**Suppl. Table 2**: List of the abbreviations for metabolite names used in the reaction list of *A. oryzae* (Suppl. Table 1) and their full name. An “m” denotes that the metabolite is found in the mitochondria. A “p” indicates that the metabolite is found in the peroxisome whereas an “e” is used to mark an extracellular metabolite.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Abbreviation** | | **Full name of metabolite** | | | |
| 1368THN | | 1,3,6,8-THN |
| 138THN | | 1,3,8-THN |
| 13GLUCAN | | 1,3-beta-D-Glucan |
| 13GLUCANe | | 1,3-beta-D-Glucan (Extracellular) |
| 13PDG | | 1,3-Bisphospho-D-glycerate |
| 14MNAN | | 1,4 beta Mannan |
| 18DHN | | 1,8-DHN |
| 2D3DGALT | | 2-Dehydro-3-deoxy-D-galactonate |
| 2MACOp | | 2-Methyl-cis-aconitate (Peroxisome) |
| 2MCITp | | 2-Methylcitrate (Peroxisome) |
| 2MICITp | | 2-Methylisocitrate (Peroxisome) |
| 2N6H | | 2-octaprenyl-6-hydroxyphenol |
| 2NMHMBm | | 3-demethylubiquinone-8 (Mitochondria) |
| 2NPMBm | | 2-octaprenyl-6-methoxy-1,4-benzoquinone (Mitochondria) |
| 2NPMMBm | | 2-octaprenyl-3-methyl-6-methoxy-1,4-benzoquinone (Mitochondria) |
| 2NPMP | | 2-octaprenyl-6-methoxyphenol |
| 2NPMPm | | 2-octaprenyl-6-methoxyphenol (Mitochondria) |
| 2NPPP | | 2-octaprenylphenol |
| 2PG | | 2-Phospho-D-glycerate |
| 3DDAH7P | | 2-Dehydro-3-deoxy-D-arabino-heptonate 7-phosphate |
| 3PG | | 3-Phospho-D-glycerate |
| 3PSER | | 3-Phosphoserine |
| 3PSME | | 5-O-(1-Carboxyvinyl)-3-phosphoshikimate |
| 3SULALA | | 3-sulfinoalanine |
| 4CMCOA | | 4-coumaroyl-COA |
| 4CMRE | | 4-hydroxycinnamate |
| 4HBZ | | 4-hydroxybenzoate |
| 4HPP | | 4-Hydroxyphenyl pyruvate |
| 4PPNCYS | | 4-Phosphopantothenoyl-L-cysteine |
| 4PPNTE | | Pantetheine 4'-phosphate |
| 4PPNTO | | D-4'-Phosphopantothenate |
| 5MTA | | 5'-Methylthioadenosine |
| 5OXOPRO | | 5-oxo-L-proline |
| 5THR1P | | S-methyl-5-thio-α-D-ribose 1-phosphate |
| 6CARHEX | | 6-carboxyhexanoate |
| 7DECHORES | | Cholesta-5,7-dien-3-beta-ol |
| A6RP | | 5-amino-6-ribityluracil |
| A6RP5P | | 5-amino-6-(5-phosphoribosylamino) uracil |
| A6RP5P2 | | 5-amino-6-(5-phosphoribitylamino) uracil |
| AACACP | | 3-oxoacyl-[acyl-carrier protein] |
| AACCOA | | Acetoacetyl coenzyme A |
| AACCOAm | | Acetoacetyl coenzyme A (Mitochondria) |
| AACCOAp | | Acetoacetyl coenzyme A (Peroxisome) |
| ABUTm | | 2-Aceto-2-hydroxy butyrate (Mitochondria) |
| AC | | Acetate |
| ACACP | | Acyl-[acyl-carrier protein] |
| ACAL | | Acetaldehyde |
| ACALm | | Acetaldehyde (Mitochondria) |
| ACAR | | O-Acetylcarnitine | |
| ACARm | | O-Acetylcarnitine (Mitochondria) | |
| ACCOA | | Acetyl coenzyme A | |
| ACCOAm | | Acetyl coenzyme A (Mitochondria) | |
| ACCOAp | | Acetyl coenzyme A (Peroxisome) | |
| ACe | | Acetate (Extracellular) | |
| ACET | | Acetone | |
| ACETm | | Acetone (Mitochondria) | |
| ACLACm | | 2-Acetolactate (Mitochondria) | |
| ACm | | Acetate (Mitochondria) | |
| ACOA | | Acyl coenzyme A | |
| ACOm | | Cis-Aconitate (Mitochondria) | |
| ACP | | Acetate (Peroxisome) | |
| ACPC | | 1-aminocyclopropane-1-carboxylate | |
| ACPm | | Acyl-carrier protein (Mitochondria) | |
| ACTAC | | Acetoacetate | |
| ACTACm | | Acetoacetate (Mitochondria) | |
| ACTP | | Acetyl phosphate | |
| ACTPm | | Acetyl phosphate (Mitochondria) | |
| ACYBUT | | Gamma-Amino-gamma-cyanobutanoate | |
| AD | | Adenine | |
| ADCHOR | | 4-Amino-4-deoxychorismate | |
| ADe | | Adenine (Extracellular) | |
| ADN | | Adenosine | |
| ADP | | ADP | |
| ADPm | | ADP (Mitochondria) | |
| ADPRIB | | ADP-ribose | |
| ADPRIBm | | ADP-ribose (Mitochondria) | |
| AFB1 | | Aflatoxin B1 | |
| AFB2 | | Aflatoxin B2 | |
| AFG1 | | Aflatoxin G1 | |
| AFG2 | | Aflatoxin G2 | |
| AGL3P | | Acyl-sn-glycerol 3-phosphate | |
| AGMT | | Agmatine | |
| AHHMD | | 2-Amino-7,8-dihydro-4-hydroxy-6-(diphosphooxymethyl)pteridine | |
| AHHMP | | 2-Amino-4-hydroxy-6-hydroxymethyl-7,8-dihydropteridine | |
| AHM | | 4-amino-5-hydroxymethyl-2-methylpyrimidine | |
| AHMP | | 4-amino-5-phosphomethyl-2-methylpyrimidine | |
| AHMPP | | 4-amino-2-methyl-5-diphosphomethylpyrimidine | |
| AHTD | | 2-Amino-4-hydroxy-6-(erythro-1,2,3-trihydroxypropyl)-dihydropteridine triphosphate | |
| AICAR | | AICAR | |
| AIR | | Aminoimidazole ribotide | |
| AKA | | 2-Oxoadipate | |
| AKG | | 2-Oxoglutarate | |
| AKGe | | 2-Oxoglutarate (Extracellular) | |
| AKGm | | 2-Oxoglutarate (Mitochondria) | |
| AKGp | | 2-Oxoglutarate (Peroxisome) | |
| AKP | | 2-Dehydropantoate | |
| AKPm | | 2-Dehydropantoate (Mitochondria) | |
| ALA | | L-Alanine | |
| ALAe | | L-Alanine (Extracellular) | |

|  |  |
| --- | --- |
| ALAGLY | R-S-Alanylglycine |
| ALAm | L-Alanine (Mitochondria) |
| ALTRNA | L-Arginyl-tRNA |
| AM6SA | 2-Aminomuconate 6-semialdehyde |
| AMA | L-2-Aminoadipate |
| AMAC | Aminoacetone |
| AMACm | Aminoacetone (Mitochondria) |
| AMASA | L-2-Aminoadipate 6-semialdehyde |
| AMIACE | Aminoacetaldehyde |
| AMIEVUL | 5-aminolevulinate |
| AMIEVULm | 5-aminolevulinate (Mitochondria) |
| AMOXOBU | 2-amino-3oxobutanoate |
| AMP | AMP |
| AMPm | AMP (Mitochondria) |
| AMPp | AMP (Peroxisome) |
| AMUCO | 2-Aminomuconate |
| AN | Anthranilate |
| AOL | D-Arabitol |
| AOLe | D-Arabitol (Extracellular) |
| AONA | 8-Amino-7-oxononanoate |
| AONAm | 8-Amino-7-oxononanoate (Mitochondria) |
| APEBU | 4-(2-aminophenyl)-2,4-dioxobutanoate |
| APOCEm | Apocytochrome C (Mitochondria) |
| APROA | 3-Aminopropanal |
| APROP | Alpha-amino-propiononitrile |
| APRUT | N-Acetylputrescine |
| APS | Adenylylsulfate |
| ARAB | D-Arabinose |
| ARABe | D-Arabinose (Extracellular) |
| ARABINe | Arabinan (Extracellular) |
| ARABLAC | D-Arabinono-1,4-lactone |
| ARG | L-Arginine |
| ARGe | L-Arginine (Extracellular) |
| ARGSUCC | N-(L-Arginino)succinate |
| ASER | O-Acetyl-L-serine |
| ASERm | O-Acetyl-L-serine (Mitochondria) |
| ASN | L-Asparagine |
| ASNe | L-Asparagine (Extracellular) |
| ASNm | L-Asparagine (Mitochondria) |
| ASNTRNA | L-Asparaginyl-tRNA |
| ASNTRNAm | L-Asparaginyl-tRNA (Mitochondria) |
| ASP | L-Aspartate |
| ASPe | L-Aspartate (Extracellular) |
| ASPERMD | N1-Acetylspermidine |
| ASPm | L-Aspartate (Mitochondria) |
| ASPSA | L-Aspartate 4-semialdehyde |
| ASPTRNA | L-Aspartyl-tRNA |
| ASPTRNAm | L-Aspartyl-tRNA (Mitochondria) |
| ASUC | N6-(1,2-Dicarboxyethyl)-AMP |
| AT3P2 | Acyldihydroxyacetone phosphate |
| ATN | Allantoin |
| ATP | ATP |
| ATPm | ATP (Mitochondria) |

