Vladimir Chupakhin

List of Publications by Year
in descending order

22	608	840585 11	752573 20
papers	citations	h-index	g-index

23	23	23	1047
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Development and implementation of an enterprise-wide predictive model for early absorption, distribution, metabolismÂand excretion properties. Future Medicinal Chemistry, 2021, 13, 1639-1654.	1.1	7
2	Industry-scale application and evaluation of deep learning for drug target prediction. Journal of Cheminformatics, 2020, 12, 26.	2.8	23
3	Repurposing High-Throughput Image Assays Enables Biological Activity Prediction for Drug Discovery. Cell Chemical Biology, 2018, 25, 611-618.e3.	2.5	176
4	HyperLoom. , 2018, , .		13
5	HyperLoom Possibilities for Executing Scientific Workflows on the Cloud. Advances in Intelligent Systems and Computing, 2018, , 397-406.	0.5	2
6	Discovery of N-(Pyridin-4-yl)-1,5-naphthyridin-2-amines as Potential Tau Pathology PET Tracers for Alzheimerâ€™s Disease. Journal of Medicinal Chemistry, 2017, 60, 1272-1291.	2.9	31
7	ExCAPE-DB: an integrated large scale dataset facilitating Big Data analysis in chemogenomics. Journal of Cheminformatics, 2017, 9, 17.	2.8	116
8	Macau: Scalable Bayesian factorization with high-dimensional side information using MCMC. , 2017, , .		23
9	Synthesis of novel bridged dinitrogen heterocycles and their evaluation as potential fragments for the design of biologically active compounds. Tetrahedron, 2014, 70, 7854-7864.	1.0	18
10	Simple Ligandâ€“Receptor Interaction Descriptor (SILIRID) for alignment-free binding site comparison. Computational and Structural Biotechnology Journal, 2014, 10, 33-37.	1.9	25
11	Asymmetric synthesis and molecular docking study of enantiomerically pure pyrrolidine derivatives with potential antithrombin activity. Tetrahedron: Asymmetry, 2013, 24, 838-843.	1.8	15
12	Determination of binding points of methylene blue and cationic phenoxazine dyes on human butyrylcholinesterase. Archives of Biochemistry and Biophysics, 2013, 532, 32-38.	1.4	10
13	Synthesis of PDE IV inhibitors. First asymmetric synthesis of two of GlaxoSmithKline's highly potent Rolipram analogues. Organic and Biomolecular Chemistry, 2013, 11, 8082.	1.5	17
14	Predicting Ligand Binding Modes from Neural Networks Trained on Proteinâ€“Ligand Interaction Fingerprints. Journal of Chemical Information and Modeling, 2013, 53, 763-772.	2.5	47
15	Design of small-molecule thrombin inhibitors based on the cis-5-phenylproline scaffold. Russian Chemical Bulletin, 2011, 60, 685-693.	0.4	7
16	Design, synthesis and biotest of a bicyclo[3.3.1]nonane analogue of 2-amino-5,6-dihydro-4H-1,3-thiazine. Mendeleev Communications, 2010, 20, 323-325.	0.6	18
17	Ionotropic GABA receptors: modelling and design of selective ligands. Journal of Cheminformatics, 2010, 2, .	2.8	0
18	Molecular modeling of ligandâ€“receptor interactions in GABAC receptor. Journal of Molecular Graphics and Modelling, 2009, 27, 813-821.	1.3	21

#	Article	IF	Citations
19	Computer-aided design of selective ligands of the benzodiazepine-binding site of the GABAA receptor. Doklady Chemistry, 2008, 422, 227-230.	0.2	7
20	Modeling and analysis of ligand-receptor interactions in the GABAC receptor. Doklady Biochemistry and Biophysics, 2007, 412, 25-28.	0.3	7
21	Design of potential NO-synthase inhibitors on the basis of 2-amino-5,6-dihydro-4H-1,3-thiazine derivatives. Moscow University Chemistry Bulletin, 2007, 62, 243-245.	0.2	4
22	Modeling the open and closed forms of GABAA receptor: Analysis of ligand-receptor interactions for the GABA-binding site. Doklady Biochemistry and Biophysics, 2006, 408, 169-174.	0.3	10