Eric R. May, Ph.D.

Associate Professor Department of Molecular and Cell Biology

University of Connecticut 91 N. Eagleville Rd, Unit 3125 Storrs, CT 06269 email: <u>eric.may@uconn.edu</u> phone: 203-695-1807 web:<u>http://maylab.uconn.edu</u>

ACADEMIC TRAINING

2/2008-8/2012	University of Michigan, Ann Arbor, MI Postdoctoral Fellow (NSF Postdoctoral Fellow 2009-2011)
12/2006	University of Florida, Gainesville, FL Ph.D. Chemical Engineering
5/2001	Bucknell University, Lewisburg, PA B.S. Chemical Engineering

PROFESSIONAL EXPERIENCE

8/2018-Present	Associate Professor of Molecular and Cell Biology University of Connecticut, Storrs, CT
8/2012-8/2018	Assistant Professor of Molecular and Cell Biology University of Connecticut, Storrs, CT
8/2012 - Present	Graduate Faculty of Chemical Engineering Graduate Faculty of Biomedical Engineering University of Connecticut, Storrs, CT
2/2008-8/2012 8/2009-8/2011	Postdoctoral Fellow NSF Postdoctoral Fellow University of Michigan, Ann Arbor, MI Department of Chemistry and Biophysics Program Advisor: Charles L Brooks III Research Project: Structure, Dynamics and Mechanics of Virus Capsids
8/2001-12/2006	Graduate Research Assistant University of Florida, Gainesville, FL Department of Chemical Engineering Advisor: Atul Narang Dissertation: Molecular Modeling of Biomembrane Deformations-The Role of Lipids

HONORS, AWARDS AND FELLOWSHIPS

- 2018 ACS OpenEye Outstanding Junior Faculty Award in Computational Chemistry
- 2013-2015 NIH NIAID Research Scholar Development Award (K22)
- 2011 National Postdoctoral Association Travel Award
- 2011 CECAM Travel Award, Multiscale Computational Biomechanics, Zurich, Switzerland
- 2010 Mathematical Virology Selected Speaker Travel Award, Ambleside, UK
- 2009-2011 National Science Foundation Postdoctoral Fellowship in Biology
- 2009 National Institutes of Health Postdoctoral Fellowship Ruth L Kirschstein NRSA (Declined due to NSF fellowship)
- 2009 Best Physical Science and Engineering Poster, Michigan UROP Spring Symposium
- 2009 Gordon Research Conference on Physical Virology Travel Grant, Galveston, TX
- 2008 Alfred P. Sloan Foundation/ACS Postdoctoral Workshop Sponsorship, Clemson University
- 2006 UF Graduate Association of Chemical Engineers AIChE Travel Grant
- 2006 UF Graduate Student Council Travel Grant
- 2001 Dow Chemicals Graduate Fellowship, University of Florida

PUBLICATIONS

- 41. A.K. Jana, M. Sharawy, **E.R. May**, "Non-equilibrium Virus Particle Dynamics: Microsecond MD Simulations of the Complete Flock House Virus Capsid Under Different Conditions", *submitted to J. Struct. Biol. Special issue on Computational Structural Biology*.
- 40. V.K. Golla, K.J. Boyd, **E.R. May**, "Curvature Sensing Lipid Dynamics in a Mitochondrial Inner Membrane Model", *submitted*.
- 39. W. Mitchell, J.D. Tamucci, E.L. Ng, S. Liu, A.V. Birk, H.H. Szeto, **E.R. May**, A.T. Alexandrescu, N.N. Alder. "Structure-Activity Relationships in the Design of Mitochondria-Targeted Peptide Therapeutics", *eLife*, 2022, 11:e75531.
- 38. M. Sharawy, N.B. Pigni, **E.R. May**, J.A. Gascon, "A favorable path to domain separation in the orange carotenoid protein", *Prot. Sci.*, 2022, 31(4):850-853.
- 37. A.K. Jana, **E.R. May**. "Atomistic Dynamics of a Viral Infection Process: Release of Membrane Lytic Peptides from a Non-Enveloped Virus", *Sci. Adv.*, 2021, 7(16):eabe1761.
- 36. A.K. Jana, **E.R. May**. "Structural and dynamic asymmetry in icosahedrally symmetric virus capsids", *Curr. Opin. Virol.*, 2020. 45:8-16.
- 35. W. Mitchell, E.A. Ng, J.D. Tamucci, K.J. Boyd, M. Sathappa, A. Coscia, M. Pan, X. Han, N.A. Eddy, E.R. May, H.H. Szeto, N.N. Alder. "The mitochondria-targeted peptide SS-31 binds lipid bilayers and modulates surface electrostatics as a key component of its mechanism of action", J. Biol. Chem., 2020, 295(21):7452-7469.
- 34. S. Juliano, L.F. Serafim, S.S. Duay, M.H. Chavez, G. Sharma, M. Rooney, F. Comert, S. Pierce, A. Radulescu, M.L. Cotten, M. Mihailescu, E.R. May, A.I. Greenwood, R. Prabhakar, A.M. Angeles-Boza. "A Potent Host Defense Peptide Triggers DNA Damage and is Active against Multi-Drug Resistant Gram-Negative Pathogens", ACS Infect. Dis., 2020, 6(5):1250-1263.
- 33. J.G. Pattis, **E.R. May.** "Markov State Model of Lassa Virus Nucleoprotein Reveals Large Structural Changes during the Trimer to Monomer Transition", *Structure*, 28:1-7, 2020.
- 32. S. Nangia, K.J. Boyd, E.R. May. "Molecular dynamics study of membrane permeabilization by wild-type and mutant lytic peptides from the non-enveloped Flock House virus", *BBA-Biomembranes*, 2020, 1862(2):183102.

