

Henry Lee Woodcock

List of Publications by Year in descending order

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78
papers

16,174
citations

156536

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81351

76
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83
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83
docs citations

83
times ranked

21776
citing authors

#	ARTICLE	IF	CITATIONS
1	<sc>CIFDock</sc>: A novel <sc>CHARMM</sc>-based flexible receptor-“flexible ligand docking protocol. <i>Journal of Computational Chemistry</i> , 2022, 43, 84-95.	1.5	4
2	Not Drug-like, but Like Drugs: Cnidaria Natural Products. <i>Marine Drugs</i> , 2022, 20, 42.	2.2	5
3	Optimizing the Calculation of Free Energy Differences in Nonequilibrium Work SQM/MM Switching Simulations. <i>Journal of Physical Chemistry B</i> , 2022, 126, 2798-2811.	1.2	5
4	Tuaimenal A, a Meroterpenoid from the Irish Deep-Sea Soft Coral <i>Duva florida</i>, Displays Inhibition of the SARS-CoV-2 3CLpro Enzyme. <i>Journal of Natural Products</i> , 2022, 85, 1315-1323.	1.5	6
5	Obtaining QM/MM binding free energies in the SAMPL8 drugs of abuse challenge: indirect approaches. <i>Journal of Computer-Aided Molecular Design</i> , 2022, 36, 263-277.	1.3	4
6	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	1.2	518
7	Comparison between ab initio and polarizable molecular dynamics simulations of 1-butyl-3-methylimidazolium tetrafluoroborate and chloride in water. <i>Journal of Molecular Liquids</i> , 2021, 337, 116521.	2.3	14
8	Characterization and engineering of a two-enzyme system for plastics depolymerization. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 25476-25485.	3.3	262
9	Hierarchical Markov State Model Building to Describe Molecular Processes. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 1816-1826.	2.3	5
10	Enantiomerization of Axially Chiral Biphenyls: Polarizable MD Simulations in Water and Butylmethylether. <i>International Journal of Molecular Sciences</i> , 2020, 21, 6222.	1.8	4
11	Mechanism of proton transfer in class A β -lactamase catalysis and inhibition by avibactam. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 5818-5825.	3.3	35
12	β -Azaprolone and Its Oxidized Variants. <i>Journal of Organic Chemistry</i> , 2020, 85, 4207-4219.	1.7	8
13	Use of Interaction Energies in QM/MM Free Energy Simulations. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4632-4645.	2.3	21
14	Modeling Boronic Acid Based Fluorescent Saccharide Sensors: Computational Investigation of <sc>d</sc>-Fructose Binding to Dimethylaminomethylphenylboronic Acid. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2150-2158.	2.5	7
15	The Good, the Bad, and the Ugly: α -HiPen, a New Dataset for Validating (S)QM/MM Free Energy Simulations. <i>Molecules</i> , 2019, 24, 681.	1.7	9
16	Characterization and engineering of a plastic-degrading aromatic polyesterase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E4350-E4357.	3.3	632
17	Origins of the Mechanochemical Coupling of Peptide Bond Formation to Protein Synthesis. <i>Journal of the American Chemical Society</i> , 2018, 140, 5077-5087.	6.6	36
18	Synthesis and β -sheet propensity of constrained N-amino peptides. <i>Bioorganic and Medicinal Chemistry</i> , 2018, 26, 1162-1166.	1.4	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. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 983-999.	1.3	21
20	Accelerating QM/MM Free Energy Computations via Intramolecular Force Matching. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 6327-6335.	2.3	40
21	Mechanistic Studies of 1-Deoxy-D-Xylulose-5-Phosphate Synthase from <i>Deinococcus radiodurans</i> . <i>Biochemistry & Molecular Biology Journal</i> , 2018, 04, .	0.3	9
22	Convergence of single-step free energy perturbation. <i>Molecular Physics</i> , 2017, 115, 1200-1213.	0.8	46
23	Disaggregation is a Mechanism for Emission Turn-On of <i>ortho</i> -Aminomethylphenylboronic Acid-Based Saccharide Sensors. <i>Journal of the American Chemical Society</i> , 2017, 139, 5568-5578.	6.6	60
24	Elucidating a chemical defense mechanism of Antarctic sponges: A computational study. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 71, 104-115.	1.3	30
25	Methods for Efficiently and Accurately Computing Quantum Mechanical Free Energies for Enzyme Catalysis. <i>Methods in Enzymology</i> , 2016, 577, 75-104.	0.4	6
26	The conserved active site histidine-glutamate pair of ferrochelatase coordinately catalyzes porphyrin metalation. <i>Journal of Porphyrins and Phthalocyanines</i> , 2016, 20, 556-569.	0.4	2
27	Thiamin Diphosphate Activation in 1-Deoxy-xylulose 5-Phosphate Synthase: Insights into the Mechanism and Underlying Intermolecular Interactions. <i>Journal of Physical Chemistry B</i> , 2016, 120, 9922-9934.	1.2	22
28	Computation of Hydration Free Energies Using the Multiple Environment Single System Quantum Mechanical/Molecular Mechanical Method. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 332-344.	2.3	42
29	Identification of Ecdysone Hormone Receptor Agonists as a Therapeutic Approach for Treating Filarial Infections. <i>PLoS Neglected Tropical Diseases</i> , 2016, 10, e0004772.	1.3	16
30	Ruthenium(II)Bis(2,2'-Bipyridine) Interactions with Nucleobases- Models for DNA Binding. <i>Biophysical Journal</i> , 2015, 108, 149a-150a.	0.2	0
31	Ligand-Induced Proton Transfer and Low-Barrier Hydrogen Bond Revealed by X-ray Crystallography. <i>Journal of the American Chemical Society</i> , 2015, 137, 8086-8095.	6.6	74
32	Photoacoustic calorimetry study of ligand photorelease from the Ru(II)bis(2,2'-bipyridine)(6,6'-dimethyl-2,2'-bipyridine) complex in aqueous solution. <i>Chemical Physics Letters</i> , 2015, 619, 214-218.	1.2	4
33	ProBIS-CHARMMing: Web Interface for Prediction and Optimization of Ligands in Protein Binding Sites. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 2308-2314.	2.5	54
34	Use of Nonequilibrium Work Methods to Compute Free Energy Differences Between Molecular Mechanical and Quantum Mechanical Representations of Molecular Systems. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 4850-4856.	2.1	55
35	Development and implementation of (Q)SAR modeling within the CHARMMing web-user interface. <i>Journal of Computational Chemistry</i> , 2015, 36, 62-67.	1.5	5
36	Efficiently computing pathway free energies: New approaches based on chain-of-replica and Non-Boltzmann Bennett reweighting schemes. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2015, 1850, 944-953.	1.1	28

