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EDUCATION

- 1997 Ph.D., Yale University, New Haven, Connecticut Physical Chemistry
Dissertation: *Methodological Development and Bioorganic Applications of Computational Simulations*
- 1992 M.S., Yale University, New Haven, Connecticut Physical Chemistry
- 1991 B.S., *Magna Cum Laude*, North Central College, Naperville, Illinois Mathematics, Chemistry, and Physics
Thesis: *Relative Effectiveness of Certain Instrumental Methods for Detecting Cocaine and Heroin*

PROFESSIONAL EXPERIENCE

FACULTY

- 2011-present Professor of Medicinal Chemistry, College of Pharmacy, University of Michigan, Ann Arbor
Professor of Chemistry, College of LSA, University of Michigan, Ann Arbor
- 2002-present Associated Faculty of the Bioinformatics Graduate Program, University of Michigan, Ann Arbor
- 2001-present Associated Faculty of the Biophysics Research Division, University of Michigan, Ann Arbor
- 2016-present Member, Executive Board, College of Pharmacy, University of Michigan, Ann Arbor
- 2016-present Member, Executive Board, Rackham Graduate School, University of Michigan, Ann Arbor
- 2010-2013 Member, Executive Board, College of Pharmacy, University of Michigan, Ann Arbor
- 2006-2011 Associate Professor of Medicinal Chemistry, College of Pharmacy, University of Michigan, Ann Arbor
- 2006-2011 Associate Professor of Chemistry, College of LSA, University of Michigan, Ann Arbor
- 2001-2006 Assistant Professor of Chemistry, College of LSA, University of Michigan, Ann Arbor
- 2000-2006 John Gideon Searle Assistant Professor of Medicinal Chemistry, College of Pharmacy, University of Michigan, Ann Arbor
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- 2017 Organizer, DREAM Challenge for Multi-Targeting Drugs
- 2008-2015 Director, Community Structure-Activity Resource (CSAR)
- 2013 Consultant to Sterne, Kessler, Goldstein, and Fox PLLC, Washington, D.C.
- 2012-present Editorial Advisory Board, *Journal of Chemical Information and Modeling*
- 2006-present Editorial Advisory Board, *Chemical Biology & Drug Design*
- 2014-2017 Editorial Advisory Board, *Journal of Medicinal Chemistry*
- 2008-2014 Editorial Board, *Proteins: Structure, Function, and Bioinformatics*
- 2006-2008 Associate Editor, *Proteins: Structure, Function, and Bioinformatics*
- 2003-2007 Associate Editor, *Annual Reports in Computational Chemistry* (COMP division of ACS)

POSTDOCTORATE, GRADUATE, AND UNDERGRADUATE

- 1997-2000 Postdoctoral Fellow with Prof. J. Andrew McCammon, University of California, San Diego
- 1992-1996 Graduate Research Assistant with Prof. William L. Jorgensen, Yale University

- 1990 Summer Research Fellow with Prof. Henry F. Schaefer III, Center for Computational Quantum Chemistry, University of Georgia, Athens
- 1989-1990 Technician, Amoco Research and Development, Naperville, IL
- 1988-1989 Research Assistant with Dr. Solomon Zaromb, Argonne National Laboratory

HONORS

FACULTY

- 2011 Fellow of AAAS, Chemistry Division
- 2009-2010 Novartis Chemistry Lectureship, Novartis Pharma AG
- 2008 Corwin Hansch Award, The Cheminformatics and QSAR Society
- 2007 Teaching Excellence Award, College of Pharmacy, University of Michigan, Ann Arbor
- 2006 NSF CAREER Award
- 2006 Wiley International Journal of Quantum Chemistry Young Investigator Award
- 2005 Student Appreciation Award for Excellence in Teaching, College of Pharmacy, University of Michigan, Ann Arbor
- 2002 Beckman Young Investigator Award, Arnold and Mabel Beckman Foundation

POSTDOCTORATE, GRADUATE, AND UNDERGRADUATE

- 1997-2000 Postdoctoral Fellowship, American Cancer Society
- 1997-2000 Postdoctoral Fellowship, LJIS Training Program (Burroughs Wellcome Fund)
- 1991-1992 Predoctoral Biophysical Training Grant (NIH), Yale University
- 1991 Honorable Mention, National Science Foundation Predoctoral Fellowship
- 1991 Outstanding Senior Chemistry Major, North Central College
- 1990 National Recipient of Gladys Anderson Emerson Chemistry Award, Iota Sigma Pi
- 1990 Seybold Undergraduate Math Award, North Central College
- 1987-1991 Presidential Full Scholarship, North Central College

OTHER SPECIAL RECOGNITION

- 2018 My PharmD student Noah Leja received the outstanding P4 research award for his work on our MixMD method (College-Wide Competition).
- 2016 Paper highlighted by Faculty of 1000 (F1000): Ghanakota and Carlson. *J. Med. Chem.* **2016**, 59, 10383-10339.
- 2016 Paper highlighted on the journal's cover: Graham, Tweedy, and Carlson. *Prot. Sci.* **2016**, 25, 1021-1029
- 2014 My graduate student Sarah Graham was accepted to the program for a Translational Research Education Certificate (TREC) and awarded \$5000 toward her stipend (University-Wide Competition)
- 2014 My graduate student Sarah Graham received a Rackham Graduate Student Research Grant of \$3000 toward equipment for her thesis project (University-Wide Competition)
- 2014 My postdoc Aqeel Ahmed was awarded a \$100k fellowship from the Postdoctoral Translational Scholars Program of MICHR, the Michigan Institute for Clinical and Health Research (UL1 TR000433)
- 2014 My REU student Sara Tweedy (Harvey Mudd) won the award for best undergraduate poster in the COMP division at the ACS National Meeting in Dallas (National Competition)
- 2014 My graduate student Phani Ghanakota was a finalist for the NVIDA Award in the COMP division at the ACS National Meeting in Dallas (National Competition)

