CURRICULUM VITAE for Catherine Leigh Allen, PhD

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EDUCATION AND DEGREES

- **Ph.D., Chemistry with Pharmacology certificate.** "Insights into the Structure and Mechanism of Anhydromuramic Acid Kinase (AnmK): A Novel Peptidoglycan Recycling Enzyme with Dual Hydrolase and Kinase Functionality." Advisor: Dewey G. McCafferty, Ph.D. 06/24/2011, Duke University, Durham, NC. Cumulative GPA: 4.0

- **B.S. with Honors, Chemistry with a concentration in Biochemistry, Cum laude; Minor in Psychology**. "Structural and Mutagenic Analyses of the M. jannaschii L7Ae Loop 9 RNA-Binding Region." 05/15/2006, Wake Forest University, Winston-Salem, NC. Cumulative GPA: 3.59; Dean's List 8 out of 8 semesters.

PROFESSIONAL EXPERIENCE

- Postdoctoral Associate *02/2014–present*
  Structural and Molecular Biochemistry, North Carolina State University, Mentor: John Cavanagh, Ph.D.
  - Developed an expression and purification scheme as well as crystallization experiments for the HK17 response regulator.
  - Provided crystallographic assistance with various x-ray structure projects including Sin proteins and VraR.
  - Performed dynamics experiments on 3 DNA-binding transition state regulators and their mutants.
  - Crystallized QseB, a quorum-sensing regulatory protein, as well as its N-terminal construct.
  - Obtained crystals of QseB in the presence of two potential inhibitors.

- Contract Editor *08/2010-present*
  American Journal Experts, Durham, NC.
  - Responsible for editing English grammar and mechanics of papers written by non-native English speakers.
  - Editing responsibilities include checking the writer's consistency, figures and field-specific jargon.
  - Currently edited nearly 300 research papers, grants and thesis chapters.
  - By editing certain papers well, earned access to related fields of expertise; now edit almost all science and medical science disciplines.

- Postdoctoral Research Scientist *07/2011–01/2014*
  Structural Biology, Hauptman-Woodward Medical Research Institute, Mentor: Andrew M. Gulick, Ph.D.
  - Developed an expression and purification scheme for seven proteins involved in an uncharacterized NRPS cluster of *Acinetobacter baumannii.*
  - Solved the crystal structure of a unique self-standing PCP domain.
  - Obtained initial crystals and data on a four-domain, 147 kD NRPS protein.
  - Determined substrate specificity using a radioactive ^{32}PPi assay, assayed activity using a modified spectrophotometric NADH consumption assay and assessed compound binding using thermal shift assays.
  - Collaborated with the Murkin Lab from SUNY Buffalo to elucidate numerous crystal structures of *Mycobacterium tuberculosis* DXR protein and its mutants with various inhibitors.
  - Performed method development for a soft agar-based motility assay for knockout strains.

- Graduate Research Assistant *06/2006–06/2011*
  Chemistry, Duke University, Mentor: Dewey G. McCafferty, Ph.D.
  - Developed the cloning, expression and purification scheme for anhydromuramic acid kinase (AnmK), an enzyme involved in peptidoglycan recycling.

- Gained experience with multiple purification resins (IMAC, GF, hydroxyapatite, ATP-Sepharose, phenyl Sepharose, etc.), Äkta devices and other purification techniques (*e.g.*, ammonium sulfate precipitation).
- Completed the synthesis of the substrate for AnmK as well as a pseudosubstrate.
- Utilized robotic systems to prepare and monitor both initial crystal screening and optimization trays.
- Solved *de novo* structure of AnmK using SAD phasing.
- Subsequently solved multiple other structures including the doubly substrate-bound form of AnmK and a transition state mimic using ADP-vanadate.
- Designed an assay to measure the biological activity of AnmK utilizing TLC and ^{32}P-labeled ATP.
- Developed a methodology to easily detect the phosphosugar reaction products using both NMR spectroscopy and mass spectrometry.

- Undergraduate Research Assistant *07/2005–05/2006*

  Biochemistry, Wake Forest University, Mentor: Bernard A. Brown II, Ph.D.
  - Expressed and purified various mutant proteins to homogeneity for crystallography.
  - Set up both hanging and sitting drop vapor diffusion crystal trays and various optimization trays.
  - Assisted in the molecular replacement structure solution and refinement of four mutant proteins.
  - Completed an Honors thesis titled "Structural and Mutagenic Analyses of the *M. jannaschii* L7Ae Loop 9 RNA-Binding Region."

