Vincent A Voelz

List of Publications by Year
in descending order

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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	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
2	The protein folding problem: when will it be solved?. Current Opinion in Structural Biology, 2007, 17, 342-346.	5.7	208
3	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
4	Taming the complexity of protein folding. Current Opinion in Structural Biology, 2011, 21, 4-11.	5.7	156
5	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
6	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
7	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
8	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
9	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
10	Bridging Microscopic and Macroscopic Mechanisms of p53-MDM2 Binding with Kinetic Network Models. Biophysical Journal, 2017, 113, 785-793.	0.5	77
11	Peptoid conformational free energy landscapes from implicitâ€solvent molecular simulations in AMBER. Biopolymers, 2011, 96, 639-650.	2.4	54
12	A Molecular Interpretation of 2D IR Protein Folding Experiments with Markov State Models. Biophysical Journal, 2014, 106, 1359-1370.	0.5	48
13	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
14	Blind Test of Physics-Based Prediction of Protein Structures. Biophysical Journal, 2009, 96, 917-924.	0.5	46
15	Molecular Dynamics Simulation of Site-Directed Spin Labeling: Experimental Validation in Muscle Fibers. Biophysical Journal, 2002, 83, 1854-1866.	0.5	45
16	Molecular Simulation of Conformational Pre-Organization in Cyclic RGD Peptides. Journal of Chemical Information and Modeling, 2015, 55, 806-813.	5.4	43
17	Site-Specific Immuno-PET Tracer to Image PD-L1. Molecular Pharmaceutics, 2019, 16, 2028-2036.	4.6	41
18	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

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19	Insights into Peptoid Helix Folding Cooperativity from an Improved Backbone Potential. Journal of Physical Chemistry B, 2015, 119, 15407-15417.	2.6	39
20	Assigning confidence to molecular property prediction. Expert Opinion on Drug Discovery, 2021, 16, 1009-1023.	5.0	34
21	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
22	Adaptive Markov state model estimation using short reseeding trajectories. Journal of Chemical Physics, 2020, 152, 024103.	3.0	32
23	Predicting Peptide Structures in Native Proteins from Physical Simulations of Fragments. PLoS Computational Biology, 2009, 5, e1000281.	3.2	30
24	Probing antibody internal dynamics with fluorescence anisotropy and molecular dynamics simulations. MAbs, 2013, 5, 306-322.	5.2	30
25	Exploring zipping and assembly as a protein folding principle. Proteins: Structure, Function and Bioinformatics, 2006, 66, 877-888.	2.6	27
26	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
27	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
28	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
29	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
30	Bayesian inference of conformational state populations from computational models and sparse experimental observables. Journal of Computational Chemistry, 2014, 35, 2215-2224.	3.3	22
31	Surprisal Metrics for Quantifying Perturbed Conformational Dynamics in Markov State Models. Journal of Chemical Theory and Computation, 2014, 10, 5716-5728.	5.3	22
32	Precisely tuneable energy transfer system using peptoid helix-based molecular scaffold. Scientific Reports, 2017, 7, 4786.	3.3	22
33	Information Content of Molecular Structures. Biophysical Journal, 2003, 85, 174-190.	0.5	19
34	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
35	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
36	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

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37	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
38	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
39	Calculation of rate spectra from noisy time series data. Proteins: Structure, Function and Bioinformatics, 2012, 80, 342-351.	2.6	14
40	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
41	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
42	Control of porphyrin interactions via structural changes of a peptoid scaffold. Organic and Biomolecular Chemistry, 2017, 15, 9670-9679.	2.8	11
43	Unprotected peptide macrocyclization and stapling via a fluorine-thiol displacement reaction. Nature Communications, 2022, 13, 350.	12.8	10
44	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
45	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
46	Metal Cation-Binding Mechanisms of Q-Proline Peptoid Macrocycles in Solution. Journal of Chemical Information and Modeling, 2021, 61, 2818-2828.	5.4	7
47	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
48	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
49	Reconciling Simulations and Experiments With BICePs: A Review. Frontiers in Molecular Biosciences, 2021, 8, 661520.	3.5	6
50	Metal-Binding Q-Proline Macrocycles. Journal of Organic Chemistry, 2021, 86, 4867-4876.	3.2	6
51	Markov State Models to Elucidate Ligand Binding Mechanism. Methods in Molecular Biology, 2021, 2266, 239-259.	0.9	5
52	A Cooperative Molecular Modeling Exerciseâ€"The Hypersurface as Classroom. Journal of Chemical Education, 2001, 78, 1202.	2.3	3
53	Estimation of binding rates and affinities from multiensemble Markov models and ligand decoupling. Journal of Chemical Physics, 2022, 156, 134115.	3.0	3
54	Microcanonical coarse-graining of the kinetic Ising model. Journal of Chemical Physics, 2020, 152, 084104.	3.0	2

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55	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
56	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