

Faramarz Mehrnejad

List of Publications by Year in descending order

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62
papers

895
citations

393982

19
h-index

525886

27
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64
all docs

64
docs citations

64
times ranked

1373
citing authors

#	ARTICLE	IF	CITATIONS
1	The process of L-asparaginase encapsulation by poly (lactic-co-glycolic acid) and methoxy poly (ethylene glycol): A molecular dynamics simulation study. <i>Materials Today Communications</i> , 2022, 31, 103435.	0.9	1
2	Human serum albumin adsorption on cellulose nanocrystal: A spectroscopy and molecular dynamics simulation research. <i>Applied Surface Science</i> , 2022, 597, 153749.	3.1	2
3	Molecular insights into the crystalline nanocellulose and human lysozyme interactions: An experimental and theoretical research. <i>International Journal of Biological Macromolecules</i> , 2022, 213, 83-95.	3.6	2
4	Atomistic insight into the luminal allosteric regulation of vesicular glutamate transporter 2 by chloride and protons: An all-atom molecular dynamics simulation study. <i>Proteins: Structure, Function and Bioinformatics</i> , 2022, 90, 2045-2057.	1.5	2
5	Effect of the Met148Leu mutation on the structure and dynamics of the rusticyanin protein from <i>Acidithiobacillus</i> sp. FJ2. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 4122-4132.	2.0	3
6	Refinement of coding SNPs in the human aryl hydrocarbon receptor gene using ISNPranker: An integrative-SNP ranking web-tool. <i>Computational Biology and Chemistry</i> , 2021, 90, 107416.	1.1	2
7	Insight into the Microcosm of the Human Growth Hormone and Its Interactions with Polymers and Copolymers: A Molecular Dynamics Perspective. <i>Langmuir</i> , 2021, 37, 90-104.	1.6	1
8	Effect of the lipid composition and cholesterol on the membrane selectivity of low generations PAMAM dendrimers: A molecular dynamics simulation study. <i>Applied Surface Science</i> , 2021, 540, 148274.	3.1	7
9	Molecular Insights into Pore Formation Mechanism, Membrane Perturbation, and Water Permeation by the Antimicrobial Peptide Pleurocidin: A Combined All-Atom and Coarse-Grained Molecular Dynamics Simulation Study. <i>Journal of Physical Chemistry B</i> , 2021, 125, 7163-7176.	1.2	14
10	Molecular modeling prediction of albumin-based nanoparticles and experimental preparation, characterization, and in-vitro release kinetics of prednisolone from the nanoparticles. <i>Journal of Drug Delivery Science and Technology</i> , 2021, 64, 102588.	1.4	6
11	Design and synthesis of polyacrylic acid/deoxycholic acid-modified chitosan copolymer and a close inspection of human growth hormone-copolymer interactions: An experimental and computational study. <i>Colloids and Surfaces B: Biointerfaces</i> , 2021, 206, 111956.	2.5	4
12	Insights into the Molecular-Level details of betaine interactions with Laccase under various thermal conditions. <i>Journal of Molecular Liquids</i> , 2021, 339, 116832.	2.3	6
13	Encapsulation of an endostatin peptide in liposomes: Stability, release, and cytotoxicity study. <i>Colloids and Surfaces B: Biointerfaces</i> , 2020, 185, 110552.	2.5	33
14	Compatibilization of clays and hydrophobic polymers: the case of montmorillonite and polyetheretherketone. <i>Polymer Bulletin</i> , 2020, 77, 5505-5527.	1.7	5
15	Molecular level insight into stability, activity, and structure of Laccase in aqueous ionic liquid and organic solvents: An experimental and computational research. <i>Journal of Molecular Liquids</i> , 2020, 317, 113925.	2.3	13
16	Molecular Insight into the Interaction between Camptothecin and Acyclic Cucurbit[4]urils as Efficient Nanocontainers in Comparison with Cucurbit[7]uril: Molecular Docking and Molecular Dynamics Simulation. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 1791-1803.	2.5	10
17	Structural Studies on an Anti-Angiogenic Peptide Using Molecular Modeling. <i>Iranian Journal of Biotechnology</i> , 2020, 18, e2553.	0.3	0
18	Effects of single-walled carbon nanotube on the conformation of human hepcidin: molecular dynamics simulation and binding free energy calculations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 2125-2132.	2.0	3

