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XCMS: processing mass spectrometry data for metabolite profiling using nonlinear peak alignment, matching, and identification

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2233	SMART: Statistical Metabolomics Analysis An R Tool.		
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2228	Toxicokinetics of Brominated Azo Dyes in the Early Life Stages of Zebrafish (<i>Danio rerio</i>) Is Prone to Aromatic Substituent Changes.		
2227	Metabolomics data analysis, visualization, and integration. 2007 , 406, 409-36		23
2226	Chromatographic alignment of ESI-LC-MS proteomics data sets by ordered bijective interpolated warping. <i>Analytical Chemistry</i> , 2006 , 78, 6140-52	7.8	173
2225	Storage and Processing of Mass Spectrometry Data.		
2224	Endocannabinoid metabolism in the absence of fatty acid amide hydrolase (FAAH): discovery of phosphorylcholine derivatives of N-acyl ethanolamines. 2006 , 45, 11267-77		37
2223	MET-IDEA: data extraction tool for mass spectrometry-based metabolomics. <i>Analytical Chemistry</i> , 2006 , 78, 4334-41	7.8	220
2222	Nonlinear data alignment for UPLC-MS and HPLC-MS based metabolomics: quantitative analysis of endogenous and exogenous metabolites in human serum. <i>Analytical Chemistry</i> , 2006 , 78, 3289-95	7.8	252
2221	A FAAH-regulated class of N-acyl taurines that activates TRP ion channels. 2006 , 45, 9007-15		171
2220	LC-MS in Metabonomics: Optimization of Experimental Conditions for the Analysis of Metabolites in Human Urine. 2006 , 29, 2475-2497		26
2219	Proteome informatics I: bioinformatics tools for processing experimental data. 2006 , 6, 5435-44		95
2218	Gas chromatography mass spectrometry-based metabolite profiling in plants. 2006 , 1, 387-96		1409
2217	An enzyme that regulates ether lipid signaling pathways in cancer annotated by multidimensional profiling. 2006 , 13, 1041-50		154
2216	Mass spectrometry reveals specific and global molecular transformations during viral infection. 2006 , 5, 2405-16		39
2215	Metabolic profiling technologies for biomarker discovery in biomedicine and drug development. 2006 , 7, 1055-75		78
2214	Phospholipid capture combined with non-linear chromatographic correction for improved serum metabolite profiling. 2006 , 2, 145-154		24
2213	Systems biology, metabolic modelling and metabolomics in drug discovery and development. 2006 , 11, 1085-92		236

2212	MathDAMP: a package for differential analysis of metabolite profiles. 2006 , 7, 530		125
2211	Current literature in mass spectrometry. 2006 , 41, 1520-31		
2210	Proteomic-based biomarker discovery with emphasis on cerebrospinal fluid and multiple sclerosis. 2006 , 7, 147-58		15
2209	PEPPER, a platform for experimental proteomic pattern recognition. 2006 , 5, 1927-41		119
2208	Biological LC/MS Preprocessing and Analysis with jABC, jETI and xcms. 2006 ,		4
2207	2D NMR metabonomic analysis: a novel method for automated peak alignment. 2007 , 23, 2926-33		20
2206	Computational methods for the comparative quantification of proteins in label-free LCn-MS experiments. 2008 , 9, 156-65		62
2205	A molecular timetable for apical bud formation and dormancy induction in poplar. 2007 , 19, 2370-90		362
2204	Maternal PPAR gamma protects nursing neonates by suppressing the production of inflammatory milk. 2007 , 21, 1895-908		89
2203	A Fast and Accurate Algorithm for the Quantification of Peptides from Mass Spectrometry Data. 2007 , 473-487		6
2202	Metabolomics and metabolite profiling: past heroes and future developments. 2007 , 13, 45-50		36
2201	Mobilization of pro-inflammatory lipids in obese Plscr3-deficient mice. 2007 , 8, R38		16
2200	Analytical aspects of plant metabolite profiling platforms: current standings and future aims. 2007 , 6, 480-97		79
2199	Evolutionary Computation, Machine Learning and Data Mining in Bioinformatics. 2007 ,		2
2198	A new algorithm using cross-assignment for label-free quantitation with LC-LTQ-FT MS. 2007 , 6, 2186-94		45
2197	Closed-loop, multiobjective optimization of two-dimensional gas chromatography/mass spectrometry for serum metabolomics. <i>Analytical Chemistry</i> , 2007 , 79, 464-76	7.8	87
2196	Bioinformatics Research and Development. 2007 ,		3
2195	Relative quantification of carboxylic acid metabolites by liquid chromatography-mass spectrometry using isotopic variants of cholamine. <i>Analytical Chemistry</i> , 2007 , 79, 5143-9	7.8	62

2194	Personalized medicine and proteomics: lessons from non-small cell lung cancer. 2007 , 6, 2925-35		51
2193	Tools in metabonomics: an integrated validation approach for LC-MS metabolic profiling of mercapturic acids in human urine. <i>Analytical Chemistry</i> , 2007 , 79, 2918-26	7.8	76
2192	Metabolomics identifies perturbations in human disorders of propionate metabolism. 2007 , 53, 2169-76		134
2191	Untargeted analysis of mass spectrometry data for elucidation of metabolites and function of enzymes. <i>Analytical Chemistry</i> , 2007 , 79, 3355-62	7.8	19
2190	Research in Computational Molecular Biology. 2007 ,		1
2189	From exogenous to endogenous: the inevitable imprint of mass spectrometry in metabolomics. 2007 , 6, 459-68		241
2188	Pharmacometabonomic phenotyping reveals different responses to xenobiotic intervention in rats. 2007 , 6, 1364-70		86
2187	Accurate mass measurements in proteomics. 2007 , 107, 3621-53		92
2186	Analytical methods from the perspective of method standardization. 2007 , 11-52		16
2185	MetHouse: Raw and Preprocessed Mass Spectrometry Data. 2007 , 4, 107-114		4
2184	Highly-parallel metabolomics approaches using LC-MS for pharmaceutical and environmental analysis. 2007 , 26, 625-636		43
2183	Metabolomics technologies and metabolite identification. 2007 , 26, 855-866		271
2182	Data processing for mass spectrometry-based metabolomics. 2007 , 1158, 318-28		478
2181	An objective comparison of pre-processing methods for enhancement of liquid chromatography-mass spectrometry data. 2007 , 1172, 135-50		23
2180	A gender-specific discriminator in Sprague-Dawley rat urine: the deployment of a metabolic profiling strategy for biomarker discovery and identification. 2007 , 362, 182-92		45
2179	A comprehensive urinary metabolomic approach for identifying kidney cancer. 2007 , 363, 185-95		405
2178	Application of ethyl chloroformate derivatization for gas chromatography-mass spectrometry based metabonomic profiling. 2007 , 583, 277-83		141
2177	Mass spectral profiling: an effective tool for quality control of herbal medicines. 2007 , 604, 89-98		37

2176	Automated reduction and interpretation of multidimensional mass spectra for analysis of complex peptide mixtures. 2007 , 260, 20-30	12
2175	Ultra-performance liquid chromatography/time-of-flight mass spectrometry based metabolomics of raw and steamed Panax notoginseng. 2007 , 21, 519-28	153
2174	Chemoselective probes for metabolite enrichment and profiling. 2007 , 4, 429-35	77
2173	Untargeted large-scale plant metabolomics using liquid chromatography coupled to mass spectrometry. 2007 , 2, 778-91	640
2172	Metabolite profile analysis: from raw data to regression and classification. 2008 , 132, 150-61	52
2171	The EIpeptiDi tool: enhancing peptide discovery in ICAT-based LC MS/MS experiments. 2007 , 8, 255	7
2170	A dynamic programming approach for the alignment of signal peaks in multiple gas chromatography-mass spectrometry experiments. 2007 , 8, 419	53
2169	On consensus biomarker selection. 2007 , 8 Suppl 5, S5	23
2168	Tools for computational processing of LC-MS datasets: a user's perspective. 2007 , 86, 281-90	23
2167	High-precision frequency measurements: indispensable tools at the core of the molecular-level analysis of complex systems. 2007 , 389, 1311-27	218
2166	Analytical tools and approaches for metabolite identification in early drug discovery. 2007 , 24, 248-57	43
2165	Biomarkers for neuroAIDS: the widening scope of metabolomics. 2007 , 2, 72-80	28
2164	Processing MALDI Mass Spectra to Improve Mass Spectral Direct Tissue Analysis. 2007 , 260, 212-221	172
2163	LC-MS-based metabonomics analysis. 2008 , 866, 64-76	127
2162	Gas chromatography/mass spectrometry in metabolic profiling of biological fluids. 2008 , 871, 202-11	235
2161	Plant metabolomics: analytical platforms and integration with functional genomics. 2008 , 7, 479-497	51
2160	Assignment of MS-based metabolomic datasets via compound interaction pair mapping. 2008 , 4, 94-103	22
2159	Accurate mass error correction in liquid chromatography time-of-flight mass spectrometry based metabolomics. 2008 , 4, 171-182	29

2158	Probing genetic algorithms for feature selection in comprehensive metabolic profiling approach. 2008 , 22, 1312-24	22
2157	Utility of separation science in metabolomic studies. 2008 , 31, 1936-47	54
2156	Multiparametric analysis of amino acids and organic acids in rat brain tissues using GC/MS. 2008 , 31, 2831-8	20
2155	Metabolic profiling of serum using Ultra Performance Liquid Chromatography and the LTQ-Orbitrap mass spectrometry system. 2008 , 871, 288-98	151
2154	GC-MS methods for metabolic profiling of microbial fermentation products of dietary polyphenols in human and in vitro intervention studies. 2008 , 871, 212-9	90
2153	Efficient mining of myxobacterial metabolite profiles enabled by liquid chromatography-electrospray ionisation-time-of-flight mass spectrometry and compound-based principal component analysis. 2008 , 624, 97-106	56
2152	Metabolomic investigation of the response of the model plant Arabidopsis thaliana to cadmium exposure: Evaluation of data pretreatment methods for further statistical analyses. 2008 , 91, 67-77	19
2151	Feature detection and alignment of hyphenated chromatographic-mass spectrometric data. Extraction of pure ion chromatograms using Kalman tracking. 2008 , 1192, 139-46	55
2150	Extending the breadth of metabolite profiling by gas chromatography coupled to mass spectrometry. 2008 , 27, 261-269	178
2149	LC-MS-based methodology for global metabolite profiling in metabonomics/metabolomics. 2008 , 27, 251-260	266
2148	Liquid chromatography-mass spectrometry in metabolite profiling. 2008 , 34, 159-69	6
2147	Metabolite annotations based on the integration of mass spectral information. 2008 , 54, 949-62	249
2146	The role of laccase in prostaglandin production by Cryptococcus neoformans. 2008 , 68, 1428-37	49
2145	Quality control for plant metabolomics: reporting MSI-compliant studies. 2008 , 53, 691-704	457
2144	OpenMS - an open-source software framework for mass spectrometry. 2008 , 9, 163	474
2143	Critical assessment of alignment procedures for LC-MS proteomics and metabolomics measurements. 2008 , 9, 375	137
2142	Envelope: interactive software for modeling and fitting complex isotope distributions. 2008 , 9, 446	9
2141	Highly sensitive feature detection for high resolution LC/MS. 2008 , 9, 504	697

2140	Corra: Computational framework and tools for LC-MS discovery and targeted mass spectrometry-based proteomics. 2008 , 9, 542		58
2139	Bio-JETI: a service integration, design, and provisioning platform for orchestrated bioinformatics processes. 2008 , 9 Suppl 4, S12		36
2138	An iterative block-shifting approach to retention time alignment that preserves the shape and area of gas chromatography-mass spectrometry peaks. 2008 , 9 Suppl 9, S15		24
2137	Correlating the transcriptome, proteome, and metabolome in the environmental adaptation of a hyperthermophile. 2008 , 7, 1027-35		60
2136	Detection of bladder cancer in human urine by metabolomic profiling using high performance liquid chromatography/mass spectrometry. 2008 , 179, 2422-6		119
2135	An assessment of software solutions for the analysis of mass spectrometry based quantitative proteomics data. 2008 , 7, 51-61		387
2134	NMR-based metabolic profiling and metabonomic approaches to problems in molecular toxicology. 2008 , 21, 9-27		267
2133	GC-MS-Based Metabolomics. 2008 , 317-340		13
2132	XCMS2: processing tandem mass spectrometry data for metabolite identification and structural characterization. <i>Analytical Chemistry</i> , 2008 , 80, 6382-9	7.8	205
2131	Expression of hepatitis B virus proteins in transgenic mice alters lipid metabolism and induces oxidative stress in the liver. 2008 , 48, 12-9		65
2130	Current trends and future requirements for the mass spectrometric investigation of microbial, mammalian and plant metabolomes. 2008 , 5, 011001		205
2129	Gene expression and metabolism in tomato fruit surface tissues. 2008 , 147, 823-51		254
2128	Integrated GC-MS and LC-MS plasma metabonomics analysis of ankylosing spondylitis. 2008 , 133, 1214-20		60
2127	Redirection of flavonoid biosynthesis through the down-regulation of an anthocyanidin glucosyltransferase in ripening strawberry fruit. 2008 , 146, 1528-39		135
2126	MeltDB: a software platform for the analysis and integration of metabolomics experiment data. 2008 , 24, 2726-32		89
2125	TagFinder for the quantitative analysis of gas chromatography--mass spectrometry (GC-MS)-based metabolite profiling experiments. 2008 , 24, 732-7		450
2124	Multi-platform investigation of the metabolome in a leptin receptor defective murine model of type 2 diabetes. 2008 , 4, 1015-23		19
2123	Advanced data-mining strategies for the analysis of direct-infusion ion trap mass spectrometry data from the association of perennial ryegrass with its endophytic fungus, <i>Neotyphodium lolii</i> . 2008 , 146, 1501-14		39

2122	Discovering oxysterols in plasma: a window on the metabolome. 2008 , 7, 3602-12		63
2121	A global metabolite profiling approach to identify protein-metabolite interactions. 2008 , 130, 14111-3		36
2120	Comparative metabolic profiling reveals secondary metabolites correlated with soybean salt tolerance. 2008 , 56, 11132-8		51
2119	Label-free comparative analysis of proteomics mixtures using chromatographic alignment of high-resolution muLC-MS data. <i>Analytical Chemistry</i> , 2008 , 80, 961-71	7.8	57
2118	Comparing capillary electrophoresis-mass spectrometry fingerprints of urine samples obtained after intake of coffee, tea, or water. <i>Analytical Chemistry</i> , 2008 , 80, 8946-55	7.8	37
2117	Multiple organic anion transporters contribute to net renal excretion of uric acid. 2008 , 33, 180-92		178
2116	Metabolome analysis of biosynthetic mutants reveals a diversity of metabolic changes and allows identification of a large number of new compounds in Arabidopsis. 2008 , 147, 2107-20		122
2115	Organic anion transporter 3 contributes to the regulation of blood pressure. 2008 , 19, 1732-40		65
2114	Computational quantification of peptides from LC-MS data. 2008 , 15, 685-704		11
2113	Biomarker Methods in Drug Discovery and Development. 2008 ,		4
2112	Metabolomics relative quantitation with mass spectrometry using chemical derivatization and isotope labeling. 2008 , 22, 327-343		15
2111	Quantitative strategies to fuel the merger of discovery and hypothesis-driven shotgun proteomics. 2009 , 8, 114-25		14
2110	Simple data-reduction method for high-resolution LC-MS data in metabolomics. 2009 , 1, 1551-7		46
2109	QbD for Raw Materials. 193-209		5
2108	Metabolic fingerprinting reveals developmental regulation of metabolites during early zebrafish embryogenesis. 2009 , 13, 397-405		19
2107	A chemical screen for biological small molecule-RNA conjugates reveals CoA-linked RNA. 2009 , 106, 7768-73		77
2106	Challenges in applying chemometrics to LC-MS-based global metabolite profile data. 2009 , 1, 805-19		13
2105	ChromA: signal-based retention time alignment for chromatography-mass spectrometry data. 2009 , 25, 2080-1		28

2104	Gene and metabolite regulatory network analysis of early developing fruit tissues highlights new candidate genes for the control of tomato fruit composition and development. 2009 , 149, 1505-28	159
2103	Retention time alignment algorithms for LC/MS data must consider non-linear shifts. 2009 , 25, 758-64	62
2102	Fruit-surface flavonoid accumulation in tomato is controlled by a SIMYB12-regulated transcriptional network. 2009 , 5, e1000777	170
2101	Two-stage model-based clustering for liquid chromatography mass spectrometry data analysis. 2009 , 8, Article 15	5
2100	apLCMS--adaptive processing of high-resolution LC/MS data. 2009 , 25, 1930-6	219
2099	Metabolite signal identification in accurate mass metabolomics data with MZedDB, an interactive m/z annotation tool utilising predicted ionisation behaviour 'rules'. 2009 , 10, 227	123
2098	multiplierz: an extensible API based desktop environment for proteomics data analysis. 2009 , 10, 364	59
2097	Comparison of public peak detection algorithms for MALDI mass spectrometry data analysis. 2009 , 10, 4	169
2096	TargetSearch--a Bioconductor package for the efficient preprocessing of GC-MS metabolite profiling data. 2009 , 10, 428	153
2095	Decon2LS: An open-source software package for automated processing and visualization of high resolution mass spectrometry data. 2009 , 10, 87	173
2094	'Metabolite-likeness' as a criterion in the design and selection of pharmaceutical drug libraries. 2009 , 14, 31-40	103
2093	Unraveling the secrets of protein-metabolite interactions. 2009 , 10, 799-801	
2092	CE-MS in metabolomics. 2009 , 30, 276-91	231
2091	The role of mass spectrometry-based metabolomics in medical countermeasures against radiation. 2010 , 29, 503-21	37
2090	Analysis of phenolic choline esters from seeds of Arabidopsis thaliana and Brassica napus by capillary liquid chromatography/electrospray- tandem mass spectrometry. 2009 , 44, 466-76	19
2089	Analytical and statistical approaches to metabolomics research. 2009 , 32, 2183-99	161
2088	An automatic peak finding method for LC-MS data using Gaussian second derivative filtering. 2009 , 32, 3906-18	28
2087	Salicylic acid and salicylic acid glucoside in xylem sap of Brassica napus infected with Verticillium longisporum. 2009 , 122, 571-9	49

2086	A chemometric study of chromatograms of tea extracts by correlation optimization warping in conjunction with PCA, support vector machines and random forest data modeling. 2009 , 642, 257-65	56
2085	Metabonomics study of liver cancer based on ultra performance liquid chromatography coupled to mass spectrometry with HILIC and RPLC separations. 2009 , 650, 3-9	180
2084	HD desktop: an integrated platform for the analysis and visualization of H/D exchange data. 2009 , 20, 601-10	93
2083	Mass-spectrometry-based metabolomics: limitations and recommendations for future progress with particular focus on nutrition research. 2009 , 5, 435-458	412
2082	The correspondence problem for metabonomics datasets. 2009 , 394, 151-62	59
2081	Development of a metabonomic approach based on LC-ESI-HRMS measurements for profiling of metabolic changes induced by recombinant equine growth hormone in horse urine. 2009 , 394, 2119-28	33
2080	Alignment of capillary electrophoresis-mass spectrometry datasets using accurate mass information. 2009 , 395, 2527-33	43
2079	IsoScore: automated localization of biotransformations by mass spectrometry using product ion scoring of virtual regioisomers. 2009 , 23, 39-50	27
2078	High-resolution extracted ion chromatography, a new tool for metabolomics and lipidomics using a second-generation orbitrap mass spectrometer. 2009 , 23, 1411-8	78
2077	Metabolomics profiling of extracellular metabolites in recombinant Chinese Hamster Ovary fed-batch culture. 2009 , 23, 3763-71	60
2076	Extraction of pure components from overlapped signals in gas chromatography-mass spectrometry (GC-MS). 2009 , 2, 6	22
2075	MS/MS spectral tag-based annotation of non-targeted profile of plant secondary metabolites. 2009 , 57, 555-77	191
2074	Expression of a bacterial bi-functional chorismate mutase/prephenate dehydratase modulates primary and secondary metabolism associated with aromatic amino acids in Arabidopsis. 2009 , 60, 156-67	70
2073	An integrated metabonomic method for profiling of metabolic changes in carbon tetrachloride induced rat urine. 2009 , 256, 191-200	29
2072	Overexpression of isocitrate lyase-glyoxylate bypass influence on metabolism in Aspergillus niger. 2009 , 11, 107-16	29
2071	A signal filtering method for improved quantification and noise discrimination in fourier transform ion cyclotron resonance mass spectrometry-based metabolomics data. 2009 , 20, 1087-95	59
2070	Joint GC-MS and LC-MS platforms for comprehensive plant metabolomics: repeatability and sample pre-treatment. 2009 , 877, 3572-80	102
2069	Web-based resources for mass-spectrometry-based metabolomics: a user's guide. 2009 , 70, 450-6	127

2068	Integrated omics approaches in plant systems biology. 2009 , 13, 532-8		172
2067	Metabolomic studies of experimental diabetic urine samples by 1H NMR spectroscopy and LC/MS method. 2009 , 97, 11-17		18
2066	Options for veterinary drug analysis using mass spectrometry. 2009 , 1216, 8016-34		90
2065	Analysis and applications of nanoparticles in the separation sciences: A case of gold nanoparticles. 2009 , 1216, 9034-47		112
2064	Metabolite analysis of human fecal water by gas chromatography/mass spectrometry with ethyl chloroformate derivatization. 2009 , 393, 163-75		110
2063	The Application of Chromatography-Mass Spectrometry: Methods to Metabonomics. 2009 , 69, 23-32		37
2062	MetaboliteDetector: comprehensive analysis tool for targeted and nontargeted GC/MS based metabolome analysis. <i>Analytical Chemistry</i> , 2009 , 81, 3429-39	7.8	287
2061	Peptidomics of prolyl endopeptidase in the central nervous system. 2009 , 48, 11971-81		37
2060	The metabolomic responses of <i>Caenorhabditis elegans</i> to cadmium are largely independent of metallothionein status, but dominated by changes in cystathionine and phytochelatins. 2009 , 8, 3512-9		95
2059	Elucidation of functions of human cytochrome P450 enzymes: identification of endogenous substrates in tissue extracts using metabolomic and isotopic labeling approaches. <i>Analytical Chemistry</i> , 2009 , 81, 3071-8	7.8	34
2058	Mechanistic aspects and novel biomarkers of responder and non-responder phenotypes in galactosamine-induced hepatitis. 2009 , 8, 5175-87		35
2057	Response and recovery in the plasma metabolome tracks the acute LCMV-induced immune response. 2009 , 8, 3578-87		31
2056	Secondary metabolomics: natural products mass spectrometry goes global. 2009 , 4, 599-601		21
2055	Quantitative metabolome profiling of colon and stomach cancer microenvironment by capillary electrophoresis time-of-flight mass spectrometry. 2009 , 69, 4918-25		699
2054	Mass spectrometry-based technologies for high-throughput metabolomics. 2009 , 1, 1665-84		53
2053	Mass spectrometry tools and metabolite-specific databases for molecular identification in metabolomics. 2009 , 134, 1322-32		215
2052	Identification of an overabundant cholesterol precursor in hepatitis B virus replicating cells by untargeted lipid metabolite profiling. 2009 , 131, 5030-1		34
2051	Explorative analysis of urine by capillary electrophoresis-mass spectrometry in chronic patients with complex regional pain syndrome. 2009 , 8, 5559-67		34

2050	Nontargeted urinary metabolite profiling of a mouse model of Crohn's disease. 2009 , 8, 2045-57		56
2049	Metabonomic characterization of aging and investigation on the anti-aging effects of total flavones of Epimedium. 2009 , 5, 1204-13		46
2048	MetaboAnalyst: a web server for metabolomic data analysis and interpretation. 2009 , 37, W652-60		1202
2047	Plant Metabolic Networks. 2009 ,		3
2046	Regulation of alkyl-dihydrothiazole-carboxylates (ATCs) by iron and the pyochelin gene cluster in <i>Pseudomonas aeruginosa</i> . 2009 , 4, 617-23		27
2045	Variable Shift and Alignment. 2009 , 85-108		7
2044	Variability analysis of human plasma and cerebral spinal fluid reveals statistical significance of changes in mass spectrometry-based metabolomics data. <i>Analytical Chemistry</i> , 2009 , 81, 8538-44	7.8	104
2043	MetAlign: interface-driven, versatile metabolomics tool for hyphenated full-scan mass spectrometry data preprocessing. <i>Analytical Chemistry</i> , 2009 , 81, 3079-86	7.8	536
2042	Plant Systems Biology. 2009 ,		3
2041	Utility of mass spectrometry for proteome analysis: part II. Ion-activation methods, statistics, bioinformatics and annotation. 2009 , 6, 171-97		13
2040	Plant phenotype demarcation using nontargeted LC-MS and GC-MS metabolite profiling. 2009 , 57, 7338-47		68
2039	Development of a robust and repeatable UPLC-MS method for the long-term metabolomic study of human serum. <i>Analytical Chemistry</i> , 2009 , 81, 1357-64	7.8	306
2038	Metabonomic study of ochratoxin a toxicity in rats after repeated administration: phenotypic anchoring enhances the ability for biomarker discovery. 2009 , 22, 1221-31		62
2037	Metabolomics analysis reveals large effects of gut microflora on mammalian blood metabolites. 2009 , 106, 3698-703		1696
2036	Development of a metabolomic approach based on liquid chromatography-high resolution mass spectrometry to screen for clenbuterol abuse in calves. 2009 , 134, 1637-46		95
2035	Pattern Recognition and Pathway Analysis with Genetic Algorithms in Mass Spectrometry Based Metabolomics. 2009 , 2, 638-666		14
2034	Current technological challenges in biomarker discovery and validation. 2010 , 16, 101-21		17
2033	Peptidomics of the prolyl peptidases. 2010 , 12, 483-91		30

2032	Postulating Modes of Action of Compounds with Antimicrobial Activities through Metabolomics Analysis. 2010 , 71, 253-258		11
2031	Metabolomic analysis via reversed-phase ion-pairing liquid chromatography coupled to a stand alone orbitrap mass spectrometer. <i>Analytical Chemistry</i> , 2010 , 82, 3212-21	7.8	380
2030	Exploratory analysis of human urine by LC-ESI-TOF MS after high intake of olive oil: understanding the metabolism of polyphenols. 2010 , 398, 463-75		76
2029	Warping and alignment technologies for inter-sample feature correspondence in 1D H-NMR, chromatography-, and capillary electrophoresis-mass spectrometry data. 2010 , 1, 105-116		8
2028	Challenges in Computational Analysis of Mass Spectrometry Data for Proteomics. 2010 , 25, 107-123		22
2027	Metabolomics: moving to the clinic. 2010 , 5, 4-17		118
2026	L'Analyse métabolomique par spectrométrie de masse: un nouvel outil pour la biochimie clinique ? 2010 , 34, 10-15		
2025	Differential metabolomics software for capillary electrophoresis-mass spectrometry data analysis. 2010 , 6, 27-41		44
2024	Capillary electrophoresis mass spectrometry-based saliva metabolomics identified oral, breast and pancreatic cancer-specific profiles. 2010 , 6, 78-95		621
2023	Development and validation of a UPLC/MS method for a nutritional metabolomic study of human plasma. 2010 , 6, 207-218		56
2022	The MetabolomeExpress Project: enabling web-based processing, analysis and transparent dissemination of GC/MS metabolomics datasets. 2010 , 11, 376		97
2021	Quantification and deconvolution of asymmetric LC-MS peaks using the bi-Gaussian mixture model and statistical model selection. 2010 , 11, 559		31
2020	Large scale physiological readjustment during growth enables rapid, comprehensive and inexpensive systems analysis. 2010 , 4, 64		21
2019	Naturstoffe und ihre biologischen Angriffsziele: proteomische und metabolische Markierungsstrategien. 2010 , 122, 2740-2759		40
2018	Natural products and their biological targets: proteomic and metabolomic labeling strategies. 2010 , 49, 2680-98		153
2017	Knowledge discovery in metabolomics: an overview of MS data handling. 2010 , 33, 290-304		142
2016	Lipidomics era: accomplishments and challenges. 2010 , 29, 877-929		139
2015	Dealing with the unknown: metabolomics and metabolite atlases. 2010 , 21, 1471-6		135

2014	Screening in veterinary drug analysis and sports doping control based on full-scan, accurate-mass spectrometry. 2010 , 29, 1250-1268	74
2013	The glycerophospho metabolome and its influence on amino acid homeostasis revealed by brain metabolomics of GDE1(-/-) mice. 2010 , 17, 831-40	31
2012	Improved parametric time warping for proteomics. 2010 , 104, 65-74	57
2011	MI-Pack: Increased confidence of metabolite identification in mass spectra by integrating accurate masses and metabolic pathways. 2010 , 104, 75-82	72
2010	Deconvolution using signal segmentation. 2010 , 104, 132-139	18
2009	Target list building for volatile metabolite profiling of fruit. 2010 , 1217, 6718-23	17
2008	Comparative evaluation of software for retention time alignment of gas chromatography/time-of-flight mass spectrometry-based metabolomic data. 2010 , 1217, 8308-16	43
2007	Image analysis tools and emerging algorithms for expression proteomics. 2010 , 10, 4226-57	36
2006	Surface-activated chemical ionization time-of-flight mass spectrometry and labeling-free approach: two powerful tools for the analysis of complex plant functional proteome profiles. 2010 , 24, 1155-60	5
2005	Liquid chromatography/mass spectrometry for investigating the biochemical effects induced by aristolochic acid in rats: the plasma metabolome. 2010 , 24, 1312-8	25
2004	Development of a targeted adductomic method for the determination of polycyclic aromatic hydrocarbon DNA adducts using online column-switching liquid chromatography/tandem mass spectrometry. 2010 , 24, 2329-40	28
2003	Mass spectrometry-based metabolomics application to identify quantitative resistance-related metabolites in barley against Fusarium head blight. 2010 , 11, 769-82	111
2002	An integrative approach for identifying a metabolic phenotype predictive of individualized pharmacokinetics of tacrolimus. 2010 , 87, 426-36	59
2001	Metabolic oxidation regulates embryonic stem cell differentiation. 2010 , 6, 411-7	396
2000	Analytical platform for metabolome analysis of microbial cells using methyl chloroformate derivatization followed by gas chromatography-mass spectrometry. 2010 , 5, 1709-29	278
1999	Global metabolic profiling procedures for urine using UPLC-MS. 2010 , 5, 1005-18	676
1998	Activity-based protein profiling for biochemical pathway discovery in cancer. 2010 , 10, 630-8	251
1997	Mass spectrometry-based metabolomics, analysis of metabolite-protein interactions, and imaging. 2010 , 49, 557-65	51

1996	Metabolome analysis of response to oxidative stress in rice suspension cells overexpressing cell death suppressor Bax inhibitor-1. 2010 , 51, 9-20		73
1995	ADEPTS: advanced peptide de novo sequencing with a pair of tandem mass spectra. 2010 , 8, 981-94		25
1994	Robust early pregnancy prediction of later preeclampsia using metabolomic biomarkers. 2010 , 56, 741-9		215
1993	Metabolic Engineering in <i>Fragaria x ananassa</i> for the Production of Epiafzelechin and Phenylpropanoids. 2010 , 293-300		
1992	Metabolome analysis revealed increase in S-methylcysteine and phosphatidylisopropanolamine synthesis upon L-cysteine deprivation in the anaerobic protozoan parasite <i>Entamoeba histolytica</i> . 2010 , 285, 39160-70		39
1991	Metabolome and photochemical analysis of rice plants overexpressing Arabidopsis NAD kinase gene. 2010 , 152, 1863-73		67
1990	Metabolomics-based discovery of diagnostic biomarkers for onchocerciasis. 2010 , 4, e834		56
1989	Analysis of LC-MS data for characterizing the metabolic changes in response to radiation. 2010 , 9, 2786-93		28
1988	Untargeted metabolomics. 2010 , Chapter 30, Unit 30.1.1-24		45
1987	Urinary metabonomic study on colorectal cancer. 2010 , 9, 1627-34		178
1986	Combining genetic diversity, informatics and metabolomics to facilitate annotation of plant gene function. 2010 , 5, 1210-27		169
1985	Peek a peak: a glance at statistics for quantitative label-free proteomics. 2010 , 7, 249-61		35
1984	Proposal for field sampling of plants and processing in the lab for environmental metabolic fingerprinting. 2010 , 6, 6		23
1983	Mass spectrometry-based methods for the determination of sulfur and related metabolite concentrations in cell extracts. 2010 , 473, 41-76		12
1982	A statistically rigorous test for the identification of parent-fragment pairs in LC-MS datasets. <i>Analytical Chemistry</i> , 2010 , 82, 1766-78	7.8	21
1981	Ultra performance liquid chromatography-mass spectrometry profiling of bile acid metabolites in biofluids: application to experimental toxicology studies. <i>Analytical Chemistry</i> , 2010 , 82, 5282-9	7.8	79
1980	Does the mass spectrometer define the marker? A comparison of global metabolite profiling data generated simultaneously via UPLC-MS on two different mass spectrometers. <i>Analytical Chemistry</i> , 2010 , 82, 8226-34	7.8	51
1979	Metabolite identification in <i>Synechococcus</i> sp. PCC 7002 using untargeted stable isotope assisted metabolite profiling. <i>Analytical Chemistry</i> , 2010 , 82, 9034-42	7.8	59

1978	Using a spike-in experiment to evaluate analysis of LC-MS data. 2010 ,		
1977	Metabolite differentiation and discovery lab (MeDDL): a new tool for biomarker discovery and mass spectral visualization. <i>Analytical Chemistry</i> , 2010 , 82, 4386-95	7.8	17
1976	Exploring disease through metabolomics. 2010 , 5, 91-103		173
1975	Cyclization of a cellular dipentaenone by <i>Streptomyces coelicolor</i> cytochrome P450 154A1 without oxidation/reduction. 2010 , 132, 15173-5		31
1974	Expanding the dipeptidyl peptidase 4-regulated peptidome via an optimized peptidomics platform. 2010 , 132, 3819-30		53
1973	Signature-discovery approach for sample matching of a nerve-agent precursor using liquid chromatography-mass spectrometry, XCMS, and chemometrics. <i>Analytical Chemistry</i> , 2010 , 82, 4165-73	7.8	156
1972	CE-MS for metabolic profiling of volume-limited urine samples: application to accelerated aging TTD mice. 2010 , 9, 4869-74		45
1971	Selective chemical intervention in the proteome of <i>Caenorhabditis elegans</i> . 2010 , 9, 6060-70		1
1970	Comprehensive lipidomics analysis of bioactive lipids in complex regulatory networks. <i>Analytical Chemistry</i> , 2010 , 82, 8176-85	7.8	80
1969	Evaluation of accurate mass and relative isotopic abundance measurements in the LTQ-orbitrap mass spectrometer for further metabolomics database building. <i>Analytical Chemistry</i> , 2010 , 82, 5490-501	7.8	109
1968	Fourier transform mass spectrometry for metabolome analysis. 2010 , 135, 2203-19		61
1967	Practical metabolomics in drug discovery. 2010 , 5, 249-63		21
1966	Common and divergent physiological, hormonal and metabolic responses of <i>Arabidopsis thaliana</i> and <i>Thellungiella halophila</i> to water and salt stress. 2010 , 167, 1342-50		74
1965	Anchoring metabolic changes to phenotypic effects in the chlorophyte <i>Scenedesmus vacuolatus</i> under chemical exposure. 2010 , 69 Suppl, S28-30		12
1964	Opening up the "Black Box": metabolic phenotyping and metabolome-wide association studies in epidemiology. 2010 , 63, 970-9		113
1963	Global analysis of circulating metabolites in hibernating ground squirrels. 2010 , 5, 265-73		28
1962	Monoacylglycerol lipase regulates a fatty acid network that promotes cancer pathogenesis. 2010 , 140, 49-61		697
1961	Extensive in vivo metabolite-protein interactions revealed by large-scale systematic analyses. 2010 , 143, 639-50		162

1960	Metabolomic analysis and visualization engine for LC-MS data. <i>Analytical Chemistry</i> , 2010 , 82, 9818-26	7.8	381
1959	The responses of <i>Arabidopsis thaliana</i> to cadmium exposure explored via metabolite profiling. 2010 , 78, 840-5		64
1958	Mass spectrometry-based metabolomics of yeast. 2010 , 470, 393-426		39
1957	Evaluation of peak picking quality in LC-MS metabolomics data. <i>Analytical Chemistry</i> , 2010 , 82, 9177-87	7.8	52
1956	Optimization and evaluation of metabolite extraction protocols for untargeted metabolic profiling of liver samples by UPLC-MS. <i>Analytical Chemistry</i> , 2010 , 82, 7779-86	7.8	144
1955	Correction of mass calibration gaps in liquid chromatography-mass spectrometry metabolomics data. 2010 , 26, 2488-9		119
1954	Development of a quantitative metabolomic approach to study clinical human fecal water metabolome based on trimethylsilylation derivatization and GC/MS analysis. <i>Analytical Chemistry</i> , 2010 , 82, 6447-56	7.8	108
1953	Application of plasma lipidomics in studying the response of patients with essential hypertension to antihypertensive drug therapy. 2011 , 7, 3271-9		48
1952	Differential macrophage polarization promotes tissue remodeling and repair in a model of ischemic retinopathy. 2011 , 1, 76		66
1951	Metabolomic analysis of liver and skeletal muscle tissues in C57BL/6J and DBA/2J mice exposed to 2,3,7,8-tetrachlorodibenzo-p-dioxin. 2011 , 7, 1956-65		28
1950	A brief review of signal processing issues in mass spectrometry-based proteomics studies. 2011 ,		
1949	A metabolomics strategy for detecting protein-metabolite interactions to identify natural nuclear receptor ligands. 2011 , 7, 1046-9		16
1948	Correlation between antioxidative activities and metabolite changes during Cheonggukjang fermentation. 2011 , 75, 732-9		46
1947	Meta-analysis of LC-MS based metabolomic experiments. 2011 ,		
1946	A correlation between antioxidant activity and metabolite release during the blanching of <i>Chrysanthemum coronarium</i> L. 2011 , 75, 674-80		10
1945	Time-course changes in potential biomarkers detected using a metabolomic approach in Walker 256 tumor-bearing rats. 2011 , 10, 1953-61		17
1944	Monoalkylglycerol ether lipids promote adipogenesis. 2011 , 133, 5178-81		25
1943	Hierarchical alignment and full resolution pattern recognition of 2D NMR spectra: application to nematode chemical ecology. <i>Analytical Chemistry</i> , 2011 , 83, 1649-57	7.8	57

