

xin-yuan Shi

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

90
papers

889
citations

17
h-index

23
g-index

112
ext. papers

1,138
ext. citations

3.2
avg, IF

4.21
L-index

#	Paper	IF	Citations
90	Formulation design and mechanism study of hydrogel based on computational pharmaceutics theories. <i>Journal of Molecular Graphics and Modelling</i> , 2022 , 110, 108051	2.8	
89	Process optimization in ginseng fermentation by and study on bile acid-binding ability of fermentation products. <i>Preparative Biochemistry and Biotechnology</i> , 2021 , 51, 120-126	2.4	1
88	Saponin surfactants used in drug delivery systems: A new application for natural medicine components. <i>International Journal of Pharmaceutics</i> , 2021 , 603, 120709	6.5	9
87	Effects of fermented ginseng on the gut microbiota and immunity of rats with antibiotic-associated diarrhea. <i>Journal of Ethnopharmacology</i> , 2021 , 267, 113594	5	17
86	Investigation on drug entrapment location in liposomes and transfersomes based on molecular dynamics simulation. <i>Journal of Molecular Modeling</i> , 2021 , 27, 111	2	4
85	Monascus ruber fermented Panax ginseng ameliorates lipid metabolism disorders and modulate gut microbiota in rats fed a high-fat diet. <i>Journal of Ethnopharmacology</i> , 2021 , 278, 114300	5	4
84	The ncRNA-Mediated Overexpression of Ferroptosis-Related Gene EMC2 Correlates With Poor Prognosis and Tumor Immune Infiltration in Breast Cancer.. <i>Frontiers in Oncology</i> , 2021 , 11, 777037	5.3	0
83	The Application of Coarse-Grained Molecular Dynamics to the Evaluation of Liposome Physical Stability. <i>AAPS PharmSciTech</i> , 2020 , 21, 138	3.9	3
82	Analysis of chemical constituents and six compounds in Qu-feng-sheng-shi Granules via HPLC-ESI-Q/TOF-MS and HPLC-UV technique. <i>Biomedical Chromatography</i> , 2020 , 34, e4829	1.7	2
81	Multiscale study on the enhancing effect and mechanism of borneolum on transdermal permeation of drugs with different log P values and molecular sizes. <i>International Journal of Pharmaceutics</i> , 2020 , 580, 119225	6.5	3
80	Paecilomyces cicadae-fermented Radix astragali activates podocyte autophagy by attenuating PI3K/AKT/mTOR pathways to protect against diabetic nephropathy in mice. <i>Biomedicine and Pharmacotherapy</i> , 2020 , 129, 110479	7.5	13
79	Raw Material Variability and Its Impact on the Online Adaptive Control of Cohesive Powder Blend Homogeneity Using NIR Spectroscopy. <i>Processes</i> , 2019 , 7, 568	2.9	3
78	Coarse-grained molecular dynamics simulations of the effect of edge activators on the skin permeation behavior of transfersomes. <i>Colloids and Surfaces B: Biointerfaces</i> , 2019 , 183, 110462	6	9
77	A Multiscale Study on the Effect of Sodium Cholate on the Deformation Ability of Elastic Liposomes. <i>AAPS PharmSciTech</i> , 2019 , 20, 311	3.9	4
76	Real-Time Release Testing of Herbal Extract Powder by Near-Infrared Spectroscopy considering the Uncertainty around Specification Limits. <i>Journal of Spectroscopy</i> , 2019 , 2019, 1-10	1.5	2
75	A multiscale study of the penetration-enhancing mechanism of menthol. <i>Journal of Traditional Chinese Medical Sciences</i> , 2019 , 6, 347-354	0.6	0
74	A compression behavior classification system of pharmaceutical powders for accelerating direct compression tablet formulation design. <i>International Journal of Pharmaceutics</i> , 2019 , 572, 118742	6.5	20

