Davidâ€d L Minh

List of Publications by Year
in descending order

52 papers	1,123 citations	471371 17 h-index	414303 32 g-index
59 all docs	59 docs citations	59 times ranked	1445 citing authors

#	Article	IF	Citations
1	Identification of the riboflavin cofactor-binding site in the Vibrio cholerae ion-pumping NQR complex: A novel structural motif in redox enzymes. Journal of Biological Chemistry, 2022, 298, 102182.	1.6	0
2	Electrostatics and water occlusion regulate covalentlyâ€bound flavin mononucleotide cofactors of Vibrio cholerae respiratory complex <scp>NQR</scp>. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1376-1385.	1.5	3
3	Alchemical Grid Dock (AlGDock): Binding Free Energy Calculations between Flexible Ligands and Rigid Receptors. Journal of Computational Chemistry, 2020, 41, 715-730.	1.5	12
4	On Restraints in Endâ€Point Proteinâ€“Ligand Binding Free Energy Calculations. Journal of Computational Chemistry, 2020, 41, 573-586.	1.5	11
5	On the polarization of ligands by proteins. Physical Chemistry Chemical Physics, 2020, 22, 12044-12057.	1.3	8
6	A Structural Model for Baxâ†2-Mediated Activation of Caspase 8-Dependent Apoptosis. International Journal of Molecular Sciences, 2020, 21, 5476.	1.8	2
7	Robosample: A rigid-body molecular simulation program based on robot mechanics. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129616.	1.1	5
8	Implicit ligand theory for relative binding free energies: II. An estimator based on control variates. Journal of Physics Communications, 2020, 4, 115010.	0.5	2
9	On Restraints in End-Point Protein-Ligand Binding Free Energy Calculations. Biophysical Journal, 2019, 116, 47a.	0.2	0
10	Conserved residue His-257 of Vibrio cholerae flavin transferase ApbE plays a critical role in substrate binding and catalysis. Journal of Biological Chemistry, 2019, 294, 13800-13810.	1.6	10
11	Role of Subunit D in Ubiquinone-Binding Site of Vibrio cholerae NQR: Pocket Flexibility and Inhibitor Resistance. ACS Omega, 2019, 4, 19324-19331.	1.6	6
12	Nonequilibrium path-ensemble averages for symmetric protocols. Journal of Chemical Physics, 2019, 151, 194103.	1.2	0
13	Alchemical Grid Dock (AlGDock) calculations in the D3R Grand Challenge 3. Journal of Computer-Aided Molecular Design, 2019, 33, 61-69.	1.3	5
14	Power transformations improve interpolation of grids for molecular mechanics interaction energies. Journal of Computational Chemistry, 2018, 39, 1200-1207.	1.5	2
15	Using the fast fourier transform in binding free energy calculations. Journal of Computational Chemistry, 2018, 39, 621-636.	1.5	19
16	Implicit ligand theory for relative binding free energies. Journal of Chemical Physics, 2018, 148, 104114.	1.2	6
17	Design, Synthesis, and Biological Evaluation of Polyaminocarboxylate Ligandâ€Based Theranostic Conjugates for Antibodyâ€Targeted Cancer Therapy and Nearâ€Infrared Optical Imaging. ChemMedChem, 2018, 13, 2606-2617.	1.6	7
18	Bayesian analysis of isothermal titration calorimetry for binding thermodynamics. PLoS ONE, 2018, 13, e0203224.	1.1	24

