Michael Gilson

List of Publications by Year
in descending order

133 papers	18,527 citations	20817 60 h-index	12946 131 g-index
166 all docs	166 docs citations	166 times ranked	13395 citing authors

#	Article	IF	Citations
1	BindingDB: a web-accessible database of experimentally determined protein-ligand binding affinities. Nucleic Acids Research, 2007, 35, D198-D201.	14.5	1,493
2	The statistical-thermodynamic basis for computation of binding affinities: a critical review. Biophysical Journal, 1997, 72, 1047-1069.	0.5	1,087
3	Calculating the electrostatic potential of molecules in solution: Method and error assessment. Journal of Computational Chemistry, 1988, 9, 327-335.	3.3	1,017
4	BindingDB in 2015: A public database for medicinal chemistry, computational chemistry and systems pharmacology. Nucleic Acids Research, 2016, 44, D1045-D1053.	14.5	1,002
5	Prediction of Ph-dependent Properties of Proteins. Journal of Molecular Biology, 1994, 238, 415-436.	4.2	807
6	Calculation of Protein-Ligand Binding Affinities. Annual Review of Biophysics and Biomolecular Structure, 2007, 36, 21-42.	18.3	807
7	Calculation of the total electrostatic energy of a macromolecular system: Solvation energies, binding energies, and conformational analysis. Proteins: Structure, Function and Bioinformatics, 1988, 4, 7-18.	2.6	794
8	Electrostatics and diffusion of molecules in solution: simulations with the University of Houston Brownian Dynamics program. Computer Physics Communications, 1995, 91, 57-95.	7.5	622
9	A synthetic host-guest system achieves avidin-biotin affinity by overcoming enthalpyâ€“entropy compensation. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 20737-20742.	7.1	534
10	Calculation of electrostatic potentials in an enzyme active site. Nature, 1987, 330, 84-86.	27.8	458
11	The dielectric constant of a folded protein. Biopolymers, 1986, 25, 2097-2119.	2.4	455
12	The Determinants of pKas in Proteins. Biochemistry, 1996, 35, 7819-7833.	2.5	439
13	Theory of Free Energy and Entropy in Noncovalent Binding. Chemical Reviews, 2009, 109, 4092-4107.	47.7	334
14	New Ultrahigh Affinity Hostâ’Guest Complexes of Cucurbit[7]uril with Bicyclo[2.2.2]octane and Adamantane Guests: Thermodynamic Analysis and Evaluation of M2 Affinity Calculations. Journal of the American Chemical Society, 2011, 133, 3570-3581.	13.7	306
15	Energetics of charge-charge interactions in proteins. Proteins: Structure, Function and Bioinformatics, 1988, 3, 32-52.	2.6	277
16	Open "back door" in a molecular dynamics simulation of acetylcholinesterase. Science, 1994, 263, 1276-1278.	12.6	277
17	Multiple-site titration and molecular modeling: Two rapid methods for computing energies and forces for ionizable groups in proteins. Proteins: Structure, Function and Bioinformatics, 1993, 15, 266-282.	2.6	273
18	Predicting Binding Free Energies: Frontiers and Benchmarks. Annual Review of Biophysics, 2017, 46, 531-558.	10.0	265

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19	Grid inhomogeneous solvation theory: Hydration structure and thermodynamics of the miniature receptor cucurbit[7]uril. Journal of Chemical Physics, 2012, 137, 044101.	3.0	258
20	Virtual Screening of Molecular Databases Using a Support Vector Machine. Journal of Chemical Information and Modeling, 2005, 45, 549-561.	5.4	241
21	Calculation of Cyclodextrin Binding Affinities: Energy, Entropy, and Implications for Drug Design. Biophysical Journal, 2004, 87, 3035-3049.	0.5	217
22	Free Energy, Entropy, and Induced Fit in Hostâ˜'Guest Recognition:Â Calculations with the Second-Generation Mining Minima Algorithm. Journal of the American Chemical Society, 2004, 126, 13156-13164.	13.7	211