- 31. J. Krucinska, M.N. Lombardo, H. Erlandsen, A. Hazeen, S. S. Duay, J.G. Pattis, V.L. Robinson, E.R. May, D.L. Wright. "Functional and structural basis of E. coli enolase inhibition by SF2312: a mimic of the carbanion intermediate", *Sci. Rep.*, 2019, 9:17106.
- 30. H. Deng, S. Ke, R. Callender, G. Balakrishnan, T.G. Spiro, E.R. May, C.L. Brooks, III, "Computational Studies of Catalytic Loop Dynamics in Yersinia Protein Tyrosine Phosphatase Using Pathway Optimization Methods", J. Phys. Chem. B., 2019, 123(37):7840-7851.
- 29. C.B. Mayo, H. Erlandsen, D.J. Mouser, A.G. Feinstein, V.L. Robinson, E.R. May, J.L. Cole. "Structural Basis of Protein Kinase R Autophosphorylation", *Biochemistry*, 2019, 58(27):2967-2977.
- 28. S.S. Duay, G. Sharma, R. Prabhakar, A.M. Angeles-Boza, E.R. May, "Molecular Dynamics Investigation into the Effect of Zinc(II) on the Structure and Membrane Interactions of the Antimicrobial Peptide Clavanin A", J. Phys. Chem. B, 2019, 123(15):3163-3176.
- 27. J.G. Pattis, S. Kamal, B. Li, E.R. May, "Catalytic Domains of Phosphodiesterase 5, 6, and 5/6 Chimera Display Differential Dynamics and Ligand Dissociation Energy Barriers", J. Phys. Chem. B, 2019, 123(4):825-835.
- 26. K.J. Boyd, E.R. May, "BUMPy: A model-independent tool for constructing lipid bilayers of varying curvature and composition", J. Chem. Theory Comput, 2018, 14(12):6642-6652.
- 25. R. Friedman, S. Khalid, C. Aponte-Santamaria, et al., "Understanding conformational dynamics of complex lipid mixtures relevant to biology", J. Membr. Biol., 2018, 251(5-6), 609-631.
- 24. K.J. Boyd, N.N. Alder, E.R. May, "Molecular Dynamics Analysis of Cardiolipin and Monolysocardiolipin on Bilayer Properties" *Biophys. J.*, 2018, 114(9):2116-2127.
- 23. S. Nangia, J.G. Pattis, E.R. May, "Folding a Viral Peptide in Different Membrane Environments: Pathway and Sampling Analyses", *J. Biol. Phys.*, 2018, 44(2):195-209. PMID: 29644513
- K. Malhotra, A. Modak, S. Nangia, T.H. Daman, U. Gunsel, V.L. Robinson, D. Mokranjac, E.R. May, N.N. Alder, "Cardiolipin mediates membrane and channel interactions of the mitochondrial TIM23 protein import complex receptor Tim50" *Sci. Adv.*, 2017, 3(9):e1700532. PMID: 28879236
- K.J. Boyd, N.N. Alder, E.R. May, "Buckling Under Pressure: Curvature Based Lipid Segregation and Stability Modulation in Cardiolipin Containing Bilayers" *Langmuir*, 2017, 33(27):6937–6946. PMID: 28628337
- S. Nangia, E.R. May, "Influence of Membrane Composition on the Binding and Folding of a Membrane Lytic Peptide from the Non-Enveloped Flock House Virus" *BBA-Biomembranes*, 2017, 1859(7):1190-1199. PMID:28395954
- 19. M.D. Ward, S. Nangia, E.R. May, "Evaluation of the Hybrid Resolution PACE Model for the Study of Folding, Insertion and Pore Formation of Membrane Associated Peptides" J. Comput. Chem., 2017, 38(16):1462-1471. PMID:28102001
- 18. J.G. Pattis, E.R. May, "Influence of RNA binding on the structure and dynamics of Lassa nucleoprotein" *Biophys. J.*, 2016, 110(6):1246-54. PMID:27028635
- 17. A. Aggarwal, E.R. May, C.L. Brooks III, W.S. Klug, "Nonuniform elastic properties of macromolecules and effect of prestrain on their continuum nature" *Phys. Rev. E.: Stat. Nonlin. Soft Matter Phys*, 2016, 93:012417. PMID:26871111
- 16. K.J. Boyd, P. Bansal, J. Feng, E.R. May, "Stability of Norwalk virus capsid protein interfaces evaluated by in-silico nanoindentation" *Front. Bioeng. Biotechnol.* 2015, 3:103. PMID:26284238
- A.J. Wowor, Y. Yan, S.M. Auclair, D. Yu, J. Zhang, E.R. May, M.L. Gross, D.A. Kendall, J.L. Cole, "Analysis of SecA Dimerization in Free Solution" *Biochemistry*, 2014, 53(19):3248-60. PMID:24786965
- 14. E.R. May, "Recent Developments in Molecular Simulation Approaches to Study Spherical Virus Capsids" *Mol. Simulat.*, 2014, 40(10-11):878-888. PMID:25197162
- 13. E.R. May, K.Arora, C.L. Brooks III, "pH Induced Stability Switching of the Bacteriophage HK97 Maturation Pathway" J. Am. Chem. Soc., 2014, 136(8):3097-3107. PMID:24495192

- J. Snijder, V.S. Reddy, E.R. May, W.H. Roos, G.R. Nemerow, G.J.L. Wuite, "Integrin and Defensin Modulate the Mechanical Properties of Adenovirus" J. Virol., 2013, 87(5):2756-2766. PMID:23269786
- 11. E.R. May, C.L. Brooks III, "On the Morphology of Viral Capsids: Elastic Properties and Buckling Transitions" J. Phys. Chem. B, 2012, 116(29):8604-9. PMID:22409201
- 10. E.R. May, J. Feng, C.L. Brooks III, "Exploring the Symmetry and Mechanism of Virus Capsid Maturation via an Ensemble of Pathways" *Biophys. J.*, 2012, 102(3):606-612. PMID:22325284
- 9. W.H. Roos, I. Gertsman, E.R. May, C.L. Brooks III, J.E. Johnson, G.J.L. Wuite, "The Mechanics of Bacteriophage Maturation" *Proc. Natl. Acad. Sci. U.S.A.*, 2012, 109(7):2342-7. PMID:22308333
- 8. E.R. May, K. Arora, R.V. Mannige, H.D. Nguyen, C.L. Brooks III, "Multiscale Approaches to Studying Virus Structure, Assembly and Dynamics", In *Computational Modeling of Biological Systems: From Molecules to Pathways*, 2102, N. Dokholyan (Ed.), Springer-Verlag, New York.
- 7. E.R. May, A. Aggarwal, W.S. Klug, C.L. Brooks III, "Viral Capsid Equilibrium Dynamics Reveals Nonuniform Elastic Properties" *Biophys. J.*, 2011, 100(11):L59-61. PMID:21641297
- 6. E.R. May, C.L. Brooks III, "Determination of Viral Capsid Elastic Properties from Equilibrium Thermal Fluctuations" *Phys. Rev. Lett.*, 2011, 106(18):188101. PMID:21635128
- 5. R.S. Armen, E.R. May, M. Taufer, "Protein Docking", In *Encyclopedia of Parallel Computing*, 2011, D. Padua (Ed.) Springer.
- 4. E.R. May, R.S. Armen, A.M. Mannan, C.L. Brooks III, "The Flexible C-terminal Arm of the Lassa Arenavirus Z-Protein Mediates Interactions with Multiple Binding Partners" *Proteins*, 2010, 78(10):2251-64. PMID:20544962
- 3. E.R. May, D.I. Kopelevich, A. Narang, "Coarse-Grained Molecular Dynamics Simulations of Phase Transitions in Mixed Lipid Systems Containing LPA, DOPA, and DOPE Lipids" *Biophys. J.*, 2008, 94(3):878-90. PMID:17921207
- E.R. May, A. Narang, D.I. Kopelevich, "Role of Molecular Tilt in Thermal Fluctuations of Lipid Membranes" *Phys. Rev. E: Stat. Nonlin. Soft Matter Phys.*, 2007, 76(2 Pt 1):021913. PMID:17930071
- 1. E.R. May, A. Narang, D.I. Kopelevich, "Molecular Modeling of Key Elastic Properties for Inhomogeneous Lipid Bilayers" *Mol. Simulat.*, 2007, 33:787-79.

PRESENTATIONS

Invited Talks and Seminars

- 6/27/23 [upcoming]American Society of Virology Annual Meeting, Plenary Talk, Athens GA.
- 10/21/22 Department of Chemistry and Biochemistry, University of Delaware, Newark, DE.
- 6/10/21 ACS Middle Atlantic Meeting of the American Chemical Society, Biophysical Chemistry Session {virtual}
- 12/4/20 Department of Chemistry and Chemical Biology, University of New Mexico, Albuquerque, NM {virtual}
- 5/3/19 Laufer Center for Physical and Quantitative Biology. Stony Brook University, Stony Brook, NY
- 4/25/19 Department of Chemistry, University of Connecticut, Storrs, CT
- 4/10/19 Department of Physics, University of Vermont, Burlington, VT
- 1/21/19 Gordon Research Conference on Physical Virology, Ventura, CA
- 10/8/18 Gibbs Conference on Biological Thermodynamics, Carbondale, IL
- 7/24/18 FASEB Virus Structure and Assembly, Steamboat Springs, Co
- 1/12/18 CECAM Workshop Frontiers in Computational Biophysics: understanding conformational dynamics of complex lipid mixtures relevant to biology, Lugano, Switzerland
- 7/18/17 Workshop on Physical Virology, International Centre for Theoretical Physics, Trieste, Italy

