Jahan B Ghasemi

List of Publications by Year
in descending order

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157 papers	3,032 citations	201575 27 h-index	254106 43 g-index
160 all docs	160 docs citations	160 times ranked	3427 citing authors

#	Article	IF	Citations
1	Design, synthesis, and nanoengineered modification of spherical graphene surface by layered double hydroxide (LDH) for removal of As(III) from aqueous solutions. Chinese Journal of Chemical Engineering, 2023, 53, 374-380.	1.7	9
2	Using the extract of pomegranate peel as a natural indicator for colorimetric detection and simultaneous determination of Fe³⁺ and Fe²⁺ by partial least squaresâ€“artificial neural network. Journal of Chemometrics, 2023, 37, .	0.7	1
3	Simultaneous removal of crystal violet and methyl green in water samples by functionalised SBA-15. International Journal of Environmental Analytical Chemistry, 2022, 102, 5919-5935.	1.8	9
4	A new Fe3+ colorimetric sensor: Nitrophenyl bispyrazole derivative synthesis using Fe3O4@SiO2@Si-Pr-NH-(CH2)2-NH2 and its DFT study. Materials Chemistry and Physics, 2022, 275, 125285.	2.0	11
5	An Onâ€“off Supramolecular Fluorescence Switch for Detection of Pb2+ Ions and Vitamin C. Journal of Fluorescence, 2022, 32, 165-173.	1.3	1
6	A new fluorescence probe for simultaneous determination of Fe2+ and Fe3+ by orthogonal signal correction-principal component regression. Journal of Molecular Structure, 2022, 1252, 131978.	1.8	10
7	Black titania; novel researches in synthesis and applications. Inorganic Chemistry Communication, 2022, 135, 109092.	1.8	8
8	A new fluorescence probe for detection of Cu+2 in blood samples: Circuit logic gate. Analytical Biochemistry, 2022, 639, 114525.	1.1	9
9	Preparation of a nonenzymatic electrochemical sensor based on a g-C₃N₄/MWO₄ (M: Cu, Mn, Co, Ni) composite for the determination of H₂O₂. New Journal of Chemistry, 2022, 46, 3766-3776.	1.4	10
10	A novel Z-scheme oxygen-doped g-C3N4 nanosheet/NaBiS2 nanoribbon for efficient photocatalytic H2O2 production and organic pollutants degradation. Journal of Physics and Chemistry of Solids, 2022, 163, 110588.	1.9	26
11	Pomegranate Punica granatum peel waste as a naked-eye natural colorimetric sensor for the detection and determination of Fe+3 and Iâ¯ ions in water. Chemosphere, 2022, 294, 133759.	4.2	13
12	Solvent-free one-pot synthesis of 4-aryl-3,5-dimethyl-1,4,7,8-tetrahydrodipyrazolo[3,4-b:4â€²,3â€²-e]pyridines using Fe3O4@SiO2@(BuSO3H)3 catalytic Fe3+ system as selective colorimetric. Research on Chemical Intermediates, 2022, 48, 2111-2133.	1.3	5
13	A novel fluorescence sensor based on a tripodal carboxylic acid for detection and measurement of Cu2+ in tomato: Experimental and computational studies. Food and Chemical Toxicology, 2022, 164, 112964.	1.8	4
14	Design and synthesis of g-C3N4/(Cu/TiO2) nanocomposite for the visible light photocatalytic degradation of endosulfan in aqueous solutions. Journal of Molecular Structure, 2022, 1258, 132650.	1.8	16
15	In-situ construction of ZnO/Sb2MoO6 nano-heterostructure for efficient visible-light photocatalytic conversion of N2 to NH3. Surfaces and Interfaces, 2022, 30, 101844.	1.5	8
16	Multiwavelength spectrophotometric-thermodynamic studies of complexation reactions of newly synthesized triazenes with Hg2+, Pb2+, Zn2+, and Cd2+ in MeOH, EtOH, DMF, and DMSO. Journal of Molecular Liquids, 2022, 357, 119145.	2.3	2
17	Fabrication of S-scheme heterojunction g-C3N4-nanosheet/ZnMoO4 nanocomposite with high efficiency in photocatalytic N2 fixation and Cr(VI) detoxification. Journal of Materials Science, 2022, 57, 9145-9163.	1.7	17
