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METLIN: a metabolite mass spectral database

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1845	Electrospun Nanofiber Mats as Smart Surfaces for Desorption Electrospray Ionization Mass Spectrometry (DESI MS)-Based Analysis and Imprint Imaging.		
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1447	High-resolution mass spectrometry associated with data mining tools for the detection of pollutants and chemical characterization of honey samples. <b>2014</b> , 62, 11335-45	38
1446	MIDAS: a database-searching algorithm for metabolite identification in metabolomics. <b>2014</b> , 86, 9496-503	80
1445	MS2Analyzer: A software for small molecule substructure annotations from accurate tandem mass spectra. <b>2014</b> , 86, 10724-31	67
1444	The role of capillary electrophoresis in metabolic profiling studies employing multiple analytical techniques. <b>2014</b> , 61, 223-235	20
1443	Integrated plasma and urine metabolomics coupled with HPLC/QTOF-MS and chemometric analysis on potential biomarkers in liver injury and hepatoprotective effects of Er-Zhi-Wan. <b>2014</b> , 406, 7367-78	34
1442	Structural mass spectrometry of tissue extracts to distinguish cancerous and non-cancerous breast diseases. <b>2014</b> , 10, 2827-37	9
1441	Objective set of criteria for optimization of sample preparation procedures for ultra-high throughput untargeted blood plasma lipid profiling by ultra performance liquid chromatography-mass spectrometry. <b>2014</b> , 86, 5766-74	153
1440	Interactive XCMS Online: simplifying advanced metabolomic data processing and subsequent statistical analyses. <b>2014</b> , 86, 6931-9	254
1439	The impact of DNA methylation technologies on drug toxicology. <b>2014</b> , 10, 637-46	8

1438	The food metabolome: a window over dietary exposure. <b>2014</b> , 99, 1286-308	335
1437	Importance of sulfur-containing metabolites in discriminating fecal extracts between normal and type-2 diabetic mice. <b>2014</b> , 13, 4220-31	24
1436	Natural products in Glycyrrhiza glabra (licorice) rhizome imaged at the cellular level by atmospheric pressure matrix-assisted laser desorption/ionization tandem mass spectrometry imaging. <b>2014</b> , 80, 161-71	54
1435	Emerging Applications of Metabolomics to Polyphenols and CVD Biomarker Discovery. <b>2014</b> , 1025-1044	
1434	Exploring metabolic pathways and regulation through functional chemoproteomic and metabolomic platforms. <b>2014</b> , 21, 1171-84	16
1433	Phenotypic mapping of metabolic profiles using self-organizing maps of high-dimensional mass spectrometry data. <b>2014</b> , 86, 6563-71	34
1432	Credentialing features: a platform to benchmark and optimize untargeted metabolomic methods. <b>2014</b> , 86, 9583-9	61
1431	Metabonomics of human colorectal cancer: new approaches for early diagnosis and biomarker discovery. <b>2014</b> , 13, 3857-70	82
1430	Response of organic N monomers in a sub-alpine soil to a dryWet cycle. <b>2014</b> , 77, 233-242	19
1429	Patch clamp electrophysiology and capillary electrophoresis-mass spectrometry metabolomics for single cell characterization. <b>2014</b> , 86, 3203-8	102
1428	Automated LC-HRMS(/MS) approach for the annotation of fragment ions derived from stable isotope labeling-assisted untargeted metabolomics. <b>2014</b> , 86, 7320-7	20
1427	Untargeted metabolomics as a screening tool for estimating compliance to a dietary pattern. <b>2014</b> , 13, 1405-18	98
1426	MET-COFEA: a liquid chromatography/mass spectrometry data processing platform for metabolite compound feature extraction and annotation. <b>2014</b> , 86, 6245-53	47
1425	Transcriptome-metabolome wide association study (TMWAS) of maneb and paraquat neurotoxicity reveals network level interactions in toxicologic mechanism. <b>2014</b> , 1, 435-444	42
1424	Mass accuracy improvement of reversed-phase liquid chromatography/electrospray ionization mass spectrometry based urinary metabolomic analysis by post-run calibration using sodium formate cluster ions. <b>2014</b> , 28, 1813-20	14
1423	The utility of metabolomics in natural product and biomarker characterization. <b>2014</b> , 1840, 3460-3474	59
1422	Lipid characterization of individual porcine oocytes by dual mode DESI-MS and data fusion. <b>2014</b> , 848, 51-60	44