|  |  |
| --- | --- |
| ATPp | ATP (Peroxisome) |
| ATT | Allantoate |
| ATTp | Allantoate (Peroxisome) |
| AVF | Averufin |
| AVN | Averantin |
| bALA | Beta-alanine |
| BASP | 4-Phospho-L-aspartate |
| BCCP | Biotin carboxyl-carrier protein |
| bDG6P | Beta-D-Glucose 6-phosphate |
| bDGLC | Beta-D-Glucose |
| bDGLCe | Beta-D-Glucose (Extracellular) |
| BETALD | Betaine aldehyde |
| BT | Biotin |
| BTAMP | Biotinyl-5-AMP |
| C100 | Decanoic acid |
| C100ACP | Decanoyl-[Acyl carrier protein] |
| C100COA | Decanoyl-Coenzyme A |
| C100COAm | Decanoyl-Coenzyme A (Mitochondria) |
| C10DACP | Decanoyl-dehydro-[acyl-carrier protein] |
| C10DCOAm | Decanoyl-dehydro-Coenzyme A (Mitochondria) |
| C10HACP | Decanoyl-Hydroxy-[acyl-carrier protein] |
| C10HCOAm | Decanoyl-Hydroxy-Coenzyme A (Mitochondria) |
| C10OACP | Decanoyl-oxo-[acyl-carrier protein] |
| C10OCOAm | Decanoyl-oxo-Coenzyme A (Mitochondria) |
| C120 | Dodecanoic acid |
| C120ACP | Dodecanoyl-[acyl-carrier protein] |
| C120COA | Dodecanoyl-Coenzyme A |
| C120COAm | Dodecanoyl-Coenzyme A (Mitochondria) |
| C12DACP | Dodecanoyl-dehydro-[acyl-carrier protein] |
| C12DCOAm | Dodecanoyl-dehydro-Coenzyme A (Mitochondria) |
| C12HACP | Dodecanoyl-Hydroxy-[acyl-carrier protein] |
| C12HCOAm | Dodecanoyl-Hydroxy-Coenzyme A (Mitochondria) |
| C12OACP | Dodecanoyl-oxo-[acyl-carrier protein] |
| C12OCOAm | Dodecanoyl-oxo-Coenzyme A (Mitochondria) |
| C140 | Myristic acid |
| C140ACP | Myristoyl-[acyl-carrier protein] |
| C140COA | Myristoyl-Coenzyme A |
| C140COAm | Myristoyl-Coenzyme A (Mitochondria) |
| C14DACP | Myristoyl-dehydro-[acyl-carrier protein] |
| C14DCOAm | Myristoyl-dehydro-Coenzyme A (Mitochondria) |
| C14HACP | Myristoyl-Hydroxy-[acyl-carrier protein] |
| C14HCOAm | Myristoyl-Hydroxy-Coenzyme A (Mitochondria) |
| C14OACP | Myristoyl-oxo-[acyl-carrier protein] |
| C14OCOAm | Myristoyl-oxo-Coenzyme A (Mitochondria) |
| C160 | Palmitate |
| C160ACP | Hexadecanoyl-[acyl-carrier protein] |
| C160COA | Hexadecanoyl-Coenzyme A |
| C160COAm | Hexadecanoyl-Coenzyme A (Mitochondria) |
| C161 | Palmitoic acid |
| C161ACP | Palmitoyl-[acyl-carrier protein] |
| C161COA | Palmitoyl-Coenzyme A |
| C162 | Hexadecadienoic acid |
| C162ACP | Hexadecadienoic acid-[acyl-carrier protein] |

|  |  |
| --- | --- |
| C162COA | Hexadecadienoyl-Coenzyme A |
| C16A | Palmitate\_aldehydes |
| C16DACP | Hexadecanoyl-dehydro-[acyl-carrier protein] |
| C16DCOAm | Hexadecanoyl-dehydro-Coenzyme A (Mitochondria) |
| C16HACP | Hexadecanoyl-Hydroxy-[acyl-carrier protein] |
| C16HCOAm | Hexadecanoyl-Hydroxy-Coenzyme A (Mitochondria) |
| C16OACP | Hexadecanoyl-oxo-[acyl-carrier protein] |
| C16OCOAm | Hexadecanoyl-oxo-Coenzyme A (Mitochondria) |
| C180 | Stearate |
| C180ACP | Stearoyl-[acyl-carrier protein] |
| C180COA | Stearoyl-Coenzyme A |
| C180COAm | Stearoyl-Coenzyme A (Mitochondria) |
| C181 | Oleic acid |
| C181ACP | Oleoyl-[acyl-carrier protein] |
| C181COA | Oleoyl-Coenzyme A |
| C182 | Linoleic acid |
| C182ACP | Linolenoyl-[acyl-carrier protein] |
| C182COA | Linolenoyl-Coenzyme A |
| C183 | Octadecatrienoic acid |
| C183ACP | Octadecatrienoic acid-[acyl-carrier protein] |
| C183COA | Octadecatrienoic acid-Coenzyme A |
| C18DACP | Stearoyl-dehydro-[acyl-carrier protein] |
| C18DCOAm | Stearoyl-dehydro-Coenzyme A (Mitochondria) |
| C18HACP | Stearoyl-Hydroxy-[acyl-carrier protein] |
| C18HCOAm | Stearoyl-Hydroxy-Coenzyme A (Mitochondria) |
| C18OACP | Stearoyl-oxo-[acyl-carrier protein] |
| C18OCOAm | Stearoyl-oxo-Coenzyme A (Mitochondria) |
| C40 | Butyric acid |
| C40ACP | Butyryl-[acyl-carrier protein] |
| C40COA | Butyryl-Coenzyme A |
| C40COAm | Butyryl-Coenzyme A (Mitochondria) |
| C4DACP | Butyryl-dehydro-[acyl-carrier protein] |
| C4DCOAm | Butyryl-dehydro-Coenzyme A (Mitochondria) |
| C4HACP | Butyryl-Hydroxy-[acyl-carrier protein] |
| C4HCOA | Butyryl-Hydroxy-Coenzyme A |
| C4HCOAm | Butyryl-Hydroxy-Coenzyme A (Mitochondria) |
| C60 | Hexanoic acid |
| C60ACP | Hexanoyl-[acyl-carrier protein] |
| C60COA | Hexanoyl-Coenzyme A |
| C60COAm | Hexanoyl-Coenzyme A (Mitochondria) |
| C6DACP | Hexanoyl-dehydro-[acyl-carrier protein] |
| C6DCOAm | Hexanoyl-dehydro-Coenzyme A (Mitochondria) |
| C6HACP | Hexanoyl-Hydroxy-[acyl-carrier protein] |
| C6HCOAm | Hexanoyl-Hydroxy-Coenzyme A (Mitochondria) |
| C6OACP | Hexanoyl-oxo-[acyl-carrier protein] |
| C6OCOAm | Hexanoyl-oxo-Coenzyme A (Mitochondria) |
| C80 | Octanoic acid |
| C80ACP | Octanoyl-[acyl-carrier protein] |
| C80COA | Octanoyl-Coenzyme A |
| C80COAm | Octanoyl-Coenzyme A (Mitochondria) |
| C8DACP | Octanoyl-dehydro-[acyl-carrier protein] |
| C8DCOAm | Octanoyl-dehydro-Coenzyme A (Mitochondria) |
| C8HACP | Octanoyl-Hydroxy-[acyl-carrier protein] |

