Dr. Henry Lee Woodcock III

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(A) Professional Preparation:

Appalachian State University	Chemistry	BS, 1998
University of Georgia	Chemistry (Phys./Comp./Theory)	PhD, 2003
National Institutes of Health	Postdoctoral fellow	2003–2006
National Institutes of Health	Lenfant Biomedical Fellow	2006–2009

(B) Appointments:

Professor	University of South Florida	2021–present
Associate Professor	University of South Florida	2015–2021
Assistant Professor	University of South Florida	2009–2015
Pre-IRTA Research Fellowship	National Institutes of Health	2002–2003
Summer Research Fellowship	National Institutes of Health	2001–2001
Research and Teaching Assistant	University of Georgia	1999–2002
Research Assistant	UNC Wilmington	1999–1999
Teaching Assistant	Appalachian State University	1998–1998

(C) Honors:

1. Faculty Outstanding Research Achievement Awards, 2021
2. Top 100 Altmetric Author (2020, altmetric.com/top100/2020): Characterization and engineering of a two-enzyme system for plastics depolymerization (#39).
3. Faculty Outstanding Research Achievement Award (USF Office of Research and Innovation, 2019).
4. Top 100 Altmetric Author (2018, altmetric.com/top100/2018): Characterization and engineering of a plastic-degrading aromatic polyesterase (#88).
5. Global Research Achievement Award (USF World, 2018).
6. Excellence in Innovation Award (USF, 2016).
7. OpenEye Outstanding Junior Faculty Award (2014, OpenEye Junior Faculty Award).
8. ACS Computers in Chemistry Division Alternative Counselor (2013–2014).
9. Faculty Fellow, University of South Florida (2012–2014, Faculty Fellows).
10. National Institutes of Health (NHLBI) Career Transition Award (2007).
11. Lenfant Biomedical Fellowship, National Heart, Lung and Blood Institute (2006).
12. Fellows Retreat Research Award, National Heart, Lung and Blood Institute (2006).
13. Intramural Research Training Award, National Institutes of Health (2003–2006).

(D) Products *(Total Citations: 15,183, H-Index: 34)*:

80. N. E Avalon, J. Nafie, T. Smalley, C. De Marco, S. G. Dietrick, R. M. Young, L. C. Warrensford, A. R. Pittman, F. L. Kearns, J. M. Binning, J. P. Dalton, M. P. Johnson, H. Lee Woodcock, A. L. Allcock, B. J. Baker; Tuaimenal A, a meroterpene from the Irish deep-sea soft coral Drifa sp., displays antiviral and antiproliferative bioactivity. *ChemRxiv*, **2022**, (10.26434/chemrxiv-2022-bjcfb-v2).

79. S. L. Vankayala, L. C. Warrensford, A. R. Pittman, B. C. Pollard, F. L. Kearns, J. D. Larkin, H. Lee Woodcock;* CIFDock: A novel CHARMM-based flexible receptor–flexible ligand docking protocol. *J. Comput. Chem.*, **2022**, 43(2), 84 (10.1002/jcc.26759).

78. C. Laguionie-Marchais, A. L. Allcock, B. J. Baker, E. A. Conneely, S. G. Dietrick, F. L. Kearns, K. McKeever, R. M. Young, C. A. Sierra, S. Soldatou, H. Lee Woodcock, M. P. Johnson; Not Drug-like, but Like Drugs: Cnidaria Natural Products. *Marine Drugs*, **2022**; 20(1):42 (10.3390/md20010042).

77. E Epifanovsky, A. Gilbert, X. Pan, Y. Shao, H. Lee Woodcock. Technical Report: Integrated Web User Interface for Multi-Scale Chemical Physics Simulations (DE-SC0011297). United States: N. p., **2021**.

76. A. Szabadi, R. Elfgen, R. Macchieraldo, F. L. Kearns, H. Lee Woodcock, B. Kirchner, C. Schroder;* 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 (10.1016/j.molliq.2021.116521).

