Wen-Sheng Cai

List of Publications by Year
in descending order

160 papers	3,304 citations	159358 30 h-index	243296 44 g-index
160 all docs	160 docs citations	160 times ranked	3565 citing authors

#	Article	IF	Citations
1	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
2	Hyperactive Antifreeze Proteins Promote Ice Growth before Binding to It. Journal of Chemical Information and Modeling, 2022, 62, 5165-5174.	2.5	9
3	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
4	Chemometrics: An Excavator in Temperature-Dependent Near-Infrared Spectroscopy. Molecules, 2022, 27, 452.	1.7	11
5	Computer-aided design of molecular machines: techniques, paradigms and difficulties. Physical Chemistry Chemical Physics, 2022, 24, 1286-1299.	1.3	6
6	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
7	A Companion Guide to the String Method with Swarms of Trajectories: Characterization, Performance, and Pitfalls. Journal of Chemical Theory and Computation, 2022, 18, 1406-1422.	2.3	14
8	Do antifreeze proteins generally possess the potential to promote ice growth?. Physical Chemistry Chemical Physics, 2022, 24, 7901-7908.	1.3	8
9	Mechanism and biomass association of glucuronoyl esterase: an Î±/Î² hydrolase with potential in biomass conversion. Nature Communications, 2022, 13, 1449.	5.8	15
10	Accurate determination of protein:ligand standard binding free energies from molecular dynamics simulations. Nature Protocols, 2022, 17, 1114-1141.	5.5	56
11	Analyzing the Water Confined in Hydrogel Using Near-Infrared Spectroscopy. Applied Spectroscopy, 2022, 76, 773-782.	1.2	5
12	Water structures revealed by near-infrared spectroscopy. Chinese Journal of Analytical Chemistry, 2022, 50, 100094.	0.9	1
13	MLCV: Bridging Machine-Learning-Based Dimensionality Reduction and Free-Energy Calculation. Journal of Chemical Information and Modeling, 2022, 62, 1-8.	2.5	23
14	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
15	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
16	Understanding the water structures by nearâ€infrared and Raman spectroscopy. Journal of Raman Spectroscopy, 2022, 53, 1686-1693.	1.2	8
17	Avoiding non-equilibrium effects in adaptive biasing force calculations. Molecular Simulation, 2021, 47, 390-394.	0.9	8
18	An ultralow-temperature aqueous zinc-ion battery. Journal of Materials Chemistry A, 2021, 9, 7042-7047.	5.2	87

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19	Accurate Estimation of Protein-ligand Binding Free Energies Based on Geometric Restraints. Acta Chimica Sinica, 2021, 79, 472.	0.5	1
20	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
21	BFEE2: Automated, Streamlined, and Accurate Absolute Binding Free-Energy Calculations. Journal of Chemical Information and Modeling, 2021, 61, 2116-2123.	2.5	35
22	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
23	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
24	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
25	Repurposing Existing Molecular Machines through Accurate Regulation of Cooperative Motions. Journal of Physical Chemistry Letters, 2021, 12, 613-619.	2.1	12
26	Regulation of aquaporin-3 water permeability by hyaluronan. Physical Chemistry Chemical Physics, 2021, 23, 25706-25711.	1.3	5
27	Modulation of membrane permeability by carbon dioxide. Journal of Computational Chemistry, 2020, 41, 421-426.	1.5	4
28	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
29	The Binding of Palonosetron and Other Antiemetic Drugs to the Serotonin 5-HT3 Receptor. Structure, 2020, 28, 1131-1140.e4.	1.6	20
30	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
31	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
32	Boosting Free-Energy Perturbation Calculations with GPU-Accelerated NAMD. Journal of Chemical Information and Modeling, 2020, 60, 5301-5307.	2.5	37
33	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
34	Finding an Optimal Pathway on a Multidimensional Free-Energy Landscape. Journal of Chemical Information and Modeling, 2020, 60, 5366-5374.	2.5	51
35	Unveiling the Hidden Movements in the Shuttling of Rotaxanes. Chemical Research in Chinese Universities, 2020, 36, 748-754.	1.3	2
36	Free-Energy Landscape of Stepwise, Directional Motion in Multiple Molecular Switches. Journal of Physical Chemistry C, 2020, 124, 6448-6453.	1.5	3

