

# Abby L. Parrill-Baker

## DEGREES

DEGREE	DISCIPLINE	INSTITUTION	YEAR
Ph. D.	Chemistry Dissertation: Applications of Artificial Intelligence in Drug Design	University of Arizona	1996
M.S.	Chemistry Thesis: Supplemementing Traditional Chemical Education on the World Wide Web	University of Arizona	1996
B.S. with Honors	Chemistry	Central Michigan University	1992

## ADMINISTRATIVE EXPERIENCE

**Interim Provost**, University of Memphis, July 1, 2022 – June 30, 2023

- Lead the Division of Academic Affairs: 12 academic colleges and schools, the graduate school, the honors college, the university libraries, Lambuth campus, educational initiatives spanning early childhood-12<sup>th</sup> grade, continuing education and workforce development, institutional effectiveness and accreditation, institutional research, commencement, registrar, global initiatives, enrollment services, admissions operations, and former division of student affairs functions (student academic success, and dean of students who oversees student involvement, student accountability, student wellness and behavioral intervention)
  - Hired 2 deans (to lead Graduate School and Herff College of Engineering) and 4 interim deans (to lead Herff College of Engineering prior to start of recently hired dean, Fogelman College of Business and Economics, College of Arts and Sciences, College of Communication and Fine Arts)
  - Onboarded 8 new or interim deans (those hired as well as deans of the School of Public Health and the Loewenberg College of Nursing)
  - Instated annual professional development theme for 2023: Cultural Inclusivity
- Collaborate with President’s senior leadership team on institution-wide directions/concerns/issues/decisions/projects/responses and strategic planning
- Collaborate with Division of Research and Innovation to maintain/sustain Carnegie R1 status.
- Collaborate with University Advancement on fundraising initiatives
- Convene cross-institutional working groups on key issues relevant across academic affairs, examples include:
  - Transfer processes/policies/communications – example key outcome: MaxCredit Pledge (marketing material for new transfer students committing to maximize credit for past academic work and life experiences), designed to minimize time to degree completion and lower transfer barriers by consolidating all credit options into a single review
  - Earned admission pathways – example key outcome: pilot Tiger Prep Academy program for summer 2023 (adapted from highly successful LiFE Prep Academy designed for FedEx employee transition to college programs), self-paced mastery-based program teaches skills for academic success, life in general, and professional development – no risk model allows waitlisted applicants to participate at no charge as continuing education students, successful completion earns both admission and 12 pre-assessed experiential learning credits (cost incurred at time of completion can be fully or partially covered by scholarship depending on earned admission timeline), lack of completion has no financial or GPA consequences
- Serve on Tennessee Higher Education Commission task force to redefine academic program post-approval monitoring

**Dean,** College of Arts and Sciences (CAS), University of Memphis, May 1, 2019 – June 30, 2022 and July 1, 2023 - present

- Lead the College of Arts and Sciences, which consists of three grand divisions (natural sciences, social sciences, humanities) and the reserve officer training corps (ROTC) units which collectively are staffed by 550 faculty members, 450 graduate assistants, and 150 staff members
- Reclassified assistant director of interdisciplinary program position to director of interdisciplinary programs, and charged hire to assess workforce needs in interdisciplinary areas: key outcome was development of environmental science concentrations in several academic programs
- Manage CAS budget of ~\$62M
- Recruit and retain chairs, directors, and staff at the college level, and work collaboratively with chairs and directors to recruit and retain faculty and staff at the department level
- Evaluate chairs, directors, and CAS staff (~35 direct reports)
- Collaborate with Division of Research and Innovation to contribute to University achievement of Carnegie R1 status
- Collaborate with Deans of other units on interdisciplinary programs and projects
- Collaborate with Development on fundraising initiatives
- Support diversity, equity and inclusion as part of NSF ADVANCE (ASPIRED) project team
- Member of Core team for STEM Research and Classroom Building project
- Manage change through the pandemic, particularly supporting faculty and student transition to online teaching and learning

**Interim Dean,** College of Arts and Sciences, University of Memphis, February 1, 2019-April 31, 2019

- Lead interdisciplinary team to complete NIH Biomedical Research Facilities (C03) proposal (and revised proposal)
- Prepare of CAS budget presentation in collaboration with CAS senior staff and with input from CAS chairs/directors
- Collaboratively work with the Advancement Division, Disability Resources for Students, and Career Services on new programs and/or problem resolution

**Associate Dean,** College of Arts and Sciences, University of Memphis, 2014-2019

- Research development (Faculty Research Grant program, collaborative grant team assembly, Dean's representative on the University Research Council)
- Faculty development (Professional Development Award Program, collaborative faculty development workshops with Office of Research and Engineering and Herff College of Engineering)
- Dean's liaison with the College of Arts and Sciences External Advisory Board
- Dean's liaison to the Peer Power Foundation (led to Peer Power Institute at the University of Memphis)
- Contributor, STEM building proposal team, STEM building recommended for funding to the State of Tennessee by the Tennessee Higher Education Commission
- Work with Dean's senior staff to develop college actions for the University strategic plan

**Chair,** Department of Chemistry, University of Memphis, 2010-2014

- Lead team of six full-time staff, fifteen tenure-track and one non tenure-track faculty
- Managed departmental budget of about \$2.5M
- Networked with chemical industry leaders in Memphis to create student internship opportunities and solicit donations of funds and instrumentation

**Chair,** Board of Directors, The PRIZM Ensemble, 2016 - 2022

- Collaborate with the Board of Directors and Executive Director to ensure all programs align with the organization mission: PRIZM Builds Diverse Community through Chamber Music Education, Youth Development, and Performance.
- Lead strategic planning efforts
- Provide oversight of Executive Director (hire, promote professional development, manage annual performance review process, review budget and spending)

- Fundraising (donor stewardship activities, phone-a-thon contributor, routinely promote organization, grant writing)

## ACADEMIC/SCIENTIFIC EXPERIENCE

RANK/POSITION	DEPARTMENT	ORGANIZATION	PERIOD
Assistant/Associate/ Full Professor	Chemistry	University of Memphis	1998/2002/2006-
Visiting Scientist	Structural Biology	St. Jude Children's Research Hospital	2004-2005
Adjunct Assistant Professor	Medicinal Chemistry	University of Mississippi	2000-
Adjunct Assistant Professor	Pharmaceutical Sciences	University of Tennessee, Memphis	2000-
Lumsden Valrance Lecturer	Chemistry	Michigan State University	1996-1998
Instructor	Chemistry	Columbia Review (MCAT Review)	1993-1996
Graduate Teaching Assistant	Chemistry	University of Arizona	1992-1996
Co-op. Education Student	Analytical Chemistry	The DOW Chemical Co.	1990-1992

## HONORS/AWARDS

HONOR/AWARD	INSTITUTION/COMPANY/ORGANIZATION	YEAR
Commencement Speaker	University of Memphis	2017
Willard Sparks Eminent Faculty Award	University of Memphis Board of Visitors	2017
Distinguished Research Award	University of Memphis Alumni Association	2011
Distinguished Research Award	College of Arts and Sciences, The University of Memphis	2008
Olin Atkins Professorship	University of Memphis	2007-2010
Award for Teaching Excellence	College of Arts and Sciences, The University of Memphis	2007
Research Paper Competition Award	University of Memphis Sigma Xi Chapter	2001
Early Career Research Award	University of Memphis College of Arts and Sciences	2000
Golden Apple Award (teaching excellence)	Michigan State University Chapter of the American Medical Student Association	1997
Outstanding Student Presentation	International Cannabis Research Society Symposium on Cannabis and Cannabinoids	1995
Presentation Award	University of Arizona Student Showcase	1995
Excellence in Teaching	Department of Chemistry – University of Arizona	1994
Gregson Scholarship	Department of Chemistry – University of Arizona	1994
Meritorious Performance in Teaching	University of Arizona Foundation	1993
Excellence in Teaching	Department of Chemistry – University of Arizona	1993
Entrance Scholarship	Department of Chemistry – University of Arizona	1992
Outstanding College Chemistry Student	Midland American Chemical Society Section	1992
Special Recognition Award	The DOW Chemical Company	1992
Special Recognition Award	The DOW Chemical Company	1991
National Merit Scholar	National Merit Scholar	1988

## TEACHING EXPERIENCE

University of Memphis

- Developed and taught first online general education chemistry course (lecture and at-home laboratory)
- Developed and taught first online graduate chemistry course
- Developed and taught undergraduate and graduate organic, medicinal, computational, and biochemistry courses
- Developed and taught an honors forum course

University of Mississippi

- Graduate computational medicinal chemistry courses (adjunct)

Michigan State University

- Undergraduate organic courses
- University of Arizona
- Undergraduate laboratory courses and recitations

## STUDENT ADVISING/MENTORING:

Former and Current	Name	Timeframe
High School	11 students mentored in summer projects	2007-2012
Undergraduate	Over 80 students mentored for periods of 1 semester-2 years, including	1998-present
Masters	5 students earned thesis MS degrees	2004-present
Doctoral	19 students defended doctoral dissertations 1 student currently co-mentored	2001-present
Postdoctoral	5 postdoctoral scholars mentored	1998-2017

## RESEARCH/SCHOLARSHIP/CREATIVE ACTIVITIES:

### PUBLICATIONS

#### Books (authored, edited)

1. Parrill, A.L., Lipkowitz, K., eds., *Reviews in Computational Chemistry*, Volume 32, Wiley, **2022**.
2. Parrill, A.L., Lipkowitz, K., eds., *Reviews in Computational Chemistry*, Volume 31, Wiley, **2018**.
3. Parrill, A.L., Lipkowitz, K., eds., *Reviews in Computational Chemistry*, Volume 30, Wiley, **2017**.
4. Parrill, A.L., Lipkowitz, K., eds., *Reviews in Computational Chemistry*, Volume 29, Wiley, **2016**.
5. Parrill, A.L., Lipkowitz, K., eds., *Reviews in Computational Chemistry*, Volume 28, Wiley, **2015**.
6. Reddy, M.R.; Parrill, A.L., eds., *Rational Drug Design: Novel Methodology and Practical Applications*, ACS Symposium Series, Vol 719, 1999.

#### Refereed journal publications (Invited publications indicated by bold numbers)

7. Szwabowski, G.L.; Daigle, B.; Baker, D.L.; Parrill, A.L., "Structure-based Pharmacophore Modeling 2. Developing a Novel Framework for Structure-based Pharmacophore Model Generation and Selection", *J. Mol. Graph. Model.*, **2023**, online ahead of print, <https://doi.org/10.1016/j.jmgm.2023.108488>.
8. Szwabowski, G.L.; Baker, D.L.; Parrill, A.L., "Application of Computational Methods for Class A GPCR Ligand Discovery", *J. Mol. Graph. Model.*, **2023**, online ahead of print, doi: 10.1016/j.jmgm.2023.108434.
9. Szwabowski, G. L.; Cole, J.A.; Baker, D.L.; Parrill, A.L., "Structure-based Pharmacophore Modeling 1. Automated Random Pharmacophore Modle Generation", *J. Mol. Graph. Model.*, **2023**, online ahead of print, doi: 10.1016/j.jmgm.2023.108429.
10. Slayden, A.V.; Dyer, C.L.; Ma, D.; Li, W.; Bukiya, A.N.; Parrill, A.L.; Dopico, A.M., "Discovery of agonist-antagonist pairs for the modulation of Ca [2]<sup>+</sup> and voltage-gated K<sup>+</sup> channels of large conductance that contain beta1 subunits", *Bioorg. Med. Chem.*, **2022**, 68, 116876.
11. Thomas, B.N.; Parrill, A.L.; Baker, D.L.; "Self-docking and cross-docking simulations of G protein-coupled receptor-ligand complexes: Impact of ligand type and receptor activation state", *J. Mol. Graph. Model.*, **2022**, 112, 108119.
12. Castleman, P.; Szwabowski, G.; Bowman, D.; Cole, J.; Parrill, A.L.; Baker, D.L.; "Ligand-based G Protein Coupled Receptor Pharmacophore Modeling: Assessing the Role of Ligand Function in Model Development", *J. Mol. Graph. Model.*, **2022**, 111, 108107.
13. Szwabowski, G.L.; Castleman, P.N.; Sears, C.K.; Wink, L.H.; Cole, J.A.; Baker, D.L.; Parrill, A.L.; "Benchmarking GPCR Homology Model Template Selection in Combination with De Novo Loop Generation", *J. Computer-Aided Mol. Des.*, **2020**, 34(10), 1027-1044.
14. Morstein, J.; Dacheux, M.A.; Norman, D.D.; Shemet, A.; Donthamsetti, P.C.; Citir, M.; Frank, J.A.; Schultz, C.; Isacoff, E.Y.; Parrill, A.L.; Tigyi, G.J.; Trauner, D. "Optical Control of Lysophosphatidic Acid Signaling", *J. Am. Chem. Soc.*, **2020**, 142(24), 10612-10616.
15. Banerjee, S.; Norman, D.D.; Deng, S.; Fakayode, S.L.; Lee, S.C.; Parrill, A.L.; Li, W.; Miller, D.D.; Tigyi, G.J. "Molecular Modelling Guided Design, Synthesis and QSAR Analysis of New Small Molecule Non-Lipid Autotaxin Inhibitors", *Bioorg. Chem.*; **2020**, 103:104188
16. Wink, L.H.; Baker, D.L.; Cole, J.A.; Parrill, A.L. "A Benchmark Study of Loop Modeling Methods Applied to G Protein-Coupled Receptors", *J. Computer-Aided Mol. Design*, **2019**, 33:6, 573-595.
17. Morstein, J.; Hill, R.Z.; Novak, A.J.E., Feng, S.; Norman, D.D.; Donthamsetti, P.C.; Frank, J.A.; Harayama, T.; Williams, B.M.; Parrill, A.L.; Tigyi, G.J.; Riezman, H.; Isacoff, E.Y.; Bautista, D.; Trauner, D. "Optical Control of Sphingosine-1-phosphate Formation and Function", *Nature Chemical Biology*, **2019**, 15:6, 623-631.
18. Castleman, P.N.; Sears, C.K.; Cole, J.A.; Baker, D.L.; Parrill, A.L. "GPCR homology model template selection benchmarking: Global versus local similarity measures", *J. Mol. Graph. Model.*, **2019**, 86:235-246 DOI: 10.1016/j.jmgm.2018.10.016.

