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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

2020-present Chair of the Department of Medicinal Chemistry, Director of the Interdepartmental Graduate Program in Medicinal Chemistry

2011-present Professor of Medicinal Chemistry, College of Pharmacy, University of Michigan, Ann Arbor
Professor of Biophysics and Chemistry, College of LSA, University of Michigan, Ann Arbor

2002-present Associated Faculty of the Bioinformatics Graduate Program, University of Michigan, Ann Arbor

2016-2019 Member, Executive Board, College of Pharmacy, University of Michigan, Ann Arbor

2016-2019 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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2017-2019 Organizing Team, 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*

2014-2017 Editorial Advisory Board, *Journal of Medicinal Chemistry*

2008-2014 Editorial Board, *Proteins: Structure, Function, and Bioinformatics*

2006-2013 Editorial Advisory Board, *Chemical Biology & Drug Design*

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

2019 Paper highlighted by Faculty of 1000 (F1000.com): RD Smith, JJ Clark, A Ahmed, ZJ Orban, JB Dunbar Jr., HA Carlson. *J. Mol. Biol.* **2019**, *431*, 2423-2433.

2019 Interviewed for comments about polypharmacology, quoted in *"*When there's more than one way to target a cancer" *Nature Medicine* **2019**, *25*, 1181-1182.

2019 Paper highlighted by Faculty of 1000 (F1000.com): JJ Clark, ML Benson, RD Smith, HA Carlson. *PLoS Comput. Biol.* **2019**, *15*, e1006705

2019 My Assistant Research Scientist Richard Smith won a poster award at the 4th Drug Discovery Reinvented Conference (International Competition)

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.com): 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.com): 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.com): 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 graduate 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/thescepticalchymist/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 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.

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

Rackham Faculty Allies Grant (PI: Carlson) **PREVIOUS** **5/1/2019-4/30/2020**
University of Michigan, Ann Arbor Total direct costs: $20,000
College of Pharmacy Graduate Programs in Medicinal Chemistry, Pharmaceutical Sciences, and Clinical Pharmacy Translational Science

This proposal outlines a series of initiatives designed to enhance diversity, equity, and inclusion (DEI) across the three graduate programs within the College of Pharmacy: Medicinal Chemistry, Pharmaceutical Sciences, and Clinical Pharmacy. We have designed a program to enhance the transition to graduate school, improve the retention, and solidify the completion rate. The program is composed of a series of five workshops for

students (one that includes faculty). We also have several initiatives to enhance their professional/academic development through DEI outreach activities.

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.

UL1 TR000433 (PI: Shanley) **PREVIOUS** **6/1/2014-5/31/2016**
NIH/National Center for Advancing Translational Sciences Total direct costs: $99,317
MICHR Translational Research Postdoctoral Award (Ahmed)
Using Computational Biology to Repurpose Existing Drugs

The goal of this project is to mine existing data from the Center for Chemical Genomics and the Honest Broker's Office to identify potential drugs for repurposing.

Role: Mentor

UL1 TR000433 (PI: Shanley) **PREVIOUS** **1/1/2015-4/30/2015**
NIH/National Center for Advancing Translational Sciences Total direct costs: $5,000
MICHR TREC Fellowship (Graham)
Antibiotic Resistance in the Clinic

The goal of this project is to expose graduate student Sarah Graham to translational research in antibiotic resistance. Genome sequencing is used to identify various single-site mutations that arise in the clinic. The work with bacteria from patient samples is guided by Prof. Betsy Foxman of the School of Public Health.

Role: Mentor

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

The major goal of this project is to provide solid techniques – based on multiple protein structures (MPS) – for incorporating protein flexibility into structure-based drug discovery. Development of a mixed solvent MD approach and application to HIV-1 protease and BACE1 are key specific aims.

U01 GM086873 (PI: Carlson) **PREVIOUS** **10/01/2008 – 9/30/2014**
NIH/NIGMS Annual direct costs: $657,895 ($376,600 to HAC)
Public/Private Collaboration for High-Quality Protein-Ligand Data

Development of the NIGMS's sole docking and scoring resource, inclusive of running docking exercises for the wider scientific community. The resource is called CSAR (the Community Structure-Activity Resource, www.csardock.org)

U01 GM086873-S1 (PI: Carlson) **PREVIOUS** **9/30/2009 – 8/31/2014**
NIH/NIGMS Total direct costs: $695,000
Public/Private Collaboration for High-Quality Protein-Ligand Data – Admin Supplement
Additional funds for equipment and a visiting scientist to augment the parent U01. Also, bridging funds to complete projects before review of CSAR center.

