Ramin Ekhteiari Salmas

List of Publications by Year
in descending order

58 papers	1,376 citations	279701 23 h-index	377752 34 g-index
58 all docs	58 docs citations	58 times ranked	2028 citing authors

#	Article	IF	Citations
1	Acetylcholinesterase and carbonic anhydrase inhibitory properties of novel urea and sulfamide derivatives incorporating dopaminergic 2-aminotetralin scaffolds. Bioorganic and Medicinal Chemistry, 2016, 24, 2318-2329.	1.4	131
2	Carbonic anhydrase inhibitory properties of novel benzylsulfamides using molecular modeling and experimental studies. Bioorganic Chemistry, 2014, 56, 75-82.	2.0	113
3	Combinatorial peptide library screening for discovery of diverse Î±-glucosidase inhibitors using molecular dynamics simulations and binary QSAR models. Journal of Biomolecular Structure and Dynamics, 2019, 37, 726-740.	2.0	74
4	The synthesis of novel sulfamides derived from Î²-benzylphenethylamines as acetylcholinesterase, butyrylcholinesterase and carbonic anhydrase enzymes inhibitors. Bioorganic Chemistry, 2017, 74, 238-250.	2.0	64
5	Binding Interactions of Dopamine and Apomorphine in D2High and D2Low States of Human Dopamine D2 Receptor Using Computational and Experimental Techniques. ACS Chemical Neuroscience, 2016, 7, 185-195.	1.7	45
6	Synthesis, anticholinesterase activity and molecular modeling study of novel carbamate-substituted thymol/carvacrol derivatives. Bioorganic and Medicinal Chemistry, 2017, 25, 1352-1363.	1.4	45
7	Virtual screening of eighteen million compounds against dengue virus: Combined molecular docking and molecular dynamics simulations study. Journal of Molecular Graphics and Modelling, 2016, 66, 99-107.	1.3	42
8	Investigating the molecular mechanism of staphylococcal DNA gyrase inhibitors: A combined ligand-based and structure-based resources pipeline. Journal of Molecular Graphics and Modelling, 2018, 85, 122-129.	1.3	42
9	Investigation of Inhibition Mechanism of Chemokine Receptor CCR5 by Micro-second Molecular Dynamics Simulations. Scientific Reports, 2015, 5, 13180.	1.6	40
10	Carbonic anhydrase inhibitors: Design, synthesis, kinetic, docking and molecular dynamics analysis of novel glycine and phenylalanine sulfonamide derivatives. Bioorganic and Medicinal Chemistry, 2015, 23, 7353-7358.	1.4	39
11	Characterization, in Vivo Evaluation, and Molecular Modeling of Different Propofolâ€“Cyclodextrin Complexes To Assess Their Drug Delivery Potential at the Bloodâ€“Brain Barrier Level. Journal of Chemical Information and Modeling, 2016, 56, 1914-1922.	2.5	39
12	Effects of propolis, caffeic acid phenethyl ester, and pollen on renal injury in hypertensive rat: An experimental and theoretical approach. Cell Biochemistry and Function, 2017, 35, 304-314.	1.4	35
13	Fullerene-based inhibitors of HIV-1 protease. Journal of Peptide Science, 2015, 21, 862-870.	0.8	31
14	Modeling and protein engineering studies of active and inactive states of human dopamine D2 receptor (D2R) and investigation of drug/receptor interactions. Molecular Diversity, 2015, 19, 321-332.	2.1	29
15	Molecular modeling and in vitro approaches towards cholinesterase inhibitory effect of some natural xanthohumol, naringenin, and acyl phloroglucinol derivatives. Phytomedicine, 2018, 42, 25-33.	2.3	29
16	Evaluation of the potential toxicity of unmodified and modified cyclodextrins on murine blood-brain barrier endothelial cells. Journal of Toxicological Sciences, 2016, 41, 175-184.	0.7	28
17	Synthesis, biological activity and multiscale molecular modeling studies for coumaryl-carboxamide derivatives as selective carbonic anhydrase IX inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2017, 32, 1042-1052.	2.5	28
18	Synthesis, bioactivity and binding energy calculations of novel 3-ethoxysalicylaldehyde based thiosemicarbazone derivatives. Bioorganic Chemistry, 2020, 100, 103924.	2.0	27

