Michael K Gilson

List of Publications by Year
in descending order

152 papers	19,950 citations	13854 67 h-index	11047 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. Nucleic Acids Research, 2007, 35, D198-D201.	6.5	1,493
2	Calculating the electrostatic potential of molecules in solution: Method and error assessment. Journal of Computational Chemistry, 1988, 9, 327-335.	1.5	1,017
3	BindingDB in 2015: A public database for medicinal chemistry, computational chemistry and systems pharmacology. Nucleic Acids Research, 2016, 44, D1045-D1053.	6.5	1,002
4	Prediction of Ph-dependent Properties of Proteins. Journal of Molecular Biology, 1994, 238, 415-436.	2.0	807
5	Calculation of Protein-Ligand Binding Affinities. Annual Review of Biophysics and Biomolecular Structure, 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. Proteins: Structure, Function and Bioinformatics, 1988, 4, 7-18.	1.5	794
7	Electrostatics and diffusion of molecules in solution: simulations with the University of Houston Brownian Dynamics program. Computer Physics Communications, 1995, 91, 57-95.	3.0	622
8	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.	3.3	534
9	Calculation of electrostatic potentials in an enzyme active site. Nature, 1987, 330, 84-86.	13.7	458
10	The dielectric constant of a folded protein. Biopolymers, 1986, 25, 2097-2119.	1.2	455
11	The Determinants of pKas in Proteins. Biochemistry, 1996, 35, 7819-7833.	1.2	439
12	Accelerated Poisson-Boltzmann calculations for static and dynamic systems. Journal of Computational Chemistry, 2002, 23, 1244-1253.	1.5	421
13	Ligand configurational entropy and protein binding. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 1534-1539.	3.3	350
14	Theory of Free Energy and Entropy in Noncovalent Binding. Chemical Reviews, 2009, 109, 4092-4107.	23.0	334
15	Computation of electrostatic forces on solvated molecules using the Poisson-Boltzmann equation. The Journal of Physical Chemistry, 1993, 97, 3591-3600.	2.9	324
16	On the calculation of electrostatic interactions in proteins. Journal of Molecular Biology, 1985, 184, 503-516.	2.0	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. Journal of the American Chemical Society, 2011, 133, 3570-3581.	6.6	306
18	Energetics of charge-charge interactions in proteins. Proteins: Structure, Function and Bioinformatics, 1988, 3, 32-52.	1.5	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. Proteins: Structure, Function and Bioinformatics, 1993, 15, 266-282.	1.5	273
20	Predicting Binding Free Energies: Frontiers and Benchmarks. Annual Review of Biophysics, 2017, 46, 531-558.	4.5	265
21	Grid inhomogeneous solvation theory: Hydration structure and thermodynamics of the miniature receptor cucurbit[7]uril. Journal of Chemical Physics, 2012, 137, 044101.	1.2	258
22	Virtual Screening of Molecular Databases Using a Support Vector Machine. Journal of Chemical Information and Modeling, 2005, 45, 549-561.	2.5	241
23	Calculation of Cyclodextrin Binding Affinities: Energy, Entropy, and Implications for Drug Design. Biophysical Journal, 2004, 87, 3035-3049.	0.2	217
24	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.	6.6	211
25	Dynamic architecture of a protein kinase. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, E4623-31.	3.3	205
26	Theory of electrostatic interactions in macromolecules. Current Opinion in Structural Biology, 1995, 5, 216-223.	2.6	203
27	Lessons learned from comparing molecular dynamics engines on the SAMPL5 dataset. Journal of Computer-Aided Molecular Design, 2017, 31, 147-161.	1.3	187
28	D3R grand challenge 2015: Evaluation of proteinâ€“ligand pose and affinity predictions. Journal of Computer-Aided Molecular Design, 2016, 30, 651-668.	1.3	178
29	SuperTarget goes quantitative: update on drug-target interactions. Nucleic Acids Research, 2012, 40, D1113-D1117.	6.5	174
30	The SAMPL4 hostâ€“guest blind prediction challenge: an overview. Journal of Computer-Aided Molecular Design, 2014, 28, 305-317.	1.3	162
31	Extraction of configurational entropy from molecular simulations via an expansion approximation. Journal of Chemical Physics, 2007, 127, 024107.	1.2	161
32	Evaluating the Accuracy of the Quasiharmonic Approximation. Journal of Chemical Theory and Computation, 2005, 1, 1017-1028.	2.3	160
33	The Binding Database: data management and interface design. Bioinformatics, 2002, 18, 130-139.	1.8	142
34	Overview of the SAMPL5 hostâ€“guest challenge: Are we doing better?. Journal of Computer-Aided Molecular Design, 2017, 31, 1-19.	1.3	140
35	Computing ionization states of proteins with a detailed charge model. Journal of Computational Chemistry, 1996, 17, 1633-1644.	1.5	139
36	Supramolecular Assembly Promotes the Electrocatalytic Reduction of Carbon Dioxide by Re(I) Bipyridine Catalysts at a Lower Overpotential. Journal of the American Chemical Society, 2014, 136, 14598-14607.	6.6	128

