

# Dr. Chris Neale, BSc, PhD

Curriculum Vitae

October 24, 2016

2152A 37th st.  
Los Alamos NM, USA, 87544  
(518) 961-2904  
candrewn@gmail.com

Los Alamos National Laboratory  
Center for Nonlinear Studies  
TA-3, Bldg 1690, Room 123  
(505) 667-8715

## RESEARCH INTERESTS

- Mechanisms of signal transduction.
- Structure-dynamics-function relationships in macromolecules.
- Developing new techniques for simulating biochemically relevant timescales.

## RESEARCH EXPERIENCE AND EDUCATION

- **2016-Present.** Director's fellow, Los Alamos National Laboratory, New Mexico.
- **2015-Present.** Postdoctoral Researcher, Los Alamos National Laboratory, Center for Nonlinear Studies, New Mexico. Advisor: Angel García.
- **2013-2015.** Postdoctoral Researcher, Rensselaer Polytechnic Institute, New York. Advisor: Angel García.
- **2012.** Postdoctoral Researcher, McMaster University, Ontario. Advisor: Russell Bishop.
- **2005-2012.** Ph.D. (Biochemistry), University of Toronto, Ontario. Advisor: Régis Pomès.
- **2004-2005.** Computer Programmer, Hospital for Sick Children, Ontario. Advisor: Julie Forman-Kay.
- **2003.** Lab Technician, Dalhousie University, Nova Scotia. Advisor: George Robertson.
- **2002.** Lab Technician, Ontario Cancer Institute, Ontario. Advisor: Robert Rottapel.
- **1999, 2000.** Cooperative Education placement, AstraZeneca Pharmaceuticals, Quebec. Advisor: Jack Cao.
- **1996-2001.** B.Sc. (Biology), Honors, University of Waterloo, Ontario.

## AWARDS AND ACCOMPLISHMENTS

- 22 peer-reviewed publications, 10 as first author, 1 as co-first author.
- **2015.** Best Postdoc Presentation award, Canadian Society for Chemistry National Meeting, Computational Chemistry: Methods and Applications Symposium, Ontario.
- **2014.** Article selected for *Biophysical Journal* Best of 2014 issue.
- **2010.** Best Student Paper award, Canadian High Performance Computing Symposium, Ontario.
- **2008.** Exceptional Trainee award, Hospital for Sick Children, Ontario.

## GRANTS AND FELLOWSHIPS

- **2014-2017.** Canadian Institutes of Health Research Postdoctoral Fellowship, \$150,000.
- **2007-2011.** Hospital for Sick Children Research Training Center Scholarship, \$36,000.
- **2006-2011.** University of Toronto Fellowship, \$60,000.

- **2010.** University of Toronto School of Graduate Studies Conference Grant, \$500.

#### COMPUTATIONAL GRANTS

- **2016.** Department of Energy Leadership Computing INCITE proposal co-PI. Principal applicant: Arvind Ramanathan (*submitted*).
- **2013-2016.** Extreme Science and Engineering Discovery Environment (XSEDE) application lead author. PI: Angel García; allocations valued at \$400,000 / year.
- **2013.** XSEDE startup allocation. PI: Chris Neale; allocated 200,000 core hours.
- **2010, 2011.** Compute Canada National Resource Allocation Committee (NRAC) application lead author. PI: Régis Pomès; allocations valued at \$2,000,000 / year.
- **2008.** Shared Hierarchical Academic Research Computing Network: Fellowships and Dedicated Resources (SHARCNET round VIII). Allocated 604,000 core hours, valued at \$25,000.

