Wendy D Cornell

List of Publications by Year in Descending Order

12 papers	13,603 citations	10 h-index	14 g-index
14 ext. papers	14,423 ext. citations	8 avg, IF	5.21 L-index

#	Paper	IF	Citations
12	Combining Docking Pose Rank and Structure with Deep Learning Improves Protein-Ligand Binding Mode Prediction over a Baseline Docking Approach. *Journal of Chemical Information and Modeling*, **2020**, 60, 4170-4179	6.1	30
11	Drug-like density: a method of quantifying the "bindability" of a protein target based on a very large set of pockets and drug-like ligands from the Protein Data Bank. *Journal of Chemical Information and Modeling*, **2010**, 50, 2029-40	6.1	78
10	Multiple protein structures and multiple ligands: effects on the apparent goodness of virtual screening results. *Journal of Computer-Aided Molecular Design*, **2008**, 22, 257-65	4.2	46
9	Comparison of topological, shape, and docking methods in virtual screening. *Journal of Chemical Information and Modeling*, **2007**, 47, 1504-19	6.1	349
8	The effects of basis set and blocking groups on the conformational energies of glycyl and alanyl dipeptides A Hartree-Fock and MP2 study. *Computational and Theoretical Chemistry*, **1997**, 392, 101-109		18
7	Application of a simple diagonal force field to the simulation of cyclopentane conformational dynamics. *Journal of Computational Chemistry*, **1996**, 17, 1541-1548	3.5	4
6	Application of a simple diagonal force field to the simulation of cyclopentane conformational dynamics **1996**, 17, 1541		1
5	A Second Generation Force Field for the Simulation of Proteins, Nucleic Acids, and Organic Molecules. *Journal of the American Chemical Society*, **1995**, 117, 5179-5197	16.4	10990
4	Application of the multimolecule and multiconformational RESP methodology to biopolymers: Charge derivation for DNA, RNA, and proteins. *Journal of Computational Chemistry*, **1995**, 16, 1357-1377	3.5	820
3	Calculation of molecular geometries, relative conformational energies, dipole moments, and molecular electrostatic potential fitted charges of small organic molecules of biochemical interest by density functional theory. *Journal of Computational Chemistry*, **1995**, 16, 1483-1506	3.5	90
2	A quantum Mechanical Investigation of the Conformational Energetics of the Alanine and Glycine Dipeptides in the Gas Phase and in Aqueous Solution. *Journal of the American Chemical Society*, **1994**, 116, 9250-9256	16.4	146
1	Application of RESP charges to calculate conformational energies, hydrogen bond energies, and free energies of solvation. *Journal of the American Chemical Society*, **1993**, 115, 9620-9631	16.4	1031