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37	â€œMining Minimaâ€â€‰ Direct Computation of Conformational Free Energy. Journal of Physical Chemistry A, 1997, 101, 1609-1618.	1.1	124
38	Substrate-driven chemotactic assembly in an enzyme cascade. Nature Chemistry, 2018, 10, 311-317.	6.6	121
39	Blind prediction of hostâ€“guest binding affinities: a new SAMPL3 challenge. Journal of Computer-Aided Molecular Design, 2012, 26, 475-487.	1.3	117
40	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.	2.3	117
41	Escaping Atom Types in Force Fields Using Direct Chemical Perception. Journal of Chemical Theory and Computation, 2018, 14, 6076-6092.	2.3	110
42	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.	3.3	109
43	Hostâ˜Guest Complexes with Proteinâ˜Ligand-like Affinities: Computational Analysis and Design. Journal of the American Chemical Society, 2009, 131, 4012-4021.	6.6	108
44	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.	2.3	107
45	Overview of the SAMPL6 hostâ€“guest binding affinity prediction challenge. Journal of Computer-Aided Molecular Design, 2018, 32, 937-963.	1.3	106
46	HIV-1 Protease Inhibitors from Inverse Design in the Substrate Envelope Exhibit Subnanomolar Binding to Drug-Resistant Variants. Journal of the American Chemical Society, 2008, 130, 6099-6113.	6.6	105
47	Evaluating the Substrate-Envelope Hypothesis: Structural Analysis of Novel HIV-1 Protease Inhibitors Designed To Be Robust against Drug Resistance. Journal of Virology, 2010, 84, 5368-5378.	1.5	104
48	Tork: Conformational analysis method for molecules and complexes. Journal of Computational Chemistry, 2003, 24, 1987-1998.	1.5	102
49	Blind prediction of cyclohexaneâ€“water distribution coefficients from the SAMPL5 challenge. Journal of Computer-Aided Molecular Design, 2016, 30, 927-944.	1.3	99
50	Comparison of generalized born and poisson models: Energetics and dynamics of HIV protease. Journal of Computational Chemistry, 2000, 21, 295-309.	1.5	98
51	Non-bonded force field model with advanced restrained electrostatic potential charges (RESP2). Communications Chemistry, 2020, 3, .	2.0	98
52	Efficient calculation of configurational entropy from molecular simulations by combining the mutualâ€information expansion and nearestâ€neighbor methods. Journal of Computational Chemistry, 2008, 29, 1605-1614.	1.5	97
53	Molecular dynamics simulation with a continuum electrostatic model of the solvent. Journal of Computational Chemistry, 1995, 16, 1081-1095.	1.5	96
54	Computational Calorimetry: High-Precision Calculation of Hostâ€“Guest Binding Thermodynamics. Journal of Chemical Theory and Computation, 2015, 11, 4377-4394.	2.3	96

