Xueguang Shao

List of Publications by Year
in descending order

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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	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	Do antifreeze proteins generally possess the potential to promote ice growth?. Physical Chemistry Chemical Physics, 2022, 24, 7901-7908.	1.3	8
8	Mechanism and biomass association of glucuronoyl esterase: an Î±/Î² hydrolase with potential in biomass conversion. Nature Communications, 2022, 13, 1449.	5.8	15
9	Accurate determination of protein:ligand standard binding free energies from molecular dynamics simulations. Nature Protocols, 2022, 17, 1114-1141.	5.5	56
10	Analyzing the Water Confined in Hydrogel Using Near-Infrared Spectroscopy. Applied Spectroscopy, 2022, 76, 773-782.	1.2	5
11	MLCV: Bridging Machine-Learning-Based Dimensionality Reduction and Free-Energy Calculation. Journal of Chemical Information and Modeling, 2022, 62, 1-8.	2.5	23
12	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
13	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
14	Understanding the water structures by nearâ€infrared and Raman spectroscopy. Journal of Raman Spectroscopy, 2022, 53, 1686-1693.	1.2	8
15	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
16	Avoiding non-equilibrium effects in adaptive biasing force calculations. Molecular Simulation, 2021, 47, 390-394.	0.9	8
17	Accurate Estimation of Protein-ligand Binding Free Energies Based on Geometric Restraints. Acta Chimica Sinica, 2021, 79, 472.	0.5	1
18	Direct non-trilinear decomposition for analyzing high-dimensional data with imperfect trilinearity. Chemometrics and Intelligent Laboratory Systems, 2021, 210, 104244.	1.8	5

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19	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
20	BFEE2: Automated, Streamlined, and Accurate Absolute Binding Free-Energy Calculations. Journal of Chemical Information and Modeling, 2021, 61, 2116-2123.	2.5	35
21	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
22	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
23	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
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	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	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
28	Modulation of membrane permeability by carbon dioxide. Journal of Computational Chemistry, 2020, 41, 421-426.	1.5	4
29	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
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	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
33	Finding an Optimal Pathway on a Multidimensional Free-Energy Landscape. Journal of Chemical Information and Modeling, 2020, 60, 5366-5374.	2.5	51
34	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
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	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
42	Tumbling of Anisole Units in Calixarene Promotes Its Shuttling in Rotaxanes. Journal of Physical Chemistry C, 2019, 123, 18050-18055.	1.5	4
43	Taming Rugged Free Energy Landscapes Using an Average Force. Accounts of Chemical Research, 2019, 52, 3254-3264.	7.6	98
44	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
45	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
46	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
47	Temperature-dependent near-infrared spectroscopy for studying the interactions in protein aqueous solutions. NIR News, 2019, 30, 15-17.	1.6	1
48	Water as a probe for serumâ€“based diagnosis by temperatureâ€“ dependent nearâ€“infrared spectroscopy. Talanta, 2019, 204, 359-366.	2.9	26
49	pH-Controlled Fluorescence Probes for Rotaxane Isomerization. Journal of Physical Chemistry C, 2019, 123, 11304-11309.	1.5	9
50	Chemometric methods for extracting information from temperature-dependent near-infrared spectra. Science China Chemistry, 2019, 62, 583-591.	4.2	24
51	Changes in Microenvironment Modulate the B- to A-DNA Transition. Journal of Chemical Information and Modeling, 2019, 59, 2324-2330.	2.5	11
52	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
53	A variable importance criterion for variable selection in near-infrared spectral analysis. Science China Chemistry, 2019, 62, 271-279.	4.2	17
54	Curvature of Buckybowl Corannulene Enhances Its Binding to Proteins. Journal of Physical Chemistry C, 2019, 123, 922-930.	1.5	8

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55	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
56	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
57	Water-Controlled Switching in Rotaxanes. Journal of Physical Chemistry C, 2018, 122, 9229-9234.	1.5	16
58	Mutual factor analysis for quantitative analysis by temperature dependent near infrared spectra. Talanta, 2018, 183, 142-148.	2.9	26
59	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
60	Experimental and Chemometric Optimization to Enhance the Performance of Near-infrared Diffuse Reflectance Spectroscopy. Analytical Letters, 2018, 51, 537-546.	1.0	3
61	Combination of heuristic optimal partner bands for variable selection in nearâ€infrared spectral analysis. Journal of Chemometrics, 2018, 32, e2971.	0.7	11
62	Modified linear model correction: A calibration transfer method without standard samples. NIR News, 2018, 29, 24-27.	1.6	5
63	Selecting temperature-dependent variables in near-infrared spectra for aquaphotomics. Chemometrics and Intelligent Laboratory Systems, 2018, 183, 23-28.	1.8	9
64	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
65	Zooming across the Free-Energy Landscape: Shaving Barriers, and Flooding Valleys. Journal of Physical Chemistry Letters, 2018, 9, 4738-4745.	2.1	100
66	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
67	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
68	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
69	Temperature Dependent Near Infrared Spectroscopy for Understanding the Hydrogen Bonding of Amines. Acta Chimica Sinica, 2018, 76, 298.	0.5	6
70	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
71	Free-energy landscapes of the coupled conformational transition and inclusion processes of altro-cyclodextrins. Molecular Simulation, 2017, 43, 977-984.	0.9	5
72	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