23	Dynamic architecture of a protein kinase. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, E4623-31.	7.1	205
24	Lessons learned from comparing molecular dynamics engines on the SAMPL5 dataset. Journal of Computer-Aided Molecular Design, 2017, 31, 147-161.	2.9	187
25	D3R grand challenge 2015: Evaluation of proteinâ€“ligand pose and affinity predictions. Journal of Computer-Aided Molecular Design, 2016, 30, 651-668.	2.9	178
26	BindingDB: A Web-Accessible Molecular Recognition Database. Combinatorial Chemistry and High Throughput Screening, 2001, 4, 719-725.	1.1	172
27	The SAMPL4 hostâ€“guest blind prediction challenge: an overview. Journal of Computer-Aided Molecular Design, 2014, 28, 305-317.	2.9	162
28	Extraction of configurational entropy from molecular simulations via an expansion approximation. Journal of Chemical Physics, 2007, 127, 024107.	3.0	161
29	D3R Grand Challenge 2: blind prediction of proteinâ€“ligand poses, affinity rankings, and relative binding free energies. Journal of Computer-Aided Molecular Design, 2018, 32, 1-20.	2.9	156
30	The Binding Database: data management and interface design. Bioinformatics, 2002, 18, 130-139.	4.1	142
31	Overview of the SAMPL5 hostâ€“guest challenge: Are we doing better?. Journal of Computer-Aided Molecular Design, 2017, 31, 1-19.	2.9	140
32	â€œMining Minimaâ€¦â€‰ Direct Computation of Conformational Free Energy. Journal of Physical Chemistry A, 1997, 101, 1609-1618.	2.5	124
33	Substrate-driven chemotactic assembly in an enzyme cascade. Nature Chemistry, 2018, 10, 311-317.	13.6	121
34	Blind prediction of hostâ€“guest binding affinities: a new SAMPL3 challenge. Journal of Computer-Aided Molecular Design, 2012, 26, 475-487.	2.9	117
35	Thermodynamics of Water in an Enzyme Active Site: Grid-Based Hydration Analysis of Coagulation Factor Xa. Journal of Chemical Theory and Computation, 2014, 10, 2769-2780.	5.3	117
36	Escaping Atom Types in Force Fields Using Direct Chemical Perception. Journal of Chemical Theory and Computation, 2018, 14, 6076-6092.	5.3	110

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37	Entropyâ€“enthalpy transduction caused by conformational shifts can obscure the forces driving proteinâ€“ligand binding. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 20006-20011.	7.1	109
38	Hostâ˜'Guest Complexes with Proteinâ˜'Ligand-like Affinities: Computational Analysis and Design. Journal of the American Chemical Society, 2009, 131, 4012-4021.	13.7	108
39	Quantum Mechanical Calculation of Noncovalent Interactions: A Large-Scale Evaluation of PMx, DFT, and SAPT Approaches. Journal of Chemical Theory and Computation, 2014, 10, 1563-1575.	5.3	107
40	Overview of the SAMPL6 hostâ€“guest binding affinity prediction challenge. Journal of Computer-Aided Molecular Design, 2018, 32, 937-963.	2.9	106
41	D3R Grand Challenge 3: blind prediction of proteinâ€“ligand poses and affinity rankings. Journal of Computer-Aided Molecular Design, 2019, 33, 1-18.	2.9	104
42	Tork: Conformational analysis method for molecules and complexes. Journal of Computational Chemistry, 2003, 24, 1987-1998.	3.3	102
43	Blind prediction of cyclohexaneâ€“water distribution coefficients from the SAMPL5 challenge. Journal of Computer-Aided Molecular Design, 2016, 30, 927-944.	2.9	99
44	Comparison of generalized born and poisson models: Energetics and dynamics of HIV protease. Journal of Computational Chemistry, 2000, 21, 295-309.	3.3	98
45	Non-bonded force field model with advanced restrained electrostatic potential charges (RESP2). Communications Chemistry, 2020, 3, .	4.5	98
