

Kyrylo Klimenko

List of Publications by Year in descending order

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Version: 2024-02-01

14
papers

117
citations

1684188
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1281871
11
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14
all docs

14
docs citations

14
times ranked

137
citing authors

#	ARTICLE	IF	CITATIONS
1	Chemical Space Mapping and Structure-Activity Analysis of the ChEMBL Antiviral Compound Set. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 1438-1454.	5.4	31
2	QSAR modelling of a large imbalanced aryl hydrocarbon activation dataset by rational and random sampling and screening of 80,086 REACH pre-registered and/or registered substances. <i>PLoS ONE</i> , 2019, 14, e0213848.	2.5	19
3	Novel enhanced applications of QSPR models: Temperature dependence of aqueous solubility. <i>Journal of Computational Chemistry</i> , 2016, 37, 2045-2051.	3.3	15
4	Virtual screening, synthesis and biological evaluation of DNA intercalating antiviral agents. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2017, 27, 3915-3919.	2.2	15
5	The Solubility of Gases in Ionic Liquids: A Chemoinformatic Predictive and Interpretable Approach. <i>ChemPhysChem</i> , 2021, 22, 2190-2200.	2.1	9
6	Water Solubility Trends in Ionic Liquids: The Quantitative Structure-Property Relationship Model versus Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2021, 125, 11491-11497.	2.6	5
7	R- based Tool for a Pairwise Structure-Activity Relationship Analysis. <i>Molecular Informatics</i> , 2018, 37, e1700094.	2.5	4
8	QSPR Modeling of Liquid-Liquid Equilibria in Two-Phase Systems of Water and Ionic Liquid. <i>Molecular Informatics</i> , 2020, 39, e2000001.	2.5	4
9	SelinfDB: A Database of Selectivity at Infinite Dilution for Liquid-Liquid Extraction. <i>Industrial & Engineering Chemistry Research</i> , 2021, 60, 8209-8217.	3.7	4
10	In silico identification of endogenous and exogenous agonists of Estrogen-related receptor β . <i>Computational Toxicology</i> , 2019, 10, 105-112.	3.3	3
11	QSAR modeling of different minimum potency levels for in vitro human CAR activation and inhibition and screening of 80,086 REACH and 54,971 U.S. substances. <i>Computational Toxicology</i> , 2020, 14, 100121.	3.3	3
12	Examining the evidence of non-monotonic dose-response in Androgen Receptor agonism high-throughput screening assay. <i>Toxicology and Applied Pharmacology</i> , 2021, 410, 115338.	2.8	3
13	Aminoalkoxyfluorenones and aminoalkoxybiphenyls: DNA binding modes. <i>Bioorganic Chemistry</i> , 2019, 86, 52-60.	4.1	1
14	QSPR modeling of selectivity at infinite dilution of ionic liquids. <i>Journal of Cheminformatics</i> , 2021, 13, 83.	6.1	1