## metabolomics

	NCT Number	Title	Authors	Description	Identifier	Dates
1	pubmed:36075173	Metabolomics reveals the effect of hypobaric treatment on energy metabolism in vibration-injured 'Huangguan' pears	Fangxu Xu Guode Li	Mechanical damage caused by vibration during transportation can destroy organization structure and reduce the fruit quality. The objective was to reveal the mechanism of hypobaric treatment on energy metabolism in vibration-injured 'Huangguan' pears based on metabolomics. Results showed that hypobaric treatment delayed the decline of adenosine triphosphate (ATP) content, energy charge (EC), H^(+)-ATPase and Ca^(2+)-ATPase activities comparing to untreated samples. Metabolomics data indicated	pmid:36075173 doi:10.1016/j.foodchem.2022.134057	Thu, 08 Sep 2022 06:00:00 -0400
2	pubmed:36075302	Overexpression of bacteriophage T4 and T7 endolysins differentially regulate the metabolic fingerprint of host Escherichia coli	Manikyaprabhu Kairamkonda Meenakshi Sharma Payal Gupta Krishna Mohan Poluri	Bioactive proteins are often overexpressed in different host systems for biotechnological/biomedical applications. Endolysins are natural bactericidal proteins that cleave the bacterial peptidoglycan membrane, and have the potential to be the next-generation enzybiotics. Therefore, the present study aims to elucidate the impact of two endolysins (T4L, T7L) overexpression on metabolic fingerprint of E. coli using NMR spectroscopy. The <sup>1</sup> H NMR-based metabolomics analysis revealed global metabolite	pmid:36075302 doi:10.1016/j.ijbiomac.2022.09.012	Thu, 08 Sep 2022 06:00:00 -0400
3	pubmed:36075303	Antibacterial mechanism of polysaccharides from the leaves of Lindera aggregata (Sims) Kosterm. by metabolomics based on HPLC/MS	Mingfeng Weng Shumin You Jiewei Luo Zhenyu Lin Ting Chen Xin Peng Bin Qiu	Lindera aggregata (Sims) Kosterm. is a traditional Chinese herb, which has been proven to have excellent antibacterial activity. In this work, we firstly extracted the polysaccharides from the leaves of Lindera aggregata (Sims) Kosterm. (LLPs), and explored their antibacterial activity and related mechanisms. The experimental results show that LLPs are a good antibacterial agent, which can damage the cell structure of bacteria and lead to the leakage of intracellular lysates. Compared with	pmid:36075303 doi:10.1016/j.ijbiomac.2022.09.009	Thu, 08 Sep 2022 06:00:00 -0400
4	pubmed:36075482	A screening test proposal for congenital defects based on maternal serum metabolomics profile	Jacopo Troisi Martina Lombardi Giovanni Scala Pierpaolo Cavallo Rennae S Tayler Steven J K Symes Sean M Richards David C Adair Alessio Fasano Lesley M McCowan Maurizio Guida	CONCLUSION: In conclusion, the present study provides a clinical validation of a metabolomics-based prenatal screening test to detect the presence of congenital defects. Further investigations are needed in order to enable the identification of the type of malformation as well as to confirm these findings on even larger study populations.	pmid:36075482 doi:10.1016/j.ajog.2022.08.050	Thu, 08 Sep 2022 06:00:00 -0400

	NCT Number	Title	Authors	Description	Identifier	Dates
5	pubmed:36075922	The emergence of psychoanalytical electrochemistry: the translation of MDD biomarker discovery to diagnosis with electrochemical sensing	Priyanka M Nadar Mckenna A Merrill Katherine Austin Stephen M Strakowski Jeffrey M Halpern	The disease burden and healthcare costs of psychiatric diseases along with the pursuit to understand their underlying biochemical mechanisms have led to psychiatric biomarker investigations. Current advances in evaluating candidate biomarkers for psychiatric diseases, such as major depressive disorder (MDD), focus on determining a specific biomarker signature or profile. The origins of candidate biomarkers are heterogenous, ranging from genomics, proteomics, and metabolomics, while incorporating	pmid:36075922 doi:10.1038/s41398-022-02138-y	Thu, 08 Sep 2022 06:00:00 -0400
6	pubmed:36075959	Metabolomic alterations in the blood plasma of older adults with mild cognitive impairment and Alzheimer's disease (from the Nakayama Study)	Tomoki Ozaki Yuta Yoshino Ayumi Tachibana Hideaki Shimizu Takaaki Mori Tomohiko Nakayama Kazuaki Mawatari Shusuke Numata Jun-Ichi Iga Akira Takahashi Tetsuro Ohmori Shu-Ichi Ueno	Alzheimer's disease (AD) is a progressive disease, and the number of AD patients is increasing every year as the population ages. One of the pathophysiological mechanisms of AD is thought to be the effect of metabolomic abnormalities. There have been several studies of metabolomic abnormalities of AD, and new biomarkers are being investigated. Metabolomic studies have been attracting attention, and the aim of this study was to identify metabolomic biomarkers associated with AD and mild cognitive	pmid:36075959 doi:10.1038/s41598-022-19670-y	Thu, 08 Sep 2022 06:00:00 -0400
7	pubmed:36075960	Paternal low protein diet perturbs intergenerational metabolic homeostasis in a tissue-specific manner in mice	Hannah L Morgan Samuel Furse Irundika H K Dias Kiran Shabir Marcos Castellanos Iqbal Khan Sean T May Nadine Holmes Matthew Carlile Fei Sang Victoria Wright Albert Koulman Adam J Watkins	The underlying mechanisms driving paternally-programmed metabolic disease in offspring remain poorly defined. We fed male C57BL/6 mice either a control normal protein diet (NPD; 18% protein) or an isocaloric low protein diet (LPD; 9% protein) for a minimum of 8 weeks. Using artificial insemination, in combination with vasectomised male mating, we generated offspring using either NPD or LPD sperm but in the presence of NPD or LPD seminal plasma. Offspring from either LPD sperm or seminal fluid	pmid:36075960 doi:10.1038/s42003-022-03914-8	Thu, 08 Sep 2022 06:00:00 -0400
8	pubmed:36076171	Unraveling metabolic patterns and molecular mechanisms underlying storability in sugar beet	Anna-Lena Gippert Silvia Madritsch Patrick Woryna Sandra Otte Martina Mayrhofer Herbert Eigner Adriana Garibay-Hernández John C D'Auria Eva M Molin Hans-Peter Mock	CONCLUSIONS: Our results indicate that increased levels of 15 free amino acids, pyroglutamic acid and two semi-polar compounds, including ferulic acid, were associated with a better storability of sugar beet taproots. Predictive metabolic patterns were already apparent at harvest. With respect to elongated storage, we highlighted the role of free amino acids in the taproot. Using complementary transcriptomic data, we could identify potential underlying mechanisms of sugar beet storability. These	pmid:36076171 doi:10.1186/s12870-022-03784-6	Thu, 08 Sep 2022 06:00:00 -0400
9	pubmed:36076172	Variation in morpho-physiological and metabolic responses to low nitrogen stress across the sorghum association panel	Marcin W Grzybowski Mackenzie Zwiener Hongyu Jin Nuwan K Wijewardane Abbas Atefi Michael J Naldrett Sophie Alvarez Yufeng Ge James C Schnable	CONCLUSION: Our results highlight that grain yield in sorghum, unlike many morphophysiological traits, exhibits substantial variability of genotype specific responses to long term low severity nitrogen deficit stress. Metabolic response to long term nitrogen stress shown higher proportion of variability explained by genotype specific responses than did morpho-pysiological traits and several metabolites were correlated with yield. This suggest, that it might be possible to build predictive	pmid:36076172 doi:10.1186/s12870-022-03823-2	Thu, 08 Sep 2022 06:00:00 -0400

