CHRISTINA BERGONZO

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EDUCATION

Post-Doctoral Research, July 2012-present
Cheatham Laboratory
University of Utah, Salt Lake City, UT
Researching structural biology and computational biophysics using large-scale HPC resources.

Doctor of Philosophy, Chemistry, August 2012
Simmerling Laboratory
Stony Brook University, Stony Brook, NY
Related course work: Quantum Chemistry, Biophysical Chemistry, Inorganic Chemistry, Chemical Biology, Topics in Theoretical Chemistry, Theoretical Chemistry: Application, Current Topics in Biological Chemistry

Bachelor of Science, Chemistry, May 2006
Manhattan College, Riverdale, NY
Major: Chemistry
Minor: Mathematics
Related course work: Advanced Organic Chemistry, Physical Chemistry, Analytical Chemistry, Advanced Inorganic Chemistry, Advanced Spectroscopy, Physics, Biochemistry, Calculus, Differential Equations, Probability and Statistics, Partial Differential Equations

HONORS AND AWARDS

- Postdoctoral Travel Assistance Award, University of Utah Graduate School, Summer 2014
- Chemistry Award for Outstanding Doctoral Student, Stony Brook University Department of Chemistry Graduate Student Awards, Spring 2012
- Chemical Computing Group Excellence Award, Spring ACS 2011
- NSF IGERT Trainee, Summer 2007 – 2011
- American Chemical Society Member, 2007 – present
- Sigma Xi Research Honor Society, Spring 2006
- Gamma Sigma Epsilon Chemistry Honor Society, Spring 2006
- Manhattan College Presidential Scholarship, Fall 2002 – Spring 2006
- Manhattan College Chemistry Department Scholarship, Fall 2002 – Spring 2006

TEACHING EXPERIENCE

Molecular Modeling Teaching Assistant, University of Utah (Spring 2013)
General Chemistry Recitation Teaching Assistant, Stony Brook University (Spring 2007)
Physical Chemistry Laboratory Teaching Assistant, Stony Brook University (Fall 2006)
Organic Laboratory Assistant, Manhattan College (Summer 2004, Summer 2005)

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RESEARCH INTERESTS

Post-graduate Research: Computational dynamics of RNA.
My current research includes developing methods for multi-dimensional replica exchange simulations of RNA tetranucleotide, tetraloop, and hairpin systems to understand RNA conformational preferences under various force field conditions. This work will be extended to develop and refine a fixed charge nucleic acid force field. Additionally, I am working to understand the biologically relevant structure shift as a function of ion environment for the Varkud Satellite Ribozyme stem loop V. This involves critical analysis of monovalent and divalent ion parameters, as well as re-refinement of NMR structures.

Graduate Research: Computational investigation of biological systems.
My research investigated the various mechanisms at work in the base excision repair pathway of oxidative damage to DNA by the glycosylase Fpg. Specifically, damage recognition, base flipping into the enzyme's active site, and translocation of the enzyme along DNA. My research led to the implementation of nudged elastic band and Hamiltonian replica exchange molecular dynamics in AMBER. These method development projects have also been applied to HIV protease to examine biologically relevant motions on long timescales.

Undergraduate Research (Summer 2005 – Summer 2006): Computational Chemistry calculations of conjugated pi systems using Titan, Spartan, Gaussian, and PyMol. Calculations of activation energy in reactants and transition states of Bergman cyclization reactions using Spartan, GaussView, and Gaussian 03.

SKILLS/ABILITIES

- Expertise in all-atom Molecular Dynamics simulations and data analysis, including but not limited to nudged elastic band, replica exchange (multi-dimensional), umbrella sampling.
- Computational experience with various local and national HPC centers, including NCSA Blue Waters and XSEDE resources Comet, Stampede, Maverick, as well as decommissioned sites NYBlue Blue Gene at Brookhaven National Laboratory, Mercury IA-64 Cluster at NCSA Illinois, Kraken Cray XT3-4-5 and Keeneland at NICS Tennessee.
- Proficient in AMBER suite, VMD, Chimera, Titan, Spartan, Gaussian 03, Maple, Microsoft Office Suite, AppleWorks Suite, Adobe Creative Commons Suite.
- Work daily in UNIX environment: proficient in bash and awk scripting.
- Working knowledge of Fortran 90, C, Python, MPI programming, and R.