- 2014 Paper highlighted by Faculty of 1000 (F1000): Ung et al. *J. Med. Chem.* **2014**, *57*, 6468-6478.
- 2014 Paper highlighted as 2013's 15th most-read paper in *JCIM*: Damm-Ganamet et al. *J. Chem. Info. Model.* **2013**, *53*: 1853-1870 (web release: April 2nd 2013)
- 2013 Paper highlighted by Faculty of 1000 (F1000): Damm-Ganamet et al. *J. Chem. Info. Model.* **2013**, *53*: 1853-1870.
- 2013 Paper highlighted as 2012's 10th most-read paper in *JCIM*: Smith et al. *J. Chem. Info. Model.* **2012**, *52*: 2098-2106 (web release: June 19th 2012)
- 2012 Paper highlighted on the journal's cover: Khazanov et al. *Prot. Struct. Func. Bioinf.* **2012**, *80*, 2523-2535
- 2011 My student Peter M.-U. Ung received the departmental award for outstanding research
- 2011 Paper highlighted on the journal's back cover: Spronk and Carlson. *Prot. Struct. Func. Bioinf.* **2011**, *79*, 2247-2259
- 2010 My graduate student Katrina Lexa was chosen for a Chemical Computing Group Excellence Award for the 239th ACS National Meeting in San Francisco (National Competition)
- 2010 My student Katrina Lexa received the departmental award for outstanding research
- 2009 Enzyme vs non-enzyme analysis (Carlson et al. *J. Med. Chem.* **2008**, *51*, 6432-6441) highlighted in *Current Opinion in Drug Discovery and Development* ("Paper Alert" **2009** *12*, 1-15)
- 2008 News highlights of our U01 award for CSAR (Community Structure-Activity Resource) at NIGMS and other news outlets like *C&E News* ("Computer-Aided Drug Design Gets Boost" **2008**, *86* (42), 39)
- 2008 News highlights of "eye" inhibitors (Damm et al. *Biopolymers* **2008**, *89*, 643-652) in Biomedical Beat – A Monthly Digest of Research News from NIGMS (6/18/2008), The Washington Post (5/28/2008), ScienceDaily, and several other medical and biotech news webservices
- 2008 Paper highlighted on the journal's cover: Damm et al. *Biopolymers* **2008**, *89*, 643-652
- 2008 HDM2 research (Bowman et al. *J. Am. Chem. Soc.* **2007**, *129*, 12809-12814) highlighted in *SciBX: Science-Business eXchange* ("Expanding protein-protein chemical space" January **2008**, 7-8)
- 2007 Graduate student Katrina Lexa chosen for an AFPE Predoctoral Fellowship (National Competition)
- 2007 Graduate student Kelly Damm chosen for a Rackham Predoctoral Fellowship (U Michigan Competition)
- 2007 Comparison of NMR vs crystal structures for structure-based drug design (Damm and Carlson. *J. Am. Chem. Soc.* **2007**, *129*, 8225-8235) highlighted on Nature's blog "The Skeptical Chymist" [http://blogs.nature.com/theskepticalchymist/2007/07/i_cant_live_without_my_radiofr.html]
- 2005 Database research highlighted in *C&E News* article "Spellbinding Data" [**2005**, *83*, 33-34]
- 2005 Interviewed for comments about ZINC, quoted in "Open Source For Virtual Screening" *C&E News* **2005**, *83*, 8
- 2004 Graduate student Kelly Damm chosen for an AFPE Predoctoral Fellowship (National Competition)
- 2004 Drug discovery research highlighted in "Dealing with Flexible Receptors" *C&E News* **2004**, *82*, 46-47
- 2004 Graduate student Kristin Meagher chosen for an ACS Medicinal Chemistry Predoctoral Fellowship Award (National Competition)
- 2004 Paper highlighted in *Nature Reviews Drug Discovery* [**2004**, *3*, 910]: Meagher and Carlson. *J. Am. Chem. Soc.* **2004**, *126*, 13276-13281
- 2004 Paper highlighted on the journal's cover: Zampella et al. *Inorg. Chem.* **2004**, *43*, 4127-4136
- 2001 Graduate student Kristin Meagher chosen for an AFPE Predoctoral Fellowship (National Competition)
- 2000 Paper highlighted in *Modern Drug Discovery* [**2000**, *3*, 15]: Carlson et al. *J. Med. Chem.* **2000**, *43*, 2100-2114

RESEARCH SUPPORT

R01 GM124283 (PI: Carlson) **CURRENT** **9/1/2017-8/31/2021**
 NIH/NIGMS Annual direct costs: \$230,000

Binding MOAD: A Database of Protein-Ligand Information

The main objectives of this proposal are to (1) grow the MOAD database and maintain pace with the PDB, (2) expand the website with new tools for cross-linking similar ligands and binding sites, and (3) harden the BindingMOAD.org website.

R01 GM125881 (PI: Soellner) **CURRENT** **12/1/2017-11/30/2021**
 NIH/NIGMS Annual direct costs to HAC: \$37,000

Conformational Control of Kinases

Despite the emerging role of noncatalytic kinase signaling, efforts to understand the importance of kinase conformation on signaling pathways have been hampered by a lack of tools to assess and modulate the global conformation of PKs. As a result, we recently developed a 'selective proteolysis' technique to rapidly determine global kinase conformation that is adaptable to many PKs (including c-Src). Additionally, we recently reported that an emerging class of kinase inhibitors, termed 'conformation-selective' kinase inhibitors, can modulate the noncatalytic functions of protein kinases via stabilization of specific kinase conformations. Here, we propose to use our selective-proteolysis technique to develop genetic and chemical tools to study the relationship of kinase conformation on noncatalytic kinase signaling. These experiments will be supported by molecular dynamics simulations

Role: Collaborator, design and oversee execution of computational studies

R01 GM065372 yrs 11-14 (PI: Carlson) **CURRENT** **2/1/2018-1/30/2022**
 NIH/National Institute of General Medical Sciences (NIGMS) Annual direct costs: \$207,000

Mapping Protein Surfaces in Computational Drug Design

This proposal outlines two areas for developing MixMD, our method for mixed-solvent molecular dynamics simulations. Specific Aim 1 develops methods for calculating the free energies, entropies, and enthalpies of the hotspot probes. Specific Aim 2 will address a series of key challenges in structure-based drug discovery. First, MixMD will be used to identify bridging water molecules in binding sites. Second, the accessibility of difficult, cryptic sites will be examined. Lastly, MixMD data will be used to predict druggabilities of binding sites.

MCubed (PI: Carlson) **PREVIOUS** **10/1/2015-4/29/2017**
 University of Michigan, Ann Arbor Total direct costs: \$60,000

Identifying druggable hotspots for proteins involved in cell-cycle control

Innovative computer-modeling methods will be used to pursue new anti-cancer therapies. Carlson has created MixMD, a molecular dynamics method for mapping druggable sites on protein surfaces. The method is particularly promising for identifying new allosteric sites. Grant's enhanced sampling methods are needed to make MixMD faster and more efficient, especially when many allosteric mechanisms cause conformational changes in the protein target. Experimental follow through will be guided by Young. He studies the regulation of proteins that function as molecular switches within cell-signaling networks: kinases, nuclear hormone receptors, and de-ubiquitinases. These kinds of regulatory proteins are particularly susceptible to allosteric control, and several anti-cancer drugs used clinically are allosteric regulators. Identifying new regulatory sites should lead to new drugs for resistant forms of cancer.

