lipids. In animal tissues, the alkyl and alkenyl moieties in both non-polar and phospholipids tend to be rather simple in composition with 16:0, 18:0 and 18:1 (double bond in position 9) predominating. Ether analogues of triacylglycerols, i.e. 1-alkyldiacyl-sn-glycerols, are present at trace levels only if at all in most animal tissues, but they can be major components of some marine lipids.

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## PC(18:2(9Z,12Z)/14:1(9Z)) -- Introduction

SYNONYM: PC(32:3); GPCho(18:2/14:1); Phosphatidylcholine(18:2/14:1); 1-linoleoyl-2-myristoleoyl-sn-glycero-3-phosphocholine; Phosphatidylcholine(32:3); Lecithin; PC(18:2(9Z,12Z)/14:1(9Z)); GPCho(32:3); 1-(9Z,12Z-octadecadienoyl)-2-(9Z-tetradecenoyl)-sn-glycero-3-phosphocholine; PC(18:2/14:1)

HMDB: HMDB0008131; HMDB08131

CAS:

PC(18:2(9Z,12Z)/14:1(9Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(18:2(9Z,12Z)/14:1(9Z)), in particular, consists of one chain of linoleic acid at the C-1 position and one chain of myristoleic acid at the C-2 position. The linoleic acid moiety is derived from seed oils, while the myristoleic acid moiety is derived from milk fats. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

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Haro C, Montes-Borrego M, Rangel-Zuniga OA, Alcala-Diaz JF, Gomez-Delgado F, Perez-Martinez P, Delgado-Lista J, Quintana-Navarro GM, Tinahones FJ, Landa BB, Lopez-Miranda J, Camargo A, Perez-Jimenez F: Two Healthy Diets Modulate Gut Microbial Community Improving Insulin Sensitivity in a Human Obese Population. *J Clin Endocrinol Metab.* 2016 Jan;101(1):233-42. doi: 10.1210/jc.2015-3351. Epub 2015 Oct 27. PMID: 26505825

Vioque J, Weinbrenner T, Asensio L, Castello A, Young IS, Fletcher A: Plasma concentrations of carotenoids and vitamin C are better correlated with dietary intake in normal weight than overweight and obese elderly subjects. *Br J Nutr.* 2007 May;97(5):977-86. PMID: 17408529

Burrows TL, Warren JM, Colyvas K, Garg ML, Collins CE: Validation of overweight children's fruit and vegetable intake using plasma carotenoids. *Obesity (Silver Spring).* 2009 Jan;17(1):162-8. doi: 10.1038/oby.2008.495. Epub 2008 Nov 6. PMID: 18997681

Reinehr T, Wolters B, Knop C, Lass N, Hellmuth C, Harder U, Peissner W, Wahl S, Grallert H, Adamski J, Illig T, Prehn C, Yu Z, Wang-Sattler R, Koletzko B: Changes in the serum metabolite profile in obese children with weight loss. *Eur J Nutr.* 2015 Mar;54(2):173-81. doi: 10.1007/s00394-014-0698-8. Epub 2014 Apr 17. PMID: 24740590

Wahl S, Yu Z, Kleber M, Singmann P, Holzapfel C, He Y, Mittelstrass K, Polonikov A, Prehn C, Romisch-Margl W, Adamski J, Suhre K, Grallert H, Illig T, Wang-Sattler R, Reinehr T: Childhood obesity is associated with changes in the



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serum metabolite profile. *Obes Facts.* 2012;5(5):660-70. doi: 10.1159/000343204. Epub 2012 Oct 4. PMID: 23108202

Cho K, Moon JS, Kang JH, Jang HB, Lee HJ, Park SI, Yu KS, Cho JY: Combined untargeted and targeted metabolomic profiling reveals urinary biomarkers for discriminating obese from normal-weight adolescents. *Pediatr Obes.* 2017 Apr;12(2):93-101. doi: 10.1111/jopo.12114. Epub 2016 Feb 22. PMID: 26910390

## PC(18:2(9Z,12Z)/15:0) -- Introduction

SYNONYM: Phosphatidylcholine(33:2); GPCho(33:2); Phosphatidylcholine(18:2/15:0); PC(33:2); GPCho(18:2/15:0); Lecithin; PC(18:2/15:0); 1-linoleoyl-2-pentadecanoyl-sn-glycero-3-phosphocholine; 1-(9Z,12Z-octadecadienoyl)-2-pentadecanoyl-sn-glycero-3-phosphocholine; PC(18:2(9Z,12Z)/15:0)

HMDB: HMDB0008132; HMDB08132

CAS:

PC(18:2(9Z,12Z)/15:0) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(18:2(9Z,12Z)/15:0), in particular, consists of one chain of linoleic acid at the C-1 position and one chain of pentadecanoic acid at the C-2 position. The linoleic acid moiety is derived from seed oils, while the pentadecanoic acid moiety is derived from dairy products and milk fat. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

## PC(18:3(6Z,9Z,12Z)/18:1(11Z)) -- Introduction

SYNONYM: PC(18:3/18:1); 1-g-linolenoyl-2-vaccenoyl-sn-glycero-3-phosphocholine; PC(18:3(6Z,9Z,12Z)/18:1(11Z)); Phosphatidylcholine(36:4); GPCho(18:3/18:1); Lecithin; PC(36:4); Phosphatidylcholine(18:3/18:1); 1-(6Z,9Z,12Z-octadecatrienoyl)-2-(11Z-octadecenoyl)-sn-glycero-3-phosphocholine; GPCho(36:4)

HMDB: HMDB0008169; HMDB08169

CAS:

PC(18:3(6Z,9Z,12Z)/18:1(11Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(18:3(6Z,9Z,12Z)/18:1(11Z)), in particular, consists of one chain of g-linolenic acid at the C-1 position and one chain of vaccenic acid at the C-2 position. The g-linolenic acid moiety is derived from animal fats, while the vaccenic acid moiety is derived from butter fat and animal fat. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

## PC(18:3(6Z,9Z,12Z)/18:1(11Z)) -- Pregnancy

Andreolini F, Borra C, Caccamo F, Di Corcia A, Nicoletti I, Samperi R, Improta F: Estriol and its conjugates in late



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Ribar S, Mesaric M, Sedic M: Sphingoid bases as possible diagnostic parameters. Croat Med J. 2003 Apr;44(2):165-70. PMID: 12698507

Khan HA, Sobki SH, Alhomida AS: Fluctuations in fasting blood glucose and serum fructosamine in pregnant women monitored on successive antenatal visits. Clin Exp Med. 2006 Oct;6(3):134-7. PMID: 17061063

Yang XL, Wu XR: The dynamic changes of several reproductive hormones during termination of early pregnancy by RU486 in combination with PG-05 in Chinese women. Adv Contracept. 1988 Dec;4(4):319-26. PMID: 3252730

Yang YJ, Lee J, Choi MH, Chung BC: Direct determination of estriol 3- and 16-glucuronides in pregnancy urine by column-switching liquid chromatography with electrospray tandem mass spectrometry. Biomed Chromatogr. 2003 Jun;17(4):219-25. PMID: 12833386

Huang PC, Kuo PL, Guo YL, Liao PC, Lee CC: Associations between urinary phthalate monoesters and thyroid hormones in pregnant women. Hum Reprod. 2007 Oct;22(10):2715-22. Epub 2007 Aug 17. PMID: 17704099

Mikkelsen TB, Osler M, Olsen SF: Validity of protein, retinol, folic acid and n-3 fatty acid intakes estimated from the food-frequency questionnaire used in the Danish National Birth Cohort. Public Health Nutr. 2006 Sep;9(6):771-8. PMID: 16925883

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Brantsaeter AL, Haugen M, Julshamn K, Alexander J, Meltzer HM: Evaluation of urinary iodine excretion as a biomarker for intake of milk and dairy products in pregnant women in the Norwegian Mother and Child Cohort Study (MoBa). Eur J Clin Nutr. 2009 Mar;63(3):347-54. Epub 2007 Dec 5. PMID: 18059417

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### PC(18:3(6Z,9Z,12Z)/18:1(11Z)) – Obesity

Tuma P, Samcova E, Balinova P: Determination of 3-methylhistidine and 1-methylhistidine in untreated urine samples by capillary electrophoresis. J Chromatogr B Analyt Technol Biomed Life Sci. 2005 Jul 5;821(1):53-9. PMID: 15899597

Serlie MJ, Meijer AJ, Groener JE, Duran M, Endert E, Fliers E, Aerts JM, Sauerwein HP: Short-term manipulation of plasma free fatty acids does not change skeletal muscle concentrations of ceramide and glucosylceramide in lean and



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overweight subjects. *J Clin Endocrinol Metab.* 2007 Apr;92(4):1524-9. Epub 2007 Jan 30. PMID: 17264178

Vice E, Privette JD, Hickner RC, Barakat HA: Ketone body metabolism in lean and obese women. *Metabolism.* 2005 Nov;54(11):1542-5. PMID: 16253646

Brind J, Strain G, Miller L, Zumoff B, Vogelman J, Orentreich N: Obese men have elevated plasma levels of estrone sulfate. *Int J Obes.* 1990 Jun;14(6):483-6. PMID: 2401584

Driskell JA, Chrisley BM, Reynolds LK, Moak SW: Plasma B6 vitamer and plasma and urinary 4-pyridoxic acid concentrations of middle-aged obese black women. *J Chromatogr.* 1991 Aug 23;568(2):333-40. PMID: 1783639

Haro C, Montes-Borrego M, Rangel-Zuniga OA, Alcala-Diaz JF, Gomez-Delgado F, Perez-Martinez P, Delgado-Lista J, Quintana-Navarro GM, Tinahones FJ, Landa BB, Lopez-Miranda J, Camargo A, Perez-Jimenez F: Two Healthy Diets Modulate Gut Microbial Community Improving Insulin Sensitivity in a Human Obese Population. *J Clin Endocrinol Metab.* 2016 Jan;101(1):233-42. doi: 10.1210/jc.2015-3351. Epub 2015 Oct 27. PMID: 26505825

Vioque J, Weinbrenner T, Asensio L, Castello A, Young IS, Fletcher A: Plasma concentrations of carotenoids and vitamin C are better correlated with dietary intake in normal weight than overweight and obese elderly subjects. *Br J Nutr.* 2007 May;97(5):977-86. PMID: 17408529

Burrows TL, Warren JM, Colyvas K, Garg ML, Collins CE: Validation of overweight children's fruit and vegetable intake using plasma carotenoids. *Obesity (Silver Spring).* 2009 Jan;17(1):162-8. doi: 10.1038/oby.2008.495. Epub 2008 Nov 6. PMID: 18997681

Reinehr T, Wolters B, Knop C, Lass N, Hellmuth C, Harder U, Peissner W, Wahl S, Grallert H, Adamski J, Illig T, Prehn C, Yu Z, Wang-Sattler R, Koletzko B: Changes in the serum metabolite profile in obese children with weight loss. *Eur J Nutr.* 2015 Mar;54(2):173-81. doi: 10.1007/s00394-014-0698-8. Epub 2014 Apr 17. PMID: 24740590

Wahl S, Yu Z, Kleber M, Singmann P, Holzapfel C, He Y, Mittelstrass K, Polonikov A, Prehn C, Romisch-Margl W, Adamski J, Suhre K, Grallert H, Illig T, Wang-Sattler R, Reinehr T: Childhood obesity is associated with changes in the serum metabolite profile. *Obes Facts.* 2012;5(5):660-70. doi: 10.1159/000343204. Epub 2012 Oct 4. PMID: 23108202

Cho K, Moon JS, Kang JH, Jang HB, Lee HJ, Park SI, Yu KS, Cho JY: Combined untargeted and targeted metabolomic profiling reveals urinary biomarkers for discriminating obese from normal-weight adolescents. *Pediatr Obes.* 2017 Apr;12(2):93-101. doi: 10.1111/jopo.12114. Epub 2016 Feb 22. PMID: 26910390

## PC(18:3(9Z,12Z,15Z)/14:1(9Z)) -- Introduction

SYNONYM: Phosphatidylcholine(18:3/14:1); GPCho(32:4); PC(18:3(9Z,12Z,15Z)/14:1(9Z)); PC(32:4); GPCho(18:3/14:1); Lecithin; PC(18:3/14:1); 1-a-linolenoyl-2-myristoleoyl-sn-glycero-3-phosphocholine; 1-(9Z,12Z,15Z-octadeatrienoyl)-2-(9Z-tetradecenoyl)-sn-glycero-3-phosphocholine; Phosphatidylcholine(32:4)

HMDB: HMDB0008197; HMDB08197

CAS:

PC(18:3(9Z,12Z,15Z)/14:1(9Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(18:3(9Z,12Z,15Z)/14:1(9Z)), in particular, consists of one chain of a-linolenic acid at the C-1 position and one chain of myristoleic acid at the C-2 position. The a-linolenic acid moiety is derived from seed oils, especially canola and soybean oil, while the myristoleic acid moiety is derived from milk fats. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.



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This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

## PC(18:3(9Z,12Z,15Z)/20:5(5Z,8Z,11Z,14Z,17Z)) -- Introduction

SYNONYM: Phosphatidylcholine(18:3/20:5); PC(18:3(9Z,12Z,15Z)/20:5(5Z,8Z,11Z,14Z,17Z)); PC(38:8); GPCho(18:3/20:5); Lecithin; PC(18:3/20:5); 1-a-linolenoyl-2-eicosapentaenoyl-sn-glycero-3-phosphocholine; Phosphatidylcholine(38:8); 1-(9Z,12Z,15Z-octadecatrienoyl)-2-(5Z,8Z,11Z,14Z,17Z-eicosapentaenoyl)-sn-glycero-3-phosphocholine; GPCho(38:8)

HMDB: HMDB0008215; HMDB08215

CAS:

PC(18:3(9Z,12Z,15Z)/20:5(5Z,8Z,11Z,14Z,17Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(18:3(9Z,12Z,15Z)/20:5(5Z,8Z,11Z,14Z,17Z)), in particular, consists of one chain of a-linolenic acid at the C-1 position and one chain of eicosapentaenoic acid at the C-2 position. The a-linolenic acid moiety is derived from seed oils, especially canola and soybean oil, while the eicosapentaenoic acid moiety is derived from fish oils, liver and kidney. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

## PC(18:4(6Z,9Z,12Z,15Z)/18:1(11Z)) -- Introduction

SYNONYM: GPCho(36:5); Phosphatidylcholine(36:5); Lecithin; 1-stearidonoyl-2-vaccenoyl-sn-glycero-3-phosphocholine; PC(36:5); PC(18:4/18:1); GPCho(18:4/18:1); PC(18:4(6Z,9Z,12Z,15Z)/18:1(11Z)); 1-(6Z,9Z,12Z,15Z-octadecatetraenoyl)-2-(11Z-octadecenoyl)-sn-glycero-3-phosphocholine; Phosphatidylcholine(18:4/18:1)

HMDB: HMDB0008235; HMDB08235

CAS:

PC(18:4(6Z,9Z,12Z,15Z)/18:1(11Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(18:4(6Z,9Z,12Z,15Z)/18:1(11Z)), in particular, consists of one chain of stearidonic acid at the C-1 position and one chain of vaccenic acid at the C-2 position. The stearidonic acid moiety is derived from seed oils, while the vaccenic acid moiety is derived from butter fat and animal fat. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.



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## PC(18:4(6Z,9Z,12Z,15Z)/18:1(11Z)) -- Pregnancy

Andreolini F, Borra C, Caccamo F, Di Corcia A, Nicoletti I, Samperi R, Improta F: Estriol and its conjugates in late pregnancy determined by extraction with Carbopack B and liquid chromatography with fluorometric detection. Clin Chem. 1985 Oct;31(10):1698-702. PMID: 2994907

Ball P, Emons G, Haupt O, Hoppen HO, Knuppen R: Radioimmunoassay of 2-hydroxyestrone. Steroids. 1978 Feb;31(2):249-58. PMID: 663967

Ribar S, Mesaric M, Sedic M: Sphingoid bases as possible diagnostic parameters. Croat Med J. 2003 Apr;44(2):165-70. PMID: 12698507

Khan HA, Sobki SH, Alhomida AS: Fluctuations in fasting blood glucose and serum fructosamine in pregnant women monitored on successive antenatal visits. Clin Exp Med. 2006 Oct;6(3):134-7. PMID: 17061063

Yang XL, Wu XR: The dynamic changes of several reproductive hormones during termination of early pregnancy by RU486 in combination with PG-05 in Chinese women. Adv Contracept. 1988 Dec;4(4):319-26. PMID: 3252730

Yang YJ, Lee J, Choi MH, Chung BC: Direct determination of estriol 3- and 16-glucuronides in pregnancy urine by column-switching liquid chromatography with electrospray tandem mass spectrometry. Biomed Chromatogr. 2003 Jun;17(4):219-25. PMID: 12833386

Huang PC, Kuo PL, Guo YL, Liao PC, Lee CC: Associations between urinary phthalate monoesters and thyroid hormones in pregnant women. Hum Reprod. 2007 Oct;22(10):2715-22. Epub 2007 Aug 17. PMID: 17704099

Mikkelsen TB, Osler M, Olsen SF: Validity of protein, retinol, folic acid and n-3 fatty acid intakes estimated from the food-frequency questionnaire used in the Danish National Birth Cohort. Public Health Nutr. 2006 Sep;9(6):771-8. PMID: 16925883

Shiraishi M, Haruna M, Matsuzaki M, Murayama R, Sasaki S, Murashima S: Validity and reproducibility of folate and vitamin B(12) intakes estimated from a self-administered diet history questionnaire in Japanese pregnant women. Nutr J. 2012 Mar 15;11:15. doi: 10.1186/1475-2891-11-15. PMID: 22420377

Brantsaeter AL, Haugen M, Julshamn K, Alexander J, Meltzer HM: Evaluation of urinary iodine excretion as a biomarker for intake of milk and dairy products in pregnant women in the Norwegian Mother and Child Cohort Study (MoBa). Eur J Clin Nutr. 2009 Mar;63(3):347-54. Epub 2007 Dec 5. PMID: 18059417

Bahado-Singh RO, Akolekar R, Mandal R, Dong E, Xia J, Kruger M, Wishart DS, Nicolaides K: Metabolomics and first-trimester prediction of early-onset preeclampsia. J Matern Fetal Neonatal Med. 2012 Oct;25(10):1840-7. doi: 10.3109/14767058.2012.680254. Epub 2012 Apr 28. PMID: 22494326

Bahado-Singh RO, Akolekar R, Mandal R, Dong E, Xia J, Kruger M, Wishart DS, Nicolaides K: First-trimester metabolomic detection of late-onset preeclampsia. Am J Obstet Gynecol. 2013 Jan;208(1):58.e1-7. doi: 10.1016/j.ajog.2012.11.003. Epub 2012 Nov 13. PMID: 23159745

Bahado-Singh RO, Akolekar R, Mandal R, Dong E, Xia J, Kruger M, Wishart DS, Nicolaides K: Metabolomic analysis for first-trimester Down syndrome prediction. Am J Obstet Gynecol. 2013 May;208(5):371.e1-8. doi: 10.1016/j.ajog.2012.12.035. Epub 2013 Jan 8. PMID: 23313728

Bahado-Singh RO, Akolekar R, Chelliah A, Mandal R, Dong E, Kruger M, Wishart DS, Nicolaides K: Metabolomic analysis for first-trimester trisomy 18 detection. Am J Obstet Gynecol. 2013 Jul;209(1):65.e1-9. doi: 10.1016/j.ajog.2013.03.028. Epub 2013 Mar 25. PMID: 23535240

Bahado-Singh RO, Ertl R, Mandal R, Bjorndahl TC, Syngelaki A, Han B, Dong E, Liu PB, Alpay-Savasan Z, Wishart DS, Nicolaides KH: Metabolomic prediction of fetal congenital heart defect in the first trimester. Am J Obstet Gynecol. 2014 Sep;211(3):240.e1-240.e14. doi: 10.1016/j.ajog.2014.03.056. Epub 2014 Apr 1. PMID: 24704061

## PC(18:4(6Z,9Z,12Z,15Z)/18:1(11Z)) -- Obesity

Tuma P, Samcova E, Balinova P: Determination of 3-methylhistidine and 1-methylhistidine in untreated urine samples by capillary electrophoresis. J Chromatogr B Analyt Technol Biomed Life Sci. 2005 Jul 5;821(1):53-9. PMID: 15899597



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Serlie MJ, Meijer AJ, Groener JE, Duran M, Endert E, Fliers E, Aerts JM, Sauerwein HP: Short-term manipulation of plasma free fatty acids does not change skeletal muscle concentrations of ceramide and glucosylceramide in lean and overweight subjects. *J Clin Endocrinol Metab.* 2007 Apr;92(4):1524-9. Epub 2007 Jan 30. PMID: 17264178

Vice E, Privette JD, Hickner RC, Barakat HA: Ketone body metabolism in lean and obese women. *Metabolism.* 2005 Nov;54(11):1542-5. PMID: 16253646

Brind J, Strain G, Miller L, Zumoff B, Vogelman J, Orentreich N: Obese men have elevated plasma levels of estrone sulfate. *Int J Obes.* 1990 Jun;14(6):483-6. PMID: 2401584

Driskell JA, Chrisley BM, Reynolds LK, Moak SW: Plasma B6 vitamer and plasma and urinary 4-pyridoxic acid concentrations of middle-aged obese black women. *J Chromatogr.* 1991 Aug 23;568(2):333-40. PMID: 1783639

Haro C, Montes-Borrego M, Rangel-Zuniga OA, Alcala-Diaz JF, Gomez-Delgado F, Perez-Martinez P, Delgado-Lista J, Quintana-Navarro GM, Tinahones FJ, Landa BB, Lopez-Miranda J, Camargo A, Perez-Jimenez F: Two Healthy Diets Modulate Gut Microbial Community Improving Insulin Sensitivity in a Human Obese Population. *J Clin Endocrinol Metab.* 2016 Jan;101(1):233-42. doi: 10.1210/jc.2015-3351. Epub 2015 Oct 27. PMID: 26505825

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Reinehr T, Wolters B, Knop C, Lass N, Hellmuth C, Harder U, Peissner W, Wahl S, Grallert H, Adamski J, Illig T, Prehn C, Yu Z, Wang-Sattler R, Koletzko B: Changes in the serum metabolite profile in obese children with weight loss. *Eur J Nutr.* 2015 Mar;54(2):173-81. doi: 10.1007/s00394-014-0698-8. Epub 2014 Apr 17. PMID: 24740590

Wahl S, Yu Z, Kleber M, Singmann P, Holzapfel C, He Y, Mittelstrass K, Polonikov A, Prehn C, Romisch-Margl W, Adamski J, Suhre K, Grallert H, Illig T, Wang-Sattler R, Reinehr T: Childhood obesity is associated with changes in the serum metabolite profile. *Obes Facts.* 2012;5(5):660-70. doi: 10.1159/000343204. Epub 2012 Oct 4. PMID: 23108202

Cho K, Moon JS, Kang JH, Jang HB, Lee HJ, Park SI, Yu KS, Cho JY: Combined untargeted and targeted metabolomic profiling reveals urinary biomarkers for discriminating obese from normal-weight adolescents. *Pediatr Obes.* 2017 Apr;12(2):93-101. doi: 10.1111/jopo.12114. Epub 2016 Feb 22. PMID: 26910390

## PC(18:4(6Z,9Z,12Z,15Z)/18:2(9Z,12Z)) -- Introduction

SYNONYM: GPCho(18:4/18:2); Phosphatidylcholine(36:6); Phosphatidylcholine(18:4/18:2); PC(18:4/18:2); PC(18:4(6Z,9Z,12Z,15Z)/18:2(9Z,12Z)); Lecithin; 1-stearidonyl-2-linoleoyl-sn-glycero-3-phosphocholine; PC(36:6); 1-(6Z,9Z,12Z,15Z-octadecatetraenoyl)-2-(9Z,12Z-octadecadienoyl)-sn-glycero-3-phosphocholine; GPCho(36:6)

HMDB: HMDB0008237; HMDB08237

CAS:

PC(18:4(6Z,9Z,12Z,15Z)/18:2(9Z,12Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(18:4(6Z,9Z,12Z,15Z)/18:2(9Z,12Z)), in particular, consists of one chain of stearidonic acid at the C-1 position and one chain of linoleic acid at the C-2 position. The stearidonic acid moiety is derived from seed oils, while the linoleic acid moiety is derived from seed oils. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-



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diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

### PC(18:4(6Z,9Z,12Z,15Z)/18:2(9Z,12Z)) -- Pregnancy

Andreolini F, Borra C, Caccamo F, Di Corcia A, Nicoletti I, Samperi R, Improta F: Estriol and its conjugates in late pregnancy determined by extraction with Carbopack B and liquid chromatography with fluorometric detection. Clin Chem. 1985 Oct;31(10):1698-702. PMID: 2994907

Ball P, Emons G, Haupt O, Hoppen HO, Knuppen R: Radioimmunoassay of 2-hydroxyestrone. Steroids. 1978 Feb;31(2):249-58. PMID: 663967

Ribar S, Mesaric M, Sedic M: Sphingoid bases as possible diagnostic parameters. Croat Med J. 2003 Apr;44(2):165-70. PMID: 12698507

Khan HA, Sobki SH, Alhomida AS: Fluctuations in fasting blood glucose and serum fructosamine in pregnant women monitored on successive antenatal visits. Clin Exp Med. 2006 Oct;6(3):134-7. PMID: 17061063

Yang XL, Wu XR: The dynamic changes of several reproductive hormones during termination of early pregnancy by RU486 in combination with PG-05 in Chinese women. Adv Contracept. 1988 Dec;4(4):319-26. PMID: 3252730

Yang YJ, Lee J, Choi MH, Chung BC: Direct determination of estriol 3- and 16-glucuronides in pregnancy urine by column-switching liquid chromatography with electrospray tandem mass spectrometry. Biomed Chromatogr. 2003 Jun;17(4):219-25. PMID: 12833386

Huang PC, Kuo PL, Guo YL, Liao PC, Lee CC: Associations between urinary phthalate monoesters and thyroid hormones in pregnant women. Hum Reprod. 2007 Oct;22(10):2715-22. Epub 2007 Aug 17. PMID: 17704099

Mikkelsen TB, Osler M, Olsen SF: Validity of protein, retinol, folic acid and n-3 fatty acid intakes estimated from the food-frequency questionnaire used in the Danish National Birth Cohort. Public Health Nutr. 2006 Sep;9(6):771-8. PMID: 16925883

Shiraishi M, Haruna M, Matsuzaki M, Murayama R, Sasaki S, Murashima S: Validity and reproducibility of folate and vitamin B(12) intakes estimated from a self-administered diet history questionnaire in Japanese pregnant women. Nutr J. 2012 Mar 15;11:15. doi: 10.1186/1475-2891-11-15. PMID: 22420377

Brantsaeter AL, Haugen M, Julshamn K, Alexander J, Meltzer HM: Evaluation of urinary iodine excretion as a biomarker for intake of milk and dairy products in pregnant women in the Norwegian Mother and Child Cohort Study (MoBa). Eur J Clin Nutr. 2009 Mar;63(3):347-54. Epub 2007 Dec 5. PMID: 18059417

Bahado-Singh RO, Akolekar R, Mandal R, Dong E, Xia J, Kruger M, Wishart DS, Nicolaides K: Metabolomics and first-trimester prediction of early-onset preeclampsia. J Matern Fetal Neonatal Med. 2012 Oct;25(10):1840-7. doi: 10.3109/14767058.2012.680254. Epub 2012 Apr 28. PMID: 22494326

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Bahado-Singh RO, Akolekar R, Mandal R, Dong E, Xia J, Kruger M, Wishart DS, Nicolaides K: Metabolomic analysis for first-trimester Down syndrome prediction. Am J Obstet Gynecol. 2013 May;208(5):371.e1-8. doi: 10.1016/j.ajog.2012.12.035. Epub 2013 Jan 8. PMID: 23313728

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### PC(18:4(6Z,9Z,12Z,15Z)/18:2(9Z,12Z)) -- Obesity



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Tuma P, Samcova E, Balinova P: Determination of 3-methylhistidine and 1-methylhistidine in untreated urine samples by capillary electrophoresis. *J Chromatogr B Analyt Technol Biomed Life Sci.* 2005 Jul 5;821(1):53-9. PMID: 15899597

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Vioque J, Weinbrenner T, Asensio L, Castello A, Young IS, Fletcher A: Plasma concentrations of carotenoids and vitamin C are better correlated with dietary intake in normal weight than overweight and obese elderly subjects. *Br J Nutr.* 2007 May;97(5):977-86. PMID: 17408529

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## PC(20:1(11Z)/14:0) -- Introduction

**SYNONYM:** PC(34:1); Phosphatidylcholine(34:1); 1-eicosenoyl-2-myristoyl-sn-glycero-3-phosphocholine; GPCho(20:1/14:0); Lecithin; GPCho(34:1); PC(20:1/14:0); PC(20:1(11Z)/14:0); 1-(11-eicosenoyl)-2-tetradecanoyl-sn-glycero-3-phosphocholine; Phosphatidylcholine(20:1/14:0)

**HMDB:** HMDB0008295; HMDB08295

**CAS:**

PC(20:1(11Z)/14:0) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(20:1(11Z)/14:0), in particular, consists of one chain of eicosenoic acid at the C-1 position and one chain of myristic acid at the C-2 position. The eicosenoic acid moiety is derived from vegetable oils and cod oils, while the myristic acid moiety is derived from nutmeg and butter. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes.



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PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

### PC(20:1(11Z)/14:0) – Pregnancy

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Bahado-Singh RO, Akolekar R, Chelliah A, Mandal R, Dong E, Kruger M, Wishart DS, Nicolaides K: Metabolomic analysis for first-trimester trisomy 18 detection. *Am J Obstet Gynecol*. 2013 Jul;209(1):65.e1-9. doi: 10.1016/j.ajog.2013.03.028. Epub 2013 Mar 25. PMID: 23535240

Bahado-Singh RO, Ertl R, Mandal R, Bjorndahl TC, Syngelaki A, Han B, Dong E, Liu PB, Alpay-Savasan Z, Wishart DS,



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Nicolaides KH: Metabolomic prediction of fetal congenital heart defect in the first trimester. Am J Obstet Gynecol. 2014 Sep;211(3):240.e1-240.e14. doi: 10.1016/j.ajog.2014.03.056. Epub 2014 Apr 1. PMID: 24704061

## PC(20:1(11Z)/14:0) -- Obesity

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Vice E, Privette JD, Hickner RC, Barakat HA: Ketone body metabolism in lean and obese women. Metabolism. 2005 Nov;54(11):1542-5. PMID: 16253646

Brind J, Strain G, Miller L, Zumoff B, Vogelman J, Orentreich N: Obese men have elevated plasma levels of estrone sulfate. Int J Obes. 1990 Jun;14(6):483-6. PMID: 2401584

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Vioque J, Weinbrenner T, Asensio L, Castello A, Young IS, Fletcher A: Plasma concentrations of carotenoids and vitamin C are better correlated with dietary intake in normal weight than overweight and obese elderly subjects. Br J Nutr. 2007 May;97(5):977-86. PMID: 17408529

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## PC(20:2(11Z,14Z)/14:0) -- Introduction

SYNONYM: 1-eicosadienoyl-2-myristoyl-sn-glycero-3-phosphocholine; Lecithin; Phosphatidylcholine(34:2); Phosphatidylcholine(20:2/14:0); PC(20:2(11Z,14Z)/14:0); PC(20:2/14:0); GPCho(34:2); GPCho(20:2/14:0); 1-(11Z,14Z-eicosadienoyl)-2-tetradecanoyl-sn-glycero-3-phosphocholine; PC(34:2)

HMDB: HMDB0008328; HMDB08328

CAS:

PC(20:2(11Z,14Z)/14:0) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(20:2(11Z,14Z)/14:0), in particular, consists of one chain of eicosadienoic acid at the C-1 position and one chain of myristic acid at the C-2 position. The eicosadienoic acid



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moiety is derived from fish oils and liver, while the myristic acid moiety is derived from nutmeg and butter. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

### PC(20:2(11Z,14Z)/14:0) -- Pregnancy

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### PC(20:2(11Z,14Z)/20:4(5Z,8Z,11Z,14Z)) -- Introduction

SYNONYM: 1-eicosadienoyl-2-arachidonoyl-sn-glycero-3-phosphocholine; Phosphatidylcholine(20:2/20:4); GPCho(20:2/20:4); GPCho(40:6); PC(20:2/20:4); Lecithin; Phosphatidylcholine(40:6); PC(40:6); 1-(11Z,14Z-eicosadienoyl)-2-(5Z,8Z,11Z,14Z-eicosatetraenoyl)-sn-glycero-3-phosphocholine; PC(20:2(11Z,14Z)/20:4(5Z,8Z,11Z,14Z))

HMDB: HMDB0008345; HMDB08345

CAS:



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PC(20:2(11Z,14Z)/20:4(5Z,8Z,11Z,14Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common.

PC(20:2(11Z,14Z)/20:4(5Z,8Z,11Z,14Z)), in particular, consists of one chain of eicosadienoic acid at the C-1 position and one chain of arachidonic acid at the C-2 position. The eicosadienoic acid moiety is derived from fish oils and liver, while the arachidonic acid moiety is derived from animal fats and eggs. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

### PC(20:2(11Z,14Z)/20:4(5Z,8Z,11Z,14Z)) – Pregnancy

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### PC(20:3(8Z,11Z,14Z)/14:0) -- Introduction

SYNONYM: PC(20:3(8Z,11Z,14Z)/14:0); PC(20:3/14:0); GPCho(20:3/14:0); Phosphatidylcholine(20:3/14:0); Lecithin;

Phosphatidylcholine(34:3); 1-homo-g-linolenoyl-2-myristoyl-sn-glycero-3-phosphocholine; GPCho(34:3); 1-(8Z,11Z,14Z-eicosatrienoyl)-2-tetradecanoyl-sn-glycero-3-phosphocholine; PC(34:3)

HMDB: HMDB0008394; HMDB08394

CAS:

PC(20:3(8Z,11Z,14Z)/14:0) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(20:3(8Z,11Z,14Z)/14:0), in particular, consists of one chain of homo-g-linolenic acid at the C-1 position and one chain of myristic acid at the C-2 position. The homo-g-linolenic acid moiety is derived from fish oils, liver and kidney, while the myristic acid moiety is derived from nutmeg and butter. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

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## PC(20:4(5Z,8Z,11Z,14Z)/20:4(8Z,11Z,14Z,17Z)) -- Introduction

SYNONYM: 1-Arachidonoyl-2-eicsoate; 1-Arachidonoyl-2-eicsoatetraenoyl-sn-glycero-3-phosphocholine; 1-Arachidonoyl-2-eicosoic acid; gpcho(20:4/20:4); gpcho(20:4n6/20:4n3); gpcho(20:4W6/20:4W3); gpcho(40:8); Lecithin; PC(20:4/20:4); PC(20:4n6/20:4n3); PC(20:4W6/20:4W3); PC(40:8); Phosphatidylcholine(20:4/20:4); Phosphatidylcholine(20:4n6/20:4n3); Phosphatidylcholine(20:4W6/20:4W3); Phosphatidylcholine(40:8); 1-(5Z,8Z,11Z,14Z-eicosatetraenoyl)-2-(8Z,11Z,14Z,17Z-eicosapentaenoyl)-sn-glycero-3-phosphocholine; PC(20:4(5Z,8Z,11Z,14Z)/20:4(8Z,11Z,14Z,17Z))

HMDB: HMDB0008444; HMDB08444

CAS:

PC(20:4(5Z,8Z,11Z,14Z)/20:4(8Z,11Z,14Z,17Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(20:4(5Z,8Z,11Z,14Z)/20:4(8Z,11Z,14Z,17Z)), in particular, consists of one chain of arachidonic acid at the C-1 position and one chain of eicosatetraenoic acid at the C-2 position. The arachidonic acid moiety is derived from animal fats and eggs, while the eicosatetraenoic acid moiety is derived from fish oils. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

## PC(20:4(8Z,11Z,14Z,17Z)/14:0) -- Introduction

SYNONYM: PC(20:4(8Z,11Z,14Z,17Z)/14:0); GPCho(34:4); PC(20:4/14:0); Phosphatidylcholine(20:4/14:0); PC(34:4); Lecithin; GPCho(20:4/14:0); 1-eicosatetraenoyl-2-myristoyl-sn-glycero-3-phosphocholine; 1-(8Z,11Z,14Z,17Z-eicosapentaenoyl)-2-tetradecanoyl-sn-glycero-3-phosphocholine; Phosphatidylcholine(34:4)

HMDB: HMDB0008459; HMDB08459

CAS:

PC(20:4(8Z,11Z,14Z,17Z)/14:0) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(20:4(8Z,11Z,14Z,17Z)/14:0), in particular, consists of one chain of eicosatetraenoic acid at the C-1 position and one chain of myristic acid at the C-2 position. The eicosatetraenoic acid moiety is derived from fish oils, while the myristic acid moiety is derived from nutmeg and butter. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

## PC(20:4(8Z,11Z,14Z,17Z)/14:0) -- Pregnancy



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Andreolini F, Borra C, Caccamo F, Di Corcia A, Nicoletti I, Samperi R, Improta F: Estriol and its conjugates in late pregnancy determined by extraction with Carbopack B and liquid chromatography with fluorometric detection. Clin Chem. 1985 Oct;31(10):1698-702. PMID: 2994907

Ball P, Emons G, Haupt O, Hoppen HO, Knuppen R: Radioimmunoassay of 2-hydroxyestrone. Steroids. 1978 Feb;31(2):249-58. PMID: 663967

Ribar S, Mesaric M, Sedic M: Sphingoid bases as possible diagnostic parameters. Croat Med J. 2003 Apr;44(2):165-70. PMID: 12698507

Khan HA, Sobki SH, Alhomida AS: Fluctuations in fasting blood glucose and serum fructosamine in pregnant women monitored on successive antenatal visits. Clin Exp Med. 2006 Oct;6(3):134-7. PMID: 17061063

Yang XL, Wu XR: The dynamic changes of several reproductive hormones during termination of early pregnancy by RU486 in combination with PG-05 in Chinese women. Adv Contracept. 1988 Dec;4(4):319-26. PMID: 3252730

Yang YJ, Lee J, Choi MH, Chung BC: Direct determination of estriol 3- and 16-glucuronides in pregnancy urine by column-switching liquid chromatography with electrospray tandem mass spectrometry. Biomed Chromatogr. 2003 Jun;17(4):219-25. PMID: 12833386

Huang PC, Kuo PL, Guo YL, Liao PC, Lee CC: Associations between urinary phthalate monoesters and thyroid hormones in pregnant women. Hum Reprod. 2007 Oct;22(10):2715-22. Epub 2007 Aug 17. PMID: 17704099

Mikkelsen TB, Osler M, Olsen SF: Validity of protein, retinol, folic acid and n-3 fatty acid intakes estimated from the food-frequency questionnaire used in the Danish National Birth Cohort. Public Health Nutr. 2006 Sep;9(6):771-8. PMID: 16925883

Shiraishi M, Haruna M, Matsuzaki M, Murayama R, Sasaki S, Murashima S: Validity and reproducibility of folate and vitamin B(12) intakes estimated from a self-administered diet history questionnaire in Japanese pregnant women. Nutr J. 2012 Mar 15;11:15. doi: 10.1186/1475-2891-11-15. PMID: 22420377

Brantsaeter AL, Haugen M, Julshamn K, Alexander J, Meltzer HM: Evaluation of urinary iodine excretion as a biomarker for intake of milk and dairy products in pregnant women in the Norwegian Mother and Child Cohort Study (MoBa). Eur J Clin Nutr. 2009 Mar;63(3):347-54. Epub 2007 Dec 5. PMID: 18059417

Bahado-Singh RO, Akolekar R, Mandal R, Dong E, Xia J, Kruger M, Wishart DS, Nicolaides K: Metabolomics and first-trimester prediction of early-onset preeclampsia. J Matern Fetal Neonatal Med. 2012 Oct;25(10):1840-7. doi: 10.3109/14767058.2012.680254. Epub 2012 Apr 28. PMID: 22494326

Bahado-Singh RO, Akolekar R, Mandal R, Dong E, Xia J, Kruger M, Wishart DS, Nicolaides K: First-trimester metabolomic detection of late-onset preeclampsia. Am J Obstet Gynecol. 2013 Jan;208(1):58.e1-7. doi: 10.1016/j.ajog.2012.11.003. Epub 2012 Nov 13. PMID: 23159745

Bahado-Singh RO, Akolekar R, Mandal R, Dong E, Xia J, Kruger M, Wishart DS, Nicolaides K: Metabolomic analysis for first-trimester Down syndrome prediction. Am J Obstet Gynecol. 2013 May;208(5):371.e1-8. doi: 10.1016/j.ajog.2012.12.035. Epub 2013 Jan 8. PMID: 23313728

Bahado-Singh RO, Akolekar R, Chelliah A, Mandal R, Dong E, Kruger M, Wishart DS, Nicolaides K: Metabolomic analysis for first-trimester trisomy 18 detection. Am J Obstet Gynecol. 2013 Jul;209(1):65.e1-9. doi: 10.1016/j.ajog.2013.03.028. Epub 2013 Mar 25. PMID: 23535240

Bahado-Singh RO, Ertl R, Mandal R, Bjorndahl TC, Syngelaki A, Han B, Dong E, Liu PB, Alpay-Savasan Z, Wishart DS, Nicolaides KH: Metabolomic prediction of fetal congenital heart defect in the first trimester. Am J Obstet Gynecol. 2014 Sep;211(3):240.e1-240.e14. doi: 10.1016/j.ajog.2014.03.056. Epub 2014 Apr 1. PMID: 24704061

## PC(20:4(8Z,11Z,14Z,17Z)/14:0) -- Obesity

Tuma P, Samcova E, Balinova P: Determination of 3-methylhistidine and 1-methylhistidine in untreated urine samples by capillary electrophoresis. J Chromatogr B Analyt Technol Biomed Life Sci. 2005 Jul 5;821(1):53-9. PMID: 15899597

Serlie MJ, Meijer AJ, Groener JE, Duran M, Endert E, Fliers E, Aerts JM, Sauerwein HP: Short-term manipulation of



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plasma free fatty acids does not change skeletal muscle concentrations of ceramide and glucosylceramide in lean and overweight subjects. *J Clin Endocrinol Metab.* 2007 Apr;92(4):1524-9. Epub 2007 Jan 30. PMID: 17264178

Vice E, Privette JD, Hickner RC, Barakat HA: Ketone body metabolism in lean and obese women. *Metabolism.* 2005 Nov;54(11):1542-5. PMID: 16253646

Brind J, Strain G, Miller L, Zumoff B, Vogelman J, Orentreich N: Obese men have elevated plasma levels of estrone sulfate. *Int J Obes.* 1990 Jun;14(6):483-6. PMID: 2401584

Driskell JA, Chrisley BM, Reynolds LK, Moak SW: Plasma B6 vitamer and plasma and urinary 4-pyridoxic acid concentrations of middle-aged obese black women. *J Chromatogr.* 1991 Aug 23;568(2):333-40. PMID: 1783639

Haro C, Montes-Borrego M, Rangel-Zuniga OA, Alcala-Diaz JF, Gomez-Delgado F, Perez-Martinez P, Delgado-Lista J, Quintana-Navarro GM, Tinahones FJ, Landa BB, Lopez-Miranda J, Camargo A, Perez-Jimenez F: Two Healthy Diets Modulate Gut Microbial Community Improving Insulin Sensitivity in a Human Obese Population. *J Clin Endocrinol Metab.* 2016 Jan;101(1):233-42. doi: 10.1210/jc.2015-3351. Epub 2015 Oct 27. PMID: 26505825

Vioque J, Weinbrenner T, Asensio L, Castello A, Young IS, Fletcher A: Plasma concentrations of carotenoids and vitamin C are better correlated with dietary intake in normal weight than overweight and obese elderly subjects. *Br J Nutr.* 2007 May;97(5):977-86. PMID: 17408529

Burrows TL, Warren JM, Colyvas K, Garg ML, Collins CE: Validation of overweight children's fruit and vegetable intake using plasma carotenoids. *Obesity (Silver Spring).* 2009 Jan;17(1):162-8. doi: 10.1038/oby.2008.495. Epub 2008 Nov 6. PMID: 18997681

Reinehr T, Wolters B, Knop C, Lass N, Hellmuth C, Harder U, Peissner W, Wahl S, Grallert H, Adamski J, Illig T, Prehn C, Yu Z, Wang-Sattler R, Koletzko B: Changes in the serum metabolite profile in obese children with weight loss. *Eur J Nutr.* 2015 Mar;54(2):173-81. doi: 10.1007/s00394-014-0698-8. Epub 2014 Apr 17. PMID: 24740590

Wahl S, Yu Z, Kleber M, Singmann P, Holzapfel C, He Y, Mittelstrass K, Polonikov A, Prehn C, Romisch-Margl W, Adamski J, Suhre K, Grallert H, Illig T, Wang-Sattler R, Reinehr T: Childhood obesity is associated with changes in the serum metabolite profile. *Obes Facts.* 2012;5(5):660-70. doi: 10.1159/000343204. Epub 2012 Oct 4. PMID: 23108202

Cho K, Moon JS, Kang JH, Jang HB, Lee HJ, Park SI, Yu KS, Cho JY: Combined untargeted and targeted metabolomic profiling reveals urinary biomarkers for discriminating obese from normal-weight adolescents. *Pediatr Obes.* 2017 Apr;12(2):93-101. doi: 10.1111/ijpo.12114. Epub 2016 Feb 22. PMID: 26910390

## PC(20:4(8Z,11Z,14Z,17Z)/18:1(11Z)) -- Introduction

SYNONYM: PC(20:4(8Z,11Z,14Z,17Z)/18:1(11Z)); 1-eicsoatetraenoyl-2-vaccenoyl-sn-glycero-3-phosphocholine; PC(20:4/18:1); Phosphatidylcholine(38:5); GPCho(38:5); Lecithin; GPCho(20:4/18:1); Phosphatidylcholine(20:4/18:1); 1-(8Z,11Z,14Z,17Z-eicosapentaenoyl)-2-(11Z-octadecenoyl)-sn-glycero-3-phosphocholine; PC(38:5)

HMDB: HMDB0008465; HMDB08465

CAS:

PC(20:4(8Z,11Z,14Z,17Z)/18:1(11Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(20:4(8Z,11Z,14Z,17Z)/18:1(11Z)), in particular, consists of one chain of eicsoatetraenoic acid at the C-1 position and one chain of vaccenic acid at the C-2 position. The eicsoatetraenoic acid moiety is derived from fish oils, while the vaccenic acid moiety is derived from butter fat and animal fat. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or



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PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

### PC(20:4(8Z,11Z,14Z,17Z)/18:1(11Z)) -- Pregnancy

Andreolini F, Borra C, Caccamo F, Di Corcia A, Nicoletti I, Samperi R, Improta F: Estriol and its conjugates in late pregnancy determined by extraction with Carbo pack B and liquid chromatography with fluorometric detection. *Clin Chem*. 1985 Oct;31(10):1698-702. PMID: 2994907

Ball P, Emons G, Haupt O, Hoppen HO, Knuppen R: Radioimmunoassay of 2-hydroxyestrone. *Steroids*. 1978 Feb;31(2):249-58. PMID: 663967

Ribar S, Mesarić M, Sedić M: Sphingoid bases as possible diagnostic parameters. *Croat Med J*. 2003 Apr;44(2):165-70. PMID: 12698507

Khan HA, Sobki SH, Alhomida AS: Fluctuations in fasting blood glucose and serum fructosamine in pregnant women monitored on successive antenatal visits. *Clin Exp Med*. 2006 Oct;6(3):134-7. PMID: 17061063

Yang XL, Wu XR: The dynamic changes of several reproductive hormones during termination of early pregnancy by RU486 in combination with PG-05 in Chinese women. *Adv Contracept*. 1988 Dec;4(4):319-26. PMID: 3252730

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Bahado-Singh RO, Akolekar R, Mandal R, Dong E, Xia J, Kruger M, Wishart DS, Nicolaides K: Metabolomic analysis for first-trimester Down syndrome prediction. *Am J Obstet Gynecol*. 2013 May;208(5):371.e1-8. doi: 10.1016/j.ajog.2012.12.035. Epub 2013 Jan 8. PMID: 23313728

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Bahado-Singh RO, Ertl R, Mandal R, Bjorndahl TC, Syngelaki A, Han B, Dong E, Liu PB, Alpay-Savasan Z, Wishart DS, Nicolaides KH: Metabolomic prediction of fetal congenital heart defect in the first trimester. *Am J Obstet Gynecol*. 2014 Sep;211(3):240.e1-240.e14. doi: 10.1016/j.ajog.2014.03.056. Epub 2014 Apr 1. PMID: 24704061



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## PC(20:4(8Z,11Z,14Z,17Z)/18:1(11Z)) -- Obesity

Tuma P, Samcova E, Balinova P: Determination of 3-methylhistidine and 1-methylhistidine in untreated urine samples by capillary electrophoresis. *J Chromatogr B Analyt Technol Biomed Life Sci.* 2005 Jul 5;821(1):53-9. PMID: 15899597

Serlie MJ, Meijer AJ, Groener JE, Duran M, Endert E, Fliers E, Aerts JM, Sauerwein HP: Short-term manipulation of plasma free fatty acids does not change skeletal muscle concentrations of ceramide and glucosylceramide in lean and overweight subjects. *J Clin Endocrinol Metab.* 2007 Apr;92(4):1524-9. Epub 2007 Jan 30. PMID: 17264178

Vice E, Privette JD, Hickner RC, Barakat HA: Ketone body metabolism in lean and obese women. *Metabolism.* 2005 Nov;54(11):1542-5. PMID: 16253646

Brind J, Strain G, Miller L, Zumoff B, Vogelman J, Orentreich N: Obese men have elevated plasma levels of estrone sulfate. *Int J Obes.* 1990 Jun;14(6):483-6. PMID: 2401584

Driskell JA, Chrisley BM, Reynolds LK, Moak SW: Plasma B6 vitamer and plasma and urinary 4-pyridoxic acid concentrations of middle-aged obese black women. *J Chromatogr.* 1991 Aug 23;568(2):333-40. PMID: 1783639

Haro C, Montes-Borrego M, Rangel-Zuniga OA, Alcala-Diaz JF, Gomez-Delgado F, Perez-Martinez P, Delgado-Lista J, Quintana-Navarro GM, Tinahones FJ, Landa BB, Lopez-Miranda J, Camargo A, Perez-Jimenez F: Two Healthy Diets Modulate Gut Microbial Community Improving Insulin Sensitivity in a Human Obese Population. *J Clin Endocrinol Metab.* 2016 Jan;101(1):233-42. doi: 10.1210/jc.2015-3351. Epub 2015 Oct 27. PMID: 26505825

Vioque J, Weinbrenner T, Asensio L, Castello A, Young IS, Fletcher A: Plasma concentrations of carotenoids and vitamin C are better correlated with dietary intake in normal weight than overweight and obese elderly subjects. *Br J Nutr.* 2007 May;97(5):977-86. PMID: 17408529

Burrows TL, Warren JM, Colyvas K, Garg ML, Collins CE: Validation of overweight children's fruit and vegetable intake using plasma carotenoids. *Obesity (Silver Spring).* 2009 Jan;17(1):162-8. doi: 10.1038/oby.2008.495. Epub 2008 Nov 6. PMID: 18997681

Reinehr T, Wolters B, Knop C, Lass N, Hellmuth C, Harder U, Peissner W, Wahl S, Grallert H, Adamski J, Illig T, Prehn C, Yu Z, Wang-Sattler R, Koletzko B: Changes in the serum metabolite profile in obese children with weight loss. *Eur J Nutr.* 2015 Mar;54(2):173-81. doi: 10.1007/s00394-014-0698-8. Epub 2014 Apr 17. PMID: 24740590

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Cho K, Moon JS, Kang JH, Jang HB, Lee HJ, Park SI, Yu KS, Cho JY: Combined untargeted and targeted metabolomic profiling reveals urinary biomarkers for discriminating obese from normal-weight adolescents. *Pediatr Obes.* 2017 Apr;12(2):93-101. doi: 10.1111/jopo.12114. Epub 2016 Feb 22. PMID: 26910390

## PC(20:4(8Z,11Z,14Z,17Z)/20:3(8Z,11Z,14Z)) -- Introduction

SYNONYM: Phosphatidylcholine(20:4/20:3); PC(20:4(8Z,11Z,14Z,17Z)/20:3(8Z,11Z,14Z)); GPCho(40:7); Lecithin; Phosphatidylcholine(40:7); GPCho(20:4/20:3); PC(40:7); PC(20:4/20:3); 1-(8Z,11Z,14Z,17Z-eicosapentaenoyl)-2-(8Z,11Z,14Z-eicosatrienoyl)-sn-glycero-3-phosphocholine; 1-eicsoatetraenoyl-2-homo-g-linolenoyl-sn-glycero-3-phosphocholine

HMDB: HMDB0008475; HMDB08475

CAS:

PC(20:4(8Z,11Z,14Z,17Z)/20:3(8Z,11Z,14Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common.