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55	Solvation thermodynamic mapping of molecular surfaces in AmberTools: GIST. Journal of Computational Chemistry, 2016, 37, 2029-2037.	1.5	95
56	The Physical Basis of Nucleic Acid Base Stacking in Water. Biophysical Journal, 2001, 80, 140-148.	0.2	87
57	The SAMPL6 SAMPLing challenge: assessing the reliability and efficiency of binding free energy calculations. Journal of Computer-Aided Molecular Design, 2020, 34, 601-633.	1.3	86
58	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
59	Bridging Calorimetry and Simulation through Precise Calculations of Cucurbiturilâ€“Guest Binding Enthalpies. Journal of Chemical Theory and Computation, 2014, 10, 4069-4078.	2.3	83
60	Screening Drug-Like Compounds by Docking to Homology Models:Â A Systematic Study. Journal of Chemical Information and Modeling, 2006, 46, 365-379.	2.5	82
61	Comparison of Continuum and Explicit Models of Solvation:Â Potentials of Mean Force for Alanine Dipeptide. The Journal of Physical Chemistry, 1996, 100, 1439-1441.	2.9	81
62	Public Domain Databases for Medicinal Chemistry. Journal of Medicinal Chemistry, 2012, 55, 6987-7002.	2.9	81
63	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.	1.3	81
64	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.	2.3	80
65	Configurational Entropy in Proteinâ€“Peptide Binding:. Journal of Molecular Biology, 2009, 389, 315-335.	2.0	79
66	Calculation of Molecular Configuration Integrals. Journal of Physical Chemistry B, 2003, 107, 1048-1055.	1.2	76
67	Strength of Solvent-Exposed Salt-Bridges. Journal of Physical Chemistry B, 1999, 103, 727-736.	1.2	71
68	Biological Applications of Electrostatic Calculations and Brownian Dynamics Simulations. Reviews in Computational Chemistry, 2007, , 229-267.	1.5	70
69	The binding database: Overview and user's guide. Biopolymers, 2001, 61, 127-141.	1.2	69
70	A new class of models for computing receptor-ligand binding affinities. Chemistry and Biology, 1997, 4, 87-92.	6.2	67
71	Symmetry Numbers for Rigid, Flexible, and Fluxional Molecules: Theory and Applications. Journal of Physical Chemistry B, 2010, 114, 16304-16317.	1.2	65
72	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.	3.3	65

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73	Small Molecule pKa Prediction with Continuum Electrostatics Calculations. Journal of the American Chemical Society, 1994, 116, 10298-10299.	6.6	64
74	Theoretical and Experimental Analysis of Ionization Equilibria in Ovomucoid Third Domainâ€. Biochemistry, 1998, 37, 8643-8652.	1.2	63
75	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.	1.2	62
76	Modeling Proteinâ^'Ligand Binding by Mining Minima. Journal of Chemical Theory and Computation, 2010, 6, 3540-3557.	2.3	60
77	Calculation of Hostâ€“Guest Binding Affinities Using a Quantum-Mechanical Energy Model. Journal of Chemical Theory and Computation, 2012, 8, 2023-2033.	2.3	60
78	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.	6.6	59
79	Overcoming dissipation in the calculation of standard binding free energies by ligand extraction. Journal of Computational Chemistry, 2013, 34, 2360-2371.	1.5	57
80	The fundamental role of flexibility on the strength of molecular binding. Soft Matter, 2012, 8, 6385.	1.2	56
81	pKaShifts in Small Molecules and HIV Protease:Â Electrostatics and Conformation. Journal of the American Chemical Society, 1998, 120, 6138-6146.	6.6	55
82	Thermodynamic linkage between the binding of protons and inhibitors to HIVâ€1 protease. Protein Science, 1999, 8, 180-195.	3.1	55
83	Ligand-receptor docking with the Mining Minima optimizer. Journal of Computer-Aided Molecular Design, 2001, 15, 157-171.	1.3	51
84	Enhanced docking with the mining minima optimizer: Acceleration and side-chain flexibility. Journal of Computational Chemistry, 2002, 23, 1656-1670.	1.5	51
85	On the Theory of Noncovalent Binding. Biophysical Journal, 2004, 87, 23-36.	0.2	51
86	Design of Mutation-resistant HIV Protease Inhibitors with the Substrate Envelope Hypothesis. Chemical Biology and Drug Design, 2007, 69, 298-313.	1.5	51
87	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.	2.3	51
88	Synthetic Adenine Receptors:Â Direct Calculation of Binding Affinity and Entropy. Journal of the American Chemical Society, 2000, 122, 2934-2937.	6.6	49
89	Automation of absolute protein-ligand binding free energy calculations for docking refinement and compound evaluation. Scientific Reports, 2021, 11, 1116.	1.6	49
90	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.	2.3	49

