

Michael K Gilson

List of Publications by Year in descending order

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152
papers

19,950
citations

13865

67
h-index

11052

137
g-index

161
all docs

161
docs citations

161
times ranked

13985
citing authors

#	ARTICLE	IF	CITATIONS
1	BindingDB: a web-accessible database of experimentally determined protein-ligand binding affinities. <i>Nucleic Acids Research</i> , 2007, 35, D198-D201.	14.5	1,493
2	Calculating the electrostatic potential of molecules in solution: Method and error assessment. <i>Journal of Computational Chemistry</i> , 1988, 9, 327-335.	3.3	1,017
3	BindingDB in 2015: A public database for medicinal chemistry, computational chemistry and systems pharmacology. <i>Nucleic Acids Research</i> , 2016, 44, D1045-D1053.	14.5	1,002
4	Prediction of Ph-dependent Properties of Proteins. <i>Journal of Molecular Biology</i> , 1994, 238, 415-436.	4.2	807
5	Calculation of Protein-Ligand Binding Affinities. <i>Annual Review of Biophysics and Biomolecular Structure</i> , 2007, 36, 21-42.	18.3	807
6	Calculation of the total electrostatic energy of a macromolecular system: Solvation energies, binding energies, and conformational analysis. <i>Proteins: Structure, Function and Bioinformatics</i> , 1988, 4, 7-18.	2.6	794
7	Electrostatics and diffusion of molecules in solution: simulations with the University of Houston Brownian Dynamics program. <i>Computer Physics Communications</i> , 1995, 91, 57-95.	7.5	622
8	A synthetic host-guest system achieves avidin-biotin affinity by overcoming enthalpyâ€“entropy compensation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 20737-20742.	7.1	534
9	Calculation of electrostatic potentials in an enzyme active site. <i>Nature</i> , 1987, 330, 84-86.	27.8	458
10	The dielectric constant of a folded protein. <i>Biopolymers</i> , 1986, 25, 2097-2119.	2.4	455
11	The Determinants of pKas in Proteins. <i>Biochemistry</i> , 1996, 35, 7819-7833.	2.5	439
12	Accelerated Poisson-Boltzmann calculations for static and dynamic systems. <i>Journal of Computational Chemistry</i> , 2002, 23, 1244-1253.	3.3	421
13	Ligand configurational entropy and protein binding. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 1534-1539.	7.1	350
14	Theory of Free Energy and Entropy in Noncovalent Binding. <i>Chemical Reviews</i> , 2009, 109, 4092-4107.	47.7	334
15	Computation of electrostatic forces on solvated molecules using the Poisson-Boltzmann equation. <i>The Journal of Physical Chemistry</i> , 1993, 97, 3591-3600.	2.9	324
16	On the calculation of electrostatic interactions in proteins. <i>Journal of Molecular Biology</i> , 1985, 184, 503-516.	4.2	315
17	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. <i>Journal of the American Chemical Society</i> , 2011, 133, 3570-3581.	13.7	306
18	Energetics of charge-charge interactions in proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 1988, 3, 32-52.	2.6	277