- Undergraduate Research Assistant *05/2003–12/2004*

  Organic Chemistry, Wake Forest University, Mentor: S. Bruce King, Ph.D.
  - Assisted with a novel method of N-hydroxyurea synthesis for use in making nitric oxide donors and corresponding carbohydrate derivatives to target breast cancer.
  - Designed a synthetic scheme and began the synthesis of a new family of N-hydroxyurea, NO-releasing dendrimers.

PROFESSIONAL ACTIVITIES

- Vice president, Broadening Excellence in Experimental Research *Fall 2012–Spring 2014*

  A club formed at Hauptman-Woodward to help mentor young graduate students, stay current with cutting edge literature, foster communication and discuss difficult experimental techniques.
- Research In Progress (RIP) *Spring 2012–Spring 2014*

  Biweekly meeting of UB postdocs in the biomedical sciences. Meetings consisted of a postdoc's presentation, followed by discussion of both their work and talk. Outside speakers also came to discuss career development.

PROFESSIONAL MEMBERSHIPS

American Crystallographic Association American Chemical Society American Association for the Advancement of Science

AWARDS AND HONORS

- Scholarship for the Becoming A Leader In The Life Sciences course at the NYS Center of Excellence in Bioinformatics and Life Sciences, Fall 2011.
- First Place Poster Award at the NC American Chemical Society Meeting, Graduate Student Division, September 2010.
- Burroughs Wellcome Fellowship, August 2009; A prestigious award offered by the Duke University Department of Chemistry to students that have demonstrated exceptional independent research ability and promising academic and professional development.
- Hobbs Endowment Fellowship, September 2009.
- Pharmacological Science Training Program (PSTP) Fellowship, May 2007; A competitive fellowship awarded through the Duke University Pharmacology and Cancer Biology Department.
- John W. Nowell Undergraduate Award in Chemistry, Wake Forest University, May 2006; Awarded to the best undergraduate student overall in chemistry.
- Blackbyrd Scholarship in Chemistry, Fall 2005– Spring 2006

MENTORING EXPERIENCE

As a Postdoctoral Fellow (NC State)

- Mentored 2 graduate students (Ryan and Logan), 4 undergraduate students and various high school/summer students.

As a Postdoctoral Fellow (Hauptman-Woodward)

- Mentored 3 graduate students (Jesse, Brad, Carter), 3 graduate rotation students (Dorothy, Kirstie, Gregg), 1 undergraduate student (Krista), multiple summer students and 1 research technician (Eric).

As a Graduate Research Assistant

- Supervised 2 biochemistry rotation students, assisted with 2 undergraduates working on a short-term research project and mentored an undergraduate student for his extended independent research project.
- Tutored various undergraduate students in General Chemistry, Biochemistry and Organic Chemistry starting in the 2008/2009 school year through the Spring 2011 semester.
- Acted as PI and mentor on a trip to the Advanced Photon Source at Argonne National Lab with a graduate student from another lab.

TEACHING EXPERIENCE

- CHM 152 Organic Chemistry Lab, Duke 2011
- CHM 31 Gen Chem Recitation, Duke 2010, 2011
- CHM 22 General Chemistry Lab, Duke 2007
- CHM 21 Gen Chem Recitation, Duke 2006
- CHM/BIO 371 Biochemistry 2 Lab, Wake 2006

LEADERSHIP/ADMINISTRATIVE EXPERIENCE

- Organized and raised funding for a National ACS Cellulose & Renewable Materials (CELL) division symposium: "The Structural Biology of Carbohydrate-Active Enzymes." San Diego, CA, March 27, 2012.

