#### Jeremy Hatton Mills

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### Education

**Ph.D.** 2010 Chemistry, The Scripps Research Institute, La Jolla, CA Graduate Advisor: Peter G. Schultz Thesis Title: Protein Engineering with Natural and Unnatural Amino Acids

**B.S.** 2001 Chemistry, Vanderbilt University, Nashville, TN Undergraduate Research Advisor: Ned A. Porter

#### **Academic Appointments**

Arizona State University	
School of Molecular Sciences	
The Biodesign Center for Molecular Design and Biomimetics	
Assistant Professor	2015—Present
University of Washington	
NRSA Postdoctoral Fellow, University of Washington	2010-2015
Postdoctoral Research Advisor: David Baker	2010 2010

#### **Fellowships and Awards**

#### 2011-2013 Ruth L. Kirschstein National Research Service Award F32 Fellowship

#### I. SCHOLARSHIP

#### A. Current Extramural Research Funding

Funding Agency	Total Amount	Funding Period	
NIH	\$1,516,802	2020-2024	
R01 Expanding the Fluorescent Toolkit With non-Canonical Amino Acids			
PI: Jeremy Mills			

NSF \$926,529 2019-2022 ABI Innovation: Development of enhanced computational enzyme design methods using a metaanalysis of enzyme dynamics PI: Jeremy Mills Co-PI: S. Banu Ozkan (ASU, Physics)

# NIH\$250,0002019-2021R21 Genetically Encodable Epitopes to Overcome Size and Resolution Limits in Cryo-EMNullCullCull

PI: Jeremy Mills Co-PI: Brent Nannenga (ASU, SEMTE)

# \$550,000

Collaborative Research: Dissecting photoconversion in fluorescent proteins one frame at a time

2018-2020

PI: Jeremy Mills\*, Former PI: Rebekka Wachter (ASU, emerita)

\*Professor Wachter applied for and received this grant, which was transferred to me upon her retirement.

# Edson Initiative for Dementia Care and Solutions\$112,5002020-2021Structural Characterization of Toxic Amyloidogenic Oligomers by Cryo-EMPI: Jeremy Mills, Brent Nannenga (ASU, SEMTE), Michael Sierks (ASU, SEMTE)\*\*This is seed funding from the Edson Family that is managed and allocated by The BiodesignInstitute at ASU. Each of the PIs listed above contributed to the proposal submission and co-<br/>advise the postdocs working on this project.

#### NIH \$63,755 2019-2023 R01 Renewal: Expanding the bioluminescent toolbox for multi-cellular imaging of tumor heterogeneity

PI: Jennifer Prescher, University of California Irvine, Co-Investigator: **Jeremy Mills**\* \*This grant was awarded to Prof. Prescher and UCI. One month of summer salary was budgeted for Co-I Mills, who serves as a collaborator on efforts related to this project.

# **B.** Publications

**Key:** \*Indicates corresponding author; #Indicates postdoctoral fellow in my laboratory; *Italicized names* are graduate students in other groups; <u>Underlined names</u> are graduate students in my group; ^Indicates undergraduates in my group.

# **Journal Articles**

# Publications as an ASU faculty member

(19) <u>Gleason, P.R.</u>, Nannenga, B.L.\*, **Mills, J.H.**\* "Rapid structural analysis of a synthetic non-canonical amino acid by microelectron diffraction" *Frontiers in Molecular Biosciences*, **2020** *in press* 

(18) Henderson, J.N#., Simmons, C.R., Fahmi, N.E., Jeffs, J.W., Borges, C.R., **Mills, J.H.\*** "Structural Insights into how Protein Environments Tune the Spectroscopic Properties of a Non canonical Amino Acid Fluorophore" *Biochemistry*, **2020**, *59*, 3401.

(17) Yao, Z., Zhang, B.S., Steinhardt, R.C., **Mills, J.H.**, Prescher, J.A. "Multicomponent Bioluminescence Imaging With a  $\pi$ -Extended luciferin" *Journal of the American Chemical Society*, **2020**, *142*, 14080.

(16) <u>Gleason, P.R., Kelly, P.I.</u>, Grisingher, D.W.<sup>^</sup>, **Mills, J.H.**\* "An Intrinsic FRET Sensor of Protein-Ligand Interactions". *Organic & Biomolecular Chemistry* **2020**, *18*, 4079.