18	Determination and degradation of carbamazepine using g-C3N4@CuS nanocomposite as sensitive fluorescence sensor and efficient photocatalyst. Inorganic Chemistry Communication, 2022, 141, 109512.	1.8	12

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19	Simultaneous electrochemical determination of morphine and methadone by using CMK-5 mesoporous carbon and multivariate calibration. Scientific Reports, 2022, 12, 8270.	1.6	11
20	Dihydropyrano quinoline derivatives functionalized nanoporous silica as novel fluorescence sensor for Fe3+ in aqueous solutions(aq). Journal of Molecular Structure, 2022, 1265, 133408.	1.8	2
21	Spiroindeno-pyridineindoles (SIPIs) as new visible colorimetric pH indicators. Chemosphere, 2022, 306, 135630.	4.2	0
22	Design and synthesis of novel pyrazole-phenyl semicarbazone derivatives as potential Î±-glucosidase inhibitor: Kinetics and molecular dynamics simulation study. International Journal of Biological Macromolecules, 2021, 166, 1082-1095.	3.6	33
23	In situ preparation of g-C3N4 nanosheet/FeOCl: Achievement and promoted photocatalytic nitrogen fixation activity. Journal of Colloid and Interface Science, 2021, 587, 538-549.	5.0	59
24	Photocatalytic degradation of different pollutants by the novel gCN-NS/Black-TiO2 heterojunction photocatalyst under visible light: Introducing a photodegradation model and optimization by response surface methodology (RSM). Materials Chemistry and Physics, 2021, 258, 123912.	2.0	60
25	Application of genetic algorithm and multivariate methods for the detection and measurement of milkâ€surfactant adulteration by attenuated total reflection and nearâ€infrared spectroscopy. Journal of the Science of Food and Agriculture, 2021, 101, 2696-2703.	1.7	13
26	10-(4-Phenylpiperazine-1-carbonyl)acridin-9(10H)-ones and related compounds: Synthesis, antiproliferative activity and inhibition of tubulin polymerization. Bioorganic and Medicinal Chemistry Letters, 2021, 32, 127687.	1.0	2
27	Use of Molecular Docking as a Decision-Making Tool in Drug Discovery. , 2021, , 229-243.		7
28	High-impressive separation of photoinduced charge carriers on step-scheme ZnO/ZnSnO3/Carbon dots heterojunction with efficient activity in photocatalytic NH3 production. Journal of the Taiwan Institute of Chemical Engineers, 2021, 118, 140-151.	2.7	32
29	In silico exploration of novel protease inhibitors against coronavirus 2019 (COVID-19). Informatics in Medicine Unlocked, 2021, 23, 100516.	1.9	7
30	A combined structure-based pharmacophore modeling and 3D-QSAR study on a series of N-heterocyclic scaffolds to screen novel antagonists as human DHFR inhibitors. Structural Chemistry, 2021, 32, 1571-1588.	1.0	1
31	SBA-Pr-Imine-Furan as an environmental adsorbent of Pd(II) in aqueous solutions. Environmental Challenges, 2021, 3, 100032.	2.0	11
32	Novel visible-light-responsive Black-TiO2/CoTiO3 Z-scheme heterojunction photocatalyst with efficient photocatalytic performance for the degradation of different organic dyes and tetracycline. Journal of the Taiwan Institute of Chemical Engineers, 2021, 121, 168-183.	2.7	34
33	One-pot synthesis of hematite-alumina hollow sphere composite by ultrasonic spray pyrolysis technique with high adsorption capacity toward PAHs. Advanced Powder Technology, 2021, 32, 1060-1069.	2.0	11
34	Synthesis and characterization of novel ZnO/NiCr2O4 nanocomposite for water purification by degradation of tetracycline and phenol under visible light irradiation. Materials Research Bulletin, 2021, 139, 111247.	2.7	30
35	Direct monitoring of diclofenac using a supramolecular fluorescent approach based on Î²-cyclodextrin nanosponge. Journal of Molecular Liquids, 2021, 336, 116104.	2.3	13
36	Design and synthesis of novel quinazolinone-pyrazole derivatives as potential Î±-glucosidase inhibitors: Structure-activity relationship, molecular modeling and kinetic study. Bioorganic Chemistry, 2021, 114, 105127.	2.0	28

