

Jahan Bakhsh Ghasemi

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.

321 papers	4,812 citations	35 h-index	47 g-index
342 ext. papers	5,622 ext. citations	3.6 avg, IF	6.27 L-index

#	Paper	IF	Citations
321	A novel Z-scheme oxygen-doped g-C3N4 nanosheet/NaBiS2 nanoribbon for efficient photocatalytic H2O2 production and organic pollutants degradation. <i>Journal of Physics and Chemistry of Solids</i> , 2022 , 163, 110588	3.9	2
320	Pomegranate Punica granatum peel waste as a naked-eye natural colorimetric sensor for the detection and determination of Fe and I ions in water.. <i>Chemosphere</i> , 2022 , 294, 133759	8.4	2
319	SBA-ionic liquid as an efficient adsorbent of palladium, silver, and gold ions. <i>Journal of the Iranian Chemical Society</i> , 2022 , 1	2	0
318	Ti3C2 MXene/Ag2ZnGeO4 Schottky heterojunctions with enhanced photocatalytic performances: Efficient charge separation and mechanism studies. <i>Separation and Purification Technology</i> , 2022 , 278, 119560	8.3	2
317	A new Fe3+ colorimetric sensor: Nitrophenyl bispyrazole derivative synthesis using Fe3O4@SiO2@Si-Pr-NH-(CH2)2-NH2 and its DFT study. <i>Materials Chemistry and Physics</i> , 2022 , 275, 125285	4.4	3
316	Design, Synthesis, and Nanoengineered Modification of Spherical Graphene Surface by LDH for Removal of As(III) from Aqueous Solutions. <i>Chinese Journal of Chemical Engineering</i> , 2022 ,	3.2	1
315	Solvent-free one-pot synthesis of 4-aryl-3,5-dimethyl-1,4,7,8-tetrahydropyrazolo[3,4-b:4',3'-e]pyridines using Fe3O4@SiO2@(BuSO3H)3 catalytic Fe3+ system as selective colorimetric. <i>Research on Chemical Intermediates</i> , 2022 , 48, 2111	2.8	2
314	A novel fluorescence sensor based on a tripodal carboxylic acid for detection and measurement of Cu in tomato: Experimental and computational studies.. <i>Food and Chemical Toxicology</i> , 2022 , 112964	4.7	0
313	Design and synthesis of g-C3N4/(Cu/TiO2) nanocomposite for the visible light photocatalytic degradation of endosulfan in aqueous solutions. <i>Journal of Molecular Structure</i> , 2022 , 1258, 132650	3.4	2
312	In-situ construction of ZnO/Sb2MoO6 nano-heterostructure for efficient visible-light photocatalytic conversion of N2 to NH3. <i>Surfaces and Interfaces</i> , 2022 , 30, 101844	4.1	0
311	Multiwavelength spectrophotometric-thermodynamic studies of complexation reactions of newly synthesized triazenes with Hg2+, Pb2+, Zn2+, and Cd2+ in MeOH, EtOH, DMF, and DMSO. <i>Journal of Molecular Liquids</i> , 2022 , 357, 119145	6	0
310	Determination and degradation of carbamazepine using g-C3N4@CuS nanocomposite as sensitive fluorescence sensor and efficient photocatalyst. <i>Inorganic Chemistry Communication</i> , 2022 , 141, 109512	3.1	1
309	Simultaneous electrochemical determination of morphine and methadone by using CMK-5 mesoporous carbon and multivariate calibration.. <i>Scientific Reports</i> , 2022 , 12, 8270	4.9	0
308	Dihydropyrano quinoline derivatives functionalized nanoporous silica as novel fluorescence sensor for Fe3+ (aq). <i>Journal of Molecular Structure</i> , 2022 , 133408	3.4	0
307	A new fluorescence probe for simultaneous determination of Fe2+ and Fe3+ by orthogonal signal correction-principal component regression. <i>Journal of Molecular Structure</i> , 2021 , 1252, 131978	3.4	0
306	Black Titania; Novel researches in Synthesis and Applications. <i>Inorganic Chemistry Communication</i> , 2021 , 109092	3.1	
305	Multicomponent Synthesis and Investigations Fluorescence Activity of Chromenone-Pyrazole Compounds. <i>Journal of Fluorescence</i> , 2021 , 1	2.4	0

304	A new fluorescence probe for detection of Cu in blood samples: Circuit logic gate.. <i>Analytical Biochemistry</i> , 2021 , 639, 114525	3.1	1
303	A theoretical and experimental study of polyaniline/GCE and DNA G-quadruplex conformation as an impedimetric biosensor for the determination of potassium ions.. <i>Chemosphere</i> , 2021 , 133460	8.4	0
