Adam W. Van Wynsberghe

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Clinton, NY 13323

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Professional Experience

2015-Present — Associate Professor
Hamilton College, Clinton, NY
Department of Chemistry

2012-2013 — Visiting Assistant Research Scientist (Sabbatical Leave from Hamilton College)
University of California-San Diego
Department of Chemistry and Biochemistry

2009-2015 — Assistant Professor
Hamilton College, Clinton, NY
Department of Chemistry

2007-2009 — NIH Post-Doctoral Fellow
University of California-San Diego
Department of Chemistry and Biochemistry
Advisor: Dr. J. Andrew McCammon

2007 — Associate Lecturer
University of Wisconsin-Madison
Department of Chemistry

Education

2001-2007 — Ph.D., Biophysics
University of Wisconsin-Madison
Dissertation: Investigation into functional motions of biological macromolecules from a computational and theoretical perspective.
Advisor: Dr. Qiang Cui

1997-2001 — B.A. (Summa Cum Laude, Phi Beta Kappa, University Honors)
Major: ACS Biochemistry, Minor: Mathematics
Ohio Wesleyan University, Delaware, OH

Research Experience

2009-Current — Principal Investigator
Directs computational biophysical chemistry laboratory at a primarily undergraduate institution. Research activities include investigations into enzyme catalysis, protein-protein interactions, and protein-ligand interactions.
Department of Chemistry, Hamilton College

2007-2009 NIH Post-Doctoral Fellow
Specialized in Brownian Dynamics simulations of macromolecular assemblies.
Advisor: Dr. J. Andrew McCammon, University of California-San Diego

2001-2007 WARF Prize Fellow, NSF Pre-Doctoral Fellow, Graduate Research Assistant
Doctoral Research: Used theoretical and computational techniques to study macromolecular motions over both fast and slow timescales. Specialized in Normal Mode Analysis and Molecular Dynamics simulations.
Advisor: Dr. Qiang Cui, University of Wisconsin-Madison

2000 Undergraduate Summer Research Intern
Used molecular biology techniques to study the contribution of the internal guidance sequence to substrate binding in the Group I intron
Advisor: Dr. Dan Herschlag, Stanford University

1999-2001 Independent Study Undergraduate Research Student
Assigned microwave spectra of environmentally interesting molecules α- and β-pinene; assisted in construction and setup of a Beowulf cluster for theoretical chemistry research
Advisor: Dr. Dale Brugh, Ohio Wesleyan University

1999-2000 NSF-REU Summer Research Student
Used FT-Mircowave Spectroscopy to determine the structure of 1,2-dichloro-3,3,4,4-tetrafluorocyclobutene in order to investigate the effect of halogenation on adjacent chemical bonds.
Advisor: Dr. Robert Kuczkowski, University of Michigan

1997-1999 Independent Study Undergraduate Research Student
Used classical biochemistry techniques to isolate and characterize an enzyme with keratinase activity.
Advisor: Dr. David Lever, Ohio Wesleyan University

Teaching Experience

2009-Current Assistant/Associate Professor
Department of Chemistry, Hamilton College

-Instructor of record for lecture and laboratory courses

Lecture: Physical Chemistry (Quantum Mechanics), General Chemistry, Physical Chemistry (Statistical and Classical Thermodynamics and Kinetics), Advanced General Chemistry (Environmental Focus)

Laboratory: General Chemistry, Physical Chemistry (Spectroscopy), Physical Chemistry (Thermo and Kinetics), Biological Chemistry, Advanced General Chemistry (Environmental Focus)

2009-Current Undergraduate Research Mentor
Department of Chemistry, Hamilton College

-Primary supervisor for research lab in computational biophysical chemistry

2008-2009 Undergraduate Research Mentor
Chemistry and Biochemistry, University of California-San Diego
-Supervised day to day research activities of undergraduates while a Postdoctoral fellow

2007 Associate Lecturer
CHEM 104, General Chemistry, University of Wisconsin-Madison
-Instructor of record for second semester general chemistry course.

