William L Jorgensen

List of Publications by Year
in descending order

418 papers	97,352 citations	2669 95 h-index	243 303 g-index
426 all docs	426 docs citations	426 times ranked	60185 citing authors

#	Article	IF	Citations
1	Comparison of simple potential functions for simulating liquid water. Journal of Chemical Physics, 1983, 79, 926-935.	1.2	34,333
2	Development and Testing of the OPLS All-Atom Force Field on Conformational Energetics and Properties of Organic Liquids. Journal of the American Chemical Society, 1996, 118, 11225-11236.	6.6	12,123
3	The OPLS [optimized potentials for liquid simulations] potential functions for proteins, energy minimizations for crystals of cyclic peptides and crambin. Journal of the American Chemical Society, 1988, 110, 1657-1666.	6.6	4,463
4	Evaluation and Reparametrization of the OPLS-AA Force Field for Proteins via Comparison with Accurate Quantum Chemical Calculations on Peptidesâ€. Journal of Physical Chemistry B, 2001, 105, 6474-6487.	1.2	3,513
5	OPLS3: A Force Field Providing Broad Coverage of Drug-like Small Molecules and Proteins. Journal of Chemical Theory and Computation, 2016, 12, 281-296.	2.3	2,349
6	Optimized intermolecular potential functions for liquid hydrocarbons. Journal of the American Chemical Society, 1984, 106, 6638-6646.	6.6	2,069
7	A five-site model for liquid water and the reproduction of the density anomaly by rigid, nonpolarizable potential functions. Journal of Chemical Physics, 2000, 112, 8910-8922.	1.2	1,984
8	The Many Roles of Computation in Drug Discovery. Science, 2004, 303, 1813-1818.	6.0	1,294
9	Quantum and statistical mechanical studies of liquids. 10. Transferable intermolecular potential functions for water, alcohols, and ethers. Application to liquid water. Journal of the American Chemical Society, 1981, 103, 335-340.	6.6	1,145
10	Aromatic-aromatic interactions: free energy profiles for the benzene dimer in water, chloroform, and liquid benzene. Journal of the American Chemical Society, 1990, 112, 4768-4774.	6.6	1,099
11	Potential energy functions for atomic-level simulations of water and organic and biomolecular systems. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 6665-6670.	3.3	1,064
12	Performance of B3LYP Density Functional Methods for a Large Set of Organic Molecules. Journal of Chemical Theory and Computation, 2008, 4, 297-306.	2.3	931
13	Accurate and Reliable Prediction of Relative Ligand Binding Potency in Prospective Drug Discovery by Way of a Modern Free-Energy Calculation Protocol and Force Field. Journal of the American Chemical Society, 2015, 137, 2695-2703.	6.6	931
14	LigParGen web server: an automatic OPLS-AA parameter generator for organic ligands. Nucleic Acids Research, 2017, 45, W331-W336.	6.5	829
15	Temperature and size dependence for Monte Carlo simulations of TIP4P water. Molecular Physics, 1985, 56, 1381-1392.	0.8	706
16	Prediction of drug solubility from structure. Advanced Drug Delivery Reviews, 2002, 54, 355-366.	6.6	691
17	Monte Carlo simulation of differences in free energies of hydration. Journal of Chemical Physics, 1985, 83, 3050-3054.	1.2	683
18	OPLS all-atom force field for carbohydrates. Journal of Computational Chemistry, 1997, 18, 1955-1970.	1.5	619

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19	Improved Peptide and Protein Torsional Energetics with the OPLS-AA Force Field. Journal of Chemical Theory and Computation, 2015, 11, 3499-3509.	2.3	611