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19	Multiple-site titration and molecular modeling: Two rapid methods for computing energies and forces for ionizable groups in proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 1993, 15, 266-282.	2.6	273
20	Predicting Binding Free Energies: Frontiers and Benchmarks. <i>Annual Review of Biophysics</i> , 2017, 46, 531-558.	10.0	265
21	Grid inhomogeneous solvation theory: Hydration structure and thermodynamics of the miniature receptor cucurbit[7]uril. <i>Journal of Chemical Physics</i> , 2012, 137, 044101.	3.0	258
22	Virtual Screening of Molecular Databases Using a Support Vector Machine. <i>Journal of Chemical Information and Modeling</i> , 2005, 45, 549-561.	5.4	241
23	Calculation of Cyclodextrin Binding Affinities: Energy, Entropy, and Implications for Drug Design. <i>Biophysical Journal</i> , 2004, 87, 3035-3049.	0.5	217
24	Free Energy, Entropy, and Induced Fit in Host-Guest Recognition: Calculations with the Second-Generation Mining Minima Algorithm. <i>Journal of the American Chemical Society</i> , 2004, 126, 13156-13164.	13.7	211
25	Dynamic architecture of a protein kinase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, E4623-31.	7.1	205
26	Theory of electrostatic interactions in macromolecules. <i>Current Opinion in Structural Biology</i> , 1995, 5, 216-223.	5.7	203
27	Lessons learned from comparing molecular dynamics engines on the SAMPL5 dataset. <i>Journal of Computer-Aided Molecular Design</i> , 2017, 31, 147-161.	2.9	187
28	D3R grand challenge 2015: Evaluation of protein-ligand pose and affinity predictions. <i>Journal of Computer-Aided Molecular Design</i> , 2016, 30, 651-668.	2.9	178
29	SuperTarget goes quantitative: update on drug-target interactions. <i>Nucleic Acids Research</i> , 2012, 40, D1113-D1117.	14.5	174
30	The SAMPL4 host-guest blind prediction challenge: an overview. <i>Journal of Computer-Aided Molecular Design</i> , 2014, 28, 305-317.	2.9	162
31	Extraction of configurational entropy from molecular simulations via an expansion approximation. <i>Journal of Chemical Physics</i> , 2007, 127, 024107.	3.0	161
32	Evaluating the Accuracy of the Quasiharmonic Approximation. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 1017-1028.	5.3	160
33	The Binding Database: data management and interface design. <i>Bioinformatics</i> , 2002, 18, 130-139.	4.1	142
34	Overview of the SAMPL5 host-guest challenge: Are we doing better?. <i>Journal of Computer-Aided Molecular Design</i> , 2017, 31, 1-19.	2.9	140
35	Computing ionization states of proteins with a detailed charge model. <i>Journal of Computational Chemistry</i> , 1996, 17, 1633-1644.	3.3	139
36	Supramolecular Assembly Promotes the Electrocatalytic Reduction of Carbon Dioxide by Re(I) Bipyridine Catalysts at a Lower Overpotential. <i>Journal of the American Chemical Society</i> , 2014, 136, 14598-14607.	13.7	128

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37	â€œMining Minimaâ€: Direct Computation of Conformational Free Energy. <i>Journal of Physical Chemistry A</i> , 1997, 101, 1609-1618.	2.5	124
38	Substrate-driven chemotactic assembly in an enzyme cascade. <i>Nature Chemistry</i> , 2018, 10, 311-317.	13.6	121
39	Blind prediction of hostâ€guest binding affinities: a new SAMPL3 challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2012, 26, 475-487.	2.9	117
40	Thermodynamics of Water in an Enzyme Active Site: Grid-Based Hydration Analysis of Coagulation Factor Xa. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2769-2780.	5.3	117
41	Escaping Atom Types in Force Fields Using Direct Chemical Perception. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 6076-6092.	5.3	110
42	Entropyâ€enthalpy transduction caused by conformational shifts can obscure the forces driving proteinâ€ligand binding. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 20006-20011.	7.1	109
43	Hostâ€Guest Complexes with Proteinâ€Ligand-like Affinities: Computational Analysis and Design. <i>Journal of the American Chemical Society</i> , 2009, 131, 4012-4021.	13.7	108
44	Quantum Mechanical Calculation of Noncovalent Interactions: A Large-Scale Evaluation of PMx, DFT, and SAPT Approaches. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1563-1575.	5.3	107
45	Overview of the SAMPL6 hostâ€guest binding affinity prediction challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 937-963.	2.9	106
46	HIV-1 Protease Inhibitors from Inverse Design in the Substrate Envelope Exhibit Subnanomolar Binding to Drug-Resistant Variants. <i>Journal of the American Chemical Society</i> , 2008, 130, 6099-6113.	13.7	105
47	Evaluating the Substrate-Envelope Hypothesis: Structural Analysis of Novel HIV-1 Protease Inhibitors Designed To Be Robust against Drug Resistance. <i>Journal of Virology</i> , 2010, 84, 5368-5378.	3.4	104
48	Tork: Conformational analysis method for molecules and complexes. <i>Journal of Computational Chemistry</i> , 2003, 24, 1987-1998.	3.3	102
49	Blind prediction of cyclohexaneâ€water distribution coefficients from the SAMPL5 challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2016, 30, 927-944.	2.9	99
50	Comparison of generalized born and poisson models: Energetics and dynamics of HIV protease. <i>Journal of Computational Chemistry</i> , 2000, 21, 295-309.	3.3	98
51	Non-bonded force field model with advanced restrained electrostatic potential charges (RESP2). <i>Communications Chemistry</i> , 2020, 3, .	4.5	98
52	Efficient calculation of configurational entropy from molecular simulations by combining the mutualâ€information expansion and nearestâ€neighbor methods. <i>Journal of Computational Chemistry</i> , 2008, 29, 1605-1614.	3.3	97
53	Molecular dynamics simulation with a continuum electrostatic model of the solvent. <i>Journal of Computational Chemistry</i> , 1995, 16, 1081-1095.	3.3	96
54	Computational Calorimetry: High-Precision Calculation of Hostâ€Guest Binding Thermodynamics. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4377-4394.	5.3	96