2005 Teaching Assistant
CHEM 109H, General Chemistry, University of Wisconsin-Madison
-Responsible for content and oversight of weekly discussion and laboratory section

2001-2006 Undergraduate Research Mentor
Chemistry, University of Wisconsin-Madison
-Supervised day to day research activities of independent study and summer research undergraduates while a graduate student

Honors and Awards

2016 Class of 1963 Faculty Fellowship
2015 Class of 1966 Career Development Award
2014 John R. Hatch, Class of 1925, Excellence in Teaching Award
2012 National Biomedical Computational Resource Summer Institute Scholarship
2008-2009 NIH (NIGMS) Ruth L. Kirschstein NRSA Post-Doctoral Fellowship
2003-2005 National Science Foundation Pre-Doctoral Fellowship
2001 Department of Defense Pre-Doctoral Fellowship (declined)
2001 Honorable Mention, Howard Hughes Medical Institute Pre-Doctoral Fellowship
2001-2002 University of Wisconsin-Madison WARF Prize Fellowship
2001 Slocum Prize in the Sciences (Highest Overall GPA), Ohio Wesleyan University
2001 Outstanding Senior Chemistry Major, Ohio Wesleyan University
2001 Phi Beta Kappa Honor Society, Ohio Wesleyan University
2000 Barry M. Goldwater Scholarship
2000 Ernest B. Yeager Award, Society for Applied Spectroscopy, Cleveland Section
2000 Ralph E. Hall Chemistry Fellowship, Ohio Wesleyan University
2000 Outstanding Junior Chemistry Major, Ohio Wesleyan University
2000 Chi Gamma Nu Chemistry Honor Society, Ohio Wesleyan University
2000 Phi Sigma Biological Sciences Honor Society, Ohio Wesleyan Univsersity
1999 Outstanding Poster, Central Ohio Undergraduate Research Symposium
1999 Charles Schafer Chemistry Scholarship, Ohio Wesleyan University
1999 Phi Society Sophomore Honor Society, Ohio Wesleyan University
1999 Pi Mu Epsilon Mathematics Honor Society, Ohio Wesleyan University
1998 Phi Eta Sigma Freshman Honor Society, Ohio Wesleyan University
1997-2001 Presidential Scholarship, Ohio Wesleyan University
1997 National Merit Finalist

Committee Service

2016-Present Committee on Academic Policy
2015-Present Planning Committee

2014-Present	Coordinator, Clare Boothe Luce Program, Hamilton College
2014-Present	Director, Chemical Physics Program
2012-2014	President, Hamilton College chapter of Phi Beta Kappa
2010-2012	Vice-President, Hamilton College chapter of Phi Beta Kappa
2010-Present	Scientific Misconduct Review Board
2013-2014; 2010-2011	Organizer, Chemistry Department Seminar Series
2009-Present	Chemical Physics Program Committee
2009-Present	High Performance Computing Advisory Group

Other Professional Activities

Reviewer	Analyst
Reviewer	Chemical Biology and Drug Design
Reviewer	Journal of the American Chemical Society
Reviewer	Journal of Chemical Education
Reviewer	Journal of Molecular Graphics and Modelling
Reviewer	Journal of Molecular Modeling
Reviewer	Journal of Physical Chemistry
Reviewer	PLoS Computational Biology
Reviewer	PROTEINS: Structure, Function, and Bioinformatics.
Reviewer	ACS-Petroleum Research Fund
Reviewer	NSF-CAREER
Panelist	NSF-MRI
Reviewer	NSF-RUI
Reviewer	Research Corporation, CCSA
2006	Cover Art Designer, *Molecular and Cellular Biophysics*, Meyer Jackson, Cambridge University Press, Cambridge.
2000-2001	Co-President of Chemistry Student Board, Ohio Wesleyan University Department of Chemistry

Affiliations

2010-2011	Sigma Xi
2007-2015	Biophysical Society
2004-Present	American Chemical Society

Grant Activity

National Science Foundation: CC* Cyber Team, $1,500,000, *Not Funded*, Co-PI, A Collaboration that Enables New Approaches to Computationally-Intensive Research at Liberal Arts Institutions

National Science Foundation: Major Research Instrumentation, $225,000, 2016-2019, Contributor, MRI: Addition of High Performance Computers for the Molecular Education and Research Consortium in Undergraduate computational chemistRY (MERCURY).

Hamilton College: Class of 1963 Faculty Fellowship, $3,500, 2016, PI, Development of a water quality theme for Chemistry 125.

Hamilton College: Class of 1966 Career Development Award, $4,800, 2015, PI, Development of BPS and PFOA Detection Methodology.

XSEDE Allocation: TG-MCB130192, 100,000 Service Units, 2013-2014, PI, A Study of Sialic Acid-Neuraminidase Binding Events through MM/PBSA Free-Energy Calculations. *Co-Pi was Hamilton College Undergraduate Leah Krause '14.

