metabolomics

	NCT Number	Title	Authors	Description	Identifier	Dates
1	pubmed:36108373	Fructus ligustri lucidi suppresses inflammation and restores the microbiome profile in murine colitis models	Wei Yu Shihong Sun Keer Zhang Huiying Li Mengjiao Xin Yanzhi Liu Jing Yan	CONCLUSION: FLL is a potent anti-colitis drug by suppressing inflammation and rescuing dysbiosis.	pmid:36108373 doi:10.1016/j.phymed.2022.154438	Thu, 15 Sep 2022 06:00:00 -0400
2	pubmed:36108463	Tripterygium glycoside tablet attenuates renal function impairment in diabetic nephropathy mice by regulating triglyceride metabolism	Jing Zhang Si-Lan Li Wen Lin Rong-Hua Pan Yue Dai Yu-Feng Xia	Tripterygium glycoside tablet (TGT) has been used clinically to alleviate diabetic nephropathy (DN) for decades. However, the mechanism of its anti-DN has not been fully clarified. The aim of this study was to elucidate molecular mechanism of TGT in repairing renal function injury. The results of biochemical parameters and renal histopathology implied that TGT intervention could attenuate creatinine, albumin excretion rate and histological injury of kidney in DN mouse model. Moreover,	pmid:36108463 doi:10.1016/j.jpba.2022.115028	Thu, 15 Sep 2022 06:00:00 -0400
3	pubmed:36108548	Metabolomic changes in lactating multiparous naturally MAP-infected Holstein- Friesian dairy cows suggest changes in mitochondrial energy pathways	E N Taylor M Beckmann G Hewinson D Rooke L A Sinclair L A J Mur	Mycobacterium avium subspecies paratuberculosis (MAP) is the causative organism of Johne's Disease, a chronic intestinal infection of ruminants. Infected cows begin shedding MAP within the asymptomatic, subclinical stage of infection before clinical signs, such as weight loss, diarrhoea and reduced milk yields develop within the clinical stages of disease. Herein, we examine the milk metabolomic profiles of naturally MAP-infected Holstein-Friesian cows. The study used biobanked milk samples	pmid:36108548 doi:10.1016/j.rvsc.2022.09.001	Thu, 15 Sep 2022 06:00:00 -0400
4	pubmed:36108615	Acute Kidney Injury and Diastolic Dysfunction: Opportunity for Targeted Intervention?	Danielle E Soranno Katja M Gist	CONCLUSIONS: Ischemic AKI results in long-term cardiovascular sequelae with sex as an important biological variable in outcomes. Histone deacetylase inhibition affects cardiovascular outcomes after AKI.	pmid:36108615 doi:10.1159/000526010	Thu, 15 Sep 2022 06:00:00 -0400
5	pubmed:36108692	Effects of dandelion (Taraxacum sp.,) supplements on lactation performance, antioxidative activity, and plasma metabolome in primiparous dairy cows	Yan Li Jie Mei Jiaqi Wang Hongyun Liu	CONCLUSION: Dandelion supplementation could improve lactation performance and elevate the plasma carbohydrate and amino acids metabolism and antioxidative activity. Supplementation of 200 g/d dandelion is recommended for lactating dairy cows.	pmid:36108692 doi:10.5713/ab.22.0061	Thu, 15 Sep 2022 06:00:00 -0400
6	pubmed:36108695	Metabolomic profiling of postmortem aged muscle in Japanese Brown beef cattle revealed an interbreed difference from Japanese Black beef	Susumu Muroya Riko Nomura Hirotaka Nagai Koichi Ojima Kazutsugu Matsukawa	CONCLUSION: Glycolysis, purine metabolism, fatty acid catabolism, and protein degradation were the most common pathways in beef during postmortem aging. The differentially expressed metabolites and the relevant metabolisms in JBRT beef may contribute to the development of a characteristic flavor.	pmid:36108695 doi:10.5713/ab.22.0202	Thu, 15 Sep 2022 06:00:00 -0400

	NCT Number	Title	Authors	Description	Identifier	Dates
