

Ronald M Levy

List of Publications by Citations

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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	Integrated Modeling Program, Applied Chemical Theory (IMPACT). <i>Journal of Computational Chemistry</i> , 2005 , 26, 1752-80	3.5	941
110	AGBNP: an analytic implicit solvent model suitable for molecular dynamics simulations and high-resolution modeling. <i>Journal of Computational Chemistry</i> , 2004 , 25, 479-99	3.5	294
109	On the nonpolar hydration free energy of proteins: surface area and continuum solvent models for the solute-solvent interaction energy. <i>Journal of the American Chemical Society</i> , 2003 , 125, 9523-30	16.4	223
108	Computer simulations with explicit solvent: recent progress in the thermodynamic decomposition of free energies and in modeling electrostatic effects. <i>Annual Review of Physical Chemistry</i> , 1998 , 49, 531-67	15.7	223
107	Computer simulations of the dielectric properties of water: Studies of the simple point charge and transferrable intermolecular potential models. <i>Journal of Chemical Physics</i> , 1989 , 91, 1242-1251	3.9	168
106	Simplified amino acid alphabets for protein fold recognition and implications for folding. <i>Protein Engineering, Design and Selection</i> , 2000 , 13, 149-52	1.9	166
105	Gaussian fluctuation formula for electrostatic free-energy changes in solution. <i>Journal of Chemical Physics</i> , 1991 , 95, 3627-3633	3.9	165
104	Temperature weighted histogram analysis method, replica exchange, and transition paths. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 6722-31	3.4	161
103	On finite-size effects in computer simulations using the Ewald potential. <i>Journal of Chemical Physics</i> , 1995 , 103, 6133-6142	3.9	144
102	Comparative performance of several flexible docking programs and scoring functions: enrichment studies for a diverse set of pharmaceutically relevant targets. <i>Journal of Chemical Information and Modeling</i> , 2007 , 47, 1599-608	6.1	128
101	The Binding Energy Distribution Analysis Method (BEDAM) for the Estimation of Protein-Ligand Binding Affinities. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 2961-2977	6.4	122
100	Free energy surfaces of beta-hairpin and alpha-helical peptides generated by replica exchange molecular dynamics with the AGBNP implicit solvent model. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004 , 56, 310-21	4.2	114
99	Solvent models for protein-ligand binding: Comparison of implicit solvent poisson and surface generalized born models with explicit solvent simulations. <i>Journal of Computational Chemistry</i> , 2001 , 22, 591-607	3.5	108
98	Conformational analysis of the DFG-out kinase motif and biochemical profiling of structurally validated type II inhibitors. <i>Journal of Medicinal Chemistry</i> , 2015 , 58, 466-79	8.3	107
97	Thermodynamics of the Hydration Shell. 1. Excess Energy of a Hydrophobic Solute. <i>The Journal of Physical Chemistry</i> , 1994 , 98, 10640-10649		107
96	Theory of binless multi-state free energy estimation with applications to protein-ligand binding. <i>Journal of Chemical Physics</i> , 2012 , 136, 144102	3.9	106
95	The AGBNP2 Implicit Solvation Model. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 2544-2564	6.4	101

