

# Vincent A Voelz

## List of Publications by Citations

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58

papers

2,113

citations

23

h-index

45

g-index

65

ext. papers

2,454

ext. citations

6.3

avg, IF

5.11

L-index

#	Paper	IF	Citations
58	Molecular simulation of ab initio protein folding for a millisecond folder NTL9(1-39). <i>Journal of the American Chemical Society</i> , <b>2010</b> , 132, 1526-8	16.4	410
57	The protein folding problem: when will it be solved?. <i>Current Opinion in Structural Biology</i> , <b>2007</b> , 17, 342-8	8.1	182
56	Taming the complexity of protein folding. <i>Current Opinion in Structural Biology</i> , <b>2011</b> , 21, 4-11	8.1	139
55	Markov state model reveals folding and functional dynamics in ultra-long MD trajectories. <i>Journal of the American Chemical Society</i> , <b>2011</b> , 133, 18413-9	16.4	129
54	Atomistic folding simulations of the five-helix bundle protein (685). <i>Journal of the American Chemical Society</i> , <b>2011</b> , 133, 664-7	16.4	125
53	Slow unfolded-state structuring in Acyl-CoA binding protein folding revealed by simulation and experiment. <i>Journal of the American Chemical Society</i> , <b>2012</b> , 134, 12565-77	16.4	113
52	Unfolded-state dynamics and structure of protein L characterized by simulation and experiment. <i>Journal of the American Chemical Society</i> , <b>2010</b> , 132, 4702-9	16.4	80
51	De novo structure prediction and experimental characterization of folded peptoid oligomers. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2012</b> , 109, 14320-5	11.5	74
50	SARS-CoV-2 simulations go exascale to predict dramatic spike opening and cryptic pockets across the proteome. <i>Nature Chemistry</i> , <b>2021</b> , 13, 651-659	17.6	62
49	Bridging Microscopic and Macroscopic Mechanisms of p53-MDM2 Binding with Kinetic Network Models. <i>Biophysical Journal</i> , <b>2017</b> , 113, 785-793	2.9	51
48	A molecular interpretation of 2D IR protein folding experiments with Markov state models. <i>Biophysical Journal</i> , <b>2014</b> , 106, 1359-70	2.9	44
47	Computational screening and selection of cyclic peptide hairpin mimetics by molecular simulation and kinetic network models. <i>Journal of Chemical Information and Modeling</i> , <b>2014</b> , 54, 1425-32	6.1	44
46	Peptoid conformational free energy landscapes from implicit-solvent molecular simulations in AMBER. <i>Biopolymers</i> , <b>2011</b> , 96, 639-50	2.2	43
45	Blind test of physics-based prediction of protein structures. <i>Biophysical Journal</i> , <b>2009</b> , 96, 917-24	2.9	42
44	Molecular dynamics simulation of site-directed spin labeling: experimental validation in muscle fibers. <i>Biophysical Journal</i> , <b>2002</b> , 83, 1854-66	2.9	42
43	Molecular Simulation of Conformational Pre-Organization in Cyclic RGD Peptides. <i>Journal of Chemical Information and Modeling</i> , <b>2015</b> , 55, 806-13	6.1	33
42	A Maximum-Caliber Approach to Predicting Perturbed Folding Kinetics Due to Mutations. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 5768-5776	6.4	33

41	SARS-CoV-2 Simulations Go Exascale to Capture Spike Opening and Reveal Cryptic Pockets Across the Proteome <b>2020</b> ,		28
40	Insights into Peptoid Helix Folding Cooperativity from an Improved Backbone Potential. <i>Journal of Physical Chemistry B</i> , <b>2015</b> , 119, 15407-17	3.4	27
39	Predicting peptide structures in native proteins from physical simulations of fragments. <i>PLoS Computational Biology</i> , <b>2009</b> , 5, e1000281	5	27
38	Exploring zipping and assembly as a protein folding principle. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2007</b> , 66, 877-88	4.2	26
37	Site-Specific Immuno-PET Tracer to Image PD-L1. <i>Molecular Pharmaceutics</i> , <b>2019</b> , 16, 2028-2036	5.6	24
36	Probing antibody internal dynamics with fluorescence anisotropy and molecular dynamics simulations. <i>MAbs</i> , <b>2013</b> , 5, 306-22	6.6	24
35	Diverted Total Synthesis of Carolacton-Inspired Analogs Yields Three Distinct Phenotypes in <i>Streptococcus mutans</i> Biofilms. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 7188-7191	16.4	22
34	Kinetic network models of tryptophan mutations in $\beta$ hairpins reveal the importance of non-native interactions. <i>Journal of Chemical Theory and Computation</i> , <b>2015</b> , 11, 2801-12	6.4	21
33	Microsecond simulations of mdm2 and its complex with p53 yield insight into force field accuracy and conformational dynamics. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2015</b> , 83, 1665-76	4.2	21
32	Surprisal Metrics for Quantifying Perturbed Conformational Dynamics in Markov State Models. <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 5716-28	6.4	20
31	Fluorinated Aromatic Monomers as Building Blocks To Control $\beta$ Peptoid Conformation and Structure. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 3430-3434	16.4	19
30	Information content of molecular structures. <i>Biophysical Journal</i> , <b>2003</b> , 85, 174-90	2.9	19
29	Bayesian inference of conformational state populations from computational models and sparse experimental observables. <i>Journal of Computational Chemistry</i> , <b>2014</b> , 35, 2215-24	3.5	18
28	Precisely tuneable energy transfer system using peptoid helix-based molecular scaffold. <i>Scientific Reports</i> , <b>2017</b> , 7, 4786	4.9	17
27	Using Kinetic Network Models To Probe Non-Native Salt-Bridge Effects on $\beta$ Helix Folding. <i>Journal of Physical Chemistry B</i> , <b>2016</b> , 120, 926-35	3.4	15
26	Calculation of rate spectra from noisy time series data. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2012</b> , 80, 342-51	4.2	13
25	Markov models of the apo-MDM2 lid region reveal diffuse yet two-state binding dynamics and receptor poses for computational docking. <i>Scientific Reports</i> , <b>2016</b> , 6, 31631	4.9	12
24	Adaptive Markov state model estimation using short reseeding trajectories. <i>Journal of Chemical Physics</i> , <b>2020</b> , 152, 024103	3.9	11

