Wolfgang Damm

List of Publications by Year
in descending order

24 papers	8,979 citations	361413 20 h-index	642732 23 g-index
25 all docs	25 docs citations	25 times ranked	11787 citing authors

#	Article	IF	Citations
1	OPLS3: A Force Field Providing Broad Coverage of Drug-like Small Molecules and Proteins. Journal of Chemical Theory and Computation, 2016, 12, 281-296.	5.3	2,349
2	Prediction of Absolute Solvation Free Energies using Molecular Dynamics Free Energy Perturbation and the OPLS Force Field. Journal of Chemical Theory and Computation, 2010, 6, 1509-1519.	5.3	1,360
3	Integrated Modeling Program, Applied Chemical Theory (IMPACT). Journal of Computational Chemistry, 2005, 26, 1752-1780.	3.3	1,194
4	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.	13.7	931
5	OPLS3e: Extending Force Field Coverage for Drug-Like Small Molecules. Journal of Chemical Theory and Computation, 2019, 15, 1863-1874.	5.3	698
6	OPLS all-atom force field for carbohydrates. Journal of Computational Chemistry, 1997, 18, 1955-1970.	3.3	619
7	OPLS4: Improving Force Field Accuracy on Challenging Regimes of Chemical Space. Journal of Chemical Theory and Computation, 2021, 17, 4291-4300.	5.3	582
8	Polarizable force fields. Current Opinion in Structural Biology, 2001, 11, 236-242.	5.7	474
9	Improving the Prediction of Absolute Solvation Free Energies Using the Next Generation OPLS Force Field. Journal of Chemical Theory and Computation, 2012, 8, 2553-2558.	5.3	239
10	A Polarizable Force Field and Continuum Solvation Methodology for Modeling of Proteinâ^'Ligand Interactions. Journal of Chemical Theory and Computation, 2005, 1, 694-715.	5.3	100
11	1,2-Stereoinduction in acyclic radicals: allylic strain effects. Tetrahedron Letters, 1992, 33, 1863-1866.	1.4	62
12	Explicit-Solvent Molecular Dynamics Simulations of the Polysaccharide Schizophyllan in Water. Biophysical Journal, 2007, 93, 442-455.	0.5	61
13	Cram's rule for radical reactions. Tetrahedron Letters, 1991, 32, 6097-6100.	1.4	49
14	The Curtin-Hammett principle: Stereoselective radical additions to alkenes. Tetrahedron Letters, 1996, 37, 351-354.	1.4	44
15	Explicit-Solvent Molecular Dynamics Simulations of the Î²(1â†'3)- and Î²(1â†'6)-Linked Disaccharides Î²-Laminarabiose and Î²-Gentiobiose in Water. Journal of Physical Chemistry B, 2004, 108, 5815-5826.	2.6	32
16	High Energy Density in Azobenzene-based Materials for Photo-Thermal Batteries via Controlled Polymer Architecture and Polymer-Solvent Interactions. Scientific Reports, 2017, 7, 17773.	3.3	31
17	Transition states for the hydrogen atom abstraction reaction by ga-oxygen substituted radicals: Felkin-Anh Rule in Radical Chemistry. Tetrahedron Letters, 1993, 34, 431-434.	1.4	29
18	Mechanistic Studies in the Radical Induced DNA Strand Cleavageâ€"Formation and Reactivity of the Radical Cation Intermediate. Tetrahedron, 2000, 56, 4117-4128.	1.9	27

#	Article	IF	Citations
19	OPLS allâ€atom force field for carbohydrates. Journal of Computational Chemistry, 1997, 18, 1955-1970.	3.3	26
20	The Felkin-Anh Rule in Radical Chemistry: 1,2-Stereoinduction in Radical Addition to Alkenes. Synlett, 1992, 1992, 441-443.	1.8	24
21	Stereoselective reactions of Î±-imide substituted radicals. Tetrahedron, 1994, 50, 7029-7048.	1.9	19
22	Reversible peptide folding: Dependence on molecular force field used. Journal of Computational Chemistry, 2000, 21, 774-787.	3.3	19
23	Advancing Free-Energy Calculations of Metalloenzymes in Drug Discovery via Implementation of LFMM Potentials. Journal of Chemical Theory and Computation, 2020, 16, 6926-6937.	5.3	8
24	OPLS all-atom force field for carbohydrates. , 1997, 18, 1955.		2