94	Thermodynamics of the Hydration Shell. 2. Excess Volume and Compressibility of a Hydrophobic Solute. <i>The Journal of Physical Chemistry</i> , 1996 , 100, 2681-2688		98
93	A Model for Studying Drying at Hydrophobic Interfaces: Structural and Thermodynamic Properties <i>Journal of Physical Chemistry B</i> , 2001 , 105, 6745-6753	3.4	96
92	On Finite-Size Corrections to the Free Energy of Ionic Hydration. <i>Journal of Physical Chemistry B</i> , 1997 , 101, 5622-5623	3.4	89
91	Simulating replica exchange simulations of protein folding with a kinetic network model. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007 , 104, 15340-5	11.5	89
90	Recent theoretical and computational advances for modeling protein-ligand binding affinities. <i>Advances in Protein Chemistry and Structural Biology</i> , 2011 , 85, 27-80	5.3	86
89	Advances in all atom sampling methods for modeling protein-ligand binding affinities. <i>Current Opinion in Structural Biology</i> , 2011 , 21, 161-6	8.1	86
88	Protein dynamics and NMR relaxation: comparison of simulations with experiment. <i>Nature</i> , 1982 , 300, 197-198	50.4	85
87	Intrinsic pKas of ionizable residues in proteins: an explicit solvent calculation for lysozyme. <i>Proteins: Structure, Function and Bioinformatics</i> , 1994 , 20, 85-97	4.2	84
86	Conserving energy during molecular dynamics simulations of water, proteins, and proteins in water. <i>Journal of Computational Chemistry</i> , 1990 , 11, 1169-1180	3.5	82
85	Vibrational relaxation and Bloch-Redfield theory. <i>Journal of Chemical Physics</i> , 1992 , 97, 703-706	3.9	79
84	Conformational equilibria and free energy profiles for the allosteric transition of the ribose-binding protein. <i>Journal of Molecular Biology</i> , 2005 , 353, 196-210	6.5	66
83	Dielectric and thermodynamic response of a generalized reaction field model for liquid state simulations. <i>Journal of Chemical Physics</i> , 1993 , 99, 9847-9852	3.9	65
82	Protein backbone structure determination using only residual dipolar couplings from one ordering medium. <i>Journal of Biomolecular NMR</i> , 2001 , 21, 335-47	3	61
81	Crankshaft motions of the polypeptide backbone in molecular dynamics simulations of human type-alpha transforming growth factor. <i>Journal of Biomolecular NMR</i> , 1995 , 6, 221-6	3	60
80	Large scale affinity calculations of cyclodextrin host-guest complexes: Understanding the role of reorganization in the molecular recognition process. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 3136-3150	6.4	58
79	Conformational equilibrium of cytochrome P450 BM-3 complexed with N-palmitoylglycine: a replica exchange molecular dynamics study. <i>Journal of the American Chemical Society</i> , 2006 , 128, 5786-91	16.4	55
78	Viewing the born model for ion hydration through a microscope. <i>International Journal of Quantum Chemistry</i> , 1988 , 34, 179-190	2.1	54
77	Thermodynamic Decomposition of Hydration Free Energies by Computer Simulation: Application to Amines, Oxides, and Sulfides. <i>Journal of Physical Chemistry B</i> , 1997 , 101, 10527-10534	3.4	53