- 3/13/16 ACS National Meeting, From Dynamics to Function & Back Again: Adventures in Simulating Biomolecules Symposium, San Diego, CA
- 10/10/15 12th Annual North Eastern Structure Symposium, University of Connecticut, Storrs, CT
- 3/6/14 Department of Molecular Biology and Biophysics, University of Connecticut Health Center, Farmington, CT
- 9/4/13 JAX-UConn/BECAT/UCHC Joint Workshop on Computational Biology and Bioinformatics, University of Connecticut, Storrs, CT
- 5/17/13 BECAT High Performance Computing Workshop, School of Engineering, University of Connecticut, Storrs, CT
- 10/19/12 Department of Biomedical Engineering, University of Connecticut, Storrs, CT
- 10/19/12 BECAT High Performance Computing Workshop, School of Engineering, University of Connecticut, Storrs, CT
- 9/8/12 Departmental Retreat for Molecular & Cell Biology, Physiology & Neurobiology Departments University of Connecticut, Bolton, CT
- 7/14/12 London Mathematical Society Grand Biological Challenges for Mathematicians Meeting Durham University, Durham, U.K.
- 4/10/12 Department of Chemical Engineering, University of Massachusetts Lowell, Lowell, MA
- 3/23/12 Department of Chemical Engineering, Tennessee Technological University, Cookeville, TN
- 3/8/12 Department of Chemistry, The City University of New York, College of Staten Island, New York, NY
- 3/1/12 Department of Physics, The George Washington University, Washington, DC
- 2/28/12 Department of Chemical Engineering, University of New Hampshire, Durham, NH
- 2/23/12 Department of Physics, University of Massachusetts Boston, Boston, MA
- 2/22/12 Department of Chemical, Materials & Biomolecular Engineering University of Connecticut, Storrs, CT
- 2/16/12 Department of Biochemistry & Molecular Biology, The Pennsylvania State University, University Park, PA
- 2/2/12 Department of Molecular & Cell Biology, University of Connecticut, Storrs, CT
- 4/19/11 Physics of Complex Systems Section, Vrije University Amsterdam, Amsterdam, NL
- 9/12/07 Biophysics Group, Department of Structural & Chemical Biology, Mount Sinai Medical School, New York, NY
- 8/30/07 Brooks Group, Department of Molecular Biology, The Scripps Research Institute, La Jolla, CA
- 8/2/07 U.S. Army Research Labs, High Performance Technologies, Aberdeen, MD
- 7/16/07 Center for Cancer Research Nanobiology Program, NIH NCI, Frederick, MD
- 8/15/06 Gene Network Sciences, Cambridge, MA

Conference Talks

- 24. K.L. Lee, E.R. May, "Computational Investigation into Mutational Allosteric Effects on Tau Protein-Antibody Binding", The Protein Society 35th Anniversary Symposium, Online, July 13, 2021.
- 23. S.S. Duay, A.M. Angeles-Boza, E.R. May, "Exploring the pH-dependent interactions of the antimicrobial peptide Clavanin A with *E. coli* outer membrane using molecular dynamics simulations", Molecular Biophysics in the Northeast 2019, Boston, MA, Nov. 9th, 2019.
- 22. W. Mitchell, E.A. Ng, K. Boyd, J.D. Tamucci, E.R. May, N. Eddy, H.S. Szeto, N.N. Alder, "Biophysical approaches to elucidate the mechanism of action of the mitochondrial therapeutic SS-31 (Elamipretide)", 15th Annual North Eastern Structure Symposium (NESS), Farmington, CT, Oct. 20, 2018.

- 21. S. Nangia, J.G. Pattis, E.R. May, "Molecular dynamics study of the Flock House virus membrane active peptide: Evaluation of binding, folding, oligomerization and pore formation mechanisms and energetics", ACS National Meeting, Boston, MA, Aug. 20, 2018.
- 20. K.J. Boyd, N.N. Alder, E.R. May, "A pivotal plane based approach for the construction of lipid bilayers of arbitrary shape and composition", CECAM Workshop: Frontiers in Computational Biophysics: understanding conformational dynamics of complex lipid mixtures relevant to biology, Lugano, Switzerland, Jan. 10, 2018.
- 19. E.R. May, "Modeling Interactions of Lytic Peptides from the Non-Enveloped Flock House Virus Capsid with Biomembranes", XXV Biennial Conference on Phage/Virus Assembly, Ellicott City, MD, Aug. 21, 2017.
- J.G. Pattis, E.R. May, "Long Timescale Simulations of Monomeric Lassa Virus Nucleoprotein Reveals Insights into Its RNA Binding Mechanism and Ribonucleoprotein Contacts", XXV Biennial Conference on Phage/Virus Assembly, Ellicott City, MD, Aug. 23, 2017.
- 17. S. Nangia, E.R. May, "Structure and Dynamics of Viral Lytic Peptides in Membrane Environments", ACS National Meeting, San Diego, CA, Mar. 13, 2016.
- 16. E.R. May, "Dynamics of Viral Lytic Peptides in Aqueous and Membrane Environments", 12th Annual North Eastern Structure Symposium (NESS), Storrs, CT, Oct. 10, 2015.
- 15. N.N. Alder, K. Malhotra, S. Nangia, T. Daman E.R. May, D. Mokranjac, "Investigating Subunit Interactions and Structural Dynamics of the Mitochondrial Protein Transport Machinery Using *in organello* and Model Membrane Systems", EMBO Conference: Mechanisms of Regulation of Protein Translocation, Dubrovnik, Croatia, Mar. 21, 2015.
- A.R. Brice, S. Nangia, E.R. May, "Molecular Simulations of the Capsid Release and Membrane Binding Processes of Flock House Lytic Peptides", 59th Annual Meeting of the Biophysical Society, Baltimore, MD, Feb. 8, 2015.
- 13. G. Dionne, A.M. Shaqra, A.E. Every, B.S. Moorthy, E.R. May, G.S. Anand, V.L. Robinson, "Guanine nucleotide-dependent Conformational Selection Regulates Distinct Alternate Ribosome Bound States of the Translation Factor BipA", Translational Control Meeting, Cold Spring Harbor, NY, Sept. 3, 2014.
- 12. E.R. May, "Conformational Dynamics of Flock House Virus Membrane Active Peptides", 4th Mathematical Virology Workshop, York, UK, Aug. 21, 2014.
- 11. K. Malhotra, S. Nangia, E.R. May, N.N. Alder, "Subunit Interactions and Structural Dynamics of the Mitochondrial TIM23 Protein Transport Complex", Gordon Research Conference on Protein Transport Across Cell Membranes, Galveston, TX, Mar. 9-14, 2014.
- 10. E.R. May, C.L. Brooks III, "Mechanical Properties of Viral Capsids From Equilibrium Thermal Fluctuations" AIChE 2011 Annual Meeting, Minneapolis, MN, Oct. 20, 2011.
- 9. E.R. May, C.L. Brooks III, "Exploring Virus Maturation Pathways Through Computer Simulations", AIChE 2011 Annual Meeting, Minneapolis, MN, Oct. 19, 2011.
- 8. E.R. May, "Multiscale Approaches for Studying Viral Capsid Maturation", CECAM Workshop on Multiscale Computational Biomechanics, Zurich, Switzerland, Apr. 13, 2011.
- 7. E.R. May, C.L. Brooks III, "Exploring the Maturation Pathway of HK97 through Computer Simulations", Gordon Research Conference on Physical Virology, Ventura, CA, Jan. 18, 2011.
- 6. E.R. May, C.L. Brooks III, "Determination of Viral Capsid Elastic Properties From Equilibrium Thermal Fluctuation" AIChE 2010 Annual Meeting, Salt Lake City, UT, Nov. 11, 2010.
- E.R. May, C.L. Brooks III, "Calculation of viral capsid elastic properties from equilibrium thermal fluctuations" 3rd Mathematical Virology Workshop, Ambleside UK, Aug. 19, 2010.
- 4. E.R. May, A. Narang, D.I. Kopelevich, "Role of Molecular Tilt in Thermal Fluctuations of Lipid Bilayers" AIChE 2007 Annual Meeting, Salt Lake City, UT, Nov. 5, 2007.

