

Mohammad Reza Bozorgmehr

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91
papers

1,021
citations

17
h-index

28
g-index

100
ext. papers

1,212
ext. citations

3.1
avg, IF

4.93
L-index

#	Paper	IF	Citations
91	How a protein can remain stable in a solvent with high content of urea: insights from molecular dynamics simulation of <i>Candida antarctica</i> lipase B in urea : choline chloride deep eutectic solvent. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 14882-93	3.6	138
90	Simultaneous detection and determination of mercury (II) and lead (II) ions through the achievement of novel functional nucleic acid-based biosensors. <i>Biosensors and Bioelectronics</i> , 2018 , 116, 130-147	11.8	77
89	Synthesis of nano curcumin using black pepper oil by O/W Nanoemulsion Technique and investigation of their biological activities. <i>LWT - Food Science and Technology</i> , 2018 , 92, 92-100	5.4	39
88	A simple paper-based aptasensor for ultrasensitive detection of lead (II) ion. <i>Analytica Chimica Acta</i> , 2019 , 1071, 70-77	6.6	35
87	Structural behavior of <i>Candida antarctica</i> lipase B in water and supercritical carbon dioxide: A molecular dynamic simulation study. <i>Journal of Supercritical Fluids</i> , 2012 , 63, 180-186	4.2	32
86	Investigation of the behavior of HSA upon binding to amlodipine and propranolol: Spectroscopic and molecular modeling approaches. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 85, 79-84	4.4	31
85	Analysis of ligand binding to proteins using molecular dynamics simulations. <i>Journal of Theoretical Biology</i> , 2008 , 254, 294-300	2.3	31
84	Enzyme is stabilized by a protection layer of ionic liquids in supercritical CO ₂ : Insights from molecular dynamic simulation. <i>Journal of Supercritical Fluids</i> , 2012 , 69, 1-7	4.2	30
83	Quantum chemical studies of chitosan nanoparticles as effective drug delivery systems for 5-fluorouracil anticancer drug. <i>Journal of Molecular Liquids</i> , 2020 , 302, 112495	6	30
82	The influence of the flavonoid quercetin on the interaction of propranolol with human serum albumin: Experimental and theoretical approaches. <i>Journal of Luminescence</i> , 2014 , 154, 229-240	3.8	29
81	Calculation of solubility of methimazole, phenazopyridine and propranolol in supercritical carbon dioxide. <i>Journal of Supercritical Fluids</i> , 2008 , 43, 390-397	4.2	29
80	Synthesis, characterization and interaction of N,NRdipyridoxyl (1,4-butanediamine) Co(III) salen complex with DNA and HSA. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012 , 97, 74-82	4.4	28
79	Conformational switch of insulin-binding aptamer into G-quadruplex induced by K ⁺ and Na ⁺ : an experimental and theoretical approach. <i>Journal of Biomolecular Structure and Dynamics</i> , 2015 , 33, 1153-63	3.6	27
78	Molecular crowding effects on conformation and stability of G-quadruplex DNA structure: insights from molecular dynamics simulation. <i>Journal of Theoretical Biology</i> , 2015 , 364, 103-12	2.3	26
77	Comprehensive quantum chemical insight into the mechanistic understanding of the surface functionalization of carbon nanotube as a nanocarrier with cladribine anticancer drug. <i>Applied Surface Science</i> , 2018 , 462, 720-729	6.7	24
76	Soybean oil-based nanoemulsion systems in absence and presence of curcumin: Molecular dynamics simulation approach. <i>Journal of Molecular Liquids</i> , 2018 , 264, 242-252	6	21
75	How Can a Free Amino Acid Stabilize a Protein? Insights from Molecular Dynamics Simulation. <i>Journal of Solution Chemistry</i> , 2015 , 44, 45-53	1.8	17

