



## PUBLICATIONS

### A. Journal Articles

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* Ghirlanda as senior (corresponding) author	underline indicates graduate students in Ghirlanda group	# indicates postdocs in Ghirlanda group	^ indicates undergraduates in Ghirlanda group	Italics indicates students in other groups
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50. Sommer DJ, Alcalá-Torano R, Dizicheh ZB, **Ghirlanda G**. Design of Redox-Active Peptides: Towards Functional Materials. *Adv Exp Med Biol*. 2016;940:215-243.

49. Alcalá-Torano R, Sommer DJ, Bahrami Dizicheh Z, **Ghirlanda G**. “Design Strategies for Redox Active Metalloenzymes: Applications in Hydrogen Production.” *Methods Enzymol*. 2016;580:389-416. doi: 10.1016/bs.mie.2016.06.001. Epub 2016 Jul 1.

48. Woodrum BW., Maxwell J., Babkov A., Hill R.B., O’Keefe B., and Ghirlanda G.\* “A designed dimer of CV-N displays enhanced antiviral activity” *Viruses*. 2016 Jun 6;8(6). pii: E158. doi: 10.3390/v8060158.

47. T. L. Olson, E. Espiritu, S. Edwardraja, C. Simmons, J. C. Williams, G. Ghirlanda, and J. P. Allen (2015) “Design of dinuclear manganese cofactors for bacterial reaction centers” *Biochim. Biophys. Acta*, special issue on “Biodesign for Bioenergetics”, *Biochim Biophys Acta*. 2015 pii: S0005-2728(15)00191-7.

46. *Zhen Li*, Ashini Bolia, Jason D. Maxwell, Andrey A. Bobkov, Giovanna Ghirlanda\*, Banu Ozkan, Claudio J. Margulis “A rigid hinge region is necessary for high affinity binding to cyanovirin and associated constructs” *Biochemistry*. 2015 Nov 24;54(46):6951-60.

45. *Sizemore S.M.*, *Cope S.M.*, Roy A., Ghirlanda G. and Vaiana S.M. “End-to-end distance and internal dynamics of calcitonin gene related peptide: a comparison with amylin” *Biophys J*. 2015 109(5):1038-48

44. Sommer DJ., *Vaughn, M.D.*, Clark B.^, and Ghirlanda G.\*, “Hydrogen Production by Co-Cyt b<sub>562</sub>”, *Biochim Biophys Acta*. 2015 Sep 12. pii: S0005-2728(15)00189-9.

43. Flores M., Olsen T.L., *Wang D.*, Edwardraja S., Shinde SB., Williams J.C., Ghirlanda G., and Allen J.P. “The Copper Environment in Artificial Metalloproteins Probed by EPR Spectroscopy”, *Journal of Physical Chemistry B*, Special Issue (Festschrift) in Honor of Professor Wolfgang Lubitz *J Phys Chem B*. 2015 ;119(43):13825-33

42. Sommer DJ., Roy A., Astashkin A., and Ghirlanda G. \*, “Modulation of Cluster Incorporation Specificity in a De Novo Iron-Sulfur Cluster Binding Peptide” *Biopolymers*. 2015 Mar 23. doi: 10.1002/bip.22635, Special Issue in honor of Bill DeGrado on his 60<sup>th</sup> birthday, in press (Impact Factor: 2.84)

41. *Flory JD*, Johnson T., Simmons C.R., Ghirlanda G., Liu Y., Yan H., and Fromme P. “Purification and Assembly of Cy5 labeled  $\gamma$ -PNAs into a 3D DNA nanocage” *Artif DNA PNA XNA*. 2014 Dec 15;5(3):1-8. doi: 10.4161/1949095X.2014.992181 (Impact Factor= n/a)