- 3. E.R. May, D.I. Kopelevich, A. Narang, "Biomembrane Deformations: Molecular Modeling of Key Elastic Properties for Inhomogeneous Lipid Bilayers" AIChE 2006 Annual Meeting, San Francisco, CA, Nov. 17, 2006.
- 2. E.R. May, "Molecular Modeling of Biomembrane Deformations The Role of Lipids" GRACE Graduate Symposium, Gainesville, FL, Apr. 26, 2006.
- 1. E.R. May, "Multi-Scale Modeling of Biomembrane Deformations" GRACE Graduate Symposium, Gainesville, FL, Mar. 9, 2005.

Conference Posters

- 78. G. Montovano, M. Sharawy, A.E. Santi, E.R. May, G.S. Anand, V.L. Robinson, "Differential Ribosome Binding by the Translation Factor BipA is Regulated Through Guanine Nucleotide-Dependent Conformational Selection", Translational Control Meeting, Cold Spring Harbor, NY, Sept. 8, 2022.
- 77. G. Montovano, T.S. Buckley, M. Sharawy, E.R. May, G.S. Anand, V.L. Robinson, "Guanine Nucleotide-Dependent Conformational Selection Regulates Distinct Alternate Ribosome Bound States of the Translation Factor BipA", ASBMB Annual Meeting, Philadelphia, PA, April 4, 2022.
- 76. A.G. Feinstein, E.R. May, J.L. Cole, "Investigation into the effect of dimerization on PKR activation energetics and dynamics with enhanced sampling molecular dynamics", 66th Annual Meeting of the Biophysical Society, San Francisco, CA, Feb 23, 2022.
- 75. V.K Golla, K.J. Boyd, E.R. May, "Curvature-based lipid partitioning and localization in a mitochondrial inner membrane model", 66th Annual Meeting of the Biophysical Society, San Francisco, CA, Feb 23, 2022.
- 74. M. Sharawy, N.B. Pigni, E.R. May, J.A. Gascon, "A favorable path to domain separation in the orange carotenoid protein", 66th Annual Meeting of the Biophysical Society, San Francisco, CA, Feb 21, 2022.
- 73. J.D. Tamucci, W. Mitchell, E.L. Ng, S.Liu, H.H. Szeto, A.T. Alexandrescu, N.N. Alder, E.R. May, "QSAR investigation into SS peptides' interaction with lipid bilayers and their effects on transmembrane ion leakage in the presence of transmembrane potentials", 66th Annual Meeting of the Biophysical Society, San Francisco, CA, Feb 21, 2022.
- 72. M. Sharawy, N. Pigni, E.R. May, J. Gascon, "A Favorable Path to Domain Separation in the Orange Carotenoid Protein", The Protein Society 35th Anniversary Symposium, Online, July 13, 2021.
- 71. J.D. Tamucci, N.N. Alder, E.R. May, "Computational Investigation into the Effect of SS-31 on Membrane Ion Distributions, Pore Formation and Ion Leakage in the Presence of Transmembrane Potentials", 65th Annual Meeting of the Biophysical Society, Online, Feb 25, 2021.
- 70. M. Sharawy, A. Louyakis, J.P. Gogarten, E.R. May, "CTAG vs. GATC: Structural Basis for Representational Differences in Reverse Palindromic DNA Tetranucleotide Sequences", 65th Annual Meeting of the Biophysical Society, Online, Feb 25, 2021.
- 69. V.L. Robinson, G. Dionne, K.J. Boyd, A.M. Shaqra, H.erlandsen, M. Ghosh, G.S. Anand, E.R. May, "A Conserved Arginine in Switch I Is Critical for ppGpp Binding to the Prokaryotic Translational GTPase BipA", 65th Annual Meeting of the Biophysical Society, Online, Feb 24, 2021.
- 68. G. Dionne, A.M. Shaqra, K.J. Boyd, M. Ghosh, H. Erlandsen, G.S. Anand, E.R. May, V.L. Robinson, "A Conserved Arginine in Switch I is Critical for ppGpp Binding to the Prokaryotic Translational GTPase BipA", NESS 2020, The North Eastern Structure Symposium, Online, Oct. 24, 2020.
- 67. A.G. Feinstein, J.C. Cole, E.R. May, "Investigation into the Effect of Dimerization on PKR Activation with Enhanced Sampling Molecular Dynamics Methods", NESS 2020, The North Eastern Structure Symposium, Online, Oct. 24, 2020.

- 66. J.G. Pattis, E.R. May, "Large Structural Changes During the Lassa Virus Nucleoprotein Trimer to Monomer Transition Revealed by Markov State Modeling", Molecular Biophysics in the Northeast 2019, Boston, MA, Nov. 9, 2019.
- 65. A.K. Jana, E.R. May, "Investigating Cell Entry Mechanisms of Non- enveloped Viruses using Computer Simulations", Molecular Biophysics in the Northeast 2019, Boston, MA, Nov. 9, 2019.
- 64. N.N. Alder, W. Mitchell, E. Ng, K.J. Boyd, J.D. Tamucci, E.R. May, N. Eddy, H. Szeto, "Biophysical Approaches Toward Understanding the Molecular Mechanism of Action of the Mitochondrial Therapeutic SS-31", 63th Annual Meeting of the Biophysical Society, Baltimore, MD, Mar. 6, 2019.
- 63. J.G. Pattis, E.R. May, "Markov State Modeling Reveals Accessibility to the RNA Binding Pocket in Monomeric Lassa Virus Nucleoprotein", 63th Annual Meeting of the Biophysical Society, Baltimore, MD, Mar. 5, 2019.
- 62. K.J. Boyd, N.N. Alder, E.R. May, "Interplay of Curvature, Lipid Segregation and Stability Modulation in Complex Lipid Bilayers", 63th Annual Meeting of the Biophysical Society, Baltimore, MD, Mar. 5, 2019.
- 61. A. Jana, S. Nangia, E.R. May, "Entry Related Dynamics of the Flock House Virus Capsid and Lytic Peptides", 63th Annual Meeting of the Biophysical Society, Baltimore, MD, Mar. 3, 2019.
- 60. Antimicrobial Peptides GRC
- 59. J.D. Tamucci, K.J. Boyd, N.N. Alder, E.R. May, "Characterizing the Binding Mechanism to Lipid Bilayers and Effects on Local Lipid Dynamics of SS-31, a Tetra-Peptide Therapeutic Agent for Mitochondrial Disorders", 15th Annual North Eastern Structure Symposium (NESS), Farmington, CT, Oct. 20, 2018. * Won Poster Award *
- 58. J.G. Pattis, E.R. May, "Exploring the High Dimensional Free Energy Landscape of Protein Conformations Using Markov State Models and Adaptive Umbrella Sampling", 15th Annual North Eastern Structure Symposium (NESS), Farmington, CT, Oct. 20, 2018.
- 57. S. Nangia, J.G. Pattis, K.J. Boyd, E.R. May, "Study of the binding, folding, oligomerization and pore formation by the membrane lytic peptide from Flock House Virus using Molecular Dynamics simulations" 15th Annual North Eastern Structure Symposium (NESS), Farmington, CT, Oct. 20, 2018. * Won Poster Award *
- 56. A. Jana, E.R. May, "Influence of Acidic pH on Liberation of Membrane Disrupting peptides from the Non-Enveloped Flock House Virus Capsid", 15th Annual North Eastern Structure Symposium (NESS), Farmington, CT, Oct. 20, 2018.
- 55. A.G. Feinstein, J.L. Cole, E.R. May, "Molecular Dynamics Investigations into a Novel Front-to-Front Dimer of Human Protein Kinase R", 15th Annual North Eastern Structure Symposium (NESS), Farmington, CT, Oct. 20, 2018.
- 54. S.S. Duay, A.M. Angeles-Boza, E.R. May, "Zinc(II) Stabilizes Helicity and Enhances E. coli Model Membrane Contacts in the C-Terminal Region of the Antimicrobial Peptide Clavanin A", 15th Annual North Eastern Structure Symposium (NESS), Farmington, CT, Oct. 20, 2018.
- 53. S.S. Duay, A.M. Angeles-Boza, E.R. May, "Molecular Dynamics Study of the Role of Zinc Ions in Clavanin A Interaction with E. coli Membrane", ACS National Meeting, Boston, MA. August 21, 2018.
- 52. S.S. Duay, A.M. Angeles-Boza, E.R. May, "Zinc(II) Stabilizes Helicity and Provides More E. coli Model Membrane Contacts to the C-Terminal Region of the Antimicrobial Peptide Clavanin A", Gordon Research Conference on Computational Chemistry, West Dover, VT, July 22-27, 2018.
- 51. K.J. Boyd, E.R. May. "BUMPy: A flexible tool for creating curved lipid membranes for molecular simulations with accurate determination of interleaflet ratios." FASEB: Molecular Biophysics of Membranes. Orlean, NY June 17-22, 2018.

