

# Yi-Zeng Liang

## List of Publications by Year in descending order

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126  
papers

6,558  
citations

71061

41  
h-index

66879

78  
g-index

129  
all docs

129  
docs citations

129  
times ranked

5335  
citing authors

#	ARTICLE	IF	CITATIONS
1	Baseline correction using adaptive iteratively reweighted penalized least squares. <i>Analyst, The</i> , 2010, 135, 1138.	1.7	752
2	Chromatographic fingerprint analysis—a rational approach for quality assessment of traditional Chinese herbal medicine. <i>Journal of Chromatography A</i> , 2006, 1112, 171-180.	1.8	413
3	Quality control of herbal medicines. <i>Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences</i> , 2004, 812, 53-70.	1.2	354
4	An intelligent background—correction algorithm for highly fluorescent samples in Raman spectroscopy. <i>Journal of Raman Spectroscopy</i> , 2010, 41, 659-669.	1.2	241
5	Information theory applied to chromatographic fingerprint of herbal medicine for quality control. <i>Journal of Chromatography A</i> , 2003, 1002, 25-40.	1.8	216
6	Random frog: An efficient reversible jump Markov Chain Monte Carlo-like approach for variable selection with applications to gene selection and disease classification. <i>Analytica Chimica Acta</i> , 2012, 740, 20-26.	2.6	209
7	Monte Carlo cross-validation for selecting a model and estimating the prediction error in multivariate calibration. <i>Journal of Chemometrics</i> , 2004, 18, 112-120.	0.7	197
8	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
9	Development of high-performance liquid chromatographic fingerprints for distinguishing Chinese Angelica from related umbelliferae herbs. <i>Journal of Chromatography A</i> , 2005, 1073, 383-392.	1.8	170
10	libPLS: An integrated library for partial least squares regression and linear discriminant analysis. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2018, 176, 34-43.	1.8	164
11	Using variable combination population analysis for variable selection in multivariate calibration. <i>Analytica Chimica Acta</i> , 2015, 862, 14-23.	2.6	158
12	An efficient method of wavelength interval selection based on random frog for multivariate spectral calibration. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 111, 31-36.	2.0	150
13	A bootstrapping soft shrinkage approach for variable selection in chemical modeling. <i>Analytica Chimica Acta</i> , 2016, 908, 63-74.	2.6	142
14	A novel variable selection approach that iteratively optimizes variable space using weighted binary matrix sampling. <i>Analyst, The</i> , 2014, 139, 4836.	1.7	127
15	Correction of retention time shifts for chromatographic fingerprints of herbal medicines. <i>Journal of Chromatography A</i> , 2004, 1029, 173-183.	1.8	118
16	Traditional Chinese medicine and separation science. <i>Journal of Separation Science</i> , 2008, 31, 2113-2137.	1.3	117
17	Pretreatments of chromatographic fingerprints for quality control of herbal medicines. <i>Journal of Chromatography A</i> , 2006, 1134, 253-259.	1.8	111
18	Model population analysis for variable selection. <i>Journal of Chemometrics</i> , 2010, 24, 418-423.	0.7	110

