J.L. Thomaston, Ph.D.
jl.thomaston@gmail.com

Education:

Ph. D. University of California, San Francisco (UCSF),
Chemistry and Chemical Biology, Dept. of Pharmaceutical Chemistry
Advisor: William DeGrado
Thesis: X-ray Crystal Structures of the Influenza M2 Proton Channel
B.A Swarthmore College

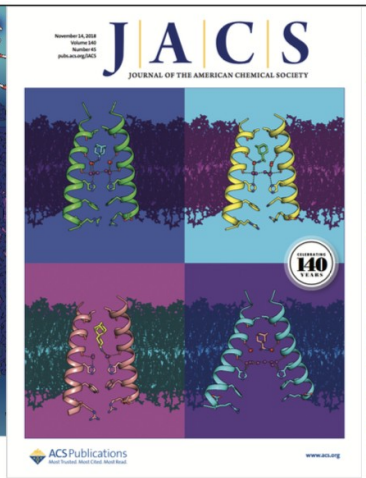
Honors and Awards:

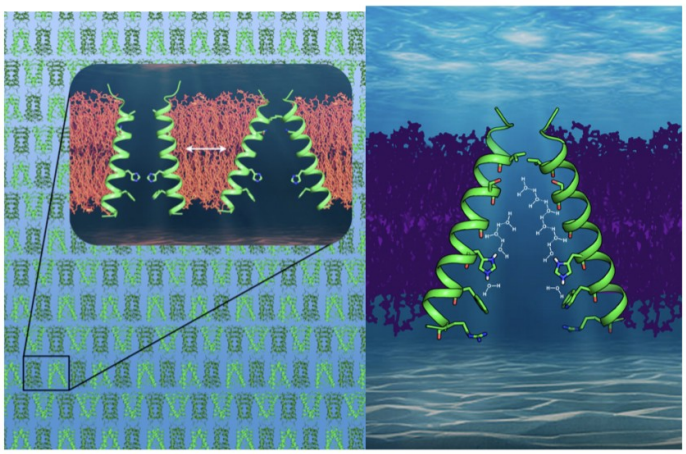
Marie Skłodowska-Curie Individual Fellowship 2019
International Conference on Crystallization of Biological Macromolecules Travel Award 2018
Margaret C. Etter Student Lecture Award, American Crystallographic Association 68th Annual Meeting 2018
Best Young Researchers Forum Award, 9th International Conference on Structural Biology 2017
Neville B. Smith Poster Award, Advanced Light Source User Meeting 2017

Research Experience:

Postdoctoral Fellow, Department of Pharmaceutical Chemistry,
University of California, San Francisco (UCSF)
Postdoctoral Fellow, Department of Biochemistry and Immunology,
Trinity College Dublin
Graduate Student Researcher, Chemistry and Chemical Biology Graduate Program,
Department of Pharmaceutical Chemistry University of California, San Francisco (UCSF)

Cover Art:





Publications:

1. Kratochvil HT, Watkins LC, Mravic M, **Thomaston JL**, Nicoludis JM, Liu L, Voth GA, DeGrado WF. "Transient Water Wires Mediate Selective Proton Conduction in Designed Channel Proteins." **Nature Chemistry** 2023, 15: 1012-1021. **Cited by 7.**

2. **Thomaston JL,** Samways ML, Konstantinidi A, Ma C, Hu Y, Bruce Macdonald HE, Wang J, Essex JW, DeGrado WF, Kolocouris AK. "Rimantadine binds to and inhibits the influenza A M2 proton channel without enantiomeric specificity." **Biochemistry** 2021, 60(32): 2471-2482. **Cited by 14.**

3. **Thomaston JL**, Konstantinidi A, Liu L, Lambrinidis G, Tan J, Caffrey M, Wang J, DeGrado WF, Kolocouris A. "X-ray crystal structures of the influenza M2 proton channel drug-resistant V27A mutant bound to a spiro-adamantyl amine inhibitor reveal the mechanism of adamantane resistance." **Biochemistry**, 2020, 59(4): 627-634. **Cited by 29.** ***Featured on the cover.***