PC(20:4(8Z,11Z,14Z,17Z)/20:3(8Z,11Z,14Z)), in particular, consists of one chain of eicsoatetraenoic acid at the C-1 position and one chain of homo-g-linolenic acid at the C-2 position. The eicsoatetraenoic acid moiety is derived from fish oils, while the homo-g-linolenic acid moiety is derived from fish oils, liver and kidney. Phospholipids, are ubiquitous in nature and



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are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

## PC(20:4(8Z,11Z,14Z,17Z)/P-18:0) -- Introduction

**SYNONYM:** Glycerophosphocholine; 1-(8Z,11Z,14Z,17Z-Eicosapentaenoyl)-2-(1Z-octadecenyl)-sn-glycero-3-phosphocholine; Glycerophosphocholine(20:4(8Z,11Z,14Z,17Z)/p-18:0); PC(20:4); gpcho(20:4); Phosphatidylcholine(20:4); PC(20:4/P-18:0); gpcho(20:4/P-18:0); Phosphatidylcholine(20:4/p-18:0)

**HMDB:** HMDB0008489; HMDB08489

**CAS:**

PC(20:4(8Z,11Z,14Z,17Z)/P-18:0) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(20:4(8Z,11Z,14Z,17Z)/P-18:0), in particular, consists of one chain of eicosatetraenoic acid at the C-1 position and one chain of plasmalogen 18:0 at the C-2 position. The eicosatetraenoic acid moiety is derived from fish oils, while the plasmalogen 18:0 moiety is derived from animal fats, liver and kidney. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC. Plasmalogens are glycerol ether phospholipids. They are of two types, alkyl ether (-O-CH<sub>2</sub>-) and alkenyl ether (-O-CH=CH-). Dihydroxyacetone phosphate (DHAP) serves as the glycerol precursor for the synthesis of plasmalogens. Three major classes of plasmalogens have been identified: choline, ethanolamine and serine derivatives. Ethanolamine plasmalogen is prevalent in myelin. Choline plasmalogen is abundant in cardiac tissue. Usually, the highest proportion of the plasmalogen form is in the ethanolamine class with rather less in choline, and commonly little or none in other phospholipids such as phosphatidylinositol. In choline plasmalogens of most tissues, a higher proportion is often of the O-alkyl rather than the O-alkenyl form, but the reverse tends to be true in heart lipids. In animal tissues, the alkyl and alkenyl moieties in both non-polar and phospholipids tend to be rather simple in composition with 16:0, 18:0 and 18:1 (double bond in position 9) predominating. Ether analogues of triacylglycerols, i.e. 1-alkyldiacyl-sn-glycerols, are present at trace levels only if at all in most animal tissues, but they can be major components of some marine lipids.

This compound belongs to the class of organic compounds known as 1-acyl,2-(1z-alkenyl)-glycerophosphocholines. These are glycerophosphocholines that carry exactly one acyl chain attached to the glycerol moiety through an ester linkage at the O1-position, and one 1Z-alkenyl chain attached through an ether linkage at the O2-position.

## PC(20:4(8Z,11Z,14Z,17Z)/P-18:0) -- Pregnancy

Andreolini F, Borra C, Caccamo F, Di Corcia A, Nicoletti I, Samperi R, Improta F: Estriol and its conjugates in late pregnancy determined by extraction with Carbopack B and liquid chromatography with fluorometric detection. Clin Chem. 1985 Oct;31(10):1698-702. PMID: 2994907

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Tuma P, Samcova E, Balinova P: Determination of 3-methylhistidine and 1-methylhistidine in untreated urine samples by capillary electrophoresis. *J Chromatogr B Analyt Technol Biomed Life Sci.* 2005 Jul 5;821(1):53-9. PMID: 15899597

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Vice E, Privette JD, Hickner RC, Barakat HA: Ketone body metabolism in lean and obese women. *Metabolism.* 2005 Nov;54(11):1542-5. PMID: 16253646

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## PC(20:5(5Z,8Z,11Z,14Z,17Z)/14:0) -- Introduction

**SYNONYM:** Phosphatidylcholine(34:5); 1-eicosapentaenoyl-2-myristoyl-sn-glycero-3-phosphocholine; PC(20:5(5Z,8Z,11Z,14Z,17Z)/14:0); Phosphatidylcholine(20:5/14:0); PC(34:5); GPCho(20:5/14:0); Lecithin; GPCho(34:5); 1-(5Z,8Z,11Z,14Z,17Z-eicosapentaenoyl)-2-tetradecanoyl-sn-glycero-3-phosphocholine; PC(20:5/14:0)

**HMDB:** HMDB0008492; HMDB08492

**CAS:**

PC(20:5(5Z,8Z,11Z,14Z,17Z)/14:0) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(20:5(5Z,8Z,11Z,14Z,17Z)/14:0), in particular, consists of one chain of eicosapentaenoic acid at the C-1 position and one chain of myristic acid at the C-2 position. The eicosapentaenoic acid moiety is derived from fish oils, liver and kidney, while the myristic acid moiety is derived from nutmeg and butter. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

## PC(20:5(5Z,8Z,11Z,14Z,17Z)/15:0) -- Introduction

**SYNONYM:** PC(20:5(5Z,8Z,11Z,14Z,17Z)/15:0); GPCho(35:5); PC(35:5); 1-eicosapentaenoyl-2-pentadecanoyl-sn-glycero-3-phosphocholine; Lecithin; PC(20:5/15:0); Phosphatidylcholine(35:5); GPCho(20:5/15:0); 1-(5Z,8Z,11Z,14Z,17Z-eicosapentaenoyl)-2-pentadecanoyl-sn-glycero-3-phosphocholine; Phosphatidylcholine(20:5/15:0)



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HMDB: HMDB0008494; HMDB08494

CAS:

PC(20:5(5Z,8Z,11Z,14Z,17Z)/15:0) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(20:5(5Z,8Z,11Z,14Z,17Z)/15:0), in particular, consists of one chain of eicosapentaenoic acid at the C-1 position and one chain of pentadecanoic acid at the C-2 position. The eicosapentaenoic acid moiety is derived from fish oils, liver and kidney, while the pentadecanoic acid moiety is derived from dairy products and milk fat. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

### PC(22:2(13Z,16Z)/14:1(9Z)) -- Introduction

SYNONYM: PC(22:2(13Z,16Z)/14:1(9Z)); GPCho(22:2/14:1); GPCho(36:3); PC(22:2/14:1); PC(36:3); Lecithin; Phosphatidylcholine(36:3); 1-docosadienoyl-2-myristoleoyl-sn-glycero-3-phosphocholine; 1-(13Z,16Z-docosadienoyl)-2-(9Z-tetradecenoyl)-sn-glycero-3-phosphocholine; Phosphatidylcholine(22:2/14:1)

HMDB: HMDB0008591; HMDB08591

CAS:

PC(22:2(13Z,16Z)/14:1(9Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(22:2(13Z,16Z)/14:1(9Z)), in particular, consists of one chain of docosadienoic acid at the C-1 position and one chain of myristoleic acid at the C-2 position. The docosadienoic acid moiety is derived from animal fats, while the myristoleic acid moiety is derived from milk fats. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

### PC(22:2(13Z,16Z)/14:1(9Z)) -- Pregnancy

Andreolini F, Borra C, Caccamo F, Di Corcia A, Nicoletti I, Samperi R, Improta F: Estriol and its conjugates in late pregnancy determined by extraction with Carbopack B and liquid chromatography with fluorometric detection. Clin Chem. 1985 Oct;31(10):1698-702. PMID: 2994907

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Ribar S, Mesaric M, Sedic M: Sphingoid bases as possible diagnostic parameters. Croat Med J. 2003 Apr;44(2):165-70. PMID: 12698507

Khan HA, Sobki SH, Alhomida AS: Fluctuations in fasting blood glucose and serum fructosamine in pregnant women monitored on successive antenatal visits. *Clin Exp Med.* 2006 Oct;6(3):134-7. PMID: 17061063

Yang XL, Wu XR: The dynamic changes of several reproductive hormones during termination of early pregnancy by RU486 in combination with PG-05 in Chinese women. *Adv Contracept.* 1988 Dec;4(4):319-26. PMID: 3252730

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Huang PC, Kuo PL, Guo YL, Liao PC, Lee CC: Associations between urinary phthalate monoesters and thyroid hormones in pregnant women. *Hum Reprod.* 2007 Oct;22(10):2715-22. Epub 2007 Aug 17. PMID: 17704099

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Brantsaeter AL, Haugen M, Julshamn K, Alexander J, Meltzer HM: Evaluation of urinary iodine excretion as a biomarker for intake of milk and dairy products in pregnant women in the Norwegian Mother and Child Cohort Study (MoBa). *Eur J Clin Nutr.* 2009 Mar;63(3):347-54. Epub 2007 Dec 5. PMID: 18059417

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## PC(22:4(7Z,10Z,13Z,16Z)/14:0) -- Introduction

SYNONYM: PC(22:4/14:0); PC(22:4(7Z,10Z,13Z,16Z)/14:0); Phosphatidylcholine(36:4); GPCho(22:4/14:0); Lecithin; GPCho(36:4); 1-adrenoyl-2-myristoyl-sn-glycero-3-phosphocholine; PC(36:4); 1-(7Z,10Z,13Z,16Z-docosatetraenoyl)-2-tetradecanoyl-sn-glycero-3-phosphocholine; Phosphatidylcholine(22:4/14:0)

HMDB: HMDB0008623; HMDB08623

CAS:

PC(22:4(7Z,10Z,13Z,16Z)/14:0) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(22:4(7Z,10Z,13Z,16Z)/14:0), in particular, consists of one chain of adrenic acid at the C-1 position and one chain of myristic acid at the C-2 position. The adrenic acid moiety is derived from animal fats, while the myristic acid moiety is derived from nutmeg and butter. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

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Andreolini F, Borra C, Caccamo F, Di Corcia A, Nicoletti I, Samperi R, Improta F: Estriol and its conjugates in late pregnancy determined by extraction with Carbopack B and liquid chromatography with fluorometric detection. Clin Chem. 1985 Oct;31(10):1698-702. PMID: 2994907

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Tuma P, Samcova E, Balinova P: Determination of 3-methylhistidine and 1-methylhistidine in untreated urine samples by capillary electrophoresis. J Chromatogr B Analyt Technol Biomed Life Sci. 2005 Jul 5;821(1):53-9. PMID: 15899597

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Cho K, Moon JS, Kang JH, Jang HB, Lee HJ, Park SI, Yu KS, Cho JY: Combined untargeted and targeted metabolomic profiling reveals urinary biomarkers for discriminating obese from normal-weight adolescents. *Pediatr Obes.* 2017 Apr;12(2):93-101. doi: 10.1111/jpo.12114. Epub 2016 Feb 22. PMID: 26910390

## PC(22:4(7Z,10Z,13Z,16Z)/22:5(4Z,7Z,10Z,13Z,16Z)) -- Introduction

**SYNONYM:** Phosphatidylcholine(22:4/22:5); PC(22:4/22:5); GPCho(22:4/22:5); Lecithin; PC(44:9); Phosphatidylcholine(44:9); PC(22:4(7Z,10Z,13Z,16Z)/22:5(4Z,7Z,10Z,13Z,16Z)); GPCho(44:9); 1-(7Z,10Z,13Z,16Z-docosatetraenoyl)-2-(4Z,7Z,10Z,13Z,16Z-docosapentaenoyl)-sn-glycero-3-phosphocholine; 1-adrenoyl-2-osbondoyl-sn-glycero-3-phosphocholine

HMDB: HMDB0008647; HMDB08647

CAS:

PC(22:4(7Z,10Z,13Z,16Z)/22:5(4Z,7Z,10Z,13Z,16Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(22:4(7Z,10Z,13Z,16Z)/22:5(4Z,7Z,10Z,13Z,16Z)), in particular, consists of one chain of adrenic acid at the C-1 position and one chain of docosapentaenoic acid at the C-2 position. The adrenic acid moiety is derived from animal fats, while the docosapentaenoic acid moiety is derived from animal fats and brain. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

## PC(22:4(7Z,10Z,13Z,16Z)/P-18:0) -- Introduction

**SYNONYM:** Glycerophosphocholine; 1-(7Z,10Z,13Z,16Z-Docosatetraenoyl)-2-(1Z-octadecenyl)-sn-glycero-3-phosphocholine; Glycerophosphocholine(22:4(7Z,10Z,13Z,16Z)/p-18:0); PC(22:4); gpcho(22:4); Phosphatidylcholine(22:4); PC(22:4/P-18:0); gpcho(22:4/P-18:0); Phosphatidylcholine(22:4/p-18:0)

HMDB: HMDB0008653; HMDB08653

CAS:

PC(22:4(7Z,10Z,13Z,16Z)/P-18:0) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(22:4(7Z,10Z,13Z,16Z)/P-18:0), in particular, consists of one chain of adrenic acid at the C-1 position and one chain of plasmalogen 18:0 at the C-2 position. The adrenic acid moiety is derived from animal fats, while the plasmalogen 18:0 moiety is derived from animal fats, liver and kidney. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or



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PE to PC. Plasmalogens are glycerol ether phospholipids. They are of two types, alkyl ether (-O-CH<sub>2</sub>-) and alkenyl ether (-O-CH=CH-). Dihydroxyacetone phosphate (DHAP) serves as the glycerol precursor for the synthesis of plasmalogens. Three major classes of plasmalogens have been identified: choline, ethanolamine and serine derivatives. Ethanolamine plasmalogen is prevalent in myelin. Choline plasmalogen is abundant in cardiac tissue. Usually, the highest proportion of the plasmalogen form is in the ethanolamine class with rather less in choline, and commonly little or none in other phospholipids such as phosphatidylinositol. In choline plasmalogens of most tissues, a higher proportion is often of the O-alkyl rather than the O-alkenyl form, but the reverse tends to be true in heart lipids. In animal tissues, the alkyl and alkenyl moieties in both non-polar and phospholipids tend to be rather simple in composition with 16:0, 18:0 and 18:1 (double bond in position 9) predominating. Ether analogues of triacylglycerols, i.e. 1-alkyldiacyl-sn-glycerols, are present at trace levels only if at all in most animal tissues, but they can be major components of some marine lipids.

This compound belongs to the class of organic compounds known as 1-acyl,2-(1z-alkenyl)-glycerophosphocholines. These are glycerophosphocholines that carry exactly one acyl chain attached to the glycerol moiety through an ester linkage at the O1-position, and one 1Z-alkenyl chain attached through an ether linkage at the O2-position.

### PC(22:4(7Z,10Z,13Z,16Z)/P-18:0) – Pregnancy

Andreolini F, Borra C, Caccamo F, Di Corcia A, Nicoletti I, Samperi R, Improta F: Estriol and its conjugates in late pregnancy determined by extraction with Carbopack B and liquid chromatography with fluorometric detection. Clin Chem. 1985 Oct;31(10):1698-702. PMID: 2994907

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Ribar S, Mesaric M, Sedic M: Sphingoid bases as possible diagnostic parameters. Croat Med J. 2003 Apr;44(2):165-70. PMID: 12698507

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Yang XL, Wu XR: The dynamic changes of several reproductive hormones during termination of early pregnancy by RU486 in combination with PG-05 in Chinese women. Adv Contracept. 1988 Dec;4(4):319-26. PMID: 3252730

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### PC(22:4(7Z,10Z,13Z,16Z)/P-18:0) – Obesity

Tuma P, Samcova E, Balinova P: Determination of 3-methylhistidine and 1-methylhistidine in untreated urine samples by capillary electrophoresis. J Chromatogr B Analyt Technol Biomed Life Sci. 2005 Jul 5;821(1):53-9. PMID: 15899597

Serlie MJ, Meijer AJ, Groener JE, Duran M, Endert E, Fliers E, Aerts JM, Sauerwein HP: Short-term manipulation of plasma free fatty acids does not change skeletal muscle concentrations of ceramide and glucosylceramide in lean and overweight subjects. J Clin Endocrinol Metab. 2007 Apr;92(4):1524-9. Epub 2007 Jan 30. PMID: 17264178

Vice E, Privette JD, Hickner RC, Barakat HA: Ketone body metabolism in lean and obese women. Metabolism. 2005 Nov;54(11):1542-5. PMID: 16253646

Brind J, Strain G, Miller L, Zumoff B, Vogelman J, Orentreich N: Obese men have elevated plasma levels of estrone sulfate. Int J Obes. 1990 Jun;14(6):483-6. PMID: 2401584

Driskell JA, Chrisley BM, Reynolds LK, Moak SW: Plasma B6 vitamer and plasma and urinary 4-pyridoxic acid concentrations of middle-aged obese black women. J Chromatogr. 1991 Aug 23;568(2):333-40. PMID: 1783639

Haro C, Montes-Borrego M, Rangel-Zuniga OA, Alcala-Diaz JF, Gomez-Delgado F, Perez-Martinez P, Delgado-Lista J, Quintana-Navarro GM, Tinahones FJ, Landa BB, Lopez-Miranda J, Camargo A, Perez-Jimenez F: Two Healthy Diets Modulate Gut Microbial Community Improving Insulin Sensitivity in a Human Obese Population. J Clin Endocrinol Metab. 2016 Jan;101(1):233-42. doi: 10.1210/jc.2015-3351. Epub 2015 Oct 27. PMID: 26505825

Vioque J, Weinbrenner T, Asensio L, Castello A, Young IS, Fletcher A: Plasma concentrations of carotenoids and vitamin C are better correlated with dietary intake in normal weight than overweight and obese elderly subjects. Br J Nutr. 2007 May;97(5):977-86. PMID: 17408529

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Wahl S, Yu Z, Kleber M, Singmann P, Holzapfel C, He Y, Mittelstrass K, Polonikov A, Prehn C, Romisch-Margl W, Adamski J, Suhre K, Grallert H, Illig T, Wang-Sattler R, Reinehr T: Childhood obesity is associated with changes in the serum metabolite profile. Obes Facts. 2012;5(5):660-70. doi: 10.1159/000343204. Epub 2012 Oct 4. PMID: 23108202

Cho K, Moon JS, Kang JH, Jang HB, Lee HJ, Park SI, Yu KS, Cho JY: Combined untargeted and targeted metabolomic profiling reveals urinary biomarkers for discriminating obese from normal-weight adolescents. Pediatr Obes. 2017 Apr;12(2):93-101. doi: 10.1111/jpo.12114. Epub 2016 Feb 22. PMID: 26910390

### PC(22:5(4Z,7Z,10Z,13Z,16Z)/20:5(5Z,8Z,11Z,14Z,17Z)) -- Introduction

SYNONYM: GPCho(22:5/20:5); PC(22:5(4Z,7Z,10Z,13Z,16Z)/20:5(5Z,8Z,11Z,14Z,17Z)); PC(22:5/20:5); PC(42:10); GPCho(42:10); Lecithin; 1-*osbondoyl*-2-eicosapentaenoyl-sn-glycero-3-phosphocholine; Phosphatidylcholine(22:5/20:5); 1-(4Z,7Z,10Z,13Z,16Z-docosapentaenoyl)-2-(5Z,8Z,11Z,14Z,17Z-eicosapentaenoyl)-sn-glycero-3-phosphocholine; Phosphatidylcholine(42:10)



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HMDB: HMDB0008675; HMDB08675

CAS:

PC(22:5(4Z,7Z,10Z,13Z,16Z)/20:5(5Z,8Z,11Z,14Z,17Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common.

PC(22:5(4Z,7Z,10Z,13Z,16Z)/20:5(5Z,8Z,11Z,14Z,17Z)), in particular, consists of one chain of docosapentaenoic acid at the C-1 position and one chain of eicosapentaenoic acid at the C-2 position. The docosapentaenoic acid moiety is derived from animal fats and brain, while the eicosapentaenoic acid moiety is derived from fish oils, liver and kidney. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

### **PC(22:5(4Z,7Z,10Z,13Z,16Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)) -- Introduction**

SYNONYM: 1-Docosapentaenoyl-2-docosahexaenoyl-sn-glycero-3-phosphocholine; 1-Osbondoyl-2-docosahexaenoyl-sn-glycero-3-phosphocholine; gpcho(22:5/22:6); gpcho(22:5n6/22:6n3); gpcho(22:5W6/22:6W3); gpcho(44:11); Lecithin; PC(22:5/22:6); PC(22:5n6/22:6n3); PC(22:5W6/22:6W3); PC(44:11); Phosphatidylcholine(22:5/22:6); Phosphatidylcholine(22:5n6/22:6n3); Phosphatidylcholine(22:5W6/22:6W3); Phosphatidylcholine(44:11); PC(22:5(4Z,7Z,10Z,13Z,16Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)); 1-(4Z,7Z,10Z,13Z,16Z-docosapentaenoyl)-2-(4Z,7Z,10Z,13Z,16Z,19Z-docosahexaenoyl)-sn-glycero-3-phosphocholine

HMDB: HMDB0008682; HMDB08682

CAS:

PC(22:5(4Z,7Z,10Z,13Z,16Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common.

PC(22:5(4Z,7Z,10Z,13Z,16Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)), in particular, consists of one chain of docosapentaenoic acid at the C-1 position and one chain of docosahexaenoic acid at the C-2 position. The docosapentaenoic acid moiety is derived from animal fats and brain, while the docosahexaenoic acid moiety is derived from fish oils. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

### **PC(22:5(7Z,10Z,13Z,16Z,19Z)/14:0) -- Introduction**

SYNONYM: 1-docosapentaenoyl-2-myristoyl-sn-glycero-3-phosphocholine; GPCho(22:5/14:0); Phosphatidylcholine(22:5/14:0); GPCho(36:5); Phosphatidylcholine(36:5); Lecithin; PC(36:5); PC(22:5(7Z,10Z,13Z,16Z,19Z)/14:0); 1-(7Z,10Z,13Z,16Z,19Z-docosapentaenoyl)-2-tetradecanoyl-sn-glycero-3-phosphocholine; PC(22:5/14:0)



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HMDB: HMDB0008689; HMDB08689

CAS:

PC(22:5(7Z,10Z,13Z,16Z,19Z)/14:0) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(22:5(7Z,10Z,13Z,16Z,19Z)/14:0), in particular, consists of one chain of docosapentaenoic acid at the C-1 position and one chain of myristic acid at the C-2 position. The docosapentaenoic acid moiety is derived from fish oils, while the myristic acid moiety is derived from nutmeg and butter. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

### PC(22:5(7Z,10Z,13Z,16Z,19Z)/14:0) – Pregnancy

Andreolini F, Borra C, Caccamo F, Di Corcia A, Nicoletti I, Samperi R, Improta F: Estriol and its conjugates in late pregnancy determined by extraction with Carbopack B and liquid chromatography with fluorometric detection. Clin Chem 1985 Oct;31(10):1698-702. PMID: 2994907

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Ribar S, Mesaric M, Sedic M: Sphingoid bases as possible diagnostic parameters. Croat Med J. 2003 Apr;44(2):165-70. PMID: 12698507

Khan HA, Sobki SH, Alhomida AS: Fluctuations in fasting blood glucose and serum fructosamine in pregnant women monitored on successive antenatal visits. Clin Exp Med. 2006 Oct;6(3):134-7. PMID: 17061063

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Yang YJ, Lee J, Choi MH, Chung BC: Direct determination of estriol 3- and 16-glucuronides in pregnancy urine by column-switching liquid chromatography with electrospray tandem mass spectrometry. Biomed Chromatogr. 2003 Jun;17(4):219-25. PMID: 12833386

Huang PC, Kuo PL, Guo YL, Liao PC, Lee CC: Associations between urinary phthalate monoesters and thyroid hormones in pregnant women. Hum Reprod. 2007 Oct;22(10):2715-22. Epub 2007 Aug 17. PMID: 17704099

Mikkelsen TB, Osler M, Olsen SF: Validity of protein, retinol, folic acid and n-3 fatty acid intakes estimated from the food-frequency questionnaire used in the Danish National Birth Cohort. Public Health Nutr. 2006 Sep;9(6):771-8. PMID: 16925883

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Brantsaeter AL, Haugen M, Julshamn K, Alexander J, Meltzer HM: Evaluation of urinary iodine excretion as a biomarker for intake of milk and dairy products in pregnant women in the Norwegian Mother and Child Cohort Study (MoBa). Eur J Clin Nutr. 2009 Mar;63(3):347-54. Epub 2007 Dec 5. PMID: 18059417

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Bahado-Singh RO, Akolekar R, Mandal R, Dong E, Xia J, Kruger M, Wishart DS, Nicolaides K: First-trimester



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metabolomic detection of late-onset preeclampsia. Am J Obstet Gynecol. 2013 Jan;208(1):58.e1-7. doi: 10.1016/j.ajog.2012.11.003. Epub 2012 Nov 13. PMID: 23159745

Bahado-Singh RO, Akolekar R, Mandal R, Dong E, Xia J, Kruger M, Wishart DS, Nicolaides K: Metabolomic analysis for first-trimester Down syndrome prediction. Am J Obstet Gynecol. 2013 May;208(5):371.e1-8. doi: 10.1016/j.ajog.2012.12.035. Epub 2013 Jan 8. PMID: 23313728

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### PC(22:5(7Z,10Z,13Z,16Z,19Z)/14:1(9Z)) -- Introduction

SYNONYM: 1-Docosapentaenoyl-2-myristoleoyl-sn-glycero-3-phosphocholine; gpcho(22:5/14:1); gpcho(22:5n3/14:1n5);



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gpcho(22:5W3/14:1W5); gpcho(36:6); Lecithin; PC Aa C36:6; PC(22:5/14:1); PC(22:5n3/14:1n5); PC(22:5W3/14:1W5); PC(36:6); Phosphatidylcholine(22:5/14:1); Phosphatidylcholine(22:5n3/14:1n5); Phosphatidylcholine(22:5W3/14:1W5); Phosphatidylcholine(36:6); PC(22:5(7Z,10Z,13Z,16Z,19Z)/14:1(9Z)); 1-(7Z,10Z,13Z,16Z,19Z-docosapentaenoyl)-2-(9Z-tetradecenoyl)-sn-glycero-3-phosphocholine

HMDB: HMDB0008690; HMDB08690

CAS:

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Cho K, Moon JS, Kang JH, Jang HB, Lee HJ, Park SI, Yu KS, Cho JY: Combined untargeted and targeted metabolomic profiling reveals urinary biomarkers for discriminating obese from normal-weight adolescents. *Pediatr Obes.* 2017 Apr;12(2):93-101. doi: 10.1111/ijpo.12114. Epub 2016 Feb 22. PMID: 26910390

## PC(22:5(7Z,10Z,13Z,16Z,19Z)/16:0) -- Introduction

SYNONYM: 1-Docosapentaenoyl-2-palmitoyl-sn-glycero-3-phosphocholine; gpcho(22:5/16:0); gpcho(22:5n3/16:0); gpcho(22:5W3/16:0); gpcho(38:5); Lecithin; PC Aa C38:5; PC(22:5/16:0); PC(22:5n3/16:0); PC(22:5W3/16:0); PC(38:5); Phosphatidylcholine(22:5/16:0); Phosphatidylcholine(22:5n3/16:0); Phosphatidylcholine(22:5W3/16:0); Phosphatidylcholine(38:5); PC(22:5(7Z,10Z,13Z,16Z,19Z)/16:0); 1-(7Z,10Z,13Z,16Z,19Z-docosapentaenoyl)-2-hexadecanoyl-sn-glycero-3-phosphocholine

HMDB: HMDB0008692; HMDB08692

CAS:

PC(22:5(7Z,10Z,13Z,16Z,19Z)/16:0) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(22:5(7Z,10Z,13Z,16Z,19Z)/16:0), in particular, consists of one chain of docosapentaenoic acid at the C-1 position and one chain of palmitic acid at the C-2 position. The docosapentaenoic acid moiety is derived from fish oils, while the palmitic acid moiety is derived from fish oils, milk fats, vegetable oils and animal fats. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

## PC(22:5(7Z,10Z,13Z,16Z,19Z)/16:0) – Pregnancy

Andreolini F, Borra C, Caccamo F, Di Corcia A, Nicoletti I, Samperi R, Improta F: Estriol and its conjugates in late pregnancy determined by extraction with Carbopack B and liquid chromatography with fluorometric detection. *Clin Chem.* 1985 Oct;31(10):1698-702. PMID: 2994907

Ball P, Emons G, Haupt O, Hoppen HO, Knuppen R: Radioimmunoassay of 2-hydroxyestrone. *Steroids.* 1978 Feb;31(2):249-58. PMID: 663967

Ribar S, Mesaric M, Sedic M: Sphingoid bases as possible diagnostic parameters. *Croat Med J.* 2003 Apr;44(2):165-70. PMID: 12698507

Khan HA, Sobki SH, Alhomida AS: Fluctuations in fasting blood glucose and serum fructosamine in pregnant women monitored on successive antenatal visits. *Clin Exp Med.* 2006 Oct;6(3):134-7. PMID: 17061063

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Mikkelsen TB, Osler M, Olsen SF: Validity of protein, retinol, folic acid and n-3 fatty acid intakes estimated from the food-



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frequency questionnaire used in the Danish National Birth Cohort. *Public Health Nutr.* 2006 Sep;9(6):771-8. PMID: 16925883

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Brantsaeter AL, Haugen M, Julshamn K, Alexander J, Meltzer HM: Evaluation of urinary iodine excretion as a biomarker for intake of milk and dairy products in pregnant women in the Norwegian Mother and Child Cohort Study (MoBa). *Eur J Clin Nutr.* 2009 Mar;63(3):347-54. Epub 2007 Dec 5. PMID: 18059417

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## PC(22:5(7Z,10Z,13Z,16Z,19Z)/16:1(9Z)) -- Introduction

**SYNONYM:** PC(22:5/16:1); GPCho(38:6); Lecithin; GPCho(22:5/16:1); Phosphatidylcholine(38:6); Phosphatidylcholine(22:5/16:1); PC(22:5(7Z,10Z,13Z,16Z,19Z)/16:1(9Z)); 1-docosapentaenoyl-2-palmitoleoyl-sn-glycero-3-phosphocholine; 1-(7Z,10Z,13Z,16Z,19Z-docosapentaenoyl)-2-(9Z-hexadecenoyl)-sn-glycero-3-phosphocholine; PC(38:6)

**HMDB:** HMDB0008693; HMDB08693

**CAS:**

PC(22:5(7Z,10Z,13Z,16Z,19Z)/16:1(9Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common.

PC(22:5(7Z,10Z,13Z,16Z,19Z)/16:1(9Z)), in particular, consists of one chain of docosapentaenoic acid at the C-1 position and one chain of palmitoleic acid at the C-2 position. The docosapentaenoic acid moiety is derived from fish oils, while the palmitoleic acid moiety is derived from animal fats and vegetable oils. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

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## PC(22:5(7Z,10Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z)) -- Introduction

**SYNONYM:** 1-Docosapentaenoyl-2-g-linolenoyl-sn-glycero-3-phosphocholine; 1-Docosapentaenoyl-2-gamma-linolenoyl-sn-glycero-3-phosphocholine; gpcho(22:5/18:3); gpcho(22:5n3/18:3n6); gpcho(22:5W3/18:3W6); gpcho(40:8); Lecithin; PC(22:5/18:3); PC(22:5n3/18:3n6); PC(22:5W3/18:3W6); PC(40:8); Phosphatidylcholine(22:5/18:3); Phosphatidylcholine(22:5n3/18:3n6); Phosphatidylcholine(22:5W3/18:3W6); Phosphatidylcholine(40:8); PC(22:5(7Z,10Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z)); 1-(7Z,10Z,13Z,16Z,19Z-docosapentaenoyl)-2-(6Z,9Z,12Z-octadecatrienoyl)-sn-glycero-3-phosphocholine

HMDB: HMDB0008698; HMDB08698

CAS:

PC(22:5(7Z,10Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common.

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This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

## PC(22:5(7Z,10Z,13Z,16Z,19Z)/20:1(11Z)) -- Introduction

**SYNONYM:** 1-Docosapentaenoyl-2-eicosenoyl-sn-glycero-3-phosphocholine; gpcho(22:5/20:1); gpcho(22:5n3/20:1n9); gpcho(22:5W3/20:1W9); gpcho(42:6); Lecithin; PC Aa C42:6; PC(22:5/20:1); PC(22:5n3/20:1n9); PC(22:5W3/20:1W9); PC(42:6); Phosphatidylcholine(22:5/20:1); Phosphatidylcholine(22:5n3/20:1n9); Phosphatidylcholine(22:5W3/20:1W9); Phosphatidylcholine(42:6); 1-(7Z,10Z,13Z,16Z,19Z-docosapentaenoyl)-2-(11-eicosenoyl)-sn-glycero-3-phosphocholine; PC(22:5(7Z,10Z,13Z,16Z,19Z)/20:1(11Z))

HMDB: HMDB0008702; HMDB08702



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CAS:

PC(22:5(7Z,10Z,13Z,16Z,19Z)/20:1(11Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common.

PC(22:5(7Z,10Z,13Z,16Z,19Z)/20:1(11Z)), in particular, consists of one chain of docosapentaenoic acid at the C-1 position and one chain of eicosenoic acid at the C-2 position. The docosapentaenoic acid moiety is derived from fish oils, while the eicosenoic acid moiety is derived from vegetable oils and cod oils. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

### PC(22:5(7Z,10Z,13Z,16Z,19Z)/20:1(11Z)) -- Pregnancy

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## PC(22:5(7Z,10Z,13Z,16Z,19Z)/20:4(5Z,8Z,11Z,14Z)) -- Introduction

**SYNONYM:** 1-Docosapentaenoyl-2-arachidonoyl-sn-glycero-3-phosphocholine; gpcho(22:5/20:4); gpcho(22:5n3/20:4n6); gpcho(22:5W3/20:4W6); gpcho(42:9); Lecithin; PC(22:5/20:4); PC(22:5n3/20:4n6); PC(22:5W3/20:4W6); PC(42:9); Phosphatidylcholine(22:5/20:4); Phosphatidylcholine(22:5n3/20:4n6); Phosphatidylcholine(22:5W3/20:4W6); Phosphatidylcholine(42:9); PC(22:5(7Z,10Z,13Z,16Z,19Z)/20:4(5Z,8Z,11Z,14Z)); 1-(7Z,10Z,13Z,16Z,19Z-docosapentaenoyl)-2-(5Z,8Z,11Z,14Z-eicosatetraenoyl)-sn-glycero-3-phosphocholine

**HMDB:** HMDB0008706; HMDB08706

**CAS:**

PC(22:5(7Z,10Z,13Z,16Z,19Z)/20:4(5Z,8Z,11Z,14Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common.

PC(22:5(7Z,10Z,13Z,16Z,19Z)/20:4(5Z,8Z,11Z,14Z)), in particular, consists of one chain of docosapentaenoic acid at the C-1 position and one chain of arachidonic acid at the C-2 position. The docosapentaenoic acid moiety is derived from fish oils, while the arachidonic acid moiety is derived from animal fats and eggs. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

## PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/16:1(9Z)) -- Introduction

**SYNONYM:** GPCho(22:6/16:1); Phosphatidylcholine(22:6/16:1); GPCho(38:7); PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/16:1(9Z)); Lecithin; Phosphatidylcholine(38:7); PC(22:6/16:1); 1-docosahexaenoyl-2-palmitoleoyl-sn-glycero-3-phosphocholine; 1-(4Z,7Z,10Z,13Z,16Z,19Z-docosahexaenoyl)-2-(9Z-hexadecenoyl)-sn-glycero-3-phosphocholine; PC(38:7)

**HMDB:** HMDB0008726; HMDB08726

**CAS:**

PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/16:1(9Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the



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C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/16:1(9Z)), in particular, consists of one chain of docosahexaenoic acid at the C-1 position and one chain of palmitoleic acid at the C-2 position. The docosahexaenoic acid moiety is derived from fish oils, while the palmitoleic acid moiety is derived from animal fats and vegetable oils. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

### **PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:1(11Z)) -- Introduction**

SYNONYM: Phosphatidylcholine(22:6/18:1); 1-docosahexaenoyl-2-vaccenoyl-sn-glycero-3-phosphocholine; GPCho(40:7); Lecithin; Phosphatidylcholine(40:7); PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:1(11Z)); PC(40:7); PC(22:6/18:1); 1-(4Z,7Z,10Z,13Z,16Z,19Z-docosahexaenoyl)-2-(11Z-octadecenoyl)-sn-glycero-3-phosphocholine; GPCho(22:6/18:1)

HMDB: HMDB0008728; HMDB08728

CAS:

PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:1(11Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common.

PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:1(11Z)), in particular, consists of one chain of docosahexaenoic acid at the C-1 position and one chain of vaccenic acid at the C-2 position. The docosahexaenoic acid moiety is derived from fish oils, while the vaccenic acid moiety is derived from butter fat and animal fat. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

### **PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:1(11Z)) -- Introduction**

SYNONYM: 1-Docosahexaenoyl-2-eicosenoyl-sn-glycero-3-phosphocholine; gpcho(22:6/20:1); gpcho(22:6n3/20:1n9); gpcho(22:6W3/20:1W9); gpcho(42:7); Lecithin; PC(22:6/20:1); PC(22:6n3/20:1n9); PC(22:6W3/20:1W9); PC(42:7); Phosphatidylcholine(22:6/20:1); Phosphatidylcholine(22:6n3/20:1n9); Phosphatidylcholine(22:6W3/20:1W9); Phosphatidylcholine(42:7); PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:1(11Z)); 1-(4Z,7Z,10Z,13Z,16Z,19Z-docosahexaenoyl)-2-(11-eicosenoyl)-sn-glycero-3-phosphocholine

HMDB: HMDB0008735; HMDB08735

CAS:

PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:1(11Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common.



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PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:1(11Z)), in particular, consists of one chain of docosahexaenoic acid at the C-1 position and one chain of eicosenoic acid at the C-2 position. The docosahexaenoic acid moiety is derived from fish oils, while the eicosenoic acid moiety is derived from vegetable oils and cod oils. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

### **PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:4(5Z,8Z,11Z,14Z)) -- Introduction**

SYNONYM: Phosphatidylcholine(42:10); PC(22:6/20:4); PC(42:10); GPCho(22:6/20:4); GPCho(42:10); Lecithin; 1-docosahexaenoyl-2-arachidonoyl-sn-glycero-3-phosphocholine; Phosphatidylcholine(22:6/20:4); 1-(4Z,7Z,10Z,13Z,16Z,19Z-docosahexaenoyl)-2-(5Z,8Z,11Z,14Z-eicosatetraenoyl)-sn-glycero-3-phosphocholine; PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:4(5Z,8Z,11Z,14Z))

HMDB: HMDB0008739; HMDB08739

CAS:

PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:4(5Z,8Z,11Z,14Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common.

PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:4(5Z,8Z,11Z,14Z)), in particular, consists of one chain of docosahexaenoic acid at the C-1 position and one chain of arachidonic acid at the C-2 position. The docosahexaenoic acid moiety is derived from fish oils, while the arachidonic acid moiety is derived from animal fats and eggs. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

### **PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:1(13Z)) -- Introduction**

SYNONYM: PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:1(13Z)); GPCho(44:7); GPCho(22:6/22:1); Phosphatidylcholine(44:7); Lecithin; PC(44:7); 1-docosahexaenoyl-2-erucoyl-sn-glycero-3-phosphocholine; Phosphatidylcholine(22:6/22:1); 1-(4Z,7Z,10Z,13Z,16Z,19Z-docosahexaenoyl)-2-(13Z-docosenoyl)-sn-glycero-3-phosphocholine; PC(22:6/22:1)

HMDB: HMDB0008743; HMDB08743

CAS:

PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:1(13Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common.

PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:1(13Z)), in particular, consists of one chain of docosahexaenoic acid at the C-1 position and one chain of erucic acid at the C-2 position. The docosahexaenoic acid moiety is derived from fish oils, while the



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erucic acid moiety is derived from seed oils and avocados. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

### **PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)) -- Introduction**

SYNONYM: 1,2-Didocosahexaenoyl-rac-glycero-3-phosphocholine; gpcho(22:6/22:6); gpcho(22:6n3/22:6n3); gpcho(22:6W3/22:6W3); gpcho(44:12); Lecithin; PC(22:6/22:6); PC(22:6n3/22:6n3); PC(22:6W3/22:6W3); PC(44:12); Phosphatidylcholine(22:6/22:6); Phosphatidylcholine(22:6n3/22:6n3); Phosphatidylcholine(22:6W3/22:6W3); Phosphatidylcholine(44:12); PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)); 1,2-di(4Z,7Z,10Z,13Z,16Z,19Z-docosahexaenoyl)-rac-glycero-3-phosphocholine

HMDB: HMDB0008748; HMDB08748

CAS:

PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common.

PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)), in particular, consists of two chains of docosahexaenoic acid at the C-1 and C-2 positions. The docosahexaenoic acid moieties are derived from fish oils. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

### **PC(24:1(15Z)/18:4(6Z,9Z,12Z,15Z)) -- Introduction**

SYNONYM: 1-Nervonoyl-2-stearidonoyl-sn-glycero-3-phosphocholine; gpcho(24:1/18:4); gpcho(24:1n9/18:4n3); gpcho(24:1W9/18:4W3); gpcho(42:5); Lecithin; PC Aa C42:5; PC(24:1/18:4); PC(24:1n9/18:4n3); PC(24:1W9/18:4W3); PC(42:5); Phosphatidylcholine(24:1/18:4); Phosphatidylcholine(24:1n9/18:4n3); Phosphatidylcholine(24:1W9/18:4W3); Phosphatidylcholine(42:5); PC(24:1(15Z)/18:4(6Z,9Z,12Z,15Z)); 1-(15Z-tetracosanoyl)-2-(6Z,9Z,12Z,15Z-octadecatetraenoyl)-sn-glycero-3-phosphocholine

HMDB: HMDB0008799; HMDB08799

CAS:

PC(24:1(15Z)/18:4(6Z,9Z,12Z,15Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(24:1(15Z)/18:4(6Z,9Z,12Z,15Z)), in particular, consists of one chain of nervonic acid at the C-1 position and one chain of stearidonic acid at the C-2 position. The nervonic acid moiety is derived from fish oils, while the stearidonic acid moiety is derived from seed oils. Phospholipids, are ubiquitous



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in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC.

This compound belongs to the class of organic compounds known as phosphatidylcholines. These are glycerophosphocholines in which the two free -OH are attached to one fatty acid each through an ester linkage.

### PC(24:1(15Z)/18:4(6Z,9Z,12Z,15Z)) -- Pregnancy

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### PC(24:1(15Z)/18:4(6Z,9Z,12Z,15Z)) -- Obesity

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Cho K, Moon JS, Kang JH, Jang HB, Lee HJ, Park SI, Yu KS, Cho JY: Combined untargeted and targeted metabolomic profiling reveals urinary biomarkers for discriminating obese from normal-weight adolescents. Pediatr Obes. 2017 Apr;12(2):93-101. doi: 10.1111/jopo.12114. Epub 2016 Feb 22. PMID: 26910390

### PE(16:0/18:2(9Z,12Z)) -- Introduction

SYNONYM: 1-C16:0-2-C18:2(Omega-6)-phosphatidylethanolamine zwitterion; 1-Hexadecanoyl-2-(9Z,12Z)-octadecadienoyl-sn-glycero-3-phosphoethanolamine zwitterion; 1-Hexadecanoyl-2-(9Z,12Z-octadecadienoyl)-sn-glycero-3-phosphoethanolamine; 1-Hexadecanoyl-2-linoleoyl-sn-glycero-3-phosphoethanolamine zwitterion; 1-Palmitoyl-2-linoleoyl-gpe; 1-Palmitoyl-2-linoleoyl-gpe (16:0/18:2); 1-Palmitoyl-2-linoleoyl-sn-glycero-3-phosphoethanolamine zwitterion; GPE(16:0/18:2(9Z,12Z)); GPE(16:0/18:2); GPEtn(34:2); PE(16:0/18:2); 1-palmitoyl-2-linoleoyl-sn-glycero-3-phosphoethanolamine; Phophatidylethanolamine(16:0/18:2); GPEtn(16:0/18:2); PE(34:2); Phophatidylethanolamine(34:2); PE(16:0/18:2(9Z,12Z))

HMDB: HMDB0008928; HMDB0005322; HMDB05322; HMDB08928



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CAS:

PE(16:0/18:2(9Z,12Z)) is a phosphatidylethanolamine (PE or GPEtn). It is a glycerophospholipid in which a phosphorylethanolamine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphoethanolamines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PE(16:0/18:2(9Z,12Z)), in particular, consists of one chain of palmitic acid at the C-1 position and one chain of linoleic acid at the C-2 position. The palmitic acid moiety is derived from fish oils, milk fats, vegetable oils and animal fats, while the linoleic acid moiety is derived from seed oils. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PEs are neutral zwitterions at physiological pH. They mostly have palmitic or stearic acid on carbon 1 and a long chain unsaturated fatty acid (e.g. 18:2, 20:4 and 22:6) on carbon 2. PE synthesis can occur via two pathways. The first requires that ethanolamine be activated by phosphorylation and then coupled to CDP. The ethanolamine is then transferred from CDP-ethanolamine to phosphatidic acid to yield PE. The second involves the decarboxylation of PS.

This compound belongs to the class of organic compounds known as phosphatidylethanolamines. These are glycerophosphoethanolamines in which two fatty acids are bonded to the glycerol moiety through ester linkages.

