

CHRISTINA H. MCCULLEY

A computational chemist specializing in biological and organic systems

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SKILLS

Simulation Software – Amber, Yasara, Gaussian/GaussView, Spartan 10, Maestro 12.2

Analysis Software - Chimera, VMD, CYLView, ChemDraw, Blender, PyMol, Microsoft Office, MestReNova, FRED, VIDA,

EDUCATION

Doctor of Philosophy, Organic Chemistry	June 2019
University of California Davis, CA- 'Computational Chemistry and its Utility in Understanding Organic Reaction Mechanisms'	
Bachelor of Science, Chemistry (Honors)	May 2012
California State University, Chico	
Bachelor of Science, Applied Mathematics	May 2012
California State University, Chico	

RESEARCH EXPERIENCE

Postdoctoral Researcher , Department of Chemistry, Wayne State University	January 2022-Present
<ul style="list-style-type: none">• Determined dissociation mechanism of reversibly photodissociable fluorescent protein dimer with classical molecular dynamics (MD). (Paper #1)• Designed a new computational NMR analysis utilizing MD and density functional theory (DFT) to determine epimer conformations of a cyclic peptide.• Provided rational design insights for a set of glycosaminoglycan-based drugs with docking and MD on heparanase protein systems and off-targets.	
Postdoctoral Researcher , Department of Chemistry, Aarhus University, Center for Catalysis	September 2019-2021
<ul style="list-style-type: none">• Led collaborative projects with chemistry graduate students, including a 1,3-Dipolar [6+4] Cycloaddition project. (Paper #3)• Suggested organocatalytic strategies for cycloaddition and stereoselective aldehyde chlorination reactions based on computed energy profiles. (Paper #2)• Gained experience presenting research to a broad and international audience at Aarhus University Jorgensen group research meetings.	
Graduate Student Researcher , Department of Chemistry, UC Davis	January 2015- June 2019
<ul style="list-style-type: none">• Led projects in collaboration with synthesis collaborators, both academic and industry, on work examining the synthesis of tetrasubstituted olefins and establishing the mechanistic pathway of platinum-promoted polyene polycyclizations. (Papers #6 and #7)• Utilized Gaussian 09 and Spartan 10 to computationally gain structural elucidation and mechanistic insight in multiple projects, including predicting terpenoid oxidation states and the mechanistic pathway of pupukeanane sesquiterpenes. (Papers #4 and #5)• Analyzed reaction mechanisms utilizing molecular dynamics (Protdyn) in examining the transition states of platinum-promoted polyene polycyclizations.• Utilized computational methodology to produce theoretical NMR results for experimental comparison when examining 2,3-Sigmatropic Rearrangements.• Mentored in their projects and trained three undergraduate researchers.• Managed, edited, and update the Tantillo group instructional manual 2017- 2020.• Acted as Graduate student representative on the Chemical Biology Program executive committee, 2016-2019.• Developed introductory skills in cellular growth, proliferation, and maintenance while cross-training in a biomedical engineering laboratory at UCD.	
Undergraduate Summer Researcher , Utah State University, Logan	June- August 2011
Synthesized and performed antibacterial study of a sorbistin analog.	
Undergraduate Summer Research Project Fellow , Humboldt State University, California	May- August 2010
Determined effect of substituents computationally on phallotoxins and the organic conductor 7,7,8,8-tetracyanoquinodimethane.	
<ul style="list-style-type: none">• Presented the project at the Humboldt State University Summer Researcher Symposium	
Undergraduate Researcher , California State University, Chico	May 2008 - May 2012
Performed synthesis of gallicynoic acids/computationally determined mechanism of the thermal rearrangements of allylic sulfonates to sulfones.	