	NCT Number	Title	Authors	Description	Identifier	Dates
10	pubmed:36076248	Drug dosing in children with obesity: a narrative updated review	Francesca Gaeta Valeria Conti Angela Pepe Pietro Vajro Amelia Filippelli Claudia Mandato	Childhood obesity and its associated comorbidities are highly prevalent diseases that may add to any other possible health problem commonly affecting the pediatric age. Uncertainties may arise concerning drug dosing when children with obesity need pharmacologic therapies. In general, in pediatric practice, there is a tendency to adapt drug doses to a child's total body weight. However, this method does not consider the pharmacological impact that a specific drug can have under a two-fold point	pmid:36076248 doi:10.1186/s13052-022-01361-z	Thu, 08 Sep 2022 06:00:00 -0400
11	pubmed:36076384	Integrated metabolomics and high-throughput sequencing to explore the dynamic correlations between flavor related metabolites and bacterial succession in the process of Mongolian cheese production	Xin Zhang Yuanrong Zheng Jing Feng Ran Zhou Ming Ma	Untargeted metabolomics was used to investigate the changes in small molecules of non-volatile metabolites and related mechanisms in the production process of Mongolian cheese. In addition, the changes in volatile compounds, free amino acids and bacterial community succession were also studied. A total of 37 differential metabolites were screened at 5 different stages of the production process by multivariate analysis of metabolomics datasets. The differential metabolites associated with amino	pmid:36076384 doi:10.1016/j.foodres.2022.111672	Fri, 09 Sep 2022 06:00:00 -0400
12	pubmed:36076393	The key metabolites associated with nutritional components in purple glutinous rice	Qiangqiang Xiong Jiao Zhang Qiang Shi Yanhong Zhang Changhui Sun Ao Li Wenjie Lu Jinlong Hu Nianbing Zhou Haiyan Wei Shuai Wang Hongcheng Zhang Jinyan Zhu	nutrients are closely related to consumer health. In this study, the contents of 22 amino acids in four glutinous rice varieties were quantified by LC-MS-targeted metabolomics, and the relationships between nutritional components and metabolites were analysed. The results demonstrated that gingerglycolipid B and pantothenic acid were significantly negatively correlated with Ala. The Lys and Cys-Cys contents of ZN18 and YZN were significantly higher than those of YCN and ZN20. Citric acid was	pmid:36076393 doi:10.1016/j.foodres.2022.111686	Fri, 09 Sep 2022 06:00:00 -0400
13	pubmed:36076417	Metabolite identification in fresh wheat grains of different colors and the influence of heat processing on metabolites via targeted and non-targeted metabolomics	Jianchao Feng Beiming Xu Dongyun Ma Zirui Hao Yuku Jia Chenyang Wang Lifang Wang	Phenolic antioxidants are phytochemical components in wheat grains that provide a variety of potential health benefits. The metabolites and antioxidant activity of fresh, mature, and heat-treated, wheat grains with black, blue, purple, and white grain coats were identified by targeted and non-targeted metabolomics. The total phenolic (TPC) and flavonoid contents (TFC) and antioxidant activity (AOA) increased with the darkening of grain color, the general trend being black > purple > blue >	pmid:36076417 doi:10.1016/j.foodres.2022.111728	Fri, 09 Sep 2022 06:00:00 -0400
14	pubmed:36076420	Noni (Morinda citrifolia L.) fruit phenolic extract supplementation ameliorates NAFLD by modulating insulin resistance, oxidative stress, inflammation, liver metabolism and gut microbiota	Ruimin Wang Lu Wang Haibo Wu Lin Zhang Xiaoping Hu Congfa Li Sixin Liu	The liver-protective activity of phenolics has been consistently reported, but the underlying protective mechanism of phenolic extract from noni fruit (NFE) against high-fatdiet (HFD)-induced nonalcoholic fatty liver disease (NAFLD) remains unclear. Mice were fed with HFD or combination of HFD and NFE for 10 weeks, and then the gut microbiota and liver metabolites were compared. In this study, NFE supplementation alleviated HFD-induced liver injury and metabolic comorbidities, as evidenced by	pmid:36076420 doi:10.1016/j.foodres.2022.111732	Fri, 09 Sep 2022 06:00:00 -0400

	NCT Number	Title	Authors	Description	Identifier	Dates
15	pubmed:36076430	Green tea extract alters gut microbiota and their metabolism of adults with metabolic syndrome in a host-free human colonic model	Shiqi Zhang Mengyang Xu Xiaowei Sun Haifei Shi Jiangjiang Zhu	CONCLUSIONS: Overall, our study revealed the impact of GTE treatment on gut microbiota composition and metabolism changes in MetS microbiota in vitro, which may provide information for further mechanistic investigation of GTE in modulating gut dysbiosis in MetS.	pmid:36076430 doi:10.1016/j.foodres.2022.111762	Fri, 09 Sep 2022 06:00:00 -0400
16	pubmed:36076438	Anti-inflammatory/anti-oxidant properties and the UPLC-QTOF/MS-based metabolomics discrimination of three yellow camellia species	Mingming Zhao Ke-Gang Linghu Linxuan Xiao Tianyi Hua Guanding Zhao Qiling Chen Shihang Xiong Liyu Shen Jinyu Yu Xiaotao Hou Erwei Hao Zhengcai Du Jiagang Deng Gang Bai Xiaojia Chen Ling Li Peng Li Hua Yu	The species of Camellia nitidissima Chi (CC) and C. euphlebia Merr. ex Sealy (CE) are two most important plant sources for commercialized herbal tea (Jinhuacha) worldwide. However, some other species of camellia genus are also sold as alternatives in market due to the great commercial value. In this study, the similarity and difference of CC and CE as well as C.insularis (CI) are comprehensively compared both in chemistry and pharmacology. Based on the ultraperformance liquid chromatography	pmid:36076438 doi:10.1016/j.foodres.2022.111628	Fri, 09 Sep 2022 06:00:00 -0400
17	pubmed:36076442	Interactions between polysaccharides and gut microbiota: A metabolomic and microbial review	Dandan Zhang Juan Liu Hao Cheng Hongliang Wang Yuzhu Tan Wuwen Feng Cheng Peng	In recent years, gut microbiota has become a hot topic because of its important role in health and diseases. Gut microbiota can produce a series of metabolites such as short chain fatty acids (SCFAs), secondary bile acids, tryptophan and indole derivatives. Over the past decade, a large number of studies have shown that oral polysaccharides can be transported to the colon and interact with gut microbiota. However, comprehensive summarization of the interactions between polysaccharides and gut	pmid:36076442 doi:10.1016/j.foodres.2022.111653	Fri, 09 Sep 2022 06:00:00 -0400
18	pubmed:36076459	Widely targeted metabolomic profiling combined with transcriptome analysis provides new insights into amino acid biosynthesis in green and red pepper fruits	Xitong Fei Haichao Hu Yingli Luo Qianqian Shi Anzhi Wei	The type and content of amino acids in pepper are important indicators to reflect its nutritional value, largely affecting the purchasing behavior of consumers.  Understanding the biosynthesis of amino acids in pepper fruit is beneficial to the development of pepper functional food.  Widely targeted metabolomics, transcriptome analysis, correlation analysis, weighted gene co-expression network analysis (WGCNA), and canonical correlation analysis (CCA) were used to evaluate the quality	pmid:36076459 doi:10.1016/j.foodres.2022.111718	Fri, 09 Sep 2022 06:00:00 -0400
19	pubmed:36076520	Blocking AMPK signalling to acetyl-CoA carboxylase increases cisplatin-induced acute kidney injury and suppresses the benefit of metformin	Geoff Harley Marina Katerelos Kurt Gleich David P de Souza Vinod K Narayana Bruce E Kemp David A Power Peter F Mount	BACKGROUND: Acute kidney injury (AKI) is accompanied by dysregulation of cellular energy metabolism and accumulation of intracellular lipid. Phosphorylation of acetyl-CoA carboxylase (ACC) by AMP-activated protein kinase (AMPK) inhibits fatty acid synthesis and promotes fatty acid oxidation (FAO), vital for kidney tubular epithelial cells (TECs). The diabetes drug metformin is protective in models of AKI; however, it is not known whether ACC phosphorylation plays a role.	pmid:36076520 doi:10.1016/j.biopha.2022.113377	Fri, 09 Sep 2022 06:00:00 -0400

