William L Jorgensen

List of Publications by Year
in descending order

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418 papers	97,352 citations	2671 95 h-index	244 303 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

#	Article	IF	Citations
163	Receptor agonists of macrophage migration inhibitory factor. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 7033-7036.	1.0	45
164	Pulled from a protein's embrace. Nature, 2010, 466, 42-43.	13.7	44
165	Estimation of Binding Affinities for Selective Thrombin Inhibitors via Monte Carlo Simulations. Journal of Medicinal Chemistry, 2001, 44, 1043-1050.	2.9	43
166	Small molecular modulation of macrophage migration inhibitory factor in the hyperoxia-induced mouse model of bronchopulmonary dysplasia. Respiratory Research, 2013, 14, 27.	1.4	43
167	Covalent inhibitors for eradication of drug-resistant HIV-1 reverse transcriptase: From design to protein crystallography. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 9725-9730.	3.3	43
168	Structure-guided design of a perampanel-derived pharmacophore targeting the SARS-CoV-2 main protease. Structure, 2021, 29, 823-833.e5.	1.6	43
169	Sampling methods for Monte Carlo simulations of nâ€butane in dilute solution. Journal of Chemical Physics, 1981, 75, 1944-1952.	1.2	42
170	Free energies of hydration for organic molecules from Monte Carlo simulations. Journal of Computer - Aided Molecular Design, 1995, 3, 123-138.	1.0	41
171	Optical Rotatory Dispersion of 2,3-Hexadiene and 2,3-Pentadiene. Journal of Physical Chemistry A, 2008, 112, 2415-2422.	1.1	41
172	Effect of hydration on the structure of an SN2 transition state. The Journal of Physical Chemistry, 1986, 90, 4651-4654.	2.9	40
173	Optimization of diarylamines as non-nucleoside inhibitors of HIV-1 reverse transcriptase. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 668-671.	1.0	40
174	Molecular dynamics and Monte Carlo simulations for proteinâ€“ligand binding and inhibitor design. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 966-971.	1.1	40
175	Improving MM-GB/SA Scoring through the Application of the Variable Dielectric Model. Journal of Chemical Theory and Computation, 2011, 7, 3859-3865.	2.3	39
176	Enhanced Monte Carlo Sampling through Replica Exchange with Solute Tempering. Journal of Chemical Theory and Computation, 2014, 10, 565-571.	2.3	39
177	Picomolar Inhibitors of HIV-1 Reverse Transcriptase: Design and Crystallography of Naphthyl Phenyl Ethers. ACS Medicinal Chemistry Letters, 2014, 5, 1259-1262.	1.3	39
178	Endothelial CD74 mediates macrophage migration inhibitory factor protection in hyperoxic lung injury. FASEB Journal, 2015, 29, 1940-1949.	0.2	39
179	Structural and Energetic Analyses of the Effects of the K103N Mutation of HIV-1 Reverse Transcriptase on Efavirenz Analogues. Journal of Medicinal Chemistry, 2004, 47, 2389-2392.	2.9	38
180	NO-MNDO:â€‰ Reintroduction of the Overlap Matrix into MNDO. Journal of Chemical Theory and Computation, 2006, 2, 413-419.	2.3	38