National Science Foundation: Major Research Instrumentation, $200,000, 2012-2015, Contributor, MRI: Acquisition of a High Performance Computer for the Molecular Education and Research Consortium in Undergraduate computational chemistRY (MERCURY)

Research Corporation: Cottrell College Science Award, $35,000 plus $30,000 Hamilton College match, 2010-2012, PI, Accurate Evaluation of Association Rate Constants of Influenza Neuraminidase Inhibitors.

National Science Foundation: Major Research Instrumentation, $177,950, 2010-2012, PI MRI-R2: Acquisition of a High Performance Computing cluster with a fast interconnect to enable shared-use, college-wide computational investigations at Hamilton College.

Teragrid Allocation: TG-MCB090196, 200,000 Service Units, 2009-2010, PI, Investigations of Ribonuclease A Catalysis.

Publications *(* denotes undergraduate co-author)*

Krause, L. M.*, J. Sørensen, A. R. Wu*, J. E. Adelman*, D. J. Mermelstein*, R. E. Amaro, and **A. W. Van Wynsberghe**, Investigation of the pathways of influenza neuraminidase ligand binding using MM/GBSA Free Energy Calculations. *In Preparation*

O'Grady, C. E.*, P. Talpey*, T. E. Elgren, and **A. W. Van Wynsberghe**, A comparison of student outcomes and attitudes from the use of a bio-molecular docking exercise in the general and biochemistry laboratories. *In Preparation.*

O'Grady, C. E.*, P. Talpey*, T. E. Elgren, and **A. W. Van Wynsberghe**, 2014. The development and implementation of a bio-molecular docking exercise for the general chemistry laboratory. In *Annual Reports in Computational Chemistry, Vol. 10.* Ralph Wheeler, editor. Elsevier, United Kingdom, pp. 167-187.

Kinnel, R. B., **A. W. Van Wynsberghe**, I. J. Rosenstein, K. S. Brewer, M. Cotten, G. C. Shields, C. J. Borton, S. Z. Senior, G. S. Rahn, and T. E. Elgren, 2013. A Departmental Focus on High Impact Undergraduate Research Experiences. In *Developing and Maintaining a Successful Undergraduate Research Program.* T. W. Chapp and M. A. Benvenuto, editors. ACS Symposium Series; American Chemical Society: Washington, D.C., vol. 1156:5-22.

Tsutakawa, S. E., **A. W. Van Wynsberghe**, B. D. Freudenthal, C. P. Weinacht, L. Gakhar, M. T. Washington, Z. Zhuang, J. A. Tainer, and I. Ivanov, 2011. Solution X-ray scattering combined with computational modeling reveals multiple conformations of covalently-bound ubiquitin on PCNA. *Proc. Natl. Acad. Sci.* 108(43):17672-17677.

Sinko, W., C. de Oliveira, S. Williams, **A. Van Wynsberghe**, J. Durrant, R. Cao, E. Oldfield, and J. A. McCammon, 2011. Applying Molecular Dynamics Simulations to Identify Rarely Sampled Ligand bound Conformational States of Undecaprenyl Pyrophosphate Synthase, an Antibacterial Target. *Chem. Biol. Drug Des.* 77(6):412-420.

Van Wynsberghe, A. W. and Q. Cui, 2010. Conservation and Variation of Structural Flexibility in Protein Families. *Structure.* 18:281-283.
(Corresponding Author)

Sung, J. C.*, **A. W. Van Wynsberghe**, R. E. Amaro, W. W. Li, and J. A. McCammon, 2010. The role of secondary sialic acid binding sites in influenza N1 neuraminidase. *J. Amer. Chem. Soc.* 132(9):2883-2885.
(Corresponding Author)

Van Wynsberghe, A. W., L. Ma, X. Chen, and Q. Cui, 2008. Functional Motions in Biomolecules: Insights from Computational Studies at Multiple Scales. In *Computational Structural Biology*. T. Schwede and M. Peitsch, editors. World Scientific Publishing.

Kondrashov, D., **A. Van Wynsberghe**, R. M. Bannen, Q. Cui, and G. N. Phillips, Jr., 2007. Protein Structural Variation in Computational Models and Crystallographic Data. *Structure*. 15:169-177.
(Feature Article)

Van Wynsberghe, A., and Q. Cui, 2006. Interpreting correlated motions using normal mode analysis. *Structure*. 14:1647-1653.