7	pubmed:36108722	Metabolome-wide association study of the relationship between chlorpyrifos exposure and first trimester serum metabolite levels in pregnant Thai farmworkers	Donghai Liang Jonathan Batross Nancy Fiedler Tippawan Prapamontol Panrapee Suttiwan Parinya Panuwet Warangkana Naksen Brittney O Baumert Volha Yakimavets Youran Tan Priya D'Souza Ampica Mangklabruks Supattra Sittiwang Kristsanachai Kaewthit Kanyapak Kohsuwan Nattawadee Promkam Sureewan Pingwong P Barry Ryan Dana Boyd Barr SAWASDEE birth cohort investigative team	INTRODUCTION: Organophosphate (OP) insecticides, including chlorpyrifos, have been linked with numerous harmful health effects on maternal and child health. Limited data are available on the biological mechanisms and endogenous pathways underlying the toxicity of chlorpyrifos exposures on pregnancy and birth outcomes. In this study, we measured a urinary chlorpyrifos metabolite and used high-resolution metabolomics (HRM) to identify biological perturbations associated with chlorpyrifos exposure	pmid:36108722 doi:10.1016/j.envres.2022.114319	Thu, 15 Sep 2022 06:00:00 -0400
8	pubmed:36108837	Maternal exposure to polystyrene nanoparticles retarded fetal growth and triggered metabolic disorders of placenta and fetus in mice	Guangquan Chen Shiyi Xiong Qiao Jing Cornelis A M van Gestel Nico M van Straalen Dick Roelofs Luming Sun Qiu Hao	Microplastics can enter the human body via direct body contact or the food chain, increasing the likelihood of adverse impacts on pregnancy and fetal development. We investigated the potential effects and modes of action of polystyrene nanoplastics (PS-NPs) in placenta and fetus using mice as a model species. Maternal PS-NP exposure (100 nm; 1 and 10 mg/L) via drinking water induced a significant decline in fetal weights at the higher exposure concentration. Abnormal morphologies of cells in the	pmid:36108837 doi:10.1016/j.scitotenv.2022.158666	Thu, 15 Sep 2022 06:00:00 -0400
9	pubmed:36109618	Metabolomic and exposomic biomarkers of risk of future neurodevelopmental delay in human milk	Kefeng Li Kerri Bertrand Jane C Naviaux Jonathan M Monk Alan Wells Lin Wang Sai Sachin Lingampelly Robert K Naviaux Christina Chambers	CONCLUSIONS: Once validated in larger studies, the chemical analysis of human milk might be added as an option in well-baby checks to help identify children at risk of NDD before the first symptoms appear.	pmid:36109618 doi:10.1038/s41390-022-02283-6	Thu, 15 Sep 2022 06:00:00 -0400
10	pubmed:36109686	Removing unwanted variation from large-scale RNA sequencing data with PRPS	Ramyar Molania Momeneh Foroutan Johann A Gagnon-Bartsch Luke C Gandolfo Aryan Jain Abhishek Sinha Gavriel Olshansky Alexander Dobrovic Anthony T Papenfuss Terence P Speed	Accurate identification and effective removal of unwanted variation is essential to derive meaningful biological results from RNA sequencing (RNA-seq) data, especially when the data come from large and complex studies. Using RNA-seq data from The Cancer Genome Atlas (TCGA), we examined several sources of unwanted variation and demonstrate here how these can significantly compromise various downstream analyses, including cancer subtype identification, association between gene expression and	pmid:36109686 doi:10.1038/s41587-022-01440-w	Thu, 15 Sep 2022 06:00:00 -0400
11	pubmed:36109783	Potential role of tea drinking in preventing hyperuricaemia in rats: biochemical and molecular evidence	Siyao Sang Lufei Wang Taotao Liang Mingjie Su Hui Li	CONCLUSION: These findings indicate that green tea cannot reduce the serum uric acid level of hyperuricaemic rats. Yellow tea can significantly improve hyperuricaemia by regulating the inflammatory response, autophagy, and apoptosis. This study provides a potential candidate for the treatment of hyperuricaemia and a basis for selecting therapeutic tea for patients with hyperuricaemia.	pmid:36109783 doi:10.1186/s13020-022-00664-x	Thu, 15 Sep 2022 06:00:00 -0400

