Emilio Gallicchio

List of Publications by Citations

80 papers	4,584 citations	33 h-index	67 g-index
87 ext. papers	5,003 ext. citations	5.2 avg, IF	5.46 L-index

#	Paper	IF	Citations
80	Integrated Modeling Program, Applied Chemical Theory (IMPACT). *Journal of Computational Chemistry*, **2005**, 26, 1752-80	3.5	941
79	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
78	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
77	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
76	The SGB/NP hydration free energy model based on the surface generalized born solvent reaction field and novel nonpolar hydration free energy estimators. *Journal of Computational Chemistry*, **2002**, 23, 517-29	3.5	212
75	Temperature weighted histogram analysis method, replica exchange, and transition paths. *Journal of Physical Chemistry B*, **2005**, 109, 6722-31	3.4	161
74	Protein folding pathways from replica exchange simulations and a kinetic network model. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 6801-6	11.5	127
73	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
72	Distinguishing native conformations of proteins from decoys with an effective free energy estimator based on the OPLS all-atom force field and the Surface Generalized Born solvent model. *Proteins: Structure, Function and Bioinformatics*, **2002**, 48, 404-22	4.2	117
71	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
70	Entropy□nthalpy Compensation in Solvation and Ligand Binding Revisited. *Journal of the American Chemical Society*, **1998**, 120, 4526-4527	16.4	113
69	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
68	Theory of binless multi-state free energy estimation with applications to protein-ligand binding. *Journal of Chemical Physics*, **2012**, 136, 144102	3.9	106
67	The AGBNP2 Implicit Solvation Model. *Journal of Chemical Theory and Computation*, **2009**, 5, 2544-2564	6.4	101
66	A Model for Studying Drying at Hydrophobic Interfaces: Structural and Thermodynamic Properties□*Journal of Physical Chemistry B*, **2001**, 105, 6745-6753	3.4	96
65	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
64	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

63	Advances in all atom sampling methods for modeling protein-ligand binding affinities. *Current Opinion in Structural Biology*, **2011**, 21, 161-6	8.1	86
62	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
61	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
60	Prediction of Protein Loop Conformations using the AGBNP Implicit Solvent Model and Torsion Angle Sampling. *Journal of Chemical Theory and Computation*, **2008**, 4, 855-868	6.4	55
59	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
58	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
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	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
55	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
54	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
53	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
52	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
51	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
50	In silico vaccine design based on molecular simulations of rhinovirus chimeras presenting HIV-1 gp41 epitopes. *Journal of Molecular Biology*, **2009**, 385, 675-91	6.5	37
49	Asynchronous replica exchange for molecular simulations. *Journal of Computational Chemistry*, **2008**, 29, 788-94	3.5	34
48	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
47	The non-polar solvent potential of mean force for the dimerization of alanine dipeptide: the role of solute-solvent van der Waals interactions. *Biophysical Chemistry*, **2004**, 109, 251-60	3.5	31
46	Recovering kinetics from a simplified protein folding model using replica exchange simulations: a kinetic network and effective stochastic dynamics. *Journal of Physical Chemistry B*, **2009**, 113, 11702-9	3.4	27

45	Asynchronous Replica Exchange Software for Grid and Heterogeneous Computing. *Computer Physics Communications*, **2015**, 196, 236-246	4.2	25
44	The linear interaction energy method for the prediction of protein stability changes upon mutation. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 111-25	4.2	25
43	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
42	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
41	Large-scale asynchronous and distributed multidimensional replica exchange molecular simulations and efficiency analysis. *Journal of Computational Chemistry*, **2015**, 36, 1772-85	3.5	19
40	Conformational dynamics of substrate in the active site of cytochrome P450 BM-3/NPG complex: insights from NMR order parameters. *Journal of the American Chemical Society*, **2007**, 129, 474-5	16.4	18
39	Molecular dynamics study of non-nucleoside reverse transcriptase inhibitor 4-[[4-[[4-[(E)-2-cyanoethenyl]-2,6-dimethylphenyl]amino]-2-pyrimidinyl]amino]benzonitrile (TMC278/rilpivirine) aggregates: correlation between amphiphilic properties of the drug and oral bioavailability. *Journal of Medicinal Chemistry*, **2009**, 52, 5896-905	8.3	17
38	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
37	Perturbation potentials to overcome order/disorder transitions in alchemical binding free energy calculations. *Journal of Chemical Physics*, **2019**, 151, 124116	3.9	16
36	A unique binding mode of the eukaryotic translation initiation factor 4E for guiding the design of novel peptide inhibitors. *Protein Science*, **2015**, 24, 1370-82	6.3	16
35	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
34	Exploring structural variability in X-ray crystallographic models using protein local optimization by torsion-angle sampling. *Acta Crystallographica Section D: Biological Crystallography*, **2008**, 64, 383-96		15
33	Role of Ligand Reorganization and Conformational Restraints on the Binding Free Energies of DAPY Non-Nucleoside Inhibitors to HIV Reverse Transcriptase. *Computational Molecular Bioscience*, **2012**, 2, 7-22	1.1	15
32	Antigenic characteristics of rhinovirus chimeras designed in silico for enhanced presentation of HIV-1 gp41 epitopes [corrected]. *Journal of Molecular Biology*, **2010**, 397, 752-66	6.5	14
31	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
30	Chimeric rhinoviruses displaying MPER epitopes elicit anti-HIV neutralizing responses. *PLoS ONE*, **2013**, 8, e72205	3.7	12
29	Free Energy-Based Virtual Screening and Optimization of RNase H Inhibitors of HIV-1 Reverse Transcriptase. *ACS Omega*, **2016**, 1, 435-447	3.9	12
28	Amide-containing β-hydroxytropolones as inhibitors of hepatitis B virus replication. *Antiviral Research*, **2020**, 177, 104777	10.8	11