20	Free energy calculations: a breakthrough for modeling organic chemistry in solution. Accounts of Chemical Research, 1989, 22, 184-189.	7.6	610
21	OPLS All-Atom Model for Amines:Â Resolution of the Amine Hydration Problem. Journal of the American Chemical Society, 1999, 121, 4827-4836.	6.6	591
22	Energy component analysis for dilute aqueous solutions of lithium(1+), sodium(1+), fluoride(1-), and chloride(1-) ions. Journal of the American Chemical Society, 1984, 106, 903-910.	6.6	586
23	Efficient Drug Lead Discovery and Optimization. Accounts of Chemical Research, 2009, 42, 724-733.	7.6	576
24	OPLS potential functions for nucleotide bases. Relative association constants of hydrogen-bonded base pairs in chloroform. Journal of the American Chemical Society, 1991, 113, 2810-2819.	6.6	570
25	Revised TIPS for simulations of liquid water and aqueous solutions. Journal of Chemical Physics, 1982, 77, 4156-4163.	1.2	483
26	Gas-phase and liquid-state properties of esters, nitriles, and nitro compounds with the OPLS-AA force field. Journal of Computational Chemistry, 2001, 22, 1340-1352.	1.5	438
27	Prediction of Properties from Simulations:Â Free Energies of Solvation in Hexadecane, Octanol, and Water. Journal of the American Chemical Society, 2000, 122, 2878-2888.	6.6	435
28	1.14*CM1A-LBCC: Localized Bond-Charge Corrected CM1A Charges for Condensed-Phase Simulations. Journal of Physical Chemistry B, 2017, 121, 3864-3870.	1.2	413
29	Temperature dependence of TIP3P, SPC, and TIP4P water from NPT Monte Carlo simulations: Seeking temperatures of maximum density. Journal of Computational Chemistry, 1998, 19, 1179-1186.	1.5	403
30	Perfluoroalkanes:Â Conformational Analysis and Liquid-State Properties from ab Initio and Monte Carlo Calculations. Journal of Physical Chemistry A, 2001, 105, 4118-4125.	1.1	401
31	Ab Initio Study of Hydrogen-Bonded Complexes of Small Organic Molecules with Water. Journal of Physical Chemistry A, 1998, 102, 3782-3797.	1.1	396
32	Molecular modeling of organic and biomolecular systems usingBOSS andMCPRO. Journal of Computational Chemistry, 2005, 26, 1689-1700.	1.5	380
33	Theoretical examination of the SN2 reaction involving chloride ion and methyl chloride in the gas phase and aqueous solution. Journal of the American Chemical Society, 1985, 107, 154-163.	6.6	372
34	Halide, Ammonium, and Alkali Metal Ion Parameters for Modeling Aqueous Solutions. Journal of Chemical Theory and Computation, 2006, 2, 1499-1509.	2.3	355
35	Prediction of drug solubility from Monte Carlo simulations. Bioorganic and Medicinal Chemistry Letters, 2000, 10, 1155-1158.	1.0	327
36	Methyl Effects on Proteinâ€“Ligand Binding. Journal of Medicinal Chemistry, 2012, 55, 4489-4500.	2.9	310

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37	Diffusion constant of the TIP5P model of liquid water. Journal of Chemical Physics, 2001, 114, 363.	1.2	307
38	Efficient computation of absolute free energies of binding by computer simulations. Application to the methane dimer in water. Journal of Chemical Physics, 1988, 89, 3742-3746.	1.2	301
39	Free Energies of Hydration and Pure Liquid Properties of Hydrocarbons from the OPLS All-Atom Model. The Journal of Physical Chemistry, 1994, 98, 13077-13082.	2.9	300
40	Development of an All-Atom Force Field for Heterocycles. Properties of Liquid Pyrrole, Furan, Diazoles, and Oxazoles. Journal of Physical Chemistry B, 1998, 102, 8049-8059.	1.2	300
41	Monte Carlo simulations of the hydration of ammonium and carboxylate ions. The Journal of Physical Chemistry, 1986, 90, 2174-2182.	2.9	299
