

Sathesh Bhat

List of Publications by Year in descending order

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Version: 2024-02-01

16
papers

1,293
citations

759233

12
h-index

940533

16
g-index

20
all docs

20
docs citations

20
times ranked

2308
citing authors

#	ARTICLE	IF	CITATIONS
1	AutoDesigner, a <i>De Novo</i> Design Algorithm for Rapidly Exploring Large Chemical Space for Lead Optimization: Application to the Design and Synthesis of α -Amino Acid Oxidase Inhibitors. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 1905-1915.	5.4	12
2	Discovery of a Novel Class of α -Amino Acid Oxidase Inhibitors Using the Schrödinger Computational Platform. <i>Journal of Medicinal Chemistry</i> , 2022, 65, 6775-6802.	6.4	10
3	From computer-aided drug discovery to computer-driven drug discovery. <i>Drug Discovery Today: Technologies</i> , 2021, 39, 111-117.	4.0	32
4	Combining Cloud-Based Free-Energy Calculations, Synthetically Aware Enumerations, and Goal-Directed Generative Machine Learning for Rapid Large-Scale Chemical Exploration and Optimization. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 4311-4325.	5.4	34
5	Reaction-Based Enumeration, Active Learning, and Free Energy Calculations To Rapidly Explore Synthetically Tractable Chemical Space and Optimize Potency of Cyclin-Dependent Kinase 2 Inhibitors. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3782-3793.	5.4	81
6	Free Energy Calculation Guided Virtual Screening of Synthetically Feasible Ligand R-Group and Scaffold Modifications: An Emerging Paradigm for Lead Optimization. <i>Annual Reports in Medicinal Chemistry</i> , 2017, 50, 237-262.	0.9	4
7	Inhibition of acetyl-CoA carboxylase suppresses fatty acid synthesis and tumor growth of non-small-cell lung cancer in preclinical models. <i>Nature Medicine</i> , 2016, 22, 1108-1119.	30.7	357
8	Acetyl-CoA carboxylase inhibition by ND-630 reduces hepatic steatosis, improves insulin sensitivity, and modulates dyslipidemia in rats. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, E1796-805.	7.1	223
9	Discovery of MK-8831, A Novel Spiro-Proline Macrocycle as a Pan-Genotypic HCV-NS3/4a Protease Inhibitor. <i>ACS Medicinal Chemistry Letters</i> , 2016, 7, 111-116.	2.8	31
10	Novel Quinoline-Based P2-P4 Macrocyclic Derivatives As Pan-Genotypic HCV NS3/4a Protease Inhibitors. <i>ACS Medicinal Chemistry Letters</i> , 2014, 5, 264-269.	2.8	22
11	2-Aryl benzimidazoles: Human SCD1-specific stearoyl coenzyme-A desaturase inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2010, 20, 6366-6369.	2.2	21
12	Exploring Inhibitor Binding at the ω Subsites of Cathepsin L. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 1361-1368.	6.4	27
13	Crystal Structure of StaL, a Glycopeptide Antibiotic Sulfotransferase from <i>Streptomyces toyocaensis</i> . <i>Journal of Biological Chemistry</i> , 2007, 282, 13073-13086.	3.4	22
14	Solvated Interaction Energy (SIE) for Scoring Protein-Ligand Binding Affinities. 1. Exploring the Parameter Space. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 122-133.	5.4	358
15	Coupled atomic charge selectivity for optimal ligand-charge distributions at protein binding sites. <i>Journal of Computational Chemistry</i> , 2006, 27, 1899-1907.	3.3	9
16	Molecular surface generation using a variable-radius solvent probe. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005, 62, 244-261.	2.6	48