	NCT Number	Title	Authors	Description	Identifier	Dates
20	pubmed:36076540	The mechanism of formononetin/calycosin compound optimizing the effects of temozolomide on C6 malignant glioma based on metabolomics and network pharmacology	Songya Li Jiayi Li Yani Fan Tao Huang Yanfen Zhou Hongwei Fan Qi Zhang Runze Qiu	The complex of formononetin and calycosin (FMN/CAL) shows a synergistic effect on temozolomide in the treatment of malignant glioma, however the mechanism is unclear. We investigated the mechanism through means of metabolomics, network pharmacology and molecular biology. FMN/CAL enhanced the inhibition of TMZ on the growth and infiltration of C6 glioma. The metabolomic results showed that the TMZ sensitization of FMN/CAL mainly involved 5 metabolic pathways and 4 metabolites in cells, 1	pmid:36076540 doi:10.1016/j.biopha.2022.113418	Fri, 09 Sep 2022 06:00:00 -0400
21	pubmed:36076543	Inhaled volatile -caryophyllene is incorporated into the aortic wall and attenuates nicotine-induced aorta degeneration via a CB2 receptor-dependent pathway	Chihiro Kishi Mayo Higashihara Yuki Takemoto Moeka Kamei Yuri Yoshioka Shinichi Matsumura Kazuya Yamada Takanori Kobayashi Yoshiharu Matahira Tatsuya Moriyama Nobuhiro Zaima	-caryophyllene (BCP) is a volatile bicyclic sesquiterpenoid found in essential oils obtained from several spices such as black pepper, oregano, basil, rosemary, cinnamon, and clove. BCP is a selective agonist of cannabinoid receptor 2 (CB2 receptor), and orally administered BCP exhibits various biological activities, including anti-inflammatory, antioxidant, and neuroprotective effects. However, it is still unclear how volatile BCP affects living organisms. We previously reported that inhaled	pmid:36076543 doi:10.1016/j.biopha.2022.113423	Fri, 09 Sep 2022 06:00:00 -0400
22	pubmed:36076557	Egg white protein hydrolysate ameliorated sepsis-induced inflammatory injuries in kidney and liver based on metabolomics analysis	Gao Huan Yang Tao Wang Yu Zhai Jinghui Zhang Yueming Song Yanqing	Sepsis caused by infection could induce systemic inflammation and various organ damages. Bioactivities of peptides derived from eggs were proved by lots of researchers; hence they might be further developed for therapeutic use. In this study, the hydrolysate named "PEP" was obtained by enzymatic hydrolysis and purification. Rats were divided into control, LPS, PEP1 and PEP2 groups. The rat model was established using lipopolysaccharide (LPS) at 10 mg/kg by intraperitoneal injection. The results	pmid:36076557 doi:10.1016/j.biopha.2022.113442	Fri, 09 Sep 2022 06:00:00 -0400
23	pubmed:36076827	Impact of Feeding Probiotics on Blood Parameters, Tail Fat Metabolites, and Volatile Flavor Components of Sunit Sheep	Ting Liu Taiwu Zhang Yanni Zhang Le Yang Yan Duan Lin Su Jianjun Tian Lina Sun Bohui Wang Ye Jin	Sheep crude tail fat has unique nutritional values and is used as a raw material for high-quality natural oil. The purpose of this study was to investigate the effects of probiotics on the metabolites and flavor of sheep crude tail fat. In this study, 12 Sunit sheep were randomly divided into an experimental group (LTF, basal feed + Lactiplantibacillusplantarum powder) and a control group (CTF, basal feed). The results of sheep crude tail fat analysis showed that blood lipid parameters were	pmid:36076827 doi:10.3390/foods11172644	Fri, 09 Sep 2022 06:00:00 -0400
24	pubmed:36076885	Effects of Auricularia auricula Polysaccharides on Gut Microbiota and Metabolic Phenotype in Mice	Qian Liu Xin An Yuan Chen Yuxuan Deng Haili Niu Ruisen Ma Haoan Zhao Wei Cao Xiaoru Wang Meng Wang	Personalized diets change the internal metabolism of organisms, which, in turn, affects the health of the body; this study was performed to explore the regulatory effects of polysaccharides extracted from Auricularia auricula on the overall metabolism and gut microbiota in normal C57BL/6J mice. The study was conducted using metabolomic and microbiomic methods to provide a scientific basis for further development and use of Auricularia auricula resources in the Qinba Mountains and in nutritional	pmid:36076885 doi:10.3390/foods11172700	Fri, 09 Sep 2022 06:00:00 -0400

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25	pubmed:36076892	NMR-Based Metabolomics to Decipher the Molecular Mechanisms in the Action of Gut- Modulating Foods	Weiwei He Hanne Christine Bertram	Metabolomics deals with uncovering and characterizing metabolites present in a biological system, and is a leading omics discipline as it provides the nearest link to the biological phenotype. Within food and nutrition, metabolomics applied to fecal samples and bio-fluids has become an important tool to obtain insight into how food and food components may exert gutmodulating effects. This review aims to highlight how nuclear magnetic resonance (NMR)-based metabolomics in food and nutrition	pmid:36076892 doi:10.3390/foods11172707	Fri, 09 Sep 2022 06:00:00 -0400
26	pubmed:36076949	Comparative Transcriptomic and Metabolic Analyses Reveal the Coordinated Mechanisms in <i>Pinus koraiensis</i> under Different Light Stress Conditions	Yuxi Li Xinxin Zhang Kewei Cai Qinhui Zhang Luping Jiang Hanxi Li Yuzhe Lv Guanzheng Qu Xiyang Zhao	Light is one of the most important environmental cues that affects plant development and regulates its behavior. Light stress directly inhibits physiological responses and plant tissue development and even induces mortality in plants. Korean pine (Pinus koraiensis) is an evergreen conifer species widely planted in northeast China that has important economic and ecological value. However, the effects of light stress on the growth and development of Korean pine are still unclear. In this study,	pmid:36076949 doi:10.3390/ijms23179556	Fri, 09 Sep 2022 06:00:00 -0400
27	pubmed:36076993	Transcriptome and Metabolome Analyses Revealed the Response Mechanism of Sugar Beet to Salt Stress of Different Durations	Jie Cui Junliang Li Cuihong Dai Liping Li	Salinity is one of the most serious threats to agriculture worldwide. Sugar beet is an important sugar-yielding crop and has a certain tolerance to salt; however, the genome-wide dynamic response to salt stress remains largely unknown in sugar beet. In the present study, physiological and transcriptome analyses of sugar beet leaves and roots were compared under salt stress at five time points. The results showed that different salt stresses influenced phenotypic characteristics, leaf relative	pmid:36076993 doi:10.3390/ijms23179599	Fri, 09 Sep 2022 06:00:00 -0400
28	pubmed:36077057	Gut Microbiome and Metabolome Modulation by Maternal High-Fat Diet and Thermogenic Challenge	Henry A Paz Anna-Claire Pilkington Ying Zhong Sree V Chintapalli James Sikes Renny S Lan Kartik Shankar Umesh D Wankhade	The gut microbiota plays a critical role in energy homeostasis and its dysbiosis is associated with obesity. Maternal high-fat diet (HFD) and -adrenergic stimuli alter the gut microbiota independently; however, their collective regulation is not clear. To investigate the combined effect of these factors on offspring microbiota, 20-week-old offspring from control diet (17% fat)- or HFD (45% fat)-fed dams received an injection of either vehicle or 3-adrenergic agonist CL316,243 (CL) for 7 days	pmid:36077057 doi:10.3390/ijms23179658	Fri, 09 Sep 2022 06:00:00 -0400
29	pubmed:36077135	Integrated Analysis of Transcriptome and Metabolome Reveals the Regulation of Chitooligosaccharide on Drought Tolerance in Sugarcane (Saccharum spp. Hybrid) under Drought Stress	Shan Yang Na Chu Hongkai Zhou Jiashuo Li Naijie Feng Junbo Su Zuhu Deng Xuefeng Shen Dianfeng Zheng	Sugarcane (Saccharum spp. hybrid) is an important crop for sugar and biofuels, and often suffers from water shortages during growth. Currently, there is limited knowledge concerning the molecular mechanism involved in sugarcane response to drought stress (DS) and whether chitooligosaccharide could alleviate DS. Here, we carried out a combined transcriptome and metabolome of sugarcane in three different treatment groups: control group (CG), DS group, and DS + chitooligosaccharide group (COS). A	pmid:36077135 doi:10.3390/ijms23179737	Fri, 09 Sep 2022 06:00:00 -0400