1942	Impurity profiling to match a nerve agent to its precursor source for chemical forensics applications. <i>Analytical Chemistry</i> , 2011 , 83, 9564-72	7.8	38
1941	PeakML/mzMatch: a file format, Java library, R library, and tool-chain for mass spectrometry data analysis. <i>Analytical Chemistry</i> , 2011 , 83, 2786-93	7.8	210
1940	Technical and biological variation in UPLC-MS-based untargeted metabolic profiling of liver extracts: application in an experimental toxicity study on galactosamine. <i>Analytical Chemistry</i> , 2011 , 83, 1116-23	7.8	49
1939	Chemotype-dependent metabolic response to methyl jasmonate elicitation in <i>Artemisia annua</i> . 2011 , 77, 1048-53		18
1938	Threshold-avoiding proteomics pipeline. <i>Analytical Chemistry</i> , 2011 , 83, 7786-94	7.8	14
1937	Serum 27-nor-5 β -cholestane-3,7,12,24,25 pentol glucuronide discovered by metabolomics as potential diagnostic biomarker for epithelium ovarian cancer. 2011 , 10, 2625-32		86
1936	Inhibition of glycosphingolipid biosynthesis induces cytokinesis failure. 2011 , 133, 10010-3		30
1935	Automated workflows for accurate mass-based putative metabolite identification in LC/MS-derived metabolomic datasets. 2011 , 27, 1108-12		156
1934	Offspring metabolomic response to maternal protein restriction in a rat model of intrauterine growth restriction (IUGR). 2011 , 10, 3292-302		48
1933	Endocannabinoid hydrolysis generates brain prostaglandins that promote neuroinflammation. 2011 , 334, 809-13		490
1932	Metabolomic approaches toward understanding nitrogen metabolism in plants. 2011 , 62, 1439-53		155
1931	Metab: an R package for high-throughput analysis of metabolomics data generated by GC-MS. 2011 , 27, 2316-8		103
1930	The analysis of native proteins and peptides in the clinical lab using mass spectrometry. 2011 , 31, 397-405		2
1929	Cross-platform analysis of longitudinal data in metabolomics. 2011 , 7, 3214-22		18
1928	Mass Spectrometry in Metabolomics. 2011 , 271-298		0
1927	Procedures for large-scale metabolic profiling of serum and plasma using gas chromatography and liquid chromatography coupled to mass spectrometry. 2011 , 6, 1060-83		1527
1926	Exploring the metabolic state of microorganisms using metabolomics. 2011 , 3, 2443-58		18
1925	Processing and analysis of GC/LC-MS-based metabolomics data. 2011 , 708, 277-98		56

1924	Metabolomic data processing, analysis, and interpretation using MetaboAnalyst. 2011 , Chapter 14, Unit 14.10		124
1923	The Small-Molecule Dimension: Mass-Spectrometry-Based Metabolomics, Enzyme Assays, and Imaging. 2011 , 675-682		
1922	Metabolomic profiling to identify potential serum biomarkers for schizophrenia and risperidone action. 2011 , 10, 5433-43		103
1921	Metabolomics in drug target discovery. 2011 , 76, 235-46		61
1920	Bioinformatics for qualitative and quantitative proteomics. 2011 , 719, 331-49		3
1919	metaXCMS: second-order analysis of untargeted metabolomics data. <i>Analytical Chemistry</i> , 2011 , 83, 696-700		86
1918	Statistical Data Analysis in Metabolomics. 2011 , 163-180		2
1917	Cross-platform comparison of <i>Caenorhabditis elegans</i> tissue extraction strategies for comprehensive metabolome coverage. <i>Analytical Chemistry</i> , 2011 , 83, 3730-6	7.8	98
1916	A targeted lipidomics approach to the study of eicosanoid release in synovial joints. 2011 , 13, R123		26
1915	UPLC-MS-based metabolite analysis in tomato. 2012 , 860, 129-44		21
1914	Stability-based biomarker selection. 2011 , 705, 15-23		40
1913	Riboneogenesis in yeast. 2011 , 145, 969-80		86
1912	Development of topotecan loaded lipid nanoparticles for chemical stabilization and prolonged release. 2011 , 79, 189-96		108
1911	Quantitative analysis of glycerophospholipids by LC-MS: acquisition, data handling, and interpretation. 2011 , 1811, 748-57		58
1910	Liquid chromatographic-mass spectrometric analysis of phospholipids. Chromatography, ionization and quantification. 2011 , 1811, 763-75		61
1909	High-throughput profiling of microbial extracts. 2011 , 74, 983-8		32
1908	Functional analysis of protein targets by metabolomic approaches. 2012 , 324, 137-62		
1907	Data processing pipelines for comprehensive profiling of proteomics samples by label-free LC-MS for biomarker discovery. 2011 , 83, 1209-24		25

1906	Hippocampal metabolomics reveals 2,3,7,8-tetrachlorodibenzo-p-dioxin toxicity associated with ageing in Sprague-Dawley rats. 2011 , 85, 1007-12	13
1905	Screening of 4-androstenedione misuse in cattle by LC-MS/MS profiling of glucuronide and sulfate steroids in urine. 2011 , 86, 186-94	25
1904	Databases on food phytochemicals and their health-promoting effects. 2011 , 59, 4331-48	151
1903	Discovery of a protein-metabolite interaction between unsaturated fatty acids and the nuclear receptor Nur77 using a metabolomics approach. 2011 , 133, 17168-71	41
1902	Metabolite profiling of Arabidopsis seedlings in response to exogenous sinalbin and sulfur deficiency. 2011 , 72, 1767-78	21
1901	. 2011 ,	5
1900	A Non-targeted Approach to Chemical Discrimination Between Green Tea Dietary Supplements and Green Tea Leaves by HPLC/MS. 2011 , 94, 487-497	13
1899	European Analytical Criteria: Past, Present, and Future. 2011 , 94, 360-372	23
1898	Meta-analysis of global metabolomics and proteomics data to link alterations with phenotype. 2011 , 26, 151-154	
1897	Ultra performance liquid chromatography and high resolution mass spectrometry for the analysis of plant lipids. 2011 , 2, 54	134
1896	Potential biomarkers in mouse myocardium of doxorubicin-induced cardiomyopathy: a metabolomic method and its application. 2011 , 6, e27683	48
1895	Metabolomics reveals reduction of metabolic oxidation in women with polycystic ovary syndrome after pioglitazone-flutamide-metformin polytherapy. 2011 , 6, e29052	34
1894	Mass and relative elution time profiling: two-dimensional analysis of sphingolipids in Alzheimer's disease brains. 2011 , 438, 165-75	39
1893	Elucidation of cellular metabolism via metabolomics and stable-isotope assisted metabolomics. 2011 , 12, 1075-86	43
1892	Metabolic profiling in disease diagnosis, toxicology and personalized healthcare. 2011 , 12, 976-95	10
1891	Patterns of Nucleotide Diversity and Association Mapping. 2011 , 267-303	1
1890	Pathophysiology of sickle cell disease is mirrored by the red blood cell metabolome. 2011 , 117, e57-66	75
1889	JA-Ile signalling in Solanum nigrum is not required for defence responses in nature. 2011 , 34, 2159-71	10

1888	Elemental formula annotation of polar and lipophilic metabolites using (13) C, (15) N and (34) S isotope labelling, in combination with high-resolution mass spectrometry. 2011 , 68, 364-76		240
1887	Extensive metabolic cross-talk in melon fruit revealed by spatial and developmental combinatorial metabolomics. 2011 , 190, 683-96		101
1886	Mining for treatment-specific and general changes in target compounds and metabolic fingerprints in response to herbivory and phytohormones in <i>Plantago lanceolata</i> . 2011 , 191, 1069-1082		32
1885	Web-based inference of biological patterns, functions and pathways from metabolomic data using MetaboAnalyst. 2011 , 6, 743-60		718
1884	Identifying developmental toxicity pathways for a subset of ToxCast chemicals using human embryonic stem cells and metabolomics. 2011 , 257, 111-21		86
1883	Descriptive review of current NMR-based metabolomic data analysis packages. 2011 , 59, 263-70		42
1882	Where systems biology meets postharvest. 2011 , 62, 223-237		46
1881	Metabonomics-based omics study and atherosclerosis. 2011 , 1, 30		10
1880	A comparative lipidomics platform for chemotaxonomic analysis of <i>Mycobacterium tuberculosis</i> . 2011 , 18, 1537-49		143
1879	Differential global profiling as a new analytical strategy for revealing micropollutant treatment by-products: application to ethinylestradiol and chlorination water treatment. 2011 , 83, 1553-9		12
1878	MassUntangler: a novel alignment tool for label-free liquid chromatography-mass spectrometry proteomic data. 2011 , 1218, 8859-68		11
1877	iMatch: a retention index tool for analysis of gas chromatography-mass spectrometry data. 2011 , 1218, 6522-30		33
1876	icoshift: An effective tool for the alignment of chromatographic data. 2011 , 1218, 7832-40		177
1875	Study of the interdependency of the data sampling ratio with retention time alignment and principal component analysis for gas chromatography. 2011 , 1218, 9091-101		15
1874	Expanding coverage of the metabolome for global metabolite profiling. <i>Analytical Chemistry</i> , 2011 , 83, 2152-61	7.8	207
1873	Optimized preprocessing of ultra-performance liquid chromatography/mass spectrometry urinary metabolic profiles for improved information recovery. <i>Analytical Chemistry</i> , 2011 , 83, 5864-72	7.8	201
1872	Metabolic differentiation of neuronal phenotypes by single-cell capillary electrophoresis-electrospray ionization-mass spectrometry. <i>Analytical Chemistry</i> , 2011 , 83, 6810-7	7.8	111
1871	Bioinformatics for Omics Data. 2011 ,		14

1870	Pathway profiling in <i>Mycobacterium tuberculosis</i> : elucidation of cholesterol-derived catabolite and enzymes that catalyze its metabolism. 2011 , 286, 43668-43678	77
1869	Metabolomics technology to phenotype resistance in barley against <i>Gibberella zeae</i> . 2011 , 130, 29-43	54
1868	Identification of metabolites related to mechanisms of resistance in barley against <i>Fusarium graminearum</i> , based on mass spectrometry. 2011 , 77, 355-70	74
1867	Metabolomics in pesticide research and development: review and future perspectives. 2011 , 7, 35-53	89
1866	Generation and processing of urinary and plasmatic metabolomic fingerprints to reveal an illegal administration of recombinant equine growth hormone from LC-HRMS measurements. 2011 , 7, 84-93	33
1865	Bioinformatics tools for cancer metabolomics. 2011 , 7, 329-343	97
1864	Urinary Metabolites of Isoliquiritigenin in Wistar Rats using UHPLC-ESI-MS-based Xenometabolomics. 2011 , 74, 341-348	10
1863	Differentiation of <i>Panax quinquefolius</i> grown in the USA and China using LC/MS-based chromatographic fingerprinting and chemometric approaches. 2011 , 399, 1877-89	43
1862	Normalization in MALDI-TOF imaging datasets of proteins: practical considerations. 2011 , 401, 167-81	159
1861	Identification strategy for unknown pollutants using high-resolution mass spectrometry: androgen-disrupting compounds identified through effect-directed analysis. 2011 , 400, 3141-9	59
1860	Identification of serum biomarkers of hepatocarcinoma through liquid chromatography/mass spectrometry-based metabolomic method. 2011 , 401, 1899-904	70
1859	Exploration of sulfur metabolism in the yeast <i>Kluyveromyces lactis</i> . 2011 , 91, 1409-23	24
1858	LC/MS-based non-targeted metabolomics for the investigation of general toxicity of 2,3,7,8-tetrachlorodibenzo-p-dioxin in C57BL/6J and DBA/2J mice. 2011 , 301, 29-36	16
1857	Automated optimization and construction of chemometric models based on highly variable raw chromatographic data. 2011 , 697, 8-15	24
1856	Qualitative metabolome analysis of human cerebrospinal fluid by ¹³ C/ ¹² C-isotope dansylation labeling combined with liquid chromatography Fourier transform ion cyclotron resonance mass spectrometry. 2011 , 22, 339-47	43
1855	Citramalic acid and salicylic acid in sugar beet root exudates solubilize soil phosphorus. 2011 , 11, 121	67
1854	AMDORAP: non-targeted metabolic profiling based on high-resolution LC-MS. 2011 , 12, 259	16
1853	An integrated workflow for robust alignment and simplified quantitative analysis of NMR spectrometry data. 2011 , 12, 405	52

1852	Metabolomic analysis of a synthetic metabolic switch in <i>Streptomyces coelicolor</i> A3(2). 2011 , 11, 4622-31	20
1851	Evaluation of urinary ribonucleoside profiling for clinical biomarker discovery using constant neutral loss scanning liquid chromatography/tandem mass spectrometry. 2011 , 25, 2071-82	13
1850	Comparison of different liquid chromatography stationary phases in LC-HRMS metabolomics for the detection of recombinant growth hormone doping control. 2011 , 34, 3493-501	22
1849	Classification and differential metabolite discovery of liver diseases based on plasma metabolic profiling and support vector machines. 2011 , 34, 3029-36	21
1848	Separation strategies for untargeted metabolomics. 2011 , 34, 3460-9	93
1847	The evolving field of imaging mass spectrometry and its impact on future biological research. 2011 , 46, 209-22	99
1846	Mass spectrometry-based holistic analytical approaches for metabolite profiling in systems biology studies. 2011 , 30, 884-906	147
1845	Metabolomics in Plant Biotechnology. 2011 , 373-388	
1844	Using metabolomic analysis to understand inflammatory bowel diseases. 2011 , 17, 1021-9	47
1843	Metabolites as global regulators: a new view of protein regulation: systematic investigation of metabolite-protein interactions may help bridge the gap between genome-wide association studies and small molecule screening studies. 2011 , 33, 485-9	28
1842	Exploring liquid chromatography-mass spectrometry fingerprints of urine samples from patients with prostate or urinary bladder cancer. 2011 , 108, 33-48	15
1841	Algorithms and tools for the preprocessing of LCMS metabolomics data. 2011 , 108, 23-32	117
1840	Evaluation of automated sample preparation, retention time locked gas chromatography-mass spectrometry and data analysis methods for the metabolomic study of <i>Arabidopsis</i> species. 2011 , 1218, 3247-54	28
1839	Applications of liquid chromatography coupled to mass spectrometry-based metabolomics in clinical chemistry and toxicology: A review. 2011 , 44, 119-35	168
1838	Metabolomics in systems microbiology. 2011 , 22, 17-25	99
1837	Ion-pairing reversed-phase liquid chromatography fractionation in combination with isotope labeling reversed-phase liquid chromatography-mass spectrometry for comprehensive metabolome profiling. 2011 , 1218, 3689-94	32
1836	Approaches to deorphanization of human and microbial cytochrome P450 enzymes. 2011 , 1814, 139-45	25
1835	Metabolomics-based identification of apoptosis-inducing metabolites in recombinant fed-batch CHO culture media. 2011 , 151, 218-24	47

1834	Mass spectrometry-based metabolomics applied to the chemical safety of food. 2011 , 30, 292-301	82
1833	Identification of serum biomarkers for lung cancer using magnetic bead-based SELDI-TOF-MS. 2011 , 32, 1537-42	16
1832	From data processing to multivariate validation--essential steps in extracting interpretable information from metabolomics data. 2011 , 12, 996-1004	26
1831	Comparison of Auto and Manual Integration for Peptidomics Data Based on High Performance Liquid Chromatography Coupled with Mass Spectrometry. 2011 , 340, 266-272	
1830	X-linked cholestasis in mouse due to mutations of the P4-ATPase ATP11C. 2011 , 108, 7890-5	49
1829	Orphans in the human cytochrome P450 superfamily: approaches to discovering functions and relevance in pharmacology. 2011 , 63, 684-99	79
1828	Global regulation of the response to sulfur availability in the cheese-related bacterium <i>Brevibacterium aurantiacum</i> . 2011 , 77, 1449-59	23
1827	AStream: an R package for annotating LC/MS metabolomic data. 2011 , 27, 1339-40	41
1826	Elemental composition determination based on MS(n). 2011 , 27, 2376-83	57
1825	Systemic gut microbial modulation of bile acid metabolism in host tissue compartments. 2011 , 108 Suppl 1, 4523-30	495
1824	Analyzing In Vivo Metabolite-Protein Interactions By Large-Scale Systematic Analyses. 2011 , 3, 181-196	5
1823	SIMA: simultaneous multiple alignment of LC/MS peak lists. 2011 , 27, 987-93	24
1822	MarVis-Filter: ranking, filtering, adduct and isotope correction of mass spectrometry data. 2012 , 2012, 263910	27
1821	Untargeted metabolomics reveals a lack of synergy between nifurtimox and eflornithine against <i>Trypanosoma brucei</i> . 2012 , 6, e1618	80
1820	Metabolome classification of commercial <i>Hypericum perforatum</i> (St. John's Wort) preparations via UPLC-qTOF-MS and chemometrics. 2012 , 78, 488-96	57
1819	Dramatic increase in glycerol biosynthesis upon oxidative stress in the anaerobic protozoan parasite <i>Entamoeba histolytica</i> . 2012 , 6, e1831	47
1818	Metabonomic Investigation on Rats' Dynamic Responses to Cantonese Herbal Tea Intake. 2012 , 554-556, 1742-1746	
1817	Generation of retinal pigment epithelial cells from small molecules and OCT4 reprogrammed human induced pluripotent stem cells. 2012 , 1, 96-109	74

1816	Metabolomics: a valuable tool for stem cell monitoring in regenerative medicine. 2012 , 9, 1713-24	25
1815	Surrogate genetics and metabolic profiling for characterization of human disease alleles. 2012 , 190, 1309-23	36
1814	Evaluation of normalization methods for analysis of LC-MS data. 2012 ,	5
1813	Normalization of LC-MS data using Gaussian process. 2012 ,	3
1812	Metabonomics in Understanding Drug Metabolism and Toxicology. 2012 , 1	
1811	Metabonomic profiles delineate the effect of traditional Chinese medicine sini decoction on myocardial infarction in rats. 2012 , 7, e34157	75
1810	The metabolomic approach identifies a biological signature of low-dose chronic exposure to cesium 137. 2012 , 53, 33-43	21
1809	Metabolomics reveals increased isoleukotoxin diol (12,13-DHOME) in human plasma after acute Intralipid infusion. 2012 , 53, 1979-86	29
1808	Current State of HPLC-MS Data Processing and Analysis in Proteomics and Metabolomics. 2012 , 9, 80-93	2
1807	Changes in bowel microbiota induced by feeding weanlings resistant starch stimulate transcriptomic and physiological responses. 2012 , 78, 6656-64	24
1806	Crosstalk between above- and belowground herbivores is mediated by minute metabolic responses of the host <i>Arabidopsis thaliana</i> . 2012 , 63, 6199-210	50
1805	Mass Spectrometry-Based Approach in Ginseng Research: A Promising Way to Metabolomics. 2012 , 8, 43-66	21
1804	Computational Methods and Algorithms for Mass Spectrometry Based Differential Proteomics: Recent Advances, Perspectives and Open Problems. 2012 , 9, 143-159	
1803	Implementation of molecular phenotyping approaches in the personalized surgical patient journey. 2012 , 255, 881-9	30
1802	Bioinformatic Approaches to Processing and Annotation of High-Resolution Mass Spectrometry Data. 159-173	
1801	Systematic applications of metabolomics in metabolic engineering. 2012 , 2, 1090-122	14
1800	Integration of datasets from different analytical techniques to assess the impact of nutrition on human metabolome. 2012 , 2, 156	32
1799	Bioinformatics Tools for Mass Spectroscopy-Based Metabolomic Data Processing and Analysis. 2012 , 7, 96-108	234

1798	Overview of Metabolomics Basics. 2012 , 79-137	0
1797	A systems biology view of responses to lignin biosynthesis perturbations in Arabidopsis. 2012 , 24, 3506-29	252
1796	Metabolic biomarkers of prenatal alcohol exposure in human embryonic stem cell-derived neural lineages. 2012 , 36, 1314-24	19
1795	Global profiling strategies for mapping dysregulated metabolic pathways in cancer. 2012 , 16, 565-77	91
1794	A review on second- and third-order multivariate calibration applied to chromatographic data. 2012 , 910, 22-30	75
1793	Tentative identification of phenolic compounds in olive pomace extracts using liquid chromatography-tandem mass spectrometry with a quadrupole-quadrupole-time-of-flight mass detector. 2012 , 60, 11542-50	55
1792	Thresholding for biomarker selection in multivariate data using Higher Criticism. 2012 , 8, 2339-46	7
1791	Serum metabolic profiling study of hepatocellular carcinoma infected with hepatitis B or hepatitis C virus by using liquid chromatography-mass spectrometry. 2012 , 11, 5433-42	51
1790	Sensitive ionization of non-volatile analytes using protein solutions as spray liquid in desorption electrospray ionization mass spectrometry. 2012 , 26, 2770-6	2
1789	Root metabolic response of rice (<i>Oryza sativa</i> L.) genotypes with contrasting tolerance to zinc deficiency and bicarbonate excess. 2012 , 236, 959-73	40
1788	Discovery of early urinary biomarkers in preclinical study of gentamicin-induced kidney injury and recovery in rats. 2012 , 8, 1181-1193	8
1787	Spatial and temporal variation in metabolic fingerprints of field-growing <i>Myriophyllum spicatum</i> . 2012 , 102, 34-43	10
1786	Metabolomic profiling reveals suppression of oxylipin biosynthesis during the early stages of legume-rhizobia symbiosis. 2012 , 586, 3150-8	33
1785	Urinary volatile compounds as biomarkers for lung cancer. 2012 , 76, 679-84	60
1784	Hydrophilic interaction and reversed-phase ultraperformance liquid chromatography TOF-MS for serum metabonomic analysis of myocardial infarction in rats and its applications. 2012 , 8, 548-56	38
1783	Implementation of a semi-automated strategy for the annotation of metabolomic fingerprints generated by liquid chromatography-high resolution mass spectrometry from biological samples. 2012 , 137, 4958-67	27
1782	D-optimal design of an untargeted HS-SPME-GC-TOF metabolite profiling method. 2012 , 137, 3725-31	11
1781	Metabolite identification using automated comparison of high-resolution multistage mass spectral trees. <i>Analytical Chemistry</i> , 2012 , 84, 5524-34	7.8 79

1780	CAMERA: an integrated strategy for compound spectra extraction and annotation of liquid chromatography/mass spectrometry data sets. <i>Analytical Chemistry</i> , 2012 , 84, 283-9	7.8	663
1779	IDEOM: an Excel interface for analysis of LC-MS-based metabolomics data. 2012 , 28, 1048-9		214
1778	Determination of total concentration of chemically labeled metabolites as a means of metabolome sample normalization and sample loading optimization in mass spectrometry-based metabolomics. <i>Analytical Chemistry</i> , 2012 , 84, 10723-31	7.8	76
1777	Analysis of urinary metabolic signatures of early hepatocellular carcinoma recurrence after surgical removal using gas chromatography-mass spectrometry. 2012 , 11, 4361-72		56
1776	Identification of intracellular <i>Spiroplasma melliferum</i> metabolites by the HPLC-MS method. 2012 , 77, 864-77		2
1775	LC-MS-based metabolomics. 2012 , 8, 470-81		317
1774	Microbial strain prioritization using metabolomics tools for the discovery of natural products. <i>Analytical Chemistry</i> , 2012 , 84, 4277-83	7.8	141
1773	Expression of a bacterial feedback-insensitive 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase of the shikimate pathway in <i>Arabidopsis</i> elucidates potential metabolic bottlenecks between primary and secondary metabolism. 2012 , 194, 430-439		84
1772	Intra- and interlaboratory reproducibility of ultra performance liquid chromatography-time-of-flight mass spectrometry for urinary metabolic profiling. <i>Analytical Chemistry</i> , 2012 , 84, 2424-32	7.8	36
1771	XCMS Online: a web-based platform to process untargeted metabolomic data. <i>Analytical Chemistry</i> , 2012 , 84, 5035-9	7.8	799
1770	Liquid chromatography-mass spectrometry based global metabolite profiling: a review. 2012 , 711, 7-16		372
1769	Chemometric evaluation of different experimental conditions on wheat (<i>Triticum aestivum</i> L.) development using liquid chromatography mass spectrometry (LC-MS) profiles of benzoxazinone derivatives. 2012 , 731, 24-31		7
1768	Instrument and process independent binning and baseline correction methods for liquid chromatography-high resolution-mass spectrometry deconvolution. 2012 , 740, 12-9		16
1767	Fibrinogen alpha chain O-glycopeptides as possible markers of urinary tract infection. 2012 , 75, 1067-73		26
1766	Metabolomic profiling of beer reveals effect of temperature on non-volatile small molecules during short-term storage. 2012 , 135, 1284-9		27
1765	Discrimination between malignant and benign ovarian tumors by plasma metabolomic profiling using ultra performance liquid chromatography/mass spectrometry. 2012 , 413, 861-8		68
1764	Global Foodomics strategy to investigate the health benefits of dietary constituents. 2012 , 1248, 139-53		96
1763	Global metabolic response in the bile of pejerrey (<i>Odontesthes bonariensis</i> , Pisces) sublethally exposed to the pyrethroid cypermethrin. 2012 , 76, 46-54		8

1762	Metabonomics. 2012 , 545-562	1
1761	Targeted and non-targeted analysis of membrane lipids using mass spectrometry. 2012 , 108, 149-72	3
1760	Metabolomics in food analysis: application to the control of forbidden substances. 2012 , 4 Suppl 1, 59-69	34
1759	Effect of dietary polyphenols on K562 leukemia cells: a Foodomics approach. 2012 , 33, 2314-27	46
1758	CE/LC-MS multiplatform for broad metabolomic analysis of dietary polyphenols effect on colon cancer cells proliferation. 2012 , 33, 2328-36	73
1757	PyMS: a Python toolkit for processing of gas chromatography-mass spectrometry (GC-MS) data. Application and comparative study of selected tools. 2012 , 13, 115	48
1756	Combining peak- and chromatogram-based retention time alignment algorithms for multiple chromatography-mass spectrometry datasets. 2012 , 13, 214	29
1755	EasyLCMS: an asynchronous web application for the automated quantification of LC-MS data. 2012 , 5, 428	10
1754	MetabR: an R script for linear model analysis of quantitative metabolomic data. 2012 , 5, 596	25
1753	High-Throughput Molecular Lipidomics. 2012 , 35-51	2
1752	Metabolome analysis of gram-positive bacteria such as <i>Staphylococcus aureus</i> by GC-MS and LC-MS. 2012 , 815, 377-98	19
1751	Metabolic profiling in Maturity-onset diabetes of the young (MODY) and young onset type 2 diabetes fails to detect robust urinary biomarkers. 2012 , 7, e40962	13
1750	Chemical and biochemical applications of MALDI TOF-MS based on analyzing the small organic compounds. 2013 , 331, 165-92	15
1749	Identification and accurate quantitation of biological oligosaccharide mixtures. <i>Analytical Chemistry</i> , 2012 , 84, 7793-801	7.8 17
1748	An accelerated workflow for untargeted metabolomics using the METLIN database. 2012 , 30, 826-8	378
1747	Serine is a natural ligand and allosteric activator of pyruvate kinase M2. 2012 , 491, 458-462	394
1746	Metabolite discovery of helacidum in rat urine with XCMS based on the data of ultra performance liquid chromatography coupled to time-of-flight mass spectrometry. 2012 , 907, 146-53	4
1745	Learned recognition of maternal signature odors mediates the first suckling episode in mice. 2012 , 22, 1998-2007	109

1744	Liquid chromatography-mass spectrometry calibration transfer and metabolomics data fusion. <i>Analytical Chemistry</i> , 2012 , 84, 9848-57	7.8	31
1743	Strategy for optimizing LC-MS data processing in metabolomics: a design of experiments approach. <i>Analytical Chemistry</i> , 2012 , 84, 6869-76	7.8	79
1742	A metabolomic approach to the study of wine micro-oxygenation. 2012 , 7, e37783		66
1741	Annotation of the human adult urinary metabolome and metabolite identification using ultra high performance liquid chromatography coupled to a linear quadrupole ion trap-Orbitrap mass spectrometer. <i>Analytical Chemistry</i> , 2012 , 84, 6429-37	7.8	94
1740	LC-MS data processing with MAVEN: a metabolomic analysis and visualization engine. 2012 , Chapter 14, Unit14.11		257
1739	Differential profiling of volatile organic compound biomarker signatures utilizing a logical statistical filter-set and novel hybrid evolutionary classifiers. 2012 ,		1
1738	Stable isotope-assisted metabolomics for network-wide metabolic pathway elucidation. <i>Analytical Chemistry</i> , 2012 , 84, 8442-7	7.8	98
1737	Innovative microwave-assisted oximation and silylation procedures for metabolomic analysis of plasma samples using gas chromatography-mass spectrometry. 2012 , 1254, 14-22		15
1736	The metabolome of induced pluripotent stem cells reveals metabolic changes occurring in somatic cell reprogramming. 2012 , 22, 168-77		388
1735	Mass spectrometry-based metabolomics to elucidate functions in marine organisms and ecosystems. 2012 , 10, 849-80		67
1734	Relative quantification of biomarkers using mixed-isotope labeling coupled with MS. 2012 , 4, 2525-41		11
1733	Fragmentation trees for the structural characterisation of metabolites. 2012 , 26, 2275-86		34
1732	A RubisCO-like protein links SAM metabolism with isoprenoid biosynthesis. 2012 , 8, 926-32		60
1731	Functional Genomics. 2012 ,		2
1730	Plant metabolomics: Applications and opportunities for agricultural biotechnology. 2012 , 67-81		17
1729	Using nanotopography and metabolomics to identify biochemical effectors of multipotency. 2012 , 6, 10239-49		99
1728	Development of isotope labeling LC-MS for human salivary metabolomics and application to profiling metabolome changes associated with mild cognitive impairment. <i>Analytical Chemistry</i> , 2012 , 84, 10802-11	7.8	66
1727	Molecular analysis of model gut microbiotas by imaging mass spectrometry and nanodesorption electrospray ionization reveals dietary metabolite transformations. <i>Analytical Chemistry</i> , 2012 , 84, 9259-67	7.8	50

1726	Optimizing the use of quality control samples for signal drift correction in large-scale urine metabolic profiling studies. <i>Analytical Chemistry</i> , 2012 , 84, 2670-7	7.8	104
1725	Metabolic profiling of the protozoan parasite <i>Entamoeba invadens</i> revealed activation of unpredicted pathway during encystation. 2012 , 7, e37740		48
1724	An ultra-fast metabolite prediction algorithm. 2012 , 7, e39158		2
1723	Phevalin (aureusimine B) production by <i>Staphylococcus aureus</i> biofilm and impacts on human keratinocyte gene expression. 2012 , 7, e40973		23
1722	Chemical communication between the endophytic fungus <i>Paraconiothyrium variabile</i> and the phytopathogen <i>Fusarium oxysporum</i> . 2012 , 7, e47313		66
1721	The Effect of LC-MS Data Preprocessing Methods on the Selection of Plasma Biomarkers in Fed vs. Fasted Rats. 2012 , 2, 77-99		50
1720	A Guideline to Univariate Statistical Analysis for LC/MS-Based Untargeted Metabolomics-Derived Data. 2012 , 2, 775-95		167
1719	. 2012 ,		5
1718	Software Techniques for Enabling High-Throughput Analysis of Metabolomic Datasets. 2012 ,		8
1717	Surface-activated chemical ionization-electrospray ionization source improves biomarker discovery with mass spectrometry. 2012 , 26, 1213-8		7
1716	Semi-targeted metabolomic approaches to validate potential markers of health for micronutrients: analytical perspectives. 2012 , 8, 1114-1129		6
1715	Statistical strategies for relating metabolomics and proteomics data: a real case study in nutrition research area. 2012 , 8, 1090-1101		9
1714	Metabolomic analysis and identification of a role for the orphan human cytochrome P450 2W1 in selective oxidation of lysophospholipids. 2012 , 53, 1610-7		32
1713	Separating the wheat from the chaff: a prioritisation pipeline for the analysis of metabolomics datasets. 2012 , 8, 29-36		38
1712	Systematic evaluation of extraction methods for multiplatform-based metabotyping: application to the <i>Fasciola hepatica</i> metabolome. <i>Analytical Chemistry</i> , 2012 , 84, 6963-72	7.8	39
1711	UPLC-MS metabolic profiling of second trimester amniotic fluid and maternal urine and comparison with NMR spectral profiling for the identification of pregnancy disorder biomarkers. 2012 , 8, 1243-54		78
1710	A metabolomic approach identifies differences in maternal serum in third trimester pregnancies that end in poor perinatal outcome. 2012 , 19, 863-75		52
1709	Innovation: Metabolomics: the apogee of the omics trilogy. 2012 , 13, 263-9		1517

1708	Meta-analysis of untargeted metabolomic data from multiple profiling experiments. 2012 , 7, 508-16	135
1707	Assessment of compatibility between extraction methods for NMR- and LC/MS-based metabolomics. <i>Analytical Chemistry</i> , 2012 , 84, 5838-44	7.8 69
1706	Myxoprincomid: Entdeckung eines Naturstoffs mithilfe einer umfassenden Analyse des sekundären Metaboloms von <i>Myxococcus xanthus</i> . 2012 , 124, 836-841	6
1705	Combined in silico modeling and metabolomics analysis to characterize fed-batch CHO cell culture. 2012 , 109, 1415-29	148
1704	A <i>Papaver somniferum</i> 10-gene cluster for synthesis of the anticancer alkaloid noscapine. 2012 , 336, 1704-8	243
1703	Prospects for a statistical theory of LC/TOFMS data. 2012 , 23, 779-91	3
1702	Charge state coalescence during electrospray ionization improves peptide identification by tandem mass spectrometry. 2012 , 23, 1390-9	43
1701	LC-MS based global metabolite profiling of grapes: solvent extraction protocol optimisation. 2012 , 8, 175-185	60
1700	Metabolite profiling and fingerprinting of commercial cultivars of <i>Humulus lupulus</i> L. (hop): a comparison of MS and NMR methods in metabolomics. 2012 , 8, 492-507	75
1699	The metabolome of human placental tissue: investigation of first trimester tissue and changes related to preeclampsia in late pregnancy. 2012 , 8, 579-597	46
1698	MSClust: a tool for unsupervised mass spectra extraction of chromatography-mass spectrometry ion-wise aligned data. 2012 , 8, 714-718	134
1697	Aligning extracted LC-MS peak lists via density maximization. 2012 , 8, 175-185	44
1696	MET-IDEA version 2.06; improved efficiency and additional functions for mass spectrometry-based metabolomics data processing. 2012 , 8, 105-110	25
1695	Metabolic dynamics during autumn cold acclimation within and among populations of Sitka spruce (<i>Picea sitchensis</i>). 2012 , 194, 192-205	50
1694	Multiscale peak alignment for chromatographic datasets. 2012 , 1223, 93-106	46
1693	Virtual separation of phytochemical constituents by their adduct-ion patterns in full mass spectra. 2012 , 1227, 181-93	12
1692	Comparative metabolite profiling and fingerprinting of medicinal licorice roots using a multiplex approach of GC-MS, LC-MS and 1D NMR techniques. 2012 , 76, 60-72	193
1691	Analysis of volatile organic compounds released from human lung cancer cells and from the urine of tumor-bearing mice. 2012 , 12, 7	72

