Afshin Fassihi

List of Publications by Year
in descending order

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80 papers	1,784 citations	236925 25 h-index	315739 38 g-index
81 all docs	81 docs citations	81 times ranked	2346 citing authors

#	Article	IF	Citations
1	Accelerating Big Data Analysis through LASSO-Random Forest Algorithm in QSAR Studies. Bioinformatics, 2022, 38, 469-475.	4.1	17
2	A Comparative DFT Study on the Antioxidant Activity of Some Novel 3â€Hydroxypyridineâ€4â€One Derivatives. Chemistry and Biodiversity, 2022, 19, e202100703.	2.1	5
3	Design, synthesis, in silico studies, and antiproliferative evaluations of novel indolin-2-one derivatives containing 3-hydroxy-4-pyridinone fragment. Bioorganic and Medicinal Chemistry Letters, 2022, 70, 128784.	2.2	3
4	New 2-alkylthio-1-benzylimidazole-5-carboxylic acid derivatives targeting gp41: design, synthesis and in vitro anti-HIV activity evaluation. Current HIV Research, 2022, 20, .	0.5	0
5	MTX-Loaded Dual Thermoresponsive and pH-Responsive Magnetic Hydrogel Nanocomposite Particles for Combined Controlled Drug Delivery and Hyperthermia Therapy of Cancer. Molecular Pharmaceutics, 2021, 18, 275-284.	4.6	45
6	Synthesis, antioxidant activity, and density functional theory study of some novel 4-[(benzo[d]thiazol-2-ylimino)methyl]phenol derivatives: a comparative approach for the explanation of their radical scavenging activities. Research in Pharmaceutical Sciences, 2021, 16, 35.	1.8	6
7	3D U-Net: A voxel-based method in binding site prediction of protein structure. Journal of Bioinformatics and Computational Biology, 2021, 19, 2150006.	0.8	11
8	Synthesis, Molecular Docking and Molecular Dynamics Simulation of 2- Thioxothiazolidin-4-One Derivatives against Gp41. Current HIV Research, 2021, 19, 47-60.	0.5	2
9	Molecular dynamics simulation and 3D-pharmacophore analysis of new quinoline-based analogues with dual potential against EGFR and VEGFR-2. International Journal of Biological Macromolecules, 2020, 142, 94-113.	7.5	18
10	Dual thermo- and pH-responsive poly(N-isopropylacrylamide-co-(2-dimethylamino) ethyl) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 387 Td (n Bulletin, 2020, 77, 3129-3142.	3.3	13
11	Synthesis, anti-HIV-1 and antiproliferative evaluation of novel 4-nitroimidazole derivatives combined with 5-hydroxy-4-pyridinone moiety. Journal of Molecular Structure, 2020, 1202, 127344.	3.6	9
12	Protein kinase inhibitorsâ€™ classification using K-Nearest neighbor algorithm. Computational Biology and Chemistry, 2020, 86, 107269.	2.3	33
13	Synthesis and evaluation of antioxidant activity of some novel hydroxypyridinone derivatives: a DFT approach for explanation of their radical scavenging activity. Research in Pharmaceutical Sciences, 2020, 15, 515.	1.8	17
14	Identification of Novel 3-Hydroxy-pyran-4-One Derivatives as Potent HIV-1 Integrase Inhibitors Using in silico Structure-Based Combinatorial Library Design Approach. Frontiers in Chemistry, 2019, 7, 574.	3.6	32
15	Preparation of some novel imidazopyridine derivatives of indole as anticancer agents: one-pot multicomponent synthesis, biological evaluation and docking studies. Research on Chemical Intermediates, 2019, 45, 5261-5290.	2.7	5
16	Design and Synthesis of Novel Cytotoxic Indoleâ€Thiosemicarbazone Derivatives: Biological Evaluation and Docking Study. Chemistry and Biodiversity, 2019, 16, e1800470.	2.1	14
17	Anti-cancer, anti-oxidant and molecular docking studies of thiosemicarbazone indole-based derivatives. Research on Chemical Intermediates, 2019, 45, 2827-2854.	2.7	29
18	Gp41 inhibitory activity prediction of theaflavin derivatives using ligand/structure-based virtual screening approaches. Computational Biology and Chemistry, 2019, 79, 119-126.	2.3	6