302	Design, synthesis, biological evaluation, and molecular modeling studies of pyrazole-benzofuran hybrids as new β -glucosidase inhibitor. <i>Scientific Reports</i> , 2021 , 11, 20776	4.9	2
301	An On-off Supramolecular Fluorescence Switch for Detection of Pb Ions and Vitamin C. <i>Journal of Fluorescence</i> , 2021 , 1	2.4	1
300	SBA-Pr-Imine-Furan as an environmental adsorbent of Pd(II) in aqueous solutions. <i>Environmental Challenges</i> , 2021 , 3, 100032	2.6	6
299	Novel visible-light-responsive Black-TiO ₂ /CoTiO ₃ Z-scheme heterojunction photocatalyst with efficient photocatalytic performance for the degradation of different organic dyes and tetracycline. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2021 , 121, 168-183	5.3	9
298	g-C ₃ N ₄ nanosheet adorned with Ag ₃ BiO ₃ as a perovskite: An effective photocatalyst for efficient visible-light photocatalytic processes. <i>Materials Science in Semiconductor Processing</i> , 2021 , 125, 105651	4.3	15
297	Synthesis of Ag(I)@FumPrBzrBenzimidazole and Its Optical and Catalytic Activities in Click Reactions. <i>ChemistrySelect</i> , 2021 , 6, 6168-6180	1.8	0
296	Synthesis and characterization of novel ZnO/NiCr ₂ O ₄ nanocomposite for water purification by degradation of tetracycline and phenol under visible light irradiation. <i>Materials Research Bulletin</i> , 2021 , 139, 111247	5.1	11
295	Design and synthesis of novel pyrazole-phenyl semicarbazone derivatives as potential β -glucosidase inhibitor: Kinetics and molecular dynamics simulation study. <i>International Journal of Biological Macromolecules</i> , 2021 , 166, 1082-1095	7.9	13
294	Z-scheme g-C ₃ N ₄ nanosheet/MgBi ₂ O ₆ systems with the visible light response for impressive photocatalytic organic contaminants degradation. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021 , 406, 113023	4.7	13
293	In situ preparation of g-CN nanosheet/FeOCl: Achievement and promoted photocatalytic nitrogen fixation activity. <i>Journal of Colloid and Interface Science</i> , 2021 , 587, 538-549	9.3	25
292	Photocatalytic degradation of different pollutants by the novel gCN-NS/Black-TiO ₂ heterojunction photocatalyst under visible light: Introducing a photodegradation model and optimization by response surface methodology (RSM). <i>Materials Chemistry and Physics</i> , 2021 , 258, 123912	4.4	27
291	Application of genetic algorithm and multivariate methods for the detection and measurement of milk-surfactant adulteration by attenuated total reflection and near-infrared spectroscopy. <i>Journal of the Science of Food and Agriculture</i> , 2021 , 101, 2696-2703	4.3	4
290	10-(4-Phenylpiperazine-1-carbonyl)acridin-9(10H)-ones and related compounds: Synthesis, antiproliferative activity and inhibition of tubulin polymerization. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2021 , 32, 127687	2.9	
289	Use of Molecular Docking as a Decision-Making Tool in Drug Discovery 2021 , 229-243		3
288	High-impressive separation of photoinduced charge carriers on step-scheme ZnO/ZnSnO ₃ /Carbon dots heterojunction with efficient activity in photocatalytic NH ₃ production. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2021 , 118, 140-151	5.3	14
287	exploration of novel protease inhibitors against coronavirus 2019 (COVID-19). <i>Informatics in Medicine Unlocked</i> , 2021 , 23, 100516	5.3	5

286	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. <i>Structural Chemistry</i> , 2021 , 32, 1571-1588	1.8	
285	g-C ₃ N ₄ -nanosheet/ZnCr ₂ O ₄ S-scheme heterojunction photocatalyst with enhanced visible-light photocatalytic activity for degradation of phenol and tetracycline. <i>Separation and Purification Technology</i> , 2021 , 118511	8.3	10