|  |  |
| --- | --- |
| C8HCOAm | Octanoyl-Hydroxy-Coenzyme A (Mitochondria) |
| C8OACP | Octanoyl-oxo-[acyl-carrier protein] |
| C8OCOAm | Octanoyl-oxo-Coenzyme A (Mitochondria) |
| Ca | Calcium |
| CAASP | N-Carbamoyl-L-aspartate |
| CABM | Carbamate |
| CAIR | 1-(5-Phospho-D-ribosyl)-5-amino-4-imidazolecarboxylate |
| CALH | 2-(3-Carboxy-3-aminopropyl)-L-histidine |
| Cam | Calcium (Mitochondria) |
| cAMP | 3',5'-Cyclic AMP |
| CAP | Carbamoyl phosphate |
| CAPm | Carbamoyl phosphate (Mitochondria) |
| CAR | Carnitine |
| CARBO | carboxylate |
| CARm | Carnitine (Mitochondria) |
| CB15LCT | Cellobiono-1,5-lactone |
| CB15LCTe | Cellobiono-1,5-lactone (Extracellular) |
| CBCCP | Carboxybiotin-carboxyl-carrier-protein |
| CBHCAP | 3-Isopropylmalate |
| cCMP | 3',5'-Cyclic CMP |
| cdAMP | 3',5'-Cyclic dAMP |
| CDP | CDP |
| CDPCHO | CDPcholine |
| CDPDG | CDPdiacylglycerol |
| CDPDGm | CDPdiacylglycerol (Mitochondria) |
| CDPETN | CDPethanolamine |
| CELLOB | Cellobiose |
| CELLOBe | Cellobiose (Extracellular) |
| CELLOTe | Cellotriose (Extracellular) |
| CELLUe | Cellulose (Extracellular) |
| CER1 | Ceramide |
| CER2 | Dihydroceramide |
| CER3 | Phytoceramide |
| CGLY | Cys-Gly |
| cGMP | 3',5'-Cyclic GMP |
| CHCOA | 6-Carboxyhexanoyl-CoA |
| CHIB | Chitobiose |
| CHIBe | Chitobiose (Extracellular) |
| CHIT | Chitin |
| CHITe | Chitin (Extracellular) |
| CHITO | Chitosan |
| CHITOe | Chitosan (Extracellular) |
| CHO | Choline |
| CHOe | Choline (Extracellular) |
| CHOR | Chorismate |
| CHOREOL | Cholesterol |
| CHOREOLESTR | Cholesterol Ester |
| CHORESTA | Cholesta-7,24-dien-3β-ol |
| cIMP | 3',5'-Cyclic IMP |
| CINNAM | Cinnamate |
| CIT | Citrate |
| CITe | Citrate (Extracellular) |
| CITm | Citrate (Mitochondria) |

|  |  |  |
| --- | --- | --- |
| CITR | | L-Citrulline |
| CITRm | | L-Citrulline (Mitochondria) |
| CLm | | Cardiolipin (Mitochondria) |
| CML | | Citramalate |
| CMP | | CMP |
| CMPm | | CMP (Mitochondria) |
| CMUSA | | 2-Amino-3-carboxymuconate semialdehyde |
| CO2 | | Carbon dioxide |
| CO2e | | Carbon dioxide (Extracellular) |
| CO2m | | Carbon dioxide (Mitochondria) |
| CO2p | | Carbon dioxide (Peroxisome) |
| COA | | Coenzyme A |
| COAm | | Coenzyme A (Mitochondria) |
| COAp | | Coenzyme A (Peroxisome) |
| CPAD5P | | 1-(2-Carboxyphenylamino)-1-deoxy-D-ribulose 5-phosphate |
| CPGIII | | Coproporphyrinogen III |
| CPGIIIm | | Coproporphyrinogen III (Mitochondria) |
| CRONYLCOA | | crotonyl coA |
| CRONYLCOAm | | Crotonyl CoA (Mitochondria) |
| CTP | | CTP |
| CTPm | | CTP (Mitochondria) |
| Cu | | Copper |
| Cum | | Copper (Mitochondria) |
| CYMECm | | Cytochrome C (Mitochondria) |
| CYNE | | Cyanate |
| CYS | | L-Cysteine |
| CYSE | | L-Cysteate |
| CYSm | | L-Cysteine (Mitochondria) |
| CYST | | L-Cystine |
| CYTD | | Cytidine |
| CYTS | | Cytosine |
| CYTSe | | Cytosine (Extracellular) |
| D45PI | | 1-Phosphatidyl-D-myo-inositol 4,5-bisphosphate |
| D6PGC | | 6-Phospho-D-gluconate |
| D6PGL | | D-Glucono-1,5-lactone 6-phosphate |
| D6RP5P | | 2,5-diamino-6-hydroxy-4-(5-phosphoribosylamino)pyrimidine |
| D8RL | | 6,7-dimethyl-8-(1-D-ribityl)lumazine |
| DA | | Deoxyadenosine |
| DADP | | dADP |
| DAGLY | | Diacylglycerol |
| DALA | | D-Alanine |
| DAMP | | dAMP |
| DANNA | | 7,8-diaminononanoate |
| DANNAm | | 7,8-diaminononanoate (Mitochondria) |
| DAPRP | | 1,3-Diaminopropane |
| DASP | | D-aspartate |
| DATP | | dATP |
| DB4P | | 3,4 dihydroxy-2-butanone-4-P |
| DC | | Deoxycytidine |
| DCDP | | dCDP |
| DCMP | | dCMP |
| DCTP | | dCTP |
| DEHXG | | 3-dehydro-2-deoxy-D-gluconate |
| DEORIPI | 2-deoxy-D-ribose 5-phosphate | | |
| DEXG | 2-deoxy-D-gluconate | | |
| DG | Deoxyguanosine | | |
| DGDG | Digalactosyl diglyceride | | |
| DGDP | dGDP | | |
| DGLC | D-Glucose | | |
| DGLCe | D-Glucose (Extracellular) | | |
| DGLYCODEX | Debranched glycogen phosphorylase-limited dextrin | | |
| DGMP | dGMP | | |
| DGPP | Diacylglycerol pyrophosphate | | |
| DGTP | dGTP | | |
| DHDMST | Dihydrodemethylsterigmatocystin | | |
| DHF | Dihydrofolate | | |
| DHFm | Dihydrofolate (Mitochondria) | | |
| DHMVAm | (R)-2,3-dihydroxy-3-methylbutanoate (Mitochondria) | | |
| DHOMST | Dihydro-O-methylsterigmatocystin | | |
| DHP | 2-Amino-4-hydroxy-6-(D-erythro-1,2,3-trihydroxypropyl)-7,8-dihydropteridine | | |
| DHPT | Dihydropteroate | | |
| DHSK | 3-Dehydroshikimate | | |
| DHSP | Sphinganine 1-phosphate | | |
| DHSPH | 3-Dehydrosphinganine | | |
| DHST | Dihydrosterigmatocystin | | |
| DHVALm | (R)-3-Hydroxy-3-methyl-2-oxobutanoate (Mitochondria) | | |
| DIDIPC | (S)-dihydrodipicolinate | | |
| DIHINDOLE | Dihydroxyindole | | |
| DIHURA | 5,6-dihydrouracil | | |
| DIMEGLY | N,N-dimethylglycine | | |
| DIMEGLYm | N,N-dimethylglycine (Mitochondria) | | |
| DIMGP | D-erythro-1-(Imidazol-4-yl)glycerol 3-phosphate | | |
| DIN | Deoxyinosine | | |
| DMNAD | Deamido-NAD | | |
| DMPP | Dimethylallyl diphosphate | | |
| DMST | Demethylsterigmatocystin | | |
| DMZYMST | 4,4-Dimethylzymosterol | | |
| DOPA | L-Dopa | | |
| DOPAe | L-Dopa (Extracellular) | | |
| DOQUI | Dopaquinone | | |
| DOQUIe | Dopaquinone (Extracellular) | | |
| DOROA | (S)-Dihydroorotate | | |
| DOROAm | (S)-Dihydroorotate (Mitochondria) | | |
| DPCOA | Dephospho-CoA | | |
| DPRO | D-proline | | |
| DPTH | 2-[3-Carboxy-3-(methylammonio)propyl]-L-histidine | | |
| DQT | 3-Dehydroquinate | | |
| DR1P | Deoxy-ribose 1-phosphate | | |
| DSAM | S-Adenosylmethioninamine | | |
| DT | Thymidine | | |
| DTB | Dethiobiotin | | |
| DTDP | dTDP | | |
| DTMP | dTMP | | |
| DTMPm | dTMP (Mitochondria) | | |

|  |  |
| --- | --- |
| DTTP | dTTP |
| DU | Deoxyuridine |
| DUDP | dUDP |
| DUMP | dUMP |
| DUMPm | dUMP (Mitochondria) |
| DUTP | dUTP |
| E4P | D-Erythrose 4-phosphate |
| ECYSm | [Enzyme]-cysteine (Mitochondria) |
| EPST | Episterol |
| ERGOSE | Sterol ester |
| ERGOST | Ergosterol |
| ERIDICOL | Eriodictyol |
| ERTEOL | Ergosta-5,7,22,24(28)-tetraenol |
| ERTROL | Ergosta-5,7,24(28)-trienol |
| ESULFCYSm | [Enzyme]-S-sulfanylcysteine (Mitochondria) |
| ETH | Ethanol |
| ETHe | Ethanol (Extracellular) |
| ETHm | Ethanol (Mitochondria) |
| F26P | D-Fructose 2,6-bisphosphate |
| F6P | Beta-D-Fructose 6-phosphate |
| FAD | FAD |
| FADH2m | FADH2 (Mitochondria) |
| FADm | FAD (Mitochondria) |
| FALD | Formaldehyde |
| FALDm | Formaldehyde (Mitochondria) |
| FDP | Beta-D-Fructose 1,6-bisphosphate |
| FERIm | Ferricytochrome C (Mitochondria) |
| FEROm | Ferrocytochrome C (Mitochondria) |
| FERRIN | Ferreirin |
| FEST | Fecosterol |
| FGAM | 2-(Formamido)-N1-(5'-phosphoribosyl)acetamidine |
| FGAR | 5'-Phosphoribosyl-N-formylglycinamide |
| FGT | S-Formylglutathione |
| FKYN | L-Formylkynurenine |
| FMN | FMN |
| FMNe | FMN (Extracellular) |
| FMNm | FMN (Mitochondria) |
| FOFMETm | N-formylmethionyl-tRNAfMet (Mitochondria) |
| FOR | Formate |
| FORe | Formate (Extracellular) |
| FORGLU | N-formimidoyl-L-glutamate |
| FORm | Formate (Mitochondria) |
| FORMIE | Formamide |
| FPP | Trans,trans-Farnesyl diphosphate |
| FRU | D-Fructose |
| FRUe | D-Fructose (Extracellular) |
| FRUTN | D-fructuronate |
| FTHF | 10-Formyltetrahydrofolate |
| FTHFm | 10-Formyltetrahydrofolate (Mitochondria) |
| FUACAC | 4-Fumarylacetoacetate |
| FUM | Fumarate |
| FUMe | Fumarate (Extracellular) |
| FUMm | Fumarate (Mitochondria) |