#	Article	IF	Citations
181	Discovery of Wild-Type and Y181C Mutant Non-nucleoside HIV-1 Reverse Transcriptase Inhibitors Using Virtual Screening with Multiple Protein Structures. Journal of Chemical Information and Modeling, 2009, 49, 1272-1279.	2.5	38
182	Identification and Characterization of JAK2 Pseudokinase Domain Small Molecule Binders. ACS Medicinal Chemistry Letters, 2017, 8, 618-621.	1.3	38
183	Advances and Insights for Small Molecule Inhibition of Macrophage Migration Inhibitory Factor. Journal of Medicinal Chemistry, 2018, 61, 8104-8119.	2.9	37
184	Optimization of Triarylpyridinone Inhibitors of the Main Protease of SARS-CoV-2 to Low-Nanomolar Antiviral Potency. ACS Medicinal Chemistry Letters, 2021, 12, 1325-1332.	1.3	37
185	Estimation of Binding Affinities for Celecoxib Analogues with COX-2 via Monte Carlo-Extended Linear Response. Bioorganic and Medicinal Chemistry Letters, 2002, 12, 267-270.	1.0	36
186	Eastern extension of azoles as non-nucleoside inhibitors of HIV-1 reverse transcriptase; cyano group alternatives. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 2485-2488.	1.0	36
187	Medium Effects on the Decarboxylation of a Biotin Model in Pure and Mixed Solvents from QM/MM Simulations. Journal of Organic Chemistry, 2006, 71, 4896-4902.	1.7	35
188	Polarized Protein-Specific Charges from Atoms-in-Molecule Electron Density Partitioning. Journal of Chemical Theory and Computation, 2013, 9, 2981-2991.	2.3	35
189	Enhanced Monte Carlo Methods for Modeling Proteins Including Computation of Absolute Free Energies of Binding. Journal of Chemical Theory and Computation, 2018, 14, 3279-3288.	2.3	35
190	Foundations of Biomolecular Modeling. Cell, 2013, 155, 1199-1202.	13.5	34
191	Selective Anion Complexation by a Calix[4]pyrrole Investigated by Monte Carlo Simulations. Journal of Organic Chemistry, 1999, 64, 7439-7444.	1.7	33
192	Computation of Accurate Activation Barriers for Methyl-Transfer Reactions of Sulfonium and Ammonium Salts in Aqueous Solution. Journal of Chemical Theory and Computation, 2007, 3, 1028-1035.	2.3	33
193	Virtual Screening and Optimization Yield Low-Nanomolar Inhibitors of the Tautomerase Activity of Plasmodium falciparum Macrophage Migration Inhibitory Factor. Journal of Medicinal Chemistry, 2012, 55, 10148-10159.	2.9	33
194	Optimization of diarylazines as anti-HIV agents with dramatically enhanced solubility. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 5213-5216.	1.0	33
195	Extension into the entrance channel of HIV-1 reverse transcriptaseâ€"Crystallography and enhanced solubility. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 5209-5212.	1.0	33
196	Cooperative Effects and Optimal Halogen Bonding Motifs for Self-Assembling Systems. Journal of Physical Chemistry A, 2014, 118, 2820-2826.	1.1	33
197	A Fluorescence Polarization Assay for Binding to Macrophage Migration Inhibitory Factor and Crystal Structures for Complexes of Two Potent Inhibitors. Journal of the American Chemical Society, 2016, 138, 8630-8638.	6.6	32
198	Investigations of Neurotrophic Inhibitors of FK506 Binding Protein via Monte Carlo Simulations. Journal of Medicinal Chemistry, 1998, 41, 3928-3939.	2.9	31

#	Article	IF	Citations
199	Efficient exploration of conformational space using the stochastic search method: application to ?-peptide oligomers. Journal of Computational Chemistry, 2001, 22, 1646-1654.	1.5	31
200	E/Z Energetics for Molecular Modeling and Design. Journal of Chemical Theory and Computation, 2010, 6, 2762-2769.	2.3	31
201	Systematic Study of Effects of Structural Modifications on the Aqueous Solubility of Drug-like Molecules. ACS Medicinal Chemistry Letters, 2017, 8, 124-127.	1.3	31
202	Quantification of Solvent Effects on the Acidities of Z and E Esters from Fluid Simulations. Journal of the American Chemical Society, 1994, 116, 10630-10638.	6.6	30
203	Generalized alteration of structure and parameters: A new method for free-energy perturbations in systems containing flexible degrees of freedom. Journal of Computational Chemistry, 1995, 16, 311-327.	1.5	30
204	Macrophage Migration Inhibitory Factor Is Detrimental in Pneumococcal Pneumonia and a Target for Therapeutic Immunomodulation. Journal of Infectious Diseases, 2015, 212, 1677-1682.	1.9	30
205	Improved Description of Sulfur Charge Anisotropy in OPLS Force Fields: Model Development and Parameterization. Journal of Physical Chemistry B, 2017, 121, 6626-6636.	1.2	30
206	From in silico hit to long-acting late-stage preclinical candidate to combat HIV-1 infection. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E802-E811.	3.3	30
207	Molecular Dynamics Simulations of a Conformationally Mobile Peptide-Based Catalyst for Atroposelective Bromination. ACS Catalysis, 2018, 8, 9968-9979.	5.5	30
208	Computational Binding Studies of Orthogonal Cyclosporin-Cyclophilin Pairs. Angewandte Chemie International Edition in English, 1997, 36, 1466-1469.	4.4	29
209	Activity predictions for efavirenz analogues with the K103N mutant of HIV reverse transcriptase. Bioorganic and Medicinal Chemistry Letters, 2003, 13, 3337-3340.	1.0	29
210	Effects of Arg90 Neutralization on the Enzyme-Catalyzed Rearrangement of Chorismate to Prephenate. Journal of Chemical Theory and Computation, 2005, 1, 617-625.	2.3	28
211	Thorpeâ"Ingold Acceleration of Oxirane Formation Is Mostly a Solvent Effect. Journal of the American Chemical Society, 2010, 132, 8766-8773.	6.6	28
212	Discovery of dimeric inhibitors by extension into the entrance channel of HIV-1 reverse transcriptase. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 1565-1568.	1.0	28
213	Structural studies provide clues for analog design of specific inhibitors of Cryptosporidium hominis thymidylate synthaseâ€"dihydrofolate reductase. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 4158-4161.	1.0	28
214	Monte Carlo calculations on HIV-1 reverse transcriptase complexed with the non-nucleoside inhibitor 8-Cl TIBO: contribution of the L100I and Y181C variants to protein stability and biological activity. Protein Engineering, Design and Selection, 2000, 13, 413-421.	1.0	27
215	Origin of the Inversion of the Acidity Order for Haloacetic Acids on Going from the Gas Phase to Solution. Journal of Physical Chemistry A, 2000, 104, 7625-7628.	1.1	27
216	Energy Profiles for Organic Reactions in Solution. Advances in Chemical Physics, 2007, , 469-488.	0.3	26