42	Development of an all-atom force field for heterocycles. Properties of liquid pyridine and diazenes. Computational and Theoretical Chemistry, 1998, 424, 145-155.	1.5	296
43	PDDG/PM3 and PDDG/MNDO: Improved semiempirical methods. Journal of Computational Chemistry, 2002, 23, 1601-1622.	1.5	289
44	Perspective on Free-Energy Perturbation Calculations for Chemical Equilibria. Journal of Chemical Theory and Computation, 2008, 4, 869-876.	2.3	286
45	Developing a Dynamic Pharmacophore Model for HIV-1 Integrase. Journal of Medicinal Chemistry, 2000, 43, 2100-2114.	2.9	271
46	SN2 reaction profiles in the gas phase and aqueous solution. Journal of the American Chemical Society, 1984, 106, 3049-3050.	6.6	255
47	Contribution of Conformer Focusing to the Uncertainty in Predicting Free Energies for Proteinâ˜Ligand Binding. Journal of Medicinal Chemistry, 2006, 49, 5880-5884.	2.9	244
48	An Extended Linear Response Method for Determining Free Energies of Hydration. The Journal of Physical Chemistry, 1995, 99, 10667-10673.	2.9	242
49	Performance of the AMBER94, MMFF94, and OPLS-AA Force Fields for Modeling Organic Liquids. The Journal of Physical Chemistry, 1996, 100, 18010-18013.	2.9	242
50	Treatment of Halogen Bonding in the OPLS-AA Force Field: Application to Potent Anti-HIV Agents. Journal of Chemical Theory and Computation, 2012, 8, 3895-3901.	2.3	232
51	Monte Carlo simulations of liquid acetonitrile with a three-site model. Molecular Physics, 1988, 63, 547-558.	0.8	227
52	Cis-trans energy difference for the peptide bond in the gas phase and in aqueous solution. Journal of the American Chemical Society, 1988, 110, 4212-4216.	6.6	223
53	Energetics of Displacing Water Molecules from Protein Binding Sites: Consequences for Ligand Optimization. Journal of the American Chemical Society, 2009, 131, 15403-15411.	6.6	222
54	Advances in Quantum and Molecular Mechanical (QM/MM) Simulations for Organic and Enzymatic Reactions. Accounts of Chemical Research, 2010, 43, 142-151.	7.6	221

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55	Theoretical studies of medium effects on conformational equilibria. The Journal of Physical Chemistry, 1983, 87, 5304-5314.	2.9	218
56	Rusting of the lock and key model for protein-ligand binding. Science, 1991, 254, 954-955.	6.0	211
57	The many faces of halogen bonding: a review of theoretical models and methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 523-540.	6.2	188
58	Free Energies of Hydration from a Generalized Born Model and an All-Atom Force Field. Journal of Physical Chemistry B, 2004, 108, 16264-16270.	1.2	187
59	Potent Noncovalent Inhibitors of the Main Protease of SARS-CoV-2 from Molecular Sculpting of the Drug Perampanel Guided by Free Energy Perturbation Calculations. ACS Central Science, 2021, 7, 467-475.	5.3	182
60	Free energy of TIP4P water and the free energies of hydration of CH4 and Cl- from statistical perturbation theory. Chemical Physics, 1989, 129, 193-200.	0.9	180
61	Identification of 14 Known Drugs as Inhibitors of the Main Protease of SARS-CoV-2. ACS Medicinal Chemistry Letters, 2020, 11, 2526-2533.	1.3	176
62	Prediction of the Water Content in Protein Binding Sites. Journal of Physical Chemistry B, 2009, 113, 13337-13346.	1.2	175
63	Steric Retardation of SN2 Reactions in the Gas Phase and Solution. Journal of the American Chemical Society, 2004, 126, 9054-9058.	6.6	174