46	Molecular dynamics simulation with a continuum electrostatic model of the solvent. Journal of Computational Chemistry, 1995, 16, 1081-1095.	3.3	96
47	Computational Calorimetry: High-Precision Calculation of Hostâ€“Guest Binding Thermodynamics. Journal of Chemical Theory and Computation, 2015, 11, 4377-4394.	5.3	96
48	The inclusion of electrostatic hydration energies in molecular mechanics calculations. Journal of Computer-Aided Molecular Design, 1991, 5, 5-20.	2.9	95
49	Solvation thermodynamic mapping of molecular surfaces in AmberTools: GIST. Journal of Computational Chemistry, 2016, 37, 2029-2037.	3.3	95
50	The SAMPL6 SAMPLing challenge: assessing the reliability and efficiency of binding free energy calculations. Journal of Computer-Aided Molecular Design, 2020, 34, 601-633.	2.9	86
51	Fast Assignment of Accurate Partial Atomic Charges:â€‰ An Electronegativity Equalization Method that Accounts for Alternate Resonance Forms. Journal of Chemical Information and Computer Sciences, 2003, 43, 1982-1997.	2.8	84
52	Bridging Calorimetry and Simulation through Precise Calculations of Cucurbiturilâ€“Guest Binding Enthalpies. Journal of Chemical Theory and Computation, 2014, 10, 4069-4078.	5.3	83
53	Public Domain Databases for Medicinal Chemistry. Journal of Medicinal Chemistry, 2012, 55, 6987-7002.	6.4	81
54	D3R grand challenge 4: blind prediction of proteinâ€“ligand poses, affinity rankings, and relative binding free energies. Journal of Computer-Aided Molecular Design, 2020, 34, 99-119.	2.9	81

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55	Development and Benchmarking of Open Force Field v1.0.0â€"the Parsley Small-Molecule Force Field. Journal of Chemical Theory and Computation, 2021, 17, 6262-6280.	5.3	80
56	Calculation of Molecular Configuration Integrals. Journal of Physical Chemistry B, 2003, 107, 1048-1055.	2.6	76
57	Biological Applications of Electrostatic Calculations and Brownian Dynamics Simulations. Reviews in Computational Chemistry, 2007, , 229-267.	1.5	70
58	The binding database: Overview and user's guide. Biopolymers, 2001, 61, 127-141.	2.4	69
59	Destabilization of an alpha-helix-bundle protein by helix dipoles.. Proceedings of the National Academy of Sciences of the United States of America, 1989, 86, 1524-1528.	7.1	68
60	Symmetry Numbers for Rigid, Flexible, and Fluxional Molecules: Theory and Applications. Journal of Physical Chemistry B, 2010, 114, 16304-16317.	2.6	65
61	Testing inhomogeneous solvation theory in structure-based ligand discovery. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E6839-E6846.	7.1	65
62	Theoretical and Experimental Analysis of Ionization Equilibria in Ovomucoid Third Domainâ€. Biochemistry, 1998, 37, 8643-8652.	2.5	63
63	HYDROPHOBE Challenge: A Joint Experimental and Computational Study on the Hostâ€"Guest Binding of Hydrocarbons to Cucurbiturils, Allowing Explicit Evaluation of Guest Hydration Free-Energy Contributions. Journal of Physical Chemistry B, 2017, 121, 11144-11162.	2.6	62
64	Antitumor Activity of 1,18-Octadecanedioic Acid-Paclitaxel Complexed with Human Serum Albumin. Journal of the American Chemical Society, 2019, 141, 11765-11769.	13.7	61
65	Calculation of Hostâ€"Guest Binding Affinities Using a Quantum-Mechanical Energy Model. Journal of Chemical Theory and Computation, 2012, 8, 2023-2033.	5.3	60
66	Improving the Efficiency and Activity of Electrocatalysts for the Reduction of CO₂ through Supramolecular Assembly with Amino Acid-Modified Ligands. Journal of the American Chemical Society, 2016, 138, 8184-8193.	13.7	59