R01 GM65372 yrs 06-10 (PI: Carlson) **PREVIOUS** **4/1/2010-3/31/2015**
 NIH/NIGMS Annual direct costs: \$190,000

Multiple Protein Structures in Computational Drug Design

Multiple Protein Structures in Computational Drug Design

The major goal of this project is to provide a solid technique – based on multiple protein structures (MPS) – for incorporating protein flexibility into structure-based drug discovery. The specific aims are to (1) optimize the protocol for using MPS from computer simulations and experimental sources, (2) extrapolate the use of MPS to exploit a subfamily of homologous proteins in the development of broad-spectrum therapeutics, and (3) apply the method to systems of biomedical importance. Collaborations with enzymologists are proposed to aid the development of novel inhibitors in the later stages of the project.

Young Investigator Award (PI: Carlson)

Arnold and Mabel Beckman Foundation

PREVIOUS

9/01/2002 – 8/31/2005

Annual direct costs: \$80,000

Incorporating Protein Flexibility and Bioinformatics into Drug Design

The major goal of this project was to create software for the development and mining of a protein-ligand database.

PATENTS

1. HA Carlson, KL Damm, KL Meagher. Compositions and Methods Relating to HIV Protease Inhibition. U.S. Provisional Patent Application No. 60/972,505 (filed on Sept 14, 2007), Patent Cooperation Treaty #WO/2009/036341 (filed on Sept 12, 2008)

PUBLICATIONS (ORCID iD: 0000-0002-7495-1699) (GOOGLE SCHOLAR: H-INDEX = 37, I10-INDEX=62)

82. S Shankar, JC-Y Tien, RF Siebenaler, VL Dommeti, S Zelenka-Wang, J Waninger, KM Juckette, A Xu, M Mody, S Eyunni, S Chugh, Y Zhang, A Goodrum, G Tsaloff, IJ Apel, L Wang, J Siddiqui, RD Smith, X Cao, HA Carlson, J Tesmer, J Shi, C Kumar-Sinha, AM Chinnaiyan. An essential role for *Argonaute 2* in EGFR-KRAS signaling in pancreatic cancer development. *Science* **2018**, in review.
81. SE Graham, N Leja, HA Carlson. MixMD Probeview: Robust binding site prediction from cosolvent simulations. *J. Chem. Info. Model.* **2018**, *58*, 1426-1433.
80. SE Graham, HA Carlson. Predicting displaceable water sites using mixed-solvent molecular dynamics. *J. Chem. Info. Model.* **2018**, *58*, 305-314.
79. A Schlessinger, R Abagyan, HA Carlson, KK Dang, J Guinney, RL Cagan. Multi-targeting drug community challenge. *Cell Chem. Biol.* **2017**, *24*, 1434-1435.
78. RD Smith, J Lu, HA Carlson. Are there physicochemical differences between allosteric and competitive ligands? *PLoS Comput. Biol.* **2017**, *13(11)*, e1005813. <https://doi.org/10.1371/journal.pcbi.1005813>
77. P Ghanakota, HA Carlson. Comparing pharmacophore models derived from crystallography and NMR ensembles. *J. Comput.-Aided Mol. Des.* **2017**, *31*, 979-993.
76. S Gathiaka, S Liu, M Chiu, H Yang, JA Stuckey, YN Kang, J Delproposito, G Kubish, JB Dunbar Jr., HA Carlson, SK Burley, WP Walters, RE Amaro, VA Feher, MK Gilson. D3R Grand Challenge 2015: Evaluation of protein-ligand pose and affinity predictions. *J. Comput.-Aided Mol. Des.* **2016**, *30*, 651-668.

Paper #75 was highlighted by Faculty of 1000 (F1000)

75. P Ghanakota, HA Carlson. Driving structure-based drug discovery through cosolvent molecular dynamics. *J. Med. Chem.* **2016**, *59*, 10383-10339.
74. J Lu, HA Carlson. ChemTreeMap: An interactive map of biochemical similarity in molecular datasets. *Bioinformatics* **2016**, *32*, 3584-3592.

73. P Ghanakota, HA Carlson. Moving beyond active-site detection: MixMD applied to allosteric systems. *J. Phys. Chem. B* **2016**, *120*, 8685-8695.
72. SE Graham, L Zhang, I Ali, YK Cho, MD Ismail, HA Carlson, B Foxman. Prevalence of CTX-M extended-spectrum β -lactamases and sequence type 131 in Korean blood, urine, and rectal *Escherichia coli* isolates. *Infect. Genet. Evol.* **2016**, *41*, 292-295.
71. SE Graham, SE Tweedy, HA Carlson. Dynamic behavior of the post-SET loop region of NSD1: Implications for histone binding and drug development. *Protein Sci.* **2016**, *25*, 1021-1029.

Papers #68-70 were highlighted on the cover of a special issue of *JCIM*

70. HA Carlson. Lessons learned over four benchmark exercises from the Community Structure-Activity Resource. *J. Chem. Info. Model.* **2016**, *56*, 951-954.
69. HA Carlson, RD Smith, KL Damm-Ganamet, JA Stuckey, A Ahmed, MA Convery, DO Somers, M Kranz, PA Elkins, G Cui, CE Peishoff, MH Lambert, JB Dunbar Jr. CSAR 2014: A benchmark exercise using unpublished data from pharma. *J. Chem. Info. Model.* **2016**, *56*, 1063-1077.
68. RD Smith, KL Damm-Ganamet, JB Dunbar Jr, A Ahmed, K Chinnaswamy, JE Delproposto, GM Kubish, CE Tinberg, SD Khare, J Dou, L Doyle, JA Stuckey, D Baker, HA Carlson. CSAR benchmark exercise 2013: Evaluation of results from a combined computational protein design, docking and scoring/ranking challenge. *J. Chem. Info. Model.* **2016**, *56*, 1022-1031.
67. PMU Ung, P Ghanakota, SE Graham, KW Lexa, HA Carlson. Identifying binding hot spots on protein surfaces by mixed-solvent molecular dynamics: HIV-1 protease as a test case. *Biopolymers* **2016**, *105*, 21-34.
66. H Xu, JD Majmudar, P Ghanakota, D Davda, KH Kim, HA Carlson, HD Showalter, BR Martin, GL Amidon. Substrate-competitive activity-based profiling of ester prodrug activating enzymes. *Mol. Pharmaceutics* **2015**, *12*, 3399-3407.
65. A Ahmed, RD Smith, JJ Clark, JB Dunbar Jr., HA Carlson. Recent improvements to Binding MOAD: a resource for protein-ligand binding affinities and structures. *Nucl. Acids Res.* **2015**, *43*, D465-D469.