74	Joule-Thomson inversion curve prediction by using equation of state. <i>Chinese Chemical Letters</i> , 2007 , 18, 1154-1158	8.1	17
73	A comparison among three equations of state in predicting the solubility of some solids in supercritical carbon dioxide. <i>Korean Journal of Chemical Engineering</i> , 2007 , 24, 102-105	2.8	17
72	An efficient and high-yielding one-pot synthesis of 1H-pyrazolo[1,2-b]phthalazine-5,10-diones catalyzed by sodium hydrogen carbonate under solvent-free conditions. <i>Oriental Journal of Chemistry</i> , 2015 , 31, 2153-2158	0.8	17
71	Molecular mechanism study of surface functionalization of silica nanoparticle as an anticancer drug nanocarrier in aqueous solution. <i>Journal of Molecular Liquids</i> , 2019 , 282, 392-400	6	15
70	Influence of Taxifolin on the Human Serum Albumin-Proprietary Interaction: Multiple Spectroscopic and Chemometrics Investigations and Molecular Dynamics Simulation. <i>Journal of Solution Chemistry</i> , 2016 , 45, 265-285	1.8	14
69	Simultaneous extraction and preconcentration of aniline, phenol, and naphthalene using magnetite-graphene oxide composites before gas chromatography determination. <i>Journal of Separation Science</i> , 2016 , 39, 3046-53	3.4	14
68	Transport properties of mixtures composed of acetone, water, and supercritical carbon dioxide by molecular dynamics simulation. <i>Journal of Supercritical Fluids</i> , 2017 , 130, 321-326	4.2	13
67	Effects of synergistic and non-synergistic anions on the iron binding site from serum transferrin: A molecular dynamic simulation analysis. <i>Journal of Molecular Graphics and Modelling</i> , 2017 , 78, 176-186	2.8	12
66	Spectroscopic and DFT investigation of interactions between cyclophosphamide and aspirin with lysozyme as binary and ternary systems. <i>Journal of Biomolecular Structure and Dynamics</i> , 2015 , 33, 1669-81	3.6	12
65	DFT study of SiO ₂ nanoparticles as a drug delivery system: structural and mechanistic aspects. <i>Structural Chemistry</i> , 2019 , 30, 715-726	1.8	12
64	Structural properties of the truncated and wild types of Taka-amylase: A molecular dynamics simulation and docking study. <i>Journal of Molecular Catalysis B: Enzymatic</i> , 2013 , 95, 36-40		11
63	Theoretical design and experimental study of new aptamers with the improved target-affinity: New insights into the Pb ²⁺ -specific aptamers as a case study. <i>Journal of Molecular Liquids</i> , 2019 , 289, 111159	6	10
62	The study of sodium dodecyl sulfate self-assembly behavior at three different concentrations in the presence and absence of lysozyme: Molecular dynamics simulation approach. <i>Journal of Molecular Liquids</i> , 2014 , 199, 184-189	6	10
61	Fast Synthesis and Antibacterial Evaluation of Benzimidazo[2,1-b]quinazolin-1-ones: Another Successful Application of Newly Prepared SO ₃ H-Functionalized Ionic Liquids as Catalysts. <i>Organic Preparations and Procedures International</i> , 2017 , 49, 236-248	1.1	9
60	Quantum chemical modeling of iron oxide magnetic nanoparticles functionalized with cytarabine. <i>Chemical Physics Letters</i> , 2019 , 719, 12-21	2.5	9
59	The effect of glycosylation on the transferrin structure: A molecular dynamic simulation analysis. <i>Journal of Theoretical Biology</i> , 2016 , 404, 73-81	2.3	9
58	Comparative study of the effects of the structurally similar flavonoids quercetin and taxifolin on the therapeutic behavior of alprazolam. <i>Canadian Journal of Chemistry</i> , 2016 , 94, 458-469	0.9	9
57	Synthesis of 1H,7H,12bH-Pyrano[3',4': 5,6]pyrano[3,4-c][1]benzopyran-1-one via Domino Knoevenagel/Hetero-Diels-Alder Reaction with Theoretical Investigations. <i>Helvetica Chimica Acta</i> , 2012 , 95, 52-60	2	9

