Ronald M Levy

List of Publications by Year in Descending Order

111 papers	6,043 citations	43 h-index	76 g-index
118 ext. papers	6,607 ext. citations	5.6 avg, IF	5.72 L-index

#	Paper	IF	Citations
111	Limits to detecting epistasis in the fitness landscape of HIV.. *PLoS ONE*, **2022**, 17, e0262314	3.7	0
110	Structure-based virtual screening workflow to identify antivirals targeting HIV-1 capsid.. *Journal of Computer-Aided Molecular Design*, **2022**, 36, 193	4.2	1
109	The generative capacity of probabilistic protein sequence models. *Nature Communications*, **2021**, 12, 6302	17.4	4
108	Molecular Dynamics Free Energy Simulations Reveal the Mechanism for the Antiviral Resistance of the M66I HIV-1 Capsid Mutation. *Viruses*, **2021**, 13,	6.2	5
107	Protein Loop Conformational Free Energy Changes via an Alchemical Path without Reaction Coordinates. *Journal of Physical Chemistry Letters*, **2021**, 12, 4368-4377	6.4	0
106	Mi3-GPU: MCMC-based Inverse Ising Inference on GPUs for protein covariation analysis. *Computer Physics Communications*, **2021**, 260,	4.2	6
105	Computational design of small molecular modulators of protein-protein interactions with a novel thermodynamic cycle: Allosteric inhibitors of HIV-1 integrase. *Protein Science*, **2021**, 30, 438-447	6.3	4
104	Solvation Thermodynamics from the Perspective of Endpoints DFT. *Journal of Physical Chemistry B*, **2020**, 124, 11771-11782	3.4	0
103	Cavity Particle in Aqueous Solution with a Hydrophobic Solute: Structure, Energetics, and Functionals. *Journal of Physical Chemistry B*, **2020**, 124, 5220-5237	3.4	1
102	Insights into the energy landscapes of chromosome organization proteins from coevolutionary sequence variation and structural modeling. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 2241-2242	11.5	
101	Ligand Binding Thermodynamic Cycles: Hysteresis, the Locally Weighted Histogram Analysis Method, and the Overlapping States Matrix. *Journal of Chemical Theory and Computation*, **2020**, 16, 67-79	6.4	6
100	Exploring the Free-Energy Landscape and Thermodynamics of Protein-Protein Association. *Biophysical Journal*, **2020**, 119, 1226-1238	2.9	6
99	Absolute Protein Binding Free Energy Simulations for Ligands with Multiple Poses, a Thermodynamic Path That Avoids Exhaustive Enumeration of the Poses. *Journal of Computational Chemistry*, **2020**, 41, 56-68	3.5	9
98	Spatially-Decomposed Free Energy of Solvation Based on the Endpoint Density-Functional Method. *Journal of Chemical Theory and Computation*, **2019**, 15, 2896-2912	6.4	9
97	Influence of multiple-sequence-alignment depth on Potts statistical models of protein covariation. *Physical Review E*, **2019**, 99, 032405	2.4	10
96	The UWHAM and SWHAM Software Package. *Scientific Reports*, **2019**, 9, 2803	4.9	7
95	HIV-1 integrase tetramers are the antiviral target of pyridine-based allosteric integrase inhibitors. *ELife*, **2019**, 8,	8.9	26

