Xueguang Shao

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/13157/publications.pdf

Version: 2024-02-01

300 papers	7,614 citations	57719 44 h-index	102432 66 g-index
301 all docs	301 docs citations	301 times ranked	5272 citing authors

#	Article	IF	Citations
1	A variable selection method based on uninformative variable elimination for multivariate calibration of near-infrared spectra. Chemometrics and Intelligent Laboratory Systems, 2008, 90, 188-194.	1.8	438
2	A consensus least squares support vector regression (LS-SVR) for analysis of near-infrared spectra of plant samples. Talanta, 2007, 72, 217-222.	2.9	138
3	A wavelength selection method based on randomization test for near-infrared spectral analysis. Chemometrics and Intelligent Laboratory Systems, 2009, 97, 189-193.	1.8	128
4	A general approach to derivative calculation using wavelet transform. Chemometrics and Intelligent Laboratory Systems, 2003, 69, 157-165.	1.8	121
5	Extended Adaptive Biasing Force Algorithm. An On-the-Fly Implementation for Accurate Free-Energy Calculations. Journal of Chemical Theory and Computation, 2016, 12, 3506-3513.	2.3	113
6	A dynamic lattice searching method for fast optimization of Lennard-Jones clusters. Journal of Computational Chemistry, 2004, 25, 1693-1698.	1.5	100
7	Zooming across the Free-Energy Landscape: Shaving Barriers, and Flooding Valleys. Journal of Physical Chemistry Letters, 2018, 9, 4738-4745.	2.1	100
8	Taming Rugged Free Energy Landscapes Using an Average Force. Accounts of Chemical Research, 2019, 52, 3254-3264.	7.6	98
9	Molecular Dynamics Study of the Inclusion of Cholesterol into Cyclodextrins. Journal of Physical Chemistry B, 2006, 110, 6372-6378.	1.2	94
10	Quantitative Determination of the Components in Overlapping Chromatographic Peaks Using Wavelet Transform. Analytical Chemistry, 1997, 69, 1722-1725.	3.2	91
11	A comparison of accelerated solvent extraction, Soxhlet extraction, and ultrasonic-assisted extraction for analysis of terpenoids and sterols in tobacco. Analytical and Bioanalytical Chemistry, 2005, 383, 1003-1008.	1.9	90
12	An Efficient Method Based on Lattice Construction and the Genetic Algorithm for Optimization of Large Lennard-Jones Clusters. Journal of Physical Chemistry A, 2004, 108, 3586-3592.	1.1	89
13	Synthesis of dendritic silver nanostructures and their application in hydrogen peroxide electroreduction. Electrochimica Acta, 2011, 56, 3170-3174.	2.6	87
14	Determination of tobacco alkaloids by gas chromatographyâ€“mass spectrometry using cloud point extraction as a preconcentration step. Analytica Chimica Acta, 2006, 561, 83-87.	2.6	84
15	A Background and noise elimination method for quantitative calibration of near infrared spectra. Analytica Chimica Acta, 2004, 511, 37-45.	2.6	80
16	Extraction of Mass Spectra and Chromatographic Profiles from Overlapping GC/MS Signal with Background. Analytical Chemistry, 2004, 76, 5143-5148.	3.2	78
17	Multivariate calibration methods in near infrared spectroscopic analysis. Analytical Methods, 2010, 2, 1662.	1.3	76
18	Continuous Wavelet Transform Applied to Removing the Fluctuating Background in Near-Infrared Spectra. Journal of Chemical Information and Computer Sciences, 2004, 44, 907-911.	2.8	75

#	Article	IF	Citations
19	A method for near-infrared spectral calibration of complex plant samples with wavelet transform and elimination of uninformative variables. Analytical and Bioanalytical Chemistry, 2004, 378, 1382-1387.	1.9	74
20	An improved boosting partial least squares method for near-infrared spectroscopic quantitative analysis. Analytica Chimica Acta, 2010, 666, 32-37.	2.6	74
21	Structural Distribution of Lennard-Jones Clusters Containing 562 to 1000 Atoms. Journal of Physical Chemistry A, 2004, 108, 9516-9520.	1.1	71
22	A new regression method based on independent component analysis. Talanta, 2006, 69, 676-680.	2.9	67
23	Preparation of Dendritic Nanostructures of Silver and Their Characterization for Electroreduction. Langmuir, 2012, 28, 5218-5226.	1.6	66
24	Breaking through the Size Control Dilemma of Silver Chalcogenide Quantum Dots via Trialkylphosphine-Induced Ripening: Leading to Ag₂Te Emitting from 950 to 2100 nm. Journal of the American Chemical Society, 2021, 143, 12867-12877.	6.6	65
25	Structural Variation of Silver Clusters from Ag13 to Ag160. Journal of Physical Chemistry A, 2007, 111, 5048-5056.	1.1	64
26	Synthesis of silver nanowires and their applications in the electrochemical detection of halide. Talanta, 2011, 84, 673-678.	2.9	60
27	A fast annealing evolutionary algorithm for global optimization. Journal of Computational Chemistry, 2002, 23, 427-435.	1.5	56
28	Inclusion Mechanism of Steroid Drugs into Î²-Cyclodextrins. Insights from Free Energy Calculations. Journal of Physical Chemistry B, 2009, 113, 7836-7843.	1.2	56
29	Accurate determination of protein:ligand standard binding free energies from molecular dynamics simulations. Nature Protocols, 2022, 17, 1114-1141.	5.5	56
30	A connectivity table for cluster similarity checking in the evolutionary optimization method. Chemical Physics Letters, 2004, 389, 309-314.	1.2	54
31	Proteinâ€“ligand recognition using spherical harmonic molecular surfaces: towards a fast and efficient filter for large virtual throughput screening. Journal of Molecular Graphics and Modelling, 2002, 20, 313-328.	1.3	53
32	Water can be a probe for sensing glucose in aqueous solutions by temperature dependent near infrared spectra. Analytica Chimica Acta, 2017, 957, 47-54.	2.6	53
33	Structural Optimization of Silver Clusters up to 80 Atoms with Gupta and Sutton-Chen Potentials. Journal of Chemical Theory and Computation, 2005, 1, 762-768.	2.3	52
34	Can the anomalous aqueous solubility of Î²-cyclodextrin be explained by its hydration free energy alone?. Physical Chemistry Chemical Physics, 2008, 10, 3236.	1.3	52
35	A primary study on resolution of overlapping GC-MS signal using mean-field approach independent component analysis. Chemometrics and Intelligent Laboratory Systems, 2006, 82, 137-144.	1.8	51
36	BFEE: A User-Friendly Graphical Interface Facilitating Absolute Binding Free-Energy Calculations. Journal of Chemical Information and Modeling, 2018, 58, 556-560.	2.5	51