19. Gacasan, S.; Baker, D.L.; Parrill, A.L. "G Protein-Coupled Receptors: The Evolution of Structural Insight", *AIMS Biophysics*, **2017**, 4(3): 491-527.
20. Banerjee, S.; Norman, D.D.; Lee, S.C.; Parrill, A.L.; Pham, T.C.T.; Baker, D.L.; Tigyi, G.; Miller, D.D. "Highly Potent Non-Carboxylic Acid Autotaxin Inhibitors Reduce Melanoma Metastasis and Chemotherapeutic Resistance of Breast Cancer Stem Cells", *J. Med. Chem.*, **2017**, 60(4), 1309-1324. DOI: 10.1021/acs.jmedchem.6b01270
21. Ragle, L.E.; Palanisamy, D.J.; Joe, M.J.; Stein, R.S.; Norman, D.D.; Tigyi, G.; Baker, D.L.; Parrill, A.L. "Discovery and Synthetic Optimization of a Novel Scaffold for Hydrophobic Tunnel-Targeted Autotaxin Inhibition", *Bioorg. Med. Chem.*, **2016**, 24(19), 4660-4674.
22. Ragle, L.E.; Baker, D.L.; Parrill, A.L. "Structure-activity relationships of autotaxin inhibition", **2016**, *Current Topics in Biochemical Research*, 17, 1-18.
23. Parrill, A.L. "Synthetic Lipids and their Role in Defining Macromolecular Assemblies", *Chem. Phys. Lipids*, **2015**, 191, 38-47.
24. McMillan, J.E.; Bukiya, A.N.; Terrell, C.L.; Patil, S.A.; Miller, D.D.; Dopico, A.M.; Parrill, A.L. "Multi-generational pharmacophore modeling for ligands to the cholane steroid-recognition site in the  $\beta 1$  modulatory subunit of the BKCa channel", *J. Mol. Graph. Model.*, **2014**, 54C:174-183. doi: 10.1016/j.jmgm.2014.10.008
25. Bukiya, A.N.; McMillan, J.; Liu, J.; Shivakumar, B.; Parrill, A.L.; Dopico, A.M. "Activation of Calcium- and Voltage-Gated Potassium Channels of Large Conductance by Leukotriene B<sub>4</sub>", *J Biol Chem.* **2014** Nov 4. pii: jbc.M114.577825. PMID: 25371198
26. Parrill, A.L. "Design of Anticancer LPA Agonists and Antagonists", *Future Medicinal Chemistry*, **2014**, 6(8), 871-883.
27. Fells, J.I.; Lee, S.C.; Norman, D.D., Tsukahara, R.; Kirby, J.R.; Nelson, S.; Seibel, W.; Papoian, R.; Patil, R.; Miller, D.D.; Parrill, A.L.; Pham, T.C.; Bittman, R.; Tigyi, G. "Targeting the hydrophobic pocket of autotaxin with virtual screening of inhibitors identifies a common aromatic sulfonamide structural motif", *FEBS J.*, **2014**, 281(4), 1017-1028.
28. Norman, D.D.; Ibezim, A.; Scott, W.E.; White, S.; Parrill, A.L.; Baker, D.L. "Autotaxin Inhibition: Development and Application of Computational Tools to Identify Site-Selective Lead Compounds", *Bioorg. & Med. Chem.*, **2013**, 21(17), 5548-5560.
29. Fells, J.I.; Lee, S.C.; Fujiwara, Y.; Norman, D.D.; Lim, K.G.; Tsukahara, R.; Liu, J.; Patil, R.; Miller, D.D.; Kirby, R.J.; Nelson, S.; Seibel, W.; Papoian, R.; Parrill, A.L.; Baker, D.L.; Bittman, R.; Tigyi, G. "Hits of a High-Throughput Screen Identify the Hydrophobic Pocket of Autotaxin/Lysophospholipase D as an Inhibitory Surface", *Mol. Pharmacol.*, **2013**, 84(3), 415-424.
30. Bukiya, A.; McMillan, J.; Fedinec, A.; Patil, S.; Miller, D.; Leffler, C.; Parrill, A.; Dopico, A. "Cerebrovascular Dilation Via Selective Targeting of the Cholane Steroid-Recognition Site in the BK Channel  $\beta 1$  Subunit by a Novel Nonsteroidal Agent", *Mol. Pharmacol.*, **2013**, 83(5), 1030-1044.
31. Ren, F.; Bhana, S.; Norman, D.; Johnson, J.; Xu, L.; Baker, D.; Parrill, A.; Huang, X. "Gold nanorods carrying paclitaxel for photothermal - chemotherapy of cancer", *Bioconjugate Chem.*, **2013**, *Bioconjug. Chem.*, 24(3), 376-386.
32. Parrill, A.L. "Computational Design and Experimental Characterization of GPCR Segment Models", *Methods Enzymol.*, **2013**, 522, 81-95.
33. Young, J.K.; Clayton, B.T.; Kikonyogo, A.; Pham, T.C.T.; Parrill, A.L. "Structure Characterization of an LPA<sub>1</sub> Second Extracellular Loop Mimetic with a Self-Assembling Coiled-Coil Folding Constraint", *Int. J. Mol. Sci.*, **2013**, 14, 2788-2807. Doi:10.3390/ijms14022788
34. Parrill, A.L.; Tigyi, G. "Integrating the puzzle pieces: The current atomistic picture of phospholipid-G protein coupled receptor interactions", *Biochim. Biophys. Acta*, **2013**, 1831(1), 2-12. PMID: 22982815
35. Baker, D.L.; Parrill, A.L. "Polymer Concepts Illustrated in the Context of Biopolymers", in *Introduction of Macromolecular Science/Polymeric Materials into the Foundational Course in Organic Chemistry*, Chapter 7, **2013**, 85-93, *ACS Symposium Series*, Volume 1151. doi: 10.1021/bk-2013-1151
36. Ruddick, K.; Parrill, A.L. "JCE Classroom Activity #113: An Interlocking Building Block Activity in Writing Formulas of Ionic Compounds", *J. Chem. Educ.*, **2012**, 89(11), 1436-1438. DOI: 10.1021/ed200513y
37. Ruddick, K.; Parrill, A.L.; Petersen, R. "Introductory Molecular Orbital Theory: An Honors General Chemistry Computational Lab as Implemented in ChemBio3D Ultra 12.0", *J. Chem. Educ.*, **2012**, 89(11), 1358-1363. DOI: 10.1021/ed2003719
38. Kiss, G.N.; Fells, J.I.; Gupte, R.; Lee, S.C.; Liu, J.; Nusser, N.; Lim, K.G.; Ray, R.M.; Lin, F.T.; Parrill, A.L.; Sumegi, B.; Miller, D.D.; Tigyi, G.J. "Virtual Screening for LPA<sub>2</sub>-Specific Agonists Identifies a Nonlipid Compound with Antiapoptotic Actions", *Mol. Pharmacol.*, **2012**, 82(6), 1162-1173. PMID: 22968304
39. Parrill, A.L.; Lima, S.; Spiegel, S. "Structure of the first sphingosine 1-phosphate receptor", *Sci. Signal.*, **2012**, 5, pe23.
40. Singh, A.K.; McMillan, J.; Bukiya, A.N.; Burton, B.; Parrill, A.L.; Dopico, A.M. "Multiple cholesterol recognition/interaction amino acid consensus (CRAC) motifs in the cytosolic C tail of the slo1 subunit determine cholesterol sensitivity of Ca<sup>2+</sup> and voltage-gated K<sup>+</sup> (BK) channels", *J. Biol. Chem.*, **2012**, 287:20509-20521, DOI:10.1074/jbc.M112.356261.
41. Parrill, A.L. "Comparative modeling of lipid receptors", Chapter 12 in *Membrane Protein Structure: Methods and Protocols*, *Methods in Molecular Biology Series*, edited by N. Vaidehi and Klein-Seetharaman, J.; 2012, vol. 914, 207-218. DOI 10.1007/978-1-62703-023-6\_12.
42. Bukiya, A.N.; Singh, A.K.; Parrill, A.L.; Dopico, A.M. "The steroid interaction site in transmembrane domain 2 of the large conductance, voltage- and calcium-gated potassium (BK) channel accessory  $\beta 1$  subunit", *Proc. Natl. Acad. Sci. USA*, **2011**, 108:50, 20207-20212. PMID: 22123969
43. Parrill, A.L.; Wanjala, I.W.; Pham, T.C.T.; Baker, D.L. "Computational Identification and Experimental Characterization of Substrate Binding Determinants of Nucleotide Pyrophosphatase/Phosphodiesterase 7", *BMC Biochemistry*, **2011**, 12:65. doi:10.1186/1471-2091-12-65

44. Mize, C.D.; Abbott, A.M.; Gacasan, S.B.; Parrill, A.L.; Baker, D.L. "Ligand-Based Autotaxin Pharmacophore Models Reflect Structure-Based Docking Results", *J. Mol. Graph. Modelling*, **2011**, 31, 76-86.
45. Valentine, W.J.; Godwin, V.I.; Osborne, D.A.; Liu, J.; Fujiwara, Y.; Van Brocklyn, J.; Bittman, R.; Parrill, A.L.; Tigyi, G. "FTY720 (Gilenya) phosphate selectivity of sphingosine 1-phosphate receptor subtype 1 (S1P<sub>1</sub>) G protein-coupled receptor requires motifs in intracellular loop 1 and transmembrane domain 2", *J. Biol. Chem.*, **2011**, 286(35), 30513-30525. <http://www.jbc.org/cgi/doi/10.1074/jbc.M111.263442>.
46. Gupte, R.; Patil, R.; Liu, J.; Wang, Y.; Lee, S.C.; Fujiwara, Y.; Fells, J.; Bolen, A.L.; Emmons-Thompson, K.; Yates, C.R.; Siddam, A.; Panupinthu, N.; Pham, T.C.; Baker, D.L.; Parrill, A.L.; Mills, G.B.; Tigyi, G.; Miller, D.D. "Benzyl and Naphthalene-Methyl Phosphonic Acid Inhibitors of Autotaxin with Anti-invasive and Anti-metastatic Actions", *Chem. Med. Chem.*, **2011**, 6(5), 922-935.
47. Parrill, A.L.; Bautista, D.L. "GPCR Conformations: Implications for Rational Drug Design", *Pharmaceuticals* **2011**, 4, 7-43.
48. Parrill, A.L. "LPA receptor agonists and antagonists: WO2010051053", *Expert Opinion Ther. Patents*, **2011**, 21(2), 281-286.
49. Parrill, A.L.; Baker, D.L. "Autotaxin Inhibitors: A Perspective on First Medicinal Chemistry Efforts", *Expert Opinion Ther. Patents*, **2010**, 20(12), 1619-1625.
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51. Gupte, R.; Siddam, A.; Lu, Y.; Li, W.; Fujiwara, Y.; Panupinthu, N.; Pham, T.C.; Baker, D.L.; Parrill, A.L.; Mills, G.B.; Tigyi, G. "Synthesis and Pharmacological Evaluation of the Stereoisomers of 3-Carba Cyclic-Phosphatidic Acid", *Bioorg. Med. Chem. Letters*, **2010**, 20(24), 7525-7528.
52. Tsukahara, T.; Tsukahara, R.; Fujiwara, Y.; Yue, J.; Cheng, Y.; Guo, H.; Bolen, A.L.; Zhang, C.; Balazs, L.; Re, F.; Du, G.; Frohman, M.A.; Baker, D.L.; Parrill, A.L.; Uchiyama, A.; Kobayashi, T.; Tigyi, G. "Phospholipase D2-dependent Inhibition of the Nuclear Hormone Receptor PPAR $\gamma$  by Cyclic Phosphatidic Acid", *Mol. Cell*, **2010**, 39(3), 421-432.
53. Valentine, W.J.; Kiss, G.N.; Liu, J.; E, S.; Gotoh, M.; Murakami-Murofushi, K.; Pham, T.C.; Baker, D.L.; Parrill, A.L.; Lu, X.; Sun, C.; Bittman, R.; Pyne, N.J.; Tigyi, G. "(S)-FTY720-vinylphosphonate, an analogue of the immunosuppressive agent FTY720, is a pan-antagonist of sphingosine 1-phosphate GPCR signaling and inhibits autotaxin activity", *Cell Signal.*, **2010**, 22(10):1543-1553.
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55. Fells, J.I.; Tsukahara, R.; Liu, J.; Tigyi, G.; Parrill, A.L. "2D Binary QSAR Modeling of LPA<sub>3</sub> Receptor Antagonism", *J. Mol. Graph. Modelling*, **2010**, 28(8), 828-833.
56. North, J.E.; Howard, A.L.; Wanjala, I.W.; Pham, T.C.T.; Baker, D.L.; Parrill, A.L. "Pharmacophore Development and Application Toward the Identification of Novel, Small-Molecule Autotaxin Inhibitors", *J. Med. Chem.*, **2010**, 53(8), 3095-3105.
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**Refereed conference publications - note that many of these duplicate publications from the preceeding section**

