Sajjad Gharaghani

List of Publications by Year
in descending order

60	1,428	393982 19	344852 36
papers	citations	h-index	g-index

66	66	66	1837
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A Survey on semi-supervised feature selection methods. Pattern Recognition, 2017, 64, 141-158.	5.1	357
2	Investigation of the interaction between amodiaquine and human serum albumin by fluorescence spectroscopy and molecular modeling. European Journal of Medicinal Chemistry, 2012, 54, 255-263.	2.6	111
3	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.	2.3	78
4	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, 7746-7754.	1.4	77
5	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.	1.7	62
6	Spectrophotometric determination of synthetic colorants using PSOâ€“GA-ANN. Food Chemistry, 2017, 220, 377-384.	4.2	60
7	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.	3.6	38
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, 773-794.	1.0	34
9	Melatonin Therapy Modulates Cerebral Metabolism and Enhances Remyelination by Increasing PDK4 in a Mouse Model of Multiple Sclerosis. Frontiers in Pharmacology, 2019, 10, 147.	1.6	34
10	Chiral halogenated Schiff base compounds: green synthesis, anticancer activity and DNA-binding study. Journal of Molecular Structure, 2018, 1161, 497-511.	1.8	33
11	A robust graph-based semi-supervised sparse feature selection method. Information Sciences, 2020, 531, 13-30.	4.0	33
12	Prediction of selectivity coefficients of univalent anions for anion-selective electrode using support vector machine. Electrochimica Acta, 2008, 53, 4276-4282.	2.6	31
13	QSAR prediction of HIV-1 protease inhibitory activities using docking derived molecular descriptors. Journal of Theoretical Biology, 2015, 369, 13-22.	0.8	30
14	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, 246-260.	1.7	30
15	Scoring multiple features to predict drug disease associations using information fusion and aggregation. SAR and QSAR in Environmental Research, 2016, 27, 609-628.	1.0	27
16	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.	2.3	24
17	AutoDTI++: deep unsupervised learning for DTI prediction by autoencoders. BMC Bioinformatics, 2021, 22, 204.	1.2	24
18	Docking, molecular dynamics simulation studies, and structure-based QSAR model on cytochrome P450 2A6 inhibitors. Structural Chemistry, 2012, 23, 341-350.	1.0	20

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19	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.	1.1	20
20	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.	1.4	20
21	Pharmacophore model, docking, QSAR, and molecular dynamics simulation studies of substituted cyclic imides and herbal medicines as COX-2 inhibitors. Heliyon, 2021, 7, e06605.	1.4	19
22	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.	1.8	15
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.	2.6	15
24	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.	2.3	14
25	Hybrid docking-QSAR studies of DPP-IV inhibition activities of a series of aminomethyl-piperidones. Computational Biology and Chemistry, 2016, 64, 335-345.	1.1	13
26	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.	1.1	12
27	NDDSA: A network- and domain-based method for predicting drug-side effect associations. Information Processing and Management, 2020, 57, 102357.	5.4	12
28	Feature selection based on graph Laplacian by using compounds with known and unknown activities. Journal of Chemometrics, 2017, 31, e2899.	0.7	10
29	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.	2.3	10
30	Chemometric studies of thymol binding with bovine serum albumin: A developing strategy for the successful investigation of pharmacological activity. Bioelectrochemistry, 2018, 124, 172-184.	2.4	10
31	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.	3.6	10
32	Electrochemical investigation of the inhibition effect of carvacrol on xanthine oxidase activity merging with theoretical studies. Process Biochemistry, 2019, 83, 86-95.	1.8	10
33	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.	3.6	9
34	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, 2043-2092.	0.6	8
35	Synthesis of new triazole tethered derivatives of curcumin and their antibacterial and antifungal properties. Journal of the Iranian Chemical Society, 2019, 16, 465-477.	1.2	8
36	Design of potential anti-tumor PARP-1 inhibitors by QSAR and molecular modeling studies. Molecular Diversity, 2021, 25, 263-277.	2.1	8

