

Bethany G. Caulkins
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Employment:

Keck Science Dept. of Pitzer, Scripps and Claremont McKenna Colleges Claremont, CA	Assistant Professor of Chemistry	July 2021 – Present
Keck Science Dept. of Pitzer, Scripps and Claremont McKenna Colleges Claremont, CA	Visiting Assistant Professor of Chemistry	August 2018 – June 2021
University of California, Riverside Riverside, CA	Lecturer, Physical Chemistry	June 2019 – July 2019
University of Southern California Los Angeles, CA	Postdoctoral Researcher	August 2017 – July 2018

Education:

University of California, Riverside Riverside, California	Ph.D.	September 2011 – June 2017
California State University, San Bernardino San Bernardino, California	B.S.	September 2009 – June 2011
Antelope Valley College Lancaster, California	A.S. A.A.	January 2006 – May 2009

Major Fields of Study:

Physical Chemistry, Bioanalytical Chemistry, and Biophysical Chemistry

Research Experience:

Keck Science Department – *Claremont, CA* August 2018 – Present
Visiting Assistant Professor of Chemistry

As a visiting faculty member, I have had the pleasure of advising two summer research students, both of whom are Latina, first-generation college students, as well as co-advised two more thesis students. Students focused on learning how to express and purify tryptophan synthase (TS), a pyridoxal-5'-phosphate (PLP)-dependent enzyme, with different isotopic labeling schemes. We were able to remove the natural PLP from the enzyme to exchange back in ^{15}N -PLP for future solid-state rotational echo double resonance (REDOR) experiments to be performed in collaboration with the Mueller Lab at UC Riverside, where I have maintained an active research presence since graduation. This experience is intended to provide a strong foundation with PLP-dependent enzymes as our research expands to another PLP-dependent enzyme, serine racemase (SR). SR has been obtained and initial experiments to determine the crystallization parameters for the enzyme have been undertaken. These experiments will be continued in the Fall semester by a thesis student working with me.

In addition to the TS project undertaken with undergraduate students, I have also started a collaboration with Professor Charles Taylor at Pomona College in Claremont, CA. We have developed solid-state NMR techniques for the analysis of synthesized chitin and chitosan, the main structural feature of arthropod exoskeletons, fungal cell walls, and cephalopod endoskeletons. Generally, chitin is isolated from crab and shrimp cells. These molecules hold high promise as functional biomaterials with a wide range of applications, and a synthetic route to these polysaccharides could prove valuable to many fields. We have been able to establish fingerprints for each molecule and are now expanding into solution-state methods for even faster identification.

University of Southern California – *Los Angeles, CA*
Postdoctoral Researcher

August 2017 – July 2018

PI: Professor Ansgar Siemer

Huntington's Disease (HD) is caused by a mutation in the poly-glutamine region of the exon 1 (Ex1) portion of the Huntingtin protein (Htt). HttEx1 consists of a 17-residue N-terminus followed by a polyglutamine (polyQ) region and a proline-rich domain (PRD) at the C-terminus. People who do not exhibit the disease display a polyQ region of less than 35 glutamine residues, while those who fall victim to HD display polyQ regions of greater than 35 residues, which encourages amyloid fibril formation. Exon 1 is found in the inclusion bodies of postmortem brains of HD patients who have the mutated Htt protein. This research focused on the expression and purification of HttEx1 followed by fibrillization of the protein for study with solid-state NMR. The goals of the project include the structural characterization of HttEx1 monomer, mapping the binding sites of small molecules and antibodies to HttEx1 in both monomer and aggregate form, and determination of the mechanism of aggregation and the structure of fibrils. These goals require use of different solution and solid-state NMR experiments, like insensitive nuclei enhanced by polarization transfer (INEPT), cross polarization (CP), and the myriad of 2-dimensional NMR experiments available for structure determination (*i.e.* NCOCa).

University of California – Riverside, *Riverside, CA*
Graduate Research Assistant

September 2011 – June 2017

PI: Professor Leonard J. Mueller

This research centered on the transformations of amino acids catalyzed by the pyridoxal-5'-phosphate (PLP) cofactor. I have extensive experience in the study of tryptophan synthase (TS) from *S. typhimurium*, which uses PLP to catalyze the synthesis of L-Trp. This work has focused on elucidating the role of acid-base chemistry in the reactions performed by PLP and requires chemical-level details of the active site environment, including the protonation states of key ionizable sites on the cofactor, substrate, and active site residues. I am an expert in the expression and purification of TS, the crystallization of TS, site-specific labeling of key amino acid residues, and solid-state NMR techniques appropriate for an enzyme in this size regime; these include basic cross polarization, double cross-polarization, and rotational echo double resonance (REDOR) experiments. These skills make me both practiced at working with TS and poised to expand these techniques to studies of additional PLP-dependent enzymes.