284	Molecular dynamics simulation, 3D-pharmacophore and scaffold hopping analysis in the design of multi-target drugs to inhibit potential targets of COVID-19. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021 , 1-22	3.6	1
283	Direct monitoring of diclofenac using a supramolecular fluorescent approach based on Cyclodextrin nanosponge. <i>Journal of Molecular Liquids</i> , 2021 , 336, 116104	6	5
282	Design and synthesis of novel quinazolinone-pyrazole derivatives as potential β -glucosidase inhibitors: Structure-activity relationship, molecular modeling and kinetic study. <i>Bioorganic Chemistry</i> , 2021 , 114, 105127	5.1	9
281	Facile and green preparation of colorimetric and fluorescent sensors for mercury, silver, and carbonate ions visual detecting: Spectroscopy and theoretical studies. <i>Journal of Molecular Structure</i> , 2021 , 1241, 130626	3.4	7
280	Orthogonality constrained inverse regression to improve model selectivity and analyte predictions from vibrational spectroscopic measurements. <i>Analytica Chimica Acta</i> , 2021 , 1185, 339073	6.6	1
279	Near-infrared spectroscopy and machine learning-based classification and calibration methods in detection and measurement of anionic surfactant in milk. <i>Journal of Food Composition and Analysis</i> , 2021 , 104, 104170	4.1	1
278	Exploratory and machine learning analysis of the stability constants of HgII- triazene ligands complexes. <i>Main Group Chemistry</i> , 2021 , 1-13	0.6	
277	Novel p β Heterojunction Nanocomposite: TiO ₂ QDs/ZnBi ₂ O ₄ Photocatalyst with Considerably Enhanced Photocatalytic Activity under Visible-Light Irradiation. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 27519-27528	3.8	24
276	Synthesis, characterization, and photocatalytic performance of Ag/AgFeO ₂ decorated on g-C ₃ N ₄ -nanosheet under the visible light irradiation. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2020 , 115, 279-292	5.3	20
275	Acrylamide content of collected food products from Tehran's market: a risk assessment study. <i>Environmental Science and Pollution Research</i> , 2020 , 27, 30558-30570	5.1	21
274	DeepCDA: deep cross-domain compound-protein affinity prediction through LSTM and convolutional neural networks. <i>Bioinformatics</i> , 2020 , 36, 4633-4642	7.2	29
273	Preparation of hierarchical g-C ₃ N ₄ @TiO ₂ hollow spheres for enhanced visible-light induced catalytic CO ₂ reduction. <i>Solar Energy</i> , 2020 , 205, 465-473	6.8	36
272	Deposited CuBi ₂ O ₄ and Bi ₃ ClO ₄ nanoparticles on g-C ₃ N ₄ nanosheet: a promising visible light-induced photocatalyst toward the removal of tetracycline hydrochloride and rhodamine B. <i>Journal of Materials Science</i> , 2020 , 55, 7775-7791	4.3	11
271	Molecular and clinical profile of congenital fibrinogen disorders in Iran, identification of two novel mutations. <i>International Journal of Laboratory Hematology</i> , 2020 , 42, 619-627	2.5	2
270	Fluorescence turn off-on probe (Cyclodextrin-hydroxyquinoline) for monitoring of Cd ions and tetracycline. <i>Methods and Applications in Fluorescence</i> , 2020 , 8, 025009	3.1	6
269	Investigation and determination of acrylamide in 24 types of roasted nuts and seeds using microextraction method coupled with gas chromatography/mass spectrometry: central composite design. <i>Journal of Food Measurement and Characterization</i> , 2020 , 14, 1249-1260	2.8	8

268	Developing a highly selective method for preconcentration and determination of cobalt in water and nut samples using 1-(2-pyridylazo)-2-naphthol and UV-visible spectroscopy. <i>Journal of the Science of Food and Agriculture</i> , 2020 , 100, 2272-2279	4.3	7
267	Sulfidic GO-grafted glass stir-bar as a noble metal ions adsorbent. <i>Microchemical Journal</i> , 2020 , 157, 104878	4.78	3
266	. <i>IEEE Sensors Journal</i> , 2020 , 20, 10138-10144	4	3