NSF

(15) Koh, M., Yao, A., Gleason, P.R., **Mills, J.H.,** Schultz, P.G. "A General Strategy for Engineering Noncanonical Amino Acid Dependent Bacterial Growth" *Journal of the American Chemical Society*, Articles ASAP. Impact Factor 13.85

(14) Almhjell, P.J.<sup>^</sup>, **Mills, J.H.**\* "Metal-chelating non-canonical amino acids in metalloprotein engineering and design" *Current Opinion in Structural Biology*, 2018, (51), 170. Impact Factor 7.18

(13) **Mills, J.H.**<sup>‡</sup>; Sheffler, W.<sup>‡</sup>; Ener, M.E.; Almhjell, P.J.^; Oberdorfer, G.; Pereira, J.H.; Banumathi, S.; Zwart, P.; Baker, D.; "Computational design of a homotrimeric metalloprotein with a trisbipyridyl core" *Proc. Natl. Acad. Sci. USA*, **2016**, 113 (52), 15012. <sup>‡</sup><u>Equal first authorship contribution for J.H.M. and W.S.</u> Impact Factor: 9.43

### **Postdoctoral Publications**

(12) Pearson, A.D.<sup>‡</sup>; **Mills, J.H.**<sup>‡</sup>; Song, Y.; Nasertorabi, F.; Han, G.W.; Baker, D.; Stevens, R.C.; Schultz, P.G. "Crystal Structure of a Kinetically Persistent Transition State in a Computationally Designed Protein Bottle" *Science*, **2015**, 347, 863. <sup>‡</sup><u>Equal first authorship contribution for A.D.P.</u> and J.H.M. Impact Factor: 37.20

(11) **Mills, J.H.**; Khare, S.D.; Bolduc, J.M.; Forouhar, F.; Mulligan, V.K.; Lew, S.; Seetharaman, J.; Tong, L.; Stoddard, B.L.; Baker, D. "Computational Design of Unnatural Amino Acid Dependent Metalloprotein with Atomic Level Accuracy" *Journal of the American Chemical Society* **2013**, *135* (36), 13393. Impact Factor: 13.85

(10) Gordon, S.R.; Stanley, E.J.; Wolf, S.; Toland, A.; Wu, S.J.; Hadidi, D.; **Mills, J.H.**; Baker, D.; Pultz, I.S.; Siegel, J.B.; "Computational Design of an α-Gliadin Peptidase" *Journal of the American Chemical Society* **2012**, *134* (50), 20513. Impact Factor: 13.85

(9) Harger, M.; Zheng, L.; Moon, A.; Ager, C.; An, J.H.; Choe, C.; Lai, Y.; Mo, B.; Zong, D.; Smith, M.D.; Egbert, R.G.; **Mills, J.H.**; Baker, D.; Pultz, I.S.; Siegel, J.B. "Expanding the Product Profile of a Microbial Alkane Biosynthetic Pathway" *ACS Synthetic Biology* **2012**, *2* (1), 59. Impact Factor 5.38

(8) Wu, S.J.; Eiben, C.B.; Carra, J.H.; Huang, I.; Zong, D.; Liu, P.; Wu, C.T.; Nivala, J.; Dunbar, J.; Huber, T.; Senft, J.; Schokman, R.; Smith, M.D.; **Mills, J.H.**; Friedlander, A.M.; Baker, D.; Siegel, J.B.; "Improvement of a Potential Anthrax Therapeutic by Computational Protein Design" *Journal of Biological Chemistry* **2011**, *286* (37), 32586. Impact Factor: 4.57

# **Graduate School and Earlier Publications**

(7) **Mills, J.H.**; Lee, H.S; Liu, C.C.; Wang, J.; Schultz, P.G. "A Genetically Encoded Direct Sensor of Antibody-Antigen Interactions" *ChemBioChem* **2009**, 10 (13), 2162. Impact Factor: 2.84

(6) Liu, C.C.; Mack A.V.; Brustad E.M.; **Mills J.H.**; Groff D.; Smider V.V.; Schultz P.G. "Evolution of Proteins with Genetically Encoded 'Chemical Warheads'" *Journal of the American Chemical Society* **2009**, *131* (28), 9616. Impact Factor: 13.85

(5) Liu, C.C.; Mack A.V.; Tsao M.L.; **Mills, J.H.**; Lee, H.S.; Choe, H.; Farzan, M.; Schultz, P.G.; Smider, V.V. "Protein Evolution with an Expanded Genetic Code" *Proceedings of the National Academy of Sciences U.S.A.* **2008**, *105* (46), 17688. Impact Factor: 9.43

(4) Kavrakova, I.K.; **Mills, J.H.** "Lewis Acid Promoted Kharasch-type Additions of 3bromoacetyl-2-oxazolidinone to Cycloalkenes" *Journal of Chemical Research* **2005**, *2005* (1), 59.

