Busecan Aksoydan

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Reducing Virulence and Biofilm of Pseudomonas aeruginosa by Potential Quorum Sensing Inhibitor Carotenoid: Zeaxanthin. Microbial Ecology, 2017, 74, 466-473.	2.8	56
2	Proposing Novel MAO-B Hit Inhibitors Using Multidimensional Molecular Modeling Approaches and Application of Binary QSAR Models for Prediction of Their Therapeutic Activity, Pharmacokinetic and Toxicity Properties. ACS Chemical Neuroscience, 2018, 9, 1768-1782.	3.5	33
3	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.	5.2	28
4	Near-physiological-temperature serial crystallography reveals conformations of SARS-CoV-2 main protease active site for improved drug repurposing. Structure, 2021, 29, 1382-1396.e6.	3.3	28
5	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.	3.5	23
6	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.	5.5	21
7	Structure-based design of hERG-neutral antihypertensive oxazalone and imidazolone derivatives. Journal of Molecular Graphics and Modelling, 2018, 79, 103-117.	2.4	18
8	Host–Guest Interactions between Candesartan and Its Prodrug Candesartan Cilexetil in Complex with 2-Hydroxypropyl-β-cyclodextrin: On the Biological Potency for Angiotensin II Antagonism. Molecular Pharmaceutics, 2019, 16, 1255-1271.	4.6	17
9	Current status of multiscale simulations on GPCRs. Current Opinion in Structural Biology, 2019, 55, 93-103.	5.7	17
10	Oligomerization and cooperativity in GPCRs from the perspective of the angiotensin AT1 and dopamine D2 receptors. Neuroscience Letters, 2019, 700, 30-37.	2.1	17
11	Biological Insights of the Dopaminergic Stabilizer ACR16 at the Binding Pocket of Dopamine D2 Receptor. ACS Chemical Neuroscience, 2017, 8, 826-836.	3.5	15
12	Screening of Clinically Approved and Investigation Drugs as Potential Inhibitors of SARS oVâ€2: A Combined <i>in silico</i> and <i>inâ€vitro</i> Study. Molecular Informatics, 2022, 41, e2100062.	2.5	9
13	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.	2.4	8
14	In silico characterization of adipokinetic hormone receptor and screening for pesticide candidates against stick insect, Carausius morosus. Journal of Molecular Graphics and Modelling, 2020, 101, 107720.	2.4	8
15	Integrated Binary QSAR-Driven Virtual Screening and In Vitro Studies for Finding Novel hMAO-B-Selective Inhibitors. Journal of Chemical Information and Modeling, 2020, 60, 4047-4055.	5.4	7
16	Molecular simulations reveal the impact of RAMP1 on ligand binding and dynamics of calcitonin gene-related peptide receptor (CGRPR) heterodimer. Computers in Biology and Medicine, 2022, 141, 105130.	7.0	3
17	Virtual drug repurposing study for the CGRPR identifies pentagastrin and leuprorelin as putative candidates. Journal of Molecular Graphics and Modelling, 2022, 116, 108254.	2.4	2
18	Publisher's note. Journal of Molecular Graphics and Modelling, 2017, 77, 240.	2.4	1

#	Article	IF	CITATIONS
19	Application of Multiscale Simulation Tools on GPCRs. An Example with Angiotensin II Type 1 Receptor. Methods in Molecular Biology, 2018, 1824, 431-448.	0.9	0