265	Enantioseparation and quantitative determination of ibuprofen using vancomycin-mediated capillary electrophoresis combined with molybdenum disulfide-assisted dispersive solid-phase extraction: optimization using experimental design. <i>Journal of the Iranian Chemical Society</i> , 2020 , 47, 1447-1457	2	2
264	Three Dimensional Quantitative Structure Activity Relationship and Pharmacophore Modeling of Tacrine Derivatives as Acetylcholinesterase Inhibitors in Alzheimer's Treatment. <i>Medicinal Chemistry</i> , 2020 , 16, 155-168	1.8	
263	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020 , 227, 117621	4.4	7
262	A dual-emission fluorescence probe for simultaneous quantification of CN ⁻ and CrO ₄ ²⁻ ions based on modified g-C ₃ N ₄ . <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2020 , 389, 112261	4.7	6
261	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. <i>Journal of Molecular Liquids</i> , 2020 , 300, 112350	6	6
260	Multi-view self-attention for interpretable drug-target interaction prediction. <i>Journal of Biomedical Informatics</i> , 2020 , 110, 103547	10.2	6
259	A highly sensitive fluorescence measurement of amphetamine using 8-hydroxyquinoline- β -cyclodextrin grafted on graphene oxide. <i>Diamond and Related Materials</i> , 2020 , 109, 108032	3.5	5
258	Acenaphtoquinoline as a selective fluorescent sensor for Hg (II) detection: experimental and theoretical studies. <i>Heliyon</i> , 2020 , 6, e04986	3.6	8
257	Simultaneous removal of crystal violet and methyl green in water samples by functionalised SBA-15. <i>International Journal of Environmental Analytical Chemistry</i> , 2020 , 1-17	1.8	5
256	Novel fused 1,2,3-triazolo-benzodiazepine derivatives as potent anticonvulsant agents: design, synthesis, in vivo, and in silico evaluations. <i>Molecular Diversity</i> , 2020 , 24, 179-189	3.1	8
255	Molecular dynamics simulation and 3D-pharmacophore analysis of new quinoline-based analogues with dual potential against EGFR and VEGFR-2. <i>International Journal of Biological Macromolecules</i> , 2020 , 142, 94-113	7.9	8
254	Anthracene modified graphene oxide-silica as an optical sensor for selective detection of Cu ²⁺ and I ⁻ ions. <i>International Journal of Environmental Analytical Chemistry</i> , 2020 , 100, 686-701	1.8	6
253	Application of the area correlation constraint in the MCR-ALS quantitative analysis of complex mixture samples. <i>Analytica Chimica Acta</i> , 2020 , 1113, 52-65	6.6	12
252	Lansoprazole-Based Colorimetric Chemosensor for Efficient Binding and Sensing of Carbonate Ion: Spectroscopy and DFT Studies. <i>Frontiers in Chemistry</i> , 2020 , 8, 626472	5	2
251	A highly selective Ag ⁺ sensor based on 8-hydroxyquinoline functionalized graphene oxide -silica nanosheet and its logic gate behaviour. <i>Journal of Materials Science: Materials in Electronics</i> , 2019 , 30, 17693-17705	2.1	5

250	SBA-Pr-SO ₃ H-catalyzed synthesis of bispyrazole compounds as anti-bacterial agents and inhibitors of phosphorylated RET tyrosine kinase. <i>Journal of the Iranian Chemical Society</i> , 2019 , 16, 1401-1409	2	5
249	Design of pyrimidine-based scaffolds as potential anticancer agents for human DHFR: three-dimensional quantitative structure–activity relationship by docking derived grid-independent descriptors. <i>Journal of the Iranian Chemical Society</i> , 2019 , 16, 2365-2378	2	1
248	Synthesis, experimental, quantum chemical and molecular dynamics study of carbon steel corrosion inhibition effect of two Schiff bases in HCl solution. <i>Journal of Molecular Liquids</i> , 2019 , 285, 626-639	6	44
247	Design and Synthesis of Novel Cytotoxic Indole-Thiosemicarbazone Derivatives: Biological Evaluation and Docking Study. <i>Chemistry and Biodiversity</i> , 2019 , 16, e1800470	2.5	7
246	Anti-cancer, anti-oxidant and molecular docking studies of thiosemicarbazone indole-based derivatives. <i>Research on Chemical Intermediates</i> , 2019 , 45, 2827-2854	2.8	19