1. Sardar, V.M.; Bautista, D.L.; Fischer, D.J.; Yokoyama, K.; Nusser, N.; Virag, T.; Wang, D.; Baker, D.L.; Tigyi, G. and Parrill, A.L. "Molecular Basis for Lysophosphatidic Acid Receptor Antagonist Selectivity", *Biochim. Biophys. Acta*, *1582*(1-3), 310-318.
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#### **Nonrefereed publications and patent applications**

- Miller, D.D.; Tigyi, G.T.; Banerjee, S.; Parrill-Baker, A.L., "Autotaxin Inhibitors", United States Patent Number 11,124,490, filed 6/2/2017, issued 9/21/2021.
- Parrill-Baker, A.L.; Baker, D.L. "Autotaxin Inhibitors", United States Patent Number 8,969,590, filed 9/18/2012, issued 3/3/2015.
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## **PRESENTATIONS**

### **INVITED PRESENTATIONS**

#### **Conferences**

- Parrill, A.L. "A Career Built on Collaborative Investigations of Membrane Protein Structure, Function, and Ligand Discovery", Women in Chemistry Symposium, Southeast Regional Meeting of the American Chemical Society, Birmingham, AL, November 10-13<sup>th</sup>, 2021.
- Parrill, A.L. "Collaborative Investigations of Membrane Protein Structure and Function", Diversity Awareness Symposium Highlighting Research and Collaboration, Saturday, April 27<sup>th</sup>, 2013
- Parrill, A.L. "Rational Approaches to Discovery of Autotaxin Inhibitors", 2011 FASEB Summer Research Conference on "Lysophospholipid Mediators in Health and Disease", Lucca, Italy, August 14-19<sup>th</sup>, 2011.
- Parrill, A.L. "Computer-Guided Discovery of Autotaxin Inhibitors", 2<sup>nd</sup> Western Canadian Medicinal Chemistry Workshop (WCMCW), Saskatoon, Canada, September 24-26, 2010.
- Parrill, A.L. "Discovering Autotaxin Inhibitors", Bioactive Lipids Meeting, Cancun, Mexico, October 25-28, 2009.
- Parrill, A.L. "Development, Validation, and Application of Binary QSAR Models to Identify and Optimize Leads to Interface with Bioactive Phospholipid Function", Chemical Computing Group North American User Group Meeting 2009, Montreal, Quebec, Canada, June 25-26<sup>th</sup>, 2009.

7. Parrill, A.L. "In-Silico Discovery of Potent, Non-Lipid Lysophosphatidic Acid Receptor Antagonists", 2007 FASEB Summer Research Conference on "Lysophospholipid Mediators in Health & Disease", Tucson, AZ, June 9-14, 2007.
8. Parrill, A.L. "Molecular Insights into Lysophosphatidic Acid Receptor Agonism", BioScience2005 - from genes to systems, Glasgow, Scotland, July 17-21, 2005.
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16. Parrill, A. L. "Computational Studies of HIV Integrase Inhibition", 10<sup>th</sup> Annual Great Lakes College Chemistry Conference, Michigan State University, April 8, 2000.
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18. Parrill, A.L.; Nakhleh, M.; Donovan, W. "Student Motivation: The Leveling Impact of Activities Outside the Box", 218<sup>th</sup> National Meeting and Exposition, New Orleans, LA August 1999.
19. Parrill, A. L., Dewan, M., Ellsworth, J. Donovan, W., Nakhleh, M. "Facilitating Chemical Education with Computers: Interactive Materials for Students and Organizational Tools for Teachers", Central Regional ACS Meeting, Columbus, OH, June 21-23, 1999.
20. Parrill, A.L.; Harrison, J.F. "Incorporating Computational Chemistry and Molecular Modeling into the Curriculum: The Short Version of a Very Long Story", 15<sup>th</sup> Biennial Conference on Chemical Education, Waterloo, Ontario, Canada, August 1998.
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#### **Other (universities/industry)**

24. Parrill, Abby L., "GPR88 Receptor Ligand Discovery: Tools to Guide Drug Discovery for Schizophrenia", Department of Chemistry seminar, University of Central Arkansas, January 25, 2019.
25. Parrill, Abby L., "G-Protein Coupled Receptor Studies: From Structural Details to Functional Definition", Outstanding Women in Science Seminar Series, University of Alabama-Birmingham, Tuesday, February 7, 2017.
26. Parrill, Abby L. "Undergraduate Investigations of G Protein-Coupled Receptor Structures and Ligand Interactions", Freed-Hardeman University, Thursday, November 10, 2016.
27. Parrill, Abby L. "Undergraduate Investigations of G Protein-Coupled Receptor Structures and Ligand Interactions", Rust College, Thursday, October 20, 2016.
28. Parrill, Abby L. "Evolving Approaches to Characterization of the Structure-Function Relationship in Lipid Receptors", Lipids at Wayne seminar series, Wayne State University, Wednesday, March 4<sup>th</sup>, 2015.
29. Parrill, Abby L. "Progress Toward a Transferable Water Soluble GPCR Design", Department of Chemistry Seminar, University of Missouri St. Louis, Monday, October 27<sup>th</sup>, 2014.
30. Parrill, Abby L. "Rational Approaches to Autotaxin Inhibition", Department of Chemistry Seminar, Union University, Friday, April 20<sup>th</sup>, 2012.
31. Parrill, Abby L. "Rational Approaches to Autotaxin Inhibition", Department of Chemistry Seminar, Jacksonville State University, Wednesday, October 19<sup>th</sup>, 2011.
32. Parrill, Abby L. "Rational Approaches to Autotaxin Inhibition", Department of Chemistry Seminar, Auburn University, Thursday, October 20<sup>th</sup>, 2011.
33. Parrill, Abby L. "Computer-Guided Discovery of Autotaxin Inhibitors", Department of Chemical Biology Seminar, St. Jude Children's Research Hospital, Friday, December 17<sup>th</sup>, 2010.

34. Parrill, Abby L. "Computer-Guided Discovery of Autotaxin Inhibitors", McGovern Lecture, University of Houston, December 9<sup>th</sup>, 2010.
35. Parrill, Abby L. "Computer-Guided Discovery of Autotaxin Inhibitors", Department of Chemistry Seminar, University of Mississippi, October 9<sup>th</sup>, 2010.
36. Parrill, Abby L. "Computer-Guided Discovery of Autotaxin Inhibitors", Department of Pharmaceutical Sciences Seminar, University of Tennessee Health Sciences Center, August 30<sup>th</sup>, 2010.
37. Parrill, Abby L. "Rational Approaches to Autotaxin Inhibition", Department of Pharmacology Seminar, University of Tennessee Health Sciences Center, Wednesday, March 24<sup>th</sup>, 2010.
38. Parrill, Abby L. "Targeted Intervention in Phospholipid Function", Department of Medicinal Chemistry Seminar, University of Utah, Monday, April 20, 2009.
39. Parrill, Abby L. "Targeted Intervention in Phospholipid Function", Department of Chemistry Seminar, Duquesne University, Monday, February 23, 2009.
40. Parrill, Abby L. "Targeted Intervention in Phospholipid Function", Department of Medicinal Chemistry Seminar, The University of Mississippi, Tuesday, September 16, 2008.
41. Parrill, Abby L. "Targeted Intervention in Phospholipid Function", Department of Pharmacology Seminar, The University of Pittsburgh, Tuesday, September 9, 2008.
42. Parrill, A.L. "Integrating Experimental and Computational Approaches to Characterize S1P Receptor Structure and Ligand Recognition", National Institutes of Health, National Institute of Diabetes and Digestive and Kidney Diseases, Genetics of Development and Disease Branch, Wednesday, June 10, 2008.
43. Parrill, A.L. "Integrating Experimental and Computational Approaches to Characterize S1P Receptor Structure and Ligand Recognition", University of California Davis, Thursday, April 24, 2008.
44. Parrill, A.L. "Integrating Experimental and Computational Approaches to Characterize S1P Receptor Structure and Ligand Recognition", Exelixis, South San Francisco, CA, Friday, April 25, 2008.
45. Parrill, A.L. "Integrating Experimental and Computational Approaches for Therapeutic Lead Discovery", Plenary Lecture, The University of Memphis Department of Chemistry Undergraduate Research Conference, February 23, 2008.
46. Parrill, A.L. "In-Silico Discovery of Potent, Non-Lipid Lysophosphatidic Acid Receptor Antagonists", University of North Carolina Greensboro, Friday, September 28, 2007.
47. Parrill, A.L. "Structural Biology of Membrane Proteins: Complementary Experimental and Theoretical Approaches", Hood College, Wednesday, February 21, 2007.
48. Parrill, A.L. "Structural Characterization of Membrane Proteins: Complementary Experimental and Theoretical Approaches", University of Tennessee Health Sciences Center, Friday, May 12, 2006.
49. Parrill, A.L. "Modeling LPA Production and Action", National Institutes of Health, Wednesday, October 19, 2005.
50. Parrill, A.L. "Computational and Experimental Characterization of Phospholipid Growth Factor Receptor Structures", University of Tennessee Health Sciences Center, Pharmaceutical Sciences Departmental Seminar, Monday, April 25, 2005.
51. Parrill, A.L. "Computational and Experimental Characterization of Phospholipid Growth Factor Receptor Structures", Vanderbilt University, Institute for Chemical Biology Seminar, Wednesday, April 20, 2005.
52. Parrill, A.L. "Distinct and Conserved Residues Mediate Sphingosine-1-Phosphate Recognition by Sphingosine-1-Phosphate Receptors", University of Mississippi, Chemistry Departmental Seminar, Thursday, September 9, 2004.
53. Parrill, A.L. "Distinct and Conserved Residues Mediate Sphingosine-1-Phosphate Recognition by Sphingosine-1-Phosphate Receptors", University of Alabama, Chemistry Departmental Seminar, Thursday, November 11, 2004.
54. Parrill, A.L. "Distinct and Conserved Residues Mediate Sphingosine-1-Phosphate Recognition by Sphingosine-1-Phosphate Receptors", Murray State University, Chemistry Departmental Seminar, Monday, December 6, 2004.
55. Parrill, A. L. "Model-Driven Structural Characterization of Phospholipid Growth Factor Receptors", Western Kentucky University, Chemistry Departmental Seminar, Friday, January 30, 2004.
56. Parrill, A. L. "Model-Driven Structural Characterization of Phospholipid Growth Factor Receptors", St. Jude Children's Research Hospital – Structural Biology Seminar, Tuesday, January 20, 2004.
57. Parrill, A. L. "Structural Studies on Membrane Bound Receptors", Mississippi College – Chemistry Departmental Seminar, Monday, November 3, 2003.
58. Parrill, A. L. "Characterizing Membrane Protein Structure using Computational Modeling and Site-Directed Mutagenesis", Rhodes College – Departmental Seminar, Monday, October 1, 2001.
59. Parrill, A. L. "G Protein Coupled Receptors: Insights into Ligand Recognition and Selectivity from Molecular Modeling", University of Memphis and University of Tennessee Health Science Center – Joint Program in Biomedical Engineering Seminar, Friday, October 12, 2001.
60. Parrill, A. L. "G Protein Coupled Receptors: Insights into Ligand Recognition and Selectivity from Molecular Modeling", University of Memphis – Departmental Seminar, Friday, September 28, 2001.
61. Parrill, A. L. "Modeling and Validation of the EDG Receptors", University of Alberta – Signal Transduction Research Group Seminar, Thursday, August 9, 2001.
62. Parrill, A. L. "The Chemistry of Artificial Sweeteners", Collierville High School, Thursday, April 12, 2001.
63. Parrill, A. L. "Modeling HIV Integrase Inhibition", Austin Peay State University – Departmental Seminar, Thursday, March 22, 2001.
64. Parrill, A. L. "Ligand Recognition in the Endothelial Differentiation Gene Receptor Family", Ceretek, Friday, March 9, 2001.

