

Van V Vu

List of Publications by Year in descending order

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80
papers

3,327
citations

201385

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161609

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85
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85
docs citations

85
times ranked

3361
citing authors

#	ARTICLE	IF	CITATIONS
1	Amyloid Oligomers: A Joint Experimental/Computational Perspective on Alzheimer's Disease, Parkinson's Disease, Type II Diabetes, and Amyotrophic Lateral Sclerosis. <i>Chemical Reviews</i> , 2021, 121, 2545-2647.	23.0	406
2	Cellulose Degradation by Polysaccharide Monooxygenases. <i>Annual Review of Biochemistry</i> , 2015, 84, 923-946.	5.0	246
3	Autodock Vina Adopts More Accurate Binding Poses but Autodock4 Forms Better Binding Affinity. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 204-211.	2.5	233
4	A family of starch-active polysaccharide monooxygenases. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 13822-13827.	3.3	222
5	Determinants of Regioselective Hydroxylation in the Fungal Polysaccharide Monooxygenases. <i>Journal of the American Chemical Society</i> , 2014, 136, 562-565.	6.6	198
6	Inhibition of Aggregation of Amyloid Peptides by Beta-Sheet Breaker Peptides and Their Binding Affinity. <i>Journal of Physical Chemistry B</i> , 2011, 115, 7433-7446.	1.2	173
7	Computational Determination of Potential Inhibitors of SARS-CoV-2 Main Protease. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 5771-5780.	2.5	118
8	Human deoxyhypusine hydroxylase, an enzyme involved in regulating cell growth, activates O ₂ with a nonheme diiron center. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 14814-14819.	3.3	105
9	Curcumin Binds to A β ₁₋₄₀ Peptides and Fibrils Stronger Than Ibuprofen and Naproxen. <i>Journal of Physical Chemistry B</i> , 2012, 116, 10165-10175.	1.2	85
10	Effect of the Tottori Familial Disease Mutation (D7N) on the Monomers and Dimers of A β ₄₀ and A β ₄₂ . <i>ACS Chemical Neuroscience</i> , 2013, 4, 1446-1457.	1.7	83
11	An Unusual Peroxo Intermediate of the Arylamine Oxygenase of the Chloramphenicol Biosynthetic Pathway. <i>Journal of the American Chemical Society</i> , 2015, 137, 1608-1617.	6.6	71
12	Fast and accurate determination of the relative binding affinities of small compounds to HIV-1 protease using non-equilibrium work. <i>Journal of Computational Chemistry</i> , 2016, 37, 2734-2742.	1.5	70
13	Benchmark of Popular Free Energy Approaches Revealing the Inhibitors Binding to SARS-CoV-2 Mpro. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2302-2312.	2.5	66
14	Effective Estimation of Ligand-Binding Affinity Using Biased Sampling Method. <i>ACS Omega</i> , 2019, 4, 3887-3893.	1.6	52
15	Top-leads from natural products for treatment of Alzheimer's disease: docking and molecular dynamics study. <i>Molecular Simulation</i> , 2013, 39, 279-291.	0.9	50
16	Copper active site in polysaccharide monooxygenases. <i>Coordination Chemistry Reviews</i> , 2018, 368, 134-157.	9.5	47
17	Tetrameric A β ₄₀ and A β ₄₂ β -Barrel Structures by Extensive Atomistic Simulations. I. In a Bilayer Mimicking a Neuronal Membrane. <i>Journal of Physical Chemistry B</i> , 2019, 123, 3643-3648.	1.2	42
18	Anti-arrhythmic Medication Propafenone a Potential Drug for Alzheimer's Disease Inhibiting Aggregation of A β : In Silico and in Vitro Studies. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 1344-1356.	2.5	41