Paper #64 was highlighted in Faculty of 1000 (F1000)

64. PMU Ung, JB Dunbar, JE Gestwicki, HA Carlson. An allosteric modulator of HIV-1 protease shows equipotent inhibition of wild-type and drug-resistant proteases. *J. Med. Chem.* **2014**, *57*, 6468-6478.
63. KW Lexa, GB Goh, HA Carlson. Parameter choice matters: Validating probe parameters for use in mixed-solvent simulations. *J. Chem. Info. Model.* **2014**, *54*, 2190-2199.
62. PM-U Ung, AD Thompson, L Chang, JE Gestwicki, HA Carlson. Identification of key hinge residues important for nucleotide-dependent allostery in *E. coli* Hsp70/DnaK. *PLoS Comput. Biol.* **2013**, *9(11)*: e1003279. DOI:10.1371/journal.pcbi.1003279.
61. NA Khazanov, HA Carlson. Exploring the composition of protein-ligand binding sites on a large scale. *PLoS Comput. Biol.* **2013**, *9(11)*: e1003321. DOI:10.1371/journal.pcbi.1003321.

Papers #58-60 were highlighted on the cover of a special issue of *JCIM*

60. HA Carlson. Check your confidence: Size really *does* matter. *J. Chem. Info. Model.* **2013**, *53*, 1837-1841.
59. JB Dunbar Jr., RD Smith, KL Damm-Ganamet, A Ahmed, EX Esposito, J Delproposto, K Chinnaswamy, Y-N Kang, G Kubish, JE Gestwicki, JA Stuckey, HA Carlson. CSAR dataset release 2012: Ligands, affinities, complexes, and docking decoys. *J. Chem. Info. Model.* **2013**, *53*, 1842-1852.

Paper #58 was 2013's 15th most-read paper in *JCIM*, and it was highlighted by Faculty of 1000 (F1000)

58. KL Damm-Ganamet, RD Smith, JB Dunbar Jr., JA Stuckey, HA Carlson. CSAR Benchmark Exercise 2011-2012: Evaluation of results from docking and relative ranking of blinded congeneric series. *J. Chem. Info. Model.* **2013**, *53*, 1853-1870.
57. KW Lexa, HA Carlson. Improving protocols for protein mapping through proper comparison to crystallography data. *J. Chem. Info. Model.* **2013**, *53*, 391-402.
56. AE Davidson, FM Siddiqui, M Lopez, P Lunt, HA Carlson, BE Moore, S Love, DE Born, H Roper, A Majumdar, S Jayadev, HR Underjill, CO Smith, M von der Hagen, A Hubner, P Jardine, A Merrison, E Curtis, T Cullip, H Jungbluth, MO Cox, TL Winder, H Abdel Salam, JZ Li, SA Moore, JJ Dowling. Novel deletion of lysine 7 expands the clinical, histopathological and genetic spectrum of TPM2-related myopathies. *Brain* **2013**, *136*: 508-521.

Paper #55 was 2012's 10th most-read paper in *JCIM*, despite appearing only half-way through the year

55. RD Smith, AE Engdahl, JB Dunbar Jr., HA Carlson. Biophysical limits of protein-ligand binding. *J. Chem. Info. Model.* **2012**, *52*: 2098-2106.

Paper #54 was highlighted on the cover of *Proteins: Structure, Function, and Bioinformatics*

54. NA Khazanov, KL Damm-Ganamet, DX Quang, HA Carlson. Overcoming sequence misalignments with weighted structural superposition. *Prot. Struct. Func. Bioinf.* **2012**, *80*, 2523-2535.
53. KW Lexa, HA Carlson. Protein flexibility in docking and surface mapping. *Q. Rev. Biophys.* **2012**, *45*: 301-343.

Papers #49-52 were highlighted on the cover of a special issue of *JCIM*

52. HA Carlson, JB Dunbar Jr. A call to arms: What you can do for computational drug discovery. *J. Chem. Info. Model.* **2011**, *51*, 2025-2026.
51. Correction to CSAR Benchmark Exercise of 2010: Selection of the protein-ligand complexes [DOI:10.1021/ci200082t]. *J. Chem. Info. Model.* **2011**, *51*, 2146.
50. RD Smith, JB Dunbar Jr, PM-U Ung, EX Esposito, C-Y Yang, S Wang, HA Carlson. CSAR Benchmark Exercise of 2010: Combined evaluation across all submitted scoring functions. *J. Chem. Info. Model.* **2011**, *51*, 2115-2131.
49. JB Dunbar Jr, RD Smith, CY Yang, PMU Ung, KW Lexa, NA Khazanov, JA Stuckey, S Wang, HA Carlson. CSAR Benchmark Exercise of 2010: Selection of the protein-ligand complexes. *J. Chem. Info. Model.* **2011**, *51*, 2036-2046.
48. KW Lexa, HA Carlson. Binding to the open conformation of HIV-1 protease. *Prot. Struct. Func. Bioinf.* **2011**, *79*, 2282-2290.

Paper #47 was highlighted on the back cover of *Proteins: Structure, Function, and Bioinformatics*

47. SA Spronk, HA Carlson. The role of tyrosine 71 in modulating the flap conformations of BACE1. *Prot. Struct. Func. Bioinf.* **2011**, *79*, 2247-2259.
46. L Chang, Y Miyata, PMU Ung, EB Bertelsen, TJ McQuade, HA Carlson, ERP Zuiderweg, JE Gestwicki. Chemical screens against a reconstituted multi-protein complex: Myricetin blocks DnaJ regulation of DnaK through an allosteric mechanism. *Chem. & Biol.* **2010**, *18*, 210-221.
45. KW Lexa, HA Carlson. Full protein flexibility is essential for proper hot-spot mapping. *J. Am. Chem. Soc.* **2011**, *133*, 200-202.
44. AA Reinke, PM Ung, JJ Quintero, HA Carlson, JE Gestwicki. Chemical probes that selectively recognize the earliest A β oligomers in complex mixtures. *J. Am. Chem. Soc.* **2010**, *132*, 17655-17657.