76	Conformational Transitions and Convergence of Absolute Binding Free Energy Calculations. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 47-60	6.4	52
75	An optimized harmonic reference system for the evaluation of discretized path integrals. <i>Journal of Chemical Physics</i> , 1984 , 80, 4488-4495	3.9	52
74	Insights into the dynamics of HIV-1 protease: a kinetic network model constructed from atomistic simulations. <i>Journal of the American Chemical Society</i> , 2011 , 133, 9387-94	16.4	48
73	Virtual screening of integrase inhibitors by large scale binding free energy calculations: the SAMPL4 challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2014 , 28, 475-90	4.2	45
72	Distinguishing binders from false positives by free energy calculations: fragment screening against the flap site of HIV protease. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 976-88	3.4	45
71	On the local and nonlocal components of solvation thermodynamics and their relation to solvation shell models. <i>Journal of Chemical Physics</i> , 1998 , 109, 4864-4872	3.9	45
70	Initial fluorescence depolarization of tyrosines in proteins. <i>Journal of the American Chemical Society</i> , 1982 , 104, 2073-2075	16.4	45
69	Kinetic network study of the diversity and temperature dependence of Trp-Cage folding pathways: combining transition path theory with stochastic simulations. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 1512-23	3.4	43
68	Potts Hamiltonian models of protein co-variation, free energy landscapes, and evolutionary fitness. <i>Current Opinion in Structural Biology</i> , 2017 , 43, 55-62	8.1	41
67	Prediction of SAMPL3 host-guest affinities with the binding energy distribution analysis method (BEDAM). <i>Journal of Computer-Aided Molecular Design</i> , 2012 , 26, 505-16	4.2	40
66	Linear Interaction Energy (LIE) Models for Ligand Binding in Implicit Solvent: Theory and Application to the Binding of NNRTIs to HIV-1 Reverse Transcriptase. <i>Journal of Chemical Theory and Computation</i> , 2007 , 3, 256-77	6.4	40
65	The mechanism of H171T resistance reveals the importance of NEprotonated His171 for the binding of allosteric inhibitor BI-D to HIV-1 integrase. <i>Retrovirology</i> , 2014 , 11, 100	3.6	34
64	Prediction of pKa Shifts without Truncation of Electrostatic Interactions: An Explicit Solvent Calculation for Succinic Acid. <i>The Journal of Physical Chemistry</i> , 1996 , 100, 6389-6392		34
63	Asynchronous replica exchange for molecular simulations. <i>Journal of Computational Chemistry</i> , 2008 , 29, 788-94	3.5	34
62	Structural propensities of kinase family proteins from a Potts model of residue co-variation. <i>Protein Science</i> , 2016 , 25, 1378-84	6.3	34
61	Simple continuous and discrete models for simulating replica exchange simulations of protein folding. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 6083-93	3.4	33
60	Inference of Epistatic Effects Leading to Entrenchment and Drug Resistance in HIV-1 Protease. <i>Molecular Biology and Evolution</i> , 2017 , 34, 1291-1306	8.3	32
59	Deep sequencing of protease inhibitor resistant HIV patient isolates reveals patterns of correlated mutations in Gag and protease. <i>PLoS Computational Biology</i> , 2015 , 11, e1004249	5	27

58	HIV-1 integrase tetramers are the antiviral target of pyridine-based allosteric integrase inhibitors. <i>ELife</i> , 2019 , 8,	8.9	26
57	Asynchronous Replica Exchange Software for Grid and Heterogeneous Computing. <i>Computer Physics Communications</i> , 2015 , 196, 236-246	4.2	25
56	Correlated electrostatic mutations provide a reservoir of stability in HIV protease. <i>PLoS Computational Biology</i> , 2012 , 8, e1002675	5	25
55	Simulating Replica Exchange: Markov State Models, Proposal Schemes, and the Infinite Swapping Limit. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 8289-301	3.4	25
54	Allosteric HIV-1 integrase inhibitors promote aberrant protein multimerization by directly mediating inter-subunit interactions: Structural and thermodynamic modeling studies. <i>Protein Science</i> , 2016 , 25, 1911-1917	6.3	24
53	Pairwise and higher-order correlations among drug-resistance mutations in HIV-1 subtype B protease. <i>BMC Bioinformatics</i> , 2009 , 10 Suppl 8, S10	3.6	24
52	Comparing alchemical and physical pathway methods for computing the absolute binding free energy of charged ligands. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 17081-17092	3.6	24
51	How long does it take to equilibrate the unfolded state of a protein?. <i>Protein Science</i> , 2013 , 22, 1459-65	6.3	23
50	Parameterization of an effective potential for protein-ligand binding from host-guest affinity data. <i>Journal of Molecular Recognition</i> , 2016 , 29, 10-21	2.6	20
49	A Stochastic Solution to the Unbinned WHAM Equations. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 3834-40	6.4	19
48	Large-scale asynchronous and distributed multidimensional replica exchange molecular simulations and efficiency analysis. <i>Journal of Computational Chemistry</i> , 2015 , 36, 1772-85	3.5	19
47	The Role of Interfacial Water in Protein-Ligand Binding: Insights from the Indirect Solvent Mediated Potential of Mean Force. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 512-526	6.4	18
46	Functional Group Contributions to Partial Molar Compressibilities of Alcohols in Water. <i>Journal of Physical Chemistry B</i> , 2000 , 104, 4210-4217	3.4	17
45	BEDAM binding free energy predictions for the SAMPL4 octa-acid host challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2015 , 29, 315-25	4.2	16
44	Molecular electrostatic potentials and partial atomic charges from correlated wave functions: Applications to the electronic ground and excited states of 3-methylindole. <i>Journal of Computational Chemistry</i> , 1992 , 13, 979-989	3.5	16
43	A combined treatment of hydration and dynamical effects for the modeling of host-guest binding thermodynamics: the SAMPL5 blinded challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2017 , 31, 29-44	4.2	15
42	A New Class of Allosteric HIV-1 Integrase Inhibitors Identified by Crystallographic Fragment Screening of the Catalytic Core Domain. <i>Journal of Biological Chemistry</i> , 2016 , 291, 23569-23577	5.4	15
41	Coevolutionary Landscape of Kinase Family Proteins: Sequence Probabilities and Functional Motifs. <i>Biophysical Journal</i> , 2018 , 114, 21-31	2.9	14