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19	Molecular Basis for Membrane Selectivity of Antimicrobial Peptide Pleurocidin in the Presence of Different Eukaryotic and Prokaryotic Model Membranes. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3262-3276.	2.5	22
20	A cyclic peptide reproducing the $\alpha 1$ helix of VEGF-B binds to VEGFR-1 and VEGFR-2 and inhibits angiogenesis and tumor growth. <i>Biochemical Journal</i> , 2019, 476, 645-663.	1.7	26
21	Paclitaxel interaction with cucurbit [7]uril and acyclic Cucurbit[4]uril nanocontainers: A computational approach. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 90, 210-218.	1.3	3
22	The role of intermolecular interactions on the encapsulation of human insulin into the chitosan and cholesterol-grafted chitosan polymers. <i>Carbohydrate Polymers</i> , 2019, 208, 345-355.	5.1	17
23	Molecular Self-Assembly Strategy for Encapsulation of an Amphipathic α -Helical Antimicrobial Peptide into the Different Polymeric and Copolymeric Nanoparticles. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 550-563.	2.5	26
24	Computational insights into pH-dependence of structure and dynamics of pyrazinamidase: A comparison of wild type and mutants. <i>Journal of Cellular Biochemistry</i> , 2019, 120, 2502-2514.	1.2	3
25	The Molecular Basis of the Sodium Dodecyl Sulfate Effect on Human Ubiquitin Structure: A Molecular Dynamics Simulation Study. <i>Scientific Reports</i> , 2018, 8, 2150.	1.6	37
26	Protein adsorption onto polysaccharides: Comparison of chitosan and chitin polymers. <i>Carbohydrate Polymers</i> , 2018, 191, 191-197.	5.1	36
27	Understanding the interactions of human follicle stimulating hormone with single-walled carbon nanotubes by molecular dynamics simulation and free energy analysis. <i>European Biophysics Journal</i> , 2018, 47, 49-57.	1.2	6
28	The combinatorial effects of osmolytes and alcohols on the stability of pyrazinamidase: Methanol affects the enzyme stability through hydrophobic interactions and hydrogen bonds. <i>International Journal of Biological Macromolecules</i> , 2018, 108, 1339-1347.	3.6	19
29	Ig-like Domain in Endoglucanase Cel9A from <i>Alicyclobacillus acidocaldarius</i> Makes Dependent the Enzyme Stability on Calcium. <i>Molecular Biotechnology</i> , 2018, 60, 698-711.	1.3	6
30	The potential impact of carboxylic-functionalized multi-walled carbon nanotubes on trypsin: A Comprehensive spectroscopic and molecular dynamics simulation study. <i>PLoS ONE</i> , 2018, 13, e0198519.	1.1	19
31	Molecular insights into the interactions of GF $\alpha 17$ with the gram-negative and gram-positive bacterial lipid bilayers. <i>Journal of Cellular Biochemistry</i> , 2018, 119, 9205-9216.	1.2	11
32	Insight to the molecular mechanisms of the osmolyte effects on <i>Mycobacterium tuberculosis</i> pyrazinamidase stability using experimental studies, molecular dynamics simulations, and free energy calculation. <i>International Journal of Mycobacteriology</i> , 2018, 7, 268.	0.3	8
33	Effects of metal-ion replacement on pyrazinamidase activity: A quantum mechanical study. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 73, 24-29.	1.3	5
34	Chitosan nanoparticles-trypsin interactions: Bio-physicochemical and molecular dynamics simulation studies. <i>International Journal of Biological Macromolecules</i> , 2017, 103, 902-909.	3.6	22
35	Efficient megalin targeted delivery to renal proximal tubular cells mediated by modified-polymyxin B-polyethylenimine based nano-gene-carriers. <i>Materials Science and Engineering C</i> , 2017, 79, 770-782.	3.8	42
36	Identification of the Crucial Residues in the Early Insertion of Pardaxin into Different Phospholipid Bilayers. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 929-941.	2.5	13