- 50. K.J. Boyd, N.N. Alder, E.R. May, "Curvature based lipid segregation and stability modulation in bilayer containing cardiolipin and monolysocardiolipin", ACS National Meeting, New Orleans, LA, Mar. 20, 2018.
- 49. S.S. Duay, A.M. Angeles-Boza, E.R. May, "Molecular Dynamics Study of the Role of Zinc Ions in Clavanin A Interactions with *E. coli* Membrane", R.T. Major Symposium, Storrs, CT Mar. 8 2018.
 * Won Poster Award *
- 48. J.G. Pattis, M.D. Ward, E.R. May, "Insights into the Lassa Virus Nucleoprotein RNA Binding Mechanism And Ribonucleoprotein Contacts", 14th Annual North Eastern Structure Symposium (NESS), Storrs, CT, Oct. 28, 2017. *** Won Poster award ***
- 47. A.G. Feinstein, J.L. Cole, E.R. May, "Molecular Dynamics Investigations into a Front-To-Front Dimer of Human PKR", 14th Annual North Eastern Structure Symposium (NESS), Storrs, CT, Oct. 28, 2017.
- 46. W. Mitchell, E. Ng, K.J. Boyd, J.D. Tamucci, M. Sathappa, A. Coscia, D. Morales, K.-C. Shih, E.R. May, H.S. Szeto, N. Eddy, N.N. Alder, "The Mechanism of Action Of SS-31 (Elamipretide): A Novel Therapeutic For Mitochondrial Dysfunction", 14th Annual North Eastern Structure Symposium (NESS), Storrs, CT, Oct. 28, 2017.
- 45. C.B. Mayo, H. Erlandsen, A. Feinstein, E.R. May, J.L. Cole, "Mechanism for activation of the antiviral kinase PKR", FASEB SRC: Protein kinases and protein phosphorylation. Cambridge, UK. August 6-11, 2017.
- 44. M.D. Ward, S. Nangia, E.R. May, "Evaluation of the Hybrid Resolution PACE Model for the Study of Folding, Insertion and Pore Formation of Membrane Associated Peptides", 61th Annual Meeting of the Biophysical Society, New Orleans, LA, Feb. 15, 2017.
- 43. M. Sathappa, W. Mitchell, A. Coscia, K.J. Boyd, E.R. May, H.H. Szeto, N.N. Alder, "Investigation of the Interactions of the SS-31 Peptides with Cardiolipin Variants: A Potential Therapeutic for Barth Syndrome", 61th Annual Meeting of the Biophysical Society, New Orleans, LA, Feb. 14, 2017.
- 42. S. Nangia, A.R. Brice, E.R. May, "Molecular Dynamics Studies of Non-Enveloped Virus Cell Entry Mechanisms", 61th Annual Meeting of the Biophysical Society, New Orleans, LA, Feb. 14, 2017.
- 41. J.G. Pattis, M.D. Ward, E.R. May, "Computational Investigation into the Solution Structure of Monomeric Lassa Virus Nucleoprotein and Insights into its RNA Binding Mechanism", 61th Annual Meeting of the Biophysical Society, New Orleans, LA, Feb. 13, 2017.
- 40. K.J. Boyd, N.N. Alder, E.R. May, "Molecular Dynamics Investigation into the Distribution of Cardiolipin Variants in Flat and Buckled Heterogeneous Bilayers", 61th Annual Meeting of the Biophysical Society, New Orleans, LA, Feb. 13, 2017.
- 39. M.K. Skoryk, K.J. Boyd, E.R. May, N.N. Alder, "Lipid-Dependence of the Membrane Interactions of the Tim23 Channel Subunit of the Mitochondrial Protein Import Machinery", 61th Annual Meeting of the Biophysical Society, New Orleans, LA, Feb. 12, 2017.
- 37. J.G. Pattis, E.R. May, "Computational Investigation of the Solution Structure of Monomeric Lassa Virus Nucleoprotein", 13th Annual North Eastern Structure Symposium (NESS), Farmington, CT, Oct. 14, 2016.
- 36. M.D. Ward, S. Nangia, E.R. May, "Evaluation of the Hybrid Resolution PACE Model for the Study of Folding, Insertion and Pore Formation of Membrane Associated Peptides", 13th Annual North Eastern Structure Symposium (NESS), Farmington, CT, Oct. 14, 2016.
- 35. K. J. Boyd, N.N. Alder, E.R. May, "Investigating the Role of Cardiolipin in Bilayer Organization and Protein Binding Properties of Mitochondrial Membranes", 13th Annual North Eastern Structure Symposium (NESS), Farmington, CT, Oct. 14, 2016.
- 34. S. Nangia, E.R. May, "Multi-scale modeling of Flock House Virus gamma peptide-membrane interactions and potential pore formation", 13th Annual North Eastern Structure Symposium (NESS), Farmington, CT, Oct. 14, 2016.

