metabolomics

	NCT Number	Title	Authors	Description	Identifier	Dates
1	pubmed:36067594	Treatment effects of Radix ginseng-Schisandra chinensis herb pair on Alzheimer's disease: An investigation of MS-based metabolomics investigation	Aimin Wang Minjie Shi Junpeng Xing Shu Liu Zhiqiang Liu Fengrui Song	Traditional Chinese medicine (TCM) plays a synergistic and comprehensive pharmacodynamic role of multi-channel and multi-target through its multi-components, showing unique therapeutic advantages in chronic and multi-gene complex diseases. Herb pair is a unique combination of two relatively fixed herbs, which embodies the integrity of TCM theory. In this study, untargeted fecal metabolomics based on MS was used to investigate the action mechanism of Radix ginseng and Schisandra chinensis (GS)...	pmid:36067594 doi:10.1016/j.jpba.2022.115007	Tue, 06 Sep 2022 06:00:00 -0400
2	pubmed:36067623	Insights into the interaction of cyclooxygenase and lipoxygenase with natural compound 3,4',5,7-Tetrahydroxyflavone based on multi-spectroscopic and metabolomics	Jie Yi Haixia Che Jiping Ren Hong Yu Kexin Song Xiaoying Wang Xiaoting Zhao Xianyao Wang Qian Li	Hypoxia induce right ventricular dysfunction in human heart, but the molecular mechanism remains limited. As known, cyclooxygenases (COX) and lipoxygenases (LOX) play a key role in the cardiovascular system under hypoxia. 3,4',5,7-Tetrahydroxyflavone (THF), which widely exists in a variety of plants and vegetables, is famous for good ability to relieve cardiac injury, but the mechanism remains to be further understood. In this study, we firstly estimated the preventive role of THF against...	pmid:36067623 doi:10.1016/j.saa.2022.121800	Tue, 06 Sep 2022 06:00:00 -0400
3	pubmed:36067630	Visualizing biomarkers and their association with clinical outcomes: A machine learning approach	Hui Zheng Robert E Gerszten Kathleen E Corey	CONCLUSION: This is an effective approach to visualize biomarkers and their correlations, allowing rapid visual identification of biomarkers and marker clusters with potentially higher degree of association with the outcome.	pmid:36067630 doi:10.1016/j.compbiomed.2022.106005	Tue, 06 Sep 2022 06:00:00 -0400
4	pubmed:36067864	Integrated analysis of effect of daisaikoto, a traditional Japanese medicine, on the metabolome and gut microbiome in a mouse model of nonalcoholic fatty liver disease	Shiori Ishizawa Akinori Nishi Noriko Kaifuchi Chika Shimobori Miwa Nahata Chihiro Yamada Seiichi Iizuka Katsuya Ohbuchi Mitsue Nishiyama Naoki Fujitsuka Toru Kono Masahiro Yamamoto	Dysregulation of lipid metabolism and diabetes are risk factors for nonalcoholic fatty liver disease (NAFLD), and the gut-liver axis and intestinal microbiome are known to be highly associated with the pathogenesis of this disease. In Japan, the traditional medicine daisaikoto (DST) is prescribed for individuals affected by hepatic dysfunction. Herein, we evaluated the therapeutic potential of DST for treating NAFLD through modification of the liver and stool metabolome and microbiome by using...	pmid:36067864 doi:10.1016/j.gene.2022.146856	Tue, 06 Sep 2022 06:00:00 -0400
5	pubmed:36068052	A re-calibration procedure for interoperable lipid collision cross section values measured by traveling wave ion mobility spectrometry	Anaïs C George Isabelle Schmitz-Afonso Vincent Marie Benoit Colsch François Fenaille Carlos Afonso Corinne Loutelier-Bourhis	Collision cross sections (CCS) have been described as relevant molecular descriptors in metabolomics and lipidomics analyses for ascertaining compound identity. Ion mobility spectrometry (IMS) allows to determine CCS with different techniques, such as drift tube ion mobility spectrometry (DTIMS), traveling wave ion mobility spectrometry (TWIMS) or trapped ion mobility spectrometry (TIMS). In contrast with DTIMS where CCS can be obtained directly with measured drift times and mathematical...	pmid:36068052 doi:10.1016/j.aca.2022.340236	Tue, 06 Sep 2022 06:00:00 -0400