#	Article	IF	Citations
37	Finding an Optimal Pathway on a Multidimensional Free-Energy Landscape. Journal of Chemical Information and Modeling, 2020, 60, 5366-5374.	2.5	51
38	An adaptive immune optimization algorithm for energy minimization problems. Journal of Chemical Physics, 2004, 120, 11401-11406.	1.2	50
39	Optimization of bimetallic Cuâ€“Au and Agâ€“Au clusters by using a modified adaptive immune optimization algorithm. Journal of Computational Chemistry, 2009, 30, 1992-2000.	1.5	50
40	Standardization of near infrared spectra measured on multi-instrument. Analytica Chimica Acta, 2014, 836, 18-23.	2.6	50
41	Linear model correction: A method for transferring a near-infrared multivariate calibration model without standard samples. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 169, 197-201.	2.0	50
42	Simultaneous Wavelength Selection and Outlier Detection in Multivariate Regression of Near-Infrared Spectra. Analytical Sciences, 2005, 21, 161-166.	0.8	49
43	Simultaneous determination of mercury, lead and cadmium ions in water using near-infrared spectroscopy with preconcentration by thiol-functionalized magnesium phyllosilicate clay. Talanta, 2011, 84, 679-683.	2.9	49
44	Wavelet transform and its applications in high performance liquid chromatography (HPLC) analysis. Chemometrics and Intelligent Laboratory Systems, 1999, 45, 249-256.	1.8	48
45	Glucose induced variation of water structure from temperature dependent near infrared spectra. RSC Advances, 2016, 6, 105729-105736.	1.7	48
46	Solubilizing Carbon Nanotubes through Noncovalent Functionalization. Insight from the Reversible Wrapping of Alginic Acid around a Single-Walled Carbon Nanotube. Journal of Physical Chemistry B, 2010, 114, 5783-5789.	1.2	46
47	Variable selection by modified IPW (iterative predictor weighting)-PLS (partial least squares) in continuous wavelet regression models. Analyst, The, 2004, 129, 664.	1.7	44
48	Outlier detection in near-infrared spectroscopic analysis by using Monte Carlo cross-validation. Science in China Series B: Chemistry, 2008, 51, 751-759.	0.8	44
49	Quantitative determination by temperature dependent near-infrared spectra. Talanta, 2010, 82, 1017-1021.	2.9	44
50	The Extended Generalized Adaptive Biasing Force Algorithm for Multidimensional Free-Energy Calculations. Journal of Chemical Theory and Computation, 2017, 13, 1566-1576.	2.3	44
51	Understanding the function of water during the gelation of globular proteins by temperature-dependent near infrared spectroscopy. Physical Chemistry Chemical Physics, 2018, 20, 20132-20140.	1.3	44
52	Rapid and nondestructive analysis of pharmaceutical products using near-infrared diffuse reflectance spectroscopy. Journal of Pharmaceutical and Biomedical Analysis, 2012, 70, 288-294.	1.4	43
53	Multiblock partial least squares regression based on wavelet transform for quantitative analysis of near infrared spectra. Chemometrics and Intelligent Laboratory Systems, 2010, 100, 22-27.	1.8	41
54	Application of latent projective graph in variable selection for near infrared spectral analysis. Chemometrics and Intelligent Laboratory Systems, 2012, 114, 44-49.	1.8	41

#	Article	IF	Citations
55	High order derivative to investigate the complexity of the near infrared spectra of aqueous solutions. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 213, 83-89.	2.0	40
56	Resolution of multicomponent overlapping chromatogram using an immune algorithm and genetic algorithm. Chemometrics and Intelligent Laboratory Systems, 2000, 50, 91-99.	1.8	39
57	Determination of Chlorogenic Acid in Plant Samples by Using Near-Infrared Spectrum with Wavelet Transform Preprocessing. Analytical Sciences, 2004, 20, 451-454.	0.8	37
58	A random tunneling algorithm for the structural optimization problem. Physical Chemistry Chemical Physics, 2002, 4, 4782-4788.	1.3	36
59	Free-Energy Landscape of the Helical Wrapping of a Carbon Nanotube by a Polysaccharide. Journal of Physical Chemistry C, 2011, 115, 1851-1856.	1.5	36
60	Simultaneous determination of heavy metal ions in water using near-infrared spectroscopy with preconcentration by nano-hydroxyapatite. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 96, 289-294.	2.0	36
61	A dynamic lattice searching method with constructed core for optimization of large lennard-jones clusters. Journal of Computational Chemistry, 2007, 28, 1427-1433.	1.5	35
62	A dynamic lattice searching method with interior operation for unbiased optimization of large Lennardâ€Jones clusters. Journal of Computational Chemistry, 2008, 29, 1772-1779.	1.5	35
63	The lubricating role of water in the shuttling of rotaxanes. Chemical Science, 2017, 8, 5087-5094.	3.7	35
64	Chemometric algorithms for analyzing high dimensional temperature dependent near infrared spectra. Chemometrics and Intelligent Laboratory Systems, 2017, 170, 109-117.	1.8	35
65	BFEE2: Automated, Streamlined, and Accurate Absolute Binding Free-Energy Calculations. Journal of Chemical Information and Modeling, 2021, 61, 2116-2123.	2.5	35
66	Determination of the component number in overlapping multicomponent chromatogram using wavelet transform. Chemometrics and Intelligent Laboratory Systems, 1998, 43, 147-155.	1.8	33
67	A method based on stochastic resonance for the detection of weak analytical signal. Talanta, 2003, 61, 863-869.	2.9	33
68	Sequential extraction of mass spectra and chromatographic profiles from overlapping gas chromatographyâ€“mass spectroscopy signals. Journal of Chromatography A, 2008, 1190, 358-364.	1.8	33
69	Application of the wavelet transform method in quantitative analysis of Raman spectra. Journal of Raman Spectroscopy, 2001, 32, 207-209.	1.2	32
70	An efficient approach for theoretical study on the low-energy isomers of large fullerenes C90â€“C140. Journal of Chemical Physics, 2005, 122, 184318.	1.2	32
71	From Material Science to Avant-Garde Cuisine. The Art of Shaping Liquids into Spheres. Journal of Physical Chemistry B, 2014, 118, 11747-11756.	1.2	32
72	Extraction of extended X-ray absorption fine structure information from the experimental data using the wavelet transform. Analytical Communications, 1998, 35, 135-137.	2.2	31