## PE(16:0/18:3(9Z,12Z,15Z)) -- Introduction

SYNONYM: GPEtn(34:3); PE(16:0/18:3); GPEtn(16:0/18:3); PE(34:3); 1-palmitoyl-2-a-linolenoyl-sn-glycero-3-phosphoethanolamine; Phophatidylethanolamine(34:3); PE(16:0/18:3(9Z,12Z,15Z)); 1-hexadecanoyl-2-(9Z,12Z,15Z-octadeatrienoyl)-sn-glycero-3-phosphoethanolamine; Phophatidylethanolamine(16:0/18:3)

HMDB: HMDB0008930; HMDB08930

CAS:

PE(16:0/18:3(9Z,12Z,15Z)) is a phosphatidylethanolamine (PE or GPEtn). It is a glycerophospholipid in which a phosphorylethanolamine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphoethanolamines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PE(16:0/18:3(9Z,12Z,15Z)), in particular, consists of one chain of palmitic acid at the C-1 position and one chain of a-linolenic acid at the C-2 position. The palmitic acid moiety is derived from fish oils, milk fats, vegetable oils and animal fats, while the a-linolenic acid moiety is derived from seed oils, especially canola and soybean oil. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PEs are neutral zwitterions at physiological pH. They mostly have palmitic or stearic acid on carbon 1 and a long chain unsaturated fatty acid (e.g. 18:2, 20:4 and 22:6) on carbon 2. PE synthesis can occur via two pathways. The first requires that ethanolamine be activated by phosphorylation and then coupled to CDP. The ethanolamine is then transferred from CDP-ethanolamine to phosphatidic acid to yield PE. The second involves the decarboxylation of PS.

This compound belongs to the class of organic compounds known as phosphatidylethanolamines. These are glycerophosphoethanolamines in which two fatty acids are bonded to the glycerol moiety through ester linkages.

## PE(16:0/20:4(5Z,8Z,11Z,14Z)) -- Introduction

SYNONYM: 1-Hexadecanoyl-2-(5Z,8Z,11Z,14Z-eicosatetraenoyl)-sn-glycero-3-phosphoethanolamine; 1-Hexadecanoyl-2-(5Z,8Z,11Z,14Z-icosatetraenoyl)-sn-glycero-3-phosphoethanolamine zwitterion; 1-Hexadecanoyl-2-arachidonoyl-sn-glycero-3-phosphoethanolamine zwitterion; 1-Palmitoyl-2-(5Z,8Z,11Z,14Z-eicosatetraenoyl)-sn-glycero-3-phosphoethanolamine zwitterion; 1-Palmitoyl-2-arachidonoyl-sn-glycero-3-phosphoethanolamine zwitterion; GPEtn(36:4); GPEtn(16:0/20:4); Phophatidylethanolamine(16:0/20:4); PE(16:0/20:4); PE(36:4); PE(16:0/20:4(5Z,8Z,11Z,14Z)); 1-palmitoyl-2-arachidonoyl-sn-glycero-3-phosphoethanolamine; Phophatidylethanolamine(36:4)

HMDB: HMDB0008937; HMDB0005323; HMDB05323; HMDB08937



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CAS:

PE(16:0/20:4(5Z,8Z,11Z,14Z)) is a phosphatidylethanolamine (PE or GPEtn). It is a glycerophospholipid in which a phosphorylethanolamine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphoethanolamines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common.

PE(16:0/20:4(5Z,8Z,11Z,14Z)), in particular, consists of one chain of palmitic acid at the C-1 position and one chain of arachidonic acid at the C-2 position. The palmitic acid moiety is derived from fish oils, milk fats, vegetable oils and animal fats, while the arachidonic acid moiety is derived from animal fats and eggs. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PEs are neutral zwitterions at physiological pH. They mostly have palmitic or stearic acid on carbon 1 and a long chain unsaturated fatty acid (e.g. 18:2, 20:4 and 22:6) on carbon 2. PE synthesis can occur via two pathways. The first requires that ethanolamine be activated by phosphorylation and then coupled to CDP. The ethanolamine is then transferred from CDP-ethanolamine to phosphatidic acid to yield PE. The second involves the decarboxylation of PS.

This compound belongs to the class of organic compounds known as phosphatidylethanolamines. These are glycerophosphoethanolamines in which two fatty acids are bonded to the glycerol moiety through ester linkages.

### PE(16:0/20:4(5Z,8Z,11Z,14Z)) -- Metastatic melanoma

Frankel AE, Coughlin LA, Kim J, Froehlich TW, Xie Y, Frenkel EP, Koh AY: Metagenomic Shotgun Sequencing and Unbiased Metabolomic Profiling Identify Specific Human Gut Microbiota and Metabolites Associated with Immune Checkpoint Therapy Efficacy in Melanoma Patients. *Neoplasia*. 2017 Oct;19(10):848-855. doi: 10.1016/j.neo.2017.08.004. Epub 2017 Sep 15. PMID: 28923537

### PE(18:2(9Z,12Z)/14:0) -- Introduction

SYNONYM: GPEtn(18:2/14:0); PE(32:2); PE(18:2(9Z,12Z)/14:0); PE(18:2/14:0); 1-linoleoyl-2-myristoyl-sn-glycero-3-phosphoethanolamine; GPEtn(32:2); Phophatidylethanolamine(32:2); 1-(9Z,12Z-octadecadienoyl)-2-tetradecanoyl-sn-glycero-3-phosphoethanolamine; Phophatidylethanolamine(18:2/14:0)

HMDB: HMDB0009085; HMDB09085

CAS:

PE(18:2(9Z,12Z)/14:0) is a phosphatidylethanolamine (PE or GPEtn). It is a glycerophospholipid in which a phosphorylethanolamine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphoethanolamines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PE(18:2(9Z,12Z)/14:0), in particular, consists of one chain of linoleic acid at the C-1 position and one chain of myristic acid at the C-2 position. The linoleic acid moiety is derived from seed oils, while the myristic acid moiety is derived from nutmeg and butter. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PEs are neutral zwitterions at physiological pH. They mostly have palmitic or stearic acid on carbon 1 and a long chain unsaturated fatty acid (e.g. 18:2, 20:4 and 22:6) on carbon 2. PE synthesis can occur via two pathways. The first requires that ethanolamine be activated by phosphorylation and then coupled to CDP. The ethanolamine is then transferred from CDP-ethanolamine to phosphatidic acid to yield PE. The second involves the decarboxylation of PS.

This compound belongs to the class of organic compounds known as phosphatidylethanolamines. These are glycerophosphoethanolamines in which two fatty acids are bonded to the glycerol moiety through ester linkages.

### PE(18:2(9Z,12Z)/20:4(5Z,8Z,11Z,14Z)) -- Introduction

SYNONYM: GPEtn(38:6); 1-linoleoyl-2-arachidonoyl-sn-glycero-3-phosphoethanolamine;



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Phosphatidylethanolamine(18:2/20:4); GPEtn(18:2/20:4); PE(18:2(9Z,12Z)/20:4(5Z,8Z,11Z,14Z)); PE(18:2/20:4); PE(38:6); 1-(9Z,12Z-octadecadienoyl)-2-(5Z,8Z,11Z,14Z-eicosatetraenoyl)-sn-glycero-3-phosphoethanolamine; Phosphatidylethanolamine(38:6)

HMDB: HMDB0009102; HMDB09102

CAS:

PE(18:2(9Z,12Z)/20:4(5Z,8Z,11Z,14Z)) is a phosphatidylethanolamine (PE or GPEtn). It is a glycerophospholipid in which a phosphorylethanolamine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphoethanolamines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common.

PE(18:2(9Z,12Z)/20:4(5Z,8Z,11Z,14Z)), in particular, consists of one chain of linoleic acid at the C-1 position and one chain of arachidonic acid at the C-2 position. The linoleic acid moiety is derived from seed oils, while the arachidonic acid moiety is derived from animal fats and eggs. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PEs are neutral zwitterions at physiological pH. They mostly have palmitic or stearic acid on carbon 1 and a long chain unsaturated fatty acid (e.g. 18:2, 20:4 and 22:6) on carbon 2. PE synthesis can occur via two pathways. The first requires that ethanolamine be activated by phosphorylation and then coupled to CDP. The ethanolamine is then transferred from CDP-ethanolamine to phosphatidic acid to yield PE. The second involves the decarboxylation of PS.

This compound belongs to the class of organic compounds known as phosphatidylethanolamines. These are glycerophosphoethanolamines in which two fatty acids are bonded to the glycerol moiety through ester linkages.

## PE(20:5(5Z,8Z,11Z,14Z,17Z)/18:1(11Z)) -- Introduction

SYNONYM: PE(20:5/18:1); PE(20:5(5Z,8Z,11Z,14Z,17Z)/18:1(11Z)); GPEtn(20:5/18:1); Phosphatidylethanolamine(20:5/18:1); 1-eicosapentaenoyl-2-vaccenoyl-sn-glycero-3-phosphoethanolamine; GPEtn(38:6); PE(38:6); 1-(5Z,8Z,11Z,14Z,17Z-eicosapentaenoyl)-2-(11Z-octadecenoyl)-sn-glycero-3-phosphoethanolamine; Phosphatidylethanolamine(38:6)

HMDB: HMDB0009454; HMDB09454

CAS:

PE(20:5(5Z,8Z,11Z,14Z,17Z)/18:1(11Z)) is a phosphatidylethanolamine (PE or GPEtn). It is a glycerophospholipid in which a phosphorylethanolamine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphoethanolamines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common.

PE(20:5(5Z,8Z,11Z,14Z,17Z)/18:1(11Z)), in particular, consists of one chain of eicosapentaenoic acid at the C-1 position and one chain of vaccenic acid at the C-2 position. The eicosapentaenoic acid moiety is derived from fish oils, liver and kidney, while the vaccenic acid moiety is derived from butter fat and animal fat. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PEs are neutral zwitterions at physiological pH. They mostly have palmitic or stearic acid on carbon 1 and a long chain unsaturated fatty acid (e.g. 18:2, 20:4 and 22:6) on carbon 2. PE synthesis can occur via two pathways. The first requires that ethanolamine be activated by phosphorylation and then coupled to CDP. The ethanolamine is then transferred from CDP-ethanolamine to phosphatidic acid to yield PE. The second involves the decarboxylation of PS.

This compound belongs to the class of organic compounds known as phosphatidylethanolamines. These are glycerophosphoethanolamines in which two fatty acids are bonded to the glycerol moiety through ester linkages.

## PE(20:5(5Z,8Z,11Z,14Z,17Z)/P-18:0) -- Introduction

SYNONYM: Glycerophosphoethanolamine; 1-(5Z,8Z,11Z,14Z,17Z-Eicosapentaenoyl)-2-(1Z-octadecenyl)-sn-glycero-3-



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phosphoethanolamine; Glycerophosphoethanolamine(20:5(5Z,8Z,11Z,14Z,17Z)/p-18:0); PE(20:5); GPEtn(20:5); Phophatidylethanolamine(20:5); PE(20:5/P-18:0); GPEtn(20:5/P-18:0); Phophatidylethanolamine(20:5/p-18:0)

HMDB: HMDB0009478; HMDB09478

CAS:

PE(20:5(5Z,8Z,11Z,14Z,17Z)/P-18:0) is a phosphatidylethanolamine (PE or GPEtn). It is a glycerophospholipid in which a phosphorylethanolamine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphoethanolamines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common.

PE(20:5(5Z,8Z,11Z,14Z,17Z)/P-18:0), in particular, consists of one chain of eicosapentaenoic acid at the C-1 position and one chain of plasmalogen 18:0 at the C-2 position. The eicosapentaenoic acid moiety is derived from fish oils, liver and kidney, while the plasmalogen 18:0 moiety is derived from animal fats, liver and kidney. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PEs are neutral zwitterions at physiological pH. They mostly have palmitic or stearic acid on carbon 1 and a long chain unsaturated fatty acid (e.g. 18:2, 20:4 and 22:6) on carbon 2. PE synthesis can occur via two pathways. The first requires that ethanolamine be activated by phosphorylation and then coupled to CDP. The ethanolamine is then transferred from CDP-ethanolamine to phosphatidic acid to yield PE. The second involves the decarboxylation of PS. Plasmalogens are glycerol ether phospholipids. They are of two types, alkyl ether (-O-CH<sub>2</sub>-) and alkenyl ether (-O-CH=CH-). Dihydroxyacetone phosphate (DHAP) serves as the glycerol precursor for the synthesis of plasmalogens. Three major classes of plasmalogens have been identified: choline, ethanolamine and serine derivatives. Ethanolamine plasmalogen is prevalent in myelin. Choline plasmalogen is abundant in cardiac tissue. Usually, the highest proportion of the plasmalogen form is in the ethanolamine class with rather less in choline, and commonly little or none in other phospholipids such as phosphatidylinositol. In choline plasmalogens of most tissues, a higher proportion is often of the O-alkyl rather than the O-alkenyl form, but the reverse tends to be true in heart lipids. In animal tissues, the alkyl and alkenyl moieties in both non-polar and phospholipids tend to be rather simple in composition with 16:0, 18:0 and 18:1 (double bond in position 9) predominating. Ether analogues of triacylglycerols, i.e. 1-alkyldiacyl-sn-glycerols, are present at trace levels only if at all in most animal tissues, but they can be major components of some marine lipids.

This compound belongs to the class of organic compounds known as glycerophosphoethanolamines. These are glycerolipids characterized by an ethanolamine ester of glycerophosphoric acid. As is the case with diacylglycerols, glycerophosphoethanolamines can have many different combinations of fatty acids of varying lengths and saturation attached to the C-1 and C-2 atoms.

## PE(22:2(13Z,16Z)/14:1(9Z)) -- Introduction

SYNONYM: PE(36:3); Phophatidylethanolamine(22:2/14:1); GPEtn(22:2/14:1); Phophatidylethanolamine(36:3); 1-docosadienoyl-2-myristoleoyl-sn-glycero-3-phosphoethanolamine; GPEtn(36:3); PE(22:2/14:1); 1-(13Z,16Z-docosadienoyl)-2-(9Z-tetradecenoyl)-sn-glycero-3-phosphoethanolamine; PE(22:2(13Z,16Z)/14:1(9Z))

HMDB: HMDB0009548; HMDB09548

CAS:

PE(22:2(13Z,16Z)/14:1(9Z)) is a phosphatidylethanolamine (PE or GPEtn). It is a glycerophospholipid in which a phosphorylethanolamine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphoethanolamines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common.

PE(22:2(13Z,16Z)/14:1(9Z)), in particular, consists of one chain of docosadienoic acid at the C-1 position and one chain of myristoleic acid at the C-2 position. The docosadienoic acid moiety is derived from animal fats, while the myristoleic acid moiety is derived from milk fats. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PEs are neutral zwitterions at physiological pH. They mostly have palmitic or



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stearic acid on carbon 1 and a long chain unsaturated fatty acid (e.g. 18:2, 20:4 and 22:6) on carbon 2. PE synthesis can occur via two pathways. The first requires that ethanolamine be activated by phosphorylation and then coupled to CDP. The ethanolamine is then transferred from CDP-ethanolamine to phosphatidic acid to yield PE. The second involves the decarboxylation of PS.

This compound belongs to the class of organic compounds known as phosphatidylethanolamines. These are glycerophosphoethanolamines in which two fatty acids are bonded to the glycerol moiety through ester linkages.

### PE(22:4(7Z,10Z,13Z,16Z)/14:0) -- Introduction

SYNONYM: PE(22:4(7Z,10Z,13Z,16Z)/14:0); GPEtn(22:4/14:0); PE(22:4/14:0); PE(36:4); Phophatidylethanolamine(22:4/14:0); GPEtn(36:4); 1-adrenoyl-2-myristoyl-sn-glycero-3-phosphoethanolamine; 1-(7Z,10Z,13Z,16Z-docosatetraenoyl)-2-tetradecanoyl-sn-glycero-3-phosphoethanolamine; Phophatidylethanolamine(36:4)

HMDB: HMDB0009580; HMDB09580

CAS:

PE(22:4(7Z,10Z,13Z,16Z)/14:0) is a phosphatidylethanolamine (PE or GPEtn). It is a glycerophospholipid in which a phosphatidylethanolamine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphoethanolamines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common.

PE(22:4(7Z,10Z,13Z,16Z)/14:0), in particular, consists of one chain of adrenic acid at the C-1 position and one chain of myristic acid at the C-2 position. The adrenic acid moiety is derived from animal fats, while the myristic acid moiety is derived from nutmeg and butter. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PEs are neutral zwitterions at physiological pH. They mostly have palmitic or stearic acid on carbon 1 and a long chain unsaturated fatty acid (e.g. 18:2, 20:4 and 22:6) on carbon 2. PE synthesis can occur via two pathways. The first requires that ethanolamine be activated by phosphorylation and then coupled to CDP. The ethanolamine is then transferred from CDP-ethanolamine to phosphatidic acid to yield PE. The second involves the decarboxylation of PS.

This compound belongs to the class of organic compounds known as phosphatidylethanolamines. These are glycerophosphoethanolamines in which two fatty acids are bonded to the glycerol moiety through ester linkages.

### PE(22:5(4Z,7Z,10Z,13Z,16Z)/14:0) -- Introduction

SYNONYM: Phophatidylethanolamine(36:5); GPEtn(22:5/14:0); GPEtn(36:5); Phophatidylethanolamine(22:5/14:0); 1-oxobondoyl-2-myristoyl-sn-glycero-3-phosphoethanolamine; PE(36:5); PE(22:5(4Z,7Z,10Z,13Z,16Z)/14:0); 1-(4Z,7Z,10Z,13Z,16Z-docosapentaenoyl)-2-tetradecanoyl-sn-glycero-3-phosphoethanolamine; PE(22:5/14:0)

HMDB: HMDB0009613; HMDB09613

CAS:

PE(22:5(4Z,7Z,10Z,13Z,16Z)/14:0) is a phosphatidylethanolamine (PE or GPEtn). It is a glycerophospholipid in which a phosphatidylethanolamine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphoethanolamines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common.

PE(22:5(4Z,7Z,10Z,13Z,16Z)/14:0), in particular, consists of one chain of docosapentaenoic acid at the C-1 position and one chain of myristic acid at the C-2 position. The docosapentaenoic acid moiety is derived from animal fats and brain, while the myristic acid moiety is derived from nutmeg and butter. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PEs are neutral zwitterions at physiological pH. They mostly have palmitic or stearic acid on carbon 1 and a long chain unsaturated fatty acid (e.g. 18:2, 20:4 and 22:6) on carbon 2. PE synthesis can occur via two pathways. The first requires that ethanolamine be activated by phosphorylation and



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then coupled to CDP. The ethanolamine is then transferred from CDP-ethanolamine to phosphatidic acid to yield PE. The second involves the decarboxylation of PS.

This compound belongs to the class of organic compounds known as phosphatidylethanolamines. These are glycerophosphoethanolamines in which two fatty acids are bonded to the glycerol moiety through ester linkages.

### PE(22:5(4Z,7Z,10Z,13Z,16Z)/18:2(9Z,12Z)) -- Introduction

SYNONYM: PE(40:7); Phosphatidylethanolamine(22:5/18:2); Phosphatidylethanolamine(40:7); PE(22:5/18:2); GPEtn(22:5/18:2); 1-*osbondoyl*-2-linoleoyl-sn-glycero-3-phosphoethanolamine; GPEtn(40:7); 1-(4Z,7Z,10Z,13Z,16Z-docosapentaenoyl)-2-(9Z,12Z-octadecadienoyl)-sn-glycero-3-phosphoethanolamine; PE(22:5(4Z,7Z,10Z,13Z,16Z)/18:2(9Z,12Z))

HMDB: HMDB0009621; HMDB09621

CAS:

PE(22:5(4Z,7Z,10Z,13Z,16Z)/18:2(9Z,12Z)) is a phosphatidylethanolamine (PE or GPEtn). It is a glycerophospholipid in which a phosphorylethanolamine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphoethanolamines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common.

PE(22:5(4Z,7Z,10Z,13Z,16Z)/18:2(9Z,12Z)), in particular, consists of one chain of docosapentaenoic acid at the C-1 position and one chain of linoleic acid at the C-2 position. The docosapentaenoic acid moiety is derived from animal fats and brain, while the linoleic acid moiety is derived from seed oils. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PEs are neutral zwitterions at physiological pH. They mostly have palmitic or stearic acid on carbon 1 and a long chain unsaturated fatty acid (e.g. 18:2, 20:4 and 22:6) on carbon 2. PE synthesis can occur via two pathways. The first requires that ethanolamine be activated by phosphorylation and then coupled to CDP. The ethanolamine is then transferred from CDP-ethanolamine to phosphatidic acid to yield PE. The second involves the decarboxylation of PS.

This compound belongs to the class of organic compounds known as phosphatidylethanolamines. These are glycerophosphoethanolamines in which two fatty acids are bonded to the glycerol moiety through ester linkages.

### PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:1(11Z)) -- Introduction

SYNONYM: GPEtn(22:6/18:1); 1-docosahexaenoyl-2-vaccenoyl-sn-glycero-3-phosphoethanolamine; PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:1(11Z)); Phosphatidylethanolamine(40:7); PE(22:6/18:1); Phosphatidylethanolamine(22:6/18:1); GPEtn(40:7); 1-(4Z,7Z,10Z,13Z,16Z,19Z-docosahexaenoyl)-2-(11Z-octadecenoyl)-sn-glycero-3-phosphoethanolamine; PE(40:7)

HMDB: HMDB0009685; HMDB09685

CAS:

PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:1(11Z)) is a phosphatidylethanolamine (PE or GPEtn). It is a glycerophospholipid in which a phosphorylethanolamine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphoethanolamines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common.

PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:1(11Z)), in particular, consists of one chain of docosahexaenoic acid at the C-1 position and one chain of vaccenic acid at the C-2 position. The docosahexaenoic acid moiety is derived from fish oils, while the vaccenic acid moiety is derived from butter fat and animal fat. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PEs are neutral zwitterions at physiological pH. They mostly have palmitic or stearic acid on carbon 1 and a long chain unsaturated fatty acid (e.g. 18:2, 20:4 and 22:6) on carbon 2. PE synthesis can occur via two pathways. The first requires that ethanolamine be activated by



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phosphorylation and then coupled to CDP. The ethanolamine is then transferred from CDP-ethanolamine to phosphatidic acid to yield PE. The second involves the decarboxylation of PS.

This compound belongs to the class of organic compounds known as phosphatidylethanolamines. These are glycerophosphoethanolamines in which two fatty acids are bonded to the glycerol moiety through ester linkages.

## PI(18:1(11Z)/20:4(5Z,8Z,11Z,14Z)) -- Introduction

SYNONYM: PI(18:1/20:4); Phosphatidylinositol(18:1/20:4); PIno(38:5); PI(38:5); PIno(18:1/20:4); Phosphatidylinositol(38:5); 1-vaccenoyl-2-arachidonoyl-sn-glycero-3-phosphoinositol; 1-(11Z-octadecenoyl)-2-(5Z,8Z,11Z,14Z-eicosatetraenoyl)-sn-glycero-3-phospho-(1'-myo-inositol); 1-(11Z-octadecenoyl)-2-(5Z,8Z,11Z,14Z-eicosatetraenoyl)-sn-glycero-3-phosphoinositol; PI(18:1(11Z)/20:4(5Z,8Z,11Z,14Z))

HMDB: HMDB0009832; HMDB09832

CAS:

PI(18:1(11Z)/20:4(5Z,8Z,11Z,14Z)) is a phosphatidylinositol. Phosphatidylinositols are important lipids, both as a key membrane constituent and as a participant in essential metabolic processes, both directly and via a number of metabolites. Phosphatidylinositols are acidic (anionic) phospholipids that consist of a phosphatidic acid backbone, linked via the phosphate group to inositol (hexahydroxycyclohexane). Phosphatidylinositols can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 18 and 20 carbons are the most common. PI(18:1(11Z)/20:4(5Z,8Z,11Z,14Z)), in particular, consists of one chain of vaccenic acid at the C-1 position and one chain of arachidonic acid at the C-2 position. The vaccenic acid moiety is derived from butter fat and animal fat, while the arachidonic acid moiety is derived from animal fats and eggs. The inositol group that is part of every phosphatidylinositol lipid is covalently linked to the phosphate group that acts as a bridge to the lipid tail. In most organisms, the stereochemical form of this inositol is myo-D-inositol (with one axial hydroxyl in position 2 with the remainder equatorial), although other forms can be found in certain plant phosphatidylinositols. Phosphatidylinositol is especially abundant in brain tissue, where it can amount to 10% of the phospholipids, but it is present in all tissues and cell types. There is usually less of it than of phosphatidylcholine, phosphatidylethanolamine and phosphatidylserine. In animal tissues, phosphatidylinositol is the primary source of the arachidonic acid required for biosynthesis of eicosanoids, including prostaglandins, via the action of the enzyme phospholipase A2. Phosphatidylinositol can be phosphorylated by a number of different kinases that place the phosphate moiety on positions 4 and 5 of the inositol ring, although position 3 can also be phosphorylated by a specific kinase. Seven different isomers are known, but the most important in both quantitative and biological terms are phosphatidylinositol 4-phosphate and phosphatidylinositol 4,5-bisphosphate. Phosphatidylinositol and the phosphatidylinositol phosphates are the main source of diacylglycerols that serve as signaling molecules, via the action of phospholipase C enzymes. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PIs contain almost exclusively stearic acid at carbon 1 and arachidonic acid at carbon 2. PIs composed exclusively of non-phosphorylated inositol exhibit a net charge of -1 at physiological pH. Molecules with phosphorylated inositol (such as PIP, PIP2, PIP3, etc.) are termed polyphosphoinositides. The polyphosphoinositides are important intracellular transducers of signals emanating from the plasma membrane. The synthesis of PI involves CDP-activated 1,2-diacylglycerol condensation with myo-inositol.

This compound belongs to the class of organic compounds known as phosphatidylinositols. These are glycerophosphoinositols where the glycerol is esterified with two fatty acids.

## PI(18:2(9Z,12Z)/18:2(9Z,12Z)) -- Introduction

SYNONYM: PI(36:4); PI(18:2(9Z,12Z)/18:2(9Z,12Z)); Phosphatidylinositol(36:4); PIno(36:4); PIno(18:2/18:2); 1,2-di(9Z,12Z-octadecadienoyl)-rac-glycero-3-phospho-(1'-myo-inositol); PI(18:2/18:2); Phosphatidylinositol(18:2/18:2); 1,2-di(9Z,12Z-octadecadienoyl)-rac-glycero-3-phosphoinositol; 1,2-dilinoleoyl-rac-glycero-3-phosphoinositol

HMDB: HMDB0009850; HMDB09850

CAS:

PI(18:2(9Z,12Z)/18:2(9Z,12Z)) is a phosphatidylinositol. Phosphatidylinositols are important lipids, both as a key membrane constituent and as a participant in essential metabolic processes, both directly and via a number of metabolites.



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Phosphatidylinositols are acidic (anionic) phospholipids that consist of a phosphatidic acid backbone, linked via the phosphate group to inositol (hexahydroxycyclohexane). Phosphatidylinositols can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 18 and 20 carbons are the most common. PI(18:2(9Z,12Z)/18:2(9Z,12Z)), in particular, consists of one chain of linoleic acid at the C-1 position and one chain of linoleic acid at the C-2 position. The linoleic acid moiety is derived from seed oils, while the linoleic acid moiety is derived from seed oils. The inositol group that is part of every phosphatidylinositol lipid is covalently linked to the phosphate group that acts as a bridge to the lipid tail. In most organisms, the stereochemical form of this inositol is myo-D-inositol (with one axial hydroxyl in position 2 with the remainder equatorial), although other forms can be found in certain plant phosphatidylinositols. Phosphatidylinositol is especially abundant in brain tissue, where it can amount to 10% of the phospholipids, but it is present in all tissues and cell types. There is usually less of it than of phosphatidylcholine, phosphatidylethanolamine and phosphatidylserine. In animal tissues, phosphatidylinositol is the primary source of the arachidonic acid required for biosynthesis of eicosanoids, including prostaglandins, via the action of the enzyme phospholipase A2. Phosphatidylinositol can be phosphorylated by a number of different kinases that place the phosphate moiety on positions 4 and 5 of the inositol ring, although position 3 can also be phosphorylated by a specific kinase. Seven different isomers are known, but the most important in both quantitative and biological terms are phosphatidylinositol 4-phosphate and phosphatidylinositol 4,5-bisphosphate. Phosphatidylinositol and the phosphatidylinositol phosphates are the main source of diacylglycerols that serve as signaling molecules, via the action of phospholipase C enzymes. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PIs contain almost exclusively stearic acid at carbon 1 and arachidonic acid at carbon 2. PIs composed exclusively of non-phosphorylated inositol exhibit a net charge of -1 at physiological pH. Molecules with phosphorylated inositol (such as PIP, PIP2, PIP3, etc.) are termed polyphosphoinositides. The polyphosphoinositides are important intracellular transducers of signals emanating from the plasma membrane. The synthesis of PI involves CDP-activated 1,2-diacylglycerol condensation with myo-inositol.

This compound belongs to the class of organic compounds known as phosphatidylinositols. These are glycerophosphoinositols where the glycerol is esterified with two fatty acids.

### PI(20:2(11Z,14Z)/18:2(9Z,12Z)) -- Introduction

SYNONYM: PI(20:2(11Z,14Z)/18:2(9Z,12Z)); 1-(11Z,14Z-eicosadienoyl)-2-(9Z,12Z-octadecadienoyl)-sn-glycero-3-phospho-(1'-myo-inositol); Phosphatidylinositol(20:2/18:2); PI(38:4); PI<sub>NO</sub>(38:4); PI<sub>NO</sub>(20:2/18:2); 1-eicosadienoyl-2-linoleoyl-sn-glycero-3-phosphoinositol; Phosphatidylinositol(38:4); 1-(11Z,14Z-eicosadienoyl)-2-(9Z,12Z-octadecadienoyl)-sn-glycero-3-phosphoinositol; PI(20:2/18:2)

HMDB: HMDB0009877; HMDB09877

CAS:

PI(20:2(11Z,14Z)/18:2(9Z,12Z)) is a phosphatidylinositol. Phosphatidylinositols are important lipids, both as a key membrane constituent and as a participant in essential metabolic processes, both directly and via a number of metabolites. Phosphatidylinositols are acidic (anionic) phospholipids that consist of a phosphatidic acid backbone, linked via the phosphate group to inositol (hexahydroxycyclohexane). Phosphatidylinositols can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 18 and 20 carbons are the most common. PI(20:2(11Z,14Z)/18:2(9Z,12Z)), in particular, consists of one chain of eicosadienoic acid at the C-1 position and one chain of linoleic acid at the C-2 position. The eicosadienoic acid moiety is derived from fish oils and liver, while the linoleic acid moiety is derived from seed oils. The inositol group that is part of every phosphatidylinositol lipid is covalently linked to the phosphate group that acts as a bridge to the lipid tail. In most organisms, the stereochemical form of this inositol is myo-D-inositol (with one axial hydroxyl in position 2 with the remainder equatorial), although other forms can be found in certain plant phosphatidylinositols. Phosphatidylinositol is especially abundant in brain tissue, where it can amount to 10% of the phospholipids, but it is present in all tissues and cell types. There is usually less of it than of phosphatidylcholine, phosphatidylethanolamine and phosphatidylserine. In animal tissues, phosphatidylinositol is the primary source of the arachidonic acid required for biosynthesis of eicosanoids, including prostaglandins, via the action of the enzyme phospholipase A2. Phosphatidylinositol can be phosphorylated by a number of different kinases that place the phosphate moiety on positions 4 and 5 of the inositol ring, although position 3 can also be phosphorylated by a specific kinase. Seven different isomers are known, but the most important in both quantitative and biological terms are phosphatidylinositol 4-phosphate and phosphatidylinositol 4,5-bisphosphate. Phosphatidylinositol and the phosphatidylinositol phosphates are the main source of diacylglycerols that serve as signaling molecules, via the action of phospholipase C enzymes. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-



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1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PIs contain almost exclusively stearic acid at carbon 1 and arachidonic acid at carbon 2. PIs composed exclusively of non-phosphorylated inositol exhibit a net charge of -1 at physiological pH. Molecules with phosphorylated inositol (such as PIP, PIP2, PIP3, etc.) are termed polyphosphoinositides. The polyphosphoinositides are important intracellular transducers of signals emanating from the plasma membrane. The synthesis of PI involves CDP-activated 1,2-diacylglycerol condensation with myo-inositol.

This compound belongs to the class of organic compounds known as phosphatidylinositols. These are glycerophosphoinositols where the glycerol is esterified with two fatty acids.

## 5-KETE -- Introduction

SYNONYM: (6E,8Z,11Z,14Z)-5-Oxoicosa-6,8,11,14-tetraenoic acid; 5-keto-ETE; 5-Ketoeicosatetraenoic acid; 5-oxo, 6t,8C,11C,14C-20:4; 5-oxo-6(e),8(Z),11(Z),14(Z)-Eicosatetraenoic acid; 5-oxo-6E,8Z,11Z,14Z-Eicosatetraenoic acid; 5-oxo-Icosa-6,8,11,14-tetraenoic acid; 5-Oxoeicosatetraenoic acid; 5-OxoETE; 5-Oxoicosatetraenoic acid; Eicos-5,8,12,14-tetraenoic acid; (6E,8Z,11Z,14Z)-5-Oxoicosa-6,8,11,14-tetraenoate; 5-Ketoeicosatetraenoate; 5-oxo-6(e),8(Z),11(Z),14(Z)-Eicosatetraenoate; 5-oxo-6E,8Z,11Z,14Z-Eicosatetraenoate; 5-oxo-Icosa-6,8,11,14-tetraenoate; 5-Oxoeicosatetraenoate; 5-Oxoicosatetraenoate; Eicos-5,8,12,14-tetraenoate; 5-keto-6,8,11,14-Eicosatetraenoate; 5-keto-6,8,11,14-Eicosatetraenoic acid; 5-oxo-Eicosatetraenoate; 5-oxo-6,8,11,14-Eicosatetraenoate; 5-oxo-6,8,11,14-Eicosatetraenoic acid; 5-oxo-Eicosatetraenoic acid; 5-oxo-6,8,11,14-ETE; 5-oxo-6,8,11,14-Eicosatetraenoic acid, e,Z,Z,Z isomer

HMDB: HMDB0010217; HMDB10217

CAS: 126432-17-5

5-oxo-6E,8Z,11Z,14Z-eicosatetraenoic acid (5-oxo-ETE), 5-lipoxygenase product is a potent chemoattractant for neutrophils and eosinophils. Its actions are mediated by the oxoeicosanoid (OXE) receptor, a member of the G protein-coupled receptor family.(PMID:18292294).

This compound belongs to the class of organic compounds known as long-chain fatty acids. These are fatty acids with an aliphatic tail that contains between 13 and 21 carbon atoms.

## LysoPC(16:0) -- Introduction

SYNONYM: (2R)-2-Hydroxy-3-(hexadecanoxy)propyl 2-(trimethylazaniumyl)ethyl phosphate; 1-16:0-LysoPC; 1-16:0-Lysophosphatidylcholine; 1-Hexadecanoyl-2-lysophosphatidylcholine; 1-Palmitoyl-2-hydroxy-sn-glycero-3-phosphocholine; 1-Palmitoyl-2-lysophosphatidylcholine; 1-Palmitoyl-GPC; 1-Palmitoyl-GPC (16:0); 1-Palmitoyl-phosphatidylcholine; 1-Palmitoyl-sn-glycero-3-phosphocholine; 1-Palmitoylphosphatidylcholine; 16:0 lyso-PC; GPC(16:0); GPC(16:0/0:0); LPC 16:0/0:0; LPC(16:0); LPC(16:0/0:0); LyPC(16:0); LyPC(16:0/0:0); LysoPC 16:0/0:0; LysoPC(16:0/0:0); Lysophosphatidylcholine(16:0); Lysophosphatidylcholine(16:0/0:0); PC(16:0/0:0); (2R)-2-Hydroxy-3-(hexadecanoxy)propyl 2-(trimethylazaniumyl)ethyl phosphoric acid; 1-Palmitoyl-glycero-3-phosphocholine; 1-Palmitoyl-lysophosphatidylcholine; LysoPC a C16:0; 1-Pam-2-lysoptdcho; LysoPC(16:0); 1-hexadecanoyl-glycero-3-phosphocholine

HMDB: HMDB0010382; HMDB10382

CAS:

LysoPC(16:0) is a lysophospholipid (LyP). It is a monoglycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. Lysophosphatidylcholines can have different combinations of fatty acids of varying lengths and saturation attached at the C-1 (sn-1) position. Fatty acids containing 16, 18 and 20 carbons are the most common. LysoPC(16:0), in particular, consists of one chain of palmitic acid at the C-1 position. The palmitic acid moiety is derived from fish oils, milk fats, vegetable oils and animal fats. Lysophosphatidylcholine is found in small amounts in most tissues. It is formed by hydrolysis of phosphatidylcholine by the enzyme phospholipase A2, as part of the de-acylation/re-acylation cycle that controls its overall molecular species composition. It can also be formed inadvertently during extraction of lipids from tissues if the phospholipase is activated by careless handling. In blood plasma significant amounts of lysophosphatidylcholine are formed by a specific enzyme system, lecithin:cholesterol acyltransferase (LCAT), which is secreted from the liver. The enzyme catalyzes the transfer of the fatty acids of position sn-2 of phosphatidylcholine to the free cholesterol in plasma, with formation of cholesterol esters and lysophosphatidylcholine. Lysophospholipids have a role in lipid signaling by acting on lysophospholipid receptors (LPL-R). LPL-R's are members of the G protein-coupled receptor family



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of integral membrane proteins.

This compound belongs to the class of organic compounds known as 1-acyl-sn-glycero-3-phosphocholines. These are glycerophosphocholines in which the glycerol is esterified with a fatty acid at O-1 position, and linked at position 3 to a phosphocholine.

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## LysoPC(18:1(11Z)) -- Introduction

SYNONYM: 1-Vaccenoyl-glycero-3-phosphocholine; LPC(18:1); LysoPC(18:1); Lysophosphatidylcholine(18:1); LPC(18:1/0:0); LPC(18:1n7/0:0); LPC(18:1W7/0:0); LyPC(18:1); LyPC(18:1/0:0); LyPC(18:1n7/0:0); LyPC(18:1W7/0:0); LysoPC a C18:1; LysoPC(18:1/0:0); LysoPC(18:1n7/0:0); LysoPC(18:1W7/0:0); Lysophosphatidylcholine(18:1/0:0); Lysophosphatidylcholine(18:1n7/0:0); Lysophosphatidylcholine(18:1W7/0:0); LysoPC(18:1(11Z)); 1-(11Z-octadecenoyl)-glycero-3-phosphocholine

HMDB: HMDB0010385; HMDB10385

CAS:

LysoPC(18:1(11Z)) is a lysophospholipid (LyP). It is a monoglycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. Lysophosphatidylcholines can have different combinations of fatty acids of varying lengths and saturation attached at the C-1 (sn-1) position. Fatty acids containing 16, 18 and 20 carbons are the most common. LysoPC(18:1(11Z)), in particular, consists of one chain of vaccenic acid at the C-1 position. The vaccenic acid moiety is derived from butter fat and animal fat. Lysophosphatidylcholine is found in small amounts in most tissues. It is



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formed by hydrolysis of phosphatidylcholine by the enzyme phospholipase A2, as part of the de-acylation/re-acylation cycle that controls its overall molecular species composition. It can also be formed inadvertently during extraction of lipids from tissues if the phospholipase is activated by careless handling. In blood plasma significant amounts of lysophosphatidylcholine are formed by a specific enzyme system, lecithin:cholesterol acyltransferase (LCAT), which is secreted from the liver. The enzyme catalyzes the transfer of the fatty acids of position sn-2 of phosphatidylcholine to the free cholesterol in plasma, with formation of cholesterol esters and lysophosphatidylcholine. Lysophospholipids have a role in lipid signaling by acting on lysophospholipid receptors (LPL-R). LPL-R's are members of the G protein-coupled receptor family of integral membrane proteins.

This compound belongs to the class of organic compounds known as 1-acyl-sn-glycero-3-phosphocholines. These are glycerophosphocholines in which the glycerol is esterified with a fatty acid at O-1 position, and linked at position 3 to a phosphocholine.

### LysoPC(18:1(11Z)) -- Pregnancy

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### **LysoPC(18:3(6Z,9Z,12Z)) -- Introduction**

SYNONYM: 1-g-Linolenoyl-glycero-3-phosphocholine; 1-gamma-Linolenoyl-glycero-3-phosphocholine; LPC(18:3);

LPC(18:3/0:0); LPC(18:3n6/0:0); LPC(18:3W6/0:0); LyPC(18:3); LyPC(18:3/0:0); LyPC(18:3n6/0:0);  
 LyPC(18:3W6/0:0); LysoPC(18:3); LysoPC(18:3/0:0); LysoPC(18:3n6/0:0); LysoPC(18:3W6/0:0);  
 Lysophosphatidylcholine(18:3); Lysophosphatidylcholine(18:3/0:0); Lysophosphatidylcholine(18:3n6/0:0);  
 Lysophosphatidylcholine(18:3W6/0:0); LysoPC(18:3(6Z,9Z,12Z)); 1-(6Z,9Z,12Z-octadecatrienoyl)-glycero-3-phosphocholine

HMDB: HMDB0010387; HMDB10387

CAS:

LysoPC(18:3(6Z,9Z,12Z)) is a lysophospholipid (LyP). It is a monoglycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. Lysophosphatidylcholines can have different combinations of fatty acids of varying lengths and saturation attached at the C-1 (sn-1) position. Fatty acids containing 16, 18 and 20 carbons are the most common. LysoPC(18:3(6Z,9Z,12Z)), in particular, consists of one chain of g-linolenic acid at the C-1 position. The g-linolenic acid moiety is derived from animal fats. Lysophosphatidylcholine is found in small amounts in most tissues. It is formed by hydrolysis of phosphatidylcholine by the enzyme phospholipase A2, as part of the de-acylation/re-acylation cycle that controls its overall molecular species composition. It can also be formed inadvertently during extraction of lipids from tissues if the phospholipase is activated by careless handling. In blood plasma significant amounts of lysophosphatidylcholine are formed by a specific enzyme system, lecithin:cholesterol acyltransferase (LCAT), which is secreted from the liver. The enzyme catalyzes the transfer of the fatty acids of position sn-2 of phosphatidylcholine to the free cholesterol in plasma, with formation of cholesterol esters and lysophosphatidylcholine. Lysophospholipids have a role in lipid signaling by acting on lysophospholipid receptors (LPL-R). LPL-R's are members of the G protein-coupled receptor family of integral membrane proteins.

This compound belongs to the class of organic compounds known as 1-acyl-sn-glycero-3-phosphocholines. These are glycerophosphocholines in which the glycerol is esterified with a fatty acid at O-1 position, and linked at position 3 to a phosphocholine.

## **LysoPC(20:0/0:0) -- Introduction**

SYNONYM: 1-Arachidonyl-glycero-3-phosphocholine; 1-Arachidoyl-sn-glycero-3-phosphocholine; 1-Eicosanoyl-sn-glycero-3-phosphocholine; LPC(20:0); LPC(20:0/0:0); LysoPC(20:0/0:0); Lysophosphatidylcholine(20:0); Lysophosphatidylcholine(20:0/0:0); PC(20:0/0:0); LyPC(20:0); LyPC(20:0/0:0); LysoPC(20:0); 1-eicosanoyl-glycero-3-phosphocholine

HMDB: HMDB0010390; HMDB10390

CAS: 108341-80-6

LysoPC(20:0/0:0) is a lysophospholipid (LyP). It is a monoglycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. Lysophosphatidylcholines can have different combinations of fatty acids of varying lengths and saturation attached at the C-1 (sn-1) position. Fatty acids containing 16, 18 and 20 carbons are the most common. LysoPC(20:0/0:0), in particular, consists of one chain of arachidic acid at the C-1 position. The arachidic acid moiety is derived from peanut oil. Lysophosphatidylcholine is found in small amounts in most tissues. It is formed by hydrolysis of phosphatidylcholine by the enzyme phospholipase A2, as part of the de-acylation/re-acylation cycle that controls its overall molecular species composition. It can also be formed inadvertently during extraction of lipids from tissues if the phospholipase is activated by careless handling. In blood plasma significant amounts of lysophosphatidylcholine are formed by a specific enzyme system, lecithin:cholesterol acyltransferase (LCAT), which is secreted from the liver. The enzyme catalyzes the transfer of the fatty acids of position sn-2 of phosphatidylcholine to the free cholesterol in plasma, with formation of cholesterol esters and lysophosphatidylcholine. Lysophospholipids have a role in lipid signaling by acting on lysophospholipid receptors (LPL-R). LPL-R's are members of the G protein-coupled receptor family of integral membrane proteins.

This compound belongs to the class of organic compounds known as 1-acyl-sn-glycero-3-phosphocholines. These are glycerophosphocholines in which the glycerol is esterified with a fatty acid at O-1 position, and linked at position 3 to a phosphocholine.

## **LysoPC(20:3(5Z,8Z,11Z)) -- Introduction**

SYNONYM: 1-Meadoyl-glycero-3-phosphocholine; LPC 20:3(5Z,8Z,11Z)/0:0; LPC(20:3(5Z,8Z,11Z)/0:0); LysoPC

20:3(5Z,8Z,11Z)/0:0; LysoPC(20:3(5Z,8Z,11Z)/0:0); Lysophosphatidylcholine(20:3(5Z,8Z,11Z)/0:0); PC 20:3(5Z,8Z,11Z)/0:0; PC(20:3(5Z,8Z,11Z)/0:0); LPC(20:3); LPC(20:3/0:0); LPC(20:3n9/0:0); LPC(20:3W9/0:0); LyPC(20:3); LyPC(20:3/0:0); LyPC(20:3n9/0:0); LyPC(20:3W9/0:0); LysoPC a C20:3; LysoPC(20:3); LysoPC(20:3/0:0); LysoPC(20:3n9/0:0); LysoPC(20:3W9/0:0); Lysophosphatidylcholine(20:3); Lysophosphatidylcholine(20:3/0:0); Lysophosphatidylcholine(20:3n9/0:0); Lysophosphatidylcholine(20:3W9/0:0); LysoPC(20:3(5Z,8Z,11Z)); 1-(5Z,8Z,11Z-eicosatrienoyl)-glycero-3-phosphocholine

HMDB: HMDB0010393; HMDB10393

CAS: 1199257-41-4

LysoPC(20:3(5Z,8Z,11Z)) is a lysophospholipid (LyP). It is a monoglycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. Lysophosphatidylcholines can have different combinations of fatty acids of varying lengths and saturation attached at the C-1 (sn-1) position. Fatty acids containing 16, 18 and 20 carbons are the most common. LysoPC(20:3(5Z,8Z,11Z)), in particular, consists of one chain of mead acid at the C-1 position. The mead acid moiety is derived from fish oils, liver and kidney. Lysophosphatidylcholine is found in small amounts in most tissues. It is formed by hydrolysis of phosphatidylcholine by the enzyme phospholipase A2, as part of the de-acylation/re-acylation cycle that controls its overall molecular species composition. It can also be formed inadvertently during extraction of lipids from tissues if the phospholipase is activated by careless handling. In blood plasma significant amounts of lysophosphatidylcholine are formed by a specific enzyme system, lecithin:cholesterol acyltransferase (LCAT), which is secreted from the liver. The enzyme catalyzes the transfer of the fatty acids of position sn-2 of phosphatidylcholine to the free cholesterol in plasma, with formation of cholesterol esters and lysophosphatidylcholine. Lysophospholipids have a role in lipid signaling by acting on lysophospholipid receptors (LPL-R). LPL-R's are members of the G protein-coupled receptor family of integral membrane proteins.

This compound belongs to the class of organic compounds known as 1-acyl-sn-glycero-3-phosphocholines. These are glycerophosphocholines in which the glycerol is esterified with a fatty acid at O-1 position, and linked at position 3 to a phosphocholine.