1690	Using a spike-in experiment to evaluate analysis of LC-MS data. 2012 , 10, 13		12
1689	Ion annotation-assisted analysis of LC-MS based metabolomic experiment. 2012 , 10 Suppl 1, S8		7
1688	A benchmark spike-in data set for biomarker identification in metabolomics. 2012 , 26, 16-24		26
1687	Gas chromatography coupled to mass spectrometry-based metabolomic to screen for anabolic practices in cattle: identification of 5 α -androst-2-en-17-one as new biomarker of 4-androstenedione misuse. 2012 , 47, 131-40		23
1686	Myxoprincomide: a natural product from <i>Myxococcus xanthus</i> discovered by comprehensive analysis of the secondary metabolome. 2012 , 51, 811-6		77
1685	Recent advances of metabolomics in plant biotechnology. 2012 , 6, 1-15		102
1684	Cord blood metabolomic profiling in intrauterine growth restriction. 2012 , 402, 1109-21		93
1683	Existing bioinformatics tools for the quantitation of post-translational modifications. 2012 , 42, 129-38		11
1682	Computational mass spectrometry for small molecules. 2013 , 5, 12		105
1681	Combination of injection volume calibration by creatinine and MS signals' normalization to overcome urine variability in LC-MS-based metabolomics studies. <i>Analytical Chemistry</i> , 2013 , 85, 7659-65 ^{7.8}	43	
1680	Mass spectrometry to evaluate the effect of the ripening process on phenols of virgin olive oils. 2013 , 115, 1053-1061		8
1679	Toward 'omic scale metabolite profiling: a dual separation-mass spectrometry approach for coverage of lipid and central carbon metabolism. <i>Analytical Chemistry</i> , 2013 , 85, 6876-84	7.8	204
1678	Review: toxicometabolomics. 2013 , 33, 1365-83		129
1677	Cell Senescence. 2013 ,		3
1676	Exploring Metabolome with GC/MS. 2013 , 67, 303-329		2
1675	MultiAlign: a multiple LC-MS analysis tool for targeted omics analysis. 2013 , 14, 49		23
1674	xMSanalyzer: automated pipeline for improved feature detection and downstream analysis of large-scale, non-targeted metabolomics data. 2013 , 14, 15		201
1673	Methodological approaches to help unravel the intracellular metabolome of <i>Bacillus subtilis</i> . 2013 , 12, 69		36

1672	Metabolomics, peptidomics and proteomics applications of capillary electrophoresis-mass spectrometry in Foodomics: a review. 2013 , 802, 1-13	80
1671	Personal genomes, quantitative dynamic omics and personalized medicine. 2013 , 1, 71-90	26
1670	A tool to evaluate correspondence between extraction ion chromatographic peaks and peptide-spectrum matches in shotgun proteomics experiments. 2013 , 13, 2386-97	3
1669	Legume Genomics. 2013 ,	4
1668	Plasma metabolome analysis by integrated ionization rapid-resolution liquid chromatography/tandem mass spectrometry. 2013 , 27, 2071-80	20
1667	Metabolomics Tools for Natural Product Discovery. 2013 ,	12
1666	Daminozide Alters Anthocyanin Metabolism in Ray Florets of Bronze Chrysanthemum (<i>Chrysanthemum morifolium</i> Ramat.). 2013 , 32, 453-460	7
1665	Metabolomics identifies a biological response to chronic low-dose natural uranium contamination in urine samples. 2013 , 9, 1168-1180	24
1664	How metabolomics can contribute to bio-processes: a proof of concept study for biomarkers discovery in the context of nitrogen-starved microalgae grown in photobioreactors. 2013 , 9, 1286-1300	20
1663	Precursor mass prediction by clustering ionization products in LC-MS-based metabolomics. 2013 , 9, 1301-1310	12
1662	Comparative analysis of volatile metabolomics signals from melanoma and benign skin: a pilot study. 2013 , 9, 998-1008	60
1661	Computational annotation of plant metabolomics profiles via a novel network-assisted approach. 2013 , 9, 904-918	12
1660	Differential mobility analysis-mass spectrometry coupled to XCMS algorithm as a novel analytical platform for metabolic profiling. 2013 , 9, 30-43	9
1659	Nearline acquisition and processing of liquid chromatography-tandem mass spectrometry data. 2013 , 9, 84-91	23
1658	Assessment of data pre-processing methods for LC-MS/MS-based metabolomics of uterine cervix cancer. 2013 , 138, 2669-77	25
1657	Overview of <i>Dekkera bruxellensis</i> behaviour in an ethanol-rich environment using untargeted and targeted metabolomic approaches. 2013 , 51, 670-678	15
1656	Potential of Fourier Transform Mass Spectrometry for High-Throughput Metabolomics Analysis. 2013 , 67, 219-302	4
1655	Mass Spectrometry Metabolomic Data Handling for Biomarker Discovery. 2013 , 425-445	10

1654	Strategies for Data Handling and Statistical Analysis in Metabolomics Studies. 2013 , 493-555		2
1653	Functional Genomics, Proteomics, Metabolomics and Bioinformatics for Systems Biology. 2013 , 3-41		4
1652	Role of plant β -glucosidases in the dual defense system of iridoid glycosides and their hydrolyzing enzymes in <i>Plantago lanceolata</i> and <i>Plantago major</i> . 2013 , 94, 99-107		38
1651	Relevance of the cyclophosphamide-induced cystitis model for pharmacological studies targeting inflammation and pain of the bladder. 2013 , 707, 32-40		46
1650	Batch Normalizer: a fast total abundance regression calibration method to simultaneously adjust batch and injection order effects in liquid chromatography/time-of-flight mass spectrometry-based metabolomics data and comparison with current calibration methods. <i>Analytical Chemistry</i> , 2013 , 85, 1037-46	7.8	79
1649	A new approach to untargeted integration of high resolution liquid chromatography-mass spectrometry data. 2013 , 801, 34-42		8
1648	New approach for chemometric analysis of mass spectrometry data. <i>Analytical Chemistry</i> , 2013 , 85, 3053-58	7.8	11
1647	Comparative proteomic and metabolomic analysis of <i>Staphylococcus warneri</i> SG1 cultured in the presence and absence of butanol. 2013 , 12, 4478-89		26
1646	Investigation of the relationship between the metabolic profile of tobacco leaves in different planting regions and climate factors using a pseudotargeted method based on gas chromatography/mass spectrometry. 2013 , 12, 5072-83		30
1645	A diurnal serum lipid integrates hepatic lipogenesis and peripheral fatty acid use. 2013 , 502, 550-4		259
1644	Measurement of DNA concentration as a normalization strategy for metabolomic data from adherent cell lines. <i>Analytical Chemistry</i> , 2013 , 85, 9536-42	7.8	72
1643	The protein quality control system manages plant defence compound synthesis. 2013 , 504, 148-52		91
1642	A comparison of five lipid extraction solvent systems for lipidomic studies of human LDL. 2013 , 54, 1812-24		159
1641	Applications of MALDI-TOF Spectroscopy. 2013 ,		1
1640	Liquid Chromatography Coupled to Mass Spectrometry-Based Metabolomics and the Concept of Biomarker. 2013 , 67, 159-218		5
1639	Proteomics & metabolomics: Mapping biochemical regulations. 2013 , 5, 321-326		12
1638	Phytochemical, phylogenetic, and anti-inflammatory evaluation of 43 <i>Urtica</i> accessions (stinging nettle) based on UPLC-Q-TOF-MS metabolomic profiles. 2013 , 96, 170-83		77
1637	Jasmonate Signaling. 2013 ,		3

1636	A novel chromatographic peak alignment method coupled with trilinear decomposition for three dimensional chromatographic data analysis to obtain the second-order advantage. 2013 , 138, 627-34		28
1635	Multi-profile Bayesian alignment model for LC-MS data analysis with integration of internal standards. 2013 , 29, 2774-80		15
1634	Plant metabolomics: from experimental design to knowledge extraction. 2013 , 1069, 279-312		6
1633	A network-based approach for predicting key enzymes explaining metabolite abundance alterations in a disease phenotype. 2013 , 7, 62		14
1632	A flexible statistical model for alignment of label-free proteomics data--incorporating ion mobility and product ion information. 2013 , 14, 364		5
1631	First mass spectrometry metabolic fingerprinting of bacterial metabolism in a model cheese. 2013 , 141, 1032-40		31
1630	Pseudotargeted metabolomics method and its application in serum biomarker discovery for hepatocellular carcinoma based on ultra high-performance liquid chromatography/triple quadrupole mass spectrometry. <i>Analytical Chemistry</i> , 2013 , 85, 8326-33	7.8	139
1629	Metabolomics in Herbal Medicine Research. 2013 , 155-174		5
1628	Integrative Analysis of Secondary Metabolism and Transcript Regulation in Arabidopsis Thaliana. 2013 , 175-195		
1627	Metabolomics driven analysis of artichoke leaf and its commercial products via UHPLC-q-TOF-MS and chemometrics. 2013 , 95, 177-87		75
1626	Research towards a systematic signature discovery process. 2013 ,		4
1625	Application of machine learning to proteomics data: classification and biomarker identification in postgenomics biology. 2013 , 17, 595-610		124
1624	Tomato fruits expressing a bacterial feedback-insensitive 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase of the shikimate pathway possess enhanced levels of multiple specialized metabolites and upgraded aroma. 2013 , 64, 4441-52		46
1623	Identification of biomarkers for unstable angina by plasma metabolomic profiling. 2013 , 9, 3059-67		26
1622	Global metabolic profiling of animal and human tissues via UPLC-MS. 2013 , 8, 17-32		405
1621	Comparative analysis of sample preparation methods to handle the complexity of the blood fluid metabolome: when less is more. <i>Analytical Chemistry</i> , 2013 , 85, 341-8	7.8	104
1620	Prioritization of putative metabolite identifications in LC-MS/MS experiments using a computational pipeline. 2013 , 13, 248-60		7
1619	Lipidomic profiling of model organisms and the world's major pathogens. 2013 , 95, 109-15		25

1618	Identification of potential biomarkers for ovarian cancer by urinary metabolomic profiling. 2013 , 12, 505-12	123
1617	High performance analysis of the cyanobacterial metabolism via liquid chromatography coupled to a LTQ-Orbitrap mass spectrometer: evidence that glucose reprograms the whole carbon metabolism and triggers oxidative stress. 2013 , 9, 21-32	27
1616	Assigning precursor-product ion relationships in indiscriminant MS/MS data from non-targeted metabolite profiling studies. 2013 , 9, 33-43	32
1615	Metabolomic study of Chilean biomining bacteria <i>Acidithiobacillus ferrooxidans</i> strain Wenelen and <i>Acidithiobacillus thiooxidans</i> strain Licanantay. 2013 , 9, 247-257	33
1614	Liquid chromatography quadrupole time-of-flight mass spectrometry characterization of metabolites guided by the METLIN database. 2013 , 8, 451-60	288
1613	An automated pipeline for high-throughput label-free quantitative proteomics. 2013 , 12, 1628-44	123
1612	Chlorination of bisphenol A: non-targeted screening for the identification of transformation products and assessment of estrogenicity in generated water. 2013 , 93, 2814-22	23
1611	Application of fast Fourier transform cross-correlation and mass spectrometry data for accurate alignment of chromatograms. 2013 , 1286, 175-82	25
1610	Resistant starch intake partly restores metabolic and inflammatory alterations in the liver of high-fat-diet-fed rats. 2013 , 24, 1920-30	35
1609	Exploring the utility of high-resolution MS with post-acquisition data mining for simultaneous exogenous and endogenous metabolite profiling. 2013 , 5, 1211-28	12
1608	Metabolic engineering of <i>Arabidopsis</i> for butanetriol production using bacterial genes. 2013 , 20, 109-20	21
1607	Impact of defoliation on the regrowth capacity and the shoot metabolite profile of <i>Plantago lanceolata</i> L. 2013 , 71, 325-33	11
1606	Antibacterial activity and phytochemical profile of fermented <i>Camellia sinensis</i> (fuzhuan tea). 2013 , 53, 945-949	44
1605	Myocardial lipidomics profiling delineate the toxicity of traditional Chinese medicine <i>Aconiti Lateralis radix praeparata</i> . 2013 , 147, 349-56	48
1604	Monitoring metabolic responses to chemotherapy in single cells and tumors using nanostructure-initiator mass spectrometry (NIMS) imaging. 2013 , 1, 4	37
1603	Feasibility of identifying the tobacco-related global metabolome in blood by UPLC-QTOF-MS. 2013 , 12, 679-91	30
1602	Gas Chromatography and Comprehensive Two-Dimensional Gas Chromatography Hyphenated with Mass Spectrometry for Targeted and Nontargeted Metabolomics. 2013 , 69-92	
1601	LC-MS-Based Nontargeted Metabolomics. 2013 , 93-115	3

1600	The Potential of Ultrahigh Resolution MS (FTICR-MS) in Metabolomics. 2013 , 117-136	2
1599	The Art and Practice of Lipidomics. 2013 , 137-176	5
1598	Ms-Based Metabolomics in Nutrition and Health Research. 2013 , 245-270	1
1597	Chemical approaches to study metabolic networks. 2013 , 465, 427-40	13
1596	Current metabolomics: technological advances. 2013 , 116, 9-16	143
1595	A global approach to analysis and interpretation of metabolic data for plant natural product discovery. 2013 , 30, 565-83	88
1594	Mass spectrometry of structurally modified DNA. 2013 , 113, 2395-436	96
1593	Sum of the parts: mass spectrometry-based metabolomics. 2013 , 52, 3829-40	48
1592	NNMT promotes epigenetic remodeling in cancer by creating a metabolic methylation sink. 2013 , 9, 300-6	233
1591	New insights into sulfur metabolism in yeasts as revealed by studies of <i>Yarrowia lipolytica</i> . 2013 , 79, 1200-11	30
1590	Identification of endogenous substrates of orphan cytochrome P450 enzymes through the use of untargeted metabolomics approaches. 2013 , 987, 71-7	6
1589	Ultra high performance liquid chromatography as a tool for the discovery and the analysis of biomarkers of diseases: a review. 2013 , 927, 37-53	52
1588	References. 2013 , 313-326	
1587	Metabolomics and Its Role in the Study of Mammalian Systems. 2013 , 345-377	1
1586	Profiling the metabolic signature of senescence. 2013 , 965, 355-71	4
1585	Metabolic Profiling of Plants by GC/MS. 2013 , 1-23	11
1584	Induced resistance in maize is based on organ-specific defence responses. 2013 , 74, 213-25	99
1583	Label-free quantitative proteomics trends for protein-protein interactions. 2013 , 81, 91-101	47

1582	Serum metabolomics reveals lipid metabolism variation between coronary artery disease and congestive heart failure: a pilot study. 2013 , 18, 314-21		16
1581	Comprehensive analysis of LC/MS data using pseudocolor plots. 2013 , 24, 230-7		4
1580	Simultaneous extraction of metabolome and lipidome with methyl tert-butyl ether from a single small tissue sample for ultra-high performance liquid chromatography/mass spectrometry. 2013 , 1298, 9-16		144
1579	Chronic ethanol consumption alters mammalian gastrointestinal content metabolites. 2013 , 12, 3297-306		84
1578	Metabolomics and PDO. 2013 , 60, 123-143		5
1577	Metabolomics as a potential new approach for investigating human reproductive disorders. 2013 , 12, 2914-20		35
1576	Global metabolite profiling of human colorectal cancer xenografts in mice using HPLC-MS/MS. 2013 , 12, 2980-6		10
1575	Detection and structural elucidation of esterified oxylipids in human synovial fluid by electrospray ionization-fourier transform ion-cyclotron mass spectrometry and liquid chromatography-ion trap-MS(3): detection of esterified hydroxylated docosapentaenoic acid containing phospholipids. <i>Analytical Chemistry</i> , 2013 , 85, 6003-10	7.8	13
1574	Differential chemical profiling to identify ozonation by-products of estrone-sulfate and first characterization of estrogenicity in generated drinking water. 2013 , 47, 3791-802		12
1573	Integrated metabolomics approach facilitates discovery of an unpredicted natural product suite from <i>Streptomyces coelicolor</i> M145. 2013 , 8, 2009-16		53
1572	Metabolo-proteomics to discover plant biotic stress resistance genes. 2013 , 18, 522-31		81
1571	Liquid Chromatographic Methods Combined with Mass Spectrometry in Metabolomics. 2013 , 145-161		2
1570	A new metabolomic workflow for early detection of Alzheimer's disease. 2013 , 1302, 65-71		67
1569	Integrated LC-MS/MS system for plant metabolomics. 2013 , 4, e201301011		21
1568	Distinct lipid compositions of two types of human prostasomes. 2013 , 13, 1660-6		95
1567	Metabolite profiling of plant tissues by liquid chromatography Fourier transform ion cyclotron resonance mass spectrometry. 2013 , 1011, 277-86		6
1566	Cytotoxic effect of commercial <i>Humulus lupulus</i> L. (hop) preparations - In comparison to its metabolomic fingerprint. 2013 , 4, 417-21		11
1565	Quantitative metabolomic and lipidomic profiling reveals aberrant amino acid metabolism in type 2 diabetes. 2013 , 9, 307-17		41

1564	A metabolomic view of how the human gut microbiota impacts the host metabolome using humanized and gnotobiotic mice. 2013 , 7, 1933-43		222
1563	Molecular network analysis of phosphotyrosine and lipid metabolism in hepatic PTP1b deletion mice. 2013 , 5, 940-63		13
1562	Glia co-culture with neurons in microfluidic platforms promotes the formation and stabilization of synaptic contacts. 2013 , 13, 3008-21		80
1561	Metabolite profiling driven analysis of <i>Salsola</i> species and their anti-acetylcholinesterase potential. 2013 , 27, 2320-7		15
1560	Combining targeted and nontargeted data analysis for liquid chromatography/high-resolution mass spectrometric analyses. 2013 , 36, 971-9		7
1559	Computational tools for the secondary analysis of metabolomics experiments. 2013 , 4, e201301003		51
1558	LC-MS metabolomics from study design to data-analysis - using a versatile pathogen as a test case. 2013 , 4, e201301002		34
1557	Gaussian process regression model for normalization of LC-MS data using scan-level information. 2013 , 11, S13		13
1556	Metabolic phenotype of the healthy rodent model using in-vial extraction of dried serum, urine, and cerebrospinal fluid spots. <i>Analytical Chemistry</i> , 2013 , 85, 7257-63	7.8	12
1555	Plasma lipidomic profiling method based on ultrasound extraction and liquid chromatography mass spectrometry. <i>Analytical Chemistry</i> , 2013 , 85, 12085-92	7.8	62
1554	Hybrid feature detection and information accumulation using high-resolution LC-MS metabolomics data. 2013 , 12, 1419-27		62
1553	RAMSY: ratio analysis of mass spectrometry to improve compound identification. <i>Analytical Chemistry</i> , 2013 , 85, 10771-9	7.8	25
1552	Novel MS-based approaches and applications in food metabolomics. 2013 , 52, 100-111		68
1551	Metabolome classification of <i>Brassica napus</i> L. organs via UPLC-QTOF-PDA-MS and their anti-oxidant potential. 2013 , 24, 277-87		46
1550	High-resolution metabolic mapping of cell types in plant roots. 2013 , 110, E1232-41		102
1549	Cytochrome P450 107U1 is required for sporulation and antibiotic production in <i>Streptomyces coelicolor</i> . 2013 , 530, 101-7		9
1548	Nonlinear alignment of chromatograms by means of moving window fast Fourier transform cross-correlation. 2013 , 36, 1677-84		10
1547	A view from above: cloud plots to visualize global metabolomic data. <i>Analytical Chemistry</i> , 2013 , 85, 798-804		72

1546	Maternal and cord blood LC-HRMS metabolomics reveal alterations in energy and polyamine metabolism, and oxidative stress in very-low birth weight infants. 2013 , 12, 2764-78	42
1545	Time-saving design of experiment protocol for optimization of LC-MS data processing in metabolomic approaches. <i>Analytical Chemistry</i> , 2013 , 85, 7109-16	7.8 36
1544	Plant Metabolomics: From Holistic Data to Relevant Biomarkers. 2013 , 20, 1056-1090	11
1543	Metabolic profiling provides a system understanding of hypothyroidism in rats and its application. 2013 , 8, e55599	28
1542	NetWeAvers: an R package for integrative biological network analysis with mass spectrometry data. 2013 , 29, 2946-7	4
1541	Honing in on phenotypes: comprehensive two-dimensional gas chromatography of herbivory-induced volatile emissions and novel opportunities for system-level analyses. 2013 , 5, plt002	5
1540	A Trypanosoma brucei kinesin heavy chain promotes parasite growth by triggering host arginase activity. 2013 , 9, e1003731	37
1539	mzMatch-ISO: an R tool for the annotation and relative quantification of isotope-labelled mass spectrometry data. 2013 , 29, 281-3	67
1538	Metabolomics of cereals under biotic stress: current knowledge and techniques. 2013 , 4, 82	89
1537	Graph-based peak alignment algorithms for multiple liquid chromatography-mass spectrometry datasets. 2013 , 29, 2469-76	7
1536	Predicting network activity from high throughput metabolomics. 2013 , 9, e1003123	431
1535	CHAPTER 4:Liquid Chromatographic Techniques in Metabolomics. 2013 , 64-86	1
1534	CHAPTER 6:Capillary Electromigration Techniques in Metabolomics. 2013 , 114-137	1
1533	Bovine cumulus cells protect maturing oocytes from increased fatty acid levels by massive intracellular lipid storage. 2013 , 88, 164	76
1532	MetaboLights--an open-access general-purpose repository for metabolomics studies and associated meta-data. 2013 , 41, D781-6	483
1531	The MetaboLights repository: curation challenges in metabolomics. 2013 , 2013, bat029	40
1530	Deciphering herbivory-induced gene-to-metabolite dynamics in Nicotiana attenuata tissues using a multifactorial approach. 2013 , 162, 1042-59	30
1529	MeltDB 2.0-advances of the metabolomics software system. 2013 , 29, 2452-9	63

1528	eMZed: an open source framework in Python for rapid and interactive development of LC/MS data analysis workflows. 2013 , 29, 963-4	35
1527	Stool microbiome and metabolome differences between colorectal cancer patients and healthy adults. 2013 , 8, e70803	407
1526	ABHD12 controls brain lysophosphatidylserine pathways that are deregulated in a murine model of the neurodegenerative disease PHARC. 2013 , 110, 1500-5	129
1525	Food safety and contamination assessment using metabolomics. 2013 , 40-53	1
1524	Selective intrauterine growth restriction in monozygotic twin pregnancies: markers of endothelial damage and metabolomic profile. 2013 , 16, 816-26	22
1523	Urinary metabolomic markers of aminoglycoside nephrotoxicity in newborn rats. 2013 , 73, 585-91	34
1522	Reprogramming the phenylpropanoid metabolism in seeds of oilseed rape by suppressing the orthologs of reduced epidermal fluorescence1. 2013 , 161, 1656-69	22
1521	Metabolomic discrimination between patients with stable angina, non-ST elevation myocardial infarction, and acute myocardial infarct. 2013 , 34, n/a-n/a	
1520	Establishment and assessment of a new human embryonic stem cell-based biomarker assay for developmental toxicity screening. 2013 , 98, 343-63	60
1519	A genome-wide assessment of variability in human serum metabolism. 2013 , 34, 515-24	38
1518	True ion pick (TIPick): a denoising and peak picking algorithm to extract ion signals from liquid chromatography/mass spectrometry data. 2013 , 48, 234-42	24
1517	Constructing a mass measurement error surface to improve automatic annotations in liquid chromatography/mass spectrometry based metabolomics. 2013 , 27, 2425-31	22
1516	GPA: An algorithm for LC/MS based glycan profile annotation. 2013 ,	2
1515	Pre-processing liquid chromatography/high-resolution mass spectrometry data: extracting pure mass spectra by deconvolution from the invariance of isotopic distribution. 2013 , 27, 917-23	5
1514	Rapid diagnosis of TB using GC-MS and chemometrics. 2013 , 5, 3079-97	17
1513	Metabolomics: an essential tool to understand the function of peroxisome proliferator-activated receptor alpha. 2013 , 41, 410-8	11
1512	Global and targeted metabolomics of esophageal squamous cell carcinoma discovers potential diagnostic and therapeutic biomarkers. 2013 , 12, 1306-18	85
1511	Metabolomics analysis for biomarker discovery: advances and challenges. 2013 , 20, 257-71	165

1510	Analysis of the exhalome: a diagnostic tool of the future. 2013 , 144, 746-749	33
1509	Forensic identification of seal oils using lipid profiles and statistical models. 2013 , 58, 336-43	3
1508	Untargeted metabolomics from biological sources using ultraperformance liquid chromatography-high resolution mass spectrometry (UPLC-HRMS). 2013 , e50433	18
1507	Tackling CASMI 2012: Solutions from MetFrag and MetFusion. 2013 , 3, 623-36	8
1506	Alterations in exhaled breath metabolite-mixtures in two rat models of lipopolysaccharide-induced lung injury. 2013 , 115, 1487-95	24
1505	Influence of Biological and Technical Covariates on Non-targeted Metabolite Profiling in a Large-scale Epidemiological Study. 2013 , 1, 220-226	
1504	Metabolomic study of a diagnostic model for the metabolites of stool fat. 2013 , 61, 9-16	1
1503	Comparative lipid profiling of the cnidarian <i>Aiptasia pallida</i> and its dinoflagellate symbiont. 2013 , 8, e57975	29
1502	Metabolomics reveals the origins of antimicrobial plant resins collected by honey bees. 2013 , 8, e77512	47
1501	Biomarker Discovery and Translation in Metabolomics. 2013 , 1, 227-240	67
1500	Genome-wide transcriptome and antioxidant analyses on gamma-irradiated phases of <i>deinococcus radiodurans</i> R1. 2014 , 9, e85649	32
1499	A pilot study exploring the use of breath analysis to differentiate healthy cattle from cattle experimentally infected with <i>Mycobacterium bovis</i> . 2014 , 9, e89280	32
1498	New biomarkers of coffee consumption identified by the non-targeted metabolomic profiling of cohort study subjects. 2014 , 9, e93474	86
1497	The application of Gaussian mixture models for signal quantification in MALDI-TOF mass spectrometry of peptides. 2014 , 9, e111016	10
1496	Metabolomics as a tool for discovery of biomarkers of autism spectrum disorder in the blood plasma of children. 2014 , 9, e112445	93
1495	ALLocator: an interactive web platform for the analysis of metabolomic LC-ESI-MS datasets, enabling semi-automated, user-revised compound annotation and mass isotopomer ratio analysis. 2014 , 9, e113909	22
1494	MetaDB a Data Processing Workflow in Untargeted MS-Based Metabolomics Experiments. 2014 , 2, 72	24
1493	Application of stable isotope-assisted metabolomics for cell metabolism studies. 2014 , 4, 142-65	36

1492	Metabolomics for biomarker discovery in gastroenterological cancer. 2014 , 4, 547-71	20
1491	Integrative Analysis Workflow for Untargeted Metabolomics in Translational Research. 2014 , 04,	1
1490	Gas Chromatography in Metabolomics Study. 2014 ,	6
1489	. 2014 ,	8
1488	Electrophoresis, Chromatography, and Mass Spectrometry. 2014 , 147-166	
1487	Systematic structural characterization of metabolites in Arabidopsis via candidate substrate-product pair networks. 2014 , 26, 929-45	93
1486	Reciprocal responses in the interaction between Arabidopsis and the cell-content-feeding chelicerate herbivore spider mite. 2014 , 164, 384-99	83
1485	Evaluation of horse urine sample preparation methods for metabolomics using LC coupled to HRMS. 2014 , 6, 785-803	11
1484	Lactobacillus acidophilus NCFM affects vitamin E acetate metabolism and intestinal bile acid signature in monocolonized mice. 2014 , 5, 296-303	15
1483	Identifying and quantifying metabolites by scoring peaks of GC-MS data. 2014 , 15, 374	8
1482	Investigating the drought-stress response of hybrid poplar genotypes by metabolite profiling. 2014 , 34, 1203-19	60
1481	Detection of an endogenous urinary biomarker associated with CYP2D6 activity using global metabolomics. 2014 , 15, 1947-62	25
1480	Large-scale metabolomic profiling identifies novel biomarkers for incident coronary heart disease. 2014 , 10, e1004801	175
1479	Benznidazole biotransformation and multiple targets in Trypanosoma cruzi revealed by metabolomics. 2014 , 8, e2844	76
1478	Disruption of the ammonium transporter AMT1.1 alters basal defenses generating resistance against Pseudomonas syringae and Plectosphaerella cucumerina. 2014 , 5, 231	32
1477	Sustained mitogen-activated protein kinase activation reprograms defense metabolism and phosphoprotein profile in Arabidopsis thaliana. 2014 , 5, 554	45
1476	Evaluating plant immunity using mass spectrometry-based metabolomics workflows. 2014 , 5, 291	42
1475	Preparing to fight back: generation and storage of priming compounds. 2014 , 5, 295	78

1474	MSPrep--summarization, normalization and diagnostics for processing of mass spectrometry-based metabolomic data. 2014 , 30, 133-4		41
1473	Metabolomics. 2014 , 106-118		
1472	Proteins with high turnover rate in barley leaves estimated by proteome analysis combined with in planta isotope labeling. 2014 , 166, 91-108		87
1471	Metabolomics in rheumatic diseases. 2014 , 9, 353-369		5
1470	Mass spectrometric analysis of L-cysteine metabolism: physiological role and fate of L-cysteine in the enteric protozoan parasite <i>Entamoeba histolytica</i> . 2014 , 5, e01995		27
1469	Feature extraction based on trimmed complex network representation for metabolomic data classification. 2014 ,		
1468	Comparative evaluation of eight software programs for alignment of gas chromatography-mass spectrometry chromatograms in metabolomics experiments. 2014 , 1374, 199-206		42
1467	Rapid-throughput glycomics applied to human milk oligosaccharide profiling for large human studies. 2014 , 406, 7925-35		41
1466	ChelomEx: Isotope-assisted discovery of metal chelates in complex media using high-resolution LC-MS. <i>Analytical Chemistry</i> , 2014 , 86, 11298-305	7.8	31
1465	A role of peripheral myelin protein 2 in lipid homeostasis of myelinating Schwann cells. 2014 , 62, 1502-12		41
1464	Emerging Trends for Stimulating the Discovery of Natural Products. 2014 , 115-161		3
1463	The metabolic enzyme AdhE controls the virulence of <i>Escherichia coli</i> O157:H7. 2014 , 93, 199-211		40
1462	Application of nontargeted metabolite profiling to discover novel markers of quality traits in an advanced population of malting barley. 2014 , 12, 147-60		37
1461	Self-organizing maps: a versatile tool for the automatic analysis of untargeted imaging datasets. 2014 , 14, 853-61		19
1460	Current state-of-the-art of nontargeted metabolomics based on liquid chromatography-mass spectrometry with special emphasis in clinical applications. 2014 , 1374, 1-13		81
1459	Large-scale profiling of metabolic dysregulation in ovarian cancer. 2015 , 136, 516-26		74
1458	High resolution mass spectrometry based techniques at the crossroads of metabolic pathways. 2014 , 33, 471-500		117
1457	WITHDRAWN: Recent advances in chemometric methods for plant metabolomics: A review. 2014 ,		3

1456	Different metabolic and genetic responses in citrus may explain relative susceptibility to <i>Tetranychus urticae</i> . 2014 , 70, 1728-41	41
1455	The roots of plant defenses: integrative multivariate analyses uncover dynamic behaviors of gene and metabolic networks of roots elicited by leaf herbivory. 2014 , 77, 880-92	22
1454	Future methods for the diagnosis of inflammatory bowel disease. 2014 , 32, 463-7	2
1453	Transcript and metabolite profiling for the evaluation of tobacco tree and poplar as feedstock for the bio-based industry. 2014 ,	3
1452	Evaluation of human plasma sample preparation protocols for untargeted metabolic profiles analyzed by UHPLC-ESI-TOF-MS. 2014 , 406, 7641-52	22
1451	Metabolomics applied in bioenergy. 2014 , 1,	13
1450	An R package to analyse LC/MS metabolomic data: MAIT (Metabolite Automatic Identification Toolkit). 2014 , 30, 1937-9	55
1449	Assessing the metabolic effects of calcineurin inhibitors in renal transplant recipients by urine metabolic profiling. 2014 , 98, 195-201	15
1448	ProbMetab: an R package for Bayesian probabilistic annotation of LC-MS-based metabolomics. 2014 , 30, 1336-7	46
1447	Orders of magnitude extension of the effective dynamic range of TDC-based TOFMS data through maximum likelihood estimation. 2014 , 25, 1824-7	4
1446	The integrated disease network. 2014 , 6, 1069-79	20
1445	Integrating omics technologies to study pulmonary physiology and pathology at the systems level. 2014 , 33, 1239-60	10
1444	Oxidation of endogenous N-arachidonoylserotonin by human cytochrome P450 2U1. 2014 , 289, 10476-10487	24
1443	Determination of antiprotozoal drug mechanisms by metabolomics approaches. 2014 , 141, 83-92	37
1442	Three-stage continuous culture system with a self-generated anaerobia to study the regionalized metabolism of the human gut microbiota. 2014 , 96, 111-8	24
1441	Dividing cells regulate their lipid composition and localization. 2014 , 156, 428-39	192
1440	Analysis of volatile human urinary metabolome by solid-phase microextraction in combination with gas chromatography-mass spectrometry for biomarker discovery: application in a pilot study to discriminate patients with renal cell carcinoma. 2014 , 50, 1993-2002	42
1439	Current practice of liquid chromatography-mass spectrometry in metabolomics and metabonomics. 2014 , 87, 12-25	278

1438	The Risa R/Bioconductor package: integrative data analysis from experimental metadata and back again. 2014 , 15 Suppl 1, S11	15
1437	Meta-analysis of global metabolomic data identifies metabolites associated with life-span extension. 2014 , 10, 737-743	23
1436	Sauvignon blanc metabolomics: grape juice metabolites affecting the development of varietal thiols and other aroma compounds in wines. 2014 , 10, 556-573	59
1435	Metabolite profiling and fingerprinting of Hypericum species: a comparison of MS and NMR metabolomics. 2014 , 10, 574-588	70
1434	A novel stable isotope labelling assisted workflow for improved untargeted LC-HRMS based metabolomics research. 2014 , 10, 754-769	57
1433	Evaluation of specific gravity as normalization strategy for cattle urinary metabolome analysis. 2014 , 10, 627-637	25
1432	Genotypes of <i>Fraxinus excelsior</i> with different susceptibility to the ash dieback pathogen <i>Hymenoscyphus pseudoalbidus</i> and their response to the phytotoxin viridiol - a metabolomic and microscopic study. 2014 , 102, 115-25	18
1431	Targeting novel chemical and constitutive primed metabolites against <i>Plectosphaerella cucumerina</i> . 2014 , 78, 227-40	41
1430	Metabolomics driven analysis of six <i>Nigella</i> species seeds via UPLC-qTOF-MS and GC-MS coupled to chemometrics. 2014 , 151, 333-42	90
1429	Bovine serum albumin as a molecular sensor for the discrimination of complex metabolite samples. 2014 , 818, 61-6	5
1428	Lipidomics: potential role in risk prediction and therapeutic monitoring for diabetes and cardiovascular disease. 2014 , 143, 12-23	114
1427	Metabolite Imager: customized spatial analysis of metabolite distributions in mass spectrometry imaging. 2014 , 10, 337-348	23
1426	Metabolomic insights into system-wide coordination of vertebrate metamorphosis. 2014 , 14, 5	23
1425	State-of-the-art non-targeted metabolomics in the study of chronic kidney disease. 2014 , 10, 425-442	26
1424	Proteomics and Metabolomics of Marine Organisms: Current Strategies and Knowledge. 2014 , 457-472	1
1423	Combination of metabolomic and phospholipid-profiling approaches for the study of Alzheimer's disease. 2014 , 104, 37-47	92
1422	NMR and LC/MS-based global metabolomics to identify serum biomarkers differentiating hepatocellular carcinoma from liver cirrhosis. 2014 , 135, 658-68	82
1421	Mass spectrometry in plant metabolomics strategies: from analytical platforms to data acquisition and processing. 2014 , 31, 784-806	124

1420	Ceramides and sphingomyelinases in senile plaques. 2014 , 65, 193-201		36
1419	A strategy for rapid analysis of xenobiotic metabolome of Sini decoction in vivo using ultra-performance liquid chromatography-electrospray ionization quadrupole-time-of-flight mass spectrometry combined with pattern recognition approach. 2014 , 96, 187-96		17
1418	MASSyPup--an 'out of the box' solution for the analysis of mass spectrometry data. 2014 , 49, 37-42		14
1417	Metabolome analysis for discovering biomarkers of gastroenterological cancer. 2014 , 966, 59-69		32
1416	Plant Isoprenoids. 2014 ,		5
1415	High-resolution mass spectrometry applied to the study of metabolome modifications in various chicken tissues after amoxicillin administration. 2014 , 153, 405-13		19
1414	High specificity in plant leaf metabolic responses to arbuscular mycorrhiza. 2014 , 5, 3886		87
1413	Peak aggregation as an innovative strategy for improving the predictive power of LC-MS metabolomic profiles. <i>Analytical Chemistry</i> , 2014 , 86, 2320-5	7.8	8
1412	Comparison of three generic vancomycin products using liquid chromatography-mass spectrometry and an online tool. 2014 , 71, 1029-38		6
1411	After the feature presentation: technologies bridging untargeted metabolomics and biology. 2014 , 28, 143-8		34
1410	A metabolomics-based method for studying the effect of yfcC gene in Escherichia coli on metabolism. 2014 , 451, 48-55		16
1409	metaMS: an open-source pipeline for GC-MS-based untargeted metabolomics. 2014 , 966, 109-16		57
1408	Metabolomics. 2014 , 181-205		11
1407	MetaboLyzer: a novel statistical workflow for analyzing Postprocessed LC-MS metabolomics data. <i>Analytical Chemistry</i> , 2014 , 86, 506-13	7.8	73
1406	Ion fusion of high-resolution LC-MS-based metabolomics data to discover more reliable biomarkers. <i>Analytical Chemistry</i> , 2014 , 86, 3793-800	7.8	33
1405	Chemometrics for the analysis of chromatographic data in metabolomics investigations. 2014 , 28, 681-687		21
1404	Identification of novel micropollutants in wastewater by a combination of suspect and nontarget screening. 2014 , 184, 25-32		182
1403	Hirmi Valley liver disease: a disease associated with exposure to pyrrolizidine alkaloids and DDT. 2014 , 60, 96-102		35

