

# Hong-Mei Lu

## List of Publications by Year in descending order

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93  
papers

2,805  
citations

236925  
25  
h-index

197818  
49  
g-index

101  
all docs

101  
docs citations

101  
times ranked

3148  
citing authors

#	ARTICLE	IF	CITATIONS
1	Deep-Learning-Based Drug-Target Interaction Prediction. <i>Journal of Proteome Research</i> , 2017, 16, 1401-1409.	3.7	381
2	A strategy that iteratively retains informative variables for selecting optimal variable subset in multivariate calibration. <i>Analytica Chimica Acta</i> , 2014, 807, 36-43.	5.4	177
3	A bootstrapping soft shrinkage approach for variable selection in chemical modeling. <i>Analytica Chimica Acta</i> , 2016, 908, 63-74.	5.4	142
4	Anti-inflammatory effect of <i>Houttuynia cordata</i> injection. <i>Journal of Ethnopharmacology</i> , 2006, 104, 245-249.	4.1	141
5	Deep learning-based component identification for the Raman spectra of mixtures. <i>Analyst</i> , The, 2019, 144, 1789-1798.	3.5	130
6	Comparative evaluation of software for deconvolution of metabolomics data based on GC-TOF-MS. <i>TrAC - Trends in Analytical Chemistry</i> , 2008, 27, 215-227.	11.4	129
7	Large-scale prediction of drug-target interactions using protein sequences and drug topological structures. <i>Analytica Chimica Acta</i> , 2012, 752, 1-10.	5.4	88
8	Variation in Chemical Composition and Antibacterial Activities of Essential Oils from Two Species of <i>Houttuynia THUNB.</i> <i>Chemical and Pharmaceutical Bulletin</i> , 2006, 54, 936-940.	1.3	65
9	Multiscale peak detection in wavelet space. <i>Analyst</i> , The, 2015, 140, 7955-7964.	3.5	65
10	DeepMirTar: a deep-learning approach for predicting human miRNA targets. <i>Bioinformatics</i> , 2018, 34, 3781-3787.	4.1	65
11	Exploring metabolic syndrome serum profiling based on gas chromatography mass spectrometry and random forest models. <i>Analytica Chimica Acta</i> , 2014, 827, 22-27.	5.4	61
12	Prediction of Liquid Chromatographic Retention Time with Graph Neural Networks to Assist in Small Molecule Identification. <i>Analytical Chemistry</i> , 2021, 93, 2200-2206.	6.5	60
13	Predicting a Molecular Fingerprint from an Electron Ionization Mass Spectrum with Deep Neural Networks. <i>Analytical Chemistry</i> , 2020, 92, 8649-8653.	6.5	59
14	Identification of green tea varieties and fast quantification of total polyphenols by near-infrared spectroscopy and ultraviolet-visible spectroscopy with chemometric algorithms. <i>Analytical Methods</i> , 2015, 7, 787-792.	2.7	55
15	Calibration transfer via an extreme learning machine auto-encoder. <i>Analyst</i> , The, 2016, 141, 1973-1980.	3.5	55
16	Identification and quality assessment of <i>Houttuynia cordata</i> injection using GC-MS fingerprint: A standardization approach. <i>Journal of Ethnopharmacology</i> , 2006, 105, 436-440.	4.1	53
17	Multiscale peak alignment for chromatographic datasets. <i>Journal of Chromatography A</i> , 2012, 1223, 93-106.	3.7	50
18	Deep MS/MS-Aided Structural-Similarity Scoring for Unknown Metabolite Identification. <i>Analytical Chemistry</i> , 2019, 91, 5629-5637.	6.5	47