40. Sommer D.J., Roy A., Schmidt R., Brown C., Gust D., Astashkine A., and Ghirlanda G.\*, A De Novo Designed 2[4Fe-4S] Ferredoxin Mimic Mediates Electron Transfer (2014) *Journal of the American Chemical Society*, 136, 17343–17349 (*featured as Spotlights*). (Impact Factor= 11.44)
39. Sommer DJ, Vaughn MD, and Ghirlanda G\*. “Protein Secondary-shell Interactions Enhance the Photoinduced Hydrogen Production of Cobalt Protoporphyrin IX” (2014) *Chemical Communications* 50(100):15852-5. doi: 10.1039/c4cc06700b. (*featured on inside cover*) (Impact Factor: 6.89)
38. Shinde S., Binder J., Goyal B<sup>#</sup>, DeMunari S., Woodrum B.W., Levitus M, and Ghirlanda, G.\* “A Designed Buried Salt Bridge in a Heterodimeric Membrane Protein” (2014) *Biopolymers*. 102(6):437-43. doi: 10.1002/bip.22564. (Impact Factor= 2.84)
37. Wang D., Ghirlanda G., Allen JP “Water oxidation by a nickel-glycine catalyst” (2014) *Journal of the American Chemical Society*, 136(29), 10198-201. (Impact Factor= 11.44)
36. Flory J.D., Simmons C., Lin S., Johnson T., Andreoni A., Ghirlanda G., Liu Y., Yan H., and Fromme P. “PNA driven engineering (incorporation, assembly, conjugation) of native proteins into DNA nanocages” (2014) *Journal of the American Chemical Society*, 136 (23), 8283–8295. (Impact Factor= 11.44)
35. Bolia A., Woodrum B., Cereda A.<sup>#</sup>, Wang X., Ozkan S.B., Ghirlanda, G.\* “Computational analysis and experimental validation of the glycan-protein interaction in Cyanovirin”, *Biophysical Journal* (2014) 106, 1142-51 (Impact Factor= 3.832)
34. Faiella M.<sup>#</sup>, Roy A., Sommer D.J., and Ghirlanda G.\*: ”Design of functional proteins: towards artificial hydrogenases” *Biopolymers-J.Pep. Sci.*, (2013) 100, 558-571 (Impact Factor: 2.84)
33. Roy A., Serrau I., Astashkin A., and Ghirlanda, G.\*: “De novo design of an artificial bis-[Fe4S4]-binding protein” (2013) *Biochemistry*, 52, 7586-94 (Impact Factor= 3.194)
32. Cope S., Shinde S., Best R., Ghirlanda G., and Vaiana S. “Cyclic N-terminal fragment of amylin forms non-amyloid fibers” (2013) *Biophysical Journal*, 105(7); 1661-1669 (Impact Factor= 3.832)
31. Ghirlanda G., “A Recipe for Ligand-Binding Proteins”, *News & Views*, (2013) *Nature* 501; 177-178 (Impact Factor= 42.351)
30. Woodrum BW, Maxwell J.D., Bolia A., Ozkan S.B., and Ghirlanda G.\*, "The antiviral lectin cyanovirin-N: probing multivalency and glycan recognition through experimental and computational approaches" (2013) *Biochemical Society Transactions*, 41; 1170-1176. (Impact Factor= 3.238)
29. Flory J.D., Shinde S., Lin S., Liu Y., Yan H., Ghirlanda G., and Fromme P.:” PNA-peptide Assembly in a 3D DNA Nanoscaffold at Room Temperature” (2013) *Journal of the American Chemical Society* 135(18):6985-93 (Impact Factor= 11.44)

28. Roy A., Madden C. and Ghirlanda G\*. "Photo-induced hydrogen production in a helical peptide incorporating a [FeFe] hydrogenase active site mimic. *Chem Commun.* (2012) 48(79):9816-8 (Impact Factor= 6.89) *Featured on inside cover*
27. Shinde S., Cordova J.M., Woodrum B.W., and Ghirlanda G\*. "Modulation of Redox Potential in a Minimalist Heme-Binding Membrane Protein" (2012) *J Biol Inorg Chem.* 17, 557-564 (Impact Factor: 3.184)
26. Guarise C., Shinde S., Kibler K., Ghirlanda G., Prins L.J, and Scrimin P.M. "A multivalent HIV-1 fusion inhibitor based on small helical foldamers" (2012) *Tetrahedron*, 68, 4346-4352. *Chemistry of Foldamers special issue* (Impact Factor: 2.817)
25. Halsey, C. M., Xiong, J., Oshokoya, O. O., Johnson, J. A., Shinde, S., Beatty, J. T., Ghirlanda, G., Jiji R., and Cooley J.W. (2011). "Simultaneous Observation of Peptide Backbone Lipid Solvation and  $\alpha$ -Helical Structure by Deep-UV Resonance Raman Spectroscopy" *ChemBioChem.* 12, 2125-28 (Impact Factor: 3.06)
24. Ghirlanda, G.\* "Design of membrane proteins: towards functional systems", *Current Opinions in Chemical Biology* (2009) 13, 643-47 (Impact Factor: 7.652)
23. Liu, Y.; Carroll, J. R.; Holt, L. A.; McMahon, J.; Giomarelli, B.; Ghirlanda, G.\* (2009) "Multivalent Interactions with gp120 Are Required for the Anti-HIV Activity of Cyanovirin" *Biopolymers* 92(3):194-200 (Impact Factor= 2.84)
22. Ghirlanda, G.\* (2008): "News and Views: Old enzymes, New tricks", *Nature* 453, 164-166 (Impact Factor= 42.351)
21. Bogani F., Spiriti J., van der Vaart A. \*, Ghirlanda G.\* (2008): "O-glycosylation and protein stability: experimental and simulation data" *Biophysical Chemistry*, 154, 157-167 (Impact Factor: 2.319)
20. Fromme, R., Katiliene, Z. #, Fromme, P. and Ghirlanda, G\* (2008): "Conformational gating of dimannose binding to the antiviral protein cyanovirin revealed by the crystal structure at 1.35 Å resolution" *Protein Science*, 17, 939-944 (Impact Factor= 2.861)
19. Fromme, R., Katiliene, Z. #, Giomarelli B., Mori, T., McMahon, J., Fromme, P. and Ghirlanda, G\*. (2007): "A Monovalent Mutant of Cyanovirin-N Provides Insight into the Role of Multiple Interactions with gp120 for Antiviral Activity". *Biochemistry* 46(32):9199-207 (Impact Factor= 3.194)
18. Cordova J.M., Noack P., Hilcove S.A. ^, Lear J.D., and Ghirlanda, G.\* (2007) "Engineering Function in a Membrane Protein: A Heme-Binding Mutant of GpA"; *Journal of the American Chemical Society* 129(3):512-518 (Impact Factor= 11.44)
17. Bogani F., McConnelly E., Joshi L., Chang Y., and Ghirlanda G.\* (2006), "Rational Design of an Immunomodulatory Glycoprotein" *Journal of the American Chemical Society* 128(22):7142-3 (Impact Factor= 11.44)
16. Ghirlanda G. \*, Osyczka, A, Liu, W., Antolovich, M. ,Smith, K. M., Dutton, P. L., Wand, A. J., and DeGrado, W. F. (2004). De Novo Design of a D<sub>2</sub>-Symmetrical Protein that Reproduces the Diheme Four-Helix Bundle in Cytochrome *bc*<sub>1</sub>. *Journal of the American Chemical Society* 126, 8141-8147 (Impact Factor= 11.44)

