William L Jorgensen

List of Publications by Citations

299 papers	80,293 citations	92 h-index	283 g-index
426 ext. papers	89,207 ext. citations	7.6 avg, IF	8.04 L-index

#	Paper	IF	Citations
299	Comparison of simple potential functions for simulating liquid water. *Journal of Chemical Physics*, **1983**, 79, 926-935	3.9	27805
298	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	16.4	9849
297	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, 1657-66	16.4	3825
296	Evaluation and Reparametrization of the OPLS-AA Force Field for Proteins via Comparison with Accurate Quantum Chemical Calculations on Peptides. *Journal of Physical Chemistry B*, **2001**, 105, 6474-6487	3.4	2979
295	Optimized intermolecular potential functions for liquid hydrocarbons. *Journal of the American Chemical Society*, **1984**, 106, 6638-6646	16.4	1815
294	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	3.9	1778
293	OPLS3: A Force Field Providing Broad Coverage of Drug-like Small Molecules and Proteins. *Journal of Chemical Theory and Computation*, **2016**, 12, 281-96	6.4	1555
292	The many roles of computation in drug discovery. *Science*, **2004**, 303, 1813-8	33.3	1088
291	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	16.4	1024
290	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	16.4	961
289	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, 6665-70	11.5	770
288	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, 2695-703	16.4	633
287	Temperature and size dependence for Monte Carlo simulations of TIP4P water. *Molecular Physics*, **1985**, 56, 1381-1392	1.7	630
286	Monte Carlo simulation of differences in free energies of hydration. *Journal of Chemical Physics*, **1985**, 83, 3050-3054	3.9	607
285	Performance of B3LYP Density Functional Methods for a Large Set of Organic Molecules. *Journal of Chemical Theory and Computation*, **2008**, 4, 297-306	6.4	601
284	Free energy calculations: a breakthrough for modeling organic chemistry in solution. *Accounts of Chemical Research*, **1989**, 22, 184-189	24.3	550
283	Prediction of drug solubility from structure. *Advanced Drug Delivery Reviews*, **2002**, 54, 355-66	18.5	541

282	OPLS all-atom force field for carbohydrates. *Journal of Computational Chemistry*, **1997**, 18, 1955-1970	3.5	535
281	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	16.4	534
280	OPLS All-Atom Model for Amines: Resolution of the Amine Hydration Problem. *Journal of the American Chemical Society*, **1999**, 121, 4827-4836	16.4	528
279	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	16.4	496
278	Efficient drug lead discovery and optimization. *Accounts of Chemical Research*, **2009**, 42, 724-33	24.3	487
277	Revised TIPS for simulations of liquid water and aqueous solutions. *Journal of Chemical Physics*, **1982**, 77, 4156-4163	3.9	456
276	Improved Peptide and Protein Torsional Energetics with the OPLSAA Force Field. *Journal of Chemical Theory and Computation*, **2015**, 11, 3499-509	6.4	391
275	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	3.5	380
274	Ab Initio Study of Hydrogen-Bonded Complexes of Small Organic Molecules with Water. *Journal of Physical Chemistry A*, **1998**, 102, 3782-3797	2.8	376
273	Prediction of Properties from Simulations: Free Energies of Solvation in Hexadecane, Octanol, and Water. *Journal of the American Chemical Society*, **2000**, 122, 2878-2888	16.4	370
272	LigParGen web server: an automatic OPLS-AA parameter generator for organic ligands. *Nucleic Acids Research*, **2017**, 45, W331-W336	20.1	366
271	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	16.4	343
270	Perfluoroalkanes: Conformational Analysis and Liquid-State Properties from ab Initio and Monte Carlo Calculations. *Journal of Physical Chemistry A*, **2001**, 105, 4118-4125	2.8	340
269	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	3.5	338
268	Molecular modeling of organic and biomolecular systems using BOSS and MCPRO. *Journal of Computational Chemistry*, **2005**, 26, 1689-700	3.5	324
267	Halide, Ammonium, and Alkali Metal Ion Parameters for Modeling Aqueous Solutions. *Journal of Chemical Theory and Computation*, **2006**, 2, 1499-509	6.4	298
266	Diffusion constant of the TIP5P model of liquid water. *Journal of Chemical Physics*, **2001**, 114, 363	3.9	286
265	Prediction of drug solubility from Monte Carlo simulations. *Bioorganic and Medicinal Chemistry Letters*, **2000**, 10, 1155-8	2.9	281