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37	Facile and green preparation of colorimetric and fluorescent sensors for mercury, silver, and carbonate ions visual detecting: Spectroscopy and theoretical studies. Journal of Molecular Structure, 2021, 1241, 130626.	1.8	21
38	Near-infrared spectroscopy and machine learning-based classification and calibration methods in detection and measurement of anionic surfactant in milk. Journal of Food Composition and Analysis, 2021, 104, 104170.	1.9	14
39	Design, synthesis, biological evaluation, and molecular modeling studies of pyrazole-benzofuran hybrids as new Î±-glucosidase inhibitor. Scientific Reports, 2021, 11, 20776.	1.6	15
40	Multicomponent Synthesis and Investigations Fluorescence Activity of Chromenoneâ€“Pyrazole Compounds. Journal of Fluorescence, 2021, , 1.	1.3	1
41	Molecular dynamics simulation and 3D-pharmacophore analysis of new quinoline-based analogues with dual potential against EGFR and VEGFR-2. International Journal of Biological Macromolecules, 2020, 142, 94-113.	3.6	18
42	Anthracene modified graphene oxide-silica as an optical sensor for selective detection of Cu²⁺ and I^{â^'} ions. International Journal of Environmental Analytical Chemistry, 2020, 100, 686-701.	1.8	7
43	Spectrophotometric-chemometrics study of the effect of solvent composition and temperature on the spectral shape and shift of copper and nickel phthalocyanines in different aqueous-nonaqueous mixed solvents. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 227, 117621.	2.0	11
44	A dual-emission fluorescence probe for simultaneous quantification of CNâ^' and Cr2O72â^' ions based on modified g-C3N4. Journal of Photochemistry and Photobiology A: Chemistry, 2020, 389, 112261.	2.0	15
45	Chemometrics-spectroscopic study of the effect of temperature and pre-micellar to post-micellar forms of various surfactants on the dimerization of nickel and copper phthalocyanines. Journal of Molecular Liquids, 2020, 300, 112350.	2.3	8
46	A highly sensitive fluorescence measurement of amphetamine using 8-hydroxyquinoline-Î²-cyclodextrin grafted on graphene oxide. Diamond and Related Materials, 2020, 109, 108032.	1.8	10
47	Acenaphtoquinoxaline as a selective fluorescent sensor for Hg (II) detection: experimental and theoretical studies. Heliyon, 2020, 6, e04986.	1.4	12
48	Novel pâ€“n Heterojunction Nanocomposite: TiO₂ QDs/ZnBi₂O₄ Photocatalyst with Considerably Enhanced Photocatalytic Activity under Visible-Light Irradiation. Journal of Physical Chemistry C, 2020, 124, 27519-27528.	1.5	54
49	Synthesis, characterization, and photocatalytic performance of Ag/AgFeO2 decorated on g-C3N4-nanosheet under the visible light irradiation. Journal of the Taiwan Institute of Chemical Engineers, 2020, 115, 279-292.	2.7	35
50	Preparation of hierarchical g-C3N4@TiO2 hollow spheres for enhanced visible-light induced catalytic CO2 reduction. Solar Energy, 2020, 205, 465-473.	2.9	59
51	Deposited CuBi2O4 and Bi3ClO4 nanoparticles on g-C3N4 nanosheet: a promising visible light-induced photocatalyst toward the removal of tetracycline hydrochloride and rhodamine B. Journal of Materials Science, 2020, 55, 7775-7791.	1.7	27
52	Fluorescence turn off-on probe (Î²-cyclodextrin-hydroxyquinoline) for monitoring of Cd²⁺ ions and tetracycline. Methods and Applications in Fluorescence, 2020, 8, 025009.	1.1	10
53	Simultaneous Quantification of Nine Major Water-Soluble Inorganic Ions Using a Potentiometric Electronic Tongue in Cheese Samples. IEEE Sensors Journal, 2020, 20, 10138-10144.	2.4	5