67	Overcoming dissipation in the calculation of standard binding free energies by ligand extraction. Journal of Computational Chemistry, 2013, 34, 2360-2371.	3.3	57
68	pKaShifts in Small Molecules and HIV Protease:Â Electrostatics and Conformation. Journal of the American Chemical Society, 1998, 120, 6138-6146.	13.7	55
69	Thermodynamic linkage between the binding of protons and inhibitors to HIVâ€1 protease. Protein Science, 1999, 8, 180-195.	7.6	55
70	Discovering de novo peptide substrates for enzymes using machine learning. Nature Communications, 2018, 9, 5253.	12.8	55
71	Ligand-receptor docking with the Mining Minima optimizer. Journal of Computer-Aided Molecular Design, 2001, 15, 157-171.	2.9	51
72	On the Theory of Noncovalent Binding. Biophysical Journal, 2004, 87, 23-36.	0.5	51

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73	Evaluating Force Field Performance in Thermodynamic Calculations of Cyclodextrin Hostâ€“Guest Binding: Water Models, Partial Charges, and Host Force Field Parameters. Journal of Chemical Theory and Computation, 2017, 13, 4253-4269.	5.3	51
74	Protein folding and binding: from biology to physics and back again. Current Opinion in Structural Biology, 2011, 21, 1-3.	5.7	49
75	Automation of absolute protein-ligand binding free energy calculations for docking refinement and compound evaluation. Scientific Reports, 2021, 11, 1116.	3.3	49
76	Attach-Pull-Release Calculations of Ligand Binding and Conformational Changes on the First BRD4 Bromodomain. Journal of Chemical Theory and Computation, 2017, 13, 3260-3275.	5.3	49
77	Structural insights into the gating of DNA passage by the topoisomerase II DNA-gate. Nature Communications, 2018, 9, 3085.	12.8	47
78	Evaluation and Minimization of Uncertainty in ITC Binding Measurements: Heat Error, Concentration Error, Saturation, and Stoichiometry. Biochimica Et Biophysica Acta - General Subjects, 2017, 1861, 485-498.	2.4	45
79	Enhanced Diffusion and Chemotaxis of Enzymes. Annual Review of Biophysics, 2020, 49, 87-105.	10.0	43
80	Identification of Symmetries in Molecules and Complexes. Journal of Chemical Information and Computer Sciences, 2004, 44, 1301-1313.	2.8	42
81	Solvation Structure and Thermodynamic Mapping (SSTMap): An Open-Source, Flexible Package for the Analysis of Water in Molecular Dynamics Trajectories. Journal of Chemical Theory and Computation, 2018, 14, 418-425.	5.3	40
82	Continuous Evaluation of Ligand Protein Predictions: A Weekly Community Challenge for Drug Docking. Structure, 2019, 27, 1326-1335.e4.	3.3	39
83	Thermodynamic and Differential Entropy under a Change of Variables. Entropy, 2010, 12, 578-590.	2.2	37
84	Binding Enthalpy Calculations for a Neutral Hostâ€“Guest Pair Yield Widely Divergent Salt Effects across Water Models. Journal of Chemical Theory and Computation, 2015, 11, 4555-4564.	5.3	36
85	Spatial Decomposition of Translational Waterâ€“Water Correlation Entropy in Binding Pockets. Journal of Chemical Theory and Computation, 2016, 12, 414-429.	5.3	34
86	Enthalpic Breakdown of Water Structure on Protein Active-Site Surfaces. Journal of Physical Chemistry B, 2016, 120, 8743-8756.	2.6	33
87	The SAMPL5 hostâ€“guest challenge: computing binding free energies andÂenthalpies from explicit solvent simulations by the attach-pull-release (APR) method. Journal of Computer-Aided Molecular Design, 2017, 31, 133-145.	2.9	33
88	Simulating Water Exchange to Buried Binding Sites. Journal of Chemical Theory and Computation, 2019, 15, 2684-2691.	5.3	33
89	The SAMPL4 hydration challenge: evaluation of partial charge sets with explicit-water molecular dynamics simulations. Journal of Computer-Aided Molecular Design, 2014, 28, 277-287.	2.9	31