#	Article	IF	Citations
73	Variable selection based on locally linear embedding mapping for near-infrared spectral analysis. Chemometrics and Intelligent Laboratory Systems, 2014, 131, 31-36.	1.8	31
74	Correcting Multivariate Calibration Model for near Infrared Spectral Analysis without Using Standard Samples. Journal of Near Infrared Spectroscopy, 2015, 23, 285-291.	0.8	31
75	Multilevel analysis of temperature dependent near-infrared spectra. Talanta, 2015, 131, 170-174.	2.9	31
76	Parallel Random Tunneling Algorithm for Structural Optimization of Lennard-Jones Clusters up toN= 330. Journal of Chemical Information and Computer Sciences, 2004, 44, 193-199.	2.8	30
77	Structural Transition from Icosahedra to Decahedra of Large Lennard-Jones Clusters. Journal of Physical Chemistry A, 2005, 109, 5193-5197.	1.1	29
78	Resolving multi-component overlapping GC-MS signals by immune algorithms. TrAC - Trends in Analytical Chemistry, 2009, 28, 1312-1321.	5.8	29
79	A weighted multiscale regression for multivariate calibration of near infrared spectra. Analyst, The, 2009, 134, 261-266.	1.7	29
80	Selecting significant genes by randomization test for cancer classification using gene expression data. Journal of Biomedical Informatics, 2013, 46, 594-601.	2.5	29
81	A WAVELET TRANSFORM AND ITS APPLICATION TO SPECTROSCOPIC ANALYSIS. Applied Spectroscopy Reviews, 2002, 37, 429-450.	3.4	28
82	Geometry Optimization and Conformational Analysis of (C60)N Clusters Using a Dynamic Lattice-Searching Method. ChemPhysChem, 2005, 6, 261-266.	1.0	28
83	Edge effects control helical wrapping of carbon nanotubes by polysaccharides. Nanoscale, 2012, 4, 2584.	2.8	28
84	Immune algorithms in analytical chemistry. TrAC - Trends in Analytical Chemistry, 2003, 22, 59-69.	5.8	27
85	Removing uncertain variables based on ensemble partial least squares. Analytica Chimica Acta, 2007, 598, 19-26.	2.6	27
86	Rapid analysis of multicomponent pesticide mixture by GCâ€“MS with the aid of chemometric resolution. Talanta, 2011, 83, 1247-1253.	2.9	27
87	Quantitative determination by temperature dependent near-infrared spectra: A further study. Talanta, 2011, 85, 420-424.	2.9	27
88	Cancer classification based on microarray gene expression data using a principal component accumulation method. Science China Chemistry, 2011, 54, 802-811.	4.2	27
89	Resolution of the NMR Spectrum Using Wavelet Transform. Applied Spectroscopy, 2000, 54, 731-738.	1.2	26
90	Optimization of Lennard-Jones atomic clusters. Computational and Theoretical Chemistry, 2002, 579, 229-234.	1.5	26

#	Article	IF	Citations
91	Elimination of interference information by a new hybrid algorithm for quantitative calibration of near infrared spectra. Analyst, The, 2003, 128, 1200.	1.7	26
92	Structural analysis of carbon clusters by using a global optimization algorithm with Brenner potential. Computational and Theoretical Chemistry, 2004, 678, 113-122.	1.5	26
93	Structural Characterization of Micelles Formed of Cholesteryl-Functionalized Cyclodextrins. Langmuir, 2011, 27, 91-97.	1.6	26
94	Simultaneous determination of phenol and p-nitrophenol in wastewater using near-infrared diffuse reflectance spectroscopy with adsorption preconcentration. Analytical Methods, 2011, 3, 703.	1.3	26
95	Mutual factor analysis for quantitative analysis by temperature dependent near infrared spectra. Talanta, 2018, 183, 142-148.	2.9	26
96	Water as a probe for serumâ€“based diagnosis by temperatureâ€“ dependent nearâ€“infrared spectroscopy. Talanta, 2019, 204, 359-366.	2.9	26
97	A new stochastic resonance algorithm to improve the detection limits for trace analysis. Chemometrics and Intelligent Laboratory Systems, 2003, 66, 41-49.	1.8	25
98	The true nature of rotary movements in rotaxanes. Chemical Science, 2016, 7, 457-462.	3.7	25
99	A Partial Least Squaresâ€Based Consensus Regression Method for the Analysis of Nearâ€Infrared Complex Spectral Data of Plant Samples. Analytical Letters, 2006, 39, 2073-2083.	1.0	24
100	Spatial Arrangement of Î±-Cyclodextrins in a Rotaxane. Insights from Free-Energy Calculations. Journal of Physical Chemistry B, 2008, 112, 5268-5271.	1.2	24
101	Variable space boosting partial least squares for multivariate calibration of near-infrared spectroscopy. Chemometrics and Intelligent Laboratory Systems, 2016, 158, 174-179.	1.8	24
102	Understanding the Molecular Interaction in Solutions by Chemometric Resolution of Nearâ^'Infrared Spectra. ChemistrySelect, 2017, 2, 10027-10032.	0.7	24
103	Chemometric methods for extracting information from temperature-dependent near-infrared spectra. Science China Chemistry, 2019, 62, 583-591.	4.2	24
104	Understanding the role of water in the aggregation of poly(N,N-dimethylaminoethyl) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 Chemistry Chemical Physics, 2019, 21, 5780-5789.	1.3	24
105	A two-level strategy for standardization of near infrared spectra by multi-level simultaneous component analysis. Analytica Chimica Acta, 2019, 1050, 25-31.	2.6	24
106	A Novel Algorithm of the Wavelet Packets Transform and its Application to DE-Noising of Analytical Signals. Analytical Letters, 1999, 32, 743-760.	1.0	23
107	Formation of the central vacancy in icosahedral Lennard-Jones clusters. Chemical Physics, 2004, 305, 69-75.	0.9	23
108	A strategy for enhancing the quantitative determination ability of the diffuse reflectance near-infrared spectroscopy. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 72, 115-119.	2.0	23

