Son Tung Ngo

List of Publications by Year
in descending order

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77	2,467	257450 24	223800 46
papers	citations	h-index	g-index

97	97	97	2457
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Amyloid Oligomers: A Joint Experimental/Computational Perspective on Alzheimerâ€™s Disease, Parkinsonâ€™s Disease, Type II Diabetes, and Amyotrophic Lateral Sclerosis. Chemical Reviews, 2021, 121, 2545-2647.	47.7	406
2	Autodock Vina Adopts More Accurate Binding Poses but Autodock4 Forms Better Binding Affinity. Journal of Chemical Information and Modeling, 2020, 60, 204-211.	5.4	233
3	Inhibition of Aggregation of Amyloid Peptides by Beta-Sheet Breaker Peptides and Their Binding Affinity. Journal of Physical Chemistry B, 2011, 115, 7433-7446.	2.6	173
4	Computational Determination of Potential Inhibitors of SARS-CoV-2 Main Protease. Journal of Chemical Information and Modeling, 2020, 60, 5771-5780.	5.4	118
5	Nano-plastics and their analytical characterisation and fate in the marine environment: From source to sea. Science of the Total Environment, 2020, 732, 138792.	8.0	96
6	Curcumin Binds to AÎ²_{1â€“40} Peptides and Fibrils Stronger Than Ibuprofen and Naproxen. Journal of Physical Chemistry B, 2012, 116, 10165-10175.	2.6	85
7	Effect of the Tottori Familial Disease Mutation (D7N) on the Monomers and Dimers of AÎ²₄₀ and AÎ²₄₂. ACS Chemical Neuroscience, 2013, 4, 1446-1457.	3.5	83
8	Fast and accurate determination of the relative binding affinities of small compounds to HIV-1 protease using non-equilibrium work. Journal of Computational Chemistry, 2016, 37, 2734-2742.	3.3	70
9	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.	5.4	66
10	Effective Estimation of Ligand-Binding Affinity Using Biased Sampling Method. ACS Omega, 2019, 4, 3887-3893.	3.5	52
11	Top-leads from natural products for treatment of Alzheimer's disease: docking and molecular dynamics study. Molecular Simulation, 2013, 39, 279-291.	2.0	50
12	Copper active site in polysaccharide monooxygenases. Coordination Chemistry Reviews, 2018, 368, 134-157.	18.8	47
13	Tetrameric AÎ²40 and AÎ²42 Î²-Barrel Structures by Extensive Atomistic Simulations. I. In a Bilayer Mimicking a Neuronal Membrane. Journal of Physical Chemistry B, 2019, 123, 3643-3648.	2.6	42
14	Anti-arrhythmic Medication Propafenone a Potential Drug for Alzheimerâ€™s Disease Inhibiting Aggregation of AÎ²: In Silico and in Vitro Studies. Journal of Chemical Information and Modeling, 2016, 56, 1344-1356.	5.4	41
15	In silico and in vitro characterization of anti-amyloidogenic activity of vitamin K3 analogues for Alzheimer's disease. Biochimica Et Biophysica Acta - General Subjects, 2013, 1830, 2960-2969.	2.4	38
16	Replica exchange molecular dynamics study of the amyloid beta (11â€“40) trimer penetrating a membrane. RSC Advances, 2017, 7, 7346-7357.	3.6	38
17	EGCG inhibits the oligomerization of amyloid beta (16-22) hexamer: Theoretical studies. Journal of Molecular Graphics and Modelling, 2017, 76, 1-10.	2.4	38
18	Replica exchange molecular dynamics study of the truncated amyloid beta (11â€“40) trimer in solution. Physical Chemistry Chemical Physics, 2017, 19, 1909-1919.	2.8	36