### **LysoPC(20:3(5Z,8Z,11Z)) -- Pregnancy**

Andreolini F, Borra C, Caccamo F, Di Corcia A, Nicoletti I, Samperi R, Improta F: Estriol and its conjugates in late pregnancy determined by extraction with Carbopack B and liquid chromatography with fluorometric detection. Clin Chem. 1985 Oct;31(10):1698-702. PMID: 2994907

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Yang XL, Wu XR: The dynamic changes of several reproductive hormones during termination of early pregnancy by RU486 in combination with PG-05 in Chinese women. Adv Contracept. 1988 Dec;4(4):319-26. PMID: 3252730

Yang YJ, Lee J, Choi MH, Chung BC: Direct determination of estriol 3- and 16-glucuronides in pregnancy urine by column-switching liquid chromatography with electrospray tandem mass spectrometry. Biomed Chromatogr. 2003 Jun;17(4):219-25. PMID: 12833386

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Brantsaeter AL, Haugen M, Julshamn K, Alexander J, Meltzer HM: Evaluation of urinary iodine excretion as a biomarker for intake of milk and dairy products in pregnant women in the Norwegian Mother and Child Cohort Study (MoBa). *Eur J Clin Nutr.* 2009 Mar;63(3):347-54. Epub 2007 Dec 5. PMID: 18059417

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Bahado-Singh RO, Akolekar R, Chelliah A, Mandal R, Dong E, Kruger M, Wishart DS, Nicolaides K: Metabolomic analysis for first-trimester trisomy 18 detection. *Am J Obstet Gynecol.* 2013 Jul;209(1):65.e1-9. doi: 10.1016/j.ajog.2013.03.028. Epub 2013 Mar 25. PMID: 23535240

Bahado-Singh RO, Ertl R, Mandal R, Bjorndahl TC, Syngelaki A, Han B, Dong E, Liu PB, Alpay-Savasan Z, Wishart DS, Nicolaides KH: Metabolomic prediction of fetal congenital heart defect in the first trimester. *Am J Obstet Gynecol.* 2014 Sep;211(3):240.e1-240.e14. doi: 10.1016/j.ajog.2014.03.056. Epub 2014 Apr 1. PMID: 24704061

## LysoPC(20:4(5Z,8Z,11Z,14Z)) -- Introduction

SYNONYM: 1-(5Z,8Z,11Z,14Z-Eicosatetraenoyl)-sn-glycero-3-phosphocholine; 1-Arachidonoyl-glycero-3-phosphocholine; 1-Arachidonoyl-GPC; GPC(20:4n6); LPC 20:4(5Z,8Z,11Z,14Z)/0:0; LPC(20:4(5Z,8Z,11Z,14Z)/0:0); LysoPC 20:4(5Z,8Z,11Z,14Z)/0:0; LysoPC(20:4(5Z,8Z,11Z,14Z)/0:0); Lysophosphatidylcholine(20:4(5Z,8Z,11Z,14Z)/0:0); PC 20:4(5Z,8Z,11Z,14Z)/0:0; PC(20:4(5Z,8Z,11Z,14Z)/0:0); LPC(20:4); LPC(20:4/0:0); LPC(20:4n6/0:0); LPC(20:4W6/0:0); LyPC(20:4); LyPC(20:4/0:0); LyPC(20:4n6/0:0); LyPC(20:4W6/0:0); LysoPC a C20:4; LysoPC(20:4); LysoPC(20:4/0:0); LysoPC(20:4n6/0:0); LysoPC(20:4W6/0:0); Lysophosphatidylcholine(20:4); Lysophosphatidylcholine(20:4/0:0); Lysophosphatidylcholine(20:4n6/0:0); Lysophosphatidylcholine(20:4W6/0:0); LysoPC(20:4(5Z,8Z,11Z,14Z)); 1-(5Z,8Z,11Z,14Z-eicosatetraenoyl)-glycero-3-phosphocholine

HMDB: HMDB0010395; HMDB10395

CAS:

LysoPC(20:4(5Z,8Z,11Z,14Z)) is a lysophospholipid (LyP). It is a monoglycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. Lysophosphatidylcholines can have different combinations of fatty acids of varying lengths and saturation attached at the C-1 (sn-1) position. Fatty acids containing 16, 18 and 20 carbons are the most common. LysoPC(20:4(5Z,8Z,11Z,14Z)), in particular, consists of one chain of arachidonic acid at the C-1 position. The arachidonic acid moiety is derived from animal fats and eggs. Lysophosphatidylcholine is found in small amounts in most tissues. It is formed by hydrolysis of phosphatidylcholine by the enzyme phospholipase A2, as part of the deacylation/re-acylation cycle that controls its overall molecular species composition. It can also be formed inadvertently during extraction of lipids from tissues if the phospholipase is activated by careless handling. In blood plasma significant amounts of lysophosphatidylcholine are formed by a specific enzyme system, lecithin:cholesterol acyltransferase (LCAT), which is secreted from the liver. The enzyme catalyzes the transfer of the fatty acids of position sn-2 of phosphatidylcholine to the free cholesterol in plasma, with formation of cholesterol esters and lysophosphatidylcholine. Lysophospholipids have a role in lipid signaling by acting on lysophospholipid receptors (LPL-R). LPL-R's are members of the G protein-coupled receptor family of integral membrane proteins.

## LysoPC(20:4(5Z,8Z,11Z,14Z)) -- Pregnancy

Andreolini F, Borra C, Caccamo F, Di Corcia A, Nicoletti I, Samperi R, Improta F: Estriol and its conjugates in late pregnancy determined by extraction with Carbopack B and liquid chromatography with fluorometric detection. *Clin Chem.*



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## LyoPC(22:0) -- Introduction

SYNONYM: 1-Behenoyl-glycero-3-phosphocholine; LPC(22:0); LPC(22:0/0:0); LyPC(22:0); LyPC(22:0/0:0); LysoPC(22:0/0:0); Lysophosphatidylcholine(22:0); Lysophosphatidylcholine(22:0/0:0); 1-docosanoyl-glycero-3-phosphocholine; LysoPC(22:0)

HMDB: HMDB0010398; HMDB10398

CAS:

LyoPC(22:0) is a lysophospholipid (LyP). It is a monoglycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. Lysophosphatidylcholines can have different combinations of fatty acids of varying lengths and saturation attached at the C-1 (sn-1) position. Fatty acids containing 16, 18 and 20 carbons are the most common. LyoPC(22:0), in particular, consists of one chain of behenic acid at the C-1 position. The behenic acid moiety is derived from groundnut oil. Lysophosphatidylcholine is found in small amounts in most tissues. It is formed by hydrolysis of phosphatidylcholine by the enzyme phospholipase A2, as part of the de-acylation/re-acylation cycle that controls its overall molecular species composition. It can also be formed inadvertently during extraction of lipids from tissues if the phospholipase is activated by careless handling. In blood plasma significant amounts of lysophosphatidylcholine are formed by a specific enzyme system, lecithin:cholesterol acyltransferase (LCAT), which is secreted from the liver. The enzyme catalyzes the transfer of the fatty acids of position sn-2 of phosphatidylcholine to the free cholesterol in plasma, with formation of cholesterol esters and lysophosphatidylcholine. Lysophospholipids have a role in lipid signaling by acting on lysophospholipid receptors (LPL-R). LPL-R's are members of the G protein-coupled receptor family of integral membrane proteins.

This compound belongs to the class of organic compounds known as 1-acyl-sn-glycero-3-phosphocholines. These are glycerophosphocholines in which the glycerol is esterified with a fatty acid at O-1 position, and linked at position 3 to a phosphocholine.



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## LysoPC(24:0) -- Introduction

SYNONYM: 1-Lignoceroyl-glycero-3-phosphocholine; LyPC(24:0); Lysophosphatidylcholine(24:0); LPC(24:0); LPC(24:0/0:0); LyPC(24:0/0:0); LysoPC a C24:0; LysoPC(24:0/0:0); Lysophosphatidylcholine(24:0/0:0); LysoPC(24:0); 1-tetracosanoyl-glycero-3-phosphocholine

HMDB: HMDB0010405; HMDB10405

CAS:

LysoPC(24:0) is a lysophospholipid (LyP). It is a monoglycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. Lysophosphatidylcholines can have different combinations of fatty acids of varying lengths and saturation attached at the C-1 (sn-1) position. Fatty acids containing 16, 18 and 20 carbons are the most common. LysoPC(24:0), in particular, consists of one chain of lignoceric acid at the C-1 position. The lignoceric acid moiety is derived from groundnut oil. Lysophosphatidylcholine is found in small amounts in most tissues. It is formed by hydrolysis of phosphatidylcholine by the enzyme phospholipase A2, as part of the de-acylation/re-acylation cycle that controls its overall molecular species composition. It can also be formed inadvertently during extraction of lipids from tissues if the phospholipase is activated by careless handling. In blood plasma significant amounts of lysophosphatidylcholine are formed by a specific enzyme system, lecithin:cholesterol acyltransferase (LCAT), which is secreted from the liver. The enzyme catalyzes the transfer of the fatty acids of position sn-2 of phosphatidylcholine to the free cholesterol in plasma, with formation of cholesterol esters and lysophosphatidylcholine. Lysophospholipids have a role in lipid signaling by acting on lysophospholipid receptors (LPL-R). LPL-R's are members of the G protein-coupled receptor family of integral membrane proteins.

This compound belongs to the class of organic compounds known as 1-acyl-sn-glycero-3-phosphocholines. These are glycerophosphocholines in which the glycerol is esterified with a fatty acid at O-1 position, and linked at position 3 to a phosphocholine.

## LysoPC(P-16:0) -- Introduction

SYNONYM: 1-(1-Enyl-palmitoyl)-glycero-3-phosphocholine; LPC P-16:0/0:0; LPC(P-16:0/0:0); LysoPC P-16:0/0:0; LysoPC(P-16:0/0:0); Lysophosphatidylcholine(P-16:0/0:0); PC P-16:0/0:0; Lysoplasmenylethanolamine; Lysoplamalogens

HMDB: HMDB0010407; HMDB10407

CAS:

LysoPC(P-16:0) is a lysophospholipid (LyP). It is a monoglycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. Lysophosphatidylcholines can have different combinations of fatty acids of varying lengths and saturation attached at the C-1 (sn-1) position. Fatty acids containing 16, 18 and 20 carbons are the most common. LysoPC(P-16:0), in particular, consists of one chain of plasmalogen 16:0 at the C-1 position. The plasmalogen 16:0 moiety is derived from animal fats, liver and kidney. Lysophosphatidylcholine is found in small amounts in most tissues. It is formed by hydrolysis of phosphatidylcholine by the enzyme phospholipase A2, as part of the de-acylation/re-acylation cycle that controls its overall molecular species composition. It can also be formed inadvertently during extraction of lipids from tissues if the phospholipase is activated by careless handling. In blood plasma significant amounts of lysophosphatidylcholine are formed by a specific enzyme system, lecithin:cholesterol acyltransferase (LCAT), which is secreted from the liver. The enzyme catalyzes the transfer of the fatty acids of position sn-2 of phosphatidylcholine to the free cholesterol in plasma, with formation of cholesterol esters and lysophosphatidylcholine. Lysophospholipids have a role in lipid signaling by acting on lysophospholipid receptors (LPL-R). LPL-R's are members of the G protein-coupled receptor family of integral membrane proteins. Plasmalogens are glycerol ether phospholipids. They are of two types, alkyl ether (-O-CH<sub>2</sub>-) and alkenyl ether (-O-CH=CH-). Dihydroxyacetone phosphate (DHAP) serves as the glycerol precursor for the synthesis of plasmalogens. Three major classes of plasmalogens have been identified: choline, ethanolamine and serine derivatives. Ethanolamine plasmalogen is prevalent in myelin. Choline plasmalogen is abundant in cardiac tissue. Usually, the highest proportion of the plasmalogen form is in the ethanolamine class with rather less in choline, and commonly little or none in other phospholipids such as phosphatidylinositol. In choline plasmalogens of most tissues, a higher proportion is often of the O-alkyl rather than the O-alkenyl form, but the reverse tends to be true in heart lipids. In animal tissues, the alkyl and alkenyl moieties in both non-polar and phospholipids tend to be rather simple in composition with 16:0, 18:0 and 18:1 (double bond in position 9) predominating. Ether analogues of triacylglycerols, i.e. 1-alkyldiacyl-sn-glycerols, are present at trace levels only if at all in most animal tissues, but they can be major components of some marine lipids.

This compound belongs to the class of organic compounds known as 1-(1z-alkenyl)-glycero-3-phosphocholines. These



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are glycerophosphocholines that carry exactly one 1Z-alkenyl chain attached at the O1 position of a glycerol moiety through an ether linkage.

## 2-Phenylacetamide -- Introduction

SYNONYM: alpha-Phenylacetamide; alpha-Toluamide; Benzeneacetamide; Phenyl-beta-acetylamine; Phenylacetamide; Phenylacetic acid amide; a-Phenylacetamide;  $\beta$ -phenylacetamide; a-Toluamide;  $\beta$ -toluamide; Phenyl-b-acetylamine; Phenyl- $\beta^2$ -acetylamine; Phenylacetate amide; (alpha-)2-Phenylacetamide; 2-Phenyl-acetamide; alpha-Toluimidic acid; beta-Phenyl-acetylamine

HMDB: HMDB0010715; HMDB10715

CAS: 103-81-1

2-Phenylacetamide is an intermediate in phenylalanine metabolism and styrene degradation(KEGG ID C02505). It is the third to last step in the synthesis of phenylacetylglutamine and is converted from phenylalanine via the enzyme phenylalanine 2-monooxygenase [EC:1.13.12.9]. It is then converted to phenylacetate via the enzyme amidase [EC:3.5.1.4].

This compound belongs to the class of organic compounds known as phenylacetamides. These are amide derivatives of phenylacetic acids.

## PC(P-16:0/18:4(6Z,9Z,12Z,15Z)) -- Introduction

SYNONYM: 1-(1-Enyl-palmitoyl)-2-stearidonoyl-sn-glycero-3-phosphocholine; gpcho(16:0/18:4); gpcho(16:0/18:4n3); gpcho(16:0/18:4W3); gpcho(34:4); Lecithin; PC Aa C34:3; PC(16:0/18:4); PC(16:0/18:4n3); PC(16:0/18:4W3); PC(34:3); Phosphatidylcholine(16:0/18:4); Phosphatidylcholine(16:0/18:4n3); Phosphatidylcholine(16:0/18:4W3); Phosphatidylcholine(34:4)

HMDB: HMDB0011214; HMDB11214

CAS:

PC(P-16:0/18:4(6Z,9Z,12Z,15Z)) is a phosphatidylcholine (PC or GPCho). It is a glycerophospholipid in which a phosphorylcholine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphocholines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PC(P-16:0/18:4(6Z,9Z,12Z,15Z)), in particular, consists of one chain of plasmalogen 16:0 at the C-1 position and one chain of stearidonic acid at the C-2 position. The plasmalogen 16:0 moiety is derived from animal fats, liver and kidney, while the stearidonic acid moiety is derived from seed oils of hemp, blackcurrant and echium, and the cyanobacterium spirulina. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC. Plasmalogens are glycerol ether phospholipids. They are of two types, alkyl ether (-O-CH<sub>2</sub>-) and alkenyl ether (-O-CH=CH-). Dihydroxyacetone phosphate (DHAP) serves as the glycerol precursor for the synthesis of plasmalogens. Three major classes of plasmalogens have been identified: choline, ethanolamine and serine derivatives. Ethanolamine plasmalogen is prevalent in myelin. Choline plasmalogen is abundant in cardiac tissue. Usually, the highest proportion of the plasmalogen form is in the ethanolamine class with rather less in choline, and commonly little or none in other phospholipids such as phosphatidylinositol. In choline plasmalogens of most tissues, a higher proportion is often of the O-alkyl rather than the O-alkenyl form, but the reverse tends to be true in heart lipids. In animal tissues, the alkyl and alkenyl moieties in both non-polar and phospholipids tend to be rather simple in composition with 16:0, 18:0 and 18:1 (double bond in position 9) predominating. Ether analogues of triacylglycerols, i.e. 1-alkyldiacyl-sn-glycerols, are present at trace levels only if at all in most animal tissues, but they can be major components of some marine lipids. Phosphatidylcholines are a class of phospholipids which incorporate choline as a headgroup. They are a major component of biological membranes and can be isolated from either egg yolk (in Greek lekithos) or soy beans from which they are mechanically extracted or chemically extracted using hexane. Phosphatidylcholines are such a major component of lecithin, that, in some contexts, the terms are sometime used as synonyms. However, lecithin extract consists of a mixture of phosphatidylcholine and other compounds. It is also used along with sodium taurocholate for simulating fed- and fasted-state



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biorelevant media in dissolution studies of highly-lipophilic drugs. Phosphatidylcholine is a major constituent of cell membranes, and also plays a role in membrane-mediated cell signalling. Phospholipase D catalyzes the hydrolysis of phosphatidylcholine to form phosphatidic acid (PA), releasing the soluble choline headgroup into the cytosol. Some medical researchers are experimenting with using Phosphatidylcholine in a type of injection that will break down fat cells; to be used as an alternative to liposuction known as Injection lipolysis. (Wikipedia). While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PCs can be synthesized via three different routes. In one route, choline is activated first by phosphorylation and then by coupling to CDP prior to attachment to phosphatidic acid. PCs can also be synthesized by the addition of choline to CDP-activated 1,2-diacylglycerol. A third route to PC synthesis involves the conversion of either PS or PE to PC. Plasmalogens are glycerol ether phospholipids. They are of two types, alkyl ether (-O-CH<sub>2</sub>-) and alkenyl ether (-O-CH=CH-). Dihydroxyacetone phosphate (DHAP) serves as the glycerol precursor for the synthesis of plasmalogens. Three major classes of plasmalogens have been identified: choline, ethanolamine and serine derivatives. Ethanolamine plasmalogen is prevalent in myelin. Choline plasmalogen is abundant in cardiac tissue. Usually, the highest proportion of the plasmalogen form is in the ethanolamine class with rather less in choline, and commonly little or none in other phospholipids such as phosphatidylinositol. In choline plasmalogens of most tissues, a higher proportion is often of the O-alkyl rather than the O-alkenyl form, but the reverse tends to be true in heart lipids. In animal tissues, the alkyl and alkenyl moieties in both non-polar and phospholipids tend to be rather simple in composition with 16:0, 18:0 and 18:1 (double bond in position 9) predominating. Ether analogues of triacylglycerols, i.e. 1-alkyldiacyl-sn-glycerols, are present at trace levels only if at all in most animal tissues, but they can be major components of some marine lipids.

### PC(P-16:0/18:4(6Z,9Z,12Z,15Z)) – Pregnancy

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## PE(P-18:1(11Z)/18:4(6Z,9Z,12Z,15Z)) -- Introduction

SYNONYM: 1-(1-Enyl-vaccenoyl)-2-stearidonoyl-sn-glycero-3-phosphoethanolamine; GPEtn(18:1/18:4); GPEtn(18:1n7/18:4n3); GPEtn(18:1W7/18:4W3); GPEtn(36:5); PE(18:1/18:4); PE(18:1N7/18:4N3); PE(18:1W7/18:4W3); PE(36:5); Phophatidylethanolamine(18:1/18:4); Phophatidylethanolamine(18:1n7/18:4n3); Phophatidylethanolamine(18:1W7/18:4W3); Phophatidylethanolamine(36:5)

HMDB: HMDB0011412; HMDB11412

CAS:

PE(P-18:1(11Z)/18:4(6Z,9Z,12Z,15Z)) is a phosphatidylethanolamine (PE or GPEtn). It is a glycerophospholipid in which a phosphorylethanolamine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphoethanolamines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PE(P-18:1(11Z)/18:4(6Z,9Z,12Z,15Z)), in particular, consists of one chain of plasmalogen 18:1n7 at the C-1 position and one chain of stearidonic acid at the C-2 position. The plasmalogen 18:1n7 moiety is derived from animal fats, liver and kidney, while the stearidonic acid moiety is derived from seed oils. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PEs are neutral zwitterions at physiological pH. They mostly have palmitic or stearic acid on carbon 1 and a long chain unsaturated fatty acid (e.g. 18:2, 20:4 and 22:6) on carbon 2. PE synthesis can occur via two pathways. The first requires that ethanolamine be activated by phosphorylation and then coupled to CDP. The ethanolamine is then transferred from CDP-ethanolamine to phosphatidic acid to yield PE. The second involves the decarboxylation of PS. Plasmalogens are glycerol ether phospholipids. They are of two types, alkyl ether (-O-CH<sub>2</sub>-) and alkenyl ether (-O-CH=CH-). Dihydroxyacetone phosphate (DHAP) serves as the glycerol precursor for the synthesis of plasmalogens. Three major classes of plasmalogens have been identified: choline, ethanolamine and serine derivatives. Ethanolamine plasmalogen is prevalent in myelin. Choline plasmalogen is abundant in cardiac tissue. Usually, the highest proportion of the plasmalogen form is in the ethanolamine class with rather less in choline, and commonly little or none in other phospholipids such as phosphatidylinositol. In choline plasmalogens of most tissues, a higher proportion is often of the O-alkyl rather than the O-alkenyl form, but the reverse tends to be true in heart lipids. In animal tissues, the alkyl and alkenyl moieties in both non-polar and phospholipids tend to be rather simple in composition with 16:0, 18:0 and 18:1 (double bond in position 9) predominating. Ether analogues of triacylglycerols, i.e. 1-alkyldiacyl-sn-glycerols, are present at trace levels only if at all in most animal tissues, but they can be major components of some marine lipids.

This compound belongs to the class of organic compounds known as 1-(1z-alkenyl),2-acylglycerophosphoethanolamines. These are glycerophosphoethanolamines that carry exactly one acyl chain attached to the glycerol moiety through an ester linkage at the O2-position, and one 1Z-alkenyl chain attached through an ether linkage at the O1-position.

## PE(P-18:1(11Z)/22:5(4Z,7Z,10Z,13Z,16Z)) -- Introduction

SYNONYM: 1-(1-Enyl-vaccenoyl)-2-docosapentaenoyl-sn-glycero-3-phosphoethanolamine; 1-(1-Enyl-vaccenoyl)-2-oxbondoyl-sn-glycero-3-phosphoethanolamine; GPEtn(18:1/22:5); GPEtn(18:1n7/22:5n6); GPEtn(18:1W7/22:5W6); GPEtn(40:6); PE(18:1/22:5); PE(18:1N7/22:5N6); PE(18:1W7/22:5W6); PE(40:6); Phophatidylethanolamine(18:1/22:5); Phophatidylethanolamine(18:1n7/22:5n6); Phophatidylethanolamine(18:1W7/22:5W6); Phophatidylethanolamine(40:6)

HMDB: HMDB0011425; HMDB11425

CAS:

PE(P-18:1(11Z)/22:5(4Z,7Z,10Z,13Z,16Z)) is a phosphatidylethanolamine (PE or GPEtn). It is a glycerophospholipid in which a phosphorylethanolamine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphoethanolamines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PE(P-18:1(11Z)/22:5(4Z,7Z,10Z,13Z,16Z)), in particular, consists of one chain of plasmalogen 18:1n7 at the C-1 position and one chain of docosapentaenoic acid at the C-2 position. The plasmalogen 18:1n7 moiety is derived from animal fats, liver and kidney, while the docosapentaenoic acid moiety is derived from animal fats and brain. Phospholipids, are ubiquitous in nature



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and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PEs are neutral zwitterions at physiological pH. They mostly have palmitic or stearic acid on carbon 1 and a long chain unsaturated fatty acid (e.g. 18:2, 20:4 and 22:6) on carbon 2. PE synthesis can occur via two pathways. The first requires that ethanolamine be activated by phosphorylation and then coupled to CDP. The ethanolamine is then transferred from CDP-ethanolamine to phosphatidic acid to yield PE. The second involves the decarboxylation of PS. Plasmalogens are glycerol ether phospholipids. They are of two types, alkyl ether (-O-CH<sub>2</sub>-) and alkenyl ether (-O-CH=CH-). Dihydroxyacetone phosphate (DHAP) serves as the glycerol precursor for the synthesis of plasmalogens. Three major classes of plasmalogens have been identified: choline, ethanolamine and serine derivatives. Ethanolamine plasmalogen is prevalent in myelin. Choline plasmalogen is abundant in cardiac tissue. Usually, the highest proportion of the plasmalogen form is in the ethanolamine class with rather less in choline, and commonly little or none in other phospholipids such as phosphatidylinositol. In choline plasmalogens of most tissues, a higher proportion is often of the O-alkyl rather than the O-alkenyl form, but the reverse tends to be true in heart lipids. In animal tissues, the alkyl and alkenyl moieties in both non-polar and phospholipids tend to be rather simple in composition with 16:0, 18:0 and 18:1 (double bond in position 9) predominating. Ether analogues of triacylglycerols, i.e. 1-alkyldiacyl-sn-glycerols, are present at trace levels only if at all in most animal tissues, but they can be major components of some marine lipids.

This compound belongs to the class of organic compounds known as 1-(1Z-alkenyl),2-acylglycerophosphoethanolamines. These are glycerophosphoethanolamines that carry exactly one acyl chain attached to the glycerol moiety through an ester linkage at the O2-position, and one 1Z-alkenyl chain attached through an ether linkage at the O1-position.

## PE(P-18:1(11Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)) -- Introduction

SYNONYM: 1-(1-Enyl-vaccenoyl)-2-docosahexaenoyl-sn-glycero-3-phosphoethanolamine; GPEtn(18:1/22:6); GPEtn(18:1n7/22:6n3); GPEtn(18:1W7/22:6W3); GPEtn(40:7); PE(18:1/22:6); PE(18:1N7/22:6N3); PE(18:1W7/22:6W3); PE(40:7); Phophatidylethanolamine(18:1/22:6); Phophatidylethanolamine(18:1n7/22:6n3); Phophatidylethanolamine(18:1W7/22:6W3); Phophatidylethanolamine(40:7)

HMDB: HMDB0011427; HMDB11427

CAS:

PE(P-18:1(11Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)) is a phosphatidylethanolamine (PE or GPEtn). It is a glycerophospholipid in which a phosphatidylethanolamine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphoethanolamines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PE(P-18:1(11Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)), in particular, consists of one chain of plasmalogen 18:1n7 at the C-1 position and one chain of docosahexaenoic acid at the C-2 position. The plasmalogen 18:1n7 moiety is derived from animal fats, liver and kidney, while the docosahexaenoic acid moiety is derived from fish oils. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PEs are neutral zwitterions at physiological pH. They mostly have palmitic or stearic acid on carbon 1 and a long chain unsaturated fatty acid (e.g. 18:2, 20:4 and 22:6) on carbon 2. PE synthesis can occur via two pathways. The first requires that ethanolamine be activated by phosphorylation and then coupled to CDP. The ethanolamine is then transferred from CDP-ethanolamine to phosphatidic acid to yield PE. The second involves the decarboxylation of PS. Plasmalogens are glycerol ether phospholipids. They are of two types, alkyl ether (-O-CH<sub>2</sub>-) and alkenyl ether (-O-CH=CH-). Dihydroxyacetone phosphate (DHAP) serves as the glycerol precursor for the synthesis of plasmalogens. Three major classes of plasmalogens have been identified: choline, ethanolamine and serine derivatives. Ethanolamine plasmalogen is prevalent in myelin. Choline plasmalogen is abundant in cardiac tissue. Usually, the highest proportion of the plasmalogen form is in the ethanolamine class with rather less in choline, and commonly little or none in other phospholipids such as phosphatidylinositol. In choline plasmalogens of most tissues, a higher proportion is often of the O-alkyl rather than the O-alkenyl form, but the reverse tends to be true in heart lipids. In animal tissues, the alkyl and alkenyl moieties in both non-polar and phospholipids tend to be rather simple in composition with 16:0, 18:0 and 18:1 (double bond in position 9) predominating. Ether analogues of triacylglycerols, i.e. 1-alkyldiacyl-sn-glycerols, are present at trace levels only if at all in most animal tissues, but they can be major components of some marine



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lipids.

This compound belongs to the class of organic compounds known as 1-(1Z-alkenyl),2-acylglycerophosphoethanolamines. These are glycerophosphoethanolamines that carry exactly one acyl chain attached to the glycerol moiety through an ester linkage at the O2-position, and one 1Z-alkenyl chain attached through an ether linkage at the O1-position.

### PE(P-18:1(9Z)/20:5(5Z,8Z,11Z,14Z,17Z)) -- Introduction

SYNONYM: 1-(1-Enyl-oleoyl)-2-eicosapentaenoyl-sn-glycero-3-phosphoethanolamine; GPEtn(18:1/20:5); GPEtn(18:1n9/20:5n3); GPEtn(18:1W9/20:5W3); GPEtn(38:6); PE(18:1/20:5); PE(18:1n9/20:5N3); PE(18:1W9/20:5W3); PE(38:6); Phophatidylethanolamine(18:1/20:5); Phophatidylethanolamine(18:1n9/20:5n3); Phophatidylethanolamine(18:1W9/20:5W3); Phophatidylethanolamine(38:6)

HMDB: HMDB0011453; HMDB11453

CAS:

PE(P-18:1(9Z)/20:5(5Z,8Z,11Z,14Z,17Z)) is a phosphatidylethanolamine (PE or GPEtn). It is a glycerophospholipid in which a phosphorylethanolamine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphoethanolamines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PE(P-18:1(9Z)/20:5(5Z,8Z,11Z,14Z,17Z)), in particular, consists of one chain of plasmalogen 18:1n9 at the C-1 position and one chain of eicosapentaenoic acid at the C-2 position. The plasmalogen 18:1n9 moiety is derived from animal fats, liver and kidney, while the eicosapentaenoic acid moiety is derived from fish oils, liver and kidney. Phospholipids, are ubiquitous in nature and are key components of the lipid bilayer of cells, as well as being involved in metabolism and signaling. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. PEs are neutral zwitterions at physiological pH. They mostly have palmitic or stearic acid on carbon 1 and a long chain unsaturated fatty acid (e.g. 18:2, 20:4 and 22:6) on carbon 2. PE synthesis can occur via two pathways. The first requires that ethanolamine be activated by phosphorylation and then coupled to CDP. The ethanolamine is then transferred from CDP-ethanolamine to phosphatidic acid to yield PE. The second involves the decarboxylation of PS. Plasmalogens are glycerol ether phospholipids. They are of two types, alkyl ether (-O-CH<sub>2</sub>-) and alkenyl ether (-O-CH=CH-). Dihydroxyacetone phosphate (DHAP) serves as the glycerol precursor for the synthesis of plasmalogens. Three major classes of plasmalogens have been identified: choline, ethanolamine and serine derivatives. Ethanolamine plasmalogen is prevalent in myelin. Choline plasmalogen is abundant in cardiac tissue. Usually, the highest proportion of the plasmalogen form is in the ethanolamine class with rather less in choline, and commonly little or none in other phospholipids such as phosphatidylinositol. In choline plasmalogens of most tissues, a higher proportion is often of the O-alkyl rather than the O-alkenyl form, but the reverse tends to be true in heart lipids. In animal tissues, the alkyl and alkenyl moieties in both non-polar and phospholipids tend to be rather simple in composition with 16:0, 18:0 and 18:1 (double bond in position 9) predominating. Ether analogues of triacylglycerols, i.e. 1-alkyldiacyl-sn-glycerols, are present at trace levels only if at all in most animal tissues, but they can be major components of some marine lipids.

This compound belongs to the class of organic compounds known as 1-(1Z-alkenyl),2-acylglycerophosphoethanolamines. These are glycerophosphoethanolamines that carry exactly one acyl chain attached to the glycerol moiety through an ester linkage at the O2-position, and one 1Z-alkenyl chain attached through an ether linkage at the O1-position.

### LysoPE(0:0/20:5(5Z,8Z,11Z,14Z,17Z)) -- Introduction

SYNONYM: (5Z,8Z,11Z,14Z,17Z-Eicosapentaenoyl)-lysophosphatidylethanolamine; 1-Hydroxy-2-eicosapentaenoyl-sn-glycero-3-phosphoethanolamine; LPE(0:0/20:5); LPE(0:0/20:5n3); LPE(0:0/20:5W3); LPE(20:5); lyso-PE(0:0/20:5); lysoph-PE(0:0/20:5n3); lyso-PE(0:0/20:5W3); lyso-PE(20:5); LysoPE(0:0/20:5); LysoPE(0:0/20:5n3); LysoPE(0:0/20:5W3); LysoPE(20:5); Lysophosphatidylethanolamine(0:0/20:5); Lysophosphatidylethanolamine(0:0/20:5n3); Lysophosphatidylethanolamine(0:0/20:5W3); Lysophosphatidylethanolamine(20:5); LysoPE(0:0/20:5(5Z,8Z,11Z,14Z,17Z)); 1-hydroxy-2-(5Z,8Z,11Z,14Z,17Z-eicosapentaenoyl)-sn-glycero-3-phosphoethanolamine

HMDB: HMDB0011489; HMDB11489



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CAS:

LysoPE(0:0/20:5(5Z,8Z,11Z,14Z,17Z)) is a lysophosphatidylethanolamine or a lysophospholipid. The term 'lysophospholipid' (LPL) refers to any phospholipid that is missing one of its two O-acyl chains. Thus, LPLs have a free alcohol in either the sn-1 or sn-2 position. The prefix 'lyso-' comes from the fact that lysophospholipids were originally found to be hemolytic however it is now used to refer generally to phospholipids missing an acyl chain. LPLs are usually the result of phospholipase A-type enzymatic activity on regular phospholipids such as phosphatidylcholine or phosphatidic acid, although they can also be generated by the acylation of glycerophospholipids or the phosphorylation of monoacylglycerols. Some LPLs serve important signaling functions such as lysophosphatidic acid. Lysophosphatidylethanolamines (LPEs) can function as plant growth regulators with several diverse uses. (LPEs) are approved for outdoor agricultural use to accelerate ripening and improve the quality of fresh produce. They are also approved for indoor use to preserve stored crops and commercial cut flowers. As a breakdown product of phosphatidylethanolamine (PE), LPE is present in cells of all organisms.

This compound belongs to the class of organic compounds known as 2-acyl-sn-glycero-3-phosphoethanolamines. These are glycerophosphoethanolamines in which the glycerol is esterified with a fatty acid at O-2 position, and linked at position 3 to a phosphoethanolamine.

## LysoPE(18:1(9Z)/0:0) -- Introduction

SYNONYM: 1-(9Z)-Octadecenoyl-sn-glycero-3-phosphoethanolamine zwitterion; 1-(9Z-Octadecenoyl)-sn-glycero-3-phosphoethanolamine; 1-18:1-LysoPE; 1-18:1-Lysophosphatidylethanolamine; 1-C18:1(Omega-9)-lysophosphatidylethanolamine zwitterion; (9Z-Octadecenoyl)-lysophosphatidylethanolamine; 1-Oleoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine; LPE(18:1); LPE(18:1:0:0); LPE(18:1n9/0:0); LPE(18:1W9/0:0); lyso-PE(18:1); lyso-PE(18:1:0:0); lyso-PE(18:1n9/0:0); lyso-PE(18:1W9/0:0); LysoPE(18:1); LysoPE(18:1:0:0); LysoPE(18:1n9/0:0); LysoPE(18:1W9/0:0); Lysophosphatidylethanolamine(18:1); Lysophosphatidylethanolamine(18:1:0:0); Lysophosphatidylethanolamine(18:1n9/0:0); Lysophosphatidylethanolamine(18:1W9/0:0); LysoPE(18:1(9Z)/0:0); 1-(9Z-octadecenoyl)-2-hydroxy-sn-glycero-3-phosphoethanolamine

HMDB: HMDB0011506; HMDB11506

CAS: 89576-29-4

LysoPE(18:1(9Z)/0:0) is a lysophosphatidylethanolamine or a lysophospholipid. The term 'lysophospholipid' (LPL) refers to any phospholipid that is missing one of its two O-acyl chains. Thus, LPLs have a free alcohol in either the sn-1 or sn-2 position. The prefix 'lyso-' comes from the fact that lysophospholipids were originally found to be hemolytic however it is now used to refer generally to phospholipids missing an acyl chain. LPLs are usually the result of phospholipase A-type enzymatic activity on regular phospholipids such as phosphatidylcholine or phosphatidic acid, although they can also be generated by the acylation of glycerophospholipids or the phosphorylation of monoacylglycerols. Some LPLs serve important signaling functions such as lysophosphatidic acid. Lysophosphatidylethanolamines (LPEs) can function as plant growth regulators with several diverse uses. (LPEs) are approved for outdoor agricultural use to accelerate ripening and improve the quality of fresh produce. They are also approved for indoor use to preserve stored crops and commercial cut flowers. As a breakdown product of phosphatidylethanolamine (PE), LPE is present in cells of all organisms.

This compound belongs to the class of organic compounds known as 1-acyl-sn-glycero-3-phosphoethanolamines. These are glycerophosphoethanolamines in which the glycerol is esterified with a fatty acid at O-1 position, and linked at position 3 to a phosphoethanolamine.

## LysoPE(18:1(9Z)/0:0) -- Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. *Tohoku J Exp Med.* 1995 May;176(1):61-8. PMID: 7482520

Cheng Y, Xie G, Chen T, Qiu Y, Zou X, Zheng M, Tan B, Feng B, Dong T, He P, Zhao L, Zhao A, Xu LX, Zhang Y, Jia W: Distinct urinary metabolic profile of human colorectal cancer. *J Proteome Res.* 2012 Feb 3;11(2):1354-63. doi: 10.1021/pr201001a. Epub 2011 Dec 28. PMID: 22148915

Monleon D, Morales JM, Barrasa A, Lopez JA, Vazquez C, Celda B: Metabolite profiling of fecal water extracts from human colorectal cancer. *NMR Biomed.* 2009 Apr;22(3):342-8. doi: 10.1002/nbm.1345. PMID: 19006102



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Weir TL, Manter DK, Sheflin AM, Barnett BA, Heuberger AL, Ryan EP: Stool microbiome and metabolome differences between colorectal cancer patients and healthy adults. *PLoS One.* 2013 Aug 6;8(8):e70803. doi: 10.1371/journal.pone.0070803. Print 2013. PMID: 23940645

Phua LC, Chue XP, Koh PK, Cheah PY, Ho HK, Chan EC: Non-invasive fecal metabonomic detection of colorectal cancer. *Cancer Biol Ther.* 2014 Apr;15(4):389-97. doi: 10.4161/cbt.27625. Epub 2014 Jan 14. PMID: 24424155

Ritchie SA, Ahiahou PW, Jayasinghe D, Heath D, Liu J, Lu Y, Jin W, Kavianpour A, Yamazaki Y, Khan AM, Hossain M, Su-Myat KK, Wood PL, Krenitsky K, Takemasa I, Miyake M, Sekimoto M, Monden M, Matsubara H, Nomura F, Goodenow DB: Reduced levels of hydroxylated, polyunsaturated ultra long-chain fatty acids in the serum of colorectal cancer patients: implications for early screening and detection. *BMC Med.* 2010 Feb 15;8:13. doi: 10.1186/1741-7015-8-13. PMID: 20156336

Qiu Y, Cai G, Su M, Chen T, Zheng X, Xu Y, Ni Y, Zhao A, Xu LX, Cai S, Jia W: Serum metabolite profiling of human colorectal cancer using GC-TOFMS and UPLC-QTOFMS. *J Proteome Res.* 2009 Oct;8(10):4844-50. doi: 10.1021/pr9004162. PMID: 19678709

Ni Y, Xie G, Jia W: Metabonomics of human colorectal cancer: new approaches for early diagnosis and biomarker discovery. *J Proteome Res.* 2014 Sep 5;13(9):3857-70. doi: 10.1021/pr500443c. Epub 2014 Aug 14. PMID: 25105552

Ikeda A, Nishiumi S, Shinohara M, Yoshie T, Hatano N, Okuno T, Bamba T, Fukusaki E, Takenawa T, Azuma T, Yoshida M: Serum metabolomics as a novel diagnostic approach for gastrointestinal cancer. *Biomed Chromatogr.* 2012 May;26(5):548-58. doi: 10.1002/bmc.1671. Epub 2011 Jul 20. PMID: 21773981

Goedert JJ, Sampson JN, Moore SC, Xiao Q, Xiong X, Hayes RB, Ahn J, Shi J, Sinha R: Fecal metabolomics: assay performance and association with colorectal cancer. *Carcinogenesis.* 2014 Sep;35(9):2089-96. doi: 10.1093/carcin/bgu131. Epub 2014 Jul 18. PMID: 25037050

Sinha R, Ahn J, Sampson JN, Shi J, Yu G, Xiong X, Hayes RB, Goedert JJ: Fecal Microbiota, Fecal Metabolome, and Colorectal Cancer Interrelations. *PLoS One.* 2016 Mar 25;11(3):e0152126. doi: 10.1371/journal.pone.0152126. eCollection 2016. PMID: 27015276

Lin Y, Ma C, Liu C, Wang Z, Yang J, Liu X, Shen Z, Wu R: NMR-based fecal metabolomics fingerprinting as predictors of earlier diagnosis in patients with colorectal cancer. *Oncotarget.* 2016 May 17;7(20):29454-64. doi: 10.18632/oncotarget.8762. PMID: 27107423

Brown DG, Rao S, Weir TL, O'Malia J, Bazan M, Brown RJ, Ryan EP: Metabolomics and metabolic pathway networks from human colorectal cancers, adjacent mucosa, and stool. *Cancer Metab.* 2016 Jun 6;4:11. doi: 10.1186/s40170-016-0151-y. eCollection 2016. PMID: 27275383

Wang X, Wang J, Rao B, Deng L: Gut flora profiling and fecal metabolite composition of colorectal cancer patients and healthy individuals. *Exp Ther Med.* 2017 Jun;13(6):2848-2854. doi: 10.3892/etm.2017.4367. Epub 2017 Apr 20. PMID: 28587349

Silke Matysik, Caroline Ivonne Le Roy, Gerhard Liebisch, Sandrine Paule Claus. Metabolomics of fecal samples: A practical consideration. *Trends in Food Science & Technology.* Vol. 57, Part B, Nov. 2016, p.244-255: <http://www.sciencedirect.com/science/article/pii/S0924224416301984> PMID: 7482520

## LysoPE(18:2(9Z,12Z)/0:0) -- Introduction

SYNONYM: (9Z,12Z-Octadecadienoyl)-lysophosphatidylethanolamine; 1-(9Z,12Z-Octadecadienoyl)-glycero-3-phosphoethanolamine; 1-Linoleoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine; lyso-PE(18:2n6/0:0); LysoPE(18:2W6/0:0); PE(18:2(9Z,12Z)/0:0); LPE(18:2); LPE(18:2/0:0); LPE(18:2n6/0:0); LPE(18:2W6/0:0); lyso-PE(18:2); lyso-PE(18:2/0:0); lyso-PE(18:2W6/0:0); LysoPE(18:2); LysoPE(18:2/0:0); LysoPE(18:2n6/0:0); Lysophosphatidylethanolamine(18:2); Lysophosphatidylethanolamine(18:2/0:0); Lysophosphatidylethanolamine(18:2n6/0:0); Lysophosphatidylethanolamine(18:2W6/0:0); LysoPE(18:2(9Z,12Z)/0:0); 1-(9Z,12Z-octadecadienoyl)-2-hydroxy-sn-glycero-3-phosphoethanolamine

HMDB: HMDB0011507; HMDB11507

CAS: 85046-18-0



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LyoPE(18:2(9Z,12Z)/0:0) is a lysophosphatidylethanolamine or a lysophospholipid. The term 'lysophospholipid' (LPL) refers to any phospholipid that is missing one of its two O-acyl chains. Thus, LPLs have a free alcohol in either the sn-1 or sn-2 position. The prefix 'lyso-' comes from the fact that lysophospholipids were originally found to be hemolytic however it is now used to refer generally to phospholipids missing an acyl chain. LPLs are usually the result of phospholipase A-type enzymatic activity on regular phospholipids such as phosphatidylcholine or phosphatidic acid, although they can also be generated by the acylation of glycerophospholipids or the phosphorylation of monoacylglycerols. Some LPLs serve important signaling functions such as lysophosphatidic acid. Lysophosphatidylethanolamines (LPEs) can function as plant growth regulators with several diverse uses. (LPEs) are approved for outdoor agricultural use to accelerate ripening and improve the quality of fresh produce. They are also approved for indoor use to preserve stored crops and commercial cut flowers. As a breakdown product of phosphatidylethanolamine (PE), LPE is present in cells of all organisms.

This compound belongs to the class of organic compounds known as 1-acyl-sn-glycero-3-phosphoethanolamines. These are glycerophosphoethanolamines in which the glycerol is esterified with a fatty acid at O-1 position, and linked at position 3 to a phosphoethanolamine.

### **LyoPE(18:2(9Z,12Z)/0:0) -- Colorectal cancer**

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. *Tohoku J Exp Med.* 1995 May;176(1):61-8. PMID: 7482520

Cheng Y, Xie G, Chen T, Qiu Y, Zou X, Zheng M, Tan B, Feng B, Dong T, He P, Zhao L, Zhao A, Xu LX, Zhang Y, Jia W: Distinct urinary metabolic profile of human colorectal cancer. *J Proteome Res.* 2012 Feb 3;11(2):1354-63. doi: 10.1021/pr201001a. Epub 2011 Dec 28. PMID: 22148915

Monleon D, Morales JM, Barrasa A, Lopez JA, Vazquez C, Celda B: Metabolite profiling of fecal water extracts from human colorectal cancer. *NMR Biomed.* 2009 Apr;22(3):342-8. doi: 10.1002/nbm.1345. PMID: 19006102

Weir TL, Manter DK, Sheflin AM, Barnett BA, Heuberger AL, Ryan EP: Stool microbiome and metabolome differences between colorectal cancer patients and healthy adults. *PLoS One.* 2013 Aug 6;8(8):e70803. doi: 10.1371/journal.pone.0070803. Print 2013. PMID: 23940645

Phua LC, Chue XP, Koh PK, Cheah PY, Ho HK, Chan EC: Non-invasive fecal metabonomic detection of colorectal cancer. *Cancer Biol Ther.* 2014 Apr;15(4):389-97. doi: 10.4161/cbt.27625. Epub 2014 Jan 14. PMID: 24424155

Ritchie SA, Ahiahou PW, Jayasinghe D, Heath D, Liu J, Lu Y, Jin W, Kavianpour A, Yamazaki Y, Khan AM, Hossain M, Su-Myat KK, Wood PL, Krenitsky K, Takemasa I, Miyake M, Sekimoto M, Monden M, Matsubara H, Nomura F, Goodenow DB: Reduced levels of hydroxylated, polyunsaturated ultra long-chain fatty acids in the serum of colorectal cancer patients: implications for early screening and detection. *BMC Med.* 2010 Feb 15;8:13. doi: 10.1186/1741-7015-8-13. PMID: 20156336

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Goedert JJ, Sampson JN, Moore SC, Xiao Q, Xiong X, Hayes RB, Ahn J, Shi J, Sinha R: Fecal metabolomics: assay performance and association with colorectal cancer. *Carcinogenesis.* 2014 Sep;35(9):2089-96. doi: 10.1093/carcin/bgu131. Epub 2014 Jul 18. PMID: 25037050

Sinha R, Ahn J, Sampson JN, Shi J, Yu G, Xiong X, Hayes RB, Goedert JJ: Fecal Microbiota, Fecal Metabolome, and Colorectal Cancer Interrelations. *PLoS One.* 2016 Mar 25;11(3):e0152126. doi: 10.1371/journal.pone.0152126. eCollection 2016. PMID: 27015276

Lin Y, Ma C, Liu C, Wang Z, Yang J, Liu X, Shen Z, Wu R: NMR-based fecal metabolomics fingerprinting as predictors of earlier diagnosis in patients with colorectal cancer. *Oncotarget.* 2016 May 17;7(20):29454-64. doi: 10.18632/oncotarget.8762. PMID: 27107423

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Wang X, Wang J, Rao B, Deng L: Gut flora profiling and fecal metabolite composition of colorectal cancer patients and healthy individuals. *Exp Ther Med.* 2017 Jun;13(6):2848-2854. doi: 10.3892/etm.2017.4367. Epub 2017 Apr 20. PMID: 28587349

Silke Matysik, Caroline Ivonne Le Roy, Gerhard Liebisch, Sandrine Paule Claus. Metabolomics of fecal samples: A practical consideration. *Trends in Food Science & Technology.* Vol. 57, Part B, Nov. 2016, p.244-255:  
<http://www.sciencedirect.com/science/article/pii/S0924224416301984> PMID: 7482520

## Adenosine 2'-phosphate -- Introduction

SYNONYM: 2'-Adenylic acid; Adenosine-2'-monophosphate; AMP 2'-Phosphate; 2'-AMP; 2'-Adenosine monophosphate; Adenosine 2' phosphate; Adenosine monophosphate; Adenosine phosphate disodium; Phosphate dipotassium, adenosine; 5'-Phosphate, adenosine; AMP; Acid, 2'-adenylic; Acid, 5'-adenylic; Adenosine 5' phosphate; Adenosine 5'-phosphate; Adenosine phosphate dipotassium; Phosphaden; Phosphate disodium, adenosine; 2' Adenosine monophosphate; 5'-Adenylic acid; Adenosine 3' phosphate; Dipotassium, adenosine phosphate; Disodium, adenosine phosphate; 2' Adenylic acid; 5' Adenylic acid; Adenosine 3'-phosphate; Adenylic acid; Monophosphate, 2'-adenosine

HMDB: HMDB0011617; HMDB11617

CAS: 130-49-4

Adenosine 2'-phosphate is converted enzymatically from adenosine 2',3'-cyclic phosphate via the enzyme 2',3'-cyclic-nucleotide 3'-phosphodiesterase (EC 3.1.4.37). In the brain, this enzyme acts on 2',3'-cyclic AMP more rapidly than on the UMP or CMP derivatives. In the liver, this enzyme acts on 2',3'-cyclic CMP more rapidly than on the purine derivatives; it also hydrolyses the corresponding 3',5'-cyclic phosphates, more slowly. This latter enzyme has been called cyclic-CMP phosphodiesterase. (KEGG). This enzyme belongs to the family of hydrolases, specifically those acting on phosphoric diester bonds. The systematic name of this enzyme class is nucleoside-2',3'-cyclic-phosphate 2'-nucleotidohydrolase. (Wikipedia).

This compound belongs to the class of organic compounds known as pentose phosphates. These are carbohydrate derivatives containing a pentose substituted by one or more phosphate groups.

## L-Iditol -- Introduction

SYNONYM: (2S,3R,4R,5S)-Hexane-1,2,3,4,5,6-hexol; L-Idit; Cordycepic acid; D-Dulcitol; D-Galactitol; Dulcite; Dulcitol; Dulcose; Galactitol; Glucitol; Hexahydric alcohol; Hexahydroxyhexane; Hexitol; iso-Sorbide; Isotol; Karion; L-Gulitol; Manna sugar; Mannit; Mannite; Meglumine; Mitobronitol; Sionit; Sionon; Siosan; Sorbo; Sorbol; Iditol

HMDB: HMDB0011632; HMDB11632

CAS: 488-45-9

Iditol is a sugar alcohol which accumulates in galactokinase deficiency (Wikipedia). Chemically, Iditol is an alcohol and a sugar, or a polyol.