4. **Thomaston JL**, Wu Y, Polizzi NF, Li L, Wang J, DeGrado WF. "X-ray crystal structure of the influenza A M2 proton channel S31N mutant in two conformational states: an open and shut case." **Journal of the American Chemical Society,** 2019, 141(29): 11481-11488. **Cited by 23.**

5. Mravic M, **Thomaston JL**, Tucker M, Solomon PE, Liu L, DeGrado WF. "Packing of apolar side chains enables accurate design of highly stable membrane proteins" **Science**, 2019, 363(6434): 1418-1423. **Cited by 105.**

6. **Thomaston JL**, Polizzi NF, Konstantinidi A, Wang J, Kolocouris A, DeGrado WF. "Inhibitors of the M2 proton channel engage and disrupt transmembrane networks of hydrogen-bonded waters." **Journal of the American Chemical Society**, 2018, 140(45): 15219-26. **Cited by 105.**
Featured on the JACS cover and in ALS Science Briefs December 7, 2018: Toward a Blueprint for Anti-influenza Drugs. https://als.lbl.gov/toward-a-

7. **Thomaston JL**, Woldeyes RA, Nakane T, Yamashita A, Tanaka T, Koiwai K, Brewster AS, Barad BA, Chen Y, Lemmin T, Uervirojnangkoorn M, Arima T, Kobayashi J, Masuda T, Suzuki M, Sugahara M, Sauter NK, Tanaka R, Nureki O, Tono K, Joti Y, Nango E, Iwata S, Yumoto F, Fraser JS, DeGrado WF. "XFEL structures of the M2 proton channel of influenza A reveal pH-dependent water networks under room temperature conditions." **Proceedings of the National Academy of Sciences**, 2017, 114(51): 13357-62. **Cited by 72.**

8. **Thomaston JL**, DeGrado WF. "Crystal structure of the drug-resistant S31N influenza M2 proton channel." **Protein Science**, 2016, 25(8): 1551-4. **Cited by 44.**

9. Baxter EL, Aguila L, Alonso-Mori R, Barnes CO, Bonagura CA, Brehmer W, Brunger A, Calero G, Caradoc-Davies TT, Chatterjee R, DeGrado WF, Fraser JS, Ibrahim M, Kern J, Kobilka BK, Kruse AC, Larsson KM, Lemke HT, Lyubimov AY, Manglik A, McPhillips SE, Norgren E, Pang SS, Soltis SM, Song J, **Thomaston J**, Tsai Y, Weis WI, Woldeyes RA, Yachandra V, Yano J, Zouni A, Cohen AE. "High-density grids for efficient data collection from multiple crystals." **Acta Cryst D Structural Biology,** 2016, 72(1): 2-11. **Cited by 74.**

10. **Thomaston JL**, Alfonso-Prieto M, Woldeyes R, Fraser JS, Klein ML, Fiorin G, DeGrado WF. "High resolution structures of the M2 proton channel from influenza A virus reveal dynamic pathways for proton stabilization and transduction." **Proceedings of the National Academy of Sciences**, 2015, 112(46): 14260-5. **Cited by 102.**
Featured in ALS Science Briefs March 7, 2016: Improving Anti-Influenza Medications.
https://als.lbl.gov/improving-

11. Huang S, Green B, Thompson M, Chen R, **Thomaston J**, DeGrado WF, and Howard KP. "C-terminal juxtamembrane region of full-length M2 protein forms a membrane surface associated amphipathic helix" **Protein Science**, 2015, 24(3): 426–429. **Cited by 21**.

