Mohammad Reza Bozorgmehr

List of Publications by Year
in descending order

99 papers	1,442 citations	361045 20 h-index	377514 34 g-index
100 all docs	100 docs citations	100 times ranked	1806 citing authors

#	Article	IF	Citations
1	How a protein can remain stable in a solvent with high content of urea: insights from molecular dynamics simulation of Candida antarctica lipase B in ureaâ€‰:â€‰choline chloride deep eutectic solvent. Physical Chemistry Chemical Physics, 2014, 16, 14882.	1.3	191
2	Simultaneous detection and determination of mercury (II) and lead (II) ions through the achievement of novel functional nucleic acid-based biosensors. Biosensors and Bioelectronics, 2018, 116, 130-147.	5.3	115
3	Synthesis of nano curcumin using black pepper oil by O/W Nanoemulsion Technique and investigation of their biological activities. LWT - Food Science and Technology, 2018, 92, 92-100.	2.5	68
4	A simple paper-based aptasensor for ultrasensitive detection of lead (II) ion. Analytica Chimica Acta, 2019, 1071, 70-77.	2.6	61
5	Quantum chemical studies of chitosan nanoparticles as effective drug delivery systems for 5-fluorouracil anticancer drug. Journal of Molecular Liquids, 2020, 302, 112495.	2.3	43
6	Structural behavior of Candida antarctica lipase B in water and supercritical carbon dioxide: A molecular dynamic simulation study. Journal of Supercritical Fluids, 2012, 63, 180-186.	1.6	41
7	Analysis of ligand binding to proteins using molecular dynamics simulations. Journal of Theoretical Biology, 2008, 254, 294-300.	0.8	36
8	Enzyme is stabilized by a protection layer of ionic liquids in supercritical CO2: Insights from molecular dynamic simulation. Journal of Supercritical Fluids, 2012, 69, 1-7.	1.6	36
9	Investigation of the behavior of HSA upon binding to amlodipine and propranolol: Spectroscopic and molecular modeling approaches. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 85, 79-84.	2.0	36
10	The influence of the flavonoid quercetin on the interaction of propranolol with human serum albumin: Experimental and theoretical approaches. Journal of Luminescence, 2014, 154, 229-240.	1.5	34
11	Comprehensive quantum chemical insight into the mechanistic understanding of the surface functionalization of carbon nanotube as a nanocarrier with cladribine anticancer drug. Applied Surface Science, 2018, 462, 720-729.	3.1	34
12	Calculation of solubility of methimazole, phenazopyridine and propranolol in supercritical carbon dioxide. Journal of Supercritical Fluids, 2008, 43, 390-397.	1.6	31
13	Synthesis, characterization and interaction of N,Nâ€²-dipyridoxyl (1,4-butanediamine) Co(III) salen complex with DNA and HSA. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 97, 74-82.	2.0	31
14	Molecular crowding effects on conformation and stability of G-quadruplex DNA structure: Insights from molecular dynamics simulation. Journal of Theoretical Biology, 2015, 364, 103-112.	0.8	30
15	Conformational switch of insulin-binding aptamer into G-quadruplex induced by K⁺and Na⁺: an experimental and theoretical approach. Journal of Biomolecular Structure and Dynamics, 2015, 33, 1153-1163.	2.0	29
16	Soybean oil-based nanoemulsion systems in absence and presence of curcumin: Molecular dynamics simulation approach. Journal of Molecular Liquids, 2018, 264, 242-252.	2.3	28
17	How Can a Free Amino Acid Stabilize a Protein? Insights from Molecular Dynamics Simulation. Journal of Solution Chemistry, 2015, 44, 45-53.	0.6	25
18	Development of a New Magnetic Dispersive Solid-Phase Microextraction Coupled with GC-MS for the Determination of Five Organophosphorus Pesticides from Vegetable Samples. Food Analytical Methods, 2021, 14, 674-686.	1.3	23

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19	Jouleâ€“Thomson inversion curve prediction by using equation of state. Chinese Chemical Letters, 2007, 18, 1154-1158.	4.8	22