40	Conformational populations of ligand-sized molecules by replica exchange molecular dynamics and temperature reweighting. <i>Journal of Computational Chemistry</i> , 2010 , 31, 1357-67	3.5	14
39	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. <i>Journal of Computational Chemistry</i> , 2017 , 38, 1198-1208	3.5	13
38	Locally weighted histogram analysis and stochastic solution for large-scale multi-state free energy estimation. <i>Journal of Chemical Physics</i> , 2016 , 144, 034107	3.9	13
37	Relationship between Solvation Thermodynamics from IST and DFT Perspectives. <i>Journal of Physical Chemistry B</i> , 2017 , 121, 3825-3841	3.4	12
36	Epistasis and entrenchment of drug resistance in HIV-1 subtype B. <i>ELife</i> , 2019 , 8,	8.9	11
35	Influence of multiple-sequence-alignment depth on Potts statistical models of protein covariation. <i>Physical Review E</i> , 2019 , 99, 032405	2.4	10
34	Large scale free energy calculations for blind predictions of protein-ligand binding: the D3R Grand Challenge 2015. <i>Journal of Computer-Aided Molecular Design</i> , 2016 , 30, 743-751	4.2	10
33	Evaluating polarizable potentials on distributed memory parallel computers: Program development and applications. <i>Journal of Computational Chemistry</i> , 1995 , 16, 1141-1152	3.5	10
32	Binding Energy Distribution Analysis Method: Hamiltonian Replica Exchange with Torsional Flattening for Binding Mode Prediction and Binding Free Energy Estimation. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 2459-70	6.4	10
31	Spatially-Decomposed Free Energy of Solvation Based on the Endpoint Density-Functional Method. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 2896-2912	6.4	9
30	Absolute Protein Binding Free Energy Simulations for Ligands with Multiple Poses, a Thermodynamic Path That Avoids Exhaustive Enumeration of the Poses. <i>Journal of Computational Chemistry</i> , 2020 , 41, 56-68	3.5	9
29	Connecting free energy surfaces in implicit and explicit solvent: an efficient method to compute conformational and solvation free energies. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 2868-78	6.4	8
28	First Passage Times, Lifetimes, and Relaxation Times of Unfolded Proteins. <i>Physical Review Letters</i> , 2015 , 115, 048101	7.4	8
27	Analysis of side-chain conformational distributions in neutrophil peptide-5 NMR structures. <i>Biopolymers</i> , 1990 , 29, 1807-22	2.2	8
26	The UWHAM and SWHAM Software Package. <i>Scientific Reports</i> , 2019 , 9, 2803	4.9	7
25	The Excess Chemical Potential of Water at the Interface with a Protein from End Point Simulations. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 4700-4707	3.4	7
24	Improving Prediction Accuracy of Binding Free Energies and Poses of HIV Integrase Complexes Using the Binding Energy Distribution Analysis Method with Flattening Potentials. <i>Journal of Chemical Information and Modeling</i> , 2018 , 58, 1356-1371	6.1	6
23	Conformational Free Energy Changes via an Alchemical Path without Reaction Coordinates. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 4428-4435	6.4	6

