

# F Marty Ytreberg

## List of Publications by Year in descending order

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Version: 2024-02-01

44  
papers

963  
citations

430874

18  
h-index

477307

29  
g-index

49  
all docs

49  
docs citations

49  
times ranked

1271  
citing authors

#	ARTICLE	IF	CITATIONS
1	Comparison of free energy methods for molecular systems. Journal of Chemical Physics, 2006, 125, 184114.	3.0	129
2	Single-ensemble nonequilibrium path-sampling estimates of free energy differences. Journal of Chemical Physics, 2004, 120, 10876-10879.	3.0	99
3	Efficient use of nonequilibrium measurement to estimate free energy differences for molecular systems. Journal of Computational Chemistry, 2004, 25, 1749-1759.	3.3	74
4	Absolute FKBP binding affinities obtained via nonequilibrium unbinding simulations. Journal of Chemical Physics, 2009, 130, 164906.	3.0	53
5	Fast Calculation of Protein-Protein Binding Free Energies Using Umbrella Sampling with a Coarse-Grained Model. Journal of Chemical Theory and Computation, 2018, 14, 991-997.	5.3	38
6	Understanding the structural ensembles of a highly extended disordered protein. Molecular BioSystems, 2012, 8, 308-319.	2.9	37
7	Initiating a watch list for Ebola virus antibody escape mutations. PeerJ, 2016, 4, e1674.	2.0	36
8	Simple estimation of absolute free energies for biomolecules. Journal of Chemical Physics, 2006, 124, 104105.	3.0	33
9	C5-Functionalized DNA, LNA, and LNA: Positional Control of Polarity-Sensitive Fluorophores Leads to Improved SNP Typing. Chemistry - A European Journal, 2011, 17, 3157-3165.	3.3	33
10	Calculated properties of field-induced aggregates in ferrofluids. Physical Review E, 2000, 61, 4107-4110.	2.1	32
11	Reducing the bias and uncertainty of free energy estimates by using regression to fit thermodynamic integration data. Journal of Computational Chemistry, 2009, 30, NA-NA.	3.3	27
12	A Novel Mouse Dscam Mutation Inhibits Localization and Shedding of DSCAM. PLoS ONE, 2012, 7, e52652.	2.5	27
13	Predicting the viability of beta-lactamase: How folding and binding free energies correlate with beta-lactamase fitness. PLoS ONE, 2020, 15, e0233509.	2.5	26
14	Understanding Bernoulli's principle through simulations. American Journal of Physics, 2011, 79, 214-216.	0.7	25
15	Expanding the watch list for potential Ebola virus antibody escape mutations. PLoS ONE, 2019, 14, e0211093.	2.5	25
16	Effect of Gold Nanoparticle Conjugation on Peptide Dynamics and Structure. Entropy, 2012, 14, 630-641.	2.2	24
17	First-Step Mutations for Adaptation at Elevated Temperature Increase Capsid Stability in a Virus. PLoS ONE, 2011, 6, e25640.	2.5	24
18	Parallel Mutations Result in a Wide Range of Cooperation and Community Consequences in a Two-Species Bacterial Consortium. PLoS ONE, 2016, 11, e0161837.	2.5	23

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19	Impact of the K24N mutation on the transactivation domain of p53 and its binding to murine double-minute clone 2. <i>Proteins: Structure, Function and Bioinformatics</i> , 2013, 81, 1738-1747.	2.6	20
20	Computational estimation of rainbow trout estrogen receptor binding affinities for environmental estrogens. <i>Toxicology and Applied Pharmacology</i> , 2011, 250, 322-326.	2.8	18
21	Peptide Conformational Equilibria Computed via a Single-Stage Shifting Protocol. <i>Journal of Physical Chemistry B</i> , 2005, 109, 9096-9103.	2.6	16
22	Implementing and Assessing an Alchemical Method for Calculating Protein-Protein Binding Free Energy. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2457-2464.	5.3	16
23	Predicting peak spectral sensitivities of vertebrate cone visual pigments using atomistic molecular simulations. <i>PLoS Computational Biology</i> , 2018, 14, e1005974.	3.2	15
24	Changing Folding and Binding Stability in a Viral Coat Protein: A Comparison between Substitutions Accessible through Mutation and Those Fixed by Natural Selection. <i>PLoS ONE</i> , 2014, 9, e112988.	2.5	13
25	EfgA is a conserved formaldehyde sensor that leads to bacterial growth arrest in response to elevated formaldehyde. <i>PLoS Biology</i> , 2021, 19, e3001208.	5.6	13
26	Assessment of software methods for estimating protein-protein relative binding affinities. <i>PLoS ONE</i> , 2020, 15, e0240573.	2.5	11
27	A black-box re-weighting analysis can correct flawed simulation data. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 7982-7987.	7.1	10
28	The cis conformation of proline leads to weaker binding of a p53 peptide to MDM2 compared to trans. <i>Archives of Biochemistry and Biophysics</i> , 2015, 575, 22-29.	3.0	10
29	Using chemical shifts to generate structural ensembles for intrinsically disordered proteins with converged distributions of secondary structure. <i>Intrinsically Disordered Proteins</i> , 2015, 3, e984565.	1.9	10
30	Paired Simulations and Experimental Investigations into the Calcium-Dependent Conformation of Albumin. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 1282-1293.	5.4	7
31	The effects of nanoscale geometry and spillover on room temperature storage of hydrogen on silica nanosprings. <i>Journal Physics D: Applied Physics</i> , 2013, 46, 505307.	2.8	6
32	New Perspectives on Ebola Virus Evolution. <i>PLoS ONE</i> , 2016, 11, e0160410.	2.5	6
33	Molecular Modeling Predicts Novel Antibody Escape Mutations in the Respiratory Syncytial Virus Fusion Glycoprotein. <i>Journal of Virology</i> , 2022, 96, .	3.4	6
34	Computational Study of Small Molecule Binding for Both Tethered and Free Conditions. <i>Journal of Physical Chemistry B</i> , 2010, 114, 5431-5434.	2.6	5
35	Demonstrated Convergence of the Equilibrium Ensemble for a Fast United-Residue Protein Model. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1860-1866.	5.3	4
36	Computational Study of Evolutionary Selection Pressure on Rainbow Trout Estrogen Receptors. <i>PLoS ONE</i> , 2010, 5, e9392.	2.5	4

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37	Second mechanism for transitions in a reaction diffusion system. <i>Physical Review E</i> , 1999, 59, 3376-3381.	2.1	3
38	Searching for a mechanistic description of pairwise epistasis in protein systems. <i>Proteins: Structure, Function and Bioinformatics</i> , 2022, 90, 1474-1485.	2.6	3
39	Protein Stability in Titan's Subsurface Water Ocean. <i>Astrobiology</i> , 2020, 20, 190-198.	3.0	1
40	Effects of the binding of calcium ions on the structure and dynamics of the $\hat{1}$ X174 virus investigated using molecular dynamics. <i>Journal of Biological Physics</i> , 2012, 38, 397-404.	1.5	0
41	Title is missing!. , 2020, 15, e0233509.		0
42	Title is missing!. , 2020, 15, e0233509.		0
43	Title is missing!. , 2020, 15, e0233509.		0
44	Title is missing!. , 2020, 15, e0233509.		0