This compound belongs to the class of organic compounds known as sugar alcohols. These are hydrogenated forms of carbohydrate in which the carbonyl group (aldehyde or ketone, reducing sugar) has been reduced to a primary or secondary hydroxyl group.

## L-Iditol -- Irritable bowel syndrome

Bearcroft CP, Perrett D, Farthing MJ: Postprandial plasma 5-hydroxytryptamine in diarrhoea predominant irritable bowel syndrome: a pilot study. *Gut.* 1998 Jan;42(1):42-6. PMID: 9505884



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Brydon WG, Nyhlin H, Eastwood MA, Merrick MV: Serum 7 alpha-hydroxy-4-cholest-3-one and selenohomocholytaurine (SeHCAT) whole body retention in the assessment of bile acid induced diarrhoea. Eur J Gastroenterol Hepatol. 1996 Feb;8(2):117-23. PMID: 8723414

Ponnusamy K, Choi JN, Kim J, Lee SY, Lee CH: Microbial community and metabolomic comparison of irritable bowel syndrome faeces. J Med Microbiol. 2011 Jun;60(Pt 6):817-27. doi: 10.1099/jmm.0.028126-0. Epub 2011 Feb 17. PMID: 21330412

Le Gall G, Noor SO, Ridgway K, Scovell L, Jamieson C, Johnson IT, Colquhoun IJ, Kemsley EK, Narbad A: Metabolomics of fecal extracts detects altered metabolic activity of gut microbiota in ulcerative colitis and irritable bowel syndrome. J Proteome Res. 2011 Sep 2;10(9):4208-18. doi: 10.1021/pr2003598. Epub 2011 Aug 8. PMID: 21761941

Hong YS, Hong KS, Park MH, Ahn YT, Lee JH, Huh CS, Lee J, Kim IK, Hwang GS, Kim JS: Metabonomic understanding of probiotic effects in humans with irritable bowel syndrome. J Clin Gastroenterol. 2011 May-Jun;45(5):415-25. doi: 10.1097/MCG.0b013e318207f76c. PMID: 21494186

Walton C, Fowler DP, Turner C, Jia W, Whitehead RN, Griffiths L, Dawson C, Waring RH, Ramsden DB, Cole JA, Cauchi M, Bessant C, Hunter JO: Analysis of volatile organic compounds of bacterial origin in chronic gastrointestinal diseases. Inflamm Bowel Dis. 2013 Sep;19(10):2069-78. doi: 10.1097/MIB.0b013e31829a91f6. PMID: 23867873

Zeber-Lubecka N, Kulecka M, Ambroziewicz F, Paziewska A, Goryca K, Karczmarski J, Rubel T, Wojtowicz W, Mlynarz P, Marczak L, Tomecki R, Mikula M, Ostrowski J: Limited prolonged effects of rifaximin treatment on irritable bowel syndrome-related differences in the fecal microbiome and metabolome. Gut Microbes. 2016 Sep 2;7(5):397-413. doi: 10.1080/19490976.2016.1215805. Epub 2016 Jul 26. PMID: 27662586

## p-Cresol glucuronide -- Introduction

SYNONYM: 4-Methylphenyl beta-D-glucopyranosiduronate; 4-Methylphenyl beta-D-glucopyranosiduronic acid; Cresol glucuronide; Cresyl glucuronide; Cresylglucuronide; P-Cresyl glucuronide; P-Cresyl-beta-D-glucuronide; P-Cresylglucuronide; pCG; 4-Cresylglucuronide

HMDB: HMDB0011686; HMDB11686

CAS:

p-Cresol glucuronide is a glucuronide derivative of p-Cresol that is typically excreted in the urine. P-Cresol (the precursor of p-cresol sulfate (PCS) and p-cresol glucuronide (PCG)) is mainly generated as an end product of tyrosine biotransformation by anaerobic intestinal bacteria. During passage through the colonic mucosa and liver, sulfatation and glucuronidation generates p-Cresol sulfate (as the most preponderant metabolite) and p-Cresol glucuronide (at markedly lower concentrations) (PMID: 23826225). Cresols are known as methylphenols. Cresols are used to dissolve other chemicals, such as disinfectants and deodorizers. They are also used to make specific chemicals that kill insect pests. Cresol solutions are used as household cleaners and disinfectants such as Lysol. Cresol solutions can also be found in photographic developers. In the past, cresol solutions have been used as antiseptics in surgery, but they have been largely displaced in this role by less toxic compounds. Cresols are found in many foods and in wood and tobacco smoke, crude oil, coal tar, and in brown mixtures such as creosote, cresolene and cresylic acids, which are wood preservatives. Microbes in the soil and water produce cresols when they break down materials in the environment. Most exposures to cresols are at very low levels that are not harmful. When cresols are breathed, ingested, or applied to the skin at very high levels, they can be very harmful. Effects observed in people include irritation and burning of skin, eyes, mouth, and throat; abdominal pain and vomiting. Cresols are also a chemical component found in Sharpey Markers. P-cresol is a major component in pig odor.

This compound belongs to the class of organic compounds known as phenolic glycosides. These are organic compounds containing a phenolic structure attached to a glycosyl moiety. Some examples of phenolic structures include lignans, and flavonoids. Among the sugar units found in natural glycosides are D-glucose, L-Fructose, and L rhamnose.

## SM(d17:1/24:1(15Z)) -- Introduction

SYNONYM: SPH(D17:1/24:1(15Z)); Sphingomyelin (D17:1/24:1(15Z))

HMDB: HMDB0011696; HMDB11696



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CAS:

Sphingomyelin SM(d17:1/24:1(15Z)) or SM(d17:1/24:1(15Z)) is a sphingomyelin. Sphingomyelin (SM or SPH) is a type of sphingolipid found in animal cell membranes, especially in the membranous myelin sheath which surrounds some nerve cell axons. It usually consists of phosphorylcholine and ceramide. In humans, sphingomyelin is the only membrane phospholipid not derived from glycerol. Like all sphingolipids, SPH has a ceramide core (sphingosine bonded to a fatty acid via an amide linkage). In addition it contains one polar head group, which is either phosphocholine or phosphoethanolamine. The plasma membrane of cells is highly enriched in sphingomyelin and is considered largely to be found in the exoplasmic leaflet of the cell membrane. However, there is some evidence that there may also be a sphingomyelin pool in the inner leaflet of the membrane. Moreover, neutral sphingomyelinase-2 - an enzyme that breaks down sphingomyelin into ceramide has been found to localise exclusively to the inner leaflet further suggesting that there may be sphingomyelin present there. Sphingomyelin can accumulate in a rare hereditary disease called Niemann-Pick Disease, types A and B. Niemann-Pick disease is a genetically-inherited disease caused by a deficiency in the enzyme Sphingomyelinase, which causes the accumulation of Sphingomyelin in spleen, liver, lungs, bone marrow, and the brain, causing irreversible neurological damage. SMs play a role in signal transduction. Sphingomyelins are synthesized by the transfer of phosphorylcholine from phosphatidylcholine to a ceramide in a reaction catalyzed by sphingomyelin synthase.

This compound belongs to the class of organic compounds known as phosphocholines. These are compounds containing a [2-(trimethylazaniumyl)ethoxy]phosphonic acid or derivative.

## N2-gamma-Glutamylglutamine -- Introduction

SYNONYM: gamma-L-Glu-L-GLN; g-L-Glu-L-GLN;  $\hat{\text{l}}^3$ -L-glu-L-GLN; g-Glutamyl glutamine;  $\hat{\text{l}}^3$ -glutamyl glutamine; gamma-Glu-GLN; gamma-Glutamylglutamine;  $\hat{\text{l}}^3$ -Glu-Gln;  $\hat{\text{l}}^3$ -Glutamylglutamine;  $\hat{\text{l}}^3$ -L-Glutamyl-L-glutamine; N2- $\hat{\text{l}}^3$ -Glutamylglutamine; N2-L- $\hat{\text{l}}^3$ -Glutamylglutamine; N2-L- $\hat{\text{l}}^3$ -Glutamyl-L-glutamine; gamma-L-Glutamyl-L-glutamine; L-gamma-Glutamyl-L-glutamine; N2-L-gamma-Glutamylglutamine; N2-L-gamma-Glutamyl-L-glutamine; N2-gamma-Glutamylglutamine

HMDB: HMDB0011738; HMDB11738

CAS: 10148-81-9

N2-gamma-Glutamylglutamine is a dipeptide obtained from condensation of the gamma-carboxy group of glutamic acid with the  $\hat{\text{l}}^{\pm}$ -amino group of glutamine. Some dipeptides are known to have physiological or cell-signaling effects although most are simply short-lived intermediates on their way to specific amino acid degradation pathways following further proteolysis.

This compound belongs to the class of organic compounds known as dipeptides. These are organic compounds containing a sequence of exactly two alpha-amino acids joined by a peptide bond.

## N2-gamma-Glutamylglutamine -- Crohn's disease

Lapidus A, Akerlund JE, Einarsson C: Gallbladder bile composition in patients with Crohn's disease. World J Gastroenterol. 2006 Jan 7;12(1):70-4. PMID: 16440420

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## gamma-Glutamyltyrosine -- Introduction

SYNONYM: N-L-gamma-Glutamyl-L-tyrosine; Glutyrosine; gamma-Glutamyl-L-tyrosine;  $\hat{\beta}$ -Glu-Tyr;  $\hat{\beta}$ -L-Glu-L-Tyr;  $\hat{\beta}$ -



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Glutamyltyrosine;  $\hat{\text{I}}^3$ -L-Glutamyl-L-tyrosine; L- $\hat{\text{I}}^3$ -Glutamyl-L-tyrosine; N- $\hat{\text{I}}^3$ -Glutamyltyrosine; N-L- $\hat{\text{I}}^3$ -Glutamyltyrosine; N-L- $\hat{\text{I}}^3$ -Glutamyl-L-tyrosine; gamma-Glu-Tyr; gamma-L-Glu-L-Tyr; gamma-L-Glutamyl-L-tyrosine; L-gamma-Glutamyl-L-tyrosine; N-gamma-Glutamyltyrosine; N-L-gamma-Glutamyltyrosine; gamma-Glutamyltyrosine; N- $\hat{\text{I}}^3$ -L-Glutamyl-L-tyrosine; N-gamma-L-Glutamyl-L-tyrosine

HMDB: HMDB0011741; HMDB0029161; HMDB11741; HMDB29161

CAS: 7432-23-7

gamma-Glutamyltyrosine is a dipeptide composed of gamma-glutamate and tyrosine, and is a proteolytic breakdown product of larger proteins. It belongs to the family of N-acyl-alpha amino acids and derivatives. These are compounds containing an alpha amino acid which bears an acyl group at its terminal nitrogen atom. gamma-Glutamyltyrosine is an incomplete breakdown product of protein digestion or protein catabolism. Some dipeptides are known to have physiological or cell-signaling effects although most are simply short-lived intermediates on their way to specific amino acid degradation pathways following further proteolysis.

This compound belongs to the class of organic compounds known as tyrosine and derivatives. These are compounds containing tyrosine or a derivative thereof resulting from reaction of tyrosine at the amino group or the carboxy group, or from the replacement of any hydrogen of glycine by a heteroatom.

## 2-Piperidinone -- Introduction

SYNONYM: 2-oxo-Piperidine; 2-Oxopiperidine; 5-Pentanolactam; alpha-Piperidone; delta-Valerolactam; Piperidinone; Piperidon; Piperidone; Piperidone-2; a-Piperidone;  $\hat{\text{I}}\pm$ -piperidone;  $\hat{\text{I}}'$ -valerolactam; 2-Piperidone; 5-amino-Lactam-pentanoate; 5-amino-Lactam-pentanoic acid; Valerolactim; Piperidin-2-one

HMDB: HMDB0011749; HMDB11749

CAS: 675-20-7

2-Piperidinone is a derivative of piperidine which is an organic compound. Piperidine is a colorless fuming liquid with an odor described as ammoniacal, pepper-like, the name comes from the genus name *Piper*, which is the Latin word for pepper. Piperidine is a widely used building block and chemical reagent in the synthesis of organic compounds, including pharmaceuticals. The piperidine structural motif is present in numerous natural alkaloids. These include piperine, which gives black pepper the hot taste. This gave the compound its name.(Wikipedia).

This compound belongs to the class of organic compounds known as piperidinones. These are compounds containing a piperidine ring which bears a ketone.

## 2-Piperidinone -- Colorectal cancer

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Kolho KL, Pessia A, Jaakkola T, de Vos WM, Velagapudi V: Faecal and Serum Metabolomics in Paediatric Inflammatory Bowel Disease. *J Crohns Colitis.* 2017 Mar 1;11(3):321-334. doi: 10.1093/ecco-jcc/jlw158. PMID: 27609529

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Ahmed I, Greenwood R, Costello B, Ratcliffe N, Probert CS: Investigation of faecal volatile organic metabolites as novel diagnostic biomarkers in inflammatory bowel disease. *Aliment Pharmacol Ther.* 2016 Mar;43(5):596-611. doi: 10.1111/apt.13522. Epub 2016 Jan 25. PMID: 26806034

Lee T, Clavel T, Smirnov K, Schmidt A, Lagkouvardos I, Walker A, Lucio M, Michalke B, Schmitt-Kopplin P, Fedorak R, Haller D: Oral versus intravenous iron replacement therapy distinctly alters the gut microbiota and metabolome in patients with IBD. *Gut.* 2017 May;66(5):863-871. doi: 10.1136/gutjnl-2015-309940. Epub 2016 Feb 4. PMID: 26848182

Kolho KL, Pessia A, Jaakkola T, de Vos WM, Velagapudi V: Faecal and Serum Metabolomics in Paediatric Inflammatory Bowel Disease. *J Crohns Colitis.* 2017 Mar 1;11(3):321-334. doi: 10.1093/ecco-jcc/jlw158. PMID: 27609529

Azario I, Pievani A, Del Priore F, Antolini L, Santi L, Corsi A, Cardinale L, Sawamoto K, Kubaski F, Gentner B, Bernardo ME, Valsecchi MG, Riminiucci M, Tomatsu S, Aiuti A, Biondi A, Serafini M: Neonatal umbilical cord blood transplantation halts skeletal disease progression in the murine model of MPS-I. *Sci Rep.* 2017 Aug 25;7(1):9473. doi: 10.1038/s41598-017-09958-9. PMID: 28842642

## SM(d18:1/14:0) -- Introduction

SYNONYM: C14 Sphingomyelin; N-(Myristoyl)sphing-4-enine-1-phosphocholine; N-(Tetradecanoyl)sphing-4-enine-1-phosphocholine; SM(32:1); Sphingomyelin (D18:1/14:0); N-(Tetradecanoyl)-sphing-4-enine-1-phosphocholine

HMDB: HMDB0012097; HMDB12097

CAS:

Sphingomyelins are synthesized by the transfer of phosphorylcholine from phosphatidylcholine to a ceramide in a reaction catalyzed by sphingomyelin synthase.

This compound belongs to the class of organic compounds known as phosphosphingolipids. These are sphingolipids with a structure based on a sphingoid base that is attached to a phosphate head group. They differ from phosphonosphingolipids which have a phosphonate head group.

## SM(d18:1/18:1(9Z)) -- Introduction



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SYNONYM: N-(9Z-Octadecenoyl)-sphing-4-enine-1-phosphocholine; N-(9Z-Octadecenoyl)-sphingosine-1-phosphocholine; C18:1 Sphingomyelin; SPH(D18:1/18:1(11Z)); Sphingomyelin; Sphingomyelin (D18:1/18:1(11Z)); N-Oleoyl-sphingomyelin; N-Oleoylsphingomyelin

HMDB: HMDB0012101; HMDB12101

CAS:

Sphingomyelin (d18:1/18:1(9Z)) or SM(d18:1/18:1(9Z)) is a type of sphingolipid found in animal cell membranes, especially in the membranous myelin sheath which surrounds some nerve cell axons. It usually consists of phosphorylcholine and ceramide. In humans, sphingomyelin is the only membrane phospholipid not derived from glycerol. Like all sphingolipids, SPH has a ceramide core (sphingosine bonded to a fatty acid via an amide linkage). In addition it contains one polar head group, which is either phosphocholine or phosphoethanolamine. The plasma membrane of cells is highly enriched in sphingomyelin and is considered largely to be found in the exoplasmic leaflet of the cell membrane. However, there is some evidence that there may also be a sphingomyelin pool in the inner leaflet of the membrane. Moreover, neutral sphingomyelinase-2 - an enzyme that breaks down sphingomyelin into ceramide has been found to localise exclusively to the inner leaflet further suggesting that there may be sphingomyelin present there. Sphingomyelin can accumulate in a rare hereditary disease called Niemann-Pick Disease, types A and B. Niemann-Pick disease is a genetically-inherited disease caused by a deficiency in the enzyme Sphingomyelinase, which causes the accumulation of Sphingomyelin in spleen, liver, lungs, bone marrow, and the brain, causing irreversible neurological damage. SMs play a role in signal transduction. Sphingomyelins are synthesized by the transfer of phosphorylcholine from phosphatidylcholine to a ceramide in a reaction catalyzed by sphingomyelin synthase.

This compound belongs to the class of organic compounds known as phosphosphingolipids. These are sphingolipids with a structure based on a sphingoid base that is attached to a phosphate head group. They differ from phosphonospingolipids which have a phosphonate head group.

### SM(d18:1/18:1(9Z)) -- Obesity

Tuma P, Samcova E, Balinova P: Determination of 3-methylhistidine and 1-methylhistidine in untreated urine samples by capillary electrophoresis. J Chromatogr B Analyt Technol Biomed Life Sci. 2005 Jul 5;821(1):53-9. PMID: 15899597

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Vice E, Privette JD, Hickner RC, Barakat HA: Ketone body metabolism in lean and obese women. Metabolism. 2005 Nov;54(11):1542-5. PMID: 16253646

Brind J, Strain G, Miller L, Zumoff B, Vogelman J, Orentreich N: Obese men have elevated plasma levels of estrone sulfate. Int J Obes. 1990 Jun;14(6):483-6. PMID: 2401584

Driskell JA, Chrisley BM, Reynolds LK, Moak SW: Plasma B6 vitamer and plasma and urinary 4-pyridoxic acid concentrations of middle-aged obese black women. J Chromatogr. 1991 Aug 23;568(2):333-40. PMID: 1783639

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Vioque J, Weinbrenner T, Asensio L, Castello A, Young IS, Fletcher A: Plasma concentrations of carotenoids and vitamin C are better correlated with dietary intake in normal weight than overweight and obese elderly subjects. Br J Nutr. 2007 May;97(5):977-86. PMID: 17408529

Burrows TL, Warren JM, Colyvas K, Garg ML, Collins CE: Validation of overweight children's fruit and vegetable intake using plasma carotenoids. Obesity (Silver Spring). 2009 Jan;17(1):162-8. doi: 10.1038/oby.2008.495. Epub 2008 Nov 6. PMID: 18997681

Reinehr T, Wolters B, Knop C, Lass N, Hellmuth C, Harder U, Peissner W, Wahl S, Grallert H, Adamski J, Illig T, Prehn C, Yu Z, Wang-Sattler R, Koletzko B: Changes in the serum metabolite profile in obese children with weight loss. Eur J Nutr.



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2015 Mar;54(2):173-81. doi: 10.1007/s00394-014-0698-8. Epub 2014 Apr 17. PMID: 24740590

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Cho K, Moon JS, Kang JH, Jang HB, Lee HJ, Park SI, Yu KS, Cho JY: Combined untargeted and targeted metabolomic profiling reveals urinary biomarkers for discriminating obese from normal-weight adolescents. *Pediatr Obes.* 2017 Apr;12(2):93-101. doi: 10.1111/jpo.12114. Epub 2016 Feb 22. PMID: 26910390

## SM(d18:1/20:0) -- Introduction

SYNONYM: (2S,3R,4E)-3-Hydroxy-2-(icosanoylamino)octadec-4-en-1-yl 2-(trimethylammonio)ethyl phosphate; C20 Sphingomyelin; N-(Eicosanoyl)-sphing-4-enine-1-phosphocholine; N-Arachidoylsphing-4-enine-1-phosphocholine; N-Arachidoylsphingosine-1-phosphocholine; N-Eicosanoylsphing-4-enine-1-phosphocholine; N-Eicosanoylsphingosine-1-phosphocholine; N-Icosanoylsphing-4-enine-1-phosphocholine; Sphingomyelin (D18:1/20:0); (2S,3R,4E)-3-Hydroxy-2-(icosanoylamino)octadec-4-en-1-yl 2-(trimethylammonio)ethyl phosphoric acid; Sphingomyelin

HMDB: HMDB0012102; HMDB12102

CAS:

Sphingomyelin (d18:1/20:0) or SM(d18:1/20:0) is a type of sphingolipid found in animal cell membranes, especially in the membranous myelin sheath which surrounds some nerve cell axons. In humans, sphingomyelin is the only membrane phospholipid not derived from glycerol. Like all sphingolipids, SPH has a ceramide core (sphingosine bonded to a fatty acid via an amide linkage). In addition it contains one polar head group, which is either phosphocholine or phosphoethanolamine. The plasma membrane of cells is highly enriched in sphingomyelin and is considered largely to be found in the exoplasmic leaflet of the cell membrane. However, there is some evidence that there may also be a sphingomyelin pool in the inner leaflet of the membrane. Moreover, neutral sphingomyelinase-2 - an enzyme that breaks down sphingomyelin into ceramide has been found to localise exclusively to the inner leaflet further suggesting that there may be sphingomyelin present there. Sphingomyelin can accumulate in a rare hereditary disease called Niemann-Pick Disease, types A and B. Niemann-Pick disease is a genetically-inherited disease caused by a deficiency in the enzyme Sphingomyelinase, which causes the accumulation of Sphingomyelin in spleen, liver, lungs, bone marrow, and the brain, causing irreversible neurological damage. SMs play a role in signal transduction. Sphingomyelins are synthesized by the transfer of phosphorylcholine from phosphatidylcholine to a ceramide in a reaction catalyzed by sphingomyelin synthase.

This compound belongs to the class of organic compounds known as phosphosphingolipids. These are sphingolipids with a structure based on a sphingoid base that is attached to a phosphate head group. They differ from phosphonospingolipids which have a phosphonate head group.

## SM(d18:1/24:1(15Z)) -- Introduction

SYNONYM: C24:1 Sphingomyelin; N-(15Z-Tetracosenoyl)-sphing-4-enine-1-phosphocholine; N-(15Z-Tetracosenoyl)sphing-4-enine-1-phosphocholine

HMDB: HMDB0012107; HMDB12107

CAS:

Sphingomyelin (d18:1/24:1(15Z)) or SM(d18:1/24:1(15Z)) is a type of sphingolipid found in animal cell membranes, especially in the membranous myelin sheath which surrounds some nerve cell axons. It usually consists of phosphorylcholine and ceramide. In humans, sphingomyelin is the only membrane phospholipid not derived from glycerol. Like all sphingolipids, SPH has a ceramide core (sphingosine bonded to a fatty acid via an amide linkage). In addition it contains one polar head group, which is either phosphocholine or phosphoethanolamine. The plasma membrane of cells is highly enriched in sphingomyelin and is considered largely to be found in the exoplasmic leaflet of the cell membrane. However, there is some evidence that there may also be a sphingomyelin pool in the inner leaflet of the membrane. Moreover, neutral sphingomyelinase-2 - an enzyme that breaks down sphingomyelin into ceramide has been found to localise exclusively to the inner leaflet further suggesting that there may be sphingomyelin present there. Sphingomyelin can accumulate in a rare hereditary disease called Niemann-Pick Disease, types A and B. Niemann-Pick disease is a genetically-inherited disease caused by a deficiency in the enzyme Sphingomyelinase, which causes the accumulation of Sphingomyelin in spleen, liver,



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This compound belongs to the class of organic compounds known as phosphosphingolipids. These are sphingolipids with a structure based on a sphingoid base that is attached to a phosphate head group. They differ from phosphonosphingolipids which have a phosphonate head group.

### SM(d18:1/24:1(15Z)) -- Obesity

Tuma P, Samcova E, Balinova P: Determination of 3-methylhistidine and 1-methylhistidine in untreated urine samples by capillary electrophoresis. *J Chromatogr B Analyt Technol Biomed Life Sci*. 2005 Jul 5;821(1):53-9. PMID: 15899597

Serlie MJ, Meijer AJ, Groener JE, Duran M, Endert E, Fliers E, Aerts JM, Sauerwein HP: Short-term manipulation of plasma free fatty acids does not change skeletal muscle concentrations of ceramide and glucosylceramide in lean and overweight subjects. *J Clin Endocrinol Metab*. 2007 Apr;92(4):1524-9. Epub 2007 Jan 30. PMID: 17264178

Vice E, Privette JD, Hickner RC, Barakat HA: Ketone body metabolism in lean and obese women. *Metabolism*. 2005 Nov;54(11):1542-5. PMID: 16253646

Brind J, Strain G, Miller L, Zumoff B, Vogelman J, Orentreich N: Obese men have elevated plasma levels of estrone sulfate. *Int J Obes*. 1990 Jun;14(6):483-6. PMID: 2401584

Driskell JA, Chrisley BM, Reynolds LK, Moak SW: Plasma B6 vitamer and plasma and urinary 4-pyridoxic acid concentrations of middle-aged obese black women. *J Chromatogr*. 1991 Aug 23;568(2):333-40. PMID: 1783639

Haro C, Montes-Borrego M, Rangel-Zuniga OA, Alcala-Diaz JF, Gomez-Delgado F, Perez-Martinez P, Delgado-Lista J, Quintana-Navarro GM, Tinahones FJ, Landa BB, Lopez-Miranda J, Camargo A, Perez-Jimenez F: Two Healthy Diets Modulate Gut Microbial Community Improving Insulin Sensitivity in a Human Obese Population. *J Clin Endocrinol Metab*. 2016 Jan;101(1):233-42. doi: 10.1210/jc.2015-3351. Epub 2015 Oct 27. PMID: 26505825

Vioque J, Weinbrenner T, Asensio L, Castello A, Young IS, Fletcher A: Plasma concentrations of carotenoids and vitamin C are better correlated with dietary intake in normal weight than overweight and obese elderly subjects. *Br J Nutr*. 2007 May;97(5):977-86. PMID: 17408529

Burrows TL, Warren JM, Colyvas K, Garg ML, Collins CE: Validation of overweight children's fruit and vegetable intake using plasma carotenoids. *Obesity (Silver Spring)*. 2009 Jan;17(1):162-8. doi: 10.1038/oby.2008.495. Epub 2008 Nov 6. PMID: 18997681

Reinehr T, Wolters B, Knop C, Lass N, Hellmuth C, Harder U, Peissner W, Wahl S, Grallert H, Adamski J, Illig T, Prehn C, Yu Z, Wang-Sattler R, Koletzko B: Changes in the serum metabolite profile in obese children with weight loss. *Eur J Nutr*. 2015 Mar;54(2):173-81. doi: 10.1007/s00394-014-0698-8. Epub 2014 Apr 17. PMID: 24740590

Wahl S, Yu Z, Kleber M, Singmann P, Holzapfel C, He Y, Mittelstrass K, Polonikov A, Prehn C, Romisch-Margl W, Adamski J, Suhre K, Grallert H, Illig T, Wang-Sattler R, Reinehr T: Childhood obesity is associated with changes in the serum metabolite profile. *Obes Facts*. 2012;5(5):660-70. doi: 10.1159/000343204. Epub 2012 Oct 4. PMID: 23108202

Cho K, Moon JS, Kang JH, Jang HB, Lee HJ, Park SI, Yu KS, Cho JY: Combined untargeted and targeted metabolomic profiling reveals urinary biomarkers for discriminating obese from normal-weight adolescents. *Pediatr Obes*. 2017 Apr;12(2):93-101. doi: 10.1111/jopo.12114. Epub 2016 Feb 22. PMID: 26910390

### SM(d18:1/24:1(15Z)) -- Metastatic melanoma

Frankel AE, Coughlin LA, Kim J, Froehlich TW, Xie Y, Frenkel EP, Koh AY: Metagenomic Shotgun Sequencing and Unbiased Metabolomic Profiling Identify Specific Human Gut Microbiota and Metabolites Associated with Immune Checkpoint Therapy Efficacy in Melanoma Patients. *Neoplasia*. 2017 Oct;19(10):848-855. doi: 10.1016/j.neo.2017.08.004. Epub 2017 Sep 15. PMID: 28923537

### 2-Amino-4-oxo-6-(1',2',3'-trihydroxypropyl)-diquinoid-7,8-dihydroxypterin -- Introduction



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**SYNONYM:**

HMDB: HMDB0012144; HMDB12144

**CAS:**

2-Amino-4-oxo-6-(1',2',3'-trihydroxypropyl)-diquinoid-7,8-dihydroxypterin is a pterin derivative. Pterin is a heterocyclic compound composed of a pyrazine ring and a pyrimidine ring with Several tautomers; the pyrimidine ring has a carbonyl oxygen and an amino group. As a group, pterins are compounds that are derivatives of 2-amino-4-oxopteridine, with additional functional groups attached to the pyrazine ring. Pterins were first discovered in the pigments of butterfly wings and perform many roles in coloration in the biological world. Pterins also function as cofactors in enzyme catalysis (Wikipedia). Some pterin derivatives (biopterin, 6-formylpterin, 6-carboxypterin) accumulate in the skin of patients affected by vitiligo, a depigmentation disorder, where the protection against UV radiation fails due to the lack of melanin. Pterins participate in biologically important photosensitization processes; for example, pterins act as sensitizers in photochemical reactions that induce DNA damage<sup>4,5</sup> and are able to generate singlet molecular oxygen<sup>6</sup> and other reactive oxygen species (PMID: 19199487).

This compound belongs to the class of organic compounds known as biopterins and derivatives. These are coenzymes containing a 2-amino-pteridine-4-one derivative. They are mainly synthesized in several parts of the body, including the pineal gland.

## Hydroxybupropion -- Introduction

SYNONYM: 4-Hydroxy bupropion; B.W.306u; BW-306U; BW 306U; BW-306-U

HMDB: HMDB0012235; HMDB12235

**CAS:**

Hydroxybupropion is found in the bupropion degradation pathway. Bupropion reacts with NADPH and O<sub>2</sub> to produce hydroxybupropion, with NADP<sup>+</sup> and H<sub>2</sub>O as byproducts.

This compound belongs to the class of organic compounds known as alkyl-phenylketones. These are aromatic compounds containing a ketone substituted by one alkyl group, and a phenyl group.

## S-Prenyl-L-cysteine -- Introduction

SYNONYM: 2-amino-3-Prenylmercaptopropionic acid; 2-amino-3-Prenylthiopropionic acid; 3-((3-Methyl-2-but-enyl)thio)-L-alanine; Prenisteine; Prenyl-L-cysteine; S-(3-Methyl-2-but-enyl-L-cysteine)

HMDB: HMDB0012286; HMDB12286

CAS: 5287-46-7

S-Prenyl-L-cysteine is catalysed by prenylcysteine oxidase to form L-cysteine. A flavoprotein (FAD). Cleaves the thioether bond of S-prenyl-L-cysteines, such as S-farnesylcysteine and S-geranylgeranylcysteine. N-Acetyl-prenylcysteine and prenylcysteinyl peptides are not substrates. This reaction may represent the final step in the degradation of prenylated proteins in mammalian tissues. The enzyme is originally thought to be a simple lyase so it had been classified as. EC 4.4.1.18.

This compound belongs to the class of organic compounds known as cysteine and derivatives. These are compounds containing cysteine or a derivative thereof resulting from reaction of cysteine at the amino group or the carboxy group, or from the replacement of any hydrogen of glycine by a heteroatom.

## PS(18:0/20:4(5Z,8Z,11Z,14Z)) -- Introduction

SYNONYM: 1-Octadecanoyl-2-(5Z,8Z,11Z,14Z)-eicosatetraenoyl-sn-glycero-3-phosphoserine; 1-Octadecanoyl-2-(5Z,8Z,11Z,14Z)-icosatetraenoyl-sn-glycero-3-phosphoserine; Phosphatidylserine(18:0/20:4); Phosphatidylserine(18:0/20:4n6); Phosphatidylserine(18:0/20:4W6); Phosphatidylserine(38:4); PS(18:0/20:4); PS(18:0/20:4N6); PS(18:0/20:4W6); PS(38:4); pSer(18:0/20:4); pSer(18:0/20:4n6); pSer(18:0/20:4W6); pSer(38:4); 1-Stearoyl-2-arachidonoyl-sn-glycero-3-phosphoserine; PS(18:0/20:4(5Z,8Z,11Z,14Z)); 1-octadecanoyl-2-(5Z,8Z,11Z,14Z-eicosatetraenoyl)-sn-glycero-3-phosphoserine



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HMDB: HMDB0012383; HMDB12383

CAS:

PS(18:0/20:4(5Z,8Z,11Z,14Z)) is a phosphatidylserine (PS or GPSer). It is a glycerophospholipid in which a phosphorylserine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, glycerophosphoserines can have many different combinations of fatty acids of varying lengths and saturation attached at the C-1 and C-2 positions. Fatty acids containing 16, 18 and 20 carbons are the most common. PS(18:0/20:4(5Z,8Z,11Z,14Z)), in particular, consists of one chain of stearic acid at the C-1 position and one chain of arachidonic acid at the C-2 position. The stearic acid moiety is derived from animal fats, coco butter and sesame oil, while the arachidonic acid moiety is derived from animal fats and eggs. Phosphatidylserine or 1,2-diacyl-sn-glycero-3-phospho-L-serine is distributed widely among animals, plants and microorganisms. It is usually less than 10% of the total phospholipids, the greatest concentration being in myelin from brain tissue. However, it may comprise 10 to 20 mol% of the total phospholipid in the plasma membrane and endoplasmic reticulum of the cell. Phosphatidylserine is an acidic (anionic) phospholipid with three ionizable groups, i.e. the phosphate moiety, the amino group and the carboxyl function. As with other acidic lipids, it exists in nature in salt form, but it has a high propensity to chelate to calcium via the charged oxygen atoms of both the carboxyl and phosphate moieties, modifying the conformation of the polar head group. This interaction may be of considerable relevance to the biological function of phosphatidylserine, especially during bone formation for example. As phosphatidylserine is located entirely on the inner monolayer surface of the plasma membrane (and of other cellular membranes) and it is the most abundant anionic phospholipids. Therefore phosphatidylserine may make the largest contribution to interfacial effects in membranes involving non-specific electrostatic interactions. This normal distribution is disturbed during platelet activation and cellular apoptosis. In human plasma, 1-stearoyl-2-oleoyl and 1-stearoyl-2-arachidonoyl species predominate, but in brain (especially grey matter), retina and many other tissues 1-stearoyl-2-docosahexaenoyl species are very abundant. Indeed, the ratio of n-3 to n-6 fatty acids in brain phosphatidylserine is very much higher than in most other lipids. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. Phosphatidylserines typically carry a net charge of -1 at physiological pH. They mostly have palmitic or stearic acid on carbon 1 and a long chain unsaturated fatty acid (e.g. 18:2, 20:4 and 22:6) on carbon 2. PS biosynthesis involves an exchange reaction of serine for ethanolamine in PE.

This compound belongs to the class of organic compounds known as phosphatidylserines. These are glycerophosphoserines in which two fatty acids are bonded to the glycerol moiety through ester linkages. As is the case with diacylglycerols, phosphatidylserines can have many different combinations of fatty acids of varying lengths and saturation attached to the C-1 and C-2 positions.

## Beta-Carboline -- Introduction

SYNONYM: 2,9-Diazfluorene; 2-Azacarbazole; 9H-beta-Carboline; 9H-pyrido(3,4-b)Indole; 9H-pyrido[3,4-b]Indole; Carbazoline; Norharman; Norharmane; b-Carboline;  $\hat{b}$ -carboline; 9H-b-Carboline; 9H- $\hat{b}$ -carboline

HMDB: HMDB0012897; HMDB12897

CAS: 244-63-3

b-Carboline (9H-pyrido[3,4-b]indole) is an organic amine that is the prototype of a class of compounds known as b-carbolines.

This compound belongs to the class of organic compounds known as beta carbolines. These are compounds containing a 9H-pyrido[3,4-b]indole moiety.

## 16(17)-EpDPE -- Introduction

SYNONYM: 16(17)-Epoxy-4Z,7Z,10Z,13Z,19Z-docosapentaenoic acid; 16,17-EDP; 16,17-Epoxydocosapentaenoic acid; 16(17)-Epoxy-4Z,7Z,10Z,13Z,19Z-docosapentaenoate; 16,17-Epoxydocosapentaenoate; 16(17)-EpDoPE

HMDB: HMDB0013621; HMDB13621

CAS:

16(17)-EpETE is the DHA homolog of 14(15)-EpETrE, derived via epoxidation of the 16,17-double bond of



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docosahexaenoic acid (DHA). The EDHF (endothelium-derived hyperpolarizing factor) activity of 16(17)-EpDPE has not yet been determined. The epoxyenase metabolites of DHA have also been detected in a murine inflammation model (PMID: 12391014). EDHF is an unidentified mediator released from vascular endothelial cells in response to acetylcholine and bradykinin which is distinct from the NOS- (nitric oxide) and COX-derived (prostacyclin) vasodilators (PMID: 9504399, 10519554). Cytochrome P450 (CYP450) metabolism of polyunsaturated fatty acids produces epoxides such as 14(15)-EpETrE which are prime candidates for the actual active mediator (PMID: 9401962). However, the CYP450 metabolites of eicosapentaenoic acid (EPA) and docosahexaenoic acid (DHA) have been little studied relative to arachidonate epoxyenase metabolites.

This compound belongs to the class of organic compounds known as long-chain fatty acids. These are fatty acids with an aliphatic tail that contains between 13 and 21 carbon atoms.

### **1,3,5-Trihydroxybenzene -- Introduction**

SYNONYM: 1,3,5-Benzenetriol; 1,3,5-Trihydroxybenzene; Benzene-1,3,5-triol; S-Trihydroxybenzene; 1,3, 5-Trihydroxybenzene; 1,3,5-Benzenetriol (acd/name 4.0); 1,3,5-Trihydroxybenzene; 1,3,5-Trihydroxycyclohexatriene; 1,3,5-Triol; 3,5-Dihydroxyphenol; 5-Benzene-1,3,5-triol; 5-Hydroxyresorcinol; 5-Oxyresorcinol; 5-Oxyresorcinolphloroglucin; Benzene, trihydroxy; Benzene-S-triol; Dilospan S; Floroglucin; Floroglucinol; Phloroglucin; Phloroglucine; Phloroglucinol (1,3,5-benzenetriol); Spasfon-lyoc; Sym-trihydroxybenzene

HMDB: HMDB0013675; HMDB13675

CAS: 108-73-6

Phloroglucinol is a benzenetriol. It is an organic compound that is used in the synthesis of pharmaceuticals and explosives. This molecule exists in two forms, or tautomers, 1,3,5-trihydroxybenzene, which has phenol-like, and 1,3,5-cyclohexanetrione (phloroglucin), which has ketone-like character. These two tautomers are in equilibrium. Phloroglucinol is a useful intermediate because it is polyfunctional.

This compound belongs to the class of organic compounds known as phloroglucinols and derivatives. These are compounds containing a phloroglucinol (benzene-1,3,5-triol) moiety, which consists of a benzene ring bearing one hydroxyl group at positions 1,3, and 5.

### **1,3-Diisopropylbenzene -- Introduction**

SYNONYM: 13-Diisopropylbenzene; 1-Isopropyl-3-methylbenzene; 1-Isopropyl-3-methylbenzene (acd/name 4.0); 1-Methyl-3-isopropylbenzene; 3-Isopropyltoluene; 3-Methyl-1-isopropylbenzene; m-Isopropyltoluene

HMDB: HMDB0013806; HMDB13806

CAS: 99-62-7

Cymene, or p-cymene, is a naturally occurring aromatic organic compound. It is classified as a hydrocarbon related to a monoterpenes. Its structure consists of a benzene ring para-substituted with a methyl group and an isopropyl group. It is insoluble in water, but miscible with ethanol and ether. Cymene is a constituent of a number of essential oils, most commonly the oil of cumin and thyme. There are two less common geometric isomers. o-Cymene, in which the alkyl groups are ortho-substituted, and m-cymene, in which they are meta-substituted. p-Cymene is the only natural isomer. [Wikipedia]

This compound belongs to the class of organic compounds known as cumenes. These are aromatic compounds containing a prop-2-ylbenzene moiety.

### **1,3-Diisopropylbenzene -- Perillyl alcohol administration for cancer treatment**

Zheng YF, Kong HW, Xiong JH, Lv S, Xu GW: Clinical significance and prognostic value of urinary nucleosides in breast cancer patients. Clin Biochem. 2005 Jan;38(1):24-30. PMID: 15607313

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Zhang Z, Chen H, Chan KK, Budd T, Ganapathi R: Gas chromatographic-mass spectrometric analysis of perillyl alcohol and



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metabolites in plasma. J Chromatogr B Biomed Sci Appl. 1999 May 14;728(1):85-95. PMID: 10379660

Cauley JA, Zmuda JM, Danielson ME, Ljung BM, Bauer DC, Cummings SR, Kuller LH: Estrogen metabolites and the risk of breast cancer in older women. Epidemiology. 2003 Nov;14(6):740-4. PMID: 14569192

Grace PB, Mistry NS, Carter MH, Leathem AJ, Teale P: High throughput quantification of phytoestrogens in human urine and serum using liquid chromatography/tandem mass spectrometry (LC-MS/MS). J Chromatogr B Analyt Technol Biomed Life Sci. 2007 Jun 15;853(1-2):138-46. Epub 2007 Mar 18. PMID: 17403619

Sugimoto M, Wong DT, Hirayama A, Soga T, Tomita M: Capillary electrophoresis mass spectrometry-based saliva metabolomics identified oral, breast and pancreatic cancer-specific profiles. Metabolomics. 2010 Mar;6(1):78-95. Epub 2009 Sep 10. PMID: 20300169

Silva CL, Passos M, Camara JS: Solid phase microextraction, mass spectrometry and metabolomic approaches for detection of potential urinary cancer biomarkers--a powerful strategy for breast cancer diagnosis. Talanta. 2012 Jan 30;89:360-8. doi: 10.1016/j.talanta.2011.12.041. Epub 2011 Dec 22. PMID: 22284503

Lv W, Yang T: Identification of possible biomarkers for breast cancer from free fatty acid profiles determined by GC-MS and multivariate statistical analysis. Clin Biochem. 2012 Jan;45(1-2):127-33. doi: 10.1016/j.clinbiochem.2011.10.011. Epub 2011 Oct 26. PMID: 22061338

Nam H, Chung BC, Kim Y, Lee K, Lee D: Combining tissue transcriptomics and urine metabolomics for breast cancer biomarker identification. Bioinformatics. 2009 Dec 1;25(23):3151-7. doi: 10.1093/bioinformatics/btp558. Epub 2009 Sep 25. PMID: 19783829

Woo HM, Kim KM, Choi MH, Jung BH, Lee J, Kong G, Nam SJ, Kim S, Bai SW, Chung BC: Mass spectrometry based metabolomic approaches in urinary biomarker study of women's cancers. Clin Chim Acta. 2009 Feb;400(1-2):63-9. doi: 10.1016/j.cca.2008.10.014. Epub 2008 Oct 30. PMID: 19010317

## Thioguanine -- Introduction

SYNONYM: 2-amino 6MP; 2-amino-1,7-dihydro-6H-Purine-6-thione; 2-amino-1,9-Dihydropurine-6-thione; 2-amino-6-Mercaptopurine; 2-amino-6-Merkaptopurin; 2-amino-6-Purinethiol; 2-Aminopurin-6-thiol; 2-Aminopurine-6(1H)-thione; 2-Aminopurine-6-thiol; 6-mercpto-2-Aminopurine; 6-Mercaptoguanine; 6-TG; 6-Thioguanine; TG; ThG; Thioguanine; Tioguanin; Tioguanina; Tioguaninum; 6 Thioguanine; glaxo Wellcome brand OF thioguanine; GlaxoSmithKline brand OF thioguanine; Lanvis; ThioguaninGSK; Thioguanine hemihydrate; Tioguanina wellcome; Wellcome brand OF thioguanine; 2 amino 6 Purinethiol; GlaxoSmithKline brand OF tioguanine; Thioguanine tabloid; glaxo Wellcome brand OF tioguanine; Tabloid; Thioguanine anhydrous; Anhydrous, thioguanine; Thioguanin GSK; Thioguanin-GSK; Thioguanine monosodium salt; Tioguanine glaxosmithkline brand

HMDB: HMDB0014496; HMDB14496

CAS: 154-42-7

Thioguanine is only found in individuals that have used or taken this drug. It is an antineoplastic compound which also has antimetabolite action. The drug is used in the therapy of acute leukemia. [PubChem]Thioguanine competes with hypoxanthine and guanine for the enzyme hypoxanthine-guanine phosphoribosyltransferase (HGPRTase) and is itself converted to 6-thioguanilyc acid (TGMP), which reaches high intracellular concentrations at therapeutic doses. TGMP interferes with the synthesis of guanine nucleotides by its inhibition of purine biosynthesis by pseudofeedback inhibition of glutamine-5-phosphoribosylpyrophosphate amidotransferase, the first enzyme unique to the de novo pathway of purine ribonucleotide synthesis. TGMP also inhibits the conversion of inosinic acid (IMP) to xanthylc acid (XMP) by competition for the enzyme IMP dehydrogenase. Thioguanine nucleotides are incorporated into both the DNA and the RNA by phosphodiester linkages, and some studies have shown that incorporation of such false bases contributes to the cytotoxicity of thioguanine. Its tumor inhibitory properties may be due to one or more of its effects on feedback inhibition of de novo purine synthesis; inhibition of purine nucleotide interconversions; or incorporation into the DNA and RNA. The overall result of its action is a sequential blockade of the utilization and synthesis of the purine nucleotides.

This compound belongs to the class of organic compounds known as purinethiones. These are purines in which the purine moiety bears a thioether.



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## Alanyl-Arginine -- Introduction

SYNONYM: a-R Dipeptide; Ala-arg; Alanine arginine dipeptide; Alanine-arginine dipeptide; Alanylarginine; AR dipeptide; L-Alanyl-L-arginine

HMDB: HMDB0028681; HMDB28681

CAS:

Alanyl-Arginine is a dipeptide composed of alanine and arginine. It is an incomplete breakdown product of protein digestion or protein catabolism. Some dipeptides are known to have physiological or cell-signaling effects although most are simply short-lived intermediates on their way to specific amino acid degradation pathways following further proteolysis. This dipeptide has not yet been identified in human tissues or biofluids and so it is classified as an 'Expected' metabolite.

This compound belongs to the class of organic compounds known as dipeptides. These are organic compounds containing a sequence of exactly two alpha-amino acids joined by a peptide bond.

## Arginyl-Leucine -- Introduction

SYNONYM: Arg-leu; Arginine leucine dipeptide; Arginine-leucine dipeptide; Arginylleucine; L-Arginyl-L-leucine; R-L Dipeptide; RL Dipeptide

HMDB: HMDB0028713; HMDB28713

CAS:

Arginyl-Leucine is a dipeptide composed of arginine and leucine. It is an incomplete breakdown product of protein digestion or protein catabolism. Some dipeptides are known to have physiological or cell-signaling effects although most are simply short-lived intermediates on their way to specific amino acid degradation pathways following further proteolysis. This dipeptide has not yet been identified in human tissues or biofluids and so it is classified as an 'Expected' metabolite.

This compound belongs to the class of organic compounds known as dipeptides. These are organic compounds containing a sequence of exactly two alpha-amino acids joined by a peptide bond.