1402	Metabolic phenotyping and systems biology approaches to understanding metabolic syndrome and fatty liver disease. 2014 , 146, 46-62	124
1401	A simple breath sampling method in intubated and mechanically ventilated critically ill patients. 2014 , 191, 67-74	27
1400	Normalization to specific gravity prior to analysis improves information recovery from high resolution mass spectrometry metabolomic profiles of human urine. <i>Analytical Chemistry</i> , 2014 , 86, 10925-31	53
1399	Brain region mapping using global metabolomics. 2014 , 21, 1575-84	54
1398	Unravelling the Triterpenoid Saponin Biosynthesis of the African Shrub <i>Maesa lanceolata</i> . 2014 ,	
1397	Comparative LC-MS-based metabolite profiling of the ancient tropical rainforest tree <i>Symphonia globulifera</i> . 2014 , 108, 102-8	12
1396	Profiling of secondary metabolites in root exudates of <i>Arabidopsis thaliana</i> . 2014 , 108, 35-46	121
1395	Developmental changes in leaf phenolics composition from three artichoke cvs. (<i>Cynara scolymus</i>) as determined via UHPLC-MS and chemometrics. 2014 , 108, 67-76	29
1394	The fungal leaf endophyte <i>Paraconiothyrium variabile</i> specifically metabolizes the host-plant metabolome for its own benefit. 2014 , 108, 95-101	46
1393	GC-MS-based metabolite profiling of <i>Cosmos caudatus</i> leaves possessing alpha-glucosidase inhibitory activity. 2014 , 79, C1130-6	43
1392	A novel strategy for quantitative analysis of the formulated complex system using chromatographic fingerprints combined with some chemometric techniques. 2014 , 1370, 179-86	9
1391	CYP83A1 is required for metabolic compatibility of <i>Arabidopsis</i> with the adapted powdery mildew fungus <i>Erysiphe cruciferarum</i> . 2014 , 202, 1310-1319	31
1390	Adaption of the global test idea to proteomics data with missing values. 2014 , 30, 1424-30	7
1389	Arbuscular mycorrhiza-induced shifts in foliar metabolism and photosynthesis mirror the developmental stage of the symbiosis and are only partly driven by improved phosphate uptake. 2014 , 27, 1403-12	24
1388	Taximin, a conserved plant-specific peptide is involved in the modulation of plant-specialized metabolism. 2014 , 12, 971-83	23
1387	A new approach combining LC-MS and multivariate statistical analysis for revealing changes in histone modification levels. 2014 , 10, 2974-83	2
1386	Metabolome analysis based on capillary electrophoresis-mass spectrometry. 2014 , 61, 215-222	66
1385	A nano ultra-performance liquid chromatography-high resolution mass spectrometry approach for global metabolomic profiling and case study on drug-resistant multiple myeloma. <i>Analytical Chemistry</i> , 2014 , 86, 3667-75	7.8 47

1384	Chemometrics in foodomics: Handling data structures from multiple analytical platforms. 2014 , 60, 71-79		65
1383	Investigation into dissolved neutral sugars and their microbial conversion in natural and artificially produced dissolved organic matter using ion chromatography with pulsed amperometric detection and reversed-phase liquid chromatography-high resolution mass spectrometry. 2014 , 6, 107-114		5
1382	Structural mass spectrometry of tissue extracts to distinguish cancerous and non-cancerous breast diseases. 2014 , 10, 2827-37		9
1381	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. <i>Analytical Chemistry</i> , 2014 , 86, 5766-74	7.8	153
1380	The hereditary spastic paraplegia-related enzyme DDHD2 is a principal brain triglyceride lipase. 2014 , 111, 14924-9		100
1379	Region-specific metabolic alterations in the brain of the APP/PS1 transgenic mice of Alzheimer's disease. 2014 , 1842, 2395-402		62
1378	Interactive XCMS Online: simplifying advanced metabolomic data processing and subsequent statistical analyses. <i>Analytical Chemistry</i> , 2014 , 86, 6931-9	7.8	254
1377	Metabolomics and traditional Chinese medicine. 2014 , 61, 207-214		54
1376	The food metabolome: a window over dietary exposure. 2014 , 99, 1286-308		335
1375	Current advances in systems and integrative biology. 2014 , 11, 35-46		24
1374	Profiling the chemical content of Ficus lyrata extracts via UPLC-PDA-qTOF-MS and chemometrics. 2014 , 28, 1549-56		10
1373	Development and quantitative evaluation of a high-resolution metabolomics technology. <i>Analytical Chemistry</i> , 2014 , 86, 2175-84	7.8	135
1372	Development of a universal metabolome-standard method for long-term LC-MS metabolome profiling and its application for bladder cancer urine-metabolite-biomarker discovery. <i>Analytical Chemistry</i> , 2014 , 86, 6540-7	7.8	76
1371	Exploring metabolic pathways and regulation through functional chemoproteomic and metabolomic platforms. 2014 , 21, 1171-84		16
1370	Phenotypic mapping of metabolic profiles using self-organizing maps of high-dimensional mass spectrometry data. <i>Analytical Chemistry</i> , 2014 , 86, 6563-71	7.8	34
1369	Credentialing features: a platform to benchmark and optimize untargeted metabolomic methods. <i>Analytical Chemistry</i> , 2014 , 86, 9583-9	7.8	61
1368	Evaluation of unintended effects in the composition of tomatoes expressing a human immunoglobulin A against rotavirus. 2014 , 62, 8158-68		6
1367	Serum and adipose tissue amino acid homeostasis in the metabolically healthy obese. 2014 , 13, 3455-66		81

1366	TracMass 2--a modular suite of tools for processing chromatography-full scan mass spectrometry data. <i>Analytical Chemistry</i> , 2014 , 86, 3435-42	7.8	30
1365	Chemometric strategy for automatic chromatographic peak detection and background drift correction in chromatographic data. 2014 , 1359, 262-70		35
1364	Flux profiling of photosynthetic carbon metabolism in intact plants. 2014 , 9, 1803-24		45
1363	MET-COFEA: a liquid chromatography/mass spectrometry data processing platform for metabolite compound feature extraction and annotation. <i>Analytical Chemistry</i> , 2014 , 86, 6245-53	7.8	47
1362	Comparative evaluation of preprocessing freeware on chromatography/mass spectrometry data for signature discovery. 2014 , 1358, 155-64		66
1361	Chromatographic fingerprint analysis of metabolites in natural and artificial agarwood using gas chromatography-mass spectrometry combined with chemometric methods. 2014 , 967, 264-73		39
1360	Pairwise alignment of chromatograms using an extended Fisher-Rao metric. 2014 , 841, 10-6		6
1359	Differential incorporation of glucose into biomass during Warburg metabolism. 2014 , 53, 4755-7		17
1358	Great interspecies and intraspecies diversity of dairy propionibacteria in the production of cheese aroma compounds. 2014 , 191, 60-8		20
1357	Stronger findings from mass spectral data through multi-peak modeling. 2014 , 15, 208		6
1356	Structure-revealing data fusion. 2014 , 15, 239		61
1355	IsoMS: automated processing of LC-MS data generated by a chemical isotope labeling metabolomics platform. <i>Analytical Chemistry</i> , 2014 , 86, 4675-9	7.8	86
1354	Pregnancy-induced metabolic phenotype variations in maternal plasma. 2014 , 13, 1527-36		65
1353	Intensity drift removal in LC/MS metabolomics by common variance compensation. 2014 , 30, 2899-905		46
1352	Development of isotope labeling liquid chromatography mass spectrometry for mouse urine metabolomics: quantitative metabolomic study of transgenic mice related to Alzheimer's disease. 2014 , 13, 4457-69		35
1351	Discrimination of conventional and organic white cabbage from a long-term field trial study using untargeted LC-MS-based metabolomics. 2014 , 406, 2885-97		32
1350	Comprehensive and simultaneous coverage of lipid and polar metabolites for endogenous cellular metabolomics using HILIC-TOF-MS. 2014 , 406, 3723-33		54
1349	Improving peak detection in high-resolution LC/MS metabolomics data using preexisting knowledge and machine learning approach. 2014 , 30, 2941-8		36

1348	Nanotopographical effects on mesenchymal stem cell morphology and phenotype. 2014 , 115, 380-90		86
1347	Metabolomic fingerprints of 21 date palm fruit varieties from Egypt using UPLC/PDA/ESI-qTOF-MS and GC-MS analyzed by chemometrics. 2014 , 64, 218-226		71
1346	Transcriptomic and metabolomic analysis of copper stress acclimation in <i>Ectocarpus siliculosus</i> highlights signaling and tolerance mechanisms in brown algae. 2014 , 14, 116		73
1345	Interactions between the jasmonic and salicylic acid pathway modulate the plant metabolome and affect herbivores of different feeding types. 2014 , 37, 1574-85		95
1344	Design and analysis of metabolomics studies in epidemiologic research: a primer on -omic technologies. 2014 , 180, 129-39		123
1343	Comprehensive foodomics study on the mechanisms operating at various molecular levels in cancer cells in response to individual rosemary polyphenols. <i>Analytical Chemistry</i> , 2014 , 86, 9807-15	7.8	48
1342	Inflammation triggers production of dimethylsphingosine from oligodendrocytes. 2014 , 279, 113-21		16
1341	Schizophrenia: Blood-Serum-Plasma Metabolomics. 2014 , 27-27		
1340	Liver metabolomics reveals increased oxidative stress and fibrogenic potential in gfrp transgenic mice in response to ionizing radiation. 2014 , 13, 3065-74		20
1339	Validated modeling for German white wine varietal authentication based on headspace solid-phase microextraction online coupled with gas chromatography mass spectrometry fingerprinting. 2014 , 62, 6844-51		33
1338	X13CMS: global tracking of isotopic labels in untargeted metabolomics. <i>Analytical Chemistry</i> , 2014 , 86, 1632-9	7.8	116
1337	Metabolomic profiling of bronchoalveolar lavage fluids by isotope labeling liquid chromatography mass spectrometry: a promising approach to studying experimental asthma. 2014 , 10, 1305-1317		11
1336	Study of metabolite differences of flue-cured tobacco from different regions using a pseudotargeted gas chromatography with mass spectrometry selected-ion monitoring method. 2014 , 37, 2177-84		12
1335	Massifquant: open-source Kalman filter-based XC-MS isotope trace feature detection. 2014 , 30, 2636-43		29
1334	Annotation of the human serum metabolome by coupling three liquid chromatography methods to high-resolution mass spectrometry. 2014 , 966, 34-47		74
1333	Metabolomics research on time-selected combination of Liuwei Dihuang and Jinkui Shenqi pills in treating kidney deficiency and aging by chemometric methods. 2014 , 130, 50-57		7
1332	Metabolomic data streaming for biology-dependent data acquisition. 2014 , 32, 524-7		33
1331	RAMClust: a novel feature clustering method enables spectral-matching-based annotation for metabolomics data. <i>Analytical Chemistry</i> , 2014 , 86, 6812-7	7.8	156

1330	Infrared biospectroscopy for a fast qualitative evaluation of sample preparation in metabolomics. 2014 , 127, 181-90	7
1329	Metabolomic study of raw and processed <i>Atractylodes macrocephala</i> Koidz by LC-MS. 2014 , 98, 74-84	36
1328	Data processing methods and quality control strategies for label-free LC-MS protein quantification. 2014 , 1844, 29-41	45
1327	Using R and Bioconductor for proteomics data analysis. 2014 , 1844, 42-51	44
1326	The metabolomics of alpha-synuclein (SNCA) gene deletion and mutation in mouse brain. 2014 , 10, 114-122	11
1325	Topographically targeted osteogenesis of mesenchymal stem cells stimulated by inclusion bodies attached to polycaprolactone surfaces. 2014 , 9, 207-20	21
1324	A metabolic phenotyping approach to characterize the effects of cantonese herbal tea on restraint stressed rats. 2014 , 37, 1466-74	9
1323	Liquid Chromatography and Liquid Chromatography-Mass Spectrometry of Plants: Techniques and Applications. 2014 , 1-9	
1322	Metabolic differences in ripening of <i>Solanum lycopersicum</i> 'Ailsa Craig' and three monogenic mutants. 2014 , 1, 140029	9
1321	Quality evaluation of extracted ion chromatograms and chromatographic peaks in liquid chromatography/mass spectrometry-based metabolomics data. 2014 , 15 Suppl 11, S5	13
1320	Haystack, a web-based tool for metabolomics research. 2014 , 15 Suppl 11, S12	9
1319	Automated label-free quantification of metabolites from liquid chromatography-mass spectrometry data. 2014 , 13, 348-59	55
1318	An algorithm for processing and analysis of Gas Chromatography-Mass Spectrometry (GC-MS) signals for early detection of Parkinson's disease. 2014 ,	
1317	Three plasma metabolite signatures for diagnosing high altitude pulmonary edema. 2015 , 5, 15126	22
1316	Acylcarnitines are anticoagulants that inhibit factor Xa and are reduced in venous thrombosis, based on metabolomics data. 2015 , 126, 1595-600	30
1315	A new peak detection algorithm for MALDI mass spectrometry data based on a modified Asymmetric Pseudo-Voigt model. 2015 , 16 Suppl 12, S12	3
1314	Metabolomics reveals impaired maturation of HDL particles in adolescents with hyperinsulinaemic androgen excess. 2015 , 5, 11496	10
1313	Arteriovenous Blood Metabolomics: A Readout of Intra-Tissue Metabostasis. 2015 , 5, 12757	47

1312	Metabolomic analysis with GC-MS to reveal potential metabolites and biological pathways involved in Pb & Cd stress response of radish roots. 2015 , 5, 18296	73
1311	Seeing the full picture of metabolism. 2015 , 12, 14-14	
1310	QCScreen: a software tool for data quality control in LC-HRMS based metabolomics. 2015 , 16, 341	14
1309	WarpGroup: increased precision of metabolomic data processing by consensus integration bound analysis. 2016 , 32, 268-75	20
1308	Metabolomic profiling of <i>Burkholderia pseudomallei</i> using UHPLC-ESI-Q-TOF-MS reveals specific biomarkers including 4-methyl-5-thiazoleethanol and unique thiamine degradation pathway. 2015 , 5, 26	10
1307	Missing value imputation strategies for metabolomics data. 2015 , 36, 3050-60	77
1306	High-throughput concentration-response analysis for omics datasets. 2015 , 34, 2167-80	27
1305	Antiphospholipid Antibodies Alter Cell-Death-Regulating Lipid Metabolites in First and Third Trimester Human Placentae. 2015 , 74, 181-99	3
1304	Mechanistic insights revealed by lipid profiling in monogenic insulin resistance syndromes. 2015 , 7, 63	21
1303	<i>Tetranychus urticae</i> -triggered responses promote genotype-dependent conspecific repellence or attractiveness in citrus. 2015 , 207, 790-804	35
1302	Mechanistic Evidence of <i>Viscum schimperi</i> (Viscaceae) Antihyperglycemic Activity: From a Bioactivity-guided Approach to Comprehensive Metabolite Profiling. 2015 , 29, 1737-43	3
1301	Release of ecologically relevant metabolites by the cyanobacterium <i>Synechococcus elongates</i> CCMP 1631. 2015 , 17, 3949-63	53
1300	Metabolomics approaches for resolving and harnessing chemical diversity in grapes, yeast and wine. 2015 , 21, 723-740	16
1299	MZDASoft: a software architecture that enables large-scale comparison of protein expression levels over multiple samples based on liquid chromatography/tandem mass spectrometry. 2015 , 29, 1841-8	6
1298	Development of a suspect and non-target screening approach to detect veterinary antibiotic residues in a complex biological matrix using liquid chromatography/high-resolution mass spectrometry. 2015 , 29, 2361-73	22
1297	. 2015 ,	9
1296	Bioinformatics Tools for Metabolomic Data Processing and Analysis Using Untargeted Liquid Chromatography Coupled With Mass Spectrometry. 2015 , 72,	8
1295	Liquid Chromatography-Mass Spectrometry Metabolic and Lipidomic Sample Preparation Workflow for Suspension-Cultured Mammalian Cells using Jurkat T lymphocyte Cells. 2015 , 8, 126-132	25

1294	LCMS data acquisition and validation in metabolomics. 2015 , 20-34	
1293	Maui-VIA: A User-Friendly Software for Visual Identification, Alignment, Correction, and Quantification of Gas Chromatography-Mass Spectrometry Data. 2014 , 2, 84	18
1292	Analytical methods in untargeted metabolomics: state of the art in 2015. 2015 , 3, 23	377
1291	Joint Analysis of Dependent Features within Compound Spectra Can Improve Detection of Differential Features. 2015 , 3, 129	2
1290	Analysis of Metabolomics Datasets with High-Performance Computing and Metabolite Atlases. 2015 , 5, 431-42	28
1289	Pilot dietary intervention with heat-stabilized rice bran modulates stool microbiota and metabolites in healthy adults. 2015 , 7, 1282-300	57
1288	Metabolic transition in mycorrhizal tomato roots. 2015 , 6, 598	80
1287	Metabolomic and high-throughput sequencing analysis-modern approach for the assessment of biodeterioration of materials from historic buildings. 2015 , 6, 979	67
1286	Rumen microbial communities influence metabolic phenotypes in lambs. 2015 , 6, 1060	55
1285	Longitudinal omics modeling and integration in clinical metabonomics research: challenges in childhood metabolic health research. 2015 , 2, 44	16
1284	Oleic acid metabolism via a conserved cytochrome P450 system-mediated β -hydroxylation in the bark beetle-associated fungus <i>Grosmannia clavigera</i> . 2015 , 10, e0120119	12
1283	Plasma metabolomic profiling of patients with diabetes-associated cognitive decline. 2015 , 10, e0126952	11
1282	Discovery of Infection Associated Metabolic Markers in Human African Trypanosomiasis. 2015 , 9, e0004200	21
1281	Signal Partitioning Algorithm for Highly Efficient Gaussian Mixture Modeling in Mass Spectrometry. 2015 , 10, e0134256	28
1280	Plasma Metabolic Profiles in Women are Menopause Dependent. 2015 , 10, e0141743	24
1279	[Metabolome and mass spectrometry: new biomedical analysis perspectives]. 2015 , 73, 126-30	3
1278	New insights about phenotypic heterogeneity within argue against its division into subspecies. 2015 , 95, 465-477	7
1277	N-lactoyl-amino acids are ubiquitous metabolites that originate from CNDP2-mediated reverse proteolysis of lactate and amino acids. 2015 , 112, 6601-6	32

1276	Hippocampal Proteomic and Metabonomic Abnormalities in Neurotransmission, Oxidative Stress, and Apoptotic Pathways in a Chronic Phencyclidine Rat Model. 2015 , 14, 3174-87	13
1275	An Integrated Computational Platform for Metabolomics Data Analysis. 2015 , 37-47	1
1274	Untargeted metabolomics analysis revealed changes in the composition of glycerolipids and phospholipids in <i>Bacillus subtilis</i> under 1-butanol stress. 2015 , 99, 5971-83	19
1273	Integration of untargeted metabolomics with transcriptomics reveals active metabolic pathways. 2014 , 2014, 503	9
1272	Comprehensive lipidome profiling of Sauvignon blanc grape juice. 2015 , 180, 249-256	19
1271	Urinary metabonomics elucidate the therapeutic mechanism of <i>Orthosiphon stamineus</i> in mouse crystal-induced kidney injury. 2015 , 166, 323-32	22
1270	IPO: a tool for automated optimization of XCMS parameters. 2015 , 16, 118	175
1269	Expanding the chemical space of polyketides through structure-guided mutagenesis of <i>Vitis vinifera</i> stilbene synthase. 2015 , 115, 136-43	23
1268	Purification of LC/GC-MS based biomolecular expression profiles using a topic model. 2015 ,	0
1267	SANIST: a rapid mass spectrometric SACL/ESI data acquisition and elaboration platform for verifying potential candidate biomarkers. 2015 , 29, 1703-10	11
1266	Metabolite profiling of symbiont and host during thermal stress and bleaching in a model cnidarian-dinoflagellate symbiosis. 2016 , 219, 516-27	40
1265	Metabolome analysis of 20 taxonomically related benzylisoquinoline alkaloid-producing plants. 2015 , 15, 220	36
1264	ATP-binding Cassette Subfamily C Member 5 (ABCC5) Functions as an Efflux Transporter of Glutamate Conjugates and Analogs. 2015 , 290, 30429-40	36
1263	LC fractionation followed by pyrolysis GC/MS for the in-depth study of aroma compounds formed during tobacco combustion. 2015 , 116, 68-74	9
1262	Unraveling the triterpenoid saponin biosynthesis of the African shrub <i>Maesa lanceolata</i> . 2015 , 8, 122-35	50
1261	A reinvigorated era of bacterial secondary metabolite discovery. 2015 , 24, 104-11	8
1260	Comparison of peak-picking workflows for untargeted liquid chromatography/high-resolution mass spectrometry metabolomics data analysis. 2015 , 29, 119-27	37
1259	Metabolite profiling for the identification of altered metabolic pathways in Alzheimer's disease. 2015 , 107, 75-81	101

1258	The organic anion transporter (OAT) family: a systems biology perspective. 2015 , 95, 83-123		239
1257	Deciphering metabolic abnormalities associated with Alzheimer's disease in the APP/PS1 mouse model using integrated metabolomic approaches. 2015 , 110, 119-128		34
1256	Ion trace detection algorithm to extract pure ion chromatograms to improve untargeted peak detection quality for liquid chromatography/time-of-flight mass spectrometry-based metabolomics data. <i>Analytical Chemistry</i> , 2015 , 87, 3048-55	7.8	19
1255	"Omics" in pharmaceutical research: overview, applications, challenges, and future perspectives. 2015 , 13, 3-21		43
1254	Visualization of proteomics data using R and bioconductor. 2015 , 15, 1375-89		34
1253	Selective paired ion contrast analysis: a novel algorithm for analyzing postprocessed LC-MS metabolomics data possessing high experimental noise. <i>Analytical Chemistry</i> , 2015 , 87, 3177-86	7.8	21
1252	LC-MS-based urinary metabolite signatures in idiopathic Parkinson's disease. 2015 , 14, 467-78		77
1251	Integrated comparative metabolite profiling via MS and NMR techniques for Senna drug quality control analysis. 2015 , 407, 1937-49		39
1250	Predicting cytotoxicity of complex mixtures in high cancer incidence regions of the Huai River Basin based on GC-MS spectrum with partial least squares regression. 2015 , 137, 391-7		5
1249	Metabolomics reveals significant impairments in the immune system of the APP/PS1 transgenic mice of Alzheimer's disease. 2015 , 36, 577-87		22
1248	An untargeted gas chromatography mass spectrometry metabolomics platform for marine polychaetes. 2015 , 1384, 133-41		10
1247	The re-emergence of natural products for drug discovery in the genomics era. 2015 , 14, 111-29		1375
1246	Robust alignment of chromatograms by statistically analyzing the shifts matrix generated by moving window fast Fourier transform cross-correlation. 2015 , 38, 965-74		2
1245	Bayesian Normalization Model for Label-Free Quantitative Analysis by LC-MS. 2015 , 12, 914-27		4
1244	Metabonomics and Gut Microbiota in Nutrition and Disease. 2015 ,		2
1243	Workflow4Metabolomics: a collaborative research infrastructure for computational metabolomics. 2015 , 31, 1493-5		240
1242	LC-MS/MS fingerprinting as an efficient approach to highlight fine differences in cheese metabolome during ripening. 2015 , 11, 1117-1130		26
1241	Lipidomic profiling reveals significant alterations in lipid biochemistry in hypothyroid rat cerebellum and the therapeutic effects of Sini decoction. 2015 , 159, 262-73		10

1240	Small glycosylated lignin oligomers are stored in Arabidopsis leaf vacuoles. 2015 , 27, 695-710	62
1239	Experiment design beyond gut feeling: statistical tests and power to detect differential metabolites in mass spectrometry data. 2015 , 11, 851-860	18
1238	Predicting retention time in hydrophilic interaction liquid chromatography mass spectrometry and its use for peak annotation in metabolomics. 2015 , 11, 696-706	60
1237	Lipidome and metabolome analysis of fresh tobacco leaves in different geographical regions using liquid chromatography-mass spectrometry. 2015 , 407, 5009-20	16
1236	Effect of Suboptimal Sampling and Handling Conditions on Urinary Metabolic Profiles. 2015 , 78, 429-434	2
1235	Effect of pre- and postnatal growth and post-weaning activity on glucose metabolism in the offspring. 2015 , 224, 171-82	18
1234	Can we trust untargeted metabolomics? Results of the metabo-ring initiative, a large-scale, multi-instrument inter-laboratory study. 2015 , 11, 807-821	84
1233	A large diversity of lactic acid bacteria species is involved in the fermentation of wheat used for the manufacture of lemzeiet. 2015 , 241, 137-149	3
1232	First insights into serum metabolomics of trenbolone/estradiol implanted bovines; screening model to predict hormone-treated and control animals status. 2015 , 11, 1184-1196	15
1231	Cyclic fatty acids found in frying oils are detoxified via classical drug metabolic pathway but also by oxidation and eliminated as conjugates in rats. 2015 , 50, 381-96	3
1230	Potential of mass spectrometry metabolomics for chemical food safety. 2015 , 7, 133-46	23
1229	Free fatty acid levels in fluid of dominant follicles at the preferred insemination time in dairy cows are not affected by early postpartum fatty acid stress. 2015 , 98, 2322-36	13
1228	Adopting Multivariate Nonparametric Tools to Determine Genotype-Phenotype Interactions in Health and Disease. 2015 , 45-62	1
1227	Trends in the application of chemometrics to foodomics studies. 2015 , 44, 4-31	48
1226	A Global Map of Lipid-Binding Proteins and Their Ligandability in Cells. 2015 , 161, 1668-80	140
1225	Linking mutagenic activity to micropollutant concentrations in wastewater samples by partial least square regression and subsequent identification of variables. 2015 , 138, 176-82	22
1224	A tandem liquid chromatography-mass spectrometry (LC-MS) method for profiling small molecules in complex samples. 2015 , 11, 1552-1562	11
1223	An integrated targeted metabolomic platform for high-throughput metabolite profiling and automated data processing. 2015 , 11, 1575-1586	58

1222	A GC-MS-based metabolomics investigation on scallop (<i>Chlamys farreri</i>) during semi-anhydrous living-preservation. 2015 , 31, 185-195		16
1221	MetTailor: dynamic block summary and intensity normalization for robust analysis of mass spectrometry data in metabolomics. 2015 , 31, 3645-52		2
1220	Quantifying Diet-Induced Metabolic Changes of the Human Gut Microbiome. 2015 , 22, 320-31		275
1219	Metabolomic investigation of systemic manifestations associated with Alzheimer's disease in the APP/PS1 transgenic mouse model. 2015 , 11, 2429-40		27
1218	Natural Gas Residual Fluids: Sources, Endpoints, and Organic Chemical Composition after Centralized Waste Treatment in Pennsylvania. 2015 , 49, 8347-55		61
1217	Plasma metabolic signatures reveal the regulatory effect of exercise training in db/db mice. 2015 , 11, 2588-96		13
1216	Genetic diversity of stilbene metabolism in <i>Vitis sylvestris</i> . 2015 , 66, 3243-57		55
1215	Probabilistic Model for Untargeted Peak Detection in LC-MS Using Bayesian Statistics. <i>Analytical Chemistry</i> , 2015 , 87, 7345-55	7.8	22
1214	Collision-Induced Dissociation Mass Spectrometry: A Powerful Tool for Natural Product Structure Elucidation. <i>Analytical Chemistry</i> , 2015 , 87, 10668-78	7.8	57
1213	Metabolome progression during early gut microbial colonization of gnotobiotic mice. 2015 , 5, 11589		24
1212	Metabolic fingerprinting of <i>Lactobacillus paracasei</i> : a multi-criteria evaluation of methods for extraction of intracellular metabolites. 2015 , 407, 6095-104		6
1211	Identification of specific metabolites in culture supernatant of <i>Mycobacterium tuberculosis</i> using metabolomics: exploration of potential biomarkers. 2015 , 4, e6		38
1210	Lipidomic analysis links mycobactin synthase K to iron uptake and virulence in <i>M. tuberculosis</i> . 2015 , 11, e1004792		28
1209	Starvation-induced collective behavior in <i>C. elegans</i> . 2015 , 5, 10647		24
1208	Mitigating the effects of variable speed on drive-by infrastructure monitoring. 2015 ,		1
1207	Metabolic Effect Level Index Links Multivariate Metabolic Fingerprints to Ecotoxicological Effect Assessment. 2015 , 49, 8096-104		22
1206	Analysis of the Human Adult Urinary Metabolome Variations with Age, Body Mass Index, and Gender by Implementing a Comprehensive Workflow for Univariate and OPLS Statistical Analyses. 2015 , 14, 3322-35		443
1205	mzDB: a file format using multiple indexing strategies for the efficient analysis of large LC-MS/MS and SWATH-MS data sets. 2015 , 14, 771-81		16

1204	Metabolomics of plant phosphorus-starvation response. 2015 , 215-236	
1203	Retention time correction in gas chromatography by modeling concentration related effects, applied to the analysis of fatty acid methyl esters. 2015 , 1394, 118-27	4
1202	Oxidized phosphatidylcholines suggest oxidative stress in patients with medium-chain acyl-CoA dehydrogenase deficiency. 2015 , 139, 62-6	29
1201	Applying metabolomic analyses to the practice of embryology: physiology, development and assisted reproductive technology. 2015 , 27, 602-20	32
1200	Characterizing volatiles and attractiveness of five brassicaceous plants with potential for a 'push-pull' strategy toward the cabbage root fly, <i>Delia radicum</i> . 2015 , 41, 330-9	24
1199	Postprandial metabolic events in mini-pigs: new insights from a combined approach using plasma metabolomics, tissue gene expression, and enzyme activity. 2015 , 11, 964-979	6
1198	Impact of collection conditions on the metabolite content of human urine samples as analyzed by liquid chromatography coupled to mass spectrometry and nuclear magnetic resonance spectroscopy. 2015 , 11, 1095-1105	30
1197	Systems Biology Approaches Applied to Regenerative Medicine. 2015 , 3, 37-45	6
1196	An extended siderophore suite from <i>Synechococcus</i> sp. PCC 7002 revealed by LC-ICPMS-ESIMS. 2015 , 7, 877-84	38
1195	Optimized Analytical Procedures for the Untargeted Metabolomic Profiling of Human Urine and Plasma by Combining Hydrophilic Interaction (HILIC) and Reverse-Phase Liquid Chromatography (RPLC)-Mass Spectrometry. 2015 , 14, 1684-95	138
1194	The reproducibility of liquid chromatography separation technology and its potential impact on large scale plant metabolomics experiments. 2015 , 991, 41-5	4
1193	Effect of storage time on metabolite profile and alpha-glucosidase inhibitory activity of <i>Cosmos caudatus</i> leaves - GCMS based metabolomics approach. 2015 , 23, 433-441	22
1192	Identification of diagnostic biomarkers and metabolic pathway shifts of heat-stressed lactating dairy cows. 2015 , 125, 17-28	58
1191	Structuring Microbial Metabolic Responses to Multiplexed Stimuli via Self-Organizing Metabolomics Maps. 2015 , 22, 661-70	36
1190	Metabolomics reveals distinct methylation reaction in MeJA elicited <i>Nigella sativa</i> callus via UPLCMS and chemometrics. 2015 , 122, 453-463	10
1189	Fast parametric time warping of peak lists. 2015 , 31, 3063-5	24
1188	Metabolomics-derived insights into the manipulation of terpenoid synthesis in <i>Centella asiatica</i> cells by methyl jasmonate. 2015 , 9, 125-136	19
1187	Untargeted metabolic profiling identifies interactions between Huntington's disease and neuronal manganese status. 2015 , 7, 363-70	24

1186	Metabolomics in chemical ecology. 2015 , 32, 937-55		75
1185	A short review of applications of liquid chromatography mass spectrometry based metabolomics techniques to the analysis of human urine. 2015 , 140, 2907-15		37
1184	A chemometric-assisted method based on gas chromatography-mass spectrometry for metabolic profiling analysis. 2015 , 1399, 65-73		17
1183	The importance of mass spectrometric dereplication in fungal secondary metabolite analysis. 2015 , 6, 71		55
1182	Unravelling the architecture and dynamics of tropane alkaloid biosynthesis pathways using metabolite correlation networks. 2015 , 116, 94-103		13
1181	Assessment of protein modifications in liver of rats under chronic treatment with paracetamol (acetaminophen) using two complementary mass spectrometry-based metabolomic approaches. 2015 , 120, 194-203		9
1180	Plasma metabolic profiling after cortical spreading depression in a transgenic mouse model of hemiplegic migraine by capillary electrophoresis--mass spectrometry. 2015 , 11, 1462-71		21
1179	Metabolites profiling of <i>Chrysanthemum pacificum</i> Nakai parts using UPLC-PDA-MS coupled to chemometrics. 2015 , 29, 1342-9		5
1178	Optimizing the lipidomics workflow for clinical studies--practical considerations. 2015 , 407, 4973-93		55
1177	ABHD4 regulates multiple classes of N-acyl phospholipids in the mammalian central nervous system. 2015 , 54, 2539-49		35
1176	Environmental metabolomics: Databases and tools for data analysis. 2015 , 177, 366-373		45
1175	Phytochemical, antioxidant and antidiabetic evaluation of eight <i>Bauhinia</i> L. species from Egypt using UHPLC-PDA-qTOF-MS and chemometrics. 2015 , 119, 41-50		53
1174	Evaluation of changes induced in rice metabolome by Cd and Cu exposure using LC-MS with XCMS and MCR-ALS data analysis strategies. 2015 , 407, 8835-47		32
1173	FlavonQ: an automated data processing tool for profiling flavone and flavonol glycosides with ultra-high-performance liquid chromatography-diode array detection-high resolution accurate mass-mass spectrometry. <i>Analytical Chemistry</i> , 2015 , 87, 9974-81	7.8	20
1172	The cumulus cell layer protects the bovine maturing oocyte against fatty acid-induced lipotoxicity. 2015 , 92, 16		54
1171	The Progress of Metabolomics Study in Traditional Chinese Medicine Research. 2015 , 43, 1281-310		23
1170	SIMAT: GC-SIM-MS data analysis tool. 2015 , 16, 259		7
1169	From sample treatment to biomarker discovery: A tutorial for untargeted metabolomics based on GC-(EI)-Q-MS. 2015 , 900, 21-35		101

1168	Annotation of the <i>Staphylococcus aureus</i> Metabolome Using Liquid Chromatography Coupled to High-Resolution Mass Spectrometry and Application to the Study of Methicillin Resistance. 2015 , 14, 4863-75	18
1167	Changing in lipid profile induced by the mutation of <i>Foxn1</i> gene: A lipidomic analysis of Nude mice skin. 2015 , 118, 234-43	13
1166	Potential of serum metabolites for diagnosing post-stroke cognitive impairment. 2015 , 11, 3287-96	36
1165	Metabolomics Study of Urine in Autism Spectrum Disorders Using a Multiplatform Analytical Methodology. 2015 , 14, 5273-82	80
1164	An untargeted metabolomics-driven approach based on LC-TOF/MS and LC-MS/MS for the screening of xenobiotics and metabolites of Zhi-Zi-Da-Huang decoction in rat plasma. 2015 , 115, 315-22	36
1163	Accumulation of non-outer segment proteins in the outer segment underlies photoreceptor degeneration in Bardet-Biedl syndrome. 2015 , 112, E4400-9	84
1162	Regulation of mitochondrial ceramide distribution by members of the BCL-2 family. 2015 , 56, 1501-10	16
1161	Pollutants in Buildings, Water and Living Organisms. 2015 ,	4
1160	Multiscale peak detection in wavelet space. 2015 , 140, 7955-64	38
1159	Hydrophilic interaction (HILIC) and reverse phase liquid chromatography (RPLC) High resolution MS for characterizing lipids profile disruption in serum of anabolic implanted bovines. 2015 , 11, 1884-1895	18
1158	Wine science in the metabolomics era. 2015 , 74, 1-20	59
1157	Mechanistic evidence of <i>Passiflora edulis</i> (Passifloraceae) anxiolytic activity in relation to its metabolite fingerprint as revealed via LC-MS and chemometrics. 2015 , 6, 3807-17	23
1156	Monitoring the Response of the Human Urinary Metabolome to Brief Maximal Exercise by a Combination of RP-UPLC-MS and (1)H NMR Spectroscopy. 2015 , 14, 4610-22	32
1155	Formation of oligopeptides in high yield under simple programmable conditions. 2015 , 6, 8385	110
1154	Analysis of the reaction products from micro-vial pyrolysis of the mixture glucose/proline and of a tobacco leaf extract: Search for Amadori intermediates. 2015 , 1422, 27-33	1
1153	Discovery and resupply of pharmacologically active plant-derived natural products: A review. 2015 , 33, 1582-1614	1267
1152	Polyphenol metabolome in human urine and its association with intake of polyphenol-rich foods across European countries. 2015 , 102, 905-13	100
1151	MET-XAlign: a metabolite cross-alignment tool for LC/MS-based comparative metabolomics. <i>Analytical Chemistry</i> , 2015 , 87, 9114-9	7.8 24

