Henry Lee Woodcock

List of Publications by Year
in descending order

78	16,174	136940 32	71682 76
papers	citations	h-index	g-index

83	83	83	19230
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	<scp>CIFDock</scp>: A novel <scp>CHARMM</scp>â€based flexible receptorâ€“flexible ligand docking protocol. Journal of Computational Chemistry, 2022, 43, 84-95.	3.3	4
2	Not Drug-like, but Like Drugs: Cnidaria Natural Products. Marine Drugs, 2022, 20, 42.	4.6	5
3	Optimizing the Calculation of Free Energy Differences in Nonequilibrium Work SQM/MM Switching Simulations. Journal of Physical Chemistry B, 2022, 126, 2798-2811.	2.6	5
4	Tuaimenal A, a Meroterpene from the Irish Deep-Sea Soft Coral Duva florida, Displays Inhibition of the SARS-CoV-2 3CLpro Enzyme. Journal of Natural Products, 2022, 85, 1315-1323.	3.0	6
5	Obtaining QM/MM binding free energies in the SAMPL8 drugs of abuse challenge: indirect approaches. Journal of Computer-Aided Molecular Design, 2022, 36, 263-277.	2.9	4
6	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.0	518
7	Comparison between ab initio and polarizable molecular dynamics simulations of 1-butyl-3-methylimidazolium tetrafluoroborate and chloride in water. Journal of Molecular Liquids, 2021, 337, 116521.	4.9	14
8	Characterization and engineering of a two-enzyme system for plastics depolymerization. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 25476-25485.	7.1	262
9	Hierarchical Markov State Model Building to Describe Molecular Processes. Journal of Chemical Theory and Computation, 2020, 16, 1816-1826.	5.3	5
10	Enantiomerization of Axially Chiral Biphenyls: Polarizable MD Simulations in Water and Butylmethylether. International Journal of Molecular Sciences, 2020, 21, 6222.	4.1	4
11	Mechanism of proton transfer in class A Î²-lactamase catalysis and inhibition by avibactam. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 5818-5825.	7.1	35
12	Î´-Azaproline and Its Oxidized Variants. Journal of Organic Chemistry, 2020, 85, 4207-4219.	3.2	8
13	Use of Interaction Energies in QM/MM Free Energy Simulations. Journal of Chemical Theory and Computation, 2019, 15, 4632-4645.	5.3	21
14	Modeling Boronic Acid Based Fluorescent Saccharide Sensors: Computational Investigation of <scp>d</scp>-Fructose Binding to Dimethylaminomethylphenylboronic Acid. Journal of Chemical Information and Modeling, 2019, 59, 2150-2158.	5.4	7
15	The Good, the Bad, and the Ugly: â€œHiPenâ€, a New Dataset for Validating (S)QM/MM Free Energy Simulations. Molecules, 2019, 24, 681.	3.8	9
16	Characterization and engineering of a plastic-degrading aromatic polyesterase. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E4350-E4357.	7.1	632
17	Origins of the Mechanochemical Coupling of Peptide Bond Formation to Protein Synthesis. Journal of the American Chemical Society, 2018, 140, 5077-5087.	13.7	36
18	Synthesis and Î²-sheet propensity of constrained N-amino peptides. Bioorganic and Medicinal Chemistry, 2018, 26, 1162-1166.	3.0	12