15. Ghirlanda G., Hilcove S.A., Pidikiti R., Johansson J.S., Lear J.D., DeGrado W.F.<sup>b</sup>, Eckenhoff R.G. (2004) Volatile anesthetic modulation of oligomerization equilibria in a hexameric model peptide. *FEBS Letters* 578(1-2), 140-4.

### **Postdoctoral Publications (University of Pennsylvania)**

14. G. Ghirlanda, J.D. Lear, N.L. Ogihara, D. Eisenberg\*, and W.F. DeGrado\*, "An Hierarchic Approach to the Design of an Hexameric Helical Barrels", *Journal of Molecular Biology*, (2002), 319, 243-253.

13. B. North, C.M. Summa, G. Ghirlanda and W.F. DeGrado\*, "D<sub>n</sub>-Symmetrical Tertiary Templates for the Design of Tubular Proteins", *Journal of Molecular Biology*, (2001), 311, 1081-1090.

12. N.L. Ogihara, G. Ghirlanda, J.W. Bryson, M. Gingery, W.F. DeGrado\*, and D. Eisenberg\*, "Design of three dimensional domain-swapped dimers and fibrous oligomers", *Proceedings of the National Academy of Science*, (2001) 98, 1404-1409

11. Yi Tang, G. Ghirlanda, N. Vahidei, J. Kua, D.T. Mainz, W.A. Goddard III, W.F. DeGrado\*, and D.A. Tirrell\*, "Stabilization of Leucine Zipper Coiled Coils by Introduction of Trifluoroleucine", *Biochemistry*, (2001) 40, 2790-2796.

10. Yi Tang, G. Ghirlanda, W.A. Petka, T. Nakajima, W.F. DeGrado\*, and D.A. Tirrell\*, "Fluorinated Coiled-coils Proteins Prepared in vivo Display Enhanced Thermal and Chemical Stability", *Angewandte der Chemie Int. Ed.*, (2001) 113, 1494-1496

9. G. Ghirlanda, J.D. Lear, A. Lombardi, and W.F. DeGrado\*, "From synthetic coiled coils to functional proteins: automated design of a receptor for the Calmodulin-binding domain of calcineurin", *Journal of Molecular Biology*, (1998), 281, 379-391.

8. A. Lombardi, J.W. Bryson, G. Ghirlanda and W.F. DeGrado\* "Design of a Synthetic Receptor for the Calmodulin-Binding Domain of Calcineurin", *Journal of the American Chemical Society* (1997), 119, 12378-12379.

### **Graduate School Publications (University of Padova, Italy)**

7. G. Ghirlanda, P. Scrimin\*, P. Tecilla, and A. Toffoletti, "Amphiphilic Cu(II) Complexes modeled after the metal-complexation subunit of Bleomycin antibiotics", *Langmuir*, (1998), 14, 1646-1655.

6. Felluga F, Scrimin P\*, Ghirlanda G, Tecilla P., Tonellato U\*. and Veronese A, "Control of permeation of ions across vesicles", *Gazz. Chim. Ital.*, (1997), 127, 551-557.

5. P. Scrimin\*, G. Ghirlanda, P. Tecilla and R.A. Moss\* "Comparative Reactivities of Phosphate Ester Cleavages by Metallomicelles, *Langmuir*, (1996), 12 (26), 6235.

4. G. Ghirlanda, P. Scrimin\*, A. Kaifer, and L.A. Echegoyen\*, "Self-assembled monolayers of Cu(II)-metallo surfactants on GC and HOPG", *Langmuir*, (1996), 12 (15), 3695-3702.

3. G. Ghirlanda, P. Scrimin\*, and L.A. Echegoyen\*, "Influence of Aggregation on Redox Potentials of Amphiphilic Cu(II) Complexes Modeled after Bleomycin Antibiotics", *Langmuir*, (1996), 12, 5188-5196.