	NCT Number	Title	Authors	Description	Identifier	Dates
30	pubmed:36077145	The Diurnal Blood Metabolome and Effects of Vitamin D Supplementation: A Randomised Crossover Trial in Postmenopausal Women	Rasmus Espersen Banny Silva Barbosa Correia Lars Rejnmark Hanne Christine Bertram	A way to maintain an adequate vitamin D status is through supplementation. Demonstration of blood-metabolome rhythmicity of vitamin D(3) post-dosing effects is lacking in the pharmacometabonomics area. Thus, the overall aim of this study was to investigate the diurnal changes in the blood metabolome and how these are affected by vitamin D(3) supplementation. The study was conducted as a crossover study, and the treatment included 200 µg (8000 IU) of vitamin D(3) as compared with placebo with a	pmid:36077145 doi:10.3390/ijms23179748	Fri, 09 Sep 2022 06:00:00 -0400
31	pubmed:36077177	Blood Levels of Endocannabinoids, Oxylipins, and Metabolites Are Altered in Hemodialysis Patients	Bruce A Watkins Allon N Friedman Jeffrey Kim Kamil Borkowski Shaun Kaiser Oliver Fiehn John W Newman	Hemodialysis patients (HDPs) have higher blood pressure, higher levels of inflammation, a higher risk of cardiovascular disease, and unusually low plasma n-3 polyunsaturated fatty acid (PUFA) levels compared to healthy subjects. The objective of our investigation was to examine the levels of endocannabinoids (eCBs) and oxylipins (OxLs) in female HDPs compared to healthy matched female controls, with the underlying hypothesis that differences in specific PUFA levels in hemodialysis patients would	pmid:36077177 doi:10.3390/ijms23179781	Fri, 09 Sep 2022 06:00:00 -0400
32	pubmed:36077200	Bioenergetic and Metabolic Impairments in Induced Pluripotent Stem Cell-Derived Cardiomyocytes Generated from Duchenne Muscular Dystrophy Patients	Lubna Willi Ifat Abramovich Jonatan Fernandez-Garcia Bella Agranovich Margarita Shulman Helena Milman Polina Baskin Binyamin Eisen Daniel E Michele Michael Arad Ofer Binah Eyal Gottlieb	Duchenne muscular dystrophy (DMD) is caused by mutations in the dystrophin gene and dilated cardiomyopathy (DCM) is a major cause of morbidity and mortality in DMD patients. We tested the hypothesis that DCM is caused by metabolic impairments by employing induced pluripotent stem cell-derived cardiomyocytes (iPSC-CMs) generated from four DMD patients; an adult male, an adult female, a 7-year-old (7y) male and a 13-year-old (13y) male, all compared to two healthy volunteers. To test the	pmid:36077200 doi:10.3390/ijms23179808	Fri, 09 Sep 2022 06:00:00 -0400
33	pubmed:36077214	Dysregulated Metabolic Pathways in Subjects with Obesity and Metabolic Syndrome	Fayaz Ahmad Mir Ehsan Ullah Raghvendra Mall Ahmad Iskandarani Tareq A Samra Farhan Cyprian Aijaz Parray Meis Alkasem Ibrahem Abdalhakam Faisal Farooq Abdul-Badi Abou-Samra	CONCLUSIONS: Metabolites and pathways associated with chronic inflammation are differentially expressed in subjects with obesity and metabolic syndrome compared to subjects with obesity but without the clinical features of metabolic syndrome.	pmid:36077214 doi:10.3390/ijms23179821	Fri, 09 Sep 2022 06:00:00 -0400
34	pubmed:36077267	Ionomic Combined with Transcriptomic and Metabolomic Analyses to Explore the Mechanism Underlying the Effect of Melatonin in Relieving Nutrient Stress in Apple	Yang Cao Peihua Du Jiahao Ji Xiaolong He Jiran Zhang Yuwei Shang Huaite Liu Jizhong Xu Bowen Liang	Nutrient stress harms plant growth and yield. Melatonin is a biologically active, multifunctional hormone that relieves abiotic stress in plants. Although previous studies have shown that melatonin plays an important role in improving nutrient-use efficiency, the mechanism of its regulation of nutrient stress remains unclear. In this study, melatonin was applied to apple plants under nutrient stress, and morphological indices, physiological and biochemical indices, and stomatal morphology were	pmid:36077267 doi:10.3390/ijms23179855	Fri, 09 Sep 2022 06:00:00 -0400

	NCT Number	Title	Authors	Description	Identifier	Dates
35	pubmed:36077288	A Novel Pathway of Chlorimuron-Ethyl Biodegradation by Chenggangzhangella methanolivorans Strain CHL1 and Its Molecular Mechanisms	Zhixiong Yu Yumeng Dai Tingting Li Wu Gu Yi Yang Xiang Li Pai Peng Lijie Yang Xinyu Li Jian Wang Zhencheng Su Xu Li Mingkai Xu Huiwen Zhang	Chlorimuron-ethyl is a widely used herbicide in agriculture. However, uncontrolled chlorimuron-ethyl application causes serious environmental problems. Chlorimuron-ethyl can be effectively degraded by microbes, but the underlying molecular mechanisms are not fully understood. In this study, we identified the possible pathways and key genes involved in chlorimuron-ethyl degradation by the Chenggangzhangella methanolivorans strain CHL1, a Methylocystaceae strain with the ability to degrade	pmid:36077288 doi:10.3390/ijms23179890	Fri, 09 Sep 2022 06:00:00 -0400
36	pubmed:36077297	Sunitinib versus Pazopanib Dilemma in Renal Cell Carcinoma: New Insights into the In Vitro Metabolic Impact, Efficacy, and Safety	Filipa Amaro Carolina Pisoeiro Maria João Valente Maria de Lourdes Bastos Paula Guedes de Pinho Márcia Carvalho Joana Pinto	Sunitinib and pazopanib are tyrosine kinase inhibitors (TKIs) used as first-line therapy for metastatic renal cell carcinoma (RCC). Although these TKIs are associated with similar survival outcomes, some differences have been reported in their safety profiles. In this work, traditional toxicological endpoints (cell viability and growth, oxidative stress, and nuclear morphology) and <sup>1</sup> H NMR spectroscopy-based metabolomics analysis were used to provide new insights into the cytotoxicity and	pmid:36077297 doi:10.3390/ijms23179898	Fri, 09 Sep 2022 06:00:00 -0400
37	pubmed:36077322	Peppers in Diet: Genome-Wide Transcriptome and Metabolome Changes in Drosophila melanogaster	Carlos Lopez-Ortiz Mary Edwards Purushothaman Natarajan Armando Pacheco-Valenciana Padma Nimmakayala Donald A Adjeroh Cristian Sirbu Umesh K Reddy	The habanero pepper (Capsicum chinense) is an increasingly important spice and vegetable crop worldwide because of its high capsaicin content and pungent flavor. Diets supplemented with the phytochemicals found in habanero peppers might cause shifts in an organism's metabolism and gene expression. Thus, understanding how these interactions occur can reveal the potential health effects associated with such changes. We performed transcriptomic and metabolomic analyses of Drosophila melanogaster	pmid:36077322 doi:10.3390/ijms23179924	Fri, 09 Sep 2022 06:00:00 -0400
38	pubmed:36077370	Multiomics Molecular Research into the Recalcitrant and Orphan Quercus ilex Tree Species: Why, What for, and How	Ana María Maldonado-Alconada María Ángeles Castillejo María-Dolores Rey Mónica Labella-Ortega Marta Tienda-Parrilla Tamara Hernández-Lao Irene Honrubia-Gómez Javier Ramírez-García Víctor M Guerrero-Sanchez Cristina López-Hidalgo Luis Valledor Rafael M Navarro-Cerrillo Jesús V Jorrin-Novo	The holm oak (Quercus ilex L.) is the dominant tree species of the Mediterranean forest and the Spanish agrosilvopastoral ecosystem, "dehesa." It has been, since the prehistoric period, an important part of the Iberian population from a social, cultural, and religious point of view, providing an ample variety of goods and services, and forming the basis of the economy in rural areas. Currently, there is renewed interest in its use for dietary diversification and sustainable food production. It	pmid:36077370 doi:10.3390/ijms23179980	Fri, 09 Sep 2022 06:00:00 -0400
39	pubmed:36077436	Precision Medicine: Determination of Ribavirin Urinary Metabolites in Relation to Drug Adverse Effects in HCV Patients	Ottavia Giampaoli Fabio Sciubba Elisa Biliotti Mariangela Spagnoli Riccardo Calvani Alberta Tomassini Giorgio Capuani Alfredo Miccheli Gloria Taliani	The most commonly used antiviral treatment against hepatitis C virus is a combination of direct-acting antivirals (DAAs) and ribavirin (RBV), which leads to a shortened duration of therapy and a sustained virologic response until 98%. Nonetheless, several dose-related side effects of RBV could limit its applications. This study aims to measure the urinary concentration of RBV and its main metabolites in order to evaluate the drug metabolism ability of HCV patients and to evaluate the adverse	pmid:36077436 doi:10.3390/ijms231710043	Fri, 09 Sep 2022 06:00:00 -0400