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55	Solvation thermodynamic mapping of molecular surfaces in AmberTools: GIST. <i>Journal of Computational Chemistry</i> , 2016, 37, 2029-2037.	3.3	95
56	The Physical Basis of Nucleic Acid Base Stacking in Water. <i>Biophysical Journal</i> , 2001, 80, 140-148.	0.5	87
57	The SAMPL6 SAMPLing challenge: assessing the reliability and efficiency of binding free energy calculations. <i>Journal of Computer-Aided Molecular Design</i> , 2020, 34, 601-633.	2.9	86
58	Fast Assignment of Accurate Partial Atomic Charges: An Electronegativity Equalization Method that Accounts for Alternate Resonance Forms. <i>Journal of Chemical Information and Computer Sciences</i> , 2003, 43, 1982-1997.	2.8	84
59	Bridging Calorimetry and Simulation through Precise Calculations of Cucurbituril Guest Binding Enthalpies. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4069-4078.	5.3	83
60	Screening Drug-Like Compounds by Docking to Homology Models: A Systematic Study. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 365-379.	5.4	82
61	Comparison of Continuum and Explicit Models of Solvation: Potentials of Mean Force for Alanine Dipeptide. <i>The Journal of Physical Chemistry</i> , 1996, 100, 1439-1441.	2.9	81
62	Public Domain Databases for Medicinal Chemistry. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 6987-7002.	6.4	81
63	D3R grand challenge 4: blind prediction of protein-ligand poses, affinity rankings, and relative binding free energies. <i>Journal of Computer-Aided Molecular Design</i> , 2020, 34, 99-119.	2.9	81
64	Development and Benchmarking of Open Force Field v1.0.0 the Parsley Small-Molecule Force Field. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6262-6280.	5.3	80
65	Configurational Entropy in Protein-Peptide Binding. <i>Journal of Molecular Biology</i> , 2009, 389, 315-335.	4.2	79
66	Calculation of Molecular Configuration Integrals. <i>Journal of Physical Chemistry B</i> , 2003, 107, 1048-1055.	2.6	76
67	Strength of Solvent-Exposed Salt-Bridges. <i>Journal of Physical Chemistry B</i> , 1999, 103, 727-736.	2.6	71
68	Biological Applications of Electrostatic Calculations and Brownian Dynamics Simulations. <i>Reviews in Computational Chemistry</i> , 2007, , 229-267.	1.5	70
69	The binding database: Overview and user's guide. <i>Biopolymers</i> , 2001, 61, 127-141.	2.4	69
70	A new class of models for computing receptor-ligand binding affinities. <i>Chemistry and Biology</i> , 1997, 4, 87-92.	6.0	67
71	Symmetry Numbers for Rigid, Flexible, and Fluxional Molecules: Theory and Applications. <i>Journal of Physical Chemistry B</i> , 2010, 114, 16304-16317.	2.6	65
72	Testing inhomogeneous solvation theory in structure-based ligand discovery. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E6839-E6846.	7.1	65