R01 GM088546-S1 (PI: Soellner) **PREVIOUS** **9/1/2011-8/31/2013**
NIH/NIGMS Annual direct costs to HAC: $56,000
Methodology for Identification of Substrate-Competitive Kinase Inhibitors – Admin Supplement
Additional funds are requested to use computational methods to explain unusual structure-activity relationships and altered modes of inhibition across a congeneric series of compounds.
Role: Collaborator, design and oversee execution of computational studies

MCB 0546073 (PI: Carlson) **PREVIOUS** **8/1/2006-7/31/2012**
NSF (MCB/DBI divisions) Annual direct costs: $106,250
CAREER: Protein-Ligand Databases in the Lab and Classroom
The goal of this research is to curate and mine Binding MOAD (Mother of All Databases), the largest collection of protein-ligand complexes augmented with binding affinity data. The specific aims are to (1) elucidate biophysical principles of molecular recognition using Binding MOAD, (2) provide the Binding MOAD website as an educational resource, and (3) expand and disseminate Binding MOAD to the scientific community.

CCMB Pilot Research Grant (CoPIs: Carlson&Gestwicki) **PREVIOUS** **1/1/2007-12/31/2009**
UMich Center for Computational Medicine and Biology Direct costs to HAC: $46,500
New Mechanisms of Inhibiting HIV-1 Protease
Funding to experimentally verify potential inhibitors of HIVp, identified through cheminformatics analysis and synthesized under the Valteich/Upjohn efforts below.
Role: Informatics PI (requires joint PIs from informatics and biology divisions)

P20 HG003890-S1 (PI: Shedden) **PREVIOUS** **8/1/2007-7/31/2008**
NIH/National Human Genome Research Institute (NHGRI) Annual direct costs for HAC: $35,000
MACE- Michigan Alliance for Cheminformatic Exploration
The Michigan Alliance for Cheminformatic Exploration (MACE) is an effort to integrate and build upon the cheminformatics and bioinformatics capabilities already in place at the University of Michigan. The Binding MOAD database will be used to provide protein-binding information for various chemical entities.
Role: Co-PI, incorporate protein-ligand data

R01 GM65372 yrs 01-05 (PI: Carlson) **PREVIOUS** **4/01/2002 – 3/31/2008**
NIH/National Institute of General Medical Sciences (NIGMS) Annual direct costs: $150,000
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) **PREVIOUS** **9/01/2002 – 8/31/2005**
Arnold and Mabel Beckman Foundation 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 = 41, I10-INDEX=74)

89. WKB Chan, HA Carlson, JR Traynor. Mixed-solvent molecular dynamics simulation-based discovery of a putative allosteric site on regulator of G protein signaling 4. *J. Comput. Chem.*, in revisions.

88. Z Xiong, M Jeon, RJ Allaway, J Kang, D Park, J Lee, H Jeon, M Ko, H Jiang, M Zheng, AC Tan, X Guo, The Multi-Targeting Drug DREAM Challenge Community, KK Dang, A Tropsha, C Hecht, TK Das, HA Carlson, R Abagyan, J Guinney, A Schlessinger, R Cagan. Crowdsourced identification of multi-1 target kinase inhibitors for RET- and TAU2-based disease: the Multi-Targeting Drug DREAM Challenge. *PLoS Comput. Biol.*, in review.

87. RD Smith, HA Carlson. Identification of cryptic binding sites using MixMD with standard and accelerated molecular dynamics. *J. Chem. Info. Model.* **2021**, *61*, 1287-1299.

86. LN Makley, OT Johnson, P Ghanakota, JN Rauch, D Osborn, TS Wu, T Cierpicki, HA Carlson, JE Gestwicki. Chemical Validation of a Druggable Site on Hsp27/HSPB1 using *In Silico* Solvent Mapping and Biophysical Methods. *Bioorg. & Med. Chem*. **2021**, *34*, 115990. *https://doi.org/10.1016/j.bmc.2020.115990*

85. JJ Clark, ZJ Orban, HA Carlson. Predicting binding sites from unbound vs. bound protein structures. *Sci. Reports* **2020**, *10*, 15856. *https://doi.org/10.1038/s41598-020-72906-7*

Paper #84 was highlighted by Faculty of 1000 (F1000.com, now F1000Prime)

84. RD Smith, JJ Clark, A Ahmed, ZJ Orban, JB Dunbar Jr., HA Carlson. Updates to Binding MOAD (Mother of All Databases): Polypharmacology tools and their utility in drug repurposing. *J. Mol. Biol.* **2019**, *431*, 2423-2433.