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19	Informative metabolites identification by variable importance analysis based on random variable combination. <i>Metabolomics</i> , 2015, 11, 1539-1551.	3.0	41
20	Comprehensive metabolic profiles of seminal plasma with different forms of male infertility and their correlation with sperm parameters. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2020, 177, 112888.	2.8	39
21	A potential tool for diagnosis of male infertility: Plasma metabolomics based on GC-MS. <i>Talanta</i> , 2016, 147, 82-89.	5.5	38
22	Exploring metabolic syndrome serum free fatty acid profiles based on GC-SIM-MS combined with random forests and canonical correlation analysis. <i>Talanta</i> , 2015, 135, 108-114.	5.5	37
23	Representative subset selection and outlier detection via isolation forest. <i>Analytical Methods</i> , 2016, 8, 7225-7231.	2.7	33
24	Separation of nine compounds from <i>Salvia plebeia</i> R.Br. using two-step high-speed counter-current chromatography with different elution modes. <i>Journal of Separation Science</i> , 2014, 37, 2118-2125.	2.5	31
25	Absolute quantitative imaging of sphingolipids in brain tissue by exhaustive liquid microjunction surface sampling-liquid chromatography-mass spectrometry. <i>Journal of Chromatography A</i> , 2020, 1609, 460436.	3.7	26
26	A novel kernel Fisher discriminant analysis: Constructing informative kernel by decision tree ensemble for metabolomics data analysis. <i>Analytica Chimica Acta</i> , 2011, 706, 97-104.	5.4	25
27	KPIC2: An Effective Framework for Mass Spectrometry-Based Metabolomics Using Pure Ion Chromatograms. <i>Analytical Chemistry</i> , 2017, 89, 7631-7640.	6.5	25
28	Metabolomics reveals the effect of Xuefu Zhuyu Decoction on plasma metabolism in rats with acute traumatic brain injury. <i>Oncotarget</i> , 2017, 8, 94692-94710.	1.8	24
29	UPLC-ESI-IT-TOF-MS metabolomic study of the therapeutic effect of Xuefu Zhuyu decoction on rats with traumatic brain injury. <i>Journal of Ethnopharmacology</i> , 2019, 245, 112149.	4.1	24
30	Qualitative analysis of major constituents from Xue Fu Zhu Yu Decoction using ultra high performance liquid chromatography with hybrid ion trap time-of-flight mass spectrometry. <i>Journal of Separation Science</i> , 2016, 39, 3457-3468.	2.5	23
31	Characterizing semen abnormality male infertility using non-targeted blood plasma metabolomics. <i>PLoS ONE</i> , 2019, 14, e0219179.	2.5	23
32	Supercritical CO <sub>2</sub> extraction of emodin and physcion from <i>Polygonum cuspidatum</i> and subsequent isolation by semipreparative chromatography. <i>Journal of Separation Science</i> , 2006, 29, 2136-2142.	2.5	22
33	Rapid Authentication of <i>Dendrobium officinale</i> by Near-Infrared Reflectance Spectroscopy and Chemometrics. <i>Analytical Letters</i> , 2015, 48, 817-829.	1.8	21
34	The rapid determination of total polyphenols content and antioxidant activity in <i>Dendrobium officinale</i> using near-infrared spectroscopy. <i>Analytical Methods</i> , 2016, 8, 4584-4589.	2.7	21
35	Direct calibration transfer to principal components via canonical correlation analysis. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2018, 181, 21-28.	3.5	21
36	MeOx-TMS derivatization for GC-MS metabolic profiling of urine and application in the discrimination between normal C57BL/6J and type 2 diabetic KK-Ay mice. <i>Analytical Methods</i> , 2014, 6, 4380-4387.	2.7	20

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37	Application of near infrared spectroscopy for the rapid determination of epimedin A, B, C and icariin in Epimedium. RSC Advances, 2015, 5, 5046-5052.	3.6	20
38	Tentative Fingerprint-Efficacy Study of Houltuynia cordata Injection in Quality Control of Traditional Chinese Medicine. Chemical and Pharmaceutical Bulletin, 2006, 54, 725-730.	1.3	19
39	Retention time prediction in hydrophilic interaction liquid chromatography with graph neural network and transfer learning. Journal of Chromatography A, 2021, 1656, 462536.	3.7	17
40	Mixture analysis using reverse searching and non-negative least squares. Chemometrics and Intelligent Laboratory Systems, 2014, 137, 10-20.	3.5	16
41	A green method for the quantification of polysaccharides in Dendrobium officinale. RSC Advances, 2015, 5, 105057-105065.	3.6	16
42	Recursive Wavelet Peak Detection of Analytical Signals. Chromatographia, 2016, 79, 1247-1255.	1.3	15
43	Enhancing coverage in LC-MS-based untargeted metabolomics by a new sample preparation procedure using mixed-mode solid-phase extraction and two derivatizations. Analytical and Bioanalytical Chemistry, 2019, 411, 6189-6202.	3.7	15
44	Fast and Low-Cost Surface-Enhanced Raman Scattering (SERS) Method for On-Site Detection of Flumetsulam in Wheat. Molecules, 2020, 25, 4662.	3.8	15
45	Establishment of reliable mass spectra and retention indices library: Identification of fatty acids in human plasma without authentic standards. Talanta, 2012, 88, 311-317.	5.5	14
46	Prediction of Peptide Fragment Ion Mass Spectra by Data Mining Techniques. Analytical Chemistry, 2014, 86, 7446-7454.	6.5	14
47	Using nonrandom two-liquid model for solvent system selection in counter-current chromatography. Journal of Chromatography A, 2014, 1355, 80-85.	3.7	14
48	Feature extraction from resolution perspective for gas chromatography-mass spectrometry datasets. RSC Advances, 2016, 6, 113997-114004.	3.6	14
49	Scalable calibration transfer without standards <i>via</i> dynamic time warping for near-infrared spectroscopy. Analytical Methods, 2019, 11, 4481-4493.	2.7	14
50	Interpretation of type 2 diabetes mellitus relevant GC-MS metabolomics fingerprints by using random forests. Analytical Methods, 2013, 5, 4883-4889.	2.7	13
51	Systematic and practical solvent system selection strategy based on the nonrandom two-liquid segment activity coefficient model for real-life counter-current chromatography separation. Journal of Chromatography A, 2015, 1393, 47-56.	3.7	13
52	Plasma Metabolomics Analysis Based on GC-MS in Infertile Males with Kidney-Yang Deficiency Syndrome. Evidence-based Complementary and Alternative Medicine, 2017, 2017, 1-11.	1.2	13
53	Fully automatic resolution of untargeted GC-MS data with deep learning assistance. Talanta, 2022, 244, 123415.	5.5	13
54	GC-MS profiling of leukemia cells: an optimized preparation protocol for the intracellular metabolome. Analytical Methods, 2018, 10, 1266-1274.	2.7	12