64	Molecular Dynamics Simulations of the Unfolding of Barnase in Water and 8 M Aqueous Urea. Biochemistry, 1997, 36, 7313-7329.	1.2	173
65	Monte Carlo simulations of pure liquid substituted benzenes with OPLS potential functions. Journal of Computational Chemistry, 1993, 14, 206-215.	1.5	172
66	QM/MM Simulations for Dielsâ˜'Alder Reactions in Water:Â Contribution of Enhanced Hydrogen Bonding at the Transition State to the Solvent Effectâ€. Journal of Physical Chemistry B, 2002, 106, 8078-8085.	1.2	172
67	Binding Affinities for Sulfonamide Inhibitors with Human Thrombin Using Monte Carlo Simulations with a Linear Response Method. Journal of Medicinal Chemistry, 1997, 40, 1539-1549.	2.9	166
68	Monte Carlo simulations of the hydration of substituted benzenes with OPLS potential functions. Journal of Computational Chemistry, 1993, 14, 195-205.	1.5	165
69	Elucidation of Fatty Acid Amide Hydrolase Inhibition by Potent Î±-Ketoheterocycle Derivatives from Monte Carlo Simulations. Journal of the American Chemical Society, 2005, 127, 17377-17384.	6.6	163
70	Do denaturants interact with aromatic hydrocarbons in water?. Journal of the American Chemical Society, 1993, 115, 9271-9275.	6.6	156
71	Accuracy of free energies of hydration for organic molecules from 6-31g*-derived partial charges. Journal of Computational Chemistry, 1993, 14, 1240-1249.	1.5	154
72	Monte Carlo simulations of liquid acetic acid and methyl acetate with the OPLS potential functions. The Journal of Physical Chemistry, 1991, 95, 3315-3322.	2.9	149

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73	Monte Carlo vs Molecular Dynamics for Conformational Sampling. The Journal of Physical Chemistry, 1996, 100, 14508-14513.	2.9	148
74	Monte Carlo simulations of liquid alkyl ethers with the OPLS potential functions. Journal of Computational Chemistry, 1990, 11, 958-971.	1.5	141
75	Analysis of Binding Affinities for Celecoxib Analogues with COX-1 and COX-2 from Combined Docking and Monte Carlo Simulations and Insight into the COX-2/COX-1 Selectivity. Journal of the American Chemical Society, 2000, 122, 9455-9466.	6.6	135
76	Solvent effects on the barrier to isomerization for a tertiary amide from ab initio and Monte Carlo calculations. Journal of the American Chemical Society, 1992, 114, 7535-7542.	6.6	133
77	Accuracy of free energies of hydration using CM1 and CM3 atomic charges. Journal of Computational Chemistry, 2004, 25, 1322-1332.	1.5	131
78	Comparison of SCC-DFTB and NDDO-Based Semiempirical Molecular Orbital Methods for Organic Molecules. Journal of Physical Chemistry A, 2006, 110, 13551-13559.	1.1	131
79	A Remote Arene-Binding Site on Prostate Specific Membrane Antigen Revealed by Antibody-Recruiting Small Molecules. Journal of the American Chemical Society, 2010, 132, 12711-12716.	6.6	131
80	Computational approaches to molecular recognition. Current Opinion in Chemical Biology, 1997, 1, 449-457.	2.8	124
81	New Linear Interaction Method for Binding Affinity Calculations Using a Continuum Solvent Model. Journal of Physical Chemistry B, 2001, 105, 10388-10397.	1.2	124
82	Computer-aided design of non-nucleoside inhibitors of HIV-1 reverse transcriptase. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 663-667.	1.0	122
83	Discovery of Human Macrophage Migration Inhibitory Factor (MIF)-CD74 Antagonists via Virtual Screening. Journal of Medicinal Chemistry, 2009, 52, 416-424.	2.9	122
84	Computationally-Guided Optimization of a Docking Hit to Yield Catechol Diethers as Potent Anti-HIV Agents. Journal of Medicinal Chemistry, 2011, 54, 8582-8591.	2.9	122