264	Monte Carlo simulations of the hydration of ammonium and carboxylate ions. *The Journal of Physical Chemistry*, **1986**, 90, 2174-2182		280
263	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		272
262	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	3.4	270
261	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	3.9	269
260	PDDG/PM3 and PDDG/MNDO: improved semiempirical methods. *Journal of Computational Chemistry*, **2002**, 23, 1601-22	3.5	268
259	Development of an all-atom force field for heterocycles. Properties of liquid pyridine and diazenes. *Computational and Theoretical Chemistry*, **1998**, 424, 145-155		260
258	Methyl effects on protein-ligand binding. *Journal of Medicinal Chemistry*, **2012**, 55, 4489-500	8.3	252
257	Developing a dynamic pharmacophore model for HIV-1 integrase. *Journal of Medicinal Chemistry*, **2000**, 43, 2100-14	8.3	248
256	SN2 reaction profiles in the gas phase and aqueous solution. *Journal of the American Chemical Society*, **1984**, 106, 3049-3050	16.4	234
255	Perspective on Free-Energy Perturbation Calculations for Chemical Equilibria. *Journal of Chemical Theory and Computation*, **2008**, 4, 869-876	6.4	226
254	An Extended Linear Response Method for Determining Free Energies of Hydration. *The Journal of Physical Chemistry*, **1995**, 99, 10667-10673		226
253	Performance of the AMBER94, MMFF94, and OPLS-AA Force Fields for Modeling Organic Liquids. *The Journal of Physical Chemistry*, **1996**, 100, 18010-18013		220
252	Monte Carlo simulations of liquid acetonitrile with a three-site model. *Molecular Physics*, **1988**, 63, 547-558	1.7	211
251	Contribution of conformer focusing to the uncertainty in predicting free energies for protein-ligand binding. *Journal of Medicinal Chemistry*, **2006**, 49, 5880-4	8.3	210
250	Treatment of Halogen Bonding in the OPLS-AA Force Field; Application to Potent Anti-HIV Agents. *Journal of Chemical Theory and Computation*, **2012**, 8, 3895-3801	6.4	206
249	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	16.4	202
248	Advances in quantum and molecular mechanical (QM/MM) simulations for organic and enzymatic reactions. *Accounts of Chemical Research*, **2010**, 43, 142-51	24.3	201
247	Energetics of displacing water molecules from protein binding sites: consequences for ligand optimization. *Journal of the American Chemical Society*, **2009**, 131, 15403-11	16.4	196

246	Theoretical studies of medium effects on conformational equilibria. *The Journal of Physical Chemistry*, **1983**, 87, 5304-5314		194
245	1.14*CM1A-LBCC: Localized Bond-Charge Corrected CM1A Charges for Condensed-Phase Simulations. *Journal of Physical Chemistry B*, **2017**, 121, 3864-3870	3.4	185
244	Rusting of the lock and key model for protein-ligand binding. *Science*, **1991**, 254, 954-5	33.3	176
243	Free Energies of Hydration from a Generalized Born Model and an All-Atom Force Field. *Journal of Physical Chemistry B*, **2004**, 108, 16264-16270	3.4	164
242	The many faces of halogen bonding: a review of theoretical models and methods. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 523-540	7.9	163
241	Molecular dynamics simulations of the unfolding of barnase in water and 8 M aqueous urea. *Biochemistry*, **1997**, 36, 7313-29	3.2	162
240	Binding affinities for sulfonamide inhibitors with human thrombin using Monte Carlo simulations with a linear response method. *Journal of Medicinal Chemistry*, **1997**, 40, 1539-49	8.3	162
239	Steric retardation of SN2 reactions in the gas phase and solution. *Journal of the American Chemical Society*, **2004**, 126, 9054-8	16.4	157
238	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	2.3	157
237	QM/MM Simulations for Diels□Alder Reactions in Water: Contribution of Enhanced Hydrogen Bonding at the Transition State to the Solvent Effect□*Journal of Physical Chemistry B*, **2002**, 106, 8078-8085	3.4	154
236	Prediction of the water content in protein binding sites. *Journal of Physical Chemistry B*, **2009**, 113, 13337-46	3.4	153
235	Do denaturants interact with aromatic hydrocarbons in water?. *Journal of the American Chemical Society*, **1993**, 115, 9271-9275	16.4	145
234	Monte Carlo simulations of pure liquid substituted benzenes with OPLS potential functions. *Journal of Computational Chemistry*, **1993**, 14, 206-215	3.5	145
233	Elucidation of fatty acid amide hydrolase inhibition by potent alpha-ketoheterocycle derivatives from Monte Carlo simulations. *Journal of the American Chemical Society*, **2005**, 127, 17377-84	16.4	143
232	Accuracy of free energies of hydration for organic molecules from 6-31g*-derived partial charges. *Journal of Computational Chemistry*, **1993**, 14, 1240-1249	3.5	142
231	Monte Carlo simulations of the hydration of substituted benzenes with OPLS potential functions. *Journal of Computational Chemistry*, **1993**, 14, 195-205	3.5	140
230	Monte Carlo simulations of liquid acetic acid and methyl acetate with the OPLS potential functions. *The Journal of Physical Chemistry*, **1991**, 95, 3315-3322		132
229	Monte Carlo simulations of liquid alkyl ethers with the OPLS potential functions. *Journal of Computational Chemistry*, **1990**, 11, 958-971	3.5	131