20	DFT study of SiO2 nanoparticles as a drug delivery system: structural and mechanistic aspects. Structural Chemistry, 2019, 30, 715-726.	1.0	21
21	Application of response surface modeling and chemometrics methods for the determination of Atenolol, Metoprolol and Propranolol in blood sample using dispersive liquidâ€“liquid microextraction combined with HPLC-DAD. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2019, 1132, 121823.	1.2	20
22	Molecular mechanism study of surface functionalization of silica nanoparticle as an anticancer drug nanocarrier in aqueous solution. Journal of Molecular Liquids, 2019, 282, 392-400.	2.3	20
23	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. Oriental Journal of Chemistry, 2015, 31, 2153-2158.	0.1	20
24	A comparison among three equations of state in predicting the solubility of some solids in supercritical carbon dioxide. Korean Journal of Chemical Engineering, 2007, 24, 102-105.	1.2	19
25	Simultaneous extraction and preconcentration of aniline, phenol, and naphthalene using magnetiteâ€“graphene oxide composites before gas chromatography determination. Journal of Separation Science, 2016, 39, 3046-3053.	1.3	18
26	Transport properties of mixtures composed of acetone, water, and supercritical carbon dioxide by molecular dynamics simulation. Journal of Supercritical Fluids, 2017, 130, 321-326.	1.6	17
27	Influence ofÂTaxifolinÂon the Human Serum Albuminâ€“PropranololÂInteraction:ÂMultiple Spectroscopic and Chemometrics Investigations and Molecular Dynamics Simulation. Journal of Solution Chemistry, 2016, 45, 265-285.	0.6	16
28	Theoretical design and experimental study of new aptamers with the improved target-affinity: New insights into the Pb2+-specific aptamers as a case study. Journal of Molecular Liquids, 2019, 289, 111159.	2.3	16
29	The effect of glycosylation on the transferrin structure: A molecular dynamic simulation analysis. Journal of Theoretical Biology, 2016, 404, 73-81.	0.8	15
30	Effects of synergistic and non-synergistic anions on the iron binding site from serum transferrin: A molecular dynamic simulation analysis. Journal of Molecular Graphics and Modelling, 2017, 78, 176-186.	1.3	15
31	Microextraction and gas chromatographyâ€“flame ionization determination of five antiepileptic drugs in biological samples using amino acid-based deep eutectic ionic liquids. Journal of Molecular Liquids, 2020, 317, 113979.	2.3	15
32	Spectroscopic and DFT investigation of interactions between cyclophosphamide and aspirin with lysozyme as binary and ternary systems. Journal of Biomolecular Structure and Dynamics, 2015, 33, 1669-1681.	2.0	14
33	Quantum chemical analysis of 5-aminolevulinic acid anticancer drug delivery systems: Carbon nanotube, â€“COOH functionalized carbon nanotube and iron oxide nanoparticle. Journal of Molecular Liquids, 2021, 340, 117182.	2.3	14
34	Structural properties of the truncated and wild types of Taka-amylase: A molecular dynamics simulation and docking study. Journal of Molecular Catalysis B: Enzymatic, 2013, 95, 36-40.	1.8	12
35	The study of sodium dodecyl sulfate self-assembly behavior at three different concentrations in the presence and absence of lysozyme: Molecular dynamics simulation approach. Journal of Molecular Liquids, 2014, 199, 184-189.	2.3	11
36	Quantum chemical modeling of iron oxide magnetic nanoparticles functionalized with cytarabine. Chemical Physics Letters, 2019, 719, 12-21.	1.2	11

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37	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. Journal of Molecular Graphics and Modelling, 2019, 86, 199-208.	1.3	11
38	The investigation of the G-quadruplex aptamer selectivity to Pb²⁺ ion: a joint molecular dynamics simulation and density functional theory study. Journal of Biomolecular Structure and Dynamics, 2020, 38, 3659-3675.	2.0	11
