Ronald M Levy

List of Publications by Year
in descending order

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111 papers	7,140 citations	57719 44 h-index	60583 81 g-index
118 all docs	118 docs citations	118 times ranked	6728 citing authors

#	Article	IF	Citations
1	Integrated Modeling Program, Applied Chemical Theory (IMPACT). Journal of Computational Chemistry, 2005, 26, 1752-1780.	1.5	1,194
2	AGBNP: An analytic implicit solvent model suitable for molecular dynamics simulations and high-resolution modeling. Journal of Computational Chemistry, 2004, 25, 479-499.	1.5	314
3	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, 531-567.	4.8	251
4	On the Nonpolar Hydration Free Energy of Proteins:Â Surface Area and Continuum Solvent Models for the Soluteâ^'Solvent Interaction Energy. Journal of the American Chemical Society, 2003, 125, 9523-9530.	6.6	251
5	Simplified amino acid alphabets for protein fold recognition and implications for folding. Protein Engineering, Design and Selection, 2000, 13, 149-152.	1.0	207
6	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.	1.2	183
7	Gaussian fluctuation formula for electrostatic freeâ€energy changes in solution. Journal of Chemical Physics, 1991, 95, 3627-3633.	1.2	176
8	Temperature Weighted Histogram Analysis Method, Replica Exchange, and Transition Pathsâ€. Journal of Physical Chemistry B, 2005, 109, 6722-6731.	1.2	173
9	On finiteâ€size effects in computer simulations using the Ewald potential. Journal of Chemical Physics, 1995, 103, 6133-6142.	1.2	156
10	Conformational Analysis of the DFG-Out Kinase Motif and Biochemical Profiling of Structurally Validated Type II Inhibitors. Journal of Medicinal Chemistry, 2015, 58, 466-479.	2.9	154
11	Comparative Performance of Several Flexible Docking Programs and Scoring Functions:â€‰ Enrichment Studies for a Diverse Set of Pharmaceutically Relevant Targets. Journal of Chemical Information and Modeling, 2007, 47, 1599-1608.	2.5	148
12	Binding Energy Distribution Analysis Method (BEDAM) for Estimation of Proteinâ^'Ligand Binding Affinities. Journal of Chemical Theory and Computation, 2010, 6, 2961-2977.	2.3	143
13	Theory of binless multi-state free energy estimation with applications to protein-ligand binding. Journal of Chemical Physics, 2012, 136, 144102.	1.2	137
14	Free energy surfaces of Î²-hairpin and Î±-helical peptides generated by replica exchange molecular dynamics with the AGBNP implicit solvent model. Proteins: Structure, Function and Bioinformatics, 2004, 56, 310-321.	1.5	124
15	Solvent models for protein-ligand binding: Comparison of implicit solvent poisson and surface generalized born models with explicit solvent simulations. Journal of Computational Chemistry, 2001, 22, 591-607.	1.5	113
16	Thermodynamics of the Hydration Shell. 1. Excess Energy of a Hydrophobic Solute. The Journal of Physical Chemistry, 1994, 98, 10640-10649.	2.9	112
17	The AGBNP2 Implicit Solvation Model. Journal of Chemical Theory and Computation, 2009, 5, 2544-2564.	2.3	111
18	Protein dynamics and NMR relaxation: comparison of simulations with experiment. Nature, 1982, 300, 197-198.	13.7	107