#	Article	IF	Citations
109	High-throughput approach for analysis of multicomponent gas chromatographicâ€“mass spectrometric signals. Journal of Chromatography A, 2009, 1216, 1469-1475.	1.8	23
110	Analysis of Scopoletin and Caffeic Acid in Tobacco by GCâ€“MS After a Rapid Derivatization Procedure. Chromatographia, 2009, 69, 743-748.	0.7	23
111	Extraction of chemical information from complex analytical signals by a non-negative independent component analysis. Analyst, The, 2009, 134, 2095.	1.7	23
112	Detecting influential observations by cluster analysis and Monte Carlo cross-validation. Analyst, The, 2010, 135, 2841.	1.7	23
113	Adsorption Behavior of Hydrophobin Proteins on Polydimethylsiloxane Substrates. Journal of Physical Chemistry B, 2012, 116, 12227-12234.	1.2	23
114	Threading or Tumbling? Insight into the Self-Inclusion Mechanism of an altro-Î±-Cyclodextrin Derivative. Journal of Physical Chemistry C, 2014, 118, 19380-19386.	1.5	23
115	Investigating the Structural Change in Protein Aqueous Solution Using Temperature-Dependent Near-Infrared Spectroscopy and Continuous Wavelet Transform. Applied Spectroscopy, 2017, 71, 472-479.	1.2	23
116	Accurate Description of Cationâ˜Ï€ Interactions in Proteins with a Nonpolarizable Force Field at No Additional Cost. Journal of Chemical Theory and Computation, 2020, 16, 6397-6407.	2.3	23
117	Knowledge-based genetic algorithm for resolving the near-infrared spectrum and understanding the water structures in aqueous solution. Chemometrics and Intelligent Laboratory Systems, 2020, 206, 104150.	1.8	23
118	MLCV: Bridging Machine-Learning-Based Dimensionality Reduction and Free-Energy Calculation. Journal of Chemical Information and Modeling, 2022, 62, 1-8.	2.5	23
119	Resolution of multicomponent chromatograms by window factor analysis with wavelet transform preprocessing. Journal of Chemometrics, 1998, 12, 85-93.	0.7	22
120	A new hybrid strategy for constructing a robust calibration model for near-infrared spectral analysis. Analytical and Bioanalytical Chemistry, 2005, 381, 795-805.	1.9	22
121	An approach by using near-infrared diffuse reflectance spectroscopy and resin adsorption for the determination of copper, cobalt and nickel ions in dilute solution. Talanta, 2009, 79, 339-343.	2.9	22
122	How Do Î±-Cyclodextrins Self-Organize on a Polymer Chain?. Journal of Physical Chemistry C, 2012, 116, 17913-17918.	1.5	22
123	Intelligent background correction using an adaptive lifting wavelet. Chemometrics and Intelligent Laboratory Systems, 2013, 125, 11-17.	1.8	22
124	Quantitative analysis of 17 amino acids in tobacco leaves using an amino acid analyzer and chemometric resolution. Journal of Separation Science, 2015, 38, 2053-2058.	1.3	22
125	Global Optimization of Lennard-Jones Clusters by a Parallel Fast Annealing Evolutionary Algorithm. Journal of Chemical Information and Computer Sciences, 2002, 42, 1099-1103.	2.8	21
126	Wavelet unfolded partial least squares for near-infrared spectral quantitative analysis of blood and tobacco powder samples. Analyst, The, 2011, 136, 4217.	1.7	21

#	Article	IF	Citations
127	Solvent-Controlled Shuttling in a Molecular Switch. Journal of Physical Chemistry C, 2012, 116, 4471-4476.	1.5	21
128	Understanding the Interaction Between Oligopeptide and Water in Aqueous Solution Using Temperature-Dependent Near-Infrared Spectroscopy. Applied Spectroscopy, 2018, 72, 1354-1361.	1.2	21
129	Removal of major interference sources in aqueous near-infrared spectroscopy techniques. Analytical and Bioanalytical Chemistry, 2004, 379, 143-148.	1.9	20
130	A dynamic lattice searching method with rotation operation for optimization of large clusters. Chemical Physics, 2009, 363, 72-77.	0.9	20
131	Multivariate calibration of near-infrared spectra by using influential variables. Analytical Methods, 2012, 4, 467.	1.3	20
132	Rapid determination of four tobacco specific nitrosamines in burley tobacco by near-infrared spectroscopy. Analytical Methods, 2012, 4, 1371.	1.3	20
133	Cyclodextrin-Mediated Recruitment and Delivery of Amphotericin B. Journal of Physical Chemistry C, 2013, 117, 11750-11756.	1.5	20
134	AN APPLICATION OF THE CONTINUOUS WAVELET TRANSFORM TO RESOLUTION OF MULTICOMPONENT OVERLAPPING ANALYTICAL SIGNALS. Analytical Letters, 2001, 34, 267-280.	1.0	19
135	SHEF: a vHTS geometrical filter using coefficients of spherical harmonic molecular surfaces. Journal of Molecular Modeling, 2008, 14, 393-401.	0.8	19
136	Interaction between tau and water during the induced aggregation revealed by near-infrared spectroscopy. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 230, 118046.	2.0	19
137	Prediction of Low-Energy Isomers of Large Fullerenes from C132 to C160. Journal of Physical Chemistry A, 2006, 110, 9247-9253.	1.1	18
138	Representative subset selection in modified iterative predictor weighting (mIPW) â€" PLS models for parsimonious multivariate calibration. Chemometrics and Intelligent Laboratory Systems, 2007, 87, 312-318.	1.8	18
139	Geometry optimization and structural distribution of silver clusters from Ag170 to Ag310. Chemical Physics Letters, 2008, 460, 315-318.	1.2	18
140	Filter design for molecular factor computing using wavelet functions. Analytica Chimica Acta, 2015, 880, 26-31.	2.6	18
141	Complex Movements in Rotaxanes: Shuttling Coupled with Conformational Transition of Cyclodextrins. Journal of Physical Chemistry C, 2016, 120, 19479-19486.	1.5	18
142	Chiral recognition of aromatic compounds by Î²-cyclodextrin based on bimodal complexation. Journal of Molecular Modeling, 2005, 11, 186-193.	0.8	17
143	An adaptive strategy for selecting representative calibration samples in the continuous wavelet domain for near-infrared spectral analysis. Analytical and Bioanalytical Chemistry, 2007, 387, 1041-1048.	1.9	17
144	A dual model strategy to transfer multivariate calibration models for near-infrared spectral analysis. Spectroscopy Letters, 2016, 49, 348-354.	0.5	17