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19	Determination of volatile components in peptic powder by gas chromatography-mass spectrometry and chemometric resolution. <i>Journal of Chromatography A</i> , 2001, 909, 237-247.	1.8	105
20	Quality control and discrimination of <i>Pericarpium Citri Reticulatae</i> and <i>Pericarpium Citri Reticulatae Viride</i> based on high-performance liquid chromatographic fingerprints and multivariate statistical analysis. <i>Analytica Chimica Acta</i> , 2007, 588, 207-215.	2.6	102
21	A new method for wavelength interval selection that intelligently optimizes the locations, widths and combinations of the intervals. <i>Analyst, The</i> , 2015, 140, 1876-1885.	1.7	97
22	Gas chromatography-mass spectrometry and chemometric resolution applied to the determination of essential oils in <i>Cortex Cinnamomi</i> . <i>Journal of Chromatography A</i> , 2001, 905, 193-205.	1.8	90
23	Recipe for revealing informative metabolites based on model population analysis. <i>Metabolomics</i> , 2010, 6, 353-361.	1.4	74
24	Purification, partial characterization and antioxidant activity of polysaccharides from <i>Glycyrrhiza uralensis</i> . <i>International Journal of Biological Macromolecules</i> , 2015, 79, 681-686.	3.6	73
25	Quality evaluation of fingerprints of herbal medicine with chromatographic data. <i>Analytica Chimica Acta</i> , 2004, 514, 69-77.	2.6	70
26	Morphological weighted penalized least squares for background correction. <i>Analyst, The</i> , 2013, 138, 4483.	1.7	70
27	Peak alignment using wavelet pattern matching and differential evolution. <i>Talanta</i> , 2011, 83, 1108-1117.	2.9	65
28	Multiscale peak detection in wavelet space. <i>Analyst, The</i> , 2015, 140, 7955-7964.	1.7	65
29	A new strategy to prevent over-fitting in partial least squares models based on model population analysis. <i>Analytica Chimica Acta</i> , 2015, 880, 32-41.	2.6	63
30	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
31	Chemometrics applied to quality control and metabolomics for traditional Chinese medicines. <i>Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences</i> , 2016, 1015-1016, 82-91.	1.2	58
32	Calibration transfer via an extreme learning machine auto-encoder. <i>Analyst, The</i> , 2016, 141, 1973-1980.	1.7	55
33	Generalized PLS regression. <i>Journal of Chemometrics</i> , 2001, 15, 135-148.	0.7	53
34	Alternative moving window factor analysis for comparison analysis between complex chromatographic data. <i>Journal of Chromatography A</i> , 2006, 1107, 273-285.	1.8	50
35	Fingerprint developing of coffee flavor by gas chromatography-mass spectrometry and combined chemometrics methods. <i>Analytica Chimica Acta</i> , 2007, 588, 216-223.	2.6	50
36	Multiscale peak alignment for chromatographic datasets. <i>Journal of Chromatography A</i> , 2012, 1223, 93-106.	1.8	50

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37	Robust principal component analysis by projection pursuit. <i>Journal of Chemometrics</i> , 1993, 7, 527-541.	0.7	49
38	Recipe for uncovering predictive genes using support vector machines based on model population analysis. <i>IEEE/ACM Transactions on Computational Biology and Bioinformatics</i> , 2011, 8, 1633-1641.	1.9	49
39	LC-DAD-APCI-MS-based screening and analysis of the absorption and metabolite components in plasma from a rabbit administered an oral solution of danggui. <i>Analytical and Bioanalytical Chemistry</i> , 2005, 383, 247-254.	1.9	44
40	A simple idea on applying large regression coefficient to improve the genetic algorithm-PLS for variable selection in multivariate calibration. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2014, 130, 76-83.	1.8	44
41	Mass spectral profiling: An effective tool for quality control of herbal medicines. <i>Analytica Chimica Acta</i> , 2007, 604, 89-98.	2.6	43
42	Informative metabolites identification by variable importance analysis based on random variable combination. <i>Metabolomics</i> , 2015, 11, 1539-1551.	1.4	41
43	Determination of the number of components in mixtures using a new approach incorporating chemical information. <i>Journal of Chemometrics</i> , 1999, 13, 15-30.	0.7	39
44	Development of the chromatographic fingerprint of <i>Scutellaria barbata</i> D. Don by GC-MS combined with Chemometrics methods. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2011, 55, 391-396.	1.4	39
45	Comparisons of Five Algorithms for Chromatogram Alignment. <i>Chromatographia</i> , 2013, 76, 1067-1078.	0.7	38
46	Model population analysis in chemometrics. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2015, 149, 166-176.	1.8	37
47	Chromatographic Fingerprinting and Metabolomics for Quality Control of TCM. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2010, 13, 943-953.	0.6	36
48	A modified random forest approach to improve multi-class classification performance of tobacco leaf grades coupled with NIR spectroscopy. <i>RSC Advances</i> , 2016, 6, 30353-30361.	1.7	35
49	High-performance liquid chromatography with atmospheric pressure chemical ionization and electrospray ionization mass spectrometry for analysis of <i>Angelica sinensis</i> . <i>Phytochemical Analysis</i> , 2007, 18, 265-274.	1.2	34
50	Chemical composition and inhibitory effect on hepatic fibrosis of Danggui Buxue Decoction. <i>FÄ-toterapÄ-Äç</i> , 2010, 81, 793-798.	1.1	34
51	Representative subset selection and outlier detection via isolation forest. <i>Analytical Methods</i> , 2016, 8, 7225-7231.	1.3	33
52	<i>In silico</i> evaluation of $\log D_{7.4}$ and comparison with other prediction methods. <i>Journal of Chemometrics</i> , 2015, 29, 389-398.	0.7	30
53	Variable selection for discriminating herbal medicines with chromatographic fingerprints. <i>Analytica Chimica Acta</i> , 2006, 572, 265-271.	2.6	29
54	Application of fast Fourier transform cross-correlation and mass spectrometry data for accurate alignment of chromatograms. <i>Journal of Chromatography A</i> , 2013, 1286, 175-182.	1.8	26