#	Article	IF	Citations
217	JAK2 JH2 Fluorescence Polarization Assay and Crystal Structures for Complexes with Three Small Molecules. ACS Medicinal Chemistry Letters, 2017, 8, 614-617.	1.3	26
218	OPLS allâ€atom force field for carbohydrates. Journal of Computational Chemistry, 1997, 18, 1955-1970.	1.5	26
219	Improved convergence of binding affinities with free energy perturbation: application to nonpeptide ligands with pp60src SH2 domain. , 2001, 15, 681-695.		25
220	Monte Carlo Backbone Sampling for Nucleic Acids Using Concerted Rotations Including Variable Bond Angles. Journal of Physical Chemistry B, 2004, 108, 16883-16892.	1.2	24
221	Rationale for the observed COX-2/COX-1 selectivity of celecoxib from Monte Carlo simulations. Bioorganic and Medicinal Chemistry Letters, 2001, 11, 1541-1544.	1.0	23
222	Improved semiempirical heats of formation through the use of bond and group equivalents. Journal of Computational Chemistry, 2002, 23, 498-510.	1.5	23
223	Analyses of Activity for Factor Xa Inhibitors Based on Monte Carlo Simulations. Journal of Medicinal Chemistry, 2003, 46, 5691-5699.	2.9	23
224	Synthesis and Evaluation of Selected Key Methyl Ether Derivatives of Vancomycin Aglycon. Journal of Medicinal Chemistry, 2010, 53, 7229-7235.	2.9	23
225	Irregularities in enzyme assays: The case of macrophage migration inhibitory factor. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 2764-2767.	1.0	23
226	Viability of molecular modeling with pentium-based PCs. Journal of Computational Chemistry, 1996, 17, 1385-1386.	1.5	22
227	Origin of the Activity Drop with the E50D Variant of Catalytic Antibody 34E4 for Kemp Elimination. Journal of Physical Chemistry B, 2009, 113, 497-504.	1.2	22
228	Potent Inhibitors Active against HIV Reverse Transcriptase with K101P, a Mutation Conferring Rilpivirine Resistance. ACS Medicinal Chemistry Letters, 2015, 6, 1075-1079.	1.3	22
229	Design, Conformation, and Crystallography of 2-Naphthyl Phenyl Ethers as Potent Anti-HIV Agents. ACS Medicinal Chemistry Letters, 2016, 7, 1156-1160.	1.3	22
230	On the Mechanism and Rate of Spontaneous Decomposition of Amino Acids. Journal of Physical Chemistry B, 2011, 115, 13624-13632.	1.2	21
231	Benzisothiazolones as modulators of macrophage migration inhibitory factor. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 4545-4549.	1.0	21
232	Structureâ€Based Evaluation of C5 Derivatives in the Catechol Diether Series Targeting <scp>HIV</scp>â€1 Reverse Transcriptase. Chemical Biology and Drug Design, 2014, 83, 541-549.	1.5	21
233	Explicit Representation of Cationâ‹¯Ï€ Interactions in Force Fields with 1/r⁴ Nonbonded Terms. Journal of Chemical Theory and Computation, 2020, 16, 7184-7194.	2.3	21
234	SCRF/Monte Carlo Study of Solvent Effects on a Polar [2+2] Cycloaddition. The Journal of Physical Chemistry, 1996, 100, 17490-17500.	2.9	20