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55	Deep-Learning-Assisted multivariate curve resolution. Journal of Chromatography A, 2021, 1635, 461713.	3.7	12
56	Nonlinear alignment of chromatograms by means of moving window fast Fourier transform cross-correlation. Journal of Separation Science, 2013, 36, 1677-1684.	2.5	11
57	Evaluation and prediction of the antioxidant activity of Epimedium from multi-wavelength chromatographic fingerprints and chemometrics. Analytical Methods, 2014, 6, 1036.	2.7	11
58	Pure ion chromatogram extraction via optimal k-means clustering. RSC Advances, 2016, 6, 56977-56985.	3.6	10
59	Fast pure ion chromatograms extraction method for LC-MS. Chemometrics and Intelligent Laboratory Systems, 2017, 170, 68-74.	3.5	10
60	Quantitative mass spectrometry imaging of amino acids with isomer differentiation in brain tissue via exhaustive liquid microjunction surface sampling—tandem mass tags labeling—ultra performance liquid chromatography—mass spectrometry. Journal of Chromatography A, 2020, 1621, 461086.	3.7	10
61	Deep Learning-Based Method for Compound Identification in NMR Spectra of Mixtures. Molecules, 2022, 27, 3653.	3.8	10
62	Separation of Glycolipids/Sphingolipids from Glycerophospholipids on TiO <sub>2</sub> Coating in Aprotic Solvent for Rapid Comprehensive Lipidomic Analysis with Liquid Microjunction Surface Sampling-Mass Spectrometry. Analytical Chemistry, 2020, 92, 11250-11259.	6.5	9
63	Model population analysis in model evaluation. Chemometrics and Intelligent Laboratory Systems, 2018, 172, 223-228.	3.5	8
64	Mixture analysis using non-negative elastic net for Raman spectroscopy. Journal of Chemometrics, 2020, 34, e3293.	1.3	8
65	Unitary and binary chromatographic fingerprints analysis of Epimedium. Analytical Methods, 2013, 5, 5331.	2.7	7
66	MARS 2: A computational tool to resolve and extract features from large-scale GC-MS datasets. Chemometrics and Intelligent Laboratory Systems, 2019, 191, 12-20.	3.5	7
67	Quantitative Mass Spectrometry Imaging of Metabolomes and Lipidomes for Tracking Changes and Therapeutic Response in Traumatic Brain Injury Surrounding Injured Area at Chronic Phase. ACS Chemical Neuroscience, 2021, 12, 1363-1375.	3.5	7
68	Determination of Fatty Acids in Rice Oil by Gas Chromatography—Mass Spectrometry (GC—MS) with Geographic and Varietal Discrimination by Supervised Orthogonal Partial Least Squares Discriminant Analysis (OPLS-DA). Analytical Letters, 2022, 55, 675-687.	1.8	7
69	Investigation of Scrambled Ions in Tandem Mass Spectra, Part 2. On the Influence of the Ions on Peptide Identification. Journal of the American Society for Mass Spectrometry, 2013, 24, 857-867.	2.8	6
70	Feature Extraction for LC—MS via Hierarchical Density Clustering. Chromatographia, 2019, 82, 1449-1457.	1.3	6
71	Exploring asthenozoospermia seminal plasma amino acid disorder based on GC-SIM-MS combined with chemometrics methods. Analytical Methods, 2019, 11, 2895-2902.	2.7	6
72	Determination of 18 photoinitiators in food paper packaging materials by FastPrep-based extraction combined with GC—MS. Food Chemistry, 2022, 377, 131980.	8.2	6