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19	Tetrameric AÎ²40 and AÎ²42 Î²-Barrel Structures by Extensive Atomistic Simulations. II. In Aqueous Solution. Journal of Physical Chemistry B, 2019, 123, 6750-6756.	2.6	31
20	Substrate selectivity in starch polysaccharide monooxygenases. Journal of Biological Chemistry, 2019, 294, 12157-12166.	3.4	31
21	Oversampling Free Energy Perturbation Simulation in Determination of the Ligandâ€Binding Free Energy. Journal of Computational Chemistry, 2020, 41, 611-618.	3.3	30
22	Rapid prediction of possible inhibitors for SARS-CoV-2 main protease using docking and FPL simulations. RSC Advances, 2020, 10, 31991-31996.	3.6	30
23	Determination of the absolute binding free energies of HIV-1 protease inhibitors using non-equilibrium molecular dynamics simulations. Chemical Physics Letters, 2017, 676, 12-17.	2.6	27
24	Probable Transmembrane Amyloid Î±-Helix Bundles Capable of Conducting Ca²⁺ Ions. Journal of Physical Chemistry B, 2019, 123, 2645-2653.	2.6	26
25	Estimation of the Binding Free Energy of AC1NX476 toÂHIVâ€1 Protease Wild Type and Mutations Using FreeÂEnergy Perturbation Method. Chemical Biology and Drug Design, 2015, 86, 546-558.	3.2	24
26	The Effects of A21G Mutation on Transmembrane Amyloid Beta (11â€“40) Trimer: An In Silico Study. Journal of Physical Chemistry B, 2017, 121, 8467-8474.	2.6	24
27	Prediction of AChE-ligand affinity using the umbrella sampling simulation. Journal of Molecular Graphics and Modelling, 2019, 93, 107441.	2.4	24
28	Oligomerization of Peptides LVEALYL and RGFFYT and Their Binding Affinity to Insulin. PLoS ONE, 2013, 8, e65358.	2.5	21
29	Assessing potential inhibitors of SARS-CoV-2 main protease from available drugs using free energy perturbation simulations. RSC Advances, 2020, 10, 40284-40290.	3.6	21
30	Stability of AÎ²11â€“40 Trimers with Parallel and Antiparallel Î²-Sheet Organizations in a Membrane-Mimicking Environment by Replica Exchange Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2020, 124, 617-626.	2.6	21
31	Binding of inhibitors to the monomeric and dimeric SARS-CoV-2 Mpro. RSC Advances, 2021, 11, 2926-2934.	3.6	19
32	Improving <scp>ligandâ€ranking</scp> of <scp>AutoDock</scp> Vina by changing the empirical parameters. Journal of Computational Chemistry, 2022, 43, 160-169.	3.3	19
33	Insights into the binding and covalent inhibition mechanism of PF-07321332 to SARS-CoV-2 M^{pro}. RSC Advances, 2022, 12, 3729-3737.	3.6	19
34	Controlling the absorption strength in bidirectional terahertz metamaterial absorbers with patterned graphene. Computational Materials Science, 2019, 166, 276-281.	3.0	18
35	Impact of A2T and D23N Mutations on Tetrameric AÎ²42 Barrel within a Dipalmitoylphosphatidylcholine Lipid Bilayer Membrane by Replica Exchange Molecular Dynamics. Journal of Physical Chemistry B, 2020, 124, 1175-1182.	2.6	18
36	Impact of the Astaxanthin, Betanin, and EGCG Compounds on Small Oligomers of Amyloid AÎ²₄₀ Peptide. Journal of Chemical Information and Modeling, 2020, 60, 1399-1408.	5.4	17

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37	Adequate prediction for inhibitor affinity of AÎ²₄₀ protofibril using the linear interaction energy method. RSC Advances, 2019, 9, 12455-12461.	3.6	16
38	How do magnetic, structural, and electronic criteria of aromaticity relate to HOMO â€“ LUMO gap? An evaluation for graphene quantum dot and its derivatives. Chemical Physics, 2020, 539, 110951.	1.9	16
39	In silico studies of solvated F19W amyloid Î² (11â€“40) trimer. RSC Advances, 2017, 7, 42379-42386.	3.6	15
40	Fast pulling of ligand approach for the design of Î²-secretase 1 inhibitors. Chemical Physics Letters, 2017, 671, 142-146.	2.6	14
41	In vitroandin silicodetermination of glutaminyl cyclase inhibitors. RSC Advances, 2019, 9, 29619-29627.	3.6	14
42	Estimating the <scp>ligandâ€binding</scp> affinity via <scp>Î»â€dependent</scp> umbrella sampling simulations. Journal of Computational Chemistry, 2021, 42, 117-123.	3.3	14
43	Effect of Cholesterol Molecules on AÎ²1-42 Wild-Type and Mutants Trimers. Molecules, 2022, 27, 1395.	3.8	13
44	Evaluation of the absolute affinity of neuraminidase inhibitor using steered molecular dynamics simulations. Journal of Molecular Graphics and Modelling, 2017, 77, 137-142.	2.4	12
45	Influence of various force fields in estimating the binding affinity of acetylcholinesterase inhibitors using fast pulling of ligand scheme. Chemical Physics Letters, 2018, 701, 65-71.	2.6	12
46	Interaction of carbohydrate binding module 20 with starch substrates. RSC Advances, 2019, 9, 24833-24842.	3.6	12
47	Gold@silica catalyst: Porosity of silica shells switches catalytic reactions. Chemical Physics Letters, 2019, 728, 80-86.	2.6	12
48	Cholesterol Molecules Alter the Energy Landscape of Small AÎ²1â€“42 Oligomers. Journal of Physical Chemistry B, 2021, 125, 2299-2307.	2.6	12
49	Conjugated polymers: A systematic investigation of their electronic and geometric properties using density functional theory and semi-empirical methods. Synthetic Metals, 2018, 246, 128-136.	3.9	11
50	Etersalate prevents the formations of 6AÎ²16-22 oligomer: An in silico study. PLoS ONE, 2018, 13, e0204026.	2.5	11
51	Searching and designing potential inhibitors for SARS-CoV-2 Mpro from natural sources using atomistic and deep-learning calculations. RSC Advances, 2021, 11, 38495-38504.	3.6	11
52	Identifying Possible AChE Inhibitors from Drug-like Molecules via Machine Learning and Experimental Studies. ACS Omega, 2022, 7, 20673-20682.	3.5	11
53	Atomistic investigation of an Iowa Amyloid-Î² trimer in aqueous solution. RSC Advances, 2018, 8, 41705-41712.	3.6	9
54	Systematic Investigation of the Structure, Stability, and Spin Magnetic Moment of CrM_n Clusters (M = Cu, Ag, Au, and n = 2â€“20) by DFT Calculations. ACS Omega, 2021, 6, 20341-20350.	3.5	9