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12	pubmed:36110042	Activation of anthocyanin biosynthesis in high light - what is the initial signal?	Galileo Estopare Araguirang Andreas S Richter	Due to their sessile nature, plants cannot escape adverse environmental conditions and evolved mechanisms to cope with sudden environmental changes. The reaction to variations in abiotic factors, also summarised as acclimation response, affects all layers of cellular functions and involves rapid modification of enzymatic activities, the metabolome, proteome and transcriptome on different time scales. One trait of plants acclimating to high light (HL) is the rapid transcriptional activation of	pmid:36110042 doi:10.1111/nph.18488	Fri, 16 Sep 2022 06:00:00 -0400
13	pubmed:36110305	Effects of different harvest frequencies on microbial community and metabolomic properties of annual ryegrass silage	Zhihui Fu Lin Sun Meiling Hou Junfeng Hao Qiang Lu Tingyu Liu Xiuzhen Ren Yushan Jia ZhiJun Wang Gentu Ge	In this study, we analyzed the fermentation quality, microbial community, and metabolome characteristics of ryegrass silage from different harvests (first harvest-AK, second harvest-BK, and third harvest-CK) and analyzed the correlation between fermentative bacteria and metabolites. The bacterial community and metabolomic characteristics were analyzed by single-molecule real-time (SMRT) sequencing and ultra-high-performance liquid chromatography-mass spectrometry (UHPLC-MS/MS), respectively	pmid:36110305 pmc:PMC9468666 doi:10.3389/fmicb.2022.971449	Fri, 16 Sep 2022 06:00:00 -0400
14	pubmed:36110355	Root-associated bacteria modulate the specialised metabolome of <i>Lithospermum officinale</i> L	Alicia Varela Alonso Henry D Naranjo Angélique Rat Nebojša Rodi Christina I Nannou Dimitra A Lambropoulou Andreana N Assimopoulou Stéphane Declerck Philipp Rödel Carolin Schneider Anne Willems	Bacteria influence plant growth and development and therefore are attractive resources for applications in agriculture. However, little is known about the impact of these microorganisms on secondary metabolite (SM) production by medicinal plants. Here we assessed, for the first time, the effects of bacteria on the modulation of SM production in the medicinal plant Lithospermum officinale (Boraginaceae family) with a focus on the naphthoquinones alkannin/shikonin and their derivatives (A/Sd). The	pmid:36110355 pmc:PMC9468582 doi:10.3389/fpls.2022.908669	Fri, 16 Sep 2022 06:00:00 -0400
15	pubmed:36110409	Prognostic value of plasma phenylalanine and gut microbiota-derived metabolite phenylacetylglutamine in coronary in-stent restenosis	Yuan Fu Yixing Yang Chen Fang Xinming Liu Ying Dong Li Xu Mulei Chen Kun Zuo Lefeng Wang	CONCLUSION: Plasma Phe and PAGIn are valuable indices for predicting coronary ISR, and gut microbes may be a promising intervention target to prevent ISR progression.	pmid:36110409 pmc:PMC9468445 doi:10.3389/fcvm.2022.944155	Fri, 16 Sep 2022 06:00:00 -0400
16	pubmed:36110515	Exploring potential mechanism of ciwujia tablets for insomnia by UPLC-Q-TOF-MS/MS, network pharmacology, and experimental validation	Hongda Liu Le Yang Chunlei Wan Zhineng Li Guangli Yan Ying Han Hui Sun Xijun Wang	Insomnia, whether chronic or intermittent, is a common central nervous system disease. Ciwujia Tablet (CWT) is a well-known traditional Chinese medicine (TCM) made from the extract of Eleutherococcus senticosus (Rupr. & Maxim.) Maxim. This medication is commonly used for treating insomnia in China, but the lack of in-depth research focused on the chemical ingredients of CWT creates a gap in knowledge regarding its effective constituents against insomnia. Considering that the therapeutic material	pmid:36110515 pmc:PMC9468710 doi:10.3389/fphar.2022.990996	Fri, 16 Sep 2022 06:00:00 -0400