Van Wynsberghe, A. W., and Q. Cui. 2005. Comparison of mode analyses at different resolutions applied to nucleic acid systems. *Biophys. J.* 89:2939-2949.
(Cover Article)

Li, G., **A. Van Wynsberghe**, O. N. A. Demerdash, and Q. Cui. 2005. Normal Mode Analysis of Macromolecules: From Enzyme Active Sites to Molecular Machines. In *Normal Mode Analysis: Theory and Applications to Biological and Chemical Systems*. Q. Cui and I. Bahar, editors. CRC Press, Boca Raton.

Felitsky, D. J., J. G. Cannon, M. W. Capp, J. Hong, **A. W. Van Wynsberghe**, C. F. Anderson, and M. T. Record. 2004. The exclusion of glycine betaine from anionic biopolymer surface: Why glycine betaine is an effective osmoprotectant but also a compatible solute. *Biochem.* 43:14732-14743.

Van Wynsberghe, A., G. H. Li, and Q. Cui. 2004. Normal-mode analysis suggests protein flexibility modulation throughout RNA polymerase's functional cycle. *Biochem.* 43:13083-13096.
(Corresponding Author)

Van Wynsberghe, A. W., S. A. Peebles, R. A. Peebles, and R. L. Kuczkowski. 2000. Rotational spectrum and structure of 1,2-dichloro-3,3,4,4-tetrafluorocyclobutene: Comparison of spectroscopy, diffraction, and ab initio results. *J. Phys. Chem. A* 104:8702-8708.

Invited Presentations

Van Wynsberghe, A. W., 2016. Development of a multi-scale sampling methodology to examine the favored ligand-binding pathways of influenza neuraminidase.
Syracuse University, Chemistry Departmental Seminar

Van Wynsberghe, A. W., 2016. Development of a multi-scale sampling methodology to examine the favored ligand-binding pathways of influenza neuraminidase.
Union College, Chemistry Departmental Seminar

Kang, G. M.*, D. J. Mermelstein*, R. B. Clayton*, and **A. W. Van Wynsberghe**, 2015. Investigation of different binding kinetics among the neuraminidase inhibitors.
SciMix Poster Session, 249th ACS National Meeting, Denver, CO.

Van Wynsberghe, A. W., 2014. Multi-Scale Simulations of ligand-binding pathways to influenza neuraminidase
Siena College, Chemistry and Biochemistry Departmental Seminar

Van Wynsberghe, A. W., 2013. Simulations of ligand binding pathways: directed diffusion with Hamilton College undergraduates: Molecular Dynamics and Markov State Models
University of California-San Diego, Amaro Laboratory Group Meeting

Van Wynsberghe, A. W., 2012. Simulations of ligand binding pathways: directed diffusion with Hamilton College undergraduates: Brownian Dynamics
University of California-San Diego, Modeling Diffusional Encounter and Subsequent Events Mini-Symposium

Van Wynsberghe, A. W., 2012. Hitting the Target: Simulations of the ligand binding pathways of influenza neuraminidase.
Colgate University, Chemistry Department Seminar Series

Van Wynsberghe, A. and Q. Cui, 2004. Nucleic acid conformational flexibility and function: Molecular dynamics and normal mode analyses of the hammerhead ribozyme.
228th ACS National Meeting, Philadelphia, PA

Van Wynsberghe, A., S. A. Peebles, R. A. Peebles, and R. L. Kuczkowski, 2000. Determining molecular structure with FT-microwave spectroscopy: expectations and surprises. 44th Meeting of the Cleveland Section of the Society for Applied Spectroscopy, Cleveland, OH
(Ernest B. Yeager Award lecture)

Contributed Presentations

Kang, J* and **A. W. Van Wynsberghe**, 2017. Computational Investigation of the Binding Pathways of Zanamivir to H274Y Neuraminidase.
Poster- 16th MERCURY Conference, Greenville, SC.

Nash, K. L.*, R. W. Wenner*, and **A. W. Van Wynsberghe**, 2017. Exploration of the Binding Kinetics of Zanamivir to WT Neuraminidase via MM/GBSA Analysis of Molecular Dynamics Simulations.
Poster- 16th MERCURY Conference, Greenville, SC.

Park, A* and **A. W. Van Wynsberghe**, 2017. Characterization of Binding Pathways of Peramivir to H274Y Neuraminidase.
Poster- 16th MERCURY Conference, Greenville, SC.

Dacres, D. F.*, E. M. Lewis*, R. W. Wenner*, and **A. W. Van Wynsberghe**, 2017. Simulating the binding pathways of sialic acid and oseltamivir to H274Y neuraminidase with molecular dynamics solutions.
Poster- 253rd ACS National Meeting, San Francisco, CA.