75. E. Epifanovsky et al.; Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package, *J. Chem. Phys.*, **2021**, 155, 084801 (10.1063/5.0055522).

74. B. C. Knott, E. Erickson, M. D. Allen, J. E. Gado, R. Graham, F. L. Kearns, I. Pardo, E. Topuzlu, J. J. Anderson, H. P. Austin, G. Dominick, C. W. Johnson, N. A. Rorrer, C. J. Szostkiewicz, V. Copiee, C. M. Payne, H. Lee Woodcock, B. S. Donohoe, G. T. Beckham,* J. E. McGeehan;* Characterization and engineering of a two-enzyme system for plastics depolymerization. *Proc. Nat. Acad. Sci.*, **2020**, (10.1073/pnas.2006753117).

73. V. Zeindlhofer, P. S. Hudson, A. M. Palvolgyi, M. Welsch, M. Almarashi, H. Lee Woodcock, B. R. Brooks, K. Bica-Schroder, C. Schroder;* Enantiomerization of Axially Chiral Biphenyls: Polarizable MD Simulations in Water and Butylmethylether. *Int. J. Mol. Sci.*, **2020**, 21(17), 6222, (10.3390/ijms21176222).

72. Y. M. Elbatrawi, K.P. Pedretty, N. Giddings, H. Lee Woodcock, J. R Del Valle;* δ-Azaproline and its oxidized variants. *J. Org. Chem.*, **2020**, 85, 4207–4219. (10.1021/acs.joc.9b03384).

71. O. A. Pemberton, R. E. Noor, V. Kumar, R. Sanishvili, M. T. Kemp, F. L. Kearns, H. Lee Woodcock, Ioannis Gelis,* Y. Chen;* Mechanism of proton transfer in class A β-lactamase catalysis and inhibition by avibactam. *Proc. Nat. Acadm. Sci.*, **2020**, 117, 5818–5825. (10.1073/pnas.1922203117).

70. D. Wolfe, J. Persichetti, A. Sharma, P. S. Hudson, H. Lee Woodcock, E. O'Brien;* Hierarchical Markov State Model Building to Describe Molecular Processes, *J. Chem. Theory. Comput.*, **2020**, 16, 1816–1826. (10.1021/acs.jctc.9b00955).

69. J. N. Kuhn, H. Lee Woodcock, M. A. Barakat, M. A. Alghamdi; Metal Chelating Composites, Methods of Using Composites, and Methods of Making Composites. U.S. patent number 10,343,143, July **2019**.

68. P. S. Hudson, H. Lee Woodcock,*, S. Boresch;* On the use of interaction energies in QM/MM free energy simulations. *J. Chem. Theory Comput.*, **2019**, 15, 4632–4645. (10.1021/acs.jctc.9b00084).

67. F. L. Kearns, C. Robart, M. T. Kemp, S. L. Vankayala, B. M. Chapin, E. V. Anslyn, H. Lee Woodcock,* J. D. Larkin;* Modeling Boronic Acid Based Fluorescent Saccharide Sensors: Com-

putational Investigation of d-Fructose Binding to Dimethylaminomethylphenylboronic Acid (DMPBA). *J. Chem. Inf. Model.*, **2019**, 59, 2150–2158. *Special issue honoring Women in Computaitonal Chemistry.* (10.1021/acs.jcim.8b00987).

66. F. L. Kearns, L. Warrensford, S. Boresch,* H. Lee Woodcock;* The Good, the Bad, and the Ugly: "HiPen", a New Dataset for Validating (S)QM/MM Free Energy Simulations. *Molecules*, **2019**, 24, 681–708. (10.3390/molecules24040681).

65. P. S. Hudson, S. Boresch, D. M. Rogers,* H. Lee Woodcock;* Accelerating QM/MM Free Energy Computations via Intramolecular Force Matching. *J. Chem. Theory Comput.*, **2018**, 14, 6327–6335. (10.1021/acs.jctc.8b00517).