73	Dissipative Particle Dynamics Study on Platycodin B Solubilization Enhancing Effect Towards Five Drug Components. <i>Chemical Research in Chinese Universities</i> , 2019 , 35, 65-70	2.2	1
72	Optimal Selection of Incoming Materials from the Inventory for Achieving the Target Drug Release Profile of High Drug Load Sustained-Release Matrix Tablet. <i>AAPS PharmSciTech</i> , 2019 , 20, 76	3.9	3
71	SeDeM expert system for directly compressed tablet formulation: A review and new perspectives. <i>Powder Technology</i> , 2019 , 342, 517-527	5.2	20
70	Bi-directional solid fermentation products of <i>Trametes robiniophila</i> Murr with <i>Radix Isatidis</i> inhibit proliferation and metastasis of breast cancer cells. <i>Journal of the Chinese Medical Association</i> , 2018 , 81, 520-530	2.8	10
69	Metabolomics data fusion between near infrared spectroscopy and high-resolution mass spectrometry: A synergetic approach to boost performance or induce confusion. <i>Talanta</i> , 2018 , 189, 641-648	6.2	15
68	Permeation-enhancing effects and mechanisms of borneol and menthol on ligustrazine: A multiscale study using in vitro and coarse-grained molecular dynamics simulation methods. <i>Chemical Biology and Drug Design</i> , 2018 , 92, 1830-1837	2.9	7
67	Structural Insights into the Thermophilic Adaption Mechanism of Endo-1,4- β -Xylanase from <i>Caldicellulosiruptor owensensis</i> . <i>Journal of Agricultural and Food Chemistry</i> , 2018 , 66, 187-193	5.7	18
66	Identification of cordycepin biosynthesis-related genes through de novo transcriptome assembly and analysis in. <i>Royal Society Open Science</i> , 2018 , 5, 181247	3.3	11
65	Setting up multivariate specifications on critical raw material attributes to ensure consistent drug dissolution from high drug-load sustained-release matrix tablet. <i>Drug Development and Industrial Pharmacy</i> , 2018 , 44, 1733-1743	3.6	5
64	Overall uncertainty measurement for near infrared analysis of cryptotanshinone in tanshinone extract. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017 , 170, 39-47	4.4	2
63	Influence of Temperature on Transdermal Penetration Enhancing Mechanism of Borneol: A Multi-Scale Study. <i>International Journal of Molecular Sciences</i> , 2017 , 18,	6.3	6
62	Novelty application of multi-omics correlation in the discrimination of sulfur-fumigation and non-sulfur-fumigation <i>Ophiopogonis Radix</i> . <i>Scientific Reports</i> , 2017 , 7, 9971	4.9	9
61	A facile approach to fabricate waterborne, nanosized polyaniline-graft-(sulfonated polyurethane) as environmental antistatic coating. <i>Journal of Applied Polymer Science</i> , 2017 , 134, 45412	2.9	7
60	Scale-up of a high shear wet granulation process using a nucleation regime map approach. <i>Particuology</i> , 2017 , 31, 87-94	2.8	15
59	Latent variable modeling to analyze the effects of process parameters on the dissolution of paracetamol tablet. <i>Bioengineered</i> , 2017 , 8, 61-70	5.7	6
58	A Molecular Interpretation on the Different Penetration Enhancement Effect of Borneol and Menthol towards 5-Fluorouracil. <i>International Journal of Molecular Sciences</i> , 2017 , 18,	6.3	9
57	PAT: From Western solid dosage forms to Chinese materia medica preparations using NIR-CI. <i>Drug Testing and Analysis</i> , 2016 , 8, 71-85	3.5	6
56	A Multiscale Study on the Penetration Enhancement Mechanism of Menthol to Osthole. <i>Journal of Chemical Information and Modeling</i> , 2016 , 56, 2234-2242	6.1	11