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19	Recent Advances in the Design and Development of Nonâ€nucleoside Reverse Transcriptase Inhibitor Scaffolds. ChemMedChem, 2019, 14, 52-77.	3.2	18
20	Structureâ€“activity relationship of polyamine conjugates for uptake via polyamine transport system. Structural Chemistry, 2019, 30, 175-184.	2.0	9
21	Design, Synthesis and Molecular Docking Studies of Some Tetrahydropyrimidine Derivatives as Possible Fascin Inhibitors. Chemistry and Biodiversity, 2019, 16, e1800339.	2.1	5
22	Synthesis, Molecular Modelling and Biological Studies of 3-hydroxypyrane- 4-one and 3-hydroxy-pyridine-4-one Derivatives as HIV-1 Integrase Inhibitors. Medicinal Chemistry, 2019, 15, 755-770.	1.5	22
23	Design, Synthesis, and Antiâ€<scp>HIV</scp>â€1 Evaluation of a Novel Series of 1,2,3,4â€Tetrahydropyrimidineâ€5â€Carboxylic Acid Derivatives. Chemistry and Biodiversity, 2018, 15, e1700502.	2.1	8
24	Deep neural network in QSAR studies using deep belief network. Applied Soft Computing Journal, 2018, 62, 251-258.	7.2	77
25	<scp>HIV</scp>â€1 Entry Inhibitors: A Review of Experimental and Computational Studies. Chemistry and Biodiversity, 2018, 15, e1800159.	2.1	14
26	Novel Catechol Derivatives of Arylimidamides as Antileishmanial Agents. Chemistry and Biodiversity, 2018, 15, e1800228.	2.1	1
27	Synthesis and antileishmanial activity of antimony (V) complexes of hydroxypyranone and hydroxypyridinone ligands. Research in Pharmaceutical Sciences, 2018, 13, 111.	1.8	7
28	Synthesis, Biological Evaluation, and Molecular Docking Studies of Novel 4â€[4â€Arylpyridinâ€1(4H)â€yl]benzoic Acid Derivatives as Antiâ€<scp>HIV</scp>â€1 Agents. Chemistry and Biodiversity, 2017, 14, e1700295.	2.1	17
29	The role of different sampling methods in improving biological activity prediction using deep belief network. Journal of Computational Chemistry, 2017, 38, 195-203.	3.3	28
30	Antiâ€HIVâ€1 Activity Prediction of Novel Gp41 Inhibitors Using Structureâ€Based Virtual Screening and Molecular Dynamics Simulation. Molecular Informatics, 2017, 36, 1600060.	2.5	18
31	Cardioprotection Potential of Some Hydroxypyridine Iron Chelators Against H2O2-Induced H9C2 Cell Injury. Turkiye Klinikleri Cardiovascular Sciences, 2017, 29, 10-16.	0.1	0
32	Cuminaldehyde as the Major Component of Cuminum cyminum, a Natural Aldehyde with Inhibitory Effect on Alphaâ€Synuclein Fibrillation and Cytotoxicity. Journal of Food Science, 2015, 80, H2336-45.	3.1	82
33	Hantzsch-Type Dihydropyridines and Biginelli-Type Tetra-hydropyrimidines: A Review of their Chemotherapeutic Activities. Journal of Pharmacy and Pharmaceutical Sciences, 2015, 18, 1.	2.1	38
34	Insights into the human A1 adenosine receptor from molecular dynamics simulation: structural study in the presence of lipid membrane. Medicinal Chemistry Research, 2015, 24, 3645-3659.	2.4	16
35	Elucidation of Molecular Mechanisms Behind the Self-Assembly Behavior of Chitosan Amphiphilic Derivatives Through Experiment and Molecular Modeling. Pharmaceutical Research, 2015, 32, 3899-3915.	3.5	7
36	Design, synthesis and anti-HIV-1 evaluation of a series of 5-hydroxypyridine-4-one derivatives as possible integrase inhibitors. Medicinal Chemistry Research, 2015, 24, 4113-4127.	2.4	9