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73	Small Molecule pKa Prediction with Continuum Electrostatics Calculations. <i>Journal of the American Chemical Society</i> , 1994, 116, 10298-10299.	13.7	64
74	Theoretical and Experimental Analysis of Ionization Equilibria in Ovomuroid Third Domain. <i>Biochemistry</i> , 1998, 37, 8643-8652.	2.5	63
75	HYDROPHOBE Challenge: A Joint Experimental and Computational Study on the Host-Guest Binding of Hydrocarbons to Cucurbiturils, Allowing Explicit Evaluation of Guest Hydration Free-Energy Contributions. <i>Journal of Physical Chemistry B</i> , 2017, 121, 11144-11162.	2.6	62
76	Modeling Protein-Ligand Binding by Mining Minima. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 3540-3557.	5.3	60
77	Calculation of Guest Binding Affinities Using a Quantum-Mechanical Energy Model. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2023-2033.	5.3	60
78	Improving the Efficiency and Activity of Electrocatalysts for the Reduction of CO ₂ through Supramolecular Assembly with Amino Acid-Modified Ligands. <i>Journal of the American Chemical Society</i> , 2016, 138, 8184-8193.	13.7	59
79	Overcoming dissipation in the calculation of standard binding free energies by ligand extraction. <i>Journal of Computational Chemistry</i> , 2013, 34, 2360-2371.	3.3	57
80	The fundamental role of flexibility on the strength of molecular binding. <i>Soft Matter</i> , 2012, 8, 6385.	2.7	56
81	pKaShifts in Small Molecules and HIV Protease: Electrostatics and Conformation. <i>Journal of the American Chemical Society</i> , 1998, 120, 6138-6146.	13.7	55
82	Thermodynamic linkage between the binding of protons and inhibitors to HIV-1 protease. <i>Protein Science</i> , 1999, 8, 180-195.	7.6	55
83	Ligand-receptor docking with the Mining Minima optimizer. <i>Journal of Computer-Aided Molecular Design</i> , 2001, 15, 157-171.	2.9	51
84	Enhanced docking with the mining minima optimizer: Acceleration and side-chain flexibility. <i>Journal of Computational Chemistry</i> , 2002, 23, 1656-1670.	3.3	51
85	On the Theory of Noncovalent Binding. <i>Biophysical Journal</i> , 2004, 87, 23-36.	0.5	51
86	Design of Mutation-resistant HIV Protease Inhibitors with the Substrate Envelope Hypothesis. <i>Chemical Biology and Drug Design</i> , 2007, 69, 298-313.	3.2	51
87	Evaluating Force Field Performance in Thermodynamic Calculations of Cyclodextrin Host-Guest Binding: Water Models, Partial Charges, and Host Force Field Parameters. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4253-4269.	5.3	51
88	Synthetic Adenine Receptors: Direct Calculation of Binding Affinity and Entropy. <i>Journal of the American Chemical Society</i> , 2000, 122, 2934-2937.	13.7	49
89	Automation of absolute protein-ligand binding free energy calculations for docking refinement and compound evaluation. <i>Scientific Reports</i> , 2021, 11, 1116.	3.3	49
90	Attach-Pull-Release Calculations of Ligand Binding and Conformational Changes on the First BRD4 Bromodomain. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3260-3275.	5.3	49

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91	Evaluation of the substrate envelope hypothesis for inhibitors of HIV-1 protease. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 68, 561-567.	2.6	48
92	Evaluation and Minimization of Uncertainty in ITC Binding Measurements: Heat Error, Concentration Error, Saturation, and Stoichiometry. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2017, 1861, 485-498.	2.4	45
93	Identification of Symmetries in Molecules and Complexes. <i>Journal of Chemical Information and Computer Sciences</i> , 2004, 44, 1301-1313.	2.8	42
94	Solvation Structure and Thermodynamic Mapping (SSTMap): An Open-Source, Flexible Package for the Analysis of Water in Molecular Dynamics Trajectories. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 418-425.	5.3	40
95	Interpreting trends in the binding of cyclic ureas to HIV-1 protease. <i>Journal of Molecular Biology</i> , 2001, 309, 507-517.	4.2	39
96	Concepts in Receptor Optimization: Targeting the RGD Peptide. <i>Journal of the American Chemical Society</i> , 2006, 128, 4675-4684.	13.7	39
97	Dielectric Screening Treatment of Electrostatic Solvation. <i>Journal of Physical Chemistry B</i> , 1997, 101, 11226-11236.	2.6	37
98	Thermodynamic and Differential Entropy under a Change of Variables. <i>Entropy</i> , 2010, 12, 578-590.	2.2	37
99	Nucleic acid base-pairing and N-methylacetamide self-association in chloroform: affinity and conformation. <i>Biophysical Chemistry</i> , 1999, 78, 183-193.	2.8	36
100	Correlation as a Determinant of Configurational Entropy in Supramolecular and Protein Systems. <i>Journal of Physical Chemistry B</i> , 2014, 118, 6447-6455.	2.6	36
101	Binding Enthalpy Calculations for a Neutral Host-Guest Pair Yield Widely Divergent Salt Effects across Water Models. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4555-4564.	5.3	36
102	Competition between Intra- and Intermolecular Hydrogen Bonding: Effect on para/ortho Adsorptive Selectivity for Substituted Phenols. <i>Industrial & Engineering Chemistry Research</i> , 2000, 39, 463-472.	3.7	34
103	Spatial Decomposition of Translational Water-Water Correlation Entropy in Binding Pockets. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 414-429.	5.3	34
104	Enthalpic Breakdown of Water Structure on Protein Active-Site Surfaces. <i>Journal of Physical Chemistry B</i> , 2016, 120, 8743-8756.	2.6	33
105	The SAMPL5 host-guest challenge: computing binding free energies and enthalpies from explicit solvent simulations by the attach-pull-release (APR) method. <i>Journal of Computer-Aided Molecular Design</i> , 2017, 31, 133-145.	2.9	33
106	Simulating Water Exchange to Buried Binding Sites. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2684-2691.	5.3	33
107	The SAMPL4 hydration challenge: evaluation of partial charge sets with explicit-water molecular dynamics simulations. <i>Journal of Computer-Aided Molecular Design</i> , 2014, 28, 277-287.	2.9	31
108	Toward Improved Force-Field Accuracy through Sensitivity Analysis of Host-Guest Binding Thermodynamics. <i>Journal of Physical Chemistry B</i> , 2015, 119, 10145-10155.	2.6	30

