

# Hong-Mei Lu

## List of Publications by Year in descending order

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93  
papers

2,805  
citations

236612

25  
h-index

197535

49  
g-index

101  
all docs

101  
docs citations

101  
times ranked

3148  
citing authors

#	ARTICLE	IF	CITATIONS
1	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.	1.0	3
2	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). <i>Analytical Letters</i> , 2022, 55, 675-687.	1.0	7
3	Determination of 18 photoinitiators in food paper packaging materials by FastPrep-based extraction combined with GC–MS. <i>Food Chemistry</i> , 2022, 377, 131980.	4.2	6
4	Fully automatic resolution of untargeted GC-MS data with deep learning assistance. <i>Talanta</i> , 2022, 244, 123415.	2.9	13
5	Quantitative Mass Spectrometry Imaging with Liquid Microjunction Surface Sampling. <i>Methods in Molecular Biology</i> , 2022, 2437, 181-194.	0.4	1
6	Deep Learning-Based Method for Compound Identification in NMR Spectra of Mixtures. <i>Molecules</i> , 2022, 27, 3653.	1.7	10
7	Deep-Learning-Assisted multivariate curve resolution. <i>Journal of Chromatography A</i> , 2021, 1635, 461713.	1.8	12
8	Standardization of Raman spectra using variable penalty dynamic time warping. <i>Analytical Methods</i> , 2021, 13, 3414-3423.	1.3	2
9	Prediction of Liquid Chromatographic Retention Time with Graph Neural Networks to Assist in Small Molecule Identification. <i>Analytical Chemistry</i> , 2021, 93, 2200-2206.	3.2	60
10	Quantitative Mass Spectrometry Imaging of Metabolomes and Lipidomes for Tracking Changes and Therapeutic Response in Traumatic Brain Injury Surrounding Injured Area at Chronic Phase. <i>ACS Chemical Neuroscience</i> , 2021, 12, 1363-1375.	1.7	7
11	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.	1.7	2
12	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.	1.9	1
13	Retention time prediction in hydrophilic interaction liquid chromatography with graph neural network and transfer learning. <i>Journal of Chromatography A</i> , 2021, 1656, 462536.	1.8	17
14	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.	2.9	5
15	Chromatographic Profiling with Machine Learning Discriminates the Maturity Grades of <i>Nicotiana tabacum</i> L. Leaves. <i>Separations</i> , 2021, 8, 9.	1.1	2
16	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.	1.4	39
17	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.	1.8	26
18	Fast and Low-Cost Surface-Enhanced Raman Scattering (SERS) Method for On-Site Detection of Flumetsulam in Wheat. <i>Molecules</i> , 2020, 25, 4662.	1.7	15

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19	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. <i>Analytical Chemistry</i> , 2020, 92, 11250-11259.	3.2	9
20	Two-Way Data Analysis: Multivariate Curve Resolution: Noniterative Resolution Methods. , 2020, , 137-152.		1
21	Mixture analysis using non-negative elastic net for Raman spectroscopy. <i>Journal of Chemometrics</i> , 2020, 34, e3293.	0.7	8
22	Predicting a Molecular Fingerprint from an Electron Ionization Mass Spectrum with Deep Neural Networks. <i>Analytical Chemistry</i> , 2020, 92, 8649-8653.	3.2	59
23	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.	0.8	5
24	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.	2.9	5
25	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. <i>Journal of Chromatography A</i> , 2020, 1621, 461086.	1.8	10
26	Detection of cimetidine in human plasma by surface-enhanced Raman scattering. <i>Micro and Nano Letters</i> , 2020, 15, 514-518.	0.6	0
27	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.	0.6	5
28	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.	2.0	24
29	Enhancing coverage in LC-MS-based untargeted metabolomics by a new sample preparation procedure using mixed-mode solid-phase extraction and two derivatizations. <i>Analytical and Bioanalytical Chemistry</i> , 2019, 411, 6189-6202.	1.9	15
30	Scalable calibration transfer without standards via dynamic time warping for near-infrared spectroscopy. <i>Analytical Methods</i> , 2019, 11, 4481-4493.	1.3	14
31	Feature Extraction for LC-MS via Hierarchical Density Clustering. <i>Chromatographia</i> , 2019, 82, 1449-1457.	0.7	6
32	Characterizing semen abnormality male infertility using non-targeted blood plasma metabolomics. <i>PLoS ONE</i> , 2019, 14, e0219179.	1.1	23
33	Deep learning-based component identification for the Raman spectra of mixtures. <i>Analyst</i> , The, 2019, 144, 1789-1798.	1.7	130
34	Exploring asthenozoospermia seminal plasma amino acid disorder based on GC-SIM-MS combined with chemometrics methods. <i>Analytical Methods</i> , 2019, 11, 2895-2902.	1.3	6
35	MARS 2: A computational tool to resolve and extract features from large-scale GC-MS datasets. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2019, 191, 12-20.	1.8	7
36	Deep MS/MS-Aided Structural-Similarity Scoring for Unknown Metabolite Identification. <i>Analytical Chemistry</i> , 2019, 91, 5629-5637.	3.2	47