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19	A mononuclear carboxylate-rich oxoiron(IV) complex: a structural and functional mimic of TauD intermediate. <i>Chemical Science</i> , 2012, 3, 1680.	3.7	40
20	In silico and in vitro characterization of anti-amyloidogenic activity of vitamin K3 analogues for Alzheimer's disease. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2013, 1830, 2960-2969.	1.1	38
21	Replica exchange molecular dynamics study of the amyloid beta (11-40) trimer penetrating a membrane. <i>RSC Advances</i> , 2017, 7, 7346-7357.	1.7	38
22	EGCG inhibits the oligomerization of amyloid beta (16-22) hexamer: Theoretical studies. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 76, 1-10.	1.3	38
23	Replica exchange molecular dynamics study of the truncated amyloid beta (11-40) trimer in solution. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 1909-1919.	1.3	36
24	Characterization of Two Distinct Adducts in the Reaction of a Nonheme Diiron(II) Complex with O ₂ . <i>Inorganic Chemistry</i> , 2009, 48, 8325-8336.	1.9	33
25	Starch-degrading polysaccharide monooxygenases. <i>Cellular and Molecular Life Sciences</i> , 2016, 73, 2809-2819.	2.4	33
26	Tetrameric A β 240 and A β 242 β -Barrel Structures by Extensive Atomistic Simulations. II. In Aqueous Solution. <i>Journal of Physical Chemistry B</i> , 2019, 123, 6750-6756.	1.2	31
27	Substrate selectivity in starch polysaccharide monooxygenases. <i>Journal of Biological Chemistry</i> , 2019, 294, 12157-12166.	1.6	31
28	Oversampling Free Energy Perturbation Simulation in Determination of the Ligand Binding Free Energy. <i>Journal of Computational Chemistry</i> , 2020, 41, 611-618.	1.5	30
29	Rapid prediction of possible inhibitors for SARS-CoV-2 main protease using docking and FPL simulations. <i>RSC Advances</i> , 2020, 10, 31991-31996.	1.7	30
30	Determination of the absolute binding free energies of HIV-1 protease inhibitors using non-equilibrium molecular dynamics simulations. <i>Chemical Physics Letters</i> , 2017, 676, 12-17.	1.2	27
31	Probable Transmembrane Amyloid β -Helix Bundles Capable of Conducting Ca ²⁺ Ions. <i>Journal of Physical Chemistry B</i> , 2019, 123, 2645-2653.	1.2	26
32	Estimation of the Binding Free Energy of AC1NX476 to HIV-1 Protease Wild Type and Mutations Using Free Energy Perturbation Method. <i>Chemical Biology and Drug Design</i> , 2015, 86, 546-558.	1.5	24
33	The Effects of A21G Mutation on Transmembrane Amyloid Beta (11-40) Trimer: An In Silico Study. <i>Journal of Physical Chemistry B</i> , 2017, 121, 8467-8474.	1.2	24
34	Prediction of AChE-ligand affinity using the umbrella sampling simulation. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 93, 107441.	1.3	24
35	Active-Site Structure of a β -Hydroxylase in Antibiotic Biosynthesis. <i>Journal of the American Chemical Society</i> , 2011, 133, 6938-6941.	6.6	21
36	Oligomerization of Peptides LVEALYL and RGFFYT and Their Binding Affinity to Insulin. <i>PLoS ONE</i> , 2013, 8, e65358.	1.1	21