1421	Discovery of a class of endogenous mammalian lipids with anti-diabetic and anti-inflammatory effects. <b>2014</b> , 159, 318-32	466

1420	Discrimination of conventional and organic white cabbage from a long-term field trial study using untargeted LC-MS-based metabolomics. <b>2014</b> , 406, 2885-97	32
1419	Detection and localization of novel hordatine-like compounds and glycosylated derivates of hordatines by imaging mass spectrometry of barley seeds. <b>2014</b> , 239, 1321-35	36
1418	Improving peak detection in high-resolution LC/MS metabolomics data using preexisting knowledge and machine learning approach. <b>2014</b> , 30, 2941-8	36
1417	Identification of metabolites from liquid chromatography-coulometric array detection profiling: gas chromatography-mass spectrometry and refractionation provide essential information orthogonal to LC-MS/microNMR. <b>2014</b> , 454, 23-32	15
1416	Application of support vector machines to metabolomics experiments with limited replicates. <b>2014</b> , 10, 1121-1128	26
1415	High-performance isotope-labeling liquid chromatography mass spectrometry for investigating the effect of drinking Goji tea on urine metabolome profiling. <b>2014</b> , 57, 678-685	6
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1413	Plant metabolomics for plant chemical responses to belowground community change by climate change. <b>2014</b> , 57, 137-149	16
1412	Proteomics, lipidomics, metabolomics: a mass spectrometry tutorial from a computer scientist's point of view. <b>2014</b> , 15 Suppl 7, S9	42
1411	Comprehensive foodomics study on the mechanisms operating at various molecular levels in cancer cells in response to individual rosemary polyphenols. <b>2014</b> , 86, 9807-15	48
1410	MALDI-guided SIMS: multiscale imaging of metabolites in bacterial biofilms. <b>2014</b> , 86, 9139-45	59
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1404	Liquid chromatography time of flight mass spectrometry based environmental metabolomics for the analysis of Pseudomonas putida Bacteria in potable water. <b>2014</b> , 966, 179-86	16
1403	Regioselective solvent-phase deuteration of polyphenolic compounds informs their identification by mass spectrometry. <b>2014</b> , 452, 76-85	5

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1401	Metabolomics analysis of collagen-induced arthritis in rats and interventional effects of oral tolerance. <b>2014</b> , 458, 49-57	18
1400	Feasibility of detecting prostate cancer by ultraperformance liquid chromatography-mass spectrometry serum metabolomics. <b>2014</b> , 13, 3444-54	43
1399	Metabolomics and proteomics reveal impacts of chemically mediated competition on marine plankton. <b>2014</b> , 111, 9009-14	90
1398	A combined metabolomic and phylogenetic study reveals putatively prebiotic effects of high molecular weight arabino-oligosaccharides when assessed by in vitro fermentation in bacterial communities derived from humans. <b>2014</b> , 28, 68-77	21
1397	Alterations in energy/redox metabolism induced by mitochondrial and environmental toxins: a specific role for glucose-6-phosphate-dehydrogenase and the pentose phosphate pathway in paraquat toxicity. <b>2014</b> , 9, 2032-48	63
1396	Towards automated discrimination of lipids versus peptides from full scan mass spectra. <b>2014</b> , 4, 87-100	5
1395	Accurate dereplication of bioactive secondary metabolites from marine-derived fungi by UHPLC-DAD-QTOFMS and a MS/HRMS library. <b>2014</b> , 12, 3681-705	99
1394	Comprehensive metabolomic study of platelets reveals the expression of discrete metabolic phenotypes during storage. <b>2014</b> , 54, 2911-23	40
1393	Copper oxide nanoparticle toxicity profiling using untargeted metabolomics. <b>2016</b> , 13, 49	48
1392	Exometabolom analysis of breast cancer cell lines: Metabolic signature. <b>2015</b> , 5, 13374	18
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1390	Acylcarnitines are anticoagulants that inhibit factor Xa and are reduced in venous thrombosis, based on metabolomics data. <b>2015</b> , 126, 1595-600	30
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1388	Traveling-wave ion mobility-mass spectrometry in metabolomics: workflows and bioinformatic tools. <b>2015</b> , 68-80	2
1387	New Technologies for Studying Biofilms. <b>2015</b> , 3,	67