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17	pubmed:36110518	Analysis of the absorbed constituents and mechanism of liquidambaris fructus extract on hepatocellular carcinoma	Shuai Wang Xin-Xin Yang Tian-Jiao Li Lin Zhao Yong-Rui Bao Xian-Sheng Meng	Background: Hepatocellular carcinoma (HCC) refers to one of the top 10 cancers in terms of morbidity and mortality globally, seriously influencing people's lives. First recorded in Compendium of Materia Medica, liquidambaris fructus (LF) generates definite anti-liver tumor effect. However, its effective substances and mechanism remain to be elucidated. Methods: Serum pharmacochemistry and UPLC-QTOF-MS technologies were employed to explore the plasma of rats after intragastric administration of	pmid:36110518 pmc:PMC9468745 doi:10.3389/fphar.2022.999935	Fri, 16 Sep 2022 06:00:00 -0400
18	pubmed:36110521	Therapeutic mechanisms of mulberry leaves in type 2 diabetes based on metabolomics	Quantao Ma Yaqi Li Ruixue Zhao Ziyan Tang Jialin Li Cong Chen Xiaoyao Liu Yujie Hu Ting Wang Baosheng Zhao	Background: Type 2 diabetes (T2D) is considered as one of the most significant metabolic syndromes worldwide, and the long-term use of the drugs already on the market for T2D often gives rise to some side effects. The mulberry leaf (ML), Morus alba L., has advantages in terms of its comprehensive therapeutic efficacy, which are characterized as multicomponent, multitarget, multipathway, and matching with the complex pathological mechanisms of diabetes. Methods: T2D rats were established by a	pmid:36110521 pmc:PMC9468646 doi:10.3389/fphar.2022.954477	Fri, 16 Sep 2022 06:00:00 -0400
19	pubmed:36110550	Combined metabolomics and proteomics to reveal beneficial mechanisms of <i>Dendrobium fimbriatum</i> against gastric mucosal injury	Jing Sun Peng-Fei Liu Jia-Ni Liu Cong Lu Li-Tao Tong Yong-Quan Wang Jia-Meng Liu Bei Fan Feng-Zhong Wang	As a dietary and medicinal plant, Dendrobium fimbriatum (DF) is widely utilized in China for improving stomach disease for centuries. However, the underlying mechanisms against gastric mucosal injury have not been fully disclosed. Here, metabolomics and proteomics were integrated to clarify the in-depth molecular mechanisms using cyclophosphamide- induced gastric mucosal injury model in mice. As a result, three metabolic pathways, such as creatine metabolism, arginine and proline metabolism, and	pmid:36110550 pmc:PMC9468276 doi:10.3389/fphar.2022.948987	Fri, 16 Sep 2022 06:00:00 -0400
20	pubmed:36110954	Impact of local anesthetics on epigenetics in cancer	Lucillia Bezu Oliver Kepp Guido Kroemer	Defective silencing of tumor suppressor genes through epigenetic alterations contributes to oncogenesis by perturbing cell cycle regulation, DNA repair or cell death mechanisms. Reversal of such epigenetic changes including DNA hypermethylation provides a promising anticancer strategy. Until now, the nucleoside derivatives 5-azacytidine and decitabine are the sole DNA methyltransferase (DNMT) inhibitors approved by the FDA for the treatment of specific hematological cancers. Nevertheless, due to	pmid:36110954 pmc:PMC9468863 doi:10.3389/fonc.2022.849895	Fri, 16 Sep 2022 06:00:00 -0400
21	pubmed:36111068	Exposure to perfluoroalkyl substances and risk of hepatocellular carcinoma in a multiethnic cohort	Jesse A Goodrich Douglas Walker Xiangping Lin Hongxu Wang Tiffany Lim Rob McConnell David V Conti Lida Chatzi Veronica Wendy Setiawan	CONCLUSION: This proof-of-concept analysis shows that exposure to high PFOS levels was associated with increased risk of non-viral HCC, likely via alterations in glucose, amino acid, and bile acid metabolism. Larger studies are needed to confirm these findings.	pmid:36111068 pmc:PMC9468464 doi:10.1016/j.jhepr.2022.100550	Fri, 16 Sep 2022 06:00:00 -0400