#	Article	IF	Citations
19	Simple Entropy Terms for End-Point Binding Free Energy Calculations. Journal of Chemical Theory and Computation, 2018, 14, 6035-6049.	2.3	22
20	Characterization of the Pseudomonas aeruginosa NQR complex, a bacterial proton pump with roles in autopoisoning resistance. Journal of Biological Chemistry, 2018, 293, 15664-15677.	1.6	20
21	Efficiency of Stratification for Ensemble Docking Using Reduced Ensembles. Journal of Chemical Information and Modeling, 2018, 58, 1915-1925.	2.5	8
22	Identification of the Catalytic Ubiquinone-binding Site of Vibrio cholerae Sodium-dependent NADH Dehydrogenase. Journal of Biological Chemistry, 2017, 292, 3039-3048.	1.6	11
23	Absolute Binding Free Energies between T4 Lysozyme and 141 Small Molecules: Calculations Based on Multiple Rigid Receptor Configurations. Journal of Chemical Theory and Computation, 2017, 13, 2930-2944.	2.3	33
24	Hamiltonian Monte Carlo with Constrained Molecular Dynamics as Gibbs Sampling. Journal of Chemical Theory and Computation, 2017, 13, 4649-4659.	2.3	3
25	Effects of Catalytic Action and Ligand Binding on Conformational Ensembles of Adenylate Kinase. Biochemistry, 2017, 56, 4559-4567.	1.2	13
26	Intermediate Thermodynamic States Contribute Equally to Free Energy Convergence: A Demonstration with Replica Exchange. Journal of Chemical Theory and Computation, 2016, 12, 2154-2161.	2.3	12
27	Layer Sampling. Communications in Statistics Part B: Simulation and Computation, 2016, 45, 73-100.	0.6	1
28	Understanding the Hastings Algorithm. Communications in Statistics Part B: Simulation and Computation, 2015, 44, 332-349.	0.6	23
29	Wide-Angle X-Ray Solution Scattering for Protein-Ligand Binding: Multivariate Curve Resolution with Bayesian Confidence Intervals. Biophysical Journal, 2013, 104, 873-883.	0.2	21
30	Steady State Dynamics of Enzyme Catalytic Action in Solution. Biophysical Journal, 2013, 104, 30a.	0.2	0
31	Correction for Nilmeier et al., Nonequilibrium candidate Monte Carlo is an efficient tool for equilibrium simulation. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 9665-9665.	3.3	4
32	Comment on â€œTransient-state fluctuationlike relation for the driving force on a biomoleculeâ€• Physical Review E, 2012, 85, 053103.	0.8	1
33	Implicit ligand theory: Rigorous binding free energies and thermodynamic expectations from molecular docking. Journal of Chemical Physics, 2012, 137, 104106.	1.2	23
34	Regenerative Markov Chain Monte Carlo for Any Distribution. Communications in Statistics Part B: Simulation and Computation, 2012, 41, 1745-1760.	0.6	8
35	Density-dependent analysis of nonequilibrium paths improves free energy estimates II. A Feynmanâ€“Kac formalism. Journal of Chemical Physics, 2011, 134, 034117.	1.2	3
36	Xâ€ray solution scattering studies of the structural diversity intrinsic to protein ensembles. Biopolymers, 2011, 95, 531-542.	1.2	30

#	Article	IF	Citations
37	Estimating equilibrium ensemble averages using multiple time slices from driven nonequilibrium processes: Theory and application to free energies, moments, and thermodynamic length in single-molecule pulling experiments. Journal of Chemical Physics, 2011, 134, 024111.	1.2	15
38	Nonequilibrium candidate Monte Carlo is an efficient tool for equilibrium simulation. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, E1009-18.	3.3	91
39	Optimized replica gas estimation of absolute integrals and partition functions. Physical Review E, 2010, 82, 031132.	0.8	1
40	Method to Predict Crowding Effects by Postprocessing Molecular Dynamics Trajectories: Application to the Flap Dynamics of HIV-1 Protease. Journal of Physical Chemistry Letters, 2010, 1, 107-110.	2.1	39
41	Optimal estimators and asymptotic variances for nonequilibrium path-ensemble averages. Journal of Chemical Physics, 2009, 131, 134110.	1.2	48
42	Path integral analysis of Jarzynskiâ€™s equality: Analytical results. Physical Review E, 2009, 79, 021122.	0.8	18
43	Density-dependent analysis of nonequilibrium paths improves free energy estimates. Journal of Chemical Physics, 2009, 130, 204102.	1.2	6
44	Molecular Crowding Inhibits Intramolecular Breathing Motions in Proteins. Journal of Molecular Biology, 2008, 375, 529-546.	2.0	86
45	Springs and Speeds in Free Energy Reconstruction from Irreversible Single-Molecule Pulling Experiments. Journal of Physical Chemistry B, 2008, 112, 5892-5897.	1.2	33
46	Optimized Free Energies from Bidirectional Single-Molecule Force Spectroscopy. Physical Review Letters, 2008, 100, 180602.	2.9	83
47	Accelerated entropy estimates with accelerated dynamics. Journal of Chemical Physics, 2007, 127, 154105.	1.2	14
48	Remarkable Loop Flexibility in Avian Influenza N1 and Its Implications for Antiviral Drug Design. Journal of the American Chemical Society, 2007, 129, 7764-7765.	6.6	157
49	Multidimensional Potentials of Mean Force from Biased Experiments along a Single Coordinate. Journal of Physical Chemistry B, 2007, 111, 4137-4140.	1.2	14
50	The Influence of Macromolecular Crowding on HIV-1 Protease Internal Dynamics. Journal of the American Chemical Society, 2006, 128, 6006-6007.	6.6	96
51	Free-energy reconstruction from experiments performed under different biasing programs. Physical Review E, 2006, 74, 061120.	0.8	16
52	The Entropic Cost of Protein-Protein Association: A Case Study on Acetylcholinesterase Binding to Fasciculin-2. Biophysical Journal, 2005, 89, L25-L27.	0.2	44