64. P. S. Hudson, K. Han, H. Lee Woodcock, B. R. Brooks; Force matching as a stepping stone to QM/MM CB[8] host/guest binding free energies: a SAMPL6 cautionary tale. *J Comput Aided Mol Des*, **2018**, 32, 983–999. (10.1007/s10822-018-0165-3).

63. J. E. McGeehan,* G. T. Beckham,* H. Lee Woodcock;* Engineering a plastic-digesting enzyme: Understanding an enzyme which can digest some of our most commonly polluting plastic packaging. *Baking Europe*, Summer **2018**, 54–56.

62. H. P. Austin, M. D. Allen, B. S. Donohoe, N. A. Rorrer, F. L. Kearns, R. Silveira, B. C. Pollard, G. Dominick, R. Duman, K. El-Omari, V. Mykhaylyk, A. Wagner, W. E. Michener, A. Amore, M. S. Skaf, M. F. Crowley, A. W. Thorne, C. W. Johnson, H. Lee Woodcock,* J. E. McGeehan,* G. T. Beckham;* Characterization and engineering of a plastic-degrading aromatic polyesterase. *Proc. Nat. Acad. Sci.*, **2018**, 115 E4350–E4357 (10.1073/pnas.1718804115 | Altmetric score: 2092, 2018 Altmetric Top 100).

61. J. N. Kuhn, H. Lee Woodcock, M. A. Barakat, M. A. Alghamdi; Metal Chelating Composites, Methods of Using Composites, and Methods of Making Composites. U.S. patent number 9,950,307, **2018**.

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55. S. Boresch,* H. Lee Woodcock;* Convergence of single-step free energy perturbation. *Mol. Phys.*, **2017**; 115, 1200–1213 (10.1080/00268976.2016.1269960).

54. S. L. Vankayalaa, F. L. Kearns, B. J. Baker, J. D. Larkin, H. Lee Woodcock;* Elucidating a chemical defense mechanism of Antarctic sponges: A computational study. *J. Mol. Graph. Model.*, **2017**; 71, 104–115 (10.1016/j.jmgm.2016.11.004).

53. J. K. White, S. Handa, S. L. Vankayala, D. J. Merkler, H. L. Woodcock;* Thiamin Diphosphate Activation in 1-deoxy-D-xylulose 5-Phosphate Synthase: Insights into the Mechanism and Underlying Intermolecular Interactions. *J. Phys. Chem. B*, **2016**; 120, 9922–9934 (10.1021/acs.jpcb.6b07248).

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48. P. S. Hudson, H. L. Woodcock,* S. Boresch;* Use of Non-equilibrium Work Methods to Compute Free Energy Differences between MM and QM Representations of Molecular Systems. *J. Phys. Chem. Lett.*, **2015**; 6(23), 4850–4856. (10.1021/acs.jpclett.5b02164).

47. J. Konc BT Miller, T Stular, S. Lesnik, H. L. Woodcock, BR Brooks, D. Janezic;* ProBiS-CHARMMing: Web Interface for Prediction and Optimization of Ligands in Protein Binding Sites. *J. Chem. Inf. Model.*, **2015**; 55(11), 2308–2314.(10.1021/acs.jcim.5b00534).

