Agastya P Bhati

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/9354813/publications.pdf

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17	470	932766 10	996533 15
papers	citations	h-index	g-index

19	19	19	455
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Rapid, Accurate, Precise, and Reliable Relative Free Energy Prediction Using Ensemble Based Thermodynamic Integration. Journal of Chemical Theory and Computation, 2017, 13, 210-222.	2.3	101
2	Rapid, accurate, precise and reproducible ligandâ€“protein binding free energy prediction. Interface Focus, 2020, 10, 20200007.	1.5	77
3	Rapid and Reliable Binding Affinity Prediction of Bromodomain Inhibitors: A Computational Study. Journal of Chemical Theory and Computation, 2017, 13, 784-795.	2.3	59
4	Uncertainty Quantification in Alchemical Free Energy Methods. Journal of Chemical Theory and Computation, 2018, 14, 2867-2880.	2.3	54
5	FabSim: Facilitating computational research through automation on large-scale and distributed e-infrastructures. Computer Physics Communications, 2016, 207, 375-385.	3.0	32
6	Evaluation and Characterization of Trk Kinase Inhibitors for the Treatment of Pain: Reliable Binding Affinity Predictions from Theory and Computation. Journal of Chemical Information and Modeling, 2017, 57, 897-909.	2.5	30
7	Ensemble-Based Replica Exchange Alchemical Free Energy Methods: The Effect of Protein Mutations on Inhibitor Binding. Journal of Chemical Theory and Computation, 2019, 15, 1265-1277.	2.3	28
8	Pandemic drugs at pandemic speed: infrastructure for accelerating COVID-19 drug discovery with hybrid machine learning- and physics-based simulations on high-performance computers. Interface Focus, 2021, 11, 20210018.	1.5	23
9	TIES 20: Relative Binding Free Energy with a Flexible Superimposition Algorithm and Partial Ring Morphing. Journal of Chemical Theory and Computation, 2021, 17, 1250-1265.	2.3	14
10	Large Scale Study of Ligandâ€“Protein Relative Binding Free Energy Calculations: Actionable Predictions from Statistically Robust Protocols. Journal of Chemical Theory and Computation, 2022, 18, 2687-2702.	2.3	14
11	Alchemical Free Energy Estimators and Molecular Dynamics Engines: Accuracy, Precision, and Reproducibility. Journal of Chemical Theory and Computation, 2022, 18, 3972-3987.	2.3	12
12	Temperature Dependence of the Stability of Ion Pair Interactions, and its Implications on the Thermostability of Proteins from Thermophiles. Journal of Chemical Sciences, 2017, 129, 405-414.	0.7	10
13	Ensemble Simulations and Experimental Free Energy Distributions: Evaluation and Characterization of Isoxazole Amides as SMYD3 Inhibitors. Journal of Chemical Information and Modeling, 2022, 62, 2561-2570.	2.5	6
14	Thermodynamic and structural insights into the repurposing of drugs that bind to SARS-CoV-2 main protease. Molecular Systems Design and Engineering, 2022, 7, 123-131.	1.7	5
15	Pattern formation in Passiflora incarnata: An activator-inhibitor model. Journal of Biosciences, 2021, 46, 1.	0.5	3
16	The performance of ensemble-based free energy protocols in computing binding affinities to ROS1 kinase. Scientific Reports, 2022, 12, .	1.6	2
17	Pattern formation in : An activator-inhibitor model. Journal of Biosciences, 2021, 46, .	0.5	0