22	Trajectory Studies of NMR Relaxation in Flexible Molecules. <i>Advances in Chemistry Series</i> , 1983 , 445-468		6
21	Ligand Binding Thermodynamic Cycles: Hysteresis, the Locally Weighted Histogram Analysis Method, and the Overlapping States Matrix. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 67-79	6.4	6
20	Exploring the Free-Energy Landscape and Thermodynamics of Protein-Protein Association. <i>Biophysical Journal</i> , 2020 , 119, 1226-1238	2.9	6
19	Mi3-GPU: MCMC-based Inverse Ising Inference on GPUs for protein covariation analysis. <i>Computer Physics Communications</i> , 2021 , 260,	4.2	6
18	Stratified UWHAM and Its Stochastic Approximation for Multicanonical Simulations Which Are Far from Equilibrium. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 4660-4674	6.4	5
17	Molecular Dynamics Free Energy Simulations Reveal the Mechanism for the Antiviral Resistance of the M66I HIV-1 Capsid Mutation. <i>Viruses</i> , 2021 , 13,	6.2	5
16	The generative capacity of probabilistic protein sequence models. <i>Nature Communications</i> , 2021 , 12, 6302	17.4	4
15	Computational design of small molecular modulators of protein-protein interactions with a novel thermodynamic cycle: Allosteric inhibitors of HIV-1 integrase. <i>Protein Science</i> , 2021 , 30, 438-447	6.3	4
14	Salsa: Scalable Asynchronous Replica Exchange for Parallel Molecular Dynamics Applications		3
13	Tertiary contacts in alpha-lactalbumin at pH 7 and pH 2: a molecular dynamics study. <i>Journal of Biomolecular Structure and Dynamics</i> , 1998 , 16, 355-65	3.6	3
12	Massive-Scale Binding Free Energy Simulations of HIV Integrase Complexes Using Asynchronous Replica Exchange Framework Implemented on the IBM WCG Distributed Network. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 1382-1397	6.1	3
11	Detecting Native Protein Folds among Large Decoy Sets with the OPLS All-Atom Potential and the Surface Generalized Born Solvent Model. <i>Advances in Chemical Physics</i> , 2002 , 459-486		2
10	Using Macromolecular Dynamics Simulations to Interpret Experiments. <i>Israel Journal of Chemistry</i> , 1986 , 27, 173-179	3.4	2
9	Cavity Particle in Aqueous Solution with a Hydrophobic Solute: Structure, Energetics, and Functionals. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 5220-5237	3.4	1
8	Inference of epistatic effects leading to entrenchment and drug resistance in HIV-1 protease		1
7	Structure-based virtual screening workflow to identify antivirals targeting HIV-1 capsid.. <i>Journal of Computer-Aided Molecular Design</i> , 2022 , 36, 193	4.2	1
6	Solvation Thermodynamics from the Perspective of Endpoints DFT. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 11771-11782	3.4	0
5	Limits to detecting epistasis in the fitness landscape of HIV.. <i>PLoS ONE</i> , 2022 , 17, e0262314	3.7	0

4	Protein Loop Conformational Free Energy Changes via an Alchemical Path without Reaction Coordinates. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 4368-4377	6.4	o
3	Insights into the energy landscapes of chromosome organization proteins from coevolutionary sequence variation and structural modeling. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020 , 117, 2241-2242	11.5	
2	Using Computer Simulations To Probe the Structure and Dynamics of Biopolymers. <i>ACS Symposium Series</i> , 1987 , 82-105	0.4	
1	Recollection. <i>Protein Science</i> , 2016 , 25, 9-11	6.3	