1150	Discovery of a novel amino acid racemase through exploration of natural variation in <i>Arabidopsis thaliana</i> . 2015 , 112, 11726-31		39
1149	Six enzymes from mayapple that complete the biosynthetic pathway to the etoposide aglycone. 2015 , 349, 1224-8		230
1148	Exploratory analysis of urinary tract infection using a GC-APCI-MS platform. 2015 , 140, 2834-41		6
1147	Non-target UHPLC/MS Analysis of Emerging Contaminants in Water. 2015 , 123-167		1
1146	The effects of mineral nitrogen limitation, competition, arbuscular mycorrhiza, and their respective interactions, on morphological and chemical plant traits of <i>Plantago lanceolata</i> . 2015 , 118, 149-61		12
1145	Metabolomics techniques for nanotoxicity investigations. 2015 , 7, 1527-44		36
1144	Data from identification of diagnostic biomarkers and metabolic pathway shifts of heat-stressed lactating dairy cows. 2015 , 4, 90-5		
1143	Nephron Toxicity Profiling via Untargeted Metabolome Analysis Employing a High Performance Liquid Chromatography-Mass Spectrometry-based Experimental and Computational Pipeline. 2015 , 290, 19121-32		8
1142	Rapid Phytotransformation of Benzotriazole Generates Synthetic Tryptophan and Auxin Analogs in <i>Arabidopsis</i> . 2015 , 49, 10959-68		62
1141	LC-MS metabolomics of psoriasis patients reveals disease severity-dependent increases in circulating amino acids that are ameliorated by anti-TNF α treatment. 2015 , 14, 557-66		50
1140	Emerging field of metabolomics: big promise for cancer biomarker identification and drug discovery. 2015 , 107, 63-74		121
1139	Untargeted metabolic profiling identifies altered serum metabolites of type 2 diabetes mellitus in a prospective, nested case control study. 2015 , 61, 487-97		94
1138	MetMSLine: an automated and fully integrated pipeline for rapid processing of high-resolution LC-MS metabolomic datasets. 2015 , 31, 788-90		21
1137	Metabolomics reveals differential metabolic adjustments of normal and overweight subjects during overfeeding. 2015 , 11, 920-938		10
1136	Rediscovery rate estimation for assessing the validation of significant findings in high-throughput studies. 2015 , 16, 563-75		24
1135	Autonomous metabolomics for rapid metabolite identification in global profiling. <i>Analytical Chemistry</i> , 2015 , 87, 884-91	7.8	119
1134	Lipidomic analysis of cerebrospinal fluid by mass spectrometry-based methods. 2015 , 38, 53-64		14
1133	Classification of <i>Lactococcus lactis</i> cell envelope proteinase based on gene sequencing, peptides formed after hydrolysis of milk, and computer modeling. 2015 , 98, 68-77		8

1132	Current peptidomics: applications, purification, identification, quantification, and functional analysis. 2015 , 15, 1026-38	142
1131	Enzymatic formation of a resorcylic acid by creating a structure-guided single-point mutation in stilbene synthase. 2015 , 24, 167-73	23
1130	UHPLC-LTQ-Orbitrap MS combined with spike-in method for plasma metabolomics analysis of acute myocardial ischemia rats and pretreatment effect of Danqi Tongmai tablet. 2015 , 11, 486-96	24
1129	Prediction of advanced ovarian cancer recurrence by plasma metabolic profiling. 2015 , 11, 516-21	17
1128	LC-MS alignment in theory and practice: a comprehensive algorithmic review. 2015 , 16, 104-17	66
1127	Mass spectral similarity for untargeted metabolomics data analysis of complex mixtures. 2015 , 377, 719-717	53
1126	Metabolomic fingerprint classification of <i>Brachychiton acerifolius</i> organs via UPLC-qTOF-PDA-MS analysis and chemometrics. 2015 , 29, 116-24	12
1125	Bioinformatics: the next frontier of metabolomics. <i>Analytical Chemistry</i> , 2015 , 87, 147-56	7.8 95
1124	Mass-spectrometry-based microbial metabolomics: recent developments and applications. 2015 , 407, 669-80	42
1123	Dissolved organic matter produced by <i>Thalassiosira pseudonana</i> . 2015 , 168, 114-123	29
1122	Metabonomic profiling of bladder cancer. 2015 , 14, 587-602	36
1121	Influence of proteolytic <i>Lactococcus lactis</i> subsp. <i>cremoris</i> on ripening of reduced-fat Cheddar cheese made with camel chymosin. 2015 , 41, 38-45	7
1120	Metabolomic-based strategies for anti-parasite drug discovery. 2015 , 20, 44-55	39
1119	PLS-DA for compositional data with application to metabolomics. 2015 , 29, 21-28	53
1118	Metabolic study of enrofloxacin and metabolic profile modifications in broiler chicken tissues after drug administration. 2015 , 172, 30-9	14
1117	A methodological approach to screen diverse cheese-related bacteria for their ability to produce aroma compounds. 2015 , 46, 145-153	49
1116	Global urine fingerprinting by LC-ESI(+)-HRMS for better characterization of metabolic pathway disruption upon anabolic practices in bovine. 2015 , 11, 184-197	23
1115	Integrative taxonomic description of <i>Plakina kanaky</i> , a new polychromatic sponge species from New Caledonia (Porifera: Homoscleromorpha). 2015 , 36, 1129-1143	9

1114	The Significance of Metabolomics in Human Health. 2016 , 89-100	2
1113	Serum metabolite profiles of postoperative fatigue syndrome in rat following partial hepatectomy. 2016 , 58, 210-5	9
1112	Population Screening for Biological and Environmental Properties of the Human Metabolic Phenotype. 2016 , 167-211	18
1111	Processing and Visualization of Metabolomics Data Using R. 2016 ,	9
1110	Microbiota Influences Morphology and Reproduction of the Brown Alga <i>Ectocarpus</i> sp. 2016 , 7, 197	33
1109	In Search of Alternative Antibiotic Drugs: Quorum-Quenching Activity in Sponges and their Bacterial Isolates. 2016 , 7, 416	46
1108	Deconjugated Bile Salts Produced by Extracellular Bile-Salt Hydrolase-Like Activities from the Probiotic <i>La1</i> Inhibit Growth. 2016 , 7, 1453	41
1107	The Nitrogen Availability Interferes with Mycorrhiza-Induced Resistance against in Tomato. 2016 , 7, 1598	37
1106	biosigner: A New Method for the Discovery of Significant Molecular Signatures from Omics Data. 2016 , 3, 26	37
1105	Dereplication of Natural Products Using GC-TOF Mass Spectrometry: Improved Metabolite Identification by Spectral Deconvolution Ratio Analysis. 2016 , 3, 59	12
1104	Non-targeted Plasma Metabolome of Early and Late Lactation Gilts. 2016 , 3, 77	3
1103	Advantages and Pitfalls of Mass Spectrometry Based Metabolome Profiling in Systems Biology. 2016 , 17,	98
1102	<i>Piriformospora indica</i> Stimulates Root Metabolism of <i>Arabidopsis thaliana</i> . 2016 , 17,	25
1101	Plant-to-Plant Variability in Root Metabolite Profiles of 19 <i>Arabidopsis thaliana</i> Accessions Is Substance-Class-Dependent. 2016 , 17,	15
1100	Prediction, Detection, and Validation of Isotope Clusters in Mass Spectrometry Data. 2016 , 6,	14
1099	MetMatch: A Semi-Automated Software Tool for the Comparison and Alignment of LC-HRMS Data from Different Metabolomics Experiments. 2016 , 6,	4
1098	Elevation of Alanine Aminotransferase Activity Occurs after Activation of the Cell-Death Signaling Initiated by Pattern-Recognition Receptors ?but before Activation of Cytolytic Effectors in NK or CD8+ T Cells in the Liver During Acute HCV Infection. 2016 , 11, e0165533	10
1097	Discovery of Metabolic Biomarkers for Duchenne Muscular Dystrophy within a Natural History Study. 2016 , 11, e0153461	17

1096	Priming by Hexanoic Acid Induce Activation of Mevalonic and Linolenic Pathways and Promotes the Emission of Plant Volatiles. 2016 , 7, 495		14
1095	Accumulation of Flavonols over Hydroxycinnamic Acids Favors Oxidative Damage Protection under Abiotic Stress. 2016 , 7, 838		143
1094	Non-targeted Metabolomics in Diverse Sorghum Breeding Lines Indicates Primary and Secondary Metabolite Profiles Are Associated with Plant Biomass Accumulation and Photosynthesis. 2016 , 7, 953		45
1093	Modeling Longitudinal Metabonomics and Microbiota Interactions in C57BL/6 Mice Fed a High Fat Diet. <i>Analytical Chemistry</i> , 2016 , 88, 7617-26	7.8	8
1092	A hybrid retention time alignment algorithm for SWATH-MS data. 2016 , 16, 2272-83		4
1091	Metabolomics reveals hippocampal metabolic fluctuations of postoperative fatigue syndrome and anti-fatigue effect of <i>Carthamus tinctorius</i> L extract in rat model. 2017 , 30, 1052-1058		1
1090	Shifting <i>Nicotiana attenuata</i> 's diurnal rhythm does not alter its resistance to the specialist herbivore <i>Manduca sexta</i> . 2016 , 58, 656-68		13
1089	Analysis of human plasma metabolites across different liquid chromatography/mass spectrometry platforms: Cross-platform transferable chemical signatures. 2016 , 30, 581-93		28
1088	Metabolomics by Gas Chromatography-Mass Spectrometry: Combined Targeted and Untargeted Profiling. 2016 , 114, 30.4.1-30.4.32		291
1087	Extending the Dynamic Range in Metabolomics Experiments by Automatic Correction of Peaks Exceeding the Detection Limit. <i>Analytical Chemistry</i> , 2016 , 88, 7487-92	7.8	16
1086	The Metabolic Signature of Biomass Formation in Barley. 2016 , 57, 1943-60		23
1085	Use of metabolomics and lipidomics to evaluate the hypocholesterolemic effect of Proanthocyanidins from grape seed in a pig model. 2016 , 60, 2219-2227		18
1084	Comprehensive investigation of tobacco leaves during natural early senescence via multi-platform metabolomics analyses. 2016 , 6, 37976		43
1083	Global metabolic analyses identify key differences in metabolite levels between polymyxin-susceptible and polymyxin-resistant <i>Acinetobacter baumannii</i> . 2016 , 6, 22287		33
1082	Metabolomics analysis for hydroxy-L-proline-induced calcium oxalate nephrolithiasis in rats based on ultra-high performance liquid chromatography quadrupole time-of-flight mass spectrometry. 2016 , 6, 30142		15
1081	Metabolic pathways of lung inflammation revealed by high-resolution metabolomics (HRM) of H1N1 influenza virus infection in mice. 2016 , 311, R906-R916		61
1080	Natural variation of root exudates in <i>Arabidopsis thaliana</i> -linking metabolomic and genomic data. 2016 , 6, 29033		89
1079	Feature extraction from resolution perspective for gas chromatography-mass spectrometry datasets. 2016 , 6, 113997-114004		13

1078	Age-associated metabolic dysregulation in bone marrow-derived macrophages stimulated with lipopolysaccharide. 2016 , 6, 22637	19
1077	Metabolite Modulation in Human Plasma in the Early Phase of Acclimatization to Hypobaric Hypoxia. 2016 , 6, 22589	25
1076	Novel Chemical Ligands to Ebola Virus and Marburg Virus Nucleoproteins Identified by Combining Affinity Mass Spectrometry and Metabolomics Approaches. 2016 , 6, 29680	39
1075	Metabolic Profiling and Metabolomic Procedures for Investigating the Biodegradation of Hydrocarbons. 2016 , 111-161	2
1074	Artemisia annua mutant impaired in artemisinin synthesis demonstrates importance of nonenzymatic conversion in terpenoid metabolism. 2016 , 113, 15150-15155	42
1073	Statistical Approaches for LC-HRMS Data To Characterize, Prioritize, and Identify Transformation Products from Water Treatment Processes. 2016 , 45-65	5
1072	Production of Phloroglucinol, a Platform Chemical, in Arabidopsis using a Bacterial Gene. 2016 , 6, 38483	11
1071	Type 1 Reaction in Patients With Leprosy Corresponds to a Decrease in Proresolving Lipid Mediators and an Increase in Proinflammatory Lipid Mediators. 2017 , 215, 431-439	11
1070	A capillary electrophoresis coupled to mass spectrometry pipeline for long term comparable assessment of the urinary metabolome. 2016 , 6, 34453	21
1069	Metabolic phenotyping for monitoring ovarian cancer patients. 2016 , 6, 23334	36
1068	Microbial Metabolomics. 2016 ,	12
1067	Performance Evaluation and Online Realization of Data-driven Normalization Methods Used in LC/MS based Untargeted Metabolomics Analysis. 2016 , 6, 38881	84
1066	Metabolomics: Applications to Food Safety and Quality Research. 2016 , 225-259	4
1065	Lipidomic Profiling of Lung Pleural Effusion Identifies Unique Metabotype for EGFR Mutants in Non-Small Cell Lung Cancer. 2016 , 6, 35110	13
1064	Yeast longevity promoted by reversing aging-associated decline in heavy isotope content. 2016 , 2, 16004	16
1063	FragClust and TestClust, two informatics tools for chemical structure hierarchical clustering analysis applied to lipidomics. The example of Alzheimer's disease. 2016 , 408, 2215-26	3
1062	Updates in metabolomics tools and resources: 2014-2015. 2016 , 37, 86-110	102
1061	Pro-apoptotic activity against cancer stem cells differs between different parts of sweet sorghum. 2016 , 23, 601-613	6

1060	LC/MS-based metabolomics strategy to assess the amelioration effects of ginseng total saponins on memory deficiency induced by simulated microgravity. 2016 , 125, 329-38	22
1059	A Multi-objective Genetic Programming Biomarker Detection Approach in Mass Spectrometry Data. 2016 , 106-122	2
1058	Metabolomics reveals positive acceleration(+Gz)-induced metabolic perturbations and the protective effect of Ginkgo biloba extract in a rat model based on ultra high-performance liquid chromatography coupled with quadrupole time-of-flight mass spectrometry. 2016 , 125, 77-84	4
1057	Novel Metabolite Biomarkers of Huntington's Disease As Detected by High-Resolution Mass Spectrometry. 2016 , 15, 1592-601	21
1056	Metabolic Phenotypes of Carotid Atherosclerotic Plaques Relate to Stroke Risk: An Exploratory Study. 2016 , 52, 5-10	24
1055	Rifampin Resistance Mutations Are Associated with Broad Chemical Remodeling of Mycobacterium tuberculosis. 2016 , 291, 14248-14256	40
1054	Bioinformatics for the synthetic biology of natural products: integrating across the Design-Build-Test cycle. 2016 , 33, 925-32	48
1053	Anti-stress effects of ginseng total saponins on hindlimb-unloaded rats assessed by a metabolomics study. 2016 , 188, 39-47	20
1052	A simple multi-scale Gaussian smoothing-based strategy for automatic chromatographic peak extraction. 2016 , 1452, 1-9	22
1051	Untargeted Metabolomics Analysis Reveals a Link between ETHE1-Mediated Disruptive Redox State and Altered Metabolic Regulation. 2016 , 15, 1630-8	10
1050	Evidence for quorum sensing and differential metabolite production by a marine bacterium in response to DMSP. 2016 , 10, 2304-16	83
1049	Global Isotope Metabolomics Reveals Adaptive Strategies for Nitrogen Assimilation. 2016 , 11, 1677-85	13
1048	Quantitative and qualitative shifts in defensive metabolites define chemical defense investment during leaf development in Inga, a genus of tropical trees. 2016 , 6, 478-92	35
1047	Annotation of the human cerebrospinal fluid lipidome using high resolution mass spectrometry and a dedicated data processing workflow. 2016 , 12, 91	30
1046	Analysis of metabolomic data: tools, current strategies and future challenges for omics data integration. 2017 , 18, 498-510	91
1045	Calibration curve-free GCMS method for quantitation of amino and non-amino organic acids in biological samples. 2016 , 12, 1	13
1044	Metabolic and transcriptomic profiling of Streptococcus intermedius during aerobic and anaerobic growth. 2016 , 12, 1	12
1043	Characterization of a New Pink-Fruited Tomato Mutant Results in the Identification of a Null Allele of the SLMYB12 Transcription Factor. 2016 , 171, 1821-36	28

1042	Non-targeted UHPLC-MS metabolomic data processing methods: a comparative investigation of normalisation, missing value imputation, transformation and scaling. 2016 , 12, 93			155
1041	UHPLC-Q-TOF-MS based serum metabonomics revealed the metabolic perturbations of ischemic stroke and the protective effect of RKIP in rat models. 2016 , 12, 1831-41			20
1040	Data fusion between high resolution (1)H-NMR and mass spectrometry: a synergetic approach to honey botanical origin characterization. 2016 , 408, 4389-401			28
1039	Time Course of Molecular and Metabolic Events in the Development of Insulin Resistance in Fructose-Fed Rats. 2016 , 15, 1862-74			18
1038	Application of MALDI Mass Spectrometry in Natural Products Analysis. 2016 , 82, 671-89			23
1037	Unsupervised Identification of Isotope-Labeled Peptides. <i>Analytical Chemistry</i> , 2016 , 88, 6092-9	7.8		1
1036	Olive oil authenticity studies by target and nontarget LC-QTOF-MS combined with advanced chemometric techniques. 2016 , 408, 7955-7970			42
1035	eRah: A Computational Tool Integrating Spectral Deconvolution and Alignment with Quantification and Identification of Metabolites in GC/MS-Based Metabolomics. <i>Analytical Chemistry</i> , 2016 , 88, 9821-9829	7.8		68
1034	Automated Annotation and Evaluation of In-Source Mass Spectra in GC/Atmospheric Pressure Chemical Ionization-MS-Based Metabolomics. <i>Analytical Chemistry</i> , 2016 , 88, 9386-9390	7.8		17
1033	An LC-MS based untargeted metabolomics study identified novel biomarkers for coronary heart disease. 2016 , 12, 3425-3434			9
1032	High-Resolution Mass Spectrometry in the Effect-Directed Analysis of Water Resources. 2016 , 71, 433-457			2
1031	Nontarget Analysis of Environmental Samples Based on Liquid Chromatography Coupled to High Resolution Mass Spectrometry (LC-HRMS). 2016 , 71, 381-403			15
1030	Using MetaboAnalyst 3.0 for Comprehensive Metabolomics Data Analysis. 2016 , 55, 14.10.1-14.10.91			957
1029	Bioinformatics in Lipidomics. 2016 , 121-150			1
1028	A systems biology approach reveals major metabolic changes in the thermoacidophilic archaeon <i>Sulfolobus solfataricus</i> in response to the carbon source L-fucose versus D-glucose. 2016 , 102, 882-908			35
1027	Clade IVa Basic Helix-Loop-Helix Transcription Factors Form Part of a Conserved Jasmonate Signaling Circuit for the Regulation of Bioactive Plant Terpenoid Biosynthesis. 2016 , 57, 2564-2575			26
1026	Quantitative metabolomics of photoreceptor degeneration and the effects of stem cell-derived retinal pigment epithelium transplantaion. 2016 , 374,			9
1025	Does centrifugation matter? Centrifugal force and spinning time alter the plasma metabolome. 2016 , 12, 159			21

1024	Development and Application of Ultra-Performance Liquid Chromatography-TOF MS for Precision Large Scale Urinary Metabolic Phenotyping. <i>Analytical Chemistry</i> , 2016 , 88, 9004-13	7.8	71
1023	Compression strategies for the chemometric analysis of mass spectrometry imaging data. 2016 , 30, 575-588		24
1022	Gene discovery and genome editing to develop cisgenic crops with improved resistance against pathogen infection. 2016 , 38, 279-295		15
1021	Serum lipidomics analysis of ovariectomized rats under Curcuma comosa treatment. 2016 , 192, 273-282		12
1020	Current state and challenges for dynamic metabolic modeling. 2016 , 33, 97-104		30
1019	Metabolomics driven analysis of Erythrina lysistemon cell suspension culture in response to methyl jasmonate elicitation. 2016 , 7, 681-9		10
1018	Enabling Efficient and Confident Annotation of LC-MS Metabolomics Data through MS1 Spectrum and Time Prediction. <i>Analytical Chemistry</i> , 2016 , 88, 9226-34	7.8	56
1017	Smartphone Analytics: Mobilizing the Lab into the Cloud for Omic-Scale Analyses. <i>Analytical Chemistry</i> , 2016 , 88, 9753-9758	7.8	13
1016	Metabolization and degradation kinetics of the urban-use pesticide fipronil by white rot fungus <i>Trametes versicolor</i> . 2016 , 18, 1256-1265		36
1015	ADAP-GC 3.0: Improved Peak Detection and Deconvolution of Co-eluting Metabolites from GC/TOF-MS Data for Metabolomics Studies. <i>Analytical Chemistry</i> , 2016 , 88, 8802-11	7.8	46
1014	Metabolomic profiling of the halophyte <i>Prosopis strombulifera</i> shows sodium salt- specific response. 2016 , 108, 145-157		23
1013	Measuring relative utilization of aerobic glycolysis in breast cancer cells by positional isotopic discrimination. 2016 , 590, 3179-87		10
1012	Metabolomics analysis reveals heavy metal copper-induced cytotoxicity in HT-29 human colon cancer cells. 2016 , 6, 78445-78456		13
1011	Automated Detection of Natural Halogenated Compounds from LC-MS Profiles-Application to the Isolation of Bioactive Chlorinated Compounds from Marine-Derived Fungi. <i>Analytical Chemistry</i> , 2016 , 88, 9143-50	7.8	26
1010	Dynamic Cluster Analysis: An Unbiased Method for Identifying A + 2 Element Containing Compounds in Liquid Chromatographic High-Resolution Time-of-Flight Mass Spectrometric Data. <i>Analytical Chemistry</i> , 2016 , 88, 12461-12469	7.8	11
1009	Spherulization as a process for the exudation of chemical cues by the encrusting sponge <i>C. crambe</i> . 2016 , 6, 29474		20
1008	Urinary signature of pig carcasses with boar taint by liquid chromatography-high-resolution mass spectrometry. 2017 , 34, 218-227		2
1007	Ultra-high-performance liquid chromatography-high-resolution mass spectrometry based metabolomics as a strategy for beer characterization. 2016 , 122, 430-436		10

1006	Coordinate Regulation of Metabolite Glycosylation and Stress Hormone Biosynthesis by TT8 in Arabidopsis. 2016 , 171, 2499-515		26
1005	- Metabolomics: An Important Tool for Assessing State of Health and Risk of Disease in Nutrigenomics Research. 2016 , 248-261		
1004	Discovery of A-type procyanidin dimers in yellow raspberries by untargeted metabolomics and correlation based data analysis. 2016 , 12, 144		3
1003	Multiplatform serum metabolic phenotyping combined with pathway mapping to identify biochemical differences in smokers. 2016 , 8, 2023-43		20
1002	Large-scale untargeted LC-MS metabolomics data correction using between-batch feature alignment and cluster-based within-batch signal intensity drift correction. 2016 , 12, 173		82
1001	Computational Metabolomics: A Framework for the Million Metabolome. 2016 , 29, 1956-1975		130
1000	Metabolomics reveals dose effects of low-dose chronic exposure to uranium in rats: identification of candidate biomarkers in urine samples. 2016 , 12, 154		17
999	MetDIA: Targeted Metabolite Extraction of Multiplexed MS/MS Spectra Generated by Data-Independent Acquisition. <i>Analytical Chemistry</i> , 2016 , 88, 8757-64	7.8	71
998	Evaluation of chromatographic conditions in reversed phase liquid chromatography-mass spectrometry systems for fingerprinting of polar and amphiphilic plant metabolites. 2016 , 408, 5855-5865		2
997	Data analysis strategies for targeted and untargeted LC-MS metabolomic studies: Overview and workflow. 2016 , 82, 425-442		172
996	Discovering Regulated Metabolite Families in Untargeted Metabolomics Studies. <i>Analytical Chemistry</i> , 2016 , 88, 8082-90	7.8	56
995	Non-targeted metabolomics combined with genetic analyses identifies bile acid synthesis and phospholipid metabolism as being associated with incident type 2 diabetes. 2016 , 59, 2114-24		54
994	Training in metabolomics research. II. Processing and statistical analysis of metabolomics data, metabolite identification, pathway analysis, applications of metabolomics and its future. 2016 , 51, 535-548		37
993	SHORT-ROOT Deficiency Alleviates the Cell Death Phenotype of the Arabidopsis catalase2 Mutant under Photorespiration-Promoting Conditions. 2016 , 28, 1844-59		30
992	Optimization of LC-Orbitrap-HRMS acquisition and MZmine 2 data processing for nontarget screening of environmental samples using design of experiments. 2016 , 408, 7905-7915		16
991	Comprehensive Plasma Metabolomic Analyses of Atherosclerotic Progression Reveal Alterations in Glycerophospholipid and Sphingolipid Metabolism in Apolipoprotein E-deficient Mice. 2016 , 6, 35037		35
990	Topic modeling for untargeted substructure exploration in metabolomics. 2016 , 113, 13738-13743		163
989	Lipid profiling of polarized human monocyte-derived macrophages. 2016 , 127, 1-8		24

988	High herbivore pressure favors constitutive over induced defense. 2016 , 6, 6037-49		39
987	Metabolomic Profiling of Mice Serum during Toxoplasmosis Progression Using Liquid Chromatography-Mass Spectrometry. 2016 , 6, 19557		41
986	Avoiding hard chromatographic segmentation: A moving window approach for the automated resolution of gas chromatography-mass spectrometry-based metabolomics signals by multivariate methods. 2016 , 1474, 145-151		5
985	Global metabolomics reveals potential urinary biomarkers of esophageal squamous cell carcinoma for diagnosis and staging. 2016 , 6, 35010		26
984	Personalized Medicine. 2016 ,		2
983	Computational Methods for Integration of Biological Data. 2016 , 137-178		1
982	Prediction of Intravenous Busulfan Clearance by Endogenous Plasma Biomarkers Using Global Pharmacometabolomics. 2016 , 12, 1		12
981	A novel targeted/untargeted GC-Orbitrap metabolomics methodology applied to and biofilms. 2016 , 12, 189		28
980	A Comparative Metabolomics Approach Reveals Early Biomarkers for Metabolic Response to Acute Myocardial Infarction. 2016 , 6, 36359		52
979	Adult Frass Provides a Pheromone Signature for <i>Drosophila</i> Feeding and Aggregation. 2016 , 42, 739-747		29
978	Multivariate Curve Resolution-Alternating Least Squares Analysis of High-Resolution Liquid Chromatography-Mass Spectrometry Data. <i>Analytical Chemistry</i> , 2016 , 88, 11092-11099	7.8	22
977	Metabolomics approach reveals metabolic disorders and potential biomarkers associated with the developmental toxicity of tetrabromobisphenol A and tetrachlorobisphenol A. 2016 , 6, 35257		15
976	Untargeted Metabolomics Analysis of ABCC6-Deficient Mice Discloses an Altered Metabolic Liver Profile. 2016 , 15, 4591-4600		4
975	Colonic transit time is related to bacterial metabolism and mucosal turnover in the gut. 2016 , 1, 16093		204
974	The WEIZMASS spectral library for high-confidence metabolite identification. 2016 , 7, 12423		62
973	Mass Spectrometry for Metabolomics and Biomass Composition Analyses. 2016 , 115-141		2
972	Integrated Metabolomics Study of the Milk of Heat-stressed Lactating Dairy Cows. 2016 , 6, 24208		47
971	Technical Challenges in Mass Spectrometry-Based Metabolomics. 2016 , 5, S0052		29

970	Informed baseline subtraction of proteomic mass spectrometry data aided by a novel sliding window algorithm. 2016 , 14, 19		4
969	Scientific workflows with the jABC framework. 2016 , 18, 629-651		8
968	Metabolomics biomarker discovery using multimodal memetic algorithm and multivariate mutual information based feature selection. 2016 ,		
967	Metabolomics in transfusion medicine. 2016 , 56, 980-93		77
966	Warburg metabolism in tumor-conditioned macrophages promotes metastasis in human pancreatic ductal adenocarcinoma. 2016 , 5, e1191731		122
965	Metabolomic approach for Extra virgin olive oil origin discrimination making use of ultra-high performance liquid chromatography [Quadrupole time-of-flight mass spectrometry. 2016 , 70, 350-359		39
964	LOBSTAHS: An Adduct-Based Lipidomics Strategy for Discovery and Identification of Oxidative Stress Biomarkers. <i>Analytical Chemistry</i> , 2016 , 88, 7154-62	7.8	49
963	General strategies to increase the repeatability in non-target screening by liquid chromatography-high resolution mass spectrometry. 2016 , 935, 173-86		33
962	The use of mass spectrometry for analysing metabolite biomarkers in epidemiology: methodological and statistical considerations for application to large numbers of biological samples. 2016 , 31, 717-33		19
961	Metabolic profiling of potential lung cancer biomarkers using bronchoalveolar lavage fluid and the integrated direct infusion/ gas chromatography mass spectrometry platform. 2016 , 145, 197-206		40
960	SMART: Statistical Metabolomics Analysis-An R Tool. <i>Analytical Chemistry</i> , 2016 , 88, 6334-41	7.8	21
959	Characterisation of the metabolome of ocular tissues and post-mortem changes in the rat retina. 2016 , 149, 8-15		12
958	Environmental Metabolic Footprinting: A novel application to study the impact of a natural and a synthetic Eriketone herbicide in soil. 2016 , 566-567, 552-558		14
957	MetFrag relaunched: incorporating strategies beyond in silico fragmentation. 2016 , 8, 3		439
956	Galaxy-M: a Galaxy workflow for processing and analyzing direct infusion and liquid chromatography mass spectrometry-based metabolomics data. 2016 , 5, 10		68
955	BatMass: a Java Software Platform for LC-MS Data Visualization in Proteomics and Metabolomics. 2016 , 15, 2500-9		28
954	The wild Egyptian artichoke as a promising functional food for the treatment of hepatitis C virus as revealed via UPLC-MS and clinical trials. 2016 , 7, 3006-16		20
953	Pure ion chromatogram extraction via optimal k-means clustering. 2016 , 6, 56977-56985		8

952	Evaluating Ultra-long-Chain Fatty Acids as Biomarkers of Colorectal Cancer Risk. 2016 , 25, 1216-23	11
951	Lipidomic analysis of fibroblasts from Zellweger spectrum disorder patients identifies disease-specific phospholipid ratios. 2016 , 57, 1447-54	38
950	Introduction to Cheminformatics. 2016 , 53, 14.1.1-14.1.21	10
949	Altered metabolite accumulation in tomato fruits by coexpressing a feedback-insensitive AroG and the PhODO1 MYB-type transcription factor. 2016 , 14, 2300-2309	9
948	The Secreted Enzyme PM20D1 Regulates Lipidated Amino Acid Uncouplers of Mitochondria. 2016 , 166, 424-435	140
947	An R package for the integrated analysis of metabolomics and spectral data. 2016 , 129, 117-24	29
946	Effects of synthetic large-scale genome reduction on metabolism and metabolic preferences in a nutritionally complex environment. 2016 , 12, 1	17
945	Evaluation of non-volatile metabolites in beer stored at high temperature and utility as an accelerated method to predict flavour stability. 2016 , 200, 301-7	12
944	Urinary metabolomic profiling to identify biomarkers of a flavonoid-rich and flavonoid-poor fruits and vegetables diet in adults: the FLAVURS trial. 2016 , 12, 1	21
943	Effect of Obesity on the Preovulatory Follicle and Lipid Fingerprint of Equine Oocytes. 2016 , 94, 15	15
942	Investigations into the Use of a Protein Sensor Assay for Metabolite Analysis. 2016 , 178, 101-13	
941	Toward automated chromatographic fingerprinting: A non-alignment approach to gas chromatography mass spectrometry data. 2016 , 911, 42-58	10
940	Ligand Activation of ERR α by Cholesterol Mediates Statin and Bisphosphonate Effects. 2016 , 23, 479-91	94
939	A roadmap for the XCMS family of software solutions in metabolomics. 2016 , 30, 87-93	80
938	Data standards can boost metabolomics research, and if there is a will, there is a way. 2016 , 12, 14	85
937	A combined proteomics and metabolomics approach to assess the effects of gold nanoparticles in vitro. 2016 , 10, 736-48	55
936	Blood transcriptomics and metabolomics for personalized medicine. 2016 , 14, 1-7	52
935	Optimization of metabolomics of defined in vitro gut microbial ecosystems. 2016 , 306, 280-289	22

934	Unbiased profiling of volatile organic compounds in the headspace of Allium plants using an in-tube extraction device. 2016 , 9, 133	24
933	A novel metabolomic approach used for the comparison of planktonic cells and biofilm samples. 2016 , 12, 75	41
932	Matrix removal in state of the art sample preparation methods for serum by charged aerosol detection and metabolomics-based LC-MS. 2016 , 915, 56-63	4
931	Algorithm for comprehensive analysis of datasets from hyphenated high resolution mass spectrometric techniques using single ion profiles and cluster analysis. 2016 , 1429, 134-41	4
930	Normalization and integration of large-scale metabolomics data using support vector regression. 2016 , 12, 1	82
929	Chemometric methods in data processing of mass spectrometry-based metabolomics: A review. 2016 , 914, 17-34	170
928	Thawing as a critical pre-analytical step in the lipidomic profiling of plasma samples: New standardized protocol. 2016 , 912, 1-9	7
927	Optimization of a liquid chromatography ion mobility-mass spectrometry method for untargeted metabolomics using experimental design and multivariate data analysis. 2016 , 913, 55-62	22
926	Chemometrics applied to quality control and metabolomics for traditional Chinese medicines. 2016 , 1015-1016, 82-91	47
925	Potential of genetically engineered hybrid poplar for pyrolytic production of bio-based phenolic compounds. 2016 , 207, 229-36	21
924	Bioanalytical techniques in nontargeted clinical lipidomics. 2016 , 8, 351-64	29
923	Multivariate metabotyping of plasma predicts survival in patients with decompensated cirrhosis. 2016 , 64, 1058-1067	55
922	The use of a gas chromatography-sensor system combined with advanced statistical methods, towards the diagnosis of urological malignancies. 2016 , 10, 017106	25
921	Chronical sleep interruption-induced cognitive decline assessed by a metabolomics method. 2016 , 302, 60-8	29
920	Microbial metabolomics in open microscale platforms. 2016 , 7, 10610	67
919	Urinary metabolic profile predicts high-fat diet sensitivity in the C57Bl6/J mouse. 2016 , 31, 88-97	1
918	Fast and Reliable Quantitative Peptidomics with labelpepmatch. 2016 , 15, 1080-9	11
917	Non-targeted profiling of semi-polar metabolites in Arabidopsis root exudates uncovers a role for coumarin secretion and lignification during the local response to phosphate limitation. 2016 , 67, 1421-32	66

916	The Breakdown of Stored Triacylglycerols Is Required during Light-Induced Stomatal Opening. 2016 , 26, 707-12		76
915	Mass Spectrometry in Plant-omics. <i>Analytical Chemistry</i> , 2016 , 88, 3422-34	7.8	50
914	Comparative metabolite profiling and fingerprinting of genus <i>Passiflora</i> leaves using a multiplex approach of UPLC-MS and NMR analyzed by chemometric tools. 2016 , 408, 3125-43		48
913	Time-Series Transcriptomics Reveals That AGAMOUS-LIKE22 Affects Primary Metabolism and Developmental Processes in Drought-Stressed Arabidopsis. 2016 , 28, 345-66		65
912	Blood metabolite markers of neocortical amyloid- β burden: discovery and enrichment using candidate proteins. 2016 , 6, e719		22
911	Defining functional classes of Barth syndrome mutation in humans. 2016 , 25, 1754-70		37
910	geoRge: A Computational Tool To Detect the Presence of Stable Isotope Labeling in LC/MS-Based Untargeted Metabolomics. <i>Analytical Chemistry</i> , 2016 , 88, 621-8	7.8	43
909	Emerging applications of metabolomics in drug discovery and precision medicine. 2016 , 15, 473-84		694
908	Human Breast Milk and Infant Formulas Differentially Modify the Intestinal Microbiota in Human Infants and Host Physiology in Rats. 2016 , 146, 191-9		32
907	A Metabolomics Study of Retrospective Forensic Data from Whole Blood Samples of Humans Exposed to 3,4-Methylenedioxymethamphetamine: A New Approach for Identifying Drug Metabolites and Changes in Metabolism Related to Drug Consumption. 2016 , 15, 619-27		29
906	Effect-directed analysis supporting monitoring of aquatic environments--An in-depth overview. 2016 , 544, 1073-118		222
905	Efficient biotransformation of non-steroid anti-inflammatory drugs by endophytic and epiphytic fungi from dried leaves of a medicinal plant, <i>Plantago lanceolata</i> L.. 2016 , 108, 115-121		20
904	Metabolite profiling in 18 Saudi date palm fruit cultivars and their antioxidant potential via UPLC-qTOF-MS and multivariate data analyses. 2016 , 7, 1077-86		32
903	Mass spectral databases for LC/MS- and GC/MS-based metabolomics: State of the field and future prospects. 2016 , 78, 23-35		295
902	Untargeted Screening and Distribution of Organo-Bromine Compounds in Sediments of Lake Michigan. 2016 , 50, 321-30		34
901	Common components and specific weights analysis: A tool for metabolomic data pre-processing. 2016 , 150, 41-50		17
900	Large-scale non-targeted metabolomic profiling in three human population-based studies. 2016 , 12, 1		23
899	High resolution mass spectrometry for structural identification of metabolites in metabolomics. 2016 , 12, 1		60