#	Article	IF	Citations
145	Lysine Mutation of the Claw-Arm-Like Loop Accelerates Catalysis by Cellobiohydrolases. Journal of the American Chemical Society, 2019, 141, 14451-14459.	6.6	17
146	A variable importance criterion for variable selection in near-infrared spectral analysis. Science China Chemistry, 2019, 62, 271-279.	4.2	17
147	Stimulus-responsive surface-enhanced Raman scattering: a â€œTrojan horseâ€•strategy for precision molecular diagnosis of cancer. Chemical Science, 2020, 11, 6111-6120.	3.7	17
148	Application of Near-infrared Spectroscopy in Micro Inorganic Analysis. Acta Chimica Sinica, 2012, 70, 2109.	0.5	17
149	Molecular interactions of Î±-cyclodextrin inclusion complexes using a genetic algorithm. Computational and Theoretical Chemistry, 2001, 535, 115-119.	1.5	16
150	Thermodynamic Insights into the Dynamic Switching of a Cyclodextrin in a Bistable Molecular Shuttle. Journal of Physical Chemistry Letters, 2010, 1, 1776-1780.	2.1	16
151	Growth Pattern of Truncated Octahedra in AlN (N â‰ 310) Clusters. Journal of Physical Chemistry A, 2010, 114, 29-36.	1.1	16
152	Direct separation of faradaic and double layer charging current in potential step voltammetry. Talanta, 2013, 116, 575-580.	2.9	16
153	How Does the Solvent Modulate Shuttling in a Pillararene/Imidazolium [2]Rotaxane? Insights from Free Energy Calculations. Journal of Physical Chemistry C, 2016, 120, 6287-6293.	1.5	16
154	Water-Controlled Switching in Rotaxanes. Journal of Physical Chemistry C, 2018, 122, 9229-9234.	1.5	16
155	Global optimization of (C60)N molecular clusters. Chemical Physics Letters, 2002, 359, 27-34.	1.2	15
156	Determination of Pyrethroid Residues in Tobacco by Means of Solid Phase Microextraction and GC/MS with the Aid of Ultrasonic Assisted Extraction Using Water as Extracting Solvent. Analytical Sciences, 2006, 22, 241-244.	0.8	15
157	Consensus analysis of multiple classifiers using non-repetitive variables: Diagnostic application to microarray gene expression data. Computational Biology and Chemistry, 2007, 31, 48-56.	1.1	15
158	Quantitative Determination of the Components in Corn and Tobacco Samples by Using Near-Infrared Spectroscopy and Multiblock Partial Least Squares. Analytical Letters, 2010, 43, 1910-1921.	1.0	15
159	Configuration of the Surface Atoms in Al_N (270 â‰ N â‰ 500) Clusters. Journal of Physical Chemistry A, 2010, 114, 12813-12818.	1.1	15
160	Online near-Infrared Spectroscopy Combined with Alternating Trilinear Decomposition for Process Analysis of Industrial Production and Quality Assurance. Industrial & Engineering Chemistry Research, 2011, 50, 7677-7681.	1.8	15
161	Feasibility for quantitative determination of deoxyribonucleic acid by using near-infrared diffuse reflectance spectroscopy. Talanta, 2012, 99, 871-874.	2.9	15
162	Understanding the effect of urea on the phase transition of poly(N-isopropylacrylamide) in aqueous solution by temperature-dependent near-infrared spectroscopy. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 253, 119573.	2.0	15

#	Article	IF	Citations
163	Overcoming Free-Energy Barriers with a Seamless Combination of a Biasing Force and a Collective Variable-Independent Boost Potential. Journal of Chemical Theory and Computation, 2021, 17, 3886-3894.	2.3	15
164	Revealing the interactions of water with cryoprotectant and protein by nearâ€“infrared spectroscopy. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 266, 120417.	2.0	15
165	Classification and Quantitative Analysis of Azithromycin Tablets by Raman Spectroscopy and Chemometrics. American Journal of Analytical Chemistry, 2011, 02, 135-141.	0.3	15
166	Mechanism and biomass association of glucuronoyl esterase: an Î±/Î² hydrolase with potential in biomass conversion. Nature Communications, 2022, 13, 1449.	5.8	15
167	Development of wavelet transform voltammetric analyzer. Talanta, 2000, 50, 1175-1182.	2.9	14
168	A Conformational Analysis Method for Understanding the Energy Landscapes of Clusters. ChemPhysChem, 2007, 8, 569-577.	1.0	14
169	Performance of the semiempirical AM1, PM3, MNDO, and tight-binding methods in comparison with DFT method for the large fullerenes C116â€“C120. Computational and Theoretical Chemistry, 2007, 817, 35-41.	1.5	14
170	Fast determination of ginsenosides in ginseng by high-performance liquid chromatography with chemometric resolution. Journal of Separation Science, 2014, 37, 2126-2130.	1.3	14
171	Preparation of 4-butylaniline-bonded attapulgite for pre-concentration of bisphenol A in trace quantity. Talanta, 2015, 136, 29-34.	2.9	14
172	Discriminant analysis of Chinese patent medicines based on near-infrared spectroscopy and principal component discriminant transformation. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 149, 985-990.	2.0	14
173	Threeâ€“level simultaneous component analysis for analyzing the nearâ€“infrared spectra of aqueous solutions under multiple perturbations. Talanta, 2020, 217, 121036.	2.9	14
174	Molecular docking of Î±-cyclodextrin inclusion complexes by genetic algorithm and empirical binding free energy function. Chemical Physics Letters, 2001, 342, 387-396.	1.2	13
175	Micro-analysis by near-infrared diffuse reflectance spectroscopy with chemometric methods. Analyst, The, 2013, 138, 6617.	1.7	13
176	Solvent and Structure Effects on the Shuttling in Pillar[5]arene/Triazole Rotaxanes. Journal of Physical Chemistry C, 2017, 121, 25547-25553.	1.5	13
177	Silver mirror for enhancing the detection ability of nearâ€“infrared diffuse reflectance spectroscopy. Talanta, 2017, 162, 123-129.	2.9	13
178	An energy-based perturbation and a taboo strategy for improving the searching ability of stochastic structural optimization methods. Chemical Physics Letters, 2005, 404, 182-186.	1.2	12
179	Structural optimization of silver clusters from Ag61 to Ag120 by dynamic lattice searching method. Chemical Physics Letters, 2006, 422, 358-362.	1.2	12
180	Comparison studies of fullerenes C72, C74, C76 and C78 by tight-binding Monte Carlo and quantum chemical methods. Computational and Theoretical Chemistry, 2006, 760, 153-158.	1.5	12

