metabolomics

	NCT Number	Title	Authors	Description	Identifier	Dates
1	pubmed:36113236	Interrogating nitritation at a molecular level: Understanding the potential influence of Nitrobacter spp	Lindsey Smoot Jason Mellin Cynthia K Brinkman Inna Popova Erik R Coats	Water resource recovery facilities (WRRFs) increasingly must maximize nitrogen and phosphorus removal, but concurrently face challenges to reduce their energy usage and environmental footprint. In particular, biological nutrient removal (BNR), which targets removal of phosphorus and nitrogen, exhibits a large energy demand. However, a BNR process achieving partial oxidation of NH(3) to NO(2) (nitritation) could reduce energy demands, with secondary environmental emission benefits. Research was	pmid:36113236 doi:10.1016/j.watres.2022.119074	Fri, 16 Sep 2022 06:00:00 -0400
2	pubmed:36113270	Metabolomic transition trajectory and potential mechanisms of N-nitrosomethylbenzylamine induced esophageal squamous cell carcinoma in rats	Chao Zhao Hu Zhang Jingjing Zhou Qiwei Liu Qiang Lu Ying Zhang Xiaojin Yu Shizhi Wang Ran Liu Yuepu Pu Lihong Yin	Esophageal squamous cell carcinoma (ESCC) is an environment-relevant malignancy with a high mortality. Nitrosamines, a class of nitrogen-containing environmental carcinogens, are widely suggested as a risk factor for ESCC. However, how nitrosamines affect metabolic regulation to promote ESCC tumorigenesis is largely unknown. In this study, the transition trajectory of serum metabolism in the course of ESCC induced by N-nitrosomethylbenzylamine (NMBA) in rats was depicted by an untargeted	pmid:36113270 doi:10.1016/j.ecoenv.2022.114071	Fri, 16 Sep 2022 06:00:00 -0400
3	pubmed:36113334	Development of a multi-omics extraction method for ecotoxicology: investigation of the reproductive cycle of Gammarus fossarum	Julien Faugere Thomas Alexandre Brunet Yohann Clément Anabelle Espeyte Olivier Geffard Jérôme Lemoine Arnaud Chaumot Davide Degli-Esposti Sophie Ayciriex Arnaud Salvador	Omics study exemplified by proteomics, lipidomics or metabolomics, provides the opportunity to get insight of the molecular modifications occurring in living organisms in response to contaminants or in different physiological conditions. However, individual omics discloses only a single layer of information leading to a partial image of the biological complexity. Multiplication of samples preparation and processing can generate analytical variations resulting from several extractions and	pmid:36113334 doi:10.1016/j.talanta.2022.123806	Fri, 16 Sep 2022 06:00:00 -0400
4	pubmed:36113526	Mapping development and health effects of cooking with solid fuels in low-income and middle-income countries, 2000-18: a geospatial modelling study	Local Burden of Disease Household Air Pollution Collaborators	BACKGROUND: More than 3 billion people do not have access to clean energy and primarily use solid fuels to cook. Use of solid fuels generates household air pollution, which was associated with more than 2 million deaths in 2019. Although local patterns in cooking vary systematically, subnational trends in use of solid fuels have yet to be comprehensively analysed. We estimated the prevalence of solid-fuel use with high spatial resolution to explore subnational inequalities, assess local	pmid:36113526 doi:10.1016/S2214-109X(22)00332-1	Fri, 16 Sep 2022 06:00:00 -0400

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5	pubmed:36113578	Hippocampal metabolic recovery as a manifestation of the protective effect of ischemic preconditioning in rats	Eva Baranovicova Dagmar Kalenska Maria Kovalska Jan Lehotsky	The ever-present risk of brain ischemic events in humans and its full prevention make the detailed studies of an organism's response to ischemia at different levels essential to understanding the mechanism of the injury as well as protection. We used the four-vessel occlusion as an animal model of forebrain ischemia to investigate its impact on the metabolic alterations in both the hippocampus and the blood plasma to see changes on the systemic level. By inducing sublethal ischemic stimuli, we	pmid:36113578 doi:10.1016/j.neuint.2022.105419	Fri, 16 Sep 2022 06:00:00 -0400