PUBLICATIONS

1. Drake, E.J., Miller, B.R., Shi, C., Tarrasch, J.T., Sundlov, J.A., Allen, C.L., Skiniotis, G., Aldrich, C.A. and Gulick, A.M. (2015) Structures of Two Distinct Conformations of holo-Nonribosomal Peptide Synthetases. *Nature*, **529**, 235–238.
2. Kholodar, S.A., Allen, C.L., Gulick, A.M. and Murkin, A.S. (2015) The Role of Phosphate in a Multistep Enzymatic Reaction: Reactions of the Substrate and Intermediate in Pieces. *J Am Chem Soc*, **137** (7), 2748-2756.
3. Allen, C.L., and Gulick, A.M. (2014) Structural and bioinformatic characterization of an *Acinetobacter baumannii* type II carrier protein. *Acta Cryst*, **D70**, 1718-1725.
4. Kholodar, S.A., Tombline, G., Liu, J., Tan, Z., Allen, C.L., Gulick, A.M., and Murkin, A.S. (2014) Alteration of the Flexible Loop in 1-Deoxy-D-xylulose-5-phosphate Reductoisomerase Boosts Enthalpy-Driven Inhibition by Fosmidomycin. *Biochemistry*, **53** (21), 3423-3431.
5. Parish, D.A., Zhou, Z., Allen, C.L., Day, C.S. and King, B.S. (2005) A convenient method for the synthesis of N-hydroxyureas. Tetrahedron Letters, 46, 8841-8843.
6. Allen, C.L., Hover, B.M, and McCafferty, D.G. (2015) The Crystal Structures of Both Unbound and Substrate-Bound Forms of E. coli Anhydromuramic Acid Kinase In Support of A Concerted Mechanism. (in preparation)
7. Allen, C.L., Clancy, K.M. and McCafferty, D.G. (2015) The Transition State Model and Product Complexes of E. coli Anhydromuramic Acid Kinase and the Mechanistic Implications. (in preparation)

POSTER PRESENTATIONS AND ABSTRACTS

1. Armbruster, K.M., Allen, C.L. and Gulick, A.M. "Exploring the role of a non-ribosomal peptide synthetase cluster in *Acinetobacter baumannii* motility." 26th Annual Witebsky Center Conference on Microbial Pathogenesis, April 2014, Buffalo, NY.
2. Allen, C.L. and Gulick, A.M. "Investigation of Non-Ribosomal Peptide Synthesis-Related Genes from An Uncharacterized Operon Implicated in *Acinetobacter baumannii* Motility." (Poster) Presented at the 71st Annual Pittsburgh Diffraction Conference, Sept. 19, 2013, Hauptman-Woodward Institute, Buffalo, NY.
3. Allen, C.L. and Gulick, A.M. "Investigation of Non-Ribosomal Peptide Synthesis-Related Genes from An Uncharacterized Operon Implicated in *Acinetobacter baumannii* Motility." (Poster) Presented at Fifth Annual UB Postdoc Research Symposium, June 13, 2013, University at Buffalo, Buffalo, NY.

4. Tombline, G., Tam, Z., Allen, C.L., Liu, J., Kholodar, S.A., Gulick, A. M. and Murkin, A.S. "Tapping active-site water boosts enthalpy-driven inhibition of DXP reductoisomerase by fosmidomycin." (Poster and Presentation) Presented at the Enzymes, Coenzymes & Metabolic Pathways Gordon Conference, July 14-19, 2013, Waterville Valley Resort, Waterville Valley, NH.
5. S Kholodar, L Allen, AM Gulick, and AS Murkin. "Activation of 1-deoxy-D-xylulose-5-phosphate reductoisomerase." (Poster) Presented at the 23rd Meeting of the Enzyme Mechanisms Conference, January 3 – 4, 2013, The Loews Coronado Bay Resort, Coronado, CA.
6. Allen, C.L. and Gulick, A.M. "Investigation of Non-Ribosomal Peptide Synthesis-Related Genes from An Uncharacterized Operon Implicated in *Acinetobacter baumannii* Motility." (Poster) Presented at the 23rd Enzyme Mechanisms Conference, January 3 – 4, 2013, Loews Coronado Bay Resort, Coronado, CA.
7. S Kholodar, L Allen, AM Gulick, and AS Murkin. "Activation of 1-deoxy-D-xylulose-5-phosphate reductoisomerase by phosphite dianion." (Poster) Presented at the 38th Northeast Regional Meeting of the American Chemical Society, October 1 – 3, 2012, Rochester, NY.
8. Allen, C.L. and Gulick, A.M. "Comprehensive investigation of a novel NRPS cluster from *Acinetobacter baumannii*." (Poster) Presented at 4th Annual UB Postdocs Research Symposium, April 16, 2012, Center For Tomorrow, UB North Campus, Buffalo, NY.
9. Allen, C.L., Hover, B.M., Nicely, N.I. and McCafferty, D.G. "Crystal Structures of Both Unbound and ATP Analog-Bound Forms of E coli Anhydromuramic Acid Kinase (AnmK), An Important Enzyme in Peptidoglycan Recycling." (Poster) Presented at the 22nd Meeting of the Enzyme Mechanisms Conference, January 3 – 4, 2011, The Don CeSar Beach Resort, St. Pete Beach, FL.
10. Allen, C.L., Hover, B.M., Nicely, N.I. and McCafferty, D.G. "Crystal Structures of Both Unbound and ATP Analog-Bound Forms of E coli Anhydromuramic Acid Kinase, An Important Enzyme in Peptidoglycan Recycling." (Poster) Presented at the Fall Meeting of the North Carolina Division of the American Chemical Society, September 28, 2010, The Solution Center, RTP, NC.
11. Allen, C.L. and McCafferty, D.G. "Isolation, Expression and Partial Purification of Anhydromuramic Acid Kinase (AnmK) and Efforts Toward Carbohydrate Substrate Synthesis." (Poster) Presented at the 2008 Annual Retreat of the Department of Pharmacology and Cancer Biology, September 26 – 28, 2008, Holiday Inn SunSpree, Wrightsville Beach, NC.
12. Allen, C.L. and Brown, B.A., II. "Structural and Mutagenic Analysis of the M. jannaschii L7Ae Loop 9 RNA-Binding Region." (Poster) Presented at the 36th Mid-Atlantic Crystallography Meeting, June 1–3, 2006, Wake Forest University, Winston-Salem, NC.
13. Allen, C.L. and King, S.B. "Development of an Improved Method for the Synthesis of Polyhydroxyureas." (Poster) Presented at the 56th Southeast Regional Meeting of the American Chemical Society, November 10–13, 2004, Sheraton Imperial Conference Center, RTP, NC.
14. Allen, C.L. and King, S.B. "Development of an Improved Method for the Synthesis of Polyhydroxyureas." (Poster) Presented at the 55th Southeast Regional Meeting of the American Chemical Society, November 16–19, 2003, Renaissance Atlanta Hotel, Atlanta, GA.