## Arginyl-Leucine -- Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. *Tohoku J Exp Med.* 1995 May;176(1):61-8. PMID: 7482520

Cheng Y, Xie G, Chen T, Qiu Y, Zou X, Zheng M, Tan B, Feng B, Dong T, He P, Zhao L, Zhao A, Xu LX, Zhang Y, Jia W: Distinct urinary metabolic profile of human colorectal cancer. *J Proteome Res.* 2012 Feb 3;11(2):1354-63. doi: 10.1021/pr201001a. Epub 2011 Dec 28. PMID: 22148915

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Ritchie SA, Ahiahou PW, Jayasinghe D, Heath D, Liu J, Lu Y, Jin W, Kavianpour A, Yamazaki Y, Khan AM, Hossain M, Su-Myat KK, Wood PL, Krenitsky K, Takemasa I, Miyake M, Sekimoto M, Monden M, Matsubara H, Nomura F, Goodenow DB: Reduced levels of hydroxylated, polyunsaturated ultra long-chain fatty acids in the serum of colorectal cancer patients: implications for early screening and detection. *BMC Med.* 2010 Feb 15;8:13. doi: 10.1186/1741-7015-8-13. PMID: 20156336

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Ni Y, Xie G, Jia W: Metabonomics of human colorectal cancer: new approaches for early diagnosis and biomarker discovery. *J Proteome Res.* 2014 Sep 5;13(9):3857-70. doi: 10.1021/pr500443c. Epub 2014 Aug 14. PMID: 25105552

Ikeda A, Nishiumi S, Shinohara M, Yoshie T, Hatano N, Okuno T, Bamba T, Fukusaki E, Takenawa T, Azuma T, Yoshida M: Serum metabolomics as a novel diagnostic approach for gastrointestinal cancer. *Biomed Chromatogr.* 2012 May;26(5):548-58. doi: 10.1002/bmc.1671. Epub 2011 Jul 20. PMID: 21773981

Goedert JJ, Sampson JN, Moore SC, Xiao Q, Xiong X, Hayes RB, Ahn J, Shi J, Sinha R: Fecal metabolomics: assay performance and association with colorectal cancer. *Carcinogenesis.* 2014 Sep;35(9):2089-96. doi: 10.1093/carcin/bgu131. Epub 2014 Jul 18. PMID: 25037050

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Lin Y, Ma C, Liu C, Wang Z, Yang J, Liu X, Shen Z, Wu R: NMR-based fecal metabolomics fingerprinting as predictors of earlier diagnosis in patients with colorectal cancer. *Oncotarget.* 2016 May 17;7(20):29454-64. doi: 10.18632/oncotarget.8762. PMID: 27107423

Brown DG, Rao S, Weir TL, O'Malia J, Bazan M, Brown RJ, Ryan EP: Metabolomics and metabolic pathway networks from human colorectal cancers, adjacent mucosa, and stool. *Cancer Metab.* 2016 Jun 6;4:11. doi: 10.1186/s40170-016-0151-y. eCollection 2016. PMID: 27275383

Wang X, Wang J, Rao B, Deng L: Gut flora profiling and fecal metabolite composition of colorectal cancer patients and healthy individuals. *Exp Ther Med.* 2017 Jun;13(6):2848-2854. doi: 10.3892/etm.2017.4367. Epub 2017 Apr 20. PMID: 28587349

Silke Matysik, Caroline Ivonne Le Roy, Gerhard Liebisch, Sandrine Paule Claus. Metabolomics of fecal samples: A practical consideration. *Trends in Food Science & Technology.* Vol. 57, Part B, Nov. 2016, p.244-255: <http://www.sciencedirect.com/science/article/pii/S0924224416301984> PMID: 7482520

## Arginyl-Phenylalanine -- Introduction

SYNONYM: Arg-phe; Arginine phenylalanine dipeptide; Arginine-phenylalanine dipeptide; Arginylphenylalanine; L-Arginyl-L-phenylalanine; R-F Dipeptide; RF Dipeptide

HMDB: HMDB0028716; HMDB28716

CAS:

Arginyl-Phenylalanine is a dipeptide composed of arginine and phenylalanine. It is an incomplete breakdown product of protein digestion or protein catabolism. Some dipeptides are known to have physiological or cell-signaling effects although most are simply short-lived intermediates on their way to specific amino acid degradation pathways following further proteolysis. This dipeptide has not yet been identified in human tissues or biofluids and so it is classified as an 'Expected' metabolite.

This compound belongs to the class of organic compounds known as dipeptides. These are organic compounds containing a sequence of exactly two alpha-amino acids joined by a peptide bond.

## Arginyl-Phenylalanine -- Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. *Tohoku J Exp Med.* 1995 May;176(1):61-8. PMID: 7482520

Cheng Y, Xie G, Chen T, Qiu Y, Zou X, Zheng M, Tan B, Feng B, Dong T, He P, Zhao L, Zhao A, Xu LX, Zhang Y, Jia W: Distinct urinary metabolic profile of human colorectal cancer. *J Proteome Res.* 2012 Feb 3;11(2):1354-63. doi: 10.1021/pr201001a. Epub 2011 Dec 28. PMID: 22148915



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Weir TL, Manter DK, Sheflin AM, Barnett BA, Heuberger AL, Ryan EP: Stool microbiome and metabolome differences between colorectal cancer patients and healthy adults. *PLoS One.* 2013 Aug 6;8(8):e70803. doi: 10.1371/journal.pone.0070803. Print 2013. PMID: 23940645

Phua LC, Chue XP, Koh PK, Cheah PY, Ho HK, Chan EC: Non-invasive fecal metabonomic detection of colorectal cancer. *Cancer Biol Ther.* 2014 Apr;15(4):389-97. doi: 10.4161/cbt.27625. Epub 2014 Jan 14. PMID: 24424155

Ritchie SA, Ahiahonu PW, Jayasinghe D, Heath D, Liu J, Lu Y, Jin W, Kavianpour A, Yamazaki Y, Khan AM, Hossain M, Su-Myat KK, Wood PL, Krenitsky K, Takemasa I, Miyake M, Sekimoto M, Monden M, Matsubara H, Nomura F, Goodenow DB: Reduced levels of hydroxylated, polyunsaturated ultra long-chain fatty acids in the serum of colorectal cancer patients: implications for early screening and detection. *BMC Med.* 2010 Feb 15;8:13. doi: 10.1186/1741-7015-8-13. PMID: 20156336

Qiu Y, Cai G, Su M, Chen T, Zheng X, Xu Y, Ni Y, Zhao A, Xu LX, Cai S, Jia W: Serum metabolite profiling of human colorectal cancer using GC-TOFMS and UPLC-QTOFMS. *J Proteome Res.* 2009 Oct;8(10):4844-50. doi: 10.1021/pr9004162. PMID: 19678709

Ni Y, Xie G, Jia W: Metabonomics of human colorectal cancer: new approaches for early diagnosis and biomarker discovery. *J Proteome Res.* 2014 Sep 5;13(9):3857-70. doi: 10.1021/pr500443c. Epub 2014 Aug 14. PMID: 25105552

Ikeda A, Nishiumi S, Shinohara M, Yoshie T, Hatano N, Okuno T, Bamba T, Fukusaki E, Takenawa T, Azuma T, Yoshida M: Serum metabolomics as a novel diagnostic approach for gastrointestinal cancer. *Biomed Chromatogr.* 2012 May;26(5):548-58. doi: 10.1002/bmc.1671. Epub 2011 Jul 20. PMID: 21773981

Goedert JJ, Sampson JN, Moore SC, Xiao Q, Xiong X, Hayes RB, Ahn J, Shi J, Sinha R: Fecal metabolomics: assay performance and association with colorectal cancer. *Carcinogenesis.* 2014 Sep;35(9):2089-96. doi: 10.1093/carcin/bgu131. Epub 2014 Jul 18. PMID: 25037050

Sinha R, Ahn J, Sampson JN, Shi J, Yu G, Xiong X, Hayes RB, Goedert JJ: Fecal Microbiota, Fecal Metabolome, and Colorectal Cancer Interrelations. *PLoS One.* 2016 Mar 25;11(3):e0152126. doi: 10.1371/journal.pone.0152126. eCollection 2016. PMID: 27015276

Lin Y, Ma C, Liu C, Wang Z, Yang J, Liu X, Shen Z, Wu R: NMR-based fecal metabolomics fingerprinting as predictors of earlier diagnosis in patients with colorectal cancer. *Oncotarget.* 2016 May 17;7(20):29454-64. doi: 10.18632/oncotarget.8762. PMID: 27107423

Brown DG, Rao S, Weir TL, O'Malia J, Bazan M, Brown RJ, Ryan EP: Metabolomics and metabolic pathway networks from human colorectal cancers, adjacent mucosa, and stool. *Cancer Metab.* 2016 Jun 6;4:11. doi: 10.1186/s40170-016-0151-y. eCollection 2016. PMID: 27275383

Wang X, Wang J, Rao B, Deng L: Gut flora profiling and fecal metabolite composition of colorectal cancer patients and healthy individuals. *Exp Ther Med.* 2017 Jun;13(6):2848-2854. doi: 10.3892/etm.2017.4367. Epub 2017 Apr 20. PMID: 28587349

Silke Matysik, Caroline Ivonne Le Roy, Gerhard Liebsch, Sandrine Paule Claus. Metabolomics of fecal samples: A practical consideration. *Trends in Food Science & Technology.* Vol. 57, Part B, Nov. 2016, p.244-255: <http://www.sciencedirect.com/science/article/pii/S0924224416301984> PMID: 7482520

## Asparaginyl-Arginine -- Introduction

SYNONYM: Asn-arg; Asparagine arginine dipeptide; Asparagine-arginine dipeptide; Asparaginylarginine; L-Asparaginyl-L-arginine; N-R Dipeptide; NR Dipeptide

HMDB: HMDB0028725; HMDB28725

CAS:

Asparaginyl-Arginine is a dipeptide composed of asparagine and arginine. It is an incomplete breakdown product of



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protein digestion or protein catabolism. Some dipeptides are known to have physiological or cell-signaling effects although most are simply short-lived intermediates on their way to specific amino acid degradation pathways following further proteolysis. This dipeptide has not yet been identified in human tissues or biofluids and so it is classified as an 'Expected' metabolite.

This compound belongs to the class of organic compounds known as dipeptides. These are organic compounds containing a sequence of exactly two alpha-amino acids joined by a peptide bond.

## Asparaginyl-Hydroxyproline -- Introduction

SYNONYM: Asparagine hydroxyproline dipeptide; Asn-hpro; Asparagine-hydroxyproline dipeptide; Asparaginylhydroxyproline; L-Asparaginyl-L-hydroxyproline; N-HP Dipeptide; NHP Dipeptide

HMDB: HMDB0028732; HMDB28732

CAS:

Asparaginyl-Hydroxyproline is a dipeptide composed of asparagine and hydroxyproline. It is an incomplete breakdown product of protein digestion or protein catabolism. Some dipeptides are known to have physiological or cell-signaling effects although most are simply short-lived intermediates on their way to specific amino acid degradation pathways following further proteolysis. This dipeptide has not yet been identified in human tissues or biofluids and so it is classified as an 'Expected' metabolite.

This compound belongs to the class of organic compounds known as dipeptides. These are organic compounds containing a sequence of exactly two alpha-amino acids joined by a peptide bond.

## Asparaginyl-Hydroxyproline – Crohn's disease

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## Asparaginyl-Hydroxyproline -- Iron deficiency

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Lee T, Clavel T, Smirnov K, Schmidt A, Lagkouardos I, Walker A, Lucio M, Michalke B, Schmitt-Kopplin P, Fedorak R, Haller D: Oral versus intravenous iron replacement therapy distinctly alters the gut microbiota and metabolome in patients with IBD. *Gut.* 2017 May;66(5):863-871. doi: 10.1136/gutjnl-2015-309940. Epub 2016 Feb 4. PMID: 26848182

## Asparaginyl-Methionine -- Introduction

SYNONYM: Asn-met; Asparagine methionine dipeptide; Asparagine-methionine dipeptide; Asparaginylmethionine; L-Asparaginyl-L-methionine; N-m Dipeptide; NM Dipeptide

HMDB: HMDB0028737; HMDB28737

CAS:

Asparaginyl-Methionine is a dipeptide composed of asparagine and methionine. It is an incomplete breakdown product of protein digestion or protein catabolism. Some dipeptides are known to have physiological or cell-signaling effects although most are simply short-lived intermediates on their way to specific amino acid degradation pathways following further proteolysis. This dipeptide has not yet been identified in human tissues or biofluids and so it is classified as an 'Expected' metabolite.

This compound belongs to the class of organic compounds known as dipeptides. These are organic compounds containing a sequence of exactly two alpha-amino acids joined by a peptide bond.

## Cysteinyl-Hydroxyproline -- Introduction

SYNONYM: Cysteine hydroxyproline dipeptide; C-HP Dipeptide; CHP Dipeptide; Cys-hpro; Cysteine-hydroxyproline dipeptide; Cysteinylhydroxyproline; L-Cysteinyl-L-hydroxyproline

HMDB: HMDB0028776; HMDB28776

CAS:

Cysteinyl-Hydroxyproline is a dipeptide composed of cysteine and hydroxyproline. It is an incomplete breakdown product of protein digestion or protein catabolism. Some dipeptides are known to have physiological or cell-signaling effects although most are simply short-lived intermediates on their way to specific amino acid degradation pathways following further proteolysis. This dipeptide has not yet been identified in human tissues or biofluids and so it is classified as an 'Expected' metabolite.



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This compound belongs to the class of organic compounds known as dipeptides. These are organic compounds containing a sequence of exactly two alpha-amino acids joined by a peptide bond.

## Glutamylarginine -- Introduction

SYNONYM: Gln-Arg; L-Glutamyl-L-arginine; N2-Glutamylarginine; N2-L-Glutamyl-L-arginine; Glutamylarginine; Glutamyl-arginine; Glutamine arginine dipeptide; Glutamine-arginine dipeptide; Q-R dipeptide; QR dipeptide; L-Gln-L-Arg

HMDB: HMDB0028791; HMDB28791

CAS: 126590-89-4

Glutamylarginine is a dipeptide composed of glutamine and arginine. It is an incomplete breakdown product of protein digestion or protein catabolism. Some dipeptides are known to have physiological or cell-signaling effects although most are simply short-lived intermediates on their way to specific amino acid degradation pathways following further proteolysis.

This compound belongs to the class of organic compounds known as dipeptides. These are organic compounds containing a sequence of exactly two alpha-amino acids joined by a peptide bond.

## Hydroxyprolyl-Isoleucine -- Introduction

SYNONYM: Hydroxyproline isoleucine dipeptide; HP-I dipeptide; HPI dipeptide; hpro-Ile; Hydroxyproline-isoleucine dipeptide; Hydroxyprolylisoleucine; L-Hydroxyprolyl-L-isoleucine

HMDB: HMDB0028866; HMDB28866

CAS:

Hydroxyprolyl-Isoleucine is a dipeptide composed of hydroxyproline and isoleucine. It is an incomplete breakdown product of protein digestion or protein catabolism. Some dipeptides are known to have physiological or cell-signaling effects although most are simply short-lived intermediates on their way to specific amino acid degradation pathways following further proteolysis. This dipeptide has not yet been identified in human tissues or biofluids and so it is classified as an 'Expected' metabolite.

This compound belongs to the class of organic compounds known as peptides. These are compounds containing an amide derived from two or more amino carboxylic acid molecules (the same or different) by formation of a covalent bond from the carbonyl carbon of one to the nitrogen atom of another.

## Leucyl-Isoleucine -- Introduction

SYNONYM: L-I dipeptide; L-Leucyl-L-isoleucine; Leu-Ile; Leucine isoleucine dipeptide; Leucine-isoleucine dipeptide; Leucylisoleucine; LI dipeptide

HMDB: HMDB0028932; HMDB28932

CAS:

Leucyl-Isoleucine is a dipeptide composed of leucine and isoleucine. It is an incomplete breakdown product of protein digestion or protein catabolism. Some dipeptides are known to have physiological or cell-signaling effects although most are simply short-lived intermediates on their way to specific amino acid degradation pathways following further proteolysis. This dipeptide has not yet been identified in human tissues or biofluids and so it is classified as an 'Expected' metabolite.

This compound belongs to the class of organic compounds known as dipeptides. These are organic compounds containing a sequence of exactly two alpha-amino acids joined by a peptide bond.

## Leucyl-Isoleucine -- Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. Tohoku J Exp Med. 1995 May;176(1):61-8. PMID: 7482520



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Cheng Y, Xie G, Chen T, Qiu Y, Zou X, Zheng M, Tan B, Feng B, Dong T, He P, Zhao L, Zhao A, Xu LX, Zhang Y, Jia W: Distinct urinary metabolic profile of human colorectal cancer. *J Proteome Res.* 2012 Feb 3;11(2):1354-63. doi: 10.1021/pr201001a. Epub 2011 Dec 28. PMID: 22148915

Monleon D, Morales JM, Barrasa A, Lopez JA, Vazquez C, Celda B: Metabolite profiling of fecal water extracts from human colorectal cancer. *NMR Biomed.* 2009 Apr;22(3):342-8. doi: 10.1002/nbm.1345. PMID: 19006102

Weir TL, Manter DK, Sheflin AM, Barnett BA, Heuberger AL, Ryan EP: Stool microbiome and metabolome differences between colorectal cancer patients and healthy adults. *PLoS One.* 2013 Aug 6;8(8):e70803. doi: 10.1371/journal.pone.0070803. Print 2013. PMID: 23940645

Phua LC, Chue XP, Koh PK, Cheah PY, Ho HK, Chan EC: Non-invasive fecal metabonomic detection of colorectal cancer. *Cancer Biol Ther.* 2014 Apr;15(4):389-97. doi: 10.4161/cbt.27625. Epub 2014 Jan 14. PMID: 24424155

Ritchie SA, Ahiahonu PW, Jayasinghe D, Heath D, Liu J, Lu Y, Jin W, Kavianpour A, Yamazaki Y, Khan AM, Hossain M, Su-Myat KK, Wood PL, Krenitsky K, Takemasa I, Miyake M, Sekimoto M, Monden M, Matsubara H, Nomura F, Goodenow DB: Reduced levels of hydroxylated, polyunsaturated ultra long-chain fatty acids in the serum of colorectal cancer patients: implications for early screening and detection. *BMC Med.* 2010 Feb 15;8:13. doi: 10.1186/1741-7015-8-13. PMID: 20156336

Qiu Y, Cai G, Su M, Chen T, Zheng X, Xu Y, Ni Y, Zhao A, Xu LX, Cai S, Jia W: Serum metabolite profiling of human colorectal cancer using GC-TOFMS and UPLC-QTOFMS. *J Proteome Res.* 2009 Oct;8(10):4844-50. doi: 10.1021/pr9004162. PMID: 19678709

Ni Y, Xie G, Jia W: Metabonomics of human colorectal cancer: new approaches for early diagnosis and biomarker discovery. *J Proteome Res.* 2014 Sep 5;13(9):3857-70. doi: 10.1021/pr500443c. Epub 2014 Aug 14. PMID: 25105552

Ikeda A, Nishiumi S, Shinohara M, Yoshie T, Hatano N, Okuno T, Bamba T, Fukusaki E, Takenawa T, Azuma T, Yoshida M: Serum metabolomics as a novel diagnostic approach for gastrointestinal cancer. *Biomed Chromatogr.* 2012 May;26(5):548-58. doi: 10.1002/bmc.1671. Epub 2011 Jul 20. PMID: 21773981

Goedert JJ, Sampson JN, Moore SC, Xiao Q, Xiong X, Hayes RB, Ahn J, Shi J, Sinha R: Fecal metabolomics: assay performance and association with colorectal cancer. *Carcinogenesis.* 2014 Sep;35(9):2089-96. doi: 10.1093/carcin/bg3131. Epub 2014 Jul 18. PMID: 25037050

Sinha R, Ahn J, Sampson JN, Shi J, Yu G, Xiong X, Hayes RB, Goedert JJ: Fecal Microbiota, Fecal Metabolome, and Colorectal Cancer Interrelations. *PLoS One.* 2016 Mar 25;11(3):e0152126. doi: 10.1371/journal.pone.0152126. eCollection 2016. PMID: 27015276

Lin Y, Ma C, Liu C, Wang Z, Yang J, Liu X, Shen Z, Wu R: NMR-based fecal metabolomics fingerprinting as predictors of earlier diagnosis in patients with colorectal cancer. *Oncotarget.* 2016 May 17;7(20):29454-64. doi: 10.18632/oncotarget.8762. PMID: 27107423

Brown DG, Rao S, Weir TL, O'Malia J, Bazan M, Brown RJ, Ryan EP: Metabolomics and metabolic pathway networks from human colorectal cancers, adjacent mucosa, and stool. *Cancer Metab.* 2016 Jun 6;4:11. doi: 10.1186/s40170-016-0151-y. eCollection 2016. PMID: 27275383

Wang X, Wang J, Rao B, Deng L: Gut flora profiling and fecal metabolite composition of colorectal cancer patients and healthy individuals. *Exp Ther Med.* 2017 Jun;13(6):2848-2854. doi: 10.3892/etm.2017.4367. Epub 2017 Apr 20. PMID: 28587349

Silke Matysik, Caroline Ivonne Le Roy, Gerhard Liebisch, Sandrine Paule Claus. Metabolomics of fecal samples: A practical consideration. *Trends in Food Science & Technology.* Vol. 57, Part B, Nov. 2016, p.244-255:  
<http://www.sciencedirect.com/science/article/pii/S0924224416301984> PMID: 7482520

## Lysyl-Alanine -- Introduction

SYNONYM: K-a Dipeptide; KA dipeptide; L-Lysyl-L-alanine; Lys-ala; Lysine alanine dipeptide; Lysine-alanine dipeptide; Lysylalanine

HMDB: HMDB0028944; HMDB28944



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CAS:

Lysyl-Alanine is a dipeptide composed of lysine and alanine. It is an incomplete breakdown product of protein digestion or protein catabolism. Some dipeptides are known to have physiological or cell-signaling effects although most are simply short-lived intermediates on their way to specific amino acid degradation pathways following further proteolysis. This dipeptide has not yet been identified in human tissues or biofluids and so it is classified as an 'Expected' metabolite.

This compound belongs to the class of organic compounds known as dipeptides. These are organic compounds containing a sequence of exactly two alpha-amino acids joined by a peptide bond.

## Phenylalanyl-Isoleucine -- Introduction

SYNONYM: F-I dipeptide; FI dipeptide; L-Phenylalanyl-L-isoleucine; Phe-ile; Phenylalanine isoleucine dipeptide; Phenylalanine-isoleucine dipeptide; Phenylalanylsoleucine

HMDB: HMDB0028998; HMDB28998

CAS:

Phenylalanyl-Isoleucine is a dipeptide composed of phenylalanine and isoleucine. It is an incomplete breakdown product of protein digestion or protein catabolism. Some dipeptides are known to have physiological or cell-signaling effects although most are simply short-lived intermediates on their way to specific amino acid degradation pathways following further proteolysis. This dipeptide has not yet been identified in human tissues or biofluids and so it is classified as an 'Expected' metabolite.

This compound belongs to the class of organic compounds known as dipeptides. These are organic compounds containing a sequence of exactly two alpha-amino acids joined by a peptide bond.

## Phenylalanyl-Isoleucine -- Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. *Tohoku J Exp Med.* 1995 May;176(1):61-8. PMID: 7482520

Cheng Y, Xie G, Chen T, Qiu Y, Zou X, Zheng M, Tan B, Feng B, Dong T, He P, Zhao L, Zhao A, Xu LX, Zhang Y, Jia W: Distinct urinary metabolic profile of human colorectal cancer. *J Proteome Res.* 2012 Feb 3;11(2):1354-63. doi: 10.1021/pr201001a. Epub 2011 Dec 28. PMID: 22148915

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Weir TL, Manter DK, Sheflin AM, Barnett BA, Heuberger AL, Ryan EP: Stool microbiome and metabolome differences between colorectal cancer patients and healthy adults. *PLoS One.* 2013 Aug 6;8(8):e70803. doi: 10.1371/journal.pone.0070803. Print 2013. PMID: 23940645

Phua LC, Chue XP, Koh PK, Cheah PY, Ho HK, Chan EC: Non-invasive fecal metabonomic detection of colorectal cancer. *Cancer Biol Ther.* 2014 Apr;15(4):389-97. doi: 10.4161/cbt.27625. Epub 2014 Jan 14. PMID: 24424155

Ritchie SA, Ahiahonu PW, Jayasinghe D, Heath D, Liu J, Lu Y, Jin W, Kavianpour A, Yamazaki Y, Khan AM, Hossain M, Su-Myat KK, Wood PL, Krenitsky K, Takemasa I, Miyake M, Sekimoto M, Monden M, Matsubara H, Nomura F, Goodenow DB: Reduced levels of hydroxylated, polyunsaturated ultra long-chain fatty acids in the serum of colorectal cancer patients: implications for early screening and detection. *BMC Med.* 2010 Feb 15;8:13. doi: 10.1186/1741-7015-8-13. PMID: 20156336

Qiu Y, Cai G, Su M, Chen T, Zheng X, Xu Y, Ni Y, Zhao A, Xu LX, Cai S, Jia W: Serum metabolite profiling of human colorectal cancer using GC-TOFMS and UPLC-QTOFMS. *J Proteome Res.* 2009 Oct;8(10):4844-50. doi: 10.1021/pr9004162. PMID: 19678709

Ni Y, Xie G, Jia W: Metabonomics of human colorectal cancer: new approaches for early diagnosis and biomarker discovery. *J Proteome Res.* 2014 Sep 5;13(9):3857-70. doi: 10.1021/pr500443c. Epub 2014 Aug 14. PMID: 25105552



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Ikeda A, Nishiumi S, Shinohara M, Yoshie T, Hatano N, Okuno T, Bamba T, Fukusaki E, Takenawa T, Azuma T, Yoshida M: Serum metabolomics as a novel diagnostic approach for gastrointestinal cancer. *Biomed Chromatogr.* 2012 May;26(5):548-58. doi: 10.1002/bmc.1671. Epub 2011 Jul 20. PMID: 21773981

Goedert JJ, Sampson JN, Moore SC, Xiao Q, Xiong X, Hayes RB, Ahn J, Shi J, Sinha R: Fecal metabolomics: assay performance and association with colorectal cancer. *Carcinogenesis.* 2014 Sep;35(9):2089-96. doi: 10.1093/carcin/bgu131. Epub 2014 Jul 18. PMID: 25037050

Sinha R, Ahn J, Sampson JN, Shi J, Yu G, Xiong X, Hayes RB, Goedert JJ: Fecal Microbiota, Fecal Metabolome, and Colorectal Cancer Interrelations. *PLoS One.* 2016 Mar 25;11(3):e0152126. doi: 10.1371/journal.pone.0152126. eCollection 2016. PMID: 27015276

Lin Y, Ma C, Liu C, Wang Z, Yang J, Liu X, Shen Z, Wu R: NMR-based fecal metabolomics fingerprinting as predictors of earlier diagnosis in patients with colorectal cancer. *Oncotarget.* 2016 May 17;7(20):29454-64. doi: 10.18632/oncotarget.8762. PMID: 27107423

Brown DG, Rao S, Weir TL, O'Malia J, Bazan M, Brown RJ, Ryan EP: Metabolomics and metabolic pathway networks from human colorectal cancers, adjacent mucosa, and stool. *Cancer Metab.* 2016 Jun 6;4:11. doi: 10.1186/s40170-016-0151-y. eCollection 2016. PMID: 27275383

Wang X, Wang J, Rao B, Deng L: Gut flora profiling and fecal metabolite composition of colorectal cancer patients and healthy individuals. *Exp Ther Med.* 2017 Jun;13(6):2848-2854. doi: 10.3892/etm.2017.4367. Epub 2017 Apr 20. PMID: 28587349

Silke Matysik, Caroline Ivonne Le Roy, Gerhard Liebsch, Sandrine Paule Claus. Metabolomics of fecal samples: A practical consideration. *Trends in Food Science & Technology.* Vol. 57, Part B, Nov. 2016, p.244-255:  
<http://www.sciencedirect.com/science/article/pii/S0924224416301984> PMID: 7482520

## Prolyl-Arginine -- Introduction

SYNONYM: L-Prolyl-L-arginine; P-R Dipeptide; PR Dipeptide; pro-Arg; Proline arginine dipeptide; Proline-arginine dipeptide; Proylarginine; Proylarginine, (D-arg-L-pro)-isomer; Proylarginine, (L-arg-D-pro)-isomer

HMDB: HMDB0029011; HMDB29011

CAS:

Prolyl-Arginine is a dipeptide composed of proline and arginine. It is an incomplete breakdown product of protein digestion or protein catabolism. Some dipeptides are known to have physiological or cell-signaling effects although most are simply short-lived intermediates on their way to specific amino acid degradation pathways following further proteolysis. This dipeptide has not yet been identified in human tissues or biofluids and so it is classified as an 'Expected' metabolite.

This compound belongs to the class of organic compounds known as dipeptides. These are organic compounds containing a sequence of exactly two alpha-amino acids joined by a peptide bond.

## Serylarginine -- Introduction

SYNONYM: L-Seranyl-L-arginine; S-R Dipeptide; Ser-arg; Serine arginine dipeptide; Serine-arginine dipeptide; Serinylarginine; SR Dipeptide

HMDB: HMDB0029033; HMDB29033

CAS:

Serinyl-Arginine is a dipeptide composed of serine and arginine. It is an incomplete breakdown product of protein digestion or protein catabolism. Some dipeptides are known to have physiological or cell-signaling effects although most are simply short-lived intermediates on their way to specific amino acid degradation pathways following further proteolysis. This dipeptide has not yet been identified in human tissues or biofluids and so it is classified as an 'Expected' metabolite.

This compound belongs to the class of organic compounds known as dipeptides. These are organic compounds containing a sequence of exactly two alpha-amino acids joined by a peptide bond.



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## Serylmethionine -- Introduction

SYNONYM: L-Seranyl-L-methionine; S-m Dipeptide; Ser-met; Serine methionine dipeptide; Serine-methionine dipeptide; Serinylmethionine; SM Dipeptide; Serylmethionine; L-Seryl-L-methionine

HMDB: HMDB0029045; HMDB29045

CAS:

Seranyl-Methionine is a dipeptide composed of serine and methionine. It is an incomplete breakdown product of protein digestion or protein catabolism. Some dipeptides are known to have physiological or cell-signaling effects although most are simply short-lived intermediates on their way to specific amino acid degradation pathways following further proteolysis. This dipeptide has not yet been identified in human tissues or biofluids and so it is classified as an 'Expected' metabolite.

This compound belongs to the class of organic compounds known as dipeptides. These are organic compounds containing a sequence of exactly two alpha-amino acids joined by a peptide bond.

## Tryptophyl-Gamma-glutamate -- Introduction

SYNONYM: L-Tryptophyl-L-gamma-glutamate; TRP-Glu; Tryptophan gamma-glutamate dipeptide; Tryptophan-gamma-glutamate dipeptide; Tryptophylgamma-glutamate; W-GE dipeptide; WGE dipeptide

HMDB: HMDB0029097; HMDB29097

CAS:

Tryptophyl-Gamma-glutamate is a dipeptide composed of tryptophan and gamma-glutamate. It is an incomplete breakdown product of protein digestion or protein catabolism. Some dipeptides are known to have physiological or cell-signaling effects although most are simply short-lived intermediates on their way to specific amino acid degradation pathways following further proteolysis. This dipeptide has not yet been identified in human tissues or biofluids and so it is classified as an 'Expected' metabolite.

This compound belongs to the class of organic compounds known as glutamine and derivatives. These are compounds containing glutamine or a derivative thereof resulting from reaction of glutamine at the amino group or the carboxy group, or from the replacement of any hydrogen of glycine by a heteroatom.

## Valyl-Isoleucine -- Introduction

SYNONYM: L-Valyl-L-isoleucine; V-I dipeptide; Val-ile; Valine isoleucine dipeptide; Valine-isoleucine dipeptide; Valylisoleucine; VI dipeptide

HMDB: HMDB0029130; HMDB29130

CAS:

Valyl-Isoleucine is a dipeptide composed of valine and isoleucine. It is an incomplete breakdown product of protein digestion or protein catabolism. Some dipeptides are known to have physiological or cell-signaling effects although most are simply short-lived intermediates on their way to specific amino acid degradation pathways following further proteolysis. This dipeptide has not yet been identified in human tissues or biofluids and so it is classified as an 'Expected' metabolite.

This compound belongs to the class of organic compounds known as dipeptides. These are organic compounds containing a sequence of exactly two alpha-amino acids joined by a peptide bond.

## Valyl-Isoleucine -- Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. Tohoku J Exp Med. 1995 May;176(1):61-8. PMID: 7482520

Cheng Y, Xie G, Chen T, Qiu Y, Zou X, Zheng M, Tan B, Feng B, Dong T, He P, Zhao L, Zhao A, Xu LX, Zhang Y, Jia W: Distinct urinary metabolic profile of human colorectal cancer. J Proteome Res. 2012 Feb 3;11(2):1354-63. doi:



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Monleon D, Morales JM, Barrasa A, Lopez JA, Vazquez C, Celda B: Metabolite profiling of fecal water extracts from human colorectal cancer. *NMR Biomed.* 2009 Apr;22(3):342-8. doi: 10.1002/nbm.1345. PMID: 19006102

Weir TL, Manter DK, Sheflin AM, Barnett BA, Heuberger AL, Ryan EP: Stool microbiome and metabolome differences between colorectal cancer patients and healthy adults. *PLoS One.* 2013 Aug 6;8(8):e70803. doi: 10.1371/journal.pone.0070803. Print 2013. PMID: 23940645

Phua LC, Chue XP, Koh PK, Cheah PY, Ho HK, Chan EC: Non-invasive fecal metabonomic detection of colorectal cancer. *Cancer Biol Ther.* 2014 Apr;15(4):389-97. doi: 10.4161/cbt.27625. Epub 2014 Jan 14. PMID: 24424155

Ritchie SA, Ahiahou PW, Jayasinghe D, Heath D, Liu J, Lu Y, Jin W, Kavianpour A, Yamazaki Y, Khan AM, Hossain M, Su-Myat KK, Wood PL, Krenitsky K, Takemasa I, Miyake M, Sekimoto M, Monden M, Matsubara H, Nomura F, Goodenow DB: Reduced levels of hydroxylated, polyunsaturated ultra long-chain fatty acids in the serum of colorectal cancer patients: implications for early screening and detection. *BMC Med.* 2010 Feb 15;8:13. doi: 10.1186/1741-7015-8-13. PMID: 20156336

Qiu Y, Cai G, Su M, Chen T, Zheng X, Xu Y, Ni Y, Zhao A, Xu LX, Cai S, Jia W: Serum metabolite profiling of human colorectal cancer using GC-TOFMS and UPLC-QTOFMS. *J Proteome Res.* 2009 Oct;8(10):4844-50. doi: 10.1021/pr9004162. PMID: 19678709

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Ikeda A, Nishiumi S, Shinohara M, Yoshie T, Hatano N, Okuno T, Bamba T, Fukusaki E, Takenawa T, Azuma T, Yoshida M: Serum metabolomics as a novel diagnostic approach for gastrointestinal cancer. *Biomed Chromatogr.* 2012 May;26(5):548-58. doi: 10.1002/bmc.1671. Epub 2011 Jul 20. PMID: 21773981

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Lin Y, Ma C, Liu C, Wang Z, Yang J, Liu X, Shen Z, Wu R: NMR-based fecal metabolomics fingerprinting as predictors of earlier diagnosis in patients with colorectal cancer. *Oncotarget.* 2016 May 17;7(20):29454-64. doi: 10.18632/oncotarget.8762. PMID: 27107423

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## Valyl-Lysine -- Introduction

SYNONYM: L-Valyl-L-lysine; V-K Dipeptide; Val-lys; Valine lysine dipeptide; Valine-lysine dipeptide; Valyllysine; VK Dipeptide

HMDB: HMDB0029132; HMDB29132

CAS:



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Valyl-Lysine is a dipeptide composed of valine and lysine. It is an incomplete breakdown product of protein digestion or protein catabolism. Some dipeptides are known to have physiological or cell-signaling effects although most are simply short-lived intermediates on their way to specific amino acid degradation pathways following further proteolysis. This dipeptide has not yet been identified in human tissues or biofluids and so it is classified as an 'Expected' metabolite.

This compound belongs to the class of organic compounds known as dipeptides. These are organic compounds containing a sequence of exactly two alpha-amino acids joined by a peptide bond.

### Valyl-Lysine -- Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. *Tohoku J Exp Med.* 1995 May;176(1):61-8. PMID: 7482520

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## Valyl-Valine -- Introduction

SYNONYM: L-Valyl-L-valine; V-V Dipeptide; Val-val; Valine valine dipeptide; Valine-valine dipeptide; Valylvaline; VV Dipeptide

HMDB: HMDB0029140; HMDB29140

CAS:

Valyl-Valine is a dipeptid composed of two valine residues. It is an incomplete breakdown product of protein digestion or protein catabolism. Some dipeptides are known to have physiological or cell-signaling effects although most are simply short-lived intermediates on their way to specific amino acid degradation pathways following further proteolysis. This dipeptide has not yet been identified in human tissues or biofluids and so it is classified as an 'Expected' metabolite.

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<http://www.sciencedirect.com/science/article/pii/S0924224416301984> PMID: 7482520

## Acetylhomoserine -- Introduction

SYNONYM: 4-Acetoxy-2-aminobutanoic acid; Homoserine acetate; O-Acetyl-L-homoserine; O-Acetylhomoserine

HMDB: HMDB0029423; HMDB29423

CAS: 7540-67-2

Acetylhomoserine is found in pulses. Acetylhomoserine is found in Pisum sativum (peas)

This compound belongs to the class of organic compounds known as alpha amino acids. These are amino acids in which the amino group is attached to the carbon atom immediately adjacent to the carboxylate group (alpha carbon).

## L-Agaridoxin -- Introduction

SYNONYM:

HMDB: HMDB0029445; HMDB29445

CAS:

L-Agaridoxin is found in mushrooms. L-Agaridoxin is a constituent of Agaricus campestris (field mushroom)

This compound belongs to the class of organic compounds known as alpha amino acids. These are amino acids in which the amino group is attached to the carbon atom immediately adjacent to the carboxylate group (alpha carbon).

## Diisopropyl sulfide -- Introduction

SYNONYM: 2,2'-Thiobis-propane; 2,2'-Thiobispropane, 9ci; 2,2'-Thiodipropane; 2,4-Dimethyl-3-thiapentane; 2-(Isopropylsulfanyl)propane; Isopropyl sulfide, 8ci; Isopropyl sulphide

HMDB: HMDB0029579; HMDB29579

CAS: 625-80-9

Diisopropyl sulfide is present in simulated meat flavours derived from autolysed baker's yeast

This compound belongs to the class of organic compounds known as dialkylthioethers. These are organosulfur



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compounds containing a thioether group that is substituted by two alkyl groups.

### 3-O-Methylcoumestrol -- Introduction

SYNONYM:

HMDB: HMDB0029584; HMDB29584

CAS:

3-O-Methylcoumestrol is found in pulses. 3-O-Methylcoumestrol is isolated from alfalfa (*Medicago sativa*)

This compound belongs to the class of organic compounds known as coumestans. These are polycyclic aromatic compounds containing a coumestan moiety, which consists of a benzoxole fused to a chromen-2-one to form 1-Benzoxolo[3,2-c]chromen-6-one. They are oxidation products of pterocarpan.

### Octadecylamine -- Introduction

SYNONYM: 1-Aminooctadecane; 1-Octadecanamine; 1-Octadecylamine; Mono{octadecylamine}; N-Octadecylamine; N-Stearylamine; Stearamine; Stearyl amine; Stearylamine; 1-Octadecanamine, 9ci; Adogenen 142; Alamine 7; Alamine 7D; Amine ab; Amines, hydrogenated tallow alkyl; Armeen 1180; Armeen 118D; Armeen 18; Armeen 18D; Armid HTD; Armofilm; Crodamine 1.18D; Farmin 80; Hydrogenated tallowamine; Kemamine P 990; Kemamine P-990, P-990D; Kemamine P990; Nissan amine ab; Noram SH; Octadecan-1-amine; OCTADECANE,1-amino; Octadecylamineadogenen 142; Oktadecylamin; Steamfilm FG; Tallow amine, hydrogenated

HMDB: HMDB0029586; HMDB29586

CAS: 124-30-1

Octadecylamine is present in food through its use as a boiler water additive

This compound belongs to the class of organic compounds known as monoalkylamines. These are organic compounds containing a primary aliphatic amine group.

### 2',6'-Dihydroxy-4'-methoxyacetophenone -- Introduction

SYNONYM: 4-O-Methylphloracetophenone; 1-(2,6-Dihydroxy-4-methoxyphenyl)ethanone; 2,6-Dihydroxy-4-methoxyacetophenone; Acetophenone, 2',6'-dihydroxy-4'-methoxy- (8ci); Ethanone, 1-(2,6-dihydroxy-4-methoxyphenyl)- (9ci)

HMDB: HMDB0029646; HMDB29646

CAS: 7507-89-3

2',6'-Dihydroxy-4'-methoxyacetophenone is found in European plum. 2',6'-Dihydroxy-4'-methoxyacetophenone is isolated from the bark of *Prunus domestica* (plum)

This compound belongs to the class of organic compounds known as alkyl-phenylketones. These are aromatic compounds containing a ketone substituted by one alkyl group, and a phenyl group.

### Phlorisobutyrophenone 2-glucoside -- Introduction

SYNONYM:

HMDB: HMDB0029651; HMDB29651

CAS: 17004-75-0

Phlorisobutyrophenone 2-glucoside is found in alcoholic beverages. Phlorisobutyrophenone 2-glucoside is a constituent of hops (*Humulus lupulus*)

This compound belongs to the class of organic compounds known as phenolic glycosides. These are organic



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compounds containing a phenolic structure attached to a glycosyl moiety. Some examples of phenolic structures include lignans, and flavonoids. Among the sugar units found in natural glycosides are D-glucose, L-Fructose, and L rhamnose.

## 2-Hydroxy-6-pentadecylbenzoic acid -- Introduction

SYNONYM: Anacardic acid; Anacardate; 2-Hydroxy-6-pentadecylbenzoate; (15:0)-Anacardic acid; 2-Hydroxy-6-pentadecylbenzoic acid; 22:0-Anacardic acid; 6-Pentadecylsalicylic acid; Cyclogallipharic acid; Hydrogenated anacardic acid; Hydroginkgolic acid; 6-(8(Z),11(Z),14-Pentadecatrienyl)salicylic acid; 6-(8,11,14-Pentadecatrienyl)salicylic acid; 6-Nonadecyl salicylic acid

HMDB: HMDB0029683; HMDB29683

CAS: 16611-84-0

2-Hydroxy-6-pentadecylbenzoic acid is found in cashew nut. Synthesised by immature seeds of *Ginkgo biloba* (ginkgo). Chemically, anacardic acid is a mixture of several closely related organic compounds. Each consists of a salicylic acid substituted with an alkyl chain that has 15 or 17 carbon atoms; anacardic acid is a mixture of saturated and unsaturated molecules. The exact mixture depends on the species of the plant and the major component is C5:3 all-Z. (Wikipedia)

This compound belongs to the class of organic compounds known as salicylic acids. These are ortho-hydroxylated benzoic acids.

## 1H-Indole-3-carboxaldehyde -- Introduction

SYNONYM: Indole-3-carbaldehyde; 1H-Indole-3-carbaldehyde; 1H-Indole-3-carboxaldehyde; 3-Formylindole; 3-Indolealdehyde; 3-Indolecarbaldehyde; 3-Indolecarboxaldehyde; 3-Indolemethanal; b-Indolylaldehyde; beta-Indolylaldehyde; indol-3-Carbaldehyd; indol-3-Carbaldehyde; indol-3-Carboxaldehyde; Indole-3-aldehyde; INDOLE-3-carboxyaldehyde

HMDB: HMDB0029737; HMDB29737

CAS: 487-89-8

1H-Indole-3-carboxaldehyde is found in barley. 1H-Indole-3-carboxaldehyde is found in barley and tomato seedlings and cotto

This compound belongs to the class of organic compounds known as indoles. These are compounds containing an indole moiety, which consists of pyrrole ring fused to benzene to form 2,3-benzopyrrole.

## 3-Amino-1,4-dimethyl-5H-pyrido[4,3-b]indole -- Introduction

SYNONYM: 1,4-Dimethyl-5H-pyrido(4,3-b)indol-3-amine; 1,4-Dimethyl-5H-pyrido[4,3-b]indol-3-amine, 9ci; 1,4-Dimethyl-9H-pyrido(4,3-b)indol-3-amine; 3-amino-1,4-Dimethyl-5H-pyrido(4,3-b)indole; 3-amino-1,4-Dimethyl-g-carboline; 3-amino-1,4-Dimethyl-gamma-carboline; TRP-1; TRP-P-1; TRP-P1; Tryptophan P1; Tryptophan-P-1; Tryptophan pyrolysate 1

HMDB: HMDB0029746; HMDB29746

CAS: 62450-06-0

3-Amino-1,4-dimethyl-5H-pyrido[4,3-b]indole is a powerful mutacarcinogen found in cooked food

This compound belongs to the class of organic compounds known as gamma carbolines. These are polycyclic aromatic compounds containing a gamma-carbazole(5H-pyrido[4,3-b]indole) moiety, with a structure characterized by the presence of pyridine fused to the pyrrole ring of an indole.

## Montecristin -- Introduction

SYNONYM: 3-(11,12-Dihydroxy-15,19-dotriacontadienyl)-5-methyl-2(5H)-furanone, 9ci

HMDB: HMDB0029795; HMDB29795



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CAS: 185336-15-6

Montecristin is found in fruits. Montecristin is a constituent of *Annona muricata* (soursop)

This compound belongs to the class of organic compounds known as annonaceous acetogenins. These are waxy derivatives of fatty acids (usually C32 or C34), containing a terminal carboxylic acid combined with a 2-propanol unit at the C-2 position to form a methyl- substituted alpha,beta-unsaturated-gamma-lactone. One of their interesting structural features is a single, adjacent, or nonadjacent tetrahydrofuran (THF) or tetrahydropyran (THP) system with one or two flanking hydroxyl group(s) at the center of a long hydrocarbon chain.

## Ethyl hexadecanoate -- Introduction

SYNONYM: Ethyl cetylate; Palmitic acid ethyl ester; WE(2:0/16:0); Ethyl cetyllic acid; Ethyl hexadecanoic acid; Palmitate ethyl ester; Ethyl hexadecanoate (ethyl palmitate); Ethyl N-hexadecanoate; Ethyl palmitate; Ethylpalmitate; FEMA 2451; Hexadecanoic acid, ethyl ester; HEXADECANOIC ACID,ethyl ester MFC18 H36 O2; Palmitic acid, ethyl ester; Palmitic acid, ethyl ester (8ci)

HMDB: HMDB0029811; HMDB29811

CAS: 628-97-7

Ethyl hexadecanoate is found in alcoholic beverages. Ethyl hexadecanoate is present in various fruits, e.g. apricot, sour cherry, grapefruit, bilberry, guava fruit, melon, pineapple, Chinese quince, ceriman (*Monstera deliciosa*) etc. Also present in crispbread, clary sage, blackcurrant buds, wines, rice bran, plum brandy, fruit brandy, Bourbon vanilla, beans and salted/pickled plum

This compound belongs to the class of organic compounds known as fatty acid esters. These are carboxylic ester derivatives of a fatty acid.

## Neotrehalose -- Introduction

SYNONYM: (GLC)2; alpha,Alpha'-trehalose; alpha-D-GLCP-(11)-alpha-D-GLCP; alpha-D-Glucopyranosyl-alpha-D-glucopyranoside; alpha-D-Trehalose; alpha-Trehalose; D-(+)-Trehalose; Ergot sugar; Mycose; a,Alpha'-trehalose;  $\beta\pm$ ,alpha'-trehalose; a-D-GLCP-(11)-a-D-GLCP;  $\beta\pm$ -D-GLCP-(11)- $\beta\pm$ -D-GLCP; a-D-Glucopyranosyl-a-D-glucopyranoside;  $\beta\pm$ -D-glucopyranosyl- $\beta\pm$ -D-glucopyranoside; a-D-Trehalose;  $\beta\pm$ -D-trehalose; a-Trehalose;  $\beta\pm$ -trehalose; alpha,alpha-Trehalose; D-Trehalose-anhydrous; delta-Trehalose-anhydrous

HMDB: HMDB0029880; HMDB29880

CAS: 585-91-1

Neotrehalose is a constituent of honey

This compound belongs to the class of organic compounds known as o-glycosyl compounds. These are glycoside in which a sugar group is bonded through one carbon to another group via a O-glycosidic bond.

## (R)-Pelletierine -- Introduction

SYNONYM: (-)-Pelletierine; (R)-(-)-Pelletierine; (R)-1-(2-Piperidyl)acetone

HMDB: HMDB0030324; HMDB30324

CAS: 2858-66-4

(R)-Pelletierine is found in fruits. (R)-Pelletierine is an alkaloid from pomegranat

This compound belongs to the class of organic compounds known as piperidines. These are compounds containing a piperidine ring, which is a saturated aliphatic six-member ring with one nitrogen atom and five carbon atoms.

## Arecaidine -- Introduction



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SYNONYM: 1,2,5,6-tetrahydro-1-Methyl-3-pyridinecarboxylic acid; 1,2,5,6-tetrahydro-1-Methyl-nicotinic acid; 1,2,5,6-tetrahydro-1-Methylnicotinic acid; Arecaine; Isoguvacine; Methylguvacine; N-Methylguvacine

HMDB: HMDB0030352; HMDB30352

CAS: 499-04-7

Arecaidine is found in nuts. Arecaidine is an alkaloid from nuts of Areca catechu (betel nuts)

This compound belongs to the class of organic compounds known as alkaloids and derivatives. These are naturally occurring chemical compounds that contain mostly basic nitrogen atoms. This group also includes some related compounds with neutral and even weakly acidic properties. Also some synthetic compounds of similar structure are attributed to alkaloids. In addition to carbon, hydrogen and nitrogen, alkaloids may also contain oxygen, sulfur and more rarely other elements such as chlorine, bromine, and phosphorus.