56	Evaluation of PVT differential properties of the Lennard-Jones fluid using radial distribution functions and molecular dynamics. <i>Chemical Physics</i> , 2007 , 335, 194-200	2.3	9
55	Development of a New Magnetic Dispersive Solid-Phase Microextraction Coupled with GC-MS for the Determination of Five Organophosphorus Pesticides from Vegetable Samples. <i>Food Analytical Methods</i> , 2021 , 14, 674-686	3.4	9
54	Application of response surface modeling and chemometrics methods for the determination of Atenolol, Metoprolol and Propranolol in blood sample using dispersive liquid-liquid microextraction combined with HPLC-DAD. <i>Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences</i> , 2019 , 1132, 121823	3.2	8
53	Prediction of the Solubility of Cholesterol and its Esters in Supercritical Carbon Dioxide. <i>Chemical Engineering and Technology</i> , 2006 , 29, 1481-1486	2	8
52	Oleuropein interactions with inner and outer surface of different types of carbon nanotubes: Insights from molecular dynamic simulation. <i>Journal of Molecular Liquids</i> , 2017 , 241, 367-373	6	7
51	All atom molecular dynamics simulation study of polyethylene polymer in supercritical water, supercritical ethanol and supercritical methanol. <i>Journal of Supercritical Fluids</i> , 2014 , 86, 124-128	4.2	7
50	Microextraction and gas chromatography-flame ionization determination of five antiepileptic drugs in biological samples using amino acid-based deep eutectic ionic liquids. <i>Journal of Molecular Liquids</i> , 2020 , 317, 113979	6	7
49	Conformation changes and diffusion of α -amylase in 1-hexyle-3-methylimidazolium chloride ionic liquid: A molecular dynamics simulation perspective. <i>Journal of Molecular Liquids</i> , 2016 , 221, 463-468	6	6
48	The effect of different alcohols on the Asp23-Lys28 and Asp23-Ala42 salt bridges of the most effective peptide in Alzheimer's disease: Molecular dynamics viewpoints. <i>Journal of Molecular Graphics and Modelling</i> , 2019 , 86, 199-208	2.8	6
47	Tautomerization Reaction, Experimental and Theoretical Characterizations of the N,N'-Dipyridoxyl(4-Methyl-1,2-Phenylenediamine) Schiff Base and its Cu(II) Complex. <i>Journal of Structural Chemistry</i> , 2018 , 59, 1102-1113	0.9	6
46	An environmentally friendly sample pre-treatment method based on magnetic ionic liquids for trace determination of nitrotoluene compounds in soil and water samples by gas chromatography-mass spectrometry using response surface methodology. <i>Chemical Papers</i> , 2020 , 74, 2929-2943	1.9	5
45	Quantum Mechanical Study on the Mechanistic, Energetic, and Structural Properties of Adsorption of 6-Thioguanine onto Fe ₂ O ₃ Nanoparticles. <i>Bulletin of the Korean Chemical Society</i> , 2017 , 38, 869-874	1.2	5
44	The study of self-aggregation behavior of the bilirubin molecules in the presence and absence of carbon nanotubes: Molecular dynamics simulation approach. <i>Journal of Molecular Liquids</i> , 2015 , 208, 342-346	6	5
43	Determination of Tramadol and Fluoxetine in Biological and Water Samples by Magnetic Dispersive Solid-Phase Microextraction (MDSPME) with Gas Chromatography [Mass Spectrometry (GC-MS). <i>Analytical Letters</i> , 2021 , 54, 884-902	2.2	5
42	Does high pressure have any effect on the structure of alpha amylase and its ability to binding to the oligosaccharides having 3-7 residues? Molecular dynamics study. <i>Journal of Molecular Graphics and Modelling</i> , 2018 , 80, 85-94	2.8	4
41	Study of the effects of methanol, ethanol and propanol alcohols as Co-solvents on the interaction of methimazole, propranolol and phenazopyridine with carbon dioxide in supercritical conditions by molecular dynamics. <i>Journal of Supercritical Fluids</i> , 2018 , 140, 91-100	4.2	4
40	Synthesis of New Functionalized 1,4-Dihydroquinolines and Pyrimido[4,5-b]quinolines. <i>Russian Journal of General Chemistry</i> , 2017 , 87, 2961-2965	0.7	4
39	The investigation of the G-quadruplex aptamer selectivity to Pb ion: a joint molecular dynamics simulation and density functional theory study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020 , 38, 3659-3675	3.6	4