- 33. S. Kamal, E.R. May, "Computational Investigation into the Structure and Correlated Dynamics of PDE6 and its Inhibition by PDE6-γ", ACS National Meeting, San Diego, CA, Mar. 16, 2016.
- 32. M.D. Ward, E.R. May, "Probing the Function of Different Regions of a pH-Dependent Viral Lytic Peptide", ACS National Meeting, San Diego, CA, Mar. 16, 2016.
- 31. J.G. Pattis, E.R. May, "Solution structure of the monomeric Lassa virus nucleoprotein and insights into its RNA binding mechanism", ACS National Meeting, San Diego, CA, Mar. 16, 2016.
- 30. A.R. Brice, E.R. May, "Revealing the pH-Controlled Release Mechanism of Lytic Peptides from Non-Enveloped Virus Capsids", ACS National Meeting, San Diego, CA, Mar. 16, 2016.
- 29. N.N Alder, K. Malhotra, M. Sathappa, S.Nangia, T. Daman, D. Mokranjac, E.R. May, "Energy Coupling Mechanisms and Lipid-Mediated Subunit Interactions of the Mitochondrial Protein Transport Machinery", 60th Annual Meeting of the Biophysical Society, Los Angeles, CA, Feb. 29, 2016.
- 28. J.Pattis, E.R. May, "Computational Investigation of the Structural Dynamics of Lassa Virus Nucleoprotein and Its RNA-Binding Mechanism", 12th Annual North Eastern Structure Symposium (NESS), Storrs, CT, Oct. 10, 2015.
- 27. A.R. Brice, E.R. May, "Characterization of Flock House Virus Capsid Dynamics Responsible for Release of Lytic Peptides", 12th Annual North Eastern Structure Symposium (NESS), Storrs, CT, Oct. 10, 2015.
- 26. S. Nangia, E.R. May, "Dynamics of Viral Lytic Peptides in Aqueous and Membrane Environments", 12th Annual North Eastern Structure Symposium (NESS), Storrs, CT, Oct. 10, 2015.
- 25. K. Malhotra, S. Nangia, T. Daman, D. Mokranjac, E.R. May, N.N. Alder, "Lipid-mediated interactions of the mitochondrial presequence translocase", EMBO Conference: Mechanisms of Regulation of Protein Translocation, Dubrovnik, Croatia, Mar. 23, 2015.
- 24. N.N. Alder, K. Malhotra, S. Nangia, T. Daman E.R. May, D. Mokranjac, "Investigating Subunit Interactions and Structural Dynamics of the Mitochondrial Protein Transport Machinery Using *in organello* and Model Membrane Systems", EMBO Conference: Mechanisms of Regulation of Protein Translocation, Dubrovnik, Croatia, Mar. 23, 2015.
- 23. J. Pattis, E.R. May, "Influence of RNA Binding on the Conformational Dynamics of the Lassa Virus Nucleoprotein", 59th Annual Meeting of the Biophysical Society, Baltimore, MD, Feb. 11, 2015.
- 22. K. Malhotra, S. Nangia, D. Mokranjac, E.R. May, N.N. Alder, "Lipid-Mediated Interactions of the Mitochondrial Presequence Translocase", American Society of Cell Biology (ASCB) Annual Meeting, Philadelphia, PA, Dec. 6-10, 2014.
- 21. A. Brice, E.R. May, "Molecular Simulations of Flock House Virus Reveal Structural Changes During Release of Lytic Peptides" 11th Annual North Eastern Structure Symposium (NESS), Farmington, CT, Oct. 17, 2014.
- J. Pattis, E.R. May, "Molecular Simulation Study and Free Energy Calculations of the Lassa Virus Nucleoprotein Gating Mechanism" 11th Annual North Eastern Structure Symposium (NESS), Farmington, CT, Oct. 17, 2014.
- 19. K. Malhotra, S. Nangia, E.R. May, N.N. Alder, "Lipid-mediated interactions of the mitochondrial presequence translocase", 11th Annual North Eastern Structure Symposium (NESS), Farmington, CT, Oct. 17, 2014.
- K. Malhotra, S. Nangia, E.R. May, N.N. Alder, "Subunit Interactions and Structural Dynamics of the Mitochondrial TIM23 Protein Transport Complex", Gordon Research Conference on Protein Transport Across Cell Membranes, Galveston, TX, Mar. 9-14, 2014.
- 17. J. Pattis, E.R. May, "Molecular Simulation Study of the Gating Mechanism of the Lassa Virus Nucleoprotein" 10th Annual North Eastern Structure Symposium (NESS), Storrs, CT, Oct 4, 2013.
- J. Pattis, E.R. May, "Molecular Simulation Study of the Gating Mechanism of the Lassa Virus Nucleoprotein", XXIII Biennial Conference on Phage/Virus Assembly, Lake Arrowhead, CA, Sept. 12, 2013.

- 15. E.R. May, C.L. Brooks III, "Molecular Simulation of pH-Dependent Maturation-Associated Structural Changes in Bacteriophage HK97", 57th Annual Meeting of the Biophysical Society, Philadelphia, PA, Feb 5, 2013.
- 14. G.L. Dionne, A.M. Shaqra, A.E. Every, B.S. Moorthy, E.R. May, G.S. Anad, V.L. Robinson, "Guanine-Nucleotide Dependent Conformational Selection Regulates Distinct Alternate Ribosome Bound States of the Translation Factor BipA" 57th Annual Meeting of the Biophysical Society, Philadelphia, PA, Feb 4, 2013.
- 13. J. Snijder, V.S. Reddy, E.R. May, W.H. Roos, G.R. Nemerow, G.J.L. Wuite, "Using Atomic Force Microscopy to Analyze Adenovirus-Host Interactions", Gordon Research Conference on Physical Virology, Ventura, CA, Jan. 21, 2013.
- 12. E.R. May, C.L. Brooks III, "pH Effects on the Thermodynamic Stability of the Maturation Transition in Bacteriophage HK97", Gordon Research Conference on Physical Virology, Ventura, CA, Jan. 21, 2013.
- 11. E.R. May, C.L. Brooks III, "Insights into the Mechanism of HK97 Maturation from Molecular Dynamics Simulations", FASEB: Virus Structure and Assembly, Saxton River, VT, June 13, 2012.
- 10. E.R. May, "Multiscale Modeling of Biophysical and Biochemical Aspects of Viral Life Cycles", AIChE 2011 Annual Meeting, Minneapolis, MN, Oct. 16, 2011.
- 9. E.R. May, "Multiscale Modeling of Biophysical and Biochemical Aspects of Viral Life Cycles", Leading Innovation and Discovery Workshop at NSF, Arlington, VA, Sept. 19, 2011.
- 8. S.C. Allen, E.R. May, J. Feng, C.L. Brooks III, "Molecular Modeling Study on the Mechanical Behavior of Norovirus" UROP Spring Research Symposium, Ann Arbor, MI, Apr. 20, 2011.
- 7. A.M. Manaan, E.R. May, R.S. Armen, C.L. Brooks III, "Flexible C-terminal arm of the Lassa Arenavirus Z-protein mediates interactions with multiple binding partners" ACS National Meeting, Anaheim, CA, Mar. 28, 2011.
- 6. E.R. May, C.L. Brooks, III, "Exploring the Maturation Pathway of HK97 through Computer Simulations", Gordon Research Conference on Physical Virology, Ventura, CA, Jan. 17, 2011.
- 5. E.R. May, "Multiscale Modeling of Biophysical and Biochemical Aspects of Viral Life Cycles", AIChE 2010 Annual Meeting, Salt Lake City, UT, Nov.7, 2010.
- 4. E.R. May, R.S. Armen, A.M. Mannan, C.L. Brooks III, "Prediction of the Lassa Arenavirus Z-Protein Structure and the Binding Mode of Z with eIF4E", CBSB10 Workshop: From Computational Biophysics to Systems Biology, Traverse City, MI, June 7, 2010.
- A.M. Mannan, E.R. May, R.S. Armen, R.V. Mannige, C.L. Brooks III, "Modeling Arenavirus Nucleocapsid and Z Protein Structures", National Center for Integrative Biomedical Informatics (NCIBI) 4th Annual Research Meeting, Ann Arbor, MI, Apr. 28, 2009.
- A.M. Mannan, E.R. May, R.S. Armen, R.V. Mannige, C.L. Brooks III, "Modeling Arenavirus Nucleocapsid and Z Protein Structures", UROP Research Symposium, Ann Arbor, MI, Apr. 1, 2009.
 * Won Poster Award *
- 1. E.R. May, C.L. Brooks III, "Elastic Parameters of Viral Capsids Derived from Atomistic Molecular Dynamics" Gordon Research Conference on Physical Virology, Galveston, TX, Feb.17, 2009.