California State University – San Bernardino, *San Bernardino, CA*
Undergraduate Research Assistant

September 2010 – June 2011

Advisor: Professor David Maynard

- Analytical chemistry of early man artifacts
- Prepared anthropological samples for NMR analysis

California State University – San Bernardino, *San Bernardino, CA*
 Undergraduate Research Assistant
 Advisor: Professor John Tate

September 2010 – June 2011

- Performed and organized literature searches

USDA – ARS US Salinity Lab *Riverside, CA*

July 2010 – September 2010

Student Intern
 Advisor: Dr. Dennis Corwin

- Performed salinity analysis experiments on soil samples from farmland irrigated with recycled water

Teaching Experience:

Advanced Laboratory	Chem 127	Keck
Physical Chemistry – Quantum Chemistry and Spectroscopy	Chem 122	Keck
Survey of Physical Chemistry Lecturer	Chem 109	UCR
Chemistry of Land, Sea, and Air	Chem 70	Keck
General Chemistry Lecture and Lab	Chem 14L	Keck
Introduction to Biological NMR Guest Lecture	April 2018 and 2019	Keck
General Chemistry Lecturer	Chem 001A	UCR
Quantum Chemistry Guest Lecturer	June 2016 and June 2017	UCR
Organic Chemistry Laboratory TA	Chem 112A	UCR
Survey of Physical Chemistry TA	Chem 109	UCR
General Chemistry TA	Chem 001A, 001B, 001C	UCR
Quantum Chemistry TA	Chem 113	UCR

Professional Memberships:

American Chemical Society (ACS)	2011-present
American Association for the Advancement of Science (AAAS)	2014-present
Chemistry Graduate Student Association President, UCR	2016-2017

Awards and Honors:

Keck Science Department Faculty Mini-Grant	2020
Distinguished Teaching Award, UCR	2017
58 th ENC Student Travel Stipend	2017
ACS Division of Biological Chemistry Travel Grant	2017
Poster Award, Rocky Mountain Conference	2016
Graduate Division Dissertation Year Program Fellowship, UCR	2015
AAAS Robert I. Larus Award	2014
1 st Place Award for Oral Presentation in Chemistry and Biochemistry, AAAS Pacific Division	2014
Outstanding Teaching Assistant Award, UCR	2013
Chancellor's Distinguished Fellowship, UCR	2011
B.S. with High Honors, ACS Certified, CSUSB	2011

Publications:

- Sakhrani, V. V.; Hilario, E.; **Caulkins, B.G.**; Hatcher-Skeers, M. E.; Fan, L.; Dunn, M. F.; Mueller, L. J. Backbone Assignments and Conformational Dynamics in the *S. typhimurium* Tryptophan Synthase α -Subunit from Solution-State NMR. *J. Biomol. NMR* **2020**, <https://doi-org.ccl.idm.oclc.org/10.1007/s10858-020-00320-2>.
- Long, J; **Caulkins, B. G.**; Mentink-Vigier, F.; Riviere, G.; Mueller, L. J.; Wang, X. Direct Dynamic Nuclear Polarization of ^{15}N and ^{13}C Spins at 14.1 T Using a Trityl Radical and Magic Angle Spinning. *Solid State Nucl. Mag.* **2019**, *100*, 85-91.
- Caulkins, B. G.**; Cervantes, S. A.; Isas, J. M.; Siemer, A. B. Dynamics of the Proline-Rich C-Terminus of Huntingtin Exon-1 Fibrils. *J. Phys. Chem. B* **2018**, *122*, 9507-9515.
- Perez, L.; **Caulkins, B. G.**; Mettry, M.; Mueller, L. J.; Hooley, R. J. Lipid Bilayer Environments Control Guest Exchange Kinetics of Deep Cavitand Hosts and Enhance Disfavored Guest Conformations. *Chem. Sci.* **2018**, *9*, 1836-1845.
- Perez, L.; Mettry, M.; Hinman, S. S.; Byers, S. R.; McKeating, K. S.; **Caulkins, B. G.**; Cheng, Q.; Hooley, R. J. Selective Protein Recognition in Supported Lipid Bilayer Arrays by Tailored, Dual-Mode Deep Cavitand Hosts. *Soft Matter* **2017**, *13*, 3966-3974.
- Caulkins, B. G.**; Young, R. P.; Kudla, R. A.; Yang, C.; Bittbauer, T. J.; Bastin, B.; Marsella, M. J.; Dunn, M. F.; Mueller, L. J. NMR Crystallography of a Carbanionic Intermediate in Tryptophan Synthase: Chemical Structure, Tautomerization, and Reaction Specificity. *J. Am. Chem. Soc.* **2016**, *138*, 15214-15226
- Hilario, E.; **Caulkins, B. G.**; Huang, Y. M.; You, W.; Chang, C. A.; Mueller, L. J.; Dunn, M. F.; Fan, L. Visualizing the Tunnel in Tryptophan Synthase with Crystallography: Insights into a Selective Filter for Accommodating Indole and Rejecting Water. *BBA - Proteins Proteom.* **2016**, *1864*, 268-279.
- Huang, Y. M.; You, W.; **Caulkins, B. G.**; Dunn, M. F.; Mueller, L. J.; Chang, C. A. Protonation States and Catalysis: Molecular Dynamics Studies of Intermediates in Tryptophan Synthase. *Protein Sci.* **2016**, *25*, 166-183.
- Young, R. P.; **Caulkins, B. G.**; Borchardt D.; Bulloch, D. N.; Larive, C. K.; Dunn, M. F.; Mueller, L. J. Solution-State ^{17}O Quadrupole Central Transition NMR Spectroscopy in the Enzyme Active Site of Tryptophan Synthase. *Angew. Chem., Int. Ed.* **2016**, *55*, 1350-1354.
- Hartman, J. D; Neubauer, T. J.; **Caulkins, B. G.**; Mueller, L. J.; Beran, G. J. O. Converging Nuclear Magnetic Shielding Calculations with Respect to Basis and System Size in Protein Systems. *J. Biol. Mol. NMR* **2015**, *62*, 327-340.
- Caulkins, B. G.**; Yang, C.; Hilario, E.; Fan, L.; Dunn, M. F.; Mueller, L. J. Catalytic Roles of βLys87 in Tryptophan Synthase: ^{15}N Solid State NMR Studies. *BBA - Proteins Proteom.* **2015**, *1854*, 1194-1199.
- Caulkins, B. G.**; Bastin, B.; Yang, C.; Neubauer, T. J.; Young, R. P.; Hilario, E.; Huang, Y. M.; Chang, C. A.; Fan, L.; Dunn, M. F.; Marsella, M. J.; Mueller, L. J. Protonation States of the Tryptophan Synthase Internal Aldimine Active Site from Solid-State NMR Spectroscopy: Direct Observation of the Protonated Schiff Base Linkage to Pyridoxal-5'-Phosphate. *J. Am. Chem. Soc.* **2014**, *136*, 12824-12827.

Presentations:

Caulkins B. G.; Young, R. P.; Liu, V.; Hatcher-Skeers, M.; Dunn, M. F.; Mueller, L. J. NMR Crystallography in Tryptophan Synthase: Proton Positions, Stable Intermediates, and Transition States. Poster Presented at the **28th International Conference on Magnetic Resonance in Biological Systems**, Dublin, Ireland (August 2018).

Caulkins B. G.; Cervantes, S. A.; Bravo, J.; Langen, R.; Siemer, A.B. Solid-state NMR of Huntingtin Fibrils. Poster Presented at the **59th Rocky Mountain Conference on Magnetic Resonance**, Snowbird, UT (July 2018).

Caulkins B. G.; Cervantes, S. A.; Bravo, J.; Langen, R.; Siemer, A.B. Solid-State NMR of Huntingtin Fibrils. Oral Presentation at the **Southern California Users of Magnets Conference**, La Jolla, CA (May 2018).

Caulkins B. G.; Young, R. P.; Dunn, M. F.; Mueller, L. J. NMR Crystallography of a Carbanionic Intermediate in Tryptophan Synthase: Chemical Structure, Tautomerization, and Reaction Specificity. Poster Presented at the **25th Enzyme Mechanisms Conference**, St. Pete Beach, FL (January 2017).

Caulkins B. G.; Young, R. P.; Dunn, M. F.; Mueller, L. J. Direct Interrogation of a Quinonoid Intermediate in Tryptophan Synthase. Poster Presented at the **58th Annual Rocky Mountain Conference on Magnetic Resonance**, Breckenridge, CO (July 2016).

Caulkins, B. G.; Young, R. P.; Dunn, M. F.; Mueller, L. J. SSNMR of Catalytic Intermediates in Tryptophan Synthase: Two Aminoacrylate Species and the Importance of Protonation States in Promoting PLP Catalysis. Poster Presented at the **9th Alpine Conference on Solid State NMR**, Chamonix, France (September 2015).