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19	Recent theoretical and computational advances for modeling proteinâ€“ligand binding affinities. Advances in Protein Chemistry and Structural Biology, 2011, 85, 27-80.	1.0	102
20	Thermodynamics of the Hydration Shell. 2. Excess Volume and Compressibility of a Hydrophobic Solute. The Journal of Physical Chemistry, 1996, 100, 2681-2688.	2.9	101
21	A Model for Studying Drying at Hydrophobic Interfaces:Â Structural and Thermodynamic Propertiesâ€. Journal of Physical Chemistry B, 2001, 105, 6745-6753.	1.2	98
22	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, 15340-15345.	3.3	97
23	Intrinsic pKas of ionizable residues in proteins: An explicit solvent calculation for lysozyme. Proteins: Structure, Function and Bioinformatics, 1994, 20, 85-97.	1.5	94
24	Advances in all atom sampling methods for modeling proteinâ€“ligand binding affinities. Current Opinion in Structural Biology, 2011, 21, 161-166.	2.6	94
25	On Finite-Size Corrections to the Free Energy of Ionic Hydration. Journal of Physical Chemistry B, 1997, 101, 5622-5623.	1.2	93
26	Conserving energy during molecular dynamics simulations of water, proteins, and proteins in water. Journal of Computational Chemistry, 1990, 11, 1169-1180.	1.5	86
27	Vibrational relaxation and Blochâ€“Redfield theory. Journal of Chemical Physics, 1992, 97, 703-706.	1.2	82
28	Large Scale Affinity Calculations of Cyclodextrin Hostâ€“Guest Complexes: Understanding the Role of Reorganization in the Molecular Recognition Process. Journal of Chemical Theory and Computation, 2013, 9, 3136-3150.	2.3	77
29	Potts Hamiltonian models of protein co-variation, free energy landscapes, and evolutionary fitness. Current Opinion in Structural Biology, 2017, 43, 55-62.	2.6	73
30	Dielectric and thermodynamic response of a generalized reaction field model for liquid state simulations. Journal of Chemical Physics, 1993, 99, 9847-9852.	1.2	70
31	Crankshaft motions of the polypeptide backbone in molecular dynamics simulations of human type-Î± transforming growth factor. Journal of Biomolecular NMR, 1995, 6, 221-226.	1.6	70
32	Protein backbone structure determination using only residual dipolar couplings from one ordering medium. Journal of Biomolecular NMR, 2001, 21, 335-347.	1.6	69
33	Conformational Equilibria and Free Energy Profiles for the Allosteric Transition of the Ribose-binding Protein. Journal of Molecular Biology, 2005, 353, 196-210.	2.0	69
34	Conformational Transitions and Convergence of Absolute Binding Free Energy Calculations. Journal of Chemical Theory and Computation, 2012, 8, 47-60.	2.3	60
35	Conformational Equilibrium of Cytochrome P450 BM-3 Complexed withN-Palmitoylglycine:Â A Replica Exchange Molecular Dynamics Study. Journal of the American Chemical Society, 2006, 128, 5786-5791.	6.6	59
36	Thermodynamic Decomposition of Hydration Free Energies by Computer Simulation:â€‰ Application to Amines, Oxides, and Sulfides. Journal of Physical Chemistry B, 1997, 101, 10527-10534.	1.2	58

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37	Viewing the born model for ion hydration through a microscope. International Journal of Quantum Chemistry, 1988, 34, 179-190.	1.0	57
38	Initial fluorescence depolarization of tyrosines in proteins. Journal of the American Chemical Society, 1982, 104, 2073-2075.	6.6	55
39	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, 976-988.	1.2	54
40	An optimized harmonic reference system for the evaluation of discretized path integrals. Journal of Chemical Physics, 1984, 80, 4488-4495.	1.2	53
41	Virtual screening of integrase inhibitors by large scale binding free energy calculations: the SAMPL4 challenge. Journal of Computer-Aided Molecular Design, 2014, 28, 475-490.	1.3	53
42	Insights into the Dynamics of HIV-1 Protease: A Kinetic Network Model Constructed from Atomistic Simulations. Journal of the American Chemical Society, 2011, 133, 9387-9394.	6.6	51
43	Inference of Epistatic Effects Leading to Entrenchment and Drug Resistance in HIV-1 Protease. Molecular Biology and Evolution, 2017, 34, 1291-1306.	3.5	51
44	Structural propensities of kinase family proteins from a Potts model of residue coâ€variation. Protein Science, 2016, 25, 1378-1384.	3.1	50
45	On the local and nonlocal components of solvation thermodynamics and their relation to solvation shell models. Journal of Chemical Physics, 1998, 109, 4864-4872.	1.2	46
46	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, 1512-1523.	1.2	46
47	Linear Interaction Energy (LIE) Models for Ligand Binding in Implicit Solvent:â€‰ Theory and Application to the Binding of NNRTIs to HIV-1 Reverse Transcriptase. Journal of Chemical Theory and Computation, 2007, 3, 256-277.	2.3	45
48	Prediction of SAMPL3 host-guest affinities with the binding energy distribution analysis method (BEDAM). Journal of Computer-Aided Molecular Design, 2012, 26, 505-516.	1.3	43
49	Simulating Replica Exchange: Markov State Models, Proposal Schemes, and the Infinite Swapping Limit. Journal of Physical Chemistry B, 2016, 120, 8289-8301.	1.2	42
50	HIV-1 integrase tetramers are the antiviral target of pyridine-based allosteric integrase inhibitors. ELife, 2019, 8, .	2.8	41
51	The mechanism of H171T resistance reveals the importance of Nΐ´-protonated His171 for the binding of allosteric inhibitor BI-D to HIV-1 integrase. Retrovirology, 2014, 11, 100.	0.9	39
52	Deep Sequencing of Protease Inhibitor Resistant HIV Patient Isolates Reveals Patterns of Correlated Mutations in Gag and Protease. PLoS Computational Biology, 2015, 11, e1004249.	1.5	38
53	Prediction of pKaShifts without Truncation of Electrostatic Interactions:Â An Explicit Solvent Calculation for Succinic Acid. The Journal of Physical Chemistry, 1996, 100, 6389-6392.	2.9	35
54	Asynchronous replica exchange for molecular simulations. Journal of Computational Chemistry, 2008, 29, 788-794.	1.5	35