1386	Lipidomics comparing DCD and DBD liver allografts uncovers lysophospholipids elevated in recipients undergoing early allograft dysfunction. <b>2015</b> , 5, 17737	17
1385	Methodologies for Effect-Directed Analysis: Environmental Applications, Food Analysis, and Drug Discovery. <b>2015</b> , 109-163	1

1384	Arteriovenous Blood Metabolomics: A Readout of Intra-Tissue Metabostasis. <b>2015</b> , 5, 12757	47
1383	A multi-platform metabolomics approach identifies highly specific biomarkers of bacterial diversity in the vagina of pregnant and non-pregnant women. <b>2015</b> , 5, 14174	73
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1381	Metabolomic profiling of Burkholderia pseudomallei using UHPLC-ESI-Q-TOF-MS reveals specific biomarkers including 4-methyl-5-thiazoleethanol and unique thiamine degradation pathway. <b>2015</b> , 5, 26	10
1380	Combination of CE-MS and advanced chemometric methods for high-throughput metabolic profiling. <b>2015</b> , 36, 2324-2335	22
1379	An in silico MS/MS library for automatic annotation of novel FAHFA lipids. <b>2015</b> , 7, 53	51
1378	LC-MS untargeted metabolomic analysis of drug-induced hepatotoxicity in HepG2 cells. <b>2015</b> , 36, 2294-2302	25
1377	Isotope-labeled differential profiling of metabolites using N-benzoyloxysuccinimide derivatization coupled to liquid chromatography/high-resolution tandem mass spectrometry. <b>2015</b> , 29, 1632-40	9
1376	Release of ecologically relevant metabolites by the cyanobacterium Synechococcus elongates CCMP 1631. <b>2015</b> , 17, 3949-63	53
1375	Application of NMR Spectroscopy to Assessment of Radiation Dose and Time Lapse. <b>2015</b> , 36, 1328-1334	2
1374	High-resolution MALDI-FT-ICR MS imaging for the analysis of metabolites from formalin-fixed, paraffin-embedded clinical tissue samples. <b>2015</b> , 237, 123-32	99
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1372	Untargeted Metabolomics Reveals Predominant Alterations in Lipid Metabolism Following Light Exposure in Broccoli Sprouts. <b>2015</b> , 16, 13678-91	15
1371	Next-generation technologies for multiomics approaches including interactome sequencing. <b>2015</b> , 2015, 104209	22
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1369	Colonization Resistance of the Gut Microbiota against Clostridium difficile. <b>2015</b> , 4, 337-57	36
1368	Intake of hydrolyzed casein is associated with reduced body fat accretion and enhanced phase II metabolism in obesity prone C57BL/6J mice. <b>2015</b> , 10, e0118895	9
1367	Metabolic Consequences of Chronic Alcohol Abuse in Non-Smokers: A Pilot Study. <b>2015</b> , 10, e0129570	8

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1365	The metabolic profile of grape berry skin and a comparison of metabolomes before veraison and at harvest. <b>2015</b> , 32, 267-272	4
1364	Metabolomic analysis to define and compare the effects of PAHs and oxygenated PAHs in developing zebrafish. <b>2015</b> , 140, 502-10	45
1363	SpeckTackle: JavaScript charts for spectroscopy. <b>2015</b> , 7, 17	10
1362	Profiling ribonucleotide modifications at full-transcriptome level: a step toward MS-based epitranscriptomics. <b>2015</b> , 21, 1361-74	31
1361	Identification of Plasma Metabolites Prognostic of Acute Kidney Injury after Cardiac Surgery with Cardiopulmonary Bypass. <b>2015</b> , 14, 2897-905	14
1360	Untargeted metabolomics analysis revealed changes in the composition of glycerolipids and phospholipids in Bacillus subtilis under 1-butanol stress. <b>2015</b> , 99, 5971-83	19
1359	Metabolome-wide association study of phenylalanine in plasma of common marmosets. <b>2015</b> , 47, 589-601	36
1358	In Situ Analysis of Small Populations of Adherent Mammalian Cells Using Laser Ablation Electrospray Ionization Mass Spectrometry in Transmission Geometry. <b>2015</b> , 87, 12130-6	25
1357	ATP-binding Cassette Subfamily C Member 5 (ABCC5) Functions as an Efflux Transporter of Glutamate Conjugates and Analogs. <b>2015</b> , 290, 30429-40	36
1356	A reinvigorated era of bacterial secondary metabolite discovery. <b>2015</b> , 24, 104-11	8
1355	Metabolite identification for mass spectrometry-based metabolomics using multiple types of correlated ion information. <b>2015</b> , 87, 2143-51	55
1354	Spatially resolved metabolic phenotyping of breast cancer by desorption electrospray ionization mass spectrometry. <b>2015</b> , 75, 1828-37	105