|  |  |
| --- | --- |
| G | D-Glycerate |
| G1P | Alpha-D-Glucose 1-phosphate |
| G6P | Alpha-D-Glucose 6-phosphate |
| GA6P | D-Glucosamine 6-phosphate |
| GABA | 4-Aminobutanoate |
| GABAe | 4-Aminobutanoate (Extracellular) |
| GABAL | 4-Aminobutyraldehyde |
| GABALm | 4-Aminobutyraldehyde (Mitochondria) |
| GABAm | 4-Aminobutanoate (Mitochondria) |
| GACER | Galactocyl ceremide |
| GAL1P | Alpha-D-Galactose 1-phosphate |
| GALN14LAC | D-Galactono-1,4-lactone |
| GALNT | D-Galactonate |
| GALOL | Galactitol |
| GALUNT | D-Galacturonate |
| GALUNTe | D-Galacturonate (Extracellular) |
| GAR | 5'-Phosphoribosylglycinamide |
| GC | Gamma-L-Glutamyl-L-cysteine |
| GCYLCR | D-glucosyl-ceramide |
| GDP | GDP |
| GDPm | GDP (Mitochondria) |
| GDPMAN | GDPmannose |
| GGPP | Geranylgeranyl diphosphate |
| GL | Glycerol |
| GL3P | Sn-Glycerol 3-phosphate |
| GL3Pm | Sn-Glycerol 3-phosphate (Mitochondria) |
| GLAC | D-Galactose |
| GLACe | D-Galactose (Extracellular) |
| GLAL | Glycoaldehyde |
| GLALp | Glycoaldehyde (Peroxisome) |
| GLC | Alpha-D-Glucose |
| GLCe | Alpha-D-Glucose (Extracellular) |
| GLCN | D-Glucosamine |
| GLCN15LAC | D-Glucono-1,5-lactone |
| GLCN15LACe | D-Glucono-1,5-lactone (Extracellular) |
| GLCNe | D-Glucosamine (Extracellular) |
| GLCNT | D-Gluconate |
| GLCNTe | D-Gluconate (Extracellular) |
| GLe | Glycerol (Extracellular) |
| GLN | L-Glutamine |
| GLNe | L-Glutamine (Extracellular) |
| GLNm | L-Glutamine (Mitochondria) |
| GLTCOA | Glutaryl CoA |
| GLU | L-Glutamate |
| GLU1SAL | Glutamate-1-semialdehyde |
| GLUCN | D-glucuronate |
| GLUCRE | D-glucurononate |
| GLUe | L-Glutamate (Extracellular) |
| GLUGSAL | L-Glutamate 5-semialdehyde |
| GLUGSALm | L-Glutamate 5-semialdehyde (Mitochondria) |
| GLUm | L-Glutamate (Mitochondria) |
| GLUP | Alpha-D-Glutamyl phosphate |
| GLX | Glyoxylate |

|  |  |
| --- | --- |
| GLXm | Glyoxylate (Mitochondria) |
| GLXp | Glyoxylate (Peroxisome) |
| GLY | Glycine |
| GLYAL | D-Glyceraldehyde |
| GLYBET | Glycine betaine |
| GLYCEROCHO | Glycerophosphocholine |
| GLYCODEX | Glycogen phosphorylase-limited dextrin |
| GLYCOGEN | Glycogen |
| GLYCOGENe | Glycogen (Extracellular) |
| GLYCOLAp | Glycolate (Peroxisome) |
| GLYe | Glycine (Extracellular) |
| GLYm | Glycine (Mitochondria) |
| GLYN | Glycerone |
| GLYNIN | Glycogenin |
| GLYTRNA | Glycyl-tRNA |
| GMP | GMP |
| GN | Guanine |
| GNe | Guanine (Extracellular) |
| Gp | D-Glycerate (Peroxisome) |
| GPP | Geranyl diphosphate |
| GSN | Guanosine |
| GTP | GTP |
| GTPm | GTP (Mitochondria) |
| H | Hydrogen |
| H\_PO | Proton |
| H\_PO\_m | Proton (Mitochondria) |
| H2O | Water |
| H2O2 | Hydrogen peroxide |
| H2O2e | Hydrogen peroxide (Extracellular) |
| H2O2m | Hydrogen peroxide (Mitochondria) |
| H2O2p | Hydrogen peroxide (Peroxysome) |
| H2Oe | Water (Extracellular) |
| H2Om | Water (Mitochondria) |
| H2Op | Water (Peroxisome) |
| H2S | Hydrogen sulfide |
| H2Sm | Hydrogen sulfide (Mitochondria) |
| H2SO3 | Sulfite |
| H2SO3e | Sulfite (Extracellular) |
| H3MCOA | (S)-3-Hydroxy-3-methylglutaryl-CoA |
| H3MCOAm | (S)-3-Hydroxy-3-methylglutaryl-CoA (Mitochondria) |
| HACN | But-1-ene-1,2,4-tricarboxylate |
| HACNm | But-1-ene-1,2,4-tricarboxylate (Mitochondria) |
| HAN | 3-Hydroxyanthranilate |
| HAVN | 5-Hydroxyaverantin |
| HCIT | 2-Hydroxybutane-1,2,4-tricarboxylate |
| HCITm | 2-Hydroxybutane-1,2,4-tricarboxylate (Mitochondria) |
| HCO3 | HCO3 |
| HCO3m | HCO3 (Mitochondria) |
| HCXY | Holo-carboxylase |
| HCYS | L-Homocysteine |
| He | Hydrogen (Extracellular) |
| HEME\_Am | Heme A (Mitochondria) |
| HEME\_Om | Heme O (Mitochondria) |

|  |  |
| --- | --- |
| HHTRNA | L-Histidyl-tRNA |
| HICIT | Homoisocitrate |
| HICITm | Homoisocitrate (Mitochondria) |
| HIS | L-Histidine |
| HISe | L-Histidine (Extracellular) |
| HISOL | L-Histidinol |
| HISOLP | L-Histidinol phosphate |
| HIURTE | 3-hydroxy-isobutyrate |
| HIURTEp | 3-hydroxy-isobutyrate (Peroxisome) |
| HKYN | 3-Hydroxykynurenine |
| HKYNm | 3-Hydroxykynurenine (Mitochondria) |
| Hm | Hydrogen (Mitochondria) |
| HMTB | Hydroxymethylbilane |
| HNO2 | Nitrite |
| HNO2m | Nitrite (Mitochondria) |
| HNO3 | Nitrate |
| HNO3e | Nitrate (Extracellular) |
| HOMOGEN | Homogentisate |
| HPRO | Trans-4-Hydroxy-L-proline |
| HPROm | Trans-4-Hydroxy-L-proline (Mitochondria) |
| HPYRp | Hydroxypyruvate (Peroxisome) |
| HSER | L-Homoserine |
| HX | HX |
| HYGTA | S-(hydroxymethyl)glutathione |
| HYISOCOA | 3-hydroxy-isobutyryl COA |
| HYISOCOAm | 3-hydroxy-isobutyryl COA (Mitochondria) |
| HYISORATEm | 3-hydroxy-isobutyrate (Mitochondria) |
| HYXN | Hypoxanthine |
| IAC | Indole-3-acetate |
| IAD | Indole-3-acetamide |
| ICIT | Isocitrate |
| ICITe | Isocitrate (Extracellular) |
| ICITm | Isocitrate (Mitochondria) |
| ICITp | Isocitrate (Peroxisome) |
| IDP | IDP |
| IDPm | IDP (Mitochondria) |
| IGP | Indoleglycerol phosphate |
| IGST | 4,4-Dimethylcholesta-8,14,24-trienol |
| IIMZYMST | Intermediate\_Methylzymosterol\_II |
| IIZYMST | Intermediate\_Zymosterol\_II |
| ILE | L-Isoleucine |
| ILEe | L-Isoleucine (Extracellular) |
| ILEm | L-Isoleucine (Mitochondria) |
| IMACP | 3-(Imidazol-4-yl)-2-oxopropyl phosphate |
| IMIPRO | (S)-3-(5-oxo-4,5-dihydro-3H-imidazol-4-yl)propanoate |
| IMP | IMP |
| IMZYMST | Intermediate\_Methylzymosterol\_I |
| INS | Inosine |
| IPC | Inositol phosphorylceramide |
| IPN | Isopenicillin N |
| IPPMAL | 2-Isopropylmalate |
| IPPMALm | 2-Isopropylmalate (Mitochondria) |
| IPPP | Isopentenyl diphosphate |

