Mohammad Reza Bozorgmehr

List of Publications by Year in Descending Order

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	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	
90	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	6	0
89	-cyclodextrin-lenalidomide anticancer drug delivery nanosystem: A quantum chemical approach. *Journal of Molecular Liquids*, **2021**, 344, 117762	6	0
88	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	1.9	1
87	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	6	1
86	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	0.7	1
85	Determination of Tramadol and Fluoxetine in Biological and Water Samples by Magnetic Dispersive Solid-Phase Microextraction (MDSPME) with Gas Chromatography -Mass Spectrometry (GC-MS). *Analytical Letters*, **2021**, 54, 884-902	2.2	5
84	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	3.4	9
83	Quantum chemical analysis of 5-aminolevulinic acid anticancer drug delivery systems: Carbon nanotube, -COOH functionalized carbon nanotube and iron oxide nanoparticle. *Journal of Molecular Liquids*, **2021**, 340, 117182	6	2
82	Quantum molecular study of mesoporous silica nanoparticle as a delivery system for troxacitabine anticancer drug. *Journal of Molecular Liquids*, **2020**, 310, 113155	6	3
81	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. *Chemical Papers*, **2020**, 74, 2929-2943	1.9	5
80	The effect of sodium dodecyl sulfate concentration on the aggregation behavior of A-(1-42) peptide: Molecular dynamics simulation approach. *Journal of Molecular Liquids*, **2020**, 303, 112651	6	0
79	Effects of the deglycosylation on the structure and activity of chloroperoxidase: Molecular dynamics simulation approach. *Journal of Molecular Graphics and Modelling*, **2020**, 97, 107570	2.8	3
78	(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	0.9	0
77	Quantum chemical studies of chitosan nanoparticles as effective drug delivery systems for 5-fluorouracil anticancer drug. *Journal of Molecular Liquids*, **2020**, 302, 112495	6	30
76	Microextraction and gas chromatography-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	6	7
75	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	2	2

74	Acetyl-11-keto-β-boswellic acid derivatives effects on 5-lipoxygenase: In silico viewpoint. *Journal of Molecular Graphics and Modelling*, **2020**, 94, 107464	2.8	1
73	The investigation of the G-quadruplex aptamer selectivity to Pb ion: a joint molecular dynamics simulation and density functional theory study. *Journal of Biomolecular Structure and Dynamics*, **2020**, 38, 3659-3675	3.6	4
72	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	2	4
71	Synthesis, Experimental and Theoretical Studies on N,N?-Dipyridoxyl(4-Chloro-1,2-Phenylenediamine) Tetradentate Ligand and Its Copper(II) Complex. *Journal of Structural Chemistry*, **2019**, 60, 1243-1255	0.9	0
70	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	6	10
69	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	0.7	1
68	Mechanistic, Energetic and Structural Studies of β-Fe2O3 Nanoparticles Functionalized with Drug Artemisinin. *Russian Journal of Inorganic Chemistry*, **2019**, 64, 503-510	1.5	3
67	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	0.5	
66	A simple paper-based aptasensor for ultrasensitive detection of lead (II) ion. *Analytica Chimica Acta*, **2019**, 1071, 70-77	6.6	35
65	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	6	15
64	Quantum chemical modeling of iron oxide magnetic nanoparticles functionalized with cytarabine. *Chemical Physics Letters*, **2019**, 719, 12-21	2.5	9
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	2.8	1
62	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. *Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences*, **2019**, 1132, 121823	3.2	8
61	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	7.6	0
60	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	1.3	
59	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	0.5	
58	Role of repulsive forces on self-assembly behavior of amyloid β-peptide (1-40): Molecular dynamics simulation approach. *Physica A: Statistical Mechanics and Its Applications*, **2019**, 513, 524-535	3.3	3
57	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	2.8	6

56	DFT study of SiO2 nanoparticles as a drug delivery system: structural and mechanistic aspects. *Structural Chemistry*, **2019**, 30, 715-726	1.8	12
55	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	5.4	39
54	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. *Journal of Molecular Graphics and Modelling*, **2018**, 80, 85-94	2.8	4
53	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	1.5	0
52	Radial distribution function within the framework of the Tsallis statistical mechanics. *Physica A: Statistical Mechanics and Its Applications*, **2018**, 506, 857-867	3.3	1
51	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	6.7	24
50	Characterization and Molecular Docking Study of New 4-Acetamidoalkyl Pyrazoles As B-Raf /Cox-2 Inhibitors. *Journal of Structural Chemistry*, **2018**, 59, 335-343	0.9	
49	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	4.2	4
48	Tautomerization Reaction, Experimental and Theoretical Characterizations of the N,N?-Dipyridoxyl(4-Methyl-1,2-Phenylenediamine) Schiff Base and its Cu(II) Complex. *Journal of Structural Chemistry*, **2018**, 59, 1102-1113	0.9	6
47	A Theoretical Investigation on the Regioselectivity of the Diels–Alder Cycloaddition of 9-(Methoxymethyl) Anthracene And Citraconic Anhydride. *Journal of Structural Chemistry*, **2018**, 59, 1810-1817	0.9	1
46	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	0.9	1
45	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	11.8	77
44	Soybean oil-based nanoemulsion systems in absence and presence of curcumin: Molecular dynamics simulation approach. *Journal of Molecular Liquids*, **2018**, 264, 242-252	6	21
43	Molecular dynamics simulations on the heterocyclic cyclodecapeptide and its linear analogous in water and octanol solvents. *Journal of Molecular Liquids*, **2017**, 229, 583-590	6	2
42	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	0.7	3
41	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	6	7
40	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	1.1	9
39	Density Functional Theoretical Study on the Mechanism of Alcoholysis of Acylpalladium(II) Complexes. *Progress in Reaction Kinetics and Mechanism*, **2017**, 42, 52-61	0.5	2