#	Article	IF	Citations
235	Computation of proteinâ€“ligand binding free energies using quantum mechanical bespoke force fields. MedChemComm, 2019, 10, 1116-1120.	3.5	20
236	Illuminating HIV gp120-ligand recognition through computationally-driven optimization of antibody-recruiting molecules. Chemical Science, 2014, 5, 2311-2317.	3.7	19
237	Discovery and crystallography of bicyclic arylaminoazines as potent inhibitors of HIV-1 reverse transcriptase. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 4824-4827.	1.0	19
238	Novel non-active site inhibitor of Cryptosporidium hominis TS-DHFR identified by a virtual screen. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 418-423.	1.0	18
239	Optimization of benzyloxazoles as non-nucleoside inhibitors of HIV-1 reverse transcriptase to enhance Y181C potency. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 1110-1113.	1.0	18
240	Crystallographic and Receptor Binding Characterization of Plasmodium falciparum Macrophage Migration Inhibitory Factor Complexed to Two Potent Inhibitors. Journal of Medicinal Chemistry, 2014, 57, 8652-8656.	2.9	18
241	Biochemical Assays for the Discovery of TDP1 Inhibitors. Molecular Cancer Therapeutics, 2014, 13, 2116-2126.	1.9	18
242	Unbinding Dynamics of Non-Nucleoside Inhibitors from HIV-1 Reverse Transcriptase. Journal of Physical Chemistry B, 2019, 123, 1741-1748.	1.2	18
243	Rapid estimation of electronic degrees of freedom in Monte Carlo calculations for polarizable models of liquid water. Journal of Chemical Physics, 2001, 114, 9337-9349.	1.2	17
244	Determination of partial molar volumes from free energy perturbation theory. Physical Chemistry Chemical Physics, 2015, 17, 8407-8415.	1.3	17
245	Absolute Free Energy of Binding Calculations for Macrophage Migration Inhibitory Factor in Complex with a Druglike Inhibitor. Journal of Physical Chemistry B, 2019, 123, 8675-8685.	1.2	17
246	Selective Janus Kinase 2 (JAK2) Pseudokinase Ligands with a Diaminotriazole Core. Journal of Medicinal Chemistry, 2020, 63, 5324-5340.	2.9	17
247	Performance of Proteinâ€“Ligand Force Fields for the Flavodoxinâ€“Flavin Mononucleotide System. Journal of Physical Chemistry Letters, 2016, 7, 3032-3036.	2.1	16
248	Improved treatment of nucleosides and nucleotides in the OPLS-AA force field. Chemical Physics Letters, 2017, 683, 276-280.	1.2	16
249	Robust Free Energy Perturbation Protocols for Creating Molecules in Solution. Journal of Chemical Theory and Computation, 2019, 15, 3941-3948.	2.3	16
250	Quantum and statistical mechanical studies of liquids. Part 22. Pressure dependence of mixing enantiomeric liquids: 1,2-dichloropropane. The Journal of Physical Chemistry, 1982, 86, 2867-2873.	2.9	15
251	Vancomycin analogs: Seeking improved binding of d-Ala-d-Ala and d-Ala-d-Lac peptides by side-chain and backbone modifications. Bioorganic and Medicinal Chemistry, 2009, 17, 5874-5886.	1.4	15
252	Computationally-guided optimization of small-molecule inhibitors of the Aurora A kinaseâ€“TPX2 proteinâ€“protein interaction. Chemical Communications, 2017, 53, 9372-9375.	2.2	15

#	Article	IF	Citations
253	Structural and pharmacological evaluation of a novel non-nucleoside reverse transcriptase inhibitor as a promising long acting nanoformulation for treating HIV. Antiviral Research, 2019, 167, 110-116.	1.9	15
254	Structure-Guided Identification of DNMT3B Inhibitors. ACS Medicinal Chemistry Letters, 2020, 11, 971-976.	1.3	15
255	Covalent Inhibition of Wild-Type HIV-1 Reverse Transcriptase Using a Fluorosulfate Warhead. ACS Medicinal Chemistry Letters, 2021, 12, 249-255.	1.3	15
256	Ab initio studies of RO? ? HOR? complexes. Solvent effects on the relative acidities of water and methanol. Journal of Computational Chemistry, 1981, 2, 7-11.	1.5	14
257	Investigation of Solvent Effects on the Rate and Stereoselectivity of the Henry Reaction. Organic Letters, 2012, 14, 260-263.	2.4	14
258	Structural and Preclinical Studies of Computationally Designed Non-Nucleoside Reverse Transcriptase Inhibitors for Treating HIV infection. Molecular Pharmacology, 2017, 91, 383-391.	1.0	14
259	Optimization of Pyrazoles as Phenol Surrogates to Yield Potent Inhibitors of Macrophage Migration Inhibitory Factor. ChemMedChem, 2018, 13, 1092-1097.	1.6	14
260	Vancomycin resistance: Modeling backbone variants with d-Ala-d-Ala and d-Ala-d-Lac peptides. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 1236-1239.	1.0	13
261	Confronting Racism in Chemistry Journals. ACS Applied Materials & Interfaces, 2020, 12, 28925-28927.	4.0	13
262	Application of a BOSSâ€"Gaussian interface for <scp>QM/MM</scp> simulations of <scp>H</scp>enry and methyl transfer reactions. Journal of Computational Chemistry, 2015, 36, 2064-2074.	1.5	12
263	Metadynamics as a Postprocessing Method for Virtual Screening with Application to the Pseudokinase Domain of JAK2. Journal of Chemical Information and Modeling, 2020, 60, 4403-4415.	2.5	12
264	Aryl extensions of thienopyrimidinones as fibroblast growth factor receptor 1 kinase inhibitors. Tetrahedron Letters, 2011, 52, 2228-2231.	0.7	11
265	A nanotherapy strategy significantly enhances anticryptosporidial activity of an inhibitor of bifunctional thymidylate synthase-dihydrofolate reductase from Cryptosporidium. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 2065-2067.	1.0	11
266	QM/MM Calculations for the Cl^{â€“} + CH₃Cl S_N2 Reaction in Water Using CM5 Charges and Density Functional Theory. Journal of Physical Chemistry A, 2019, 123, 5713-5717.	1.1	11
267	Chapter 14 Solvent Effects on Organic Reactions from QM/MM Simulations. Annual Reports in Computational Chemistry, 2006, , 263-278.	0.9	10
268	A mechanistic and structural investigation of modified derivatives of the diaryltriazine class of NNRTIs targeting HIV-1 reverse transcriptase. Biochimica Et Biophysica Acta - General Subjects, 2014, 1840, 2203-2211.	1.1	10
269	Computational binding studies of human pp60c-src SH2 domain with a series of nonpeptide, phosphophenyl-containing ligands. Bioorganic and Medicinal Chemistry Letters, 2000, 10, 2067-2070.	1.0	9
270	Perspective on "Equation of state calculations by fast computing machines". Theoretical Chemistry Accounts, 2000, 103, 225-227.	0.5	9