RESEARCH SUPERVISION

University of Connecticut

Postdoctoral Fellows

Allyn Brice, Ph.D. (2013 – 2016) Shivangi Nangia, Ph.D. (2013 - 2019) Asis Jana, Ph.D. (2017 – 2020) Mahmoud Sharawy Ph.D. (2019-Present) Vinaya Kumar Golla, Ph.D. (2021-Present)

Graduate Students

Ph.D. Students
Jason Pattis (2012-2019) Ph.D. Molecular and Cell Biology
Kevin Boyd (2015-2019) Ph.D. Molecular and Cell Biology
Searle (I.C.) Duay (2017-2020) Ph.D. Chemistry (co-Advised with Alfredo Angeles-Boza)
Aaron Feinstein (2017-Present) Ph.D. Molecular and Cell Biology
Jeffery (J.D.) Tamucci (2017-Present) Ph.D. Molecular and Cell Biology
Don Stimpson (2020-Present) Ph.D. Molecular and Cell Biology (co-Advised with N. Alder)
Andong (Tony) Li (2022-Present) Ph.D. Molecular and Cell Biology (co-Advised with S. White)
Patrick Corrigan (2022-Present) Ph.D. Chemistry (co-Advised with Jessica Rouge)

M.S. Students

Deaneria Lakheram (2017-2018) M.S. Molecular and Cell Biology Michael Ward (2015-2017) M.S. Molecular and Cell Biology Prakhar Bansal (2016) M.S. Molecular and Cell Biology Shaan Kamal (2016) M.S. Molecular and Cell Biology

Undergraduates

Kevin Boyd (2012-2014) Molecular and Cell Biology '14, Honors Prakhar Bansal (2012-2016) Molecular and Cell Biology '16, University Scholar*, Honors Shaan Kamal (2013-2016) Molecular and Cell Biology '16, University Scholar*, Honors Adrian Coscia (2016-2017 Molecular and Cell Biology, '17, University Scholar*, Honors Michael Ward (2014-2015) Molecular and Cell Biology '15 Maneesh Koneru (2015-2018) Structural Biology and Biophysics '18, University Scholar*, Honors Aberdeen Taylor (2017-2019) Structural Biology and Biophysics '19 Kate Lee (2019-2022) Structural Biology and Biophysics '22, University Scholar*, Honors Milan Patel (2021-Present) Physics, MCB '23, Honors Athan Montemarano (2021-Present), MCB, '23, Honors Rey Carten (2022-Present) MCB, '24, Honors

*University Scholar is the highest distinction awarded to undergraduate students at UConn

McNair Fellows

Alejandro Meran (Summer 2014) Patricia Santos (Summer 2014) Jason DeJesus (Summer 2015) Savannah Villalba (Summer 2016) Venoude Valmyr (Summer 2017)

High School Students

Davesh Kakkar (Summer 2018, 2019) CREC Academy of Aerospace Engineering

University of Michigan

Undergraduates Shane Allen (2010-2011) Biomedical Engineering '14 Aristotle Mannan (2008-2009) Molecular, Cellular and Developmental Biology '11

AWARDS TO SUPERVISED STUDENTS

Searle Duay (2017-2020, graduate)

- RT Major Symposium outstanding poster award
- Masterton-Hurley Teaching Award (departmental)
- Bobbitt-Chou Graduate Summer Research Fellowship (departmental)

Aaron Feinstein (2017 – Present, graduate)

o Richard C. Crain, Jr. Memorial Fellowship (departmental)

Kevin Boyd (2012-2019, undergraduate, graduate)

- NSF Graduate Research Fellowship (national)
- Todd M. Schuster Award in Molecular and Cell Biology (departmental)
- Summer Undergraduate Research Fund (SURF) Award (university)
- Doctoral Dissertation Fellowship (university)

Jason Pattis (2012-2019, graduate)

- Structural Biology, Biochemistry and Biophysics Award (departmental)
- NESS Outstanding Poster Award
- o Richard C. Crain, Jr. Memorial Fellowship (departmental)

Prakhar Bansal (2013-2016, undergraduate)

- University Scholar (university)
- Todd M. Schuster Award in Molecular and Cell Biology (departmental)
- Life Science Honors Thesis Award (university)
- o Molecular and Cell Biology Outstanding Student Award (departmental)

Shivangi Nangia, (2013-2019, postdoctoral)

• NESS Outstanding Poster Award

Shaan Kamal (2014-2016, undergraduate, postgrad)

- University Scholar (university)
- IDEA Grant (university)
- Trimble Family Summer Undergraduate Research Fund Award (university)
- Life Science Honors Thesis Award (university)
- o Honors Award in Life Sciences (multi-departmental)

Michael Ward (2014-2017, undergraduate, graduate)

• NSF Graduate Research Fellowship Honorable Mention (national)

Maneesh Koneru (2015-2018, undergraduate)

- University Scholar (university)
- Summer Undergraduate Research Fund (SURF) Award (university)

Jeffrey Tamucci (2017-Present, graduate)

- Outstanding MCB TA award (departmental)
- NESS Outstanding Poster Award
- o Richard C. Crain, Jr. Memorial Fellowship (departmental)
- Summer Doctoral Dissertation Fellowship (university)

Aberdeen Taylor (2017-2019, undergraduate)

- o Todd M. Schuster Award in Molecular and Cell Biology (departmental)
- Summer Undergraduate Research Fund (SURF) Award (university)

Kate Lee (2019-2022, Undergraduate)

- o Todd M. Schuster Award in Molecular and Cell Biology (departmental)
- Summer Undergraduate Research Fund (SURF) Award (university)
- University Scholar (university)
- Goldwater Scholarship (national)

Milan Patel (2021- Present, Undergraduate)

• Summer Undergraduate Research Fund (SURF) Award (university)

Rey Carten (2022-Present, Undergraduate)

• Summer Undergraduate Research Fund (SURF) Award (university)

TEACHING EXPERIENCE

University of Connecticut

Instructor Biophysical Chemistry II, MCB 3004/5004, 3 Credits, Spring 2015-2019, 2021-2023 Instructor, Structural Dynamics of Macromolecular Machines, MCB 4014/5014, 3 Credits, Fall 2012-2015, 2017-2018, 2020-2022 (with V. Robinson)

Instructor, MCB Invited Seminar, MCB 5984, 1 Credit, Spring 2019, 2021-2023; Fall 2019-2022 (with K. Campellone)

Instructor, Graduate Seminar in Biochemistry, MCB 5099, 1 Credit, Fall 2013, Spring 2014 Biology Summer Institute Instructor, UCONN Early College Experience (ECE) (Summer 2014, 2016)

COMMITTEE AND SERVICE DUTIES

Graduate Student Committees

Ph.D. Students

Name	Major Advisor	Role	Graduated
Katherine Launer-Felty	James Cole	Examiner	Ph.D. MCB 2014
Sharado Patil	Andrei Alexandrescu	Associate Advisor	Ph.D. MCB 2014
Chris Karch	Peter Burkhard	Associate Advisor	Ph.D. MCB 2015
Ketan Malhotra	Nathan Alder	Associate Advisor	Ph.D. MCB 2016
Sally Chamberland	Nathan Alder	Associate Advisor	Ph.D. MCB 2019
Sarah Bernardis Low	Peter Burkhard	Associate Advisor	Ph.D. MCB 2019
Therese Tripler	Carolyn Teschke	Associate Advisor	Ph.D. MCB 2019
Hari Sharma	Elena Dormidontova	Associate Advisor	Ph.D. Physics 2019
David Mouser	James Cole	Associate Advisor	Ph.D. MCB 2020
Cassie Zerbe	James Cole	Associate Advisor	Ph.D. MCB 2019
Rebecca Newcomer	Andrei Alexandrescu	Associate Advisor	Ph.D. MCB 2020
Melissa Skoryk	Nathan Alder	Associate Advisor	Ph.D. MCB 2020
Stephen Hesler	James Cole	Associate Advisor	Ph.D. MCB 2021
Rishabh Kejriwal	Simon White	Associate Advisor	Ph.D. MCB 2022
Wayne Mitchell	Nathan Alder	Associate Advisor	Ph.D. MCB 2022
Steven Hesler	James Cole	Associate Advisor	Ph.D. MCB 2021
Jennifer Podgorski	Simon White	Associate Advisor	
Giancarlo Montovano	Victoria Robinson	Associate Advisor	
Erik Ammermann	Yongku Cho	Associate Advisor	

Benjamin Garrett Julia Jerolamon	Nathan Alder Nathan Alder	Associate Advisor Associate Advisor	
Masters Students	X7' (' D 1'		
Gilman Dionne	Victoria Robinson	Associate Advisor	M.S. MCB 2013