38	Temperature and molecular crowding effects on the sensitivity of T30695 aptamer toward Pb ²⁺ ion: a joint molecular dynamics simulation and experimental study. <i>Molecular Simulation</i> , 2020 , 46, 592-603	2.0	4
37	Evaluation of catalytic activity of two newly prepared functionalized sulfonic acids ionic liquids in the synthesis of carbamatoalkyl naphthols under mild conditions. <i>Russian Journal of General Chemistry</i> , 2017 , 87, 311-315	0.7	3
36	Mechanistic, Energetic and Structural Studies of Fe ₂ O ₃ Nanoparticles Functionalized with Drug Artemisinin. <i>Russian Journal of Inorganic Chemistry</i> , 2019 , 64, 503-510	1.5	3
35	Quantum molecular study of mesoporous silica nanoparticle as a delivery system for troxacitabine anticancer drug. <i>Journal of Molecular Liquids</i> , 2020 , 310, 113155	6	3
34	Effects of the deglycosylation on the structure and activity of chloroperoxidase: Molecular dynamics simulation approach. <i>Journal of Molecular Graphics and Modelling</i> , 2020 , 97, 107570	2.8	3
33	Kinetics and mechanism of the 1,3-dipolar cycloaddition of nitrilimine with thione-containing dipolarophile: a detailed DFT study. <i>Research on Chemical Intermediates</i> , 2016 , 42, 6125-6141	2.8	3
32	Evaluation of attraction terms in equations of state on the prediction of solubility of some biomolecules in supercritical carbon dioxide. <i>Chinese Chemical Letters</i> , 2009 , 20, 501-505	8.1	3
31	Role of repulsive forces on self-assembly behavior of amyloid peptide (1-40): Molecular dynamics simulation approach. <i>Physica A: Statistical Mechanics and Its Applications</i> , 2019 , 513, 524-535	3.3	3
30	Molecular dynamics simulations on the heterocyclic cyclodecapeptide and its linear analogous in water and octanol solvents. <i>Journal of Molecular Liquids</i> , 2017 , 229, 583-590	6	2
29	Density Functional Theoretical Study on the Mechanism of Alcoholysis of Acylpalladium(II) Complexes. <i>Progress in Reaction Kinetics and Mechanism</i> , 2017 , 42, 52-61	0.5	2
28	Structure-activity relationship for Fe(III)-salen-like complexes as potent anticancer agents. <i>Scientific World Journal, The</i> , 2014 , 2014, 745649	2.2	2
27	Self-association process of tetracycline antibiotic in different aqueous solutions: a joint experimental study and molecular dynamics simulation. <i>Journal of the Iranian Chemical Society</i> , 2020 , 17, 2997-3007	2	2
26	Theoretical Study on the Mechanism of Covalent Bonding of Dapsone onto Functionalised Carbon Nanotubes: Effects of Coupling Agent. <i>Progress in Reaction Kinetics and Mechanism</i> , 2016 , 41, 345-355	0.5	2
25	Quantum chemical analysis of 5-aminolevulinic acid anticancer drug delivery systems: Carbon nanotube, HOOH functionalized carbon nanotube and iron oxide nanoparticle. <i>Journal of Molecular Liquids</i> , 2021 , 340, 117182	6	2
24	Reverse Micelle Surfactant System Comprising the 1-decanoyl-rac-glycerol and the Lauryldimethylamine-N-oxide: Structure and Dynamics of Confined Water. <i>Russian Journal of Physical Chemistry A</i> , 2019 , 93, 1122-1127	0.7	1
23	Study of alpha-amylase and gold nanoparticles interaction at two different temperatures through molecular dynamics. <i>Journal of Molecular Graphics and Modelling</i> , 2019 , 88, 273-281	2.8	1
22	Radial distribution function within the framework of the Tsallis statistical mechanics. <i>Physica A: Statistical Mechanics and Its Applications</i> , 2018 , 506, 857-867	3.3	1
21	A molecular dynamics study on the liquid SbCl ₅ and SbF ₅ using force fields derived from quantum chemical calculations. <i>Physics and Chemistry of Liquids</i> , 2013 , 51, 695-703	1.5	1