PUBLICATIONS AND PRESENTATIONS

Publications

1. **McCulley, C. H.**; Walker, A. R. "Dimer interface destabilization of photodissociative Dronpa driven by asymmetric monomer dynamics", *J. Phys. Chem. B*, **2023, Submitted**, DOI: 10.26434/chemrxiv-2023-435mj
2. Mohr L.; **McCulley, C. H.**; Blom J.; Lamhauge, J. N.; Jorgensen, K. A. "Investigation of the Organocatalytic Chlorination of α -branched Aldehydes." *Chem. Eur. J.* 2021, 27, 17465-17475.
3. McLeod, D.; Cherubini-Celli, A.; Sivasothirajah, N.; **McCulley, C. H.**; Christensen, M. L.; Jorgensen, K. A. "Enantioselective 1,3-Dipolar [6+4] Cycloaddition of Pyrylium Ions and Fulvenes towards Cyclooctanoids." *Chem. Eur. J.* 2020, 26, 11417-11422.
4. **McCulley, C. H.**; T. A.; Tantillo, D. J. "Predicting Rearrangement-Competent Terpenoid Oxidation Levels" *J. Am. Chem. Soc.* 2020, 142, 6060-6065.
5. **McCulley, C. H.**; Tantillo, D. J. "Secondary Carbocations in the Biosynthesis of Pupukeanane Sesquiterpenes." *J. Phys. Chem. A* 2018, 122, 8058-8061.
6. **McCulley, C. H.**; Geier, M. J.; Hudson, B. M.; Gagne, M. R.; Tantillo, D. J. "Biomimetic Platinum-Promoted Polyene Polycyclizations: Influence of Alkene Substitution and Pre-cyclization Conformations." *J. Am. Chem. Soc.* 2017, 139, 11158-11164.
7. Lim, N.-K.; Weiss, P.; Li, B. X.; **McCulley, C. H.**; Hare, S. R.; Bensema, B. L.; Palazzo, T. A.; Tantillo, D. J.; Zhang, H.; Gosselin, F. "Synthesis of Highly Stereodefined Tetrasubstituted Acyclic All-Carbon Olefins via a Syn-Elimination Approach" *Org. Lett.* 2017 19(22) 6212.

Conferences and Symposia

- Presented a poster at ACS National Meeting 2023 San Francisco, CA.
- Invited seminar speaker for the Chemistry and Biochemistry Department at CSU, Chico, 2018.
- Invited oral presentations at UC Davis Chemical Biology Program Retreat, 2017.
- Poster presentations at 24th IUPAC International Conference on Physical Organic Chemistry, Chemical Biology in the Bay Area Day, 2018; the Miller Symposium (UC Davis), 2017 & 2018; UC Davis Chemical Biology Program Retreat, 2015 & 2016; ACS National Meeting 2009 (Salt Lake City, Utah) and 2011 (Anaheim, CA).

LEADERSHIP AND VOLUNTEER ACTIVITIES

- *Student member*, executive committee for the Miller Symposium, UC Davis Department of Chemistry, 2017 - 2019
- *Graduate student representative*, the Chemical Biology Program executive committee, UC Davis, 2016 - 2019
- *Student coordinator*, National Organic Symposium, UC Davis, June 2017
- *Graduate student in charge*, the Tantillo group instructional manual, UC Davis, 2017 - 2020
- *Student mentor*, for undergraduate students performing summer research in the Tantillo laboratory

SELECTED AWARDS AND SCHOLARSHIPS

- 24th IUPAC International Conference on Physical Organic Chemistry (ICPOC) registration grant award, 2018
- UC Davis Miller Symposium Award for Best Poster Presentation, 2018
- UC Davis Department of Chemistry Travel Grant, 2018
- Participated in the Chemical Biology Program at UCD and received a two-year research fellowship, 2015-2017
- Outstanding Graduating Senior in Chemistry, by the Department of Chemistry & Biochemistry at CSU, Chico, 2012
- Floyd L. English Natural Sciences Scholarship recipient, 2008-2011

TEACHING EXPERIENCE

Teaching Assistant, UC Davis

September 2014- June 2019

Organized discussion sections for general and organic chemistry, instructed classes of 30-40 students in computational tools used for theoretical pharmaceutical chemistry, oversaw general, organic, and advanced bio-organic chemistry experiments, hosted office hours and review sections, handled course logistics and provided feedback on original student drug design proposals and presentations. Optimized Held Teaching assistant position for organic, physical organic chemistry, theoretical pharmaceutical chemistry, and advanced bio-organic chemistry laboratory courses at UCD and for theoretical pharmaceutical chemistry (computer-aided drug design) courses at Academia Sinica, Taipei

Courses: Physical Organic Chemistry (graduate level); Pharmaceutical Chemistry 2 (upper division); Advanced Bio-organic Chemistry Laboratory (upper division); Organic Chemistry (upper division) and General Chemistry (freshman level)