|  |  |
| --- | --- |
| ISOBUCOA | Isobutyryl coA |
| ISOVACOA | Isovaleryl-CoA |
| ISOVACOAm | Isovaleryl-CoA (Mitochondria) |
| ITP | ITP |
| ITPm | ITP (Mitochondria) |
| IZYMST | Intermediate\_Zymosterol\_I |
| K | Potassium |
| Ke | Potassium (Extracellular) |
| KEMYOI | 2-keto-myo-inositol |
| Km | Potassium (Mitochondria) |
| KYN | L-Kynurenine |
| KYNm | L-Kynurenine (Mitochondria) |
| LAC | D-Lactate |
| LACAL | D-Lactaldehyde |
| LACALm | (S)-Lactaldehyde (Mitochondria) |
| LACe | D-Lactate (Extracellular) |
| LACm | (R)-Lactate (Mitochondria) |
| LACT | Lactose |
| LACTe | Lactose (Extracellular) |
| LAlaTRNA | L-alanyl-tRNA |
| LAOL | L-Arabitol |
| LARAB | L-Arabinose |
| LARABe | L-Arabinose (Extracellular) |
| LCysTRNA | L-cysteinyl-tRNA |
| LEU | L-Leucine |
| LEUe | L-Leucine (Extracellular) |
| LEUm | L-Leucine (Mitochondria) |
| LGALNT | L-Galactonate |
| LGLNTRNA | L-glutaminyl-tRNA |
| LGLNTRNAm | L-glutaminyl-tRNA (Mitochondria) |
| LGLUTRNA | L-glutamyl-tRNA |
| LGLUTRNAm | L-glutamyl-tRNA (Mitochondria) |
| LGLYAL | L-Glyceraldehyde |
| LGT | (R)-S-Lactoylglutathione |
| LILEUTRNA | L-isoleucine-tRNA |
| LILEUTRNAm | L-isoleucine-tRNA (Mitochondria) |
| LIPOm | Lipoamide (Mitochondria) |
| LLAC | L-Lactate |
| LLACe | L-Lactate (Extracellular) |
| LLACm | (S)-Lactate (Mitochondria) |
| LLCT | L-Cystathionine |
| LLDACV | N-[5-amino-5-carboxypentanoyl]-L-cysteinyl-D-valine |
| LLeuTRNA | L-leucyl-tRNA |
| LLTRNA | L-Lysyl-tRNA |
| LMETTRNA | L-methionyl-tRNA |
| LMETTRNAm | L-methionyl-tRNA (Mitochondria) |
| LNST | Lanosterol |
| LPAA | Lysophosphatidylamine |
| LPC | Lysophosphatidylcholine |
| LPDME | Lysophosphatidyl-N-dimethylethanolamine |
| LPE | Lysophosphatidylethanolamine |
| LPG | Lysophosphatidylglycerol |
| LPheTRNA | L-phenylalanyl-tRNA |

|  |  |
| --- | --- |
| LPMME | Lysophosphatidyl-N-methylethanolamine |
| LPROTRNA | L-prolyl-tRNA |
| LPS | Lysophosphatidylserine |
| LRL | L-Ribulose |
| LRL5P | L-ribulose 5-phosphate |
| LRLe | L-Ribulose (Extracellular) |
| LSECTRNA | L-selenocysteinyl-tRNA |
| LSERTRNA | L-seryl-tRNA |
| LTHETRNA | L-threonyl-tRNA |
| LTHETRNAm | L-threonyl-tRNA (Mitochondria) |
| LTST | Lathosterol |
| LTyrTRNA | L-tyrosyl-tRNA |
| LTyrTRNAm | L-tyrosyl-tRNA (Mitochondria) |
| LValTRNA | L-valyl-tRNAVal |
| LXUL | L-Xylulose |
| LXULe | L-Xylulose (Extracellular) |
| LYS | L-Lysine |
| LYSe | L-Lysine (Extracellular) |
| MACAC | Maleylacetoacetate |
| MAGLY | Monoacylglycerol |
| MAL | (S)-Malate |
| MALACP | Malonyl-[acyl-carrier protein] |
| MALCOA | Malonyl Coenzyme A |
| MALe | (S)-Malate (Extracellular) |
| MALm | (S)-Malate (Mitochondria) |
| MALp | (S)-Malate (Peroxisome) |
| MAN | D-Mannose |
| MAN1P | Alpha-D-Mannose 1-phosphate |
| MAN6P | D-Mannose 6-phosphate |
| MANe | D-Mannose (Extracellular) |
| MANNAN | Mannan |
| MANNANe | Mannan (Extracellular) |
| MANOE | D-mannonate |
| MCECOA | 2-methylaceto-acetyl CoA |
| MCRCOA | 2-methylbut-2-enoyl-CoA |
| MCRCOAm | 2-methylbut-2-enoyl-CoA (Mitochondria) |
| MELI | Melibiose |
| MELIe | Melibiose (Extracellular) |
| MENIN | Melanin |
| MESC | Mesaconate |
| MET | L-Methionine |
| METBUCOA | 2-methylbutyryl coA |
| METBYCOA | 2-methyl-2-hydroxybutyryl coA |
| METe | L-Methionine (Extracellular) |
| METHF | 5,10-Methenyltetrahydrofolate |
| METHFm | 5,10-Methenyltetrahydrofolate (Mitochondria) |
| METHOL | Methanol |
| METHOLe | Methanol (Extracellular) |
| METTHF | 5,10-Methylenetetrahydrofolate |
| METTHFm | 5,10-Methylenetetrahydrofolate (Mitochondria) |
| MGCOA | 3-methylglutaconyl-CoA |
| MGCOAm | 3-methylglutaconyl-CoA (Mitochondria) |
| MGDG | Monogalactosyl diglyceride |

|  |  |  |
| --- | --- | --- |
| MHIS | N(pai)-Methyl-L-histidine | |
| MI1P | 1L-myo-Inositol 1-phosphate | |
| MIP2C | Inositol-mannose-P-inositol-P-ceramide | |
| MIPC | Mannose-inositol-P-ceramide | |
| MLT | Maltose | |
| MLTe | Maltose (Extracellular) | |
| MLTIOSE | Maltotriose | |
| MLTOSE | Maltotetraose | |
| MMCOA | (S)-methylmalonyl-CoA | |
| MMSHYm | 2-methyl-3-oxopropanoate (Mitochondria) | |
| MNT | D-Mannitol | |
| MNT1P | D-Mannitol 1-phosphate | |
| MNTe | D-Mannitol (Extracellular) | |
| MTHF | 5-Methyltetrahydrofolate | |
| MTHFm | 5-Methyltetrahydrofolate (Mitochondria) | |
| MTHGXL | Methylglyoxal | |
| MTHGXLm | Methylglyoxal (Mitochondria) | |
| MTHPTGLU | 5-Methyltetrahydropteroyltri-L-glutamate | |
| MVL | (R)-Mevalonate | |
| MYOBISPI | Myo-inositol 1,4-bisphosphate | |
| MYOCYPI | 1D-myo-inositol 1,2-cyclic phosphate | |
| MYOI | Myo-Inositol | |
| MYOIe | Myo-Inositol (Extracellular) | |
| MZYMST | 4-Methylzymsterol | |
| N4HBZ | 3-octaprenyl-4-hydroxybenzoate | |
| Na | Sodium | |
| NAD | NAD+ | |
| NADH | NADH | |
| NADHm | NADH (Mitochondria) | |
| NADHp | NADH (Peroxisome) | |
| NADm | NAD+ (Mitochondria) | |
| NADP | NAD+ (Peroxisome) | |
| NADPH | NADPH | |
| NADPHm | NADPH (Mitochondria) | |
| NADPHp | NADPH (Peroxisome) | |
| NADPm | NADP+ (Mitochondria) | |
| NADPp | NADP+ (Peroxisome) | |
| Nae | Sodium (Extracellular) | |
| NAG | N-Acetyl-D-glucosamine | |
| NAGA1P | N-Acetyl-D-glucosamine 1-phosphate | |
| NAGA6P | N-Acetyl-D-glucosamine 6-phosphate | |
| NAGe | N-Acetyl-D-glucosamine (Extracellular) | |
| NAGLUm | N-Acetyl-L-glutamate (Mitochondria) | |
| NAGLUPm | N-Acetyl-L-glutamate 5-phosphate (Mitochondria) | |
| NAGLUSm | N-Acetyl-L-glutamate 5-semialdehyde (Mitochondria) | |
| Nam | Sodium (Mitochondria) | |
| NAORN | N2-Acetyl-L-ornithine | |
| NAORNm | N2-Acetyl-L-ornithine (Mitochondria) | |
| NCACE | Naringenin chalcone | |
| NGEN | Naringenin | |
| NH3 | Ammonia | |
| NH3e | Ammonia (Extracellular) | |
| NH3m | Ammonia (Mitochondria) | |
| NH4OH | Ammonium hydroxide |
| NICD | Nicotinamide |
| NICDm | Nicotinamide (Mitochondria) |
| NICNATE | Nicotinate |
| NICNATEm | Nicotinate (Mitochondria) |
| NICNUCLE | Nicotinate D-ribonucleotide |
| NITE | Nitriles |
| NITROPRO | 2-nitropropane |
| NITROPROm | 2-nitropropane (Mitochondria) |
| NMNm | Nicotinamide mononucleotide (Mitochondria) |
| NO | Nitric oxide |
| NOR | Norsolorinic acid |
| NPP | Octaprenyl diphosphate |
| NPRAN | N-(5-Phospho-D-ribosyl)anthranilate |
| O2 | Oxygen |
| O2e | Oxygen (Extracellular) |
| O2m | Oxygen (Mitochondria) |
| O2p | Oxygen (Peroxisome) |
| OA | Oxaloacetate |
| OAe | Oxaloacetate (Extracellular) |
| OAHSER | O-Acetyl-L-homoserine |
| OAm | Oxaloacetate (Mitochondria) |
| OAp | Oxaloacetate (Peroxisome) |
| OBUT | 2-Oxobutanoate |
| OBUTm | 2-Oxobutanoate (Mitochondria) |
| OGT | Oxidized glutathione |
| OICAP | 3-Carboxy-4-methyl-2-oxopentanoate |
| OICAPm | 3-Carboxy-4-methyl-2-oxopentanoate (Mitochondria) |
| OIVAL | (R)-2-Oxoisovalerate |
| OIVALm | (R)-2-Oxoisovalerate (Mitochondria) |
| OMP | Orotidine 5'-phosphate |
| OMST | O-methylsterigmatocystin |
| OMVAL | 2-keto-3-methyl-valerate |
| OMVALm | 2-keto-3-methyl-valerate (Mitochondria) |
| ORN | L-Ornithine |
| ORNm | L-Ornithine (Mitochondria) |
| OROA | Orotate |
| OROAm | Orotate (Mitochondria) |
| OSLHSER | O-Succinyl-L-homoserine |
| OTHIO | Oxidized thioredoxin |
| OTHIOm | Oxidized thioredoxin (Mitochondria) |
| OXAL | Oxalate |
| OXALe | Oxalate (Extracellular) |
| OXGLY | Oxaloglycolate |
| P5C | (S)-1-Pyrroline-5-carboxylate |
| P5Cm | (S)-1-Pyrroline-5-carboxylate (Mitochondria) |
| PA | Phosphatidate |
| PAA | Phosphatidylamine |
| PABA | 4-Aminobenzoate |
| PAC | Phenylacetic acid |
| PAD | 2-Phenylacetamide |

