Joshua Pottel

List of Publications by Year
in descending order

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19 papers	475 citations	759233 12 h-index	794594 19 g-index
23 all docs	23 docs citations	23 times ranked	848 citing authors

#	Article	IF	Citations
1	Docking Ligands into Flexible and Solvated Macromolecules. 8. Forming New Bondsâ”€Challenges and Opportunities. Journal of Chemical Information and Modeling, 2022, 62, 1061-1077.	5.4	6
2	COVID-19: Famotidine, Histamine, Mast Cells, and Mechanisms. Frontiers in Pharmacology, 2021, 12, 633680.	3.5	64
3	From desktop to benchtop with automated computational workflows for computer-aided design in asymmetric catalysis. Nature Catalysis, 2020, 3, 574-584.	34.4	31
4	The activities of drug inactive ingredients on biological targets. Science, 2020, 369, 403-413.	12.6	61
5	Bacterial metabolism rescues the inhibition of intestinal drug absorption by food and drug additives. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 16009-16018.	7.1	39
6	Interactions of Oral Molecular Excipients with Breast Cancer Resistance Protein, BCRP. Molecular Pharmaceutics, 2020, 17, 748-756.	4.6	16
7	The Recognition of Unrelated Ligands by Identical Proteins. ACS Chemical Biology, 2018, 13, 2522-2533.	3.4	6
8	Customizable Generation of Synthetically Accessible, Local Chemical Subspaces. Journal of Chemical Information and Modeling, 2017, 57, 454-467.	5.4	13
9	Highly Regioselective Monoacylation of Unprotected Glucopyranoside Using Transient Directingâ€Protecting Groups. European Journal of Organic Chemistry, 2017, 2017, 646-656.	2.4	12
10	A Molecular Basis for Innovation in Drug Excipients. Clinical Pharmacology and Therapeutics, 2017, 101, 320-323.	4.7	12
11	Elucidating Hyperconjugation from Electronegativity to Predict Drug Conformational Energy in a High Throughput Manner. Journal of Chemical Information and Modeling, 2016, 56, 788-801.	5.4	9
12	Medicinal Chemistry Projects Requiring Imaginative Structure-Based Drug Design Methods. Accounts of Chemical Research, 2016, 49, 1646-1657.	15.6	40
13	Metabolic Instability of Cyanothiazolidineâ€Based Prolyl Oligopeptidase Inhibitors: a Structural Assignment Challenge and Potential Medicinal Chemistry Implications. ChemMedChem, 2015, 10, 1174-1183.	3.2	9
14	Understanding P450â€mediated Bioâ€transformations into Epoxide and Phenolic Metabolites. Angewandte Chemie - International Edition, 2015, 54, 13743-13747.	13.8	17
15	Single-Point Mutation with a Rotamer Library Toolkit: Toward Protein Engineering. Journal of Chemical Information and Modeling, 2015, 55, 2657-2671.	5.4	6
16	Design, synthesis and evaluation of antiestrogen and histone deacetylase inhibitor molecular hybrids. Bioorganic and Medicinal Chemistry, 2015, 23, 7597-7606.	3.0	28
17	Docking Ligands into Flexible and Solvated Macromolecules. 6. Development and Application to the Docking of HDACs and other Zinc Metalloenzymes Inhibitors. Journal of Chemical Information and Modeling, 2014, 54, 254-265.	5.4	39
18	Stereo- and Regioselective Synthesis of Polysubstituted Chiral 1,4-Oxazepanes. Journal of Organic Chemistry, 2013, 78, 872-885.	3.2	15

#	Article	IF	Citations
19	Development of a Computational Tool to Rival Experts in the Prediction of Sites of Metabolism of Xenobiotics by P450s. Journal of Chemical Information and Modeling, 2012, 52, 2471-2483.	5.4	52