TALKS AND PRESENTATIONS

1. Allen, C.L. "Combating Iraqibacter: Using Structural Biology to Examine NRPS-Derived Bacterial Secondary Metabolites." Biomedical Postdoc *Research In Progress (RIP)* Lunch Series, January 31, 2013.
2. Allen, C.L. and McCafferty, D.G. "Anhydromuramic Acid Kinase (AnmK): Significance, Substrate and Structure." Invited talk given to monthly NSLS users seminar, April 24, 2009.
3. Allen, C.L. "Isolation, Expression and Partial Purification of Anhydromuramic Acid Kinase (AnmK) and Efforts Toward Carbohydrate Substrate Synthesis." Preliminary Exam Presentation. April 10, 2008.
4. Allen, C.L. Suryadi, J. and Brown, II, B.A. "Specificity determinants in the *M. jannaschii* L7Ae K-turn binding protein." Undergraduate honors thesis defense, April 26, 2006.

RESEARCH AND CAREER TRAINING

- "Teaching Training for Academic Careers" offered by the UB Office of Postdoctoral Scholars. January – March 2013.
- "Becoming a Leader in the Life Sciences" program offered by the UB School of Management Center for Entrepreneurial Leadership and the NYS COE in Bioinformatics & Life Sciences. Fall 2011.
- Triangle Area PHENIX Users Workshop. Duke University, April 11, 2010.
- RapiData 2009, Collection and Structure Solving: A Practical Course in Macromolecular X-Ray Diffraction Measurement. National Synchrotron Light Source, April 19 – 24, 2009.
- ACA Summer School in Macromolecular Crystallography. Illinois Institute of Technology, July 2007.

RESEARCH SKILLS

- Basic organic synthesis and product purification, including flash chromatography
- Molecular biology and protein biochemistry skills including protein cloning, mutation, and expression
- Extensive protein and small molecule purification/chromatography by FPLC and HPLC
- Spectrometry (MALDI and LC-MS) proficiency
- Assay development experience, including DSF and spectrophotometric coupled-enzyme assays
- Protein crystallization: sparse matrix screening and grid screening, condition optimization, and micro/streak seeding
- Robotics: Phoenix & Alchemist liquid handlers, Minstrel II
- Cryocrystallography techniques: cryoprotection optimization, crystal handling, mounting and annealing
- Crystallographic data collection and processing with SAD/MAD *de novo* structure solution experience
- Molecular replacement: Phaser, phenix.automr, Molrep, Balbes, EPMR
- Structure refinement: REFMAC5, phenix.refine
- Model building: Coot, phenix.autobuild
- Radiation (^{32}P and ^{3}H) and BSL2 training
- Experience with *A. baumannii* growth and motility assays
- NMR (both 1D small molecule and 2D protein) experience
- Scientific editing proficiency