(3) Yin, J.; **Mills, J.H.**; Schultz, P.G. "A Catalysis Based Selection for Peroxidase Antibodies with Increased Activity." *Journal of the American Chemical Society* **2004**, *126* (10), 3006. Impact Factor: 13.85

(2) Pratt, D.A.; **Mills, J.H.**; Porter, N.A. "Theoretical Calculations of Carbon—Oxygen Bond Dissociation Enthalpies of Peroxyl Radicals Formed in the Autoxidation of Lipids." *Journal of the American Chemical Society* **2003**, *125* (19), 5801. Impact Factor: 13.85

(1) Orihuela, C.J.; **Mills, J.H.;** Robb, C.W.; Wilson, C.J.; Watson, D.A.; Niesel, D.W. *"Streptococcus pneumoniae* PstS Production is Phosphate Responsive and Enhanced During Growth in the Murine Peritoneal Cavity." *Infection and Immunology* **2001**, *69* (12), 7565. Impact Factor: 3.73

### **C. Research Presentations**

#### Mills' Presentations at Academic Institutions (since joining ASU)

- 2019 Rational Design of Fluorescent Biosensors Using Non-Canonical Amino Acids Invited Seminar, University of Georgia, Athens, GA
- 2019 Rational Design of Fluorescent Biosensors Using Non-Canonical Amino Acids Invited Seminar, University of Arizona, Tucson, AZ
- 2018 Computational Design of Biosensors Using Fluorescent Non-Canonical Amino Acids Invited Seminar, Pacific Northwest National Laboratory, Richland, WA
- 2018 Computational Design of Proteins Containing Functional Non-Canonical Amino Acids
   Molecular, Cellular and Tissue Bioengineering Symposium, Arizona State University, Tempe, AZ
- 2017 *The Importance of Structural Analysis in Molecular Design* Invited lecture, DESY, Hamburg, Germany
- 2016 Toward on/off Fluorescent Sensors of Protein—Protein Interactions Symposium in honor of Professor Stuart Lindsay, Arizona State University, Tempe, AZ
- 2016 *Toward Computational Design of Protein Catalysts* Biodesign Institute Annual Retreat, Carefree, AZ
- 2016 Computational Design of Proteins Containing Non-canonical Amino Acids with Rosetta
   Center for Biological Physics Weekly Seminar, Arizona State University, Tempe, AZ.
- 2016 Computational Design of a Homotrimeric Metalloprotein with a Trisbipyridyl Core

Advanced Light Source, Berkeley, CA.

- 2015 Computational Design of Functional Proteins Containing Non-canonical Amino Acids University of Science and Technology, Hefei, China.
- 2015 Computational Design of Functional Proteins Containing Non-canonical Amino Acids University of California Davis, Davis, CA
- 2015 Computational Design of Functional Proteins Containing Non-canonical Amino Acids Stanford Research Institute, Menlo Park, CA
- **Group Posters (**work conducted at ASU)
- 2019 A novel approach to integrate protein dynamics into computational enzyme design methods
   <u>Bethany Kolbaba Kartchner</u>, I. John Kazan, S. Banu Ozkan, Jeremy H. Mills Fusion (Biodesign Institute Annual Retreat), Phoenix, AZ 03/2019
- 2017 Design of a two-state fluorescent biosensor using the non-canonical amino acid 7hydroxy-coumarin-yl-ethylglycine Gleason, P.R.; Mills, J.H. RosettaCon, Leavenworth, WA 08/2017
- 2017 Computational design of a metal biosensor with the noncanonical amino acid 8hydroxyquinol-alanine (Updated from 2016 poster) Kelly, P.I.; Mills, J.H. RosettaCon, Leavenworth, WA 08/2017
- 2016 Computational design of an enantioselective, C-C bond forming metalloprotein using the non-canonical amino acid bipyridylalanine <u>Gleason, P.R.; Mills, J.H., RosettaCon</u>, Leavenworth, WA 08/2016
- 2016 Computational design of a metal biosensor with the noncanonical amino acid 8hydroxyquinol-alanine Kelly, P.I.; Mills, J.H. RosettaCon, Leavenworth, WA 08/2016
- **Group Member Oral Presentations** (*work conducted at ASU*) \* designates the student that presented the work
- 2020 Next-generation protein-based fluorescent sensors <u>Patrick R. Gleason</u>\*, <u>Bethany Kolbaba Kartchner</u>, **Jeremy H. Mills**
- 2020 A novel approach to integrate protein dynamics into computational enzyme design methods using the Rosetta software suite <u>Bethany Kolbaba Kartchner</u>\*, I. John Kazan, S. Banu Ozkan, Jeremy H. Mills *Biophysical Society Annual Meeting*, San Diego, CA 02/2020
- 2019 *A novel approach to integrate protein dynamics into computational enzyme design methods*

