

Wendy D Cornell

List of Publications by Year in descending order

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Version: 2024-02-01

12
papers

15,168
citations

932766

10
h-index

1281420

11
g-index

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docs citations

14
times ranked

13999
citing authors

#	ARTICLE	IF	CITATIONS
1	Combining Docking Pose Rank and Structure with Deep Learning Improves Protein-Ligand Binding Mode Prediction over a Baseline Docking Approach. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 4170-4179.	2.5	64
2	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. <i>Journal of Chemical Information and Modeling</i> , 2010, 50, 2029-2040.	2.5	100
3	Multiple protein structures and multiple ligands: effects on the apparent goodness of virtual screening results. <i>Journal of Computer-Aided Molecular Design</i> , 2008, 22, 257-265.	1.3	52
4	Comparison of Topological, Shape, and Docking Methods in Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 1504-1519.	2.5	384
5	The effects of basis set and blocking groups on the conformational energies of glycyl and alanyl dipeptides A Hartree-Fock and MP2 study. <i>Computational and Theoretical Chemistry</i> , 1997, 392, 101-109.	1.5	19
6	Application of a simple diagonal force field to the simulation of cyclopentane conformational dynamics. <i>Journal of Computational Chemistry</i> , 1996, 17, 1541-1548.	1.5	5
7	Application of a simple diagonal force field to the simulation of cyclopentane conformational dynamics. , 1996, 17, 1541.		1
8	Application of the multimolecule and multiconformational RESP methodology to biopolymers: Charge derivation for DNA, RNA, and proteins. <i>Journal of Computational Chemistry</i> , 1995, 16, 1357-1377.	1.5	944
9	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. <i>Journal of Computational Chemistry</i> , 1995, 16, 1483-1506.	1.5	99
10	A Second Generation Force Field for the Simulation of Proteins, Nucleic Acids, and Organic Molecules. <i>Journal of the American Chemical Society</i> , 1995, 117, 5179-5197.	6.6	12,116
11	A quantum Mechanical Investigation of the Conformational Energetics of the Alanine and Glycine Dipeptides in the Gas Phase and in Aqueous Solution. <i>Journal of the American Chemical Society</i> , 1994, 116, 9250-9256.	6.6	155
12	Application of RESP charges to calculate conformational energies, hydrogen bond energies, and free energies of solvation. <i>Journal of the American Chemical Society</i> , 1993, 115, 9620-9631.	6.6	1,229