898	Non-targeted screening approaches for contaminants and adulterants in food using liquid chromatography hyphenated to high resolution mass spectrometry. 2016 , 1428, 86-96		79
897	Liquid chromatography-high-resolution mass spectrometry-based cell metabolomics: Experimental design, recommendations, and applications. 2016 , 75, 118-128		38
896	Application of Systems Theory in Longitudinal Studies on the Origin and Progression of Alzheimer's Disease. 2016 , 1303, 49-67		29
895	N(8)-acetylspermidine as a potential plasma biomarker for Snyder-Robinson syndrome identified by clinical metabolomics. 2016 , 39, 131-7		23
894	System-based proteomic and metabolomic analysis of the Df(16)A mouse identifies potential miR-185 targets and molecular pathway alterations. 2017 , 22, 384-395		15
893	Sample preparation optimization in fecal metabolic profiling. 2017 , 1047, 115-123		55
892	Metabolizing Data in the Cloud. 2017 , 35, 481-483		19
891	Co-option of the sphingolipid metabolism for the production of nitroalkene defensive chemicals in termite soldiers. 2017 , 82, 52-61		6
890	Visualization, Quantification, and Alignment of Spectral Drift in Population Scale Untargeted Metabolomics Data. <i>Analytical Chemistry</i> , 2017 , 89, 1399-1404	7.8	29
889	Omics for understanding synergistic action of validamycin A and <i>Trichoderma asperellum</i> GDFS1009 against maize sheath blight pathogen. 2017 , 7, 40140		20
888	BreathDx - molecular analysis of exhaled breath as a diagnostic test for ventilator-associated pneumonia: protocol for a European multicentre observational study. 2017 , 17, 1		50
887	Urinary metabolomics of complete Freund's adjuvant-induced hyperalgesia in rats. 2017 , 31, e3886		2
886	Eugenol specialty chemical production in transgenic poplar (<i>Populus tremula</i> L. <i>P. alba</i>) field trials. 2017 , 15, 970-981		12
885	Urine Metabolomics in Hypertension Research. 2017 , 1527, 61-68		6
884	Metabolomics: Definitions and Significance in Systems Biology. 2017 , 965, 3-17		38
883	Preprocessing and Pretreatment of Metabolomics Data for Statistical Analysis. 2017 , 965, 145-161		24
882	Rats' urinary metabolomes reveal the potential roles of functional foods and exercise in obesity management. 2017 , 8, 985-996		9
881	Integrated omics analysis of specialized metabolism in medicinal plants. 2017 , 90, 764-787		122

880	An untargeted metabolomics method for archived newborn dried blood spots in epidemiologic studies. 2017 , 13, 1		38
879	Metabolic profiling of human plasma and urine in chronic kidney disease by hydrophilic interaction liquid chromatography coupled with time-of-flight mass spectrometry: a pilot study. 2017 , 409, 2201-2211		26
878	Successes and pitfalls in automated dereplication strategy using liquid chromatography coupled to mass spectrometry data: A CASMI 2016 experience. 2017 , 21, 297-305		6
877	Metabolomics for empirical delineation of the traditional Korean fermented foods and beverages. 2017 , 61, 103-115		29
876	Amniotic Fluid and Maternal Serum Metabolic Signatures in the Second Trimester Associated with Preterm Delivery. 2017 , 16, 898-910		34
875	Employing Two-stage Derivatisation and GC-MS to Assay for Cathine and Related Stimulant Alkaloids across the Celastraceae. 2017 , 28, 257-266		6
874	Metabolic profiling identification of metabolites formed in Mediterranean mussels (<i>Mytilus galloprovincialis</i>) after diclofenac exposure. 2017 , 583, 257-268		31
873	Chemogeography of the red macroalgae <i>Asparagopsis</i> : metabolomics, bioactivity, and relation to invasiveness. 2017 , 13, 1		14
872	Joint Bounding of Peaks Across Samples Improves Differential Analysis in Mass Spectrometry-Based Metabolomics. <i>Analytical Chemistry</i> , 2017 , 89, 3517-3523	7.8	7
871	compMS2Miner: An Automatable Metabolite Identification, Visualization, and Data-Sharing R Package for High-Resolution LC-MS Data Sets. <i>Analytical Chemistry</i> , 2017 , 89, 3919-3928	7.8	23
870	Mass Spectral Feature List Optimizer (MS-FLO): A Tool To Minimize False Positive Peak Reports in Untargeted Liquid Chromatography-Mass Spectroscopy (LC-MS) Data Processing. <i>Analytical Chemistry</i> , 2017 , 89, 3250-3255	7.8	85
869	A Comprehensive Analysis of Metabolomics and Transcriptomics in Cervical Cancer. 2017 , 7, 43353		44
868	Comparative metabolomic study between African and Amazonian <i>Symphonia globulifera</i> by tandem LC/HRMS. 2017 , 20, 309-315		4
867	Comprehensive metabolite profiling of onion bulbs (<i>Allium cepa</i>) using liquid chromatography coupled with electrospray ionization quadrupole time-of-flight mass spectrometry. 2017 , 13, 1		21
866	Interplay between metabolic identities in the intestinal crypt supports stem cell function. 2017 , 543, 424-427		239
865	The interaction between the proliferating macroalga <i>Asparagopsis taxiformis</i> and the coral <i>Astroides calycularis</i> induces changes in microbiome and metabolomic fingerprints. 2017 , 7, 42625		21
864	Ultra high performance liquid chromatography-high resolution mass spectrometry plasma lipidomics can distinguish between canine breeds despite uncontrolled environmental variability and non-standardized diets. 2017 , 13, 15		22
863	Transplantation of fecal microbiota from patients with irritable bowel syndrome alters gut function and behavior in recipient mice. 2017 , 9,		246

862	Polymeric hydrophilic interaction liquid chromatography coupled with Orbitrap mass spectrometry and chemometric analysis for untargeted metabolite profiling of natural rice variants. 2017, 73, 165-173		6
861	EN-Methylamino-L-alanine (BMAA) perturbs alanine, aspartate and glutamate metabolism pathways in human neuroblastoma cells as determined by metabolic profiling. 2017, 49, 905-919		22
860	msPurity: Automated Evaluation of Precursor Ion Purity for Mass Spectrometry-Based Fragmentation in Metabolomics. <i>Analytical Chemistry</i> , 2017, 89, 2432-2439	7.8	28
859	An innovative chemometric method for processing direct introduction high resolution mass spectrometry metabolomic data: independent component discriminant analysis (ICDA). 2017, 13, 1		9
858	Discovery of Cell-Type-Specific and Disease-Related Enzymatic Activity Changes via Global Evaluation of Peptide Metabolism. 2017, 139, 3465-3472		14
857	Lipidomics in biomedical research-practical considerations. 2017, 1862, 800-803		24
856	Metabolomics reveals biotic and abiotic elicitor effects on the soft coral <i>Sarcophyton ehrenbergi</i> terpenoid content. 2017, 7, 648		20
855	Customized Consensus Spectral Library Building for Untargeted Quantitative Metabolomics Analysis with Data Independent Acquisition Mass Spectrometry and MetaboDIA Workflow. <i>Analytical Chemistry</i> , 2017, 89, 4897-4906	7.8	27
854	Indolepropionic acid and novel lipid metabolites are associated with a lower risk of type 2 diabetes in the Finnish Diabetes Prevention Study. 2017, 7, 46337		137
853	Two stage algorithm vs commonly used approaches for the suspect screening of complex environmental samples analyzed via liquid chromatography high resolution time of flight mass spectroscopy: A test study. 2017, 1501, 68-78		18
852	JA but not JA-Ile is the cell-nonautonomous signal activating JA mediated systemic defenses to herbivory in <i>Nicotiana attenuata</i> . 2017, 59, 552-571		22
851	Metabolomic approaches in the discovery of potential urinary biomarkers of drug-induced liver injury (DILI). 2017, 47, 633-649		16
850	Discrimination of pancreatic cancer and pancreatitis by LC-MS metabolomics. 2017, 13, 61		30
849	The importance of bioinformatics for connecting data-driven lipidomics and biological insights. 2017, 1862, 762-765		15
848	Knowledge integration strategies for untargeted metabolomics based on MCR-ALS analysis of CE-MS and LC-MS data. 2017, 978, 10-23		35
847	Untargeted metabolomics reveals a mild impact of remote ischemic conditioning on the plasma metabolome and β -hydroxybutyrate as a possible cardioprotective factor and biomarker of tissue ischemia. 2017, 13, 67		7
846	Inhibition of expression of the circadian clock gene <i>Period</i> causes metabolic abnormalities including repression of glycometabolism in <i>Bombyx mori</i> cells. 2017, 7, 46258		10
845	Addressing reproducibility in single-laboratory phenotyping experiments. 2017, 14, 462-464		30

844	Systems biology guided by XCMS Online metabolomics. 2017 , 14, 461-462		120
843	Metabolic Profiling of Hoodia, Chamomile, Terminalia Species and Evaluation of Commercial Preparations Using Ultrahigh-Performance Liquid Chromatography Quadrupole-Time-of-Flight Mass Spectrometry. 2017 , 83, 1297-1308		4
842	Recent advances in expanding the coverage of the lipidome. 2017 , 43, 127-133		42
841	Unsupervised Discovery and Comparison of Structural Families Across Multiple Samples in Untargeted Metabolomics. <i>Analytical Chemistry</i> , 2017 , 89, 7569-7577	7.8	33
840	KPIC2: An Effective Framework for Mass Spectrometry-Based Metabolomics Using Pure Ion Chromatograms. <i>Analytical Chemistry</i> , 2017 , 89, 7631-7640	7.8	17
839	Compound annotation in liquid chromatography/high-resolution mass spectrometry based metabolomics: robust adduct ion determination as a prerequisite to structure prediction in electrospray ionization mass spectra. 2017 , 31, 1261-1266		31
838	A Web Service Framework for Interactive Analysis of Metabolomics Data. <i>Analytical Chemistry</i> , 2017 , 89, 5713-5718	7.8	8
837	Metabolomic and Proteomic Analysis of Maize Embryonic Callus induced from immature embryo. 2017 , 7, 1004		21
836	Workflow methodology for rat brain metabolome exploration using NMR, LC-MS and GC-MS analytical platforms. 2017 , 142, 270-278		15
835	From chromatogram to analyte to metabolite. How to pick horses for courses from the massive web resources for mass spectral plant metabolomics. 2017 , 6, 1-20		43
834	Serum-based metabolomics characterization of pigs treated with ractopamine. 2017 , 13, 1		18
833	The early metabolomic response of adipose tissue during acute cold exposure in mice. 2017 , 7, 3455		31
832	Lipid homeostasis and regulated cell death. 2017 , 39, 83-89		68
831	Acute Consumption of Flavan-3-ol-Enriched Dark Chocolate Affects Human Endogenous Metabolism. 2017 , 16, 2516-2526		11
830	Lipidomics Profiling of Human Adipose Tissue Identifies a Pattern of Lipids Associated with Fish Oil Supplementation. 2017 , 16, 3168-3179		8
829	Origin-based polyphenolic fingerprinting of Theobroma cacao in unfermented and fermented beans. 2017 , 99, 550-559		58
828	PIXiE: an algorithm for automated ion mobility arrival time extraction and collision cross section calculation using global data association. 2017 , 33, 2715-2722		7
827	Non-targeted, high resolution mass spectrometry strategy for simultaneous monitoring of xenobiotics and endogenous compounds in green sea turtles on the Great Barrier Reef. 2017 , 599-600, 1251-1262		36

826	Mining mass spectrometry data: Using new computational tools to find novel organic compounds in complex environmental mixtures. 2017 , 110, 92-99		21
825	Deposition of a Sorbent into a Recession on a Solid Support To Provide a New, Mechanically Robust Solid-Phase Microextraction Device. <i>Analytical Chemistry</i> , 2017 , 89, 8021-8026	7.8	35
824	Metabolomic analysis for the study of maturation in pediatrics: Effect of confounding factors in a pilot study. 2017 , 38, 2323-2330		0
823	Mammalian Systems Biotechnology Reveals Global Cellular Adaptations in a Recombinant CHO Cell Line. 2017 , 4, 530-542.e6		65
822	Bioinformatics can boost metabolomics research. 2017 , 261, 137-141		31
821	Forecasting Chronic Diseases Using Data Fusion. 2017 , 16, 2435-2444		11
820	Rapid discovery and identification of the prototypes and their metabolites of Da-Huang-Xiao-Shi decoction in rat plasma by an integrative strategy based on liquid chromatography coupled with mass spectrometry. 2017 , 40, 2722-2731		6
819	Clustering of MS spectra using unsupervised methods to aid the identification of secondary metabolites from <i>Pseudomonas aeruginosa</i> . 2017 , 1071, 19-28		30
818	A scalable platform to identify fungal secondary metabolites and their gene clusters. 2017 , 13, 895-901		108
817	Trypsin inhibitor screening in traditional Chinese medicine by using an immobilized enzyme microreactor in capillary and molecular docking study. 2017 , 40, 3168-3174		27
816	A discovery-driven approach to elucidate urinary metabolome changes after a regular and moderate consumption of beer and nonalcoholic beer in subjects at high cardiovascular risk. 2017 , 61, 1600980		5
815	Metabolome Comparison of Bioactive and Inactive <i>Rhododendron</i> Extracts and Identification of an Antibacterial Cannabinoid(s) from <i>Rhododendron collettianum</i> . 2017 , 28, 454-464		15
814	An overview of large-dimensional covariance and precision matrix estimators with applications in chemometrics. 2017 , 31, e2880		15
813	Plasma metabolite score correlates with Hypoxia time in a newly born piglet model for asphyxia. 2017 , 12, 1-7		16
812	Early metabolic and transcriptional variations in fruit of natural white-fruited <i>Fragaria vesca</i> genotypes. 2017 , 7, 45113		31
811	metaX: a flexible and comprehensive software for processing metabolomics data. 2017 , 18, 183		168
810	Fixation of CO using the ethylmalonyl-CoA pathway in the photoheterotrophic marine bacterium <i>Dinoroseobacter shibae</i> . 2017 , 19, 2645-2660		11
809	Three serum metabolite signatures for diagnosing low-grade and high-grade bladder cancer. 2017 , 7, 46176		18

808	The Use of Metabolomics to Identify Biological Signatures of Manganese Exposure. 2017 , 61, 406-415	15
807	Strategy for comparative untargeted metabolomics reveals honey markers of different floral and geographic origins using ultrahigh-performance liquid chromatography-hybrid quadrupole-orbitrap mass spectrometry. 2017 , 1499, 78-89	36
806	Metabolomic Changes in Rat Model of Cauda Equina Injury. 2017 , 102, 449-458	3
805	Metabolomics of the tick-Borrelia interaction during the nymphal tick blood meal. 2017 , 7, 44394	16
804	New insights into the mechanistic action of methyldehydrodieugenol B towards Leishmania (L.) infantum via a multiplatform based untargeted metabolomics approach. 2017 , 13, 1	5
803	Two phylogenetically and compartmentally distinct CDP-diacylglycerol synthases cooperate for lipid biogenesis in. 2017 , 292, 7145-7159	17
802	Capillary electrophoresis mass spectrometry as a tool for untargeted metabolomics. 2017 , 9, 99-130	63
801	Impact of exercise on fecal and cecal metabolome over aging: a longitudinal study in rats. 2017 , 9, 21-36	13
800	Investigation of the derivatization conditions for GC-MS metabolomics of biological samples. 2017 , 9, 53-65	48
799	Post-acquisition spectral stitching. An alternative approach for data processing in untargeted metabolomics by UHPLC-ESI(-)-HRMS. 2017 , 1047, 106-114	3
798	Batch-processing of imaging or liquid-chromatography mass spectrometry datasets and De Novo sequencing of polyketide siderophores. 2017 , 1865, 768-775	19
797	Genome sequence and genetic diversity of European ash trees. 2017 , 541, 212-216	101
796	Targeted full-scan LC-MS metabolomics: simultaneous quantitation of knowns and feature discovery provide the best of both worlds. 2017 , 9, 5-8	3
795	Current ambient concentrations of ozone in Panama modulate the leaf chemistry of the tropical tree Ficus insipida. 2017 , 172, 363-372	6
794	Data Streaming for Metabolomics: Accelerating Data Processing and Analysis from Days to Minutes. <i>Analytical Chemistry</i> , 2017 , 89, 1254-1259	7.8 20
793	Statistical Analysis of Proteomics, Metabolomics, and Lipidomics Data Using Mass Spectrometry. 2017 ,	4
792	Metabolomics-based approach for ranking the candidate structures of unidentified peaks in capillary electrophoresis time-of-flight mass spectrometry. 2017 , 38, 1053-1059	9
791	Determination of hydroxycinnamic acids present in Rhododendron species. 2017 , 144, 216-225	14

790	Dynamic metabolic reprogramming of steroidal glycol-alkaloid and phenylpropanoid biosynthesis may impart early blight resistance in wild tomato (<i>Solanum arcanum</i> Peralta). 2017 , 95, 411-423	20
789	Genetic Mapping and Biochemical Basis of Yellow Feather Pigmentation in Budgerigars. 2017 , 171, 427-439.e2170	5
788	Comparative assessment of software for non-targeted data analysis in the study of volatile fingerprint changes during storage of a strawberry beverage. 2017 , 1522, 70-77	5
787	Fast pure ion chromatograms extraction method for LC-MS. 2017 , 170, 68-74	5
786	Bioinformatics Tools for the Interpretation of Metabolomics Data. 2017 , 3, 374-383	28
785	Cytosolic acetyl-CoA promotes histone acetylation predominantly at H3K27 in Arabidopsis. 2017 , 3, 814-824	46
784	Application of the amniotic fluid metabolome to the study of fetal malformations, using Down syndrome as a specific model. 2017 , 16, 7405-7415	12
783	Robust biomarker identification in a two-class problem based on pairwise log-ratios. 2017 , 171, 277-285	13
782	Exhaled isoprene for monitoring recovery from acute hypoxic stress. 2017 , 11, 047111	4
781	Data acquisition workflows in liquid chromatography coupled to high resolution mass spectrometry-based metabolomics: Where do we stand?. 2017 , 1526, 1-12	69
780	A preliminary study of bipolar disorder type I by mass spectrometry-based serum lipidomics. 2017 , 258, 268-273	18
779	Seasonal cycling in the gut microbiome of the Hadza hunter-gatherers of Tanzania. 2017 , 357, 802-806	423
778	Recent chemometrics advances for foodomics. 2017 , 96, 42-51	61
777	A cross-platform metabolomics workflow for volume-restricted tissue samples: application to an animal model for polycystic kidney disease. 2017 , 13, 1940-1945	2
776	Navigating freely-available software tools for metabolomics analysis. 2017 , 13, 106	131
775	AssayR: A Simple Mass Spectrometry Software Tool for Targeted Metabolic and Stable Isotope Tracer Analyses. <i>Analytical Chemistry</i> , 2017 , 89, 9616-9619	7.8 16
774	Untargeted LCMS Data Preprocessing in Metabolomics. 2017 , 1, 187-192	8
773	Revealing anti-inflammation mechanism of water-extract and oil of forsythiae fructus on carrageenan-Induced edema rats by serum metabolomics. 2017 , 95, 929-937	16

772	Evaluation of intensity drift correction strategies using MetaboDrift, a normalization tool for multi-batch metabolomics data. 2017 , 1523, 265-274		29
771	AntDAS: Automatic Data Analysis Strategy for UPLC-QTOF-Based Nontargeted Metabolic Profiling Analysis. <i>Analytical Chemistry</i> , 2017 , 89, 11083-11090	7.8	24
770	Liquid chromatography - high resolution mass spectrometry-based metabolomic approach for the detection of Continuous Erythropoiesis Receptor Activator effects in horse doping control. 2017 , 1521, 90-99		9
769	Phenylpropanoid profiling reveals a class of hydroxycinnamoyl glucaric acid conjugates in <i>Isatis tinctoria</i> leaves. 2017 , 144, 127-140		20
768	Identification of Novel Hydrogen-Substituted Polyfluoroalkyl Ether Sulfonates in Environmental Matrices near Metal-Plating Facilities. 2017 , 51, 11588-11596		42
767	Metabolomics differences between silkworms (<i>Bombyx mori</i>) reared on fresh mulberry (<i>Morus</i>) leaves or artificial diets. 2017 , 7, 10972		32
766	Stimulation of 3D osteogenesis by mesenchymal stem cells using a nanovibrational bioreactor. 2017 , 1, 758-770		58
765	Mass spectrometry methods to study protein-metabolite interactions. 2017 , 12, 1271-1280		6
764	Biomarker Quantitation Using Relative Approaches. 2017 , 183-194		
763	Revitalization of a Forward Genetic Screen Identifies Three New Regulators of Fungal Secondary Metabolism in the Genus. 2017 , 8,		29
762	Metabolomic approach to understand the acute and chronic hepatotoxicity of <i>Veratrum nigrum</i> extract in mice based on ultra-high-performance liquid chromatography coupled with quadrupole time-of-flight mass spectrometry. 2017 , 27, 687-696		4
761	Metabolomic analysis identifies altered metabolic pathways in Multiple Sclerosis. 2017 , 93, 148-155		35
760	Metabolite profiling of non-sterile rhizosphere soil. 2017 , 92, 147-162		85
759	Mass-spectra-based peak alignment for automatic nontargeted metabolic profiling analysis for biomarker screening in plant samples. 2017 , 1513, 201-209		13
758	Strains of the <i>Lactobacillus casei</i> group show diverse abilities for the production of flavor compounds in 2 model systems. 2017 , 100, 6918-6929		14
757	Biotic interactions in a Mediterranean oak forest: role of allelopathy along phenological development of woody species. 2017 , 136, 699-710		15
756	Create, run, share, publish, and reference your LC-MS, FIA-MS, GC-MS, and NMR data analysis workflows with the Workflow4Metabolomics 3.0 Galaxy online infrastructure for metabolomics. 2017 , 93, 89-101		69
755	One Step Forward for Reducing False Positive and False Negative Compound Identifications from Mass Spectrometry Metabolomics Data: New Algorithms for Constructing Extracted Ion Chromatograms and Detecting Chromatographic Peaks. <i>Analytical Chemistry</i> , 2017 , 89, 8696-8703	7.8	137

754	An alignment algorithm for LC-MS-based metabolomics dataset assisted by MS/MS information. 2017 , 990, 96-102	11
753	Emerging analytical methods for the characterization and quantification of organic contaminants in flowback and produced water. 2017 , 15, 12-23	42
752	PiMP my metabolome: an integrated, web-based tool for LC-MS metabolomics data. 2017 , 33, 4007-4009	27
751	Pre-analytic evaluation of volumetric absorptive microsampling and integration in a mass spectrometry-based metabolomics workflow. 2017 , 409, 6263-6276	28
750	Investigation of Distinction Chemical Markers for Rhubarb Authentication Based on High-Performance Liquid Chromatography-Time-of-Flight Mass Spectrometry and Multivariate Statistical Analysis. 2017 , 10, 3934-3946	5
749	Adipose tissue and metabolic and inflammatory responses to stroke are altered in obese mice. 2017 , 10, 1229-1243	16
748	Vitamin B6 is essential for serine de novo biosynthesis. 2017 , 40, 883-891	21
747	The impact of extraction protocol on the chemical profile of cannabis extracts from a single cultivar. 2021 , 11, 21801	0
746	Variation in root exudate composition influences soil microbiome membership and function.	
745	SLAW: A Scalable and Self-Optimizing Processing Workflow for Untargeted LC-MS. <i>Analytical Chemistry</i> , 2021 , 93, 15024-15032	7.8 5
744	Integrated metabolome and transcriptome analyses provide insight into colon cancer development by the gut microbiota.	
743	Integrative Analysis to Identify Race-Associated Metabolite Biomarkers for Hepatocellular Carcinoma. 2020 , 2020, 5300-5303	0
742	Dynamic binning peak detection and assessment of various lipidomics liquid chromatography-mass spectrometry pre-processing platforms.	
741	Aird: A computation-oriented mass spectrometry data format enables higher compression ratio and less decoding time.	
740	Soil chemical legacies trigger species-specific and context-dependent root responses in later arriving plants.	
739	Early metabolic priming under differing carbon sufficiency conditions influences peach fruit quality development.	
738	Rapid Development of Improved Data-dependent Acquisition Strategies.	
737	Metabolic profile discriminates and predicts Arabidopsis susceptibility to virus under field conditions.	

736	A non-targeted approach to chemical discrimination between green tea dietary supplements and green tea leaves by HPLC/MS. 2011 , 94, 487-97		6
735	Ribonucleotide reductase subunit M2B deficiency leads to mitochondrial permeability transition pore opening and is associated with aggressive clinicopathologic manifestations of breast cancer. 2018 , 10, 3635-3649		2
734	Plasma metabolic alterations and potential biomarkers in individuals at clinical high risk for psychosis. 2021 , 239, 19-28		1
733	High-resolution association mapping with libraries of immortalized lines from ancestral landraces. 2021 , 1		2
732	High-Fructose Diet Alters Intestinal Microbial Profile and Correlates with Early Tumorigenesis in a Mouse Model of Barrett's Esophagus.. 2021 , 9,		1
731	Toxicity of 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone (NNK) in early development: A wide-scope metabolomics assay in zebrafish embryos.. 2021 , 429, 127746		0
730	Modulation of the Tomato Rhizosphere Microbiome via Changes in Root Exudation Mediated by the Ethylene Receptor NR.. 2021 , 9,		0
729	Foodomics: Analytical Opportunities and Challenges. <i>Analytical Chemistry</i> , 2021 ,	7.8	5
728	Metabolomics Strategy Assisted by Transcriptomics Analysis to Identify Potential Biomarkers Associated with Tuberculosis. 2021 , 14, 4795-4807		0
727	Plasma Lipidomic and Metabolomic Profiling after Birth in Neonates Born to SARS-CoV-19 Infected and Non-Infected Mothers at Delivery: Preliminary Results.. 2021 , 11,		0
726	Targeted and Untargeted Metabolomics Profiling of Wheat Reveals Amino Acids Increase Resistance to Head Blight. 2021 , 12, 762605		4
725	Prochlorococcus extracellular vesicles: molecular composition and adsorption to diverse microbes. 2021 ,		1
724	Metabolism-mediated mechanisms underpin the differential stomatal speediness regulation among ferns and angiosperms. 2021 ,		1
723	Suspect, non-target and target screening of pharmaceuticals and personal care products (PPCPs) in a drinking water system. 2021 , 808, 151866		2
722	Long-term exposure to environmental diclofenac concentrations impairs growth and induces molecular changes in <i>Lymnaea stagnalis</i> freshwater snails. 2021 , 133065		0
721	Tobacco as a potential raw material for drug production. 2021 , 43, 1		1
720	A Validated HPLC-PDA-HRMS Method to Investigate the Biological Stability and Metabolism of Antiparasitic Triterpenic Esters. 2021 , 26,		
719	MCF-7 Drug Resistant Cell Lines Switch Their Lipid Metabolism to Triple Negative Breast Cancer Signature. 2021 , 13,		0

718	Factors that influence the quality of metabolomics data in in vitro cell toxicity studies: a systematic survey. 2021 , 11, 22119		0
717	From Centroided to Profile Mode: Machine Learning for Prediction of Peak Width in HRMS Data. <i>Analytical Chemistry</i> , 2021 ,	7.8	1
716	Plasma Metabolomics of Intermediate and Neovascular Age-Related Macular Degeneration Patients. 2021 , 10,		1
715	Metabolomics and transcriptomics of pheromone biosynthesis in an aggressive forest pest <i>Ips typographus</i> . 2021 , 140, 103680		2
714	A novel strategy for the detection of boldenone undecylenate misuse in cattle using ultra-high performance liquid chromatography coupled to high resolution orbitrap mass spectrometry: from non-targeted to targeted. 2021 ,		0
713	High-Resolution Exposomics and Metabolomics Reveals Specific Associations in Cholestatic Liver Diseases. 2021 ,		1
712	Transcriptomic and metabolomic analyses reveal the altitude adaptability and evolution of different colored flowers in alpine <i>Rhododendron</i> species. 2021 ,		0
711	MetEx, a Metabolomics Explorer Application for Natural Product Discovery. 2021 ,		0
710	A Metabolomics approach for the diagnosis Of SecondAry InfeCtions in COVID-19 (MOSAIC): a study protocol. 2021 , 21, 1204		0
709	Integrated physiological, transcriptome and metabolome analyses of the hepatopancreas of the female swimming crab <i>Portunus trituberculatus</i> under ammonia exposure. 2021 , 228, 113026		4
708	Screening of organic chemicals in surface water of the North River by high resolution mass spectrometry. 2021 , 290, 133174		4
707	In vitro interaction network of a synthetic gut bacterial community. 2021 ,		5
706	Longitudinal Metabolomics Reveals Ornithine Cycle Dysregulation Correlates With Inflammation and Coagulation in COVID-19 Severe Patients.. 2021 , 12, 723818		1
705	ProMetIS, deep phenotyping of mouse models by combined proteomics and metabolomics analysis. 2021 , 8, 311		1
704	Proteomics and Metabolomics in Cancer Diagnosis and Therapy. 2021 , 1-31		
703	Dietary fucoidan extracted from macroalgae alleviate the hepatic lipid accumulation of black seabream (). 2021 ,		0
702	Pentose Phosphate Pathway Regulates Tolerogenic Apoptotic Cell Clearance and Immune Tolerance.. 2021 , 12, 797091		0
701	Chemical profile of a novel ripened Pu-erh tea and its metabolic conversion during pile fermentation.. 2022 , 378, 132126		1

700	Breath analysis using electronic nose and gas chromatography- mass spectrometry: a pilot study on bronchial infections in bronchiectasis.. 2021 ,	1
699	A new platform for untargeted UHPLC-HRMS data analysis to address the time-shift problem.. 2022 , 1193, 339393	1
698	Uncovering transformation products of four organic contaminants of concern by photodegradation experiments and analysis of real samples from a local river.. 2021 , 293, 133408	2
697	Lipidomics in Biomarker Research. 2021 ,	1
696	Histone acetyltransferase NAA40 modulates acetyl-CoA levels and lipid synthesis.. 2022 , 20, 22	2
695	Integrating Network Analysis and Metabolomics to Reveal Mechanism of Huaganjian Decoction in Treatment of Cholestatic Hepatic Injury.. 2021 , 12, 773957	
694	Vertical Transfer of Metabolites Detectable from Newborn's Dried Blood Spot Samples Using UPLC-MS: A Chemometric Study.. 2022 , 12,	3
693	Metabolite discovery: Biochemistry's scientific driver.. 2022 , 34, 21-34	2
692	SILAC Phosphoproteomics Reveals Unique Signaling Circuits in CAR-T Cells and the Inhibition of B Cell-Activating Phosphorylation in Target Cells.. 2022 ,	1
691	Day and night isotope labelling reveal metabolic pathway specific regulation of protein synthesis rates in Arabidopsis.. 2022 ,	1
690	Bioengineered models of Parkinson's disease using patient-derived dopaminergic neurons exhibit distinct biological profiles in a 3D microenvironment.. 2022 , 79, 78	0
689	ptairMS: real-time processing and analysis of PTR-TOF-MS data for biomarker discovery in exhaled breath.. 2022 ,	1
688	Metabolomics-based non-targeted screening analysis of 34 PPCPs in bovine and piscine muscles.. 2021 ,	1
687	Antiviral metabolite 3'-Deoxy-3',4'-didehydro-cytidine is detectable in serum and identifies acute viral infections including COVID-19.. 2022 ,	1
686	Postmortem Metabolomics Reveal Acylcarnitines as Potential Biomarkers for Fatal Oxycodone-Related Intoxication.. 2022 , 12,	0
685	Combining Isotopologue Workflows and Simultaneous Multidimensional Separations to Detect, Identify, and Validate Metabolites in Untargeted Analyses.. <i>Analytical Chemistry</i> , 2022 ,	7.8 1
684	Operationalizing the Exposome Using Passive Silicone Samplers.. 2022 , 8, 1-29	0
683	Biomarkers of Mycoplasma pneumoniae pneumonia in children by urine metabolomics based on Q Exactive liquid chromatography tandem mass spectrometry.. 2021 , e9234	0

682	Aird: a computation-oriented mass spectrometry data format enables a higher compression ratio and less decoding time.. 2022 , 23, 35	1
681	Myostatin Knockout Regulates Bile Acid Metabolism by Promoting Bile Acid Synthesis in Cattle.. 2022 , 12,	3
680	Chemical Cartography Approaches to Study Trypanosomatid Infection.. 2022 ,	
679	Complex marine microbial communities partition metabolism of scarce resources over the diel cycle.. 2022 ,	1
678	FROM A NON-TARGETED METABOLOMICS APPROACH TO A TARGETED BIOMARKERS STRATEGY TO HIGHLIGHT TESTOSTERONE ABUSE IN EQUINE. ILLUSTRATION OF A METHODOLOGICAL TRANSFER BETWEEN PLATFORMS AND LABORATORIES.. 2022 ,	0
677	An integrated pathological research for precise diagnosis of schizophrenia combining LC-MS/H NMR metabolomics and transcriptomics. 2021 , 524, 84-95	0
676	Biomarker selection and a prospective metabolite-based machine learning diagnostic for lyme disease.. 2022 , 12, 1478	0
675	Proteomics and Metabolomics in Cancer Diagnosis and Therapy. 2022 , 2309-2338	
674	A Checklist for Reproducible Computational Analysis in Clinical Metabolomics Research.. 2022 , 12,	0
673	Relationship between lung function and exhaled volatile organic compounds in healthy infants.. 2022 ,	1
672	Integrated Analysis of the Cecal Microbiome and Plasma Metabolomics to Explore NaoMaiTong and Its Potential Role in Changing the Intestinal Flora and Their Metabolites in Ischemic Stroke.. 2021 , 12, 773722	1
671	Comparative metabolomics revealed key pathways associated with the synergistic killing of multidrug-resistant by a bacteriophage-polymyxin combination.. 2022 , 20, 485-495	2
670	An Interpretable Deep Learning Approach for Biomarker Detection in LC-MS Proteomics Data.. 2022 , PP,	
669	Amlodipine, an anti-hypertensive drug, alleviates non-alcoholic fatty liver disease by modulating gut microbiota. 2021 ,	2
668	UDP-glucose dehydrogenase expression is upregulated following EMT and differentially affects intracellular glycerophosphocholine and acetylaspartate levels in breast mesenchymal cell lines.. 2021 ,	0
667	Microalgae show a range of responses to exometabolites of foreign species.. 2022 , 62, None	0
666	The effects of methyl jasmonate on growth, gene expression and metabolite accumulation in <i>Isatis indigotica</i> Fort.. 2022 , 177, 114482	2
665	Model of retention time and density of gradient peak capacity for improved LC-MS method optimization: Application to metabolomics.. 2022 , 1197, 339492	

- 664 TrendProbe: Time profile analysis of emerging contaminants by LC-HRMS non-target screening and deep learning convolutional neural network.. **2022**, 428, 128194 1
- 663 Metabolomics of peripheral artery disease.. **2022**, 106, 67-89
- 662 Molecular networking in infectious disease models.. **2022**, 663, 341-375
- 661 Molecular networking-based strategies in mass spectrometry coupled with in silico dereplication of peptidic natural products and gene cluster analysis.. **2022**, 663, 273-302
- 660 Metabolome and transcriptome related dataset for pheromone biosynthesis in an aggressive forest pest .. **2022**, 41, 107912
- 659 Metabonomics reveals the main small molecules differences between green and white egg shells in ducks. **2022**, 21, 208-216
- 658 Comprehensive Peak Characterization (CPC) in Untargeted LC-MS Analysis.. **2022**, 12, 0
- 657 Developments in high-resolution mass spectrometric analyses of new psychoactive substances.. **2022**, 96, 949 2
- 656 Molecular Gatekeeper Discovery: Workflow for Linking Multiple Exposure Biomarkers to Metabolomics.. **2022**, 1
- 655 Chromosome-level genome assembly of *Aristolochia contorta* provides insights into the biosynthesis of benzyloisoquinoline alkaloids and aristolochic acids.. **2022**, 0
- 654 Alterations in the gut microbiome and metabolome profiles of septic rats treated with aminophylline.. **2022**, 20, 69 0
- 653 Systematic Evaluation of HILIC Stationary Phases for Global Metabolomics of Human Plasma.. **2022**, 12, 0
- 652 A live yeast supplementation to gestating ewes improves bioactive molecule composition in colostrum with no impact on its bacterial composition and beneficially affects immune status of the offspring.. **2022**, 11, e5 0
- 651 Recent advances in mass spectrometry analytical techniques for per- and polyfluoroalkyl substances (PFAS).. **2022**, 414, 2795 1
- 650 Metabolomics and lipidomics to identify biomarkers of effect related to exposure to NON-dioxin-like polychlorinated biphenyls in pigs.. **2022**, 296, 133957
- 649 Metabolic Profiling Reveals That the Olfactory Cues in the Duck Uropygial Gland Potentially Act as Sex Pheromones.. **2022**, 12,
- 648 Direct on-swab metabolic profiling of vaginal microbiome host interactions during pregnancy and preterm birth. **2021**, 12, 5967 6
- 647 Unique mechanistic insights into pathways associated with the synergistic activity of polymyxin B and caspofungin against multidrug-resistant .. **2022**, 20, 1077-1087 2