54	Lansoprazole-Based Colorimetric Chemosensor for Efficient Binding and Sensing of Carbonate Ion: Spectroscopy and DFT Studies. Frontiers in Chemistry, 2020, 8, 626472.	1.8	12

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55	Three Dimensional Quantitative Structure Activity Relationship and Pharmacophore Modeling of Tacrine Derivatives as Acetylcholinesterase Inhibitors in Alzheimer's Treatment. Medicinal Chemistry, 2020, 16, 155-168.	0.7	0
56	An ultrasensitive fluorescence sensor for determination of trace levels of copper in blood samples. Analytical and Bioanalytical Chemistry, 2019, 411, 5593-5603.	1.9	29
57	Inhibition activity prediction for a dataset of candidatesâ€™ drug by combining fuzzy logic with <scp>MLR</scp>/<scp>ANN QSAR</scp> models. Chemical Biology and Drug Design, 2019, 93, 1139-1157.	1.5	10
58	Boron-doped graphitic carbon nitride as a novel fluorescent probe for mercury(<scp>ii</scp>) and iron(<scp>iii</scp>): a circuit logic gate mimic. New Journal of Chemistry, 2019, 43, 12087-12093.	1.4	25
59	A highly selective Ag+ sensor based on 8-hydroxyquinoline functionalized graphene oxide -silica nanosheet and its logic gate behaviour. Journal of Materials Science: Materials in Electronics, 2019, 30, 17693-17705.	1.1	9
60	SBA-Pr-SO3H-catalyzed synthesis of bispyrazole compounds as anti-bacterial agents and inhibitors of phosphorylated RET tyrosine kinase. Journal of the Iranian Chemical Society, 2019, 16, 1401-1409.	1.2	7
61	Design of pyrimidine-based scaffolds as potential anticancer agents for human DHFR: three-dimensional quantitative structureâ€“activity relationship by docking derived grid-independent descriptors. Journal of the Iranian Chemical Society, 2019, 16, 2365-2378.	1.2	1
62	Synthesis, experimental, quantum chemical and molecular dynamics study of carbon steel corrosion inhibition effect of two Schiff bases in HCl solution. Journal of Molecular Liquids, 2019, 285, 626-639.	2.3	69
63	Highly selective silica-based fluorescent nanosensor for ferric ion (Fe3+) detection in aqueous media. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 218, 293-298.	2.0	13
64	Dispersive solid phase extraction of lead in water samples using embedded 1,5-diphenylcarbazone grafted graphene oxide in microporous magnetic chitosan coupled with flame atomic absorption spectrometry. Journal of the Iranian Chemical Society, 2019, 16, 1411-1421.	1.2	16
65	Voltammetric Electronic Tongue for the Simultaneous Determination of Three Benzodiazepines. Sensors, 2019, 19, 5002.	2.1	16
66	Exploring 3D-QSPR models of human skin permeability for a diverse dataset of chemical compounds. Journal of Receptor and Signal Transduction Research, 2019, 39, 442-450.	1.3	2
67	Efficient removal of malachite green from wastewater by using boron-doped mesoporous carbon nitride. Applied Surface Science, 2019, 469, 236-245.	3.1	71
68	Simultaneous determination of dihydroxybenzene isomers at nitrogen-doped graphene surface using fast Fourier transform square wave voltammetry and multivariate calibration. Microchemical Journal, 2019, 145, 596-605.	2.3	20
69	Probing the origin of dihydrofolate reductase inhibition via proteochemometric modeling. Journal of Chemometrics, 2019, 33, e3090.	0.7	5
70	Computer-aided molecular design of (E)-N-Aryl-2-ethene-sulfonamide analogues as microtubule targeted agents in prostate cancer. Arabian Journal of Chemistry, 2019, 12, 2150-2165.	2.3	4
71	Dynamic structure based pharmacophore modeling of the Acetylcholinesterase reveals several potential inhibitors. Journal of Biomolecular Structure and Dynamics, 2019, 37, 1800-1812.	2.0	33
72	Identification of Essential 2D and 3D Chemical Features for Discovery of the Novel Tubulin Polymerization Inhibitors. Current Topics in Medicinal Chemistry, 2019, 19, 1092-1120.	1.0	5