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55	Orthogonal projection (OP) technique applied to pattern recognition of fingerprints of the herbal medicine <i>houltuynia cordata</i> Thunb. and its final injection products. <i>Analytical and Bioanalytical Chemistry</i> , 2006, 385, 392-400.	1.9	23
56	RAPID AND SIMULTANEOUS DETERMINATION OF COPPER, CADMIUM, NICKEL, AND COBALT IN ZINC ELECTROLYTE SOLUTIONS BY COMPLEX ADSORPTION WAVE POLAROGRAPHY. <i>Instrumentation Science and Technology</i> , 2002, 20, 1-14.	0.8	21
57	Essential Oil Composition of <i>Osmanthus fragrans</i> Varieties by GC-MS and Heuristic Evolving Latent Projections. <i>Chromatographia</i> , 2009, 70, 1163-1169.	0.7	21
58	Prediction of retention indices for frequently reported compounds of plant essential oils using multiple linear regression, partial least squares, and support vector machine. <i>Journal of Separation Science</i> , 2013, 36, 2464-2471.	1.3	21
59	Variable importance analysis based on rank aggregation with applications in metabolomics for biomarker discovery. <i>Analytica Chimica Acta</i> , 2016, 911, 27-34.	2.6	20
60	A non-linear mapping-based generalized backpropagation network for unsupervised learning. <i>Journal of Chemometrics</i> , 1996, 10, 241-252.	0.7	19
61	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
62	Resolution of the essential constituents of <i>Ramulus cinnamomi</i> by an evolving chemometric approach. <i>Fresenius' Journal of Analytical Chemistry</i> , 2001, 371, 331-336.	1.5	18
63	Evaluation of separation quality in two-dimensional hyphenated chromatography. <i>Analytica Chimica Acta</i> , 2001, 450, 99-114.	2.6	18
64	A Combinational Strategy of Model Disturbance and Outlier Comparison to Define Applicability Domain in Quantitative Structural Activity Relationship. <i>Molecular Informatics</i> , 2014, 33, 503-513.	1.4	18
65	Automatic standardization method for Raman spectrometers with applications to pharmaceuticals. <i>Journal of Raman Spectroscopy</i> , 2015, 46, 147-154.	1.2	18
66	Comparing chemical fingerprints of herbal medicines using modified window target-testing factor analysis. <i>Analytical and Bioanalytical Chemistry</i> , 2005, 381, 913-924.	1.9	16
67	Determination of constituents of essential oil from <i>Angelica sinensis</i> by gas chromatography- <sup>13</sup> C mass spectrometry. <i>Central South University</i> , 2005, 12, 430-436.	0.5	16
68	Comments on the Baseline Removal Method Based on Quantile Regression and Comparison of Several Methods. <i>Chromatographia</i> , 2012, 75, 313-314.	0.7	16
69	Mixture analysis using reverse searching and non-negative least squares. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2014, 137, 10-20.	1.8	16
70	A green method for the quantification of polysaccharides in <i>Dendrobium officinale</i> . <i>RSC Advances</i> , 2015, 5, 105057-105065.	1.7	16
71	Simultaneous Determination of Enalapril and Enalaprilat in Human Plasma by LC-MS: Application to a Bioequivalence Study. <i>Chromatographia</i> , 2007, 65, 209-215.	0.7	15
72	Simultaneous determination of neutral and uronic sugars based on UV-vis spectrometry combined with PLS. <i>International Journal of Biological Macromolecules</i> , 2016, 87, 290-294.	3.6	15