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37	X-ray absorption spectroscopic characterization of the diferric-peroxo intermediate of human deoxyhypusine hydroxylase in the presence of its substrate eIF5a. <i>Journal of Biological Inorganic Chemistry</i> , 2016, 21, 605-618.	1.1	21
38	Assessing potential inhibitors of SARS-CoV-2 main protease from available drugs using free energy perturbation simulations. <i>RSC Advances</i> , 2020, 10, 40284-40290.	1.7	21
39	Stability of A β ¹⁻⁴⁰ Trimers with Parallel and Antiparallel β -Sheet Organizations in a Membrane-Mimicking Environment by Replica Exchange Molecular Dynamics Simulation. <i>Journal of Physical Chemistry B</i> , 2020, 124, 617-626.	1.2	21
40	Binding of inhibitors to the monomeric and dimeric SARS-CoV-2 Mpro. <i>RSC Advances</i> , 2021, 11, 2926-2934.	1.7	19
41	Improving ^{ligand}ranking of ^{AutoDock} Vina by changing the empirical parameters. <i>Journal of Computational Chemistry</i> , 2022, 43, 160-169.	1.5	19
42	Insights into the binding and covalent inhibition mechanism of PF-07321332 to SARS-CoV-2 M^{pro}. <i>RSC Advances</i> , 2022, 12, 3729-3737.	1.7	19
43	Impact of A2T and D23N Mutations on Tetrameric A β ²⁴⁻⁴² Barrel within a Dipalmitoylphosphatidylcholine Lipid Bilayer Membrane by Replica Exchange Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2020, 124, 1175-1182.	1.2	18
44	Impact of the Astaxanthin, Betanin, and EGCG Compounds on Small Oligomers of Amyloid A β ⁴⁰ Peptide. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 1399-1408.	2.5	17
45	Adequate prediction for inhibitor affinity of A β ⁴⁰ protofibril using the linear interaction energy method. <i>RSC Advances</i> , 2019, 9, 12455-12461.	1.7	16
46	How do magnetic, structural, and electronic criteria of aromaticity relate to HOMO – LUMO gap? An evaluation for graphene quantum dot and its derivatives. <i>Chemical Physics</i> , 2020, 539, 110951.	0.9	16
47	In silico studies of solvated F19W amyloid β ¹⁻⁴⁰ trimer. <i>RSC Advances</i> , 2017, 7, 42379-42386.	1.7	15
48	Fast pulling of ligand approach for the design of β -secretase 1 inhibitors. <i>Chemical Physics Letters</i> , 2017, 671, 142-146.	1.2	14
49	In vitro and in silico determination of glutaminyl cyclase inhibitors. <i>RSC Advances</i> , 2019, 9, 29619-29627.	1.7	14
50	Estimating the ^{ligand}binding affinity via ^Î-dependent umbrella sampling simulations. <i>Journal of Computational Chemistry</i> , 2021, 42, 117-123.	1.5	14
51	Effect of Cholesterol Molecules on A β ¹⁻⁴² Wild-Type and Mutants Trimers. <i>Molecules</i> , 2022, 27, 1395.	1.7	13
52	Evaluation of the absolute affinity of neuraminidase inhibitor using steered molecular dynamics simulations. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 77, 137-142.	1.3	12
53	Influence of various force fields in estimating the binding affinity of acetylcholinesterase inhibitors using fast pulling of ligand scheme. <i>Chemical Physics Letters</i> , 2018, 701, 65-71.	1.2	12
54	Interaction of carbohydrate binding module 20 with starch substrates. <i>RSC Advances</i> , 2019, 9, 24833-24842.	1.7	12