Kang, G. M.* and **A. W. Van Wynsberghe**, 2017. Investigation of different binding kinetics among the neuraminidase inhibitors.
Poster- 253rd ACS National Meeting, San Francisco, CA.

Lewis, E. M.*, P. F. Marris*, L. M. Krause*, and **A. W. Van Wynsberghe**, 2017. Analysis of MM/GBSA free energy calculations to investigate the binding pathways of neuraminidase.
Poster- 253rd ACS National Meeting, San Francisco, CA.
(Awarded Computers in Chemistry Undergraduate Poster Award)

Wenner, R. W.*, AB W. Abera*, B. J. Banman*, and **A. W. Van Wynsberghe**, 2017. Examining the binding pathways of peramivir to wild-type neuraminidase through molecular dynamics simulations and MM/GBSA analysis.
Poster- 253rd ACS National Meeting, San Francisco, CA.

Abera, AB W.*, B. J. Banman*, and **A. W. Van Wynsberghe**, 2016. Investigating the Binding pathways of Peramivir to Neuraminidase Through Molecular Dynamics Simulations and MM/GBSA Analysis.
Poster- 15th MERCURY Conference on Computational Chemistry, Lewisburg, PA.

Dacres, D. F.* E. M. Lewis*, R. W. Wenner*, J. F. Graziadei, and **A. W. Van Wynsberghe**, 2016. Simulating the Binding Pathways of Sialic Acid and Oseltamivir to H274Y Neuraminidase with Molecular Dynamics Simulations.
Poster- 15th MERCURY Conference on Computational Chemistry, Lewisburg, PA.

Lewis, E. M.*, P. F. Marris*, L. M. Krause, and **A. W. Van Wynsberghe**, 2016. Analysis of the Binding Pathways of Neuraminidase through MM/GBSA Post-Processing of Equilibrium Molecular Dynamics Trajectories.
Poster- 15th MERCURY Conference on Computational Chemistry, Lewisburg, PA.

Nash, K. L.* R. W. Wenner*, and **A. W. Van Wynsberghe**, 2016. Exploring the binding pathways of zanamivir to wild-type neuraminidase using molecular dynamics and MM/GBSA.
Poster- 15th MERCURY Conference on Computational Chemistry, Lewisburg, PA.

Van Wynsberghe, A. W., 2016. Development of a multi-scale sampling methodology to examine the favored ligand-binding pathways of influenza neuraminidase.
PHYS: Computer Simulations of Thermodynamics and Long-Time Kinetics of Molecular Events, 251st ACS National Meeting, San Diego, CA.

Dacres, D. F.* E. M. Lewis*, R. W. Wenner*, and **A. W. Van Wynsberghe**, 2016. Examining the Binding Pathways of Various Ligands to H274Y and Wild-Type Neuraminidase via Molecular Dynamics Simulations and MM/GBSA Analysis.
Poster- 251st ACS National Meeting, San Diego, CA.

Marris, P. F.* L. M. Krause*, J. Sørensen, and **A. W. Van Wynsberghe**, 2016. Investigating binding pathways to neuraminidase using MM/GBSA free energy analysis.
Poster- 251st ACS National Meeting, San Diego, CA.

Dacres, D. F.*, J. F. Graziadei*, P. F. Marris*, and **A. W. Van Wynsberghe**, 2015. Investigation of Sialic Acid Association Kinetics to H274 Neuraminidase Using Molecular Dynamics Simulations.
Poster- 14th MERCURY Conference on Computational Chemistry, Lewisburg, PA.

Lewis, E. M.*, R. W. Wenner*, P. F. Marris*, and **A. W. Van Wynsberghe**, 2015. Examining the Binding Pathways of Oseltamivir to H274Y Neuraminidase
Poster- 14th MERCURY Conference on Computational Chemistry, Lewisburg, PA.

Marris, P. F.*, L. M. Krause*, J. Sørensen, and **A. W. Van Wynsberghe**, 2015. Investigating binding pathways to neuraminidase using MM/GBSA free energy analysis.
Poster- 14th MERCURY Conference on Computational Chemistry, Lewisburg, PA.

Kang, G. M.*, D. J. Mermelstein*, R. B. Clayton*, and **A. W. Van Wynsberghe**, 2015. Investigation of different binding kinetics among the neuraminidase inhibitors.
Poster- 249th ACS National Meeting, Denver, CO.