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73	A roughness penalty approach and its application to noisy hyphenated chromatographic two-way data. <i>Journal of Chemometrics</i> , 1999, 13, 511-524.	0.7	14
74	Library Search of Mass Spectra with a New Matching Algorithm Based on Substructure Similarity.. <i>Analytical Sciences</i> , 2001, 17, 635-638.	0.8	14
75	Study on absorption of <i>Angelica sinensis</i> in rabbit plasma by HPLC-DAD-MS and multicomponent spectral correlative chromatography. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2006, 82, 229-235.	1.8	14
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	Sequential number-theoretic optimization (SNT0) method applied to chemical quantitative analysis. <i>Journal of Chemometrics</i> , 1997, 11, 267-281.	0.7	13
78	Chemical rank estimation for excitation-emission matrices using a morphological approach. <i>Journal of Chemometrics</i> , 1998, 12, 95-104.	0.7	13
79	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
80	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
81	Analysis of the Water Soluble Constituents of <i>Cordyceps Sinensis</i> With Heuristic Evolving Latent Projections. <i>Analytical Letters</i> , 2000, 33, 3195-3211.	1.0	12
82	Resolution and identification of the acidic fraction of a petroleum ether extract of <i>Radix Rehmanniae Preparata</i> by an evolving chemometric approach. <i>Chromatographia</i> , 2003, 57, 235-243.	0.7	11
83	Interpretation of the characteristic fragmentation mechanisms through determining the initial ionization site by natural spin density: A study on the derivatives of tryptophan and tryptamine. <i>International Journal of Mass Spectrometry</i> , 2009, 286, 112-121.	0.7	11
84	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
85	Comparative Analysis of the Volatile Components of <i>Agrimonia eupatoria</i> from Leaves and Roots by Gas Chromatography-Mass Spectrometry and Multivariate Curve Resolution. <i>Journal of Analytical Methods in Chemistry</i> , 2013, 2013, 1-9.	0.7	11
86	Two novel procedures for automatic resolution of two-way data from coupled chromatography. <i>Analyst</i> , 2001, 126, 161-168.	1.7	10
87	Development and Validation of LC-MS Method for the Determination of Hydroxyzine Hydrochloride in Human Plasma and Subsequent Application in a Bioequivalence Study. <i>Chromatographia</i> , 2007, 66, 481-486.	0.7	10
88	Simultaneous determination of adenine, uridine and adenosine in <i>cordyceps sinensis</i> and its substitutes by LC/ESI-MS. <i>Central South University</i> , 2004, 11, 295-299.	0.5	9
89	Analysis of volatile chemical components of <i>Radix Paeoniae Rubra</i> by gas chromatography-mass spectrometry and chemometric resolution. <i>Central South University</i> , 2007, 14, 57-61.	0.5	9
90	Comparative analysis of essential components between the herbal pair <i>Radix Saposhnikoviae</i> Rhizoma seu <i>Radix Notopterygii</i> and its single herbs by GC-MS combined with a chemometric resolution method. <i>Analytical Methods</i> , 2009, 1, 45.	1.3	9

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91	Variable complementary network: a novel approach for identifying biomarkers and their mutual associations. <i>Metabolomics</i> , 2012, 8, 1218-1226.	1.4	9
92	A novel strategy for quantitative analysis of the formulated complex system using chromatographic fingerprints combined with some chemometric techniques. <i>Journal of Chromatography A</i> , 2014, 1370, 179-186.	1.8	9
93	Sparse canonical correlation analysis applied to metabolomics studies for integrative analysis and biomarker discovery. <i>Journal of Chemometrics</i> , 2015, 29, 371-378.	0.7	9
94	Elastic net wavelength interval selection based on iterative rank PLS regression coefficient screening. <i>Analytical Methods</i> , 2017, 9, 672-679.	1.3	9
95	Modified secured principal component regression for detection of unexpected chromatographic features in herbal fingerprints. <i>Analyst</i> , 2006, 131, 538.	1.7	8
96	Chromatographic fingerprint analysis of Fructus Aurantii Immaturus by HPLC-DAD and chemometric methods. <i>Journal of Central South University</i> , 2011, 18, 353-360.	1.2	8
97	Retention Indices for Identification of Aroma Compounds by GC: Development and Application of a Retention Index Database. <i>Chromatographia</i> , 2015, 78, 89-108.	0.7	8
98	Chromatographic fingerprint of Semen Armeniacae Amarae based on high-performance liquid chromatogram and chemometric methods. <i>Analytical Methods</i> , 2012, 4, 299-308.	1.3	7
99	Incorporating variable importance into kernel PLS for modeling the structure-activity relationship. <i>Journal of Mathematical Chemistry</i> , 2018, 56, 713-727.	0.7	7
100	A Novel Approach to the Retrieval of the Mass Spectrum of a Mixture.. <i>Analytical Sciences</i> , 2000, 16, 603-607.	0.8	6
101	Comparative analysis of chemical components between barks and leaves of <i>Eucommia ulmoides</i> Oliver. <i>Central South University</i> , 2009, 16, 371-379.	0.5	6
102	Determination of trace elements in high purity nickel by high resolution inductively coupled plasma mass spectrometry. <i>Journal of Central South University</i> , 2012, 19, 2416-2420.	1.2	6
103	Empirical Kriging models and their applications to QSAR. <i>Journal of Chemometrics</i> , 2007, 21, 43-52.	0.7	5
104	Microwave digestion polarography for determining seven trace elements in <i>Salvia Miltiorrhiza</i> Root and compound <i>Salvia Miltiorrhiza</i> Root injection simultaneously. <i>Central South University</i> , 2007, 14, 514-519.	0.5	5
105	UPLC-MS/MS Analysis of Baicalin in the Cerebrospinal Fluid of Rabbits: Application to a Pharmacokinetic Study. <i>Chromatographia</i> , 2008, 68, 463-466.	0.7	5
106	Chemical fingerprinting of Su-He-Xiang-Wan and attribution of major characteristic peaks for its quality control by GC-MS. <i>Journal of Central South University</i> , 2013, 20, 2115-2123.	1.2	5
107	Shrunken centroids regularized discriminant analysis as a promising strategy for metabolomics data exploration. <i>Journal of Chemometrics</i> , 2015, 29, 154-164.	0.7	5
108	Two new algorithms for resolution of two-way data. <i>Journal of Chemometrics</i> , 1996, 10, 63-76.	0.7	4