65. Parrill, A. L. "Using computational chemistry to understand protein-ligand interactions", Tennessee State University, Department of Chemistry - Departmental Seminar, Thursday, September 28, 2000.
66. Parrill, A. L. "Molecular Modeling and Experimental Validation of Membrane Protein Structures", University of Missouri, St. Louis, Department of Chemistry - Departmental Seminar, Monday, September 18, 2000.
67. Parrill, A. L. "How phospholipid growth factors recognize their receptor: A computational modeling-driven approach", University of Tennessee, Memphis, Department of Physiology - Departmental Seminar, Thursday, September 14, 2000.
68. Parrill, A. L. "Modeling and Model Validation of the G Protein-Coupled Receptor, Edg-1", University of Tennessee, Memphis, Department of Pharmaceutical Sciences - Departmental Seminar, Monday, April 24, 2000.
69. Parrill, A. L. "Computational Investigations into the Mechanism of Metal Ion Influence on HIV Integrase Inhibition", University of Kentucky Department of Chemistry - Departmental Seminar, Thursday, January 27, 1999.
70. Parrill, A. L. "Dynamic Modeling of G Protein-Coupled Receptor Structural Changes Induced by Site-Directed Mutations", Murray State Department of Chemistry - Departmental Seminar, Monday, November 8, 1999.
71. Parrill, A. L. "Computational Exploration of the Anticancer Activity Mechanism for an Unusual Anthracycline", Tennessee Tech Department of Chemistry - Departmental Seminar, Friday, October 8, 1999.
72. Parrill, A.L. "Computer Modeling to Understand Antitumor Activity", Union University Department of Chemistry – Departmental Seminar, Thursday, April 15, 1999.
73. Parrill, A.L. "Computational Chemistry Applied to Understanding the Antitumor Activity of 14-Acyl Anthracyclines", University of Mississippi Department of Chemistry – Departmental Seminar, Friday, April 9, 1999.
74. Parrill, A.L. "Opportunities for Women in Science: Networking, Funding, and Training", Middle Tennessee State University – Women in Science Seminar Series, Wednesday, March 3, 1999.
75. Parrill, A.L. "Modeling Biochemical Interactions: Examples Relevant to HIV and Cancer", Middle Tennessee State University Department of Chemistry – Departmental Seminar, Thursday, March 4, 1999.
76. Parrill, A.L. "G-Protein Coupled Receptor Modeling: From Two-Dimensional Sequence to Three-Dimensional Structure", University of Memphis Department of Computer Science – Computational Biology Seminar, Tuesday, February 23, 1999.
77. Parrill, A.L. "Supplementing Experiment with Computational Chemistry to Better Understand Drug Action: The Role of Protein Kinase C in the Antitumor Activity of AD198", Arkansas State University Department of Chemistry – Departmental Seminar, Friday, February 12, 1999.
78. Parrill, A.L. "Computational Modeling of Protein-Ligand Interactions of the EDG Receptor Family and HIV-1 Integrase", University of Cincinnati Department of Chemistry – Biochemistry Divisional Seminar, Tuesday, December 1, 1998.
79. Parrill, A.L. "Modeling Protein/Ligand Interactions from Many Directions: A Look at HIV-Integrase Inhibition and the Lysophosphatidic Acid Receptor Family", University of Mississippi Department of Medicinal Chemistry – Departmental Seminar, Tuesday, November 10, 1998.
80. Parrill, A.L. "Computational Chemistry Methods and Applications in Pharmaceutical Research", University of Tennessee at Memphis Department of Pharmacology – Departmental Seminar, Friday, September 25, 1998.
81. Parrill, A.L. "Innovative Classroom Practices and Their Impact on Classroom Atmosphere", Louisiana State University Department of Chemistry – Departmental Seminar, Friday, September 11, 1998.
82. Parrill, A.L. "Innovative Classroom Practices: Their Impact on Student Learning and Assessment", Louisiana State University Teaching Series, Thursday, September 10, 1998.
83. Parrill, A.L. "Supplementing Chemical Education on the World Wide Web", Central Michigan University Department of Chemistry – Departmental Seminar, Fall, 1997.

### **OTHER PRESENTATIONS**

84. Szwabowski, G.L.; Griffing, M.C.; Guerrero, M.; Ruddick, K.R.; Cole, J.A.; Baker, D.L., Parrill A.L., "A Method of Automated Pharmacophore Model Generation Using Multiple Copy Simultaneous Search" National American Chemical Society Meeting, August 2021.
85. Orellana, K.\*; Dyer, C.\*; Parrill, A.L.; Baker, D.L., "Statistical Analysis of Protein Similarity Measures?" National American Chemical Society Meeting, August 2021.
86. Hoffman, B.\*; Wiley\*, E. R.; Baker, D.L., "Synthesis and Quantitative Analysis of Diffusible Signal Factor Analogs as Antibiofilm Agents" National American Chemical Society Meeting, August 2021.
87. Dyer, C.; Parrill, A.L.; Baker, D.L., "Hydrophobic Surface Patch Disruption to Produce Water-Soluble G-Protein Coupled Receptor Analogs" Southeast Regional Meeting of the American Chemical Society, November 2021.
88. Dyer, C.\*; Orellana, K.\*; Parrill, A.L.; Baker, D.L., "Statistical Analysis of Protein Similarity Measures", Southeast Regional Meeting of the American Chemical Society, November 2021.
89. Szwabowski, G.L.; Parrill, A.L.; Baker, D.L., "A method of automated, score-based pharmacophore generation using Multiple Copy Simultaneous Search" Southeast Regional Meeting of the American Chemical Society, November 2021.
90. Guerrero, M.; Szwabowski, G.L.; Ruddick, K.R.; Parrill, A.L.; Baker, D.L., "Experimental Validation of Computationally Generated Structure-Based Pharmacophores" Southeast Regional Meeting of the American Chemical Society, November 2021.
91. Hoffman, B. and Baker D.L., "Quantitative analysis of fatty acid diffusible signaling factors by HPLC-ESI-MS" Southeast Regional Meeting of the American Chemical Society, November 2021.
92. Wiley, E.R. and Baker, D.L., "Synthesis and characterization of novel diffusible signal factor analogs for analysis of structure activity relationships" Southeast Regional Meeting of the American Chemical Society, November 2021.

93. Ruddick, K.R., Elayan, A.M., Nelson, H.A., Lashet, C., Hanson, J., Parrill, A.L., Cole, J.A., and Baker, D.L., NanoLuc (NLuc) complementation assay elucidates role of specific G-proteins in GPR88 signaling. Experimental Biology National Meeting 2021. **CHOSEN** for additional GPCR colloquium by ASPET, ASBMB, and APS.
94. Castleman, G.L. Szwabowski, D. Bowman, J. Cole, A.L. Parrill-Baker, D.L. Baker “Pharmacophore benchmarking: The role of ligand function in pharmacophore development.” 2020 Rocky Mountain Regional Meeting of the American Chemical Society. November 2020. **AWARD:** Division of Medicinal Chemistry Award for presentation.
95. Szwabowski, G.L., Parrill, A.L., Baker, D.L., “Automated construction of fragment-based pharmacophores to elucidate novel GPCR ligands”, Rocky Mountain Regional Meeting of the American Chemical Society, November 2020
96. Dyer, C., Parrill, A.L., Baker, D.L., “Statistical Analysis of Protein-Protein Comparison Methods.” Rocky Mountain Regional Meeting of the American Chemical Society, November 2020. **AWARD:** Stanley C. Israel Regional Award for Advancing Diversity in the Chemical Sciences
97. Hoffman, B. and Baker, D.L., “Quantitative analysis of diffusible signaling factors using negative ion liquid chromatography electrospray ionization mass spectrometry (HPLCESI-MS)” Rocky Mountain Regional Meeting of the American Chemical Society, November 2020.
98. Wiley, E. R., and Baker, D. L., “Modular synthesis and characterization of diffusible signal factor analogs for the study of structure activity relationships and mechanism of action.” 2020 Rocky Mountain Regional Meeting of the American Chemical Society. Virtual. November 2020.
99. Thomas, B.N., Parrill, A.L., and Baker, D.L., “Self-docking and cross-docking simulations of G protein-coupled receptor-ligand complexes: analysis of ligand type and receptor activation state”, Rocky Mountain Regional Meeting of the American Chemical Society, November 2020.
100. Griffing, M., Baker, D.L., and Parrill, A.L. “Systematic Analysis of Ligand Binding Site Locations Within Crystallized GPCR Complexes”, American Chemical Society Rocky Mountain Region Meeting, November 2020.
101. Castleman, Paige N.; Szwabowski, Gregory L.; Baker, Daniel L.; Parrill, Abby L. “Pharmacophore benchmarking: The role of ligand function in pharmacophore development.” 2019 Southeast Regional Meeting of the American Chemical Society. Savannah, GA. 2019.
102. Szwabowski, G.L.; Castleman, P.N.; Sears, C.K.; Wink, L.H.; Cole, J.A.; Baker, D.L.; Parrill, A.L. “Benchmarking GPCR homology model template selection in combination with de novo loop generation”, 2019 Southeastern Regional Meeting of the American Chemical Society, 2019.
103. Hannie, K.D.; Parrill, A.L.; Baker, D.L., “Computational and Experimental Filtering of Potential Therapeutics using ADMET Properties,” 258th American Chemical Society National Meeting and Exposition. San Diego, CA. August 26-28th, 2019.
104. Castleman, P.N., Cole, J.A., Baker, D.L., and Parrill, A.L., “Homology Model Template Selection Benchmarking: Global Versus Local Similarity Measures”, National Meeting of the American Chemical Society, 2018.
105. Castleman, P.N., Cole, J.A., Baker, D.L., and Parrill, A.L., “Homology Model Template Selection Benchmarking: Global Versus Local Similarity Measures”, 74th Annual Meeting of the Southwest Region of the American Chemical Society, 2018.
106. Sears, C.K., Parrill, A.L., and Baker, D.L., “Development of a G Protein-Coupled Receptor Deorphanization Protocol: Application to GPR37L1”, 74th Annual Meeting of the Southwest Region of the American Chemical Society, 2018.
107. Emma G. Jackson and Abby L. Parrill, “GPR88 Modeling and Antagonist Discovery”, 67th Southeast/71st Southwest Joint Regional Meeting of the American Chemical Society, Memphis, TN, United States, November 4-7 (2015).
108. Rachel Coleman and Abby Parrill-Baker, “Modeling GPR6: A Potential Therapeutic Target in the treatment of Parkinson's Disease”, 67th Southeast/71st Southwest Joint Regional Meeting of the American Chemical Society, Memphis, TN, United States, November 4-7 (2015).
109. Natalie Galindo and Abby Parrill, “GPR31 Modeling and Pharmacophore-Guided Antagonist Discovery”, 67th Southeast/71st Southwest Joint Regional Meeting of the American Chemical Society, Memphis, TN, United States, November 4-7 (2015).
110. Jay M. Yarbro, Samantha B. Gacasan, Jesse Ziebarth, Yongmei Wang, Abby L. Parrill-Baker, Ramin Homayouni, “(NIPSNAP1) with NAD and NADH”, 67th Southeast/71st Southwest Joint Regional Meeting of the American Chemical Society, Memphis, TN, United States, November 4-7 (2015).
111. L. Ragle, D.L. Baker, A.L. Parrill, “Expanded structure-activity relationship analysis of small molecule autotaxin inhibitors” , 67th Southeast/71st Southwest Joint Regional Meeting of the American Chemical Society, Memphis, TN, United States, November 4-7 (2015).
112. S.B. Gacasan, V.I. Godwin, L. Wink, B. Nguyen, P. Kurtzweil, L. Church, S. Iqbal, A. Kikonyogo, A.L. Parrill, “Investigating function of water-soluble  $\beta$ 2 adrenoreceptor mimics using circular dichroism”, 67th Southeast/71st Southwest Joint Regional Meeting of the American Chemical Society, Memphis, TN, United States, November 4-7 (2015).
113. L. Wink, A. Kikonyogo, A.L. Parrill, “Applying comparative modeling strategies and virtual docking toward deorphanization of GPR26” , 67th Southeast/71st Southwest Joint Regional Meeting of the American Chemical Society, Memphis, TN, United States, November 4-7 (2015).
114. Parrill, A.L.; Tigyi, G. “Integrating the Puzzle Pieces of Phospholipid-receptor Interactions”, G-protein-coupled-receptors: from structural insights to functional mechanisms, co-organized by the Biochemical Society and Monash University, Prato, Italy, September 2012.
115. Pham, T. C. T.; Wanjala, I. W.; Howard, A. L.; Breland, D. K.; DeYonker, N. J.; Webster, C. E.; Parrill, A. L.; Baker, D. L. “Characterizing the structure and function of lipid preferring nucleotide pyrophosphatase phosphodiesterases using computational and experimental methods”, 63<sup>rd</sup> Southeast Regional Meeting of the American Chemical Society, Richmond, VA, United States, October 26-29, 2011.