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19	Solubility profiles, hydration and desolvation of curcumin complexed with Î³-cyclodextrin and hydroxypropyl-Î³-cyclodextrin. Journal of Molecular Structure, 2017, 1134, 91-98.	1.8	26
20	In vitro and in silico approaches to appraise Polygonum maritimum L. as a source of innovative products with anti-ageing potential. Industrial Crops and Products, 2018, 111, 391-399.	2.5	26
21	Elucidation of Conformational States, Dynamics, and Mechanism of Binding in Human Îº-Opioid Receptor Complexes. Journal of Chemical Information and Modeling, 2014, 54, 2294-2308.	2.5	25
22	Silverâ€“Sodium Ion Exchange Dynamics in LTA Zeolite Membranes. Journal of Physical Chemistry C, 2013, 117, 1663-1671.	1.5	24
23	Analysis of the Glutamate Agonist LY404,039 Binding to Nonstatic Dopamine Receptor D2 Dimer Structures and Consensus Docking. ACS Chemical Neuroscience, 2017, 8, 1404-1415.	1.7	23
24	Discovery of selective dengue virus inhibitors using combination of molecular fingerprint-based virtual screening protocols, structure-based pharmacophore model development, molecular dynamics simulations and in vitro studies. Journal of Molecular Graphics and Modelling, 2018, 79, 88-102.	1.3	23
25	In silicoinvestigation of PARP-1 catalytic domains inholoandapostates for the design of high-affinity PARP-1 inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 112-120.	2.5	21
26	Integration of multi-scale molecular modeling approaches with experiments for the in silico guided design and discovery of novel hERG-Neutral antihypertensive oxazalone and imidazolone derivatives and analysis of their potential restrictive effects on cell proliferation. European Journal of Medicinal Chemistry, 2018, 145, 273-290.	2.6	21
27	Leveraging NMR and X-ray Data of the Free Ligands to Build Better Drugs Targeting Angiotensin II Type 1 G-Protein Coupled Receptor. Current Medicinal Chemistry, 2015, 23, 36-59.	1.2	20
28	Structure-based design of hERG-neutral antihypertensive oxazalone and imidazolone derivatives. Journal of Molecular Graphics and Modelling, 2018, 79, 103-117.	1.3	18
29	Oligomerization and cooperativity in GPCRs from the perspective of the angiotensin AT1 and dopamine D2 receptors. Neuroscience Letters, 2019, 700, 30-37.	1.0	17
30	Evaluation of collagenase, elastase and tyrosinase inhibitory activities of Cotinus coggygria Scop. through in vitro and in silico approaches. South African Journal of Botany, 2020, 132, 277-288.	1.2	17
31	Virtual screening of small molecules databases for discovery of novel PARP-1 inhibitors: combination of in silico and in vitro studies. Journal of Biomolecular Structure and Dynamics, 2017, 35, 1899-1915.	2.0	16
32	Combined molecular modeling and cholinesterase inhibition studies on some natural and semisynthetic O-alkylcoumarin derivatives. Bioorganic Chemistry, 2019, 84, 355-362.	2.0	16
33	Molecular Simulations of Solved Co-crystallized X-Ray Structures Identify Action Mechanisms of PDEÎ´ Inhibitors. Biophysical Journal, 2015, 109, 1163-1168.	0.2	15
34	Biological Insights of the Dopaminergic Stabilizer ACR16 at the Binding Pocket of Dopamine D2 Receptor. ACS Chemical Neuroscience, 2017, 8, 826-836.	1.7	15
35	Kinetic andin silicostudies of hydroxy-based inhibitors of carbonic anhydrase isoforms I and II. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 31-37.	2.5	14
36	Atomistic molecular dynamics simulations of typical and atypical antipsychotic drugs at the dopamine D2 receptor (D2R) elucidates their inhibition mechanism. Journal of Biomolecular Structure and Dynamics, 2017, 35, 738-754.	2.0	14