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37	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
38	Threeâ€“level simultaneous component analysis for analyzing the nearâ€“infrared spectra of aqueous solutions under multiple perturbations. Talanta, 2020, 217, 121036.	2.9	14
39	Insights into directional movement in molecular machines from free-energy calculations. Physical Chemistry Chemical Physics, 2020, 22, 7888-7893.	1.3	1
40	Temperature-Dependent Near-Infrared Spectroscopy for Sensitive Detection of Glucose. Acta Chimica Sinica, 2020, 78, 125.	0.5	4
41	Molecular Simulations of Supramolecular Architectures. , 2020, , 1107-1133.		0
42	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
43	Molecular Simulations of Supramolecular Architectures. , 2019, , 1-27.		0
44	Tumbling of Anisole Units in Calixarene Promotes Its Shuttling in Rotaxanes. Journal of Physical Chemistry C, 2019, 123, 18050-18055.	1.5	4
45	Click RNA for Rapid Capture and Identification of Intracellular MicroRNA Targets. Analytical Chemistry, 2019, 91, 15740-15747.	3.2	6
46	Taming Rugged Free Energy Landscapes Using an Average Force. Accounts of Chemical Research, 2019, 52, 3254-3264.	7.6	98
47	Induced Night Vision by Singlet-Oxygen-Mediated Activation of Rhodopsin. Journal of Physical Chemistry Letters, 2019, 10, 7133-7140.	2.1	14
48	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
49	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
50	Temperature-dependent near-infrared spectroscopy for studying the interactions in protein aqueous solutions. NIR News, 2019, 30, 15-17.	1.6	1
51	Water as a probe for serumâ€“based diagnosis by temperatureâ€“ dependent nearâ€“infrared spectroscopy. Talanta, 2019, 204, 359-366.	2.9	26
52	pH-Controlled Fluorescence Probes for Rotaxane Isomerization. Journal of Physical Chemistry C, 2019, 123, 11304-11309.	1.5	9
53	Chemometric methods for extracting information from temperature-dependent near-infrared spectra. Science China Chemistry, 2019, 62, 583-591.	4.2	24
54	Reversible Self-Assembly of Nanoprobes in Live Cells for Dynamic Intracellular pH Imaging. ACS Nano, 2019, 13, 1421-1432.	7.3	33

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55	Changes in Microenvironment Modulate the B- to A-DNA Transition. Journal of Chemical Information and Modeling, 2019, 59, 2324-2330.	2.5	11
56	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
57	A variable importance criterion for variable selection in near-infrared spectral analysis. Science China Chemistry, 2019, 62, 271-279.	4.2	17
58	Curvature of Buckybowl Corannulene Enhances Its Binding to Proteins. Journal of Physical Chemistry C, 2019, 123, 922-930.	1.5	8
59	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
60	Water-Controlled Switching in Rotaxanes. Journal of Physical Chemistry C, 2018, 122, 9229-9234.	1.5	16
61	Mutual factor analysis for quantitative analysis by temperature dependent near infrared spectra. Talanta, 2018, 183, 142-148.	2.9	26
62	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
63	Experimental and Chemometric Optimization to Enhance the Performance of Near-infrared Diffuse Reflectance Spectroscopy. Analytical Letters, 2018, 51, 537-546.	1.0	3
64	Combination of heuristic optimal partner bands for variable selection in nearâ€infrared spectral analysis. Journal of Chemometrics, 2018, 32, e2971.	0.7	11
65	Modified linear model correction: A calibration transfer method without standard samples. NIR News, 2018, 29, 24-27.	1.6	5
66	Selecting temperature-dependent variables in near-infrared spectra for aquaphotomics. Chemometrics and Intelligent Laboratory Systems, 2018, 183, 23-28.	1.8	9
67	Accurate Estimation of the Standard Binding Free Energy of Netropsin with DNA. Molecules, 2018, 23, 228.	1.7	85
68	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
69	Zooming across the Free-Energy Landscape: Shaving Barriers, and Flooding Valleys. Journal of Physical Chemistry Letters, 2018, 9, 4738-4745.	2.1	100
70	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
71	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
72	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