228	Comparison of SCC-DFTB and NDDO-based semiempirical molecular orbital methods for organic molecules. *Journal of Physical Chemistry A*, **2006**, 110, 13551-9	2.8	127
227	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	16.4	126
226	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	16.4	123
225	Accuracy of free energies of hydration using CM1 and CM3 atomic charges. *Journal of Computational Chemistry*, **2004**, 25, 1322-32	3.5	120
224	Monte Carlo vs Molecular Dynamics for Conformational Sampling. *The Journal of Physical Chemistry*, **1996**, 100, 14508-14513		119
223	New Linear Interaction Method for Binding Affinity Calculations Using a Continuum Solvent Model. *Journal of Physical Chemistry B*, **2001**, 105, 10388-10397	3.4	116
222	A remote arene-binding site on prostate specific membrane antigen revealed by antibody-recruiting small molecules. *Journal of the American Chemical Society*, **2010**, 132, 12711-6	16.4	112
221	Computational approaches to molecular recognition. *Current Opinion in Chemical Biology*, **1997**, 1, 449-57	9.7	110
220	A Quantum Mechanical and Molecular Mechanical Method Based on CM1A Charges: Applications to Solvent Effects on Organic Equilibria and Reactions. *Journal of Physical Chemistry B*, **1998**, 102, 1787-1796	3.4	109
219	Computer-aided design of non-nucleoside inhibitors of HIV-1 reverse transcriptase. *Bioorganic and Medicinal Chemistry Letters*, **2006**, 16, 663-7	2.9	107
218	Monte Carlo simulation of n-butane in water. Conformational evidence for the hydrophobic effect. *Journal of Chemical Physics*, **1982**, 77, 5757-5765	3.9	107
217	Discovery of human macrophage migration inhibitory factor (MIF)-CD74 antagonists via virtual screening. *Journal of Medicinal Chemistry*, **2009**, 52, 416-24	8.3	106
216	Computational Investigations of Carbenium Ion Reactions Relevant to Sterol Biosynthesis. *Journal of the American Chemical Society*, **1997**, 119, 10846-10854	16.4	104
215	Macrophomate synthase: QM/MM simulations address the Diels-Alder versus Michael-Aldol reaction mechanism. *Journal of the American Chemical Society*, **2005**, 127, 3577-88	16.4	104
214	Computationally-guided optimization of a docking hit to yield catechol diethers as potent anti-HIV agents. *Journal of Medicinal Chemistry*, **2011**, 54, 8582-91	8.3	103
213	The nature of dilute solutions of sodium ion in water, methanol, and tetrahydrofuran. *Journal of Chemical Physics*, **1982**, 77, 5080-5089	3.9	101
212	An improved intermolecular potential function for simulations of liquid hydrogen fluoride. *Molecular Physics*, **1984**, 51, 119-132	1.7	99
211	Identification of 14 Known Drugs as Inhibitors of the Main Protease of SARS-CoV-2. *ACS Medicinal Chemistry Letters*, **2020**, 11, 2526-2533	4.3	98

210	Estimation of binding affinities for HEPT and nevirapine analogues with HIV-1 reverse transcriptase via Monte Carlo simulations. *Journal of Medicinal Chemistry*, **2001**, 44, 145-54	8.3	94
209	Urea: Potential Functions, log P, and Free Energy of Hydration. *Israel Journal of Chemistry*, **1993**, 33, 323-330	3.4	93
208	Free energies of solvation in chloroform and water from a linear response approach. *Journal of Physical Organic Chemistry*, **1997**, 10, 563-576	2.1	92
207	Solvent effects and mechanism for a nucleophilic aromatic substitution from QM/MM simulations. *Organic Letters*, **2004**, 6, 2881-4	6.2	92
206	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	16.4	92
205	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	3.9	89
204	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	16.4	88
203	Limited effects of polarization for Cl(H2O)n and Na+(H2O)n clusters. *Journal of Chemical Physics*, **1993**, 99, 4233-4235	3.9	87
202	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	3.9	85
201	Optimization of azoles as anti-human immunodeficiency virus agents guided by free-energy calculations. *Journal of the American Chemical Society*, **2008**, 130, 9492-9	16.4	84
200	Monte Carlo Simulations for Proteins: Binding Affinities for Trypsin-Benzamidine Complexes via Free-Energy Perturbations. *Journal of Physical Chemistry B*, **1997**, 101, 9663-9669	3.4	83
199	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, 5272-86	8.3	83
198	Prediction of activity for nonnucleoside inhibitors with HIV-1 reverse transcriptase based on Monte Carlo simulations. *Journal of Medicinal Chemistry*, **2002**, 45, 2970-87	8.3	82
197	Biomolecular Force Field Parameterization via Atoms-in-Molecule Electron Density Partitioning. *Journal of Chemical Theory and Computation*, **2016**, 12, 2312-23	6.4	82
196	Catalytic mechanism and performance of computationally designed enzymes for Kemp elimination. *Journal of the American Chemical Society*, **2008**, 130, 15907-15	16.4	80
195	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, 15372-3	16.4	80
194	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, 16904-13	16.4	79
193	Polypeptide folding using Monte Carlo sampling, concerted rotation, and continuum solvation. *Journal of the American Chemical Society*, **2004**, 126, 1849-57	16.4	76

192	Why urea eliminates ammonia rather than hydrolyzes in aqueous solution. *Journal of Physical Chemistry B*, **2007**, 111, 720-30	3.4	75
191	Conformation of alkanes in the gas phase and pure liquids. *Journal of Physical Chemistry B*, **2006**, 110, 21198-204	3.4	75
190	Effects of Water Placement on Predictions of Binding Affinities for p38 MAP Kinase Inhibitors. *Journal of Chemical Theory and Computation*, **2010**, 6, 3850-3856	6.4	73
189	Estimation of the binding affinities of FKBP12 inhibitors using a linear response method. *Bioorganic and Medicinal Chemistry*, **1999**, 7, 851-60	3.4	73
188	Characterization of biaryl torsional energetics and its treatment in OPLS all-atom force fields. *Journal of Chemical Information and Modeling*, **2013**, 53, 1191-9	6.1	70
187	Understanding Rate Accelerations for Diels-Alder Reactions in Solution Using Enhanced QM/MM Methodology. *Journal of Chemical Theory and Computation*, **2007**, 3, 1412-9	6.4	70
186	Elucidation of Rate Variations for a Diels-Alder Reaction in Ionic Liquids from QM/MM Simulations. *Journal of Chemical Theory and Computation*, **2007**, 3, 132-8	6.4	70
185	An empirical boundary potential for water droplet simulations. *Journal of Computational Chemistry*, **1995**, 16, 951-972	3.5	70
184	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	16.8	70
183	Cope elimination: elucidation of solvent effects from QM/MM simulations. *Journal of the American Chemical Society*, **2006**, 128, 6141-6	16.4	69
182	Extension of the PDDG/PM3 and PDDG/MNDO semiempirical molecular orbital methods to the halogens. *Journal of Computational Chemistry*, **2004**, 25, 138-50	3.5	69
181	Contributions of conformational compression and preferential transition state stabilization to the rate enhancement by chorismate mutase. *Journal of the American Chemical Society*, **2003**, 125, 6892-9	16.4	69
180	A comprehensive study of the rotational energy profiles of organic systems by ab initio MO theory, forming a basis for peptide torsional parameters. *Journal of Computational Chemistry*, **1995**, 16, 984-1010	3.5	69
179	Validation of a model for the complex of HIV-1 reverse transcriptase with nonnucleoside inhibitor TMC125. *Journal of the American Chemical Society*, **2003**, 125, 6016-7	16.4	66
178	Host–guest chemistry of rotaxanes and catenanes: application of a polarizable all-atom force field to cyclobis(paraquat-p-phenylene) complexes with disubstituted benzenes and biphenyls. *Journal of the Chemical Society Perkin Transactions II*, **1999**, 2365-2375		66
177	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	16.4	66
176	Basis set dependence of the structure and properties of liquid hydrogen fluoride. *Journal of Chemical Physics*, **1979**, 70, 5888-5897	3.9	66
175	Picomolar inhibitors of HIV reverse transcriptase featuring bicyclic replacement of a cyanovinylphenyl group. *Journal of the American Chemical Society*, **2013**, 135, 16705-13	16.4	64