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19	Force matching as a stepping stone to QM/MM CB[8] host/guest binding free energies: a SAMPL6 cautionary tale. Journal of Computer-Aided Molecular Design, 2018, 32, 983-999.	2.9	21
20	Accelerating QM/MM Free Energy Computations via Intramolecular Force Matching. Journal of Chemical Theory and Computation, 2018, 14, 6327-6335.	5.3	40
21	Mechanistic Studies of 1-Deoxy-D-Xylulose-5-Phosphate Synthase from Deinococcus radiodurans. Biochemistry & Molecular Biology Journal, 2018, 04, .	0.3	9
22	Convergence of single-step free energy perturbation. Molecular Physics, 2017, 115, 1200-1213.	1.7	46
23	Disaggregation is a Mechanism for Emission Turn-On of ortho-Aminomethylphenylboronic Acid-Based Saccharide Sensors. Journal of the American Chemical Society, 2017, 139, 5568-5578.	13.7	60
24	Elucidating a chemical defense mechanism of Antarctic sponges: A computational study. Journal of Molecular Graphics and Modelling, 2017, 71, 104-115.	2.4	30
25	Methods for Efficiently and Accurately Computing Quantum Mechanical Free Energies for Enzyme Catalysis. Methods in Enzymology, 2016, 577, 75-104.	1.0	6
26	The conserved active site histidine-glutamate pair of ferrochelatase coordinately catalyzes porphyrin metalation. Journal of Porphyrins and Phthalocyanines, 2016, 20, 556-569.	0.8	2
27	Thiamin Diphosphate Activation in 1-Deoxy-<scp>d</scp>-xylulose 5-Phosphate Synthase: Insights into the Mechanism and Underlying Intermolecular Interactions. Journal of Physical Chemistry B, 2016, 120, 9922-9934.	2.6	22
28	Computation of Hydration Free Energies Using the Multiple Environment Single System Quantum Mechanical/Molecular Mechanical Method. Journal of Chemical Theory and Computation, 2016, 12, 332-344.	5.3	42
29	Identification of Ecdysone Hormone Receptor Agonists as a Therapeutic Approach for Treating Filarial Infections. PLoS Neglected Tropical Diseases, 2016, 10, e0004772.	3.0	16
30	Ruthenium(II)Bis(2,2â€²-Bipyridine) Interactions with Nucleaobases- Models for DNA Binding. Biophysical Journal, 2015, 108, 149a-150a.	0.5	0
31	Ligand-Induced Proton Transfer and Low-Barrier Hydrogen Bond Revealed by X-ray Crystallography. Journal of the American Chemical Society, 2015, 137, 8086-8095.	13.7	74
32	Photoacoustic calorimetry study of ligand photorelease from the Ru(II)bis(2,2â€²-bipyridine)(6,6â€²-dimethyl-2,2â€²-bipyridine) complex in aqueous solution. Chemical Physics Letters, 2015, 619, 214-218.	2.6	4
33	ProBiS-CHARMMing: Web Interface for Prediction and Optimization of Ligands in Protein Binding Sites. Journal of Chemical Information and Modeling, 2015, 55, 2308-2314.	5.4	54
34	Use of Nonequilibrium Work Methods to Compute Free Energy Differences Between Molecular Mechanical and Quantum Mechanical Representations of Molecular Systems. Journal of Physical Chemistry Letters, 2015, 6, 4850-4856.	4.6	55
35	Development and implementation of (Q)SAR modeling within the CHARMMing web-user interface. Journal of Computational Chemistry, 2015, 36, 62-67.	3.3	5
36	Efficiently computing pathway free energies: New approaches based on chain-of-replica and Non-Boltzmann Bennett reweighting schemes. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 944-953.	2.4	28

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37	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
38	Web-Based Computational Chemistry Education with CHARMMing I: Lessons and Tutorial. PLoS Computational Biology, 2014, 10, e1003719.	3.2	14
39	Web-Based Computational Chemistry Education with CHARMMing II: Coarse-Grained Protein Folding. PLoS Computational Biology, 2014, 10, e1003738.	3.2	8
40	Web-Based Computational Chemistry Education with CHARMMing III: Reduction Potentials of Electron Transfer Proteins. PLoS Computational Biology, 2014, 10, e1003739.	3.2	10
41	Can Molecular Dynamics and QM/MM Solve the Penicillin Binding Protein Protonation Puzzle?. Journal of Chemical Information and Modeling, 2014, 54, 1412-1424.	5.4	7
42	Equilibrium and kinetics of Pb²⁺adsorption from aqueous solution by dendrimer/titania composites. Desalination and Water Treatment, 2014, 52, 5869-5875.	1.0	22
43	Fragment-Based Docking: Development of the CHARMMing Web User Interface as a Platform for Computer-Aided Drug Design. Journal of Chemical Information and Modeling, 2014, 54, 2612-2620.	5.4	21
44	Ru(II)Bis(2,2â€² Bipyridine)L Complexes as Photorelease Agents for Bioactive Molecules: Photothermal Studies of Ligand Release. Biophysical Journal, 2014, 106, 477a-478a.	0.5	0
45	Multiscale Free Energy Simulations: An Efficient Method for Connecting Classical MD Simulations to QM or QM/MM Free Energies Using Non-Boltzmann Bennett Reweighting Schemes. Journal of Chemical Theory and Computation, 2014, 10, 1406-1419.	5.3	111
46	Identification and Characterization of Noncovalent Interactions That Drive Binding and Specificity in DD-Peptidases and Î²-Lactamases. Journal of Chemical Theory and Computation, 2014, 10, 855-864.	5.3	15
47	Virtual target screening to rapidly identify potential protein targets of natural products in drug discovery. AIMS Molecular Science, 2014, 1, 81-98.	0.5	1
48	EDTA functionalized silica for removal of Cu(II), Zn(II) and Ni(II) from aqueous solution. Journal of Colloid and Interface Science, 2013, 408, 200-205.	9.4	90
49	Remediation of Cu(II), Ni(II), and Cr(III) ions from simulated wastewater by dendrimer/titania composites. Journal of Environmental Management, 2013, 117, 50-57.	7.8	78
50	How Does Catalase Release Nitric Oxide? A Computational Structureâ€“Activity Relationship Study. Journal of Chemical Information and Modeling, 2013, 53, 2951-2961.	5.4	7
51	Unlocking the Binding and Reaction Mechanism of Hydroxyurea Substrates as Biological Nitric Oxide Donors. Journal of Chemical Information and Modeling, 2012, 52, 1288-1297.	5.4	15
52	Understanding Ion Sensing in Zn(II) Porphyrins: Spectroscopic and Computational Studies of Nitrite/Nitrate Binding. Inorganic Chemistry, 2012, 51, 4756-4762.	4.0	10
53	Virtual Target Screening: Validation Using Kinase Inhibitors. Journal of Chemical Information and Modeling, 2012, 52, 2192-2203.	5.4	28
54	Iron Chelation by Polyamidoamine Dendrimers: A Second-Order Kinetic Model for Metalâ€“Amine Complexation. Journal of Physical Chemistry B, 2011, 115, 13534-13540.	2.6	40