	NCT Number	Title	Authors	Description	Identifier	Dates
40	pubmed:36077519	Integrated Analysis of Transcriptome and Metabolome Reveals Distinct Responses of Pelteobagrus fulvidraco against Aeromonas veronii Infection at Invaded and Recovering Stage	Xianhui Ning Ye Peng Peng Tang Yiran Zhang Lingling Wang Wenwen Zhang Kai Zhang Jie Ji Shaowu Yin	Yellow catfish (Pelteobagrus fulvidraco) is an important aquaculture fish susceptible to Aeromonas veronii infection, which causes acute death resulting in huge economic losses. Understanding the molecular processes of host immune defense is indispensable to disease control. Here, we conducted the integrated and comparative analyses of the transcriptome and metabolome of yellow catfish in response to A. veronii infection at the invaded stage and recovering stage. The crosstalk between A	pmid:36077519 doi:10.3390/ijms231710121	Fri, 09 Sep 2022 06:00:00 -0400
41	pubmed:36077538	Comparative Metabolome and Transcriptome Analysis of Anthocyanin Biosynthesis in White and Pink Petals of Cotton (Gossypium hirsutum L.)	Dongnan Shao Qian Liang Xuefeng Wang Qian-Hao Zhu Feng Liu Yanjun Li Xinyu Zhang Yonglin Yang Jie Sun Fei Xue	Upland cotton (Gossypium hirsutum L.) is one of the important fiber crops. Cotton flowers usually appear white (or creamcolored) without colored spots at the petal base, and turn pink on the next day after flowering. In this study, using a mutant showing pink petals with crimson spots at their base, we conducted comparative metabolome and transcriptome analyses to investigate the molecular mechanism of coloration in cotton flowers. Metabolic profiling showed that cyanidin-3-O-glucoside and	pmid:36077538 doi:10.3390/ijms231710137	Fri, 09 Sep 2022 06:00:00 -0400
42	pubmed:36077553	Identification of Potential Biomarkers and Metabolic Pathways of Different Levels of Heat Stress in Beef Calves	Won-Seob Kim Jongkyoo Kim Hong-Gu Lee	Heat stress (HS) damages the global beef industry by reducing growth performance causing high economic losses each year. However, understanding the physiological mechanisms of HS in Hanwoo calves remains elusive. The objective of this study was to identify the potential biomarkers and metabolic pathways involving different levels of heat stress in Hanwoo calves. Data were collected from sixteen Hanwoo bull calves (169.6 $\pm$ 4.6 days old, BW of 136.9 $\pm$ 6.2 kg), which were maintained at four	pmid:36077553 doi:10.3390/ijms231710155	Fri, 09 Sep 2022 06:00:00 -0400
43	pubmed:36077598	Proteomics Profiling of Osteoporosis and Osteopenia Patients and Associated Network Analysis	Mysoon M Al-Ansari Shereen M Aleidi Afshan Masood Eman A Alnehmi Mai Abdel Jabar Maha Almogren Mohammed Alshaker Hicham Benabdelkamel Anas M Abdel Rahman	Bone mass reduction due to an imbalance in osteogenesis and osteolysis is characterized by low bone mineral density (LBMD) and is clinically classified as osteopenia (ON) or osteoporosis (OP), which is more severe. Multiple biomarkers for diagnosing OP and its progression have been reported; however, most of these lack specificity. This cohort study aimed to investigate sensitive and specific LBMD-associated protein biomarkers in patients diagnosed with ON and OP. A label-free liquid	pmid:36077598 doi:10.3390/ijms231710200	Fri, 09 Sep 2022 06:00:00 -0400
44	pubmed:36077608	Characterization of the Metabolome of Breast Tissues from Non-Hispanic Black and Non-Hispanic White Women Reveals Correlations between Microbial Dysbiosis and Enhanced Lipid Metabolism Pathways in Triple-Negative Breast Tumors	Alana Smith Xueyuan Cao Qingqing Gu Ernestine Kubi Amos-Abanyie Elizabeth A Tolley Gregory Vidal Beverly Lyn-Cook Athena Starlard-Davenport	Triple-negative breast cancer (TNBC) is an aggressive form of breast cancer that is non-responsive to hormonal therapies and disproportionately impact women of African ancestry. We previously showed that TN breast tumors have a distinct microbial signature that differs from less aggressive breast tumor subtypes and normal breast tissues. However, it is unknown whether these differences in breast tumor microbiota may be driven by alterations in microbial metabolites, leading to potentially	pmid:36077608 doi:10.3390/cancers14174075	Fri, 09 Sep 2022 06:00:00 -0400

	NCT Number	Title	Authors	Description	Identifier	Dates
45	pubmed:36077725	Intestinal Klebsiella pneumoniae Contributes to Pneumonia by Synthesizing Glutamine in Multiple Myeloma	Yihui Wang Qin Yang Yinghong Zhu Xingxing Jian Jiaojiao Guo Jingyu Zhang Chunmei Kuang Xiangling Feng Gang An Lugui Qiu Guancheng Li Yanjuan He Wen Zhou	Pneumonia accounts for a significant cause of morbidity and mortality in multiple myeloma (MM) patients. It has been previously shown that intestinal Klebsiella pneumonia (K. pneumonia) enriches in MM and promotes MM progression. However, what role the altered gut microbiota plays in MM with pneumonia remains unknown. Here, we show that intestinal K. pneumonia is significantly enriched in MM with pneumonia. This enriched intestinal K. pneumonia links to the incidence of pneumonia in MM, and	pmid:36077725 doi:10.3390/cancers14174188	Fri, 09 Sep 2022 06:00:00 -0400
46	pubmed:36077791	An FDA-Approved Antifungal, Ketoconazole, and Its Novel Derivative Suppress tGLI1-Mediated Breast Cancer Brain Metastasis by Inhibiting the DNA- Binding Activity of Brain Metastasis- Promoting Transcription Factor tGLI1	Daniel Doheny Sara Manore Sherona R Sirkisoon Dongqin Zhu Noah R Aguayo Alexandria Harrison Mariana Najjar Marlyn Anguelov Anderson O'Brien Cox Cristina M Furdui Kounosuke Watabe Thomas Hollis Alexandra Thomas Roy Strowd Hui-Wen Lo	The goal of this study is to identify pharmacological inhibitors that target a recently identified novel mediator of breast cancer brain metastasis (BCBM), truncated glioma-associated oncogene homolog 1 (tGLI1). Inhibitors of tGLI1 are not yet available. To identify compounds that selectively kill tGLI1-expressing breast cancer, we screened 1527 compounds using two sets of isogenic breast cancer and braintropic breast cancer cell lines engineered to stably express the control, GLI1, or tGLI1	pmid:36077791 doi:10.3390/cancers14174256	Fri, 09 Sep 2022 06:00:00 -0400
47	pubmed:36077913	The Future of Biomarkers in Veterinary Medicine: Emerging Approaches and Associated Challenges	Tharangani R W Perera David A Skerrett-Byrne Zamira Gibb Brett Nixon Aleona Swegen	New biomarkers promise to transform veterinary practice through rapid diagnosis of diseases, effective monitoring of animal health and improved welfare and production efficiency. However, the road from biomarker discovery to translation is not always straightforward. This review focuses on molecular biomarkers under development in the veterinary field, introduces the emerging technological approaches transforming this space and the role of 'omics platforms in novel biomarker discovery. The vast	pmid:36077913 doi:10.3390/ani12172194	Fri, 09 Sep 2022 06:00:00 -0400
48	pubmed:36077948	Effect of Chinese Herbs on Serum Biochemical Parameters, Immunity Indices, Antioxidant Capacity and Metabolomics in Early Weaned Yak Calves	Cuixia Jiang Quanmin Dong Xiaoping Xin Abraham Allan Degen Luming Ding	Chinese traditional herbs are used widely as feed supplements to improve the immune response and antioxidant capacity of livestock. Twenty early-weaned 4-month-old yak calves (72.3 ± 3.65 kg) were divided randomly into four groups (n = 5 per group); three groups were provided with supplementary 80 mL/kg DMI of the root water extracts of either Angelica sinensis, Codonopsis pilosula or Glycyrrhiza uralensis, and one group (control) was not provided with a supplement. Compared to control calves,	pmid:36077948 doi:10.3390/ani12172228	Fri, 09 Sep 2022 06:00:00 -0400