|  |  |
| --- | --- |
| PADm | 2-Phenylacetamide (Mitochondria) |
| PAm | Phosphatidate (Mitochondria) |
| PANT | (R)-Pantoate |
| PANTm | (R)-Pantoate (Mitochondria) |
| PAP | Adenosine 3',5'-bisphosphate |
| PAPm | Adenosine 3',5'-bisphosphate (Mitochondria) |
| PAPS | 3'-Phosphoadenylylsulfate |
| PC | Phosphatidylcholine |
| PCACE | Protocatechuate |
| PCHO | Choline phosphate |
| PDME | Phosphatidyl-N-dimethylethanolamine |
| PDXAL | Pyridoxal |
| PDXAM | Pyridoxamine |
| PDXAM5PI | Pyridoxamine-5-phosphate |
| PDXI | Pyridoxine |
| PDXI5PI | Pyridoxine-5-phosphate |
| PDXL5PI | Pyridoxal-5-phosphate |
| PE | Phosphatidylethanolamine |
| PEm | Phosphatidylethanolamine (Mitochondria) |
| PEN | Penicillin |
| PENACID | Pennicillic acid |
| PENN | Penicillin N |
| PEP | Phosphoenolpyruvate |
| PEPm | Phosphoenolpyruvate (Mitochondria) |
| PETHM | Ethanolamine phosphate |
| PG | Phosphatidylglycerol |
| PGm | Phosphatidylglycerol (Mitochondria) |
| PGPm | Phosphatidylglycerophosphate (Mitochondria) |
| PHAC | Phenylacetate |
| PHACAL | Phenylacetaldehyde |
| PHACALm | Phenylacetaldehyde (Mitochondria) |
| PHAC-COA | Phenylacetyl-CoA |
| PHC | L-1-Pyrroline-3-hydroxy-5-carboxylate |
| PHCm | L-1-Pyrroline-3-hydroxy-5-carboxylate (Mitochondria) |
| PHE | L-Phenylalanine |
| PHEe | L-Phenylalanine (Extracellular) |
| PHEETHAL | Phenylethylalcohol |
| PHEETHALm | Phenylethylalcohol (Mitochondria) |
| PHEm | L-Phenylalanine (Mitochondria) |
| PHEMEm | Protoheme (Mitochondria) |
| PHEN | Prephenate |
| PHP | 3-Phosphonooxypyruvate |
| PHPYR | Phenylpyruvate |
| PHSER | O-Phospho-L-homoserine |
| PHSP | Phytosphingosine 1-phosphate |
| PI | Orthophosphate |
| PIe | Orthophosphate (Extracellular) |
| PIm | Orthophosphate (Mitochondria) |
| PINS | 1-Phosphatidyl-D-myo-inositol |
| PINS4P | 1-Phosphatidyl-1D-myo-inositol 4-phosphate |
| PINSP | 1-Phosphatidyl-1D-myo-inositol 3-phosphate |
| PMME | Phosphatidyl-N-methylethanolamine |
| PMVL | (R)-5-Phosphomevalonate |

|  |  |
| --- | --- |
| PNTO | (R)-Pantothenate |
| PPBG | Porphobilinogen |
| PPGIXm | Protoporphyrinogen IX |
| ppGpp | ppGpp |
| PPI | Pyrophosphate |
| PPIm | Pyrophosphate (Mitochondria) |
| PPIp | Pyrophosphate (Peroxixome) |
| PPMAL | 2-Isopropylmaleate |
| PPMVL | (R)-5-Diphosphomevalonate |
| pppGpp | pppGpp |
| PPRIXm | Protoporphyrin IX (Mitochondria) |
| PRAM | 5-Phosphoribosylamine |
| PRBAMP | N1-(5-Phospho-D-ribosyl)-AMP |
| PRBATP | N1-(5-Phospho-D-ribosyl)-ATP |
| PRECOR | Precorrin |
| PRFICA | 1-(5'-Phosphoribosyl)-5-formamido-4-imidazolecarboxamide |
| PRFP | 5-(5-Phospho-D-ribosylaminoformimino)-1-(5-phosphoribosyl)-imidazole-4carboxamide |
| PRLP | N-(5'-Phospho-D-1'-ribulosylformimino)-5-amino-1-(5"-phospho-D-ribosyl)-4imidazolecarboxamide |
| PRO | L-Proline |
| PROe | L-Proline (Extracellular) |
| PROm | L-Proline (Mitochondria) |
| PROP | Propanoate |
| PROPCOA | Propanoyl-CoA |
| PROPCOAm | Propanoyl-CoA (Mitochondria) |
| PROPCOAp | Propanoyl-CoA (Peroxisome) |
| PROPe | Propanoate (Extracellular) |
| PROPm | Propanoate (Mitochondria) |
| PRPP | 5-Phospho-alpha-D-ribose 1-diphosphate |
| PS | Phosphatidylserine |
| PSm | Phosphatidylserine (Mitochondria) |
| PSPH | Phytosphingosine |
| PTATEe | Pectate (Extracellular) |
| PTRSC | Putrescine |
| PTRSCm | Putrescine (Mitochondria) |
| PURI5P | Pseudouridine 5'-phosphate |
| PYR | Pyruvate |
| PYRe | Pyruvate (Extracellular) |
| PYRm | Pyruvate (Mitochondria) |
| PYRp | Pyruvate (Peroxisome) |
| PYTE | Phytate |
| QA | Quinolinate |
| QH2m | Ubiquinol (Mitochondria) |
| Qm | Ubiquinone (Mitochondria) |
| QT | Quinate |
| R1P | D-Ribose 1-phosphate |
| R5P | D-Ribose 5-phosphate |
| R5Pm | D-Ribose 5-phosphate (Mitochondria) |
| RAFe | Raffinose (Extracellular) |
| RGT | Glutathione |
| RIB | D-Ribose |
| RIBe | D-Ribose (Extracellular) |