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Kaduk, K. Khistyaev, J. Kim, J. Kim, R. A. King, P. Klunzinger, D. Kosenkov, T. Kowalczyk, C. M. Krauter, K. U. Lao, A. Laurent, K. V. Lawler, S. V. Levchenko, C. Y. Lin, F. Liu, E. Livshits, R. C. Lochan, A. Luenser, P. Manohar, S. F. Manzer, S.-P. Mao, N. Mardirossian, A. V. Marenich, S. A. Maurer, N. J. Mayhall, C. M. Oana, R. Olivares-Amaya, D. P. O'Neill, J. A. Parkhill, T. M. Perrine, R. Peverati, P. A. Pieniazek, A. Prociuk, D. R. Rehn, E. Rosta, N. J. Russ, N. Sergueev, S. M. Sharada, S. Sharmaa, D. W. Small, A. Sodt, T. Stein, D. Stuck, Y.-C. Su, A. J. W. Thom, T. Tsuchimochi, L. Vogt, O. Vydrov, T. Wang, M. A. Watson, J. Wenzel, A. White, C. F. Williams, V. Vanovschi, S. Yeganeh, S. R. Yost, Z.-Q. You, I. Y. Zhang, X. Zhang, Y. Zhou, B. R. Brooks, G. K. L. Chan, D. M. Chipman, C. J. Cramer, W. A. Goddard III, M. S. Gordon, W. J. Hehre, A. Klamt, H. F. Schaefer III, M. W. Schmidt, C. D. Sherrill, D. G. Truhlar, A. Warshel, X. Xua, A. Aspuru-Guzik R. Baer, A. T. Bell, N. A. Besley, J.-D. Chai, A. Dreuw, B. D. Dunietz, T. R. Furlani, S. R. Gwaltney, C-P. Hsu, Y. Jung, J. Kong, D. S. Lambrecht, W. Liang, C. Ochsenfeld, V. A. Rassolov, L. V. Slipchenko, J. E. Subotnik, T. Van Voorhis, J. M. Herbert, A. I. Krylov, P. M. W. Gill, M. Head-Gordon. Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Mol. Phys.*, **2015**; 113(2), 184-215. (10.1080/00268976.2014.952696).

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37. Y. Pevzner, D. N. Santiago, J. S. Fries, R. S. Metcalf, K. G. Daniel, L. Calcul, H. L. Woodcock, B. J. Baker, W. C. Guida, W. H. Brooks; Virtual target screening to rapidly identify potential protein targets of natural products in drug discovery. *AIMS Molec. Sci.*, **2014**; 1(2), 81–98 (10.3934/molsci.2014.2.81).

36. J. C. Hargis, J. K. White, Y. Chen, H. L. Woodcock*; Can Molecular Dynamics and QM/MM solve the Penicillin Binding Protein Protonation Puzzle?. *J. Chem. Inf. Mod.*, **2014**; 54(5), 1412–1424 (10.1021/ci5000517).

35. G. Konig, P. S. Hudson, S. Boresch,* H. L. Woodcock*; 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. *J. Chem. Theory Comput.*, **2014**; 10(4), 1406–1419 (10.1021/ct401118k).

34. J. C. Hargis, S. L. Vankayala, J. K. White, H. L. Woodcock*; Identification and characterization of non-covalent interactions that drive binding and specificity in DD-peptidases and β-lactamases. *J. Chem. Theory Comput.*, **2014**; 20(2), 855–864 (10.1021/ct400968v).

33. S. L. Vankayala, J. C. Hargis, H. L. Woodcock;* How Does Catalase Release Nitric Oxide? A Computational Structure Activity Relationship Study. *J. Chem. Inf. Mod.*, **2013**; 53(11), 2591–2961 (10.1021/ci400395c).

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31. M. H. Ramadan, M. A. Barakat, J. N. Kuhn, H. L. Woodcock; Equilibrium and Kinetics of Pb2+ removal from aqueous solution by dendrimer/titania composites. *Desalination and Water Treatment*, **2013**; 1(1), 1–7 (10.1080/19443994.2013.815584).

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1. H. Lee Woodcock, Damian Moran, Paul von Rague Schleyer and H.F. Schaefer; The Almost Bottleable Triplet Carbene: 2,6-dibromo-4-tert-butyl-2',6'-bistrifluoromethyl-4'-isopropyldiphenylcarbene; *J. Am. Chem. Soc.*; **2001**; 123(18); 4331 (10.1021/ja003552q).