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37	Docking studies of some 5-hydroxypyridine-4-one derivatives: evaluation of integrase and ribonuclease H domain of reverse transcriptase as possible targets for anti-HIV-1 activity. Medicinal Chemistry Research, 2015, 24, 2195-2212.	2.4	6
38	QSAR and docking analysis of A2B adenosine receptor antagonists based on non-xanthine scaffold. Medicinal Chemistry Research, 2015, 24, 394-407.	2.4	18
39	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.	2.4	12
40	Docking Studies of Some Novel Kojic acid Derivatives as Possible Tyrosinase Inhibitors. Biomedical and Pharmacology Journal, 2015, 8, 535-545.	0.5	11
41	A study on the anti-inflammatory effects of new derivatives of 3-hydroxy pyridine-4-one. Advanced Biomedical Research, 2014, 3, 134.	0.5	2
42	Assessment of antibacterial activity of wool fabrics dyed with natural dyes. Journal of Cleaner Production, 2014, 72, 139-145.	9.3	117
43	Wound healing by topical application of antioxidant iron chelators: kojic acid and deferiprone. International Wound Journal, 2013, 10, 260-264.	2.9	43
44	Computational evaluation of some indenopyrazole derivatives as anticancer compounds; application of QSAR and docking methodologies. Journal of Enzyme Inhibition and Medicinal Chemistry, 2013, 28, 16-32.	5.2	18
45	Physicochemical, pharmaceutical and biological approaches toward designing optimized and efficient hydrophobically modified chitosan-based polymeric micelles as a nanocarrier system for targeted delivery of anticancer drugs. Journal of Drug Targeting, 2013, 21, 693-709.	4.4	35
46	Linear and nonlinear QSAR modeling of 1,3,8-substituted-9-deazaxanthines as potential selective A2BAR antagonists. Medicinal Chemistry Research, 2013, 22, 4549-4567.	2.4	10
47	Molecular Dynamics Simulation of Chemokine Receptors in Lipid Bilayer: A Case Study on <scp>C</scp>â€“<scp>C</scp> Chemokine Receptor Type 2. Chemical Biology and Drug Design, 2013, 82, 534-545.	3.2	15
48	QSAR analysis of some 1-(3,3-diphenylpropyl)-piperidinyl amides and ureas as CCR5 inhibitors using genetic algorithm-least square support vector machine. Medicinal Chemistry Research, 2013, 22, 4384-4400.	2.4	13
49	Statistically validated QSAR study of some antagonists of the human CCR5 receptor using least square support vector machine based on the genetic algorithm and factor analysis. Medicinal Chemistry Research, 2013, 22, 1399-1414.	2.4	7
50	Inhibitory effect and structureâ€“activity relationship of some Biginelli-type pyrimidines against HSV-1. Medicinal Chemistry Research, 2013, 22, 1270-1276.	2.4	12
51	Synthesis, calcium-channel blocking activity, and conformational analysis of some novel 1,4-dihydropyridines: application of PM3 and DFT computational methods. Medicinal Chemistry Research, 2012, 21, 2749-2761.	2.4	14
52	QSAR study of some CCR5 antagonists as anti-HIV agents using radial basis function neural network and general regression neural network on the basis of principal components. Medicinal Chemistry Research, 2012, 21, 3246-3262.	2.4	16
53	Synthesis and antimicrobial activity of novel derivatives of Biginelli pyrimidines. Medicinal Chemistry Research, 2012, 21, 3973-3983.	2.4	27
54	Iron chelation afforded cardioprotection against H2O2-induced H9C2 cell injury: Application of novel 3-hydroxy pyridine-4-one derivatives. International Journal of Cardiology, 2012, 162, 60-63.	1.7	2