#	Article	IF	Citations
181	A fast surface-matching procedure for proteinâ€“ligand docking. Journal of Molecular Modeling, 2006, 12, 965-972.	0.8	12
182	A post-modification approach to independent component analysis for resolution of overlapping GC/MS signals: from independent components to chemical components. Science in China Series B: Chemistry, 2007, 50, 530-537.	0.8	12
183	Systematic search for energetically favored isomers of large fullerenes C122â€“C130 and C162â€“C180. Computational Materials Science, 2008, 41, 522-528.	1.4	12
184	Structures and stabilities of multi-terminal carbon nanotube junctions. Computational Materials Science, 2008, 43, 531-539.	1.4	12
185	Discrimination of plant samples using near-infrared spectroscopy with a principal component accumulation method. Analytical Methods, 2012, 4, 2893.	1.3	12
186	Enhancing the sensitivity of potential step voltammetry using chemometric resolution. Analyst, The, 2014, 139, 1016.	1.7	12
187	Direct quantitative analysis from the current curve data of pulse voltammetric techniques. Journal of Electroanalytical Chemistry, 2014, 725, 25-31.	1.9	12
188	ELF: An Extended-Lagrangian Free Energy Calculation Module for Multiple Molecular Dynamics Engines. Journal of Chemical Information and Modeling, 2018, 58, 1315-1318.	2.5	12
189	Accuracy of Alternate Nonpolarizable Force Fields for the Determination of Proteinâ€“Ligand Binding Affinities Dominated by Cationâ^Ï€ Interactions. Journal of Chemical Theory and Computation, 2021, 17, 3908-3915.	2.3	12
190	Repurposing Existing Molecular Machines through Accurate Regulation of Cooperative Motions. Journal of Physical Chemistry Letters, 2021, 12, 613-619.	2.1	12
191	A study on the detection of weak photoacoustic signals by stochastic resonance. Fresenius' Journal of Analytical Chemistry, 2001, 370, 1087-1090.	1.5	11
192	Fullerenes connected nanotubes: An approach to build multidimensional carbon nanocomposites. Chemical Physics, 2006, 331, 85-91.	0.9	11
193	Rapid Determination of Metabolites in Bioâ€fluid Samples by Raman Spectroscopy and Optimum Combinations of Chemometric Methods. Chinese Journal of Chemistry, 2011, 29, 2525-2532.	2.6	11
194	The effects of 7-dehydrocholesterol on the structural properties of membranes. Physical Biology, 2011, 8, 056005.	0.8	11
195	Chemometric approach for fast analysis of prometryn in human hair by GC-MS. Journal of Separation Science, 2013, 36, 2277-2282.	1.3	11
196	Optimizing the models for rapid determination of chlorogenic acid, scopoletin and rutin in plant samples by near-infrared diffuse reflectance spectroscopy. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 128, 711-715.	2.0	11
197	Immobilization of papain on nanoporous silica. RSC Advances, 2014, 4, 13304-13312.	1.7	11
198	Cooperative Recruitment of Amphotericin B Mediated by a Cyclodextrin Dimer. Journal of Physical Chemistry C, 2014, 118, 24173-24180.	1.5	11

#	Article	IF	Citations
199	Combination of heuristic optimal partner bands for variable selection in nearâ€infrared spectral analysis. Journal of Chemometrics, 2018, 32, e2971.	0.7	11
200	Changes in Microenvironment Modulate the B- to A-DNA Transition. Journal of Chemical Information and Modeling, 2019, 59, 2324-2330.	2.5	11
201	Nanomachine-Assisted Ion Transport Across Membranes: From Mechanism to Rational Design and Applications. Journal of Physical Chemistry Letters, 2021, 12, 3281-3287.	2.1	11
202	Effect of Temperature on Near-infrared Spectra ofn-Alkanes. Acta Chimica Sinica, 2016, 74, 172.	0.5	11
203	Chemometrics: An Excavator in Temperature-Dependent Near-Infrared Spectroscopy. Molecules, 2022, 27, 452.	1.7	11
204	Resolution of Overlapping Chromatographic Peaks Using a Genetic Algorithm. Analytical Letters, 2000, 33, 373-390.	1.0	10
205	RESOLUTION OF MULTICOMPONENT OVERLAPPING NMR SIGNALS USING AN IMMUNE ALGORITHM AND GENETIC ALGORITHM. Analytical Letters, 2002, 35, 2375-2387.	1.0	10
206	Bimodal Complexations of Steroids with Cyclodextrins by a Flexible Docking Algorithm. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2005, 51, 41-51.	1.6	10
207	Determination and Characterization of the Pyrolysis Products of Isoprocarb by GC MS. Journal of Chromatographic Science, 2006, 44, 141-147.	0.7	10
208	Self-assembly behavior of Î²-cyclodextrin and imipramine. A Free energy perturbation study. Chemical Physics, 2010, 371, 84-90.	0.9	10
209	Regulation of Silver Precursor Reactivity via Tertiary Phosphine to Synthesize Near-Infrared Ag₂Te with Photoluminescence Quantum Yield of up to 14.7%. Chemistry of Materials, 2021, 33, 9524-9533.	3.2	10
210	On-Line Resolution of Overlapping Chromatograms Using the Wavelet Transform.. Analytical Sciences, 1999, 15, 681-684.	0.8	9
211	Resolution of multicomponent NMR signals using wavelet compression and immune algorithm. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 1075-1082.	2.0	9
212	Application of genetic stochastic resonance algorithm to quantitative structureâ€“activity relationship study. Chemometrics and Intelligent Laboratory Systems, 2005, 75, 181-188.	1.8	9
213	Formation and stability of parallel carbon nanotube junctions. Computational and Theoretical Chemistry, 2006, 767, 87-93.	1.5	9
214	A variable differential consensus method for improving the quantitative near-infrared spectroscopic analysis. Science China Chemistry, 2012, 55, 1946-1952.	4.2	9
215	Determination of Bilirubin Using near Infrared Diffuse Reflectance Spectroscopy with Selective Concentration on Î²-Cyclodextrin. Journal of Near Infrared Spectroscopy, 2016, 24, 345-352.	0.8	9
216	Selecting temperature-dependent variables in near-infrared spectra for aquaphotomics. Chemometrics and Intelligent Laboratory Systems, 2018, 183, 23-28.	1.8	9

#	Article	IF	Citations
217	pH-Controlled Fluorescence Probes for Rotaxane Isomerization. Journal of Physical Chemistry C, 2019, 123, 11304-11309.	1.5	9
218	Understanding the complexity of the structures in alcohol solutions by temperatureâ€“dependent nearâ€“infrared spectroscopy. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 229, 117864.	2.0	9
219	Hyperactive Antifreeze Proteins Promote Ice Growth before Binding to It. Journal of Chemical Information and Modeling, 2022, 62, 5165-5174.	2.5	9
220	Insight into the stability of protein in confined environment through analyzing the structure of water by temperature-dependent near-infrared spectroscopy. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 267, 120581.	2.0	9
221	A theoretical investigation of small Si/C clusters by a combination of MM and QM method. Chemical Physics Letters, 2005, 405, 97-102.	1.2	8
222	Comparison of the Properties of Bent and Straight Single-Walled Carbon Nanotube Intramolecular Junctions. Journal of Chemical Theory and Computation, 2009, 5, 1554-1559.	2.3	8
223	Rapid discrimination of slimming capsules based on illegal additives by electronic nose and flash gas chromatography. Journal of Separation Science, 2015, 38, 621-625.	1.3	8
224	Pretreating cellulases with hydrophobins for improving bioconversion of cellulose: an experimental and computational study. Green Chemistry, 2016, 18, 6666-6674.	4.6	8
225	Near-infrared spectroscopy and chemometric modelling for rapid diagnosis of kidney disease. Science China Chemistry, 2017, 60, 299-304.	4.2	8
226	Titanium dioxide as an adsorbent to enhance the detection ability of near-infrared diffuse reflectance spectroscopy. Chinese Chemical Letters, 2019, 30, 1024-1026.	4.8	8
227	Curvature of Buckybowl Corannulene Enhances Its Binding to Proteins. Journal of Physical Chemistry C, 2019, 123, 922-930.	1.5	8
228	Avoiding non-equilibrium effects in adaptive biasing force calculations. Molecular Simulation, 2021, 47, 390-394.	0.9	8
229	Do antifreeze proteins generally possess the potential to promote ice growth?. Physical Chemistry Chemical Physics, 2022, 24, 7901-7908.	1.3	8
230	Understanding the water structures by nearâ€infrared and Raman spectroscopy. Journal of Raman Spectroscopy, 2022, 53, 1686-1693.	1.2	8
231	A Wavelet-Based Genetic Algorithm for Compression and De-Noising of Chromatograms. Analytical Letters, 1999, 32, 1899-1915.	1.0	7
232	Application of Adaptive Wavelet Algorithm to the Resolution and Quantitative Analysis of Overlapping Multicomponent Chromatogram. Analytical Letters, 2003, 36, 1261-1277.	1.0	7
233	Quantitative Prediction of Normal Boiling Points for Organic Compounds Using Gas Chromatographic Retention Times on Two Columns of Different Polarity. Chromatographia, 2004, 59, .	0.7	7
234	Studies on the interaction of Î±-cyclodextrin with phospholipid by a flexible docking algorithm. Chemometrics and Intelligent Laboratory Systems, 2006, 82, 260-268.	1.8	7