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55	Unbinding ligands from SARS-CoV-2 Mpro via umbrella sampling simulations. Royal Society Open Science, 2022, 9, 211480.	2.4	9
56	Theoretical study of the interactions between the first transmembrane segment of NS2 protein and a POPC lipid bilayer. Biophysical Chemistry, 2016, 217, 1-7.	2.8	8
57	C-Terminal Plays as the Possible Nucleation of the Self-Aggregation of the S-Shape AÎ²_{11â€“42} Tetramer in Solution: Intensive MD Study. ACS Omega, 2019, 4, 11066-11073.	3.5	8
58	Potential inhibitors for SARS-CoV-2 Mpro from marine compounds. RSC Advances, 2021, 11, 22206-22213.	3.6	8
59	Searching for AChE inhibitors from natural compounds by using machine learning and atomistic simulations. Journal of Molecular Graphics and Modelling, 2022, 115, 108230.	2.4	8
60	Effective estimation of the inhibitor affinity of HIV-1 protease via a modified LIE approach. RSC Advances, 2020, 10, 7732-7739.	3.6	7
61	Propafenone effects on the stable structures of AÎ²16-22 system. Chemical Physics Letters, 2018, 696, 55-60.	2.6	6
62	The influences of E22Q mutant on solvated 3AÎ² 11-40 peptide: A REMD study. Journal of Molecular Graphics and Modelling, 2018, 83, 122-128.	2.4	6
63	Graphene-integrated hybridized metamaterials for wide-angle tunable THz absorbers. Photonics and Nanostructures - Fundamentals and Applications, 2021, 45, 100924.	2.0	6
64	Computational investigation of possible inhibitors of the winged-helix domain of MUS81. Journal of Molecular Graphics and Modelling, 2021, 103, 107771.	2.4	5
65	Unifying approach to multilayer metamaterials absorber for bandwidth enhancement. Optics Communications, 2021, 485, 126725.	2.1	5
66	Marine derivatives preventwMUS81in silicostudies. Royal Society Open Science, 2021, 8, 210974.	2.4	5
67	Umbrella Sampling-Based Method to Compute Ligand-Binding Affinity. Methods in Molecular Biology, 2022, 2385, 313-323.	0.9	5
68	Terahertz cut-wire-pair metamaterial absorber. Journal of Applied Physics, 2021, 130, .	2.5	4
69	Design, synthesis and bioevaluation of novel 6-substituted aminoindazole derivatives as anticancer agents. RSC Advances, 2020, 10, 45199-45206.	3.6	3
70	Fine Tuning of the Copper Active Site in Polysaccharide Monooxygenases. Journal of Physical Chemistry B, 2020, 124, 1859-1865.	2.6	3
71	Impact of the Rat R5G, Y10F, and H13R Mutations on Tetrameric AÎ²42 Î²-Barrel in a Lipid Bilayer Membrane Model. Journal of Physical Chemistry B, 2021, 125, 3105-3113.	2.6	3
72	Computational Investigations of the Transmembrane Italian-Mutant (E22K) 3A(eta_{11 - 40}) in Aqueous Solution. Communications in Physics, 2018, 28, 265.	0.0	3

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73	Thermodynamics and kinetics in antibody resistance of the 501Y.V2 SARS-CoV-2 variant. RSC Advances, 2021, 11, 33438-33446.	3.6	3
74	Photofragmentation Patterns of Cobalt Oxide Cations Co_nO_m⁺ (n = 5â€“9, m = 4â€“13): From Oxygen-Deficient to Oxygen-Rich Species. Journal of Physical Chemistry A, 2020, 124, 7333-7339.	2.5	1
75	501Y.V2 spike protein resists the neutralizing antibody in atomistic simulations. Computational Biology and Chemistry, 2022, 97, 107636.	2.3	1
76	In silico Probing Ca2+ And Zn2+ Permeable Transmembrane 4AÎ²1-42 Barrel. Communications in Physics, 2020, 31, .	0.0	0
77	Initial study on SARS-CoV-2 main protease inhibition mechanism of some potential drugs using molecular docking simulation. Science and Technology, 2020, 58, 665-675.	0.2	0