(E) Research Support:

Pending:

Project/Proposal Title: Molecular mechanisms of lithium action on Kinases
Source of Support: National Institutes of Health, NIGMS
Total Award Period Covered: 09/2022 – 08/2026
Person-Months Per Year Committed to the Project: 0.5 month per year
Role: co-I

Active:

Project/Proposal Title: Design and application of robust and efficient QM/MM free energy simulation methods for biomolecular systems.
Source of Support: National Institutes of Health, NIGMS (R01GM129519)
Total Award Period Covered: 09/2018 – 08/2022
Person-Months Per Year Committed to the Project: 1.2 month per year
Role: PI

The main goal of this work is to develop a set of robust, efficient, and accurate new techniques that will make the application of QM/MM FES nearly routine. These methods will be subsequently applied to study two classes of biomolecular applications that present extreme challenges to current techniques. Namely, the accurate computation of (1) absolute pKa as a function of ligand binding and reaction and (2) free energy differences of binding as a function of tautomerism.

Project/Proposal Title: Toward understanding the chemistry and biology of microbial DXP synthase.
Source of Support: National Institutes of Health, NIGMS (R01GM143810)
Total Award Period Covered: 07/2021 – 06/2025
Person-Months Per Year Committed to the Project: 1.0 month per year
Role: co-PI

Microbial metabolism plays important roles in human health and disease. Our research will investigate a key microbial metabolic enzyme, DXP synthase, toward a long-term goal to understand its function in the human microbiome and its physiological relevance during microbial infection.

Project/Proposal Title: Data Management for Molecular Simulation: An Throughput-Oriented Approach
Source of Support: National Institutes of Health, NIGMS (R01GM140316)
Total Award Period Covered: 09/2021 – 08/2025
Person-Months Per Year Committed to the Project: 0.8 month per year
Role: Co-I

We propose a novel MD data analysis framework that can significantly improve throughput and latency of data analysis tasks. It will also benefit computer simulations as a high throughput means for researchers to study the structure, dynamics, and thermodynamics of biomolecules. This will greatly impact many fields of medical research such as discovery of new medicines, biomimetic material design, and pathology/diagnosis of genetic diseases.

Completed:

Project/Proposal Title: High-level QM/MM free energy calculations and reaction path studies at affordable computational cost.
Source of Support: National Science Foundation (CHE-1464946)
Total Award Period Covered: 05/2015 – 04/2020
Person-Months Per Year Committed to the Project: 1.00 months per year
Role: PI

Project/Proposal Title: Integrated Web User Interface for Multi-Scale Chemical Physics Simulations (Phase II SBIR).
Source of Support: Department of Energy via sub-contract from Q-Chem Inc. (DE-SC0011297TDD)
Total Award Period Covered: 04/2015 – 03/2020
Person-Months Per Year Committed to the Project: 1.00 months per year
Role: Co-PI

Project/Proposal Title: N-amino peptide-derived β-strand mimics.
Source of Support: National Science Foundation (CHE-1709927)
Total Award Period Covered: 01/2017 – 12/2020
Person-Months Per Year Committed to the Project: 0.1 month per year
Role: Senior Personnel

Project/Proposal Title: Graduate Student Fellowship
Source of Support: National Institutes of Health
Total Award Period Covered: 2018 – 2020
Role: Advisor

Project/Proposal Title: Graduate Student Fellowship
Source of Support: National Science Foundation (GRFP)
Total Award Period Covered: 2018 – 2020
Role: Advisor

Project/Proposal Title: Graduate Student Fellowship
Source of Support: Department of Energy (SCGSR)
Total Award Period Covered: 2018 – 2019
Role: Advisor

Project/Proposal Title: Multi-scale Simulations of Boronic Acids in Proteasome Inhibition (Woodcock: Senior Personnel).
Source of Support: National Institutes of Health
Total Award Period Covered: 08/2014 – 07/2019
Person-Months Per Year Committed to the Project: 0.75 month per year