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109	Toward Learned Chemical Perception of Force Field Typing Rules. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 402-423.	5.3	30
110	Comparing Ligand Interactions with Multiple Receptors via Serial Docking. <i>Journal of Chemical Information and Computer Sciences</i> , 2004, 44, 1961-1970.	2.8	29
111	Prediction of SAMPL3 host-guest binding affinities: evaluating the accuracy of generalized force-fields. <i>Journal of Computer-Aided Molecular Design</i> , 2012, 26, 517-525.	2.9	29
112	Intramolecular versus Intermolecular Hydrogen Bonding in the Adsorption of Aromatic Alcohols onto an Acrylic Ester Sorbent. <i>Journal of Physical Chemistry B</i> , 2000, 104, 4735-4744.	2.6	28
113	Structural model for an AxxxG-mediated dimer of surfactant-associated protein C. <i>FEBS Journal</i> , 2004, 271, 2086-2092.	0.2	28
114	Coordinate Systems and the Calculation of Molecular Properties. <i>Journal of Physical Chemistry A</i> , 2002, 106, 563-566.	2.5	27
115	Parameterization of an effective potential for protein-ligand binding from host-guest affinity data. <i>Journal of Molecular Recognition</i> , 2016, 29, 10-21.	2.1	27
116	A hierarchical method for generating low-energy conformers of a protein-ligand complex. , 1998, 33, 475-495.		26
117	Accounting for the Central Role of Interfacial Water in Protein-Ligand Binding Free Energy Calculations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7883-7894.	5.3	24
118	Additivity in the Analysis and Design of HIV Protease Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 737-754.	6.4	23
119	Bind3P: Optimization of a Water Model Based on Host-Guest Binding Data. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3621-3632.	5.3	23
120	Attractive Interactions between Heteroallenes and the Cucurbituril Portal. <i>Journal of the American Chemical Society</i> , 2017, 139, 8138-8145.	13.7	22
121	Accounting for apparent deviations between calorimetric and van't Hoff enthalpies. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2018, 1862, 692-704.	2.4	22
122	A molecular reconstruction approach to site-based 3D-RISM and comparison to GIST hydration thermodynamic maps in an enzyme active site. <i>PLoS ONE</i> , 2019, 14, e0219473.	2.5	22
123	Enhancing water sampling of buried binding sites using nonequilibrium candidate Monte Carlo. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 167-177.	2.9	22
124	Acetylcholinesterase: Effects of Ionic Strength and Dimerization on the Rate Constants. <i>Israel Journal of Chemistry</i> , 1994, 34, 151-158.	2.3	21
125	Binding Thermodynamics of Host-Guest Systems with SMIRNOFF99Frosst 1.0.5 from the Open Force Field Initiative. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6225-6242.	5.3	21
126	Toward the Design of Mutation-Resistant Enzyme Inhibitors: Further Evaluation of the Substrate Envelope Hypothesis. <i>Chemical Biology and Drug Design</i> , 2009, 74, 234-245.	3.2	20