83. P Ghanakota, D DasGupta, HA Carlson. Free energies and entropies of binding sites identified by MixMD cosolvent simulations. *J. Chem. Info. Model*. **2019**, *59*, 2035-2045.

Paper #82 was highlighted by Faculty of 1000 (F1000.com, now F1000Prime)

82. JJ Clark, ML Benson, RD Smith, HA Carlson. Inherent versus induced protein flexibility: Comparisons within and between apo and holo structures. *PLoS Comput. Biol.* **2019**, *15*, e1006705. *https://doi.org/10.1371/journal.pcbi.1006705*

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, RD Smith, 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 Delproposto, 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.com, now F1000Prime)

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.

Papers #71 was highlighted on the cover of *Protein Science*

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.com, now F1000Prime)

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.com)

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.

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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.

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17. LM Sandvoss, HA Carlson. Conformational behavior of β-proline oligomers. *J. Am. Chem. Soc*. **2003**, *125*, 15855-15862.

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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.
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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.
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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.
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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 ACADEMIES OF SCIENCE, ENGINEERING, AND MEDICINE

- Member, Committee on Proposal Evaluation for Allocation of Supercomputing Time for the Study of Molecular Dynamics, Tenth Round" (9/2019)

NATIONAL SCIENCE FOUNDATION

- Ad hoc reviewer

NATIONAL INSTITUTES OF HEALTH

- Member, CSR Special Emphasis Panels and ad hoc assignments on standing study sections
  - ZRG1 BST-T (55) R – U24 Biomedical Data Repositories and Knowledgebases (6/2021)
  - ZRG1 CB-V (55) – R35 MIRA review (10/2020)
  - MSFD – Macromolecular Structure and Function D Study Section – (6/2020)
  - ZRG1 AARR-D (56) R – PAR-17-340: HIV Protease Evolution and Drug Resistance (12/2018)
  - 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*

MEMBERSHIP IN PROFESSIONAL ORGANIZATIONS

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

INVITED LECTURES

2021 Commencement Keynote Speaker, First-Gen Student Ceremony, University of Michigan, Ann Arbor
2021 Amber Developers' Meeting (Virtual)
2020 Free Energy Meeting, Novartis (Virtual)
2020 University of Wisconsin, Eau Claire, Chemistry Department Seminar (Virtual)
2020 Wayne State University, Physics Department Seminar, Detroit, MI (Virtual)
2019 Merck Pharmaceuticals, West Point, PA
2019 Keynote Speaker, Supercomputing Conference, University of Pittsburgh, PA
2019 ACS Webinar, "Cosolvent Molecular Dynamics: Mapping Protein Surfaces to Discover Allosteric Sites"
2019 4th Drug Discovery Reinvented 2019, Nassau, Bahamas
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 Colombia, 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

2021 Jelena Tošović, Ph.D. (Visiting Scientist)
2020 Sunil Tripathi, Ph.D. (Postdoctoral Fellow)
2020 Anthony Dominic (Adjunct Research Investigator)
2020 Swapnil Wagle, Ph.D. (Postdoctoral Fellow)
2020 Pancham Lal Gupta, Ph.D. (Postdoctoral Fellow)
2019 Antonio Mika (Pharm.D. Student)
2018 Wallace Chan, Ph. D. (Postoctoral Fellow) Primary advisor: John Traynor, Ph.D.
2018 Debarati DasGupta, Ph.D. (Postdoctoral Fellow)
2017 Richard D. Smith, Ph.D. (Assistant Research Scientist)

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)
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Anthony Dominic (Protein Structure-Function REU Summer Student, 2019)
Senior at North Central College, Naperville, IL

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Software Developer, Credit Acceptance Corporation

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Graduate Study in Bioinformatics, University of Michigan, Ann Arbor

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MD/PhD Graduate Study, University of Michigan, Ann Arbor

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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)