	NCT Number	Title	Authors	Description	Identifier	Dates
49	pubmed:36077963	Using Untargeted LC-MS Metabolomics to Identify the Association of Biomarkers in Cattle Feces with Marbling Standard Longissimus Lumborum	Dong Chen Minchao Su He Zhu Gang Zhong Xiaoyan Wang Weimin Ma Metha Wanapat Zhiliang Tan	CONCLUSIONS: In conclusion, this study supports new opinions for the successive evaluation of marbling beef through metabolites. Furthermore, six non-invasive fecal metabolites that can evaluate beef marbling grade were found, including SM(d18:0/16:1(9Z)), PC(15:0/18:2(9Z,12Z)), ADP, PC(16:0/16:0), and 3-O-Sulfogalactosylceramide.	pmid:36077963 doi:10.3390/ani12172243	Fri, 09 Sep 2022 06:00:00 -0400
50	pubmed:36078127	Omics Analysis of Chemoresistant Triple Negative Breast Cancer Cells Reveals Novel Metabolic Vulnerabilities	Dimitris Kordias Christina E Kostara Styliani Papadaki John Verigos Eleni Bairaktari Angeliki Magklara	The emergence of drug resistance in cancer poses the greatest hurdle for successful therapeutic results and is associated with most cancer deaths. In triple negative breast cancer (TNBC), due to the lack of specific therapeutic targets, systemic chemotherapy is at the forefront of treatments, but it only benefits a fraction of patients because of the development of resistance. Cancer cells may possess an innate resistance to chemotherapeutic agents or develop new mechanisms of acquired	pmid:36078127 doi:10.3390/cells11172719	Fri, 09 Sep 2022 06:00:00 -0400
51	pubmed:36079081	(R)Evolution in Allergic Rhinitis Add-On Therapy: From Probiotics to Postbiotics and Parabiotics	Martina Capponi Alessandra Gori Giovanna De Castro Giorgio Ciprandi Caterina Anania Giulia Brindisi Mariangela Tosca Bianca Laura Cinicola Alessandra Salvatori Lorenzo Loffredo Alberto Spalice Anna Maria Zicari	Starting from the "Hygiene Hypothesis" to the "Microflora hypothesis" we provided an overview of the symbiotic and dynamic equilibrium between microbiota and the immune system, focusing on the role of dysbiosis in atopic march, particularly on allergic rhinitis. The advent of deep sequencing technologies and metabolomics allowed us to better characterize the microbiota diversity between individuals and body sites. Each body site, with its own specific environmental niches, shapes the microbiota	pmid:36079081 doi:10.3390/jcm11175154	Fri, 09 Sep 2022 06:00:00 -0400
52	pubmed:36079611	Integrated Analysis of Transcriptome and Metabolome Reveals New Insights into the Formation of Purple Leaf Veins and Leaf Edge Cracks in Brassica juncea	Kaijing Zhang Dekun Yang Yuchao Hu Martin Kagiki Njogu Jingjing Qian Li Jia Congsheng Yan Ziang Li Xing Wang Liping Wang	Purple leaf veins and leaf edge cracks comprise the typical leaf phenotype of Brassica juncea; however, the molecular mechanisms and metabolic pathways of the formation of purple leaf veins and leaf edge cracks remain unclear. In this study, transcriptome and metabolome analyses were conducted to explore the regulation pathway of purple leaf vein and leaf edge crack formation based on four mustard samples that showed different leaf colors and degrees of cracking. The results showed genes with	pmid:36079611 doi:10.3390/plants11172229	Fri, 09 Sep 2022 06:00:00 -0400
53	pubmed:36079691	Marrubium alysson L. Ameliorated Methotrexate-Induced Testicular Damage in Mice through Regulation of Apoptosis and miRNA-29a Expression: LC-MS/MS Metabolic Profiling	Reda F A Abdelhameed Asmaa I Ali Sameh S Elhady Hend E Abo Mansour Eman T Mehanna Sarah M Mosaad Salma A Ibrahim Rawan H Hareeri Jihan M Badr Nermeen A Eltahawy	Despite the efficient anti-cancer capabilities of methotrexate (MTX), it may induce myelosuppression, liver dysfunction and testicular toxicity. The purpose of this investigation was to determine whether Marrubium alysson L. (M. alysson L.) methanolic extract and its polyphenol fraction could protect mouse testicles from MTX-induced damage. We also investigated the protective effects of three selected pure flavonoid components of M. alysson L. extract. Mice were divided into seven groups (n =	pmid:36079691 doi:10.3390/plants11172309	Fri, 09 Sep 2022 06:00:00 -0400

	NCT Number	Title	Authors	Description	Identifier	Dates
54	pubmed:36079724	Gut Microbiota Dysbiosis after Traumatic Brain Injury Contributes to Persistent Microglial Activation Associated with Upregulated Lyz2 and Shifted Tryptophan Metabolic Phenotype	Zhipeng Zheng Shuai Wang Chenghao Wu Yang Cao Qiao Gu Ying Zhu Wei Zhang Wei Hu	Traumatic brain injury (TBI) is a common cause of disability and mortality, affecting millions of people every year. The neuroinflammation and immune response post-TBI initially have neuroprotective and reparative effects, but prolonged neuroinflammation leads to secondary injury and increases the risk of chronic neurodegenerative diseases. Persistent microglial activation plays a critical role in chronic neuroinflammation post-TBI. Given the bidirectional communication along the brain-gut axis,	pmid:36079724 doi:10.3390/nu14173467	Fri, 09 Sep 2022 06:00:00 -0400
55	pubmed:36079725	Metabologenomic Approach Reveals Intestinal Environmental Features Associated with Barley-Induced Glucose Tolerance Improvements in Japanese: A Randomized Controlled Trial	Yuka Goto Yuichiro Nishimoto Shinnosuke Murakami Tatsuhiro Nomaguchi Yuka Mori Masaki Ito Ryohei Nakaguro Toru Kudo Tsubasa Matsuoka Takuji Yamada Toshiki Kobayashi Shinji Fukuda	(1) Background: Consumption of barley has been known to exert beneficial effects on glucose tolerance; however, it has also been reported that there are inter-individual differences in these responses. Recent evidence has suggested that these individual differences are mediated by the gut microbiota. (2) Methods: In the present study, we aimed to understand the relationship between the intestinal environment, including intestinal microbiome and their metabolome, and glucose tolerance. A	pmid:36079725 doi:10.3390/nu14173468	Fri, 09 Sep 2022 06:00:00 -0400
56	pubmed:36079746	Impact of Clarified Apple Juices with Different Processing Methods on Gut Microbiota and Metabolomics of Rats	Lei Xu Shini Yang Kewen Wang Anjing Lu Xue Wang Zhenzhen Xu	The consumption of processed foods has increased compared to that of fresh foods in recent years, especially due to the coronavirus disease 2019 pandemic. Here, we evaluated the health effects of clarified apple juices (CAJs, devoid of pectin and additives) processed to different degrees, including not-from-concentrate (NFC) and from-concentrate (FC) CAJs. A 56-day experiment including a juice-switch after 28 days was designed. An integrated analysis of 16S rRNA sequencing and untargeted	pmid:36079746 doi:10.3390/nu14173488	Fri, 09 Sep 2022 06:00:00 -0400
57	pubmed:36079758	Early and Long-Term Effects of Abdominal Fat Reduction Using Ultrasound and Radiofrequency Treatments	Magdalena Kiedrowicz Ewa Duchnik Jolanta Wesoowska Beata Bania Magorzata Peregud-Pogorzelska Dominika Maciejewska-Markiewicz Ewa Stachowska Joanna Kruk Mariola Marchlewicz	BACKGROUND: Abdominal obesity, together with atherogenic dyslipidemia, increased blood pressure and impaired glucose tolerance, was included in the components of metabolic syndrome identifying patients at high risk of cardiovascular diseases. Subcutaneous adipose tissue is a buffer for dietary fatty acids (FAs). It was reported that the fatty acid composition of adipose tissue reflects the dietary intake of FAs in the previous 6 to 9 months. Therefore, we decided to evaluate the early and	pmid:36079758 doi:10.3390/nu14173498	Fri, 09 Sep 2022 06:00:00 -0400
58	pubmed:36079872	Mediterranean Diet and Atrial Fibrillation: Lessons Learned from the AFHRI Case- Control Study	Felix Alexander Neumann Bettina Jagemann Nataliya Makarova Christin Susanna Börschel Ghazal Aarabi Friederike Gutmann Renate B Schnabel Birgit-Christiane Zyriax	A relationship between lifestyle, diet, and atrial fibrillation (AF) remains unclear. Except for alcohol consumption, AF guidelines do not differentiate specific advice for this rhythm disorder. The aim of this study was to investigate the association between adherence to healthy dietary patterns and the presence of AF, among 104 low risk participants from the 1:1 matched casecontrol AFHRI (Atrial Fibrillation in High-Risk Individuals) study. Dietary data were obtained using a three-day food	pmid:36079872 doi:10.3390/nu14173615	Fri, 09 Sep 2022 06:00:00 -0400