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73	The lubricating role of water in the shuttling of rotaxanes. Chemical Science, 2017, 8, 5087-5094.	3.7	35
74	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
75	Chemometric algorithms for analyzing high dimensional temperature dependent near infrared spectra. Chemometrics and Intelligent Laboratory Systems, 2017, 170, 109-117.	1.8	35
76	Understanding the Molecular Interaction in Solutions by Chemometric Resolution of Nearâ^'Infrared Spectra. ChemistrySelect, 2017, 2, 10027-10032.	0.7	24
77	Determination of Bovine Hemoglobin by Near-Infrared Diffuse Reflectance Spectroscopy with Novel Adsorption Preconcentration. Analytical Letters, 2017, 50, 1196-1208.	1.0	0
78	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
79	Silver mirror for enhancing the detection ability of nearâ€“infrared diffuse reflectance spectroscopy. Talanta, 2017, 162, 123-129.	2.9	13
80	Near-infrared spectroscopy and chemometric modelling for rapid diagnosis of kidney disease. Science China Chemistry, 2017, 60, 299-304.	4.2	8
81	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
82	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
83	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
84	A dual model strategy to transfer multivariate calibration models for near-infrared spectral analysis. Spectroscopy Letters, 2016, 49, 348-354.	0.5	17
85	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
86	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
87	Complex Movements in Rotaxanes: Shuttling Coupled with Conformational Transition of Cyclodextrins. Journal of Physical Chemistry C, 2016, 120, 19479-19486.	1.5	18
88	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
89	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
90	Glucose induced variation of water structure from temperature dependent near infrared spectra. RSC Advances, 2016, 6, 105729-105736.	1.7	48

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91	Pretreating cellulases with hydrophobins for improving bioconversion of cellulose: an experimental and computational study. Green Chemistry, 2016, 18, 6666-6674.	4.6	8
92	The true nature of rotary movements in rotaxanes. Chemical Science, 2016, 7, 457-462.	3.7	25
93	Effect of Temperature on Near-infrared Spectra ofn-Alkanes. Acta Chimica Sinica, 2016, 74, 172.	0.5	11
94	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
95	Deciphering the Mechanism Involved in the Switch On/Off of Molecular Pistons. Chinese Journal of Chemistry, 2015, 33, 1199-1205.	2.6	3
96	Standard signal extraction for analyzing target analytes in real samples with complex matrices. Journal of Chemometrics, 2015, 29, 300-308.	0.7	2
97	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
98	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
99	Designing classification filters for integrated sensing and processing using optimal discriminant vectors. Chemometrics and Intelligent Laboratory Systems, 2015, 149, 22-27.	1.8	1
100	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
101	Preparation of 4-butylaniline-bonded attapulgite for pre-concentration of bisphenol A in trace quantity. Talanta, 2015, 136, 29-34.	2.9	14
102	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
103	Filter design for molecular factor computing using wavelet functions. Analytica Chimica Acta, 2015, 880, 26-31.	2.6	18
104	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
105	What causes tumbling of altro-Î±-CD derivatives? Insight from computer simulations. RSC Advances, 2015, 5, 57309-57317.	1.7	5
106	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
107	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
108	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

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109	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
110	Multilevel analysis of temperature dependent near-infrared spectra. Talanta, 2015, 131, 170-174.	2.9	31
111	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
112	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
113	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
114	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
115	Immobilization of papain on nanoporous silica. RSC Advances, 2014, 4, 13304-13312.	1.7	11
116	Enhancing the sensitivity of potential step voltammetry using chemometric resolution. Analyst, The, 2014, 139, 1016.	1.7	12
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	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
119	Complexation mechanism of cucurbit[6]uril with hexamethylene diammonium cations in saline solution. Physical Chemistry Chemical Physics, 2014, 16, 24169-24172.	1.3	6
120	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
121	Cooperative Recruitment of Amphotericin B Mediated by a Cyclodextrin Dimer. Journal of Physical Chemistry C, 2014, 118, 24173-24180.	1.5	11
122	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
123	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
124	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
125	Direct quantitative analysis from the current curve data of pulse voltammetric techniques. Journal of Electroanalytical Chemistry, 2014, 725, 25-31.	1.9	12
126	Standardization of near infrared spectra measured on multi-instrument. Analytica Chimica Acta, 2014, 836, 18-23.	2.6	50