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73	Simultaneous sensitive determination of benzenediol isomers using multiwall carbon nanotubeâ€“ionic liquid modified carbon paste electrode by a combination of artificial neural network and fast Fourier transform admittance voltammetry. New Journal of Chemistry, 2018, 42, 6479-6487.	1.4	8
74	Synthesis of magnetically modified mesoporous nanoparticles and their application in simultaneous determination of Pb(II), Cd(II) and Cu(II). Research on Chemical Intermediates, 2018, 44, 1689-1709.	1.3	19
75	Computational Multi-Target Drug Design. Methods in Pharmacology and Toxicology, 2018, , 51-90.	0.1	1
76	A detailed structural study of cytotoxicity effect of ionic liquids on the leukemia rat cell line IPC-81 by three dimensional quantitative structure toxicity relationship. Ecotoxicology and Environmental Safety, 2018, 158, 256-265.	2.9	20
77	Highâ€throughput Docking and Molecular Dynamics Simulations towards the Identification of Novel Peptidomimetic Inhibitors against CDC7. Molecular Informatics, 2018, 37, e1800022.	1.4	4
78	In Silico Studies in Drug Research Against Neurodegenerative Diseases. Current Neuropharmacology, 2018, 16, 664-725.	1.4	51
79	Computerâ€aided drug design to explore cyclodextrin therapeutics and biomedical applications. Chemical Biology and Drug Design, 2017, 89, 257-268.	1.5	28
80	Simultaneous spectrophotometric determination of crystal violet and malachite green in water samples using partial least squares regression and central composite design after preconcentration by dispersive solid-phase extraction. Environmental Monitoring and Assessment, 2017, 189, 196.	1.3	23
81	Characterization of the interaction of glycyrrhizin and glycyrrhetinic acid with bovine serum albumin by spectrophotometric-gradient flow injection titration technique and molecular modeling simulations. International Journal of Biological Macromolecules, 2017, 102, 92-103.	3.6	9
82	N-Heterocyclic (4-Phenylpiperazin-1-yl)methanones Derived from Phenoxazine and Phenothiazine as Highly Potent Inhibitors of Tubulin Polymerization. Journal of Medicinal Chemistry, 2017, 60, 749-766.	2.9	28
83	Simultaneous determination of binary solution of triphenylmethane dyes in complex matrices onto magnetic amino-rich SWCNT using second-order calibration method. Environmental Monitoring and Assessment, 2017, 189, 594.	1.3	9
84	Spectroscopic and molecular modeling studies on the interactions of some benzofuran derivatives with BSA. Monatshefte FÃ¼r Chemie, 2017, 148, 1887-1896.	0.9	2
85	Graphene oxideâ€“alizarin yellow Râ€“magnetic chitosan nanocomposite: a selective and efficient sorbent for sub-trace determination of aluminum in water samples. Analytical Methods, 2017, 9, 222-231.	1.3	16
86	Proteochemometric Modeling of the Interaction Space of Carbonic Anhydrase and its Inhibitors: An Assessment of Structureâ€based and Sequenceâ€based Descriptors. Molecular Informatics, 2017, 36, 1600102.	1.4	12
87	Predicting Degradation Half-life of Organophosphorus Pesticides in Soil Using Three-Dimensional Molecular Interaction Fields. International Journal of Quantitative Structure-Property Relationships, 2017, 2, 27-35.	1.1	1
88	Computer Aided Drug Design for Multi-Target Drug Design: SAR /QSAR, Molecular Docking and Pharmacophore Methods. Current Drug Targets, 2017, 18, 556-575.	1.0	78
89	Dual-acting of Hybrid Compounds - A New Dawn in the Discovery of Multi-target Drugs: Lead Generation Approaches. Current Topics in Medicinal Chemistry, 2017, 17, 1096-1114.	1.0	26
90	Molecular Docking Challenges and Limitations. , 2017, , 770-794.		9