	NCT Number	Title	Authors	Description	Identifier	Dates
6	pubmed:36068057	Instrument-type effects on chemical isotope labeling LC-MS metabolome analysis: Quadrupole time-of-flight MS vs. Orbitrap MS	Chu-Fan Wang Liang Li	Chemical isotope labeling (CIL) LC-MS is a powerful tool for metabolome analysis with markedly improved metabolomic coverage and quantification accuracy over the conventional LC-MS technique. In addition, with differential isotope labeling, each labeled metabolite is detected as a peak pair in the mass spectra, offering the possibility of differentiating true metabolite peaks from the singlet noise or background peaks. In this study, we examined the effects of instrument type on the...	pmid:36068057 doi:10.1016/j.aca.2022.340255	Tue, 06 Sep 2022 06:00:00 -0400
7	pubmed:36068059	Optimization of capillary electrophoresis coupled to negative mode electrospray ionization-mass spectrometry using polyvinyl alcohol coated capillaries. Application to a study on non-small cell lung cancer	Ángeles López-López Michal Ciborowski Jacek Niklinski Coral Barbas Ángeles López-Gonzálvez	Despite recent developments in separation techniques, the analysis of relatively small highly polar negatively charged analytes (e.g. small organic acids, phosphorylated sugars, and underivatized amino acids) remains challenging. Capillary electrophoresis coupled to mass spectrometry (CE-MS) has been included in the untargeted metabolomics toolbox, although mostly in positive polarity. The aim of this study was to assess the use of CE-MS to analyze highly polar and negatively charged metabolites...	pmid:36068059 doi:10.1016/j.aca.2022.340259	Tue, 06 Sep 2022 06:00:00 -0400
8	pubmed:36068068	Visual diagnosis of COVID-19 disease based on serum metabolites using a paper-based electronic tongue	Mohammad Mahdi Bordbar Hosein Samadinia Azarmidokht Sheini Jasem Aboonajmi Pegah Hashemi Hosein Khoshsafar Raheleh Halabian Akbar Khanmohammadi B Fatemeh Nobakht M Gh Hashem Sharghi Mostafa Ghanei Hasan Bagheri	This study aims to use a paper-based sensor array for point-of-care detection of COVID-19 diseases. Various chemical compounds such as nanoparticles, organic dyes and metal ion complexes were employed as sensing elements in the array fabrication, capturing the metabolites of human serum samples. The viral infection caused the type and concentration of serum compositions to change, resulting in different color responses for the infected and control samples. For this purpose, 118 serum samples of...	pmid:36068068 doi:10.1016/j.aca.2022.340286	Tue, 06 Sep 2022 06:00:00 -0400
9	pubmed:36068249	Identification of a broad lipid repertoire associated to the endothelial cell protein C receptor (EPCR)	Elena Erausquin María Morán-Garrido Jorge Sáiz Coral Barbas Gilda Dichiara-Rodríguez Alejandro Urdiciain Jacinto López-Sagaseta	Evidence is mounting that the nature of the lipid bound to the endothelial cell protein C receptor (EPCR) has an impact on its biological roles, as observed in anticoagulation and more recently, in autoimmune disease. Phosphatidylethanolamine and phosphatidylcholine species dominate the EPCR lipid cargo, yet, the extent of diversity in the EPCR-associated lipid repertoire is still unknown and remains to be uncovered. We undertook mass spectrometry analyses to decipher the EPCR lipidome, and...	pmid:36068249 doi:10.1038/s41598-022-18844-y	Tue, 06 Sep 2022 06:00:00 -0400

	NCT Number	Title	Authors	Description	Identifier	Dates
10	pubmed:36068258	Cultivating epizoic diatoms provides insights into the evolution and ecology of both epibionts and hosts	Matt P Ashworth Roksana Majewska Thomas A Frankovich Michael Sullivan Sunica Bosak Klara Filek Bart Van de Vijver Michael Arendt Jeffrey Schwenter Ronel Nel Nathan J Robinson Meagan P Gary Edward C Theriot Nicole I Stacy Daryl W Lam Justin R Perrault Charles A Manire Schonna R Manning	Our understanding of the importance of microbiomes on large aquatic animals-such as whales, sea turtles and manatees-has advanced considerably in recent years. The latest observations indicate that epibiotic diatom communities constitute diverse, polyphyletic, and compositionally stable assemblages that include both putatively obligate epizoic and generalist species. Here, we outline a successful approach to culture putatively obligate epizoic diatoms without their hosts. That some taxa can be...	pmid:36068258 doi:10.1038/s41598-022-19064-0	Tue, 06 Sep 2022 06:00:00 -0400
