Justin A. Lemkul, Ph.D.

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EDUCATION

August 2007 – May 2012
Ph.D., Biochemistry
Virginia Polytechnic Institute and State University
MILES-IGERT Graduate Certificate

August 2003 – May 2007
B.S. in Honors, Biochemistry (Summa Cum Laude)
Virginia Polytechnic Institute and State University
Minor in Chemistry, Concentration in Biotechnology

FUNDING

2014 – 2017 Ruth L. Kirschstein National Research Service Award (NIH/NIGMS F32)
"Exploring RNA Folding and Dynamics Using a Polarizable Force Field"

AWARDS AND HONORS

2016	The Wiley Computers in Chemistry Outstanding Postdoc Award (American Chemical Society COMP Division)
2013	Virginia Tech Graduate School Outstanding Dissertation in Science, Technology, Engineering, and Mathematics
2012	Virginia Tech College of Agriculture and Life Sciences Outstanding Doctoral Student
2011	Kendall W. King Memorial Scholarship (outstanding senior Biochemistry graduate student)
2009	1st Place poster (Student Biomedical category), 6th Annual VCOM Research Day
2009	James F. Eheart Travel scholarship
2008	Bruce M. Anderson Graduate Award (outstanding first-year Biochemistry graduate student)
2008 – 2010	NSF MILES-IGERT Training Grant for Research in Oxidative Processes
2007 – 2012	Institute for Critical Technology and Applied Science (ICTAS) Doctoral Scholar Graduate Fellowship
2007	James Lewis Howe Award
2006	Phi Beta Kappa National Arts and Sciences Honor Fraternity
2005, 2006	R. W. Engel Scholarship
2003 – 2007	Dean's List

EMPLOYMENT AND RESEARCH EXPERIENCE

July 2013 – Present
Ruth L. Kirschstein NRSA Postdoctoral Fellow (A.D. MacKerell, Jr.)
Department of Pharmaceutical Sciences, University of Maryland, Baltimore

- Drude polarizable and additive CGenFF force field development
- Simulations of nucleic acids using CHARMM, NAMD, and OpenMM (GPU)
- Quantum mechanical calculations using Gaussian, Molpro, and Q-Chem

May 2012 – May 2013 **Research Scientist** (D.R. Bevan)
Department of Biochemistry, Virginia Polytechnic Institute and State University
- MD simulations of the Aβ peptide in membranes
- MD simulations of PPARγ-RXRα-DNA complexes

2008 – 2012 **Graduate Research Assistant** (D.R. Bevan)
Department of Biochemistry, Virginia Polytechnic Institute and State University
- MD simulations of the Aβ peptide in membranes and water using GROMACS
- Small molecule parametrization (flavonoids)
- Free energy calculations and non-equilibrium MD
- Development of GridMAT-MD, a GPL program for membrane analysis
- Programming: Perl, Linux/Unix, C/C++, shell scripting, HTML, LaTeX

2008 **Graduate Rotation Student** (F. Schubot)
Department of Biological Sciences, Virginia Polytechnic Institute and State University
- Protein expression, purification, and crystallization of protein-DNA complexes

2007 – 2008 **Graduate Rotation Student** (P. Sobrado)
Department of Biochemistry, Virginia Polytechnic Institute and State University
- Cloning, expression, and purification of protein kinases

2004 – 2007 **Undergraduate Researcher** (D.R. Bevan)
Department of Biochemistry, Virginia Polytechnic Institute and State University
- MD simulations of DNA in AMBER and Aβ in membranes in GROMACS

2006 **Summer Undergraduate Researcher** (K.E. Saker)
Virginia-Maryland Regional College of Veterinary Medicine
- Feline care and nutrition
- Mammalian cell culture, MTT assays, flow cytometry

PUBLICATIONS

1. **J.A. Lemkul** and A.D. MacKerell, Jr. (2016) "Balancing Interactions of Mg^{2+} in Aqueous Solution and with Nucleic Acid Moieties For a Polarizable Force Field Based on the Classical Drude Oscillator Model." *J. Phys. Chem. B* In Press. DOI: 10.1021/acs.jpcb.6b09262

