# Henry Lee Woodcock

## List of Publications by Year in Descending Order



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| 72 papers | 12,659 citations | 31 h-index | 83 g-index |
| 83 ext. papers | 14,511 ext. citations | 5.6 avg, IF | 5.22 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 72 | CIFDock: A novel CHARMM-based flexible receptor-flexible ligand docking protocol. *Journal of Computational Chemistry*, **2022**, 43, 84-95 | 3.5 | 0 |
| 71 | Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. *Journal of Chemical Physics*, **2021**, 155, 084801 | 3.9 | 115 |
| 70 | 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 | 6 | 2 |
| 69 | Mechanism of proton transfer in class A β-lactamase catalysis and inhibition by avibactam. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 5818-5825 | 11.5 | 15 |
| 68 | β-Azaproline and Its Oxidized Variants. *Journal of Organic Chemistry*, **2020**, 85, 4207-4219 | 4.2 | 3 |
| 67 | 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 | 11.5 | 90 |
| 66 | Hierarchical Markov State Model Building to Describe Molecular Processes. *Journal of Chemical Theory and Computation*, **2020**, 16, 1816-1826 | 6.4 | 3 |
| 65 | Enantiomerization of Axially Chiral Biphenyls: Polarizable MD Simulations in Water and Butylmethylether. *International Journal of Molecular Sciences*, **2020**, 21, | 6.3 | 1 |
| 64 | Use of Interaction Energies in QM/MM Free Energy Simulations. *Journal of Chemical Theory and Computation*, **2019**, 15, 4632-4645 | 6.4 | 13 |
| 63 | Modeling Boronic Acid Based Fluorescent Saccharide Sensors: Computational Investigation of d-Fructose Binding to Dimethylaminomethylphenylboronic Acid. *Journal of Chemical Information and Modeling*, **2019**, 59, 2150-2158 | 6.1 | 3 |
| 62 | The Good, the Bad, and the Ugly: "HiPen", a New Dataset for Validating (S)QM/MM Free Energy Simulations. *Molecules*, **2019**, 24, | 4.8 | 6 |
| 61 | 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 | 11.5 | 369 |
| 60 | Origins of the Mechanochemical Coupling of Peptide Bond Formation to Protein Synthesis. *Journal of the American Chemical Society*, **2018**, 140, 5077-5087 | 16.4 | 28 |
| 59 | Synthesis and β-sheet propensity of constrained N-amino peptides. *Bioorganic and Medicinal Chemistry*, **2018**, 26, 1162-1166 | 3.4 | 10 |
| 58 | 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 | 4.2 | 15 |
| 57 | Accelerating QM/MM Free Energy Computations via Intramolecular Force Matching. *Journal of Chemical Theory and Computation*, **2018**, 14, 6327-6335 | 6.4 | 30 |
| 56 | Mechanistic Studies of 1-Deoxy-D-Xylulose-5-Phosphate Synthase from. *Biochemistry & Molecular Biology Journal*, **2018**, 4, | 0 | 6 |

