

# Duy Phuoc Tran

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/1538860/publications.pdf>

Version: 2024-02-01

21  
papers

481  
citations

759233

12  
h-index

839539

18  
g-index

26  
all docs

26  
docs citations

26  
times ranked

589  
citing authors

#	ARTICLE	IF	CITATIONS
1	Inhibition of the hexamerization of SARS-CoV-2 endoribonuclease and modeling of RNA structures bound to the hexamer. <i>Scientific Reports</i> , 2022, 12, 3860.	3.3	5
2	Delineating the conformational landscape of the adenosine A2A receptor during G protein coupling. <i>Cell</i> , 2021, 184, 1884-1894.e14.	28.9	97
3	Using molecular dynamics simulations to prioritize and understand AI-generated cell penetrating peptides. <i>Scientific Reports</i> , 2021, 11, 10630.	3.3	17
4	Calculation of Binding Free Energy and Kinetic Rates with Flexible Protein Docking. <i>Seibutsu Butsuri</i> , 2021, 61, 398-399.	0.1	0
5	Binding free energy of protein/ligand complexes calculated using dissociation Parallel Cascade Selection Molecular Dynamics and Markov state model. <i>Biophysics and Physicobiology</i> , 2021, 18, 305-316.	1.0	18
6	Generating Ampicillin-Level Antimicrobial Peptides with Activity-Aware Generative Adversarial Networks. <i>ACS Omega</i> , 2020, 5, 22847-22851.	3.5	52
7	Edge expansion parallel cascade selection molecular dynamics simulation for investigating large-amplitude collective motions of proteins. <i>Journal of Chemical Physics</i> , 2020, 152, 225101.	3.0	4
8	Kinetic Selection and Relaxation of the Intrinsically Disordered Region of a Protein upon Binding. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2835-2845.	5.3	14
9	Enhancing Biomolecular Sampling with Reinforcement Learning: A Tree Search Molecular Dynamics Simulation Method. <i>ACS Omega</i> , 2019, 4, 13853-13862.	3.5	25
10	Dissociation Process of a MDM2/p53 Complex Investigated by Parallel Cascade Selection Molecular Dynamics and the Markov State Model. <i>Journal of Physical Chemistry B</i> , 2019, 123, 2469-2478.	2.6	36
11	Protein-Ligand Dissociation Simulated by Parallel Cascade Selection Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 404-417.	5.3	34
12	Vibrational Energy Transfer from Heme through Atomic Contacts in Proteins. <i>Journal of Physical Chemistry B</i> , 2018, 122, 5877-5884.	2.6	30
13	<i>In silico</i> study of <i>Bombyx mori</i> fibroin enhancement by graphene in acidic environment. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 19240-19249.	2.8	6
14	Obtaining Binding Free Energy from a Path Sampling without Force Bias. <i>Biophysical Journal</i> , 2016, 110, 642a.	0.5	0
15	Parallel cascade selection molecular dynamics for efficient conformational sampling and free energy calculation of proteins. <i>AIP Conference Proceedings</i> , 2016, , .	0.4	22
16	Ligand binding to anti-cancer target CD44 investigated by molecular simulations. <i>Journal of Molecular Modeling</i> , 2016, 22, 165.	1.8	12
17	Melting of Mesoscale Lennard-Jones Crystals with Free Surfaces. <i>Journal of the Physical Society of Japan</i> , 2013, 82, 064601.	1.6	2
18	GOMoDo: A GPCRs Online Modeling and Docking Webserver. <i>PLoS ONE</i> , 2013, 8, e74092.	2.5	84

#	ARTICLE	IF	CITATIONS
19	Structural properties of simulated liquid GaAsm. Computational Materials Science, 2012, 54, 183-187.	3.0	0
20	Atomic mechanism of homogeneous melting of bcc Fe at the limit of superheating. Physica B: Condensed Matter, 2012, 407, 978-984.	2.7	17
21	Structural defects and thermodynamics of vitreous GeO2 nanoparticles. Current Applied Physics, 2011, 11, 303-310.	2.4	2