|  |  |
| --- | --- |
| RIBFLAV | Riboflavin |
| RIBFLAVe | Riboflavin (Extracellular) |
| RL | D-Ribulose |
| RL5P | D-Ribulose 5-phosphate |
| RLe | D-Ribulose (Extracellular) |
| RTHIO | Reduced thioredoxin |
| RTHIOm | Reduced thioredoxin (Mitochondria) |
| RX | RX |
| S | Sulfur |
| S23E | (S)-2,3-Epoxysqualene |
| S7P | Sedoheptulose 7-phosphate |
| SACP | N6-(L-1,3-Dicarboxypropyl)-L-lysine |
| SAH | S-Adenosyl-L-homocysteine |
| SAHm | S-Adenosyl-L-homocysteine (Mitochondria) |
| SAICAR | 1-(5'-Phosphoribosyl)-5-amino-4-(N-succinocarboxamide)-imidazole |
| SAM | S-Adenosyl-L-methionine |
| SAMm | S-Adenosyl-L-methionine (Mitochondria) |
| SAMOB | S-adenosyl-4-methylthio-2-oxobutanoate |
| SAMOBm | S-adenosyl-4-methylthio-2-oxobutanoate (Mitochondria) |
| SAPm | S-Aminomethyldihydrolipoylprotein (Mitochondria) |
| SARC | Sarcosine |
| SARCm | Sarcosine (Mitochondria) |
| SCTLE | Scytalone |
| SER | L-Serine |
| SERe | L-Serine (Extracellular) |
| SERm | L-Serine (Mitochondria) |
| SHCR | Sirohydrochlorin |
| SIHM | Siroheme |
| SLF | Sulfate |
| SLFe | Sulfate (Extracellular) |
| SME | Shikimate |
| SME3P | Shikimate-3-phosphate |
| SNPI | Selenophosphate |
| SOR | L-Sorbose |
| SORe | L-Sorbose (Extracellular) |
| SOT | D-Sorbitol |
| SOTe | D-Sorbitol (Extracellular) |
| SPH | Sphinganine |
| SPMYLIN | Sphingomyelin |
| SPRM | Spermine |
| SPRMD | Spermidine |
| SQL | Squalene |
| ST | Sterigmatocystin |
| STAR | Starch |
| STARe | Starch (Extracellular) |
| SUCC | Succinate |
| SUCCe | Succinate (Extracellular) |
| SUCCm | Succinate (Mitochondria) |
| SUCCOAm | Succinyl coenzyme A (Mitochondria) |
| SUCCp | Succinate (Peroxisome) |
| SUCCSAL | Succinate semialdehyde |
| SUCCSALm | Succinate semialdehyde (Mitochondria) |
| SUCe | Sucrose (Extracellular) |

|  |  |  |
| --- | --- | --- |
| SUFT | Sulfatide | |
| T3P1 | D-Glyceraldehyde 3-phosphate | |
| T3P2 | Glycerone phosphate | |
| T6P | Tagatose-6-phosphate | |
| TAGLY | Triacylglycerol | |
| TAR | Tartrate | |
| TARE | Tartrate | |
| TDP | D-tagatose 1,6-bisphosphate | |
| TGE | Tagatose | |
| TGEe | Tagatose (Extracellular) | |
| TGLCOA | Tigly CoA | |
| THDP | Thiamine diphosphate | |
| THF | Tetrahydrofolate | |
| THFG | Tetrahydrofolyl-[Glu] | |
| THFm | Tetrahydrofolate (Mitochondria) | |
| THME | Thiamine | |
| THMP | Thiamine monophosphate | |
| THPTGLU | Tetrahydropteroyltri-L-glutamate | |
| THR | L-Threonine | |
| THRe | L-Threonine (Extracellular) | |
| THRm | L-Threonine (Mitochondria) | |
| THY | Thymine | |
| THZ | 4-methyl-5-(2-hydroxyethyl)thiazole | |
| THZP | 4-methyl-5-(2-phosphonooxyethyl)thiazole | |
| TPI | D-myo-inositol 1,4,5-trisphosphate | |
| TPP | Thiamine diphosphate | |
| TR3DHT | L-threo-3-deoxy-hexulosonate | |
| TRE | Alpha,alpha-Trehalose | |
| TRE6P | Alpha,alpha-Trehalose 6-phosphate | |
| TREe | Alpha,alpha-Trehalose (Extracellular) | |
| TRMAS | L-threo-3-methylaspartate | |
| TRNA | TRNA | |
| TRNAm | TRNA (Mitochondria) | |
| TRP | L-Tryptophan | |
| TRPe | L-Tryptophan (Extracellular) | |
| TRPM | Tryptamine | |
| TRPTRNA | L-Tryptophanyl-tRNA | |
| TTGGP | Trans, trans cis-geranyl geranyl diphosphate | |
| TYR | L-Tyrosine | |
| TYRe | L-Tyrosine (Extracellular) | |
| TYRm | L-Tyrosine (Mitochondria) | |
| UDP | UDP | |
| UDPG | UDPglucose | |
| UDPGAL | UDPgalactose | |
| UDPGE | UDP-glucuronate | |
| UDPNAG | UDP-N-acetyl-D-glucosamine | |
| UDPNAGA | UDP-N-acetyl-D-galactosamine | |
| UGC | Ureidoglycolate | |
| UGCp | Ureidoglycolate (Peroxisome) | |
| UMP | UMP | |
| UPGIII | Uroporphyrinogen III | |
| URA | Uracil | |
| URAe | Uracil (Extracellular) | |
| URATEp | Urate (Peroxisome) |
| UREA | Urea |
| UREAC | Urea-1-carboxylate |
| UREAp | Urea (Peroxisome) |
| UREIPRO | N-carbamoyl-β-alanine |
| URI | Uridine |
| UROCA | Urocanate |
| UTP | UTP |
| VAL | L-Valine |
| VALe | L-Valine (Extracellular) |
| VALm | L-Valine (Mitochondria) |
| VEML | Vermelone |
| VERA | Versicolorin A |
| VERAL | Versiconal |
| VERB | Versicolorin B |
| VESTINE | Vestine |
| VHA | Versiconal hemiacetal acetate |
| XAN | Xanthine |
| XANp | Xanthine (Peroxixome) |
| XMP | Xanthosine 5'-phosphate |
| XOL | Xylitol |
| XOLe | Xylitol (Extracellular) |
| XTSINE | Xanthosine |
| XUL | D-Xylulose |
| XUL5P | D-Xylulose 5-phosphate |
| XULe | D-Xylulose (Extracellular) |
| XYL | D-Xylose |
| XYLAN | Xylan |
| XYLANe | Xylan (Extracellular) |
| XYLe | D-Xylose (Extracellular) |
| ZYMST | Zymosterol |

**Suppl. Table 3**: Macromolecular composition (Biomass formation) of *A. oryzae*. The measured values are from Pedersen et al. (1999) where *A. oryzae* (A1560, wild type strain) grown on glucose and ammonia for a growth rate of 0.10 1/h and a specific glucose uptake rate of 1.12 mmol glucose/(g DW.h). For Glycogen, the measured value is from Debois et al. (1995). For Glucan and Chitin, the measured values are from Pedersen et al. (1996).

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Biomass component** | **%[g/g]** | **%[mol/mol]** | **Average MW**  **[g/mol of monomers in polymer]** | **Stoichiometric coefficient**  **[mmol/ g DW]** |
| **Proteins** | 40.0 | 71.24 | 134.58 | 3.50075 |
| **Carbohydrates** | 28.0 |  |  |  |
| Glycogen | 0.1 | 0.04 | 666.6 | 0.00212 |
| Chitin | 7.0 | 8.29 | 203.2 | 0.40759 |
| Glucan | 20.8 | 30.82 | 162.1 | 1.51453 |
| **RNA** | 5.3 | 3.72 | 341.9 | 0.18259 |
| **DNA** | 0.8 | 0.58 | 332.3 | 0.02836 |
| **Lipids** | 6.8 | 2.09 | 780.43 |  |
| ***Neutral Lipids***  Triacylglycerol | 2.12 | 0.53 | 954.96 | 0.02617 |
| ***Free fatty acids*** | 0.35 | 0.28 | 301.31 | 0.01365 |
| ***Phospholipids***  Phosphatidylethanolamine | 0.97 | 0.30 | 782.50 | 0.01468 |
| Phosphatidylcholine | 2.38 | 0.68 | 834.80 | 0.03356 |
| Phosphatidylserine | 0.40 | 0.11 | 827.32 | 0.00564 |
| Phosphatidylamine | 0.58 | 0.18 | 755.24 | 0.00903 |
| **D-Mannitol** | 3.3 | 4.34 | 182.2 | 0.21333 |
| **Glycerol** | 0.7 | 1.82 | 92.1 | 0.08952 |
| **Ash** | 15.1 | - | - | - |

Average MW of biomass (g/mol) = 239.68

Elemental biomass composition = CH1.5O0.53N0.19P0.005S0.01

MW on C-mole (g/C-mol) = 25.1

**Suppl. Table 4**: Protein composition of *A. oryzae*. The measured values are from Pedersen et al. (1999).

|  |  |  |  |
| --- | --- | --- | --- |
| **Amino acid type** | **MW**  **[g/mol]** | **Composition [%mol]** | **Composition [% (g/g)]** |
| Alanine | 89.1 | 9.5 | 6.6 |
| Arginine | 174.2 | 4.4 | 6.0 |
| Asparagine | 132.1 | 4.6 | 4.7 |
| Aspartate | 133.1 | 4.6 | 4.8 |
| Cysteine | 121.2 | 1.1 | 1.0 |
| Glutamate | 147.1 | 8 | 9.2 |
| Glutamine | 146.1 | 8 | 9.1 |
| Glycine | 75.1 | 9.4 | 5.5 |
| Histidine | 155.2 | 2 | 2.4 |
| Isoleucine | 131.2 | 4.5 | 4.6 |
| Leucine | 131.2 | 6.9 | 7.1 |
| Lysine | 146.2 | 5.7 | 6.5 |
| Methionine | 149.2 | 1.4 | 1.6 |
| Phenylalanine | 165.2 | 3.1 | 4.0 |
| Proline | 115.1 | 4.7 | 4.2 |
| Serine | 105.1 | 6.6 | 5.4 |
| Threonine | 119.1 | 4.8 | 4.5 |
| Tryptophan | 204.2 | 1.8 | 2.9 |
| Tyrosine | 181.2 | 2.8 | 4.0 |
| Valine | 117.1 | 6.4 | 5.9 |