85	Monte Carlo simulation of nâ€butane in water. Conformational evidence for the hydrophobic effect. Journal of Chemical Physics, 1982, 77, 5757-5765.	1.2	119
86	Computational Investigations of Carbenium Ion Reactions Relevant to Sterol Biosynthesis. Journal of the American Chemical Society, 1997, 119, 10846-10854.	6.6	117
87	A Quantum Mechanical and Molecular Mechanical Method Based on CM1A Charges:â€‰ Applications to Solvent Effects on Organic Equilibria and Reactions. Journal of Physical Chemistry B, 1998, 102, 1787-1796.	1.2	113
88	A priori calculations of pKa's for organic compounds in water. The pKa of ethane. Journal of the American Chemical Society, 1987, 109, 6857-6858.	6.6	111
89	Macrophomate Synthase:Â QM/MM Simulations Address the Dielsâ^'Alder versus Michaelâ^'Aldol Reaction Mechanism. Journal of the American Chemical Society, 2005, 127, 3577-3588.	6.6	108
90	The nature of dilute solutions of sodium ion in water, methanol, and tetrahydrofuran. Journal of Chemical Physics, 1982, 77, 5080-5089.	1.2	107

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91	Biomolecular Force Field Parameterization via Atoms-in-Molecule Electron Density Partitioning. Journal of Chemical Theory and Computation, 2016, 12, 2312-2323.	2.3	104
92	Quantum, intramolecular flexibility, and polarizability effects on the reproduction of the density anomaly of liquid water by simple potential functions. Journal of Chemical Physics, 2001, 115, 10758-10768.	1.2	103
93	An improved intermolecular potential function for simulations of liquid hydrogen fluoride. Molecular Physics, 1984, 51, 119-132.	0.8	102
94	Urea: Potential Functions, log P, and Free Energy of Hydration. Israel Journal of Chemistry, 1993, 33, 323-330.	1.0	102
95	Estimation of Binding Affinities for HEPT and Nevirapine Analogues with HIV-1 Reverse Transcriptase via Monte Carlo Simulations. Journal of Medicinal Chemistry, 2001, 44, 145-154.	2.9	100
96	Solvent Effects and Mechanism for a Nucleophilic Aromatic Substitution from QM/MM Simulations. Organic Letters, 2004, 6, 2881-2884.	2.4	97
97	Molecular dynamics of proteins with the OPLS potential functions. Simulation of the third domain of silver pheasant ovomucoid in water. Journal of the American Chemical Society, 1990, 112, 2773-2781.	6.6	95
98	Free energies of solvation in chloroform and water from a linear response approach. Journal of Physical Organic Chemistry, 1997, 10, 563-576.	0.9	92
99	Limited effects of polarization for Clâ¯(H2O)n and Na+(H2O)n clusters. Journal of Chemical Physics, 1993, 99, 4233-4235.	1.2	90
100	Monte Carlo Simulations for Proteins:Â Binding Affinities for Trypsinâ¯Benzamidine Complexes via Free-Energy Perturbations. Journal of Physical Chemistry B, 1997, 101, 9663-9669.	1.2	88
101	Prediction of Activity for Nonnucleoside Inhibitors with HIV-1 Reverse Transcriptase Based on Monte Carlo Simulations. Journal of Medicinal Chemistry, 2002, 45, 2970-2987.	2.9	88
102	Monte Carlo backbone sampling for polypeptides with variable bond angles and dihedral angles using concerted rotations and a Gaussian bias. Journal of Chemical Physics, 2003, 118, 4261-4271.	1.2	88
103	Conformation of Alkanes in the Gas Phase and Pure Liquids. Journal of Physical Chemistry B, 2006, 110, 21198-21204.	1.2	88
104	Optimization of Azoles as Anti-Human Immunodeficiency Virus Agents Guided by Free-Energy Calculations. Journal of the American Chemical Society, 2008, 130, 9492-9499.	6.6	88