116. Norman, D. D.; Scott, W. E.; White, S.; Ibezim, A.; Parrill, A. L.; Baker, D. L. "ATX inhibition: Development of computational tools to identify hydrophobic tunnel targeted leads", 63<sup>rd</sup> Southeast Regional Meeting of the American Chemical Society, Richmond, VA, United States, October 26-29, 2011.
117. Baker, D.L.; Mize, C.; Abbott, A.; Parrill, A.L. "Design and application of computational tools for the rational design and discovery of Autotaxin inhibitors", 241<sup>st</sup> American Chemical Society National Meeting & Exposition, Anaheim, CA, United States, March 27-31, 2011.
118. Parrill, A.L.; Howard, A.L.; Wanjala, I.W.; Baker, D.L. "Insights into substrate recognition and discrimination by the phospholipid-preferring Nucleotide Pyrophosphatase/Phosphodiesterase isoforms", 241<sup>st</sup> American Chemical Society National Meeting & Exposition, Anaheim, CA, United States, March 27-31, 2011.
119. Baker, D.L.; Wanjala, I.W.; Parrill, A.L. "Characterization of substrate specifying determinants of nucleotide pyrophosphatase phosphodiesterase severn", 66<sup>th</sup> SWRM/62<sup>nd</sup> SERMACS, New Orleans, LA, November 30<sup>th</sup>-December 4<sup>th</sup>, 2010.
120. Pham, T.T.; Wanjala, I.; Howard, A.; Parrill, A.L.; Baker, D.L. "Insights into the structure and function of lipid preferring Nucleotide Pyrophosphatase Phosphodiesterase isoforms", 66<sup>th</sup> SWRM/62<sup>nd</sup> SERMACS, New Orleans, LA, November 30<sup>th</sup>-December 4<sup>th</sup>, 2010.
121. Parrill, Abby L.; North, E. Jeffrey; Hoeglund, Adrienne; Bostic, Heidi; Best, Michael D; Baker, Daniel L "Computer-Guided Discovery of Autotaxin Inhibitors", 240<sup>th</sup> ACS National Meeting & Exposition, Boston, Massachusetts, August 22-26, 2010.
122. Wanjala, Irene W.; Parrill, Abby L.; Baker, Daniel L. Structural and Functional Characterization of Alkaline Sphingomyelinase (NPP7). 38<sup>th</sup> Great Lakes Regional Meeting of the American Chemical Society, Chicago, IL, United States, May 13-16, 2009.
123. Xu, X.; Zhang, H.; Parrill, A.; Tigyi, G.; Prestwich, G. D. "Lysophosphatidic acid (LPA) antagonists treat breast and lung cancer in engineered tumor models" 237<sup>th</sup> ACS National Meeting, Salt Lake City, UT, March 22-26<sup>th</sup>, 2009.
124. Shaffer, R.; Bonilla, E.; Parrill, A.L. "Unlocking the Structure of G-Protein Coupled Receptors", 29<sup>th</sup> Annual Undergraduate Research Conference, The University of Memphis, February 28<sup>th</sup>, 2009.
125. McMillan, J.; Bukiya, A.; Dopico, A.; Parrill, A.L. "Computational Methods to Discriminate Between Active and Inactive Anti-Hypertensive Compounds", 29<sup>th</sup> Annual Undergraduate Research Conference, The University of Memphis, February 28<sup>th</sup>, 2009.
126. Ghaila, K. C.; Parrill, A.L. "A Computational Model of Nucleotide Pyrophosphatase/Phosphodiesterase 4 (NPP4) for Substrate Determination", 29<sup>th</sup> Annual Undergraduate Research Conference, The University of Memphis, February 28<sup>th</sup>, 2009.
127. Williams, J.R.; Perygin, D.H.; Parrill, A.L.; Fujiwara, Y.; Tigyi, G. "Identification of Cationic Residues Involved in Ligand Recognition at the Lysophosphatidate Receptor, LPA<sub>5</sub>", 60<sup>th</sup> Southeastern Regional Meeting of the American Chemical Society, Nashville, TN, United States, November 12-15 (2008).
128. Pham, Truc-Chi T.; Hoeglund, Adrienne; Baker, Daniel L.; Parrill, Abby. Pharmacological Characterization of Candidate Drug-Like Autotaxin Inhibitors. 60<sup>th</sup> Southeast Regional Meeting of the American Chemical Society, Nashville, TN, United States, November 12-15 (2008).
129. Wanjala, Irene W.; Parrill, Abby L.; Baker, Daniel L. Computational and Experimental Approaches for the Analysis of Alkaline Sphingomyelinase (Alk-SMase/NPP7). 60<sup>th</sup> Southeast Regional Meeting of the American Chemical Society, Nashville, TN, United States, November 12-15 (2008).
130. Williams, J.R.; Perygin, D.H.; Fujiwara, Y.; Tigyi, G.; Parrill, A.L. "Identification of Cationic Residues Involved in Ligand Recognition at the Lysophosphatidate Receptor, LPA<sub>5</sub>", 16<sup>th</sup> Annual NHLBI Cardiovascular Diversity Research Supplement Awardee Session, Saturday, 11/8/08.
131. North, E. J.; Baker, D. L.; Parrill, A. L. "Virtual and Combinatorial Advances in the Identification of Bioavailable Autotaxin Inhibitors," 60<sup>th</sup> Southeastern Regional Meeting of the American Chemical Society, Nashville, TN, November 12-15, 2008.
132. Montedonico, L.E.; Baker, D.L.; Parrill A.L. "Design and Biological Evaluation of Mechanism-Based Autotaxin Inhibitors", 60<sup>th</sup> Annual South Eastern Regional Meeting of the American Chemical Society, Nashville, TN, November 12-15, 2008.
133. Howard-Shearer, A.L.; Baker, D.L.; Parrill A.L. "Computational and Mutagenic Studies of NPP6", 60<sup>th</sup> Southeastern Regional Meeting (SERMACS), Nashville, TN, November 12-15, 2008.
134. Clayton, B. T.; Parrill, A. L. "Design of LPA<sub>1</sub> Receptor Peptide Loop Mimetics and Determination of Secondary Structure Using Circular Dichroism", 64<sup>th</sup> Southwest Regional Meeting of the American Chemical Society, Little Rock, AR, United States, October 1-4 (2008).
135. North, E. J.; Baker, D. L.; Parrill, A. L. "Autotaxin Structure Activity Relationships Identified through Lysophosphatidylcholine Analogs", 64<sup>th</sup> Southwest Regional Meeting of the American Chemical Society, Little Rock, AR, United States, October 1-4 (2008).
136. Howard-Shearer, A. L.; Baker, D. L.; Parrill, A. L. "NPP6 Model Validation by Computational Docking and Mutagenesis", 64<sup>th</sup> Southwest Regional Meeting of the American Chemical Society, Little Rock, AR, United States, October 1-4 (2008).
137. Clayton, B. T.; Parrill, A. L. "Coiled-coils promote self-assembly of LPA receptor peptide loop mimetics", 236<sup>th</sup> ACS National Meeting, Philadelphia, PA, United States, August 17-21, 2008 (2008).
138. Williams, J. R.; Fujiwara, Y.; Tigyi, G.; Balasankoula, S.; Parrill, A. L. "Optimization of the LPA<sub>5</sub> receptor model for therapeutic lead discovery", 236<sup>th</sup> ACS National Meeting, Philadelphia, PA, United States, August 17-21, 2008.
139. Hoeglund, A.B.; Parrill, A.L.; Baker, D.L. "Screening and Identification of New Classes of Autotaxin (ATX) Inhibitors by Computational Modeling", Keystone Symposia: Computer-Aided Drug Design, Steamboat Springs, CO, March 29-April 3, 2008.
140. Parrill, A.L.; Hoeglund, A.B.; Echols, U.; Nguyen, T.; Pham, T.C.T.; Baker, D.L. "Computationally-Guided Discovery of Autotaxin Inhibitors", Joint Biophysical Society 52<sup>nd</sup> Annual Meeting & 16<sup>th</sup> IUPAB International Biophysics Congress, Long Beach, CA, February 2-6, 2008.