174	Extension of the PDDG/PM3 Semiempirical Molecular Orbital Method to Sulfur, Silicon, and Phosphorus. *Journal of Chemical Theory and Computation*, **2005**, 1, 817-23	6.4	64
173	Polarization Effects for Hydrogen-Bonded Complexes of Substituted Phenols with Water and Chloride Ion. *Journal of Chemical Theory and Computation*, **2007**, 3, 1987-1992	6.4	63
172	From docking false-positive to active anti-HIV agent. *Journal of Medicinal Chemistry*, **2007**, 50, 5324-9	8.3	63
171	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	16.4	63
170	Steric and solvation effects in ionic S(N)2 reactions. *Journal of the American Chemical Society*, **2009**, 131, 16162-70	16.4	62
169	In Silico Improvement of beta3-peptide inhibitors of p53 x hDM2 and p53 x hDMX. *Journal of the American Chemical Society*, **2009**, 131, 6356-7	16.4	62
168	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, 2416-28	6.1	61
167	Limiting cardiac ischemic injury by pharmacological augmentation of macrophage migration inhibitory factor-AMP-activated protein kinase signal transduction. *Circulation*, **2013**, 128, 225-36	16.7	60
166	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	3.5	59
165	Efficient discovery of potent anti-HIV agents targeting the Tyr181Cys variant of HIV reverse transcriptase. *Journal of the American Chemical Society*, **2011**, 133, 15686-96	16.4	57
164	Optimization of N-benzyl-benzoxazol-2-ones as receptor antagonists of macrophage migration inhibitory factor (MIF). *Bioorganic and Medicinal Chemistry Letters*, **2010**, 20, 5811-4	2.9	56
163	Conformational Complexity of Succinic Acid and Its Monoanion in the Gas Phase and in Solution: Ab Initio Calculations and Monte Carlo Simulations. *Journal of the American Chemical Society*, **1998**, 120, 9672-9679	16.4	56
162	Influence of inter- and intramolecular hydrogen bonding on kemp decarboxylations from QM/MM simulations. *Journal of the American Chemical Society*, **2005**, 127, 8829-34	16.4	53
161	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	16.4	53
160	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	16.4	52
159	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	16.4	51
158	Quantum mechanical/molecular mechanical modeling finds Diels-Alder reactions are accelerated less on the surface of water than in water. *Journal of the American Chemical Society*, **2010**, 132, 3097-104	16.4	50
157	Discovery of novel fibroblast growth factor receptor 1 kinase inhibitors by structure-based virtual screening. *Journal of Medicinal Chemistry*, **2010**, 53, 1662-72	8.3	50