94	Epistasis and entrenchment of drug resistance in HIV-1 subtype B. *ELife*, **2019**, 8,	8.9	11
93	Massive-Scale Binding Free Energy Simulations of HIV Integrase Complexes Using Asynchronous Replica Exchange Framework Implemented on the IBM WCG Distributed Network. *Journal of Chemical Information and Modeling*, **2019**, 59, 1382-1397	6.1	3
92	The Excess Chemical Potential of Water at the Interface with a Protein from End Point Simulations. *Journal of Physical Chemistry B*, **2018**, 122, 4700-4707	3.4	7
91	Coevolutionary Landscape of Kinase Family Proteins: Sequence Probabilities and Functional Motifs. *Biophysical Journal*, **2018**, 114, 21-31	2.9	14
90	The Role of Interfacial Water in Protein-Ligand Binding: Insights from the Indirect Solvent Mediated Potential of Mean Force. *Journal of Chemical Theory and Computation*, **2018**, 14, 512-526	6.4	18
89	Improving Prediction Accuracy of Binding Free Energies and Poses of HIV Integrase Complexes Using the Binding Energy Distribution Analysis Method with Flattening Potentials. *Journal of Chemical Information and Modeling*, **2018**, 58, 1356-1371	6.1	6
88	Conformational Free Energy Changes via an Alchemical Path without Reaction Coordinates. *Journal of Physical Chemistry Letters*, **2018**, 9, 4428-4435	6.4	6
87	Comparing alchemical and physical pathway methods for computing the absolute binding free energy of charged ligands. *Physical Chemistry Chemical Physics*, **2018**, 20, 17081-17092	3.6	24
86	Relationship between Solvation Thermodynamics from IST and DFT Perspectives. *Journal of Physical Chemistry B*, **2017**, 121, 3825-3841	3.4	12
85	Inference of Epistatic Effects Leading to Entrenchment and Drug Resistance in HIV-1 Protease. *Molecular Biology and Evolution*, **2017**, 34, 1291-1306	8.3	32
84	Computing conformational free energy differences in explicit solvent: An efficient thermodynamic cycle using an auxiliary potential and a free energy functional constructed from the end points. *Journal of Computational Chemistry*, **2017**, 38, 1198-1208	3.5	13
83	Stratified UWHAM and Its Stochastic Approximation for Multicanonical Simulations Which Are Far from Equilibrium. *Journal of Chemical Theory and Computation*, **2017**, 13, 4660-4674	6.4	5
82	A combined treatment of hydration and dynamical effects for the modeling of host-guest binding thermodynamics: the SAMPL5 blinded challenge. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 29-44	4.2	15
81	Potts Hamiltonian models of protein co-variation, free energy landscapes, and evolutionary fitness. *Current Opinion in Structural Biology*, **2017**, 43, 55-62	8.1	41
80	Large scale free energy calculations for blind predictions of protein-ligand binding: the D3R Grand Challenge 2015. *Journal of Computer-Aided Molecular Design*, **2016**, 30, 743-751	4.2	10
79	Allosteric HIV-1 integrase inhibitors promote aberrant protein multimerization by directly mediating inter-subunit interactions: Structural and thermodynamic modeling studies. *Protein Science*, **2016**, 25, 1911-1917	6.3	24
78	Structural propensities of kinase family proteins from a Potts model of residue co-variation. *Protein Science*, **2016**, 25, 1378-84	6.3	34
77	Locally weighted histogram analysis and stochastic solution for large-scale multi-state free energy estimation. *Journal of Chemical Physics*, **2016**, 144, 034107	3.9	13