12. **Thomaston JL**, Nguyen P***,*** Brown EC***,*** Upshur MA***,*** Wang J***,*** DeGrado WF, Howard KP. "Detection of drug-induced conformational change of a transmembrane protein in lipid bilayers using site-directed spin labeling." **Protein Science**, 2013, 22(1): 65–73. **Cited by 24.**
Featured Article, Protein Science Volume 22 Issue 1.Invited Talks at International Conferences:

Invited Talks at International Conferences:

1. **32nd European Crystallographic Meeting**. Vienna, Austria. August 2019. Hot Structures session. "Structural basis of adamantane resistance in the influenza A M2 proton channel."
2. **17th International Conference on the Crystallization of Biological Macromolecules.** Shanghai, China. October 2018. "Crystallization of a transmembrane proton channel from the influenza A virus." **ICCBM Travel Award.**
3. **Environmental Molecular Sciences Laboratory (EMSL) Integration Meeting**, Richland, Washington, USA. August 2018. "Solvent dynamics in the influenza M2 proton channel: a song of ice and fire"
4. **American Crystallographic Association 68th Annual Meeting**, Toronto, Canada. July 2018. Structural Biology of Pathogens session. "Structural characterization of adamantane-resistant mutants of the influenza M2 proton channel" **Margaret C. Etter Student Lecture Award.**
5. **Biophysical Society 62nd Annual Meeting**. San Francisco, California, USA. February 2018. Ion Channels, Pharmacology, and Disease platform session. " X-ray crystal structures of the influenza A M2 proton channel bound to amantadine, rimantadine, and inhibitors"
6. **75th Annual Pittsburgh Diffraction Conference**. Pittsburgh, Pennsylvania, USA. October 2017. "XFEL structures of the influenza M2 proton channel at 1.4 Å "
7. **9th International Conference on Structural Biology**. Zürich, Switzerland. September 2017. "XFEL structures of the influenza M2 proton channel at 1.4 Å: room temperature water networks and insights into proton conduction." Best Young Researchers Forum Award.
8. **Protein Society 31st Annual Meeting**, Montreal, Québec, Canada. July 2017. Young Investigator Talk, Structural Insights Into Ion-Transporting Membrane Proteins session. "X-ray crystal structures of the influenza A M2 proton channel bound to amantadine, rimantadine, and inhibitors"
9. **American Crystallographic Association 67th Annual Meeting**, New Orleans, Louisiana, USA. May 2017. XFEL Applications to Biological Systems session. "XFEL structures of the influenza M2 proton channel at 1.4 Å: room temperature water networks and insights into proton conduction"
10. **BioXFEL STC 4th Annual International Conference**, Las Vegas, Nevada, USA. January 2017. Structural Discoveries session. "XFEL structures of the influenza M2 proton channel at 1.4 Å: room temperature water networks and insights into proton conduction"
11. **American Crystallographic Association 65th Annual Meeting**, Philadelphia, Pennsylvania, USA. July 2015. Hot Structures from Membrane Systems session. " High-resolution crystal structures of the influenza A M2 proton channel: insights into water networks"

Informal Invited Talks:

12. Institute of Atomic and Molecular Sciences, Taipei, Taiwan, January 2024.
13. European Molecular Biology Laboratory, Heidelberg, Germany. August 2023.
14. European Molecular Biology Laboratory, Grenoble, France. July 2023.

15. Xi'an Jiaotong Liverpool University (remote presentation). June 2023.
16. Chemical Biology in the Bay Area (CBBA) Day, Berkeley, California, USA. April 2018.
17. Membrane Structural and Functional Biology Group, Department of Biochemistry and Immunology, Trinity College Dublin. Dublin, Ireland. March 2017.
18. Research in Progress Seminar, Cardiovascular Research Institute, University of California, San Francisco. San Francisco, California, USA. October 2016.
19. Horizons in Structural Biology - X-rays, Electrons, and Beyond Structural Biology Workshop. San Francisco, California, USA. June 2016.
20. Mission Bay Research in Progress Seminar, University of California, San Francisco. San Francisco, California, USA. September 2016.
21. Integrative Program in Quantitative Biology (IPQB) Boot Camp, University of California, San Francisco. San Francisco, California, USA. September 2015.
22. Mission Bay Research in Progress Seminar, University of California, San Francisco. San Francisco, California, USA. June 2015.
23. Structural Biology Research Center, High Energy Research Organization (KEK). Tsukuba, Ibaraki, Japan. May 2015.
24. Structural Biology Group, Molecular Biophysics and Integrated Bioimaging Division, Lawrence Berkeley National Laboratory. Berkeley, California, USA. January 2015.
25. Research in Progress Seminar, Cardiovascular Research Institute, University of California, San Francisco. San Francisco, California, USA. August 2014.