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127	Chemometric Resolution for Rapid Determination of Prometryn in Leek Samples Using GCâ€“MS. Chromatographia, 2013, 76, 849-855.	0.7	5
128	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
129	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
130	Selecting significant genes by randomization test for cancer classification using gene expression data. Journal of Biomedical Informatics, 2013, 46, 594-601.	2.5	29
131	Micro-analysis by near-infrared diffuse reflectance spectroscopy with chemometric methods. Analyst, The, 2013, 138, 6617.	1.7	13
132	Direct separation of faradaic and double layer charging current in potential step voltammetry. Talanta, 2013, 116, 575-580.	2.9	16
133	Intelligent background correction using an adaptive lifting wavelet. Chemometrics and Intelligent Laboratory Systems, 2013, 125, 11-17.	1.8	22
134	Cyclodextrin-Mediated Recruitment and Delivery of Amphotericin B. Journal of Physical Chemistry C, 2013, 117, 11750-11756.	1.5	20
135	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
136	Chemometric approach for fast analysis of prometryn in human hair by GC-MS. Journal of Separation Science, 2013, 36, 2277-2282.	1.3	11
137	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
138	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
139	Multivariate calibration of near-infrared spectra by using influential variables. Analytical Methods, 2012, 4, 467.	1.3	20
140	Discrimination of plant samples using near-infrared spectroscopy with a principal component accumulation method. Analytical Methods, 2012, 4, 2893.	1.3	12
141	Rapid determination of four tobacco specific nitrosamines in burley tobacco by near-infrared spectroscopy. Analytical Methods, 2012, 4, 1371.	1.3	20
142	How Do Î±-Cyclodextrins Self-Organize on a Polymer Chain?. Journal of Physical Chemistry C, 2012, 116, 17913-17918.	1.5	22
143	Solvent-Controlled Shuttling in a Molecular Switch. Journal of Physical Chemistry C, 2012, 116, 4471-4476.	1.5	21
144	Adsorption Behavior of Hydrophobin Proteins on Polydimethylsiloxane Substrates. Journal of Physical Chemistry B, 2012, 116, 12227-12234.	1.2	23

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145	Preparation of Dendritic Nanostructures of Silver and Their Characterization for Electroreduction. Langmuir, 2012, 28, 5218-5226.	1.6	66
146	Feasibility for quantitative determination of deoxyribonucleic acid by using near-infrared diffuse reflectance spectroscopy. Talanta, 2012, 99, 871-874.	2.9	15
147	A variable differential consensus method for improving the quantitative near-infrared spectroscopic analysis. Science China Chemistry, 2012, 55, 1946-1952.	4.2	9
148	Edge effects control helical wrapping of carbon nanotubes by polysaccharides. Nanoscale, 2012, 4, 2584.	2.8	28
149	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
150	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
151	Application of Near-infrared Spectroscopy in Micro Inorganic Analysis. Acta Chimica Sinica, 2012, 70, 2109.	0.5	17
152	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
153	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
154	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
155	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
156	Structural Characterization of Micelles Formed of Cholesteryl-Functionalized Cyclodextrins. Langmuir, 2011, 27, 91-97.	1.6	26
157	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
158	Rapid analysis of multicomponent pesticide mixture by GCâ€“MS with the aid of chemometric resolution. Talanta, 2011, 83, 1247-1253.	2.9	27
159	Synthesis of silver nanowires and their applications in the electrochemical detection of halide. Talanta, 2011, 84, 673-678.	2.9	60
160	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
161	Quantitative determination by temperature dependent near-infrared spectra: A further study. Talanta, 2011, 85, 420-424.	2.9	27
162	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

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163	Cancer classification based on microarray gene expression data using a principal component accumulation method. Science China Chemistry, 2011, 54, 802-811.	4.2	27
164	Impact of different potentials on the structures and energies of clusters. Journal of Computational Chemistry, 2011, 32, 3075-3080.	1.5	3
165	Synthesis of dendritic silver nanostructures and their application in hydrogen peroxide electroreduction. Electrochimica Acta, 2011, 56, 3170-3174.	2.6	87
166	The effects of 7-dehydrocholesterol on the structural properties of membranes. Physical Biology, 2011, 8, 056005.	0.8	11
167	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
168	Classification and Quantitative Analysis of Azithromycin Tablets by Raman Spectroscopy and Chemometrics. American Journal of Analytical Chemistry, 2011, 02, 135-141.	0.3	15
169	Self-assembly behavior of Î²-cyclodextrin and imipramine. A Free energy perturbation study. Chemical Physics, 2010, 371, 84-90.	0.9	10
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