76	Recollection. *Protein Science*, **2016**, 25, 9-11	6.3	
75	Binding Energy Distribution Analysis Method: Hamiltonian Replica Exchange with Torsional Flattening for Binding Mode Prediction and Binding Free Energy Estimation. *Journal of Chemical Theory and Computation*, **2016**, 12, 2459-70	6.4	10
74	Simulating Replica Exchange: Markov State Models, Proposal Schemes, and the Infinite Swapping Limit. *Journal of Physical Chemistry B*, **2016**, 120, 8289-301	3.4	25
73	A New Class of Allosteric HIV-1 Integrase Inhibitors Identified by Crystallographic Fragment Screening of the Catalytic Core Domain. *Journal of Biological Chemistry*, **2016**, 291, 23569-23577	5.4	15
72	Parameterization of an effective potential for protein-ligand binding from host-guest affinity data. *Journal of Molecular Recognition*, **2016**, 29, 10-21	2.6	20
71	BEDAM binding free energy predictions for the SAMPL4 octa-acid host challenge. *Journal of Computer-Aided Molecular Design*, **2015**, 29, 315-25	4.2	16
70	Asynchronous Replica Exchange Software for Grid and Heterogeneous Computing. *Computer Physics Communications*, **2015**, 196, 236-246	4.2	25
69	Deep sequencing of protease inhibitor resistant HIV patient isolates reveals patterns of correlated mutations in Gag and protease. *PLoS Computational Biology*, **2015**, 11, e1004249	5	27
68	Connecting free energy surfaces in implicit and explicit solvent: an efficient method to compute conformational and solvation free energies. *Journal of Chemical Theory and Computation*, **2015**, 11, 2868-78	6.4	8
67	A Stochastic Solution to the Unbinned WHAM Equations. *Journal of Physical Chemistry Letters*, **2015**, 6, 3834-40	6.4	19
66	First Passage Times, Lifetimes, and Relaxation Times of Unfolded Proteins. *Physical Review Letters*, **2015**, 115, 048101	7.4	8
65	Conformational analysis of the DFG-out kinase motif and biochemical profiling of structurally validated type II inhibitors. *Journal of Medicinal Chemistry*, **2015**, 58, 466-79	8.3	107
64	Large-scale asynchronous and distributed multidimensional replica exchange molecular simulations and efficiency analysis. *Journal of Computational Chemistry*, **2015**, 36, 1772-85	3.5	19
63	Distinguishing binders from false positives by free energy calculations: fragment screening against the flap site of HIV protease. *Journal of Physical Chemistry B*, **2015**, 119, 976-88	3.4	45
62	Virtual screening of integrase inhibitors by large scale binding free energy calculations: the SAMPL4 challenge. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 475-90	4.2	45
61	The mechanism of H171T resistance reveals the importance of Nεprotonated His171 for the binding of allosteric inhibitor BI-D to HIV-1 integrase. *Retrovirology*, **2014**, 11, 100	3.6	34
60	How long does it take to equilibrate the unfolded state of a protein?. *Protein Science*, **2013**, 22, 1459-65	6.3	23
59	Large scale affinity calculations of cyclodextrin host-guest complexes: Understanding the role of reorganization in the molecular recognition process. *Journal of Chemical Theory and Computation*, **2013**, 9, 3136-3150	6.4	58

58	Theory of binless multi-state free energy estimation with applications to protein-ligand binding. *Journal of Chemical Physics*, **2012**, 136, 144102	3.9	106
57	Conformational Transitions and Convergence of Absolute Binding Free Energy Calculations. *Journal of Chemical Theory and Computation*, **2012**, 8, 47-60	6.4	52
56	Prediction of SAMPL3 host-guest affinities with the binding energy distribution analysis method (BEDAM). *Journal of Computer-Aided Molecular Design*, **2012**, 26, 505-16	4.2	40
55	Correlated electrostatic mutations provide a reservoir of stability in HIV protease. *PLoS Computational Biology*, **2012**, 8, e1002675	5	25
54	Recent theoretical and computational advances for modeling protein-ligand binding affinities. *Advances in Protein Chemistry and Structural Biology*, **2011**, 85, 27-80	5.3	86
53	Advances in all atom sampling methods for modeling protein-ligand binding affinities. *Current Opinion in Structural Biology*, **2011**, 21, 161-6	8.1	86
52	Insights into the dynamics of HIV-1 protease: a kinetic network model constructed from atomistic simulations. *Journal of the American Chemical Society*, **2011**, 133, 9387-94	16.4	48
51	Kinetic network study of the diversity and temperature dependence of Trp-Cage folding pathways: combining transition path theory with stochastic simulations. *Journal of Physical Chemistry B*, **2011**, 115, 1512-23	3.4	43
50	The Binding Energy Distribution Analysis Method (BEDAM) for the Estimation of Protein-Ligand Binding Affinities. *Journal of Chemical Theory and Computation*, **2010**, 6, 2961-2977	6.4	122
49	Conformational populations of ligand-sized molecules by replica exchange molecular dynamics and temperature reweighting. *Journal of Computational Chemistry*, **2010**, 31, 1357-67	3.5	14
48	Pairwise and higher-order correlations among drug-resistance mutations in HIV-1 subtype B protease. *BMC Bioinformatics*, **2009**, 10 Suppl 8, S10	3.6	24
47	The AGBNP2 Implicit Solvation Model. *Journal of Chemical Theory and Computation*, **2009**, 5, 2544-2564	6.4	101
46	Simple continuous and discrete models for simulating replica exchange simulations of protein folding. *Journal of Physical Chemistry B*, **2008**, 112, 6083-93	3.4	33
45	Asynchronous replica exchange for molecular simulations. *Journal of Computational Chemistry*, **2008**, 29, 788-94	3.5	34
44	Linear Interaction Energy (LIE) Models for Ligand Binding in Implicit Solvent: Theory and Application to the Binding of NNRTIs to HIV-1 Reverse Transcriptase. *Journal of Chemical Theory and Computation*, **2007**, 3, 256-77	6.4	40
43	Comparative performance of several flexible docking programs and scoring functions: enrichment studies for a diverse set of pharmaceutically relevant targets. *Journal of Chemical Information and Modeling*, **2007**, 47, 1599-608	6.1	128
42	Simulating replica exchange simulations of protein folding with a kinetic network model. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 15340-5	11.5	89
41	Conformational equilibrium of cytochrome P450 BM-3 complexed with N-palmitoylglycine: a replica exchange molecular dynamics study. *Journal of the American Chemical Society*, **2006**, 128, 5786-91	16.4	55