105	Prediction of Binding Affinities for TIBO Inhibitors of HIV-1 Reverse Transcriptase Using Monte Carlo Simulations in a Linear Response Method. Journal of Medicinal Chemistry, 1998, 41, 5272-5286.	2.9	87
106	FEP-Guided Selection of Bicyclic Heterocycles in Lead Optimization for Non-Nucleoside Inhibitors of HIV-1 Reverse Transcriptase. Journal of the American Chemical Society, 2006, 128, 15372-15373.	6.6	86
107	Why Urea Eliminates Ammonia Rather than Hydrolyzes in Aqueous Solution. Journal of Physical Chemistry B, 2007, 111, 720-730.	1.2	85
108	Characterization of Biaryl Torsional Energetics and its Treatment in OPLS All-Atom Force Fields. Journal of Chemical Information and Modeling, 2013, 53, 1191-1199.	2.5	84

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109	Catalytic Mechanism and Performance of Computationally Designed Enzymes for Kemp Elimination. Journal of the American Chemical Society, 2008, 130, 15907-15915.	6.6	83
110	Elucidation of Hydrolysis Mechanisms for Fatty Acid Amide Hydrolase and Its Lys142Ala Variant via QM/MM Simulations. Journal of the American Chemical Society, 2006, 128, 16904-16913.	6.6	82
111	Effects of Water Placement on Predictions of Binding Affinities for p38Î± MAP Kinase Inhibitors. Journal of Chemical Theory and Computation, 2010, 6, 3850-3856.	2.3	81
112	Search for Non-Nucleoside Inhibitors of HIV-1 Reverse Transcriptase Using Chemical Similarity, Molecular Docking, and MM-GB/SA Scoring. Journal of Chemical Information and Modeling, 2007, 47, 2416-2428.	2.5	79
113	Understanding Rate Accelerations for Dielsâ˜'Alder Reactions in Solution Using Enhanced QM/MM Methodology. Journal of Chemical Theory and Computation, 2007, 3, 1412-1419.	2.3	78
114	Picomolar Inhibitors of HIV Reverse Transcriptase Featuring Bicyclic Replacement of a Cyanovinylphenyl Group. Journal of the American Chemical Society, 2013, 135, 16705-16713.	6.6	78
115	Polypeptide Folding Using Monte Carlo Sampling, Concerted Rotation, and Continuum Solvation. Journal of the American Chemical Society, 2004, 126, 1849-1857.	6.6	77
116	Elucidation of Rate Variations for a Dielsâ˜'Alder Reaction in Ionic Liquids from QM/MM Simulations. Journal of Chemical Theory and Computation, 2007, 3, 132-138.	2.3	77
117	Extension of the PDDG/PM3 and PDDG/MNDO semiempirical molecular orbital methods to the halogens. Journal of Computational Chemistry, 2004, 25, 138-150.	1.5	76
118	Estimation of the binding affinities of FKBP12 inhibitors using a linear response method. Bioorganic and Medicinal Chemistry, 1999, 7, 851-860.	1.4	75
119	Importance of Polarization for Dipolar Solutes in Low-Dielectric Media: 1,2-Dichloroethane and Water in Cyclohexane. Journal of the American Chemical Society, 1995, 117, 11809-11810.	6.6	74
120	Validation of a Model for the Complex of HIV-1 Reverse Transcriptase with Nonnucleoside Inhibitor TMC125. Journal of the American Chemical Society, 2003, 125, 6016-6017.	6.6	74
121	Cope Elimination:Â Elucidation of Solvent Effects from QM/MM Simulations. Journal of the American Chemical Society, 2006, 128, 6141-6146.	6.6	74
122	Contributions of Conformational Compression and Preferential Transition State Stabilization to the Rate Enhancement by Chorismate Mutase. Journal of the American Chemical Society, 2003, 125, 6892-6899.	6.6	73
123	Polarization Effects for Hydrogen-Bonded Complexes of Substituted Phenols with Water and Chloride Ion. Journal of Chemical Theory and Computation, 2007, 3, 1987-1992.	2.3	73
