

Man Hoang Viet

List of Publications by Year in descending order

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Version: 2024-02-01

58
papers

1,715
citations

304368

22
h-index

301761

39
g-index

62
all docs

62
docs citations

62
times ranked

1816
citing authors

#	ARTICLE	IF	CITATIONS
1	A fast and high-quality charge model for the next generation general AMBER force field. Journal of Chemical Physics, 2020, 153, 114502.	1.2	195
2	Inhibition of Aggregation of Amyloid Peptides by Beta-Sheet Breaker Peptides and Their Binding Affinity. Journal of Physical Chemistry B, 2011, 115, 7433-7446.	1.2	173
3	High-Resolution Structures of the Amyloid- β 1-42 Dimers from the Comparison of Four Atomistic Force Fields. Journal of Physical Chemistry B, 2017, 121, 5977-5987.	1.2	120
4	Effects of All-Atom Molecular Mechanics Force Fields on Amyloid Peptide Assembly: The Case of A β ₁₆₋₂₂ Dimer. Journal of Chemical Theory and Computation, 2019, 15, 1440-1452.	2.3	102
5	Top Leads for Swine Influenza A/H1N1 Virus Revealed by Steered Molecular Dynamics Approach. Journal of Chemical Information and Modeling, 2010, 50, 2236-2247.	2.5	84
6	Effect of the Tottori Familial Disease Mutation (D7N) on the Monomers and Dimers of A β ₄₀ and A β ₄₂ . ACS Chemical Neuroscience, 2013, 4, 1446-1457.	1.7	83
7	Fast, Accurate, and Reliable Protocols for Routine Calculations of Protein-Ligand Binding Affinities in Drug Design Projects Using AMBER GPU-TI with ff14SB/GAFF. ACS Omega, 2020, 5, 4611-4619.	1.6	74
8	Effect of the English Familial Disease Mutation (H6R) on the Monomers and Dimers of A β ₄₀ and A β ₄₂ . ACS Chemical Neuroscience, 2014, 5, 646-657.	1.7	49
9	Effects of Water Models on Binding Affinity: Evidence from All-Atom Simulation of Binding of Tamiflu to A/H5N1 Neuraminidase. Scientific World Journal, The, 2014, 2014, 1-14.	0.8	42
10	Picosecond dissociation of amyloid fibrils with infrared laser: A nonequilibrium simulation study. Journal of Chemical Physics, 2015, 143, 155101.	1.2	41
11	Amyloid peptide A β ₄₀ inhibits aggregation of A β ₄₂ : Evidence from molecular dynamics simulations. Journal of Chemical Physics, 2012, 136, 245105.	1.2	38
12	Prediction of the Binding Affinities and Selectivity for CB1 and CB2 Ligands Using Homology Modeling, Molecular Docking, Molecular Dynamics Simulations, and MM-PBSA Binding Free Energy Calculations. ACS Chemical Neuroscience, 2020, 11, 1139-1158.	1.7	38
13	Effect of Taiwan Mutation (D7H) on Structures of Amyloid- β Peptides: Replica Exchange Molecular Dynamics Study. Journal of Physical Chemistry B, 2014, 118, 8972-8981.	1.2	36
14	Discovery of Dihydrochalcone as Potential Lead for Alzheimer's Disease: In Silico and In Vitro Study. PLoS ONE, 2013, 8, e79151.	1.1	33
15	Conformational Ensembles of the Wild-Type and S8C A β ₁₋₄₂ Dimers. Journal of Physical Chemistry B, 2017, 121, 2434-2442.	1.2	31
16	In Silico and In Vitro Study of Binding Affinity of Tripeptides to Amyloid β Fibrils: Implications for Alzheimer's Disease. Journal of Physical Chemistry B, 2015, 119, 5145-5155.	1.2	30
17	Nonequilibrium all-atom molecular dynamics simulation of the bubble cavitation and application to dissociate amyloid fibrils. Journal of Chemical Physics, 2016, 145, 174113.	1.2	30
18	Amyloid Properties of Asparagine and Glutamine in Prion-like Proteins. ACS Chemical Neuroscience, 2016, 7, 576-587.	1.7	30