2. **J.A. Lemkul**, S.K. Lakkaraju, and A.D. MacKerell, Jr. (2016) "Characterization of Mg^{2+} Distributions around RNA in Solution." *ACS Omega* 1 (4): 680-688. (PMC5088455)

3. I. Soteras, F.-Y. Lin, K. Vanommeslaeghe, **J.A. Lemkul**, K. A. Armacost, C.L. Brooks III, and A.D. MacKerell, Jr. (2016) "Parametrization of Halogen Bonds in the CHARMM General Force Field: Improved Treatment of Ligand-Protein Interactions." *Bioorg. Med. Chem.* 24 (20): 4812-4825. (PMC5053860)

4. **J.A. Lemkul**, J. Huang, B. Roux, and A.D. MacKerell, Jr. (2016) "An Empirical Polarizable Force Field Based on the Classical Drude Oscillator Model: Development History and Recent Applications." *Chem. Rev.* 116 (9): 4983-5013. (PMC4865892)

5. J. Lee, X. Cheng, J. Swails, M.S. Yeom, P. Eastman, **J.A. Lemkul**, S. Wei, J. Buckner, J.C. Jeong, Y. Qi, S. Jo, V. Pande, D.A. Case, C.L. Brooks III, A.D. MacKerell, Jr., J.B. Klauda, and W. Im. (2016) "CHARMM-GUI Input Generation for NAMD, GROMACS, AMBER, OpenMM, and CHARMM/OpenMM Simulations using the CHARMM Force Fields." *J. Chem. Theory Comput.* 12 (1): 405-413. (PMC4712441)

6. S.K. Lakkaraju, **J.A. Lemkul**, J. Huang, and A.D. MacKerell, Jr. (2016) "DIRECT-ID: An Automated Method to Identify and Quantify Conformational Variations - Application to β_2-adrenergic GPCR." *J. Comput. Chem.* 37 (4): 416-425. (PMC4756637)

7. **J.A. Lemkul**, J. Huang, and A.D. MacKerell, Jr. (2015) "Induced Dipole-Dipole Interactions Influence Unfolding Pathways of Wild-Type and Mutant Amyloid β-Peptides." *J. Phys Chem. B* 119 (51): 15574-15582. (PMC4690896)

8. **J.A. Lemkul**, B. Roux, D. van der Spoel, and A.D. MacKerell, Jr. (2015) "Implementation of Extended Lagrangian Dynamics in GROMACS for Polarizable Simulations Using the Classical Drude Oscillator Model." *J. Comput. Chem.* 36 (19): 1473-1479. (PMC4481176)

9. **J.A. Lemkul**, S.N. Lewis, J. Bassaganya-Riera, and D.R. Bevan (2015) "Phosphorylation of PPARγ Affects Collective Motions of the PPARγ-RXRα-DNA Complex." *PLOS ONE.* 10 (5): e0123984.

10. S.R. Gerben, **J.A. Lemkul**, A.M. Brown, and D.R. Bevan (2014) "Comparing Atomistic Molecular Mechanics Force Fields for a Difficult Target: A Case Study of the Amyloid β-Peptide." *J. Biomol. Struct. Dyn.* 32 (11): 1817-1832.

11. **J.A. Lemkul**, A. Savelyev, and A.D. MacKerell, Jr. (2014) "Induced Polarization Influences the Fundamental Forces in DNA Base Flipping." *J. Phys. Chem. Lett.* 5 (12): 2077-2083. (PMC4064933)

12. D.G.S. Capelluto, X. Zhao, A. Lucas, **J.A. Lemkul**, S. Xiao, X. Fu, F. Sun, D.R. Bevan, and C.V. Finkielstein (2014) "Biophysical and molecular dynamics studies of phosphatidic acid binding to the Dvl-2 DEP domain." *Biophys. J.* 106 (5): 1101-1111.

13. A.M. Brown, **J.A. Lemkul**, N. Schaum, and D.R. Bevan (2014) "Simulations of Monomeric Amyloid β-Peptide (1-40) with Varying Solution Conditions and Oxidation State of Met35: Implications for Aggregation." *Arch. Biochem. Biophys.* 545 (1): 44-62.