124	Limiting Cardiac Ischemic Injury by Pharmacological Augmentation of Macrophage Migration Inhibitory Factorâ€"AMP-Activated Protein Kinase Signal Transduction. Circulation, 2013, 128, 225-236.	1.6	73
125	An empirical boundary potential for water droplet simulations. Journal of Computational Chemistry, 1995, 16, 951-972.	1.5	72
126	A comprehensive study of the rotational energy profiles of organic systems byab initio MO theory, forming a basis for peptide torsional parameters. Journal of Computational Chemistry, 1995, 16, 984-1010.	1.5	72

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127	Steric and Solvation Effects in Ionic S_N2 Reactions. Journal of the American Chemical Society, 2009, 131, 16162-16170.	6.6	72
128	Extension of the PDDG/PM3 Semiempirical Molecular Orbital Method to Sulfur, Silicon, and Phosphorus. Journal of Chemical Theory and Computation, 2005, 1, 817-823.	2.3	70
129	Basis set dependence of the structure and properties of liquid hydrogen fluoride. Journal of Chemical Physics, 1979, 70, 5888-5897.	1.2	69
130	Monte Carlo Investigations of Selective Anion Complexation by a Bis(phenylurea)p-tert-Butylcalix[4]arene. Journal of the American Chemical Society, 1998, 120, 5104-5111.	6.6	69
131	Hostâ€“guest chemistry of rotaxanes and catenanes: application of a polarizable all-atom force field to cyclobis(paraquat-p-phenylene) complexes with disubstituted benzenes and biphenylsâ€Šâ€. Journal of the Chemical Society Perkin Transactions II, 1999, , 2365-2375.	0.9	69
132	In Silico Improvement of Î²³-Peptide Inhibitors of p53â€¢hDM2 and p53â€¢hDMX. Journal of the American Chemical Society, 2009, 131, 6356-6357.	6.6	68
133	From Docking False-Positive to Active Anti-HIV Agent. Journal of Medicinal Chemistry, 2007, 50, 5324-5329.	2.9	65
134	Efficient Discovery of Potent Anti-HIV Agents Targeting the Tyr181Cys Variant of HIV Reverse Transcriptase. Journal of the American Chemical Society, 2011, 133, 15686-15696.	6.6	64
135	Design, Synthesis, and Protein Crystallography of Biaryltriazoles as Potent Tautomerase Inhibitors of Macrophage Migration Inhibitory Factor. Journal of the American Chemical Society, 2015, 137, 2996-3003.	6.6	63
136	Optimization of N-benzyl-benzoxazol-2-ones as receptor antagonists of macrophage migration inhibitory factor (MIF). Bioorganic and Medicinal Chemistry Letters, 2010, 20, 5811-5814.	1.0	62
137	Comparison of 6-31G*-based MST/SCRF and FEP evaluations of the free energies of hydration for small neutral molecules. Journal of Computational Chemistry, 1993, 14, 1498-1503.	1.5	61
138	Quantum and statistical mechanical studies of liquids. 20. Pressure dependence of hydrogen bonding in liquid methanol. Journal of the American Chemical Society, 1982, 104, 373-378.	6.6	60
139	Discovery of Novel Fibroblast Growth Factor Receptor 1 Kinase Inhibitors by Structure-Based Virtual Screening. Journal of Medicinal Chemistry, 2010, 53, 1662-1672.	2.9	60
140	Conformational Complexity of Succinic Acid and Its Monoanion in the Gas Phase and in Solution:Â Ab Initio Calculations and Monte Carlo Simulations. Journal of the American Chemical Society, 1998, 120, 9672-9679.	6.6	58
141	Influence of Inter- and Intramolecular Hydrogen Bonding on Kemp Decarboxylations from QM/MM Simulations. Journal of the American Chemical Society, 2005, 127, 8829-8834.	6.6	57
142	Investigation of Solvent Effects for the Claisen Rearrangement of Chorismate to Prephenate:â€‰ Mechanistic Interpretation via Near Attack Conformations. Journal of the American Chemical Society, 2003, 125, 6663-6672.	6.6	56