20	Determination of benzene, toluene, ethylbenzene, and p-xylene with headspace-hollow fiber solid-phase microextraction-gas chromatography in wastewater and Buxus leaves, employing a chemometric approach. <i>Chemical Papers</i> , 2021 , 75, 4305-4316	1.9	1
19	Investigating the effect of 1-Butyl-3-methylimidazolium bromide and 1-Butyl-3-methylimidazolium methyl sulfate ionic liquids on structure and function of Chloroperoxidase by molecular dynamics simulation. <i>Journal of Molecular Liquids</i> , 2021 , 332, 115850	6	1
18	Determination of Thermodynamics Constant of Interaction among of Atenolol and Metoprolol with Human Serum Albumin: Spectroscopic and Molecular Modeling Approaches. <i>Russian Journal of Physical Chemistry A</i> , 2021 , 95, 1269-1276	0.7	1
17	Acetyl-11-keto-Eboswellic acid derivatives effects on 5-lipoxygenase: In silico viewpoint. <i>Journal of Molecular Graphics and Modelling</i> , 2020 , 94, 107464	2.8	1
16	A Theoretical Investigation on the Regioselectivity of the Diels-Alder Cycloaddition of 9-(Methoxymethyl) Anthracene And Citraconic Anhydride. <i>Journal of Structural Chemistry</i> , 2018 , 59, 1810-1817 ¹	0.9	1
15	Biosensor Properties of DA-DA Dinucleotide in the Presence of DI-L-Lysine and Single Carbon Nanotubes: Molecular Dynamics Simulation and Density Functional Theory Approach. <i>Journal of Structural Chemistry</i> , 2018 , 59, 1228-1235	0.9	1
14	Synthesis, Experimental and Theoretical Studies on N,N'-Dipyridoxyl(4-Chloro-1,2-Phenylenediamine) Tetradentate Ligand and Its Copper(II) Complex. <i>Journal of Structural Chemistry</i> , 2019 , 60, 1243-1255	0.9	0
13	The effect of sodium dodecyl sulfate concentration on the aggregation behavior of A α (1-42) peptide: Molecular dynamics simulation approach. <i>Journal of Molecular Liquids</i> , 2020 , 303, 112651	6	0
12	Mechanistic, energetic and structural studies of carbon nanotubes functionalised with dihydroartemisinin drug in gas and solution phases. <i>Physics and Chemistry of Liquids</i> , 2018 , 56, 610-618	1.5	0
11	Effect of Lysyllysine on non-covalent hybridization of single walled carbon nanotube by single-stranded DNA homodimer: in silico approach. <i>Journal of Nanostructure in Chemistry</i> , 2019 , 9, 315-321	7.6	0
10	(E)-4-(((2-amino-5-chlorophenyl)imino)methyl)-5-(hydroxy-methyl)-2-methylpyridin-3-ol and its Cu(II) complex: Synthesis, DFT calculations and AIM analysis. <i>Journal of the Serbian Chemical Society</i> , 2020 , 85, 1033-1046	0.9	0
9	Theoretical Design and Experimental Study of New Aptamers with the Enhanced Binding Affinity Relying on Colorimetric Assay for Tetracycline Detection. <i>Journal of Molecular Liquids</i> , 2021 , 349, 118196 ⁶	6	0
8	β-cyclodextrin-lenalidomide anticancer drug delivery nanosystem: A quantum chemical approach. <i>Journal of Molecular Liquids</i> , 2021 , 344, 117762	6	0
7	Mechanistic and energetic studies of superparamagnetic iron oxide nanoparticles as a cyclophosphamide anticancer drug nanocarrier: A quantum mechanical approach. <i>Progress in Reaction Kinetics and Mechanism</i> , 2019 , 44, 92-101	0.5	
6	Characterization and Molecular Docking Study of New 4-Acetamidoalkyl Pyrazoles As B-Raf /Cox-2 Inhibitors. <i>Journal of Structural Chemistry</i> , 2018 , 59, 335-343	0.9	
5	The Effect of Temperature on the Interaction of Phenanthroline-based Ligands with G-quadruplex: In Silico Viewpoint. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2019 , 22, 546-554	1.3	
4	Flavodoxin in a binary surfactant system consisting of the nonionic 1-decanoyl-rac-glycerol and the zwitterionic lauryldimethylamine-N-oxide: molecular dynamics simulation approach. <i>Papers in Physics</i> , 2012 , 12, 120004		
3	Does the single-walled carbon nanotube affect the rate constant of binding of biotin to streptavidin? Molecular dynamics simulation perspective. <i>Progress in Reaction Kinetics and Mechanism</i> , 2019 , 44, 234-243	0.5	

- 2 Non-Covalent Hybridization of Carbon Nanotube by Single-Stranded DNA Homodecamers: in-silico Approach. *Russian Journal of Physical Chemistry A*, **2022**, 96, 145-151 0.7
- 1 Synthesis of Heterocyclic Systems 3H-furo[2,3-b]imidazo[4,5-f]quinolines and 3H-furo[2,3-b]pyrazolo[4,3-f]quinolines as New Antibacterial Agents. *Pharmaceutical Chemistry Journal*, 1 0.9