Vincent A Voelz

List of Publications by Year in Descending Order

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	Unprotected peptide macrocyclization and stapling via a fluorine-thiol displacement reaction.. *Nature Communications*, **2022**, 13, 350	17.4	2
57	Estimation of binding rates and affinities from multiensemble Markov models and ligand decoupling.. *Journal of Chemical Physics*, **2022**, 156, 134115	3.9	0
56	Metal-Binding Q-Proline Macrocycles. *Journal of Organic Chemistry*, **2021**, 86, 4867-4876	4.2	3
55	Solution-State Preorganization of Cyclic β-Hairpin Ligands Determines Binding Mechanism and Affinities for MDM2. *Journal of Chemical Information and Modeling*, **2021**, 61, 2353-2367	6.1	3
54	SARS-CoV-2 simulations go exascale to predict dramatic spike opening and cryptic pockets across the proteome. *Nature Chemistry*, **2021**, 13, 651-659	17.6	62
53	Reconciling Simulations and Experiments With BICePs: A Review. *Frontiers in Molecular Biosciences*, **2021**, 8, 661520	5.6	1
52	Assigning confidence to molecular property prediction. *Expert Opinion on Drug Discovery*, **2021**, 16, 1009-1023	6.1	10
51	Metal Cation-Binding Mechanisms of Q-Proline Peptoid Macrocycles in Solution. *Journal of Chemical Information and Modeling*, **2021**, 61, 2818-2828	6.1	1
50	Stacking Gaussian processes to improve [Formula: see text] predictions in the SAMPL7 challenge. *Journal of Computer-Aided Molecular Design*, **2021**, 35, 953-961	4.2	0
49	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	6.4	1
48	Markov State Models to Elucidate Ligand Binding Mechanism. *Methods in Molecular Biology*, **2021**, 2266, 239-259	1.4	2
47	Microcanonical coarse-graining of the kinetic Ising model. *Journal of Chemical Physics*, **2020**, 152, 084104	3.9	2
46	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	6.4	9
45	SARS-CoV-2 Simulations Go Exascale to Capture Spike Opening and Reveal Cryptic Pockets Across the Proteome **2020**,		28
44	Adaptive Markov state model estimation using short reseeding trajectories. *Journal of Chemical Physics*, **2020**, 152, 024103	3.9	11
43	Exposing the Nucleation Site in β-Helix Folding: A Joint Experimental and Simulation Study. *Journal of Physical Chemistry B*, **2019**, 123, 1797-1807	3.4	8
42	Site-Specific Immuno-PET Tracer to Image PD-L1. *Molecular Pharmaceutics*, **2019**, 16, 2028-2036	5.6	24

41	Fluorinated Aromatic Monomers as Building Blocks To Control Peptoid Conformation and Structure. *Journal of the American Chemical Society*, **2019**, 141, 3430-3434	16.4	19
40	Model Selection Using BICePs: A Bayesian Approach for Force Field Validation and Parameterization. *Journal of Physical Chemistry B*, **2018**, 122, 5610-5622	3.4	9
39	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	5.4	9
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	3.4	7
37	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	16.4	22
36	Computational and Experimental Evaluation of Designed Cap Hairpins Using Molecular Simulations and Kinetic Network Models. *Journal of Chemical Information and Modeling*, **2017**, 57, 1609-1620	6.1	6
35	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	5.4	8
34	Control of porphyrin interactions via structural changes of a peptoid scaffold. *Organic and Biomolecular Chemistry*, **2017**, 15, 9670-9679	3.9	9
33	Bridging Microscopic and Macroscopic Mechanisms of p53-MDM2 Binding with Kinetic Network Models. *Biophysical Journal*, **2017**, 113, 785-793	2.9	51
32	Precisely tuneable energy transfer system using peptoid helix-based molecular scaffold. *Scientific Reports*, **2017**, 7, 4786	4.9	17
31	A Maximum-Caliber Approach to Predicting Perturbed Folding Kinetics Due to Mutations. *Journal of Chemical Theory and Computation*, **2016**, 12, 5768-5776	6.4	33
30	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	4.9	12
29	Using Kinetic Network Models To Probe Non-Native Salt-Bridge Effects on Helix Folding. *Journal of Physical Chemistry B*, **2016**, 120, 926-35	3.4	15
28	Molecular Simulation of Conformational Pre-Organization in Cyclic RGD Peptides. *Journal of Chemical Information and Modeling*, **2015**, 55, 806-13	6.1	33
27	Kinetic network models of tryptophan mutations in hairpins reveal the importance of non-native interactions. *Journal of Chemical Theory and Computation*, **2015**, 11, 2801-12	6.4	21
26	Insights into Peptoid Helix Folding Cooperativity from an Improved Backbone Potential. *Journal of Physical Chemistry B*, **2015**, 119, 15407-17	3.4	27
25	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, 1665-76	4.2	21
24	A molecular interpretation of 2D IR protein folding experiments with Markov state models. *Biophysical Journal*, **2014**, 106, 1359-70	2.9	44