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91	Evaluation of the substrate envelope hypothesis for inhibitors of HIV-1 protease. Proteins: Structure, Function and Bioinformatics, 2007, 68, 561-567.	1.5	48
92	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.	1.1	45
93	Identification of Symmetries in Molecules and Complexes. Journal of Chemical Information and Computer Sciences, 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. Journal of Chemical Theory and Computation, 2018, 14, 418-425.	2.3	40
95	Interpreting trends in the binding of cyclic ureas to HIV-1 protease. Journal of Molecular Biology, 2001, 309, 507-517.	2.0	39
96	Concepts in Receptor Optimization:Â Targeting the RGD Peptide. Journal of the American Chemical Society, 2006, 128, 4675-4684.	6.6	39
97	Dielectric Screening Treatment of Electrostatic Solvation. Journal of Physical Chemistry B, 1997, 101, 11226-11236.	1.2	37
98	Thermodynamic and Differential Entropy under a Change of Variables. Entropy, 2010, 12, 578-590.	1.1	37
99	Nucleic acid base-pairing and N-methylacetamide self-association in chloroform: affinity and conformation. Biophysical Chemistry, 1999, 78, 183-193.	1.5	36
100	Correlation as a Determinant of Configurational Entropy in Supramolecular and Protein Systems. Journal of Physical Chemistry B, 2014, 118, 6447-6455.	1.2	36
101	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.	2.3	36
102	Competition between Intra- and Intermolecular Hydrogen Bonding:Â Effect on para/ortho Adsorptive Selectivity for Substituted Phenols. Industrial & Engineering Chemistry Research, 2000, 39, 463-472.	1.8	34
103	Spatial Decomposition of Translational Waterâ€“Water Correlation Entropy in Binding Pockets. Journal of Chemical Theory and Computation, 2016, 12, 414-429.	2.3	34
104	Enthalpic Breakdown of Water Structure on Protein Active-Site Surfaces. Journal of Physical Chemistry B, 2016, 120, 8743-8756.	1.2	33
105	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.	1.3	33
106	Simulating Water Exchange to Buried Binding Sites. Journal of Chemical Theory and Computation, 2019, 15, 2684-2691.	2.3	33
107	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.	1.3	31
108	Toward Improved Force-Field Accuracy through Sensitivity Analysis of Host-Guest Binding Thermodynamics. Journal of Physical Chemistry B, 2015, 119, 10145-10155.	1.2	30

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109	Toward Learned Chemical Perception of Force Field Typing Rules. Journal of Chemical Theory and Computation, 2019, 15, 402-423.	2.3	30
110	Comparing Ligand Interactions with Multiple Receptors via Serial Docking. Journal of Chemical Information and Computer Sciences, 2004, 44, 1961-1970.	2.8	29
111	Prediction of SAMPL3 hostâ€“guest binding affinities: evaluating the accuracy of generalized force-fields. Journal of Computer-Aided Molecular Design, 2012, 26, 517-525.	1.3	29
112	Intramolecular versus Intermolecular Hydrogen Bonding in the Adsorption of Aromatic Alcohols onto an Acrylic Ester Sorbent. Journal of Physical Chemistry B, 2000, 104, 4735-4744.	1.2	28
113	Structural model for an AxxxG-mediated dimer of surfactant-associated protein C. FEBS Journal, 2004, 271, 2086-2092.	0.2	28
114	Coordinate Systems and the Calculation of Molecular Properties. Journal of Physical Chemistry A, 2002, 106, 563-566.	1.1	27
115	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
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 Proteinâ€“Ligand Binding Free Energy Calculations. Journal of Chemical Theory and Computation, 2020, 16, 7883-7894.	2.3	24
118	Additivity in the Analysis and Design of HIV Protease Inhibitors. Journal of Medicinal Chemistry, 2009, 52, 737-754.	2.9	23
119	Bind3P: Optimization of a Water Model Based on Hostâ€“Guest Binding Data. Journal of Chemical Theory and Computation, 2018, 14, 3621-3632.	2.3	23
120	Attractive Interactions between Heteroallenes and the Cucurbituril Portal. Journal of the American Chemical Society, 2017, 139, 8138-8145.	6.6	22
121	Accounting for apparent deviations between calorimetric and van't Hoff enthalpies. Biochimica Et Biophysica Acta - General Subjects, 2018, 1862, 692-704.	1.1	22
122	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.	1.1	22
123	Enhancing water sampling of buried binding sites using nonequilibrium candidate Monte Carlo. Journal of Computer-Aided Molecular Design, 2021, 35, 167-177.	1.3	22
124	Acetylcholinesterase: Effects of Ionic Strength and Dimerization on the Rate Constants. Israel Journal of Chemistry, 1994, 34, 151-158.	1.0	21
125	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.	2.3	21
126	Toward the Design of Mutationâ€Resistant Enzyme Inhibitors: Further Evaluation of the Substrate Envelope Hypothesis. Chemical Biology and Drug Design, 2009, 74, 234-245.	1.5	20