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55	Characterization of Tunable Radical Metalâ€“Carbenes: Key Intermediates in Catalytic Cyclopropanation. Organometallics, 2011, 30, 2739-2746.	2.3	73
56	Catalytic Asymmetric Aza-Darzens Reaction with a Vaulted Biphenanthrol Magnesium Phosphate Salt. Organic Letters, 2011, 13, 2188-2191.	4.6	91
57	Characterizing the Mechanism of the Double Proton Transfer in the Formamide Dimer. Journal of Physical Chemistry A, 2011, 115, 2650-2657.	2.5	33
58	Efficient Calculation of QM/MM Frequencies with the Mobile Block Hessian. Journal of Chemical Theory and Computation, 2011, 7, 496-514.	5.3	32
59	MSCALE: A General Utility for Multiscale Modeling. Journal of Chemical Theory and Computation, 2011, 7, 1208-1219.	5.3	41
60	CHARMM: The biomolecular simulation program. Journal of Computational Chemistry, 2009, 30, 1545-1614.	3.3	7,077
61	Artificial reaction coordinate â€œtunnelingâ€•in freeâ€energy calculations: The catalytic reaction of RNase H. Journal of Computational Chemistry, 2009, 30, 1634-1641.	3.3	81
62	Computation of through-space NMR shielding effects in aromatic ring Ï€-stacked complexes. Journal of Molecular Graphics and Modelling, 2008, 26, 1125-1130.	2.4	16
63	CHARMMing: A New, Flexible Web Portal for CHARMM. Journal of Chemical Information and Modeling, 2008, 48, 1920-1929.	5.4	118
64	Pathways and Populations: Stereoelectronic Insights into the Exocyclic Torsion of 5-(Hydroxymethyl)tetrahydropyran. Journal of the American Chemical Society, 2008, 130, 6345-6347.	13.7	6
65	Vibrational subsystem analysis: A method for probing free energies and correlations in the harmonic limit. Journal of Chemical Physics, 2008, 129, 214109.	3.0	58
66	Carbene Stabilization by Aryl Substituents. Is Bigger Better?. Journal of the American Chemical Society, 2007, 129, 3763-3770.	13.7	56
67	Exploring SCC-DFTB Paths for Mapping QM/MM Reaction Mechanismsâ€. Journal of Physical Chemistry A, 2007, 111, 5720-5728.	2.5	71
68	Ab Initio Modeling of Glycosyl Torsions and Anomeric Effects in a Model Carbohydrate: 2-Ethoxy Tetrahydropyran. Biophysical Journal, 2007, 93, 1-10.	0.5	48
69	Interfacing Q-Chem and CHARMM to perform QM/MM reaction path calculations. Journal of Computational Chemistry, 2007, 28, 1485-1502.	3.3	190
70	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	2.8	2,597
71	The microwave and infrared spectroscopy of benzaldehyde: Conflict between theory and experimental deductions. Journal of Chemical Physics, 2004, 120, 4247-4250.	3.0	32
72	Exploring the quantum mechanical/molecular mechanical replica path method: a pathway optimization of the chorismate to prephenate Claisen rearrangement catalyzed by chorismate mutase. Theoretical Chemistry Accounts, 2003, 109, 140-148.	1.4	100

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73	Naphthalenyl, Anthracenyl, Tetracenyl, and Pentacenyl Radicals and Their Anions. Journal of Physical Chemistry A, 2003, 107, 6311-6316.	2.5	16
74	On the Viability of Small Endohedral Hydrocarbon Cage Complexes:Â X@C4H4, X@C8H8, X@C8H14, X@C10H16, X@C12H12, and X@C16H16. Journal of the American Chemical Society, 2003, 125, 11442-11451.	13.7	45
75	Problematic Energy Differences between Cumulenes and Poly-ynes:â€‰ Does This Point to a Systematic Improvement of Density Functional Theory?. Journal of Physical Chemistry A, 2002, 106, 11923-11931.	2.5	176
76	Analysis of the Origin of Through-Space Proton NMR Deshielding by Selected Organic Functional Groups. Organic Letters, 2001, 3, 3823-3826.	4.6	44
77	The Almost Bottleable Triplet Carbene:â€‰ 2,6-dibromo-4-tert-butyl-2â€˜,6â€˜-bis(trifluoromethyl)-4â€˜-isopropyldiphenylcarbene. Journal of the American Chemical Society, 2001, 123, 4331-4335.	13.7	25
78	A Systematic Study of the X̀ƒ 2B1, Ãƒ 2A1, and B̀ƒ 2B2 States of the Neutral Radical PH2. Journal of Physical Chemistry A, 2001, 105, 5037-5045.	2.5	9