2. R. Moss, B.D Park, P. Scrimin\*, and G.Ghirlanda, "Lanthanide Cleavage of Phosphodiester Liposomes", *Journal of the Chemical Society, Chem. Commun* (1995), 1627
1. G. Ghirlanda, P. Scrimin\*, P. Tecilla, and U. Tonellato\*, "Functionalized surfactants for monitoring Cu(II) permeation across the membrane of artificial liposomes", (1993) *Journal of Organic Chemistry*, 58, 302

### Invited book chapters:

1. P. Scrimin, F. Felluga, G. Ghirlanda, P. Tecilla, U. Tonellato, and A. Veronese, "Control of Permeation of Ions Across Vesicles and Chemical Differentiation of their Bilayer Membrane", in *Molecular Recognition and Inclusion*, A.W. Coleman Ed., Kluwer Academic Publishers, The Netherlands, 1998, pp. 159-166.
2. G. Ghirlanda, L.Prins and P. Scrimin, "Catalysis by peptide-based enzyme models", in "Amino Acids, Peptides and Proteins in Organic Chemistry", H.B. Hughes Ed., Wiley VCH, 2012.
3. D.J. Sommer, R. Alcalá-Torano, Z. Barhani Dizicheh, and G.Ghirlanda "Design of electron transfer peptides: Towards Functional Materials" T. Goves and A Cartajena Eds, *Protein-based Engineered Nanostructures*, Springer, in press

### Editor:

**Book co-editor** (with Alessandro Senes, U Wisconsin-Madison), "Design of membrane proteins", in the *Methods in Molecular Biology* series (John and Jan Walker, series editors). Published December 2013

### Press coverage:

- Featured on PepTalk, April 2014 ([http://www.bachem.com/newsletter/Bachem\\_PEPTalk\\_Edition\\_64.html](http://www.bachem.com/newsletter/Bachem_PEPTalk_Edition_64.html))
- Interviewed by Italian LA7 TV as part of Marie Curie Nobel centennial celebrations.

### Patents applications

1. Chang Y., Yan H., and Ghirlanda G.: "Novel DNA-origami Nanovaccines", using DNA-based scaffolds for HIV vaccines, disclosure filed June 2011; patent pending.
2. Joshi, L and Ghirlanda, G. "Rational Design and Engineering of Proteins and Peptides for Immunomodulation", disclosure filed 2007

**PRESENTATIONS****A. Conference Presentations** (*since joining ASU; international conferences in italics*)

22. June 2016 Gordon Conference Metallocofactors, Stonehill College, MA;
21. *December 2015, PacifiChem, workshop on Protein Design, Honolulu, Hawaii, TBA*
20. *October 2015, International Symposium on Clusters and Nanomaterials, Richmond, VA*
19. August 2015, American Chemical Society meeting in Boston, TBA, two talks:  
“Metalloenzyme mechanism workshop” and “Biological Inspiration for Environmental Sustainability: Bioinspired Approaches for Energy Conversion, Storage and Materials workshop”
18. June 2015, Gordon Conference Proteins, Holderness, NH. Short talk: “Protein-Based Hybrid Catalysts for Hydrogen Production”
17. August 2014, Symposium: Frontiers in Biophysics and Chemical Biology, UCSF  
“Directed Evolution of Protein-Based Hybrid Catalysts for Hydrogen Production”
16. August 2014, American Chemical Society meeting in San Francisco, “Protein-based catalysts for hydrogen production”
15. *February 2014, Gordon Conference Peptides*, “Directed Evolution of Protein-Based Hybrid Catalysts for Hydrogen Production”
14. January 2014, Western Photosynthesis Conference, January 2014, Session Chair and invited speaker, “De novo design of artificial hydrogenases”
13. *April 2013, Protein Engineering meeting, Chester, UK*: “Computational analysis and experimental validation of the glycan-protein interaction in Cyanovirin”
12. *October 2012, PEM6, Atlanta, GA*: “Design of functional proteins: towards fuel production“
11. May 2012, “Physics, chemistry, and biology of membrane proteins” workshop, Tempe, AZ: “Design of Tailor-Made Glycan Recognition Protein Modules based on Cyanovirin”
10. *April 2012, Koln, Germany, Haereus Foundation Harvesting Light*: “De novo design of functional protein assemblies: towards hydrogen production”
9. February 2012, Denver, CO, DOE Scientific review
8. September 2011, DOE meeting @HUB Berkeley: “Design of artificial hydrogenases”
7. *September 2011, Marie Curie conference in Padova, Italy*
6. May 2011, DOE EFRC meeting: “Design of artificial hydrogenases”
5. *March 2010, Gordon Conference Peptides*, Short talk
4. November 2009, AIRE workshop, Tempe, AZ “Artificial proteins for bioenergetic processes”
3. September 2008, Lake Tahoe, CA, NSF Workshop on Physical Organic Chemistry
2. June 2008, RMACS Park City, UT “Artificial proteins for bioenergetic processes”
1. October 2006, RMACS, Tucson, AZ: “Sweet Entanglement: role of multivalent binding to oligomannosides in the antiviral activity of cyanovirin”

