Sathesh Bhat

List of Publications by Year
in descending order

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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	Solvated Interaction Energy (SIE) for Scoring Proteinâ"Ligand Binding Affinities. 1. Exploring the Parameter Space. Journal of Chemical Information and Modeling, 2007, 47, 122-133.	5.4	358
2	Inhibition of acetyl-CoA carboxylase suppresses fatty acid synthesis and tumor growth of non-small-cell lung cancer in preclinical models. Nature Medicine, 2016, 22, 1108-1119.	30.7	357
3	Acetyl-CoA carboxylase inhibition by ND-630 reduces hepatic steatosis, improves insulin sensitivity, and modulates dyslipidemia in rats. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E1796-805.	7.1	223
4	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. Journal of Chemical Information and Modeling, 2019, 59, 3782-3793.	5.4	81
5	Molecular surface generation using a variable-radius solvent probe. Proteins: Structure, Function and Bioinformatics, 2005, 62, 244-261.	2.6	48
6	Combining Cloud-Based Free-Energy Calculations, Synthetically Aware Enumerations, and Goal-Directed Generative Machine Learning for Rapid Large-Scale Chemical Exploration and Optimization. Journal of Chemical Information and Modeling, 2020, 60, 4311-4325.	5.4	34
7	From computer-aided drug discovery to computer-driven drug discovery. Drug Discovery Today: Technologies, 2021, 39, 111-117.	4.0	32
8	Discovery of MK-8831, A Novel Spiro-Proline Macrocycle as a Pan-Genotypic HCV-NS3/4a Protease Inhibitor. ACS Medicinal Chemistry Letters, 2016, 7, 111-116.	2.8	31
9	Exploring Inhibitor Binding at the Sâ€² Subsites of Cathepsin L. Journal of Medicinal Chemistry, 2008, 51, 1361-1368.	6.4	27
10	Crystal Structure of StaL, a Glycopeptide Antibiotic Sulfotransferase from Streptomyces toyocaensis. Journal of Biological Chemistry, 2007, 282, 13073-13086.	3.4	22
11	Novel Quinoline-Based P2â€"P4 Macrocyclic Derivatives As Pan-Genotypic HCV NS3/4a Protease Inhibitors. ACS Medicinal Chemistry Letters, 2014, 5, 264-269.	2.8	22
12	2-Aryl benzimidazoles: Human SCD1-specific stearoyl coenzyme-A desaturase inhibitors. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 6366-6369.	2.2	21
13	AutoDesigner, a De Novo Design Algorithm for Rapidly Exploring Large Chemical Space for Lead Optimization: Application to the Design and Synthesis of <scp>d</scp>-Amino Acid Oxidase Inhibitors. Journal of Chemical Information and Modeling, 2022, 62, 1905-1915.	5.4	12
14	Discovery of a Novel Class of <scp>d</scp>-Amino Acid Oxidase Inhibitors Using the SchrÃ¶dinger Computational Platform. Journal of Medicinal Chemistry, 2022, 65, 6775-6802.	6.4	10
15	Coupled atomic charge selectivity for optimal ligand-charge distributions at protein binding sites. Journal of Computational Chemistry, 2006, 27, 1899-1907.	3.3	9
16	Free Energy Calculation Guided Virtual Screening of Synthetically Feasible Ligand R-Group and Scaffold Modifications: An Emerging Paradigm for Lead Optimization. Annual Reports in Medicinal Chemistry, 2017, 50, 237-262.	0.9	4