Vincent A Voelz

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/2899879/publications.pdf

Version: 2024-02-01

56 papers	2,728 citations	236925 25 h-index	189892 50 g-index
65 all docs	65 docs citations	65 times ranked	3000 citing authors

#	Article	IF	Citations
1	Unprotected peptide macrocyclization and stapling via a fluorine-thiol displacement reaction. Nature Communications, 2022, 13, 350.	12.8	10
2	Estimation of binding rates and affinities from multiensemble Markov models and ligand decoupling. Journal of Chemical Physics, 2022, 156, 134115.	3.0	3
3	Solution-State Preorganization of Cyclic Î²-Hairpin Ligands Determines Binding Mechanism and Affinities for MDM2. Journal of Chemical Information and Modeling, 2021, 61, 2353-2367.	5.4	6
4	SARS-CoV-2 simulations go exascale to predict dramatic spike opening and cryptic pockets across the proteome. Nature Chemistry, 2021, 13, 651-659.	13.6	190
5	Reconciling Simulations and Experiments With BICePs: A Review. Frontiers in Molecular Biosciences, 2021, 8, 661520.	3.5	6
6	Assigning confidence to molecular property prediction. Expert Opinion on Drug Discovery, 2021, 16, 1009-1023.	5.0	34
7	Metal Cation-Binding Mechanisms of Q-Proline Peptoid Macrocycles in Solution. Journal of Chemical Information and Modeling, 2021, 61, 2818-2828.	5.4	7
8	Stacking Gaussian processes to improve $$pK_a$$ predictions in the SAMPL7 challenge. Journal of Computer-Aided Molecular Design, 2021, 35, 953-961.	2.9	2
9	Expanded Ensemble Methods Can be Used to Accurately Predict Protein-Ligand Relative Binding Free Energies. Journal of Chemical Theory and Computation, 2021, 17, 6536-6547.	5.3	7
10	Markov State Models to Elucidate Ligand Binding Mechanism. Methods in Molecular Biology, 2021, 2266, 239-259.	0.9	5
11	Metal-Binding Q-Proline Macrocycles. Journal of Organic Chemistry, 2021, 86, 4867-4876.	3.2	6
12	Adaptive Markov state model estimation using short reseeding trajectories. Journal of Chemical Physics, 2020, 152, 024103.	3.0	32
13	Microcanonical coarse-graining of the kinetic Ising model. Journal of Chemical Physics, 2020, 152, 084104.	3.0	2
14	Reconciling Simulated Ensembles of Apomyoglobin with Experimental Hydrogen/Deuterium Exchange Data Using Bayesian Inference and Multiensemble Markov State Models. Journal of Chemical Theory and Computation, 2020, 16, 1333-1348.	5.3	25
15	Exposing the Nucleation Site in Î±-Helix Folding: A Joint Experimental and Simulation Study. Journal of Physical Chemistry B, 2019, 123, 1797-1807.	2.6	13
16	Site-Specific Immuno-PET Tracer to Image PD-L1. Molecular Pharmaceutics, 2019, 16, 2028-2036.	4.6	41
17	Fluorinated Aromatic Monomers as Building Blocks To Control Î±-Peptoid Conformation and Structure. Journal of the American Chemical Society, 2019, 141, 3430-3434.	13.7	33
18	Model Selection Using BICePs: A Bayesian Approach for Force Field Validation and Parameterization. Journal of Physical Chemistry B, 2018, 122, 5610-5622.	2.6	19