Project/Proposal Title: Elucidating the Crystalline Structure of Cellulose (Woodcock: PI).
Source of Support: National Renewable Energy Laboratory Sub-contract (DOE)
Total Award Period Covered: 03/2015 – 02/2016
Person-Months Per Year Committed to the Project: 0.75 month per year

Project/Proposal Title: Treatment and recycling of industrial waste-water from different sectors in Saudi Arabia using advanced techniques (Woodcock: co-PI).
Source of Support: KAU (Sub-contract: 2107-1056-01).
Total Award Period Covered: 08/2011 – 07/2016

Person-Months Per Year Committed to the Project: 0.50 month per year

Project/Proposal Title: Modern Drug Resistance: Elucidation of Beta-Lactamase Mechanisms of Action (Woodcock: PI).
Source of Support: National Institutes of Health (NHLBI, K22 HL088341-01A1).
Total Award Period Covered: 08/2009 – 07/2014
Person-Months Per Year Committed to the Project: 1.50 month per year

Project/Proposal Title: Integrated Web User Interface for Multi-Scale Chemical Physics Simulations (Phase I SBIR, Woodcock: co-PI).
Source of Support: Department of Energy via sub-contract from Q-Chem Inc. (DE-SC0011297TDD)
Yearly Award Amount: ∼$50,000
Total Award Period Covered: 04/2014 – 03/2015
Person-Months Per Year Committed to the Project: 1.00 months per year

(F) Synergistic Activities:

1. National Program Chair for the American Chemical Society, Computers in Chemistry Division (2015 – Present).
2. ACS National Award Committee (2019-2022).
3. Co-Organizer, Macromolecular Modeling Workshop (Florida International University, April 2017 - https://casfaculty.fiu.edu/David.Chatfield/workshop):
4. Co-organizer, CECAM (Centre Europeen de Calcul Atomique et Moleculaire; www.cecam.org): Advances in Biomolecular Modelling and Simulations using CHARMM. (2012: https://www.cecam.org/workshop-805.html and 2014: https://www.cecam.org/workshop-1043.htm)
5. Computational Symposium Organizer, Florida Local ACS Meeting (FAME, 2010 – 2014).
6. Co-author of both the CHARMM and Q-Chem software suites and lead developer of the Q-Chem/CHARMM QM/MM interface, general multiscale modeling framework (MSCALE), and Replica Path and Off-Path Simulation infrastructures.
7. Initiated and lead the development of a new web portal for the CHARMM macromolecular modeling package, CHARMMing (CHARMM interface and graphics, www.charmming.org). This is an open-source project that provides a user-friendly interface for the preparation, submission, monitoring, and visualization of molecular simulations.
8. Professional Memberships: American Chemical Society, Biophysical Society, Computers in Chemistry Division of the American Chemical Society (ACS COMP), ACS Physical Chemistry Division (ACS PHYS), World Association of Theoretical and Computational Chemists (WATOC), South Eastern Theoretical Chemistry Association (SETCA)
9. Scientific Referee: *Journal of the American Chemical Society, Journal of Chemical Theory and Computation, Journal of Computational Chemistry, Journal of Chemical Information and Modeling, Journal of Physical Chemistry, PloS Computational Biology, Physical Chemistry Chemical Physics, Theoretical Chemistry Accounts, Molecular Physics, Acta Pharmacologica Sinica, Carbohydrate Research, Journal of Chemical Physics, Food Biophysics,* and numerous more.
10. Grant Referee: National Institutes of Health, National Science Foundation, Department of Energy, ACS National Award Committee, American Chemical Society Petroleum Research Fund (PRF), National Science Foundation's XSEDE Allocations Committee, ACS COMP Postdoc, Graduate, and Junior Faculty Awards.