#	Article	IF	Citations
235	A practical approach for near infrared spectral quantitative analysis of complex samples using partial least squares modeling. Science in China Series B: Chemistry, 2009, 52, 1021-1027.	0.8	7
236	Weighted partial least squares regression by variable grouping strategy for multivariate calibration of near infrared spectra. Analytical Methods, 2010, 2, 289.	1.3	7
237	Selective determination of mercury (II) ion in water by near-infrared diffuse reflection spectroscopy with the aid of preconcentration and multivariate calibration. Vibrational Spectroscopy, 2013, 68, 104-108.	1.2	7
238	Band target entropy minimization for retrieving the information of individual components from overlapping chromatographic data. Journal of Chromatography A, 2015, 1411, 110-115.	1.8	7
239	Addressing Polarization Phenomena in Molecular Machines Containing Transition Metal Ions with an Additive Force Field. Journal of Chemical Theory and Computation, 2019, 15, 1841-1847.	2.3	7
240	A Simulation on the Complexation of Cyclodextrins with Phospholipid Headgroups. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2006, 56, 225-235.	1.6	6
241	A strategy for enhancing the reliability of near-infrared spectral analysis. Vibrational Spectroscopy, 2008, 47, 113-118.	1.2	6
242	Simultaneous Identification and Quantitative Determination of Amino Acids in Mixture by NMR Spectroscopy Using Chemometric Resolution. Spectroscopy Letters, 2011, 44, 244-250.	0.5	6
243	Complexation mechanism of cucurbit[6]uril with hexamethylene diammonium cations in saline solution. Physical Chemistry Chemical Physics, 2014, 16, 24169-24172.	1.3	6
244	Temperature Dependent Near Infrared Spectroscopy for Understanding the Hydrogen Bonding of Amines. Acta Chimica Sinica, 2018, 76, 298.	0.5	6
245	Computer-aided design of molecular machines: techniques, paradigms and difficulties. Physical Chemistry Chemical Physics, 2022, 24, 1286-1299.	1.3	6
246	Electronic structures, stabilities, and spectroscopies of the fullerene derivatives C68X4 (X=H, F, Cl). Computational and Theoretical Chemistry, 2010, 945, 33-38.	1.5	5
247	Predicting the coordination geometry for Mg²⁺in the p53 DNA-binding domain: insights from computational studies. Physical Chemistry Chemical Physics, 2011, 13, 1140-1151.	1.3	5
248	Chemometric Resolution for Rapid Determination of Prometryn in Leek Samples Using GCâ€“MS. Chromatographia, 2013, 76, 849-855.	0.7	5
249	Rapid analysis of phthalic acid esters in environmental water using fast elution gas chromatography with mass spectrometry and adaptive library spectra. Journal of Separation Science, 2014, 37, 1585-1590.	1.3	5
250	Resolving overlapping GCâ€“MS signals with a multistep screening chemometric approach for the fast determination of pesticides. Journal of Separation Science, 2014, 37, 828-834.	1.3	5
251	Discrimination of Chinese patent medicines using near-infrared spectroscopy and principal component accumulation method. Analytical Methods, 2014, 6, 4692-4697.	1.3	5
252	Preparation of 4â€butylanilineâ€bonded silica gel for the solidâ€phase extraction of flavone glycosides. Journal of Separation Science, 2015, 38, 1149-1155.	1.3	5

#	Article	IF	Citations
253	Generalized window factor analysis for selective analysis of the target component in real samples with complex matrices. Journal of Chromatography A, 2015, 1407, 203-207.	1.8	5
254	What causes tumbling of altro-Î±-CD derivatives? Insight from computer simulations. RSC Advances, 2015, 5, 57309-57317.	1.7	5
255	Free-energy landscapes of the coupled conformational transition and inclusion processes of altro-cyclodextrins. Molecular Simulation, 2017, 43, 977-984.	0.9	5
256	Modified linear model correction: A calibration transfer method without standard samples. NIR News, 2018, 29, 24-27.	1.6	5
257	Conformational changes of DNA induced by a trans-azobenzene derivative via non-covalent interactions. Physical Chemistry Chemical Physics, 2018, 20, 22645-22651.	1.3	5
258	Determination of triglycerides in human serum by near-infrared diffuse reflectance spectroscopy using silver mirror as a substrate. Chinese Chemical Letters, 2019, 30, 111-114.	4.8	5
259	Direct non-trilinear decomposition for analyzing high-dimensional data with imperfect trilinearity. Chemometrics and Intelligent Laboratory Systems, 2021, 210, 104244.	1.8	5
260	Regulation of aquaporin-3 water permeability by hyaluronan. Physical Chemistry Chemical Physics, 2021, 23, 25706-25711.	1.3	5
261	Analyzing the Water Confined in Hydrogel Using Near-Infrared Spectroscopy. Applied Spectroscopy, 2022, 76, 773-782.	1.2	5
262	On-line analysis of the photoacoustic spectral signal using wavelet transform. Fresenius' Journal of Analytical Chemistry, 1999, 363, 215-218.	1.5	4
263	An On-Line Wavelet Transform for De-Noising of High Performance Liquid Chromatograms. Analytical Letters, 1999, 32, 2507-2520.	1.0	4
264	Fast Determination of Phenanthrene in Soil by Gas Chromatographyâ€Mass Spectrometry Using Chemometric Resolution and Standard Addition Method. Chinese Journal of Chemistry, 2013, 31, 545-550.	2.6	4
265	Unveiling the Underlying Mechanism for Compression and Decompression Strokes of a Molecular Engine. Journal of Physical Chemistry C, 2014, 118, 12562-12567.	1.5	4
266	Why do the structural properties of complexes formed by glucans and carbon nanotubes differ so much?. RSC Advances, 2015, 5, 95682-95689.	1.7	4
267	Tumbling of Anisole Units in Calixarene Promotes Its Shuttling in Rotaxanes. Journal of Physical Chemistry C, 2019, 123, 18050-18055.	1.5	4
268	Modulation of membrane permeability by carbon dioxide. Journal of Computational Chemistry, 2020, 41, 421-426.	1.5	4
269	Temperature-Dependent Near-Infrared Spectroscopy for Sensitive Detection of Glucose. Acta Chimica Sinica, 2020, 78, 125.	0.5	4
270	In situ insight into the self-assembly evolution of ABA-type block copolymers in water during the gelation process using infrared spectroscopy and near-infrared spectroscopy. Physical Chemistry Chemical Physics, 2022, 24, 17004-17013.	1.3	4