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109	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
110	Optimization of Liensinine, Isoliensinine and Neferine Extraction from the Embryo of the Seed of <i>Nelumbo nucifera</i> GAERTN. <i>Separation Science and Technology</i> , 2008, 43, 3637-3651.	1.3	4
111	Analysis of volatile components in herbal pair <i>herba schizonepetae-ramulus cinnamomi</i> . <i>Central South University</i> , 2008, 15, 791-795.	0.5	3
112	Stability, detonation properties and pyrolysis mechanisms of polynitrotriprismanes $C_6H_6 \cdot n(NO_2)_n$ ( $n=1 \sim 6$ ). <i>Journal of Central South University</i> , 2011, 18, 1395-1401.	1.2	3
113	QSRR Study on Flavor Compounds of Diverse Structures on Different Columns with the Help of New Chemometric Methods. <i>Chromatographia</i> , 2013, 76, 241-253.	0.7	3
114	A novel tree kernel partial least squares for modeling the structure-activity relationship. <i>Journal of Chemometrics</i> , 2013, 27, 43-49.	0.7	3
115	Application of GC-MS coupled with chemometrics for scanning serum metabolic biomarkers from renal fibrosis rat. <i>Biochemical and Biophysical Research Communications</i> , 2015, 461, 186-192.	1.0	3
116	Simultaneous separation and determination of four main isoflavonoids in <i>Astragali Radix</i> by an isocratic LC/ESI-MS method. <i>Journal of Central South University</i> , 2016, 23, 303-309.	1.2	3
117	A multi-sequential number-theoretic optimization algorithm using clustering methods. <i>Central South University</i> , 2005, 12, 283-293.	0.5	2
118	CHROMATOGRAPHIC FINGERPRINTS OF SEED EMBRYO OF <i>NELUMBO NUCIFERA</i> GAERTN BY REVERSED-PHASE AND HYDROPHILIC INTERACTION LIQUID CHROMATOGRAPHY. <i>Journal of Liquid Chromatography and Related Technologies</i> , 2012, 35, 621-633.	0.5	2
119	Trace amounts of impurities in electrolytic manganese metal by sector field inductively coupled plasma mass spectrometry. <i>Journal of Central South University</i> , 2013, 20, 3385-3390.	1.2	2
120	Simultaneous determination mercury species of <i>Su-He-Xiang-Wan</i> in rat tissues by HPLC-CVG-AFS. <i>Journal of Central South University</i> , 2013, 20, 894-901.	1.2	2
121	Semiautomated Alignment of High-Throughput Metabolite Profiles with Chemometric Tools. <i>Journal of Analytical Methods in Chemistry</i> , 2017, 2017, 1-9.	0.7	2
122	Relationship between initial efficiency and structure parameters of carbon anode material for Li-ion battery. <i>Central South University</i> , 2008, 15, 484-487.	0.5	1
123	Kernel $k$ -nearest neighbor classifier based on decision tree ensemble for SAR modeling analysis. <i>Analytical Methods</i> , 2014, 6, 6621.	1.3	1
124	Direct rapid determination of traces of sulfide in environment samples. <i>Central South University</i> , 2002, 9, 250-254.	0.5	0
125	Systematically structural identification of nitric compounds in crude oil with chemometric resolution. <i>Central South University</i> , 2005, 12, 300-305.	0.5	0
126	Structural features hidden in the degree distributions of topological graphs. <i>Journal of Mathematical Chemistry</i> , 2005, 37, 37-56.	0.7	0