14. **J.A. Lemkul** and D.R. Bevan (2013) "Aggregation of Alzheimer's Amyloid β-Peptide in Biological Membranes: A Molecular Dynamics Study." *Biochemistry.* 52 (29): 4971-4980.

15. **J.A. Lemkul** and D.R. Bevan (2012) "The Role of Molecular Simulations in the Development of Inhibitors of Amyloid β-Peptide Aggregation for the Treatment of Alzheimer's Disease." *ACS Chem. Neurosci.* 3 (11): 845-856.
    - Cover art for special issue on Alzheimer's Disease

16. **J.A. Lemkul** and D.R. Bevan (2012) "Morin Inhibits the Early Stages of Amyloid β-Peptide Aggregation by Altering Tertiary and Quaternary Interactions to Produce 'Off-Pathway' Structures." *Biochemistry.* 51 (30): 5990-6009.

17. **J.A. Lemkul** and D.R. Bevan (2011) "Lipid Composition Influences the Release of Alzheimer's Amyloid β-Peptide from Membranes." *Protein Sci.* 20 (9): 1530-1545.

18. **J.A. Lemkul** and D.R. Bevan (2011) "Characterization of Interactions Between PilA from *Pseudomonas aeruginosa* Strain K and a Model Membrane." *J. Phys. Chem. B* 115 (24): 8004-8008.

19. **J.A. Lemkul**, W.J. Allen, and D.R. Bevan (2010) "Practical Considerations for Building GROMOS-Compatible Small Molecule Topologies." *J. Chem. Inf. Model.* 50 (12): 2221-2235.

20. P. Mehere, Q. Han, **J.A. Lemkul**, C.J. Vavricka, H. Robinson, D.R. Bevan, and J. Li (2010) "Tyrosine Aminotransferase: biochemical and structural properties and molecular dynamics simulations." *Protein & Cell* 1 (11): 1023-1032.

21. **J.A. Lemkul** and D.R. Bevan (2010) "Destabilizing Alzheimer's $A\beta_{42}$ Protofibrils with Morin: Mechanistic Insights from Molecular Dynamics Simulations." *Biochemistry* 49 (18): 3935-3946.

22. **J.A. Lemkul** and D.R. Bevan (2010) "Assessing the Stability of Alzheimer's Amyloid Protofibrils Using Molecular Dynamics" *J. Phys. Chem. B* 114 (4): 1652-1660.
    - Listed as "Editor Selected Biophysical Research," October 2011

23. W.J. Allen, **J.A. Lemkul**, and D.R. Bevan (2009) "GridMAT-MD: A Grid-based Membrane Analysis Tool for Use With Molecular Dynamics." *J. Comput. Chem.* 30 (12): 1952-1958.

24. **J.A. Lemkul** and D.R. Bevan (2009) "Perturbation of membranes by the amyloid β-peptide – a molecular dynamics study." *FEBS J.* 276 (11): 3060-3075.
    - Highlighted in *FEBS J* virtual issue "Protein Misfolding, Prions, and Amyloid," January 2010

25. **J.A. Lemkul** and D.R. Bevan (2008) "A Comparative Molecular Dynamics Analysis of the Amyloid β-Peptide in a Lipid Bilayer." *Arch. Biochem. Biophys.* 470 (1): 54-63.

INVITED PRESENTATIONS

1. "Polarizable Force Field for DNA and RNA Based on the Classical Drude Oscillator Model." National Institutes of Health, Laboratory of Computational Biology. Rockville, MD, April 2016.

2. "Influence of Induced Polarization on Amyloid Peptide Misfolding in Different Solution Environments." 249th ACS National Meeting. Denver, CO, March 2015.

3. "Biomolecular Force Fields: Fundamentals and Improvements for the Next Generation." 8th Annual q-bio Summer School, University of New Mexico, Albuquerque, NM, August 2014.

4. "Insights into Protein Complexation and Drug Discovery from Steered Molecular Dynamics Simulations." 2013 GROMACS Workshop and Conference, Charlottesville, VA, September 2013.

5. "Molecular Dynamics Simulations: Using High-Performance Computing to Solve Problems in Biology, Chemistry, and Physics." Roanoke College, Salem, VA, March 2013.