11	pubmed:36068416	Tachycardiomyopathy entails a dysfunctional pattern of interrelated mitochondrial functions	Michael G Paulus Kathrin Renner Alexander G Nickel Christoph Brochhausen Katharina Limm Elmar Zügner Maria J Baier Steffen Pabel Stefan Wallner Christoph Birner Andreas Luchner Christoph Magnes Peter J Oefner Klaus J Stark Stefan Wagner Christoph Maack Lars S Maier Katrin Streckfuss-Bömeke Samuel Sossalla Alexander Dietl	Tachycardiomyopathy is characterised by reversible left ventricular dysfunction, provoked by rapid ventricular rate. While the knowledge of mitochondria advanced in most cardiomyopathies, mitochondrial functions await elucidation in tachycardiomyopathy. Pacemakers were implanted in 61 rabbits. Tachypacing was performed with 330 bpm for 10 days (n = 11, early left ventricular dysfunction) or with up to 380 bpm over 30 days (n = 24, tachycardiomyopathy, TCM). In n = 26, pacemakers remained...	pmid:36068416 doi:10.1007/s00395-022-00949-0	Tue, 06 Sep 2022 06:00:00 -0400
12	pubmed:36068740	Polyvinyl chloride microplastics induced gut barrier dysfunction, microbiota dysbiosis and metabolism disorder in adult mice	Xuebing Chen Jingshen Zhuang Qianling Chen Luyao Xu Xia Yue Dongfang Qiao	Microplastics (MPs) are a new kind of environmental pollutant that has attracted extensive attention in recent years. MPs can be ingested by multiple organisms and mainly accumulate in the intestine. However, there is still little known about the toxic effects of MPs on humans. Here, we chose the male adult mice as the research model, which were exposed to 2 μm polyvinyl chloride (PVC) MPs at a concentration of 100 mg/kg for consecutive 60 days, to study the toxicity of PVC-MPs. The changes in...	pmid:36068740 doi:10.1016/j.ecoenv.2022.113809	Wed, 07 Sep 2022 06:00:00 -0400
13	pubmed:36068784	Losartan ameliorates renal interstitial fibrosis through metabolic pathway and Smurfs-TGF-/Smad	Junju Zou Xiaotao Zhou Yuerong Ma Rong Yu	The genesis and development of renal fibrosis involve a variety of pathways closely related to inflammation, cytokines, oxidative stress and metabolic abnormalities. Renal fibrosis is the result of a complex combination of a variety of lesions. Epithelial-mesenchymal transdifferentiation (EMT) of renal tubular epithelial cells is considered the key to renal fibrosis. Losartan is a typical Angiotensin II (ANG II) receptor antagonist and relaxes blood vessels. In this study, we investigated the...	pmid:36068784 doi:10.1016/j.biopha.2022.112931	Wed, 07 Sep 2022 06:00:00 -0400

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14	pubmed:36069453	Metabolite Production in *Alkanna tinctoria* Links Plant Development with the Recruitment of Individual Members of Microbiome Thriving at the Root-Soil Interface	Cintia Csorba Nebojša Rodi Yanyan Zhao Livio Antonielli Günter Brader Angeliki Vlachou Evangelia Tsiokanos Ismahen Lalaymia Stéphane Declerck Vassilios P Papageorgiou Andreana N Assimopoulou Angela Sessitsch	Plants are naturally associated with diverse microbial communities, which play significant roles in plant performance, such as growth promotion or fending off pathogens. The roots of Alkanna tinctoria L. are rich in naphthoquinones, particularly the medicinally used enantiomers alkannin and shikonin and their derivatives. Former studies already have shown that microorganisms may modulate plant metabolism. To further investigate the potential interaction between A. tinctoria and associated...	pmid:36069453 doi:10.1128/msystems.00451-22	Wed, 07 Sep 2022 06:00:00 -0400