6	pubmed:36113793	Hemoglobin normalization outperforms other methods for standardizing dried blood spot metabolomics: A comparative study	Abhishek Jain Montana Morris Elizabeth Z Lin Sajid A Khan Xiaomei Ma Nicole C Deziel Krystal J Godri Pollitt Caroline H Johnson	Dried blood spot (DBS) metabolomics has numerous applications in newborn health screening, exposomics, and biomonitoring of environmental chemicals in pregnant women and the elderly. However, accurate metabolite quantification is hindered by several challenges: notably the "hematocrit effect" and unknown blood-spotting volumes. Different techniques have been employed to overcome these issues but there is no consensus on the optimal normalization method for DBS metabolomics, and in some cases no	pmid:36113793 doi:10.1016/j.scitotenv.2022.158716	Fri, 16 Sep 2022 06:00:00 -0400
7	pubmed:36113916	Ultrafast 2D NMR for the analysis of complex mixtures	Célia Lhoste Benjamin Lorandel Clément Praud Achille Marchand Rituraj Mishra Arnab Dey Aurélie Bernard Jean-Nicolas Dumez Patrick Giraudeau	2D NMR is extensively used in many different fields, and its potential for the study of complex biochemical or chemical mixtures has been widely demonstrated. 2D NMR gives the ability to resolve peaks that overlap in 1D spectra, while providing both structural and quantitative information. However, complex mixtures are often analysed in situations where the data acquisition time is a crucial limitation, due to an ongoing chemical reaction or a moving sample from a hyphenated technique, or to the	pmid:36113916 doi:10.1016/j.pnmrs.2022.01.002	Fri, 16 Sep 2022 06:00:00 -0400
8	pubmed:36114074	Steroidogenic factor 1 (NR5A1) induces multiple transcriptional changes during differentiation of human gonadal-like cells	Kirsi Sepponen Karolina Lundin Dawit A Yohannes Sanna Vuoristo Diego Balboa Matti Poutanen Claes Ohlsson Steinar Hustad Ersilia Bifulco Pauliina Paloviita Timo Otonkoski Olli Ritvos Kirsi Sainio Juha S Tapanainen Timo Tuuri	Nuclear receptor subfamily 5 group A member 1 (NR5A1) encodes steroidogenic factor 1 (SF1), a key regulatory factor that determines gonadal development and coordinates endocrine functions. Here, we have established a stem cell-based model of human gonadal development and applied it to evaluate the effects of NR5A1 during the transition from bipotential gonad to testicular cells. We combined directed differentiation of human induced pluripotent stem cells (46,XY) with activation of endogenous	pmid:36114074 doi:10.1016/j.diff.2022.08.001	Fri, 16 Sep 2022 06:00:00 -0400

	NCT Number	Title	Authors	Description	Identifier	Dates
9	pubmed:36114335	Discovery, isolation, heterologous expression and mode-of-action studies of the antibiotic polyketide tatiomicin from Amycolatopsis sp. DEM30355	Bernhard Kepplinger Lina Mardiana Joseph Cowell Stephanie Morton-Laing Yousef Dashti Corinne Wills Emma C L Marrs John D Perry Joe Gray Michael Goodfellow Jeff Errington Michael R Probert William Clegg Jonathan Bogaerts Wouter Herrebout Nick E E Allenby Michael J Hall	A genomic and bioactivity informed analysis of the metabolome of the extremophile Amycolatopsis sp. DEM30355 has allowed for the discovery and isolation of the polyketide antibiotic tatiomicin. Identification of the biosynthetic gene cluster was confirmed by heterologous expression in Streptomyces coelicolor M1152. Structural elucidation, including absolute stereochemical assignment, was performed using complementary crystallographic, spectroscopic and computational methods. Tatiomicin shows	pmid:36114335 doi:10.1038/s41598-022-18726-3	Fri, 16 Sep 2022 06:00:00 -0400
