John C Faver

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/2481835/publications.pdf

Version: 2024-02-01

25	826	471509	580821
papers	citations	17 h-index	25 g-index

26	26	26	893
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Formal Estimation of Errors in Computed Absolute Interaction Energies of Proteinâ"Ligand Complexes. Journal of Chemical Theory and Computation, 2011, 7, 790-797.	5.3	127
2	The BioFragment Database (BFDb): An open-data platform for computational chemistry analysis of noncovalent interactions. Journal of Chemical Physics, 2017, 147, 161727.	3.0	82
3	A Mild, DNA-Compatible Nitro Reduction Using B₂(OH)₄. Organic Letters, 2019, 21, 2194-2199.	4.6	56
4	Quantitative Comparison of Enrichment from DNA-Encoded Chemical Library Selections. ACS Combinatorial Science, 2019, 21, 75-82.	3.8	48
5	The Energy Computation Paradox and ab initio Protein Folding. PLoS ONE, 2011, 6, e18868.	2.5	48
6	Utility of the Hard/Soft Acidâ"Base Principle via the Fukui Function in Biological Systems. Journal of Chemical Theory and Computation, 2010, 6, 548-559.	5.3	43
7	Discovery and characterization of bromodomain 2â€"specific inhibitors of BRDT. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	42
8	Discovery of potent thrombin inhibitors from a protease-focused DNA-encoded chemical library. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 16782-16789.	7.1	40
9	Câ€"N Coupling of DNA-Conjugated (Hetero)aryl Bromides and Chlorides for DNA-Encoded Chemical Library Synthesis. Bioconjugate Chemistry, 2020, 31, 770-780.	3.6	39
10	DNA-encoded chemistry technology yields expedient access to SARS-CoV-2 M ^{pro} inhibitors. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	36
11	Model for the fast estimation of basis set superposition error in biomolecular systems. Journal of Chemical Physics, 2011, 135, 144110.	3.0	31
12	Identifying Oxacillinase-48 Carbapenemase Inhibitors Using DNA-Encoded Chemical Libraries. ACS Infectious Diseases, 2020, 6, 1214-1227.	3.8	27
13	The Effects of Computational Modeling Errors on the Estimation of Statistical Mechanical Variables. Journal of Chemical Theory and Computation, 2012, 8, 3769-3776.	5.3	24
14	Palladium-Catalyzed Hydroxycarbonylation of (Hetero)aryl Halides for DNA-Encoded Chemical Library Synthesis. Bioconjugate Chemistry, 2019, 30, 2209-2215.	3.6	24
15	Mass-spectrometry-based proteomic correlates of grade and stage reveal pathways and kinases associated with aggressive human cancers. Oncogene, 2021, 40, 2081-2095.	5.9	22
16	Pairwise additivity of energy components in protein-ligand binding: The HIV II protease-Indinavir case. Journal of Chemical Physics, 2011, 135, 085101.	3.0	19
17	Bringing Clarity to the Prediction of Proteinâ€"Ligand Binding Free Energies via â€œBlurringâ€. Journal of Chemical Theory and Computation, 2014, 10, 1314-1325.	5.3	19
18	Computer-Aided Drug Design: Using Numbers to Your Advantage. ACS Medicinal Chemistry Letters, 2013, 4, 812-814.	2.8	17

#	Article	IF	Citations
19	Computationally-guided optimization of small-molecule inhibitors of the Aurora A kinaseâ€“TPX2 proteinâ€“protein interaction. Chemical Communications, 2017, 53, 9372-9375.	4.1	15
20	Structure-Guided Identification of DNMT3B Inhibitors. ACS Medicinal Chemistry Letters, 2020, 11, 971-976.	2.8	15
21	Discovery of potent BET bromodomain 1 stereoselective inhibitors using DNA-encoded chemical library selections. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	15
22	Statistics-based model for basis set superposition error correction in large biomolecules. Physical Chemistry Chemical Physics, 2012, 14, 7795.	2.8	12
23	Prediction of trypsin/molecular fragment binding affinities by free energy decomposition and empirical scores. Journal of Computer-Aided Molecular Design, 2012, 26, 647-659.	2.9	11
24	Fragment-based error estimation in biomolecular modeling. Drug Discovery Today, 2014, 19, 45-50.	6.4	7
25	Indoloxytriazines as binding molecules for the JAK2 JH2 pseudokinase domain and its V617F variant. Tetrahedron Letters, 2021, 77, 153248.	1.4	7