#	Article	IF	Citations
271	Virtual screening reveals allosteric inhibitors of the Toxoplasma gondii thymidylate synthaseâ€“dihydrofolate reductase. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 1232-1235.	1.0	9
272	Hydration Properties and Solvent Effects for All-Atom Solutes in Polarizable Coarse-Grained Water. Journal of Physical Chemistry B, 2016, 120, 8102-8114.	1.2	9
273	Claisen Rearrangement of Allyl Vinyl Ether. ACS Symposium Series, 1994, , 243-259.	0.5	8
274	Solvent as Catalyst: Computational Studies of Organic Reactions in Solution. ACS Symposium Series, 1999, , 74-85.	0.5	8
275	Adding a Hydrogen Bond May Not Help: Naphthyridinone vs Quinoline Inhibitors of Macrophage Migration Inhibitory Factor. ACS Medicinal Chemistry Letters, 2017, 8, 1287-1291.	1.3	8
276	Assault on Resistance: The Use of Computational Chemistry in the Development of Anti-HIV Drugs. Current Pharmaceutical Design, 2006, 12, 1843-1856.	0.9	7
277	Structural investigation of <scp>2â€naphthyl</scp> phenyl ether inhibitors bound to <scp>WT</scp> and <scp>Y181C</scp> reverse transcriptase highlights key features of the <scp>NNRTI</scp> binding site. Protein Science, 2020, 29, 1902-1910.	3.1	7
278	Indoloxytriazines as binding molecules for the JAK2 JH2 pseudokinase domain and its V617F variant. Tetrahedron Letters, 2021, 77, 153248.	0.7	7
279	Structural Studies and Structure Activity Relationships for Novel Computationally Designed Non-nucleoside Inhibitors and Their Interactions With HIV-1 Reverse Transcriptase. Frontiers in Molecular Biosciences, 2022, 9, 805187.	1.6	7
280	Insights on JAK2 Modulation by Potent, Selective, and Cell-Permeable Pseudokinase-Domain Ligands. Journal of Medicinal Chemistry, 2022, 65, 8380-8400.	2.9	7
281	Comment on simulations of liquid ammonia based on quantum mechanical potential functions. Journal of Chemical Physics, 1981, 75, 2026-2027.	1.2	6
282	Energetic effects for observed and unobserved HIV-1 reverse transcriptase mutations of residues L100, V106, and Y181 in the presence of nevirapine and efavirenz. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 969-972.	1.0	6
283	Novel allosteric covalent inhibitors of bifunctional Cryptosporidium hominis TS-DHFR from parasitic protozoa identified by virtual screening. Bioorganic and Medicinal Chemistry Letters, 2019, 29, 1413-1418.	1.0	6
284	Conversion of a False Virtual Screen Hit into Selective JAK2 JH2 Domain Binders Using Convergent Design Strategies. ACS Medicinal Chemistry Letters, 2022, 13, 819-826.	1.3	6
285	Structure activity relationship towards design of cryptosporidium specific thymidylate synthase inhibitors. European Journal of Medicinal Chemistry, 2019, 183, 111673.	2.6	5
286	Update to Our Reader, Reviewer, and Author Communitiesâ€”April 2020. ACS Applied Materials & Interfaces, 2020, 12, 20147-20148.	4.0	5
287	Confronting Racism in Chemistry Journals. Nano Letters, 2020, 20, 4715-4717.	4.5	5
288	Longâ€acting and extendedâ€release implant and nanoformulations with a synergistic antiretroviral twoâ€drug combination controls HIV â€¡ infection in a humanized mouse model. Bioengineering and Translational Medicine, 2022, 7, e10237.	3.9	5