### **B. Presentations at Academic Institutions** (*since joining ASU*)

25. October 2016, Syracuse University, "Design of artificial hydrogenases"
24. April 2013, Johns Hopkins University, MD: "Design of functional proteins: towards mimics of hydrogenase"
23. March 2013, VirginiaTech, VA: "Design of functional proteins: towards mimics of hydrogenase"
22. February 2013, Rochester University, NY: "Design of functional proteins: towards mimics of hydrogenase"
21. February 2012, Colorado School of MinesGolden, CO: Design of functional proteins
20. September 2011, UCSF Pharmacy "Rational design of antiviral lectins"
19. February 2011, UT Houston Medical Center, "Design of functional proteins"
18. February 2011, Rice University, "Design of functional proteins"
17. February 2011, Miami University, "Design of functional proteins: towards applications in solar to fuel energy conversion.
16. March 2010, University of Wisconsin-Madison,
15. March 2010, Gordon Conference Peptides, Short talk
14. October 2009, University of Missouri-Columbia
13. October 2009, Johns Hopkins University "Multivalency effects in antiviral lectins"
12. April 2009, Wayne State University "Design of functional proteins"
11. April 2009, University of Michigan "Design of functional proteins"
10. April 2009, University of Delaware "Design of functional proteins"
9. September 2008, University of Arizona "Design of functional proteins"
8. February 08, SUNY Buffalo "Design of functional proteins"
7. October 2004: CalState at LA, CA: "Design of functional proteins"
6. April 2004: University of Redlands, CA: "Design of functional proteins"
5. March 2004: New Mexico Tech, NM: "Design of functional proteins"
4. March 2003: University of Trieste, Italy: "Novel heme-binding proteins"
3. March 2003: University of Padova, Italy: "Novel heme-binding proteins"
2. February 2003: Loyola Marimount University: "Novel heme-binding proteins"
1. April 2002: Strasbourg University, France: "Design of  $D_n$  symmetric proteins"

### **C. Group Posters (work conducted at ASU)**

- Gordon Research Seminar Bioinorganic, January 2014 Oral presentation (Dayn Sommer)
- Gordon Conference Solar Fuels, 1 poster
- Photosynthesis society international meeting, August 2013 (3 posters) (Dong Wang, Tien Olson, Justin Flory)
- Protein Society Meeting July 2013 (2 posters) (Brian Woodrum, Ashini Bolia)
- Gordon Conference Proteins June 2013 (1 poster)
- Biophysical society February 2013 (4 posters) (Sara Sizemore, Stephanie Cope, Taisong Zhang, Ashini Bolia)
- Gordon Research Seminar Bioinorganic, January 2013 Oral presentation (Anindya Roy)
- PEM6, October 2012 (3 posters)\* (Anindya Roy, Justin Flory)
- Protein Society meeting, August 2012 (2 posters)\*



- Gordon Conference Photosynthesis, July 2012\*
- St Jude BSDF Symposium, April 2012
- Biophysical Society Meeting, February 2012 (3 posters, one selected for short talk) (Stephanie Cope, Ashini Bolia, Sara Sizemore)
- Gordon conference Metals in Biology, February 2012\*
- Glycobiology Society Meeting, Seattle, November 2011 (3 posters)\* (Melissa Ruben, Sai Kumar)
- Peptide Society Meeting, San Diego, June 2011 (3 posters)\* (Anindya Roy, Sandip Shinde)
- EFRC Meeting, Washington DC, May 2011 (2 posters)
- Protein Society Meeting, San Diego, August 2010
- NIH Annual AIDS meeting, Bethesda, June 2010
- Gordon conference "Peptides", February 2010
- Protein Society Meeting, Boston, August 2009
- Protein Society Meeting, San Diego, August 2008
- Gordon conference "Biopolymers", June 2008
- Gordon conference "Bioorganic Chemistry" June 2007
- Gordon conference "Proteins", June 2007
- Gordon conference "Biopolymers", June 2006
- Protein Society Meeting, San Diego, August 2006 (3 posters)
- Metalloprotein and Protein Design, Chicago, July 2005 (3 posters)
- Gordon conference "Proteins", NH June 2005
- Protein Society meeting, San Diego, August 2004 (2 posters)
- Gordon conference "Bioorganic Chemistry", NH, June 2004
- Protein Society European symposium, Firenze, Italy, April 2003

\*: students sponsored by travel awards

#### **Students and Postdocs Honors (last 3 years)**

- Dayn Sommer, April 2015: Graduate Student Research Enhancement Fellowship, DOE
- Dayn Sommer, April 2015, Leroy Eyring Outstanding Graduate Student award
- Sara Hernandez, April-June 2015 : Spanish Government Graduate Fellowship, University of Madrid (award to visit Ghirlanda Group)
- Arnau Call-Quintana, September-December 2014: Spanish Government Graduate Fellowship, University of Girona (award to visit Ghirlanda Group)
- Dayn Sommer, January 2014: Gordon Research Seminars on Bioinorganic Chemistry, Speaker
- Anindya Roy, January 2013: Gordon Research Seminars on Bioinorganic Chemistry, Speaker
- Dr. Marina Faiella, 2013-2014, L'Oreal Women in Science Fellowship
- Anindya Roy, October 2012 PEMS 6, Best Poster award
- Anindya Roy, April 2012: Leroy Eyring Outstanding Graduate Student award