	NCT Number	Title	Authors	Description	Identifier	Dates
59	pubmed:36079890	Reconfiguration of Gut Microbiota and Reprogramming of Liver Metabolism with Phycobiliproteins Bioactive Peptides to Rehabilitate Obese Rats	Jing Liu Dongyu Zhen Changbao Hu Yawen Liu Xuanri Shen Pengcheng Fu Yanfu He	Phycobiliproteins (derived from Arthrospira platensis) bioactive peptide extracts (PPE) possess multiple pharmacological effects in the mitigation of human metabolic disorders. The role of PPE in the treatment of dietinduced obesity and the understanding of the underlying mechanism between the gut microbiome and metabolic blood circulation for obese patients remains poorly understood. In this study, we showed that PPE attenuated obesity by reducing body weight, and ameliorated glucose and lipid	pmid:36079890 doi:10.3390/nu14173635	Fri, 09 Sep 2022 06:00:00 -0400
60	pubmed:36080249	Metabolomic Analysis and MRM Verification of Coarse and Fine Skin Tissues of Liaoning Cashmere Goat	Yanan Xu Weidong Cai Rui Chen Xinjiang Zhang Zhixian Bai Yu Zhang Yuting Qin Ming Gu Yinggang Sun Yanzhi Wu Zeying Wang	One of the critical elements in evaluating the quality of cashmere is its fineness, but we still know little about how it is regulated at the metabolic level. In this paper, we use UHPLC-MS/MS detection and analysis technology to compare the difference in metabolites between coarse cashmere (CT_LCG) and fine cashmere (FT_LCG) skin of Liaoning cashmere goats. According to the data, under positive mode four metabolites were significantly up-regulated and seven were significantly down-regulated. In	pmid:36080249 doi:10.3390/molecules27175483	Fri, 09 Sep 2022 06:00:00 -0400
61	pubmed:36080275	In the Swim of Cannabis: Developmental Toxicity and Metabolomic Pathway Alterations of Zebrafish Larvae Exposed to THC for the Assessment of Its Potential Environmental and Human Health Impact	Theodoros Chatzimitakos Ieremias Chousidis Dimitrios Leonardos Constantine Stalikas Ioannis Leonardos	As the pharmacological properties and therapeutic applications of Cannabis sativa L. pace with the upsurge of interest of the scientific community in harnessing its constituent phytocannabinoids, illicit use may raise serious health issues.  Tetrahydrocannabinol (THC) is one of the most well-known phytoactive constituents of cannabis and continues to garner scientific and public attention not only because of its pharmacological value but also because overthe-counter products of THC and	pmid:36080275 doi:10.3390/molecules27175506	Fri, 09 Sep 2022 06:00:00 -0400
62	pubmed:36080285	Simultaneous UHPLC-MS Quantification of Catechins and Untargeted Metabolomic Profiling for Proof-of-Concept Authenticity Determination of <i>Maytenus</i> ssp. Samples	Rodolfo Santos Duarte Elisa Ribeiro Miranda Antunes Alexandra Christine Helena Frankland Sawaya	Due to the widespread use of Maytenus ilicifolia leaves in the treatment of gastric ulcers, herbal medicines derived from such species are distributed by the national health system in Brazil. A related species, Maytenus aquifolium, is also used for the same disorders, and both are popularly known as Espinheira-santa. Due to their popular use, the quality and efficiency of the herbal medicines derived from these species is an important public health issue. The purpose of this study was to develop	pmid:36080285 doi:10.3390/molecules27175520	Fri, 09 Sep 2022 06:00:00 -0400
63	pubmed:36080292	1H NMR Metabolomics of Chinese Human Milk at Different Stages of Lactation among Secretors and Non-Secretors	Maaria Kortesniemi Tahereh Jafari Yumei Zhang Baoru Yang	Human milk is an intricate, bioactive food promoting infant health. We studied the composition of human milk samples collected over an 8-month lactation using <sup>1</sup> H NMR metabolomics. A total of 72 human breast milk samples were collected from ten Chinese mothers at eight different time points. The concentrations of ten human milk oligosaccharides (HMOs), fucose and lactose were quantified. Six of the mothers were classified as Lewis-positive secretors (Se^(+)Le^(+)) and four as Lewis-positive	pmid:36080292 doi:10.3390/molecules27175526	Fri, 09 Sep 2022 06:00:00 -0400

	NCT Number	Title	Authors	Description	Identifier	Dates
64	pubmed:36080314	Integrating Enhanced Profiling and Chemometrics to Unveil the Potential Markers for Differentiating among the Leaves of Panax ginseng, P. quinquefolius, and P. notoginseng by Ultra-High Performance Liquid Chromatography/Ion Mobi	Feifei Yang Boxue Chen Meiting Jiang Huimin Wang Ying Hu Hongda Wang Xiaoyan Xu Xiumei Gao Wenzhi Yang	The leaves of Panax species (e.g., Panax ginseng-PGL, P. quinquefolius-PQL, and P. notoginseng-PNL) can serve as a source for healthcare products. Comprehensive characterization and unveiling of the metabolomic difference among PGL, PQL, and PNL are critical to ensure their correct use. For this purpose, enhanced profiling and chemometrics were integrated to probe into the ginsenoside markers for PGL/PQL/PNL by ultra-high performance liquid chromatography/ion mobility-quadrupole time-of-flight	pmid:36080314 doi:10.3390/molecules27175549	Fri, 09 Sep 2022 06:00:00 -0400
65	pubmed:36080331	Coordinative Changes in Metabolites in Grape Cells Exposed to Endophytic Fungi and Their Extracts	Jin-Zhuo Qu Fang Liu Xiao-Xia Pan Chang-Mei Liao Tong Li Han-Bo Zhang Ming-Zhi Yang	Endophytes and their elicitors can all be utilized in regulating crop biochemical qualities. However, living endophytes and their derived elicitors are always applied separately; little is known about the similarities and differences of their effects. To increase the efficiency of this system when applied in practice, the present work profiled simultaneously the metabolomes in grape cells exposed to endophytic fungi (EF) and their corresponding fungal extracts (CFE). As expected, grape cells	pmid:36080331 doi:10.3390/molecules27175566	Fri, 09 Sep 2022 06:00:00 -0400
66	pubmed:36080394	Development, Validation, and Use of <sup>1</sup> H-NMR Spectroscopy for Evaluating the Quality of Acerola-Based Food Supplements and Quantifying Ascorbic Acid	Asma Bourafai-Aziez Daniel Jacob Gwladys Charpentier Emmanuel Cassin Guillaume Rousselot Annick Moing Catherine Deborde	Acerola (Malpighia emarginata D.C.) is an exotic fruit with high agro-industrial potential due to its high content of ascorbic acid (AA), phenolic compounds, and carotenoid pigments. Acerola fruit is processed into concentrated juice or powder to be incorporated into food supplements. The ascorbic acid content of concentrated juice or powders must be controlled and well assessed. Therefore, the development of optimal methods and procedures for the rapid and accurate determination of the ascorbic	pmid:36080394 doi:10.3390/molecules27175614	Fri, 09 Sep 2022 06:00:00 -0400
67	pubmed:36080430	Duguetia pycnastera Sandwith (Annonaceae) Leaf Essential Oil Inhibits HepG2 Cell Growth In Vitro and In Vivo	Emmanoel V Costa César A S de Souza Alexandre F C Galvão Valdenizia R Silva Luciano de S Santos Rosane B Dias Clarissa A Gurgel Rocha Milena B P Soares Felipe M A da Silva Hector H F Koolen Daniel P Bezerra	Duguetia pycnastera Sandwith (Annonaceae) is a tropical tree that can be found in the Guyanas, Bolivia, Venezuela, and Brazil. In Brazil, it is popularly known as "ata", "envira", "envira-preta", and "envirasurucucu". In the present work, we investigated the in vitro and in vivo HepG2 cell growth inhibition capacity of D. pycnastera leaf essential oil (EO). The chemical composition of the EO was determined by GC-MS and GC-FID analyses. The alamar blue assay was used to examine the in vitro	pmid:36080430 doi:10.3390/molecules27175664	Fri, 09 Sep 2022 06:00:00 -0400
68	pubmed:36080474	Ortho-Phosphinoarenesulfonamide-Mediated Staudinger Reduction of Aryl and Alkyl Azides	Xingzhuo Li Zhenguo Wang Wenjun Luo Zixu Wang Keshu Yin Le Li	Conventional Staudinger reductions of organic azides are sluggish with aryl or bulky aliphatic azides. In addition, Staudinger reduction usually requires a large excess of water to promote the decomposition of the aza-ylide intermediate into phosphine oxide and amine products. To overcome the challenges above, we designed a novel triaryl phosphine reagent 2c with an ortho-SO(2)NH(2) substituent. Herein, we report that such phosphine reagents are able to mediate the Staudinger reduction of both	pmid:36080474 doi:10.3390/molecules27175707	Fri, 09 Sep 2022 06:00:00 -0400