55	Robust design space development for HPLC analysis of five chemical components in Panax notoginseng saponins. <i>Journal of Liquid Chromatography and Related Technologies</i> , 2016 , 39, 504-512	1.3	8
54	Rapid analysis of spatial distribution of PVPP and hardness of Yinhuang dispersible tablets by NIR-CI. <i>Journal of Innovative Optical Health Sciences</i> , 2016 , 09, 1550016	1.2	2
53	Comparison of Ensemble Strategies in Online NIR for Monitoring the Extraction Process of Pericarpium Citri Reticulatae Based on Different Variable Selections. <i>Planta Medica</i> , 2016 , 82, 154-62	3.1	8
52	Near-infrared chemical imaging for quantitative analysis of chlorpheniramine maleate and distribution homogeneity assessment in pharmaceutical formulations. <i>Journal of Innovative Optical Health Sciences</i> , 2016 , 09, 1650002	1.2	2
51	Statistical modeling methods to analyze the impacts of multiunit process variability on critical quality attributes of Chinese herbal medicine tablets. <i>Drug Design, Development and Therapy</i> , 2016 , 10, 3909-3924	4.4	5
50	Effects of Concentrations on the Transdermal Permeation Enhancing Mechanisms of Borneol: A Coarse-Grained Molecular Dynamics Simulation on Mixed-Bilayer Membranes. <i>International Journal of Molecular Sciences</i> , 2016 , 17,	6.3	14
49	Rapid analysis of dyed safflowers by color objectification and pattern recognition methods. <i>Journal of Traditional Chinese Medical Sciences</i> , 2016 , 3, 234-241	0.6	2
48	MDL and RMSEP assessment of spectral pretreatments by adding different noises in calibration/validation datasets. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016 , 163, 20-7	4.4	23
47	Determination of Geniposide in Gardenia jasminoides Ellis Fruit by Near-Infrared Spectroscopy and Chemometrics. <i>Analytical Letters</i> , 2016 , 49, 2063-2076	2.2	4
46	Establishment and reliability evaluation of the design space for HPLC analysis of six alkaloids in Coptis chinensis (Huanglian) using Bayesian approach. <i>Chinese Journal of Natural Medicines</i> , 2016 , 14, 697-708	2.8	16
45	Micro-electro-mechanical systems/near-infrared validation of different sampling modes and sample sets coupled with multiple models. <i>Planta Medica</i> , 2015 , 81, 167-74	3.1	2
44	A online NIR sensor for the pilot-scale extraction process in Fructus aurantii coupled with single and ensemble methods. <i>Sensors</i> , 2015 , 15, 8749-63	3.8	11
43	Monitoring As and Hg variation in An-Gong-Niu-Huang Wan (AGNH) intermediates in a pilot scale blending process using laser-induced breakdown spectroscopy. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 151, 547-52	4.4	8
42	Interaction of menthol with mixed-lipid bilayer of stratum corneum: A coarse-grained simulation study. <i>Journal of Molecular Graphics and Modelling</i> , 2015 , 60, 98-107	2.8	23
41	Optimization of Parameter Selection for Partial Least Squares Model Development. <i>Scientific Reports</i> , 2015 , 5, 11647	4.9	44
40	Evaluation of the value of near infrared (NIR) spectromicroscopy for the analysis of glycyrrhizic acid in licorice. <i>Chinese Journal of Natural Medicines</i> , 2015 , 13, 316-20	2.8	4
39	Evaluating the reliability of spectral variables selected by subsampling methods. <i>Journal of Chemometrics</i> , 2015 , 29, 87-95	1.6	4
38	Dealing with heterogeneous classification problem in the framework of multi-instance learning. <i>Talanta</i> , 2015 , 132, 175-81	6.2	1

37	Near Infrared Spectroscopy Model Development and Variable Importance in Projection Assignment of Particle Size and Lobetyolin Content of Codonopsis Radix. <i>Journal of Near Infrared Spectroscopy</i> , 2015 , 23, 327-335	1.5	5
36	Online near-infrared analysis coupled with MWPLS and SiPLS models for the multi-ingredient and multi-phase extraction of licorice (Gancao). <i>Chinese Medicine</i> , 2015 , 10, 38	4.7	13
35	Rapid characterization of tanshinone extract powder by near infrared spectroscopy. <i>International Journal of Analytical Chemistry</i> , 2015 , 2015, 704940	1.4	1
34	Robust PLS Prediction Model for Saikosaponin A in Bupleurum chinense DC. Coupled with Granularity-Hybrid Calibration Set. <i>Journal of Analytical Methods in Chemistry</i> , 2015 , 2015, 583841	2	1
33	Method validation for the analysis of licorice acid in the blending process by near infrared diffuse reflectance spectroscopy. <i>Analytical Methods</i> , 2015 , 7, 5830-5837	3.2	7
32	Near-infrared for on-line determination of quality parameter of Sophora japonica L. (Formula particles): From lab investigation to pilot-scale extraction process. <i>Pharmacognosy Magazine</i> , 2015 , 11, 8-13	0.8	11
31	Microanalysis of Multi-Element in Juncus effusus L. by LIBS Technique. <i>Plasma Science and Technology</i> , 2015 , 17, 904-908	1.5	7
30	Dissipative particle dynamics study on self-assembled platycodin structures: the potential biocarriers for drug delivery. <i>Journal of Molecular Graphics and Modelling</i> , 2015 , 57, 20-6	2.8	16
29	Solubilization of menthol by platycodin D in aqueous solution: an integrated study of classical experiments and dissipative particle dynamics simulation. <i>International Journal of Pharmaceutics</i> , 2015 , 480, 143-51	6.5	7
28	Estimation of multivariate detection limits of four quality parameters in licorice using MEMS-NIR spectrometry coupled with two sampling accessories. <i>Journal of Innovative Optical Health Sciences</i> , 2015 , 08, 1550009	1.2	
27	NIR assignment of isopsoralen by 2D-COS technology and model application in Yunkang Oral Liquid. <i>Journal of Innovative Optical Health Sciences</i> , 2015 , 08, 1550023	1.2	3
26	Application of Design of Experiment and Design Space (DOE-DS) Methodology for the HPLC Separation of Panax Notoginseng Saponins. <i>Open Chemical Engineering Journal</i> , 2015 , 9, 47-52	1.2	3
25	Application of TOPO to the Multistage Batch Process Optimization of Gardenia Extracts. <i>Lecture Notes in Computer Science</i> , 2015 , 267-276	0.9	
24	Rapid elemental analysis and provenance study of Blumea balsamifera DC using laser-induced breakdown spectroscopy. <i>Sensors</i> , 2014 , 15, 642-55	3.8	21
23	Absorption and quantitative characteristics of C-H bond and O-H bond of NIR. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2014 , 117, 703-709	0.7	8
22	Dissipative Particle Dynamics Simulation of Ginsenoside R _g Vesicular Solubilization Systems. <i>Journal of Computational and Theoretical Nanoscience</i> , 2014 , 11, 2046-2054	0.3	3
21	Rapid Discrimination of Chlorpheniramine Maleate and Assessment of Its Surface Content Uniformity in a Pharmaceutical Formulation by NIR-CI Coupled with Statistical Measurement. <i>Journal of Spectroscopy</i> , 2014 , 2014, 1-9	1.5	3
20	Interactions of borneol with DPPC phospholipid membranes: a molecular dynamics simulation study. <i>International Journal of Molecular Sciences</i> , 2014 , 15, 20365-81	6.3	11

