Sajjad Gharaghani

List of Publications by Year in Descending Order

59 papers	965 citations	16 h-index	29 g-index
66 ext. papers	1,192 ext. citations	3.9 avg, IF	4.73 L-index

#	Paper	IF	Citations
59	Biomolecular interactions and binding dynamics of inhibitor arachidonic acid, with tyrosinase enzyme.. *Journal of Biomolecular Structure and Dynamics*, **2022**, 1-10	3.6	0
58	BRNS + SSFSM-DTI: A hybrid method for drug-target interaction prediction based on balanced reliable negative samples and semi-supervised feature selection. *Chemometrics and Intelligent Laboratory Systems*, **2022**, 220, 104462	3.8	
57	Proteochemometrics modeling for prediction of the interactions between caspase isoforms and their inhibitors.. *Molecular Diversity*, **2022**, 1	3.1	
56	Inhibition of GSK_3□by Iridoid Glycosides of Snowberry () Effective in the Treatment of Alzheimer□s Disease Using Computational Drug Design Methods. *Frontiers in Chemistry*, **2021**, 9, 709932	5	0
55	AutoDTI++: deep unsupervised learning for DTI prediction by autoencoders. *BMC Bioinformatics*, **2021**, 22, 204	3.6	2
54	Pharmacophore model, docking, QSAR, and molecular dynamics simulation studies of substituted cyclic imides and herbal medicines as COX-2 inhibitors. *Heliyon*, **2021**, 7, e06605	3.6	3
53	Moonlighting protein prediction using physico-chemical and evolutional properties via machine learning methods. *BMC Bioinformatics*, **2021**, 22, 261	3.6	3
52	Design of potential anti-tumor PARP-1 inhibitors by QSAR and molecular modeling studies. *Molecular Diversity*, **2021**, 25, 263-277	3.1	5
51	Novel and Predictive QSAR Model for Steroidal and Nonsteroidal 5□Reductase Type II Inhibitors. *Current Drug Discovery Technologies*, **2021**, 18, 317-332	1.5	
50	A simple and robust model to predict the inhibitory activity of □glucosidase inhibitors through combined QSAR modeling and molecular docking techniques. *Molecular Diversity*, **2021**, 25, 1811-1825	3.1	3
49	Drug-designing Studies on Sulforaphane Analogues: Pharmacophore Mapping, Molecular Docking and QSAR Modeling. *Current Drug Discovery Technologies*, **2021**, 18, 139-157	1.5	4
48	Structural systems pharmacology: A framework for integrating metabolic network and structure-based virtual screening for drug discovery against bacteria.. *PLoS ONE*, **2021**, 16, e0261267	3.7	
47	Sparse feature selection in multi-target modeling of carbonic anhydrase isoforms by exploiting shared information among multiple targets. *Chemometrics and Intelligent Laboratory Systems*, **2020**, 200, 104000	3.8	2
46	In silico drug repositioning of FDA-approved drugs to predict new inhibitors for alpha-synuclein aggregation. *Computational Biology and Chemistry*, **2020**, 88, 107308	3.6	1
45	A robust graph-based semi-supervised sparse feature selection method. *Information Sciences*, **2020**, 531, 13-30	7.7	12
44	An efficient nano-biocatalyst for lignocellulosic biomass hydrolysis: Xylanase immobilization on organically modified biogenic mesoporous silica nanoparticles. *International Journal of Biological Macromolecules*, **2020**, 164, 3462-3473	7.9	20
43	NDDSA: A network- and domain-based method for predicting drug-side effect associations. *Information Processing and Management*, **2020**, 57, 102357	6.3	1