141. North, E. Jeffrey; Baker, Daniel L.; Parrill, Abby L. "Synthesis and Evaluation of Lysophosphatidylcholine Analogs as Tools to Determine Crucial Autotaxin Substrate Characteristics", 59th Southeast Regional Meeting of the American Chemical Society, Greenville, SC, October 24-27, 2007.
142. Fells, J. I. Jr.; Tsukahara, R.; Liu, J.; Fujiwara, Y.; Tigyi, G.; Parrill, Abby L. "Using Virtual Screening to Identify Bioactive Molecules", GTCbio 3rd Modern Drug Discovery & Development Summit, San Francisco, CA, November 28-30, 2007.
143. Howard, A.L.; Baker, D.L.; Parrill, A.L. "Spectroscopic and Functional Characterization of Human NPP6", 2007 FASEB Summer Research Conference on "Lysophospholipid Mediators in Health & Disease", Tucson, AZ, June 9-14, 2007.
144. North, E.J.; Baker, D.L.; Parrill, A.L. "Synthesis and Evaluation of LPC Analogues for Autotaxin Substrate Characterization", 2007 FASEB Summer Research Conference on "Lysophospholipid Mediators in Health & Disease", Tucson, AZ, June 9-14, 2007.
145. Pham, T.C.T.; Kriwacki, R.; Parrill, A.L. "Peptide Design and Structural Characterization of SIP<sub>4</sub> E1 Loop Mimetic", 2007 FASEB Summer Research Conference on "Lysophospholipid Mediators in Health & Disease", Tucson, AZ, June 9-14, 2007.
146. Tsukahara, T.; Tsukahara, R.; Cheng, Y.-H.; Zhang, C.; Balazs, L.; Du, G.; Frohman, M.A.; Baker, D.; Parrill, A.L.; Tigyi, G. "The Novel Second Messenger Cyclic Phosphatidic Acid Negatively Regulates Nuclear Hormone Receptor PPAR $\gamma$ ", 2007 FASEB Summer Research Conference on "Lysophospholipid Mediators in Health & Disease", Tucson, AZ, June 9-14, 2007.
147. Tsukahara, R.; Durgam, G.G.; Gududuru, V.; Fujiwara, Y.; Jiang, G.; Zhang, H.; Xu, Y.; Miller, D.D.; Prestwich, G.D.; Parrill, A.L.; Tigyi, G., "Identification and Classification of Selective Agonists and Antagonists of LPA Receptors", 2007 FASEB Summer Research Conference on "Lysophospholipid Mediators in Health & Disease", Tucson, AZ, June 9-14, 2007.
148. Valentine, W.J.; Mujahid, S.; Fells, J.; Yokoyama, K.; Fujiwara, Y.; Tsukahara, R.; Parrill, A.L.; Tigyi, G. "Conserved Residues Responsible for Ligand Recognition in the EDG-family Lysophosphatidic Acid Receptors", 2007 FASEB Summer Research Conference on "Lysophospholipid Mediators in Health & Disease", Tucson, AZ, June 9-14, 2007.
149. Clayton, Benjamin T.; Pham, Truc Chi; Parrill, Abby L. "Structural Characterization of Lysophosphatidic Acid G Protein-Coupled Receptors by NMR Spectroscopy", 19<sup>th</sup> Annual Univ. Memphis Student Research Forum, April 2, 2007.
150. Howard, Angela L.; Baker, Daniel L.; Parrill, Abby L. NPP6 as a Model of the Catalytic Domain of Autotaxin. 19th Annual University of Memphis Student Research Forum, April 2, 2007.
151. North, Elton Jeffrey; Baker, Daniel L.; Parrill, Abby L. Synthesis and Evaluation of Nonhydrolyzable Autotaxin Inhibitors. 19th Annual University of Memphis Student Research Forum, April 2, 2007.
152. Nau, F. J.; Parrill, A.L. "Toward Synthesis of Para-Alkyl Substituted Alcohols as Conformationally Constrained Fatty Alcohols", American Chemical Society 233<sup>rd</sup> National Meeting & Exposition, Chicago, IL, March 25-29, 2007.
153. Parrill, A.L., Fells, J.I.; Perygin, D.; Tsukahara, R.; Tigyi, G. "In-silico Discovery of Non-Lipid Lysophosphatidic Acid Receptor Antagonists", Gordon Research Conference: Molecular Pharmacology, Ventura Beach, California, January 28-February 2, 2007.
154. Fujiwara, Y.; Osborne, D.; Walker, M.; Wang, D.; Bautista, D.; Liliom, K.; Van Brocklyn, J.; Parrill, A.L.; Tigyi, G. "Identification of the Hydrophobic Ligand Binding Pocket of the SIP<sub>1</sub> Receptor", Gordon Research Conference: Molecular Pharmacology, Ventura Beach, California, January 28-February 2, 2007.
155. Tigyi, G.; E S.; Fujiwara, Y.; Tsukahara, R.; Li, C.; Naren, A.; Lin, F.; Parrill, A.L.; Deng, W. "Cellular Responses Mediated via C-terminal Macromolecular Complexes of LPA<sub>2</sub>", Gordon Research Conference: Molecular Pharmacology, Ventura Beach, California, January 28-February 2, 2007.
156. Osborne, D.A.; Fujiwara, Y.; Walker, M.D.; Wang, D.A.; Bautista, D.A.; Liliom, K.; VanBrocklyn, J.R.; Parrill, A.L.; Tigyi, G. "Identification of the Hydrophobic Binding Pocket of the SIP<sub>1</sub> Receptor", 15th Conference on Current Trends in Computational Chemistry, Jackson, MS November 3-4, 2006.
157. Afolabi, T.; Parrill, A.L. "QSAR Modeling of LPA<sub>3</sub> Receptor Activity" The 18th Annual Student Research Forum, The University of Memphis, Memphis, TN, April, 2006.
158. Afolabi, T.; Parrill, A.L. "QSAR Modeling of LPA<sub>3</sub> Receptor Activity" The 20th National Conference on Undergraduate Research, April 6-8, 2006.
159. James I. Fells, Sr., Abby L. Parrill, Ryoko Tsukahara, and Gabor Tigyi "Identifying Potential LPA<sub>3</sub> Antagonists Using In Silico Screening", 14th Conference on Current Trends in Computational Chemistry, Jackson, MS November 4-5, 2005.
160. Mor M. Naor and Abby L. Parrill "The Neighborhood Influence on Sphingosine 1-Phosphate pKa", 61st Southwest and 57th Southeast Joint Regional Meetings of the American Chemical Society, Memphis, TN, USA, Nov. 2005.
161. James I. Fells, Sr., Abby L. Parrill, Ryoko Tsukahara, and Gabor Tigyi "High-throughput Screening for LPA<sub>3</sub> Antagonist Selectivity", 57th Southeast / 61st Southwest Joint Regional American Chemical Society Meeting, Memphis, TN November 1-4, 2005.
162. Duane Miller, Gangadhar Durgam, Veeresa Gududuru, Gabor Tigyi, Abby Parrill, Eunju Hurh, Jim Dalton "Synthesis and Biological Evaluation of Lipid Ligands", 57th Southeast / 61st Southwest Joint Regional American Chemical Society Meeting, Memphis, TN November 1-4, 2005.
163. Truc-Chi T. Pham, Richard Kriwacki, Abby Parrill "Peptide Design and Structural Characterization of a GPCR Loop Mimetic", 57th Southeast / 61st Southwest Joint Regional American Chemical Society Meeting, Memphis, TN November 1-4, 2005.
164. Donna H. Perygin and Abby L. Parrill, "3-D Database Searching for the Identification of Novel LPA<sub>1</sub> Antagonists", 57th Southeast / 61st Southwest Joint Regional American Chemical Society Meeting, Memphis, TN November 1-4, 2005.
165. Baker, D.L.; Pigg, K. R.; Tsukahara, R.; Tigyi, G.; Parrill, A.L.; Li, Z.; Bittman, R. "Synthesis, Evaluation and Application of Benzophenone Analogs of Lysophosphatidic Acid and Alkyl Glycerophosphate", 2005 FASEB Summer Research Conference on "Lysolipids in Health and Disease", Snowmass, Colorado, June 11-16, 2005.

166. Tsukahara, T.; Yasuda, S.; Makarova, N.; Yuan, H.; Parrill, A.; Tigyi, G. "Analogues of Lysophosphatidic Acid are Novel Partial Agonists of PPAR $\gamma$ ", 2005 FASEB Summer Research Conference on "Lysolipids in Health and Disease", Snowmass, Colorado, June 11-16, 2005.
167. Fujiwara, Y.; Sardar, V.; Tokumura, A.; Baker, D.; Murakami-Murofushi, K.; Parrill, A.; Tigyi, G. "Identification of Residues Responsible for Ligand Recognition and Regioisomeric Selectivity of LPA Receptors Expressed in Mammalian Cells", 2005 FASEB Summer Research Conference on "Lysolipids in Health and Disease", Snowmass, Colorado, June 11-16, 2005.
168. Osborne, D.A.; Fujiwara, Y.; Cseh, S.; Holdsworth, G.; Jo, E.; Tigyi, G.; Rosen, H.; Parrill, A.L. "Synergistic Computational and Experimental Investigations of S1P Receptor Agonist Selectivity", 2005 FASEB Summer Research Conference on "Lysolipids in Health and Disease", Snowmass, Colorado, June 11-16, 2005.
169. Walker, M.D.; Liliom, K.; Wang, D.; Fujiwara, Y.; Osborne, D.A.; Parrill, A.L.; Tigyi, G. "Computational and Pharmacological Identification of the Hydrophobic Ligand Binding Pocket of the S1P<sub>1</sub> Receptor", 2005 FASEB Summer Research Conference on "Lysolipids in Health and Disease", Snowmass, Colorado, June 11-16, 2005.
170. Tigyi, G.J.; Tsukahara, T.; Tsukahara, R.; Yasuda, S.; Yuan, H.; Allison, P.; Parrill, A. "Different Residues are Required for Lysophosphatidic Acid and Rosiglitazone Binding to PPAR $\gamma$ ", Experimental Biology 2005, San Diego, CA, April 2-6, 2005.
171. Walker, M.D.; Liliom, K.; Wang, D.; Fujiwara, Y.; Osborne, D.; Parrill, A.L.; Tigyi, G. "Computational and Pharmacological Identification of the Ligand Binding Pocket of the S1P<sub>1</sub> Receptor" Experimental Biology 2005, San Diego, CA, April 2-6, 2005.
172. Looney, A.L.; Sardar, V.M.; Parrill, A.L. "Computational Design and Analysis of Novel Peptide Mimics of LPA Receptor Loops", 56<sup>th</sup> Southeast Regional American Chemical Society Meeting, Research Triangle Park, NC, November 10-13, 2004.
173. Osborne, D.A., Fells, J.I., Fujiwara, Y., Cseh, S., Tigyi, G., and Parrill, A.L. "Modeling Aromatic Agonist Selectivity at the Sphingosine-1-Phosphate (S1P) Receptors." 13<sup>th</sup> Current Trends in Computational Chemistry International Conference. November 2004.
174. Fells, J.I., Osborne, D.A., Pham, T. C., Parrill, A.L. "Computational Studies of Agonist Selectivity at the S1P<sub>4</sub> Receptor", 13<sup>th</sup> Current Trends in Computational Chemistry International Conference. November 2004.
175. Osborne, D.A., Fujiwara, Y., Cseh, S., Tigyi, G., and Parrill, A.L. "Use of Poisson-Boltzmann methodology to quantitate sphingosine-1-phosphate receptor agonism" MALTO meeting, University of Tennessee Health Science Center, May 16, 2004.
176. Pham, T. C. T.; Inagaki, Y.; Igarashi, Y.; Fujiwara, Y.; Tigyi, G.; Parrill, A.L. "3-Dimensional Models of Sphingosine 1-Phosphate Receptors", MALTO meeting, University of Tennessee Health Science Center, May 16, 2004.
177. Osborne, D.A., Fujiwara, Y., Cseh, S., Tigyi, G., and Parrill, A.L. "Quantitative Modeling of Sphingosine-1-Phosphate (S1P) Receptor Agonism: the Use of Poisson-Boltzmann Methodology to Estimate Binding Free Energies" Southeast Theoretical Chemistry Association, University of Mississippi, May 21, 2004.
178. Pham, T. C. T.; Inagaki, Y.; Igarashi, Y.; Fujiwara, Y.; Tigyi, G.; Parrill, A.L. "3-Dimensional Models of Sphingosine 1-Phosphate Receptors", Southeast Theoretical Chemistry Association, University of Mississippi, May 21, 2004.
179. Christina Turner and Abby L. Parrill, "Two Distinct Integrase Binding Pockets for HIV Integrase Inhibitors", The 16<sup>th</sup> Annual Student Research Forum, The University of Memphis, Memphis, TN, April, 2004.
180. Osborne, D.A., Fujiwara, Y., Cseh, S., Tigyi, G., and Parrill, A.L. "Modeling Agonism in the Sphingosine-1-Phosphate (S1P) Receptors" Division of Physical and Applied Sciences, The 16<sup>th</sup> Annual Student Research Forum, University of Memphis. April 2004.
181. Fells, J.I., Osborne, D.A., Pham, T. C., Parrill, A.L. "Computational Evaluation of Receptor Selectivity for Phospholipid Growth Factors", Tennessee Louis Stokes Alliance for Minority Participation Undergraduate Research Conference, Nashville, TN, April 2004.
182. Pham, T. C.; Inagaki, Y.; Igarashi, Y.; Fujiwara, Y.; Tigyi, G.; Parrill, A. L. "Modeling and Mutagenesis of the Mouse S1P<sub>4</sub> Receptor", 227<sup>th</sup> American Chemical Society National Meeting and Exposition, March 28-April 1, 2004.
183. Osborne, D. A.; Fujiwara, Cseh, S.; Wang, Y.; Tigyi, G.; Parrill, A. L. "Modeling Agonist Selectivity at the Sphingosine 1-Phosphate Receptors", 227<sup>th</sup> American Chemical Society National Meeting and Exposition, March 28-April 1, 2004.
184. Fells, J. I.; Osborne, D. A.; and Parrill, A. L. "Computational Evaluation of Receptor Selectivity for Phospholipid Growth Factors", Southeastern Conference on Undergraduate Research at Emory, December, 2003.
185. Daniel A. Osborne, Sandor Cseh, Yuko Fujiwara, Natalia Makarova, Gabor Tigyi, and Abby L. Parrill "S1P Receptors and Their Differential Interactions with S1P Agonists", FASEB Summer Research Conference, Lysophospholipids and Related Lipids in Biology and Diseases, Snowmass, CO, June 28-July 3, 2003.
186. Vineet M. Sardar and Abby L. Parrill "Molecular Dynamics Simulations of LPA Receptor-Ligand Complexes", FASEB Summer Research Conference, Lysophospholipids and Related Lipids in Biology and Diseases, Snowmass, CO, June 28-July 3, 2003.
187. Gangadhar G. Durgam, Tamas Virag, Don B. Elrod, Karoly Liliom, Vineet M. Sardar, Abby L. Parrill, Kazuaki Yokoyama, Wenlin Deng, Gabor Tigyi, and Duane D. Miller, "Fatty Alcohol Phosphates are Subtype-Selective Agonists and Antagonists of Lysophosphatidic Acid Receptors", FASEB Summer Research Conference, Lysophospholipids and Related Lipids in Biology and Diseases, Snowmass, CO, June 28-July 3, 2003.
188. Tamas Virag, Gangadhar G. Durgam, Don B. Elrod, Karoly Liliom, Vineet M. Sardar, Abby L. Parrill, Kazuaki Yokoyama, Wenlin Deng, Gabor Tigyi, and Duane D. Miller, "Fatty Alcohol Phosphates are Subtype-Selective Agonists and Antagonists of Lysophosphatidic Acid Receptors", FASEB National Meeting, 2003.
189. Daniel A. Osborne and Abby L. Parrill, "Pi-Stacking Interactions Confer Immunosuppressant Binding Selectivity in the S1P Receptors", The 15<sup>th</sup> Annual Student Research Forum, The University of Memphis, Memphis, TN, April 28, 2003.