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37	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , 2015, 113, 184-215.	0.8	2,561
38	Web-Based Computational Chemistry Education with CHARMMing I: Lessons and Tutorial. <i>PLoS Computational Biology</i> , 2014, 10, e1003719.	1.5	14
39	Web-Based Computational Chemistry Education with CHARMMing II: Coarse-Grained Protein Folding. <i>PLoS Computational Biology</i> , 2014, 10, e1003738.	1.5	8
40	Web-Based Computational Chemistry Education with CHARMMing III: Reduction Potentials of Electron Transfer Proteins. <i>PLoS Computational Biology</i> , 2014, 10, e1003739.	1.5	10
41	Can Molecular Dynamics and QM/MM Solve the Penicillin Binding Protein Protonation Puzzle?. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 1412-1424.	2.5	7
42	Equilibrium and kinetics of Pb ²⁺ adsorption from aqueous solution by dendrimer/titania composites. <i>Desalination and Water Treatment</i> , 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. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 2612-2620.	2.5	21
44	Ru(II)Bis(2,2'-Bipyridine)L Complexes as Photorelease Agents for Bioactive Molecules: Photothermal Studies of Ligand Release. <i>Biophysical Journal</i> , 2014, 106, 477a-478a.	0.2	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. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1406-1419.	2.3	111
46	Identification and Characterization of Noncovalent Interactions That Drive Binding and Specificity in DD-Peptidases and Î²-Lactamases. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 855-864.	2.3	15
47	Virtual target screening to rapidly identify potential protein targets of natural products in drug discovery. <i>AIMS Molecular Science</i> , 2014, 1, 81-98.	0.3	1
48	EDTA functionalized silica for removal of Cu(II), Zn(II) and Ni(II) from aqueous solution. <i>Journal of Colloid and Interface Science</i> , 2013, 408, 200-205.	5.0	90
49	Remediation of Cu(II), Ni(II), and Cr(III) ions from simulated wastewater by dendrimer/titania composites. <i>Journal of Environmental Management</i> , 2013, 117, 50-57.	3.8	78
50	How Does Catalase Release Nitric Oxide? A Computational Structure-Activity Relationship Study. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 2951-2961.	2.5	7
51	Unlocking the Binding and Reaction Mechanism of Hydroxyurea Substrates as Biological Nitric Oxide Donors. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 1288-1297.	2.5	15
52	Understanding Ion Sensing in Zn(II) Porphyrins: Spectroscopic and Computational Studies of Nitrite/Nitrate Binding. <i>Inorganic Chemistry</i> , 2012, 51, 4756-4762.	1.9	10
53	Virtual Target Screening: Validation Using Kinase Inhibitors. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 2192-2203.	2.5	28
54	Iron Chelation by Polyamidoamine Dendrimers: A Second-Order Kinetic Model for Metal-Amine Complexation. <i>Journal of Physical Chemistry B</i> , 2011, 115, 13534-13540.	1.2	40