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37	The effects of pollen, propolis, and caffeic acid phenethyl ester on tyrosine hydroxylase activity and total RNA levels in hypertensive rats caused by nitric oxide synthase inhibition: experimental, docking and molecular dynamic studies. Journal of Biomolecular Structure and Dynamics, 2018, 36, 609-620.	2.0	14
38	The signaling pathway of dopamine D2 receptor (D2R) activation using normal mode analysis (NMA) and the construction of pharmacophore models for D2R ligands. Journal of Biomolecular Structure and Dynamics, 2017, 35, 2040-2048.	2.0	13
39	Profiling the annual change of the neurobiological and antioxidant effects of five Origanum species in correlation with their phytochemical composition. Food Chemistry, 2022, 368, 130775.	4.2	13
40	Biochemical changes induced by grape seed extract and low level laser therapy administration during intraoral wound healing in rat liver: an experimental and in silico study. Journal of Biomolecular Structure and Dynamics, 2018, 36, 993-1008.	2.0	12
41	Discovery of Klotho peptide antagonists against Wnt3 and Wnt3a target proteins using combination of protein engineering, proteinâ€“protein docking, peptide docking and molecular dynamics simulations. Journal of Enzyme Inhibition and Medicinal Chemistry, 2017, 32, 84-98.	2.5	11
42	Discovering novel carbonic anhydrase type IX (CA IX) inhibitors from seven million compounds using virtual screening andin vitroanalysis. Journal of Enzyme Inhibition and Medicinal Chemistry, 2015, 31, 1-9.	2.5	10
43	Investigation of inhibition of human glucose 6-phosphate dehydrogenase by some 99mTc chelators byin silicoandin vitromethods. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 141-147.	2.5	9
44	First universal pharmacophore model for hERG1 K + channel activators: acthER. Journal of Molecular Graphics and Modelling, 2017, 74, 153-170.	1.3	9
45	Synthesis, anticholinesterase activity and molecular modeling studies of novel carvacrol-substituted amide derivatives. Journal of Biomolecular Structure and Dynamics, 2020, 38, 841-859.	2.0	9
46	HDXmodeller: an online webserver for high-resolution HDX-MS with auto-validation. Communications Biology, 2021, 4, 199.	2.0	9
47	Identification of novel serotonin reuptake inhibitors targeting central and allosteric binding sites: A virtual screening and molecular dynamics simulations study. Journal of Molecular Graphics and Modelling, 2017, 74, 193-202.	1.3	8
48	A QM proteinâ€“ligand investigation of antipsychotic drugs with the dopamine D2 Receptor (D2R). Journal of Biomolecular Structure and Dynamics, 2018, 36, 2668-2677.	2.0	6
49	Mutated form (G52E) of inactive diphtheria toxin CRM197: molecular simulations clearly display effect of the mutation to NAD binding. Journal of Biomolecular Structure and Dynamics, 2016, 34, 2462-2468.	2.0	4
50	Kinetic and docking studies of cytosolic/tumor-associated carbonic anhydrase isozymes I, II and IX with some hydroxylic compounds. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 1214-1220.	2.5	4
51	Structural Investigation of the Dopamine-2 Receptor Agonist Bromocriptine Binding to Dimeric D2HighR and D2LowR States. Journal of Chemical Information and Modeling, 2018, 58, 826-836.	2.5	3
52	Characterization and Management of Noise in HDX-MS Data Modeling. Analytical Chemistry, 2021, 93, 7323-7331.	3.2	3
53	Publisher Note. Journal of Molecular Graphics and Modelling, 2017, 77, 338.	1.3	2
54	Amberboin and lipidiol: X-ray crystalographic data, absolute configuration and inhibition of cholinesterase. Phytochemistry Letters, 2018, 27, 44-48.	0.6	2

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55	7-Acetoxyhorminone from Salvia multicaulis Vahl. as Promising Inhibitor of 3-Hydroxy-3-methylglutaryl Coenzyme A (HMG-CoA) Reductase. Pharmaceuticals, 2022, 15, 198.	1.7	2
56	Publisher's note. Journal of Molecular Graphics and Modelling, 2017, 77, 240.	1.3	1
57	Protein Engineering Studies for C-C Chemokine Receptor Type 2 (CCR2). Current Enzyme Inhibition, 2016, 12, 110-114.	0.3	0
58	Exploiting the Propagation of Constrained Variables for Enhanced HDX-MS Data Optimization. Analytical Chemistry, 2021, 93, 16417-16424.	3.2	0