#	Article	IF	Citations
289	Molecular and cellular studies evaluating a potent 2-cyanoindolizine catechol diether NNRTI targeting wildtype and Y181C mutant HIV-1 reverse transcriptase. Bioorganic and Medicinal Chemistry Letters, 2019, 29, 2182-2188.	1.0	4
290	Confronting Racism in Chemistry Journals. Organic Letters, 2020, 22, 4919-4921.	2.4	4
291	A Reflection on Paul von RaguÃ© Schleyer. Journal of Chemical Theory and Computation, 2015, 11, 1-1.	2.3	3
292	Understanding the structural basis of species selective, stereospecific inhibition for Cryptosporidium and human thymidylate synthase. FEBS Letters, 2019, 593, 2069-2078.	1.3	3
293	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Journal of the American Chemical Society, 2020, 142, 8059-8060.	6.6	3
294	Progress and issues for computationally guided lead discovery and optimization. , 2010, , 1-14.		2
295	Autobiography of William L. Jorgensen: Scientific History and Recollections. Journal of Physical Chemistry B, 2015, 119, 624-632.	1.2	2
296	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. ACS Nano, 2020, 14, 5151-5152.	7.3	2
297	Confronting Racism in Chemistry Journals. ACS Nano, 2020, 14, 7675-7677.	7.3	2
298	Targeting the TS dimer interface in bifunctional Cryptosporidium hominis TS-DHFR from parasitic protozoa: Virtual screening identifies novel TS allosteric inhibitors. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 127292.	1.0	2
299	Confronting Racism in Chemistry Journals. Chemical Reviews, 2020, 120, 5795-5797.	23.0	2
300	OPLS all-atom force field for carbohydrates. , 1997, 18, 1955.		2
301	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. ACS Energy Letters, 2020, 5, 1610-1611.	8.8	1
302	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Environmental Science and Technology Letters, 2020, 7, 280-281.	3.9	1
303	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Journal of Chemical Education, 2020, 97, 1217-1218.	1.1	1
304	Confronting Racism in Chemistry Journals. Journal of Physical Chemistry Letters, 2020, 11, 5279-5281.	2.1	1
305	Confronting Racism in Chemistry Journals. ACS Central Science, 2020, 6, 1012-1014.	5.3	1
306	Confronting Racism in Chemistry Journals. Journal of the American Society for Mass Spectrometry, 2020, 31, 1321-1323.	1.2	1

#	Article	IF	Citations
307	Confronting Racism in Chemistry Journals. Crystal Growth and Design, 2020, 20, 4201-4203.	1.4	1
308	Confronting Racism in Chemistry Journals. ACS Catalysis, 2020, 10, 7307-7309.	5.5	1
309	Confronting Racism in Chemistry Journals. Journal of the American Chemical Society, 2020, 142, 11319-11321.	6.6	1
310	Confronting Racism in Chemistry Journals. Journal of Physical Chemistry B, 2020, 124, 5335-5337.	1.2	1
311	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Crystal Growth and Design, 2020, 20, 2817-2818.	1.4	1
312	A Reflection on Norman Louis Allinger. Journal of Chemical Theory and Computation, 2021, 17, 2013-2013.	2.3	1
313	Confronting Racism in Chemistry Journals. ACS Biomaterials Science and Engineering, 2020, 6, 3690-3692.	2.6	1
314	Confronting Racism in Chemistry Journals. ACS Omega, 2020, 5, 14857-14859.	1.6	1
315	Confronting Racism in Chemistry Journals. Molecular Pharmaceutics, 2020, 17, 2229-2231.	2.3	1
316	Confronting Racism in Chemistry Journals. ACS Chemical Neuroscience, 2020, 11, 1852-1854.	1.7	1
317	Reply to Pandey et al.: Understanding the efficacy of a potential antiretroviral drug candidate in humanized mouse model of HIV infection. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E8114-E8115.	3.3	0
318	Confronting Racism in Chemistry Journals. ACS Pharmacology and Translational Science, 2020, 3, 559-561.	2.5	0
319	Confronting Racism in Chemistry Journals. Biochemistry, 2020, 59, 2313-2315.	1.2	0
320	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. ACS Biomaterials Science and Engineering, 2020, 6, 2707-2708.	2.6	0
321	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. ACS Central Science, 2020, 6, 589-590.	5.3	0
322	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. ACS Chemical Biology, 2020, 15, 1282-1283.	1.6	0
323	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. ACS Chemical Neuroscience, 2020, 11, 1196-1197.	1.7	0
324	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. ACS Earth and Space Chemistry, 2020, 4, 672-673.	1.2	0