Average MW of protein (g/mol) = 134.58

**Suppl. Table 5**: DNA composition of

Pedersen et al. (1999).

|  |  |  |  |
| --- | --- | --- | --- |
| **dNTP type** | **MW**  **[g/mol]** | **Composition [% (mol)]** | **Composition [% (g/g)]** |
| dAMP | 349.2 | 24.2 | 25.51 |
| dTMP | 322.2 | 24.2 | 23.53 |
| dGMP | 347.2 | 25.8 | 27.04 |
| dCMP | 307.2 | 25.8 | 23.92 |

Average MW of DNA (g/mol) = 332.3

**Remark:** Assuming the same composition in NTP and NMP

**Suppl. Table 6**: RNA composition of

Pedersen et al. (1999).

|  |  |  |  |
| --- | --- | --- | --- |
| **NTP type** | **MW**  **[g/mol]** | **Composition [% (mol)]** | **Composition [% (g/g)]** |
| AMP | 347.2 | 25.6 | 26.1 |
| UMP | 324.2 | 26.2 | 24.9 |
| GMP | 363.2 | 28.6 | 30.5 |
| CMP | 323.2 | 19.6 | 18.6 |

Average MW of RNA (g/mol) = 341.9

**Remark** Assuming the same composition in NTP and NMP **Suppl. Table 7**: Lipid composition of Sakuradani et. al (1999).

|  |  |  |  |
| --- | --- | --- | --- |
| **Lipid type** | **Average MW**  **[g/mol]** | **Composition [%mol]** | **Composition [% (g/g)]** |
| Triacylglycerol | 954.96 | 25.50 | 31.20 |
| Free fatty acids | 301.31 | 13.3 | 5.13 |
| Phosphatidylethanolamine | 782.50 | 14.3 | 14.34 |
| Phosphatidylcholine | 834.80 | 32.7 | 34.98 |
| Phosphatidylserine | 827.32 | 5.5 | 5.83 |
| Phosphatidylamine | 755.24 | 8.8 | 8.52 |

Average MW of total lipids (g/mol) = 780.43

**Suppl. Table 8**: Triacylglycerol composition of *A. oryzae*. The measured values are from Sakuradani et. al (1999).

|  |  |  |  |
| --- | --- | --- | --- |
| **Fatty acids** | **MW [g/mol]** | **Composition [%mol]** | **% [mol/100 mol of total fatty acids in lipid]** |
| C16:0 | 239.2 | 47.10 | 11.8 |
| C16:1 | 237.2 | 2.42 | 0.6 |
| C18:0 | 267.5 | 15.35 | 4.3 |
| C18:1 | 265.3 | 53.28 | 14.8 |
| C18:2 | 263.2 | 233.62 | 64.4 |
| C18:3 | 261.2 | 14.99 | 4.1 |

**Suppl. Table 9**: Phospholipid composition of *A. oryzae*. The measured values are from Sakuradani et. al (1999).

|  |  |  |  |
| --- | --- | --- | --- |
| **Fatty acids** | **MW [g/mol]** | **Composition [%mol]** | **% [mol/100 mol of total fatty acids in lipid]** |
| C16:0 | 239.2 | 58.56 | 17.3 |
| C16:1 | 237.2 | 1.44 | 0.4 |
| C18:0 | 267.5 | 5.43 | 1.8 |
| C18:1 | 265.3 | 42.61 | 13.9 |
| C18:2 | 263.2 | 197.54 | 64.2 |
| C18:3 | 261.2 | 7.44 | 2.4 |

**Suppl. Table 10**: Free fatty acid composition of *A. oryzae*. The measured values are from Sakuradani et al. (1999).

|  |  |  |  |
| --- | --- | --- | --- |
| **Fatty acids** | **MW [g/mol]** | **Composition [%mol]** | **% [mol/100 mol of total fatty acids in lipid]** |
| C16:0 | 239.2 | 27.20 | 21.6 |
| C16:1 | 237.2 | 0.51 | 0.4 |
| C18:0 | 267.5 | 3.04 | 2.7 |
| C18:1 | 265.3 | 15.34 | 13.5 |
| C18:2 | 263.2 | 66.73 | 58.3 |
| C18:3 | 261.2 | 4.04 | 3.5 |

**References:**

**Books, paper publications and databases are applied for genome-scale reconstruction**

Brown, D.W., Yu, J.H., Kelkar, H.S., Fernandes, M., Nesbitt, T.C., Keller, N.P., Adams, T.H., and Leonard, T.J: **Twenty-five coregulated transcripts define a sterigmatocystin gene cluster in *Aspergillus nidulans***. *PNAS* 1996, **93**: 1418-1422.

Carlsen M., Nielsen J., Villadsen J: **Growth and alpha-amylase production by *Aspergillus oryzae* during continuous cultivations.** *Journal of Biotechnology* 1996, 81-93.

David H, Hofmann G, Oliveira A.P, Jarmer H, Nielsen J: **Metabolic network driven analysis of genome-wide transcription data from *Aspergillus nidulans***. *Genome Biology* 2006, **7** (11).

David H, Akesson M, Nielsen J: **Reconstruction of the central carbon metabolism of *Aspergillus niger***. *European Journal of Biochemistry* 2003, **270**: 4243-4253. Debois, M., Heydorn, A., Obel, N: **Macromolecule analysis of *Aspergillus oryzae***. *Master Thesis* 1995, Technical University of Denmark.

Forster J, Famili I, Fu P, Palsson B.O, Nielsen J: **Genome-scale reconstruction of the *Saccharomyces cerevisiae* metabolic network**. *Genome Research* 2003, **13**:244-

253.

Machida M, Asai K, Sano M, Tanaka T, Kumagai T, Terai G, Kusumoto KI, Arima T, Akita O, Kashiwagi Y *et al*: **Genome sequencing and analysis of *Aspergillus oryzae***. *Nature* 2005, **438**:1157-1161.

McMurry, J. and Begley, T: **The Organic Chemistry of Biological Pathways**. *Englewood* 2005, CO: Roberts and Co. Publishers.

Pedersen H, Carlsen M, Nielsen J: **Identification of enzymes and quantification of metabolic fluxes in the wild type and in a recombinant *Aspergillus oryzae* strain**. *Applied and Environmental Microbiology* 1999, **65**:11-19.

Pedersen, H: **Metabolic flux in *Aspergillus oryzae***. *Master Thesis* 1996, Technical

University of Denmark.

Sakuradani, E, [Kobayashi M,](http://www.ncbi.nlm.nih.gov/sites/entrez?Db=pubmed&Cmd=Search&Term=%22Kobayashi%20M%22%5BAuthor%5D&itool=EntrezSystem2.PEntrez.Pubmed.Pubmed_ResultsPanel.Pubmed_DiscoveryPanel.Pubmed_RVAbstractPlus) [Shimizu S](http://www.ncbi.nlm.nih.gov/sites/entrez?Db=pubmed&Cmd=Search&Term=%22Shimizu%20S%22%5BAuthor%5D&itool=EntrezSystem2.PEntrez.Pubmed.Pubmed_ResultsPanel.Pubmed_DiscoveryPanel.Pubmed_RVAbstractPlus): **Delta 9-fatty acid desaturase from arachidonic acid producing fungus**.  *European Journal of Biochemistry* 1999, **260**:

208-216.

Hilditch, S, Berghäll, S, Kalkkinen, N, Penttilä, M, Richard, P:T**he missing link in the fungal D-galacturonate pathway; Identification of the L-threo-3-deoxyhexulosonate aldolase**. *Journal of Biological Chemistry* 2007, 1-16.

Tsai, H.F., Fujii, I., Watanabe, A., Wheeler, A.H., Chang, Y.C., Yasuoka, Y., Ebizuka, Y. and Kwon-Chung, K.J: **Pentaketide melanin biosynthesis in *Aspergillus fumigatus* requires chain-length shortening of a heptaketide precursor**. *Journal of Biological Chemistry* 2001, **276**: 29292-29298.

***Aspergillus* oryzae genome database**

[http://www.bio.nite.go.jp/dogan/MicroTop?GENOME\_ID=ao]

**BioCyc pathway database**

[http://biocyc.org/server.html]

**Comparative genome analysis database**:

[[http://ergo.integratedgenomics.com/ERGO]](http://ergo.integratedgenomics.com/ERGO)

**KEGG pathway database**:

[[http://www.kegg.com](http://www.kegg.com/)]