43. AD Schuyler, HA Carlson, EL Feldman. Computational methods for identifying a layered allosteric regulatory mechanism for ALS-causing mutations of Cu-Zn superoxide dismutase 1. *Prot. Struct. Func. Bioinf.* **2011**, 79, 417-427.
42. L Chang, AD Thompson, PM-U Ung, HA Carlson, JE Gestwicki. Mutagenesis reveals the complex relationships between ATPase rate and the chaperone activities of Escherichia coli heat shock protein 70 (Hsp70/DnaK). *J. Biol. Chem.* **2010**, 285, 21282-21291.
41. S Wisén, EB Bertelsen, AD Thompson, S Patury, PM-U Ung, L Chang, CG Evans, GM Walter, P Wipf, HA Carlson, JL Brodsky, ER Zuiderweg, JE Gestwicki. Binding of a small molecule at a protein-protein interface regulates the chaperone activity of Hsp70-Hsp40. *ACS Chem. Biol.* **2010**, 5, 611-622.
40. AD Schuyler, HA Carlson, EL Feldman. Computational methods for predicting sites of functionally important dynamics. *J. Phys. Chem. B* **2009**, 113, 6613-6622.
39. KW Lexa, KL Damm, JJ Quintero, JE Gestwicki, HA Carlson. Clarifying allosteric control of flap conformations in the 1TW7 crystal structure of HIV-1 protease. *Prot. Struct. Func. Bioinfo.* **2009**, 74, 872-880.

Paper #38 highlighted in *Current Opinion in Drug Discovery and Development* [2009 12:1-15.]

38. HA Carlson, RD Smith, NA Khazanov, PD Kirchhoff, JB Dunbar Jr, ML Benson. Differences between high- and low-affinity complexes of enzymes and non-enzymes. *J. Med. Chem.* **2008**, 51, 6432-6441.
37. MG Lerner, KL Meagher, HA Carlson. Automated clustering of probe molecules from solvent mapping of protein surfaces. *J. Comput.-Aided Mol. Des.* **2008**, 22, 727-736.

Paper #36 was highlighted on the cover of *Biopolymers*, on the NIGMS website, and several news outlets

36. KL Damm, PMU Ung, JJ Quintero, JE Gestwicki, HA Carlson. A poke in the eye: Inhibiting HIV-1 protease through its flap-recognition pocket. *Biopolymers* **2008**, 89, 643-652.
35. ML Benson, RD Smith, NA Khazanov, HA Carlson, B Dimcheff, P Dresslar. Updating Binding MOAD – Data management and information workflow. *New Math. Natur. Comput.* **2010**, 6, 49-56.
34. ML Benson, RD Smith, NA Khazanov, B Dimcheff, J Beaver, P Dresslar, JE Nerothin, HA Carlson. Binding MOAD, a high-quality protein-ligand database. *Nucleic Acids Res.* **2008**, 36, D674-D678.
33. MG Lerner, AL Bowman, HA Carlson. Incorporating dynamics in *E. coli* dihydrofolate reductase enhances structure-based drug discovery. *J. Chem. Info. Model.* **2007**, 47, 2358-2365.

Paper #32 was highlighted in *SciBX: Science–Business eXchange* [January 2008, 7-8]

32. AL Bowman, Z Nikolovska-Coleska, H Zhong, S Wang, HA Carlson. Small molecule inhibitors of the MDM2-p53 interaction discovered by ensemble-based receptor models. *J. Am. Chem. Soc.* **2007**, 129, 12809-12814.

Paper #31 was highlighted in Nature's blog "The Skeptical Chymist"

31. KL Damm, HA Carlson. Exploring experimental sources of multiple protein conformations in structure-based drug design. *J. Am. Chem. Soc.* **2007**, 129, 8225-8235.
30. AL Bowman, MG Lerner, HA Carlson. Protein flexibility and species specificity in structure-based drug discovery: Dihydrofolate reductase as a test system. *J. Am. Chem. Soc.* **2007**, 129, 3634-3640.
29. KL Meagher, MG Lerner, HA Carlson. Refining the MPS pharmacophore method: Consistency across three independent HIV-1 protease models. *J. Med. Chem.* **2006**, 49, 3478-3484.
28. KL Damm, HA Carlson. Gaussian-weighted RMSD superposition of proteins: A structural comparison for flexible proteins and predicted protein structures. *Biophys. J.* **2006**, 90, 4558-4573.

27. H Zhong, HA Carlson. Conformational studies of polyprolines. *J. Chem. Theory Comput.* **2006**, 2, 342-353.
26. RD Smith, L Hu, JA Falkner, ML Benson, JP Nerothin, HA Carlson. Exploring protein-ligand recognition with Binding MOAD. *J. Mol. Graphics Model.* **2006**, 24, 414-425.
25. X-J Tan, HA Carlson. Docking studies and ligand recognition in folylpolyglutamate synthetase. *J. Med. Chem.* **2005**, 48, 7764-7772.
24. JY Kravitz, VL Pecoraro, HA Carlson. Quantum mechanics/molecular mechanics calculations of the vanadium dependent chloroperoxidase. *J. Chem. Theory Comput.* **2005**, 1, 1265-1274.
23. KA Todorov, X-J Tan, ST Nonekowski, GA Garcia, HA Carlson. The role of aspartic acid 143 in *E. coli* tRNA-guanine transglycosylase: Insights from mutagenesis studies and computational modeling. *Biophys. J.* **2005**, 89, 1965-1977.

Paper #22 was highlighted in C&E News [2005, 83, 33-34].

22. L Hu, ML Benson, RD Smith, MG Lerner, HA Carlson. Binding MOAD (Mother of All Databases). *Prot. Struct. Func. Bioinfo.* **2005**, 60, 333-340.

Paper #21 was highlighted in Nature Reviews Drug Discovery [2004, 3, 910].

21. KL Meagher, HA Carlson. Incorporating protein flexibility in structure-based drug discovery: Using HIV-1 protease as a test case. *J. Am. Chem. Soc.* **2004**, 126, 13276-13281.
20. H Zhong, HA Carlson. Computational studies and peptidomimetic design for the human p53-MDM2 complex. *Prot. Struct. Func. Bioinfo.* **2005**, 58, 222-234.
19. KL Meagher, HA Carlson. Solvation influences flap collapse in HIV-1 protease. *Prot. Struct. Func. Bioinfo.* **2005**, 58, 119-125.