Emily Park	Victoria Robinson	Associate Advisor	M.S. MCB 2015
Srinath Pingle	James Cole	Associate Advisor	M.S. MCB 2016
Dylan Laprise	Nathan Alder	Associate Advisor	M.S. MCB 2017
Nathan Sanford	Victoria Robinson	Associate Advisor	M.S. MCB 2017
Josh Podgorski	Simon White	Associate Advisor	M.S. MCB 2022

Departmental Committees

Mentoring Committee, Chair 2022-Present Faculty Search Committee, Chair 2021-2022 Departmental Merit Calculator Committee, Chair 2021-2022 Faculty Search Committee, Member 2016-2017 Graduate Admissions Committee, Member 2014-Present Recruitment Committee, Member 2013-2016, 2018

College Committees

CLAS Big Data Task Force, Member 2019-2020

University Committees

UITS HPC Director Search Committee, Member 2020-2021

OTHER PROFESSIONAL ACTIVITIES

Grant Reviewer

Mar 2023:	NIH NIGMS MIRA review panel
Oct 2022:	NIH Biomedical Technology Development and Dissemination Center (RMI), Mail
	Reviewer
Dec 2021:	UConn InChip Seed Grant Competition
Oct 2021:	NIH Basic Research to Inform Vaccine and Therapeutic Development for Non-Polio
	Human Enteroviruses (NPEV)
Apr 2021:	UConn Research Excellence Program
Dec 2020:	Poland National Science Centre
May 2020:	Poland National Science Centre
Sept 2019:	National Academy of Sciences Committee on Molecular Dynamics Simulations
Mar 2019:	UConn Research Excellence Program
Feb 2019:	NIH NIAID B Cell Epitope BAA Review Panel
Aug 2018:	National Academy of Sciences Committee on Molecular Dynamics Simulations
May 2018:	UConn Research Excellence Program
Apr 2018:	ACS Chemical Computing Group Excellence Award for Graduate Students
Sept 2017:	Poland National Science Centre
Apr 2017:	UConn Research Excellence Program
Apr 2017:	Poland National Science Centre
Feb 2017:	Welcome Trust

Jan 2017:	NSF GRFP Reviewer
Nov 2016:	Human Frontiers in Science Program (HFSP)
Sep 2016:	Poland National Science Centre
Jan 2016:	NSF GRFP Reviewer
Apr 2015:	Poland National Science Centre
Jan 2015:	NSF GRFP Reviewer
Dec 2013:	NIH – BBM Study Section

Conference Chairing

June 2021:	ACS Middle Atlantic Meeting of the American Chemical Society (MARM20021),
	Session co-Chair, Biophysical Chemistry Session
March 2016:	ACS Spring Meeting, Session Chair, From Dynamics to Function & Back Again:
	Adventures in Simulating Biomolecules Symposium
Feb 2015:	Biophysical Society Annual Meeting, Session co-Chair, Platform: Protein Assemblies

Conference Organizing

Co-Organizer 2019 Molecular Biophysics in the Northeast (MBN) Co-Organizer 2018 New England Structure Symposium (NESS) Co-Organizer 2016 ECE Biology Summer Institute Co-Organizer 2015 New England Structure Symposium (NESS)

Editorial Work

2020-Present: Editorial Board Member for Life

- 2017-Present: Editorial Board Member for Aims Biophysics
- 2015-Present: Review Editor for *Frontiers in Endocrinology*, Molecular and Structural Endocrinology section
- 2014-2015: Guest Editor for Special Issue of Viruses on "Virus Maturation"

Journal Reviewer

ACS Chemical Biology, ACS Nano, BBA Biomembranes, Biochemistry, Bioorganic & Medicinal Chemistry, Biophysical Journal, Chemical Biology and Drug Design, Chemical Communications, Computational Biology and Chemistry, Current Opinion in Virology, Frontiers in Bioengineering and Biotechnology, Frontiers in Endocrinology, Frontiers in Medical Technology, Journal of the American Chemical Society, Journal of Biological Physics, Journal of Chemical Physics, Journal of Chemical Theory and Computation, Journal of General Virology, Journal of Molecular Biology, Journal of Molecular Graphics and Modelling, Journal of Molecular Liquids, Journal of Molecular Recognition, Journal of Physical Chemistry B, Journal of Physical Chemistry Letters, Journal of Structural Biology, Journal of Virology, Langmuir, Nanoscale, Nucleic Acids Research, Physical Biology, Physical Chemistry Chemical Physics, Physical Review E, Physical Review Letters, PLoS Computational Biology, PLoS ONE, PLoS Pathogens, PNAS Nexus, Protein Science, Proteins, Science Advances, Scientific Reports, Scientia Pharmaceutica, Soft Matter, Trends in Microbiology, Virology, Virology, Virus Adaptation and Treatment

Book Reviewer

Frontiers in Computational Chemistry, Vol. 4. Ed. Zaheer Ul-Haq Molecular Biology of Assemblies and Machines by Wolfgang Baumeister, Louise Johnson, Richard Perham, and Alasdair Steven

Science Judging

2015 Connecticut Science Fair Poster Judge for Biophysics Society, Hamden, CT 2015 New England McNair Scholars Program Conference Research Symposium, Storrs, CT

Professional Society Memberships

American Chemical Society (ACS) Biophysical Society (BPS) American Association for the Advancement of Science (AAAS)

Mentoring

McNair Fellows Program Faculty Mentor Undergraduate Research Opportunity Program (UROP), Faculty Mentor, University of Michigan Postdoc Advisory Committee for Caitlin Scott (Postdoc with Deb Kendall)

FUNDING HISTORY

Current Support

NIH R35-GM119762, Maximizing Investigators' Research Award (MIRA) Project: Structural Dynamics of Viral Proteins: Development and Application of Multiscale Computational Methods for Studying Viral Capsids, Proteins and Membrane Systems Dates: 3/1/22-2/28/27 Total Costs: \$2,213,759 Role: PI

NIH R01-AG0658979

Project: First-In-Class Peptide Therapeutics for Mitochondrial Disorders: Molecular Mechanism of Action and Optimization of Design Dates: 9/30/20-4/30/25 Total Costs: \$2,501,812 Role: co-I (PI: Alder)

NIH R01-HL165729

Project: An Intimate and Multifaceted Partnership: Cardiolipin and the Mitochondrial ADP/ATP Carrier Dates:12/10/22-11/30/26 Total Costs: \$2,073,445 Role: co-I (PI: Claypool)

Completed Support

NIH R35-GM119762, Maximizing Investigators' Research Award (MIRA) Project: STRUCTURAL DYNAMICS OF VIRAL PROTEINS: COMPUTATIONAL INVESTIGATION OF CAPSIDS, LYTIC PEPTIDES AND NUCLEOPROTEINS UNDER VARYING CONDITIONS Dates: 7/15/16-2/28/22 Total Costs: \$1,787,171 Role: PI

NIH R35-GM119762, Supplement

Project: Acquisition of GPU based High Performance Computational Equipment Dates: 6/1/18-5/31/19 Total Costs: \$77,040 Role: PI

NIH K22-AI099163, NIAID Research Scholar Development Award Project: Computational Studies of Stage Cell Entry Events by Non-enveloped Viruses Dates: 2/1/13 – 1/31/16 Total Costs: \$259,997 Role: PI

UConn Large Faculty Grant Project: Computational Study into the Structure and Dynamics of the Lassa Virus Ribonucleoprotein Complex Dates: 7/1/13-6/30/14 Direct Costs: \$20,000 Role: PI

NSF DBI-0905773, Postdoctoral Fellowship in Biology Project: Structure, Dynamics and Mechanics of Viral Proteins: A Multiscale Computational Study Dates: 9/1/09 – 8/31/11 Total Costs: \$123,000 Role: PI

NIH F32-AI080125, Ruth L. Kirschstein NRSA Postdoctoral Fellowship Project: Multiscale Modeling of Viral Capsid Maturation Transitions and Elastic Properties Dates: Declined Total Costs: \$101,764 Role: PI