10	pubmed:36114458	Probabilistic quotient's work and pharmacokinetics' contribution: countering size effect in metabolic time series measurements	Mathias Gotsmy Julia Brunmair Christoph Büschl Christopher Gerner Jürgen Zanghellini	Metabolomic time course analyses of biofluids are highly relevant for clinical diagnostics. However, many sampling methods suffer from unknown sample sizes, commonly known as size effects. This prevents absolute quantification of biomarkers. Recently, several mathematical post acquisition normalization methods have been developed to overcome these problems either by exploiting already known pharmacokinetic information or by statistical means. Here we present an improved normalization method,	pmid:36114458 doi:10.1186/s12859-022-04918-1	Fri, 16 Sep 2022 06:00:00 -0400
11	pubmed:36114515	Development of a stable semi-continuous lipid production system of an oleaginous Chlamydomonas sp. mutant using multiomics profiling	Tomoki Oyama Yuichi Kato Ryota Hidese Mami Matsuda Minenosuke Matsutani Satoru Watanabe Akihiko Kondo Tomohisa Hasunuma	CONCLUSIONS: By optimizing nitrate supply and cell density, a one-step cultivation system for Chlamydomonas sp. KAC1801 under nitrate-replete conditions was successfully developed. KAC1801 achieved a lipid productivity comparable to previously reported levels under nitrogen-limiting conditions. In the culture system of this study, metabolome and transcriptome analyses revealed a nitrogen starvation-like response in KAC1801.	pmid:36114515 doi:10.1186/s13068-022-02196-w	Fri, 16 Sep 2022 06:00:00 -0400
12	pubmed:36114669	Metabolomics-centered mining of plant metabolic diversity and function: past decade and future perspectives	Shuangqian Shen Chuansong Zhan Chenkun Yang Alisdair R Fernie Jie Luo	Plants are natural experts in organic synthesis being able to generate large numbers of specific metabolites with widely varying structures in order to adapt to variable survival challenges. Metabolomics is a research discipline that integrates the capabilities of several types of research including analytical chemistry, statistics and biochemical expertise. Its ongoing development provides solutions for the systematic understanding of quantitative changes in the levels of these metabolites and	pmid:36114669 doi:10.1016/j.molp.2022.09.007	Sat, 17 Sep 2022 06:00:00 -0400

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13	pubmed:36114745	Gankyrin and TIGAR cooperatively accelerate glucose metabolism toward PPP and TCA cycle in hepatocellular carcinoma	Chun Yang Xiao-Wen Cui Zhi-Wen Ding Tian-Yi Jiang Xiao-Fan Feng Yu-Fei Pan Yun-Kai Lin Tai-Yu Shang Qing Wang Jian Pan Jian Wang Hong-Yang Wang Li-Wei Dong	Oncogene-derived metabolic reprogramming is important for anabolic growth of cancer cells, which is now considered not to be simply rely on glycolysis and passively caused by mitochondrial damage. The present work focused on gankyrin, a relatively specific oncogene in hepatocellular carcinoma (HCC), and its impact on glycolysis and mitochondrial homeostasis. Metabolomics, RNA-seq analysis and subsequent conjoint analysis illustrated that gankyrin regulated pentose phosphate pathway (PPP),	pmid:36114745 doi:10.1111/cas.15593	Sat, 17 Sep 2022 06:00:00 -0400
14	pubmed:36115026	Lipid profiling analyses from mouse models and human infants	Laurentya Olga Ivana Bobeldijk-Pastorova Richard C Bas Florine Seidel Stuart G Snowden Samuel Furse Ken K Ong Robert Kleemann Albert Koulman	This protocol outlines a translational lipidomic approach to discover lipid biomarkers that could predict morphometric body and histological organ measurements (e.g., weight and adiposity gains) during specific stages of life (e.g., early life). We describe procedures ranging from animal experimentation and histological analyses to downstream analytical steps through lipid profiling, both in mice and humans. This protocol represents a reliable and versatile approach to translate and validate	pmid:36115026 doi:10.1016/j.xpro.2022.101679	Sat, 17 Sep 2022 06:00:00 -0400