1353	Temporal metabolomic responses of cultured HepG2 liver cells to high fructose and high glucose exposures. <b>2015</b> , 11, 707-721	14
1352	Untargeted UPLC-MS profiling pipeline to expand tissue metabolome coverage: application to cardiovascular disease. <b>2015</b> , 87, 4184-93	128
1351	Improved data-dependent acquisition for untargeted metabolomics using gas-phase fractionation with staggered mass range. <b>2015</b> , 87, 2861-8	30
1350	NMR spectroscopic search module for Spektraris, an online resource for plant natural product identificationTaxane diterpenoids from Taxus Imedia cell suspension cultures as a case study. <b>2015</b> , 113, 87-95	20
1349	Metabolomic serum profiling detects early-stage high-grade serous ovarian cancer in a mouse model. <b>2015</b> , 14, 917-27	15

1348	Ion mobility-derived collision cross section as an additional measure for lipid fingerprinting and identification. <b>2015</b> , 87, 1137-44	199
1347	Multidimensional analytical approach based on UHPLC-UV-ion mobility-MS for the screening of natural pigments. <b>2015</b> , 87, 2593-9	43
1346	Metabolic phenotyping of atherosclerotic plaques reveals latent associations between free cholesterol and ceramide metabolism in atherogenesis. <b>2015</b> , 14, 1389-99	53
1345	Faecal metabolomic fingerprint after moderate consumption of red wine by healthy subjects. <b>2015</b> , 14, 897-905	48
1344	Perturbations of tyrosine metabolism promote the indolepyruvate pathway via tryptophan in host and microbiome. <b>2015</b> , 114, 431-7	33
1343	A new strategy for MS/MS data acquisition applying multiple data dependent experiments on Orbitrap mass spectrometers in non-targeted metabolomic applications. <b>2015</b> , 11, 1068-1080	37
1342	Isofunctional enzymes PAD1 and UbiX catalyze formation of a novel cofactor required by ferulic acid decarboxylase and 4-hydroxy-3-polyprenylbenzoic acid decarboxylase. <b>2015</b> , 10, 1137-44	65
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1340	Metabolomics and diabetes: analytical and computational approaches. <b>2015</b> , 64, 718-32	110
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1337	Metabolomics in the developmental origins of obesity and its cardiometabolic consequences. <b>2015</b> , 6, 65-78	35
1336	First insights into serum metabolomics of trenbolone/estradiol implanted bovines; screening model to predict hormone-treated and control animalsstatus. <b>2015</b> , 11, 1184-1196	15
1335	Development and Application of a High-Resolution Imaging Mass Spectrometer for the Study of Plant Tissues. <b>2015</b> , 56, 1329-38	30
1334	An integrated targeted metabolomic platform for high-throughput metabolite profiling and automated data processing. <b>2015</b> , 11, 1575-1586	58
1333	Computational and statistical analysis of metabolomics data. <b>2015</b> , 11, 1492-1513	135
1332	MetTailor: dynamic block summary and intensity normalization for robust analysis of mass spectrometry data in metabolomics. <b>2015</b> , 31, 3645-52	2
1331	Dimethyl fumarate modulates antioxidant and lipid metabolism in oligodendrocytes. <b>2015</b> , 5, 169-175	45

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1329	Retention Time Prediction Improves Identification in Nontargeted Lipidomics Approaches. <b>2015</b> , 87, 7698-704	50
1328	Biomarker Development for Chronic Obstructive Pulmonary Disease. From Discovery to Clinical Implementation. <b>2015</b> , 192, 1162-70	42
1327	Novel metabolic markers for the risk of diabetes development in American Indians. <b>2015</b> , 38, 220-7	49
1326	Metabolomics of plant phosphorus-starvation response. <b>2015</b> , 215-236	
1325	Predicting drug metabolism: experiment and/or computation?. <b>2015</b> , 14, 387-404	255
1324	Targeting of the hydrophobic metabolome by pathogens. <b>2015</b> , 16, 439-60	10
1323	Metabolomic composition of normal aged and cataractous human lenses. <b>2015</b> , 134, 15-23	52
1322	Metabolome analysis via comprehensive two-dimensional liquid chromatography: identification of modified nucleosides from RNA metabolism. <b>2015</b> , 407, 3555-66	30
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1320	Influence of Desorption Conditions on Analyte Sensitivity and Internal Energy in Discrete Tissue or Whole Body Imaging by IR-MALDESI. <b>2015</b> , 26, 899-910	18