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19	Tau R3â€“R4 Domain Dimer of the Wild Type and Phosphorylated Ser356 Sequences. I. In Solution by Atomistic Simulations. <i>Journal of Physical Chemistry B</i> , 2020, 124, 2975-2983.	1.2	30
20	Calculate proteinâ€“ligand binding affinities with the extended linear interaction energy method: application on the Cathepsin S set in the D3R Grand Challenge 3. <i>Journal of Computer-Aided Molecular Design</i> , 2019, 33, 105-117.	1.3	27
21	Molecular Mechanism of the Cell Membrane Pore Formation Induced by Bubble Stable Cavitation. <i>Journal of Physical Chemistry B</i> , 2019, 123, 71-78.	1.2	25
22	High performance p-type segmented leg of misfit-layered cobaltite and half-Heusler alloy. <i>Energy Conversion and Management</i> , 2015, 99, 20-27.	4.4	23
23	Effects of All-Atom Molecular Mechanics Force Fields on Amyloid Peptide Assembly: The Case of PHF6 Peptide of Tau Protein. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6458-6471.	2.3	23
24	Rayleigh-Plesset equation of the bubble stable cavitation in water: A nonequilibrium all-atom molecular dynamics simulation study. <i>Journal of Chemical Physics</i> , 2018, 148, .	1.2	22
25	<i>in silico</i> binding profile characterization of SARS-CoV-2 spike protein and its mutants bound to human ACE2 receptor. <i>Briefings in Bioinformatics</i> , 2021, 22, .	3.2	22
26	Structure and Dynamics of DNA and RNA Double Helices of CAG and GAC Trinucleotide Repeats. <i>Biophysical Journal</i> , 2017, 113, 19-36.	0.2	19
27	E-motif formed by extrahelical cytosine bases in DNA homoduplexes of trinucleotide and hexanucleotide repeats. <i>Nucleic Acids Research</i> , 2018, 46, 942-955.	6.5	19
28	Prediction of Drugâ€“Drug Interactions Between Opioids and Overdosed Benzodiazepines Using Physiologically Based Pharmacokinetic (PBPK) Modeling and Simulation. <i>Drugs in R and D</i> , 2019, 19, 297-305.	1.1	17
29	Machine learning on ligand-residue interaction profiles to significantly improve binding affinity prediction. <i>Briefings in Bioinformatics</i> , 2021, 22, .	3.2	17
30	Structure and Dynamics of DNA and RNA Double Helices Obtained from the CCG and GGC Trinucleotide Repeats. <i>Journal of Physical Chemistry B</i> , 2018, 122, 4491-4512.	1.2	16
31	Infrared Laser-Induced Amyloid Fibril Dissociation: A Joint Experimental/Theoretical Study on the GNNQQNY Peptide. <i>Journal of Physical Chemistry B</i> , 2020, 124, 6266-6277.	1.2	16
32	Determination of van der Waals Parameters Using a Double Exponential Potential for Nonbonded Divalent Metal Cations in TIP3P Solvent. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 1086-1097.	2.3	16
33	Molecular mechanism of ultrasound interaction with a blood brain barrier model. <i>Journal of Chemical Physics</i> , 2020, 153, 045104.	1.2	15
34	Recent progress in general force fields of small molecules. <i>Current Opinion in Structural Biology</i> , 2022, 72, 187-193.	2.6	15
35	Picosecond melting of peptide nanotubes using an infrared laser: a nonequilibrium simulation study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 27275-27280.	1.3	14
36	Al ²⁴¹ Aggregates More Like Al ²⁴⁰ than Like Al ²⁴² : In Silico and in Vitro Study. <i>Journal of Physical Chemistry B</i> , 2016, 120, 7371-7379.	1.2	13