- 646 Guidelines for metabolomics-guided transposon mutagenesis for microbial natural product discovery.. **2022**, 665, 305-323
- 645 Computational Resources for Oncology Research: A Comprehensive Analysis. **2022**, 65-92 2
- 644 Data analysis in metabolomics: from information to knowledge. **2022**, 287-379
- 643 An Interoperability Framework for Multicentric Breath Metabolomic Studies.
- 642 JPA: Joint Metabolic Feature Extraction Increases the Depth of Chemical Coverage for LC-MS-Based Metabolomics and Exposomics.. **2022**, 12, 1
- 641 Alterations in Gut Microbiota Are Correlated With Serum Metabolites in Patients With Insomnia Disorder.. **2022**, 12, 722662 2
- 640 Reproducible untargeted metabolomics workflow for exhaustive MS2 data acquisition of MS1 features.. **2022**, 14, 6 1
- 639 The SARS-CoV2 envelope is distinct from host membranes, exposes pro-coagulant lipids, and can be inactivated in vivo by surfactant-containing oral rinses.
- 638 Characterization of browning during CO2 destringency treatment in astringent persimmon fruit. 1 0
- 637 Automated Annotation of Untargeted All-Ion Fragmentation LC-MS Metabolomics Data with MetaboAnnotatoR.. *Analytical Chemistry*, **2022**, 7.8 0
- 636 Shifting a Cellular Metabolic Landscape Identifies a Refractory Environment for Flavivirus Replication.
- 635 Contemporary Research Progress on the Detection of Polycyclic Aromatic Hydrocarbons.. **2022**, 19, 0
- 634 LipidMS 3.0: an R-package and a web-based tool for LC-MS/MS data processing and lipid annotation. 0
- 633 Recent advances in metabolomics analysis for early drug development.. **2022**, 3
- 632 Lipidomics Profiles in Hepatocytes from Nonalcoholic Steatohepatitis Patients Differ Markedly from In Vitro-Induced Steatotic Hepatocytes.. **2022**, 0
- 631 TidyMass: An Object-oriented Reproducible Analysis Framework for LC-MS Data. 0
- 630 Comparison of Microbial Community and Metabolites in Four Stomach Compartments of Myostatin-Gene-Edited and Non-edited Cattle.. **2022**, 13, 844962 2
- 629 Exogenous lipase administration alters gut microbiota composition and ameliorates Alzheimer's disease-like pathology in APP/PS1 mice.. **2022**, 12, 4797 1

628	Finding Correspondence between Metabolomic Features in Untargeted Liquid Chromatography-Mass Spectrometry Metabolomics Datasets.. <i>Analytical Chemistry</i> , 2022 ,	7.8	0
627	Urinary metabolomic profiling from spontaneous tolerant kidney transplanted recipients shows enrichment in tryptophan-derived metabolites.. 2022 , 103844		1
626	Multi-Omics Characterization of Type 2 Diabetes Mellitus-Induced Cognitive Impairment in the db/db Mouse Model.. 2022 , 27,		0
625	Metabolomics in clinical and forensic toxicology, sports anti-doping, and veterinary residues.. 2022 ,		1
624	Multi-omics strategies for investigating the microbiome in toxicology research.. 2022 ,		1
623	Integrative metabolomic profiling reveals aberrations in myometrium associated with adenomyosis: a pilot study.. 2022 , 20, 49		0
622	First Application of Fecal Microbiota Transplantation in Adult Asperger Syndrome With Digestive Symptoms-A Case Report.. 2022 , 13, 695481		1
621	Paramounter: Direct Measurement of Universal Parameters To Process Metabolomics Data in a "White Box".. <i>Analytical Chemistry</i> , 2022 ,	7.8	2
620	pyAIR-A New Software Tool for Breathomics Applications-Searching for Markers in TD-GC-HRMS Analysis.. 2022 , 27,		
619	StackZDPD: a novel encoding scheme for mass spectrometry data optimized for speed and compression ratio.. 2022 , 12, 5384		0
618	Multi-Omics Analyses Characterize the Gut Microbiome and Metabolome Signatures of Soldiers Under Sustained Military Training.. 2022 , 13, 827071		1
617	Amplified Drought and Seasonal Cycle Modulate Leaf Metabolome.. 2022 , 12,		0
616	Analysis of the Formation of Sauce-Flavored Daqu Using Non-targeted Metabolomics.. 2022 , 13, 857966		2
615	Deep Learning-Assisted Peak Curation for Large-Scale LC-MS Metabolomics.. <i>Analytical Chemistry</i> , 2022 ,	7.8	1
614	Rescues Glycyrrhizic Acid Loss Under Drought Stress in by Activating the Jasmonic Acid Pathway.. 2021 , 12, 798525		3
613	Application of a hybrid zwitterionic hydrophilic interaction liquid chromatography column in metabolic profiling studies.. 2022 , 1672, 463013		2
612	Metabolomics on the study of marine organisms.. 2022 , 18, 17		3
611	Untargeted metabolomics by liquid chromatography-mass spectrometry for food authentication: A review.. 2022 ,		1

610	Positive Effects of Neutrophil Elastase Inhibitor (Sivelestat) on Gut Microbiome and Metabolite Profiles of Septic Rats.. 2022 , 12, 818391	1
609	Integrative metabolomic characterization identifies plasma metabolomic signature in the diagnosis of papillary thyroid cancer.. 2022 ,	0
608	Metabolic Response in Endothelial Cells to Catecholamine Stimulation Associated with Increased Vascular Permeability.. 2022 , 23,	2
607	Distinct metabolic profiling is correlated with bisexual flowers formation resulting from exogenous ethephon induction in melon (L.).. 2022 , 10, e13088	
606	An anchored experimental design and meta-analysis approach to address batch effects in large-scale metabolomics.	
605	Effects of Dietary Protein Level on the Microbial Composition and Metabolomic Profile in Postweaning Piglets.. 2022 , 2022, 3355687	0
604	Transcriptional, epigenetic and metabolic signatures in cardiometabolic syndrome defined by extreme phenotypes.. 2022 , 14, 39	0
603	Integration of the Human Gut Microbiome and Serum Metabolome Reveals Novel Biological Factors Involved in the Regulation of Bone Mineral Density.. 2022 , 12, 853499	0
602	Synthetic Red Blood Cell-Specific Glycolytic Intermediate 2,3-Diphosphoglycerate (2,3-DPG) Inhibits Development .. 2022 , 12, 840968	0
601	Identification of Serum Biomarkers Associated With Emergence Agitation After General Anesthesia in Adult Patients: A Metabolomics Analysis.. 2022 , 9, 828867	
600	Groundwater metabolome responds to recharge in fractured sedimentary strata.	
599	Oceanographic setting influences the prokaryotic community and metabolome in deep-sea sponges.. 2022 , 12, 3356	1
598	Getting in control of persistent, mobile and toxic (PMT) and very persistent and very mobile (vPvM) substances to protect water resources: strategies from diverse perspectives. 2022 , 34,	1
597	Predictive metabolomics of multiple Atacama plant species unveils a core set of generic metabolites for extreme climate resilience.. 2022 ,	1
596	Integrated Metabolomics and Transcriptome Revealed the Effect of Fermented Residue Promoting Immunity.. 2022 , 13, 889436	
595	Serological Phenotyping Analysis Uncovers a Unique Metabolomic Pattern Associated With Early Onset of Type 2 Diabetes Mellitus.. 2022 , 9, 841209	0
594	Collision Cross Section Calculations to Aid Metabolite Annotation.. 2022 ,	2
593	Metabolomics approach to assess the effect of siphonal autotomy on metabolic characteristics of razor clam <i>Solen grandis</i> .. 2022 , 12, 5528	0

592	Proteome metabolome and transcriptome data for three Symbiodiniaceae under ambient and heat stress conditions.. 2022 , 9, 153	1
591	The effect of endophyte on phyllosphere microbes and leaf metabolites in .. 2022 , 25, 104144	2
590	Characteristic fragmentations of nitroaromatic compounds (NACs) in Orbitrap HCD and integrated strategy for recognition of NACs in environmental samples.. 2022 , 155106	1
589	Investigation of Metabolic Resistance to Soybean Aphid (Matsumura) Feeding in Soybean Cultivars.. 2022 , 13,	0
588	Spotlight on mass spectrometric non-target screening analysis: Advanced data processing methods recently communicated for extracting, prioritizing and quantifying features.	1
587	Secondary-metabolites fingerprinting of Argania spinosa kernels using liquid chromatography-mass spectrometry and chemometrics, for metabolite identification and quantification as well as for geographic classification.. 2022 , 1670, 462972	1
586	Multi-omic based production strain improvement (MOBpsi) for bio-manufacturing of toxic chemicals.. 2022 ,	0
585	Physiological, biochemical and metabolomic mechanisms of mitigation of drought stress-induced tobacco growth inhibition by spermidine. 2022 , 181, 114844	0
584	Integrated metabolomic and transcriptomic analysis identifies benzo[a]pyrene-induced characteristic metabolic reprogramming during accumulation of lipids and reactive oxygen species in macrophages.. 2022 , 154685	0
583	Non-targeted metabolomics of cooked cowpea and pigeon pea from Ghana using two distinct and complementary analytical platforms.. 2022 , 4, 100087	0
582	Potential obesogenic effects of TBBPA and its alternatives TBBPS and TCBPA revealed by metabolic perturbations in human hepatoma cells.. 2022 , 154847	1
581	1-deoxysphingolipids bind to COUP-TF to modulate lymphatic and cardiac cell development. 2021 , 56, 3128-3145.e15	0
580	Alteration of Serum Metabolites in Women of Reproductive Age with Chronic Constipation.. 2022 , 28, e934117	0
579	Responses to larval herbivory in the phenylpropanoid pathway of Ulmus minor are boosted by prior insect egg deposition. 2021 , 255, 16	1
578	Molecular species selectivity of lipid transport creates a mitochondrial sink for di-unsaturated phospholipids. 2021 , e106837	0
577	Phenylacetylglutamine, a Novel Biomarker in Acute Ischemic Stroke.. 2021 , 8, 798765	0
576	Metabolomics Work Flow and Analytics in Systems Biology.. 2021 ,	0
575	TrpNet: Understanding Tryptophan Metabolism across Gut Microbiome.. 2021 , 12,	1

574	Planting Season Impacts Sugarcane Stem Development, Secondary Metabolite Levels, and Natural Antisense Transcription.. 2021 , 10,		0
573	MEMO: Mass Spectrometry-based Sample Vectorization to Explore Chemodiverse Datasets.		
572	Metabolite Profiling of the Social Spider <i>Stegodyphus dumicola</i> Along a Climate Gradient. 2022 , 10,		0
571	Multimomics implicate gut microbiota in altered lipid and energy metabolism in Parkinson's disease.. 2022 , 8, 39		3
570	Oogenesis and lipid metabolism in the deep-sea sponge <i>Phakellia ventilabrum</i> (Linnaeus, 1767).. 2022 , 12, 6317		0
569	Pyruvate kinase, a metabolic sensor powering glycolysis, drives the metabolic control of DNA replication.. 2022 , 20, 87		1
568	BAFinder: A Software for Unknown Bile Acid Identification Using Accurate Mass LC-MS/MS in Positive and Negative Modes.. <i>Analytical Chemistry</i> , 2022 ,	7.8	0
567	DEIMoS: An Open-Source Tool for Processing High-Dimensional Mass Spectrometry Data.. <i>Analytical Chemistry</i> , 2022 ,	7.8	3
566	MEMO: Mass Spectrometry-Based Sample Vectorization to Explore Chemodiverse Datasets. 2022 , 2,		1
565	Biomarkers of PEGylated Liposomal Doxorubicin-Induced Hypersensitivity Reaction in Breast Cancer Patients Based on Metabolomics.. 2022 , 13, 827446		
564	Guide to Metabolomics Analysis: A Bioinformatics Workflow.. 2022 , 12,		1
563	The SARS-CoV2 envelope differs from host cells, exposes pro-coagulant lipids, and is disrupted in vivo by oral rinses.. 2022 , 100208		3
562	Triiron Tetrairon Phosphate (Fe ₃ (PO ₄)) Nanomaterials Enhanced Flavonoid Accumulation in Tomato Fruits.. 2022 , 12,		0
561	Development and Application of an LC-MS/MS Untargeted Exposomics Method with a Separated Pooled Quality Control Strategy.. 2022 , 27,		0
560	Plasma concentrations of lipophilic persistent organic pollutants and glucose homeostasis in youth populations.. 2022 , 212, 113296		1
559	Table_1.DOCX. 2018 ,		
558	Table_2.DOCX. 2018 ,		
557	Table_3.DOCX. 2018 ,		

556 Table_4.DOCX. 2018,

555 Data_Sheet_1.pdf. 2019,

554 Data_Sheet_2.ZIP. 2019,

553 Data_Sheet_3.PDF. 2019,

552 Table_1.XLSX. 2019,

551 Data_Sheet_1.PDF. 2020,

550 Table_1.DOCX. 2020,

549 Presentation_1.PDF. 2018,

548 Table_1.pdf. 2018,

547 Data_Sheet_1.docx. 2019,

546 Table_1.XLSX. 2019,

545 Table_2.XLSX. 2019,

544 Table_3.XLSX. 2019,

543 Table_4.XLSX. 2019,

542 Table_5.XLSX. 2019,

541 Table_1.pdf. 2020,

540 Image_1.JPEG. 2020,

539 Image_2.JPEG. 2020,

538 Image_3.PNG. 2020,

537 Table_1.XLSX. 2020,

536 Table_10.XLS. 2020,

535 Table_11.XLS. 2020,

534 Table_2.DOCX. 2020,

533 Table_3.XLS. 2020,

532 Table_4.XLS. 2020,

531 Table_5.XLS. 2020,

530 Table_6.XLS. 2020,

529 Table_7.XLS. 2020,

528 Table_8.XLS. 2020,

527 Table_9.XLS. 2020,

526 DataSheet_1.pdf. 2019,

525 Table_1.xls. 2019,

524 Table_2.xls. 2019,

523 Data_Sheet_1.docx. 2019,

522 DataSheet1.pdf. 2018,

521 DataSheet2.xlsx. 2018,

520 Data_Sheet_1.docx. **2018,**

519 Data_Sheet_2.xlsx. **2018,**

518 Data_Sheet_3.xlsx. **2018,**

517 Image1.pdf. **2018,**

516 Table1.pdf. **2018,**

515 Data_Sheet_1.docx. **2020,**

514 Image_1.TIF. **2020,**

513 Image_2.TIF. **2020,**

512 Table_1.XLSX. **2020,**

511 Data_Sheet_1.pdf. **2020,**

510 Data_Sheet_1.docx. **2018,**

509 Data_Sheet_2.xlsx. **2018,**

508 Data_Sheet_3.xlsx. **2018,**

507 Data_Sheet_4.xlsx. **2018,**

506 Data_Sheet_5.xlsx. **2018,**

505 Data_Sheet_6.xlsx. **2018,**

504 Data_Sheet_1.PDF. **2020,**

503 Table_1.DOCX. **2021,**

502 Table_2.XLSX. 2021,

501 Table_3.XLSX. 2021,

500 Image_1.TIF. 2018,

499 Image_2.TIF. 2018,

498 Image_3.JPEG. 2018,

497 Image_4.TIF. 2018,

496 Image_5.TIF. 2018,

495 Table_1.XLS. 2018,

494 Table_2.XLS. 2018,

493 Table_3.XLS. 2018,

492 Table_4.XLSX. 2018,

491 Table_5.XLSX. 2018,

490 Table_6.XLSX. 2018,

489 Table_7.XLSX. 2018,

488 Table_8.docx. 2018,

487 Data_Sheet_1.docx. 2019,

486 Data_Sheet_2.docx. 2019,

485 Data_Sheet_3.docx. 2019,

484 Table_1.xlsx. 2019,

483 Table_2.xls. 2019,

482 Table_3.xlsx. 2019,

481 Table_4.DOCX. 2019,

480 Table_5.XLSX. 2019,

479 Table_6.XLS. 2019,

478 Table_7.XLSX. 2019,

477 Data_Sheet_1.PDF. 2018,

476 Data_Sheet_2.PDF. 2018,

475 Table_1.docx. 2018,

474 Data_Sheet_1.docx. 2020,

473 Data_Sheet_1.doc. 2019,

472 Data_Sheet_1.pdf. 2020,

471 Data_Sheet_1.ZIP. 2018,

470 Image_1.TIFF. 2019,

469 Table_1.DOCX. 2019,

468 Image_1.JPEG. 2019,

467 Presentation1.pdf. 2018,

466 Image_1.JPEG. **2020,**

465 Table_1.DOCX. **2020,**

464 Table_2.DOCX. **2020,**

463 Table_3.DOCX. **2020,**

462 Table_4.DOCX. **2020,**

461 Table_5.DOCX. **2020,**

460 Table_6.DOCX. **2020,**

459 Table_7.DOCX. **2020,**

458 datasheet1.docx. **2020,**

457 Image_1.TIF. **2018,**

456 Table_1.xlsx. **2018,**

455 Table_2.xlsx. **2018,**

454 Data_Sheet_1.doc. **2018,**

453 Data_Sheet_2.PDF. **2018,**

452 Image_1.PDF. **2018,**

451 Image_2.PDF. **2018,**

450 Image_3.PDF. **2018,**

449 Image_4.PDF. **2018,**

448 Image_5.PDF. 2018,

447 Image_6.TIF. 2018,

446 Table_1.XLSX. 2018,

445 Table_2.XLSX. 2018,

444 Table_3.XLS. 2018,

443 Table_4.XLS. 2018,

442 Table_5.XLSX. 2018,

441 Image_1.pdf. 2018,

440 Image_2.pdf. 2018,

439 Image_3.pdf. 2018,

438 Image_4.pdf. 2018,

437 Image_5.pdf. 2018,

436 Image_6.pdf. 2018,

435 Image_7.pdf. 2018,

434 Table_1.pdf. 2018,

433 Table_2.pdf. 2018,

432 Table_3.pdf. 2018,

431 Table_1.XLSX. 2018,

430 Table_2.XLSX. 2018,

429 Table_3.XLSX. 2018,

428 Table_4.XLSX. 2018,

427 Data_Sheet_1.DOCX. 2018,

426 Data_Sheet_2.XLSX. 2018,

425 Data_Sheet_3.XLSX. 2018,

424 Data_Sheet_1.docx. 2019,

423 Image_1.tif. 2019,

422 DataSheet_1.xlsx. 2019,

421 DataSheet_2.xlsx. 2019,

420 DataSheet_3.xlsx. 2019,

419 Presentation_1.pdf. 2019,

418 Data_Sheet_1.zip. 2018,

417 Image_1.pdf. 2018,

416 Table_1.XLSX. 2018,

415 Table_2.CSV. 2018,

414 Table_3.CSV. 2018,

413 DataSheet_1.xlsx. 2019,

412 DataSheet_2.xlsx. **2019,**

411 Presentation_1.pdf. **2019,**

410 Data_Sheet_1.pdf. **2019,**

409 Data_Sheet_2.xls. **2019,**

408 Data_Sheet_1.docx. **2019,**

407 Table_1.xlsx. **2019,**

406 Image_1.TIF. **2019,**

405 Image_2.TIF. **2019,**

404 Image_3.TIF. **2019,**

403 Image_4.TIF. **2019,**

402 Image_5.TIF. **2019,**

401 Image_6.TIF. **2019,**

400 Table_1.DOCX. **2019,**

399 Table_2.XLSX. **2019,**

398 Table_3.XLSX. **2019,**

397 Table_4.XLSX. **2019,**

396 Glycine betaine uptake and metabolism in marine microbial communities.. **2022,**

1

395 Detecting the Sources of Chemicals in the Black Sea Using Non-Target Screening and Deep Learning Convolutional Neural Networks.

394	Evaluation of R packages to process and analyze LCMS metabolomics data. 2022 , 76,	
393	Metabolomics Reveals 5-Aminolevulinic Acid Improved the Ability of Tea Leaves (<i>Camellia sinensis</i> L.) against Cold Stress. 2022 , 12, 392	1
392	The metabolic and proteomic repertoires of periderm tissue in skin of the reticulated Sikkim cucumber fruit.	1
391	Multi-Omic Profiling of Multi-Biosamples Reveals the Role of Amino Acid and Nucleotide Metabolism in Endometrial Cancer.. 2022 , 12, 861142	0
390	Towards Unbiased Evaluation of Ionization Performance in LC-HRMS Metabolomics Method Development. 2022 , 12, 426	
389	Advances in suspect screening and non-target analysis of polar emerging contaminants in the environmental monitoring. 2022 , 116671	0
388	Sugars dominate the seagrass rhizosphere.. 2022 ,	1
387	Aquifer system and depth specific chemical patterns in fractured-rock groundwater from the Critical Zone revealed by untargeted LC-MS-based metabolomics.. 2022 , 219, 118566	0
386	Application of MS-Based Metabolomic Approaches in Analysis of Starfish and Sea Cucumber Bioactive Compounds. 2022 , 20, 320	1
385	Deep Learning-based Pseudo-Mass Spectrometry Imaging Analysis for Precision Medicine.	
384	Variation in Root Exudate Composition Influences Soil Microbiome Membership and Function.. 2022 , e0022622	2
383	Preliminary authentication of apple juices using untargeted UHPLC-HRMS analysis combined to chemometrics. 2022 , 109098	
382	Application of Metabolite Set Enrichment Analysis (MSEA) on untargeted metabolomics data prioritizes relevant pathways and detects novel biomarkers for inherited metabolic disorders.. 2022	1
381	Non-target, suspect and target screening of chemicals of emerging concern in landfill leachates and groundwater in Guangzhou, South China.. 2022 , 837, 155705	1
380	Untargeted Metabolomic Approach to Determine the Regulatory Pathways on Salicylic Acid-Mediated Stress Response in Seedlings.. 2022 , 27,	
379	Early Metabolomic Markers of Acute Low-Dose Exposure to Uranium in Rats. 2022 , 12, 421	0
378	A 'shape-orientated' algorithm employing an adapted Marr wavelet and shape matching index improves the performance of continuous wavelet transform for chromatographic peak detection and quantification.. 2022 , 1673, 463086	
377	Antidiabetic activity and metabolite profiles of ascidian <i>Halocynthia roretzi</i> . 2022 , 93, 105095	0

- 376 Untargeted metabolomics based on LCMS to elucidate the mechanism underlying nitrite degradation by *Limosilactobacillus fermentum* RC4. **2022**, 163, 113414 0
- 375 Tomato Systemin induces resistance against *Plectosphaerella cucumerina* in *Arabidopsis* through the induction of phenolic compounds and priming of tryptophan derivatives. **2022**, 111321 1
- 374 Targeted and Untargeted Mass Spectrometry-Based Metabolomics for Chemical Profiling of Three Coffee Species. **2022**, 27, 3152 0
- 373 Norm ISWSVR: A Data Integration and Normalization Approach for Large-Scale Metabolomics.. *Analytical Chemistry*, **2022**, 7.8 0
- 372 Lowering of lysophosphatidylcholines in ovariectomized rats by *Curcuma comosa*.. **2022**, 17, e0268179
- 371 Application of proteomics and metabolomics in microbiology research. **2022**, 107-129
- 370 Untargeted Metabolomic Profiling of Fungal Species Populations. **2022**, 349-365 0
- 369 The positive role of root decomposition on the bioremediation of organic pollutants contaminated soil: A case study using PCB-9 as a model compound. **2022**, 108726 0
- 368 Differentiating metabolomic responses of amphibians to multiple stressors. **2022**, 155666
- 367 A Comprehensive Database for DNA Adductomics. **2022**, 10, 0
- 366 Migration time correction for dual pressure capillary electrophoresis in semi-targeted metabolomics study. 0
- 365 Real-Ambient Exposure to Air Pollution Induces Hypertrophy of Adipose Tissue Modulated by Mitochondria-Mediated Glycolipid Metabolism in Young Mice.
- 364 Preparation and Curation of Omics Data for Genome-Wide Association Studies. **2022**, 127-150
- 363 Statistical Modeling Techniques. **2022**, 665-680
- 362 Discrimination of Geographical Origin of Agricultural Products From Small-Scale Districts by Widely Targeted Metabolomics With a Case Study on Pinggu Peach. **2022**, 9,
- 361 Interaction Between Cecal Metabolites and Liver Lipid Metabolism Pathways During Induced Molting in Laying Hens. **2022**, 13, 2
- 360 Intracellular acetyl CoA potentiates the therapeutic efficacy of anti-tumor CD8+ T cells. 1
- 359 Effects of different de-enzyming methods on microbial composition and volatile compounds of raw PuLar tea based on microbiome and metabolomics. **2022**, 101817

358	Triclosan is the Predominant Antibacterial Compound in Ontario Sewage Sludge.	2
357	Unique Probiotic Properties and Bioactive Metabolites of <i>Saccharomyces boulardii</i> .	1
356	Genome-wide association mapping within a local <i>Arabidopsis thaliana</i> population more fully reveals the genetic architecture for defensive metabolite diversity. 2022 , 377,	1
355	Volatile Organic Compounds Frequently Identified after Hyperbaric Hyperoxic Exposure: The VAPOR Library. 2022 , 12, 470	1
354	Identification of novel biomarkers for acute radiation injury using multi-omics approach and nonhuman primate model. 2022 ,	0
353	Metabolic adaptation of diatoms to hypersalinity. 2022 , 113267	0
352	Rapid target and non-target screening method for determination of emerging organic chemicals in fish. 2022 , 463185	
351	Metabolite annotation from knowns to unknowns through knowledge-guided multi-layer metabolic network.	
350	Recent developments in data acquisition, treatment and analysis with ion mobility-mass spectrometry for lipidomics. 2100328	2
349	Cyclic AMP and biofilms reveal the synergistic proliferation strategy of <i>Pseudomonas aeruginosa</i> and <i>Escherichia coli</i> under the costimulation of high concentrations of microplastics and enrofloxacin. 2022 , 156470	0
348	Metabolomics reveals primary response of wheat (<i>Triticum aestivum</i>) to irrigation with oilfield produced water. 2022 , 212, 113547	0
347	Identification of coal geographic origin by FTIR coupled with metabolomics analysis. 2022 , 125, 104224	
346	Ecosystem metabolomics of dissolved organic matter from arctic soil pore water across seasonal transitions. 2022 , 91-106	
345	Evaluating the effects of environmental perturbations in bloom forming cyanobacteria through untargeted metabolomics. 2022 , 231-244	
344	Metabolomics profiling of di-(2-propylheptyl) phthalate (DHP) biotransformation products as exposure markers: analytical strategy and application. 2022 , 1-19	
343	Metabolomic Profiles of Multidrug-Resistant <i>Salmonella Typhimurium</i> from Humans, Bovine, and Porcine Hosts. 2022 , 12, 1518	0
342	Integrated analysis of changes in soil microbiota and metabolites following long-term fertilization in a subtropical maize-wheat agroecosystem. 2022 ,	
341	Dissecting the relationship between plasma and tissue metabolome in a cohort of women with obesity: Analysis of subcutaneous and visceral adipose, muscle, and liver. 2022 , 36,	

340	An optimization method for untargeted MS-based isotopic tracing investigations of metabolism. 2022 , 18,		0
339	Batch alignment via retention orders for preprocessing large-scale multi-batch LC-MS experiments.		
338	Power of mzRAPP-Based Performance Assessments in MS1-Based Nontargeted Feature Detection. <i>Analytical Chemistry</i> , 2022 , 94, 8588-8595	7.8	1
337	An exercise-inducible metabolite that suppresses feeding and obesity. 2022 , 606, 785-790		6
336	The Potential Role of Metabolomics in Drug-Induced Liver Injury (DILI) Assessment. 2022 , 12, 564		3
335	MetEx: A Targeted Extraction Strategy for Improving the Coverage and Accuracy of Metabolite Annotation in Liquid Chromatography-High-Resolution Mass Spectrometry Data. <i>Analytical Chemistry</i> , 2022 , 94, 8561-8569	7.8	0
334	A Divergent Selection on Breast Meat Ultimate pH, a Key Factor for Chicken Meat Quality, is Associated With Different Circulating Lipid Profiles. 13,		1
333	Using MetaboAnalyst 5.0 for LC-MS spectra processing, multi-omics integration and covariate adjustment of global metabolomics data.		27
332	Trackable and scalable LC-MS metabolomics data processing using asari.		1
331	Multi-Omics Analysis of the Microbiome and Metabolome Reveals the Relationship Between the Gut Microbiota and Wooden Breast Myopathy in Broilers. 9,		0
330	The Depletion Mechanism Actuates Bacterial Aggregation by Exopolysaccharides and Determines Species Distribution & Composition in Bacterial Aggregates. 12,		1
329	A Current Encyclopedia of Bioinformatics Tools, Data Formats and Resources for Mass Spectrometry Lipidomics. 2022 , 12, 584		3
328	Molecular Mechanisms behind Safranal Toxicity to HepG2 Cells from Dual Omics. 2022 , 11, 1125		1
327	Arbuscular mycorrhizal fungi prevent the negative effect of drought and modulate the growth-defence trade-off in tomato plants.		1
326	Oxidative stress from DGAT1 oncoprotein inhibition in melanoma suppresses tumor growth when ROS defenses are also breached. 2022 , 39, 110995		0
325	Metabolomics study of the desiccation and recovery process in the resurrection plants <i>Ramonda serbica</i> and <i>R. nathaliae</i> .		
324	Metabolic profilings of rat INS-1 E-cells under changing levels of essential amino acids. 2022 , 9,		
323	Association of metabolomic and lipidomic data with Chinese and New Zealand consumer clusters showing preferential likings for lamb meat from three production systems. 2022 , 158, 111504		0

- 322 Aromatic Plants as New Candidates in Phytoremediation-OMICS Technology. **2022**, 385-414
- 321 Metabolomic fingerprinting of porcine lung tissue during pre-clinical prolonged ex vivo lung perfusion using in vivo SPME coupled with LC-HRMS. **2022**, 1
- 320 Convolutional Neural Network-Based Compound Fingerprint Prediction for Metabolite Annotation. **2022**, 12, 605
- 319 UHPLC-Q-Exactive Orbitrap MS/MS-based untargeted lipidomics reveals molecular mechanisms and metabolic pathways of lipid changes during golden pomfret (*Trachinotus ovatus*) fermentation. **2022**, 133676 0
- 318 New insights into the Van Krevelen diagram: Automated molecular formula determination from HRMS for a large chemical profiling of lichen extracts.
- 317 Metabolomic analysis of serum from pure coronary artery ectasia patients based on UPLC-QE/MS technique. **2022**,
- 316 Increased signal-to-noise ratios within experimental field trials by regressing spatially distributed soil properties as principal components. 11,
- 315 Influence of Home Indoor Dampness Exposure on Volatile Organic Compounds in Exhaled Breath of Mothers and Their Infants: The NELA Birth Cohort. **2022**, 12, 6864
- 314 Metabolism of the aquatic pollutant diclofenac in the *Lymnaea stagnalis* freshwater gastropod.
- 313 Effects of Storage Temperature on Indica-Japonica Hybrid Rice Metabolites, Analyzed Using Liquid Chromatography and Mass Spectrometry. **2022**, 23, 7421 0
- 312 Alterations of Gut Microbiome and Fecal Fatty Acids in Patients With Polycystic Ovary Syndrome in Central China. 13, 1
- 311 Lactoferrin Supplementation during Gestation and Lactation Is Efficient for Boosting Rat Pup Development. **2022**, 14, 2814
- 310 MetHoS: a platform for large-scale processing, storage and analysis of metabolomics data. **2022**, 23, 0
- 309 Adaptation of the infant gut microbiome during the complementary feeding transition. **2022**, 17, e0270213 2
- 308 Single-cell multi-omics enabled discovery of alkaloid biosynthetic pathway genes in the medical plant *Catharanthus roseus*. 0
- 307 Metabolomic Characterization of Acute Ischemic Stroke Facilitates Metabolomic Biomarker Discovery. 1
- 306 The Knock-Down of the Chloroquine Resistance Transporter PfCRT Is Linked to Oligopeptide Handling in *Plasmodium falciparum*. 1
- 305 Agronomic and metabolomics analysis of rice-Tartary buckwheat (*Fagopyrum tataricum* Gaertn) bred by hybridization. **2022**, 12, 0

- 304 MobilityTransformR: an R package for effective mobility transformation of CE-MS data. ○
- 303 Integrated transcriptomics and metabolomics analysis of the intestine of cobia (*Rachycentron canadum*) under hypoxia stress. **2022**, 25, 101261 ○
- 302 Metabolome, transcriptome and physiological analyses provide insight into the color transition of litchi pericarp. **2022**, 192, 112031 ○
- 301 Review of contemporary chemometric strategies applied on preparing GCMS data in forensic analysis. **2022**, 181, 107732 ○
- 300 Metabolomics Approach on Non-Targeted Screening of 50 PPCPs in Lettuce and Maize. **2022**, 27, 4711
- 299 MS2Query: Reliable and Scalable MS2 Mass Spectral-based Analogue Search. ○
- 298 Microbial community composition and soil metabolism in the coexisting *Cordyceps militaris* and *Ophiocordyceps highlandensis*.
- 297 AI/ML-driven advances in untargeted metabolomics and exposomics for biomedical applications. **2022**, 3, 100978 1
- 296 Impacts of Formula Supplemented with Milk Fat Globule Membrane on the Neurolipidome of Brain Regions of Piglets. **2022**, 12, 689 ○
- 295 Enhanced cytotoxicity of a novel family of ATPase inhibitors in colorectal cancer cells with high NAT2 activity. **2022**, 115184
- 294 MAVEN2: An Updated Open-Source Mass Spectrometry Exploration Platform. **2022**, 12, 684 ○
- 293 Detecting the sources of chemicals in the Black Sea using non-target screening and deep learning convolutional neural networks. **2022**, 847, 157554
- 292 Addressing big data challenges in mass spectrometry-based metabolomics. 1
- 291 Emerging metabolomic tools to study cancer metastasis. **2022**, 1 1
- 290 TidyMass an object-oriented reproducible analysis framework for LCMS data. **2022**, 13, ○
- 289 The Effects of NAA on the Tuberos Root Yield and Quality of *Rehmannia glutinosa* and Its Regulatory Mechanism by Transcriptome and Metabolome Profiling. **2022**, 44, 3291-3311
- 288 Recent advances in proteomics and metabolomics in plants. **2022**, 2, ○
- 287 A Metabolomic Approach and Traditional Physical Assessments to Compare U22 Soccer Players According to Their Competitive Level. **2022**, 11, 1103 1

- 286 Differences of novel hybrid mode flaps and traditional perforator flaps in level of metabolites using LC-MS.
- 285 Cell envelope remodeling requires high concentrations of biotin during *Mycobacterium abscessus* model lung infection. 1
- 284 LipidMS 3.0: an R-package and a web-based tool for LC-MS/MS data processing and lipid annotation. 1
- 283 Energy dissipation in early detection of cellular responses to metabolic challenges.
- 282 Comparative transcriptome and metabolome analyses identified the mode of sucrose degradation as a metabolic marker for early vegetative propagation in bulbs of *Lycoris*. 1
- 281 Deep learning-based pseudo-mass spectrometry imaging analysis for precision medicine. 0
- 280 Serum metabolomic characterization of PLA2G6-associated dystonia/parkinsonism: A case-control biomarker study. 16, 0
- 279 Untargeted Multimodal Metabolomics Investigation of the *Haemonchus contortus* Exsheathment Secretome. **2022**, 11, 2525 1
- 278 Identification of prediagnostic metabolites associated with prostate cancer risk by untargeted mass spectrometry-based metabolomics: A case-control study nested in the Northern Sweden Health and Disease Study. 0
- 277 HPLC(Q)-TOF-MS-Based Study of Plasma Metabolic Profile Differences Associated with Age in Pediatric Population Using an Animal Model. **2022**, 12, 739 0
- 276 Transcriptome and Metabolome Analyses Revealed the Response Mechanism of Sugar Beet to Salt Stress of Different Durations. **2022**, 23, 9599 1
- 275 Characterization of metabolites of elderberry juice fermented by *Lactobacillus bulgaricus* BNCC336436 and *Streptococcus thermophilus* ABT-T using LCMS/MS.
- 274 Multi-Omics Profiling Reveals Resource Allocation and Acclimation Strategies to Temperature Changes in a Marine Dinoflagellate.
- 273 Pharmacokinetic and metabolomic studies with a BIO 300 Oral Powder formulation in nonhuman primates. **2022**, 12, 1
- 272 Time-dependent metabolomics uncover dynamic metabolic adaptations in MCF-7 cells exposed to bisphenol A. **2023**, 17, 1
- 271 Modulation of gut microbiota and fecal metabolites by corn silk among high-fat diet-induced hypercholesterolemia mice. 9, 0
- 270 Association of N-Acetyl Asparagine with QTc in Diabetes: A Metabolomics Study. **2022**, 10, 1955
- 269 Combined Transcriptomic and Metabolomic Analysis Reveals the Mechanism of Flavonoid Biosynthesis in *Handroanthus chrysanthus* (Jacq.) S.O.Grose. **2022**, 13, 1285