#### PEER-REVIEWED PUBLICATIONS

Google Scholar statistics: <http://tinyurl.com/NealeScholar>

*h-index*: 14; *total citations*: 837

22. **2016.** C. Neale, R. Pomès, "Sampling errors in free energy simulations of small molecules in lipid bilayers", *BBA Biomembranes*, 1858(10):2539-2548.
21. **2016.** C. Neale, R. Pomès, A.E. García, "Peptide bond isomerization in high-temperature simulations", *J. Chem. Theory Comput.*, 12(4):1989-1999.
20. **2015.** C. Neale, H.D. Hecce, R. Pomès, A.E. García, "Can specific protein-lipid interactions stabilize an active state of the beta 2 adrenergic receptor?", *Biophys. J.*, 109(8):1652-1662.
19. **2015.** C. Neale, K. Huang, A.E. García, S. Tristram-Nagle, "Penetration of HIV-1 Tat47-57 into PC/PE bilayers assessed by MD simulation and X-ray scattering", *Membranes*, 5(3):473-494.
18. **2015.** C. Neale, N. Chakrabarti, P. Pomorski, E.F. Pai, R. Pomès, "Hydrophobic gating of ion permeation in magnesium channel CorA", *PLoS Comput. Biol.*, 11(7):e1004303. *Selected for cover*.
17. **2014.** C. Neale, J.C.Y. Hsu, C.M. Yip, R. Pomès, "Indolicidin binding induces thinning of a lipid bilayer", *Biophys. J.*, 106(8):L29-L31. *Selected for cover; selected for Best of 2014 issue*.
16. **2013.** C. Neale, C. Madill, S. Rauscher, R. Pomès, "Accelerating convergence in molecular dynamics simulations of solutes in lipid membranes by conducting a random walk along the bilayer normal", *J. Chem. Theory Comput.*, 9(8):3686-3703.
15. **2013.** C. Neale, H. Ghanei, J. Holyoake, R.E. Bishop, G.G. Privé, R. Pomès, "Detergent-mediated protein aggregation", *Chem. Phys. Lipids*, 169:72-84.
14. **2013.** M. Krzeminski, J.A. Marsh, C. Neale, W-Y. Choy, J.D. Forman-Kay, "Characterization of disordered proteins with ENSEMBLE", *Bioinformatics*, 29(3):398-399.
13. **2012.** L. Huynh, C. Neale, R. Pomès, C. Allen, "Computational approaches to the rational design of nanoemulsions, polymeric micelles, and dendrimers for drug delivery", *Nanomed.-Nanotechnol.*, 8(1):20-36.
12. **2011.** C. Neale, W.F.D. Bennett, D.P. Tieleman, R. Pomès, "Statistical convergence of equilibrium properties in simulations of molecular solutes embedded in lipid bilayers", *J. Chem. Theory Comput.*, 7(12):4175-4188.