23	Assigning confidence to molecular property prediction. <i>Expert Opinion on Drug Discovery</i> , <b>2021</b> , 16, 100961-1023	10.23	10
22	Control of porphyrin interactions via structural changes of a peptoid scaffold. <i>Organic and Biomolecular Chemistry</i> , <b>2017</b> , 15, 9670-9679	3.9	9
21	Reconciling Simulated Ensembles of Apomyoglobin with Experimental Hydrogen/Deuterium Exchange Data Using Bayesian Inference and Multiensemble Markov State Models. <i>Journal of Chemical Theory and Computation</i> , <b>2020</b> , 16, 1333-1348	6.4	9
20	Model Selection Using BICePs: A Bayesian Approach for Force Field Validation and Parameterization. <i>Journal of Physical Chemistry B</i> , <b>2018</b> , 122, 5610-5622	3.4	9
19	Simulations of the regulatory ACT domain of human phenylalanine hydroxylase (PAH) unveil its mechanism of phenylalanine binding. <i>Journal of Biological Chemistry</i> , <b>2018</b> , 293, 19532-19543	5.4	9
18	Molecular simulations and free-energy calculations suggest conformation-dependent anion binding to a cytoplasmic site as a mechanism for Na/K-ATPase ion selectivity. <i>Journal of Biological Chemistry</i> , <b>2017</b> , 292, 12412-12423	5.4	8
17	Exposing the Nucleation Site in $\beta$ -Helix Folding: A Joint Experimental and Simulation Study. <i>Journal of Physical Chemistry B</i> , <b>2019</b> , 123, 1797-1807	3.4	8
16	Elucidating the inhibition of peptidoglycan biosynthesis in <i>Staphylococcus aureus</i> by albocycline, a macrolactone isolated from <i>Streptomyces maizeus</i> . <i>Bioorganic and Medicinal Chemistry</i> , <b>2018</b> , 26, 3453-3460	3.4	7
15	Computational and Experimental Evaluation of Designed $\beta$ Cap Hairpins Using Molecular Simulations and Kinetic Network Models. <i>Journal of Chemical Information and Modeling</i> , <b>2017</b> , 57, 1609-1620	6.1	6
14	Probing the nanosecond dynamics of a designed three-stranded beta-sheet with a massively parallel molecular dynamics simulation. <i>International Journal of Molecular Sciences</i> , <b>2009</b> , 10, 1013-30	6.3	6
13	A Cooperative Molecular Modeling Exercise: The Hypersurface as Classroom. <i>Journal of Chemical Education</i> , <b>2001</b> , 78, 1202	2.4	3
12	Metal-Binding Q-Proline Macrocycles. <i>Journal of Organic Chemistry</i> , <b>2021</b> , 86, 4867-4876	4.2	3
11	Solution-State Preorganization of Cyclic $\beta$ Hairpin Ligands Determines Binding Mechanism and Affinities for MDM2. <i>Journal of Chemical Information and Modeling</i> , <b>2021</b> , 61, 2353-2367	6.1	3
10	Microcanonical coarse-graining of the kinetic Ising model. <i>Journal of Chemical Physics</i> , <b>2020</b> , 152, 084104	3.9	2
9	Unprotected peptide macrocyclization and stapling via a fluorine-thiol displacement reaction.. <i>Nature Communications</i> , <b>2022</b> , 13, 350	17.4	2
8	Bridging microscopic and macroscopic mechanisms of p53-MDM2 binding using molecular simulations and kinetic network models		2
7	Metal Cation-Binding Mechanisms of Q-Proline Peptoid Macrocycles in Solution		2
6	Markov State Models to Elucidate Ligand Binding Mechanism. <i>Methods in Molecular Biology</i> , <b>2021</b> , 2266, 239-259	1.4	2

5	Reconciling Simulations and Experiments With BICePs: A Review. <i>Frontiers in Molecular Biosciences</i> , <b>2021</b> , 8, 661520	5.6	1
4	Metal Cation-Binding Mechanisms of Q-Proline Peptoid Macrocycles in Solution. <i>Journal of Chemical Information and Modeling</i> , <b>2021</b> , 61, 2818-2828	6.1	1
3	Expanded Ensemble Methods Can be Used to Accurately Predict Protein-Ligand Relative Binding Free Energies. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 6536-6547	6.4	1
2	Stacking Gaussian processes to improve [Formula: see text] predictions in the SAMPL7 challenge. <i>Journal of Computer-Aided Molecular Design</i> , <b>2021</b> , 35, 953-961	4.2	0
1	Estimation of binding rates and affinities from multiensemble Markov models and ligand decoupling.. <i>Journal of Chemical Physics</i> , <b>2022</b> , 156, 134115	3.9	0