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73	Temperature Dependent Near Infrared Spectroscopy for Understanding the Hydrogen Bonding of Amines. Acta Chimica Sinica, 2018, 76, 298.	0.5	6
74	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
75	Free-energy landscapes of the coupled conformational transition and inclusion processes of altro-cyclodextrins. Molecular Simulation, 2017, 43, 977-984.	0.9	5
76	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
77	The lubricating role of water in the shuttling of rotaxanes. Chemical Science, 2017, 8, 5087-5094.	3.7	35
78	Understanding the thermal stability of human serum proteins with the related near-infrared spectral variables selected by Monte Carlo-uninformative variable elimination. Chinese Chemical Letters, 2017, 28, 1447-1452.	4.8	24
79	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
80	New Coarse Variables for the Accurate Determination of Standard Binding Free Energies. Journal of Chemical Theory and Computation, 2017, 13, 5173-5178.	2.3	49
81	Chemometric algorithms for analyzing high dimensional temperature dependent near infrared spectra. Chemometrics and Intelligent Laboratory Systems, 2017, 170, 109-117.	1.8	35
82	Understanding the Molecular Interaction in Solutions by Chemometric Resolution of Nearâ˜Infrared Spectra. ChemistrySelect, 2017, 2, 10027-10032.	0.7	24
83	Determination of Bovine Hemoglobin by Near-Infrared Diffuse Reflectance Spectroscopy with Novel Adsorption Preconcentration. Analytical Letters, 2017, 50, 1196-1208.	1.0	0
84	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
85	Silver mirror for enhancing the detection ability of nearâ€“infrared diffuse reflectance spectroscopy. Talanta, 2017, 162, 123-129.	2.9	13
86	Near-infrared spectroscopy and chemometric modelling for rapid diagnosis of kidney disease. Science China Chemistry, 2017, 60, 299-304.	4.2	8
87	Molecular dynamics simulation reveals how phosphorylation of tyrosine 26 of phosphoglycerate mutase 1 upregulates glycolysis and promotes tumor growth. Oncotarget, 2017, 8, 12093-12107.	0.8	14
88	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
89	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
90	A dual model strategy to transfer multivariate calibration models for near-infrared spectral analysis. Spectroscopy Letters, 2016, 49, 348-354.	0.5	17

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91	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
92	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
93	Complex Movements in Rotaxanes: Shuttling Coupled with Conformational Transition of Cyclodextrins. Journal of Physical Chemistry C, 2016, 120, 19479-19486.	1.5	18
94	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
95	Glucose induced variation of water structure from temperature dependent near infrared spectra. RSC Advances, 2016, 6, 105729-105736.	1.7	48
96	Pretreating cellulases with hydrophobins for improving bioconversion of cellulose: an experimental and computational study. Green Chemistry, 2016, 18, 6666-6674.	4.6	8
97	The true nature of rotary movements in rotaxanes. Chemical Science, 2016, 7, 457-462.	3.7	25
98	Effect of Temperature on Near-infrared Spectra ofn-Alkanes. Acta Chimica Sinica, 2016, 74, 172.	0.5	11
99	Deciphering the Mechanism Involved in the Switch On/Off of Molecular Pistons. Chinese Journal of Chemistry, 2015, 33, 1199-1205.	2.6	3
100	Standard signal extraction for analyzing target analytes in real samples with complex matrices. Journal of Chemometrics, 2015, 29, 300-308.	0.7	2
101	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
102	Sonoporation at Small and Large Length Scales: Effect of Cavitation Bubble Collapse on Membranes. Journal of Physical Chemistry Letters, 2015, 6, 413-418.	2.1	41
103	Preparation of 4-butylaniline-bonded attapulgite for pre-concentration of bisphenol A in trace quantity. Talanta, 2015, 136, 29-34.	2.9	14
104	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
105	Filter design for molecular factor computing using wavelet functions. Analytica Chimica Acta, 2015, 880, 26-31.	2.6	18
106	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
107	What causes tumbling of altro-Î±-CD derivatives? Insight from computer simulations. RSC Advances, 2015, 5, 57309-57317.	1.7	5
108	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