6. "Dimerization of the Amyloid β-Peptide in Biological Membranes." CECAM workshop – Anchoring simulations to experiments: challenges for understanding and treating Alzheimer's disease. Insitut de Biologie Physico-Chemique. Paris, France, May 2012.

7. "Advancing Therapeutics for Alzheimer's Disease with Molecular Dynamics Simulations: An Unconventional Approach to Drug Discovery." Washington & Lee University, Lexington, VA, December 2010.

8. "Computational Approaches to Alzheimer's Drug Discovery." University of Virginia, Charlottesville, VA, November 2010.

9. "Advancing Therapeutics for Alzheimer's Disease with Molecular Dynamics Simulations." 2010 meeting of the Virginia Academy of Science (88th VAS), James Madison University, Harrisonburg, VA, May 2010.

POSTERS AND CONFERENCE PRESENTATIONS

1. **J.A. Lemkul** and A.D. MacKerell, Jr. "Polarizable Force Field for DNA and RNA Based on the Classical Drude Oscillator Model." 252nd ACS National Meeting, Philadelphia, PA, August 2016. (Poster presentation.)

2. **J.A. Lemkul** and A.D. MacKerell, Jr. "Polarizable Force Field for DNA and RNA Based on the Classical Drude Oscillator Model." School of Pharmacy Research Day, Baltimore, MD, April 2016. (Poster presentation.)

3. **J.A. Lemkul**, A. Savelyev, and A.D. MacKerell, Jr. "Towards a Polarizable Force Field for RNA Based on the Classical Drude Oscillator." School of Pharmacy Research Day, Baltimore, MD, April 2015. (Poster presentation.)

4. **J.A. Lemkul**, A. Savelyev, and A.D. MacKerell, Jr. "Towards a Polarizable Force Field for RNA Based on the Classical Drude Oscillator," Biophys. J. **108** (S1): 159a. February 2015. (Poster presentation, given at the Biophysical Society 59th Annual Meeting, Baltimore, MD.)

5. **J.A. Lemkul**, A. Savelyev, and A.D. MacKerell, Jr. "Induced Polarization Influences the Fundamental Forces in DNA Base Flipping" School of Pharmacy Research Day, Baltimore, MD, April 2014. (Poster presentation.)

6. **J.A. Lemkul** and D.R. Bevan. "New Insights into the Mechanism of Alzheimer's Disease from Molecular Dynamics Simulations." Spring ICTAS Doctoral Scholars Meeting, Blacksburg, VA, April 2012. (Poster presentation).

7. **J.A. Lemkul** and D.R. Bevan. "Lipid Composition Influences the Release of Alzheimer's Amyloid β-Peptide from Membranes." Spring ICTAS Doctoral Scholars Meeting, Blacksburg, VA, April 2011. (Poster presentation).

8. **J.A. Lemkul** and D.R. Bevan. "Ganglioside GM1 Facilitates Release of Alzheimer's Aβ Peptide from Lipid Rafts." ACC Interdisciplinary Forum for Discovery in Life Sciences, Blacksburg, VA, October 2010. (Platform presentation).

9. **J.A. Lemkul** and D.R. Bevan. "Ganglioside GM1 Facilitates Release of Alzheimer's Aβ Peptide from Lipid Rafts." 2010 ICTAS Research Day, Blacksburg, VA, September 2010. (Poster presentation).

10. **J.A. Lemkul** and D.R. Bevan. "Thermodynamics of Amyloid Fibril Dissociation: Identifying Targets for Therapeutic Intervention in Alzheimer's Disease." Edward Via College of Osteopathic Medicine 6th Annual Research Day, Blacksburg, VA, October 2009. (1st Place in the Student Biomedical poster, platform presentation.)

11. **J.A. Lemkul** and D.R. Bevan. "Dissolving Alzheimer's Amyloid Plaques with Red Wine: Insights from Molecular Dynamics Simulations." Protein Sci. **18** (S1): 73. 23rd Annual Symposium of the Protein Society, Boston, MA, July 2009. (Poster presentation.)

12. **J.A. Lemkul** and D.R. Bevan. "Dissolving Alzheimer's Amyloid Plaques with Red Wine: Insights from Molecular Dynamics Simulations." 4th Annual Virginia Tech Structural Biology Symposium, Blacksburg, VA, March 2009. (Poster presentation.)