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37	Moonlighting protein prediction using physico-chemical and evolutional properties via machine learning methods. BMC Bioinformatics, 2021, 22, 261.	1.2	8
38	A Structureâ€based QSAR and Docking Study on Imidazo[1,5â€a][1,2,4]â€triazolo[1,5â€d][1,4,]benzodiazepines as Selective GABA_AÎ±5 Inverse Agonists. Chemical Biology and Drug Design, 2011, 78, 612-621.	1.5	7
39	Structural stability of Î²-lactoglobulin in the presence of cetylpyridinum bromide: spectroscopic and molecular docking studies. Journal of Biomolecular Structure and Dynamics, 2018, 36, 753-760.	2.0	7
40	Sequential and Mixed Genetic Algorithm and Learning Automata (SGALA, MGALA) for Feature Selection in QSAR. Iranian Journal of Pharmaceutical Research, 2017, 16, 533-553.	0.3	7
41	Synthesis and Antibacterial Evaluation of Novel Xanthone Sulfonamides. Journal of Chemical Research, 2015, 39, 433-437.	0.6	6
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.	1.9	6
43	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.	1.6	6
44	In Silico Drug-designing Studies on Sulforaphane Analogues: Pharmacophore Mapping, Molecular Docking and QSAR Modeling. Current Drug Discovery Technologies, 2021, 18, 139-157.	0.6	6
45	Inhibition of GSK_3Î² by Iridoid Glycosides of Snowberry (Symphoricarpos albus) Effective in the Treatment of Alzheimerâ€™s Disease Using Computational Drug Design Methods. Frontiers in Chemistry, 2021, 9, 709932.	1.8	6
46	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.	1.0	5
47	Toward a hierarchical virtual screening and toxicity risk analysis for identifying novel CA XII inhibitors. BioSystems, 2017, 162, 35-43.	0.9	4
48	Synthesis of novel norsufentanil analogs via a fourâ€component Ugi reaction and in vivo, docking, and <scp>QSAR</scp> studies of their analgesic activity. Chemical Biology and Drug Design, 2018, 91, 902-914.	1.5	4
49	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.	1.8	4
50	In silico drug repositioning of FDA-approved drugs to predict new inhibitors for alpha-synuclein aggregation. Computational Biology and Chemistry, 2020, 88, 107308.	1.1	4
51	Structural systems pharmacology: A framework for integrating metabolic network and structure-based virtual screening for drug discovery against bacteria. PLoS ONE, 2021, 16, e0261267.	1.1	4
52	An in silico approach to design peptide mimetics based on docking and molecular dynamics simulation of EGFRâ€“matuzumab complex. Journal of the Iranian Chemical Society, 2016, 13, 1805-1817.	1.2	3
53	A simple and robust model to predict the inhibitory activity of Î±-glucosidase inhibitors through combined QSAR modeling and molecular docking techniques. Molecular Diversity, 2021, 25, 1811-1825.	2.1	3
54	Multitarget fragmentâ€based design of novel inhibitors for AChE and SSAO/VAPâ€1 enzymes. Journal of Chemometrics, 2013, 27, 297-305.	0.7	2

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55	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.	1.8	2
56	Novel insights into the effect of folateâ€“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.	1.4	1
57	Novel and Predictive QSAR Model for Steroidal and Nonsteroidal 5Î±- Reductase Type II Inhibitors. Current Drug Discovery Technologies, 2021, 18, 317-332.	0.6	1
58	Biomolecular interactions and binding dynamics of inhibitor arachidonic acid, with tyrosinase enzyme. Journal of Biomolecular Structure and Dynamics, 2023, 41, 1378-1387.	2.0	1
59	Insilico Analysis of Zinc Database to Discover New Potent HIV1 Protease Inhibitors. Journal of Pharmacy and Pharmacology, 2020, 8, .	0.1	0
60	Proteochemometrics modeling for prediction of the interactions between caspase isoforms and their inhibitors. Molecular Diversity, 2022, , 1.	2.1	0