Paper #18 was highlighted on the cover of Inorganic Chemistry

18. G Zampella, JY Kravitz, CE Webster, P Fantucci, MB Hall, HA Carlson, VL Pecoraro, L De Gioia. Quantum mechanical models of the resting state of the vanadium-dependent haloperoxidase. *Inorg. Chem.* **2004**, 43, 4127-4136.
17. LM Sandvoss, HA Carlson. Conformational behavior of β -proline oligomers. *J. Am. Chem. Soc.* **2003**, 125, 15855-15862.
16. BR Huck, JD Fisk, ID Guzei, HA Carlson, SH Gellman. Secondary structural preferences of 2,2-disubstituted pyrrolidine-4-carboxylic acid oligomers: β -peptide foldamers that cannot form internal hydrogen bonds. *J. Am. Chem. Soc.* **2003**, 125, 9035-9037.
15. KL Meagher, LT Redman, HA Carlson. Development of polyphosphate parameters for use with the AMBER force field. *J. Comput. Chem.* **2003**, 24, 1016-1025.
14. HA Carlson. Protein flexibility and drug design: How to hit a moving target. *Curr. Opin. Chem. Biol.* **2002**, 6, 447-452.
13. HA Carlson. Protein flexibility is an important component of structure-based drug discovery. *Curr. Pharm. Des.* **2002**, 8, 1571-1578.
12. HA Carlson, JA McCammon. Accommodating protein flexibility in computational drug design. *Mol. Pharmacol.* **2000**, 57, 213-218.
11. HA Carlson, KM Masukawa, JA McCammon. Method for including the dynamic fluctuations of a protein in computer-aided drug design. *J. Phys. Chem. A* **1999**, 103, 10213-10219.

Paper #10 was highlighted in *Modern Drug Discovery* [2000, 3, 15]

10. HA Carlson, KM Masukawa, K Rubins, FD Bushman, WL Jorgensen, RD Lins, JM Briggs, JA McCammon. Developing a dynamic pharmacophore model for HIV-1 integrase. *J. Med. Chem.* **2000**, *43*, 2100-2114.
9. MJ Potter, PD Kirchoff, HA Carlson, JA McCammon. Molecular dynamics simulations of a cryptophane and its complexes with tetramethylammonium and neopentane using a continuum solvent model. *J. Comput. Chem.* **1999**, *20*, 956-970.
8. RD Lins, JM Briggs, TP Straatsma, HA Carlson, J Greenwald, S Choe, JA McCammon. Molecular dynamics studies on the HIV-1 integrase catalytic domain. *Biophys. J.* **1999**, *76*, 2999-3011.
7. HA Carlson, JM Briggs, JA McCammon. Calculation of the pK_a values for the ligands and side chains of *Escherichia coli* D-ala-D-ala ligase. *J. Med. Chem.* **1999**, *42*, 109-117.
6. NA McDonald, HA Carlson, WL Jorgensen. Extension of the linear response method for free energies of solvation in chloroform. *J. Phys. Org. Chem.* **1997**, *10*, 563-576.
5. HA Carlson, WL Jorgensen. Monte Carlo investigations of solvent effects on the chorismate to prephenate rearrangement. *J. Am. Chem. Soc.* **1996**, *118*, 8475-8484.
4. HA Carlson, WL Jorgensen. An extended linear response method for determining free energies of hydration. *J. Phys. Chem.* **1995**, *99*, 10667-10673.
3. HA Carlson, WL Jorgensen. Investigations into the stereochemistry of cyclophane-steroid complexes via Monte Carlo simulations. *Tetrahedron* **1995**, *51*, 449-472.
2. HA Carlson, TB Nguyen, M Orozco, WL Jorgensen. Accuracy of free energies of hydration for organic molecules from 6-31G*-derived partial charges. *J. Comput. Chem.* **1993**, *14*, 1240-1249.
1. HA Carlson, GE Quelch, HF Schaefer III. How "stable" is cyclobutene? The activation energy for the unimolecular rearrangement to butatriene. *J. Am. Chem. Soc.* **1992**, *114*, 5344-5348.

BOOK CHAPTERS

2. ML Benson, RD Smith, NA Khazanov, HA Carlson, B Dimcheff, P Dresslar. Updating Binding MOAD – Data management and information workflow. In *Information Sciences 2007: Proceedings of the 10th Joint Conference on Information Sciences*. Eds. PY Cao, H Cheng, D Hung, C Kahraman, CW Ngo, Y Ohsawa, MG Romay, MC Su, A Vasilakos, D Wang, PP Wang. World Scientific Publishing Company Pte Ltd, Singapore, **2007**, pp. 14-20.
1. KM Masukawa, HA Carlson, JA McCammon. Chapter 22. Technique for developing a pharmacophore model that accommodates inherent protein flexibility: An application to HIV-1 integrase. *Pharmacophore Perception, Development, and Use in Drug Design* Osman Güner, ed., **2000**, pp. 409-427.

NATIONAL SERVICE

NATIONAL SCIENCE FOUNDATION

- Ad hoc reviewer

NATIONAL INSTITUTES OF HEALTH

- Member, CSR Special Emphasis Panels and ad hoc assignments on standing study sections

- ZRG1 F04B-T (20) L – Biochemistry and Biophysics of Biological Macromolecules Fellowship Applications (6/2018)
- MSFD - Macromolecular Structure and Function D Study Section – (2/2016)
- R24, Legacy Resources of NIGMS (2/2015)
- ZRG1 BST-J (50) BD2K-LINCS-Perturbation Data Coordination and Integration Center (6/2014)
- ZRG1 AARR-D (40) P - HIV Protease Program Project (4/2012)
- BDMA - Biodata Management and Analysis Study Section (2/2012)
- ZGM1 PPBC-4 (LR) Limited Pilot for NIGMS Legacy Community-Wide Scientific Resources (5/2011)
- ZRG1 AARR-A (40) Structural Biology of HIV/AIDS-Related Proteins (4/2007)
- ZRG1 AARR-A (03) Structural Biology of AIDS-Responsive Drugs (11/04)
- PA-03-020 Molecular Targets for Cancer Drug Discovery: Exploratory Grants (7/03)
- ZRG1 AARR-1 (50) Structural Biology of AIDS-Related Proteins (5/2002)

AMERICAN CHEMICAL SOCIETY

- Ad hoc reviewer of PRF grants
- Organized a symposium for the 244th American Chemical Society's National Meeting in Boston (8/19/2012)
 - The CSAR 2012 Benchmark Exercise Symposium included 12 invited speakers
- Organized a symposium for the 240th American Chemical Society's National Meeting in Boston (8/23/2010)
 - The CSAR 2010 Benchmark Exercise Symposium included 14 invited speakers and open discussion panels
- Invited to organize a symposium for the 225th American Chemical Society's National Meeting in New Orleans (3/23/2003)
 - Symposium talks included 36 invited speakers
 - \$3600 grant from Petroleum Research Fund (PRF #39368-SE "Protein Flexibility, at the ACS National Meeting, March 2003, New Orleans, LA," Heather A. Carlson on the behalf of the ACS Division of Computers in Chemistry)
 - \$1855 in funds from the COMP division of the ACS
 - Obtained \$2500 donation from Chemical Computing Group
 - Obtained \$1000 donation from GlaxoSmithKline
 - Provided travel money for nine participants (junior faculty and foreign speakers)