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91	Quantitative Characterization of the Interaction Space of the Mammalian Carbonic Anhydrase Isoforms I, <scp>II</scp>,<scp> VII</scp>,<scp> IX</scp>,<scp> XII</scp>, and <scp>XIV</scp> and their Inhibitors, Using the Proteochemometric Approach. Chemical Biology and Drug Design, 2016, 88, 341-353.	1.5	16
92	QSPR approaches to elucidate the stability constants between Î²-cyclodextrin and some organic compounds: Docking based 3D conformer. Journal of Molecular Liquids, 2016, 219, 1036-1043.	2.3	6
93	Thermodynamic study of Î²-cyclodextrin-dye inclusion complexes using gradient flow injection technique and molecular modeling. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 165, 54-60.	2.0	5
94	Experimental, computational and chemometrics studies of BSA-vitamin B6 interaction by UVâ€“Vis, FT-IR, fluorescence spectroscopy, molecular dynamics simulation and hard-soft modeling methods. Bioorganic Chemistry, 2016, 68, 124-136.	2.0	62
95	Using Wavelet Analysis To Assist in Identification of Significant Events in Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2016, 56, 1282-1291.	2.5	17
96	Extraction optimization of pepsin-soluble collagen from eggshell membrane by response surface methodology (RSM). Food Chemistry, 2016, 190, 186-193.	4.2	100
97	Multivariate optimization, preconcentration and determination of mercury ions with (1-(p-acetyl) Tj ETQq1 1 0.784314 rgBT /Overloc 1111-1119.	1.3	12
98	Alignment independent 3D-QSAR, quantum calculations and molecular docking of Mer specific tyrosine kinase inhibitors as anticancer drugs. Saudi Pharmaceutical Journal, 2016, 24, 197-212.	1.2	12
99	Molecular Docking Challenges and Limitations. Advances in Medical Technologies and Clinical Practice Book Series, 2016, , 56-80.	0.3	2
100	Multivariate curve resolution alternating least squares in the quantitative determination of sulfur using overlapped S(K_{Î±})â€“Mo(L_{Î±}) emission peaks by wavelength dispersive Xâ€ray fluorescence spectrometry. X-Ray Spectrometry, 2015, 44, 75-80.	0.9	8
101	Application of multivariate optimization procedures for preconcentration and determination of Au(III) and Pt(IV) in aqueous samples with graphene oxide by X-ray fluorescence spectrometry. Environmental Monitoring and Assessment, 2015, 187, 149.	1.3	12
102	3D-QSAR and virtual screening studies in identification of new Rho kinase inhibitors with different scaffolds. Journal of the Iranian Chemical Society, 2015, 12, 1945-1959.	1.2	10
103	Computer-aided scaffold hopping to identify a novel series of casein kinase 1 delta (CK1d) inhibitors for amyotrophic lateral sclerosis. European Journal of Pharmaceutical Sciences, 2015, 78, 151-162.	1.9	12
104	Molecular docking, 2D and 3D-QSAR studies of new indole-based derivatives as HCV-NS5B polymerase inhibitors. Journal of the Iranian Chemical Society, 2015, 12, 1789-1799.	1.2	9
105	An improved ensemble learning machine for biological activity prediction of tyrosine kinase inhibitors. Journal of Chemometrics, 2015, 29, 213-223.	0.7	2
106	Application of bilinear least squares/residual bilinearization in bulk liquid membrane system for simultaneous multicomponent quantification of two synthetic dyes. Chemometrics and Intelligent Laboratory Systems, 2015, 144, 48-55.	1.8	9
107	An in silico screening study and design of potent cognition agents. Journal of Computational Science, 2015, 11, 112-120.	1.5	1
108	Multivariate statistical analysis methods in QSAR. RSC Advances, 2015, 5, 104635-104665.	1.7	66

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109	A chemometric study on the stream sediments of Meshkinshahr, NW Iran, using supervised and unsupervised classification methods. Arabian Journal of Geosciences, 2015, 8, 2853-2861.	0.6	1