### 3-Methyl-5-pentyl-2-furanundecanoic acid -- Introduction

SYNONYM: F5 acid; F5 Furan fatty acid; MonoMe(11,5)

HMDB: HMDB0031005; HMDB31005

CAS: 57818-37-8

3-methyl-5-pentyl-2-furanundecanoic acid is a furan fatty acid (F-acid). F-acids are heterocyclic fatty acids containing a central furan moiety with a carboxylalkyl chain (mostly 7, 9, 11, or 13 carbons) in the 2-position and an alkyl chain (mostly 3 or 5 carbons) in the 5-position. Despite being found in low concentrations in food lipids, they are excellent antioxidants and radical scavengers. This allows them to play an important role in preventing lipid peroxidation and protecting polyunsaturated fatty acids. They are often incorporated into phospholipids and cholesterol esters of fish and other marine organisms. 3-methyl-5-pentyl-2-furanundecanoic acid, in particular, can be described by the shorthand notation 11M5. This refers to its 11-carbon carboxylalkyl moiety, the methyl substitution in the 3-position of its furan moiety, and its 5-carbon alkyl moiety. It is a constituent of fats of the liver and gonads of fishes, e.g. pike (*Esox lucius*).

This compound belongs to the class of organic compounds known as long-chain fatty acids. These are fatty acids with an aliphatic tail that contains between 13 and 21 carbon atoms.

### Methyl pentyl disulfide -- Introduction

SYNONYM: 1-(Methyldisulfanyl)pentane; 2,3-Dithiaoctane; Amyl methyl disulfide; Disulfide, methyl pentyl; Methyl N-amyl disulfide; Methyl N-pentyl disulphide; Methyl pentyl disulfide, 9ci

HMDB: HMDB0031161; HMDB31161

CAS: 72437-68-4

Methyl pentyl disulfide is found in chives. Methyl pentyl disulfide is a constituent of chives (*Allium schoenoprasum*)

This compound belongs to the class of organic compounds known as dialkyldisulfides. These are organic compounds containing a disulfide group R-SS-R' where R and R' are both alkyl groups.

### Cohibin A -- Introduction

SYNONYM: Cohibin c

HMDB: HMDB0031168; HMDB31168

CAS: 189508-31-4

Cohibin A is found in fruits. Cohibin A is a constituent of the roots of *Annona muricata* (soursop)

This compound belongs to the class of organic compounds known as annonaceous acetogenins. These are waxy derivatives of fatty acids (usually C32 or C34), containing a terminal carboxylic acid combined with a 2-propanol unit at the



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C-2 position to form a methyl- substituted alpha,beta-unsaturated-gamma-lactone. One of their interesting structural features is a single, adjacent, or nonadjacent tetrahydrofuran (THF) or tetrahydropyran (THP) system with one or two flanking hydroxyl group(s) at the center of a long hydrocarbon chain.

## Pyrrolidine -- Introduction

SYNONYM: Azolidine; Tetrahydropyrrole; Tetramethylenimine; 1-Azacyclopentane; Azacyclopentane; FEMA 3523

HMDB: HMDB0031641; HMDB31641

CAS: 123-75-1

Pyrrolidine is found in alcoholic beverages. Pyrrolidine is widely distributed in foodstuffs in trace amounts., presumably as bacterial decarboxylation produced of proline. Pyrrolidine is present in bread, milk, cheese, carrots, celery stalks, beer, spirits, coffee, caviar and fatty fish. Pyrrolidine is a flavouring agent.Pyrrolidine is a clear liquid with an unpleasant odor that is ammoniacal, fishy, shellfish-like and seaweed-like. Pyrrolidine is found naturally in the leaves of tobacco and carrot. The pyrrolidine ring structure is present in numerous natural alkaloids such as nicotine and hygrine. It is found in many pharmaceutical drugs such as procyclidine and bepridil. It also forms the basis for the racetam compounds (e.g. piracetam, aniracetam). Pyrrolidine is a pyrrolidine ring is the central structure of the amino acids proline and hydroxyproline. (Wikipedia)

This compound belongs to the class of organic compounds known as pyrrolidines. These are compounds containing a pyrrolidine ring, which is a five-membered saturated aliphatic heterocycle with one nitrogen atom and four carbon atoms.

## N-Nitroso-pyrrolidine -- Introduction

SYNONYM: 1-Nitrosopyrrolidine; 1-nitroso-Pyrrolidine; N-nitroso-1-Pyrrolidinamine; nitroso-Pyrrolidine; Nitrosopyrrolidine; tetrahydro-N-nitroso-Pyrrole; N-Nitrosopyrrolidine; N Nitrosopyrrolidine

HMDB: HMDB0031642; HMDB31642

CAS: 930-55-2

N-Nitroso-pyrrolidine is found in animal foods. N-Nitroso-pyrrolidine is found in fried bacon

This compound belongs to the class of organic compounds known as pyrrolidines. These are compounds containing a pyrrolidine ring, which is a five-membered saturated aliphatic heterocycle with one nitrogen atom and four carbon atoms.

## (E)-Monocrotophos -- Introduction

SYNONYM: (E)-Monocrotophos; Azodrin; Dimethyl (E)-1-methyl-2-(methylcarbamoyl)vinyl phosphate; Dimethyl (E)-3-hydroxy-N-methylcrotonamide; Phosphoric acid, dimethyl (E)-1-methyl-3-(methylamino)-3-oxo-1-propenyl ester; Dimethyl (E)-1-methyl-2-(methylcarbamoyl)vinyl phosphoric acid; Phosphate, dimethyl (E)-1-methyl-3-(methylamino)-3-oxo-1-propenyl ester; 3-(Dimethoxyphosphinyloxy)N-methyl-cis-crotonamide; 3-Dimethoxyphosphinoyloxy-N-methylisocrotonamide; 3-Hydroxy-N-methyl-cis-crotonamide dimethyl phosphate; 3-Hydroxy-N-methyl-cis-crotonamide dimethyl phosphate ester; 3-Hydroxy-N-methyl-dimethylphosphate(E)-crotonamide; 3-Hydroxy-N-methyl-dimethylphosphatecis-crotonamide; Aimocron; Apadrin; Azadrin; Azodrin 202R; Azodrin insecticide; Azodrin-71; Biloborn; Bilobran; cis-1-Methyl-2-methyl carbamoyl vinyl phosphate; Corophos; Crisodin; Crisodrin; Croton 36; Crotos; Des-N-methyl dicrotophos; Dimethyl 1-methyl-2-(methylcarbamoyl)vinyl phosphate, cis; Dimethyl phosphate OF 3-hydroxy-N-methyl-cis-crotonamide; e-Monocrotophos; Glare phos 36; Hazodrin; Monocil; Monocil 40; Monocron; Monocrotophos 40 ec; Monodrin; Monokrotofosz; Monostar; N-Desmethyl bidrin; Nuvacron; Nuvacron 20; Nuvacron-20; O,O-Dimethyl cis-1-methyl-2-methylcarbamoylvinylphosphate; O,O-Dimethyl-O-(2-N-methylcarbamoyl-1-methyl-vinyl)-fosfaat; O,O-Dimetil-O-(2-N-metilcarbamoiil-1-metil-vinil)-fosfato; Pandar; Parryfos; Pillardrin; Plantdrin; Rapid X; Shell SD 9129; Susvin; Ulvair

HMDB: HMDB0031805; HMDB31805

CAS: 6923-22-4

(E)-Monocrotophos is an Agricultural insecticide with both systemic and contact action

This compound belongs to the class of organic compounds known as dialkyl phosphates. These are organic compounds



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containing a phosphate group that is linked to exactly two alkyl chain.

### 3-O-Acetylepisamarcandin -- Introduction

SYNONYM:

HMDB: HMDB0031958; HMDB31958

CAS: 61490-18-4

3-O-Acetylepisamarcandin is found in green vegetables. 3-O-Acetylepisamarcandin is isolated from Ferula assa-foetida (asafoetida)

This compound belongs to the class of organic compounds known as coumarins and derivatives. These are polycyclic aromatic compounds containing a 1-benzopyran moiety with a ketone group at the C2 carbon atom (1-benzopyran-2-one).

### Episetinidol-(4beta->8)-catechin -- Introduction

SYNONYM: Episetinidol(4b->8)catechin

HMDB: HMDB0032007; HMDB32007

CAS:

Episetinidol-(4beta->8)-catechin is found in fruits. Episetinidol-(4beta->8)-catechin is a constituent of Pithecellobium dulce (manila tamarino)

This compound belongs to the class of organic compounds known as proanthocyanidins. These are molecules containing an oligomeric moiety of C4-C8 and/or C4-C6 and/or C2-C7 oligo/polymers of flavan-3-ols.

### Lauroyl diethanolamide -- Introduction

SYNONYM: Clindrol; Lauramide dea; Lauric diethanolamide; Lauryl diethanolamide; N,N-Bis(2-hydroxyethyl)dodecanamide, 9ci. N,N-bis(2-hydroxyethyl)lauramide

HMDB: HMDB0032358; HMDB32358

CAS: 120-40-1

Lauroyl diethanolamide is used as a food additive [EAFUS] ("EAFUS: Everything Added to Food in the United States. [<http://www.eafus.com/>]")

This compound belongs to the class of organic compounds known as n-acyl amines. These are compounds containing a fatty acid moiety linked to an amine group through an ester linkage.

### Triethanolamine -- Introduction

SYNONYM: 2,2',2"-NITRILOTRIETHANOL; 2,2',2"-Nitrilotris(ethanol); H3Tea; N(CH<sub>2</sub>CH<sub>2</sub>OH)<sub>3</sub>; nitrilo-2,2',2"-Triethanol; Nitrilotriethanol; TEA; Tris(2-hydroxyethyl)amine; Tris(beta-hydroxyethyl)amine; Tris(b-hydroxyethyl)amine; Tris(<sup>1</sup>H-hydroxyethyl)amine; 2,2', 2"-Nitrilotriethanol; 2,2',2"-nitrilotriethanol; 2,2',2"-Nitrilotri-ethanol; 2,2',2"-Nitrilotri-ethanol; 2,2',2"-Nitrilotrisethanol; 2,2',2"-Nitrilotris[ethanol]; 2,2',2"-Trihydroxy-triethylamine; 2,2',2"-Trihydroxytriethylamine; 2,2',2"-Nitrilotriethanol; 2,2',2"-Nitrilotriethanol; 2,2',2"-Nitrilotriethanol; 2,2',2"-Nitrilotriethanol; 637-39-8 (Unspecified hydrochloride); 7376-31-0 (Unspecified sulfate salt); 7376-31-0 (Unspecified sulphate salt); Alkano; Alkanolamine 244; BTB; Cerumenex; Daltogen; Ethanol, 2,2',2"-nitrilotris-, homopolymer; Mobisy; Mobisy; nitrilo-2,2',2Quot -triethanol; Nitrilotris(ethanol); Poly(triethanolamine) ether; Sodium isa; Sterolamide; Sting-kill; Tea (amino alcohol); TEOA; thiofaco T-35; Tri(hydroxyethyl)amine; Triethanolamin-NG; Triethanolamin; Triethanolamin-NG; Triethanolamine condensate polymer; Triethanolamine homopolymer; Triethylolamine; Trihydroxyethylamine; Trihydroxytriethylamine; Tris(2-hydroxyethyl) amine; Tris(beta -hydroxyethyl)amine; Tris(hydroxyethyl)amine; Trola; Trolamine (NF)

HMDB: HMDB0032538; HMDB32538



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CAS: 102-71-6

Triethanolamine is used as a food additive [EAFUS] ("EAFUS: Everything Added to Food in the United States. [http://www.eafus.com/]")

This compound belongs to the class of organic compounds known as 1,2-aminoalcohols. These are organic compounds containing an alkyl chain with an amine group bound to the C1 atom and an alcohol group bound to the C2 atom.

### Triethanolamine -- Cystic fibrosis

Matsui A, Psacharopoulos HT, Mowat AP, Portmann B, Murphy GM: Radioimmunoassay of serum glycocholic acid, standard laboratory tests of liver function and liver biopsy findings: comparative study of children with liver disease. *J Clin Pathol.* 1982 Sep;35(9):1011-7. PMID: 7119120

Smith JL, Lewindon PJ, Hoskins AC, Pereira TN, Setchell KD, O'Connell NC, Shepherd RW, Ramm GA: Endogenous ursodeoxycholic acid and cholic acid in liver disease due to cystic fibrosis. *Hepatology.* 2004 Jun;39(6):1673-82. PMID: 15185309

Scalabrin G, Galimberti D, Mutti E, Scalabrini D, Veber D, De Riz M, Bamonti F, Capello E, Mancardi GL, Scarpini E: Loss of epidermal growth factor regulation by cobalamin in multiple sclerosis. *Brain Res.* 2010 May 28;1333:64-71. doi: 10.1016/j.brainres.2010.03.073. Epub 2010 Mar 27. PMID: 20347721

Adriana Nori de Macedo. Robust capillary electrophoresis methods for biomarker discovery and routine measurements in clinical and epidemiological applications. March 2017: <https://macsphere.mcmaster.ca/handle/11375/21248> PMID: 7119120

### 2-(Methylamino)benzoic acid -- Introduction

SYNONYM: N-Methyl-2-aminobenzoic acid; N-Methyl-O-aminobenzoic acid; O-(methylamino)Benzocic acid; N-Methyl-2-aminobenzoate; 2-(methylamino)Benzooate; N-Methyl-O-aminobenzoate; O-(methylamino)Benzooate; 2-(methylamino)-Benzooic acid; N-Methyl-anthranoic acid; N-Methylanthranilic acid, 8ci

HMDB: HMDB0032609; HMDB32609

CAS: 119-68-6

2-(Methylamino)benzoic acid is found in citrus. 2-(Methylamino)benzoic acid is isolated from grapefruit peel oil

This compound belongs to the class of organic compounds known as aminobenzoic acids. These are benzoic acids containing an amine group attached to the benzene moiety.

### 4,8,12,15-Octadecatetraenoic acid -- Introduction

SYNONYM:

HMDB: HMDB0032672; HMDB32672

CAS: 67329-10-6

4,8,12,15-Octadecatetraenoic acid is found in fishes. 4,8,12,15-Octadecatetraenoic acid is isolated from sardine oil

This compound belongs to the class of organic compounds known as lineolic acids and derivatives. These are derivatives of lineolic acid. Lineolic acid is a polyunsaturated omega-6 18 carbon long fatty acid, with two CC double bonds at the 9- and 12-positions.

### 3-(2-Methylpropanoyloxy)-8-(3-methylbutanoyloxy)-9,10-epoxy-p-mentha-1,3,5-triene -- Introduction

SYNONYM:

HMDB: HMDB0032700; HMDB32700



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CAS:

3-(2-Methylpropanoyloxy)-8-(3-methylbutanoyloxy)-9,10-epoxy-p-mentha-1,3,5-triene is found in fats and oils. 3-(2-Methylpropanoyloxy)-8-(3-methylbutanoyloxy)-9,10-epoxy-p-mentha-1,3,5-triene is a constituent of *Madia sativa* (Chile tarweed)

This compound belongs to the class of organic compounds known as phenol esters. These are aromatic compounds containing a benzene ring substituted by a hydroxyl group and an ester group.

## Osmaronin -- Introduction

SYNONYM:

HMDB: HMDB0032769; HMDB32769

CAS: 160551-60-0

Osmaronin is found in cereals and cereal products. Osmaronin is a constituent of the leaves of *Hordeum vulgare* (barley).

This compound belongs to the class of organic compounds known as fatty acyl glycosides of mono- and disaccharides. These are compounds composed of a mono- or disaccharide moiety linked to one hydroxyl group of a fatty alcohol or of a phosphorylated alcohol (phosphoprenols), a hydroxy fatty acid or to one carboxyl group of a fatty acid (ester linkage) or to an amino alcohol.

## 4,5-Dimethylthiazole -- Introduction

SYNONYM: (Trichloromethyl)-phosphorous dichloride; 4,5-Dimethyl-1,3-thiazole; 4,5-Dimethyl-thiazole; FEMA 3274

HMDB: HMDB0032976; HMDB32976

CAS: 3581-91-7

4,5-Dimethylthiazole is a flavouring agent.

This compound belongs to the class of organic compounds known as 4,5-disubstituted thiazoles. These are compounds containing a thiazole ring substituted at positions 4 and 5 only.

## 5-(2-Hydroxyethyl)-4-methylthiazole -- Introduction

SYNONYM: 4-Methyl-5-(2'-hydroxyethyl)-thiazole; 4-Methyl-5-(2-hydroxyethyl)-thiazole; 4-Methyl-5-thiazolethanol; Hemineurine; 2-(4-Methyl-1,3-thiazol-5-yl)ethanol; 2-(4-Methyl-5-thiazoly)ethanol; 2-(4-METHYL-thiazol-5-yl)-ethanol; 2-(4-Methylthiazol-5-yl)ethanol; 2-(4-Methylthiazole-5-yl)ethanol; 4-Methyl-5-(2-hydroxyethyl)thiazole; 4-METHYL-5-(beta-hydroxyethyl)-thiazole; 4-Methyl-5-(beta-hydroxyethyl)thiazole; 4-Methyl-5-hydroxethylthiazole; 4-Methyl-5-hydroxyethylthiazole; 4-Methyl-5-thiazolethanol; 4-Methyl-5-thiazoleethanol, 9ci; 4-Methyl-5-thiazolylethanol; 4-Methyl-5-(beta-hydroxyethyl)thiazole; 5-(2-Hydroxyethyl)-4-methylthiazole (sulfurol); 5-(beta-Hydroxyethyl)-4-methylthiazole; 5-(Hydroxyethyl)-4-methylthiazole; FEMA 3204; HET; MHT; Sulfurol; Thiamine breakdown product 4-methyl-5-thiazoleethanol- from; Thiamine thiazole; Thiazole, 5-(2-hydroxyethyl)-4-methyl; TZE; Thiamine thiazole hydrochloride; Thiamine thiazole phosphate

HMDB: HMDB0032985; HMDB32985

CAS: 137-00-8

5-(2-Hydroxyethyl)-4-methylthiazole is found in alcoholic beverages. 5-(2-Hydroxyethyl)-4-methylthiazole is a flavour ingredient. 5-(2-Hydroxyethyl)-4-methylthiazole is present in cooked beef, beer, spirits, cocoa, roast peanut, porcini (*Boletus edulis*) and malt.

This compound belongs to the class of organic compounds known as 4,5-disubstituted thiazoles. These are compounds containing a thiazole ring substituted at positions 4 and 5 only.



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## 5-(2-Hydroxyethyl)-4-methylthiazole -- Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. *Tohoku J Exp Med.* 1995 May;176(1):61-8. PMID: 7482520

Cheng Y, Xie G, Chen T, Qiu Y, Zou X, Zheng M, Tan B, Feng B, Dong T, He P, Zhao L, Zhao A, Xu LX, Zhang Y, Jia W: Distinct urinary metabolic profile of human colorectal cancer. *J Proteome Res.* 2012 Feb 3;11(2):1354-63. doi: 10.1021/pr201001a. Epub 2011 Dec 28. PMID: 22148915

Monleon D, Morales JM, Barrasa A, Lopez JA, Vazquez C, Celda B: Metabolite profiling of fecal water extracts from human colorectal cancer. *NMR Biomed.* 2009 Apr;22(3):342-8. doi: 10.1002/nbm.1345. PMID: 19006102

Weir TL, Manter DK, Sheflin AM, Barnett BA, Heuberger AL, Ryan EP: Stool microbiome and metabolome differences between colorectal cancer patients and healthy adults. *PLoS One.* 2013 Aug 6;8(8):e70803. doi: 10.1371/journal.pone.0070803. Print 2013. PMID: 23940645

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Ritchie SA, Ahiahonu PW, Jayasinghe D, Heath D, Liu J, Lu Y, Jin W, Kavianpour A, Yamazaki Y, Khan AM, Hossain M, Su-Myat KK, Wood PL, Krenitsky K, Takemasa I, Miyake M, Sekimoto M, Monden M, Matsubara H, Nomura F, Goodenow DB: Reduced levels of hydroxylated, polyunsaturated ultra long-chain fatty acids in the serum of colorectal cancer patients: implications for early screening and detection. *BMC Med.* 2010 Feb 15;8:13. doi: 10.1186/1741-7015-8-13. PMID: 20156336

Qiu Y, Cai G, Su M, Chen T, Zheng X, Xu Y, Ni Y, Zhao A, Xu LX, Cai S, Jia W: Serum metabolite profiling of human colorectal cancer using GC-TOFMS and UPLC-QTOFMS. *J Proteome Res.* 2009 Oct;8(10):4844-50. doi: 10.1021/pr9004162. PMID: 19678709

Ni Y, Xie G, Jia W: Metabonomics of human colorectal cancer: new approaches for early diagnosis and biomarker discovery. *J Proteome Res.* 2014 Sep 5;13(9):3857-70. doi: 10.1021/pr500443c. Epub 2014 Aug 14. PMID: 25105552

Ikeda A, Nishiumi S, Shinohara M, Yoshie T, Hatano N, Okuno T, Bamba T, Fukusaki E, Takenawa T, Azuma T, Yoshida M: Serum metabolomics as a novel diagnostic approach for gastrointestinal cancer. *Biomed Chromatogr.* 2012 May;26(5):548-58. doi: 10.1002/bmc.1671. Epub 2011 Jul 20. PMID: 21773981

Goedert JJ, Sampson JN, Moore SC, Xiao Q, Xiong X, Hayes RB, Ahn J, Shi J, Sinha R: Fecal metabolomics: assay performance and association with colorectal cancer. *Carcinogenesis.* 2014 Sep;35(9):2089-96. doi: 10.1093/carcin/bgu131. Epub 2014 Jul 18. PMID: 25037050

Sinha R, Ahn J, Sampson JN, Shi J, Yu G, Xiong X, Hayes RB, Goedert JJ: Fecal Microbiota, Fecal Metabolome, and Colorectal Cancer Interrelations. *PLoS One.* 2016 Mar 25;11(3):e0152126. doi: 10.1371/journal.pone.0152126. eCollection 2016. PMID: 27015276

Lin Y, Ma C, Liu C, Wang Z, Yang J, Liu X, Shen Z, Wu R: NMR-based fecal metabolomics fingerprinting as predictors of earlier diagnosis in patients with colorectal cancer. *Oncotarget.* 2016 May 17;7(20):29454-64. doi: 10.18632/oncotarget.8762. PMID: 27107423

Brown DG, Rao S, Weir TL, O'Malia J, Bazan M, Brown RJ, Ryan EP: Metabolomics and metabolic pathway networks from human colorectal cancers, adjacent mucosa, and stool. *Cancer Metab.* 2016 Jun 6;4:11. doi: 10.1186/s40170-016-0151-y. eCollection 2016. PMID: 27275383

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## Methylpyrazine -- Introduction

SYNONYM: 2-Methylpyrazine; 2-Methyl-1,4-diazine; 2-Methyl-pyrazine; FEMA 3309; Methyl-pyrazine

HMDB: HMDB0033112; HMDB33112

CAS: 109-08-0

Methylpyrazine is found in alcoholic beverages. Methylpyrazine is a flavouring agent. Methylpyrazine is present in many foods, e.g. bakery products, dairy products, meats, baked or French fried potato, roasted barley, cocoa, coffee, tea, roasted filbert, roasted pecan, peanut, soy products, rum and whisky.

This compound belongs to the class of organic compounds known as pyrazines. These are compounds containing a pyrazine ring, which is a six-member aromatic heterocycle, that consists of two nitrogen atoms (at positions 1 and 4) and four carbon atoms.

## 1-Methylpyrrolo[1,2-a]pyrazine -- Introduction

SYNONYM:

HMDB: HMDB0033171; HMDB33171

CAS: 64608-59-9

1-Methylpyrrolo[1,2-a]pyrazine is a maillard product.

This compound belongs to the class of organic compounds known as pyrrolopyrazines. These are compounds containing a pyrrolopyrazine moiety, which consists of a pyrrole ring fused to a pyrazine. Pyrrole is 5-membered ring consisting of four carbon atoms and one nitrogen atom. Pyrazine is a 6-membered ring consisting of six carbon atoms and two nitrogen centers at ring positions 1 and 4.

## 6-Chloro-N-(1-methylethyl)-1,3,5-triazine-2,4-diamine -- Introduction

SYNONYM: 2-amino-4-chloro-6-(isopropylamino)-S-Triazine; 2-chloro-4-amino-6-(isopropylamino)-S-Triazine; 4-Deethylatrazine; 6-chloro-N-Isopropyl-1,3,5-triazine-2,4-diamine; Deethylatrazin; Desethyl atrazine; 2-amino-4-chloro-6-(isopropylamino)-1,3,5-Triazine; 2-amino-4-chloro-6-isopropylamino-1,3,5-Triazine; 2-amino-4-isopropylamino-6-chloro-S-Triazine; 2-chloro-4-amino-6-isopropylamino-S-Triazine; 2-chloro-4-isopropylamino-6-amino-S-Triazine; 6-chloro-N-(1-Methylethyl)-1,3,5-triazine-2,4-diamine, 9ci; 6-chloro-N-(Propan-2-yl)-1,3,5-triazine-2,4-diamine; Atrazine desethyl; Atrazine m (des-ethyl); Atrazine-desethyl; CIAT; Deethylatrazine; Deethylatrazine; Des-ethyl atrazine; Desethyl-atrazine; Desethylatrazine; Desisopropyl propazine; 2-CIAT

HMDB: HMDB0033249; HMDB33249

CAS: 6190-65-4

6-Chloro-N-(1-methylethyl)-1,3,5-triazine-2,4-diamine is a major soil metabolite of Atrazine DK W85-F. Environmental pollutant of soil and water.

This compound belongs to the class of organic compounds known as 1,3,5-triazine-2,4-diamines. These are aromatic compounds containing a 1,3,5-triazine ring which is 2,4-disubstituted with amine groups.

## 2-(1-Propenyl)-delta1-piperideine -- Introduction

SYNONYM: 2-(1-Propenyl)-D1-piperideine

HMDB: HMDB0033365; HMDB33365

CAS: 16543-92-3

2-(1-Propenyl)-delta1-piperideine is found in fruits. 2-(1-Propenyl)-delta1-piperideine is isolated from pomegranate (leaves).



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This compound belongs to the class of organic compounds known as tetrahydropyridines. These are derivatives of pyridine in which two double bonds in the pyridine moiety are reduced by adding four hydrogen atoms.

## Oxonantenine -- Introduction

SYNONYM: 1,2-Dimethoxy-4,5,6,6a-tetrahydro-9,10-(methylenedioxy)noraporphin-7-one; 1,2-Dimethoxy-9,10-methylenedioxyoxoaporphine

HMDB: HMDB0033367; HMDB33367

CAS: 15358-38-0

Oxonantenine is found in cherimoya. Oxonantenine is an alkaloid from Laurelia sempervirens (Peruvian nutmeg).

This compound belongs to the class of organic compounds known as aporphines. These are quinoline alkaloids containing the dibenzo[de,g]quinoline ring system or a dehydrogenated derivative thereof.

## Ethyl dodecanoate -- Introduction

SYNONYM: Dodecanoic acid, ethyl ester; Dodecanoic acid,ethyl ester; Ethyl dodecylate; Ethyl ester dodecanoic acid; Ethyl laurate; Ethyl laurinate; Ethyl N-dodecanoate; Ethyl N-dodecanote; Ethyllaurate; FEMA 2441; Lauric acid ethyl ester; Lauric acid, ethyl ester; Lauric acid, ethyl ester (8ci)

HMDB: HMDB0033788; HMDB33788

CAS: 106-33-2

Ethyl dodecanoate is found in alcoholic beverages. Ethyl dodecanoate is present in various fruits, eg. apple, apricot, guava, melon, etc. Also present in wheatbread, crispbread, ginger, whisky, fruit brandies and wine. flavouring agent.

This compound belongs to the class of organic compounds known as fatty acid esters. These are carboxylic ester derivatives of a fatty acid.

## Ethyl dodecanoate -- Enteritis

Probert CS, Jones PR, Ratcliffe NM: A novel method for rapidly diagnosing the causes of diarrhoea. Gut. 2004 Jan;53(1):58-61. PMID: 14684577

## 2'-O-Methylcajanone -- Introduction

SYNONYM:

HMDB: HMDB0033806; HMDB33806

CAS: 71765-79-2

2'-O-Methylcajanone is found in pigeon pea. 2'-O-Methylcajanone is isolated from root bark of Cajanus cajan (pigeon pea).

This compound belongs to the class of organic compounds known as 3'-prenylated isoflavanones. These are isoflavanones featuring a C5-isoprenoid unit at the 3'-position.

## Chavicol -- Introduction

SYNONYM: 4-(2-Propenyl)phenol; 4-(Prop-2-enyl)-phenol; 4-Allylphenol; gamma-(P-Hydroxyphenyl)-alpha-propylene; P-Allylphenol; P-Chavicol; P-Hydroxyallylbenzene; g-(P-Hydroxyphenyl)-a-propylene;  $\beta$ -(P-hydroxyphenyl)- $\beta$ -propylene; 3-(P-Hydroxyphenyl)-1-propene; 4-(2-Propenyl)-phenol; alpha -Propylene; laquo gammaraquo -(P-Hydroxyphenyl)-alpha -propylene; P-Allyl-phenol; P-Hydroxyallylpropene; Phenol, 4-(2-propenyl)- (9ci); Phenol, P-allyl- (8ci)

HMDB: HMDB0034107; HMDB34107



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CAS: 501-92-8

Chavicol is found in allspice. Chavicol is found in many essential oils, e.g. anise and Gardenia. Chavicol is used in perfumery and flavours.

This compound belongs to the class of organic compounds known as 1-hydroxy-2-unsubstituted benzenoids. These are phenols that are unsubstituted at the 2-position.

### Ricinoleic acid -- Introduction

SYNONYM: 12-Hydroxyoleic acid; 12-Hydroxyoleate; Ricinoleate; (9Z)-(12S)-Hydroxyoctadecenoic acid; (9Z)-12-Hydroxy-9-octadecenoic acid; (9Z)-12-Hydroxyoctadec-9-enoic acid; (9Z,12R)-12-Hydroxyoctadec-9-enoic acid; (R)-12-Hydroxy-cis-9-octadecenoic acid; 12-Hydroxy-(9Z,12R)-9-octadecenoic acid; 12-Hydroxy-9-octadecenoic acid; 12-Hydroxy-cis-9-octadecenoic acid; 12-Hydroxy-oleic acid; 12-Hydroxy-[R-(Z)]-9-octadecenoic acid; D-12-Hydroxyoleic acid; Flexircin 100; L'acide ricinoleique; P -10 acid; RCL; Ricinelaidic acid; Ricinic acid; Ricinolic acid; Ricinusoleic acid; Riconoleic acid; 12-Hydroxy-9-octadecenoic acid; 12-Hydroxyoctadec-cis-9-enoic acid; Ricinoleic acid, (R-(e))-isomer

HMDB: HMDB0034297; HMDB34297

CAS: 141-22-0

Ricinoleic acid is found in corn. Ricinoleic acid occurs in castor oil and other oils e.g. grape and ergot (*Claviceps purpurea*). Ricinoleic acid (12-hydroxy-9-cis-octadecenoic acid) is an unsaturated omega-9 fatty acid that naturally occurs in mature Castor plant (*Ricinus communis* L., Euphorbiaceae) seeds or in sclerotium of ergot (*Claviceps purpurea* Tul., Clavicipitaceae). About 90% of the fatty acid content in castor oil is the triglyceride formed from ricinoleic acid. Ricinoleic acid is manufactured for industries by saponification or fractional distillation of hydrolyzed castor oil. The zinc salt is used in personal care products, such as deodorants.

This compound belongs to the class of organic compounds known as long-chain fatty acids. These are fatty acids with an aliphatic tail that contains between 13 and 21 carbon atoms.

### Piperidine -- Introduction

SYNONYM: Azacyclohexane; Azinane; Cyclopentimine; Hexahydropyridine; Pentamethyleneamine; Pentamethyleneimine; Pentamethylenimine; pip; Cypentil; FEMA 2908; hexahydro-Pyridine; Hexazane; Perhydropyridine; Piperidin; Piperidine ON rasta resin

HMDB: HMDB0034301; HMDB34301

CAS: 110-89-4

Piperidine is found in barley. Piperidine is present in black pepper (*Piper nigrum*). Piperidine is a flavouring agent. Piperidine (Azinane after the Hantzsch Widman nomenclature) is an organic compound with the molecular formula (CH<sub>2</sub>)<sub>5</sub>NH. This heterocyclic amine consists of a six-membered ring containing five methylene units and one nitrogen atom. It is a colorless fuming liquid with an odor described as ammoniacal, pepper-like; the name comes from the genus name *Piper*, which is the Latin word for pepper. Piperidine is a widely used building block and chemical reagent in the synthesis of organic compounds, including pharmaceuticals. Piperidine is a widely used secondary amine. It is widely used to convert ketones to enamines. Enamines derived from piperidine can be used in the Stork enamine alkylation reaction. Piperidine is used as a solvent and as a base. The same is true for certain derivatives: N-formylpiperidine is a polar aprotic solvent with better hydrocarbon solubility than other amide solvents, and 2,2,6,6-tetramethylpiperidine is highly sterically hindered base, useful because of its low nucleophilicity and high solubility in organic solvents.

This compound belongs to the class of organic compounds known as piperidines. These are compounds containing a piperidine ring, which is a saturated aliphatic six-membered ring with one nitrogen atom and five carbon atoms.

### Piperidine -- Perillyl alcohol administration for cancer treatment

Zheng YF, Kong HW, Xiong JH, Lv S, Xu GW: Clinical significance and prognostic value of urinary nucleosides in breast cancer patients. Clin Biochem. 2005 Jan;38(1):24-30. PMID: 15607313



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Byun JA, Lee SH, Jung BH, Choi MH, Moon MH, Chung BC: Analysis of polyamines as carbamoyl derivatives in urine and serum by liquid chromatography-tandem mass spectrometry. *Biomed Chromatogr.* 2008 Jan;22(1):73-80. PMID: 17668437

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Cauley JA, Zmuda JM, Danielson ME, Ljung BM, Bauer DC, Cummings SR, Kuller LH: Estrogen metabolites and the risk of breast cancer in older women. *Epidemiology.* 2003 Nov;14(6):740-4. PMID: 14569192

Grace PB, Mistry NS, Carter MH, Leathem AJ, Teale P: High throughput quantification of phytoestrogens in human urine and serum using liquid chromatography/tandem mass spectrometry (LC-MS/MS). *J Chromatogr B Analyt Technol Biomed Life Sci.* 2007 Jun 15;853(1-2):138-46. Epub 2007 Mar 18. PMID: 17403619

Sugimoto M, Wong DT, Hirayama A, Soga T, Tomita M: Capillary electrophoresis mass spectrometry-based saliva metabolomics identified oral, breast and pancreatic cancer-specific profiles. *Metabolomics.* 2010 Mar;6(1):78-95. Epub 2009 Sep 10. PMID: 20300169

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## Piperidine -- Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. *Tohoku J Exp Med.* 1995 May;176(1):61-8. PMID: 7482520

Cheng Y, Xie G, Chen T, Qiu Y, Zou X, Zheng M, Tan B, Feng B, Dong T, He P, Zhao L, Zhao A, Xu LX, Zhang Y, Jia W: Distinct urinary metabolic profile of human colorectal cancer. *J Proteome Res.* 2012 Feb 3;11(2):1354-63. doi: 10.1021/pr201001a. Epub 2011 Dec 28. PMID: 22148915

Monleon D, Morales JM, Barrasa A, Lopez JA, Vazquez C, Celda B: Metabolite profiling of fecal water extracts from human colorectal cancer. *NMR Biomed.* 2009 Apr;22(3):342-8. doi: 10.1002/nbm.1345. PMID: 19006102

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### Piperidine -- Periodontal disease

Sugimoto M, Wong DT, Hirayama A, Soga T, Tomita M: Capillary electrophoresis mass spectrometry-based saliva metabolomics identified oral, breast and pancreatic cancer-specific profiles. *Metabolomics.* 2010 Mar;6(1):78-95. Epub 2009 Sep 10. PMID: 20300169

### Piperidine -- Pancreatic cancer

Loser C, Folsch UR, Paprotny C, Creutzfeldt W: Polyamine concentrations in pancreatic tissue, serum, and urine of patients with pancreatic cancer. *Pancreas.* 1990 Mar;5(2):119-27. PMID: 2315288

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Xie G, Lu L, Qiu Y, Ni Q, Zhang W, Gao YT, Risch HA, Yu H, Jia W: Plasma metabolite biomarkers for the detection of pancreatic cancer. *J Proteome Res.* 2015 Feb 6;14(2):1195-202. doi: 10.1021/pr501135f. Epub 2014 Dec 8. PMID: 25429707

### Piperidine -- Metastatic melanoma



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## Epidermin -- Introduction

SYNONYM: Epidermin?; Suprofen acyl glucuronide; Suprofen glucuronide

HMDB: HMDB0034777; HMDB34777

CAS: 126050-09-7

Epidermin is found in cereals and cereal products. Epidermin is a constituent of barley (*Hordeum vulgare*)

This compound belongs to the class of organic compounds known as cyanogenic glycosides. These are glycosides in which the aglycone moiety contains a cyanide group.

## trans-p-Menthane-1,7,8-triol 8-glucoside -- Introduction

SYNONYM:

HMDB: HMDB0034784; HMDB34784

CAS: 217962-29-3

trans-p-Menthane-1,7,8-triol 8-glucoside is found in herbs and spices. trans-p-Menthane-1,7,8-triol 8-glucoside is a constituent of *Foeniculum vulgare* (fennel)

This compound belongs to the class of organic compounds known as o-glycosyl compounds. These are glycoside in which a sugar group is bonded through one carbon to another group via a O-glycosidic bond.

## Persicaxanthin -- Introduction

SYNONYM: (3S,5R,6S)-5,6-Epoxy-5,6-dihydro-12'-apo-beta,psi-carotene-3,12'-diol; 5,6-Epoxy-5,6-dihydro-12'-apo-b-carotene-3,12'-diol

HMDB: HMDB0034952; HMDB34952

CAS: 80952-82-5

Persicaxanthin is found in european plum. Persicaxanthin is isolated from plums *Prunus domestic*

This compound belongs to the class of organic compounds known as diterpenoids. These are terpene compounds formed by four isoprene units.

## Melleolide M -- Introduction

SYNONYM:

HMDB: HMDB0035068; HMDB35068

CAS:

Melleolide M is found in mushrooms. Melleolide M is a metabolite of *Armillariella mellea* (honey mushroom)

This compound belongs to the class of organic compounds known as melleolides and analogues. These are compounds with a structure characterized by the presence of a 2-hydroxy-4-methoxy-6-methylbenzoic acid derivative linked to a 3,6,6,7b-tetramethyl-cyclobuta[e]indene moiety.

## Emodin -- Introduction



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SYNONYM: 1,3,8-Trihydroxy-6-methyl-9,10-anthracenedione; 1,3,8-Trihydroxy-6-methyl-9,10-anthraquinone; 3-METHYL-1,6,8-trihydroxyanthraquinone; Schuttgelb; 1,3, 8-Trihydroxy-6-methyl-9,10-anthraquinone; 1,3,8-Trihydroxy-6-methyl-9,10-anthracenedione, 9ci; 1,3,8-Trihydroxy-6-methylantra-9,10-quinone; 4,5,7-Trihydroxy-2-methylantraquinone; 6-Methyl-1,3,8-trihydroxy-9,10-anthracenedione; 6-Methyl-1,3,8-trihydroxyanthraquinone; 9,10-Anthracenedione, 1,3,8-trihydroxy-6-methyl- (9ci); Archin; Emodol; Frangula emodin; Frangulic acid; Frangulinic acid; Rheum-emodin; Emodin, rheum; Emodin, frangula; Rheum emodin

HMDB: HMDB0035214; HMDB35214

CAS: 518-82-1

Emodin is found in dock. Emodin is present in Cascara sagrada. Emodin is a purgative resin from rhubarb, *Polygonum cuspidatum*, the buckthorn and Japanese Knotweed (*Fallopia japonica*). The term may also refer to any one of a series of principles isomeric with the emodin of rhubarb. (Wikipedia)

This compound belongs to the class of organic compounds known as hydroxyanthraquinones. These are compounds containing a hydroxyanthraquinone moiety, which consists of an anthracene bearing a quinone, and hydroxyl group.

## Cohibin C -- Introduction

SYNONYM:

HMDB: HMDB0035397; HMDB35397

CAS:

Cohibin C is found in fruits. Cohibin C is a constituent of *Annona muricata* (soursop)

This compound belongs to the class of organic compounds known as annonaceous acetogenins. These are waxy derivatives of fatty acids (usually C32 or C34), containing a terminal carboxylic acid combined with a 2-propanol unit at the C-2 position to form a methyl- substituted alpha,beta-unsaturated-gamma-lactone. One of their interesting structural features is a single, adjacent, or nonadjacent tetrahydrofuran (THF) or tetrahydropyran (THP) system with one or two flanking hydroxyl group(s) at the center of a long hydrocarbon chain.

## Cafestol -- Introduction

SYNONYM: Cafesterol; Coffeol

HMDB: HMDB0035710; HMDB35710

CAS: 469-83-0

Cafestol is found in arabica coffee. Cafestol is a constituent of coffee bean oil. Cafestol is present in boiled-type coffee beverages. Possesses hypercholesterolaemic activity. Diterpenoid constits. of coffee products are associated with cardiotoxic properties Cafestol is a diterpene molecule present in coffee

This compound belongs to the class of organic compounds known as naphthofurans. These are compounds containing a furan ring fused to a naphthalene moiety. Furan is a 5 membered- ring aromatic ring with four carbon and one oxygen atoms. Naphthalene is a polycyclic aromatic hydrocarbon made up of two fused benzene rings.

## Naematalone -- Introduction

SYNONYM: Naematalon; Nematalone

HMDB: HMDB0035781; HMDB35781

CAS: 92121-62-5

Naematalone is found in mushrooms. Naematalone is a metabolite of *Hypholoma capnoides* (conifer tuft

This compound belongs to the class of organic compounds known as sesquiterpenoids. These are terpenes with three



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consecutive isoprene units.

### Labienoxime -- Introduction

SYNONYM: 2,4,4,7-Tetramethylnona-6,8-dien-3-one oxime; 6,8-Nonadien-3-one, 2,4,4,7-tetramethyl-, oxime

HMDB: HMDB0036031; HMDB36031

CAS: 81783-01-9

Labienoxime is a fragrance ingredient with a blackcurrant-like arom

This compound belongs to the class of organic compounds known as ketoximes. These are organic compounds with the general formula  $\text{RC}(\text{R}')=\text{NOH}$  ( $\text{R}, \text{R}' = \text{organyl}$ ).

### Persicachrome -- Introduction

SYNONYM: (3S)-5,8-Epoxy-5,8-dihydro-12'-apo-beta,psi-carotene-3,12'-diol; 5,8-Epoxy-5,8-dihydro-12'-apo-b-carotene-3,12'-diol

HMDB: HMDB0036425; HMDB36425

CAS: 80931-31-3

(3S,5R,8S)-Persicachrome is found in fruits. (3S,5R,8S)-Persicachrome is a constituent of flesh of cling peaches (*Prunus persica*).

This compound belongs to the class of organic compounds known as diterpenoids. These are terpene compounds formed by four isoprene units.

### Isokobusone -- Introduction

SYNONYM: 6-Hydroxy-15-nor-7(14)-caryophyllen-3-one

HMDB: HMDB0036791; HMDB36791

CAS: 24173-72-6

Isokobusone is found in root vegetables. Isokobusone is a constituent of *Cyperus rotundus* (nutgrass).

This compound belongs to the class of organic compounds known as cyclic alcohols and derivatives. These are organic compounds containing an aliphatic ring substituted with at least one hydroxyl group.

### 2,4-Dihydroxy-7,8-dimethoxy-2H-1,4-benzoxazin-3(4H)-one 2-glucoside -- Introduction

SYNONYM:

HMDB: HMDB0037550; HMDB37550

CAS: 40246-08-0

2,4-Dihydroxy-7,8-dimethoxy-2H-1,4-benzoxazin-3(4H)-one 2-glucoside is found in cereals and cereal products. It is a constituent of wheat and sweet corn (*Zea mays*).

This compound belongs to the class of organic compounds known as o-glycosyl compounds. These are glycoside in which a sugar group is bonded through one carbon to another group via a O-glycosidic bond.

### Goyaglycoside c -- Introduction

SYNONYM: Goyaglycoside-c

HMDB: HMDB0038349; HMDB38349



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CAS:333332-49-3

Goyaglycoside d is found in bitter gourd. Goyaglycoside d is a constituent of *Momordica charantia* (bitter melon).

This compound belongs to the class of organic compounds known as cucurbitacin glycosides. These are polycyclic compounds containing a carbohydrate derivative glycosidically linked to a curcubitane nucleus.

## Methyl 2-(10-heptadecenyl)-6-hydroxybenzoate -- Introduction

SYNONYM:

HMDB: HMDB0038523; HMDB38523

CAS: 111047-31-5

Methyl 2-(10-heptadecenyl)-6-hydroxybenzoate is found in fats and oils. Methyl 2-(10-heptadecenyl)-6-hydroxybenzoate is isolated from *Ginkgo biloba* (ginkgo).

This compound belongs to the class of organic compounds known as o-hydroxybenzoic acid esters. These are benzoic acid esters where the benzene ring is ortho-substituted with a hydroxy group.

## Elenaic acid -- Introduction

SYNONYM: 3-Formyl-3,4-dihydro-5-(methoxycarbonyl)-2-methyl-2H-pyran-4-acetic acid, 9ci; Elenolic acid

HMDB: HMDB0039136; HMDB39136

CAS: 34422-12-3

Elenaic acid is found in fats and oils. Elenaic acid is isolated from olives (*Olea europaea*) leaves and fruits.

This compound belongs to the class of organic compounds known as dicarboxylic acids and derivatives. These are organic compounds containing exactly two carboxylic acid groups.

## Stigmastane-3,6-dione -- Introduction

SYNONYM:

HMDB: HMDB0039822; HMDB39822

CAS:

Stigmastane-3,6-dione is found in cereals and cereal products. Stigmastane-3,6-dione is a constituent of mature wheat straw (*Triticum aestivum*).

This compound belongs to the class of organic compounds known as stigmastanes and derivatives. These are sterol lipids with a structure based on the stigmastane skeleton, which consists of a cholestanone moiety bearing an ethyl group at the carbon atom C24.

## 2-Octyl-4-propylthiazole -- Introduction

SYNONYM:

HMDB: HMDB0040114; HMDB40114

CAS: 96693-82-2

Claimed food uses are not well documented.

This compound belongs to the class of organic compounds known as 2,4-disubstituted thiazoles. These are compounds containing a thiazole ring substituted at the positions 2 and 3.



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## Pentanenitrile -- Introduction

SYNONYM: 1-Butyl cyanide; 1-cyano-Butane; 1-Cyanobutane; Butyl cyanide; N-Butyl cyanide; N-Pentanenitrile; N-Valeronitrile; Pentanenitrile, 9ci; Pentanonitrile; Valeronitrile, 8ci

HMDB: HMDB0040173; HMDB40173

CAS: 110-59-8

Pentanenitrile is found in brassicas. Pentanenitrile is a constituent of various Brassica species.

This compound belongs to the class of organic compounds known as nitriles. These are compounds having the structure RC#N; thus C-substituted derivatives of hydrocyanic acid, HC#N.

## Azacridone A -- Introduction

SYNONYM:

HMDB: HMDB0040367; HMDB40367

CAS: 150050-14-9

Azacridone A is found in citrus. Azacridone A is an alkaloid from roots of Citrus paradisi (grapefruit).

This compound belongs to the class of organic compounds known as chromenopyridines. These are aromatic heterocyclic compounds structurally characterized by a pyridine ring fused to a chromene moiety.

## 2-O-p-Coumaroylhydroxycitric acid -- Introduction

SYNONYM:

HMDB: HMDB0040570; HMDB40570

CAS: 62345-85-1

2-O-p-Coumaroylhydroxycitric acid is found in cereals and cereal products. 2-O-p-Coumaroylhydroxycitric acid is a constituent of Zea mays (sweet corn).

This compound belongs to the class of organic compounds known as coumaric acid esters. These are aromatic compounds containing an ester derivative of coumaric acid.

## 3-Acetyl-2,5-dimethylthiophene -- Introduction

SYNONYM: 1-(2,5-Dimethyl-3-thienyl)-ethanone; 1-(2,5-Dimethyl-3-thienyl)ethanone; 1-(2,5-Dimethyl-3-thienyl)ethanone, 9ci; 2,5-Dimethyl-3-acetylthiophene; 2,5-Dimethyl-3-thienyl methyl ketone; 2,5-Dimethyl-3-thienyl methyl ketone, 8ci; 2,5-Dimethylthiophen-3-yl methyl ketone; 3-Acetyl-2,5-dimethyl thiophene; Dimethylthienylketone; FEMA 3527; Ketone, 2,5-dimethyl-3-thienyl methyl

HMDB: HMDB0040589; HMDB40589

CAS: 2530-10-1

3-Acetyl-2,5-dimethylthiophene is a flavouring ingredient.

This compound belongs to the class of organic compounds known as aryl alkyl ketones. These are ketones have the generic structure  $\text{RC}(\text{=O})\text{R}'$ , where R = aryl group and R'=alkyl group.

## 4-Hydroxy-6-methyl-3-(1-oxobutyl)-2H-pyran-2-one -- Introduction

SYNONYM:

HMDB: HMDB0040637; HMDB40637



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CAS:22073-85-4

4-Hydroxy-6-methyl-3-(1-oxobutyl)-2H-pyran-2-one is found in herbs and spices. 4-Hydroxy-6-methyl-3-(1-oxobutyl)-2H-pyran-2-one is a constituent of *Pogostemon cablin* (patchouli).