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| 55 | Convergence of single-step free energy perturbation. *Molecular Physics*, **2017**, 115, 1200-1213 | 1.7 | 34 |
| 54 | 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 | 16.4 | 50 |
| 53 | Elucidating a chemical defense mechanism of Antarctic sponges: A computational study. *Journal of Molecular Graphics and Modelling*, **2017**, 71, 104-115 | 2.8 | 24 |
| 52 | Thiamin Diphosphate Activation in 1-Deoxy-d-xylulose 5-Phosphate Synthase: Insights into the Mechanism and Underlying Intermolecular Interactions. *Journal of Physical Chemistry B*, **2016**, 120, 9922-34 | 3.4 | 16 |
| 51 | Computation of Hydration Free Energies Using the Multiple Environment Single System Quantum Mechanical/Molecular Mechanical Method. *Journal of Chemical Theory and Computation*, **2016**, 12, 332-44 | 6.4 | 36 |
| 50 | Identification of Ecdysone Hormone Receptor Agonists as a Therapeutic Approach for Treating Filarial Infections. *PLoS Neglected Tropical Diseases*, **2016**, 10, e0004772 | 4.8 | 10 |
| 49 | Methods for Efficiently and Accurately Computing Quantum Mechanical Free Energies for Enzyme Catalysis. *Methods in Enzymology*, **2016**, 577, 75-104 | 1.7 | 4 |
| 48 | The conserved active site histidine-glutamate pair of ferrochelatase coordinately catalyzes porphyrin metalation. *Journal of Porphyrins and Phthalocyanines*, **2016**, 20, 556-569 | 1.8 | 2 |
| 47 | Photoacoustic calorimetry study of ligand photorelease from the Ru(II)bis(2,2?-bipyridine)(6,6?-dimethyl-2,2?-bipyridine) complex in aqueous solution. *Chemical Physics Letters*, **2015**, 619, 214-218 | 2.5 | 4 |
| 46 | ProBiS-CHARMMing: Web Interface for Prediction and Optimization of Ligands in Protein Binding Sites. *Journal of Chemical Information and Modeling*, **2015**, 55, 2308-14 | 6.1 | 43 |
| 45 | 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, 4850-6 | 6.4 | 43 |
| 44 | Development and implementation of (Q)SAR modeling within the CHARMMing web-user interface. *Journal of Computational Chemistry*, **2015**, 36, 62-7 | 3.5 | 5 |
| 43 | 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 | 4 | 25 |
| 42 | Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215 | 1.7 | 2068 |
| 41 | Ligand-Induced Proton Transfer and Low-Barrier Hydrogen Bond Revealed by X-ray Crystallography. *Journal of the American Chemical Society*, **2015**, 137, 8086-95 | 16.4 | 58 |
| 40 | Can molecular dynamics and QM/MM solve the penicillin binding protein protonation puzzle?. *Journal of Chemical Information and Modeling*, **2014**, 54, 1412-24 | 6.1 | 7 |
| 39 | Equilibrium and kinetics of Pb2+ adsorption from aqueous solution by dendrimer/titania composites. *Desalination and Water Treatment*, **2014**, 52, 5869-5875 | | 16 |
| 38 | 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, 2612-20 | 6.1 | 17 |

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| 37 | 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 | 6.4 | 96 |
| 36 | Identification and Characterization of Noncovalent Interactions That Drive Binding and Specificity in DD-Peptidases and β-Lactamases. *Journal of Chemical Theory and Computation*, **2014**, 10, 855-864 | 6.4 | 14 |
| 35 | Web-based computational chemistry education with CHARMMing I: Lessons and tutorial. *PLoS Computational Biology*, **2014**, 10, e1003719 | 5 | 10 |
| 34 | Web-based computational chemistry education with CHARMMing II: Coarse-grained protein folding. *PLoS Computational Biology*, **2014**, 10, e1003738 | 5 | 5 |
| 33 | Web-based computational chemistry education with CHARMMing III: Reduction potentials of electron transfer proteins. *PLoS Computational Biology*, **2014**, 10, e1003739 | 5 | 5 |
| 32 | Virtual target screening to rapidly identify potential protein targets of natural products in drug discovery. *AIMS Molecular Science*, **2014**, 1, 81-98 | 0.9 | 1 |
| 31 | EDTA functionalized silica for removal of Cu(II), Zn(II) and Ni(II) from aqueous solution. *Journal of Colloid and Interface Science*, **2013**, 408, 200-5 | 9.3 | 76 |
| 30 | Remediation of Cu(II), Ni(II), and Cr(III) ions from simulated wastewater by dendrimer/titania composites. *Journal of Environmental Management*, **2013**, 117, 50-7 | 7.9 | 69 |
| 29 | How does catalase release nitric oxide? A computational structure-activity relationship study. *Journal of Chemical Information and Modeling*, **2013**, 53, 2951-61 | 6.1 | 5 |
| 28 | Unlocking the binding and reaction mechanism of hydroxyurea substrates as biological nitric oxide donors. *Journal of Chemical Information and Modeling*, **2012**, 52, 1288-97 | 6.1 | 15 |
| 27 | Understanding ion sensing in Zn(II) porphyrins: spectroscopic and computational studies of nitrite/nitrate binding. *Inorganic Chemistry*, **2012**, 51, 4756-62 | 5.1 | 9 |
| 26 | Virtual target screening: validation using kinase inhibitors. *Journal of Chemical Information and Modeling*, **2012**, 52, 2192-203 | 6.1 | 21 |
| 25 | Catalytic asymmetric aza-Darzens reaction with a vaulted biphenanthrol magnesium phosphate salt. *Organic Letters*, **2011**, 13, 2188-91 | 6.2 | 77 |
| 24 | Characterizing the mechanism of the double proton transfer in the formamide dimer. *Journal of Physical Chemistry A*, **2011**, 115, 2650-7 | 2.8 | 31 |
| 23 | Efficient Calculation of QM/MM Frequencies with the Mobile Block Hessian. *Journal of Chemical Theory and Computation*, **2011**, 7, 496-514 | 6.4 | 29 |
| 22 | MSCALE: A General Utility for Multiscale Modeling. *Journal of Chemical Theory and Computation*, **2011**, 7, 1208-1219 | 6.4 | 38 |
| 21 | Iron chelation by polyamidoamine dendrimers: a second-order kinetic model for metal-amine complexation. *Journal of Physical Chemistry B*, **2011**, 115, 13534-40 | 3.4 | 40 |
| 20 | Characterization of Tunable Radical Metal-Carbenes: Key Intermediates in Catalytic Cyclopropanation. *Organometallics*, **2011**, 30, 2739-2746 | 3.8 | 69 |