1319	Metabolome searcher: a high throughput tool for metabolite identification and metabolic pathway mapping directly from mass spectrometry and using genome restriction. <b>2015</b> , 16, 62	27
1318	High-resolution metabolomics to discover potential parasite-specific biomarkers in a Plasmodium falciparum erythrocytic stage culture system. <b>2015</b> , 14, 122	37
1317	Open-access metabolomics databases for natural product research: present capabilities and future potential. <b>2015</b> , 3, 22	89
1316	Non-target screening with high-resolution mass spectrometry: critical review using a collaborative trial on water analysis. <b>2015</b> , 407, 6237-55	358
1315	Untargeted metabolic profiling identifies interactions between Huntington's disease and neuronal manganese status. <b>2015</b> , 7, 363-70	24
1314	Development of a metabolic biosignature for detection of early Lyme disease. <b>2015</b> , 60, 1767-75	52
1313	Mass spectrometry tools and workflows for revealing microbial chemistry. <b>2015</b> , 140, 4949-66	30

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1311	Molecular cartography of the human skin surface in 3D. <b>2015</b> , 112, E2120-9	237
1310	Plasma metabolic profiling after cortical spreading depression in a transgenic mouse model of hemiplegic migraine by capillary electrophoresismass spectrometry. <b>2015</b> , 11, 1462-71	21
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1308	Metabolic fingerprint after acute and under sustained consumption of a functional beverage based on grape skin extract in healthy human subjects. <b>2015</b> , 6, 1288-98	22
1307	Exometabolomics and MSI: deconstructing how cells interact to transform their small molecule environment. <b>2015</b> , 34, 209-16	40
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1305	Insights on profiling of phorbol, deoxyphorbol, ingenol and jatrophane diterpene esters by high performance liquid chromatography coupled to multiple stage mass spectrometry. <b>2015</b> , 1422, 128-139	21
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1303	Changing in lipid profile induced by the mutation of Foxn1 gene: A lipidomic analysis of Nude mice skin. <b>2015</b> , 118, 234-43	13
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1301	Proteome and metabolome profiling of wild-type and YCA1-knock-out yeast cells during acetic acid-induced programmed cell death. <b>2015</b> , 128, 173-88	21
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1295	Developmental and Metabolic Plasticity of White-Skinned Grape Berries in Response to Botrytis cinerea during Noble Rot. <b>2015</b> , 169, 2422-43	60

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1294	Pivotal role of computers and software in mass spectrometry - SEQUEST and 20 years of tandem MS database searching. <b>2015</b> , 26, 1804-13	20
1293	Determining conserved metabolic biomarkers from a million database queries. <b>2015</b> , 31, 3721-4	7
1292	Global Metabonomic and Proteomic Analysis of Human Conjunctival Epithelial Cells (IOBA-NHC) in Response to Hyperosmotic Stress. <b>2015</b> , 14, 3982-95	22
1291	DnsID in MyCompoundID for rapid identification of dansylated amine- and phenol-containing metabolites in LC-MS-based metabolomics. <b>2015</b> , 87, 9838-45	78
1290	Effect of Copper on Fatty Acid Profiles in Non- and Semifermented Teas Analyzed by LC-MS-Based Nontargeted Screening. <b>2015</b> , 63, 8519-26	4
1289	Reference Standardization for Mass Spectrometry and High-resolution Metabolomics Applications to Exposome Research. <b>2015</b> , 148, 531-43	123
1288	Metabolomics analysis of the toxicity pathways of triphenyl phosphate in HepaRG cells and comparison to oxidative stress mechanisms caused by acetaminophen. <b>2015</b> , 29, 2045-54	28
1287	St. John's Wort Attenuates Colorectal Carcinogenesis in Mice through Suppression of Inflammatory Signaling. <b>2015</b> , 8, 786-95	4
1286	Development of nanoelectrospray high resolution isotope dilution mass spectrometry for targeted quantitative analysis of urinary metabolites: application to population profiling and clinical studies. <b>2015</b> , 7, 5122-5133	8
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1283	Combining DI-ESI-MS and NMR datasets for metabolic profiling. <b>2015</b> , 11, 391-402	55