Wenner, R. W.*, L. M. Krause*, J. F. Graziadei*, P. F. Marris*, and **A. W. Van Wynsberghe**, 2015. Calculation of the association trajectories of oseltamivir and sialic acid to wild type and H274Y viral neuraminidase.
Poster- 249th ACS National Meeting, Denver, CO.

Kang, G. M.*, D. J. Mermelstein*, R. B. Clayton*, and **A. W. Van Wynsberghe**, 2014. Investigation of Different Binding Kinetics Among the Neuraminidase Inhibitors.
Poster- 13th MERCURY Conference on Computational Chemistry, Lewisburg, PA.

Marris, P. F*, R. W. Wenner*, L. M. Krause*, J. Sørensen, A. R. Wu*, R. E. Amaro, and **A. W. Van Wynsberghe**, 2014. Investigating oseltamivir binding pathways to H274Y neuraminidase using molecular dynamics simulations and MM/GBSA analysis.
Poster- 13th MERCURY Conference on Computational Chemistry, Lewisburg, PA.

Wenner, R. W.*, P. F. Marris*, J. E. Adelman*, and **A. W. Van Wynsberghe**, 2014. Observing the Diffusion of Oseltamivir into the Active and Secondary Sites of Neuraminidase Wild Type and the H274Y Variant.
Poster- 13th MERCURY Conference on Computational Chemistry, Lewisburg, PA.

Alvarado, S. M.*, L. Krause*, A. R. Wu*, and **A. W. Van Wynsberghe**, 2013. Close-Range Behavior of Oseltamivir with Viral Neueraminidase.
Poster- 12th MERCURY Conference on Computational Chemistry, Lewisburg, PA.

Banman B. J.*, J. E. Adelman*, A. R. Wu*, and **A. W. Van Wynsberghe**, 2013. Observing the inter- and intramolecular Events of Sialic Acid Binding to the Active Site of Neuraminidase.
Poster- 12th MERCURY Conference on Computational Chemistry, Lewisburg, PA.

Ho, J. H.*, C. M. Montangon*, R. B. Clayton*, and **A. W. Van Wynsberghe**, 2013. Investigation of the effects of molecular charges and water desolvation on the complex formation of Neuraminidase and its inhibitors.
Poster- 12th MERCURY Conference on Computational Chemistry, Lewisburg, PA.

O'Grady, C. E.*, P. Talpey*, and **A. W. Van Wynsberghe**, 2013. Development of a molecular docking exercise to elucidate principles of biophysical chemistry in the general chemistry lab.
Poster- 12th MERCURY Conference on Computational Chemistry, Lewisburg, PA.

Montagnon, C. M.*, R. B. Clayton*, and **A. W. Van Wynsberghe**, 2013. Investigation of the effects of electronic desolvation on oseltamivir binding kinetics to N1 influenza neuraminidase.
Poster- 245th ACS National Meeting, New Orlenas, LA

Wu, A. R.*, L. Krause*, and **A. W. Van Wynsberghe**, 2013. Elucidation of the molecular interactions between neuraminidase and sialic acid.
Poster- 245th ACS National Meeting, New Orlenas, LA

Krause, L.*, A. Wu*, D. Mermelstein*, J. E. Adelman*, and **A. W. Van Wynsberghe**, 2012. The Effect of Starting Location and Orientation on Molecular Dynamics Simulations as Applied to the Influenza Neuraminidase-Sialic Acid System.
Poster- 7th National Biomedical Computation Resource Summer Institute, San Diego, CA

Krause, L.*, A. Wu*, D. Mermelstein*, J. E. Adelman*, and **A. W. Van Wynsberghe**, 2012. The Effect of Starting Location and Orientation on Molecular Dynamics Simulations as Applied to the Influenza Neuraminidase-Sialic Acid System.
Poster- 11th MERCURY conference on Computational Chemistry, Lewisburg, PA

Clayton, R. B.*, C. M. Montagnon*, E. L. Losito*, and **A. W. Van Wynsberghe**, 2012. Investigation of Differences in Desolvation Energy Between Ligands
Poster- 11th MERCURY conference on Computational Chemistry, Lewisburg, PA

Losito, E. L.*, L. D. Leonard*, and **A. W. Van Wynsberghe**, 2012. Role of influenza A neuraminidase electrostatics in the binding of ligands.
Poster- 243rd ACS National Meeting, San Diego, CA

Mermelstein, D. J.*, J. E. Adelman*, and **A. W. Van Wynsberghe**, 2012. Determination of an Appropriate Surface for the Transition from Brownian Dynamics to Molecular Dynamics in Sialic Acid Binding to Neuraminidase.
Poster- 243rd ACS National Meeting, San Diego, CA