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127	Computational Study of KNI-272, a Potent Inhibitor of HIV-1 Protease: On the Mechanism of Preorganization. Journal of Physical Chemistry B, 1999, 103, 1031-1044.	1.2	19
128	The electrostatic response of water to neutral polar solutes: Implications for continuum solvent modeling. Journal of Chemical Physics, 2013, 138, 224504.	1.2	19
129	Blind prediction of SAMPL4 cucurbit[7]uril binding affinities with the mining minima method. Journal of Computer-Aided Molecular Design, 2014, 28, 463-474.	1.3	18
130	ConCept:â€‰ de Novo Design of Synthetic Receptors for Targeted Ligands. Journal of Chemical Information and Modeling, 2007, 47, 425-434.	2.5	17
131	Protein-ligand binding enthalpies from near-millisecond simulations: Analysis of a preorganization paradox. Journal of Chemical Physics, 2018, 149, 072311.	1.2	17
132	A Thermodynamic Limit on the Role of Self-Propulsion in Enhanced Enzyme Diffusion. Biophysical Journal, 2019, 116, 1898-1906.	0.2	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. Journal of Chemical Theory and Computation, 2021, 17, 7366-7372.	2.3	16
134	Sampling conformations in high dimensions using low-dimensional distribution functions. Journal of Chemical Physics, 2009, 130, 134102.	1.2	15
135	Ions and Inhibitors in the Binding Site of HIV Protease: Comparison ofÂMonte Carlo Simulations and the Linearized Poisson-Boltzmann Theory. Biophysical Journal, 2009, 96, 1293-1306.	0.2	15
136	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.	1.4	15
137	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.	2.3	15
138	Force and Stress along Simulated Dissociation Pathways of Cucurbiturilâ€“Guest Systems. Journal of Chemical Theory and Computation, 2012, 8, 966-976.	2.3	14
139	Motor-like Properties of Nonmotor Enzymes. Biophysical Journal, 2018, 114, 2174-2179.	0.2	13
140	Calculation and Visualization of Atomistic Mechanical Stresses in Nanomaterials and Biomolecules. PLoS ONE, 2014, 9, e113119.	1.1	13
141	Stress Analysis at the Molecular Level: A Forced Cucurbituril-Guest Dissociation Pathway. Journal of Chemical Theory and Computation, 2010, 6, 637-646.	2.3	12
142	Sensitivity Analysis and Charge-Optimization for Flexible Ligands:â€‰ Applicability to Lead Optimization. Journal of Chemical Theory and Computation, 2006, 2, 259-270.	2.3	11
143	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.	1.4	9
144	Charge Optimization Theory for Induced-Fit Ligands. Journal of Chemical Theory and Computation, 2012, 8, 4580-4592.	2.3	8

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145	Evaluation of Representations and Response Models for Polarizable Force Fields. Journal of Physical Chemistry B, 2016, 120, 8668-8684.	1.2	6
146	Data-driven analysis of the number of Lennardâ€“Jones types needed in a force field. Communications Chemistry, 2020, 3, .	2.0	6
147	Modeling protonation equilibria in biomolecules. , 1997, , 199-222.		6
148	Modeling Molecular Recognition: Theory and Application. Journal of Biomolecular Structure and Dynamics, 2000, 17, 89-94.	2.0	5
149	Binding of Cations and Protons in the Active Site of Acetylcholinesterase. Jerusalem Symposia on Quantum Chemistry and Biochemistry, 1995, , 25-37.	0.2	5
150	Accelerated convergence of molecular free energy via superposition approximation-based reference states. Journal of Chemical Physics, 2011, 134, 134107.	1.2	4
151	Editorial: Molecular recognition databases. Biopolymers, 2001, 61, 97-98.	1.2	2
152	Virtual Screening of Molecular Databases Using a Support Vector Machine.. ChemInform, 2005, 36, no.	0.1	1