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55	Cholesterol Molecules Alter the Energy Landscape of Small A β 1-42 Oligomers. <i>Journal of Physical Chemistry B</i> , 2021, 125, 2299-2307.	1.2	12
56	Conjugated polymers: A systematic investigation of their electronic and geometric properties using density functional theory and semi-empirical methods. <i>Synthetic Metals</i> , 2018, 246, 128-136.	2.1	11
57	Etersalate prevents the formations of 6A β 16-22 oligomer: An in silico study. <i>PLoS ONE</i> , 2018, 13, e0204026.	1.1	11
58	Searching and designing potential inhibitors for SARS-CoV-2 Mpro from natural sources using atomistic and deep-learning calculations. <i>RSC Advances</i> , 2021, 11, 38495-38504.	1.7	11
59	Identifying Possible AChE Inhibitors from Drug-like Molecules via Machine Learning and Experimental Studies. <i>ACS Omega</i> , 2022, 7, 20673-20682.	1.6	11
60	Atomistic investigation of an Iowa Amyloid- β 2 trimer in aqueous solution. <i>RSC Advances</i> , 2018, 8, 41705-41712.	1.7	9
61	Fabrication of superhydrophobic surface using one-step chemical treatment. <i>Surfaces and Interfaces</i> , 2020, 21, 100673.	1.5	9
62	Systematic Investigation of the Structure, Stability, and Spin Magnetic Moment of CrM _n Clusters (M = Cu, Ag, Au, and n = 2-20) by DFT Calculations. <i>ACS Omega</i> , 2021, 6, 20341-20350.	1.6	9
63	Unbinding ligands from SARS-CoV-2 Mpro via umbrella sampling simulations. <i>Royal Society Open Science</i> , 2022, 9, 211480.	1.1	9
64	Theoretical study of the interactions between the first transmembrane segment of NS2 protein and a POPC lipid bilayer. <i>Biophysical Chemistry</i> , 2016, 217, 1-7.	1.5	8
65	C-Terminal Plays as the Possible Nucleation of the Self-Aggregation of the S-Shape A β 11-42 Tetramer in Solution: Intensive MD Study. <i>ACS Omega</i> , 2019, 4, 11066-11073.	1.6	8
66	Potential inhibitors for SARS-CoV-2 Mpro from marine compounds. <i>RSC Advances</i> , 2021, 11, 22206-22213.	1.7	8
67	Searching for AChE inhibitors from natural compounds by using machine learning and atomistic simulations. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 115, 108230.	1.3	8
68	Effective estimation of the inhibitor affinity of HIV-1 protease via a modified LIE approach. <i>RSC Advances</i> , 2020, 10, 7732-7739.	1.7	7
69	Propafenone effects on the stable structures of A β 16-22 system. <i>Chemical Physics Letters</i> , 2018, 696, 55-60.	1.2	6
70	The influences of E22Q mutant on solvated 3A β 11-40 peptide: A REMD study. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 83, 122-128.	1.3	6
71	Computational investigation of possible inhibitors of the winged-helix domain of MUS81. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 103, 107771.	1.3	5
72	Marine derivatives prevent MUS81 in silico studies. <i>Royal Society Open Science</i> , 2021, 8, 210974.	1.1	5

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73	Umbrella Sampling-Based Method to Compute Ligand-Binding Affinity. <i>Methods in Molecular Biology</i> , 2022, 2385, 313-323.	0.4	5
74	Terahertz cut-wire-pair metamaterial absorber. <i>Journal of Applied Physics</i> , 2021, 130, .	1.1	4
75	Fine Tuning of the Copper Active Site in Polysaccharide Monooxygenases. <i>Journal of Physical Chemistry B</i> , 2020, 124, 1859-1865.	1.2	3
76	Impact of the Rat R5G, Y10F, and H13R Mutations on Tetrameric $\alpha^2\beta^2$ -Barrel in a Lipid Bilayer Membrane Model. <i>Journal of Physical Chemistry B</i> , 2021, 125, 3105-3113.	1.2	3
77	Computational Investigations of the Transmembrane Italian-Mutant (E22K) α (eta_{11-40}) in Aqueous Solution. <i>Communications in Physics</i> , 2018, 28, 265.	0.0	3
78	Thermodynamics and kinetics in antibody resistance of the 501Y.V2 SARS-CoV-2 variant. <i>RSC Advances</i> , 2021, 11, 33438-33446.	1.7	3
79	Solution structure of the reduced active site of a starch-active polysaccharide monooxygenase from <i>Neurospora crassa</i> . <i>Vietnam Journal of Science Technology and Engineering</i> , 2018, 60, 9-12.	0.1	2
80	501Y.V2 spike protein resists the neutralizing antibody in atomistic simulations. <i>Computational Biology and Chemistry</i> , 2022, 97, 107636.	1.1	1