245	Investigation and determination of acrylamide in the main group of cereal products using advanced microextraction method coupled with gas chromatography-mass spectrometry. <i>Journal of Cereal Science</i> , 2019 , 87, 157-164	3.8	29
244	Highly selective silica-based fluorescent nanosensor for ferric ion (Fe) detection in aqueous media. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019 , 218, 293-298	4.4	8
243	A highly selective magnetic solid-phase extraction method for preconcentration of Cd(II) using N,N'-bis(salicylidene)ethylenediamine in water and food samples. <i>Research on Chemical Intermediates</i> , 2019 , 45, 3141-3153	2.8	14
242	An ultrasensitive fluorescence sensor for determination of trace levels of copper in blood samples. <i>Analytical and Bioanalytical Chemistry</i> , 2019 , 411, 5593-5603	4.4	17
241	Inhibition activity prediction for a dataset of candidates' drug by combining fuzzy logic with MLR/ANN QSAR models. <i>Chemical Biology and Drug Design</i> , 2019 , 93, 1139-1157	2.9	3
240	Boron-doped graphitic carbon nitride as a novel fluorescent probe for mercury(II) and iron(III): a circuit logic gate mimic. <i>New Journal of Chemistry</i> , 2019 , 43, 12087-12093	3.6	14
239	Deep Transferable Compound Representation across Domains and Tasks for Low Data Drug Discovery. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 4528-4539	6.1	13
238	Identification of Essential 2D and 3D Chemical Features for Discovery of the Novel Tubulin Polymerization Inhibitors. <i>Current Topics in Medicinal Chemistry</i> , 2019 , 19, 1092-1120	3	3
237	Pharmacophore Modeling, Synthesis, Scaffold Hopping and Biological α -Hematin Inhibition Interaction Studies for Anti-malaria Compounds. <i>Current Topics in Medicinal Chemistry</i> , 2019 , 19, 2743-2755	2.5	6
236	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. <i>Journal of the Iranian Chemical Society</i> , 2019 , 16, 1411-1421	2	11
235	Voltammetric sensing of oxacillin by using a screen-printed electrode modified with molecularly imprinted polyaniline, gold nanourchins and graphene oxide. <i>Mikrochimica Acta</i> , 2019 , 186, 798	5.8	13
234	Voltammetric Electronic Tongue for the Simultaneous Determination of Three Benzodiazepines. <i>Sensors</i> , 2019 , 19,	3.8	9
233	Exploring 3D-QSPR models of human skin permeability for a diverse dataset of chemical compounds. <i>Journal of Receptor and Signal Transduction Research</i> , 2019 , 39, 442-450	2.6	

232	Efficient removal of malachite green from wastewater by using boron-doped mesoporous carbon nitride. <i>Applied Surface Science</i> , 2019 , 469, 236-245	6.7	45
231	Simultaneous determination of dihydroxybenzene isomers at nitrogen-doped graphene surface using fast Fourier transform square wave voltammetry and multivariate calibration. <i>Microchemical Journal</i> , 2019 , 145, 596-605	4.8	16
230	Probing the origin of dihydrofolate reductase inhibition via proteochemometric modeling. <i>Journal of Chemometrics</i> , 2019 , 33, e3090	1.6	4
229	Computer-aided molecular design of (E)-N-Aryl-2-ethene-sulfonamide analogues as microtubule targeted agents in prostate cancer. <i>Arabian Journal of Chemistry</i> , 2019 , 12, 2150-2165	5.9	4
228	Dynamic structure based pharmacophore modeling of the Acetylcholinesterase reveals several potential inhibitors. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019 , 37, 1800-1812	3.6	26
227	Simultaneous sensitive determination of benzenediol isomers using multiwall carbon nanotube/ionic liquid modified carbon paste electrode by a combination of artificial neural network and fast Fourier transform admittance voltammetry. <i>New Journal of Chemistry</i> , 2018 , 42, 6479-6487	3.6	8