39	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 chromatographyâ€“mass spectrometry using response surface methodology. Chemical Papers, 2020, 74, 2929-2943.	1.0	11
40	Evaluation of Pâ€“Vâ€“T differential properties of the Lennard-Jones fluid using radial distribution functions and molecular dynamics. Chemical Physics, 2007, 335, 194-200.	0.9	10
41	Synthesis of 1H,7H,12bHâ€Pyrano[3â€²,4â€²:â€‰5,6]pyrano[3,4â€c][1]benzopyranâ€1â€one via Domino Knoevenagel/Heteroâ€Dielsï£¿Alder Reaction with Theoretical Investigations. Helvetica Chimica Acta, 2012, 95, 52-60.	1.0	10
42	Comparative study of the effects of the structurally similar flavonoids quercetin and taxifolin on the therapeutic behavior of alprazolam. Canadian Journal of Chemistry, 2016, 94, 458-469.	0.6	10
43	Fast Synthesis and Antibacterial Evaluation of Benzimidazo[2,1-b]quinazolin-1-ones: Another Successful Application of Newly Prepared SO₃H-Functionalized Ionic Liquids as Catalysts. Organic Preparations and Procedures International, 2017, 49, 236-248.	0.6	10
44	All atom molecular dynamics simulation study of polyethylene polymer in supercritical water, supercritical ethanol and supercritical methanol. Journal of Supercritical Fluids, 2014, 86, 124-128.	1.6	9
45	Temperature and molecular crowding effects on the sensitivity of T30695 aptamer toward Pb²⁺ion: a joint molecular dynamics simulation and experimental study. Molecular Simulation, 2020, 46, 592-603.	0.9	9
46	Determination of Tramadol and Fluoxetine in Biological and Water Samples by Magnetic Dispersive Solid-Phase Microextraction (MDSPME) with Gas Chromatography â€“ Mass Spectrometry (GC-MS). Analytical Letters, 2021, 54, 884-902.	1.0	9
47	Prediction of the Solubility of Cholesterol and its Esters in Supercritical Carbon Dioxide. Chemical Engineering and Technology, 2006, 29, 1481-1486.	0.9	8
48	Conformation changes and diffusion of Î±-amylase in 1-hexyle-3-methylimidazolium chloride ionic liquid: A molecular dynamics simulation perspective. Journal of Molecular Liquids, 2016, 221, 463-468.	2.3	8
49	Quantum molecular study of mesoporous silica nanoparticle as a delivery system for troxacitabine anticancer drug. Journal of Molecular Liquids, 2020, 310, 113155.	2.3	8
50	The study of self-aggregation behavior of the bilirubin molecules in the presence and absence of carbon nanotubes: Molecular dynamics simulation approach. Journal of Molecular Liquids, 2015, 208, 342-346.	2.3	7
51	Oleuropein interactions with inner and outer surface of different types of carbon nanotubes: Insights from molecular dynamic simulation. Journal of Molecular Liquids, 2017, 241, 367-373.	2.3	7
52	Tautomerization Reaction, Experimental and Theoretical Characterizations of the N,Nâ€²-Dipyridoxyl(4-Methyl-1,2-Phenylenediamine) Schiff Base and its Cu(II) Complex. Journal of Structural Chemistry, 2018, 59, 1102-1113.	0.3	7
53	Role of repulsive forces on self-assembly behavior of amyloid<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll" id="d1e748" altimg="si46.gif"><mml:mi>Î²</mml:mi></mml:math>-peptide (1-40): Molecular dynamics simulation approach. Physica A: Statistical Mechanics and Its Applications, 2019, 513, 524-535.	1.2	7
54	Synthesis of New Functionalized 1,4-Dihydroquinolines and Pyrimido[4,5-b]quinolines. Russian Journal of General Chemistry, 2017, 87, 2961-2965.	0.3	6

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55	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. Journal of Supercritical Fluids, 2018, 140, 91-100.	1.6	6
56	Quantum Mechanical Study on the Mechanistic, Energetic, and Structural Properties of Adsorption of 6â€Thioguanine onto Î³â€‹scp›Fe‹sub›2‹/sub›O‹sub›3‹/sub›‹/scp› Nanoparticles. Bulletin of the Korean Chemical Society, 2017, 38, 869-874.	1.0	5
57	Does high pressure have any effect on the structure of alpha amylase and its ability to binding to the oligosaccharides having 3â€“7 residues? Molecular dynamics study. Journal of Molecular Graphics and Modelling, 2018, 80, 85-94.	1.3	5
