Mingjun

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/7625981/publications.pdf

Version: 2024-02-01

7	145	6	7
papers	citations	h-index	g-index
10	10	10	178
all docs	docs citations	times ranked	citing authors

#	Article	IF	CITATIONS
1	Harnessing Cloud Architecture for Crystal Structure Prediction Calculations. Crystal Growth and Design, 2018, 18, 6891-6900.	3.0	41
2	Optimal designs for pairwise calculation: An application to free energy perturbation in minimizing prediction variability. Journal of Computational Chemistry, 2020, 41, 247-257.	3.3	26
3	Prediction of the Relative Free Energies of Drug Polymorphs above Zero Kelvin. Crystal Growth and Design, 2020, 20, 5211-5224.	3.0	26
4	A Cloud Computing Platform for Scalable Relative and Absolute Binding Free Energy Predictions: New Opportunities and Challenges for Drug Discovery. Journal of Chemical Information and Modeling, 2021, 61, 2720-2732.	5.4	23
5	Solid-Form Transition Temperature Prediction from a Virtual Polymorph Screening: A Reality Check. Crystal Growth and Design, 2019, 19, 7132-7137.	3.0	12
6	Scaffold Hopping Transformations Using Auxiliary Restraints for Calculating Accurate Relative Binding Free Energies. Journal of Chemical Theory and Computation, 2021, 17, 3710-3726.	5.3	12
7	Enhanced QM/MM sampling for free energy calculation of chemical reactions: A case study of double proton transfer. Journal of Chemical Physics, 2019, 150, 044111.	3.0	2