156	Optimization of pyrimidinyl- and triazinyl-amines as non-nucleoside inhibitors of HIV-1 reverse transcriptase. *Bioorganic and Medicinal Chemistry Letters*, **2006**, 16, 5664-7	2.9	49
155	Monte Carlo simulations of liquid tetrahydrofuran including pseudorotation. *Journal of Chemical Physics*, **1982**, 77, 5073-5079	3.9	49
154	Computer-aided discovery of anti-HIV agents. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 4768-4778	3.4	48
153	Exploring solvent effects upon the Menshutkin reaction using a polarizable force field. *Journal of Physical Chemistry B*, **2010**, 114, 8425-30	3.4	48
152	Exploiting structural analysis, in silico screening, and serendipity to identify novel inhibitors of drug-resistant falciparum malaria. *ACS Chemical Biology*, **2009**, 4, 29-40	4.9	48
151	Monte Carlo Investigations of Solvent Effects on the Chorismate to Prephenate Rearrangement. *Journal of the American Chemical Society*, **1996**, 118, 8475-8484	16.4	48
150	General model for estimation of the inhibition of protein kinases using Monte Carlo simulations. *Journal of Medicinal Chemistry*, **2004**, 47, 2534-49	8.3	47
149	Investigation of solvent effects for the Claisen rearrangement of chorismate to prephenate: mechanistic interpretation via near attack conformations. *Journal of the American Chemical Society*, **2003**, 125, 6663-72	16.4	46
148	Exploring Adsorption of Water and Ions on Carbon Surfaces using a Polarizable Force Field. *Journal of Physical Chemistry Letters*, **2013**, 4, 468-474	6.4	45
147	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, 2799-802	2.9	45
146	Evaluation of CM5 Charges for Condensed-Phase Modeling. *Journal of Chemical Theory and Computation*, **2014**, 10, 2802-2812	6.4	44
145	Illustrating Concepts in Physical Organic Chemistry with 3D Printed Orbitals. *Journal of Chemical Education*, **2015**, 92, 2113-2116	2.4	44
144	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	16.4	44
143	Structure-based evaluation of non-nucleoside inhibitors with improved potency and solubility that target HIV reverse transcriptase variants. *Journal of Medicinal Chemistry*, **2015**, 58, 2737-45	8.3	42
142	Estimation of binding affinities for selective thrombin inhibitors via Monte Carlo simulations. *Journal of Medicinal Chemistry*, **2001**, 44, 1043-50	8.3	42
141	Crystal structures of HIV-1 reverse transcriptase with picomolar inhibitors reveal key interactions for drug design. *Journal of the American Chemical Society*, **2012**, 134, 19501-3	16.4	41
140	Challenges for academic drug discovery. *Angewandte Chemie - International Edition*, **2012**, 51, 11680-4	16.4	41
139	Optical rotatory dispersion of 2,3-hexadiene and 2,3-pentadiene. *Journal of Physical Chemistry A*, **2008**, 112, 2415-22	2.8	40

138	Evaluation of CM5 Charges for Nonaqueous Condensed-Phase Modeling. *Journal of Chemical Theory and Computation*, **2015**, 11, 4273-82	6.4	38
137	Receptor agonists of macrophage migration inhibitory factor. *Bioorganic and Medicinal Chemistry Letters*, **2010**, 20, 7033-6	2.9	38
136	Optimization of diarylamines as non-nucleoside inhibitors of HIV-1 reverse transcriptase. *Bioorganic and Medicinal Chemistry Letters*, **2006**, 16, 668-71	2.9	38
135	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, 1272-9	6.1	37
134	Sampling methods for Monte Carlo simulations of n-butane in dilute solution. *Journal of Chemical Physics*, **1981**, 75, 1944-1952	3.9	37
133	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, 2389-92	8.3	36
132	Estimation of binding affinities for celecoxib analogues with COX-2 via Monte Carlo-extended linear response. *Bioorganic and Medicinal Chemistry Letters*, **2002**, 12, 267-70	2.9	36
131	Medium effects on the decarboxylation of a biotin model in pure and mixed solvents from QM/MM simulations. *Journal of Organic Chemistry*, **2006**, 71, 4896-902	4.2	35
130	Free energies of hydration for organic molecules from Monte Carlo simulations. *Journal of Computer - Aided Molecular Design*, **1995**, 3, 123-138		35
129	Effect of hydration on the structure of an SN2 transition state. *The Journal of Physical Chemistry*, **1986**, 90, 4651-4654		35
128	Small molecular modulation of macrophage migration inhibitory factor in the hyperoxia-induced mouse model of bronchopulmonary dysplasia. *Respiratory Research*, **2013**, 14, 27	7.3	34
127	Role of macrophage migration inhibitory factor in the regulatory T cell response of tumor-bearing mice. *Journal of Immunology*, **2012**, 189, 3905-13	5.3	34
126	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, 1028-35	6.4	33
125	NO-MNDO: Reintroduction of the Overlap Matrix into MNDO. *Journal of Chemical Theory and Computation*, **2006**, 2, 413-9	6.4	33
124	Enhanced Monte Carlo Sampling through Replica Exchange with Solute Tempering. *Journal of Chemical Theory and Computation*, **2014**, 10, 565-571	6.4	32
123	Eastern extension of azoles as non-nucleoside inhibitors of HIV-1 reverse transcriptase; cyano group alternatives. *Bioorganic and Medicinal Chemistry Letters*, **2010**, 20, 2485-8	2.9	32
122	Selective Anion Complexation by a Calix[4]pyrrole Investigated by Monte Carlo Simulations. *Journal of Organic Chemistry*, **1999**, 64, 7439-7444	4.2	32
121	Investigations of neurotrophic inhibitors of FK506 binding protein via Monte Carlo simulations. *Journal of Medicinal Chemistry*, **1998**, 41, 3928-39	8.3	31