	NCT Number	Title	Authors	Description	Identifier	Dates
69	pubmed:36081564	Alterations in the gastric microbiota and metabolites in gastric cancer: An update review	Changzhen Lei Daojun Gong Bo Zhuang Zhiwei Zhang	Gastric cancer (GC) is one of the leading causes of cancer mortality worldwide. Numerous studies have shown that the gastric microbiota can contribute to the occurrence and development of GC by generating harmful microbial metabolites, suggesting the possibility of discovering biomarkers. Metabolomics has emerged as an advanced promising analytical method for the analysis of microbiota-derived metabolites, which have greatly accelerated our understanding of host-microbiota metabolic interactions	pmid:36081564 pmc:PMC9445122 doi:10.3389/fonc.2022.960281	Fri, 09 Sep 2022 06:00:00 -0400
70	pubmed:36081629	Metabolic model of necrotizing enterocolitis in the premature newborn gut resulting from enteric dysbiosis	Giorgio Casaburi Jingjing Wei Sufyan Kazi Junlin Liu Kewei Wang Guo-Zhong Tao Po-Yu Lin James C Y Dunn Bethany M Henrick Steven A Frese Karl G Sylvester	Necrotizing enterocolitis (NEC) is a leading cause of premature newborn morbidity and mortality. The clinical features of NEC consistently include prematurity, gut dysbiosis and enteral inflammation, yet the pathogenesis remains obscure. Herein we combine metagenomics and targeted metabolomics, with functional in vivo and in vitro assessment, to define a novel molecular mechanism of NEC. One thousand six hundred and forty seven publicly available metagenomics datasets were analyzed (NEC = 245;	pmid:36081629 pmc:PMC9445129 doi:10.3389/fped.2022.893059	Fri, 09 Sep 2022 06:00:00 -0400
71	pubmed:36082289	Identification of early quassinoid biosynthesis in the invasive tree of heaven ( Ailanthus altissima) confirms evolutionary origin from protolimonoids	Ling Chuang Shenyu Liu Dave Biedermann Jakob Franke	The tree of heaven, Ailanthus altissima (MILL.) SWINGLE, is a globally invasive plant known to secrete allelopathic metabolites called quassinoids. Quassinoids are highly modified triterpenoids. So far, nothing has been known about the biochemical basis of quassinoid biosynthesis. Here, based on transcriptome and metabolome data of Ailanthus altissima, we present the first three steps of quassinoid biosynthesis, which are catalysed by an oxidosqualene cyclase and two cytochrome P450	pmid:36082289 pmc:PMC9445810 doi:10.3389/fpls.2022.958138	Fri, 09 Sep 2022 06:00:00 -0400
72	pubmed:36082450	SIRT2 promotes cell proliferation and migration through mediating ERK1/2 activation and lactosylceramide accumulation in prostate cancer	Rui Lin Yiping Yang Eran Wu Menghan Zhou Shan Wang Qingyun Zhang	CONCLUSIONS: Our data suggested that SIRT2 is overexpressed in CRPC and NEPC and could promote cell growth and migration through activating ERK1/2 pathway and inducing lactosylceramide production, indicating that SIRT2 has the potential to be a new target for the treatment of PCa.	pmid:36082450 doi:10.1002/pros.24437	Fri, 09 Sep 2022 06:00:00 -0400
73	pubmed:36083004	Effects of PB-TURSO on the transcriptional and metabolic landscape of sporadic ALS fibroblasts	Jasmine A Fels Jalia Dash Kent Leslie Giovanni Manfredi Hibiki Kawamata	OBJECTIVE: ALS is a rapidly progressive, fatal disorder caused by motor neuron degeneration, for which there is a great unmet therapeutic need. AMX0035, a combination of sodium phenylbutyrate (PB) and taurursodiol (TUDCA, TURSO), has shown promising results in early ALS clinical trials, but its mechanisms of action remain to be elucidated. Therefore, our goal was to obtain an unbiased landscape of the molecular effects of AMX0035 in ALS patient-derived cells.	pmid:36083004 doi:10.1002/acn3.51648	Fri, 09 Sep 2022 06:00:00 -0400

	NCT Number	Title	Authors	Description	Identifier	Dates
74	pubmed:36083566	Metabolomics for exposure assessment and toxicity effects of occupational pollutants: current status and future perspectives	Fatemeh Dehghani Saeed Yousefinejad Douglas I Walker Fariborz Omidi	CONCLUSION: Continued application to worker populations has the potential to enable characterization of thousands of chemical signals in biological samples, which could lead to discovery of new biomarkers of exposure for chemicals, identify possible toxicological mechanisms, and improved understanding of biological effects increasing disease risk associated with occupational exposure.	pmid:36083566 doi:10.1007/s11306-022-01930-7	Fri, 09 Sep 2022 06:00:00 -0400
75	pubmed:36083892	The microbiome-derived metabolite TMAO drives immune activation and boosts responses to immune checkpoint blockade in pancreatic cancer	Gauri Mirji Alison Worth Sajad Ahmad Bhat Mohamed El Sayed Toshitha Kannan Aaron R Goldman Hsin-Yao Tang Qin Liu Noam Auslander Chi V Dang Mohamed Abdel-Mohsen Andrew Kossenkov Ben Z Stanger Rahul S Shinde	The composition of the gut microbiome can control innate and adaptive immunity and has emerged as a key regulator of tumor growth, especially in the context of immune checkpoint blockade (ICB) therapy. However, the underlying mechanisms for how the microbiome affects tumor growth remain unclear. Pancreatic ductal adenocarcinoma (PDAC) tends to be refractory to therapy, including ICB. Using a nontargeted, liquid chromatography-tandem mass spectrometry-based metabolomic screen, we identified the	pmid:36083892 doi:10.1126/sciimmunol.abn0704	Fri, 09 Sep 2022 06:00:00 -0400
76	pubmed:36083951	The associations between ADHD, pain, inflammation, and quality of life in children and adolescents-a clinical study protocol	Nóra Kerekes Sara Lundqvist Elke Schubert Hjalmarsson Åsa Torinsson Naluai Anne-Katrin Kantzer Rajna Knez	New research shows that the prevalence of neurodevelopmental disorders, such as attention-deficit/hyperactivity disorder (ADHD), is increased in children and adolescents as well as in adults with chronic pain, compared to those without chronic pain. Children and adolescents with ADHD also have an increased incidence of various physical conditions associated with pain, and they more frequently suffer from inflammatory diseases. Moreover, parents of children with ADHD can often suffer from pain	pmid:36083951 doi:10.1371/journal.pone.0273653	Fri, 09 Sep 2022 06:00:00 -0400
77	pubmed:36084068	Whole genome sequence analysis of two subspecies of Companilactobacillus Futsaii and experimental verification of drug resistance and effect on the exploratory behavior of mice based on unique gene	Zhao Xin Xing Wei Qiuxia Jiao Qiufeng Gou Yumeng Zhang Chaoming Peng Qu Pan	This study characterized the whole genome of Companilactobacillus futsaii subsp. chongqingii CQ16Z1 isolated from Chongqing of China, performed genome sequence analysis with Companilactobacillus futsaii subsp. futsaii YM0097 isolated from Taiwan of China, and experimentally verified drug resistance and effect on the exploratory behavior of male C57BL/6 mice and analysis of gut microbiota and metabolomic studies. The genome of CQ16Z1 is 2.6 Mb. Sequence analysis between genomes showed that the	pmid:36084068 doi:10.1371/journal.pone.0274244	Fri, 09 Sep 2022 06:00:00 -0400