58	Î²-cyclodextrin-lenalidomide anticancer drug delivery nanosystem: A quantum chemical approach. Journal of Molecular Liquids, 2021, 344, 117762.	2.3	5
59	Structure-Activity Relationship for Fe(III)-Salen-Like Complexes as Potent Anticancer Agents. Scientific World Journal, The, 2014, 2014, 1-10.	0.8	4
60	Theoretical Study on the Mechanism of Covalent Bonding of Dapsone onto Functionalised Carbon Nanotubes: Effects of Coupling Agent. Progress in Reaction Kinetics and Mechanism, 2016, 41, 345-355.	1.1	4
61	Evaluation of catalytic activity of two newly prepared functionalized sulfonic acids ionic liquids in the synthesis of carbamatoalkyl naphthols under mild conditions. Russian Journal of General Chemistry, 2017, 87, 311-315.	0.3	4
62	Synthesis, Experimental and Theoretical Studies on N,Nâ€²-Dipyridoxyl(4-Chloro-1,2-Phenylenediamine) Tetradentate Ligand and Its Copper(II) Complex. Journal of Structural Chemistry, 2019, 60, 1243-1255.	0.3	4
63	Study of alpha-amylase and gold nanoparticles interaction at two different temperatures through molecular dynamics. Journal of Molecular Graphics and Modelling, 2019, 88, 273-281.	1.3	4
64	Self-association process of tetracycline antibiotic in different aqueous solutions: a joint experimental study and molecular dynamics simulation. Journal of the Iranian Chemical Society, 2020, 17, 2997-3007.	1.2	4
65	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. Chemical Papers, 2021, 75, 4305-4316.	1.0	4
66	Determination of Thermodynamics Constant of Interaction among of Atenolol and Metoprolol with Human Serum Albumin: Spectroscopic and Molecular Modeling Approaches. Russian Journal of Physical Chemistry A, 2021, 95, 1269-1276.	0.1	4
67	Theoretical Design and Experimental Study of New Aptamers with the Enhanced Binding Affinity Relying on Colorimetric Assay for Tetracycline Detection. Journal of Molecular Liquids, 2021, 349, 118196.	2.3	4
68	Evaluation of attraction terms in equations of state on the prediction of solubility of some biomolecules in supercritical carbon dioxide. Chinese Chemical Letters, 2009, 20, 501-505.	4.8	3
69	Kinetics and mechanism of the 1,3-dipolar cycloaddition of nitrilimine with thione-containing dipolarophile: a detailed DFT study. Research on Chemical Intermediates, 2016, 42, 6125-6141.	1.3	3
70	Mechanistic, energetic and structural studies of carbon nanotubes functionalised with dihydroartemisinin drug in gas and solution phases. Physics and Chemistry of Liquids, 2018, 56, 610-618.	0.4	3
71	Mechanistic, Energetic and Structural Studies of Î³-Fe2O3 Nanoparticles Functionalized with Drug Artemisinin. Russian Journal of Inorganic Chemistry, 2019, 64, 503-510.	0.3	3
72	Effects of the deglycosylation on the structure and activity of chloroperoxidase: Molecular dynamics simulation approach. Journal of Molecular Graphics and Modelling, 2020, 97, 107570.	1.3	3

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73	Molecular dynamics simulations on the heterocyclic cyclodecapeptide and its linear analogous in water and octanol solvents. Journal of Molecular Liquids, 2017, 229, 583-590.	2.3	2
74	Density Functional Theoretical Study on the Mechanism of Alcoholysis of Acylpalladium(II) Complexes. Progress in Reaction Kinetics and Mechanism, 2017, 42, 52-61.	1.1	2
75	Radial distribution function within the framework of the Tsallis statistical mechanics. Physica A: Statistical Mechanics and Its Applications, 2018, 506, 857-867.	1.2	2
76	Acetyl-11-keto-Î²-boswellic acid derivatives effects on 5-lipoxygenase: In silico viewpoint. Journal of Molecular Graphics and Modelling, 2020, 94, 107464.	1.3	2
77	The effect of sodium dodecyl sulfate concentration on the aggregation behavior of AÎ² (1â€“42) peptide: Molecular dynamics simulation approach. Journal of Molecular Liquids, 2020, 303, 112651.	2.3	2