Teaching Experience:

Probe Science Night: Trinity College, Dublin. 2019
Taught concepts of structural biology and crystallography in a public outreach demonstration targeted towards children and adults in Dublin, Ireland.

Bay Area Science Festival Discovery Days: San Francisco, California. 2015
Volunteered with the UCSF Women in Science organization to demonstrate biochemistry concepts to a public audience.

Science & Health Education Partnership,
Philip and Sala Burton High School. 2013-2014
Edison Charter Academy: San Francisco, California. 2012-2013
Guest instructor, designed lesson plans and hands-on experiments for 6th and 10th grade students in the San Francisco public school system. Lesson plans featured: crystallization, effects of pH on plant growth, drug-resistant bacteria, DNA extraction.

Pharmaceutical Chemistry Teaching Assistant: UCSF. 2013
Led recitation classes, graded coursework and exams for a 50-person course "Drugs of the Central Nervous System" in the School of Pharmacy. Held weekly office hours and led review classes for exam preparation.

General Chemistry Recitation Teacher: University of Pennsylvania. 2010-2011
Taught four semester-long, 30-person weekly recitation courses for general chemistry. Proctored and graded exams for two 200-person Chemistry 101 courses.

Biochemistry Lab Teaching Assistant: Swarthmore College. 2010
Assisted instruction of 15-person biochemistry wet lab course, taught students practical experimental and data analysis techniques, graded lab reports.

Techniques:

X-ray diffraction: single crystal diffraction at synchrotron sources under cryogenic and room temperature conditions (ALS 8.3.1, APS 24ID-C, APS 24ID-E, APS 24ID-D, DLS I-24, SLS PXI), remote data collection, data collection from pucks, serial crystallography at a synchrotron source (SSRL 12-2), diffraction of crystals under high voltage conditions (SSRL 7-1 and 12-2), serial crystallography at X-ray Free Electron Laser sources (SACLA BL3, LCLS XPP and MFX beamlines).

Software: Phenix, Coot, PyMol, CCP4 suite, Mosflm, XDS, DIALS, HKL3000, Cheetah, CrystFEL, cctbx.xfel, figure making in Adobe Photoshop and Adobe Illustrator, making animated molecular movies using PyMOL and Adobe Photoshop, basic scripting in Python and Unix.

Crystallography: protein crystallography using the lipid cubic phase, sponge phase, detergent micelles, hanging drops, sitting drops, LCP sandwich plates, large-batch microcrystal sample preparation for serial diffraction experiments, harvesting crystals, crystal soaks, crystal seeding, automated sample setup using Mosquito, LCP Mosquito, and Gryphon instruments, optimization of crystallization conditions using expansion and additive screens, automated imaging using Rock Imager.

General: protein expression in bacteria, protein purification using His-columns and FPLC (size exclusion, ion exchange), membrane protein prep, site-directed mutagenesis, cloning, PCR, gel electrophoresis, Western blot, peptide synthesis using high-temperature manual techniques and automated microwave synthesizers, cleavage from resin, HPLC purification (prep, semi-prep and analytical), mass spectrometry (LCMS and MALDI), UV-Vis spectroscopy, CD spectroscopy, EPR spectroscopy, NMR spectroscopy

Referees:

William DeGrado
Professor, University of California, San Francisco
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James Holton
Beamline Scientist, Advanced Light Source, LBNL
JMHolton@lbl.gov

Antonios Kolocouris
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National and Kapodistrian University of Athens
Email: ankol@pharm.uoa.gr