38	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	2.8	12
37	Quantum Mechanical Study on the Mechanistic, Energetic, and Structural Properties of Adsorption of 6-Thioguanine onto □Fe2O3 Nanoparticles. *Bulletin of the Korean Chemical Society*, **2017**, 38, 869-874	1.2	5
36	Transport properties of mixtures composed of acetone, water, and supercritical carbon dioxide by molecular dynamics simulation. *Journal of Supercritical Fluids*, **2017**, 130, 321-326	4.2	13
35	Synthesis of New Functionalized 1,4-Dihydroquinolines and Pyrimido[4,5-b]quinolines. *Russian Journal of General Chemistry*, **2017**, 87, 2961-2965	0.7	4
34	The effect of glycosylation on the transferrin structure: A molecular dynamic simulation analysis. *Journal of Theoretical Biology*, **2016**, 404, 73-81	2.3	9
33	Conformation changes and diffusion of □amylase in 1-hexyle-3-methylimidazolium chloride ionic liquid: A molecular dynamics simulation perspective. *Journal of Molecular Liquids*, **2016**, 221, 463-468	6	6
32	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	0.9	9
31	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	2.8	3
30	Influence of Taxifolin on the Human Serum Albumin□Propranolol Interaction: Multiple Spectroscopic and Chemometrics Investigations and Molecular Dynamics Simulation. *Journal of Solution Chemistry*, **2016**, 45, 265-285	1.8	14
29	Simultaneous extraction and preconcentration of aniline, phenol, and naphthalene using magnetite-graphene oxide composites before gas chromatography determination. *Journal of Separation Science*, **2016**, 39, 3046-53	3.4	14
28	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	0.5	2
27	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, 1153-63	3.6	27
26	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, 1669-81	3.6	12
25	Molecular crowding effects on conformation and stability of G-quadruplex DNA structure: insights from molecular dynamics simulation. *Journal of Theoretical Biology*, **2015**, 364, 103-12	2.3	26
24	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	6	5
23	How Can a Free Amino Acid Stabilize a Protein? Insights from Molecular Dynamics Simulation. *Journal of Solution Chemistry*, **2015**, 44, 45-53	1.8	17
22	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	0.8	17
21	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	3.8	29

20	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	6	10
19	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 urea : choline chloride deep eutectic solvent. *Physical Chemistry Chemical Physics*, **2014**, 16, 14882-93	3.6	138
18	Structure-activity relationship for Fe(III)-salen-like complexes as potent anticancer agents. *Scientific World Journal, The*, **2014**, 2014, 745649	2.2	2
17	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	4.2	7
16	A molecular dynamics study on the liquid SbCl5 and SbF5 using force fields derived from quantum chemical calculations. *Physics and Chemistry of Liquids*, **2013**, 51, 695-703	1.5	1
15	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		11
14	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	4.4	31
13	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	4.2	32
12	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. *Helvetica Chimica Acta*, **2012**, 95, 52-60	2	9
11	Synthesis, characterization and interaction of N,NRdipyridoxyl (1,4-butanediamine) Co(III) salen complex with DNA and HSA. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 97, 74-82	4.4	28
10	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	4.2	30
9	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	8.1	3
8	Analysis of ligand binding to proteins using molecular dynamics simulations. *Journal of Theoretical Biology*, **2008**, 254, 294-300	2.3	31
7	Calculation of solubility of methimazole, phenazopyridine and propranolol in supercritical carbon dioxide. *Journal of Supercritical Fluids*, **2008**, 43, 390-397	4.2	29
6	Joule□Thomson inversion curve prediction by using equation of state. *Chinese Chemical Letters*, **2007**, 18, 1154-1158	8.1	17
5	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	2.8	17
4	Evaluation of P□V□T differential properties of the Lennard-Jones fluid using radial distribution functions and molecular dynamics. *Chemical Physics*, **2007**, 335, 194-200	2.3	9
3	Prediction of the Solubility of Cholesterol and its Esters in Supercritical Carbon Dioxide. *Chemical Engineering and Technology*, **2006**, 29, 1481-1486	2	8

2	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*,12, 120004	
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