110	Solid phase headspace microextraction of tricyclic antidepressants using a directly prepared nanocomposite consisting of graphene, CTAB and polyaniline. Mikrochimica Acta, 2015, 182, 633-641.	2.5	22
111	Discovery of New Potential Antimalarial Compounds Using Virtual Screening of ZINC Database. Combinatorial Chemistry and High Throughput Screening, 2015, 18, 227-234.	0.6	10
112	Application of Multivariate Linear and Nonlinear Calibration and Classification Methods in Drug Design. Combinatorial Chemistry and High Throughput Screening, 2015, 18, 795-808.	0.6	12
113	Pharmacophore elucidation and 3D-QSAR analysis of a new class of highly potent inhibitors of acid ceramidase based on maximum common substructure and field fit alignment methods. Journal of the Iranian Chemical Society, 2014, 11, 1329-1336.	1.2	7
114	Second-order data obtained by beta-cyclodextrin complexes: A novel approach for multicomponent analysis with three-way multivariate calibration methods. Talanta, 2014, 128, 254-262.	2.9	5
115	Using chemometric methods for overlap correction of sodium-zinc spectral lines generated by wavelength dispersive X-ray fluorescence in mineral samples. X-Ray Spectrometry, 2014, 43, 131-137.	0.9	9
116	An Alignment Independent 3D-QSAR Modeling of Dispersibility of Single-walled Carbon Nanotubes in Different Organic Solvents. Fullerenes Nanotubes and Carbon Nanostructures, 2014, 22, 605-617.	1.0	15
117	A rapid, automated gradient flow injectionâ€“spectrophotometric technique for study of metal complexation reactions. Talanta, 2014, 128, 511-517.	2.9	10
118	Combined docking, molecular dynamics simulations and spectroscopic studies for the rational design of a dipeptide ligand for affinity chromatography separation of human serum albumin. Journal of Molecular Modeling, 2014, 20, 2446.	0.8	35
119	3D-QSAR and docking studies of the stability constants of different guest molecules with beta-cyclodextrin. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2014, 79, 401-413.	0.9	9
120	Simultaneous multicomponent spectrophotometric monitoring of methyl and propyl parabens using multivariate statistical methods after their preconcentration by robust ionic liquid-based dispersive liquidâ€“liquid microextraction. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 122, 295-303.	2.0	26
121	Toward a continuous wavelet transform-based search method for feature selection for classification of spectroscopic data. Chemometrics and Intelligent Laboratory Systems, 2013, 127, 185-194.	1.8	17
122	Quasi 4D-QSAR and 3D-QSAR study of the pan class I phosphoinositide-3-kinase (PI3K) inhibitors. Medicinal Chemistry Research, 2013, 22, 1587-1596.	1.1	11
123	3D-QSAR, CoMFA, and CoMSIA of new phenyloxazolidinones derivatives as potent HIV-1 protease inhibitors. Structural Chemistry, 2013, 24, 433-444.	1.0	13
124	Docking and pharmacophoreâ€based alignment comparative molecular field analysis threeâ€dimensional quantitative structureâ€“activity relationship analysis of dihydrofolate reductase inhibitors by linear and nonlinear calibration methods. Journal of Chemometrics, 2013, 27, 287-296.	0.7	13
125	Docking and CoMFA study on novel human CCR5 receptor antagonists. Medicinal Chemistry Research, 2013, 22, 1356-1364.	1.1	2
126	Simultaneous spectrophotometric determination of trace amount of polycyclic aromatic hydrocarbons in water samples after magnetic solid-phase extraction by using projection pursuit regression. Environmental Monitoring and Assessment, 2013, 185, 2297-2305.	1.3	26

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127	Application of principal component analysisâ€“multivariate adaptive regression splines for the simultaneous spectrofluorimetric determination of dialkyltins in micellar media. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 115, 357-363.	2.0	24