42	Chemometrics approaches based on electrochemical methods for the investigation of interaction between bovine serum albumin and carvacrol with the aim of its application to protein sensing. *Journal of Electroanalytical Chemistry*, **2019**, 845, 48-56	4.1	1
41	Electrochemical investigation of the inhibition effect of carvacrol on xanthine oxidase activity merging with theoretical studies. *Process Biochemistry*, **2019**, 83, 86-95	4.8	3
40	Melatonin Therapy Modulates Cerebral Metabolism and Enhances Remyelination by Increasing PDK4 in a Mouse Model of Multiple Sclerosis. *Frontiers in Pharmacology*, **2019**, 10, 147	5.6	17
39	Deciphering the inhibition effect of thymoquinone on xanthine oxidase activity using differential pulse voltammetry in combination with theoretical studies. *Enzyme and Microbial Technology*, **2019**, 121, 29-36	3.8	3
38	Synthesis of new triazole tethered derivatives of curcumin and their antibacterial and antifungal properties. *Journal of the Iranian Chemical Society*, **2019**, 16, 465-477	2	4
37	Chiral halogenated Schiff base compounds: green synthesis, anticancer activity and DNA-binding study. *Journal of Molecular Structure*, **2018**, 1161, 497-511	3.4	19
36	New insights into the efficiency of thymol synergistic effect with p-cymene in inhibiting advanced glycation end products: A multi-way analysis based on spectroscopic and electrochemical methods in combination with molecular docking study. *Journal of Pharmaceutical and Biomedical Analysis*, **2018**, 150, 436-451	3.5	14
35	Studies on DNA binding properties of new Schiff base ligands using spectroscopic, electrochemical and computational methods: Influence of substitutions on DNA-binding. *Journal of Molecular Liquids*, **2018**, 253, 61-71	6	42
34	Identifying the novel natural antioxidants by coupling different feature selection methods with nonlinear regressions and gas chromatography-mass spectroscopy. *Microchemical Journal*, **2018**, 139, 372-379	4.8	9
33	Structural stability of β-lactoglobulin in the presence of cetylpyridinum bromide: spectroscopic and molecular docking studies. *Journal of Biomolecular Structure and Dynamics*, **2018**, 36, 753-760	3.6	6
32	Monitoring the protective ability of thymoquinone mixture with p-cymene against bovine serum albumin (BSA) glycation: MCR-ALS analysis based on combined spectroscopic and electrochemical methods. *International Journal of Biological Macromolecules*, **2018**, 107, 2465-2474	7.9	6
31	Chemometric studies of thymol binding with bovine serum albumin: A developing strategy for the successful investigation of pharmacological activity. *Bioelectrochemistry*, **2018**, 124, 172-184	5.6	7
30	An in-depth view of potential dual effect of thymol in inhibiting xanthine oxidase activity: Electrochemical measurements in combination with four way PARAFAC analysis and molecular docking insights. *International Journal of Biological Macromolecules*, **2018**, 119, 1298-1310	7.9	7
29	A novel proteochemometrics model for predicting the inhibition of nine carbonic anhydrase isoforms based on supervised Laplacian score and k-nearest neighbour regression. *SAR and QSAR in Environmental Research*, **2018**, 29, 419-437	3.5	4
28	Synthesis of novel norsufentanil analogs via a four-component Ugi reaction and in vivo, docking, and QSAR studies of their analgesic activity. *Chemical Biology and Drug Design*, **2018**, 91, 902-914	2.9	4
27	Multi experimental and computational studies for DNA and HSA interaction of new nano-scale ultrasound-assisted synthesized Pd(II) complex as a potent anticancer drug. *Journal of Molecular Liquids*, **2018**, 264, 386-397	6	8
26	Novel insights into the effect of folate–albumin binding on the transport of ascorbic acid as an anticancer agent: chemometric analysis based on combined spectroscopic and electrochemical studies. *New Journal of Chemistry*, **2018**, 42, 11031-11045	3.6	1
25	Constraint score for semi-supervised feature selection in ligand-and receptor-based QSAR on serine/threonine-protein kinase PLK3 inhibitors. *Chemometrics and Intelligent Laboratory Systems*, **2017**, 163, 31-40	3.8	11