268	Leveraging R (LevR) for fast processing of mass spectrometry data and machine learning: Applications analyzing fingerprints and glycopeptides. 2,	0
267	Vitamin B3 Triggers Biosynthesis of Secondary Metabolite Dormancy Signals in <i>Streptococcus suis</i> . 2022 , 144, 14997-15001	0
266	Non-target metabolomics reveals the changes of small molecular substances in duck breast meat under different preservation time. 2022 , 111859	0
265	Mass Spectrometry-Based Nontargeted and Targeted Analytical Approaches in Fingerprinting and Metabolomics of Food and Agricultural Research.	0
264	Characterization of interactions of dietary cholesterol with the murine and human gut microbiome. 2022 , 7, 1390-1403	2
263	Metabolomics analysis of unresolved molecular variability in stoichiometry dynamics of a stream dissolved organic matter. 2022 , 223, 118923	0
262	Groundwater metabolome responds to recharge in fractured sedimentary strata. 2022 , 223, 118998	0
261	Integrated transcriptomic and metabolomic analysis reveal mechanisms of disease resistance in apples induced by <i>Wickerhamomyces anomalus</i> . 2022 , 173, 105005	0
260	Investigation of flavonoid components and their associated antioxidant capacity in different pigmented rice varieties. 2022 , 161, 111726	1
259	Chronic toxicity of PFAS-free AFFF alternatives in terrestrial plant <i>Brassica rapa</i> . 2022 , 850, 158100	0
258	Dissection of <i>Moringa oleifera</i> leaf metabolome in context of its different extracts, origin and in relationship to its biological effects as analysed using molecular networking and chemometrics. 2023 , 399, 133948	5
257	Novel lipid biomarkers for algal resistance to viral infection in the ocean.	0
256	Glutathione metabolism in <i>Cryptocaryon irritans</i> involved in defense against oxidative stress induced by zinc ions. 2022 , 15,	0
255	Integrated omics analysis reveals differences in gut microbiota and gut-host metabolite profiles between obese and lean chickens. 2022 , 101, 102165	1
254	Hemoglobin normalization outperforms other methods for standardizing dried blood spot metabolomics: A comparative study. 2023 , 854, 158716	0
253	Artificial intelligence in microbial natural product drug discovery: current and emerging role.	0
252	Strategies for structure elucidation of small molecules based on LCMS/MS data from complex biological samples. 2022 , 20, 5085-5097	0
251	Offline Breath Analysis: Standardization of Breath Sampling and Analysis Using Mass Spectrometry and Innovative Algorithms. 2022 ,	0

250	Cardioprotective and Synergistic Effect of Qifu Decoction Against Cardiotoxicity Induced by Doxorubicin.	0
249	Tag you're it: Application of stable isotope labeling and LC-MS to identify the precursors of specialized metabolites in plants. 2022 ,	0
248	Using targeted metabolomics to elucidate the indole auxin network in plants. 2022 ,	0
247	Plasma metabolomics in a deep vein thrombosis rat model based on ultra-high performance liquid chromatography-electrostatic field orbitrap high resolution mass spectrometry. 2022 , 40, 736-745	1
246	In Vitro Interactions between Okadaic Acid and Rat Gut Microbiome. 2022 , 20, 556	0
245	Hepatic transcriptomics and metabolomics indicated pathways associated with immune stress of broilers induced by lipopolysaccharide. 2022 , 102199	0
244	TurboPutative: A web server for data handling and metabolite classification in untargeted metabolomics. 9,	0
243	Urea Nitrogen Metabolite Can Contribute to Implementing the Ideal Protein Concept in Monogastric Animals. 2022 , 12, 2344	2
242	Systemic whitefly-induced metabolic responses in newly developed distal leaves of husk tomato plants (<i>Physalis philadelphica</i>) impairs whiteflies development.	0
241	Gramiketides, Novel Polyketide Derivatives of <i>Fusarium Graminearum</i> , Are Produced during the Infection of Wheat. 2022 , 8, 1030	0
240	Difference in Intestinal Flora and Characteristics of Plasma Metabonomics in Pneumoconiosis Patients. 2022 , 12, 917	0
239	Biosynthesis of the Isocoumarin Derivatives Fusamarins Is Mediated by the PKS8 Gene Cluster in <i>Fusarium</i> .	0
238	Data Processing and Analysis in Mass Spectrometry-Based Metabolomics. 2023 , 207-239	0
237	The interaction of MD-2 with small molecules in huanglian jiedu decoction play a critical role in the treatment of sepsis. 13,	0
236	An initial investigation of accuracy required for the identification of small molecules in complex samples using quantum chemical calculated NMR chemical shifts. 2022 , 14,	0
235	Connecting chemical exposome to human health using high-resolution mass spectrometry-based biomonitoring: Recent advances and future perspectives.	0
234	Autonomous CE Mass-Spectra Examination (ACME) for the Ocean Worlds Life Surveyor (OWLS).	0
233	Metabolic reconstitution of germ-free mice by a gnotobiotic microbiota varies over the circadian cycle. 2022 , 20, e3001743	1

- 232 openNAU: An open-source platform for normalizing, analyzing, and visualizing untargeted metabolomics data. ○
- 231 The Proteomics and Metabolomics Studies of GZU001 on Promoting the Merisis of Maize (*Zea mays* L.) Roots. ○
- 230 Impact of in Situ Simulated Climate Change on Communities and Non-Indigenous Species: Two Climates, Two Responses. ○
- 229 4D genetic networks reveal the genetic basis of metabolites and seed oil-related traits in 398 soybean RILs. **2022**, 15, ○
- 228 Metabolome and Transcriptome Profiling Reveal Carbon Metabolic Flux Changes in *Yarrowia lipolytica* Cells to Rapamycin. **2022**, 8, 939 ○
- 227 Allelopathic Potential of Mangroves from the Red River Estuary against the Rice Weed *Echinochloa crus-galli* and Variation in Their Leaf Metabolome. **2022**, 11, 2464 ○
- 226 Isolation and Lipidomic Screening of Human Milk Extracellular Vesicles. **2023**, 177-188 ○
- 225 Defining the Chemical Additives Driving In Vitro Toxicities of Plastics. ○
- 224 Genome-wide association studies of seed metabolites identify loci controlling specialized metabolites in *Arabidopsis thaliana*. ○
- 223 Targeted Metabolomics Provide Chemotaxonomic Insights of *Medicago ruthenica*, with Coupled Transcriptomics Elucidating the Mechanism Underlying Floral Coloration. **2022**, 11, 2408 ○
- 222 Bioactive Compounds from Marine Sponges and Algae: Effects on Cancer Cell Metabolome and Chemical Structures. **2022**, 23, 10680 ○
- 221 Volatile Dimethyl Disulfide from Guava Plants Regulate Developmental Performance of Asian Citrus Psyllid through Activation of Defense Responses in Neighboring Orange Plants. **2022**, 23, 10271 ○
- 220 *Neisseria* species as pathobionts in bronchiectasis. **2022**, 30, 1311-1327.e8 1
- 219 The effects of *Clostridium butyricum* on Ira rabbit growth performance, cecal microbiota and plasma metabolome. 13, ○
- 218 Databases and Tools to Investigate Protein-Metabolite Interactions. **2023**, 231-249 ○
- 217 Plasma Metabolomics Reveals Systemic Metabolic Alterations of Subclinical and Clinical Hypothyroidism. ○
- 216 Comparative analysis of the fecal microbiome and metabolomics of healthy versus captive South China tigers with mild-diarrhea. ○
- 215 A conserved metabolic signature associated with response to fast-acting antimalarial agents. ○

214	InSpectra DA Platform for Identifying Emerging Chemical Threats.	0
213	Comprehensive metabolomic characterization of the hippocampus in a ketamine mouse model of schizophrenia. 2022 , 632, 150-157	0
212	Alignstein: Optimal transport for improved LC-MS retention time alignment. 2022 , 11,	1
211	Amplified Drought Alters Leaf Litter Metabolome, Slows Down Litter Decomposition, and Modifies Home Field (Dis)Advantage in Three Mediterranean Forests. 2022 , 11, 2582	0
210	Lipidomics reveals the potential mechanism of honokiol against adenine-induced chronic kidney disease. 13,	0
209	Yellow polyketide pigment suppresses premature hatching in social amoeba. 2022 , 119,	0
208	Metabolic consequences of various fruit-based diets in a generalist insect species.	0
207	Engineering of global transcription factor FruR to redirect the carbon flow in Escherichia coli for enhancing l-phenylalanine biosynthesis. 2022 , 21,	0
206	Transcriptomics&metabolomics joint analysis: New highlight into the triterpenoid saponin biosynthesis in quinoa (Chenopodium quinoa Willd.). 13,	0
205	Integrated metabolomics and lipidomics study of patients with atopic dermatitis in response to dupilumab. 13,	1
204	Untargeted stable isotope-resolved metabolomics to assess the effect of PI3K inhibition on metabolic pathway activities in a PTEN null breast cancer cell line. 9,	0
203	Mass Spectroscopy as an Analytical Tool to Harness the Production of Secondary Plant Metabolites: The Way Forward for Drug Discovery. 2023 , 77-103	0
202	A novel set of volatile urinary biomarkers for late-life major depressive and anxiety disorders upon the progression of frailty: a pilot study. 2022 , 2,	0
201	The impact of ethnicity and intra-pancreatic fat on the postprandial metabolome response to whey protein in overweight Asian Chinese and European Caucasian women with prediabetes. 3,	0
200	Artemisia annua L. plants lacking Bornyl diPhosphate Synthase reallocate carbon from monoterpenes to sesquiterpenes except artemisinin. 13,	0
199	Hopomics: Humulus lupulus Brewing Cultivars Classification Based on LC-MS Profiling and Nested Feature Selection. 2022 , 12, 945	0
198	Characterizing the metabolic effects of the selective inhibition of gut microbial βglucuronidases in mice. 2022 , 12,	0
197	Transcriptome and Metabolome Analysis Provides Insights into the Heterosis of Yield and Quality Traits in Two Hybrid Rice Varieties (Oryza sativa L.). 2022 , 23, 12934	0

- 196 Integrated Metabolomics, Lipidomics, and Genomics Reveal the Presence of a New Biomarker, Butanediol Glucuronide, Associated with the Activation of Liver Ketogenesis and Lipid Oxidation by Tomato-Based Sofrito in Obese Rats. **2022**, 11, 2165 ○
- 195 LPCAT4 Knockdown Alters Barrier Integrity and Cellular Bioenergetics in Human Urothelium. **2022**, 23, 11871 ○
- 194 Metabolome-wide association study on ABCA7 indicates a role of ceramide metabolism in Alzheimer's disease. **2022**, 119, 1 ○
- 193 Integrated Metabolomics and Lipidomics Approach for the Study of Metabolic Network and Early Diagnosis in Cerebral Infarction. ○
- 192 Microwave Plasma Torch Mass Spectrometry for some Rare Earth Elements. **2022**, 104379 ○
- 191 Application of clusterization algorithms for analysis of semivolatile pollutants in Arkhangelsk snow. ○
- 190 Benthic exometabolites and their ecological significance on threatened Caribbean coral reefs. **2022**, 2, ○
- 189 An analytical pipeline to support robust research on the ecology, evolution, and function of floral volatiles. 10, ○
- 188 A liquid chromatography-mass spectroscopy-based untargeted metabolomic study of the rat cochlear nucleus at various stages of maturity. **2022**, 108645 ○
- 187 Multi-omics analysis reveals neuroinflammation, activated glial signaling, and dysregulated synaptic signaling and metabolism in the hippocampus of aged mice. 14, ○
- 186 Metabonomic analysis of the haemolymph reveals the dual effects of dietary selenium supplementations on growth of silkworm *Bombyx mori*. 1-16 ○
- 185 Using Organic Contaminants to Constrain the Terrestrial Journey of the Martian Meteorite Lafayette. **2022**, 22, 1351-1362 ○
- 184 Neofunctionalized carbonic anhydrases in the biosynthesis of neuroactive plant alkaloids. ○
- 183 Mechanosensitive brain tumor cells construct blood-tumor barrier to mask chemosensitivity. **2022**, ○
- 182 Rescue of social deficits by early-life melatonin supplementation through modulation of gut microbiota in a murine model of autism. **2022**, 156, 113949 ○
- 181 Multi-omics provide mechanistic insight into the Pb-induced changes in tadpole fitness-related traits and environmental water quality. **2022**, 247, 114207 1
- 180 Deep denoising autoencoder-assisted continuous scoring of peak quality in high-resolution LCMS data. **2022**, 231, 104694 ○
- 179 Plasma Metabolomic and Lipidomic Profiling of Metabolic Dysfunction-Associated Fatty Liver Disease in Humans Using an Untargeted Multiplatform Approach. **2022**, 12, 1081 1

- 178 Endophytic nitrogen-fixing bacteria DX120E inoculation altered the carbon and nitrogen metabolism in sugarcane. 13, 0
- 177 Plasma metabolomic profiles reveal sex- and maturation-dependent metabolic strategies in sea lamprey (*Petromyzon marinus*). **2022**, 18, 1
- 176 The Winchcombe meteorite, a unique and pristine witness from the outer solar system. **2022**, 8, 0
- 175 Disruption of *Zea mays* isochorismate synthase 1 decreases PHENYLALANINE AMMONIA LYASE activity and suppresses hypersensitive response-induced metabolism. 0
- 174 An interoperability framework for multicentric breath metabolomic studies. **2022**, 105557 0
- 173 Plasma metabolomics for the assessment of the progression of non-small cell lung cancer. 039361552211373 1
- 172 Metabolomics-Based Analysis of the Major Taste Contributors of Meat by Comparing Differences in Muscle Tissue between Chickens and Common Livestock Species. **2022**, 11, 3586 0
- 171 Combined Metabolomic and Transcriptomic Analysis Reveals Allantoin Enhances Drought Tolerance in Rice. **2022**, 23, 14172 0
- 170 Metabolic diversity in a collection of wild and cultivated *Brassica rapa* subspecies. 9, 0
- 169 Ecological and metabolomic responses of plants to deer exclosure in a suburban forest. **2022**, 12, 0
- 168 Dynamic Plasma Lipidomic Analysis Revealed Cholesterol Ester and Amides Associated with Sepsis Development in Critically Ill Patients after Cardiovascular Surgery with Cardiopulmonary Bypass. **2022**, 12, 1838 0
- 167 Transcriptomic and metabolomic integration to assess the response of gilthead sea bream (*Sparus aurata*) exposed to the most used insect repellent: DEET. **2022**, 120678 0
- 166 Ensemble Clustering Combined with Clustering Optimization: A Novel Workflow for Analyzing Metabolomics Data. 0
- 165 Metabolite annotation from knowns to unknowns through knowledge-guided multi-layer metabolic networking. **2022**, 13, 1
- 164 Metabolomic Study of a Rat Model of Retinal Detachment. **2022**, 12, 1077 0
- 163 Multi-omics HeCaToS dataset of repeated dose toxicity for cardiotoxic & hepatotoxic compounds. **2022**, 9, 0
- 162 Heterogeneity and Co-occurrence in the Luminal and Mucosal Gut Microbiomes and Metabolomes of Oriental Rat snake (*Ptyas mucosus*). 0
- 161 Alignment and Analysis of a Disparately Acquired Multibatch Metabolomics Study of Maternal Pregnancy Samples. 0

- 160 Pancreatic cancer cells crave glutamine for glycosylation and CA19-9 biosynthesis through hexosamine biosynthetic pathway. ○
- 159 Toward building mass spectrometry-based metabolomics and lipidomics atlases for biological and clinical research. **2022**, 116825 ○
- 158 Metabolomic and systematic biochemical analysis of sheep infected with *Fasciola hepatica*. **2023**, 313, 109852 ○
- 157 Mass spectrometry-based metabolomics for clinical study: Recent progresses and applications. **2023**, 158, 116896 ○
- 156 Study on morphological traits, nutrient compositions and comparative metabolomics of diploid and tetraploid Tartary buckwheat sprouts during sprouting. **2023**, 164, 112334 ○
- 155 Structural, metagenomic and metabolic shifts in multispecies freshwater biofilm models exposed to silver nanoparticles. **2023**, 11, 109162 ○
- 154 A novel simultaneous quantitative method for differential volatile components in herbs based on combined near-infrared and mid-infrared spectroscopy. **2023**, 407, 135096 ○
- 153 Liquid chromatography-mass spectrometry based metabolomics investigation of different tissues of *Mytilus galloprovincialis*. **2023**, 45, 101051 ○
- 152 Metabolic dysfunctions promoted by AIN-93G standard diet compared with three obesity-inducing diets in C57BL/6J mice. **2022**, 5, 436-444 ○
- 151 Ecometabolomics Studies of Bryophytes. **2022**, 1-43 ○
- 150 Compound Identification Strategies in Mass Spectrometry-Based Metabolomics and Pharmacometabolomics. **2022**, ○
- 149 Turning Metabolomics Data Processing from a Black Box to a White Box **2022**, 20-22 ○
- 148 Responses of the Macroalga *Ulva prolifera* Müller to Ocean Acidification Revealed by Complementary NMR- and MS-Based Omics Approaches. **2022**, 20, 743 ○
- 147 Caffeine-Induced Sleep Restriction Alters the Gut Microbiome and Fecal Metabolic Profiles in Mice. **2022**, 23, 14837 1
- 146 Nutritional and host environments determine community ecology and keystone species in a synthetic gut bacterial community. ○
- 145 Advances in experimental and computational methodologies for the study of microbial-surface interactions at different omics levels. 13, ○
- 144 HILIC-MS for Untargeted Profiling of the Free Glycation Product Diversity. **2022**, 12, 1179 ○
- 143 Influence of Chlorinating Agents on the Formation of Stable Biomarkers in Hair for the Retrospective Verification of Exposure. **2022**, 94, 16579-16586 ○

- 142 Flavor Profiling Using Comprehensive Mass Spectrometry Analysis of Metabolites in Tomato Soups. **2022**, 12, 1194 ○
- 141 Metabolomics and Network Pharmacology in the Exploration of the Multi-Targeted Therapeutic Approach of Traditional Medicinal Plants. **2022**, 11, 3243 ○
- 140 Identification and Characterization of Transcription Factors Involved in Geraniol Biosynthesis in *Rosa chinensis*. **2022**, 23, 14684 ○
- 139 A Comprehensive Mass Spectrometry-Based Workflow for Clinical Metabolomics Cohort Studies. **2022**, 12, 1168 ○
- 138 Metabolomics of Different Seaweeds in Functional Food Prospects. **2022**, 287-340 ○
- 137 An anchored experimental design and meta-analysis approach to address batch effects in large-scale metabolomics. 9, ○
- 136 Evidence for a chemical arms race between cuckoo wasps of the genus *Hedychrum* and their distantly related host apoid wasps. **2022**, 22, ○
- 135 Dysregulation of Amino Acid, Lipid, and Acylpyruvate Metabolism in Idiopathic Intracranial Hypertension: A Non-targeted Case Control and Longitudinal Metabolomic Study. ○
- 134 In Vitro and In Vivo Toxicometabolomics of the Synthetic Cathinone PCYP Studied by Means of LC-HRMS/MS. **2022**, 12, 1209 ○
- 133 Untargeted metabolomics analysis reveals dynamic changes in co-fermentation with human milk-derived probiotics and *Poria cocos*. 13, ○
- 132 Gilthead Seabream Liver Integrative Proteomics and Metabolomics Analysis Reveals Regulation by Different Prosurvival Pathways in the Metabolic Adaptation to Stress. **2022**, 23, 15395 ○
- 131 The interplay between the gut microbiota and metabolism during the third trimester of pregnancy. 13, ○
- 130 An Untargeted Metabolomics Workflow that Scales to Thousands of Samples for Population-Based Studies. **2022**, 94, 17370-17378 ○
- 129 FERMO: a Dashboard for Streamlined Rationalized Prioritization of Molecular Features from Mass Spectrometry Data. ○
- 128 Metabolomics analysis of plasma samples of patients with fibromyalgia and electromagnetic sensitivity using GCMS technique. **2022**, 12, ○
- 127 Untargeted and targeted metabolomics identify metabolite biomarkers for *Salmonella* Enteritidis in chicken meat. **2022**, 135294 1
- 126 LC-MS/MS based untargeted lipidomics uncovers lipid signatures of late-onset preeclampsia. **2022**, ○
- 125 Serum metabolic traits reveal therapeutic toxicities and responses of neoadjuvant chemoradiotherapy in patients with rectal cancer. **2022**, 13, ○

- 124 Mass Spectrometric Methods for Non-Targeted Screening of Metabolites: A Future Perspective for the Identification of Unknown Compounds in Plant Extracts. **2022**, 9, 415 ○
- 123 DNA Authentication and Chemical Analysis of Psilocybe Mushrooms Reveal Widespread Misdeterminations in Fungaria and Inconsistencies in Metabolites. **2022**, 88, ○
- 122 Non-target screening of emerging contaminants in landfills: A Review. **2022**, 100430 ○
- 121 DeepRTAlign: toward accurate retention time alignment for large cohort mass spectrometry data analysis. ○
- 120 Optimization of Parameters for ROI Data Compression for Nontargeted Analyses Using LC-HRMS. ○
- 119 Liver RBFOX2 regulates cholesterol homeostasis via Scarb1 alternative splicing in mice. **2022**, 4, 1812-1829 1
- 118 Metabolite Profiling and Bioassay-Guided Fractionation of Zataria multiflora Boiss. Hydroethanolic Leaf Extracts for Identification of Broad-Spectrum Pre and Postharvest Antifungal Agents. **2022**, 27, 8903 ○
- 117 How Low Can You Go? Selecting Intensity Thresholds for Untargeted Metabolomics Data Preprocessing. **2022**, 94, 17964-17971 ○
- 116 Lysophosphatidylcholines and phosphatidylcholines as biomarkers for stroke recovery. 13, ○
- 115 Plasmodium falciparum adapts its investment into replication versus transmission according to the host environment. ○
- 114 An exposome connectivity paradigm for the mechanistic assessment of the effects of prenatal and early life exposure to metals on neurodevelopment. 10, ○
- 113 Environmental Chemicals and Endogenous Metabolites in Bile of USA and Norway Patients with Primary Sclerosing Cholangitis. ○
- 112 Maize resistance to witchweed through changes in strigolactone biosynthesis. **2023**, 379, 94-99 1
- 111 AntDAS-DDA: A New Platform for Data-Dependent Acquisition Mode-Based Untargeted Metabolomic Profiling Analysis with Advantage of Recognizing In-source Fragment Ions to Improve Compound Identification. ○
- 110 Combined metabolomic and transcriptomic analysis reveals key components of OsCIPK17 overexpression improves drought tolerance in rice. 13, ○
- 109 Discretized skew-t mixture model for deconvoluting liquid chromatograph mass spectrometry data. ○
- 108 Benchmarking Outlier Detection Methods for Detecting IEM Patients in Untargeted Metabolomics Data. **2023**, 13, 97 ○
- 107 Deep learning-based method for automatic resolution of gas chromatography-mass spectrometry data from complex samples. **2023**, 1690, 463768 ○

- 106 ConInceDeep: A novel deep learning method for component identification of mixture based on Raman spectroscopy. **2023**, 234, 104757
- 105 Untargeted metabolomics reveals the combination effects and mechanisms of Huangqi-fuzi herb-pair against doxorubicin-induced cardiotoxicity. **2023**, 305, 116109
- 104 Untargeted lipidomic profiling of grapes highlights the importance of modified lipid species beyond the traditional compound classes. **2023**, 410, 135360
- 103 MODeLING.Vis: A Graphical User Interface Toolbox Developed for Machine Learning and Pattern Recognition of Biomolecular Data. **2023**, 15, 42
- 102 The P450 Sterol Side Chain Cleaving Enzyme (P450scc) for Digoxin Biosynthesis in the Foxglove Plant Belongs to the CYP87A Family.
- 101 Mapping the early life gut microbiome in neonates with critical congenital heart disease: multiomics insights and implications for host metabolic and immunological health. **2022**, 10,
- 100 Metabolomics Profiling of Di-(2-propylheptyl) Phthalate (DPHP) Biotransformation Products as Exposure Markers: Analytical Strategy and Application. **2023**, 271-289
- 99 Metabolomics and its application in fermented foods. **2023**, 361-376
- 98 Host Tree and Geography Induce Metabolic Shifts in the Epiphytic Liverwort *Radula complanata*. **2023**, 12, 571
- 97 Uracil restores susceptibility of methicillin-resistant *Staphylococcus aureus* to aminoglycosides through metabolic reprogramming. 14,
- 96 Biotin-dependent cell envelope remodelling is required for *Mycobacterium abscessus* survival in lung infection.
- 95 Metabolomic Phenotypes Reflect Patient Sex and Injury Status: A Cross-Sectional Analysis of Human Synovial Fluid.
- 94 Volatile terpenoid profiling in gin and beer a targeted approach. **2023**, 118, 105178
- 93 Identification on new contaminants of emerging concern: suspect and non-target analysis of marine environmental samples. **2023**, 439-463
- 92 Exhaled Volatile Organic Compounds for Early Prediction of Bronchopulmonary Dysplasia in Infants Born Preterm. **2023**, 113368
- 91 Investigation on the immunotoxicity induced by Emamectin benzoate on THP -1 macrophages based on metabolomics analysis.
- 90 Physiological response in *E. coli* to YdgR overexpression depends on whether the protein has an intact function. **2023**,
- 89 Valorization of soybean pulp for sustainable β -ketoisocaproate production using engineered *Bacillus subtilis* whole-cell biocatalyst. **2023**, 322, 138200

- 88 AMPK activation protects against prostate cancer by inducing a catabolic cellular state. **2023**, 42, 112396 ○
- 87 A comparison of feature extraction capabilities of advanced UHPLC-HRMS data analysis tools in plant metabolomics. **2023**, 1254, 341127 ○
- 86 Gas chromatography-mass spectrometry and liquid chromatography-mass spectrometry metabolomics platforms: Tools for plant oligosaccharides analysis. **2023**, 5, 100304 ○
- 85 Quantitative challenges and their bioinformatic solutions in mass spectrometry-based metabolomics. **2023**, 161, 117009 ○
- 84 Single-Filament Imaging Mass Spectrometry Lipidomics in *Arthrospira platensis*. ○
- 83 An automated workflow on data processing (AutoDP) for semiquantitative analysis of urine organic acids with GC-MS to facilitate diagnosis of inborn errors of metabolism. **2023**, 540, 117230 ○
- 82 Potential biomarkers for alleviation of *Streptococcus pneumoniae* pneumonia by QingFei Yin. **2023**, 51, 100234 ○
- 81 Targeting the intestinal circadian clock by meal timing ameliorates gastrointestinal inflammation. ○
- 80 The Genetic Background Is Shaping Cecal Enlargement in the Absence of Intestinal Microbiota. **2023**, 15, 636 ○
- 79 Multi-omics reveals that forage fiber promotes rumen development of pre-weaning calves compared to non-forage fiber. ○
- 78 FMO rewires metabolism to promote longevity through tryptophan and one carbon metabolism in *C. elegans*. **2023**, 14, ○
- 77 Evaluating LC-HRMS metabolomics data processing software using FAIR principles for research software. **2023**, 19, ○
- 76 Changes of gut microbiome and metabolome in the AOM/DSS mouse model of colorectal cancer with FLASH radiation. **2023**, 4, 1-10 ○
- 75 Metabolomics profiling to characterize cerebral ischemia-reperfusion injury in mice. 14, ○
- 74 Identification of essential sites of lipid peroxidation in ferroptosis. ○
- 73 NSC228155 alleviates septic cardiomyopathy via protecting mitochondria and inhibiting inflammation. **2023**, 116, 109847 ○
- 72 Secreted metabolome of porcine blastocysts encapsulated within. **2023**, 35, 375-394 ○
- 71 Root exudates and rhizosphere microbiomes jointly determine temporal shifts in plant-soil feedbacks. ○

- 70 Untargeted Metabolomics for Integrative Taxonomy: Metabolomics, DNA Marker-Based Sequencing, and Phenotype Bioimaging. **2023**, 12, 881 ○
- 69 Circulating metabolomic and lipidomic changes in subjects with new-onset type 1 diabetes after optimization of glycemic control. **2023**, 197, 110578 ○
- 68 Identification of metabolic and protein markers representative of the impact of mild nitrogen deficit on agronomic performance of maize hybrids. ○
- 67 Glutamine is a substrate for glycosylation and CA19-9 biosynthesis through hexosamine biosynthetic pathway in pancreatic cancer. **2023**, 14, ○
- 66 Urine metabolites are correlated with elevated urine inflammatory factors in rheumatoid arthritis at early stage. ○
- 65 Lipidomic profiling of rat hepatic stellate cells during activation reveals a two-stage process accompanied by increased levels of lysosomal lipids. **2023**, 299, 103042 ○
- 64 Maternal antibiotic treatment during pregnancy attenuates the transport and absorption of maternal antibody IgG through TLR4 and TLR2 receptor. 14, ○
- 63 The proteomics and metabolomics studies of GZU001 on promoting the Merisis of maize (*Zea mays* L.) roots. **2023**, 23, ○
- 62 High-quality *Cymbidium mannii* genome and multifaceted regulation of crassulacean acid metabolism in epiphytes. **2023**, 100564 ○
- 61 Glutamine deprivation induces ferroptosis in pancreatic cancer cells. **2023**, ○
- 60 Glucokinase Inactivation Ameliorates Lipid Accumulation and Exerts Favorable Effects on Lipid Metabolism in Hepatocytes. **2023**, 24, 4315 ○
- 59 Liquid Crystal Monomer: A Potential PPAR γ Antagonist. **2023**, 57, 3758-3771 ○
- 58 Metabolomic Diversity of Human Milk Cells over the Course of Lactation: A Preliminary Study. **2023**, 15, 1100 ○
- 57 Metabolomics-based response of *Salmonella* to desiccation stress and skimmed milk powder storage. 14, ○
- 56 Metabolic and inflammatory linkage of the chicken cecal microbiome to growth performance. 14, ○
- 55 Effect of Dopants and Gas-Phase Composition on Ionization Behavior and Efficiency in Dielectric Barrier Discharge Ionization. **2023**, 34, 538-549 ○
- 54 Spatial Lipidomic Profiling of Mouse Joint Tissue Demonstrates the Essential Role of PHOSPHO1 in Growth Plate Homeostasis. ○
- 53 HDPairFinder: A data processing platform for hydrogen/deuterium isotopic labeling-based nontargeted analysis of trace-level amino-containing chemicals in environmental water. **2024**, 136, 583-593 ○

- 52 Multiomics reveals glutathione metabolism as a driver of bimodality during stem cell aging. **2023**, 35, 472-486.e6 ○
- 51 Isotope-Guided Metabolomics Reveals Divergent Incorporation of Valine into Different Flavor Precursor Classes in Chives. ○
- 50 Fasting-mimicking diet synergizes with ferroptosis against quiescent, chemotherapy-resistant cells. **2023**, 90, 104496 ○
- 49 Carbon sufficiency boosts phenylpropanoid biosynthesis early in peach fruit development priming superior fruit quality. **2023**, 196, 1019-1031 ○
- 48 Integrative analysis of multimodal mass spectrometry data in MZmine 3. **2023**, 41, 447-449 1
- 47 Hyperlipidaemia elicits an atypical, T helper 1-like CD4+ T-cell response: a key role for very low-density lipoprotein. **2023**, 3, ○
- 46 Proteomics- and Metabolomics-Based Analysis of Metabolic Changes in a Swine Model of Pulmonary Hypertension. **2023**, 24, 4870 ○
- 45 Rumen microbial-driven metabolite from grazing lambs potentially regulates body fatty acid metabolism by lipid-related genes in liver. **2023**, 14, ○
- 44 Sulfotransferase 1C2 promotes hepatocellular carcinoma progression by enhancing glycolysis and fatty acid metabolism. ○
- 43 Alterations in the gut microbiome and metabolome profiles of septic mice treated with Shen FuHuang formula. 14, ○
- 42 Metabolic reprogramming by Acly inhibition using SB-204990 alters glucoregulation and modulates molecular mechanisms associated with aging. **2023**, 6, ○
- 41 Impact of in vitro phytohormone treatments on the metabolome of the leafy liverwort *Radula complanata* (L.) Dumort. **2023**, 19, ○
- 40 InSpectra DA Platform for Identifying Emerging Chemical Threats. ○
- 39 CYP4F2 is a human-specific determinant of circulating N-acyl amino acid levels. ○
- 38 Untargeted Metabolomics to Characterize the Urinary Chemical Landscape of E-Cigarette Users. **2023**, 36, 630-642 ○
- 37 *Plasmodium falciparum* adapts its investment into replication versus transmission according to the host environment. 12, ○
- 36 Metabolomics meets systems immunology. **2023**, 24, ○
- 35 Perturbation and resilience of the gut microbiome up to three months after β -lactams exposure in healthy volunteers suggest an important role of endogenous β -lactamases. ○

- 34 Metabolomics analysis reveals changes related to pseudocyst formation induced by iron depletion in *Trichomonas vaginalis*. ○
- 33 Exploring the mechanism of browning of *Rosa roxburghii* juice based on nontargeted metabolomics. ○
- 32 Exploratory data fusion of untargeted multimodal LC-HRMS with annotation by LCMS-TOF-ion mobility: White wine case study. **2023**, 29, 111-122 ○
- 31 Metabolomics in Hyperuricemia and Gout. **2023**, 1, 49-61 ○
- 30 To metabolomics and beyond: a technological portfolio to investigate cancer metabolism. **2023**, 8, ○
- 29 Untangling the Complexities of Processing and Analysis for Untargeted LC-MS Data Using Open-Source Tools. **2023**, 13, 463 ○
- 28 Mechanistic Understanding of the Discrepancies between Common Peak Picking Algorithms in Liquid ChromatographyMass Spectrometry-Based Metabolomics. **2023**, 95, 5894-5902 ○
- 27 The roles of brain lipids and polar metabolites in the hypoxia tolerance of deep-diving pinnipeds. **2023**, 226, ○
- 26 Optimizing XCMS parameters for GC-MS metabolomics data processing: a case study. **2023**, 19, ○
- 25 MS2Query: reliable and scalable MS2 mass spectra-based analogue search. **2023**, 14, ○
- 24 A mass spectrum-oriented computational method for ion mobility-resolved untargeted metabolomics. **2023**, 14, ○
- 23 Metabolomics-based strategy to assess drug hepatotoxicity and uncover the mechanisms of hepatotoxicity involved. ○
- 22 Colorectal cancer detection and treatment with engineered probiotics. ○
- 21 *Trichoderma virens* exerts herbicidal effect on *Arabidopsis thaliana* via modulation of amino acid metabolism. **2023**, 111702 ○
- 20 N-arachidonylglycine is a caloric state-dependent circulating metabolite which regulates human CD4+T cell responsiveness. **2023**, 26, 106578 ○
- 19 Combined metabolomics and gut microbiome to investigate the effects and mechanisms of Yuquan Pill on type 2 diabetes in rats. **2023**, 1222, 123713 ○
- 18 Extensive variation of leaf specialized metabolite production in sessile oak (*Quercus petraea*) populations is to a large extent genetically determined but not locally adaptive. ○
- 17 Altered serum metabolome associated with vascular calcification developed from CKD and the critical pathways. 10, ○

- 16 The Intestinal Clock Regulates Host Metabolism through the Fiber-Dependent Microbiome and Macronutrient Transcriptome. ○
- 15 In vivo solid phase microextraction for therapeutic monitoring and pharmacometabolomic fingerprinting of lung during in vivo lung perfusion of FOLFOX. **2023**, ○
- 14 Encoding LCMS-Based Untargeted Metabolomics Data into Images toward AI-Based Clinical Diagnosis. ○
- 13 Identification of common aroma contributors and the regulated metabolites of different kinds of meat. **2023**, 114737 ○
- 12 Early environmental exposure to oxytetracycline in *Danio rerio* may contribute to neurobehavioral abnormalities in adult zebrafish. **2023**, 882, 163482 ○
- 11 Membrane Adaptations and Cellular Responses of *Sulfolobus acidocaldarius* to the Allylamine Terbinafine. **2023**, 24, 7328 ○
- 10 Differences in the luminal and mucosal gut microbiomes and metabolomes of oriental rat snake (*Ptyas mucosus*). ○
- 9 A robust reprogramming strategy for generating hepatocyte-like cells usable in pharmaco-toxicological studies. **2023**, 14, ○
- 8 Plasma metabolomic response to high-carbohydrate meals of differing glycaemic load in overweight women. ○
- 7 The combination elxacaftor/tezacaftor/ivacaftor (ETI) modulates the de novo synthetic pathway of ceramides in a genotype-independent manner. **2023**, ○
- 6 Using the exposome to understand the role of the environment in gender- and sex-specific medicine. **2023**, 89-116 ○
- 5 The Untargeted Metabolomics Reveals Differences in Energy Metabolism in Patients with Different Subtypes of Ischemic Stroke. ○
- 4 Effect of fermented heat-treated rice bran on performance and possible role of intestinal microbiota in laying hens. 14, ○
- 3 Application of Lipidomics in Psychiatry: Plasma-Based Potential Biomarkers in Schizophrenia and Bipolar Disorder. **2023**, 13, 600 ○
- 2 Metabolomics characterizes early metabolic changes and markers of tolerant *Eucalyptus* ssp. clones against drought stress. **2023**, 212, 113715 ○
- 1 Integration of Metabolomic and Proteomic Data to Uncover Actionable Metabolic Pathways. **2023**, 137-148 ○