Montagnon, C. M.*, L. D. Leonard*, E. L. Losito*, and **A. W. Van Wynsberghe**, 2012. Investigation of Oseltamivir Binding Kinetics to N1 Influenza Neuraminidase.
Poster- 243rd ACS National Meeting, San Diego, CA

Wu, A. R.*, R. S. Green*, and **A. W. Van Wynsberghe**, 2012. Characterization of the Association between Neuraminidase and Sialic Acid Using Molecular Dynamics Simulations.
Poster- 243rd ACS National Meeting, San Diego, CA

Mermelstein, D. J.*, J. E. Adelman*, and **A. W. Van Wynsberghe**, 2011. Determination of an Appropriate Surface for the Transition from Brownian Dynamics to Molecular Dynamics in Sialic Acid Binding to Neuraminidase.
Poster- 10th MERCURY conference on Computational Chemistry, Lewisburg, PA

Montagnon, C. M.*, L. D. Leonard*, E. L. Losito*, J. C. Sung*, and **A. W. Van Wynsberghe**, 2011. Investigation of Oseltamivir Binding Kinetics to N1 Influenza Neuraminidase.
Poster- 10th MERCURY conference on Computational Chemistry, Lewisburg, PA

Wu, A. R.*, R. S. Green*, and **A. W. Van Wynsberghe**, 2011. Characterization of the Association between Neuraminidase and Sialic Acid Using Molecular Dynamics Simulations.
Poster- 10th MERCURY conference on Computational Chemistry, Lewisburg, PA

Adelman, J. E.*, J. C. Sung*, and **A. W. Van Wynsberghe**, 2010. A novel paradigm for finding the kinetics of the the influenza neuraminidase-sialic acid system.
Poster- 9th MERCURY conference on Computational Chemistry, Clinton, NY

Losito, E. L.*, J. C. Sung*, C. A. Rico*, and **A. W. Van Wynsberghe**, 2010. Association rate constants of peramivir and zanamivir to influenza A neuraminidase active and secondary sites.
Poster- 9th MERCURY conference on Computational Chemistry, Clinton, NY

Hagstrom, A. L.*, Sam Ha Eun Cho*, and **A. W. Van Wynsberghe**, 2010. Analysis of conformational changes in thrombin mutants and their effects on thrombomodulin binding.
Poster- 9th MERCURY conference on Computational Chemistry

Sung, J. C.*, **A. W. Van Wynsberghe**, R. E. Amaro, W. W. Li, and J. A. McCammon, 2009. The role of secondary sialic acid binding sites in influenza N1 neuraminidase.
Poster- 8th MERCURY Conference on Computational Chemistry, Clinton, NY

Sung, J.*, **A. W. Van Wynsberghe**, R. E. Amaro, and J. A. McCammon, 2009. Theoretical studies on the purpose of the surface binding site of avian influenza neuraminidase.
Poster- 237th ACS National Meeting, Salt Lake City, UT

Van Wynsberghe, A. W., I. Ivanov, and J. A. McCammon, 2009. Models of PCNA-monoubiquitin interaction complexes.
Poster- 237th ACS National Meeting, Salt Lake City, UT

Van Wynsberghe, A. W., and J. A. McCammon, 2008. Investigation of Thrombin-Thrombomodulin Association Kinetics Using Brownian Dynamics Simulations.
Poster- 52nd Biophysical Society National Meeting, Long Beach, CA

Kondrashov, D., **A. W. Van Wynsberghe**, E. J. Levin, R. M. Bannen, E. Bitto, R. Aranda, J. G. McCoy, Q. Cui, and G. N. Phillips Jr., 2007. Protein dynamics in crystallographic data and coarse-grained normal mode analysis.
Poster- 234th ACS National Meeting, Boston, MA

Van Wynsberghe, A. and Q. Cui, 2006. Identifying important residues through computational "Alanine Scanning" and the Kullback-Leibler divergence and a discussion on interpreting correlated motion using normal modes.
Poster-32nd Steenbock Symposium, Madison, WI.

Kondrashov, D. A., **A. Van Wynsberghe**, R. M. Bannen, Q. Cui, and G. N. Phillips, Jr., 2006. Optimization, validation, and application of coarse-grained models of residue interaction.
Platform- 32nd Steenbock Symposium, Madison, WI.