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22.	pubmed:36111147	A systematic review on omics data (metagenomics, metatranscriptomics, and metabolomics) in the role of microbiome in gallbladder disease	Paola Di Carlo Nicola Serra Rosa Alduina Riccardo Guarino Antonio Craxì Anna Giammanco Teresa Fasciana Antonio Cascio Consolato M Sergi	Microbiotas are the range of microorganisms (mainly bacteria and fungi) colonizing multicellular, macroscopic organisms. They are crucial for several metabolic functions affecting the health of the host. However, difficulties hamper the investigation of microbiota composition in cultivating microorganisms in standard growth media. For this reason, our knowledge of microbiota can benefit from the analysis of microbial macromolecules (DNA, transcripts, proteins, or by-products) present in various	pmid:36111147 pmc:PMC9468903 doi:10.3389/fphys.2022.888233	Fri, 16 Sep 2022 06:00:00 -0400
23	pubmed:36111548	Metabolome-Wide Association Study of Cord Blood Metabolites With Blood Pressure in Childhood and Adolescence	Mingyu Zhang Tammy M Brady Jessie P Buckley Lawrence J Appel Xiumei Hong Guoying Wang Liming Liang Xiaobin Wang Noel T Mueller	CONCLUSIONS: In our urban and predominantly racial/ethnic minority cohort, we provide evidence that metabolomic alterations in utero, in particular, acylcarnitine- and purine-metabolism metabolites, may be involved in the early life origins of hypertension.	pmid:36111548 doi:10.1161/HYPERTENSIONAHA.122.201 39	Fri, 16 Sep 2022 06:00:00 -0400
24	pubmed:36111651	Holothuria Leucospilota polysaccharides alleviate hyperlipidemia via alteration of lipid metabolism and inflammation-related gene expression	Shanshan Lu Yiqiong Yuan Fei Chen Yuanping Zheng Chuan Li Jun Cao Guanghua Xia Zhongyuan Liu Xuanri Shen Yanfu He Dayong Zhou Kexue Zhu	Hyperlipemia is becoming a chronic disease that threatens human health. At the same time, people pay more and more attention to hyperlipemia. Holothuria Leucospilota polysaccharide (HLP) has been reported to ameliorate hyperlipidemia in high-fat dietinduced rats. Therefore, this study aimed to explore further metabolomics' role in improving liver function and reveal its mechanism. After oral administration of HLP for 4 weeks, total cholesterol (TC) and triglycerides (TG) levels of the liver in	pmid:36111651 doi:10.1111/jfbc.14392	Fri, 16 Sep 2022 06:00:00 -0400
25	pubmed:36111668	Exploration of the underlying mechanisms of isoniazid/rifampicin-induced liver injury in mice using an integrated proteomics and metabolomics approach	Yanqing Song Xiaoyu Qu Lina Tao Huan Gao Yueming Zhang Jinghui Zhai Jiawei Gong Tingting Hu	The hepatotoxic mechanism resulting from coadministration of isoniazid (INH) and rifampicin (RIF) are complex and studies remain inconclusive. To systematically explore the underlying mechanisms, an integrated mass-based untargeted metabolomics and label-free quantitative proteomics approach was used to clarify the mechanism of INH/RIF-induced liver injury. Thirty male mice were randomly divided into three groups: control (receiving orally administered vehicle solution), INH (150 mg/kg) + RIF	pmid:36111668 doi:10.1002/jbt.23217	Fri, 16 Sep 2022 06:00:00 -0400