128	Identification of novel inhibitors of HIV-1 integrase using pharmacophore-based virtual screening combined with molecular docking strategies. Medicinal Chemistry Research, 2013, 22, 5545-5556.	1.1	6
129	Application of random forest regression to spectral multivariate calibration. Analytical Methods, 2013, 5, 1863.	1.3	32
130	Comparative study of Boxâ€“Behnken, central composite, and Doehlert matrix for multivariate optimization of Pb (II) adsorption onto Robinia tree leaves. Journal of Chemometrics, 2013, 27, 12-20.	0.7	158
131	3D-QSAR, docking and molecular dynamics for factor Xa inhibitors as anticoagulant agents. Molecular Simulation, 2013, 39, 453-471.	0.9	11
132	Docking, CoMFA and CoMSIA studies of a series of sulfonamides derivatives as carbonic anhydrase I inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2013, 28, 320-327.	2.5	9
133	Alignment Independent 3D-QSAR Modeling of Fullerene (C₆₀) Solubility in Different Organic Solvents. Fullerenes Nanotubes and Carbon Nanostructures, 2013, 21, 367-380.	1.0	19
134	Methods and Applications of Structure Based Pharmacophores in Drug Discovery. Current Topics in Medicinal Chemistry, 2013, 13, 1036-1047.	1.0	66
135	Docking, CoMFA and CoMSIA Studies of a Series of N-Benzoylated Phenoxazines and Phenothiazines Derivatives as Antiproliferative Agents. Bulletin of the Korean Chemical Society, 2013, 34, 899-906.	1.0	10
136	Improvement of the Prediction Power of the CoMFA and CoMSIA Models of Histamine H3 Antagonists by Different Variable Selection Methods. Scientia Pharmaceutica, 2012, 80, 547-566.	0.7	17
137	Pharmacophore Identification, Molecular Docking, Virtual Screening, and In Silico ADME Studies of Nonâ€Nucleoside Reverse Transcriptase Inhibitors. Molecular Informatics, 2012, 31, 856-866.	1.4	18
138	Molecular docking and 3D-QSAR studies of falcipain inhibitors using CoMFA, CoMSIA, and Open3DQSAR. Medicinal Chemistry Research, 2012, 21, 2788-2806.	1.1	23
139	Docking and 3D-QSAR study of stability constants of benzene derivatives as environmental pollutants with Î±-cyclodextrin. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2012, 73, 405-413.	1.6	16
140	Simultaneous spectrophotometric determination of uranium and zirconium using cloud point extraction and multivariate methods. Journal of the Iranian Chemical Society, 2012, 9, 257-262.	1.2	23
141	Ultrasound-assisted ionic liquid-based microextraction combined with least squares support vector machines regression for the simultaneous determination of aluminum, gallium, and indium in water and coal samples. Environmental Monitoring and Assessment, 2012, 184, 3971-3981.	1.3	22
142	4D-LQTA-QSAR and docking study on potent gram-negative specific LpxC inhibitors: a comparison to CoMFA modeling. Molecular Diversity, 2012, 16, 203-213.	2.1	22
143	The Influence of Growing Region on Fatty Acids and Sterol Composition of Iranian Olive Oils by Unsupervised Clustering Methods. JAOCS, Journal of the American Oil Chemists' Society, 2012, 89, 371-378.	0.8	25
144	Thermodynamic study of the dimerization equilibrium of methylene blue, methylene green and thiazole orange at various surfactant concentrations and different ionic strengths and in mixed solvents by spectral titration and chemometric analysis. Dyes and Pigments, 2012, 92, 1031-1041.	2.0	50

#	Article	IF	Citations
145	A New Variable Selection Method Based on Mutual Information Maximization by Replacing Collinear Variables for Nonlinear Quantitative Structure-Property Relationship Models. Bulletin of the Korean Chemical Society, 2012, 33, 1527-1535.	1.0	4
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