#	Article	IF	Citations
271	Preparation of Nd2O3 Thin Films by a Novel Solâ€“Gel Dipping Process. Physica Status Solidi A, 1997, 162, 623-630.	1.7	3
272	Analysis of extended X-ray absorption fine structure spectra using annealing evolutionary algorithms. Analytical Communications, 1999, 36, 313-315.	2.2	3
273	Dynamic lattice searching methods for optimization of clusters. Frontiers of Chemistry in China: Selected Publications From Chinese Universities, 2009, 4, 335-342.	0.4	3
274	Structure, Stability, and Thermochemistry of the Fullerene Derivatives C64X6 (X = H, F, Cl). Journal of Physical Chemistry A, 2009, 113, 10839-10844.	1.1	3
275	Impact of different potentials on the structures and energies of clusters. Journal of Computational Chemistry, 2011, 32, 3075-3080.	1.5	3
276	Deciphering the Mechanism Involved in the Switch On/Off of Molecular Pistons. Chinese Journal of Chemistry, 2015, 33, 1199-1205.	2.6	3
277	Determination of cysteine using near-infrared diffuse reflectance spectroscopy with enrichment via thiol-maleimide click reaction. Chemical Research in Chinese Universities, 2016, 32, 912-916.	1.3	3
278	Experimental and Chemometric Optimization to Enhance the Performance of Near-infrared Diffuse Reflectance Spectroscopy. Analytical Letters, 2018, 51, 537-546.	1.0	3
279	Free-Energy Landscape of Stepwise, Directional Motion in Multiple Molecular Switches. Journal of Physical Chemistry C, 2020, 124, 6448-6453.	1.5	3
280	Conformational Change from U- to I-Shape of Ion Transporters Facilitates K⁺ Transport across Lipid Bilayers. Journal of Physical Chemistry B, 2022, 126, 1520-1528.	1.2	3
281	Investigating the water structures in reverse micelles by temperature-dependent near infrared spectroscopy combined with independent component analysis. Journal of Near Infrared Spectroscopy, 2022, 30, 154-159.	0.8	3
282	An improved transmutation method for quantitative determination of the components in multicomponent overlapping chromatograms. Analytical and Bioanalytical Chemistry, 2004, 379, 714-9.	1.9	2
283	Quantitative Analysis of Chromium(VI) in Dilute Solution by Using Adsorption and Diffuse Reflectance Nearâ€infrared Spectroscopy. Chinese Journal of Chemistry, 2010, 28, 2009-2014.	2.6	2
284	Standard signal extraction for analyzing target analytes in real samples with complex matrices. Journal of Chemometrics, 2015, 29, 300-308.	0.7	2
285	Improved inductively coupled plasma optical emission spectroscopy analysis of trace elements in complex matrices by chemometric resolution. Journal of Analytical Atomic Spectrometry, 2015, 30, 936-940.	1.6	2
286	Unveiling the Hidden Movements in the Shuttling of Rotaxanes. Chemical Research in Chinese Universities, 2020, 36, 748-754.	1.3	2
287	Uncovering the Mechanism of Drug Resistance Caused by the T790M Mutation in EGFR Kinase From Absolute Binding Free Energy Calculations. Frontiers in Molecular Biosciences, 2022, 9, .	1.6	2
288	From multilayered graphite flakes to nanostructures: A tight-binding molecular dynamics study. Journal of Chemical Physics, 2008, 129, 224709.	1.2	1

#	Article	IF	Citations
289	Improving the Robustness and Stability of Partial Least Squares Regression for Nearâ€infrared Spectral Analysis. Chinese Journal of Chemistry, 2009, 27, 1328-1332.	2.6	1
290	Rapid determination of amino acids in ginseng by high performance liquid chromatography and chemometric resolution. Chemical Research in Chinese Universities, 2014, 30, 578-581.	1.3	1
291	Designing classification filters for integrated sensing and processing using optimal discriminant vectors. Chemometrics and Intelligent Laboratory Systems, 2015, 149, 22-27.	1.8	1
292	Predicting chromatographic retention time of C10-chlorinated paraffins in gas chromatography-mass spectrometry using quantitative structure retention relationship. Chemical Research in Chinese Universities, 2015, 31, 192-197.	1.3	1
293	Temperature-dependent near-infrared spectroscopy for studying the interactions in protein aqueous solutions. NIR News, 2019, 30, 15-17.	1.6	1
294	Accurate Estimation of Protein-ligand Binding Free Energies Based on Geometric Restraints. Acta Chimica Sinica, 2021, 79, 472.	0.5	1
295	Rapid analysis of complex samples using overlapping gas chromatography-mass spectrometry signals based on high-throughput approach. Chinese Journal of Chromatography (Se Pu), 2017, 35, 8.	0.1	1
296	Insights into directional movement in molecular machines from free-energy calculations. Physical Chemistry Chemical Physics, 2020, 22, 7888-7893.	1.3	1
297	A chemometric method to identify selective ion for resolution of overlapping gas chromatography-mass spectrometry signal. Science China Chemistry, 2013, 56, 656-663.	4.2	0
298	Determination of Bovine Hemoglobin by Near-Infrared Diffuse Reflectance Spectroscopy with Novel Adsorption Preconcentration. Analytical Letters, 2017, 50, 1196-1208.	1.0	0
299	Understanding the role of water in the aggregation of proteins and polymers in aqueous solution using near-infrared spectroscopy. NIR News, 2020, 31, 21-24.	1.6	0
300	Rapid Analysis of Pesticide Mixture by Gas Chromatography-Mass Spectrometry with a New Alternative Iterative Algorithm. Acta Chimica Sinica, 2013, 71, 729.	0.5	0