#	Article	IF	Citations
325	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. ACS Macro Letters, 2020, 9, 666-667.	2.3	0
326	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. , 2020, 2, 563-564.		0
327	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. ACS Photonics, 2020, 7, 1080-1081.	3.2	0
328	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. ACS Pharmacology and Translational Science, 2020, 3, 455-456.	2.5	0
329	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. ACS Sustainable Chemistry and Engineering, 2020, 8, 6574-6575.	3.2	0
330	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Analytical Chemistry, 2020, 92, 6187-6188.	3.2	0
331	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Chemistry of Materials, 2020, 32, 3678-3679.	3.2	0
332	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Journal of Proteome Research, 2020, 19, 1883-1884.	1.8	0
333	Confronting Racism in Chemistry Journals. Langmuir, 2020, 36, 7155-7157.	1.6	0
334	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. ACS Applied Polymer Materials, 2020, 2, 1739-1740.	2.0	0
335	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. ACS Combinatorial Science, 2020, 22, 223-224.	3.8	0
336	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. ACS Medicinal Chemistry Letters, 2020, 11, 1060-1061.	1.3	0
337	Editorial Confronting Racism in Chemistry Journals. , 2020, 2, 829-831.		0
338	Confronting Racism in Chemistry Journals. ACS Applied Energy Materials, 2020, 3, 6016-6018.	2.5	0
339	Confronting Racism in Chemistry Journals. Industrial & Engineering Chemistry Research, 2020, 59, 11915-11917.	1.8	0
340	Confronting Racism in Chemistry Journals. Journal of Natural Products, 2020, 83, 2057-2059.	1.5	0
341	Confronting Racism in Chemistry Journals. ACS Medicinal Chemistry Letters, 2020, 11, 1354-1356.	1.3	0
342	Confronting Racism in Chemistry Journals. Energy & Fuels, 2020, 34, 7771-7773.	2.5	0

#	Article	IF	Citations
343	Confronting Racism in Chemistry Journals. ACS Sensors, 2020, 5, 1858-1860.	4.0	0
344	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Biochemistry, 2020, 59, 1641-1642.	1.2	0
345	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Journal of Chemical & Engineering Data, 2020, 65, 2253-2254.	1.0	0
346	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Organic Process Research and Development, 2020, 24, 872-873.	1.3	0
347	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. ACS Omega, 2020, 5, 9624-9625.	1.6	0
348	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. ACS Applied Electronic Materials, 2020, 2, 1184-1185.	2.0	0
349	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Journal of Physical Chemistry C, 2020, 124, 9629-9630.	1.5	0
350	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Journal of Physical Chemistry Letters, 2020, 11, 3571-3572.	2.1	0
351	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. ACS Synthetic Biology, 2020, 9, 979-980.	1.9	0
352	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. ACS Applied Energy Materials, 2020, 3, 4091-4092.	2.5	0
353	Confronting Racism in Chemistry Journals. Journal of Chemical Theory and Computation, 2020, 16, 4003-4005.	2.3	0
354	Confronting Racism in Chemistry Journals. Journal of Organic Chemistry, 2020, 85, 8297-8299.	1.7	0
355	Confronting Racism in Chemistry Journals. Analytical Chemistry, 2020, 92, 8625-8627.	3.2	0
356	Confronting Racism in Chemistry Journals. Journal of Chemical Education, 2020, 97, 1695-1697.	1.1	0
357	Confronting Racism in Chemistry Journals. Organic Process Research and Development, 2020, 24, 1215-1217.	1.3	0
358	Confronting Racism in Chemistry Journals. ACS Sustainable Chemistry and Engineering, 2020, 8, .	3.2	0
359	Confronting Racism in Chemistry Journals. Chemistry of Materials, 2020, 32, 5369-5371.	3.2	0
360	Confronting Racism in Chemistry Journals. Chemical Research in Toxicology, 2020, 33, 1511-1513.	1.7	0

#	Article	IF	Citations
361	Confronting Racism in Chemistry Journals. Inorganic Chemistry, 2020, 59, 8639-8641.	1.9	0
362	Confronting Racism in Chemistry Journals. ACS Applied Nano Materials, 2020, 3, 6131-6133.	2.4	0
363	Confronting Racism in Chemistry Journals. ACS Applied Polymer Materials, 2020, 2, 2496-2498.	2.0	0
364	Confronting Racism in Chemistry Journals. ACS Chemical Biology, 2020, 15, 1719-1721.	1.6	0
365	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Journal of Chemical Theory and Computation, 2020, 16, 2881-2882.	2.3	0
366	Confronting Racism in Chemistry Journals. Biomacromolecules, 2020, 21, 2543-2545.	2.6	0
367	Confronting Racism in Chemistry Journals. Journal of Medicinal Chemistry, 2020, 63, 6575-6577.	2.9	0
368	Confronting Racism in Chemistry Journals. Macromolecules, 2020, 53, 5015-5017.	2.2	0
369	Confronting Racism in Chemistry Journals. Organometallics, 2020, 39, 2331-2333.	1.1	0
370	Confronting Racism in Chemistry Journals. Accounts of Chemical Research, 2020, 53, 1257-1259.	7.6	0
371	Confronting Racism in Chemistry Journals. Journal of Physical Chemistry A, 2020, 124, 5271-5273.	1.1	0
372	Confronting Racism in Chemistry Journals. ACS Energy Letters, 2020, 5, 2291-2293.	8.8	0
373	Confronting Racism in Chemistry Journals. Journal of Chemical Information and Modeling, 2020, 60, 3325-3327.	2.5	0
374	Confronting Racism in Chemistry Journals. Journal of Proteome Research, 2020, 19, 2911-2913.	1.8	0
375	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Journal of Agricultural and Food Chemistry, 2020, 68, 5019-5020.	2.4	0
376	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Journal of Physical Chemistry B, 2020, 124, 3603-3604.	1.2	0
377	Confronting Racism in Chemistry Journals. Bioconjugate Chemistry, 2020, 31, 1693-1695.	1.8	0
378	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. ACS Applied Nano Materials, 2020, 3, 3960-3961.	2.4	0