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127	Computational Study of KNI-272, a Potent Inhibitor of HIV-1 Protease: On the Mechanism of Preorganization. <i>Journal of Physical Chemistry B</i> , 1999, 103, 1031-1044.	2.6	19
128	The electrostatic response of water to neutral polar solutes: Implications for continuum solvent modeling. <i>Journal of Chemical Physics</i> , 2013, 138, 224504.	3.0	19
129	Blind prediction of SAMPL4 cucurbit[7]uril binding affinities with the mining minima method. <i>Journal of Computer-Aided Molecular Design</i> , 2014, 28, 463-474.	2.9	18
130	ConCept: a de Novo Design of Synthetic Receptors for Targeted Ligands. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 425-434.	5.4	17
131	Protein-ligand binding enthalpies from near-millisecond simulations: Analysis of a preorganization paradox. <i>Journal of Chemical Physics</i> , 2018, 149, 072311.	3.0	17
132	A Thermodynamic Limit on the Role of Self-Propulsion in Enhanced Enzyme Diffusion. <i>Biophysical Journal</i> , 2019, 116, 1898-1906.	0.5	17
133	Fast Equilibration of Water between Buried Sites and the Bulk by Molecular Dynamics with Parallel Monte Carlo Water Moves on Graphical Processing Units. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 7366-7372.	5.3	16
134	Sampling conformations in high dimensions using low-dimensional distribution functions. <i>Journal of Chemical Physics</i> , 2009, 130, 134102.	3.0	15
135	Ions and Inhibitors in the Binding Site of HIV Protease: Comparison of Monte Carlo Simulations and the Linearized Poisson-Boltzmann Theory. <i>Biophysical Journal</i> , 2009, 96, 1293-1306.	0.5	15
136	Connecting proteins with drug-like compounds: Open source drug discovery workflows with BindingDB and KNIME. <i>Database: the Journal of Biological Databases and Curation</i> , 2015, 2015, bav087.	3.0	15
137	Data-Driven Mapping of Gas-Phase Quantum Calculations to General Force Field Lennard-Jones Parameters. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 1115-1127.	5.3	15
138	Force and Stress along Simulated Dissociation Pathways of Cucurbituril-Guest Systems. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 966-976.	5.3	14
139	Motor-like Properties of Nonmotor Enzymes. <i>Biophysical Journal</i> , 2018, 114, 2174-2179.	0.5	13
140	Calculation and Visualization of Atomistic Mechanical Stresses in Nanomaterials and Biomolecules. <i>PLoS ONE</i> , 2014, 9, e113119.	2.5	13
141	Stress Analysis at the Molecular Level: A Forced Cucurbituril-Guest Dissociation Pathway. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 637-646.	5.3	12
142	Sensitivity Analysis and Charge-Optimization for Flexible Ligands: Applicability to Lead Optimization. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 259-270.	5.3	11
143	Probing the orientation of inhibitor and epoxy-eicosatrienoic acid binding in the active site of soluble epoxide hydrolase. <i>Archives of Biochemistry and Biophysics</i> , 2017, 613, 1-11.	3.0	9
144	Charge Optimization Theory for Induced-Fit Ligands. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4580-4592.	5.3	8

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145	Evaluation of Representations and Response Models for Polarizable Force Fields. <i>Journal of Physical Chemistry B</i> , 2016, 120, 8668-8684.	2.6	6
146	Data-driven analysis of the number of Lennard-Jones types needed in a force field. <i>Communications Chemistry</i> , 2020, 3, .	4.5	6
147	Modeling protonation equilibria in biomolecules. , 1997, , 199-222.		6
148	Modeling Molecular Recognition: Theory and Application. <i>Journal of Biomolecular Structure and Dynamics</i> , 2000, 17, 89-94.	3.5	5
149	Binding of Cations and Protons in the Active Site of Acetylcholinesterase. <i>Jerusalem Symposia on Quantum Chemistry and Biochemistry</i> , 1995, , 25-37.	0.2	5
150	Accelerated convergence of molecular free energy via superposition approximation-based reference states. <i>Journal of Chemical Physics</i> , 2011, 134, 134107.	3.0	4
151	Editorial: Molecular recognition databases. <i>Biopolymers</i> , 2001, 61, 97-98.	2.4	2
152	Virtual Screening of Molecular Databases Using a Support Vector Machine.. <i>ChemInform</i> , 2005, 36, no.	0.0	1