120	Molecular dynamics and Monte Carlo simulations for protein-ligand binding and inhibitor design. *Biochimica Et Biophysica Acta - General Subjects*, **2015**, 1850, 966-971	4	30
119	Picomolar Inhibitors of HIV-1 Reverse Transcriptase: Design and Crystallography of Naphthyl Phenyl Ethers. *ACS Medicinal Chemistry Letters*, **2014**, 5, 1259-62	4.3	30
118	Cooperative effects and optimal halogen bonding motifs for self-assembling systems. *Journal of Physical Chemistry A*, **2014**, 118, 2820-6	2.8	30
117	Extension into the entrance channel of HIV-1 reverse transcriptase--crystallography and enhanced solubility. *Bioorganic and Medicinal Chemistry Letters*, **2013**, 23, 5209-12	2.9	30
116	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, 10148-59	8.3	30
115	Improving MM-GB/SA Scoring through the Application of the Variable Dielectric Model. *Journal of Chemical Theory and Computation*, **2011**, 7, 3859-3865	6.4	29
114	Computational Binding Studies of Orthogonal Cyclosporin-Cyclophilin Pairs. *Angewandte Chemie International Edition in English*, **1997**, 36, 1466-1469		29
113	Activity predictions for efavirenz analogues with the K103N mutant of HIV reverse transcriptase. *Bioorganic and Medicinal Chemistry Letters*, **2003**, 13, 3337-40	2.9	29
112	Efficient exploration of conformational space using the stochastic search method: application to peptide oligomers. *Journal of Computational Chemistry*, **2001**, 22, 1646-1654	3.5	29
111	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	16.4	29
110	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	11.5	28
109	Optimization of diarylazines as anti-HIV agents with dramatically enhanced solubility. *Bioorganic and Medicinal Chemistry Letters*, **2013**, 23, 5213-6	2.9	28
108	Polarized Protein-Specific Charges from Atoms-in-Molecule Electron Density Partitioning. *Journal of Chemical Theory and Computation*, **2013**, 9, 2981-2991	6.4	28
107	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	11.5	28
106	Endothelial CD74 mediates macrophage migration inhibitory factor protection in hyperoxic lung injury. *FASEB Journal*, **2015**, 29, 1940-9	0.9	27
105	Development and Testing of the OPLS-AA/M Force Field for RNA. *Journal of Chemical Theory and Computation*, **2019**, 15, 2734-2742	6.4	26
104	Discovery of dimeric inhibitors by extension into the entrance channel of HIV-1 reverse transcriptase. *Bioorganic and Medicinal Chemistry Letters*, **2012**, 22, 1565-8	2.9	26
103	Effects of Arg90 Neutralization on the Enzyme-Catalyzed Rearrangement of Chorismate to Prephenate. *Journal of Chemical Theory and Computation*, **2005**, 1, 617-25	6.4	26

102	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	2.8	26
101	OPLS all-atom force field for carbohydrates **1997**, 18, 1955		26
100	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, 8630-8	16.4	25
99	Foundations of biomolecular modeling. *Cell*, **2013**, 155, 1199-202	56.2	25
98	Energy Profiles for Organic Reactions in Solution. *Advances in Chemical Physics*, **2007**, 469-488		25
97	Improved convergence of binding affinities with free energy perturbation: application to nonpeptide ligands with pp60src SH2 domain. *Journal of Computer-Aided Molecular Design*, **2001**, 15, 681-95	4.2	25
96	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	3.5	25
95	Thorpe-Ingold acceleration of oxirane formation is mostly a solvent effect. *Journal of the American Chemical Society*, **2010**, 132, 8766-73	16.4	24
94	Monte Carlo Backbone Sampling for Nucleic Acids Using Concerted Rotations Including Variable Bond Angles. *Journal of Physical Chemistry B*, **2004**, 108, 16883-16892	3.4	24
93	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, 413-21	1.9	24
92	Macrophage Migration Inhibitory Factor Is Detrimental in Pneumococcal Pneumonia and a Target for Therapeutic Immunomodulation. *Journal of Infectious Diseases*, **2015**, 212, 1677-82	7	23
91	E/Z Energetics for Molecular Modeling and Design. *Journal of Chemical Theory and Computation*, **2010**, 6, 2762-2769	6.4	23
90	Analyses of activity for factor Xa inhibitors based on Monte Carlo simulations. *Journal of Medicinal Chemistry*, **2003**, 46, 5691-9	8.3	23
89	Rationale for the observed COX-2/COX-1 selectivity of celecoxib from Monte Carlo simulations. *Bioorganic and Medicinal Chemistry Letters*, **2001**, 11, 1541-4	2.9	23
88	Advances and Insights for Small Molecule Inhibition of Macrophage Migration Inhibitory Factor. *Journal of Medicinal Chemistry*, **2018**, 61, 8104-8119	8.3	23
87	Identification and Characterization of JAK2 Pseudokinase Domain Small Molecule Binders. *ACS Medicinal Chemistry Letters*, **2017**, 8, 618-621	4.3	22
86	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	3.4	22
85	Improved semiempirical heats of formation through the use of bond and group equivalents. *Journal of Computational Chemistry*, **2002**, 23, 498-510	3.5	22