Bethany Kolbaba Kartchner\*, I. John Kazan, S. Banu Ozkan, Jeremy H. Mills *BioPhest*, Tempe, AZ 03/2019

2019 Computational design of a metal-sensing fluorescent biosensor using the genetically encoded NCAA 7-hydroxycoumarin-4-ethyl-glycine <u>Gleason, P.R.</u>\* *RosettaCon*, Leavenworth, WA 08/2019

## **D.** Awards

#### **Honors Awarded to Mentees**

Patrick Almhjell<sup>^</sup> Dean's Medal, School of Molecular Sciences, 2017

Patrick Kelly Distinguished Teaching Assistant Award, School of Molecular Sciences, 2016

Anthony Meza Distinguished Teaching Assistant Award, School of Molecular Sciences, 2016

# **II. TEACHING EXPERIENCE**

#### A. Courses Taught

I have developed curricula for courses at the graduate and undergraduate levels. Chemical Biology (CHM/BCH 520) is a graduate level, survey of relevant literature and is cross-listed for advanced undergraduate students. I have also taught CHM 234, General Organic Chemistry II. Material for CHM 234 was developed in collaboration with other faculty members in order to ensure consistency between the different sections of the course.

Course	Year(s)	Semester	Credit hours	Enrollment
<sup>a</sup> New courses developed at AS	SU; <sup>b</sup> Cross-listed	l for undergr	aduates; <sup>c</sup> Cro	oss-listed for Graduat
Students				
CHM/BCH 520 <sup><i>a</i>,<i>b</i></sup>	2015	Fall	3	6
CHM/BCH 520 <sup>b</sup>	2016	Fall	3	29
CHM 234 <sup><i>a</i></sup>	2017	Spring	3	145
CHM/BCH 520 <sup>b</sup>	2017	Fall	3	25
CHM 234	2018	Spring	3	232
СНМ 433 <sup>ь</sup> /СНМ 520	2018	Fall	3	98
CHM 234	2019	Spring	3	291
CHM 494/CHM 520	2020	Fall	3	6
CHM 433/CHM 531	2020	Spring	3	51

#### **B.** Graduate Student Mentoring

Current Graduate	Year enrolled/	Research Topics
Students	Program	

Patrick Kelly	2015 / Ph.D.	Computational design of fluorescent sensors of metal ions
Bethany Kartchner	2018 / Ph.D.	Computational design of novel enzymes
Erik Stahl	2020 / Ph.D.	Computational design of fluorescent sensors of protein-ligand interactions

Previous Graduate Students	Year finished / Degree	Thesis Title
Patrick Gleason	2020 / Ph.D.	Protein design and engineering using the fluorescent non-canonical amino acid L-(7- hydroxycoumarin-4-yl)ethyl glycine
Dominic Grisingher	2020 / M.S.	<i>Purification and characterization of TRI_05</i> <i>I13SM6I</i>
Anthony Meza	2018 / M.S.	Characterization of a non-canonical amino acid dependent metalloprotein

#### Member of Student Thesis Committee for the following graduate students (23 total):

Current, Ph.D.: Alex Buchberger (Nicholas Stephanopoulos, advisor) Nicholas Halloran (Giovanna Ghirlanda, advisor) Raghu Pradeep (Hao Yan, Nicholas Stephanopoulos, advisors) Zina Al-Sahouri (Wei Liu, advisor) Abesh Banerjee (Giovanna Ghirlanda, advisor) Mohammad Rahman (Giovanna Ghirlanda, advisor) Justus Nwachukwu (Anne Jones, Advisor) Julio Bernal-Chanchavac (Nicholas Stephanopoulos, advisor) Michelle Costantino (Giovanna Ghirlanda, advisor) Kaitlyn Parrott (Marcia Levitus, advisor)

Previous, Ph.D.: James Geiger (Wei Liu, advisor) Stefan Tekel (Karmella Haynes, advisor) Cassandra Barrett (Karmella Haynes, advisor) Lan Zhu (Wei Liu, advisor) Nicholas Sisco (Wade Van Horn, advisor) Amar Thaker, (Brent Nannenga, advisor)

Previous, M.S.: Isabella Breen (Rebekka Wachter, advisor) Kiko Rex (Xu Wang, advisor) Daniel Vargas (Karmella Haynes, advisor)

Current Barrett Honors Thesis: Jackson Vanlandingham (Yuval Mazor, advisor)

Previous Barrett Honors Thesis: Adam Akkad, (Nick Stephanopoulos, advisor) Alexis Nichols (Wei Liu, advisor) Kiko Rex (Xu Wang, advisor) Grant Severson (Nick Stephanopoulos, advisor)

#### C. Undergraduate Student Mentoring

The following ASU undergraduate students have performed research in our group for a semester or more.