11. **2010.** L. Huynh, C. Neale, R. Pomès, C. Allen, "Systematic design of unimolecular star copolymer micelles using molecular dynamics simulations", *Soft Matter*, 6:5491-5501.
10. **2010.** J.A. Cuesta-Seijo, C. Neale, M.A. Khan, J. Mokhtar, C.D. Tran, R.E. Bishop, R. Pomès, G.G. Privé, "PagP crystallized from SDS/cosolvent reveals the route for phospholipid access to the hydrocarbon ruler", *Structure*, 18(9):1210-1219.
9. **2010.** N. Chakrabarti, C. Neale, J. Payandeh, E.F. Pai, R. Pomès, "An iris-like mechanism of pore dilation in the CorA magnesium transport system", *Biophys. J.*, 98(5):784-792.
8. **2009.** S. Rauscher, C. Neale, R. Pomès, "Simulated tempering distributed replica sampling, virtual replica exchange, and other generalized-ensemble methods for conformational sampling", *J. Chem. Theory Comput.*, 5(10):2640-2662.
7. **2009.** M.S. Al-Abdul-Wahid, C. Neale, R. Pomès, R.S. Prosser, "A solution NMR approach to the measurement of amphiphile immersion depth and orientation in membrane model systems", *J. Am. Chem. Soc.*, 131:6452-6459.
6. **2008.** C. Neale, T. Rodinger, R. Pomès, "Equilibrium exchange enhances the convergence rate of umbrella sampling", *Chem. Phys. Lett.*, 460:375-381.
5. **2007.** M.A. Khan, C. Neale, C. Michaux, R. Pomès, G.G. Privé, R.W. Woody, R.E. Bishop, "Gauging a hydrocarbon ruler by an intrinsic exciton probe", *Biochemistry*, 46:4565-4579.
4. **2007.** J.A. Marsh\*, C. Neale\*, F.E. Jack, W-Y. Choy, A.Y. Lee, K.A. Crowhurst, J.D. Forman-Kay, "Improved structural characterizations of the drkN SH3 domain unfolded state suggest a compact ensemble with native-like and non-native structure", *J. Mol. Biol.*, 367:1494-1510.  
\*These authors contributed equally to this work.
3. **2006.** M. Tollinger, C. Neale, L.E. Kay, J.D. Forman-Kay, "Characterization of the hydrodynamic properties of the folding transition state of an SH3 domain by magnetization transfer NMR spectroscopy", *Biochemistry*, 45:6434-6445.
2. **2005.** L.X. Wu, J. La Rose, L. Chen, C. Neale, T. Mak, K. Okkenhaug, R. Wange, R. Rottapel, "CD28 regulates the translation of Bcl-xL via the phosphatidylinositol 3-kinase/mammalian target of rapamycin pathway", *J. Immunol.*, 174:180-194.
1. **2002.** R. Rottapel, S. Ilangumaran, C. Neale, J. La Rose, J.M-Y. Ho, M.H-H. Nguyen, D. Barber, P. Dubreuil, P. de Sepulveda, "The tumor suppressor activity of SOCS-1", *Oncogene*, 21:4351-4362.

#### INVITED TALKS

10. **2016.** Department of Chemistry, West Virginia University.
9. **2016.** Energy Landscapes: From Protein Folding to Macromolecular Assembly, Santa Fe, New Mexico.
8. **2016.** Department of Biological Sciences, University of Pittsburgh.
7. **2015.** Department of Chemistry, Dalhousie University, Nova Scotia.
6. **2015.** Bioinformatics Cluster, University of Rochester, New York.
5. **2015.** Department of Biology, Siena College, New York.
4. **2015.** Department of Pharmaceutical Sciences, Albany College of Pharmacy, New York.
3. **2013.** Department of Chemistry, Wilfrid Laurier University, Ontario.
2. **2011.** Shared Hierarchical Academic Research Computing Network seminar, University of the Ontario Institute of Technology, Oshawa, Ontario.
1. **2007.** Canadian Institutes of Health Research Symposium on Membrane Proteins, University of Toronto, Ontario.

## CONTRIBUTED TALKS

14. **2016.** Canadian Society for Chemistry National Meeting, Halifax, Nova Scotia.
13. **2015.** Canadian Biophysical Society National Meeting, Waterloo, Ontario.
12. **2015.** Canadian High Performance Computing Symposium, Montreal, Quebec.
11. **2015.** Canadian Chemistry Conference, Ottawa, Ontario. *Best Postdoc Presentation award.*
10. **2015.** Protein Folding Consortium Annual Meeting, University of California, Berkeley.
9. **2015.** American Chemical Society National Meeting, Denver, Colorado.
8. **2015.** Biophysical Society National Meeting, Baltimore, Maryland.
7. **2014.** Rensselaer Nanotechnology Center Research Symposium, Rensselaer Polytechnic Institute, New York.
6. **2014.** Workshop on Free Energy Methods in Drug Design, Vertex Pharmaceuticals, Boston, Massachusetts.
5. **2013.** Gromacs Workshop, University of Virginia.
4. **2013.** Biophysical Society National Meeting, Philadelphia.
3. **2011.** Biophysical Society National Meeting, Baltimore.
2. **2010.** Canadian High Performance Computing Symposium, Toronto. *Best Student Paper award.*
1. **2009.** Chemical Biophysics Symposium, Toronto, Ontario.