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37	GC-MS profiling of leukemia cells: an optimized preparation protocol for the intracellular metabolome. <i>Analytical Methods</i> , 2018, 10, 1266-1274.	1.3	12
38	Model population analysis in model evaluation. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2018, 172, 223-228.	1.8	8
39	Chemometrics in instrumental analysis of complex systemsâ€”in honor and memory of Yiâ€™Zeng Liang. <i>Journal of Chemometrics</i> , 2018, 32, e3095.	0.7	1
40	DeepMirTar: a deep-learning approach for predicting human miRNA targets. <i>Bioinformatics</i> , 2018, 34, 3781-3787.	1.8	65
41	Metabolic profiling putatively identifies plasma biomarkers of male infertility using UPLC-ESI-TOFMS. <i>RSC Advances</i> , 2018, 8, 25974-25982.	1.7	5
42	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.	1.4	5
43	Direct calibration transfer to principal components via canonical correlation analysis. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2018, 181, 21-28.	1.8	21
44	Deep-Learning-Based Drugâ€™Target Interaction Prediction. <i>Journal of Proteome Research</i> , 2017, 16, 1401-1409.	1.8	381
45	KPIC2: An Effective Framework for Mass Spectrometry-Based Metabolomics Using Pure Ion Chromatograms. <i>Analytical Chemistry</i> , 2017, 89, 7631-7640.	3.2	25
46	Fast pure ion chromatograms extraction method for LC-MS. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2017, 170, 68-74.	1.8	10
47	Plasma Metabolomics Analysis Based on GC-MS in Infertile Males with Kidney-Yang Deficiency Syndrome. <i>Evidence-based Complementary and Alternative Medicine</i> , 2017, 2017, 1-11.	0.5	13
48	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.	0.8	24
49	Feature extraction from resolution perspective for gas chromatography-mass spectrometry datasets. <i>RSC Advances</i> , 2016, 6, 113997-114004.	1.7	14
50	Representative subset selection and outlier detection via isolation forest. <i>Analytical Methods</i> , 2016, 8, 7225-7231.	1.3	33
51	Recursive Wavelet Peak Detection of Analytical Signals. <i>Chromatographia</i> , 2016, 79, 1247-1255.	0.7	15
52	Qualitative analysis of major constituents from Xue Fu Zhu Yu Decoction using ultra high performance liquid chromatography with hybrid ion trap timeâ€™ofâ€™flight mass spectrometry. <i>Journal of Separation Science</i> , 2016, 39, 3457-3468.	1.3	23
53	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.	1.3	21
54	Pure ion chromatogram extraction via optimal k-means clustering. <i>RSC Advances</i> , 2016, 6, 56977-56985.	1.7	10