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1281	Network-based approach for analyzing intra- and interfluid metabolite associations in human blood, urine, and saliva. <b>2015</b> , 14, 1183-94	33
1280	Biological Basis of Alcohol-Induced Cancer. <b>2015</b> ,	3
1279	Application of mass spectrometry-based metabolomics in identification of early noninvasive biomarkers of alcohol-induced liver disease using mouse model. <b>2015</b> , 815, 217-38	14
1278	Metabolome and proteome profiling of complex I deficiency induced by rotenone. <b>2015</b> , 14, 224-35	43
1277	Relative quantification of amine-containing metabolites using isobaric N,N-dimethyl leucine (DiLeu) reagents via LC-ESI-MS/MS and CE-ESI-MS/MS. <b>2015</b> , 140, 467-75	43

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1275	Mass spectral similarity for untargeted metabolomics data analysis of complex mixtures. <b>2015</b> , 377, 719-717	53
1274	Assessing drug and metabolite detection in liver tissue by UV-MALDI and IR-MALDESI mass spectrometry imaging coupled to FT-ICR MS. <b>2015</b> , 377, 448-155	43
1273	Methods in Membrane Lipids. 2015,	4
1272	A comparative LC-MS based profiling approach to analyze lipid composition in tissue culture systems. <b>2015</b> , 1232, 103-13	3
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1269	Determination of Metabolites in the Cerebellum of 2,3,7,8-Tetrachlorodibenzo-p-Dioxin Exposed Mice by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry. <b>2015</b> , 48, 594-604	
1268	Comparison of capillary electrophoresis-mass spectrometry and hydrophilic interaction chromatography-mass spectrometry for anionic metabolic profiling of urine. <b>2015</b> , 132, 1-7	25
1267	An explorative study of the effect of apple and apple products on the human plasma metabolome investigated by LCMS profiling. <b>2015</b> , 11, 27-39	14
1266	Competitive fragmentation modeling of ESI-MS/MS spectra for putative metabolite identification. <b>2015</b> , 11, 98-110	237
1265	C Metabolomics: NMR and IROA for Unknown Identification. <b>2016</b> , 4, 116-120	15
1264	Understanding Metabolomics in Biomedical Research. <b>2016</b> , 31, 7-16	37
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1262	Population Screening for Biological and Environmental Properties of the Human Metabolic Phenotype. <b>2016</b> , 167-211	18
1261	Processing and Visualization of Metabolomics Data Using R. <b>2016</b> ,	9
1260	Evidence for Strain-Specific Exometabolomic Responses of the Coccolithophore Emiliania huxleyi to Grazing by the Dinoflagellate Oxyrrhis marina. <b>2016</b> , 3,	4
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1224	Application of Clinical Bioinformatics. 2016,	8
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87	Energy dissipation in early detection of cellular responses to metabolic challenges.	
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85	Time-dependent metabolomics uncover dynamic metabolic adaptions in MCF-7 cells exposed to bisphenol A. <b>2023</b> , 17,	1
84	Enhancing Genome-Scale Model by Integrative Exometabolome and Transcriptome: Unveiling Carbon Assimilation towards Sphingolipid Biosynthetic Capability of Cordyceps militaris. <b>2022</b> , 8, 887	O
83	Untargeted metabolomics analysis based on HS-SPME-GC-MS and UPLC-Q-TOF/MS reveals the contribution of stem to the flavor of Cyclocarya paliurus herbal extract. <b>2022</b> , 167, 113819	O
82	Metabolomics analysis of unresolved molecular variability in stoichiometry dynamics of a stream dissolved organic matter. <b>2022</b> , 223, 118923	O
81	Long time stability of 35 small endogenous biomolecules in dried urine spotted on various surfaces and environmental conditions. <b>2022</b> , 339, 111420	O
80	Metabolomic and elemental profiling of blood serum in bladder cancer. 2022,	O
79	Angong Niuhuang Pill ameliorates cerebral ischemia/reperfusion injury in mice partly by restoring gut microbiota dysbiosis. 13,	O
78	Validation of Sennae Folium specification grade classification based on UPLC-Q-TOF/MS spectrum-effect relationship. <b>2022</b> , 15, 104223	0
77	Comparison of the efficacies of Huangqi-Danshen herbal pair compatibility with wild-simulated and transplanted Astragali Radix based on a novel metabolomics strategy. <b>2022</b> , 230, 104658	O