23	Computational screening and selection of cyclic peptide hairpin mimetics by molecular simulation and kinetic network models. *Journal of Chemical Information and Modeling*, **2014**, 54, 1425-32	6.1	44
22	Bayesian inference of conformational state populations from computational models and sparse experimental observables. *Journal of Computational Chemistry*, **2014**, 35, 2215-24	3.5	18
21	Surprisal Metrics for Quantifying Perturbed Conformational Dynamics in Markov State Models. *Journal of Chemical Theory and Computation*, **2014**, 10, 5716-28	6.4	20
20	Probing antibody internal dynamics with fluorescence anisotropy and molecular dynamics simulations. *MAbs*, **2013**, 5, 306-22	6.6	24
19	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, 14320-5	11.5	74
18	Slow unfolded-state structuring in Acyl-CoA binding protein folding revealed by simulation and experiment. *Journal of the American Chemical Society*, **2012**, 134, 12565-77	16.4	113
17	Calculation of rate spectra from noisy time series data. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 342-51	4.2	13
16	Markov state model reveals folding and functional dynamics in ultra-long MD trajectories. *Journal of the American Chemical Society*, **2011**, 133, 18413-9	16.4	129
15	Taming the complexity of protein folding. *Current Opinion in Structural Biology*, **2011**, 21, 4-11	8.1	139
14	Peptoid conformational free energy landscapes from implicit-solvent molecular simulations in AMBER. *Biopolymers*, **2011**, 96, 639-50	2.2	43
13	Atomistic folding simulations of the five-helix bundle protein (λ6-85). *Journal of the American Chemical Society*, **2011**, 133, 664-7	16.4	125
12	Unfolded-state dynamics and structure of protein L characterized by simulation and experiment. *Journal of the American Chemical Society*, **2010**, 132, 4702-9	16.4	80
11	Molecular simulation of ab initio protein folding for a millisecond folder NTL9(1-39). *Journal of the American Chemical Society*, **2010**, 132, 1526-8	16.4	410
10	Predicting peptide structures in native proteins from physical simulations of fragments. *PLoS Computational Biology*, **2009**, 5, e1000281	5	27
9	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, 1013-30	6.3	6
8	Blind test of physics-based prediction of protein structures. *Biophysical Journal*, **2009**, 96, 917-24	2.9	42
7	The protein folding problem: when will it be solved?. *Current Opinion in Structural Biology*, **2007**, 17, 342-8	8.1	182
6	Exploring zipping and assembly as a protein folding principle. *Proteins: Structure, Function and Bioinformatics*, **2007**, 66, 877-88	4.2	26

5	Information content of molecular structures. *Biophysical Journal*, **2003**, 85, 174-90	2.9	19
4	Molecular dynamics simulation of site-directed spin labeling: experimental validation in muscle fibers. *Biophysical Journal*, **2002**, 83, 1854-66	2.9	42
3	A Cooperative Molecular Modeling Exercise The Hypersurface as Classroom. *Journal of Chemical Education*, **2001**, 78, 1202	2.4	3
2	Bridging microscopic and macroscopic mechanisms of p53-MDM2 binding using molecular simulations and kinetic network models		2
1	Metal Cation-Binding Mechanisms of Q-Proline Peptoid Macrocycles in Solution		2