143	Exploring Adsorption of Water and Ions on Carbon Surfaces Using a Polarizable Force Field. Journal of Physical Chemistry Letters, 2013, 4, 468-474.	2.1	56
144	Computer-aided discovery of anti-HIV agents. Bioorganic and Medicinal Chemistry, 2016, 24, 4768-4778.	1.4	56

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145	Monte Carlo Investigations of Solvent Effects on the Chorismate to Prephenate Rearrangement. Journal of the American Chemical Society, 1996, 118, 8475-8484.	6.6	55
146	Quantum Mechanical/Molecular Mechanical Modeling Finds Dielsâ^'Alder Reactions Are Accelerated Less on the Surface of Water Than in Water. Journal of the American Chemical Society, 2010, 132, 3097-3104.	6.6	55
147	Exploiting Structural Analysis, in Silico Screening, and Serendipity To Identify Novel Inhibitors of Drug-Resistant Falciparum Malaria. ACS Chemical Biology, 2009, 4, 29-40.	1.6	54
148	Evaluation of CM5 Charges for Condensed-Phase Modeling. Journal of Chemical Theory and Computation, 2014, 10, 2802-2812.	2.3	54
149	Monte Carlo simulations of liquid tetrahydrofuran including pseudorotation. Journal of Chemical Physics, 1982, 77, 5073-5079.	1.2	53
150	Exploring Solvent Effects upon the Menshutkin Reaction Using a Polarizable Force Field. Journal of Physical Chemistry B, 2010, 114, 8425-8430.	1.2	53
151	Validation of a Model for the Complex of HIV-1 Reverse Transcriptase with Sustiva through Computation of Resistance Profiles. Journal of the American Chemical Society, 2000, 122, 12898-12900.	6.6	52
152	Optimization of pyrimidinyl- and triazinyl-amines as non-nucleoside inhibitors of HIV-1 reverse transcriptase. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 5664-5667.	1.0	52
153	Development and Testing of the OPLS-AA/M Force Field for RNA. Journal of Chemical Theory and Computation, 2019, 15, 2734-2742.	2.3	51
154	Illustrating Concepts in Physical Organic Chemistry with 3D Printed Orbitals. Journal of Chemical Education, 2015, 92, 2113-2116.	1.1	50
155	Evaluation of CM5 Charges for Nonaqueous Condensed-Phase Modeling. Journal of Chemical Theory and Computation, 2015, 11, 4273-4282.	2.3	49
156	Antiviral drug design: computational analyses of the effects of the L100I mutation for HIV-RT on the binding of NNRTIs. Bioorganic and Medicinal Chemistry Letters, 2001, 11, 2799-2802.	1.0	48
157	General Model for Estimation of the Inhibition of Protein Kinases Using Monte Carlo Simulations. Journal of Medicinal Chemistry, 2004, 47, 2534-2549.	2.9	48
158	Crystal Structures of HIV-1 Reverse Transcriptase with Picomolar Inhibitors Reveal Key Interactions for Drug Design. Journal of the American Chemical Society, 2012, 134, 19501-19503.	6.6	48
159	Challenges for Academic Drug Discovery. Angewandte Chemie - International Edition, 2012, 51, 11680-11684.	7.2	48
160	Structure-Based Evaluation of Non-nucleoside Inhibitors with Improved Potency and Solubility That Target HIV Reverse Transcriptase Variants. Journal of Medicinal Chemistry, 2015, 58, 2737-2745.	2.9	48
161	Role of Macrophage Migration Inhibitory Factor in the Regulatory T Cell Response of Tumor-Bearing Mice. Journal of Immunology, 2012, 189, 3905-3913.	0.4	47
162	Quantum and statistical mechanical studies of liquids. 21. The nature of dilute solutions of sodium and methoxide ions in methanol. Journal of the American Chemical Society, 1982, 104, 4584-4591.	6.6	46

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