Duy Phuoc Tran

List of Publications by Year
in descending order

21	481	759233 12	839539 18
papers	citations	h-index	g-index

26	26	26	589
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Delineating the conformational landscape of the adenosine A2A receptor during G protein coupling. Cell, 2021, 184, 1884-1894.e14.	28.9	97
2	GOMoDo: A GPCRs Online Modeling and Docking Webserver. PLoS ONE, 2013, 8, e74092.	2.5	84
3	Generating Ampicillin-Level Antimicrobial Peptides with Activity-Aware Generative Adversarial Networks. ACS Omega, 2020, 5, 22847-22851.	3.5	52
4	Dissociation Process of a MDM2/p53 Complex Investigated by Parallel Cascade Selection Molecular Dynamics and the Markov State Model. Journal of Physical Chemistry B, 2019, 123, 2469-2478.	2.6	36
5	Proteinâ€“Ligand Dissociation Simulated by Parallel Cascade Selection Molecular Dynamics. Journal of Chemical Theory and Computation, 2018, 14, 404-417.	5.3	34
6	Vibrational Energy Transfer from Heme through Atomic Contacts in Proteins. Journal of Physical Chemistry B, 2018, 122, 5877-5884.	2.6	30
7	Enhancing Biomolecular Sampling with Reinforcement Learning: A Tree Search Molecular Dynamics Simulation Method. ACS Omega, 2019, 4, 13853-13862.	3.5	25
8	Parallel cascade selection molecular dynamics for efficient conformational sampling and free energy calculation of proteins. AIP Conference Proceedings, 2016, , .	0.4	22
9	Binding free energy of protein/ligand complexes calculated using dissociation Parallel Cascade Selection Molecular Dynamics and Markov state model. Biophysics and Physicobiology, 2021, 18, 305-316.	1.0	18
10	Atomic mechanism of homogeneous melting of bcc Fe at the limit of superheating. Physica B: Condensed Matter, 2012, 407, 978-984.	2.7	17
11	Using molecular dynamics simulations to prioritize and understand AI-generated cell penetrating peptides. Scientific Reports, 2021, 11, 10630.	3.3	17
12	Kinetic Selection and Relaxation of the Intrinsically Disordered Region of a Protein upon Binding. Journal of Chemical Theory and Computation, 2020, 16, 2835-2845.	5.3	14
13	Ligand binding to anti-cancer target CD44 investigated by molecular simulations. Journal of Molecular Modeling, 2016, 22, 165.	1.8	12
14	In silico study of Bombyx mori fibroin enhancement by graphene in acidic environment. Physical Chemistry Chemical Physics, 2018, 20, 19240-19249.	2.8	6
15	Inhibition of the hexamerization of SARS-CoV-2 endoribonuclease and modeling of RNA structures bound to the hexamer. Scientific Reports, 2022, 12, 3860.	3.3	5
16	Edge expansion parallel cascade selection molecular dynamics simulation for investigating large-amplitude collective motions of proteins. Journal of Chemical Physics, 2020, 152, 225101.	3.0	4
17	Structural defects and thermodynamics of vitreous GeO2 nanoparticles. Current Applied Physics, 2011, 11, 303-310.	2.4	2
18	Melting of Mesoscale Lennard-Jones Crystals with Free Surfaces. Journal of the Physical Society of Japan, 2013, 82, 064601.	1.6	2

#	Article	IF	Citations
19	Structural properties of simulated liquid GanAsm. Computational Materials Science, 2012, 54, 183-187.	3.0	0
20	Obtaining Binding Free Energy from a Path Sampling without Force Bias. Biophysical Journal, 2016, 110, 642a.	0.5	0
21	Calculation of Binding Free Energy and Kinetic Rates with Flexible Protein Docking. Seibutsu Butsuri, 2021, 61, 398-399.	0.1	0