40	Temperature weighted histogram analysis method, replica exchange, and transition paths. *Journal of Physical Chemistry B*, **2005**, 109, 6722-31	3.4	161
39	Conformational equilibria and free energy profiles for the allosteric transition of the ribose-binding protein. *Journal of Molecular Biology*, **2005**, 353, 196-210	6.5	66
38	Integrated Modeling Program, Applied Chemical Theory (IMPACT). *Journal of Computational Chemistry*, **2005**, 26, 1752-80	3.5	941
37	Free energy surfaces of beta-hairpin and alpha-helical peptides generated by replica exchange molecular dynamics with the AGBNP implicit solvent model. *Proteins: Structure, Function and Bioinformatics*, **2004**, 56, 310-21	4.2	114
36	AGBNP: an analytic implicit solvent model suitable for molecular dynamics simulations and high-resolution modeling. *Journal of Computational Chemistry*, **2004**, 25, 479-99	3.5	294
35	On the nonpolar hydration free energy of proteins: surface area and continuum solvent models for the solute-solvent interaction energy. *Journal of the American Chemical Society*, **2003**, 125, 9523-30	16.4	223
34	Detecting Native Protein Folds among Large Decoy Sets with the OPLS All-Atom Potential and the Surface Generalized Born Solvent Model. *Advances in Chemical Physics*, **2002**, 459-486		2
33	Solvent models for protein□gand binding: Comparison of implicit solvent poisson and surface generalized born models with explicit solvent simulations. *Journal of Computational Chemistry*, **2001**, 22, 591-607	3.5	108
32	Protein backbone structure determination using only residual dipolar couplings from one ordering medium. *Journal of Biomolecular NMR*, **2001**, 21, 335-47	3	61
31	A Model for Studying Drying at Hydrophobic Interfaces: Structural and Thermodynamic Properties□*Journal of Physical Chemistry B*, **2001**, 105, 6745-6753	3.4	96
30	Simplified amino acid alphabets for protein fold recognition and implications for folding. *Protein Engineering, Design and Selection*, **2000**, 13, 149-52	1.9	166
29	Functional Group Contributions to Partial Molar Compressibilities of Alcohols in Water. *Journal of Physical Chemistry B*, **2000**, 104, 4210-4217	3.4	17
28	On the local and nonlocal components of solvation thermodynamics and their relation to solvation shell models. *Journal of Chemical Physics*, **1998**, 109, 4864-4872	3.9	45
27	Tertiary contacts in alpha-lactalbumin at pH 7 and pH 2: a molecular dynamics study. *Journal of Biomolecular Structure and Dynamics*, **1998**, 16, 355-65	3.6	3
26	Computer simulations with explicit solvent: recent progress in the thermodynamic decomposition of free energies and in modeling electrostatic effects. *Annual Review of Physical Chemistry*, **1998**, 49, 531-67	15.7	223
25	Thermodynamic Decomposition of Hydration Free Energies by Computer Simulation: Application to Amines, Oxides, and Sulfides. *Journal of Physical Chemistry B*, **1997**, 101, 10527-10534	3.4	53
24	On Finite-Size Corrections to the Free Energy of Ionic Hydration. *Journal of Physical Chemistry B*, **1997**, 101, 5622-5623	3.4	89
23	Prediction of pKa Shifts without Truncation of Electrostatic Interactions: An Explicit Solvent Calculation for Succinic Acid. *The Journal of Physical Chemistry*, **1996**, 100, 6389-6392		34