90	Toward Improved Force-Field Accuracy through Sensitivity Analysis of Host-Guest Binding Thermodynamics. Journal of Physical Chemistry B, 2015, 119, 10145-10155.	2.6	30

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91	Toward Learned Chemical Perception of Force Field Typing Rules. Journal of Chemical Theory and Computation, 2019, 15, 402-423.	5.3	30
92	Prediction of SAMPL3 hostâ€“guest binding affinities: evaluating the accuracy of generalized force-fields. Journal of Computer-Aided Molecular Design, 2012, 26, 517-525.	2.9	29
93	Parameterization of an effective potential for proteinâ€“ligand binding from hostâ€“guest affinity data. Journal of Molecular Recognition, 2016, 29, 10-21.	2.1	27
94	Alignment-Free Antimicrobial Peptide Predictors: Improving Performance by a Thorough Analysis of the Largest Available Data Set. Journal of Chemical Information and Modeling, 2021, 61, 3141-3157.	5.4	27
95	Improving Structure-Based Virtual Screening with Ensemble Docking and Machine Learning. Journal of Chemical Information and Modeling, 2021, 61, 5362-5376.	5.4	27
96	Accounting for the Central Role of Interfacial Water in Proteinâ€“Ligand Binding Free Energy Calculations. Journal of Chemical Theory and Computation, 2020, 16, 7883-7894.	5.3	24
97	Bind3P: Optimization of a Water Model Based on Hostâ€“Guest Binding Data. Journal of Chemical Theory and Computation, 2018, 14, 3621-3632.	5.3	23
98	Attractive Interactions between Heteroallenes and the Cucurbituril Portal. Journal of the American Chemical Society, 2017, 139, 8138-8145.	13.7	22
99	Accounting for apparent deviations between calorimetric and van't Hoff enthalpies. Biochimica Et Biophysica Acta - General Subjects, 2018, 1862, 692-704.	2.4	22
100	A molecular reconstruction approach to site-based 3D-RISM and comparison to GIST hydration thermodynamic maps in an enzyme active site. PLoS ONE, 2019, 14, e0219473.	2.5	22
101	Enhancing water sampling of buried binding sites using nonequilibrium candidate Monte Carlo. Journal of Computer-Aided Molecular Design, 2021, 35, 167-177.	2.9	22
102	CACHE (Critical Assessment of Computational Hit-finding Experiments): A publicâ€“private partnership benchmarking initiative to enable the development of computational methods for hit-finding. Nature Reviews Chemistry, 2022, 6, 287-295.	30.2	22
103	Acetylcholinesterase: Effects of Ionic Strength and Dimerization on the Rate Constants. Israel Journal of Chemistry, 1994, 34, 151-158.	2.3	21
104	Binding Thermodynamics of Hostâ€“Guest Systems with SMIRNOFF99Frosst 1.0.5 from the Open Force Field Initiative. Journal of Chemical Theory and Computation, 2019, 15, 6225-6242.	5.3	21
105	The electrostatic response of water to neutral polar solutes: Implications for continuum solvent modeling. Journal of Chemical Physics, 2013, 138, 224504.	3.0	19
106	Blind prediction of SAMPL4 cucurbit[7]uril binding affinities with the mining minima method. Journal of Computer-Aided Molecular Design, 2014, 28, 463-474.	2.9	18
107	Protein-ligand binding enthalpies from near-millisecond simulations: Analysis of a preorganization paradox. Journal of Chemical Physics, 2018, 149, 072311.	3.0	17
108	A Thermodynamic Limit on the Role of Self-Propulsion in Enhanced Enzyme Diffusion. Biophysical Journal, 2019, 116, 1898-1906.	0.5	17

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109	Fast Equilibration of Water between Buried Sites and the Bulk by Molecular Dynamics with Parallel Monte Carlo Water Moves on Graphical Processing Units. Journal of Chemical Theory and Computation, 2021, 17, 7366-7372.	5.3	16