**FUNDING STATUS**

<i>Funding Agency</i>	<i>Total Amount</i>	<i>Funding Period</i>
<b>Current:</b>		
<b>1. NSF Chemistry</b>	\$ 458,800	7/1/15-6/30/18
“Artificial Hydrogenases by Design: Hybrid Protein-Organometallic Catalysts”		
Supplement for international collaboration	\$ 10,000	
<b>2. NIH R21</b>	\$ 550,000	10/1/16-9/30/18
“New Tools for Glycosciences”		
<b>3. NIH RO1</b>		
PI Sara Vaiana		
“Conformational dynamic, binding and aggregation of IDPs”		
Ghirlanda	\$ 87,906	Approved
<b>4. NSF IGERT (training grant)</b>	\$ 3,498,000	7/1/12-6/30/17
(PI Vermaas, Willem)		
Solar Utilization Network (SUN)		
<b>Pending: See FAR</b>		
<b>Completed (last 5 yrs):</b>		
<b>1. NIH U54</b>		
PI: Petra Fromme	\$ 8,680,000	9/1/10-8/31/15
“Center for Structure Determination of Pathogen Associated Membrane Proteins”		
Institutional recognition to Ghirlanda Lab		10%
<b>2. NSF MCB</b>	\$837,330	8/1/11-7/30/16
PI: Ghirlanda		
Collaborative Research: A General Approach to the Design of Tailor-Made Glycan Recognition Protein Modules		
<b>3. DOE EFR</b>	\$14,754,000	8/1/09 - 4/30/15
PI: Gust (ASU)		
Subtask 3: PI Ghirlanda	25%	
Allocation to Ghirlanda Lab	10%	
EFR Center for Bio-Inspired Solar Fuel Production		
<b>4. CLAS Seed Funds</b>	\$ 50,000	1/1/13-12/31/13
Protein interaction domains (PIDs)		
Co-PI S.B. Ozkan, Physics		

5. NSF-Organic and Macromolecular Chemistry \$455,000 2/1/05 – 1/31/11  
CAREER: Towards the Rational Control of Redox Potential and Catalytic Activity of Designed  
Functional Membrane Proteins  
PI: G.Ghirlanda

## II. TEACHING EXPERIENCE

### A. Courses Taught

My teaching portfolio includes a combination of undergraduate courses, including the two-semester sequence of Organic Chemistry (off-sequence), Medicinal Chemistry, and laboratory courses, and graduate courses in my discipline (Bioorganic Chemistry, Protein Design and Evolution). In addition to the courses listed below, graduate students and undergraduates in my lab were enrolled in Research classes (BCH and CHM 392, 592, 792). Most recently, I have been implementing the online development of CHM 231

Course	Year(s)	Semester	Credit hours	Enrollment
598 Protein Design and Evolution <sup>a</sup>	2008	Fall	3	28
	2005			25
435/535 Medicinal Chemistry <sup>a, b</sup>	2005	Spring	3	25
	2007			38
	2011			65
	2014			105
	2015			72
	2016			85
598 Bioorganic Chemistry <sup>a</sup>	2006	Fall	3	27
336 Organic Chemistry lab II	2006	Spring	1	78
235 Elementary Organic Chem. lab	2007	Fall	1	120
	2005			120
501 Organic Seminar	2006	Spring	1	35
	2004			30
332 Organic Chemistry II	2004	Fall	3	190
	2003			170
	2002			150
331 Organic Chemistry I	2004	Spring	3	150
333 Organic Chemistry for majors I	2009	Fall	3	78
	2010	Fall	3	60
	2012	Fall	3	50
334 Organic Chemistry for majors II	2010	Spring	3	65
233 Organic Chemistry	2012	Fall	3	180
520 Chemical Biology <sup>a</sup>	2013	Fall	3	16
231 Elementary Organic Chemistry	2014	Fall	3	130
	2016	Fall	3	135
BCH598 Biological Design I	2009	Guest	Protein	20
	2010	lectures	design (3	
	2011		lectures)	

<sup>a</sup>New courses developed at ASU; <sup>b</sup> Cross-listed for the Masters in Medicinal Chemistry program.

## B. Graduate Student Mentoring

*Awards:* nominated for ASU FWA Outstanding Faculty Mentor Award 2015

<i>Current</i>	<i>Year enrolled/Program</i>	<i>Research Topics</i>
William Asma	2016, PhD	Design of metalloproteins
Ismail Can Kazan	2015, PhD	Computational analysis of glycan-protein interactions (with Prof. Ozkan, Physics)
Rafael Alcala-Torano*	2012, PhD	Design of metalloproteins
Zahra Barhami-Dizicheh	2013 PhD	Design of metalloproteins
Nicholas Halloran	2014 PhD	Design of metalloprotein
<b><i>PhDs awarded</i></b>	<b><i>Year of graduation</i></b>	<b><i>Thesis</i></b>
Dayn Sommer	April 2016	Design of metalloproteins
Ashini Bolia Coadvised with Prof S.B. Ozkan	August 2015	Computational studies
Anindya Roy Now postdoc with David Baker, U of Washington	April 2014	Engineering oxidoreductases: towards artificial hydrogenases
Brian Woodrum Now instructor at ASU	August 2014	Glycan-Cyanovirin-N Interactions and Designed WW Domains: Combining Experimental and Computational Studies
Melissa Ruben Now teacher at BASIS	May 2013	Directed evolution of CV-N
Sandip Shinde Now Research Scientist at Heliae	August 2010	Design of membrane hemoproteins
Jeanine M. Cordova Now Medical Liaison Director, Boheringer	August 2008	Design, characterization and modulation of a novel membrane hemoprotein
Federica Bogani Now at Intel, Portland, OR	December 2006	Creation of a bioactive glycoprotein mimetic