24	Feature selection based on graph Laplacian by using compounds with known and unknown activities. *Journal of Chemometrics*, **2017**, 31, e2899	1.6	8
23	Experimental and theoretical investigation of interaction between bovine serum albumin and the mixture of caffeic acid and salicylic acid as the antioxidants. *Electrochimica Acta*, **2017**, 255, 428-441	6.7	14
22	Studies of DNA- and HSA-binding properties of new nano-scale green synthesized Ni (II) complex as anticancer agent using spectroscopic methods, viscosity measurement, molecular docking, MD simulation and QM/MM. *Journal of Molecular Liquids*, **2017**, 248, 24-35	6	21
21	Toward a hierarchical virtual screening and toxicity risk analysis for identifying novel CA XII inhibitors. *BioSystems*, **2017**, 162, 35-43	1.9	3
20	A Survey on semi-supervised feature selection methods. *Pattern Recognition*, **2017**, 64, 141-158	7.7	221
19	Spectrophotometric determination of synthetic colorants using PSO-GA-ANN. *Food Chemistry*, **2017** , 220, 377-384	8.5	46
18	Sequential and Mixed Genetic Algorithm and Learning Automata (SGALA, MGALA) for Feature Selection in QSAR. *Iranian Journal of Pharmaceutical Research*, **2017**, 16, 533-553	1.1	7
17	Synthesis, characterization and separation of chiral and achiral diastereomers of Schiff base Pd(II) complex: A comparative study of their DNA- and HSA-binding. *Journal of Photochemistry and Photobiology B: Biology*, **2016**, 163, 246-60	6.7	26
16	Hybrid docking-QSAR studies of DPP-IV inhibition activities of a series of aminomethyl-piperidones. *Computational Biology and Chemistry*, **2016**, 64, 335-345	3.6	12
15	An in silico approach to design peptide mimetics based on docking and molecular dynamics simulation of EGFR□matuzumab complex. *Journal of the Iranian Chemical Society*, **2016**, 13, 1805-1817	2	3
14	Synthesis, characterization and biological application of four novel metal-Schiff base complexes derived from allylamine and their interactions with human serum albumin: Experimental, molecular docking and ONIOM computational study. *Journal of Photochemistry and Photobiology B: Biology*, **2016**, 162, 448-462	6.7	53
13	New and mild method for the synthesis of alprazolam and diazepam and computational study of their binding mode to GABAA receptor. *Medicinal Chemistry Research*, **2016**, 25, 1538-1550	2.2	12
12	Scoring multiple features to predict drug disease associations using information fusion and aggregation. *SAR and QSAR in Environmental Research*, **2016**, 27, 609-28	3.5	18
11	Synthesis and Antibacterial Evaluation of Novel Xanthone Sulfonamides. *Journal of Chemical Research*, **2015**, 39, 433-437	0.6	5
10	QSAR and docking studies of some 1,2,3,4-tetrahydropyrimidines: evaluation of gp41 as possible target for anti-HIV-1 activity. *Medicinal Chemistry Research*, **2015**, 24, 1707-1724	2.2	9
9	QSAR prediction of HIV-1 protease inhibitory activities using docking derived molecular descriptors. *Journal of Theoretical Biology*, **2015**, 369, 13-22	2.3	28
8	Molecular dynamics simulation study and molecular docking descriptors in structure-based QSAR on acetylcholinesterase (AChE) inhibitors. *SAR and QSAR in Environmental Research*, **2013**, 24, 773-94	3.5	29
7	Multitarget fragment-based design of novel inhibitors for AChE and SSAO/VAP-1 enzymes. *Journal of Chemometrics*, **2013**, 27, 297-305	1.6	1

6	Docking, molecular dynamics simulation studies, and structure-based QSAR model on cytochrome P450 2A6 inhibitors. *Structural Chemistry*, **2012**, 23, 341-350	1.8	19
5	Investigation of the interaction between amodiaquine and human serum albumin by fluorescence spectroscopy and molecular modeling. *European Journal of Medicinal Chemistry*, **2012**, 54, 255-63	6.8	93
4	Interactions between Activin-Like Kinase 5 (ALK5) receptor and its inhibitors and the construction of a Docking Descriptor-Based QSAR model. *Journal of the Brazilian Chemical Society*, **2012**, 23, 2043-2052	1.5	8
3	A structure-based QSAR and docking study on imidazo[1,5-a][1,2,4]-triazolo[1,5-d][1,4,]benzodiazepines as Selective GABA(A) α5 inverse agonists. *Chemical Biology and Drug Design*, **2011**, 78, 612-21	2.9	7
2	Prediction of selectivity coefficients of univalent anions for anion-selective electrode using support vector machine. *Electrochimica Acta*, **2008**, 53, 4276-4282	6.7	28
1	A novel QSAR model for prediction of apoptosis-inducing activity of 4-aryl-4-H-chromenes based on support vector machine. *Bioorganic and Medicinal Chemistry*, **2007**, 15, 7746-54	3.4	71