110	Connecting proteins with drug-like compounds: Open source drug discovery workflows with BindingDB and KNIME. Database: the Journal of Biological Databases and Curation, 2015, 2015, bav087.	3.0	15
111	Data-Driven Mapping of Gas-Phase Quantum Calculations to General Force Field Lennard-Jones Parameters. Journal of Chemical Theory and Computation, 2020, 16, 1115-1127.	5.3	15
112	Force and Stress along Simulated Dissociation Pathways of Cucurbiturilâ€“Guest Systems. Journal of Chemical Theory and Computation, 2012, 8, 966-976.	5.3	14
113	Toward Expanded Diversity of Hostâ€“Guest Interactions via Synthesis and Characterization of Cyclodextrin Derivatives. Journal of Solution Chemistry, 2018, 47, 1597-1608.	1.2	14
114	Motor-like Properties of Nonmotor Enzymes. Biophysical Journal, 2018, 114, 2174-2179.	0.5	13
115	Calculation and Visualization of Atomistic Mechanical Stresses in Nanomaterials and Biomolecules. PLoS ONE, 2014, 9, e113119.	2.5	13
116	Stress Analysis at the Molecular Level: A Forced Cucurbituril-Guest Dissociation Pathway. Journal of Chemical Theory and Computation, 2010, 6, 637-646.	5.3	12
117	Sensitivity Analysis and Charge-Optimization for Flexible Ligands:â€‰ Applicability to Lead Optimization. Journal of Chemical Theory and Computation, 2006, 2, 259-270.	5.3	11
118	Responsibility of Co-Authors. Science, 1997, 275, 11e-14.	12.6	11
119	Probing the orientation of inhibitor and epoxy-eicosatrienoic acid binding in the active site of soluble epoxide hydrolase. Archives of Biochemistry and Biophysics, 2017, 613, 1-11.	3.0	9
120	Experimental characterization of the association of Î²-cyclodextrin and eight novel cyclodextrin derivatives with two guest compounds. Journal of Computer-Aided Molecular Design, 2021, 35, 95-104.	2.9	9
121	Facile synthesis of a diverse library of mono-3-substituted Î²-cyclodextrin analogues. Supramolecular Chemistry, 2019, 31, 251-259.	1.2	8
122	Entropic effects enable life at extreme temperatures. Science Advances, 2019, 5, eaaw4783.	10.3	7
123	Evaluation of Representations and Response Models for Polarizable Force Fields. Journal of Physical Chemistry B, 2016, 120, 8668-8684.	2.6	6
124	Data-driven analysis of the number of Lennardâ€“Jones types needed in a force field. Communications Chemistry, 2020, 3, .	4.5	6
125	Mechanistic analysis of light-driven overcrowded alkene-based molecular motors by multiscale molecular simulations. Physical Chemistry Chemical Physics, 2021, 23, 8525-8540.	2.8	6
126	Stimuli Induced Uptake of Proteinâ€Like Peptide Brush Polymers. Chemistry - A European Journal, 2022, 28, .	3.3	6

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127	Editorial: Molecular recognition databases. Biopolymers, 2001, 61, 97-98.	2.4	2
128	The bioinformatics of molecular recognition. Journal of Molecular Recognition, 2002, 15, 1-1.	2.1	2
129	Dual Inhibitors of Cyclooxygenaseâ€2 and Soluble Epoxide Hydrolase: Studies of Binding Modes at the Active Sites and Timeâ€dependency of Inhibition, and Development of Waterâ€soluble Prodrugs. FASEB Journal, 2018, 32, 558.2.	0.5	1
130	Shouldn't enantiomeric purity be included in the 'minimum information about a bioactive entity? Response from the MIABE group. Nature Reviews Drug Discovery, 2012, 11, 730-730.	46.4	0
131	This issue: Drug Design Data Resource Grand Challenge 4, first of two issues. Journal of Computer-Aided Molecular Design, 2019, 33, 1009-1009.	2.9	0
132	Drug Design Data Resource, Grand Challenge 4, second of two issues. Journal of Computer-Aided Molecular Design, 2020, 34, 97-97.	2.9	0
133	Continuous Evaluation of Ligand Protein Predictions: A Weekly Community Challenge for Drug Docking. SSRN Electronic Journal, 0, , .	0.4	0