SERVICE

- XSEDE Supercomputing Conference Abstract Review Committee –2014-present
- Reviewer for Biopolymers Journal – 2015-present
- Reviewer for the Journal of the American Statistical Association – 2014-2015
- ACS National Meeting Session Presider – PHYS – August 2014
- ACS National Meeting Session Presider – COMP – August 2014, March 2011, August 2009, August 2008, April 2008

PUBLICATIONS (REVERSE CHRONOLOGICAL ORDER)

2016 (16) **Bergonzo, C.**, Hall, K.B., Cheatham, T.E. III. Divalent Ion Dependent Conformational Changes in an RNA Stem-Loop Observed by Molecular Dynamics. *J. Chem. Theory Comput.,* 2016, doi: 10.1021/acs.jctc.6b00173.

(15) Li, H., Endutkin, A., **Bergonzo, C.**, Grollman, A.P., Campbell, A.J., de los Santos, C., Zharkov, D.O., Simmerling, C. A Dynamic Checkpoint in Oxidative Lesion Discrimination by Formamidopyrimidine-DNA Glycosylase. *Nucleic Acids Research,* 2016, 44 (2) 683-694.

2015 (14) **Bergonzo, C.**, Hall, K.B., Cheatham, T.E. III. Stem-loop V of Varkud Satellite RNA Exhibits Characteristics of the Mg^{2+} Bound Structure in the Presence of Monovalent Ions. *J. Phys. Chem. B*, 2015, 119 (38) 12355-12364.

(13) **Bergonzo, C.**, Cheatham, T.E. III. Improved Force Field Parameters Lead to a Better Description of RNA Structure. *J. Chem. Theory Comput.*, 2015, 11 (9) 3969-3972.

(12) **Bergonzo, C.**, Henriksen, N.M., Roe, D.R., Cheatham, T.E. III. Highly sampled tetranucleotide and tetraloop motifs enable evaluation of common RNA force fields. RNA, 2015, 21 (9) 1578-1590.

(11) Kuznetsov, N.A. and **Bergonzo, C.**, Campbell, A.J., Li, H., Mechetin, G.V., de los Santos, C., Grollman, A.P., Fedorova, O.S., Zharkov, D.O., Simmerling, C. Active destabilization of base pairs by a DNA glycosylase wedge initiates damage recognition. *Nucleic Acids Research*. 2015, 43 (1) 272-281.

2014 (10) Roe, D.R., **Bergonzo, C.**, Cheatham III, T.E. Evaluation of Enhanced Sampling Provided By Accelerated Molecular Dynamics with Hamiltonian Replica Exchange Methods. *J. Phys. Chem. B.* 2014, 118 (13) 3543-3552.

(9) Galindo-Murillo, R., **Bergonzo, C.**, and Cheatham, T.E. III. Molecular modeling of nucleic acid structure: Setup and Analysis. *Current Protocols Nucleic Acid Chemistry*, 2014, 56:7.10.1-7.10.21.

(8) **Bergonzo, C.**, Henriksen, N.M., Roe, D.R., Swails, J.M., Roitberg, A.E., Cheatham, T.E. III. Multi-dimensional Replica Exchange Molecular Dynamics Yields a Converged Ensemble of an RNA Tetranucleotide. *J. Chem. Theory Comput.,* 2014**,** 10 (1) 492-499.

2013 (7) **Bergonzo, C.**, Galindo-Murillo, R., and Cheatham, T.E. III. Molecular modeling of nucleic acid structure: Energy and Sampling. *Current Protocols Nucleic Acid Chemistry*, 2013, 54:7.8.1-7.8.21.

(6) **Bergonzo, C.**, Galindo-Murillo, R., and Cheatham, T.E. III. Molecular modeling of nucleic acid structure: Electrostatics and solvation. *Current Protocols Nucleic Acid Chemistry*, 2013, 55:7.9.1-7.9.27

(5) Galindo-Murillo, R., **Bergonzo, C.**, and Cheatham, T.E. III. Molecular Modeling of nucleic acid structure. *Current Protocols Nucleic Acid Chemistry,* 2013, 54:7.5.1-7.5.13.