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| 19 | CHARMM: the biomolecular simulation program. *Journal of Computational Chemistry*, **2009**, 30, 1545-614 | 3.5 | 5515 |
| 18 | Artificial reaction coordinate "tunneling" in free-energy calculations: the catalytic reaction of RNase H. *Journal of Computational Chemistry*, **2009**, 30, 1634-41 | 3.5 | 73 |
| 17 | CHARMMing: a new, flexible web portal for CHARMM. *Journal of Chemical Information and Modeling* , **2008**, 48, 1920-9 | 6.1 | 105 |
| 16 | Pathways and populations: stereoelectronic insights into the exocyclic torsion of 5-(hydroxymethyl)tetrahydropyran. *Journal of the American Chemical Society*, **2008**, 130, 6345-7 | 16.4 | 6 |
| 15 | Vibrational subsystem analysis: A method for probing free energies and correlations in the harmonic limit. *Journal of Chemical Physics*, **2008**, 129, 214109 | 3.9 | 47 |
| 14 | Computation of through-space NMR shielding effects in aromatic ring pi-stacked complexes. *Journal of Molecular Graphics and Modelling*, **2008**, 26, 1125-30 | 2.8 | 16 |
| 13 | Carbene stabilization by aryl substituents. Is bigger better?. *Journal of the American Chemical Society*, **2007**, 129, 3763-70 | 16.4 | 50 |
| 12 | Exploring SCC-DFTB paths for mapping QM/MM reaction mechanisms. *Journal of Physical Chemistry A*, **2007**, 111, 5720-8 | 2.8 | 63 |
| 11 | Ab initio modeling of glycosyl torsions and anomeric effects in a model carbohydrate: 2-ethoxy tetrahydropyran. *Biophysical Journal*, **2007**, 93, 1-10 | 2.9 | 45 |
| 10 | Interfacing Q-Chem and CHARMM to perform QM/MM reaction path calculations. *Journal of Computational Chemistry*, **2007**, 28, 1485-1502 | 3.5 | 170 |
| 9 | Advances in methods and algorithms in a modern quantum chemistry program package. *Physical Chemistry Chemical Physics*, **2006**, 8, 3172-91 | 3.6 | 2371 |
| 8 | The microwave and infrared spectroscopy of benzaldehyde: conflict between theory and experimental deductions. *Journal of Chemical Physics*, **2004**, 120, 4247-50 | 3.9 | 28 |
| 7 | 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 | 1.9 | 93 |
| 6 | Naphthalenyl, Anthracenyl, Tetracenyl, and Pentacenyl Radicals and Their Anions. *Journal of Physical Chemistry A*, **2003**, 107, 6311-6316 | 2.8 | 15 |
| 5 | On the viability of small endohedral hydrocarbon cage complexes: X@C4H4, X@C8H8, X@C8H14, X@C10H16, X@C12H12, AND X@C16H16. *Journal of the American Chemical Society*, **2003**, 125, 11442-51 | 16.4 | 37 |
| 4 | Problematic Energy Differences between Cumulenes and Poly-ynes: Does This Point to a Systematic Improvement of Density Functional Theory?. *Journal of Physical Chemistry A*, **2002**, 106, 11923-11931 | 2.8 | 166 |
| 3 | Analysis of the origin of through-space proton NMR deshielding by selected organic functional groups. *Organic Letters*, **2001**, 3, 3823-6 | 6.2 | 43 |
| 2 | The almost bottleable triplet carbene: 2,6-dibromo-4-tert-butyl-2',6'-bis(trifluoromethyl)-4'-isopropyldiphenylcarbene. *Journal of the American Chemical Society*, **2001**, 123, 4331-5 | 16.4 | 25 |

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| 1 | A Systematic Study of the X 2B1, 2A1, and B 2B2 States of the Neutral Radical PH2. *Journal of Physical Chemistry A*, **2001**, 105, 5037-5045 | 2.8 | 8 |