78	DFT Study on the Covalent Adsorption of Drug Carvedilol onto COOH Functionalized Carbon Nanotubes. Oriental Journal of Chemistry, 2015, 31, 1403-1407.	0.1	2
79	A molecular dynamics study on the liquid SbCl5and SbF5using force fields derived from quantum chemical calculations. Physics and Chemistry of Liquids, 2013, 51, 695-703.	0.4	1
80	N,Nâ€²-Dipyridoxyl(1,8-diamino-3,6-dioxaoctane) Schiff-base: Synthesis, experimental and theoretical identification. Bulletin of the Chemical Society of Ethiopia, 2013, 27, .	0.5	1
81	A Theoretical Investigation on the Regioselectivity of the Dielsâ€“Alder Cycloaddition of 9-(Methoxymethyl) Anthracene And Citraconic Anhydride. Journal of Structural Chemistry, 2018, 59, 1810-1817.	0.3	1
82	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. Journal of Structural Chemistry, 2018, 59, 1228-1235.	0.3	1
83	Effect of Lysyllysine on non-covalent hybridization of single walled carbon nanotube by single-stranded DNA homodimer: in silico approach. Journal of Nanostructure in Chemistry, 2019, 9, 315-321.	5.3	1
84	Reverse Micelle Surfactant System Comprising the 1-decanoyl-rac-glycerol and the Lauryldimethylamine-N-oxide: Structure and Dynamics of Confined Water. Russian Journal of Physical Chemistry A, 2019, 93, 1122-1127.	0.1	1
85	Investigating the effect of 1-Butyl-3-methylimidazolium bromide and 1-Butyl-3-methylimidazolium methyl sulfate ionic liquids on structure and function of Chloroproxidase by molecular dynamics simulation. Journal of Molecular Liquids, 2021, 332, 115850.	2.3	1
86	DFT Study on Adsorption of Drug Artemisinin Onto Carbon Nanotubes. Journal of Computational and Theoretical Nanoscience, 2017, 14, 1778-1783.	0.4	1
87	Structure of the Cyclic, Cationic Antimicrobial Peptide (KKWWKF) in Octanol Solution: in silico Approach. Indonesian Journal of Chemistry, 2020, 20, 1283.	0.3	1
88	(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. Journal of the Serbian Chemical Society, 2020, 85, 1033-1046.	0.4	1
89	QUANTUM CHEMICAL STUDIES OF CHITOSAN NANOPARTICLES AS ANTICANCER DRUG DELIVERY SYSTEM FOR DECITABINE. Cellulose Chemistry and Technology, 2020, 54, 679-688.	0.5	1
90	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, 2022, 56, 206-214.	0.3	1

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91	Critical and synergy nodes in insulin-EGF signaling network. Clinical Biochemistry, 2011, 44, S33.	0.8	0
92	Kinetics and Mechanisms of the Diels-Alder Reaction of 9-bromomethyl Anthracene with Citraconic Anhydride: A DFT study. Oriental Journal of Chemistry, 2016, 32, 1139-1144.	0.1	0
93	Characterization and Molecular Docking Study of New 4-Acetamidoalkyl Pyrazoles As B-Raf /Cox-2 Inhibitors. Journal of Structural Chemistry, 2018, 59, 335-343.	0.3	0
94	Mechanistic and energetic studies of superparamagnetic iron oxide nanoparticles as a cyclophosphamide anticancer drug nanocarrier: A quantum mechanical approach. Progress in Reaction Kinetics and Mechanism, 2019, 44, 92-101.	1.1	0
95	Does the single-walled carbon nanotube affect the rate constant of binding of biotin to streptavidin? Molecular dynamics simulation perspective. Progress in Reaction Kinetics and Mechanism, 2019, 44, 234-243.	1.1	0
96	The Effect of Temperature on the Interaction of Phenanthroline-based Ligands with G-quadruplex: In Silico Viewpoint. Combinatorial Chemistry and High Throughput Screening, 2019, 22, 546-554.	0.6	0
97	Flavodoxin in a binary surfactant system consisting of the nonionic 1-decanoyl-rac-glycerol and the zwitterionic lauryldimethylamine-N-oxide: molecular dynamics simulation approach. Papers in Physics, 0, 12, 120004.	0.2	0
98	DFT-QTAIM Study of Gold Nanoparticles and Cyclic Peptide as Effective Drug Nanocarriers. Orbital, 2020, 12, .	0.1	0
99	Non-Covalent Hybridization of Carbon Nanotube by Single-Stranded DNA Homodecamers: in-silico Approach. Russian Journal of Physical Chemistry A, 2022, 96, 145-151.	0.1	0