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55	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.	1.8	2
56	Calibration transfer via an extreme learning machine auto-encoder. <i>Analyst, The</i> , 2016, 141, 1973-1980.	1.7	55
57	A bootstrapping soft shrinkage approach for variable selection in chemical modeling. <i>Analytica Chimica Acta</i> , 2016, 908, 63-74.	2.6	142
58	A potential tool for diagnosis of male infertility: Plasma metabolomics based on GC-MS. <i>Talanta</i> , 2016, 147, 82-89.	2.9	38
59	Influence of Light Intensity on the Yield and Quality of <i>Houttuynia cordata</i> . <i>Plant Production Science</i> , 2015, 18, 522-528.	0.9	5
60	A green method for the quantification of polysaccharides in <i>Dendrobium officinale</i> . <i>RSC Advances</i> , 2015, 5, 105057-105065.	1.7	16
61	Rapid Authentication of <i>Dendrobium officinale</i> by Near-Infrared Reflectance Spectroscopy and Chemometrics. <i>Analytical Letters</i> , 2015, 48, 817-829.	1.0	21
62	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.	2.9	37
63	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.	1.3	2
64	Systematic and practical solvent system selection strategy based on the nonrandom two-liquid segment activity coefficient model for real-life counter-current chromatography separation. <i>Journal of Chromatography A</i> , 2015, 1393, 47-56.	1.8	13
65	Informative metabolites identification by variable importance analysis based on random variable combination. <i>Metabolomics</i> , 2015, 11, 1539-1551.	1.4	41
66	Multiscale peak detection in wavelet space. <i>Analyst, The</i> , 2015, 140, 7955-7964.	1.7	65
67	Application of near infrared spectroscopy for the rapid determination of epimedin A, B, C and icariin in <i>Epimedium</i> . <i>RSC Advances</i> , 2015, 5, 5046-5052.	1.7	20
68	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.	1.3	55
69	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.	1.3	31
70	A strategy that iteratively retains informative variables for selecting optimal variable subset in multivariate calibration. <i>Analytica Chimica Acta</i> , 2014, 807, 36-43.	2.6	177
71	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.	1.3	20
72	Evaluation and prediction of the antioxidant activity of <i>Epimedium</i> from multi-wavelength chromatographic fingerprints and chemometrics. <i>Analytical Methods</i> , 2014, 6, 1036.	1.3	11

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73	Prediction of Peptide Fragment Ion Mass Spectra by Data Mining Techniques. <i>Analytical Chemistry</i> , 2014, 86, 7446-7454.	3.2	14
74	Exploring metabolic syndrome serum profiling based on gas chromatography mass spectrometry and random forest models. <i>Analytica Chimica Acta</i> , 2014, 827, 22-27.	2.6	61
75	Mixture analysis using reverse searching and non-negative least squares. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2014, 137, 10-20.	1.8	16
76	Using nonrandom two-liquid model for solvent system selection in counter-current chromatography. <i>Journal of Chromatography A</i> , 2014, 1355, 80-85.	1.8	14
77	Unitary and binary chromatographic fingerprints analysis of <i>Epimedium</i> . <i>Analytical Methods</i> , 2013, 5, 5331.	1.3	7
78	Interpretation of type 2 diabetes mellitus relevant GC-MS metabolomics fingerprints by using random forests. <i>Analytical Methods</i> , 2013, 5, 4883-4889.	1.3	13
79	A GC-MS study of the stability of rat serum metabolome during the sample preparation procedure. <i>Analytical Methods</i> , 2013, 5, 6807.	1.3	0
80	Investigation of Scrambled Ions in Tandem Mass Spectra, Part 2. On the Influence of the Ions on Peptide Identification. <i>Journal of the American Society for Mass Spectrometry</i> , 2013, 24, 857-867.	1.2	6
81	Nonlinear alignment of chromatograms by means of moving window fast Fourier transform cross-correlation. <i>Journal of Separation Science</i> , 2013, 36, 1677-1684.	1.3	11
82	Establishment of reliable mass spectra and retention indices library: Identification of fatty acids in human plasma without authentic standards. <i>Talanta</i> , 2012, 88, 311-317.	2.9	14
83	Large-scale prediction of drug-target interactions using protein sequences and drug topological structures. <i>Analytica Chimica Acta</i> , 2012, 752, 1-10.	2.6	88
84	Multiscale peak alignment for chromatographic datasets. <i>Journal of Chromatography A</i> , 2012, 1223, 93-106.	1.8	50
85	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.	2.6	25
86	Sample classification of GC-ToF-MS metabolomics data without the requirement for chromatographic deconvolution. <i>Metabolomics</i> , 2011, 7, 191-205.	1.4	5
87	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.	5.8	129
88	Anti-inflammatory effect of <i>Houttuynia cordata</i> injection. <i>Journal of Ethnopharmacology</i> , 2006, 104, 245-249.	2.0	141
89	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.	2.0	53
90	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.	0.6	65

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91	Tentative Fingerprint-Efficacy Study of <i>Houttuynia cordata</i> Injection in Quality Control of Traditional Chinese Medicine. <i>Chemical and Pharmaceutical Bulletin</i> , 2006, 54, 725-730.	0.6	19
92	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
93	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.	1.3	22