\* indicates underrepresented groups in STEM fields

Current Undergraduate Students Jose Ayala\*

Previous Undergraduate Students **Patrick Almhjell** Barrett Honors College SMS Dean's Medalist Spring 2017 Successfully defended Honors Thesis entitled Computational Design of a Self-Assembling *Metalloprotein* Currently a graduate student in Frances Arnold's Laboratory at Caltech Anthony Meza\* Currently enrolled in the Graduate Program in Chemistry at The University of Wisconsin, Madison **Dominic Grishinger** Barrett Honors College Successfully defended an honors thesis entitled Purification and characterization of TRI 05 *I13SM6I* in Spring 2020 Currently enrolled in the Graduate Program in Biophysics at UCSF **Bethany Kartchner\*** Currently a graduate student in my laboratory Hanna Monroe\* **Stephen Houx** 

**C. Postdoctoral Researchers Mentoring** Nathan Henderson, Assistant Research Scientist 2015-present

# Collaborators:

Prof. Brent Nannenga\*, Department of Chemical Engineering, ASU
Prof. Michael Sierks, Department of Chemical Engineering, ASU
Prof. S. Banu Ozkan, Department of Physics, ASU
Prof. Giovanna Ghirlanda, School of Molecular Sciences, ASU
Prof. Jennifer Prescher\*, Department of Chemistry, University of California Irvine
Prof. Peter G. Schultz\*, Department of Chemistry, The Scripps Research Institute
\*Indicates that publications have resulted from the collaborative efforts.

# **III. SERVICE**

# A. Professional service:

I have served as a peer reviewer for more than 30 manuscripts in the following journals: ACS Applied Materials & Interfaces ACS Catalysis ACS Chemical Biology ACS Omega Biochemistry Bioconjugation Chemistry Bioorganic and Medicinal Chemistry Letters Essays in Biochemistry Journal of Molecular Biology Molecular Biology and Evolution Organic & Biomolecular Chemistry Proceedings of the National Academy of Sciences Protein Science

# I have served as an *ad hoc* reviewer for the following funding agencies:

National Science Foundation Biotechnology and Biological Sciences Research Council (BBSRC, UK)

**I have served as a panel member for the following funding agencies:** *NIH SBIR/STTR BCMB-10, June 2019* 

# Service to the Rosetta Commons:

**Co-organizer RosettaCon 2018** (with Prof. Neil King, University of Washington) This annual conference is attended by more than 250 members of the Rosetta Commons including undergraduate and graduate students, postdoctoral fellows and PIs. Prof. King and I were responsible for organizing the conference. Our duties included developing the conference program (including keynote speaker selection, selection of general conference speakers based on abstracts, activity development and venue booking).

# **B.** Departmental service

#### **School of Molecular Sciences**

Member of Delegation for Graduate Recruiting in China	2015
Faculty Representative, SMS Winter Graduation Ceremonies	2015
Committee on Seminars	2015-2016
Graduate Admissions Committee, Member	2016-2017
Member of Faculty Search Committee	2016-2017
Representative of SMS at freshman orientation	2017
Faculty Advisor, Student Affiliates of the American Chemical Society	2017-present
Graduate Programs Committee, Member	2020-present

### The Biodesign Center for Molecular Design and Biomimetics / The Biodesign Institute

Activity developer, coordinator and presenter, The Night of the Open Door 2016 & 2017 Member of Faculty Search Committee 2016-2017 Member of Biodesign Travel Grant Committee 2018-2019

#### C. University service

User representative / Presenter, Advanced Light Source Yearly Review (Berkeley, CA) 2016 Advisor for the ASU iGEM team 2016-2017 Member of delegation to foster collaboration between ASU and DESY (Hamburg, Germany) 2016

#### D. Outreach activities / Service to the local Community:

Activity developer, coordinator and presenter, The Night of the Open Door, 2016-2019 Category Judge, AzSEF (state science fair of Arizona), 2016-2019 Category Judge, ISEF (International Science and Engineering Fair), 2016, 2019 Mock Judge, pre-ISEF preparation session for Phoenix area students attending ISEF, 2016-2019