PROFESSIONAL JOURNALS

Editorial Advisory Board, *Journal of Chemical Information and Modeling*
 Editorial Advisory Board, *Chemical Biology & Drug Design*

MEMBERSHIP IN PROFESSIONAL ORGANIZATIONS

American Chemical Society American Association for the Advancement of Science
 Biophysical Society

INVITED LECTURES

- 2018 Workshop on the Mathematics of Drug Design/Discovery, Field's Institute, University of Toronto, Canada
- 2018 Structural Biology Seminar, Pasteur Institute, Paris, France
- 2017 Biomolecular NMR and Computation, Gordon Research Conference, Mt. Snow, VT
- 2017 Genentech, South San Francisco, CA
- 2016 3DSIG Meeting (ISMB National Meeting) Orlando, FL

- 2016 D3R Meeting, University of California, San Diego
2015 250th ACS National Meeting, Boston, MA
2015 Drug Discovery Re-Invented 2015, Ascot, United Kingdom
2014 NSF Software Institute for Molecular Simulations: Workshop I, Berkeley, CA
2014 Ameri-QSAR symposium, COMP division, 248th ACS National Meeting, in San Francisco, CA
2014 EMBO Practical Course in Biomolecular Simulation, Paris, France
2014 Chemical Biology Initiative Annual Symposium, University of Michigan, Ann Arbor
2013 Laufer Center for Physical and Quantitative Biology, SUNY Stony Brook, NY
2013 Structure-Based Drug Design CHI Conference, Boston, MA
2013 Biomolecular NMR and Computation, Gordon Research Conference, Mt. Snow, VT
2013 Molecular Biophysics Annual Symposium, University of Michigan, Ann Arbor
2013 245th National Meeting of the American Chemical Society, New Orleans, LA
2012 Modeling Protein Interactions, University of Kansas, Lawrence, KS
2012 19th EuroQSAR Meeting, Vienna, Austria
2012 244th National Meeting of the American Chemical Society, Philadelphia, PA
2012 Gordon Research Conference on Bioorganic Chemistry, Proctor Academy, Andover, NH
2012 Keynote Award Lecture, Rall Symposium, North Central College, Naperville, IL
2012 Third Annual Michigan Data Mining Workshop, University of Michigan, Ann Arbor
2012 243rd National Meeting of the American Chemical Society, San Diego, CA
2011 Fifth Meeting on U.S. Government Chemical Databases and Open Chemistry, National Cancer Institute
2011 241st National Meeting of the American Chemical Society, Anaheim, CA
2011 Novartis Pharma AG – Boston, MA
2010 Pfizer, Groton, CT
2010 240th National Meeting of the American Chemical Society, Boston, MA
2010 PDB, Rutgers, New Brunswick, NJ
2010 AstraZeneca, Boston, MA
2010 Novartis Pharma AG - Horsham, UK
2010 Novartis Pharma AG - Basel, Switzerland
2010 Keystone - Computer Aided Drug Design, Whistler, British Columbia, Canada
2010 Therapeutic Applications of Computational Biology and Chemistry 2010 (TACBAC2010), Wellcome Center/EBI, UK
2009 Department of Computational Biology, University of Pittsburgh, PA
2008 Webinar, Solving Computational Chemistry Challenges
2008 Genentech, South San Francisco, CA
2008 Chemical Biology Colloquium Series, University of Minnesota, Twin Cities
2008 The 5th Annual North Eastern Structure Symposium (NESS) Computational Approaches to Structural Biology, University of Connecticut, Storrs, CT
2008 Department of Chemistry, Kalamazoo College, Kalamazoo, MI
2008 MOE Users' Meeting, CCG, Montreal, Canada
2008 Abbott Pharmaceuticals, Chicago, IL
2008 235th National Meeting of the American Chemical Society, New Orleans, LA
2008 Keystone Symposium, Computer-Aided Drug Design, Steamboat Springs, CO
2007 Tommy Liljefors Retirement Symposium, University of Copenhagen, Denmark
2007 Latest Advances in Drug Discovery & Development, eCheminfo InterAction Meeting, Bryn Mawr College, Philadelphia, PA
2007 Structural Biology & Computational Chemistry Symposium, Wyeth Research, Cambridge, MA
2007 10th Joint Conference on Information Sciences, Salt Lake City, UT
2007 Department of Biochemistry, University of Missouri-Columbia
2007 233rd National Meeting of the American Chemical Society, Chicago, IL

- 2006 232nd National Meeting of the American Chemical Society, San Francisco, CA
 2006 PharmaDiscovery 2006, Bethesda, MD
 2006 Departments of Physiology and Molecular Biophysics, Johns Hopkins University, Baltimore, MD
 2006 Center for Advanced Research in Biotechnology (CARB), National Institute of Standards and Technology and the University of Maryland, Rockville, MD
 2006 231st National Meeting of the American Chemical Society, Atlanta, GA
 2006 46th Sanibel Symposium, St. Simons Island, GA
 2005 Department of Biochemistry, Michigan State University, East Lansing, Michigan
 2005 Gordon Research Conference on Computer-Aided Drug Design (sent KL Meager in my place)
 2005 Molecular, Cell Biology, and Biotechnology Seminar Series, Virginia Tech, Blacksburg, VA.
 2005 Vitae Pharma, Ft. Washington, PA.
 2005 Jorgensen Symposium “30 Years in the Trenches”, Yale University
 2005 Department of Molecular Biophysics and Biochemistry, Yale University
 2005 Departments of Pharmaceutics and Medicinal Chemistry, University of Utah
 2005 229th National Meeting of the American Chemical Society, San Diego, CA
 2004 Department of Bioengineering, Notre Dame University
 2004 Department of Medicinal and Biological Chemistry, University of Toledo
 2004 International Society of Quantum Biology and Pharmacology President’s Meeting, Como, Italy
 2004 Workshop on Flexible Docking, CECAM, Lyon, France
 2003 Department of Chemistry, University of Illinois, Urbana-Champaign
 2003 Gordon Research Conference on Computer-Aided Drug Design
 2003 225th National Meeting of the American Chemical Society, New Orleans, LA
 2002 First MERCURY Conference in Computational Chemistry, Hamilton College, Clinton, NY
 2001 Department of Pharmaceutical Sciences, Wayne State University, Detroit, Michigan
 2001 American Chemical Society Central/Great Lakes Regional Meeting, Grand Rapids, Michigan
 2001 Center for Biological Modeling, Michigan State University, East Lansing, Michigan
 2000 Pfizer Inc., Ann Arbor, MI
 2000 219th American Chemical Society National Meeting, San Francisco, CA
 1999 Molecular Simulations Inc., San Diego, CA
 1998 Computational Chemistry Division's Electrostatic Interests Group, The Scripps Research Institute
 1996 Chemistry Department, ETH - Zürich
 1994 Second Canadian Computational Chemistry Conference, Queen’s University at Kingston