76	Metabolomics analysis reveals differences in milk metabolism and fermentation rate between individual Lactococcus lactis subsp. lactis strains. <b>2022</b> , 162, 111920	O
75	Engineering microbial biofactories for a sustainable future. <b>2023</b> , 25-58	O
74	Artificial intelligence in microbial natural product drug discovery: current and emerging role.	0
73	Application of Bmics technologies in tropical and subtropical fruit crops. 2022, 119-145	O
72	Metaboloma use in ophthalmology. <b>2022</b> , 81,	0
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69	A look beyond dietary (poly)phenols: The low molecular weight phenolic metabolites and their concentrations in human circulation. <b>2022</b> , 21, 3931-3962	1
68	Birth Weight and Early Postnatal Outcomes: Association with the Cord Blood Lipidome. <b>2022</b> , 14, 3760	O
67	TurboPutative: A web server for data handling and metabolite classification in untargeted metabolomics. 9,	Ο
66	Data Processing and Analysis in Mass Spectrometry-Based Metabolomics. <b>2023</b> , 207-239	O
65	An initial investigation of accuracy required for the identification of small molecules in complex samples using quantum chemical calculated NMR chemical shifts. <b>2022</b> , 14,	O
64	Effects of uteroplacental insufficiency on growth-restricted rats with altered lung development: A metabolomic analysis. 10,	О
63	Metabolomic Profiling of End-Stage Heart Failure Secondary to Chronic Chagas Cardiomyopathy. <b>2022</b> , 23, 10456	O
62	Evaluation of Metabolism of a Defined Pesticide Mixture through Multiple In Vitro Liver Models. <b>2022</b> , 10, 566	2
61	The Formation of Refractory Dissolved Organic Nitrogen From Free Amino Acids in the Ocean. <b>2022</b> , 49,	O
60	Multi-modal mass spectrometry imaging reveals single-cell metabolic states in mammalian liver.	О
59	Understanding the nutraceutical diversity through a comparative analysis of the taproot metabolomes of different edible radish types via UHPLCQTOFMS. <b>2022</b> , 134469	O
58	Databases and Tools to Investigate Protein-Metabolite Interactions. 2023, 231-249	О
57	Serum metabolites associated with wholegrain consumption using nontargeted metabolic profiling: a discovery and reproducibility study.	O
56	Data Processing in Metabolomics Capillary Electrophoresis Mass Spectrometry. 2022, 121-145	О
55	Mixed Tree Nuts, Cognition and Gut Microbiota: a 4-week, Placebo-Controlled, Randomized Crossover Trial in Healthy Non-Elderly Adults.	O
54	Chemical Imaging Reveals Diverse Functions of Tricarboxylic Acid Metabolites in Root Growth and Development.	О
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51	LargeMetabo: an out-of-the-box tool for processing and analyzing large-scale metabolomic data.	2
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47	A class of anti-inflammatory lipids decrease with aging in the central nervous system.	o
46	Metabolome-wide association study on ABCA7 indicates a role of ceramide metabolism in Alzheimer disease. <b>2022</b> , 119,	1
45	Desorption Electrospray Ionization Mass Spectrometry Imaging Allows Spatial Localization of Changes in Acetaminophen Metabolism in the Liver after Intervention with 4-Methylpyrazole. <b>2022</b> , 33, 2094-2107	1
44	Phytochemical Profile, Plant Precursors and Some Properties of Georgian Propolis. 2022, 27, 7714	2
43	An untargeted metabolomics approach to characterize dissolved organic matter in groundwater of the Samail Ophiolite.	О
42	Metabolomics profiling in acute liver transplant rejection in a pediatric population. 2022, 12,	0
41	IR-MALDI Mass Spectrometry Imaging with Plasma Post-Ionization of Nonpolar Metabolites.	О
40	Nontargeted metabolomic analysis of four different parts of Actinidia arguta by UPLC-Q-TOF-MSE. <b>2023</b> , 163, 112228	0
39	What I wish I had known before starting my PhD□	o
38	Critical assessment of chromatographic metadata in publicly available metabolomics data repositories. <b>2022</b> , 18,	0
37	Applications of machine learning in metabolomics: Disease modeling and classification. 13,	O
36	Metabolomics of asthma, COPD, and asthma-COPD overlap: an overview. 1-18	0
35	Impact of industrial freezing on quality attributes of carrot slices. <b>2022</b> , 301-308	O

34	Metabolomic Profiling to Identify Early Urinary Biomarkers and Metabolic Pathway Alterations in Autosomal Dominant Polycystic Kidney Disease.	O