This compound belongs to the class of organic compounds known as aryl alkyl ketones. These are ketones have the generic structure  $\text{RC}(=\text{O})\text{R}'$ , where R = aryl group and R'=alkyl group.

## Hydroxytyrosol 1-O-glucoside -- Introduction

SYNONYM: (-)-3,4-Dihydroxyphenethyl glucoside; 3,4-Dihydroxyphenethyl glucoside

HMDB: HMDB0041024; HMDB41024

CAS: 76873-99-9

Hydroxytyrosol 1-O-glucoside is found in fruits. Hydroxytyrosol 1-O-glucoside is a constituent of *Prunus* sp.

This compound belongs to the class of organic compounds known as o-glycosyl compounds. These are glycoside in which a sugar group is bonded through one carbon to another group via a O-glycosidic bond.

## Kanzonol K -- Introduction

SYNONYM: 2',4',5-Trihydroxy-7-methoxy-3',6-diprenylisoflavone

HMDB: HMDB0041212; HMDB41212

CAS: 156281-30-0

Kanzonol K is found in herbs and spices. Kanzonol K is a constituent of *Glycyrrhiza uralensis* (Chinese licorice).

This compound belongs to the class of organic compounds known as 6-prenylated isoflavanones. These are isoflavanones featuring a C5-isoprenoid unit at the 6-position.

## 1-Deoxy-D-glucitol -- Introduction

SYNONYM: 6-Deoxy-L-gulitol; Fucitol

HMDB: HMDB0041500; HMDB41500

CAS: 18545-96-5

1-Deoxy-D-glucitol is found in herbs and spices. 1-Deoxy-D-glucitol is a constituent of the fruit of *Foeniculum vulgare* (fennel).

This compound belongs to the class of organic compounds known as hexoses. These are monosaccharides in which the sugar unit is a six-carbon containing moiety.

## Pivaloylcarnitine -- Introduction

SYNONYM: Pivaloyl carnitine

HMDB: HMDB0041993; HMDB41993

CAS: 98299-38-8

Pivaloylcarnitine belongs to the family of Acyl Carnitines. These are organic compounds containing a fatty acid with the carboxylic acid attached to carnitine through an ester bond.

This compound belongs to the class of organic compounds known as acyl carnitines. These are organic compounds containing a fatty acid with the carboxylic acid attached to carnitine through an ester bond.



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## 2-(3,4-Dihydroxybenzoyloxy)-4,6-dihydroxybenzoate -- Introduction

SYNONYM: 2,4DIOH-6(2,4Diohbenacid)benzacid; 2-Protocatechoylphloroglucinolcarboxylate; 2-Protocatechuoyl phloroglucinolcarboxylate; 2-(3,4-Dihydroxybenzoyloxy)-4,6-dihydroxybenzoic acid; 2-Protocatechoylphloroglucinolcarboxylic acid; 2-Protocatechuoyl phloroglucinolcarboxylic acid

HMDB: HMDB0059651; HMDB59651

CAS:

2-(3,4-dihydroxybenzoyloxy)-4,6-dihydroxybenzoate is part of the Flavonoid metabolism pathway. It is a substrate for: Pirin.

This compound belongs to the class of organic compounds known as depsides and depsidones. These are polycyclic compounds that is either a polyphenolic compound composed of two or more monocyclic aromatic units linked by an ester bond (depside), or a compound containing the depsidone structure (depsidone).

## 9-Hydroxyphenanthrene -- Introduction

SYNONYM: 9-Phenanthrenol; 9-Phenanthrol

HMDB: HMDB0059801; HMDB59801

CAS:

This compound belongs to the family of Phenanthrenes and Derivatives. These are polycyclic compounds containing a phenanthrene moiety, which is a tricyclic aromatic compound with three non-linearly fused benzene.

This compound belongs to the class of organic compounds known as phenanthrols. These are compounds containing a phenanthrene (or its hydrogenated derivative) to which a hydroxyl group is attached.

## alpha-Methylstyrene -- Introduction

SYNONYM: 1-Methyl-1-phenylethylene; 2-Phenylpropene; alpha-Methylstyrene;  $\beta$ -methylstyrene; alpha-Methyl-styrene; alpha-Methylstyrol

HMDB: HMDB0059899; HMDB59899

CAS:

alpha-Methylstyrene belongs to the family of Phenylpropenes. These are compounds containing a phenylpropene moiety, which consists of a propene substituent bound to a phenyl group.

This compound belongs to the class of organic compounds known as phenylpropenes. These are compounds containing a phenylpropene moiety, which consists of a propene substituent bound to a phenyl group.

## alpha-Methylstyrene -- Crohn's disease

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PMID: 19491857

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### alpha-Methylstyrene -- Ulcerative colitis

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Kolho KL, Pessia A, Jaakkola T, de Vos WM, Velagapudi V: Faecal and Serum Metabolomics in Paediatric Inflammatory Bowel Disease. *J Crohns Colitis.* 2017 Mar 1;11(3):321-334. doi: 10.1093/ecco-jcc/jjw158. PMID: 27609529

Azario I, Pievani A, Del Priore F, Antolini L, Santi L, Corsi A, Cardinale L, Sawamoto K, Kubaski F, Gentner B, Bernardo ME, Valsecchi MG, Riminucci M, Tomatsu S, Aiuti A, Biondi A, Serafini M: Neonatal umbilical cord blood transplantation halts skeletal disease progression in the murine model of MPS-I. *Sci Rep.* 2017 Aug 25;7(1):9473. doi: 10.1038/s41598-017-09958-9. PMID: 28842642

## 4-Oxo-2-noneenal -- Introduction

SYNONYM: 4-oxo-2-Nonenal; ONE; 4-Oxonon-2-enal

HMDB: HMDB0060285; HMDB60285

CAS:

This compound belongs to the family of Medium-chain Aldehydes. These are An aldehyde with a chain length containing between 6 and 12 carbon atoms.

This compound belongs to the class of organic compounds known as medium-chain aldehydes. These are an aldehyde with a chain length containing between 6 and 12 carbon atoms.

## (2R)-2-Hydroxy-2-methylbutanenitrile -- Introduction

SYNONYM: (2R)-2-Hydroxy-2-cyanobutane; (2R)-2-Hydroxy-2-methylbutyronitrile; (R)-Butan-2-one cyanohydrin; 2-Hydroxy-2-methylbutanenitrile

HMDB: HMDB0060309; HMDB60309

CAS:

This compound belongs to the family of Tertiary Alcohols. These are compounds in which a hydroxy group, -OH, is attached to a saturated carbon atom R<sub>3</sub>COH (R ≠ H).

This compound belongs to the class of organic compounds known as tertiary alcohols. These are compounds in which a hydroxy group, -OH, is attached to a saturated carbon atom R<sub>3</sub>COH (R not H).

## 1-Methoxyphenanthrene -- Introduction

SYNONYM: Methyl 1-phenanthryl ether



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HMDB: HMDB0060323; HMDB60323

CAS:

This compound belongs to the family of Phenanthrenes and Derivatives. These are polycyclic compounds containing a phenanthrene moiety, which is a tricyclic aromatic compound with three non-linearly fused benzene.

This compound belongs to the class of organic compounds known as phenanthrenes and derivatives. These are polycyclic compounds containing a phenanthrene moiety, which is a tricyclic aromatic compound with three non-linearly fused benzene.

## Acetone cyanohydrin -- Introduction

SYNONYM: 2-Hydroxyisobutyronitrile; 2-Methylactonitrile; Acetone cyanhydrin; Acetone-cyanhydrin; alpha-Hydroxyisobutyronitrile; a-Hydroxyisobutyronitrile;  $\beta$ -hydroxyisobutyronitrile; Acetoncyanhydrine; Acetone cyanhydrin, 14C-labeled

HMDB: HMDB0060427; HMDB60427

CAS:

Acetone cyanhydrin (ACH) is an organic compound used in the production of methyl methacrylate, the monomer of the transparent plastic polymethyl methacrylate (PMMA), also known as acrylic. (Wikipedia)

This compound belongs to the class of organic compounds known as tertiary alcohols. These are compounds in which a hydroxy group, -OH, is attached to a saturated carbon atom R<sub>3</sub>COH (R not H).

## DL-Glutamate -- Introduction

SYNONYM: 2-Aminogluutaric acid; DL-Glutamic acid; DL-Glutaminic acid; E; Glu; Glutamate; Glutaminic acid; Glutaminsaeure; 2-Aminogluutarate; DL-Glutaminate; Glutamic acid; Glutamine; D-Glutamate; L Glutamate; L Glutamic acid; D Glutamate; Glutamate, potassium; Glutamic acid, (D)-isomer; L-Glutamate; L-Glutamic acid; Aluminum L glutamate; Aluminum L-glutamate; L-Glutamate, aluminum; Potassium glutamate

HMDB: HMDB0060475; HMDB60475

CAS:

This compound belongs to the family of Alpha Amino Acids. These are amino acids in which the amino group is attached to the carbon atom immediately adjacent to the carboxylate group (alpha carbon).

This compound belongs to the class of organic compounds known as glutamic acid and derivatives. These are compounds containing glutamic acid or a derivative thereof resulting from reaction of glutamic acid at the amino group or the carboxy group, or from the replacement of any hydrogen of glycine by a heteroatom.

## 9,10-epoxyoctadecanoic acid -- Introduction

SYNONYM: 8-(3-Octyloxiran-2-yl)octanoic acid; 9,10-Epoxyoctadecanoic acid; 8-(3-Octyloxiran-2-yl)octanoate; 9,10-Epoxy stearic acid; 9,10-Epoxyoctadecanoate; 9,10-Epoxy stearic acid, potassium salt; cis-9,10-Epoxy stearic acid; 9,10-Epoxy stearic acid, (trans)-isomer; 9,10-Epoxy stearic acid, 14C-acid; 9,10-Epoxy stearic acid, ammonium salt; 9,10-Epoxy stearic acid, (cis)-isomer; 9,10-Epoxy stearic acid, sodium salt

HMDB: HMDB0061650; HMDB61650

CAS:

9,10-epoxyoctadecanoic acid is an epoxy fatty acid. Epoxy fatty acids bear an oxirane ring that shares a CC-bond with the aliphatic chain. The cis-9,10-epoxyoctadecanoic acid has been found in liver microsomes and is believed to originate from CYP-catalyzed epoxidation of oleic acid.

This compound belongs to the class of organic compounds known as lineolic acids and derivatives. These are



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derivatives of lineolic acid. Lineolic acid is a polyunsaturated omega-6 18 carbon long fatty acid, with two CC double bonds at the 9- and 12-positions.

## 1-Arachidonoylglycerophosphoinositol -- Introduction

SYNONYM: 1-(5Z,8Z,11Z,14Z-Eicosatetraenoyl)-sn-glycero-3-phospho-(1'-myo-inositol); 1-Arachidonoylglycerophosphoinositol; PI(20:4(5Z,8Z,11Z,14Z)/0:0)

HMDB: HMDB0061690; HMDB61690

CAS:

1-Arachidonoylglycerophosphoinositol belongs to the family of glycerophosphoinositols, which are lipids containing a common glycerophosphate skeleton linked to at least one fatty acyl chain and an inositol moiety. Their general formula is  $O[C@H]1[C@H](O)[C@@H](O)[C@H](OP(O)(=O)OC[C@H](CO(R1))O(R2))[C@H](O)[C@@H]1O$ , where R1-R2 are fatty acid chains PI(20:4(5Z,8Z,11Z,14Z)/0:0) is made up of one 5Z,8Z,11Z,14Z-eicosatetraenoyl(R1).

This compound belongs to the class of organic compounds known as 1-acyl-sn-glycerol-3-phosphoinositols. These are glycerophosphoinositols where the glycerol is acylated only at position O-1 with a fatty acid.

## N-methylvaline -- Introduction

SYNONYM: (2S)-3-Methyl-2-(methylamino)butanoic acid; MaVal; Methylvaline; N-Methylvaline; (2S)-3-Methyl-2-(methylamino)butanoate

HMDB: HMDB0061716; HMDB61716

CAS:

N-methylvaline, also known as MeVal, D-Valine, or N-Methyl-L-valine, is an N-methylamino acid that is the N-methyl derivative of valine. It functions as a bronsted acid, a molecular entity capable of donating a hydron to an acceptor (Bronsted base) via oxoacid

This compound belongs to the class of organic compounds known as valine and derivatives. These are compounds containing valine or a derivative thereof resulting from reaction of valine at the amino group or the carboxy group, or from the replacement of any hydrogen of glycine by a heteroatom.

## 1-deoxy-1-(N6-lysino)-D-fructose -- Introduction

SYNONYM: (+)-Aspartic acid; (R,S)-Aspartic acid; 2-Aminobutanedioic acid; Asp; D; DL-Aminosuccinic acid; DL-Asparagic acid; (+)-Aspartate; Aspartate; (R,S)-Aspartate; 2-Aminobutanedioate; DL-Aminosuccinate; DL-Asparagate

HMDB: HMDB0062186; HMDB62186

CAS: 617-45-8

1-deoxy-1-(N6-lysino)-D-fructose is also known as Aspartate or (+)-Aspartic acid. 1-deoxy-1-(N6-lysino)-D-fructose is considered to be soluble (in water) and acidic

This compound belongs to the class of organic compounds known as aspartic acid and derivatives. These are compounds containing an aspartic acid or a derivative thereof resulting from reaction of aspartic acid at the amino group or the carboxy group, or from the replacement of any hydrogen of glycine by a heteroatom.

## 2-acetyl-1-alkyl-sn-glycero-3-phosphocholine -- Introduction

SYNONYM: (R)-7-(Acetoxy)-4-hydroxy-N,N,N-trimethyl-3,5,9-trioxa-4-phosphapentacosan-1-aminium hydroxide inner salt 4-oxide; 1-Hexadecyl-2-acetyl-sn-glycero-3-phosphocholine; 1-O-Hexadecyl paf; 1-O-Hexadecyl-2-acetyl-sn-glycero-3-phosphocholine; 1-O-Hexadecyl-2-acetyl-sn-glyceryl-3-phosphorylcholine; 1-O-Hexadecyl-2-O-acetyl-sn-glycero-3-phosphocholine; 1-O-Hexadecyl-2-O-acetyl-sn-glyceryl-3-phosphorylcholine; 1-O-Hexadecyl-platelet-activating factor; C16 PAF; C16-PAF; C16:0 PAF; PAF; Platelet-activating factor; Platelet-activating factor C16; 1-Hexadecyl-2-acetyl-glycerophosphocholine; APRL; Hexadecyl-paf-acether; 1-Hexadecyl-2-acetyl-glycero-3-



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phosphocholine; HD-PAF; PAF-16 CPD; HAG-PC; HAGPC; Antihypertensive polar renomedullary lipid

HMDB: HMDB0062195; HMDB62195

CAS: 74389-68-7

2-acetyl-1-alkyl-sn-glycero-3-phosphocholine is also known as 1-O-Hexadecyl paf or 1-O-Hexadecyl-platelet-activating factor. 2-acetyl-1-alkyl-sn-glycero-3-phosphocholine is considered to be practically insoluble (in water) and acidic. 2-acetyl-1-alkyl-sn-glycero-3-phosphocholine is a glycerophosphocholine lipid molecule

This compound belongs to the class of organic compounds known as 1-alkyl,2-acetylglycero-3-phosphocholines. These are glycerophosphocholines that carry exactly one acetyl chain attached to the glycerol moiety through an ester linkage at the O2-position, and one alkyl chain attached through an ether linkage at the O1-position.

## 18-carboxy dinor Leukotriene B4 -- Introduction

SYNONYM: 18-Carboxy-19,20-dinorleukotriene b4; 18-COOH-19,20-LTB4

HMDB: HMDB0062301; HMDB62301

CAS:

18-carboxy dinor Leukotriene B4, also known as 18-COOH-19,20-LTB4, is classified as a member of the Long-chain fatty acids. Long-chain fatty acids are fatty acids with an aliphatic tail that contains between 13 and 21 carbon atoms. 18-carboxy dinor Leukotriene B4 is considered to be practically insoluble (in water) and acidic

This compound belongs to the class of organic compounds known as long-chain fatty acids. These are fatty acids with an aliphatic tail that contains between 13 and 21 carbon atoms.

## 1-(5Z,8Z,11Z,14Z-eicosatetraenoyl)-sn-glycero-3-phosphate -- Introduction

SYNONYM: 1-(5Z,8Z,11Z,14Z)-Eicosatetraenoyl-sn-glycero-3-phosphate; 1-(5Z,8Z,11Z,14Z)-Icosatetraenoyl-sn-glycero-3-phosphate; 1-(5Z,8Z,11Z,14Z-Eicosatetraenoyl)-sn-glycero-3-phosphate; 1-Arachidonoyl lpa; 1-Arachidonoyl lysophosphatidic acid; LPA(20:4(5Z,8Z,11Z,14Z)/0:0); Lysophosphatidic acid (20:4(5Z,8Z,11Z,14Z)/0:0); PA(20:4(5Z,8Z,11Z,14Z)/0:0); PA(20:4/0:0); 1-(5Z,8Z,11Z,14Z)-Eicosatetraenoyl-sn-glycero-3-phosphoric acid; 1-Arachidonoyl-sn-glycerol 3-phosphoric acid; 1-(5Z,8Z,11Z,14Z)-Icosatetraenoyl-sn-glycero-3-phosphoric acid; 1-(5Z,8Z,11Z,14Z-Eicosatetraenoyl)-sn-glycero-3-phosphoric acid; 1-Arachidonoyl lysophosphatidate; Lysophosphatidate (20:4(5Z,8Z,11Z,14Z)/0:0)

HMDB: HMDB0062312; HMDB62312

CAS:

1-(5Z,8Z,11Z,14Z-eicosatetraenoyl)-sn-glycero-3-phosphate is also known as LPA(20:4(5Z,8Z,11Z,14Z)/0:0) or 1-Arachidonoyl lpa. 1-(5Z,8Z,11Z,14Z-eicosatetraenoyl)-sn-glycero-3-phosphate is considered to be practically insoluble (in water) and acidic. 1-(5Z,8Z,11Z,14Z-eicosatetraenoyl)-sn-glycero-3-phosphate is a glycerophosphate lipid molecule

This compound belongs to the class of organic compounds known as 1-acylglycerol-3-phosphates. These are lysophosphatidic acids where the glycerol is esterified with a fatty acid at O-1 position.

## Trans-urocanate -- Introduction

SYNONYM: 3-(1H-Imidazol-4-yl)-2-propenoic acid; 3-Imidazol-4-ylacrylic acid; 3-(1H-Imidazol-4-yl)-2-propenoate; Urocanate; 3-Imidazol-4-ylacrylate

HMDB: HMDB0062562; HMDB62562

CAS:

Trans-urocanate is also known as (e)-3-(Imidazol-4-yl)propenoate or trans-Urocanic acid. Trans-urocanate is considered to be soluble (in water) and acidic



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This compound belongs to the class of chemical entities known as imidazolyl carboxylic acids and derivatives. These are organic compounds containing a carboxylic acid chain (of at least 2 carbon atoms) linked to an imidazole ring.

### Trans-urocanate -- Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. *Tohoku J Exp Med.* 1995 May;176(1):61-8. PMID: 7482520

Cheng Y, Xie G, Chen T, Qiu Y, Zou X, Zheng M, Tan B, Feng B, Dong T, He P, Zhao L, Zhao A, Xu LX, Zhang Y, Jia W: Distinct urinary metabolic profile of human colorectal cancer. *J Proteome Res.* 2012 Feb 3;11(2):1354-63. doi: 10.1021/pr201001a. Epub 2011 Dec 28. PMID: 22148915

Monleon D, Morales JM, Barrasa A, Lopez JA, Vazquez C, Celda B: Metabolite profiling of fecal water extracts from human colorectal cancer. *NMR Biomed.* 2009 Apr;22(3):342-8. doi: 10.1002/nbm.1345. PMID: 19006102

Weir TL, Manter DK, Sheflin AM, Barnett BA, Heuberger AL, Ryan EP: Stool microbiome and metabolome differences between colorectal cancer patients and healthy adults. *PLoS One.* 2013 Aug 6;8(8):e70803. doi: 10.1371/journal.pone.0070803. Print 2013. PMID: 23940645

Phua LC, Chue XP, Koh PK, Cheah PY, Ho HK, Chan EC: Non-invasive fecal metabonomic detection of colorectal cancer. *Cancer Biol Ther.* 2014 Apr;15(4):389-97. doi: 10.4161/cbt.27625. Epub 2014 Jan 14. PMID: 24424155

Ritchie SA, Ahiahou PW, Jayasinghe D, Heath D, Liu J, Lu Y, Jin W, Kavianpour A, Yamazaki Y, Khan AM, Hossain M, Su-Myat KK, Wood PL, Krenitsky K, Takemasa I, Miyake M, Sekimoto M, Monden M, Matsubara H, Nomura F, Goodenow DB: Reduced levels of hydroxylated, polyunsaturated ultra long-chain fatty acids in the serum of colorectal cancer patients: implications for early screening and detection. *BMC Med.* 2010 Feb 15;8:13. doi: 10.1186/1741-7015-8-13. PMID: 20156336

Qiu Y, Cai G, Su M, Chen T, Zheng X, Xu Y, Ni Y, Zhao A, Xu LX, Cai S, Jia W: Serum metabolite profiling of human colorectal cancer using GC-TOFMS and UPLC-QTOFMS. *J Proteome Res.* 2009 Oct;8(10):4844-50. doi: 10.1021/pr9004162. PMID: 19678709

Ni Y, Xie G, Jia W: Metabonomics of human colorectal cancer: new approaches for early diagnosis and biomarker discovery. *J Proteome Res.* 2014 Sep 5;13(9):3857-70. doi: 10.1021/pr500443c. Epub 2014 Aug 14. PMID: 25105552

Ikeda A, Nishiumi S, Shinohara M, Yoshie T, Hatano N, Okuno T, Bamba T, Fukusaki E, Takenawa T, Azuma T, Yoshida M: Serum metabolomics as a novel diagnostic approach for gastrointestinal cancer. *Biomed Chromatogr.* 2012 May;26(5):548-58. doi: 10.1002/bmc.1671. Epub 2011 Jul 20. PMID: 21773981

Goedert JJ, Sampson JN, Moore SC, Xiao Q, Xiong X, Hayes RB, Ahn J, Shi J, Sinha R: Fecal metabolomics: assay performance and association with colorectal cancer. *Carcinogenesis.* 2014 Sep;35(9):2089-96. doi: 10.1093/carcin/bgj131. Epub 2014 Jul 18. PMID: 25037050

Sinha R, Ahn J, Sampson JN, Shi J, Yu G, Xiong X, Hayes RB, Goedert JJ: Fecal Microbiota, Fecal Metabolome, and Colorectal Cancer Interrelations. *PLoS One.* 2016 Mar 25;11(3):e0152126. doi: 10.1371/journal.pone.0152126. eCollection 2016. PMID: 27015276

Lin Y, Ma C, Liu C, Wang Z, Yang J, Liu X, Shen Z, Wu R: NMR-based fecal metabolomics fingerprinting as predictors of earlier diagnosis in patients with colorectal cancer. *Oncotarget.* 2016 May 17;7(20):29454-64. doi: 10.18632/oncotarget.8762. PMID: 27107423

Brown DG, Rao S, Weir TL, O'Malia J, Bazan M, Brown RJ, Ryan EP: Metabolomics and metabolic pathway networks from human colorectal cancers, adjacent mucosa, and stool. *Cancer Metab.* 2016 Jun 6;4:11. doi: 10.1186/s40170-016-0151-y. eCollection 2016. PMID: 27275383

Wang X, Wang J, Rao B, Deng L: Gut flora profiling and fecal metabolite composition of colorectal cancer patients and healthy individuals. *Exp Ther Med.* 2017 Jun;13(6):2848-2854. doi: 10.3892/etm.2017.4367. Epub 2017 Apr 20. PMID: 28587349

Silke Matysik, Caroline Ivonne Le Roy, Gerhard Liebisch, Sandrine Paule Claus. Metabolomics of fecal samples: A practical



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consideration. Trends in Food Science & Technology. Vol. 57, Part B, Nov. 2016, p.244-255:  
<http://www.sciencedirect.com/science/article/pii/S0924224416301984> PMID: 7482520

## Linoleamide -- Introduction

SYNONYM: (9Z,12Z)-Octadeca-9,12-dien-1-amide; 9,12-Octadecadienamide; Linoleate amide; Linoleic acid amide; Linoleoyl amide

HMDB: HMDB0062656; HMDB62656

CAS: 3072-13-7

Linoleamide, also known as 9,12-Octadecadienamide or Linoleic acid amide, is classified as a member of the Fatty amides. Fatty amides are carboxylic acid amide derivatives of fatty acids, that are formed from a fatty acid and an amine. Linoleamide is considered to be practically insoluble (in water) and relatively neutral. Linoleamide is a fatty amide lipid molecule

This compound belongs to the class of organic compounds known as fatty amides. These are carboxylic acid amide derivatives of fatty acids, that are formed from a fatty acid and an amine.

## Linoleamide -- Colorectal cancer

Ishiwata S, Itoh K, Yamaguchi T, Ishida N, Mizugaki M: Comparison of serum and urinary levels of modified nucleoside, 1-methyladenosine, in cancer patients using a monoclonal antibody-based inhibition ELISA. Tohoku J Exp Med. 1995 May;176(1):61-8. PMID: 7482520

Cheng Y, Xie G, Chen T, Qiu Y, Zou X, Zheng M, Tan B, Feng B, Dong T, He P, Zhao L, Zhao A, Xu LX, Zhang Y, Jia W: Distinct urinary metabolic profile of human colorectal cancer. J Proteome Res. 2012 Feb 3;11(2):1354-63. doi: 10.1021/pr201001a. Epub 2011 Dec 28. PMID: 22148915

Monleon D, Morales JM, Barrasa A, Lopez JA, Vazquez C, Celda B: Metabolite profiling of fecal water extracts from human colorectal cancer. NMR Biomed. 2009 Apr;22(3):342-8. doi: 10.1002/nbm.1345. PMID: 19006102

Weir TL, Manter DK, Sheflin AM, Barnett BA, Heuberger AL, Ryan EP: Stool microbiome and metabolome differences between colorectal cancer patients and healthy adults. PLoS One. 2013 Aug 6;8(8):e70803. doi: 10.1371/journal.pone.0070803. Print 2013. PMID: 23940645

Phua LC, Chue XP, Koh PK, Cheah PY, Ho HK, Chan EC: Non-invasive fecal metabonomic detection of colorectal cancer. Cancer Biol Ther. 2014 Apr;15(4):389-97. doi: 10.4161/cbt.27625. Epub 2014 Jan 14. PMID: 24424155

Ritchie SA, Ahiahou PW, Jayasinghe D, Heath D, Liu J, Lu Y, Jin W, Kavianpour A, Yamazaki Y, Khan AM, Hossain M, Su-Myat KK, Wood PL, Krenitsky K, Takemasa I, Miyake M, Sekimoto M, Monden M, Matsubara H, Nomura F, Goodenow DB: Reduced levels of hydroxylated, polyunsaturated ultra long-chain fatty acids in the serum of colorectal cancer patients: implications for early screening and detection. BMC Med. 2010 Feb 15;8:13. doi: 10.1186/1741-7015-8-13. PMID: 20156336

Qiu Y, Cai G, Su M, Chen T, Zheng X, Xu Y, Ni Y, Zhao A, Xu LX, Cai S, Jia W: Serum metabolite profiling of human colorectal cancer using GC-TOFMS and UPLC-QTOFMS. J Proteome Res. 2009 Oct;8(10):4844-50. doi: 10.1021/pr9004162. PMID: 19678709

Ni Y, Xie G, Jia W: Metabonomics of human colorectal cancer: new approaches for early diagnosis and biomarker discovery. J Proteome Res. 2014 Sep 5;13(9):3857-70. doi: 10.1021/pr500443c. Epub 2014 Aug 14. PMID: 25105552

Ikeda A, Nishiumi S, Shinohara M, Yoshie T, Hatano N, Okuno T, Bamba T, Fukusaki E, Takenawa T, Azuma T, Yoshida M: Serum metabolomics as a novel diagnostic approach for gastrointestinal cancer. Biomed Chromatogr. 2012 May;26(5):548-58. doi: 10.1002/bmc.1671. Epub 2011 Jul 20. PMID: 21773981

Goedert JJ, Sampson JN, Moore SC, Xiao Q, Xiong X, Hayes RB, Ahn J, Shi J, Sinha R: Fecal metabolomics: assay performance and association with colorectal cancer. Carcinogenesis. 2014 Sep;35(9):2089-96. doi: 10.1093/carcin/bgu131. Epub 2014 Jul 18. PMID: 25037050



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Sinha R, Ahn J, Sampson JN, Shi J, Yu G, Xiong X, Hayes RB, Goedert JJ: Fecal Microbiota, Fecal Metabolome, and Colorectal Cancer Interrelations. *PLoS One.* 2016 Mar 25;11(3):e0152126. doi: 10.1371/journal.pone.0152126. eCollection 2016. PMID: 27015276

Lin Y, Ma C, Liu C, Wang Z, Yang J, Liu X, Shen Z, Wu R: NMR-based fecal metabolomics fingerprinting as predictors of earlier diagnosis in patients with colorectal cancer. *Oncotarget.* 2016 May 17;7(20):29454-64. doi: 10.18632/oncotarget.8762. PMID: 27107423

Brown DG, Rao S, Weir TL, O'Malia J, Bazan M, Brown RJ, Ryan EP: Metabolomics and metabolic pathway networks from human colorectal cancers, adjacent mucosa, and stool. *Cancer Metab.* 2016 Jun 6;4:11. doi: 10.1186/s40170-016-0151-y. eCollection 2016. PMID: 27275383

Wang X, Wang J, Rao B, Deng L: Gut flora profiling and fecal metabolite composition of colorectal cancer patients and healthy individuals. *Exp Ther Med.* 2017 Jun;13(6):2848-2854. doi: 10.3892/etm.2017.4367. Epub 2017 Apr 20. PMID: 28587349

Silke Matysik, Caroline Ivonne Le Roy, Gerhard Liebisch, Sandrine Paule Claus. Metabolomics of fecal samples: A practical consideration. *Trends in Food Science & Technology.* Vol. 57, Part B, Nov. 2016, p.244-255: <http://www.sciencedirect.com/science/article/pii/S0924224416301984> PMID: 7482520

## Diethyl phthalic acid -- Introduction

SYNONYM: 1,2-Benzenedicarboxylic acid diethyl ester; 1,2-Diethyl phthalate; DEP; Diethyl 1,2-benzenedicarboxylate; Diethyl benzene-1,2-dicarboxylate; Diethyl O-phthalate; Ethyl phthalate; O-Benzenedicarboxylic acid diethyl ester; O-Bis(ethoxycarbonyl)benzene; Phthalic acid diethyl ester; Phthalsaeurediethylester; 1,2-Benzenedicarboxylate diethyl ester; Diethyl phthalic acid; 1,2-Diethyl phthalic acid; Diethyl 1,2-benzenedicarboxylic acid; Diethyl benzene-1,2-dicarboxylic acid; Diethyl O-phthalic acid; Ethyl phthalic acid; O-Benzenedicarboxylate diethyl ester; Phthalate diethyl ester

HMDB: HMDB0094660; HMDB94660

CAS:

Diethyl phthalic acid, also known as diethyl phthalate, 1,2-diethyl phthalic acid or 1,2-benzenedicarboxylic acid diethyl ester, is classified as a member of the benzoic acid esters. Benzoic acid esters are ester derivatives of benzoic acid. Diethyl phthalic acid is considered to be practically insoluble (in water) and basic. This substance is commonly used to make plastics more flexible. Products in which it is found include toothbrushes, automobile parts, tools, toys, and food packaging. Diethyl phthalic acid can be released fairly easily from these products, as it is not part of the chain of chemicals (polymers) that makes up the plastic. Diethyl phthalic acid is also used in cosmetics, insecticides, and aspirin. Phthalate esters can cause reproductive and developmental toxicity. (L1900, A2883) It is a non-carcinogenic (not listed by IARC) potentially toxic compound. (ChemoSummarizer)

This compound belongs to the class of organic compounds known as benzoic acid esters. These are ester derivatives of benzoic acid.

## Diethyl phthalic acid -- Autism

James SJ, Cutler P, Melnyk S, Jernigan S, Janak L, Gaylor DW, Neubrander JA: Metabolic biomarkers of increased oxidative stress and impaired methylation capacity in children with autism. *Am J Clin Nutr.* 2004 Dec;80(6):1611-7. PMID: 15585776

Narayan M, Srinath S, Anderson GM, Meundi DB: Cerebrospinal fluid levels of homovanillic acid and 5-hydroxyindoleacetic acid in autism. *Biol Psychiatry.* 1993 Apr 15-May 1;33(8-9):630-5. PMID: 7687150

Shaw W: Increased urinary excretion of a 3-(3-hydroxyphenyl)-3-hydroxypropionic acid (HPHPA), an abnormal phenylalanine metabolite of Clostridia spp. in the gastrointestinal tract, in urine samples from patients with autism and schizophrenia. *Nutr Neurosci.* 2010 Jun;13(3):135-43. doi: 10.1179/147683010X12611460763968. PMID: 20423563

Jaeken J, Van den Berghe G: An infantile autistic syndrome characterised by the presence of succinylpurines in body fluids. *Lancet.* 1984 Nov 10;2(8411):1058-61. PMID: 6150139

Anderson GM, Ross DL, Klykylo W, Feibel FC, Cohen DJ: Cerebrospinal fluid indoleacetic acid in autistic subjects. *J*

Autism Dev Disord. 1988 Jun;18(2):259-62. PMID: 3410814

Kusaga A, Yamashita Y, Koeda T, Hiratani M, Kaneko M, Yamada S, Matsuishi T: Increased urine phenylethylamine after methylphenidate treatment in children with ADHD. Ann Neurol. 2002 Sep;52(3):372-4. PMID: 12205654

De Angelis M, Piccolo M, Vannini L, Siragusa S, De Giacomo A, Serrazzanetti DI, Cristofori F, Guerzoni ME, Gobbetti M, Francavilla R: Fecal microbiota and metabolome of children with autism and pervasive developmental disorder not otherwise specified. PLoS One. 2013 Oct 9;8(10):e76993. doi: 10.1371/journal.pone.0076993. eCollection 2013. PMID: 24130822

### Diethyl phthalic acid -- Pervasive developmental disorder not otherwise specified

De Angelis M, Piccolo M, Vannini L, Siragusa S, De Giacomo A, Serrazzanetti DI, Cristofori F, Guerzoni ME, Gobbetti M, Francavilla R: Fecal microbiota and metabolome of children with autism and pervasive developmental disorder not otherwise specified. PLoS One. 2013 Oct 9;8(10):e76993. doi: 10.1371/journal.pone.0076993. eCollection 2013. PMID: 24130822

### PS(16:0/18:1(11Z)) -- Introduction

SYNONYM: PSer(16:0/18:1); PS(16:0/18:1(11Z)); Phosphatidylserine(16:0/18:1); PSer(34:1); Phosphatidylserine(34:1); PS(34:1); PS(16:0/18:1); 1-hexadecanoyl-2-(11Z-octadecenoyl)-sn-glycero-3-phosphoserine; 1-palmitoyl-2-vaccenoyl-sn-glycero-3-phosphoserine

HMDB: HMDB0112267

CAS:

PS(16:0/18:1(11Z)) is a phosphatidylserine. It is a glycerophospholipid in which a phosphorylserine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, phosphatidylserines can have many different combinations of fatty acids of varying lengths and saturation attached to the C-1 and C-2 atoms. PS(16:0/18:1(11Z)), in particular, consists of one hexadecanoyl chain to the C-1 atom, and one 11Z-octadecenoyl to the C-2 atom. Phosphatidylserine or 1,2-diacyl-sn-glycero-3-phospho-L-serine is distributed widely among animals, plants and microorganisms. Phosphatidylserine is an acidic (anionic) phospholipid with three ionizable groups, i.e. the phosphate moiety, the amino group and the carboxyl function. As with other acidic lipids, it exists in nature in salt form, but it has a high propensity to chelate to calcium via the charged oxygen atoms of both the carboxyl and phosphate moieties, modifying the conformation of the polar head group. This interaction may be of considerable relevance to the biological function of phosphatidylserine. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. Phosphatidylserines typically carry a net charge of -1 at physiological pH. They mostly have palmitic or stearic acid on carbon 1 and a long chain unsaturated fatty acid (e.g. 18:2, 20:4 and 22:6) on carbon 2. PS biosynthesis involves an exchange reaction of serine for ethanolamine in PE.

This compound belongs to the class of organic compounds known as phosphatidylserines. These are glycerophosphosersines in which two fatty acids are bonded to the glycerol moiety through ester linkages.

### PS(20:5(5Z,8Z,11Z,14Z,17Z)/18:0) -- Introduction

SYNONYM: 1-eicosapentaenoyl-2-stearoyl-sn-glycero-3-phosphoserine ; PS(20:5/18:0) ; PS(20:5n3/18:0) ; PS(20:5w3/18:0) ; PS(38:5) ; Pser(20:5(5Z,8Z,11Z,14Z,17Z)/18:0) ; Pser(20:5/18:0) ; Pser(20:5n3/18:0) ; Pser(20:5w3/18:0) ; Pser(38:5) ; Phosphatidylserine(20:5(5Z,8Z,11Z,14Z,17Z)/18:0) ; Phosphatidylserine(20:5/18:0) ; Phosphatidylserine(20:5n3/18:0) ; Phosphatidylserine(20:5w3/18:0) ; Phosphatidylserine(38:5) ; PS(20:5(5Z,8Z,11Z,14Z,17Z)/18:0); PSer(38:5); PS(20:5/18:0); PSer(20:5/18:0); PS(38:5); Phosphatidylserine(20:5/18:0); 1-(5Z,8Z,11Z,14Z,17Z-eicosapentaenoyl)-2-octadecanoyl-sn-glycero-3-phosphoserine; 1-eicosapentaenoyl-2-stearoyl-sn-glycero-3-phosphoserine

HMDB: HMDB0112684

CAS:

PS(20:5(5Z,8Z,11Z,14Z,17Z)/18:0) is a phosphatidylserine. It is a glycerophospholipid in which a phosphorylserine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, phosphatidylserines can have many different combinations of fatty acids of varying lengths and saturation attached to the C-1 and C-2 positions.



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PS(20:5(5Z,8Z,11Z,14Z,17Z)/18:0), in particular, consists of one chain of eicosapentaenoic acid at the C-1 position and one chain of stearic acid at the C-2 position. Phosphatidylserine or 1,2-diacyl-sn-glycero-3-phospho-L-serine is distributed widely among animals, plants, and microorganisms. Phosphatidylserine is an acidic (anionic) phospholipid with three ionizable groups (i.e. the phosphate moiety, the amino group and the carboxyl group). As with other acidic lipids, it exists in nature in salt form, but it has a high propensity to chelate calcium via the charged oxygen atoms of both the carboxyl and phosphate moieties, modifying the conformation of the polar head group. This interaction may be of considerable relevance to the biological function of phosphatidylserine. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. Phosphatidylserines typically carry a net charge of -1 at physiological pH. They mostly have a palmitic or stearic acid on carbon 1 and a long chain unsaturated fatty acid (e.g. 18:2, 20:4 and 22:6) on carbon 2. PS biosynthesis involves an exchange reaction of serine for ethanolamine in PE.

This compound belongs to the class of organic compounds known as phosphatidylserines. These are glycerophosphoserines in which two fatty acids are bonded to the glycerol moiety through ester linkages.

### **PS(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z)) -- Introduction**

SYNONYM: 1-docosahexaenoyl-2-gamma-linolenoyl-sn-glycero-3-phosphoserine ; PS(22:6/18:3) ; PS(22:6n3/18:3n6) ; PS(22:6w3/18:3w6) ; PS(40:9) ; Pser(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z)) ; Pser(22:6/18:3) ; Pser(22:6n3/18:3n6) ; Pser(22:6w3/18:3w6) ; Pser(40:9) ; Phosphatidylserine(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z)) ; Phosphatidylserine(22:6/18:3) ; Phosphatidylserine(22:6n3/18:3n6) ; Phosphatidylserine(22:6w3/18:3w6) ; Phosphatidylserine(40:9) ; PS(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z)) ; PS(22:6/18:3) ; Phosphatidylserine(22:6/18:3) ; 1-docosahexaenoyl-2-gamma-linolenoyl-sn-glycero-3-phosphoserine ; PSer(22:6/18:3) ; PSer(40:9) ; 1-(4Z,7Z,10Z,13Z,16Z,19Z-docosahexaenoyl)-2-(6Z,9Z,12Z-octadecatrienoyl)-sn-glycero-3-phosphoserine ; PS(40:9)

HMDB: HMDB0112866

CAS:

PS(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z)) is a phosphatidylserine. It is a glycerophospholipid in which a phosphorylserine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, phosphatidylserines can have many different combinations of fatty acids of varying lengths and saturation attached to the C-1 and C-2 positions. PS(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:3(6Z,9Z,12Z)), in particular, consists of one chain of docosahexaenoic acid at the C-1 position and one chain of gamma-linolenic acid at the C-2 position. Phosphatidylserine or 1,2-diacyl-sn-glycero-3-phospho-L-serine is distributed widely among animals, plants, and microorganisms. Phosphatidylserine is an acidic (anionic) phospholipid with three ionizable groups (i.e. the phosphate moiety, the amino group and the carboxyl group). As with other acidic lipids, it exists in nature in salt form, but it has a high propensity to chelate calcium via the charged oxygen atoms of both the carboxyl and phosphate moieties, modifying the conformation of the polar head group. This interaction may be of considerable relevance to the biological function of phosphatidylserine. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. Phosphatidylserines typically carry a net charge of -1 at physiological pH. They mostly have a palmitic or stearic acid on carbon 1 and a long chain unsaturated fatty acid (e.g. 18:2, 20:4 and 22:6) on carbon 2. PS biosynthesis involves an exchange reaction of serine for ethanolamine in PE.

This compound belongs to the class of organic compounds known as phosphatidylserines. These are glycerophosphoserines in which two fatty acids are bonded to the glycerol moiety through ester linkages.

### **PS(22:4(7Z,10Z,13Z,16Z)/20:5(5Z,8Z,11Z,14Z,17Z)) -- Introduction**

SYNONYM: 1-adrenoyl-2-eicosapentaenoyl-sn-glycero-3-phosphoserine ; PS(22:4/20:5) ; PS(22:4n6/20:5n3) ; PS(22:4w6/20:5w3) ; PS(42:9) ; Pser(22:4(7Z,10Z,13Z,16Z)/20:5(5Z,8Z,11Z,14Z,17Z)) ; Pser(22:4/20:5) ; Pser(22:4n6/20:5n3) ; Pser(22:4w6/20:5w3) ; Pser(42:9) ; Phosphatidylserine(22:4(7Z,10Z,13Z,16Z)/20:5(5Z,8Z,11Z,14Z,17Z)) ; Phosphatidylserine(22:4/20:5) ; Phosphatidylserine(22:4n6/20:5n3) ; Phosphatidylserine(22:4w6/20:5w3) ; Phosphatidylserine(42:9) ; PS(22:4(7Z,10Z,13Z,16Z)/20:5(5Z,8Z,11Z,14Z,17Z)) ; Phosphatidylserine(22:4/20:5) ; PSer(42:9) ; PS(42:9) ; PSer(22:4/20:5) ; PS(22:4/20:5) ; 1-(7Z,10Z,13Z,16Z-docosatetraenoyl)-2-(5Z,8Z,11Z,14Z,17Z-eicosapentaenoyl)-sn-



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glycero-3-phosphoserine; 1-adrenoyl-2-eicosapentaenoyl-sn-glycero-3-phosphoserine

HMDB: HMDB0116781

CAS:

PS(22:4(7Z,10Z,13Z,16Z)/20:5(5Z,8Z,11Z,14Z,17Z)) is a phosphatidylserine. It is a glycerophospholipid in which a phosphorylserine moiety occupies a glycerol substitution site. As is the case with diacylglycerols, phosphatidylserines can have many different combinations of fatty acids of varying lengths and saturation attached to the C-1 and C-2 atoms. PS(22:4(7Z,10Z,13Z,16Z)/20:5(5Z,8Z,11Z,14Z,17Z)), in particular, consists of one 7Z,10Z,13Z,16Z-docosatetraenoyl chain to the C-1 atom, and one 5Z,8Z,11Z,14Z,17Z-eicosapentaenoyl to the C-2 atom. Phosphatidylserine or 1,2-diacyl-sn-glycero-3-phospho-L-serine is distributed widely among animals, plants and microorganisms. Phosphatidylserine is an acidic (anionic) phospholipid with three ionizable groups, i.e. the phosphate moiety, the amino group and the carboxyl function. As with other acidic lipids, it exists in nature in salt form, but it has a high propensity to chelate to calcium via the charged oxygen atoms of both the carboxyl and phosphate moieties, modifying the conformation of the polar head group. This interaction may be of considerable relevance to the biological function of phosphatidylserine. While most phospholipids have a saturated fatty acid on C-1 and an unsaturated fatty acid on C-2 of the glycerol backbone, the fatty acid distribution at the C-1 and C-2 positions of glycerol within phospholipids is continually in flux, owing to phospholipid degradation and the continuous phospholipid remodeling that occurs while these molecules are in membranes. Phosphatidylserines typically carry a net charge of -1 at physiological pH. They mostly have palmitic or stearic acid on carbon 1 and a long chain unsaturated fatty acid (e.g. 18:2, 20:4 and 22:6) on carbon 2. PS biosynthesis involves an exchange reaction of serine for ethanolamine in PE.

This compound belongs to the class of organic compounds known as phosphatidylserines. These are glycerophosphoserines in which two fatty acids are bonded to the glycerol moiety through ester linkages.

## 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-4-one -- Introduction

SYNONYM:

HMDB: HMDB0125371

CAS:

2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-4-one is a predicted metabolite generated by BioTransformer<sup>®</sup> that is produced by the metabolism of 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-4H-chromen-4-one. It is generated by unspecified-gutmicro enzyme via a flavonoid-c-ring-reduction reaction. This flavonoid-c-ring-reduction occurs in human gut microbiota.

This compound belongs to the class of organic compounds known as flavanonols. These are compounds containing a flavan-3-one moiety, with a structure characterized by a 2-phenyl-3,4-dihydro-2H-1-benzopyran bearing a hydroxyl group and a ketone at the carbon C2 and C3, respectively.

## Mesylate -- Introduction

SYNONYM: Methansulfonsaeure; Methylsulfonic acid; Methansulphonsaeure; Methanesulfonate; Methanesulphonate; Methanesulphonic acid; Methylsulfonate; Methylsulphonate; Methylsulphonic acid; Methanesulfonic acid, chromium (2+) salt; Methanesulfonic acid, cobalt (2+) salt; Methanesulfonic acid, ammonia salt; Methanesulfonic acid, nickel (2+) salt; Methanesulfonic acid, copper (2+) salt; Methanesulfonic acid, iron (2+) salt; Methanesulfonic acid, iron (3+)salt; Methanesulfonic acid, potassium salt; Methanesulfonic acid, sodium salt; Barium methanesulfonate; Methanesulfonic acid, chromium (3+) salt; Methanesulfonic acid, silver (1+) salt; Potassium methanesulfonate

HMDB: HMDB0240280

CAS:

Mesylate, also known as methanesulfonate or mesylic acid, belongs to the class of organic compounds known as organosulfonic acids. Organosulfonic acids are compounds containing the sulfonic acid group, which has the general structure RS(=O)2OH (R is not a hydrogen atom). Mesylate exists as a solid, soluble (in water), and an extremely strong acidic compound (based on its pKa). Mesylate is also a parent compound for other transformation products, including but not limited to, methanesulfonates, S-methyl methanethiosulfonate, and (Z)-11-methyl-N-(methylsulfonyl)dodec-2-enamide.



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This compound belongs to the class of chemical entities known as organosulfonic acids. These are compounds containing the sulfonic acid group, which has the general structure RS(=O)2OH (R is not a hydrogen atom).

## Tromethamine -- Introduction

SYNONYM: 1,1,1-Tris(hydroxymethyl)methanamine; 2-amino-2-(Hydroxymethyl)-1,3-propanediol; Aminotris(hydroxymethyl)methane; THAM; Tris amino; Tris base; Tris buffer; Tris(hydroxymethyl)aminomethane; Tris-base; Trizma; Trometamol; Tromethamine; Abbott brand OF trometamol; Tris-MG(II)-KCL buffer; Trisamine; Trometamol abbott brand; Tri(hydroxymethyl)aminomethane; Tris-magnesium(II)-potassium chloride buffer

HMDB: HMDB0240288

CAS:

Tromethamine, also known as trometamol or tham, belongs to the class of organic compounds known as 1,2-aminoalcohols. These are organic compounds containing an alkyl chain with an amine group bound to the C1 atom and an alcohol group bound to the C2 atom. Tromethamine is a drug which is used for the prevention and correction of metabolic acidosis. Tromethamine exists as a solid, soluble (in water), and a very weakly acidic compound (based on its pKa). Tromethamine is also a parent compound for other transformation products, including but not limited to, bis-tris, bis-tris propane, and N-tris(hydroxymethyl)methylglycine.

This compound belongs to the class of chemical entities known as 1,2-aminoalcohols. These are organic compounds containing an alkyl chain with an amine group bound to the C1 atom and an alcohol group bound to the C2 atom.



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