84	Irregularities in enzyme assays: The case of macrophage migration inhibitory factor. *Bioorganic and Medicinal Chemistry Letters*, **2016**, 26, 2764-2767	2.9	22
83	Systematic Study of Effects of Structural Modifications on the Aqueous Solubility of Drug-like Molecules. *ACS Medicinal Chemistry Letters*, **2017**, 8, 124-127	4.3	21
82	Design, Conformation, and Crystallography of 2-Naphthyl Phenyl Ethers as Potent Anti-HIV Agents. *ACS Medicinal Chemistry Letters*, **2016**, 7, 1156-1160	4.3	21
81	Structural studies provide clues for analog design of specific inhibitors of Cryptosporidium hominis thymidylate synthase-dihydrofolate reductase. *Bioorganic and Medicinal Chemistry Letters*, **2014**, 24, 4158-61	2.9	21
80	Molecular Dynamics Simulations of a Conformationally Mobile Peptide-Based Catalyst for Atroposelective Bromination. *ACS Catalysis*, **2018**, 8, 9968-9979	13.1	21
79	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	6.4	20
78	JAK2 JH2 Fluorescence Polarization Assay and Crystal Structures for Complexes with Three Small Molecules. *ACS Medicinal Chemistry Letters*, **2017**, 8, 614-617	4.3	19
77	Potent Inhibitors Active against HIV Reverse Transcriptase with K101P, a Mutation Conferring Rilpivirine Resistance. *ACS Medicinal Chemistry Letters*, **2015**, 6, 1075-9	4.3	19
76	On the mechanism and rate of spontaneous decomposition of amino acids. *Journal of Physical Chemistry B*, **2011**, 115, 13624-32	3.4	19
75	Benzisothiazolones as modulators of macrophage migration inhibitory factor. *Bioorganic and Medicinal Chemistry Letters*, **2011**, 21, 4545-9	2.9	19
74	Improved Description of Sulfur Charge Anisotropy in OPLS Force Fields: Model Development and Parameterization. *Journal of Physical Chemistry B*, **2017**, 121, 6626-6636	3.4	18
73	Illuminating HIV gp120-Ligand Recognition through Computationally-Driven Optimization of Antibody-Recruiting Molecules. *Chemical Science*, **2014**, 5, 2311-2317	9.4	18
72	Viability of molecular modeling with pentium-based PCs. *Journal of Computational Chemistry*, **1996**, 17, 1385-6	3.5	18
71	Biochemical assays for the discovery of TDP1 inhibitors. *Molecular Cancer Therapeutics*, **2014**, 13, 2116-26	6.1	17
70	Synthesis and evaluation of selected key methyl ether derivatives of vancomycin aglycon. *Journal of Medicinal Chemistry*, **2010**, 53, 7229-35	8.3	17
69	Novel non-active site inhibitor of Cryptosporidium hominis TS-DHFR identified by a virtual screen. *Bioorganic and Medicinal Chemistry Letters*, **2009**, 19, 418-23	2.9	17
68	SCRF/Monte Carlo Study of Solvent Effects on a Polar [2+2] Cycloaddition. *The Journal of Physical Chemistry*, **1996**, 100, 17490-17500		17
67	Optimization of benzyloxazoles as non-nucleoside inhibitors of HIV-1 reverse transcriptase to enhance Y181C potency. *Bioorganic and Medicinal Chemistry Letters*, **2013**, 23, 1110-3	2.9	16

66	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	3.9	16
65	Crystallographic and receptor binding characterization of Plasmodium falciparum macrophage migration inhibitory factor complexed to two potent inhibitors. *Journal of Medicinal Chemistry*, **2014**, 57, 8652-6	8.3	15
64	Structural and Preclinical Studies of Computationally Designed Non-Nucleoside Reverse Transcriptase Inhibitors for Treating HIV infection. *Molecular Pharmacology*, **2017**, 91, 383-391	4.3	14
63	Discovery and crystallography of bicyclic arylaminoazines as potent inhibitors of HIV-1 reverse transcriptase. *Bioorganic and Medicinal Chemistry Letters*, **2015**, 25, 4824-4827	2.9	14
62	Determination of partial molar volumes from free energy perturbation theory. *Physical Chemistry Chemical Physics*, **2015**, 17, 8407-15	3.6	14
61	Structure-based evaluation of C5 derivatives in the catechol diether series targeting HIV-1 reverse transcriptase. *Chemical Biology and Drug Design*, **2014**, 83, 541-9	2.9	14
60	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	3.5	14
59	Improved Treatment of Nucleosides and Nucleotides in the OPLS-AA Force Field. *Chemical Physics Letters*, **2017**, 683, 276-280	2.5	13
58	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	10.8	13
57	Niedermolekulare Inhibitoren der Wechselwirkung zwischen der E3-Ligase VHL und HIF1□ *Angewandte Chemie*, **2012**, 124, 11630-11634	3.6	13
56	Investigation of solvent effects on the rate and stereoselectivity of the Henry reaction. *Organic Letters*, **2012**, 14, 260-3	6.2	13
55	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, 5874-86	3.4	13
54	Vancomycin resistance: modeling backbone variants with D-Ala-D-Ala and D-Ala-D-Lac peptides. *Bioorganic and Medicinal Chemistry Letters*, **2009**, 19, 1236-9	2.9	13
53	Computation of protein-ligand binding free energies using quantum mechanical bespoke force fields. *MedChemComm*, **2019**, 10, 1116-1120	5	13
52	Unbinding Dynamics of Non-Nucleoside Inhibitors from HIV-1 Reverse Transcriptase. *Journal of Physical Chemistry B*, **2019**, 123, 1741-1748	3.4	13
51	Optimization of Pyrazoles as Phenol Surrogates to Yield Potent Inhibitors of Macrophage Migration Inhibitory Factor. *ChemMedChem*, **2018**, 13, 1092-1097	3.7	12
50	Performance of Protein-Ligand Force Fields for the Flavodoxin-Flavin Mononucleotide System. *Journal of Physical Chemistry Letters*, **2016**, 7, 3032-6	6.4	12
49	Computationally-guided optimization of small-molecule inhibitors of the Aurora A kinase-TPX2 protein-protein interaction. *Chemical Communications*, **2017**, 53, 9372-9375	5.8	12