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37	Molecular Mechanism and Kinetics of Amyloid- β Aggregate Formation: A Simulation Study. ACS Chemical Neuroscience, 2019, 10, 4643-4658.	1.7	13
38	Structural Determinants of Polyglutamine Protofibrils and Crystallites. ACS Chemical Neuroscience, 2015, 6, 632-645.	1.7	12
39	Interaction mechanism between the focused ultrasound and lipid membrane at the molecular level. Journal of Chemical Physics, 2019, 150, 215101.	1.2	11
40	Molecular conformations and dynamics of nucleotide repeats associated with neurodegenerative diseases: double helices and CAG hairpin loops. Computational and Structural Biotechnology Journal, 2021, 19, 2819-2832.	1.9	11
41	Elastic moduli of normal and cancer cell membranes revealed by molecular dynamics simulations. Physical Chemistry Chemical Physics, 2022, 24, 6225-6237.	1.3	10
42	Communication: Multiple atomistic force fields in a single enhanced sampling simulation. Journal of Chemical Physics, 2015, 143, 021101.	1.2	9
43	Picosecond infrared laser-induced all-atom nonequilibrium molecular dynamics simulation of dissociation of viruses. Physical Chemistry Chemical Physics, 2016, 18, 11951-11958.	1.3	9
44	New application of <i>in silico</i> methods in identifying mechanisms of action and key components of anti-cancer herbal formulation YIV-906 (PHY906). Physical Chemistry Chemical Physics, 2019, 21, 23501-23513.	1.3	9
45	Studying submicrosecond protein folding kinetics using a photolabile caging strategy and time-resolved photoacoustic calorimetry. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2973-2983.	1.5	8
46	Breaking down cellulose fibrils with a mid-infrared laser. Cellulose, 2018, 25, 5553-5568.	2.4	8
47	Introducing Virtual Oligomerization Inhibition to Identify Potent Inhibitors of $\text{A}\beta$ Oligomerization. Journal of Chemical Theory and Computation, 2020, 16, 3920-3935.	2.3	7
48	Comparative melting and healing of B-DNA and Z-DNA by an infrared laser pulse. Journal of Chemical Physics, 2016, 144, 145101.	1.2	6
49	A multiple-step <i>in silico</i> screening protocol to identify allosteric inhibitors of Spike-hACE2 binding. Physical Chemistry Chemical Physics, 2022, 24, 4305-4316.	1.3	6
50	Molecular Mechanism of Ultrasound-Induced Structural Defects in Liposomes: A Nonequilibrium Molecular Dynamics Simulation Study. Langmuir, 2021, 37, 7945-7954.	1.6	5
51	Nonequilibrium atomistic molecular dynamics simulation of tubular nanomotor propelled by bubble propulsion. Journal of Chemical Physics, 2019, 151, 024103.	1.2	4
52	Nonequilibrium molecular dynamics simulations of infrared laser-induced dissociation of a tetrameric $\text{A}\beta$ barrel in a neuronal membrane model. Chemistry and Physics of Lipids, 2021, 234, 105030.	1.5	2
53	Joint Computational/Cell-Based Approach for Screening Inhibitors of Tau Oligomerization: A Proof-of-Concept Study. Journal of Alzheimer's Disease, 2022, 89, 107-119.	1.2	2
54	Stability and Ion Distributions Around Left- and Right-Handed DNA and RNA Duplexes: A Comparative Study. Biophysical Journal, 2016, 110, 407a.	0.2	1

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55	Incorporating structural similarity into a scoring function to enhance the prediction of binding affinities. <i>Journal of Cheminformatics</i> , 2021, 13, 11.	2.8	1
56	Tripeptides Screening Report: Proline is Important for A β 2 Fibrils Depolymerization. <i>Biophysical Journal</i> , 2014, 106, 55a-56a.	0.2	0
57	Contrasting Roles of Asparagine and Glutamine in the Aggregation of Prion-Like Proteins. <i>Biophysical Journal</i> , 2016, 110, 214a-215a.	0.2	0
58	Structural Determinants of Polyglutamine Protofibrils and Crystallites. <i>Biophysical Journal</i> , 2016, 110, 215a.	0.2	0