Bannen, R. M., V. Suresh, D. Kondrashov, **A. Van Wynsberghe**, Q. Cui, J. C., Mitchell, G. N. Phillips, Jr., and S. J. Wright., 2006. Probing dynamics and interactions of proteins using normal modes.
Poster- 32nd Steenbock Symposium, Madison, WI.

Van Wynsberghe A., G. Li, and Q. Cui, 2003. Structural analysis of protein flexibility in bacterial and viral RNA polymerases.
Poster- FASEB Summer Conference on Transcription Initiation in Prokaryotes, Saxtons River,VT

Van Wynsberghe A., G. Li, and Q. Cui, 2003. Structural analysis of protein flexibility in bacterial and viral RNA polymerases.
Poster- 47th Biophysical Society National Meeting, San Antonio, TX

Brugh, D. J., **A. Van Wynsberghe**, and R. D. Suenram, 2000. Application of Fourier Transform Microwave Spectroscopy to Pinene Detection.
Platform- Pittcon 2000, New Orleans, LA

Van Wynsberghe, A., S. A. Peebles, R. A. Peebles, and R. L. Kuczkowski, 1999. Structure determination of 1,2-dichloro-3,3,4,4-tetrafluorocycylobutene by FT-microwave spectroscopy.
Poster- Central Ohio Undergraduate Research Symposium, Columbus, OH
(Awarded Outstanding Poster)

Students Supervised *(immediate or current position)*

Hamilton College

Janice Kang, '20
Abenezer Abera, Biochemistry '19
Matthew Bleich, Chemistry and Philosophy '18
David Dacres, Chemistry '18
Alexie Diakite, Biology '18
Erin Lewis, Chemistry '18
Catherine Lyndaker, Chemistry '18
Kalvin Nash, Biochemistry and French '18
Allen Park, Chemistry '18
Leah Weaver, Chemistry '18
Geum Mi Kang, Biochemistry '17
Richard Wenner, Chemistry and Computer Science '17 (Software Engineer, Wayfair)
Patrick Marris, Mathematics '16
Bryon Banman, Chemistry '16
Jia Tsien Ho, Chemistry '16 (medical student, University of Sydney)
Lizbeth DaBramo, Chemistry, '15 (Watson Fellow; UC Berkeley Env. Engr. and Public Policy graduate student)
Jordan Graziadei, Chemistry '15 (U. of Pennsylvania School of Veterinary Medicine)
Savannah Alvarado, Hispanic Studies '15
Rob Clayton, Biochemistry '15 (Hologic, Inc.)
Clare O'Grady, Chemistry '14 (Hazard Review Specialist, The Wercs, Ltd.)

Leah Krause, Chemistry '14 (medical student, University of Minnesota Medical School)
Dan Mermelstein, Chemistry '14 (graduate student, Chemistry and Biochemistry, UC-San Diego)
Peter Talpey, Mathematics '14
Jeremy Adelman, (Barry M. Goldwater Scholar) Mathematics and Physics '13 (graduate student, Physics, UC-Davis)
Carmen Montagnon, Chemistry '13 (medical studnet, Mayo Medical School)
Alvin Wu, Biochemistry '13 (medical student, Stony Brook University of Medicine)
Anna Hagstrom, Chemistry '13-Amherst (graduate student, Chemical and Env. Engr., Yale University)
Erica Losito, Biochemistry '12 (graduate student and Carlson Fellow, Biophysics, Johns Hopkins)
Rebecca Green, Chemistry and Mathematics '11 (medical student, University of Pennsylvania School of Medicine)
Laura Leonard, Chemistry and Hispanic Studies, '11 (medical student, University of Vermont College of Medicine)
Sam Cho, Chemistry '10 (medical student, Michigan State University College of Human Medicine)
Tom Morrell, Chemistry '10 (NSF Pre-Doctoral Fellow, Chemistry, Princeton University)
Carlos Rico, Chemical Physics '10 (NSF Pre-Doctoral Fellow, Chemical Biology, Rockefeller University)

University of California-San Diego

Jeffrey Sung, Chemistry and Physics '10 (graduate student, Chemistry, University of Minnesota)

University of Wisconsin-Madison

Kate Engel, Biochemistry and Genetics '07 (graduate student, Molecular and Cell Biology, UC-Berkeley)
Mischa Wolfson, Chemistry and Computer Science '06 (graduate student, Chemistry, MIT)
Vanderlene Kung, '04 (M.D.-Ph.D. Student and NIH NRSA Fellow, Northwestern University Medical-Scientist Training Program)
Lawrence Klein, Chemistry '04 (NSF Pre-Doctoral Fellow, Biophysics, Stanford University)