33	Good practices and recommendations for using and benchmarking computational metabolomics metabolite annotation tools. <b>2022</b> , 18,	1
32	DNMT3B PWWP mutations cause hypermethylation of heterochromatin.	О
31	Plant Metabolomics: The Great Potential of Plant Metabolomics in Big Data Biology. <b>2022</b> , 50-66	O
30	Distinct Quality Changes of Asparagus during Growth by Widely Targeted Metabolomics Analysis. <b>2022</b> , 70, 15999-16009	О
29	Advanced analytical and informatic strategies for metabolite annotation in untargeted metabolomics. <b>2022</b> , 116903	O
28	Relationship between 4-Hydroxynonenal (4-HNE) as Systemic Biomarker of Lipid Peroxidation and Metabolomic Profiling of Patients with Prostate Cancer. <b>2023</b> , 13, 145	1
27	Urine Metabolome Dynamics Discriminate Influenza Vaccination Response. <b>2023</b> , 15, 242	O
26	Diagnostic biomarker panels of osteoarthritis: UPLC-QToF/MS-based serum metabolic profiling. 11, e14563	O
25	Guidelines and considerations for building multidimensional libraries for untargeted MS-based metabolomics. <b>2023</b> , 19,	O
24	Integrating Metabolomics and Gene Expression Underlying Potential Biomarkers Compounds Associated with Antioxidant Activity in Southern Grape Seeds. <b>2023</b> , 13, 210	О
23	QC-GN2oMS2: a Graph Neural Net for High Resolution Mass Spectra Prediction.	O
22	Metabolomics of diabetes and cardiovascular disease. <b>2023</b> , 239-260	О
21	Metabolomic Approaches to Study Nutritional Aspects in Cereal Crops. <b>2023</b> , 127-148	O
20	Data Science and Plant Metabolomics. <b>2023</b> , 13, 454	О
19	Ultra-performance liquid chromatography coupled with quadrupole high-resolution time-of-flight mass spectrometry for metabolite profiling and biological activity of Stellaria pallida (Dumort) Pir[] <b>2023</b> , 32, 975-989	O
18	Associations of altered hepatic gene expression in American lifestyle-induced obesity syndrome diet-fed mice with metabolic changes during NAFLD development and progression. <b>2023</b> , 115, 109307	O
17	A comparison of feature extraction capabilities of advanced UHPLC-HRMS data analysis tools in plant metabolomics. <b>2023</b> , 1254, 341127	O

16	Gas chromatography-mass spectrometry and liquid chromatography-mass spectrometry metabolomics platforms: Tools for plant oligosaccharides analysis. <b>2023</b> , 5, 100304	О
15	Toxicological effects of cyanobacterial metabolites on zebrafish larval development. <b>2023</b> , 125, 102430	O
14	Metabolomic profiling reveals bacterial metabolic adaptation strategies and new metabolites. <b>2023</b> , 74, 102287	O
13	Untargeted metabolomic analysis to explore the impact of soil amendments in a non-conventional wastewater treatment. <b>2023</b> , 870, 161890	O
12	From structural determination of natural products in complex mixtures to single cell resolution: Perspectives on advances and challenges for mass spectrometry. 2,	0
11	Divergence in metabolomic profile in clownfish and damselfish skin mucus. 11,	O
10	Stable isotope-resolved metabolomics based on mass spectrometry: Methods and their applications. <b>2023</b> , 160, 116985	0
9	Liquid Crystal Monomer: A Potential PPAR[Antagonist. <b>2023</b> , 57, 3758-3771	O
8	Identifying Plasma and Urinary Biomarkers of Fermented Food Intake and Their Associations with Cardiometabolic Health in a Dutch Observational Cohort. <b>2023</b> , 71, 4426-4439	O
7	Phytochemical Study on Seeds of Paeonia clusii subsp. rhodiaAntioxidant and Anti-Tyrosinase Properties. <b>2023</b> , 24, 4935	O
6	An untargeted exometabolomics approach to characterize dissolved organic matter in groundwater of the Samail Ophiolite. 14,	0
5	TXNIP loss expands Myc-dependent transcriptional programs by increasing Myc genomic binding. <b>2023</b> , 21, e3001778	O
4	Comparative metabolomics analysis reveals alkaloid repertoires in young and mature Mitragyna speciosa (Korth.) Havil. Leaves. <b>2023</b> , 18, e0283147	0
3	The impact of culture systems on the gut microbiota and gut metabolome of bighead carp (Hypophthalmichthys nobilis). <b>2023</b> , 5,	O
2	DT-109 ameliorates nonalcoholic steatohepatitis in nonhuman primates. <b>2023</b> ,	0
1	Plasma metabolomic response to high-carbohydrate meals of differing glycaemic load in overweight women.	O