190. Christina Turner and Abby L. Parrill, "Docking Studies of Eleven Structural Types of HIV Integrase Inhibitors Demonstrate Two Non-Overlapping Binding Sites", The 15th Annual Student Research Forum, The University of Memphis, Memphis, TN, April 28, 2003.
191. Hongbin Yuan and Abby L. Parrill, "Three-Dimensional QSAR Study of HIV-1 Integrase Inhibition", The 15th Annual Student Research Forum, The University of Memphis, Memphis, TN, April 28, 2003.
192. Daniel A. Osborne and Abby L. Parrill, "Docking Studies to Examine Immunosuppressive Phospholipid Binding Selectivity", Eleventh Conference on Current Trends in Computational Chemistry, Jackson, Mississippi, November 1-2, 2002.
193. Christina Turner, Hongbin Yuan and Abby L. Parrill, "Docking Studies of Eleven Structural Types of HIV Integrase Inhibitors Demonstrate Two Non-Overlapping Binding Sites", Eleventh Conference on Current Trends in Computational Chemistry, Jackson, Mississippi, November 1-2, 2002.
194. Lynn Wincenciak, Charles Singer, Frank Onyemauwa, Dianqing Sun, Abby L. Parrill, Peter K. Bridson, "Molecular Modeling of the Human A<sub>2A</sub> Adenosine Receptor", 54<sup>th</sup> Southeast Regional Meeting of the American Chemical Society, Charleston, SC, November 13-16, 2002.
195. Sardar, V.M.; Virag, T.; Fischer, D.J.; Elrod, D.; Bautista, D.L.; Wang, D.; Nusser, N.; Yokoyama, K.; Baker, D.L.; Miller, D.D.; Tigyi, G.; Parrill, A.L. "Molecular Modeling Studies of Lysophosphatidic Acid Receptor Antagonists", 224<sup>th</sup> ACS National Meeting, Boston, MA, August 18-22, 2002.
196. Cundari, T.; Parrill, A.; Burkey, T.J.; Anderson, M.E. "A Summer at the Interface of Theory and Experiment. The NSF-REU Site in Chemistry at The University of Memphis", 223<sup>rd</sup> ACS National Meeting, Orlando, FL, April 7-11, 2002.
197. Duke, C. B.; Parrill, A. L. "QSAR Modeling of Rat Adenosine A1 Receptor Agonists", Tennessee Academy of Science West Tennessee Collegiate Meeting, Memphis, TN, March 23, 2002.
198. Parrill, A.L.; Yuan, H. "QSAR Studies of HIV-1 Integrase Inhibition", 222<sup>nd</sup> American Chemical Society National Meeting and Exposition, Chicago, IL August 2001.
199. Mineno, T.; Parrill, A.L.; Avery, M.A. "Modeling of Plasmeprins as Novel Targets Against *Plasmodium faciparum*", 222<sup>nd</sup> American Chemical Society National Meeting and Exposition, Chicago, IL August 2001.
200. Bautista, D.; Fischer, D.J.; Nusser, N.; Virag, T.; Wang, D.; Baker, D.L.; Tigyi, G.; Parrill, A.L. "Computational Studies of a Lysophosphatidic Acid Receptor Antagonist", 2001 FASEB Summer Research Conference on "Lysophospholipids and Related Bioactive Lipids in Biology and Diseases", Tucson, Arizona, June 9-16, 2001.
201. Wang, D.; Lorincz, Z.; Bautista, D.; Parrill, A.L.; Tigyi, G. "What Determines Ligand Specificity in the EDG Family?", 2001 FASEB Summer Research Conference on "Lysophospholipids and Related Bioactive Lipids in Biology and Diseases", Tucson, Arizona, June 9-16, 2001.
202. Singer, C.; Harper, B.; Onyemauwa, F.; Bridson, P. K.; Parrill, A. L. "Molecular Modeling of Adenosine Receptors and Their Ligands" 110<sup>th</sup> Annual Meeting of the Tennessee Academy of Science, Belmont University, Nashville, Tennessee, November 17, 2000.
203. Brooks, S. D.; Rubio, J.; Parrill, A. L. "Molecular Modeling of Protein Kinase C Isoforms" 110<sup>th</sup> Annual Meeting of the Tennessee Academy of Science, Belmont University, Nashville, Tennessee, November 17, 2000.
204. Parrill, A. L.; Bautista, D. L.; Van Brocklyn, J.; Spiegel, S.; Wang, D.; Lorincz, Z.; Fischer, D.; Liliom, K.; Baker, D.; Tigyi, G. "Computational Modeling and Experimental Validation of Phospholipid Growth Factor Recognition" 35<sup>th</sup> Annual Southeastern Regional Lipid Conference, Cashiers, North Carolina, November 1-3, 2000.
205. Sims, Y.\*; Parrill, A.L. "The Impact of Metal Ions on the HIV-Integrase Enzyme", National Minority Research Symposium, Washington, D.C., October 10-13, 2000.
206. A.L. Parrill, D.L. Bautista, D.L. Baker, D-A. Wang, Z. Lörinec, D.J. Fischer, K. Liliom, G. Tigyi, J. VanBrocklyn, S. Spiegel "Defining the ligand specificity of EDG1, 2, and 6 through mutagenesis, docking, and molecular dynamics studies" 220<sup>th</sup> American Chemical Society National Meeting and Exposition, Washington, D. C., August 19-24, 2000.
207. A.L. Parrill and P.K. Bridson "Student use of computational chemistry to justify proposed drug targets in a medicinal chemistry course: Integrating computational experiments and writing assignments", 220<sup>th</sup> American Chemical Society National Meeting and Exposition, Washington, D. C., August 19-24, 2000.
208. A.L. Parrill, H. Yuan, C. Turner, G.B. Ray, "Computational evidence for two HIV-1 integrase inhibitor interaction sites", 220<sup>th</sup> American Chemical Society National Meeting and Exposition, Washington, D. C., August 19-24, 2000.
209. Parrill, A.L.; Bautista, D.L.; Lorincz, Z.; Wang, D.; Baker, D.L.; Fisher, D.J.; Van Brocklyn, J.; Spiegel, S. Tigyi, G. "Computational Modeling and Experimental Validation of the Phospholipid Receptors, EDG1 and EDG2, and their Complexes with Sphingosine-1-Phosphate and Lysophosphatidic Acid", Gordon Research Conference: Glycolipid and Sphingolipid Biology, Barga, Italy, May 14-19, 2000.
210. Bautista, D. L.; Baker, D. L.; Wang, D.; Lorinec, Z.; Fischer, D. J.; Liliom, K.; Van Brocklyn, J.; Spiegel, S.; Tigyi, G. and Parrill, A. L., "Modeling Ligand Specificity Differences of EDG1 and EDG2 Using Molecular Dynamics and Docking", American Chemical Society Middle Atlantic Regional Meeting, Newark, DE, May 12-14, 2000.
211. Bautista, D.L.; Baker, D.L.; Lorinec, Z.; Wang, D.; Fischer, D.J.; Van Brocklyn, J.; Spiegel, S.; Tigyi, G. and Parrill, A.L. "Dynamic Modeling of EDG1 Receptor Structural Changes Induced by Site-Directed Mutations", 219<sup>th</sup> American Chemical Society National Meeting and Exposition, San Francisco, CA, March 26-30, 2000.
212. Abu-Khudeir, M.; Parrill, A. L. "Differential Influence of Metal Ions in the HIV Integrase Active Site", Tennessee Academy of Sciences, Christian Brothers University, Memphis, TN, March 25, 2000.

213. Bautista, D.L.; Baker, D.L.; Wang, D.; Fischer, D.J.; Van Brocklyn, J.; Spiegel, S.; Tigyi, G. and Parrill, A.L. "Dynamic Modeling of EDG1 Receptor Structural Changes Induced by Site-Directed Mutations", Eighth Conference on Current Trends in Computational Chemistry, Vicksburg, MI, November 5-6, 1999.
214. Yuan, H. and Parrill, A.L., "QSAR Study on HIV-1 Integrase Inhibition", Eighth Conference on Current Trends in Computational Chemistry, Vicksburg, MI, November 5-6, 1999.
215. Yuan, H. and Parrill, A.L., "QSAR Development to Describe the HIV-1 Integrase Inhibition", American Chemical Society Southeast Regional Meeting, Knoxville, TN, October 17-20, 1999.
216. Parrill, A.L.; Ray, G. B.; "Docking Studies of Salicylhydrazine Inhibitors to the HIV-1 Integrase Catalytic Domain", 218<sup>th</sup> National Meeting and Exposition, New Orleans, LA August 1999.
217. Parrill, A.L.; Roaten, J.B.; Sweatman, T.W. and Israel, M. "Dynamic Models of the N-benzyladriamycin-14-valerate Complex with the C1b Domain of Protein Kinase C- $\delta$ " 218<sup>th</sup> National Meeting and Exposition, New Orleans, LA August 1999.
218. Parrill, A.L.; Baker, D.L.; Wang, D.; Fischer, D.J.; Van Brocklyn, J.; Spiegel, S.; Tigyi, G. "Structural Features of EDG1 Receptor-Ligand Complexes Revealed by Computational Modeling and Mutagenesis", Lysophospholipids and Eicosanoids in Cancer and in Cardiovascular and Neurodegenerative Diseases, a New York Academy of Sciences Conference, New York, NY, June 25-28, 1999.
219. Deng, J.; Schroeder, S.; Roaten, J.B.; Sweatman, T. and Parrill, A.L. "Simulation of the Interaction between PKC- $\delta$  Mutants and Phorbol Esters", 26<sup>th</sup> Annual MALTO Meeting, Memphis, TN, May 23-25, 1999.
220. Jolly, A.; Hirsh, A.; Yuan, H.; Ray, G. and Parrill, A.L. "Modeling the Interactions of HIV Integrase with Inhibitors", 26<sup>th</sup> Annual MALTO Meeting, Memphis, TN, May 23-25, 1999.
221. Parrill, A.L.; Baker, D.L.; Wang, D.; Fischer, D.J.; Van Brocklyn, J.; Spiegel, S.; Tigyi, G. "G-Protein Coupled Receptor Model Development - Turning Primary Sequence into Tertiary Structure", 28<sup>th</sup> Southeast Theoretical Chemistry Association Meeting, April 23-24, 1999.
222. Deng, J.; Schroeder, S.; Roaten, J.B.; Sweatman, T. and Parrill, A.L. "Simulation of the Interaction between PKC- $\delta$  Mutants and Phorbol Esters", 28<sup>th</sup> Southeast Theoretical Chemistry Association Meeting, April 23-24, 1999.
223. Jayawardene, D.; Dass, C.; Parrill, A.L. "Pharmacophoric Comparison of Methionine Enkephalin Derivatives", 28<sup>th</sup> Southeast Theoretical Chemistry Association Meeting, April 23-24, 1999.
224. Ray, G.; Yuan, H.; Jolly, A.; Hirsh, A. and Parrill, A.L. "Computational Studies of HIV Integrase and Salicylhydrazine Inhibitors", 28<sup>th</sup> Southeast Theoretical Chemistry Association Meeting, April 23-24, 1999.
225. \*Roaten, J.B., Bertics, P.J., Kazanietz, M.G., Rodrigues, P.J., Lothstein, L., Parrill, A., Sweatman, T.W. "N-Benzyladriamycin-14-valerate (AD 198): A novel C1-antagonist of protein kinase C (PKC)", American Association for Cancer Research 90<sup>th</sup> Annual Meeting, Philadelphia, PA, Spring 1999.
226. Parrill, A. L.; Ellsworth, J. "Facilitating Chemical Education with Computers: World Wide Web-based Interactive Materials and Organizational Tools for Learning Exercises", American Chemical Society 217<sup>th</sup> National Meeting and Exposition, Anaheim, CA March 1999.
227. Sweatman, T.; Roaten, J. B.; Lothstein, L.; Israel, M.; Kazanietz, M.; Parrill, A. "Protein Kinase C: A Membrane Target for Novel Anthracycline Analogs", American Chemical Society 217<sup>th</sup> National Meeting and Exposition, Anaheim, CA March 1999.
228. Nakhleh, M. B.; Donovan, W. J.; Parrill, A. L. "Evaluation of interactive technologies for chemistry web sites: Educational materials for organic chemistry (EMOC)", American Chemical Society 217<sup>th</sup> National Meeting and Exposition, Anaheim, CA Spring 1999.
229. \*Nakhleh, M. B.; Donovan, W. J.; Parrill, A. L. "Interactive Technologies for Chemistry Websites: An Evaluation of Educational Materials for Organic Chemistry (EMOC)" National Association for Research in Science Teaching 1999 National Meeting, Boston, MA Spring 1999.
230. Roaten, J.B.; Kazanietz, M.G.; Israel, M.; Sweatman, T.; Parrill, A.L. "Molecular Modeling Studies of N-Benzyladriamycin-14-valerate in Complex with the Phorbol Ester Binding C1b Domain of Protein Kinase C- $\delta$ " Seventh Conference on Current Trends in Computational Chemistry, Vicksburg, Mississippi, November 6-7, 1998.
231. Nelson, S.; Parrill, A.L.; Azadnia, A. "Development of an Extended Collaborative Learning Experiment for Organic Chemistry Laboratories" 1998 Great Lakes College Chemistry Conference.
232. Parrill, A.L. "Everyday Chemical Reactions: Promoting Interest and Learning Through Relevant Writing Assignments" Fall 1998 ConfChem, Turning Students on to Science.
233. Parrill, A.L.; Ramamoorthy, P.S.; Gervay, J. "Molecular Dynamics Docking and Relative Binding Affinity Comparison of Potential Neuraminidase Inhibitors" American Chemical Society 215<sup>th</sup> National Meeting and Exposition, Dallas, TX Spring 1998.
234. Parrill, A.L. "The Internet as a tool for streamlining the use of self-and peer assessments in large classes", American Chemical Society (ACS) 214<sup>th</sup> National Meeting and Exposition, Las Vegas, NV Fall 1997.
235. Parrill, A.L.; Butler, S.; Byrum, D.L.; Wolpa, B.; Gervay, J. "Computational Chemistry for Large Classes - A Simple Online Laboratory Which Overcomes Cost Barriers", 213<sup>th</sup> ACS National Meeting and Exposition, San Francisco, CA, Spring 1997.
236. Parrill, A.L.; "Do Students Use Non-Required Materials on the WWW to Learn Chemistry?", ACS 213<sup>th</sup> National Meeting and Exposition, San Francisco, CA, Spring 1997.
237. Parrill, A.L.; Gervay, J. "Supplementing Traditional Chemical Education on the World Wide Web" Gordon Conference - *Innovations in College Chemistry Teaching*, June30-July 5, 1996, Plymouth, NH.

