Trung Hai Nguyen

List of Publications by Year
in descending order

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29 papers	854 citations	567144 15 h-index	501076 28 g-index
32 all docs	32 docs citations	32 times ranked	1025 citing authors

#	Article	IF	Citations
1	Autodock Vina Adopts More Accurate Binding Poses but Autodock4 Forms Better Binding Affinity. Journal of Chemical Information and Modeling, 2020, 60, 204-211.	2.5	233
2	Water at hydrophobic interfaces delays proton surface-to-bulk transfer and provides a pathway for lateral proton diffusion. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 9744-9749.	3.3	104
3	Benchmark of Popular Free Energy Approaches Revealing the Inhibitors Binding to SARS-CoV-2 Mpro. Journal of Chemical Information and Modeling, 2021, 61, 2302-2312.	2.5	66
4	Origin of proton affinity to membrane/water interfaces. Scientific Reports, 2017, 7, 4553.	1.6	49
5	Absolute Binding Free Energies between T4 Lysozyme and 141 Small Molecules: Calculations Based on Multiple Rigid Receptor Configurations. Journal of Chemical Theory and Computation, 2017, 13, 2930-2944.	2.3	33
6	Cubic and noncubic multiple-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>q</mml:mi></mml:math>states in the Heisenberg antiferromagnet on the pyrochlore lattice. Physical Review B, 2011, 84, .	1.1	32
7	Oversampling Free Energy Perturbation Simulation in Determination of the Ligandâ€Binding Free Energy. Journal of Computational Chemistry, 2020, 41, 611-618.	1.5	30
8	Rapid prediction of possible inhibitors for SARS-CoV-2 main protease using docking and FPL simulations. RSC Advances, 2020, 10, 31991-31996.	1.7	30
9	Platination of the copper transporter ATP7A involved in anticancer drug resistance. Dalton Transactions, 2014, 43, 12085.	1.6	29
10	Structural Determinants of Cisplatin and Transplatin Binding to the Met-Rich Motif of Ctr1: A Computational Spectroscopy Approach. Journal of Chemical Theory and Computation, 2012, 8, 2912-2920.	2.3	27
11	Bayesian analysis of isothermal titration calorimetry for binding thermodynamics. PLoS ONE, 2018, 13, e0203224.	1.1	24
12	Using the fast fourier transform in binding free energy calculations. Journal of Computational Chemistry, 2018, 39, 621-636.	1.5	19
13	Improving <scp>ligandâ€ranking</scp> of <scp>AutoDock</scp> Vina by changing the empirical parameters. Journal of Computational Chemistry, 2022, 43, 160-169.	1.5	19
14	Insights into the binding and covalent inhibition mechanism of PF-07321332 to SARS-CoV-2 M^{pro}. RSC Advances, 2022, 12, 3729-3737.	1.7	19
15	Diffusion and dynamical heterogeneity in simulated liquid SiO2under high pressure. Journal of Physics Condensed Matter, 2007, 19, 116104.	0.7	16
16	Tetrahedral â†” octahedral network structure transition in simulated vitreous SiO2. Physics Letters, Section A: General, Atomic and Solid State Physics, 2006, 356, 246-250.	0.9	15
17	Structural Biology of Cisplatin Complexes with Cellular Targets: The Adduct with Human Copper Chaperone Atox1 in Aqueous Solution. Chemistry - A European Journal, 2014, 20, 11719-11725.	1.7	14
18	Effect of Cholesterol Molecules on Aî²1-42 Wild-Type and Mutants Trimers. Molecules, 2022, 27, 1395.	1.7	13

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19	Molecular Recognition of Platinated DNA from Chromosomal HMGB1. Journal of Chemical Theory and Computation, 2014, 10, 3578-3584.	2.3	12
20	Intermediate Thermodynamic States Contribute Equally to Free Energy Convergence: A Demonstration with Replica Exchange. Journal of Chemical Theory and Computation, 2016, 12, 2154-2161.	2.3	12
21	Interfacial water molecules at biological membranes: Structural features and role for lateral proton diffusion. PLoS ONE, 2018, 13, e0193454.	1.1	12
22	Identifying Possible AChE Inhibitors from Drug-like Molecules via Machine Learning and Experimental Studies. ACS Omega, 2022, 7, 20673-20682.	1.6	11
23	Unbinding ligands from SARS-CoV-2 Mpro via umbrella sampling simulations. Royal Society Open Science, 2022, 9, 211480.	1.1	9
24	Searching for AChE inhibitors from natural compounds by using machine learning and atomistic simulations. Journal of Molecular Graphics and Modelling, 2022, 115, 108230.	1.3	8
25	Design, Synthesis, and Biological Evaluation of Polyaminocarboxylate Ligandâ€Based Theranostic Conjugates for Antibodyâ€Targeted Cancer Therapy and Nearâ€Infrared Optical Imaging. ChemMedChem, 2018, 13, 2606-2617.	1.6	7
26	Implicit ligand theory for relative binding free energies. Journal of Chemical Physics, 2018, 148, 104114.	1.2	6
27	Thermodynamics and kinetics in antibody resistance of the 501Y.V2 SARS-CoV-2 variant. RSC Advances, 2021, 11, 33438-33446.	1.7	3
28	Implicit ligand theory for relative binding free energies: II. An estimator based on control variates. Journal of Physics Communications, 2020, 4, 115010.	0.5	2
29	Nonequilibrium path-ensemble averages for symmetric protocols. Journal of Chemical Physics, 2019, 151, 194103.	1.2	0