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109	Computer-Assisted Rational Modifications to Improve the Thermostability of Î²-Glucosidase from Penicillium piceum H16. Bioenergy Research, 2015, 8, 1384-1390.	2.2	29
110	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
111	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
112	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
113	Multilevel analysis of temperature dependent near-infrared spectra. Talanta, 2015, 131, 170-174.	2.9	31
114	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
115	Development of functional biointerfaces by surface modification of polydimethylsiloxane with bioactive chlorogenic acid. Colloids and Surfaces B: Biointerfaces, 2014, 116, 700-706.	2.5	18
116	Immobilization of papain on nanoporous silica. RSC Advances, 2014, 4, 13304-13312.	1.7	11
117	Discrimination of Chinese patent medicines using near-infrared spectroscopy and principal component accumulation method. Analytical Methods, 2014, 6, 4692-4697.	1.3	5
118	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
119	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
120	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
121	Standardization of near infrared spectra measured on multi-instrument. Analytica Chimica Acta, 2014, 836, 18-23.	2.6	50
122	Chemometric Resolution for Rapid Determination of Prometryn in Leek Samples Using GCâ€“MS. Chromatographia, 2013, 76, 849-855.	0.7	5
123	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
124	Cyclodextrin-Mediated Recruitment and Delivery of Amphotericin B. Journal of Physical Chemistry C, 2013, 117, 11750-11756.	1.5	20
125	Water Conduction through a Peptide Nanotube. Journal of Physical Chemistry C, 2013, 117, 26797-26803.	1.5	30
126	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

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127	Multivariate calibration of near-infrared spectra by using influential variables. Analytical Methods, 2012, 4, 467.	1.3	20
128	Discrimination of plant samples using near-infrared spectroscopy with a principal component accumulation method. Analytical Methods, 2012, 4, 2893.	1.3	12
129	Rapid determination of four tobacco specific nitrosamines in burley tobacco by near-infrared spectroscopy. Analytical Methods, 2012, 4, 1371.	1.3	20
130	l-3,4-dihydroxyphenylalanine-collagen modified PDMS surface for controlled cell culture. Journal of Materials Chemistry, 2012, 22, 10763.	6.7	20
131	How Do Î±-Cyclodextrins Self-Organize on a Polymer Chain?. Journal of Physical Chemistry C, 2012, 116, 17913-17918.	1.5	22
132	Solvent-Controlled Shuttling in a Molecular Switch. Journal of Physical Chemistry C, 2012, 116, 4471-4476.	1.5	21
133	Adsorption Behavior of Hydrophobin Proteins on Polydimethylsiloxane Substrates. Journal of Physical Chemistry B, 2012, 116, 12227-12234.	1.2	23
134	A Toolkit for the Analysis of Free-Energy Perturbation Calculations. Journal of Chemical Theory and Computation, 2012, 8, 2606-2616.	2.3	153
135	A variable differential consensus method for improving the quantitative near-infrared spectroscopic analysis. Science China Chemistry, 2012, 55, 1946-1952.	4.2	9
136	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
137	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
138	Quantitative determination by temperature dependent near-infrared spectra: A further study. Talanta, 2011, 85, 420-424.	2.9	27
139	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
140	Cancer classification based on microarray gene expression data using a principal component accumulation method. Science China Chemistry, 2011, 54, 802-811.	4.2	27
141	Preparation of a Pyrazosulfuron-Ethyl Imprinted Polymer with Hydrophilic External Layers by Reversible Addition-Fragmentation Chain Transfer Precipitation and Grafting Polymerization. Analytical Letters, 2011, 44, 2617-2632.	1.0	16
142	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
143	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
144	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

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145	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
146	Quantitative determination by temperature dependent near-infrared spectra. Talanta, 2010, 82, 1017-1021.	2.9	44
147	Multivariate calibration methods in near infrared spectroscopic analysis. Analytical Methods, 2010, 2, 1662.	1.3	76
148	Weighted partial least squares regression by variable grouping strategy for multivariate calibration of near infrared spectra. Analytical Methods, 2010, 2, 289.	1.3	7
149	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
150	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
151	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
152	Analysis of Scopoletin and Caffeic Acid in Tobacco by GCâ€“MS After a Rapid Derivatization Procedure. Chromatographia, 2009, 69, 743-748.	0.7	23
153	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
154	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
155	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
156	SHEF: a vHTS geometrical filter using coefficients of spherical harmonic molecular surfaces. Journal of Molecular Modeling, 2008, 14, 393-401.	0.8	19
157	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
158	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
159	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
160	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