## POSTERS

13. **2016.** Symposium on Cell Signaling, Santa Fe, New Mexico.
12. **2016.** Biophysical Society National Meeting, Los Angeles, California.
11. **2016.** Keystone Symposium – G Protein-Coupled Receptors: Structural Dynamics and Functional Implications, Keystone, Colorado.
10. **2014.** G-protein Signaling Workshop, Thomas Jefferson University, Philadelphia, Pennsylvania.
9. **2014.** Keystone Symposium – G Protein-Coupled Receptors: Structural Dynamics and Functional Implications, Snowbird, Utah.
8. **2012.** Chemical Biophysics Symposium, Toronto, Ontario.
7. **2012.** Biophysical Society National Meeting, San Diego, California.
6. **2011.** Biophysical Society National Meeting, Baltimore, Maryland.
5. **2010.** Canadian Society for Chemistry National Meeting, Toronto, Ontario.
4. **2010.** Workshop on Free Energy Methods in Drug Design, Cambridge, Massachusetts.
3. **2010.** Keystone Symposium – Computer Aided Drug Design, Whistler, British Columbia.
2. **2010.** Chemical Biophysics Symposium, Toronto, Ontario.
1. **2010.** Biophysical Society National Meeting, San Francisco, California.

## TEACHING AND MENTORING EXPERIENCE

- **2015.** Guest lecturer in "Computational Chemistry for Graduate Students", State University of New York, Albany.
- **2015.** Guest lecturer in "Freshman Seminar for the World of Chemistry Living-Learning Community", State University of New York, Albany.
- **2014-2015.** Mentored undergraduate student Jorge Alarcon Ochoa and graduate student Joel Janke in the lab of Angel García at Rensselaer Polytechnic Institute.

- **2007-2012.** Mentored six graduate students at the University of Toronto: Grace Li, Rowan Henry, David Caplan, and Kethika Kulleperuma in the lab of Régis Pomès; Loan Huynh in the lab of Christine Allen; and Jenny Hsu in the lab of Christopher Yip.
- **2007-present.** Assisted peers and encouraged the development of problem solving skills in more than 1,000 postings on the internet mailing list of the computer simulation software package GROMACS.
- **2009.** Faculty of Medicine Saturday Program for underachieving elementary school students, University of Toronto, Ontario.
- **2000.** Teaching assistant, histology laboratory, University of Waterloo, Ontario.

#### EARLY ACCESS TO HIGH PERFORMANCE COMPUTING CLUSTERS

- **2013, 2015** Computational Center for Nanotechnology Innovations (CCNI), Albany, New York
- **2012** Southern Ontario Smart Computing Innovation Platform (SOSCIP).
- **2012** Westgrid "Parallel" 10,000-core HPC cluster of Compute Canada.
- **2011** CLUMEQ "Guillimin" 14,000-core HPC cluster of Compute Canada.
- **2009** SciNet 30,000-core HPC cluster of Compute Canada.

#### SERVICE

- **2016.** Organizer, postdoc and student seminar series, Los Alamos National Laboratory, Center for Nonlinear Studies, New Mexico.
- **2015.** Session Chair, "Computational Chemistry: Methods and Applications", Canadian Chemistry Conference, Ottawa.
- **2015.** Workshop organizer and presenter, "RNA Dynamics: Going from *in vitro* to *in silico*", The RNA Institute, State University of New York (SUNY), Albany, NY, USA. (co-organizers: Alan Chen, SUNY; Jeff Noel, Rice; Paul Whitford, Northeastern).
- **2010, 2014.** Internal review of Compute Canada's strategic plan.
- **2012-present.** Reviewing activity: *Biophysical Journal*; *Chemistry and Physics of Lipids*; *Journal of Chemical Physics*; *Journal of Chemical Theory and Computation*; *Molecular Simulation*; *PLOS Computational Biology*; *PLOS ONE*; *Proteins: Structure, Function, and Bioinformatics*

#### MEDIA COVERAGE

- **2010.** *Vaughan Citizen* newspaper interview promoting Compute Canada infrastructure, "Vaughan's speedy computer".

#### WEBSITE

<http://www.chris-neale.com>