CURRENT COWORKERS

- 2016 Zach Orban (Undergraduate Student)
 2012 Jordan Clark (Graduate Student, Medicinal Chemistry)
 2010 Dr. Richard D. Smith, Ph.D. (Postdoctoral Fellow)

FORMER COWORKERS

RESEARCH AND VISITING SCIENTISTS

- Dr. James B. Dunbar, Jr. Ph.D. (Research Scientist, 2007-2017)
 Dr. Kelly Ganamet, Ph.D. (Research Scientist, 2011-2014)
 Dr. Emilio Esposito, Ph.D. (Visiting Scientist, 2010-2011)

POSTDOCTORAL FELLOWS

- Aqeel Ahmed, Ph.D. (Postdoctoral Fellow, 2012-2015)
Scientist, Bioinformatics Inc., Boston, MA
- Adam Schuyler, Ph.D. (Postdoctoral Fellow, 2007-2009) Joint advisor: Eva Feldman MD., Ph.D.
Assistant Professor, University of Connecticut Health Center
- Steven A. Spronk, Ph.D. (Postdoctoral Researcher, 2006-2008)
Scientist, Bristol-Myers Squibb
- Anna L. Bowman, D.Phil. (Postdoctoral Researcher, 2005-2007)
Research Assistant Professor, Northeastern University
- Xiao-Jian Tan, Ph.D. (Postdoctoral Researcher, 2003-2005)
Deceased
- Liegi Hu, Ph.D. (Postdoctoral Researcher, 2001-2004)
Software Development Analyst, Northrop Grumman, Atlanta
- Haizhen Zhong, Ph.D. (Postdoctoral Researcher, 2001-2003)
Professor, University of Nebraska, Omaha
- Mavinahalli N. Jagadeesh, Ph.D. (Postdoctoral Researcher, 2002-2003)
Research Scientist with Chandra Verma, Bioinformatics Institute, A*STAR, Singapore

GRADUATE STUDENTS

- Sarah Graham, Ph.D. (Ph.D. in Biophysics, 2017)
Bioinformatics Postdoc, University of Michigan, Ann Arbor
- Jing Lu, Ph.D. (Ph.D. in Bioinformatics, 2016)
Machine Learning Scientist with Veracyte, San Francisco, CA
- Phani Ghanakota, Ph.D. (Ph.D. in Medicinal Chemistry, 2015)
Scientist, Schrödinger, New York, NY
- Peter Man-Un Ung, Ph.D. (Ph.D. in Medicinal Chemistry, 2012) Secondary advisor: Jason Gestwicki, Ph.D.
Research Scientist with Avner Schlessinger, Mount Sinai School of Medicine
- Nickolay A. Khazanov, Ph.D. (Ph.D. in Bioinformatics, 2011)
Bioinformatics Scientist, Compendia Bioscience, Ann Arbor, MI
- Katrina W. Lexa, Ph.D. (Ph.D. in Medicinal Chemistry, 2011)
Scientist, Merck Pharmaceuticals
- Jerome Quintero, Ph.D. (Ph.D. in Biophysics, 2011) Secondary advisor: Jason Gestwicki, Ph.D.
Affiliate, Accentia Technologies, Cooper City, FL
- Richard D. Smith, Ph.D. (Ph.D. in Biophysics, 2010)
Assistant Research Scientist with Heather A. Carlson, University of Michigan, Ann Arbor
- Mark L. Benson, Ph.D. (Ph.D. in Bioinformatics, 2009)
Scientist, National Cancer Institute
- Jeff Werezynski, Ph.D. (Ph.D. in Biophysics, 2008 Primary advisor: Ioan Andricioaei, Ph.D.)
Assistant Professor, Illinois Institute of Technology
- Michael G. Lerner, Ph.D. (Ph.D. in Biophysics, 2007)
Associate Professor, Earlham College
- Kelly L. Damm, Ph.D. (Ph.D. in Medicinal Chemistry, 2007)
Scientist, Johnson & Johnson

Jason P. Nerothin, M.S. (Web designer and programmer, 2004-2005)
 Database manager with David Eisenberg (HHMI Investigator), UCLA

Kristin L. Meagher, Ph.D. (Ph.D. in Medicinal Chemistry, 2005)
 Research Scientist, Nuvalent, Boston, MA

Joslyn Y. Kravitz, Ph.D. (Ph. D. in Physical Chemistry, 2005) Joint advisor: VL Pecoraro Ph.D.
 AAAS Science & Technology Policy Fellow, Office of the Director, NIH

Maj. Katherine W. Abold, Ph.D. (Ph. D. in Medicinal Chemistry, 2003) Primary advisor: GA Garcia Ph.D.
 United States Air Force Academy and Senior Scientist of Patrick Air Force Base, FL

Leah M. Sandvoss (M.S. in Medicinal Chemistry, 2002)
 Scientist, Pfizer-La Jolla

PHARM D STUDENTS

Noah Leja, Pharm.D. (Research Assistant, 2016-2018)

Philip L. Williams, Pharm.D. (Research Assistant, 2008-2010)

Timothy Baccus, Pharm.D. (Research Assistant, 2008-2010)

Teren L. Bouladin, Pharm.D. (Research Assistant, 2005-2007)

Carrie W. Abramson, Pharm.D. (Research Assistant, 2005-2007)

Steven M. Stout, Pharm.D. (Research Assistant, 2005-2007)

UNDERGRADUATE STUDENTS

Daniel Geiszler (Protein Structure-Function REU Summer Student, 2016)
 Graduate Study in Bioinformatics, University of Michigan, Ann Arbor

Sara E. Tweedy (Chemistry REU Summer Student, 2013)
 MD/PhD Graduate Study, University of Michigan, Ann Arbor

Alaina E. Engdahl (Protein Structure-Function REU Summer Student, 2011)
 Graduate Study in Medicinal Chemistry, University of Michigan, Ann Arbor

Daniel X. Quang (Protein Structure-Function REU Summer Student, 2010)
 Graduate Study in Mathematical Systems Biology, UC Irvine

Derek Mendez (MARC Summer Undergraduate Researcher, 2008)
 Graduate Study in Applied Physics, Stanford University

Alexander E. Buck (Chemistry REU Summer Student, 2006)
 Graduate Study in Chemistry, University of Michigan, Ann Arbor

Luke T. Redman (B.S. in Biochemistry, 2002)