19	NIR rapid assessments of Chinese material medica: simultaneous determination of three major active components of licorice 2014 ,		1
18	Multiscale study on the interaction mechanism between ginsenoside biosurfactant and saikosaponin a. <i>Journal of Colloid and Interface Science</i> , 2013 , 396, 165-72	9.3	22
17	Application of orthogonal space regression to calibration transfer without standards. <i>Journal of Chemometrics</i> , 2013 , 27, 406-413	1.6	18
16	Multivariate detection limits of on-line NIR model for extraction process of chlorogenic acid from <i>Lonicera japonica</i> . <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2013 , 77, 16-20	3.5	40
15	NIR spectroscopy as a process analytical technology (PAT) tool for monitoring and understanding of a hydrolysis process. <i>Bioresource Technology</i> , 2013 , 137, 394-9	11	33
14	A novel model selection strategy using total error concept. <i>Talanta</i> , 2013 , 107, 248-54	6.2	18
13	Target-oriented overall process optimization (TOPO) for reducing variability in the quality of herbal medicine products. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2013 , 128, 144-152	3.8	4
12	Improving the creditability and reproducibility of variables selected from near infrared spectra 2013 ,		1
11	A Mesoscopic Simulation Study on the Solubilization of Menthol by Platycodin D. <i>Journal of Engineering Science and Technology Review</i> , 2013 , 6, 125-129	1.8	3
10	Validation of NIR Model for On-line Monitoring of Flos <i>Lonicera Japonica</i> Extraction Process with Different Batches of Materials. <i>International Journal of Online and Biomedical Engineering</i> , 2013 , 9, 44	0.8	3
9	Visualizing excipient composition and homogeneity of Compound Licorice Tablets by near-infrared chemical imaging. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 86, 631-6	4.4	19
8	Validation of a NIR quantification method for the determination of chlorogenic acid in <i>Lonicera japonica</i> solution in ethanol precipitation process. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2012 , 62, 1-6	3.5	46
7	Absorption characteristics and quantitative contribution of overtones and combination of NIR: Method development and validation. <i>Journal of Molecular Structure</i> , 2012 , 1019, 97-102	3.4	12
6	Monitoring of a pharmaceutical blending process using near infrared chemical imaging. <i>Vibrational Spectroscopy</i> , 2012 , 63, 371-379	2.1	18
5	Development and Validation of a Portable AOTF-NIR Measurement Method for the Determination of Baicalin in Yinhuang Oral Solution 2012 ,		1
4	Development and validation of NIR model using low-concentration calibration range: rapid analysis of <i>Lonicera japonica</i> solution in ethanol precipitation process. <i>Analytical Methods</i> , 2012 , 4, 1084	3.2	12
3	NIR analysis for batch process of ethanol precipitation coupled with a new calibration model updating strategy. <i>Analytica Chimica Acta</i> , 2012 , 720, 22-8	6.6	56
2	Solubilization of saikosaponin a by ginsenoside Ro biosurfactant in aqueous solution: mesoscopic simulation. <i>Journal of Colloid and Interface Science</i> , 2012 , 384, 73-80	9.3	17

- 1 NIR Determination of Three Critical Quality Attributes in Alcohol Precipitation Process of *Lonicerae Japonicae* with Uncertainty Analysis **2012**,

1