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55	Characterization of adenosine receptor in its native environment: insights from molecular dynamics simulations of palmitoylated/glycosylated, membrane-integrated human A2B adenosine receptor. Journal of Molecular Modeling, 2012, 18, 4309-4324.	1.8	15
56	Computer-aided design of novel antibacterial 3-hydroxypyridine-4-ones: application of QSAR methods based on the MOLMAP approach. Journal of Computer-Aided Molecular Design, 2012, 26, 349-361.	2.9	22
57	Application of an expert system based on Genetic Algorithmâ€“Adaptive Neuro-Fuzzy Inference System (GAâ€“ANFIS) in QSAR of cathepsin K inhibitors. Expert Systems With Applications, 2012, 39, 6182-6191.	7.6	38
58	Comparative quantitative structureâ€“activity relationship study of some 1-aminocyclopentyl-3-carboxyamides as CCR2 inhibitors using stepwise MLR, FA-MLR, and GA-PLS. Medicinal Chemistry Research, 2012, 21, 100-115.	2.4	12
59	QSAR study of anthranilic acid sulfonamides as methionine aminopeptidase-2 inhibitors. Monatshefte FÃ¼r Chemie, 2012, 143, 189-198.	1.8	4
60	Theoretical studies of 1,4-dihydropyridine-3,5-dicarboxamides as possible inhibitors of Mycobacterium tuberculosis enoyl reductase. Monatshefte FÃ¼r Chemie, 2012, 143, 19-27.	1.8	4
61	Preparation of budesonideâ€“dextran conjugates using glutarate spacer as a colon-targeted drug delivery system:in vitro/in vivoevaluation in induced ulcerative colitis. Journal of Drug Targeting, 2011, 19, 140-153.	4.4	32
62	Homology modeling of human CCR5 and analysis of its binding properties through molecular docking and molecular dynamics simulation. Biochimica Et Biophysica Acta - Biomembranes, 2011, 1808, 802-817.	2.6	54
63	Exploring a Model of a Chemokine Receptor/Ligand Complex in an Explicit Membrane Environment by Molecular Dynamics Simulation: The Human CCR1 Receptor. Journal of Chemical Information and Modeling, 2011, 51, 2717-2730.	5.4	22
64	QSAR Analysis for Some Diarylâ€substituted Pyrazoles as CCR2 Inhibitors by GAâ€Stepwise MLR. Chemical Biology and Drug Design, 2011, 77, 75-85.	3.2	22
65	Application of PC-ANN and PC-LS-SVM in QSAR of CCR1 antagonist compounds: A comparative study. European Journal of Medicinal Chemistry, 2010, 45, 1572-1582.	5.5	51
66	Effectiveness of budesonide-succinate-dextran conjugate as a novel prodrug of budesonide against acetic acid-induced colitis in rats. International Journal of Colorectal Disease, 2010, 25, 1159-1165.	2.2	49
67	Application of partial least squares and radial basis function neural networks in multivariate imaging analysis-quantitative structure activity relationship: Study of cyclin dependent kinase 4 inhibitors. Journal of Molecular Graphics and Modelling, 2010, 29, 518-528.	2.4	26
68	QSAR study of isatin analogues as in vitro anti-cancer agents. European Journal of Medicinal Chemistry, 2010, 45, 1113-1118.	5.5	50
69	Validated QSAR analysis of some diaryl substituted pyrazoles as CCR2 inhibitors by various linear and nonlinear multivariate chemometrics methods. European Journal of Medicinal Chemistry, 2010, 45, 3394-3406.	5.5	29
70	QSAR study of anthranilic acid sulfonamides as inhibitors of methionine aminopeptidase-2 using LS-SVM and GRNN based on principal components. European Journal of Medicinal Chemistry, 2010, 45, 4499-4508.	5.5	58
71	Synthesis, antimicrobial evaluation and QSAR study of some 3-hydroxypyridine-4-one and 3-hydroxypyran-4-one derivatives. European Journal of Medicinal Chemistry, 2009, 44, 2145-2157.	5.5	67
72	Synthesis and antitubercular activity of novel 4-substituted imidazolyl-2,6-dimethyl-N3,N5-bisaryl-1,4-dihydropyridine-3,5-dicarboxamides. European Journal of Medicinal Chemistry, 2009, 44, 3253-3258.	5.5	60

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73	Quantitative Structureâ€“Activity Relationship Studies on 2â€Aminoâ€6â€arylsulfonylbenzonitriles as Human Immunodeficiency Viruses Type 1 Reverse Transcriptase Inhibitors Using Descriptors Obtained from Substituents and Whole Molecular Structures. Chemical Biology and Drug Design, 2009, 74, 405-415.	3.2	5
74	Synthesis and evaluation of dextranâ€“budesonide conjugates as colon specific prodrugs for treatment of ulcerative colitis. International Journal of Pharmaceutics, 2009, 365, 69-76.	5.2	66
75	QSAR study of PETT derivatives as potent HIV-1 reverse transcriptase inhibitors. Journal of Molecular Graphics and Modelling, 2009, 28, 146-155.	2.4	7
76	N-Propynyl analogs of Î²-phenylethylidenehydrazines: Synthesis and evaluation of effects on glycine, GABA, and monoamine oxidase. Bioorganic and Medicinal Chemistry, 2008, 16, 8254-8263.	3.0	6
77	QSAR Study of Antimicrobial 3-Hydroxypyridine-4-one and 3-Hydroxypyran-4-one Derivatives Using Different Chemometric Tools. International Journal of Molecular Sciences, 2008, 9, 2407-2423.	4.1	21
78	QSAR Study of p56lck Protein Tyrosine Kinase Inhibitory Activity of Flavonoid Derivatives Using MLR and GA-PLS. International Journal of Molecular Sciences, 2008, 9, 1876-1892.	4.1	28
79	Design and biological evaluation of phenyl-substituted analogs of Î²-phenylethylidenehydrazine. Bioorganic and Medicinal Chemistry, 2005, 13, 4389-4395.	3.0	11
80	Synthesis of dialkyl 1,4â€dihydroâ€2,6â€dimethylpyridineâ€3,5â€dicarboxylates and alkyl 1,4â€dihydroâ€2,6â€dimethylâ€3â€nitropyridineâ€5â€carboxylates possessing a câ€4 2,4â€dioxoâ€1,2,3,4â€tetrahydropyrimidinâ€5â€yl (uracil) substituent to determine calcium channel modulation structureâ€activity relationships. Journal of Heterocyclic Chemistry, 2004, 41, 263-266.	2.6	6