26	pubmed:36111751	Plasma Free Amino Acid Profile in HIV-Positive Cases	Irfan Binici Hamit Hakan Alp Hasan Karsen Ismail Koyuncu Ataman Gonel Hakim Çelik Mustafa Kasm Karahocagil	CONCLUSION: The significant differences in amino acid profile between HIV-positive and healthy subjects may represent an auxiliary biomarker of cellular damage in asymptomatic HIV-positive patients that may be examined in more detail in further studies. It may also provide guidance for symptomatic cases in terms of the association between symptoms, clinical manifestations, and deficiency or excess of certain amino acids in the context of the complete metabolomics record of HIVpositive patients.	pmid:36111751 doi:10.2174/1570162X20666220428103250	Fri, 16 Sep 2022 06:00:00 -0400

	NCT Number	Title	Authors	Description	Identifier	Dates
27	pubmed:36111835	How Soft Is Secondary Electrospray Ionization?	Jérôme Kaeslin Cedric Wüthrich Stamatios Giannoukos Renato Zenobi	Secondary electrospray ionization (SESI) mass spectrometry (MS) is a direct infusion technique often used for untargeted metabolomics, e.g., for online breath analysis. SESI is thought to be a soft ionization method, which is important to avoid interference from in-source fragments and to simplify compound annotation. In this work, benzylammonium ions, formed from volatile benzylamines, with known bond dissociation enthalpies were used as thermometer ions to investigate the internal energy	pmid:36111835 doi:10.1021/jasms.2c00201	Fri, 16 Sep 2022 06:00:00 -0400
28	pubmed:36112136	Dysregulation of glutamine/glutamate metabolism in COVID-19 patients: a metabolism study in African population and mini meta-analysis	Xiao-Kun Li Bo Tu Xiao-Ai Zhang Wen Xu Jia-Hao Chen Biao Xu Jun-Jie Zheng Peng-Fei Hao Reginald Cole Mohamed Boie Jalloh Qing-Bin Lu Chang Li Stephen Sevalie Wei Liu Wei-Wei Chen	Coronavirus disease 2019 (COVID-19) remains a serious global threat. The metabolic analysis had been successfully applied in the efforts to uncover the pathological mechanisms and biomarkers of disease severity. Here we performed a quasitargeted metabolomic analysis on 56 COVID-19 patients from Sierra Leone in western Africa, revealing the metabolomic profiles and the association with disease severity, which was confirmed by the targeted metabolomic analysis of 19 pairs of COVID-19 patients. A	pmid:36112136 doi:10.1002/jmv.28150	Fri, 16 Sep 2022 06:00:00 -0400
29	pubmed:36112275	Enzymatic Sialylation of Synthetic Multivalent Scaffolds: From 3'-Sialyllactose Glycomacromolecules to Novel Neoglycosides	Patrick B Konietzny Hannelore Peters Marc L Hofer Ulla I M Gerling-Driessen Robert P de Vries Thomas Peters Laura Hartmann	Sialoglycans play a key role in many biological recognition processes and sialylated conjugates of various types have successfully been applied, e.g., as antivirals or in anti-tumor therapy. A key feature for high affinity binding of such conjugates is the multivalent presentation of sialoglycans which often possess synthetic challenges. Here, we describe the combination of solid phase polymer synthesis and enzymatic sialylation yielding 3'-sialyllactose-presenting precision glycomacromolecules	pmid:36112275 doi:10.1002/mabi.202200358	Fri, 16 Sep 2022 06:00:00 -0400
30	pubmed:36112882	Stable Isotope-Guided Metabolomics Reveals Polar-Functionalized Fatty-Acylated RiPPs from Streptomyces	Shumpei Asamizu Shinta Ijichi Shotaro Hoshino Hansaem Jo Hidenori Takahashi Yuko Itoh Sohkichi Matsumoto Hiroyasu Onaka	Ribosomally synthesized and posttranslationally modified peptides (RiPPs) with polar-functionalized fatty acyl groups are a rarely found untapped class of natural products. Although polar-functionalized fatty-acylated RiPPs (PFARs) have potential as antimicrobial agents, the repertoire is still limited. Therefore, expanding the chemical space is expected to contribute to the development of pharmaceutical agents. In this study, we performed genome mining and stable isotope-guided comparative	pmid:36112882 doi:10.1021/acschembio.2c00601	Fri, 16 Sep 2022 06:00:00 -0400