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<b><i>Masters awarded</i></b>	<b><i>Year of graduation</i></b>	<b><i>Thesis</i></b>
Jay Jursich <i>Now Chemistry instructor, ASU</i>	May 2010	Membrane hemoproteins, CO <sub>2</sub>
Yinan Liu <i>Now Analyst, American Express</i>	August 2008	Dimeric mutants of cyanovirin-N provide insight into the role of multivalent interactions with gp1: for antiviral activity
Jessica Troxel	May 2007	Expression and purification of ME1 using Bcl-XL expression
Pamela Noack <i>Now Arizona DOA</i>	May 2005	Design and synthesis of a novel membrane hemoprotein
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<b><i>Non-thesis MS awarded</i></b>	<b><i>Year of graduation</i></b>	<b><i>Research topic</i></b>
Jason Maxwell <i>Now PhD student, ASU</i>	May 2013	Expression of Cyanovirin mutants
P. Joshua Laughlin <i>Now in Dental School</i>	May 2010	Expression of Cyanovirin mutants
Jacob Carroll <i>Now in Dental School</i>	August 2008	Expression of dimeric cyanovirin-N analogs
Lindsay Holt <i>Now in hospital pharmacy</i>	December 2008	Expression of dimeric cyanovirin-N analogs

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**Member of Student Thesis Committee for the following graduate students (Total: 60):**

Current: Antaeres *Antoniuk-Pablant*, Sara Sizemore (PhD 2015), Chelsea Brown, Antaeres *Antoniuk-Pablant*, Trevor Kelsey (PhD 2015), Andrew Serban, Jacob Hilton, Dhenugen Logeswaran, MinJoo Kim, Liao Yen-Yu, Yinnan Chen, Wei Feng, Lilli Li, Lina Franco, Andrey Kanygin, Ashok Kumar, Hagit Levin, Sandipan Roy, Anshu Sharma, YangYang Tang, Sijie Yang.

**Collaborator/informal coadvisor for the following graduate students**

Michael D. Vaughn (2 papers together, 3 more in preparation); Justin Flory (3 papers); Dong Wang (2 papers); Stephanie Cope (1 paper, 1 in preparation); Sara Sizemore (2 papers in preparation)

**B. Undergraduate Student Mentoring**

The following undergraduate students have performed research in our group as part of their plan of studies (at least 3 credit hours, or 9 lab hours); several are members of underrepresented groups:

Simon Hilcove, Honors Thesis, ASU, defended May 2003, currently at Scripps as a graduate student (2 publications);

Katie Alley, Chemistry, 8/30/03-5/15/04, Dental School;

Linda Ngo, Biochemistry, 8/30/03-12/15/03;  
 Takeyoshi Nishio, Biochemistry, 1/20/04-8/15/04  
 Jeanine Cordova\*, Biochemistry, 1/20/04-5/15/04, graduate student, ASU  
 Christopher See, Biochemistry, 3/1/05-6/1/06;  
 Jenny Terry, MCB, 5/15/05-6/1/06  
 Lisa Albrecht, Biochemistry, 8/22/05-5/30/06  
 Karen Howard, Biochemistry, 1/1/2006-5/30/07, Dental School  
 Yuan He, Biochemistry, 5/15/07-8/15/07  
 Jessica Melbourn, 8/2007-5/2008  
 Andrew Brown, Biochemistry, 2008-09, graduate student, ASU  
 Loreth Vergara\*, Biochemistry, 2008-09  
 Pei Wei, Biochemistry, 2008-09, Columbia School of Public Health  
 Stephanie Jennsen, Spring 2010  
 Brian Etter, Spring 2010  
 Jason Maxwell, Spring 2010, Fall 2010  
 Anthony Woods, Fall 2010  
 Michael Birnbaum, Fall 2010 Graduate School, University of Miami Medical School  
 Shawana Piggee\*, Fall 2011-Spring 2012  
 Chong Long, Fall 2011  
 Chris Orozco\*, Fall 2011-Spring 2012  
 Garrett Coffman, Fall2012-Summer 2013, Graduate school, Indiana University  
 Amanda Romero\*, Fall 2013  
 Mirella Rodriguez\*, Fall 2013  
 Dustin Robinette\*, Fall 2013  
 Jason Allen, Fall 2013-present, *Honors thesis*, CLAS Summer fellowship  
 Brett Clark\*, Spring 2014-Fall 2014 Supported by WAESO fellowship  
 Zina Al-Sahouri Fall 2014-present  
 Denysia Allen\* Fall 2014-2016 Supported by IMSD fellowship, *Honors thesis*  
 DJ Murphy Spring 2015-Fall 2016  
 Lihn Minh Spring 15-Fall 2015  
 Sarah Pfiltzer Fall 2016

\* indicates underrepresented groups

### C. Postdoctoral Researchers Mentoring

- a. Dr. Ira M. Bennett, 7/1/03-12/31/03; Research Assistant Professor at CSPO, ASU
- b. Dr. Zivile Katiliene, 8/16-04- 4/16/06; Manager at U.Colorado-Denver Medical School
- c. Dr. Mathieu Walthers, 9/1/10- 9/1/2012; Scientist, Wolkhardt Pharmaceuticals, Chicago, IL
- d. Dr. Angelo Cereda, 6/1/10- 6/31/2011, postdoc at ASU (Jones group)
- e. Dr. Luca Bau', 1/1/11-May 2012, Postdoc at University of Oxford
- f. Dr. Selvakumar Edwardraja, 10/30/2011- May 2012, now EMBO fellow
- g. Dr Haiyan Sun, 6/15/2012-5/1/2013, Senior Scientist at Biodesign, ASU
- h. Dr. Bhupesh Goyal, 8/12-2/13, Assistant Professor at Sri Guru Granth Sahib World University, Punjab
- i. Dr. Marina Faiella, 1/10/12-7/31/2014, Scientist at Roche, Switzerland

