Alexey V Zakharov

List of Publications by Year
in descending order

31	1,779	394421 19	434195 31
papers	citations	h-index	g-index

39	39	39	2276
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	QSAR Modelling of Rat Acute Toxicity on the Basis of PASS Prediction. Molecular Informatics, 2011, 30, 241-250.	2.5	278
2	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. Environmental Health Perspectives, 2016, 124, 1023-1033.	6.0	264
3	A critical overview of computational approaches employed for COVID-19 drug discovery. Chemical Society Reviews, 2021, 50, 9121-9151.	38.1	128
4	Alarms about structural alerts. Green Chemistry, 2016, 18, 4348-4360.	9.0	103
5	QSAR Modeling of Imbalanced High-Throughput Screening Data in PubChem. Journal of Chemical Information and Modeling, 2014, 54, 705-712.	5.4	95
6	Deep learning identifies synergistic drug combinations for treating COVID-19. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	87
7	Synergistic and Antagonistic Drug Combinations against SARS-CoV-2. Molecular Therapy, 2021, 29, 873-885.	8.2	78
8	Quantitative Prediction of Antitarget Interaction Profiles for Chemical Compounds. Chemical Research in Toxicology, 2012, 25, 2378-2385.	3.3	70
9	QSAR Modeling and Prediction of Drugâ€“Drug Interactions. Molecular Pharmaceutics, 2016, 13, 545-556.	4.6	65
10	A widely-applicable high-throughput cellular thermal shift assay (CETSA) using split Nano Luciferase. Scientific Reports, 2018, 8, 9472.	3.3	65
11	Novel Consensus Architecture To Improve Performance of Large-Scale Multitask Deep Learning QSAR Models. Journal of Chemical Information and Modeling, 2019, 59, 4613-4624.	5.4	47
12	A New Approach to Radial Basis Function Approximation and Its Application to QSAR. Journal of Chemical Information and Modeling, 2014, 54, 713-719.	5.4	43
13	Discovery of TMPRSS2 Inhibitors from Virtual Screening as a Potential Treatment of COVID-19. ACS Pharmacology and Translational Science, 2021, 4, 1124-1135.	4.9	40
14	An Automated High-Throughput Metabolic Stability Assay Using an Integrated High-Resolution Accurate Mass Method and Automated Data Analysis Software. Drug Metabolism and Disposition, 2016, 44, 1653-1661.	3.3	35
15	Large-Scale Modeling of Multispecies Acute Toxicity End Points Using Consensus of Multitask Deep Learning Methods. Journal of Chemical Information and Modeling, 2021, 61, 653-663.	5.4	35
16	QSAR Modeling Using Large-Scale Databases: Case Study for HIV-1 Reverse Transcriptase Inhibitors. Journal of Chemical Information and Modeling, 2015, 55, 1388-1399.	5.4	34
17	Computational tools and resources for metabolism-related property predictions. 2. Application to prediction of half-life time in human liver microsomes. Future Medicinal Chemistry, 2012, 4, 1933-1944.	2.3	31
18	Critical Assessment of Artificial Intelligence Methods for Prediction of hERG Channel Inhibition in the â€œBig Dataâ€•Era. Journal of Chemical Information and Modeling, 2020, 60, 6007-6019.	5.4	29

#	Article	IF	Citations
19	Endonuclease FEN1 Coregulates ERÎ± Activity and Provides a Novel Drug Interface in Tamoxifen-Resistant Breast Cancer. Cancer Research, 2020, 80, 1914-1926.	0.9	23
20	SCAM Detective: Accurate Predictor of Small, Colloidally Aggregating Molecules. Journal of Chemical Information and Modeling, 2020, 60, 4056-4063.	5.4	21
21	Design, Synthesis and Pharmacological Evaluation of Novel Vanadium-Containing Complexes as Antidiabetic Agents. PLoS ONE, 2014, 9, e100386.	2.5	17
22	Rational Use of Heterogeneous Data in Quantitative Structureâ€“Activity Relationship (QSAR) Modeling of Cyclooxygenase/Lipoxygenase Inhibitors. Journal of Chemical Information and Modeling, 2019, 59, 713-730.	5.4	17
23	Predicting liver cytosol stability of small molecules. Journal of Cheminformatics, 2020, 12, 21.	6.1	16
24	Novel HIV-1 Integrase Inhibitor Development by Virtual Screening Based on QSAR Models. Current Topics in Medicinal Chemistry, 2015, 16, 441-448.	2.1	14
25	Optimization of High-Throughput Methyltransferase Assays for the Discovery of Small Molecule Inhibitors. ACS Combinatorial Science, 2020, 22, 422-432.	3.8	14
26	Development of Robust Quantitative Structure-Activity Relationship Models for CYP2C9, CYP2D6, and CYP3A4 Catalysis and Inhibition. Drug Metabolism and Disposition, 2021, 49, 822-832.	3.3	14
27	Computational Toxicology in Drug Discovery: Opportunities and Limitations. Challenges and Advances in Computational Chemistry and Physics, 2014, , 325-367.	0.6	8
28	Hybrid In Silico Approach Reveals Novel Inhibitors of Multiple SARS-CoV-2 Variants. ACS Pharmacology and Translational Science, 2021, 4, 1675-1688.	4.9	6
29	Small Molecule Inhibitors of Activation-Induced Deaminase Decrease Class Switch Recombination in B Cells. ACS Pharmacology and Translational Science, 2021, 4, 1214-1226.	4.9	5
30	Allosteric Binders of ACE2 Are Promising Anti-SARS-CoV-2 Agents. ACS Pharmacology and Translational Science, 2022, 5, 468-478.	4.9	3
31	A Genome-Edited ERÎ±-HiBiT Fusion Reporter Cell Line for the Identification of ERÎ± Modulators Via High-Throughput Screening and CETSA. Assay and Drug Development Technologies, 2021, 19, 539-549.	1.2	2