#	Article	IF	Citations
19	Simulations of the regulatory ACT domain of human phenylalanine hydroxylase (PAH) unveil its mechanism of phenylalanine binding. Journal of Biological Chemistry, 2018, 293, 19532-19543.	3.4	15
20	Elucidating the inhibition of peptidoglycan biosynthesis in Staphylococcus aureus by albocycline, a macrolactone isolated from Streptomyces maizeus. Bioorganic and Medicinal Chemistry, 2018, 26, 3453-3460.	3.0	15
21	Binding Pathways of Phenylalanine to the Dimeric Regulatory Domain of Human PAH Reveal a LID Gating Mechanism. Biophysical Journal, 2018, 114, 226a.	0.5	1
22	Diverted Total Synthesis of Carolacton-Inspired Analogs Yields Three Distinct Phenotypes in Streptococcus mutans Biofilms. Journal of the American Chemical Society, 2017, 139, 7188-7191.	13.7	27
23	Computational and Experimental Evaluation of Designed Î²-Cap Hairpins Using Molecular Simulations and Kinetic Network Models. Journal of Chemical Information and Modeling, 2017, 57, 1609-1620.	5.4	9
24	Molecular simulations and free-energy calculations suggest conformation-dependent anion binding to a cytoplasmic site as a mechanism for Na+/K+-ATPase ion selectivity. Journal of Biological Chemistry, 2017, 292, 12412-12423.	3.4	12
25	Control of porphyrin interactions via structural changes of a peptoid scaffold. Organic and Biomolecular Chemistry, 2017, 15, 9670-9679.	2.8	11
26	Bridging Microscopic and Macroscopic Mechanisms of p53-MDM2 Binding with Kinetic Network Models. Biophysical Journal, 2017, 113, 785-793.	0.5	77
27	Precisely tuneable energy transfer system using peptoid helix-based molecular scaffold. Scientific Reports, 2017, 7, 4786.	3.3	22
28	A Maximum-Caliber Approach to Predicting Perturbed Folding Kinetics Due to Mutations. Journal of Chemical Theory and Computation, 2016, 12, 5768-5776.	5.3	40
29	Markov models of the apo-MDM2 lid region reveal diffuse yet two-state binding dynamics and receptor poses for computational docking. Scientific Reports, 2016, 6, 31631.	3.3	17
30	Using Kinetic Network Models To Probe Non-Native Salt-Bridge Effects on Î±-Helix Folding. Journal of Physical Chemistry B, 2016, 120, 926-935.	2.6	16
31	Microsecond simulations of mdm2 and its complex with p53 yield insight into force field accuracy and conformational dynamics. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1665-1676.	2.6	24
32	Molecular Simulation of Conformational Pre-Organization in Cyclic RGD Peptides. Journal of Chemical Information and Modeling, 2015, 55, 806-813.	5.4	43
33	Kinetic Network Models of Tryptophan Mutations in Î²-Hairpins Reveal the Importance of Non-Native Interactions. Journal of Chemical Theory and Computation, 2015, 11, 2801-2812.	5.3	27
34	Insights into Peptoid Helix Folding Cooperativity from an Improved Backbone Potential. Journal of Physical Chemistry B, 2015, 119, 15407-15417.	2.6	39
35	Bayesian inference of conformational state populations from computational models and sparse experimental observables. Journal of Computational Chemistry, 2014, 35, 2215-2224.	3.3	22
36	Surprisal Metrics for Quantifying Perturbed Conformational Dynamics in Markov State Models. Journal of Chemical Theory and Computation, 2014, 10, 5716-5728.	5.3	22

#	Article	IF	Citations
37	A Molecular Interpretation of 2D IR Protein Folding Experiments with Markov State Models. Biophysical Journal, 2014, 106, 1359-1370.	0.5	48
38	Computational Screening and Selection of Cyclic Peptide Hairpin Mimetics by Molecular Simulation and Kinetic Network Models. Journal of Chemical Information and Modeling, 2014, 54, 1425-1432.	5.4	47
39	Probing antibody internal dynamics with fluorescence anisotropy and molecular dynamics simulations. MAbs, 2013, 5, 306-322.	5.2	30
40	De novo structure prediction and experimental characterization of folded peptoid oligomers. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 14320-14325.	7.1	88
41	Slow Unfolded-State Structuring in Acyl-CoA Binding Protein Folding Revealed by Simulation and Experiment. Journal of the American Chemical Society, 2012, 134, 12565-12577.	13.7	132
42	Calculation of rate spectra from noisy time series data. Proteins: Structure, Function and Bioinformatics, 2012, 80, 342-351.	2.6	14
43	Atomistic Folding Simulations of the Five-Helix Bundle Protein Î»_{6â˜85}. Journal of the American Chemical Society, 2011, 133, 664-667.	13.7	137
44	Markov State Model Reveals Folding and Functional Dynamics in Ultra-Long MD Trajectories. Journal of the American Chemical Society, 2011, 133, 18413-18419.	13.7	150
45	Taming the complexity of protein folding. Current Opinion in Structural Biology, 2011, 21, 4-11.	5.7	156
46	Peptoid conformational free energy landscapes from implicitâ€solvent molecular simulations in AMBER. Biopolymers, 2011, 96, 639-650.	2.4	54
47	Molecular Simulation of ab Initio Protein Folding for a Millisecond Folder NTL9(1â˜39). Journal of the American Chemical Society, 2010, 132, 1526-1528.	13.7	473
48	Unfolded-State Dynamics and Structure of Protein L Characterized by Simulation and Experiment. Journal of the American Chemical Society, 2010, 132, 4702-4709.	13.7	86
49	Predicting Peptide Structures in Native Proteins from Physical Simulations of Fragments. PLoS Computational Biology, 2009, 5, e1000281.	3.2	30
50	Probing the Nanosecond Dynamics of a Designed Three-Stranded Beta-Sheet with a Massively Parallel Molecular Dynamics Simulation. International Journal of Molecular Sciences, 2009, 10, 1013-1030.	4.1	7
51	Blind Test of Physics-Based Prediction of Protein Structures. Biophysical Journal, 2009, 96, 917-924.	0.5	46
52	The protein folding problem: when will it be solved?. Current Opinion in Structural Biology, 2007, 17, 342-346.	5.7	208
53	Exploring zipping and assembly as a protein folding principle. Proteins: Structure, Function and Bioinformatics, 2006, 66, 877-888.	2.6	27
54	Information Content of Molecular Structures. Biophysical Journal, 2003, 85, 174-190.	0.5	19

#	Article	IF	Citations
55	Molecular Dynamics Simulation of Site-Directed Spin Labeling: Experimental Validation in Muscle Fibers. Biophysical Journal, 2002, 83, 1854-1866.	0.5	45
56	A Cooperative Molecular Modeling Exerciseâ€"The Hypersurface as Classroom. Journal of Chemical Education, 2001, 78, 1202.	2.3	3