15	pubmed:36069784	*Zwartia hollandica* gen. nov., sp. nov., *Jezberella montanilacus* gen. nov., sp. nov. and *Sheuella amnicola* gen. nov., comb. nov., representing the environmental GKS98 (betIII) cluster	Martin W Hahn Alexandra Pitt Johanna Schmidt Ulrike Koll Jacqueline Wolf William B Whitman Paul L E Bodelier Meina Neumann-Schaal	We present two strains affiliated with the GKS98 cluster. This phylogenetically defined cluster is representing abundant, mainly uncultured freshwater bacteria, which were observed by many cultivation-independent studies on the diversity of bacteria in various freshwater lakes and streams. Bacteria affiliated with the GKS98 cluster were detected by cultivation-independent methods in freshwater systems located in Europe, Asia, Africa and the Americas. The two strains, LF4-65^(T) (=CCUG...	pmid:36069784 doi:10.1099/ijsem.0.005513	Wed, 07 Sep 2022 06:00:00 -0400
16	pubmed:36070101	Untargeted metabolite profiling of Enterococcus villorum SB2, isolated from the vagina of pregnant women, by HR-LCMS	Shivani Singh Gaur Uday S Annapure	Enterococcus bacteria are studied in various sectors including fermentation, food and dairy industries,as well as studied for their probiotic properties but have limited use due to their possible pathogenic behavior. The present report talks about the metabolites produced, by the previously isolated Enterococcus strain, E.villorum SB2 (accession number KX830968), from the vaginal source. The growth of the bacteria in three types of media (M17, MRS and LAPTg) was compared, where the M17 media...	pmid:36070101 doi:10.1007/s11274-022-03404-3	Wed, 07 Sep 2022 06:00:00 -0400
17	pubmed:36070186	Effects of long-term simulated microgravity on liver metabolism in rhesus macaques	Beibei Zong Yujia Wang Jingyi Wang Peng Zhang Guanghan Kan Mingyang Li Juan Feng Yifan Wang Xiaoping Chen Rong Jin Qing Ge	The liver is an essential multifunctional organ and constantly communicates with nearly all the tissues in the body. Spaceflight or simulated microgravity has a significant impact on the livers of rodent models, including lipid accumulation and inflammatory cell infiltration. Whether similar liver lipotoxicity could occur in humans is not known, even though altered circulating cholesterol profile has been reported in astronauts. Using a 42-day head-down bed rest (HDBR) model in rhesus macaques,...	pmid:36070186 doi:10.1096/fj.202200544RR	Wed, 07 Sep 2022 06:00:00 -0400

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18	pubmed:36070448	Development of a mass spectrometry-based metabolomics workflow for traceability of wild and cultivated *Cordyceps sinensis*	Bo Ding Hanxiang Li Hongbo Huang Jianjun Xie Zhiyuan Wang Wenrui Chen Yiwen Tao	Cordyceps sinensis, as an expensive traditional Chinese medicine and edible fungus mycelium, lacks an effective quality evaluation method, especially and cultivated Cordyceps sinensis. In this study, a feasible workflow method was developed for traceability evaluation of wild and cultivated Cordyceps sinensis, based on mass spectrometry-based metabolomics. Mass spectrometry data were firstly acquired from Cordyceps sinensis, samples by liquid chromatography-quadrupole and time of flight mass...	pmid:36070448 doi:10.1080/19440049.2022.2118864	Wed, 07 Sep 2022 06:00:00 -0400
19	pubmed:36070505	A Direct Infusion Probe for Rapid Metabolomics of Low-Volume Samples	Cátia Marques Liangwen Liu Kyle D Duncan Ingela Lanekoff	Targeted and nontargeted metabolomics has the potential to evaluate and detect global metabolite changes in biological systems. Direct infusion mass spectrometric analysis enables detection of all ionizable small molecules, thus simultaneously providing information on both metabolites and lipids in chemically complex samples. However, to unravel the heterogeneity of the metabolic status of cells in culture and tissue a low number of cells per sample should be analyzed with high sensitivity,...	pmid:36070505 doi:10.1021/acs.analchem.2c02918	Wed, 07 Sep 2022 06:00:00 -0400