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55	Asynchronous replica exchange software for grid and heterogeneous computing. Computer Physics Communications, 2015, 196, 236-246.	3.0	35
56	Simple Continuous and Discrete Models for Simulating Replica Exchange Simulations of Protein Folding. Journal of Physical Chemistry B, 2008, 112, 6083-6093.	1.2	34
57	Comparing alchemical and physical pathway methods for computing the absolute binding free energy of charged ligands. Physical Chemistry Chemical Physics, 2018, 20, 17081-17092.	1.3	34
58	Correlated Electrostatic Mutations Provide a Reservoir of Stability in HIV Protease. PLoS Computational Biology, 2012, 8, e1002675.	1.5	31
59	Allosteric HIVâ€1 integrase inhibitors promote aberrant protein multimerization by directly mediating interâ€subunit interactions: Structural and thermodynamic modeling studies. Protein Science, 2016, 25, 1911-1917.	3.1	30
60	The generative capacity of probabilistic protein sequence models. Nature Communications, 2021, 12, 6302.	5.8	28
61	A Stochastic Solution to the Unbinned WHAM Equations. Journal of Physical Chemistry Letters, 2015, 6, 3834-3840.	2.1	27
62	Parameterization of an effective potential for proteinâ€“ligand binding from hostâ€“guest affinity data. Journal of Molecular Recognition, 2016, 29, 10-21.	1.1	27
63	Pairwise and higher-order correlations among drug-resistance mutations in HIV-1 subtype B protease. BMC Bioinformatics, 2009, 10, S10.	1.2	26
64	The Role of Interfacial Water in Proteinâ€“Ligand Binding: Insights from the Indirect Solvent Mediated Potential of Mean Force. Journal of Chemical Theory and Computation, 2018, 14, 512-526.	2.3	25
65	Epistasis and entrenchment of drug resistance in HIV-1 subtype B. ELife, 2019, 8, .	2.8	25
66	How long does it take to equilibrate the unfolded state of a protein?. Protein Science, 2013, 22, 1459-1465.	3.1	24
67	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.	1.6	20
68	Largeâ€scale asynchronous and distributed multidimensional replica exchange molecular simulations and efficiency analysis. Journal of Computational Chemistry, 2015, 36, 1772-1785.	1.5	19
69	Coevolutionary Landscape of Kinase Family Proteins: Sequence Probabilities and Functional Motifs. Biophysical Journal, 2018, 114, 21-31.	0.2	19
70	A combined treatment of hydration and dynamical effects for the modeling of hostâ€“guest binding thermodynamics: the SAMPL5 blinded challenge. Journal of Computer-Aided Molecular Design, 2017, 31, 29-44.	1.3	18
71	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.	1.5	17
72	Functional Group Contributions to Partial Molar Compressibilities of Alcohols in Water. Journal of Physical Chemistry B, 2000, 104, 4210-4217.	1.2	17