27	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
26	Assessment of a Single Decoupling Alchemical Approach for the Calculation of the Absolute Binding Free Energies of Protein-Peptide Complexes. *Frontiers in Molecular Biosciences*, **2018**, 5, 22	5.6	10
25	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
24	Combining Alchemical Transformation with a Physical Pathway to Accelerate Absolute Binding Free Energy Calculations of Charged Ligands to Enclosed Binding Sites. *Journal of Chemical Theory and Computation*, **2020**, 16, 2803-2813	6.4	9
23	Efficient gaussian density formulation of volume and surface areas of macromolecules on graphical processing units. *Journal of Computational Chemistry*, **2017**, 38, 740-752	3.5	8
22	The generalized Boltzmann distribution is the only distribution in which the Gibbs-Shannon entropy equals the thermodynamic entropy. *Journal of Chemical Physics*, **2019**, 151, 034113	3.9	8
21	Synthetic β-Hydroxytropolones as Inhibitors of HIV Reverse Transcriptase Ribonuclease H Activity. *MedChemComm*, **2016**, 7, 1783-1788	5	8
20	Alchemical transformations for concerted hydration free energy estimation with explicit solvation. *Journal of Chemical Physics*, **2021**, 154, 054103	3.9	7
19	Inclusion of enclosed hydration effects in the binding free energy estimation of dopamine D3 receptor complexes. *PLoS ONE*, **2019**, 14, e0222902	3.7	6
18	Exploring the Free-Energy Landscape and Thermodynamics of Protein-Protein Association. *Biophysical Journal*, **2020**, 119, 1226-1238	2.9	6
17	Analytical Model of the Free Energy of Alchemical Molecular Binding. *Journal of Chemical Theory and Computation*, **2018**, 14, 6183-6196	6.4	6
16	New Dopamine D3-Selective Receptor Ligands Containing a 6-Methoxy-1,2,3,4-tetrahydroisoquinolin-7-ol Motif. *ACS Medicinal Chemistry Letters*, **2018**, 9, 990-995	4.3	6
15	3,7-Dihydroxytropolones Inhibit Initiation of Hepatitis B Virus Minus-Strand DNA Synthesis. *Molecules*, **2020**, 25,	4.8	4
14	Salsa: Scalable Asynchronous Replica Exchange for Parallel Molecular Dynamics Applications		3
13	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
12	Role of Displacing Confined Solvent in the Conformational Equilibrium of β-Cyclodextrin. *Journal of Physical Chemistry B*, **2019**, 123, 8378-8386	3.4	2
11	A grid-based algorithm in conjunction with a gaussian-based model of atoms for describing molecular geometry. *Journal of Computational Chemistry*, **2019**, 40, 1290-1304	3.5	2
10	A framework for flexible and scalable replica-exchange on production distributed CI **2013**,		2

9	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
8	Implicit solvent models for protein-ligand binding: Insights based on explicit solvent simulations **1999**,		2
7	Relative Binding Free Energy Calculations for Ligands with Diverse Scaffolds with the Alchemical Transfer Method.. *Journal of Chemical Information and Modeling*, **2022**, 62, 309-323	6.1	2
6	Alchemical Transfer Approach to Absolute Binding Free Energy Estimation. *Journal of Chemical Theory and Computation*, **2021**, 17, 3309-3319	6.4	2
5	Application of the alchemical transfer and potential of mean force methods to the SAMPL8 host-guest blinded challenge.. *Journal of Computer-Aided Molecular Design*, **2022**, 36, 63	4.2	1
4	Free Energy-Based Computational Methods for the Study of Protein-Peptide Binding Equilibria.. *Methods in Molecular Biology*, **2022**, 2405, 303-334	1.4	1
3	New tetrahydroisoquinoline-based DR ligands with an o-xylenyl linker motif. *Bioorganic and Medicinal Chemistry Letters*, **2021**, 42, 128047	2.9	0
2	FORTRAN routine to compute Born□Oppenheimer potential energy curves directly from spectroscopic data. *Journal of Computational Chemistry*, **1993**, 14, 579-586	3.5	
1	Fold Recognition using the OPLS All-Atom Potential and the Surface Generalized Born Solvent Model. *Lecture Notes in Computational Science and Engineering*, **2002**, 445-476	0.3	