Thomas E. Morrell
1200 E. California Blvd., MC 2-32, Pasadena, CA 91125
(626)-395-3827 • tmorrell@caltech.edu
orcid.org/0000-0001-9266-5146

Experience

Research Data Specialist, Caltech Library, Pasadena, CA — Jul. 2016-*present*

- Member of Digital Library Development group
- Launched campus-wide research data repository
- Programs applications to manage library and campus data
- Consults with research groups about their data management challenges
- Develops and runs software, data, and author carpentry programming workshops
- Implemented virtual reality workstation

Graduate Research Assistant, Princeton University, Princeton, NJ — Jul. 2010-Jul. 2016

- Supervisor: Haw Yang
- Initiated first computational work in group for interpreting single molecule fluorescence data
    - Developed Python software to automatically add fluorescence labeling points to proteins
    - Determined regulatory schemes for Protein Tyrosine Phosphatase B in *M. Tuberculosis*
    - Created data analysis methods for extracting motion in Insulin Degrading Enzyme
    - Simulated and discovered new conformations of Gramicidin S synthase A

Graduate Teaching Assistant, Princeton University, Princeton, NJ — Sept. 2010-May 2011

- Taught 3 recitations for general chemistry, mentored students in advanced experiments
- Designed recitation worksheets, held office hours, graded exams
- Ran laboratories for upper-level students, graded reports; designed and led independent projects
- Published independent project with students in the *Journal of Chemical Education*

Education

Master of the Arts, Chemistry — Jan. 2012
Princeton University, Princeton, NJ

- Advisor: Professor Haw Yang

Bachelor of the Arts, Chemistry, *cum laude*, honors in major — Jun. 2010
Hamilton College, Clinton, NY

- Minor: Physics

Publications

7. **Morrell, T. E.**; Rafalska-Metcalf , I. U.; Yang, H.; Chu, J-W. "Compound Molecular Logic in Accessing the Active Site of Mycobacterium tuberculosis Protein Tyrosine Phosphatase B" *J. Am. Chem. Soc.* **2018**, 10.1021/jacs.8b08070
6. Alfermann, J.; Sun, Xun; Mayerthaler, F.; **Morrell, T. E.**; Dehling, E.; Volkmann, G.; Komatsuzaki, T.; Yang, H.; Mootz, H. D. "FRET monitoring of a nonribosomal peptide synthetase" *Nat. Chem. Bio.* **2017**, 10.1038/nchembio.2435
5. Sun, X.; **Morrell, T. E.**; Yang, H. "Extraction of Protein Conformational Modes from Distance Distributions Using Structurally Imputed Bayesian Data Augmentation" *J. Phys. Chem. B* **2016**, *120*, 10469-10482. 10.1021/acs.jpcb.6b07767
4. Landry, M. L.; **Morrell, T. E.**; Karagounis, T. K.; Hsia, C. –H.; Wang, C. –Y. "Simple Synthesis of CdSe Quantum Dots" *J. Chem. Educ.* **2014**, *91*, 274. 10.1021/ed300568e
3. Temelso, B.; **Morrell, T. E.**; Shields, R. M.; Allodi, M. A.; Wood, E. K.; Kirschner, K. N.; Castonguay, T. C.; Archer, K. A.; Shields, G. C. "Quantum Mechanical Study of Sulfuric Acid Hydration: Atmospheric Implications" *J. Phys. Chem. A* **2012**, *116*, 2209. 10.1021/jp2119026
2. Shields, R. M.; Temelso, B.; Archer, K. A.; **Morrell, T. E.**; Shields, G. C. "Accurate Predictions of Water Cluster Formation, $(H_2O)_{n=2-10}$" *J. Phys. Chem. A* **2010**, *114*, 11725. 10.1021/jp104865w

1. **Morrell, T. E.**; Shields, G. C. "Atmospheric Implications for Formation of Clusters of Ammonium and 1-10 Water Molecules" *J. Phys. Chem. A* **2010**, *114*, 4266. 10.1021/jp911493

Presentations

BE/Bi 103, invited guest speaker "Research Data Management: Simple Ways to Make your Research Life Easier" Data Analysis in the Biological Sciences, Caltech, October 10, 2018. Presentation

PEARC, "Library and Research Computing Efforts and Tools to Improve Data Sharing and Archiving" Pittsburgh, Pennsylvania, June 24, 2018. Workshop + Presentation

Open Repositories, "Positioning a repository as campus research infrastructure" Bozeman, Montana, June 5, 2018. Presentation

BE/Bi 103, invited guest speaker "Research Data Management: Simple Ways to Make your Research Life Easier" Data Analysis in the Biological Sciences, Caltech, November 22, 2017. Presentation

Open Repositories, "Launching a Researcher-Focused Data Repository at Caltech using the Invenio 3 platform" Brisbane, Australia, June 25, 2017. Presentation

Open Repositories, "Building an open platform across diverse content and technologies" Brisbane, Australia, June 26, 2017. Presentation

BE/Bi/NB 203, invited guest speaker "Research Data Management: Simple Ways to Make your Research Life Easier" Introduction to Programming for the Biological Sciences Bootcamp, Caltech, June 22, 2017. 10.5281/zenodo.817555

American Chemical Society National Meeting, Invited speaker for the Symposium in Honor of George C. Shields, Denver, CO, Mar. 23, 2015.

American Chemical Society National Meeting, "Allosteric coupling of correlated local unfolding and large-amplitude conformational change in proteins." Indianapolis, IN, Sept. 11, 2013.

Instruction

Software/Data Carpentry Python for postdocs, Caltech, January 22-23; 29-30, 2019.

Software Carpentry Git/Command Line for postdocs, Caltech, November 13-14, 2018.

Author Carpentry, Caltech, October 25-26, 2018.

Software Carpentry, Caltech, August 13-16, 2018.

Author Carpentry, Wrote content and taught reproducible reporting using Rstudio. Force11 Scholarly Communications Institute, University of California, San Diego, July 30- August 3, 2018.

Software/Data Carpentry Python for postdocs, Caltech, May 7-8; 14-15, 2018.

Software Carpentry Git, Caltech, November 16, 2017.

Author Carpentry, Wrote content on sharing data and taught sharing data and publishing web content with GitHub. Force11 Scholarly Communications Institute, University of California, San Diego, August 2-3, 2017.

Data Carpentry/GitHub Desktop, Customized content to use GitHub Desktop and taught version control with git. Caltech, July 20-21, 2017.

Data Carpentry for Humanists, Customized content for audience and taught command line, git, and python sections. Caltech, May 6-7, 2017.

Data Carpentry for Graduate Students, Caltech, April 26-27, 2017.

Honors

- 2nd prize, Research Poster Competition, Princeton University — Oct. 2013
- Pickering Teaching Award, Princeton University — Jun. 2012
- Hugh Scott Taylor Prize, Physical Chemistry, Princeton University — Sept. 2010
- NSF Graduate Research Fellowship — 2010
- Donald J. Denney Prize in Physical Chemistry, Hamilton College — Jun. 2010
- Norton Prize for Chemistry Research, Hamilton College — Jun. 2010
- Elihu Root Fellowship to Pursue Graduate Work, Hamilton College — Jun. 2010
- Sigma Xi Chemistry Honor Society — Jun. 2010
- ACS/IREU Scholar — May 2009