2011 (4) **Bergonzo, C.**, Simmerling, C. An Overview of String Based Path Sampling Methods, *Annual Reports in Computational Chemistry* 2011, 7, 89-97.

(3) **Bergonzo, C.**, Campbell, A.J, de los Santos, C., Grollman, A.P., Simmerling, C. Energetic Preference of 8-oxoG Eversion Pathways in a DNA Glycosylase. *Journal of the American Chemical Society*, 2011, 133 (37) 14504-14506

2009 (2) **Bergonzo, C.**, Campbell, A.J., Walker, R.C., Simmerling, C. A partial nudged elastic band implementation for use with large or explicitly solvated systems. *International*

Journal of Quantum Chemistry, 2009. Special Issue: Proceedings of the International Symposium on Theory and Computations in Molecular and Materials Sciences, Biology, and Pharmacology. 109, 3781-3790.

(1) Song, K., Campbell, A.J., **Bergonzo, C.**, de los Santos, C., Grollman, A.P., Simmerling, C. An Improved Reaction Coordinate for Nucleic Acid Base Flipping Studies. *J. Chem. Theory Comput.*, 2009, 5 (11) 3105-3113.

RECENT PRESENTATIONS (REVERSE CHRONOLOGICAL ORDER)

2016 **Bergonzo, C.,** Cheatham, T.E. III. "Computational RNA Dynamics: The Good, the Bad, and the Ugly." Oral Presentation, Department of Medicinal Chemistry, College of Pharmacy, University of Utah, UT.

2015 **Bergonzo, C.** "Nucleic Acids Through a Virtual Microscope: The Potential and Promise of Simulation." Invited Talk, The Ohio State University, OH.

2014 **Bergonzo, C.,** Rau, M., Hall, K., Cheatham, T.E. III. **"**Conformational Ensembles of Stem-loop V of Varkud Satellite RNA are Limited by Magnesium Ions." Oral Presentation, Department of Medicinal Chemistry, College of Pharmacy, University of Utah, UT.

Bergonzo, C., Henriksen, N.M., Roe, D.R., Cheatham, T.E. III. "Evaluating Force Field Accuracy of RNA Dynamics Using Enhanced Sampling Methods." Oral Presentation, Physical Chemistry Division, ACS 248th National Meeting, San Francisco, CA.

Bergonzo, C., Henriksen, N.M., Roe, D.R., Cheatham, T.E. III. "Computational Studies of RNA Dynamics: Evaluating Force Field Accuracy." Oral Presentation, Computers in Chemistry Division, ACS 248th National Meeting, San Francisco, CA.

Bergonzo, C., Henriksen, N.M., Roe, D.R., Swails, J.M., Roitberg, A.E., Cheatham, T.E. III. "Overcoming the Sampling Problem in Force Field Evaluation via GPU-accelerated Multi-dimensional Replica Exchange Molecular Dynamics." Poster Presentation, Computers in Chemistry Division NVIDIA GPU Award Nominated Poster, ACS 248th National Meeting, San Francisco, CA.

Bergonzo, C., and Cheatham, T.E. III. "Evaluating Nucleic Acid Force Fields using Multi-dimensional Replica Exchange." Oral Presentation, International Society of Quantum Biology and Pharmacology President's Meeting, Telluride, CO.

Bergonzo, C., Cheatham, T.E. III. **"**Computational Studies of RNA Dynamics." Oral Presentation, Department of Medicinal Chemistry, College of Pharmacy, University of Utah, UT.

2013 **Bergonzo, C.**, Cheatham, T.E. III. "Using Enhanced Sampling Methods to Generate the Conformational Ensemble of GACC Tetranucleotide." Oral Presentation Combined Computational Group Meeting, University of Utah, UT.

Bergonzo, C., Cheatham, T.E. III. **"**Computational Study of RNA Dynamics." Oral Presentation, Telluride Science Research Conference: RNA Dynamics, Telluride, CO.