226	High-throughput Docking and Molecular Dynamics Simulations towards the Identification of Novel Peptidomimetic Inhibitors against CDC7. <i>Molecular Informatics</i> , 2018 , 37, e1800022	3.8	2
225	Synthesis and cholinesterase inhibitory activity of new 2-benzofuran carboxamide-benzylpyridinium salts. <i>Bioorganic Chemistry</i> , 2018 , 80, 180-188	5.1	10
224	Docking of Natural Products against Neurodegenerative Diseases: General Concepts. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2018 , 21, 152-160	1.3	10
223	Combating Diseases with Computational Strategies Used for Drug Design and Discovery. <i>Current Topics in Medicinal Chemistry</i> , 2018 , 18, 2743-2773	3	12
222	In Silico Studies in Drug Research Against Neurodegenerative Diseases. <i>Current Neuropharmacology</i> , 2018 , 16, 664-725	7.6	34
221	The Effect of Single and Double Acetylation of Lysine Residues on Structural and Dynamical Features of Human Splicing Factor TDP-43 - A Statistical Ensemble Analysis. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2018 , 21, 358-373	1.3	
220	Synthesis of magnetically modified mesoporous nanoparticles and their application in simultaneous determination of Pb(II), Cd(II) and Cu(II). <i>Research on Chemical Intermediates</i> , 2018 , 44, 1689-1709	2.8	13
219	Computational Multi-Target Drug Design. <i>Methods in Pharmacology and Toxicology</i> , 2018 , 51-90	1.1	1
218	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. <i>Ecotoxicology and Environmental Safety</i> , 2018 , 158, 256-265	7	16
217	Chemometric analysis of comprehensive two dimensional gas chromatography-mass spectrometry metabolomics data. <i>Journal of Chromatography A</i> , 2017 , 1488, 113-125	4.5	42
216	Computer-aided drug design to explore cyclodextrin therapeutics and biomedical applications. <i>Chemical Biology and Drug Design</i> , 2017 , 89, 257-268	2.9	16
215	Receptor modeling of environmental aerosol data using MLPCA-MCR-ALS. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2017 , 167, 50-62	3.8	4

214	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. <i>Environmental Monitoring and Assessment</i> , 2017 , 189, 196	3.1	16
213	Characterization of the interaction of glycyrrhizin and glycyrrhetic acid with bovine serum albumin by spectrophotometric-gradient flow injection titration technique and molecular modeling simulations. <i>International Journal of Biological Macromolecules</i> , 2017 , 102, 92-103	7.9	5
212	3D QSAR studies, pharmacophore modeling, and virtual screening of diarylpyrazole-benzenesulfonamide derivatives as a template to obtain new inhibitors, using human carbonic anhydrase II as a model protein. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2017 , 32, 688-700	5.6	11
211	N-Heterocyclic (4-Phenylpiperazin-1-yl)methanones Derived from Phenoxazine and Phenothiazine as Highly Potent Inhibitors of Tubulin Polymerization. <i>Journal of Medicinal Chemistry</i> , 2017 , 60, 749-766	8.3	22
210	An intelligent readout integrated circuit (iROIC) with on-chip local gradient operations 2017 ,		1
209	Formulation and Development of a New Prebiotic Cereal-based Dairy Dessert: Rheological, Sensory and Physical Attributes. <i>Food Science and Technology Research</i> , 2017 , 23, 637-649	0.8	4
208	Optimization of Influential Factors on the Photocatalytic Performance of TiO ₂ /Graphene Composite in Degradation of an Organic Dye by RSM Methodology. <i>Journal of Cluster Science</i> , 2017 , 28, 2979-2995	3	10
207	Simultaneous determination of binary solution of triphenylmethane dyes in complex matrices onto magnetic amino-rich SWCNT using second-order calibration method. <i>Environmental Monitoring and Assessment</i> , 2017 , 189, 594	3.1	7
206	Spectroscopic and molecular modeling studies on the interactions of some benzofuran derivatives with BSA. <i>Monatshefte für Chemie</i> , 2017 , 148, 1887-1896	1.4	1