- j. Dr. Sriram Sokalingam, 5/1/2013-5/30/2014, now postdoc at ASU, Chang group  
 k. Dr. Annabelle Gellig, 6/1/2013-7/31/2014

***Collaborators:***

- Dr. Sandra Gendler, Mayo Clinic
- Prof. A.K. Jones, ASU
- Prof. Levitus, ASU
- Prof. Yung Chang, SOLS, ASU
- Prof. B. Jacobs, SOLS, ASU
- Prof. A. van der Vaart, ASU
- Prof. S.B. Ozkan, ASU Physics
- Prof. S. Vaiana, ASU Physics
- Dr. Barry O'Keefe, National Cancer Institute, Frederick, MD
- Prof. Lokesh Joshi, Department of Bioengineering and The Biodesign Institute, ASU
- Dr. Margherita Morpurgo, Department of Pharmacy, University of Padova, Italy
- Prof. Paolo Scrimin, Department of Chemistry, University of Padova, Italy
- Dr. Fabrizio Mancin, Department of Chemistry, University of Padova, Italy
- Prof. Giacinto Scoles, SISSA, Trieste, Italy
- Prof. Claudio Margulis, Department of Chemistry, University of Iowa
- Prof. Julio Flloret, University of Girona, Spain
- Prof. Aitziber Lopez Cortajena, University of Madrid, Spain
- Prof. Jose Caaveiro, Tokyo University, Japan

### III. SERVICE

***A. Professional service:***

- Organizer, workshop on Metalloproteins, ACS meeting Boston 2015
- American Peptide Society award committee, member (2015-)
- American Chemical Society award committee, member (2014-2017)
- Protein Society Mentoring Committee, member since 2002
- Session Chair, Western Photosynthesis Conference, Asilomar 2014
- Organizer, Workshop on Biological Physics of Membrane Protein, Tempe, May 2012
- NSF Molecular and Cell Biology, Organic and Macromolecular Chemistry, and Bioengineering, *ad hoc* reviewer; panel member (13 panels since 2007)
- American Chemical Society Type G grants reviewer (1 in 2005)
- CNRS (French NSF), 2 grants
- MUIR (Italy), 2 grants
- Volkswagen Foundation, 2 grants
- Mentoring committee member, The Protein Society, 2006 - present
- Panelist on Funding workshop, Protein Society meeting, 2008, 2010, 2012
- Judge for students poster award, Protein Society meeting, 2006, 2008, 2010
- Young Scientists Symposium on career choices, European Symposium of the Protein Society, Firenze, Italy, April 2003: co-organizer and speaker.



- Gordon conference, Bioorganic Chemistry, June 2004: Discussion Leader, Protein Design
- Reviewer for peer-reviewed journals (Nature, Proceedings of the National Academy of Sciences, Proteins, Biochemistry, Macromolecules, Inorganic Chemistry, Journal of the American Chemical Society, Bioorganic and Medicinal Chemistry Letters, Biophysical Chemistry, Journal of Computational Chemistry)

### ***B. Departmental service***

- Undergraduate curriculum committee, 2002-2007, 2009-2010; established a new concentration in Medicinal Chemistry for our BS in Biochemistry (now the program with the largest enrollment in the Department).
- Course director for BS/Ms in Medicinal Chemistry; the program can be taken in accelerated form in conjunction with a BS in Biochemistry. A crucial aspect of these programs, in particular of the Masters program, is that they involve directly other entities in the Phoenix area, such as the new Medical School in the Downtown area, the Mayo clinic, the Burrows Institute, and the TGen Institute.
- Personnel and budget committee, Elected member since 2012, Chair since 2016-17
- Chemical Biology Faculty search committee, Chair, 2012-13 (one hire)
- Biomimicry Faculty search committee, member, 2013-2014, 2014-2015, 2016-17 (three hires)
- Safety committee, 2008
- Graduate students-faculty liaison, Masters program, 2008-present
- Departmental recruitment committees, member in 2003/04 (three tenure-track positions), 2004/05 (one tenure-track position), 2007/08 (one tenure-track position, three service professional positions), 2009/10 (one tenure-track position),
- Recruitment trips (University of Redlands, CA; New Mexico Tech, NM; Loyola Marymount University, CA; Cal State LA, CA; University of Padova, Italy; University of Trieste, Italy)

### ***C. Outreach activities:***

- Expanded “Science is Fun”, an outreach program established by Michael McKelvy, to include biochemistry experiments (2005-2009), as part of CAREER proposal
- CRESMET Fellows training program for high school teachers, participant, 2008-present (hosts two high school teachers from underperforming schools during summer, and continues contact during the school year; organized a graduate students visit to Casa Grande High School, and one of high school students from Casa Grande to ASU)
- Mentors high school students for summer internships or senior projects (Ali Khan and Maxime Godart, BASIS Scottsdale; Skye Russell, Basis Phoenix )
- AZ Science Outreach Foundation; designed activities, performed demonstrations with three graduate students from lab