13. **J.A. Lemkul** and D.R. Bevan. "Dissolving Alzheimer's Amyloid Plaques with Red Wine: Insights from Molecular Dynamics Simulations." 25th Annual Graduate Student Association Research Symposium, Blacksburg, VA, March 2009. (Poster presentation.)

14. **J.A. Lemkul** and D.R. Bevan. "Binding of Flavonoids to the Amyloid β-Peptide: Treating Alzheimer's Disease with Red Wine." Free Radic. Biol. Med. **45** (1): S87. Suppl. 16th Annual Meeting of the Society for Free Radical Biology and Medicine, November 2008. (Poster presentation.)

15. **J.A. Lemkul** and D.R. Bevan. "Membrane Molecular Dynamics of Alzheimer's Amyloid-β Peptide." Dean's Forum on Health, Food, and Nutrition, Blacksburg, VA, November 2007. (Poster presentation.)

16. **J.A. Lemkul** and D.R. Bevan. "Membrane Molecular Dynamics of Alzheimer's Amyloid-β Peptide." 2007 MII Technical Conference and Review, Blacksburg, VA, October 2007. (Poster presentation.)

17. **J.A. Lemkul** and D.R. Bevan. "A Molecular Dynamics Analysis of the Amyloid-β Peptide: Insights into the Molecular Mechanism of Alzheimer's Disease." Protein Science **16** (S1): 79. 21st Annual Symposium of the Protein Society, Boston, MA, July 2007. (Poster and platform presentation.)

18. **J.A. Lemkul**, A.E. Tanner, and K.E. Saker. "The Effect of Antioxidants on 8-Oxoguanine Levels in the Treatment of Feline Obesity and Human Cancer," Summer Undergraduate Research Program Symposium, Blacksburg, VA, August 2006. (Platform presentation.)

TEACHING EXPERIENCE

April 2015	**Guest Lecturer** – PHAR 621 Molecular Biophysics *Department of Pharmaceutical Sciences, University of Maryland, Baltimore*
August 2014	**Lecturer and Mentor** *8th Annual q-bio Summer School, University of New Mexico*
September 2013	**Tutorial Instructor** *2013 USA GROMACS Conference and Workshop, University of Virginia*
February 2013	**Guest Lecturer** – BCHM 4116 General Biochemistry *Department of Biochemistry, Virginia Polytechnic Institute and State University*
Fall 2011	**Course Discussion Leader** – BCHM 1014 Introduction to Biochemistry (G. Gillaspy) *Department of Biochemistry, Virginia Polytechnic Institute and State University*
December 2010	**Guest Lecturer** – BIOL 274 Structural Biology *Department of Biology, Washington & Lee University*
Fall 2009	**Co-Instructor** – BCHM 5984 Applications of Molecular Modeling *Department of Biochemistry, Virginia Polytechnic Institute and State University*
Spring 2009	**Teaching Assistant** – BCHM 4116 General Biochemistry (E.M. Gregory, Z. Tu) *Department of Biochemistry, Virginia Polytechnic Institute and State University*
2006 – 2007	**Teaching Assistant** – CHEM 1035/1036 General Chemistry (P. Amateis, P. Durrill) *Department of Chemistry, Virginia Polytechnic Institute and State University*
2004 – 2007	**Chemistry Learning Center Tutor (Alpha Chi Sigma)** *Department of Chemistry, Virginia Polytechnic Institute and State University*

JOURNAL REVIEWER

ACS Chemical Neuroscience
Advances in Bioinformatics
BBA Proteins and Proteomics
Interdisciplinary Sciences: Computational Life Sciences
International Journal of Biological Macromolecules
Journal of Biomolecular Structure and Dynamics
Journal of Chemical Information and Modeling
Journal of Chemical Physics
Journal of Chemical Theory and Computation
Journal of Molecular Modeling
The Journal of Physical Chemistry
Molecular Informatics
Molecular Simulation
Molecules
Nucleic Acids Research
PLoS Computational Biology
PLoS ONE
Proteins: Structure, Function and Bioinformatics
Research on Chemical Intermediates
RSC Advances
The Science of Nature (formerly Naturwissenschaften)