22	Thermodynamics of the Hydration Shell. 2. Excess Volume and Compressibility of a Hydrophobic Solute. *The Journal of Physical Chemistry*, **1996**, 100, 2681-2688		98
21	Crankshaft motions of the polypeptide backbone in molecular dynamics simulations of human type-alpha transforming growth factor. *Journal of Biomolecular NMR*, **1995**, 6, 221-6	3	60
20	On finite-size effects in computer simulations using the Ewald potential. *Journal of Chemical Physics* , **1995**, 103, 6133-6142	3.9	144
19	Evaluating polarizable potentials on distributed memory parallel computers: Program development and applications. *Journal of Computational Chemistry*, **1995**, 16, 1141-1152	3.5	10
18	Thermodynamics of the Hydration Shell. 1. Excess Energy of a Hydrophobic Solute. *The Journal of Physical Chemistry*, **1994**, 98, 10640-10649		107
17	Intrinsic pKas of ionizable residues in proteins: an explicit solvent calculation for lysozyme. *Proteins: Structure, Function and Bioinformatics*, **1994**, 20, 85-97	4.2	84
16	Dielectric and thermodynamic response of a generalized reaction field model for liquid state simulations. *Journal of Chemical Physics*, **1993**, 99, 9847-9852	3.9	65
15	Vibrational relaxation and Bloch-Redfield theory. *Journal of Chemical Physics*, **1992**, 97, 703-706	3.9	79
14	Molecular electrostatic potentials and partial atomic charges from correlated wave functions: Applications to the electronic ground and excited states of 3-methylindole. *Journal of Computational Chemistry*, **1992**, 13, 979-989	3.5	16
13	Gaussian fluctuation formula for electrostatic free-energy changes in solution. *Journal of Chemical Physics*, **1991**, 95, 3627-3633	3.9	165
12	Analysis of side-chain conformational distributions in neutrophil peptide-5 NMR structures. *Biopolymers*, **1990**, 29, 1807-22	2.2	8
11	Conserving energy during molecular dynamics simulations of water, proteins, and proteins in water. *Journal of Computational Chemistry*, **1990**, 11, 1169-1180	3.5	82
10	Computer simulations of the dielectric properties of water: Studies of the simple point charge and transferrable intermolecular potential models. *Journal of Chemical Physics*, **1989**, 91, 1242-1251	3.9	168
9	Viewing the born model for ion hydration through a microscope. *International Journal of Quantum Chemistry*, **1988**, 34, 179-190	2.1	54
8	Using Computer Simulations To Probe the Structure and Dynamics of Biopolymers. *ACS Symposium Series*, **1987**, 82-105	0.4	
7	Using Macromolecular Dynamics Simulations to Interpret Experiments. *Israel Journal of Chemistry*, **1986**, 27, 173-179	3.4	2
6	An optimized harmonic reference system for the evaluation of discretized path integrals. *Journal of Chemical Physics*, **1984**, 80, 4488-4495	3.9	52
5	Trajectory Studies of NMR Relaxation in Flexible Molecules. *Advances in Chemistry Series*, **1983**, 445-468		6

4	Initial fluorescence depolarization of tyrosines in proteins. *Journal of the American Chemical Society* , **1982**, 104, 2073-2075	16.4	45
3	Protein dynamics and NMR relaxation: comparison of simulations with experiment. *Nature*, **1982**, 300, 197-198	50.4	85
2	Salsa: Scalable Asynchronous Replica Exchange for Parallel Molecular Dynamics Applications		3
1	Inference of epistatic effects leading to entrenchment and drug resistance in HIV-1 protease		1