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37	Aryl hydrocarbon receptor gene transitions (c.-742C>T; c.1661G>A) and idiopathic male infertility: a case-control study with in silico and meta-analysis. <i>Environmental Science and Pollution Research</i> , 2017, 24, 20599-20615.	2.7	6
38	Follicle-stimulating hormone encapsulation in the cholesterol-modified chitosan nanoparticles via molecular dynamics simulations and binding free energy calculations. <i>European Journal of Pharmaceutical Sciences</i> , 2017, 107, 126-137.	1.9	25
39	A computational study of the electronic structure and the chemical activity of curcumin and some novel curcuminoids by density functional theory. <i>Journal of the Iranian Chemical Society</i> , 2017, 14, 357-364.	1.2	4
40	Insight into the interactions, residue snorkeling, and membrane disordering potency of a single antimicrobial peptide into different lipid bilayers. <i>PLoS ONE</i> , 2017, 12, e0187216.	1.1	27
41	The antiangiogenic and antitumor activities of the N-terminal fragment of endostatin augmented by Ile/Arg substitution: The overall structure implicated the biological activity. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2016, 1864, 1765-1774.	1.1	9
42	Effects of sorbitol and glycerol on the structure, dynamics, and stability of Mycobacterium tuberculosis pyrazinamidase. <i>International Journal of Mycobacteriology</i> , 2016, 5, S138-S139.	0.3	3
43	Effect of sorbitol and glycerol on the stability of trypsin and difference between their stabilization effects in the various solvents. <i>Biotechnology and Applied Biochemistry</i> , 2016, 63, 206-213.	1.4	33
44	An in silico approach to investigate the source of the controversial interpretations about the phenotypic results of the human AhR-gene G1661A polymorphism. <i>Journal of Theoretical Biology</i> , 2016, 393, 1-15.	0.8	29
45	HYNIC a bifunctional prosthetic group for the labelling of peptides with 99mTc and 18FDG. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2016, 307, 1125-1134.	0.7	12
46	Molecular Insight into Human Lysozyme and Its Ability to Form Amyloid Fibrils in High Concentrations of Sodium Dodecyl Sulfate: A View from Molecular Dynamics Simulations. <i>PLoS ONE</i> , 2016, 11, e0165213.	1.1	35
47	Synthesis, Radiolabeling, and Biological Evaluation of Peptide LIKKPF Functionalized with HYNIC as Apoptosis Imaging Agent. <i>Iranian Journal of Pharmaceutical Research</i> , 2016, 15, 415-24.	0.3	4
48	Structural and Dynamical Study of Bovine Carbonic Anhydrase II in the Presence of Substrate: An Essential Dynamics and Molecular Dynamics Simulation Study. <i>Biophysical Journal</i> , 2015, 108, 316a.	0.2	0
49	Biochemical Characterization and Computational Identification of Mycobacterium tuberculosis Pyrazinamidase in Some Pyrazinamide-Resistant Isolates of Iran. <i>Protein Journal</i> , 2015, 34, 181-192.	0.7	6
50	Molecular Interactions in the Systems Composed of Curcumin, Water and Single-Walled Carbon Nanotube: A Molecular Dynamics Simulation Study. <i>Journal of Computational and Theoretical Nanoscience</i> , 2015, 12, 2077-2083.	0.4	6
51	Study of Orientation and Penetration of LAH4 into Lipid Bilayer Membranes: pH and Composition Dependence. <i>Chemical Biology and Drug Design</i> , 2014, 84, 242-252.	1.5	10
52	Salinity Tolerance Ranking Of Various Wheat Landraces From The West Of The Urmia Saline Lake In Iran By Using Physiological Parameters. <i>Journal of Plant Nutrition</i> , 2014, 37, 1025-1039.	0.9	3
53	Interaction of Piscidin-1 with zwitterionic versus anionic membranes: a comparative molecular dynamics study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2013, 31, 1393-1403.	2.0	13
54	A New Efficient Protocol for Directed Differentiation of Retinal Pigmented Epithelial Cells from Normal and Retinal Disease Induced Pluripotent Stem Cells. <i>Stem Cells and Development</i> , 2012, 21, 2262-2272.	1.1	64

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55	Role of Hydrophobic Forces and Backbone Hydrogen Bonding on Helical Stability of Peptide Encapsulated Into Single Wall Carbon Nanotubes. <i>Journal of Computational and Theoretical Nanoscience</i> , 2012, 9, 783-788.	0.4	2
56	Effects of osmolytes on the helical conformation of model peptide: Molecular dynamics simulation. <i>Journal of Chemical Physics</i> , 2011, 134, 035104.	1.2	27
57	Mechanisms of amphipathic helical peptide denaturation by guanidinium chloride and urea: a molecular dynamics simulation study. <i>Journal of Computer-Aided Molecular Design</i> , 2010, 24, 829-841.	1.3	23
58	Structural studies of SNARE complex and its interaction with complexin by molecular dynamics simulation. <i>Biopolymers</i> , 2010, 93, NA-NA.	1.2	6
59	Molecular Dynamics Simulation Study of the Interaction of Piscidin 1 with DPPC Bilayers: Structure-Activity Relationship. <i>Journal of Biomolecular Structure and Dynamics</i> , 2010, 27, 551-559.	2.0	35
60	PCR-based Gene Synthesis, Molecular Cloning, High Level Expression, Purification, and Characterization of Novel Antimicrobial Peptide, Brevinin-2R, in <i>Escherichia Coli</i> . <i>Applied Biochemistry and Biotechnology</i> , 2008, 149, 109-118.	1.4	27
61	Structural and Dynamical Studies of Humanin in Water and TFE/Water Mixture: A Molecular Dynamics Simulation. <i>Journal of Biomolecular Structure and Dynamics</i> , 2008, 26, 255-262.	2.0	26
62	The structural properties of magainin in water, TFE/water, and aqueous urea solutions: Molecular dynamics simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 67, 931-940.	1.5	24