Caulkins, B. G.; Yang, C.; Dunn, M. F.; Mueller, L. J. Catalytic Roles of β Lys87 in Tryptophan Synthase: ^{15}N Solid State NMR Studies. Oral Presentation at the **56th ENC**, Asilomar, CA (April 2015).

Caulkins, B. G.; Young, R. P.; Yang, C.; Neubauer, T. J.; Dunn, M. F.; Mueller, L. J. NMR Crystallography in the Enzyme Active Site of Tryptophan Synthase. Poster Presented at the **AAAS National Meeting**, San Jose, CA (February 2015).

Caulkins, B. G.; Yang, C.; Neubauer, T. J.; Young, R. P.; Dunn, M. F.; Mueller, L. J. Structural Restraints and Mechanistic Insights from ^{13}C , ^{15}N , and ^{31}P NMR Spectroscopy of the Enzyme Active Site in Tryptophan Synthase. Oral Presentation at the **56th Annual Rocky Mountain Conference on Magnetic Resonance**, Copper Mountain, CO (July 2014).

Caulkins, B. G.; Bastin, B.; Yang, C.; Neubauer, T. J.; Young, R. P.; Hilario, E.; Fan, L.; Dunn, M. F.; Marsella, M. J.; Mueller, L. J. NMR Crystallography in the Enzyme Active Site of Tryptophan Synthase. Oral Presentation at the **AAAS 95th Pacific Division Regional Meeting**, Riverside, CA (June 2014).

Young, R. P.; Neubauer, T. J.; **Caulkins, B. G.;** Yang, C.; Niks, D.; Dunn, M. F.; Mueller, L. J. NMR Crystallography in an Enzyme Active Site: Testing the Acid Form Hypothesis in Tryptophan Synthase. Poster Presented at the **54th ENC**, Asilomar, CA (April 2013).

Caulkins, B G.; Yang, C; Neubauer, T.; Lai, J.; Niks, D.; Dunn, M. F.; Mueller, L. J. NMR Crystallography in the Enzyme Active Site of Tryptophan Synthase: Testing the Acid-Form Hypothesis of the Quinonoid Intermediate. Poster Presented at the **54th Rocky Mountain Conference on Analytical Chemistry**, Copper Mountain, CO (July 2012).

Outreach:

Date	Location	Event
Fall 2019	Keck	STEAM Program for inner-city high school students
2019-02-21	Keck	Demonstration: "Alchemy", Seventh Graders from Pomona Catholic
2016-03-04/05	UCR	Grad Student Recruitment
2016-02-09	UCR	RUSD Science Fair Judge, Elementary School
2015-12-08	Castlevue Elementary	Science Fair Judge
2015-12-02	UCR	Tour of research laboratories to freshmen undergraduate Cal Baptist students
2015-10-22	Taft Elementary	Demonstration: The Scientific Method, Fifth Grade
2015-10-16	UCR	Graduate School Open House
2015-02-10	UCR	RUSD Science Fair Judge, 12th Grade and Elementary School
2014-12-09	Castlevue Elementary	Science Fair Judge
2014-11-07	UCR	Presentation to incoming TAs on teaching philosophy
2014-02-11	UCR	RUSD Science Fair Judge, 4th and 5th Grade
2013-12-12	Castlevue Elementary	Science Fair Judge
2013-11-22	Castlevue Elementary	Demonstration: Solids/Liquids/Gases, Third Grade
2013-11-19	UCR	Dinner with speaker Dr. Joachim Kohn, Director of the New Jersey Center for Biomaterials Board of Governors Professor from Rutgers, State University of New Jersey
2013-11-08	Rancho Verde High School	Presentation to students about college, graduate school, and research
2013-10-23	Taft Elementary	Demonstration: The Scientific Method, Third Grade
2013-10-04	UCR	Presentation to incoming TAs on teaching philosophy
2013-05-30	Castlevue Elementary	Demonstration: Solids/Liquids/Gases, Second Grade
2013-03-16	Antelope Valley College	Science Olympiad Chemistry Test Assistant
2013-03-08	UCR	Grad Student Recruitment
2012-10-24	Taft Elementary	Demonstration: The Scientific Method, Third Grade
2012-03-28	Castlevue Elementary	Science Fair Judge, Fifth Grade
2012-03-16	UCR	Grad Student Recruitment
2012-03-09	UCR	Grad Student Recruitment

References:

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