48	Explicit Representation of Cation-π Interactions in Force Fields with 1/ Nonbonded Terms. *Journal of Chemical Theory and Computation*, **2020**, 16, 7184-7194	6.4	12
47	Structure-guided design of a perampanel-derived pharmacophore targeting the SARS-CoV-2 main protease. *Structure*, **2021**, 29, 823-833.e5	5.2	12
46	Selective Janus Kinase 2 (JAK2) Pseudokinase Ligands with a Diaminotriazole Core. *Journal of Medicinal Chemistry*, **2020**, 63, 5324-5340	8.3	11
45	Application of a BOSS-Gaussian interface for QM/MM simulations of Henry and methyl transfer reactions. *Journal of Computational Chemistry*, **2015**, 36, 2064-74	3.5	11
44	Identification of 14 Known Drugs as Inhibitors of the Main Protease of SARS-CoV-2 **2020**,		11
43	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	3.4	10
42	Aryl Extensions of Thienopyrimidinones as Fibroblast Growth Factor Receptor 1 Kinase Inhibitors. *Tetrahedron Letters*, **2011**, 52, 2228-2231	2	10
41	Chapter 14 Solvent Effects on Organic Reactions from QM/MM Simulations. *Annual Reports in Computational Chemistry*, **2006**, 263-278	1.8	10
40	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		10
39	Robust Free Energy Perturbation Protocols for Creating Molecules in Solution. *Journal of Chemical Theory and Computation*, **2019**, 15, 3941-3948	6.4	9
38	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, 2065-7	2.9	9
37	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, 2203-11	4	9
36	Virtual screening reveals allosteric inhibitors of the Toxoplasma gondii thymidylate synthase-dihydrofolate reductase. *Bioorganic and Medicinal Chemistry Letters*, **2014**, 24, 1232-5	2.9	9
35	Perspective on Equation of state calculations by fast computing machines. *Theoretical Chemistry Accounts*, **2000**, 103, 225-227	1.9	9
34	Adding a Hydrogen Bond May Not Help: Naphthyridinone vs Quinoline Inhibitors of Macrophage Migration Inhibitory Factor. *ACS Medicinal Chemistry Letters*, **2017**, 8, 1287-1291	4.3	8
33	Computational binding studies of human pp60c-src SH2 domain with a series of nonpeptide, phosphophenyl-containing ligands. *Bioorganic and Medicinal Chemistry Letters*, **2000**, 10, 2067-70	2.9	8
32	Assault on resistance: the use of computational chemistry in the development of anti-HIV drugs. *Current Pharmaceutical Design*, **2006**, 12, 1843-56	3.3	7
31	Hydration Properties and Solvent Effects for All-Atom Solutes in Polarizable Coarse-Grained Water. *Journal of Physical Chemistry B*, **2016**, 120, 8102-14	3.4	7

30	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	4.3	7
29	QM/MM Calculations for the Cl + CHCl S2 Reaction in Water Using CM5 Charges and Density Functional Theory. *Journal of Physical Chemistry A*, **2019**, 123, 5713-5717	2.8	6
28	Structure-Guided Identification of DNMT3B Inhibitors. *ACS Medicinal Chemistry Letters*, **2020**, 11, 971-976	4.3	6
27	Herausforderungen f□die akademische Wirkstoff-Forschung. *Angewandte Chemie*, **2012**, 124, 11848-11853	3.8	6
26	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, 969-72	2.9	6
25	Solvent as Catalyst: Computational Studies of Organic Reactions in Solution. *ACS Symposium Series*, **1999**, 74-85	0.4	6
24	Claisen Rearrangement of Allyl Vinyl Ether. *ACS Symposium Series*, **1994**, 243-259	0.4	6
23	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	2.9	5
22	Covalent Inhibition of Wild-Type HIV-1 Reverse Transcriptase Using a Fluorosulfate Warhead. *ACS Medicinal Chemistry Letters*, **2021**, 12, 249-255	4.3	5
21	Structure activity relationship towards design of cryptosporidium specific thymidylate synthase inhibitors. *European Journal of Medicinal Chemistry*, **2019**, 183, 111673	6.8	4
20	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	2.9	3
19	Structural investigation of 2-naphthyl phenyl ether inhibitors bound to WT and Y181C reverse transcriptase highlights key features of the NNRTI binding site. *Protein Science*, **2020**, 29, 1902-1910	6.3	3
18	Comment on simulations of liquid ammonia based on quantum mechanical potential functions. *Journal of Chemical Physics*, **1981**, 75, 2026-2027	3.9	3
17	Understanding the structural basis of species selective, stereospecific inhibition for Cryptosporidium and human thymidylate synthase. *FEBS Letters*, **2019**, 593, 2069-2078	3.8	2
16	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	6.1	2
15	Autobiography of William L. Jorgensen: scientific history and recollections. *Journal of Physical Chemistry B*, **2015**, 119, 624-32	3.4	2
14	OPLS all-atom force field for carbohydrates **1997**, 18, 1955		2
13	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	2.9	1

12	Progress and issues for computationally guided lead discovery and optimization1-14		1
11	Indoloxytriazines as binding molecules for the JAK2 JH2 pseudokinase domain and its V617F variant. *Tetrahedron Letters*, **2021**, 77,	2	1
10	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	5.6	1
9	Long-acting and extended-release implant and nanoformulations with a synergistic antiretroviral two-drug combination controls HIV-1 infection in a humanized mouse model.. *Bioengineering and Translational Medicine*, **2022**, 7, e10237	14.8	0
8	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	4.3	0
7	Confronting Racism in Chemistry Journals. *ACS Applied Nano Materials*, **2020**, 3, 6131-6133	5.6	
6	Confronting Racism in Chemistry Journals. *ACS Applied Polymer Materials*, **2020**, 2, 2496-2498	4.3	
5	Confronting Racism in Chemistry Journals. *Organometallics*, **2020**, 39, 2331-2333	3.8	
4	Update to Our Reader, Reviewer, and Author Communities: April 2020. *Energy & Fuels*, **2020**, 34, 5107-5108	4.1	
3	Update to Our Reader, Reviewer, and Author Communities: April 2020. *Organometallics*, **2020**, 39, 1665-1666	3.8	
2	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	11.5	
1	Confronting Racism in Chemistry Journals. *Journal of Chemical Health and Safety*, **2020**, 27, 198-200	1.7	