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55	Characterization of Tunable Radical Metal-Carbenes: Key Intermediates in Catalytic Cyclopropanation. <i>Organometallics</i> , 2011, 30, 2739-2746.	1.1	73
56	Catalytic Asymmetric Aza-Darzens Reaction with a Vaulted Biphenanthrol Magnesium Phosphate Salt. <i>Organic Letters</i> , 2011, 13, 2188-2191.	2.4	91
57	Characterizing the Mechanism of the Double Proton Transfer in the Formamide Dimer. <i>Journal of Physical Chemistry A</i> , 2011, 115, 2650-2657.	1.1	33
58	Efficient Calculation of QM/MM Frequencies with the Mobile Block Hessian. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 496-514.	2.3	32
59	MSCALE: A General Utility for Multiscale Modeling. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1208-1219.	2.3	41
60	CHARMM: The biomolecular simulation program. <i>Journal of Computational Chemistry</i> , 2009, 30, 1545-1614.	1.5	7,077
61	Artificial reaction coordinate tunneling in free energy calculations: The catalytic reaction of RNase H. <i>Journal of Computational Chemistry</i> , 2009, 30, 1634-1641.	1.5	81
62	Computation of through-space NMR shielding effects in aromatic ring π -stacked complexes. <i>Journal of Molecular Graphics and Modelling</i> , 2008, 26, 1125-1130.	1.3	16
63	CHARMMing: A New, Flexible Web Portal for CHARMM. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 1920-1929.	2.5	118
64	Pathways and Populations: Stereoelectronic Insights into the Exocyclic Torsion of 5-(Hydroxymethyl)tetrahydropyran. <i>Journal of the American Chemical Society</i> , 2008, 130, 6345-6347.	6.6	6
65	Vibrational subsystem analysis: A method for probing free energies and correlations in the harmonic limit. <i>Journal of Chemical Physics</i> , 2008, 129, 214109.	1.2	58
66	Carbene Stabilization by Aryl Substituents. Is Bigger Better?. <i>Journal of the American Chemical Society</i> , 2007, 129, 3763-3770.	6.6	56
67	Exploring SCC-DFTB Paths for Mapping QM/MM Reaction Mechanisms. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5720-5728.	1.1	71
68	Ab Initio Modeling of Glycosyl Torsions and Anomeric Effects in a Model Carbohydrate: 2-Ethoxy Tetrahydropyran. <i>Biophysical Journal</i> , 2007, 93, 1-10.	0.2	48
69	Interfacing Q-Chem and CHARMM to perform QM/MM reaction path calculations. <i>Journal of Computational Chemistry</i> , 2007, 28, 1485-1502.	1.5	190
70	Advances in methods and algorithms in a modern quantum chemistry program package. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 3172-3191.	1.3	2,597
71	The microwave and infrared spectroscopy of benzaldehyde: Conflict between theory and experimental deductions. <i>Journal of Chemical Physics</i> , 2004, 120, 4247-4250.	1.2	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. <i>Theoretical Chemistry Accounts</i> , 2003, 109, 140-148.	0.5	100

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73	Naphthalenyl, Anthracenyl, Tetracenyl, and Pentacenyl Radicals and Their Anions. <i>Journal of Physical Chemistry A</i> , 2003, 107, 6311-6316.	1.1	16
74	On the Viability of Small Endohedral Hydrocarbon Cage Complexes: $X@C_4H_4$, $X@C_8H_8$, $X@C_8H_{14}$, $X@C_{10}H_{16}$, $X@C_{12}H_{12}$, and $X@C_{16}H_{16}$. <i>Journal of the American Chemical Society</i> , 2003, 125, 11442-11451.	6.6	45
75	Problematic Energy Differences between Cumulenes and Polyynes: Does This Point to a Systematic Improvement of Density Functional Theory?. <i>Journal of Physical Chemistry A</i> , 2002, 106, 11923-11931.	1.1	176
76	Analysis of the Origin of Through-Space Proton NMR Deshielding by Selected Organic Functional Groups. <i>Organic Letters</i> , 2001, 3, 3823-3826.	2.4	44
77	The Almost Bottleable Triplet Carbene: 2,6-dibromo-4-tert-butyl-2,6-bis(trifluoromethyl)-4-isopropylidiphenylcarbene. <i>Journal of the American Chemical Society</i> , 2001, 123, 4331-4335.	6.6	25
78	A Systematic Study of the $X^1\Sigma^+$ 2B1, $\tilde{A}^1\Sigma^+$ 2A1, and $B^1\Sigma^+$ 2B2 States of the Neutral Radical PH2. <i>Journal of Physical Chemistry A</i> , 2001, 105, 5037-5045.	1.1	9