#	Article	IF	Citations
379	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Journal of Natural Products, 2020, 83, 1357-1358.	1.5	0
380	Confronting Racism in Chemistry Journals. ACS Synthetic Biology, 2020, 9, 1487-1489.	1.9	0
381	Confronting Racism in Chemistry Journals. Journal of Chemical & Engineering Data, 2020, 65, 3403-3405.	1.0	0
382	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Bioconjugate Chemistry, 2020, 31, 1211-1212.	1.8	0
383	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Journal of Chemical Health and Safety, 2020, 27, 133-134.	1.1	0
384	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Chemical Research in Toxicology, 2020, 33, 1509-1510.	1.7	0
385	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Energy & Fuels, 2020, 34, 5107-5108.	2.5	0
386	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. ACS Applied Bio Materials, 2020, 3, 2873-2874.	2.3	0
387	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Journal of Organic Chemistry, 2020, 85, 5751-5752.	1.7	0
388	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Journal of the American Society for Mass Spectrometry, 2020, 31, 1006-1007.	1.2	0
389	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Accounts of Chemical Research, 2020, 53, 1001-1002.	7.6	0
390	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Biomacromolecules, 2020, 21, 1966-1967.	2.6	0
391	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Chemical Reviews, 2020, 120, 3939-3940.	23.0	0
392	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Environmental Science & Technology, 2020, 54, 5307-5308.	4.6	0
393	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Langmuir, 2020, 36, 4565-4566.	1.6	0
394	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Molecular Pharmaceutics, 2020, 17, 1445-1446.	2.3	0
395	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. ACS Infectious Diseases, 2020, 6, 891-892.	1.8	0
396	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Journal of Medicinal Chemistry, 2020, 63, 4409-4410.	2.9	0

#	Article	IF	Citations
397	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Journal of Physical Chemistry A, 2020, 124, 3501-3502.	1.1	0
398	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Nano Letters, 2020, 20, 2935-2936.	4.5	0
399	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. ACS Sensors, 2020, 5, 1251-1252.	4.0	0
400	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Journal of Chemical Information and Modeling, 2020, 60, 2651-2652.	2.5	0
401	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Industrial & Engineering Chemistry Research, 2020, 59, 8509-8510.	1.8	0
402	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Inorganic Chemistry, 2020, 59, 5796-5797.	1.9	0
403	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Organometallics, 2020, 39, 1665-1666.	1.1	0
404	Update to Our Reader, Reviewer, and Author Communitiesâ€"April 2020. Organic Letters, 2020, 22, 3307-3308.	2.4	0
405	Confronting Racism in Chemistry Journals. ACS ES&T Engineering, 2021, 1, 3-5.	3.7	0
406	Confronting Racism in Chemistry Journals. ACS ES&T Water, 2021, 1, 3-5.	2.3	0
407	Confronting Racism in Chemistry Journals. ACS Applied Electronic Materials, 2020, 2, 1774-1776.	2.0	0
408	Confronting Racism in Chemistry Journals. Journal of Agricultural and Food Chemistry, 2020, 68, 6941-6943.	2.4	0
409	Confronting Racism in Chemistry Journals. ACS Earth and Space Chemistry, 2020, 4, 961-963.	1.2	0
410	Confronting Racism in Chemistry Journals. Environmental Science and Technology Letters, 2020, 7, 447-449.	3.9	0
411	Confronting Racism in Chemistry Journals. ACS Combinatorial Science, 2020, 22, 327-329.	3.8	0
412	Confronting Racism in Chemistry Journals. ACS Infectious Diseases, 2020, 6, 1529-1531.	1.8	0
413	Confronting Racism in Chemistry Journals. ACS Applied Bio Materials, 2020, 3, 3925-3927.	2.3	0
414	Confronting Racism in Chemistry Journals. Journal of Physical Chemistry C, 2020, 124, 14069-14071.	1.5	0

#	Article	IF	Citations
415	Confronting Racism in Chemistry Journals. ACS Macro Letters, 2020, 9, 1004-1006.	2.3	0
416	Confronting Racism in Chemistry Journals. ACS Photonics, 2020, 7, 1586-1588.	3.2	0
417	Confronting Racism in Chemistry Journals. Environmental Science & Technology, 2020, 54, 7735-7737.	4.6	0
418	Confronting Racism in Chemistry Journals. Journal of Chemical Health and Safety, 2020, 27, 198-200.	1.1	0