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73	Sample classification of GC-ToF-MS metabolomics data without the requirement for chromatographic deconvolution. <i>Metabolomics</i> , 2011, 7, 191-205.	3.0	5
74	Influence of Light Intensity on the Yield and Quality of <i>Houttuynia cordata</i> . <i>Plant Production Science</i> , 2015, 18, 522-528.	2.0	5
75	Metabolic profiling putatively identifies plasma biomarkers of male infertility using UPLC-ESI-IT-TOFMS. <i>RSC Advances</i> , 2018, 8, 25974-25982.	3.6	5
76	TarMet: a reactive GUI tool for efficient and confident quantification of MS based targeted metabolic and stable isotope tracer analysis. <i>Metabolomics</i> , 2018, 14, 68.	3.0	5
77	Development of a sensitive and rapid UHPLC-MS/MS method for simultaneous quantification of nine compounds in rat plasma and application in a comparative pharmacokinetic study after oral administration of Xuefu Zhuyu Decoction and nimodipine. <i>Biomedical Chromatography</i> , 2020, 34, e4872.	1.7	5
78	Rapid in situ quantitation of photoinitiators in packaging by two-points kinetic calibration of liquid microjunction surface sampling-mass spectrometry. <i>Talanta</i> , 2020, 216, 121017.	5.5	5
79	Per-pixel absolute quantitation for mass spectrometry imaging of endogenous lipidomes by model prediction of mass transfer kinetics in single-probe-based ambient liquid extraction. <i>Talanta</i> , 2021, 234, 122654.	5.5	5
80	Rapid and sensitive detection of neotame in instant grain beverages by paper-based silver nanoparticles substrates. <i>Micro and Nano Letters</i> , 2020, 15, 1099-1104.	1.3	5
81	Optimization of extraction and determination of emodin from <i>Polygonum cuspidatum</i> Sieb. et Zucc. products by HPLC-DAD. <i>Central South University</i> , 2006, 13, 658-662.	0.5	4
82	Rapid Characterization of Proteinaceous Binders Used in Artwork and Cultural Heritage Materials by Surface-Enhanced Raman Spectroscopy (SERS). <i>Analytical Letters</i> , 2022, 55, 555-565.	1.8	3
83	Robust alignment of chromatograms by statistically analyzing the shifts matrix generated by moving window fast Fourier transform cross-correlation. <i>Journal of Separation Science</i> , 2015, 38, 965-974.	2.5	2
84	Parallel formula generator based on branch-and-bound algorithm for elucidating high resolution mass spectra. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2016, 153, 106-109.	3.5	2
85	Standardization of Raman spectra using variable penalty dynamic time warping. <i>Analytical Methods</i> , 2021, 13, 3414-3423.	2.7	2
86	Pure Ion Chromatograms Combined with Advanced Machine Learning Methods Improve Accuracy of Discriminant Models in LC-MS-Based Untargeted Metabolomics. <i>Molecules</i> , 2021, 26, 2715.	3.8	2
87	Chromatographic Profiling with Machine Learning Discriminates the Maturity Grades of <i>Nicotiana tabacum</i> L. Leaves. <i>Separations</i> , 2021, 8, 9.	2.4	2
88	Chemometrics in instrumental analysis of complex systems—in honor and memory of Yi Zeng Liang. <i>Journal of Chemometrics</i> , 2018, 32, e3095.	1.3	1
89	Two-Way Data Analysis: Multivariate Curve Resolution: Noniterative Resolution Methods. , 2020, , 137-152.		1
90	Photocatalytic reduction-based liquid microjunction surface sampling-mass spectrometry for rapid in situ analysis of aromatic amines originating from azo dyes in packaging papers. <i>Analytical and Bioanalytical Chemistry</i> , 2021, 413, 6649-6660.	3.7	1

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91	Quantitative Mass Spectrometry Imaging with Liquid Microjunction Surface Sampling. Methods in Molecular Biology, 2022, 2437, 181-194.	0.9	1
92	A GC-MS study of the stability of rat serum metabolome during the sample preparation procedure. Analytical Methods, 2013, 5, 6807.	2.7	0
93	Detection of cimetidine in human plasma by surface-enhanced Raman scattering. Micro and Nano Letters, 2020, 15, 514-518.	1.3	0