205	Graphene oxide/izarin yellow R/magnetic chitosan nanocomposite: a selective and efficient sorbent for sub-trace determination of aluminum in water samples. <i>Analytical Methods</i> , 2017 , 9, 222-231	3.2	16
204	Proteochemometric Modeling of the Interaction Space of Carbonic Anhydrase and its Inhibitors: An Assessment of Structure-based and Sequence-based Descriptors. <i>Molecular Informatics</i> , 2017 , 36, 1600102	2.8	10
203	Predicting Degradation Half-life of Organophosphorus Pesticides in Soil Using Three-Dimensional Molecular Interaction Fields. <i>International Journal of Quantitative Structure-Property Relationships</i> , 2017 , 2, 27-35	1.2	1
202	Computer Aided Drug Design for Multi-Target Drug Design: SAR /QSAR, Molecular Docking and Pharmacophore Methods. <i>Current Drug Targets</i> , 2017 , 18, 556-575	3	58
201	Dual-acting of Hybrid Compounds - A New Dawn in the Discovery of Multi-target Drugs: Lead Generation Approaches. <i>Current Topics in Medicinal Chemistry</i> , 2017 , 17, 1096-1114	3	16
200	Comparison of three sensory characterization methods based on consumer perception for the development of a novel functional cereal-based dessert. <i>AIMS Agriculture and Food</i> , 2017 , 2, 258-278	1.2	5
199	Molecular Docking Challenges and Limitations 2017 , 770-794		3
198	Alignment independent 3D-QSAR, quantum calculations and molecular docking of Mer specific tyrosine kinase inhibitors as anticancer drugs. <i>Saudi Pharmaceutical Journal</i> , 2016 , 24, 197-212	4.4	8
197	Using Wavelet Analysis To Assist in Identification of Significant Events in Molecular Dynamics Simulations. <i>Journal of Chemical Information and Modeling</i> , 2016 , 56, 1282-91	6.1	8

196	Extraction optimization of pepsin-soluble collagen from eggshell membrane by response surface methodology (RSM). <i>Food Chemistry</i> , 2016 , 190, 186-193	8.5	78
195	Multivariate optimization, preconcentration and determination of mercury ions with (1-(p-acetyl phenyl)-3-(o-methyl benzoate)) triazene in aqueous samples using ICP-AES. <i>Analytical Methods</i> , 2016 , 8, 1111-1119	3.2	11
194	Molecular Docking Challenges and Limitations. <i>Advances in Medical Technologies and Clinical Practice Book Series</i> , 2016 , 56-80	0.3	2
193	Quantitative Characterization of the Interaction Space of the Mammalian Carbonic Anhydrase Isoforms I, II, VII, IX, XII, and XIV and their Inhibitors, Using the Proteochemometric Approach. <i>Chemical Biology and Drug Design</i> , 2016 , 88, 341-53	2.9	14
192	QSPR approaches to elucidate the stability constants between β -cyclodextrin and some organic compounds: Docking based 3D conformer. <i>Journal of Molecular Liquids</i> , 2016 , 219, 1036-1043	6	4
191	Thermodynamic study of β -cyclodextrin-dye inclusion complexes using gradient flow injection technique and molecular modeling. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016 , 165, 54-60	4.4	5
190	Experimental, computational and chemometrics studies of BSA-vitamin B6 interaction by UV-Vis, FT-IR, fluorescence spectroscopy, molecular dynamics simulation and hard-soft modeling methods. <i>Bioorganic Chemistry</i> , 2016 , 68, 124-36	5.1	46
189	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. <i>Environmental Monitoring and Assessment</i> , 2015 , 187, 149	3.1	8
188	Large-Area Semiconducting Graphene Nanomesh Tailored by Interferometric Lithography. <i>Scientific Reports</i> , 2015 , 5, 11463	4.9	22
187	3D-QSAR and virtual screening studies in identification of new Rho kinase inhibitors with different scaffolds. <i>Journal of the Iranian Chemical Society</i> , 2015 , 12, 1945-1959	2	10
186	Experimental and theoretical investigation effect of flavonols antioxidants on DNA damage. <i>Analytica Chimica Acta</i> , 2015 , 887, 82-91	6.6	15
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