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73	Conformational populations of ligandâ€sized molecules by replica exchange molecular dynamics and temperature reweighting. Journal of Computational Chemistry, 2010, 31, 1357-1367.	1.5	17
74	BEDAM binding free energy predictions for the SAMPL4 octa-acid host challenge. Journal of Computer-Aided Molecular Design, 2015, 29, 315-325.	1.3	17
75	Large scale free energy calculations for blind predictions of proteinâ€“ligand binding: the D3R Grand Challenge 2015. Journal of Computer-Aided Molecular Design, 2016, 30, 743-751.	1.3	17
76	Influence of multiple-sequence-alignment depth on Potts statistical models of protein covariation. Physical Review E, 2019, 99, 032405.	0.8	17
77	Mi3-GPU: MCMC-based inverse Ising inference on GPUs for protein covariation analysis. Computer Physics Communications, 2021, 260, 107312.	3.0	17
78	Locally weighted histogram analysis and stochastic solution for large-scale multi-state free energy estimation. Journal of Chemical Physics, 2016, 144, 034107.	1.2	16
79	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.	1.5	16
80	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.	1.5	15
81	Relationship between Solvation Thermodynamics from IST and DFT Perspectives. Journal of Physical Chemistry B, 2017, 121, 3825-3841.	1.2	14
82	First Passage Times, Lifetimes, and Relaxation Times of Unfolded Proteins. Physical Review Letters, 2015, 115, 048101.	2.9	12
83	Spatially-Decomposed Free Energy of Solvation Based on the Endpoint Density-Functional Method. Journal of Chemical Theory and Computation, 2019, 15, 2896-2912.	2.3	12
84	Exploring the Free-Energy Landscape and Thermodynamics of Protein-Protein Association. Biophysical Journal, 2020, 119, 1226-1238.	0.2	12
85	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, 2459-2470.	2.3	11
86	Conformational Free Energy Changes via an Alchemical Path without Reaction Coordinates. Journal of Physical Chemistry Letters, 2018, 9, 4428-4435.	2.1	11
87	Molecular Dynamics Free Energy Simulations Reveal the Mechanism for the Antiviral Resistance of the M66I HIV-1 Capsid Mutation. Viruses, 2021, 13, 920.	1.5	11
88	Evaluating polarizable potentials on distributed memory parallel computers: Program development and applications. Journal of Computational Chemistry, 1995, 16, 1141-1152.	1.5	10
89	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, 2868-2878.	2.3	10
90	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.	1.2	10

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91	Analysis of side-chain conformational distributions in neutrophil peptide-5 nmr structures. Biopolymers, 1990, 29, 1807-1822.	1.2	9
92	Stratified UWHAM and Its Stochastic Approximation for Multicanonical Simulations Which Are Far from Equilibrium. Journal of Chemical Theory and Computation, 2017, 13, 4660-4674.	2.3	9
93	The UWHAM and SWHAM Software Package. Scientific Reports, 2019, 9, 2803.	1.6	9
94	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.	2.3	8
95	Trajectory Studies of NMR Relaxation in Flexible Molecules. Advances in Chemistry Series, 1983, , 445-468.	0.6	7
96	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.	2.5	7
97	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.	2.5	6
98	Computational design of small molecular modulators of <scp>proteinâ€“protein</scp> interactions with a novel thermodynamic cycle: Allosteric inhibitors of <scp>HIV</scp>â€1 integrase. Protein Science, 2021, 30, 438-447.	3.1	6
99	Limits to detecting epistasis in the fitness landscape of HIV. PLoS ONE, 2022, 17, e0262314.	1.1	6
100	Structure-based virtual screening workflow to identify antivirals targeting HIV-1 capsid. Journal of Computer-Aided Molecular Design, 2022, 36, 193-203.	1.3	6
101	Protein Loop Conformational Free Energy Changes via an Alchemical Path without Reaction Coordinates. Journal of Physical Chemistry Letters, 2021, 12, 4368-4377.	2.1	5
102	Unique features of different classes of <scp>Gâ€proteinâ€coupled</scp> receptors revealed from sequence coevolutionary and structural analysis. Proteins: Structure, Function and Bioinformatics, 2022, 90, 601-614.	1.5	4
103	Tertiary Contacts in Î±a-Lactalbumin at pH 7 and pH 2: A Molecular Dynamics Study. Journal of Biomolecular Structure and Dynamics, 1998, 16, 355-365.	2.0	3
104	Salsa: Scalable Asynchronous Replica Exchange for Parallel Molecular Dynamics Applications. , 0, , .		3
105	Using Macromolecular Dynamics Simulations to Interpret Experiments. Israel Journal of Chemistry, 1986, 27, 173-179.	1.0	2
106	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.	0.3	2
107	Solvation Thermodynamics from the Perspective of Endpoints DFT. Journal of Physical Chemistry B, 2020, 124, 11771-11782.	1.2	2
108	Cavity Particle in Aqueous Solution with a Hydrophobic Solute: Structure, Energetics, and Functionals. Journal of Physical Chemistry B, 2020, 124, 5220-5237.	1.2	1

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109	Using Computer Simulations To Probe the Structure and Dynamics of Biopolymers. ACS Symposium Series, 1987, , 82-105.	0.5	0
110	Recollection. Protein Science, 2016, 25, 9-11.	3.1	0
111	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.	3.3	0