238. Parrill, A.L. "Hypermedia Tutorials Helping Students Understand Stereochemistry" National Science Teachers Association's Global Summit on Science and Science Education, San Francisco, CA December 27-29, 1996.
239. Gervay, J; Parrill, A.L. "Supplementing Traditional Chemical Education on the World Wide Web" National Science Teachers Association's Global Summit on Science and Science Education, San Francisco, CA December 27-29, 1996.
240. Parrill, A.L.; Dolata, D.P. "CLEW-Using A Genetic Algorithm to Determine Rules that Simplify Complex Pharmacological Data", ACS 211<sup>th</sup> National Meeting and Exposition, New Orleans, LA, Spring 1996.
241. Parrill, A.L.; Gervay, J. "Discovering Stereochemistry: Multi-media Discovery-Based Tutorials", ACS 211<sup>th</sup> National Meeting and Exposition, New Orleans, LA, Spring 1996.
242. Parrill, A.L.; Walters, W.P.; Dolata, D.P. "A New Pharmacophoric Mapping for Structurally Dissimilar Cannabinoids", International Cannabis Research Society 1995 Symposium, Scottsdale, AZ
243. Parrill, A.L.; Dolata, D.P.; Mamuya, N.; Roberts, G.; Gervay, J. "Comparison of Computational Methods for Determining Sialyllactone Conformations in Solution", ACS National Meeting, Anaheim, CA, 1995
244. Parrill, A.L.; Mamuya, N.; Gervay, J. "Computational Studies of Sialyllactones: Methods and Uses", First Electronic Glycoscience Conference, 1995.
245. Parrill, A.L.; Gervay, J. "Chemical Education: The Wonder of Discovery", Student Showcase '95, The University of Arizona, Tucson, AZ 85721.
246. Parrill, A.L.; Walters, W.P.; Dolata, D.P. "A Novel Pharmacophore Model of the Cannabinoids", 1995 International Cannabis Research Society Symposium on Cannabis and the Cannabinoids, Scottsdale, AZ, June, 1995.
247. Parrill, A.L.; Walters, W.P.; Dolata, D.P. "CLEW- A Learning-Based Approach to Pharmacophore Hypothesis Generation", ACS National Meeting, Anaheim, CA 1995.

## SUPPORT:

EXTERNAL (Funded)	AGENCY/SOURCE	AMOUNT	PERIOD
Regulation of arterial diameter through specific sensing of endogenous steroids and novel nonsteroidal analogs by BK channel subunits (subcontract PI, 100%)	UTHSC (subcontract from NIH grant)	\$336,667	3/19-3/23
GPR88 Ligand Discovery (PI, 60% with Dan Baker)	NIH	\$408,014	6/16-5/19
MRI: Acquisition of a 400 MHz Spectrometer (senior personnel, 5%)	NSF	\$339,585	8/15-7/18
Vasodilation of BK Channel Beta 1 (subcontract PI, 100%)	UTHSC	\$8,312	12/13-5/14
Vasodilation of BK Channel Beta 1 (subcontract PI, 100%)	UTHSC	\$5,674	9/12-12/13
LPA Receptors (subcontract PI, 100%)	UTHSC	\$5,000	1/13-8/13
REU Site: University of Memphis Interdisciplinary Research in Chemistry (PI, 50%)	National Science Foundation	\$442,744	9/12-8/15
REU Site: Collaborative Research in Chemistry at the University of Memphis (PI, 50%)	National Science Foundation	\$220,000	6/09-5/12
Identification of ATX Inhibitors as Potential Cancer Chemotherapeutic Leads (PI, 50%)	Elsa Pardee Foundation	\$100,770	1/08-12/08
MRI – Acquisition of a spectropolarimeter for Research and Education (PI, 30%)	National Science Foundation	\$137,000	8/07-7/10
MRI – Acquisition of an LC-MS for Research and Education (co-PI, 10%)	NSF	\$365,000	8/06-7/09
LPA Targets and Cancer (subcontract)	UTHSC/National Institutes of Health	\$41,986/yr	8/06-7/10
R01: Computational Approach to Ligand Discovery for LPA GPCR and PPAR	National Institutes of Health	\$1,725,813	8/06-5/11
Diversity Supplement – Rolanda London (undergraduate)	National Institutes of Health	\$32,922	7/07-5/09
Diversity Supplement – Jesica Williams (graduate)	National Institutes of Health	\$116,328	6/08-5/11
ARRA Supplement – Debra Bautista (secondary chemistry teacher)	National Institutes of Health	\$50,762	6/09-6/11
ARRA Supplement – Alexandra Kikonyogo (postdoctoral associate)	National Institutes of Health	\$262,859	7/09-6/11
CRIF: Acquisition of a 400 MHz NMR Spectrometer for Research and Education (Co-PI, 30%)	National Science Foundation	\$262,500	2/05-6/07
REU: A Summer at the Interface of Theory and Experiment	National Science Foundation	\$173,250	4/04-3/07

Characterization of Antagonist Binding to Lysophosphatidic Acid Receptors	American Heart Association	\$140,000	7/03-6/06
QM/MM Investigation of FTY720 Receptor Selectivity	National Center for Supercomputing Applications	10,000 units	1/03-1/04
Study of Phospholipid Growth Factor Receptors (Subcontract PI, 100%)	UTHSC/National Institutes of Health (NIHLB)	\$1,100,00	8/01-7/06
REU: A Summer at the Interface of Theory and Experiment (Co-PI, 50%)	National Science Foundation (REU)	\$147,040	2/00-1/02
Computer-Driven Structure-Function Analysis of Phospholipid Growth Factor Receptors - (PI, 50%)	American Heart Association	\$214,500	1/00-12/03
R15: QSAR and Docking Studies of HIV-Integrase – (PI, 30%)	National Institutes of Health (NIAID)	\$104,000	8/99-8/03
Minority Supplement: QSAR and Docking Studies of HIV-Integrase – (PI)	National Institutes of Health (NIAID)	\$24,192	8/99-8/03
Michigan State Univ. Online Curriculum Initiative and Research Scholars (MSU-OCIRS) Program (CO-PI, 10%)	Howard Hughes Medical Institute	\$1,000,000	1998-2003
Interactive Technologies for Chemistry Websites	National Science Foundation (POWRE)	\$75,000	10/97-10/99
Rational Drug Design Symposium	Petroleum Research Fund	\$2000	9/97

<b>INTERNAL</b>	<b>SOURCE</b>	<b>AMOUNT</b>	<b>PERIOD</b>
Water-Soluble GPCR (PI)	FedEx Institute of Technology	\$32,000	7/2012-2015
ATX Inhibitors – Diversification into New Chemical Entities (CO-PI, 50%)	FedEx Institute of Technology	\$18,750	1/2013-2014
A Water-Soluble G Protein Coupled Receptor Model (PI)	Faculty Research Grant	\$6500	2009-2010
Computational Chemistry Seminar Program (PI)	College of Arts and Sciences Academic Enrichment Fund	\$2000	2005-2006
Personal Development Assignment	College of Arts and Sciences	1 semester	1/04-6/04
Undergraduate Research Conference (PI, 80%)	College of Arts and Sciences Public Service Funds	\$500	1998-1999
Computational Chemistry Seminar Program (PI, 80%)	College of Arts and Sciences Academic Enrichment Fund	\$1000	1999-2000
Modeling Ligand Specificity in the EDG Receptor Family (PI)	Faculty Research Grant	\$5000	10/99-10/00
Modeling Differences between Activation and Inhibition of Protein Kinase C (PI)	New Faculty Research Initiation	\$8500	10/00-9/01
Quantitating Selectivity of a Novel Immunosuppressive Agent (PI)	Faculty Research Grant	\$6500	7/03-6/04
Computational Chemistry Seminar and Workshop Program (PI, 100%)	College of Arts and Sciences Academic Enrichment Fund	\$2000	2005-2006

## **OUTREACH:**

<b>PROJECT</b>	<b>PARTICIPANTS</b>	<b>PERIOD</b>	<b>SPONSORSHIP (if any)</b>
Battle of the Brains Judge	>100 (high school students)	2010	City of Germantown
Science Fair Judge	>100 (high school and junior high school students)	3/2001	American Chemical Society – Memphis Section
SHADES workshop to attract 8 <sup>th</sup> grade girls to science and engineering careers	35	3/11/2000	American Association of University Women - Memphis Branch
Science Fair hands-on activities	~50	3/8/2000	American Chemical Society - Memphis Section
High School Research Seminar	100	2/19/2000	American Heart Association
National Chemistry Week Library Demonstration at the Main Library-Polymers	20	11/9/1999	American Chemical Society - Memphis Section
Science Works "The Chemistry of Color"	25	6/5/1999	American Chemical Society, Children's

			Museum
International Chemistry Celebration "Colorful Chemistry"	50	5/1/1999	American Chemical Society, Memphis Botanic Gardens
Science-by-Mail	20 (students across the country)	1998-2000	Museum of Science
Science Fair Judge	115 (high school students)	3/2/99	Ross Christian Academy
Make-a-Wish Foundation visit	3 (St. Jude patient and siblings)	Fall 1998	Make-a-Wish Foundation
Science Olympiad (Michigan State Finals)	80 (high school students in Michigan)	1997-1998	MI Science Olympiad

## SERVICE:

UNIVERSITY	COMMITTEE/ACTIVITY (if Chair, add [C])	PERIOD
<b>Department</b>	Chair	2010-2014
	Undergraduate Studies Committee [C]	2001-2009
	Tenure and Promotion Committee [C]	2003-2009
	Faculty Search Committee	2004-2005
	Department WWW Development Committee	1998-1999
	Graduate Studies Committee	1998-2001
	Undergraduate Research Conference Planning	2/99
<b>College/School</b>	Faculty Research Grant Review Panel	4/00-4/01
	Pre-health Professional Evaluation Committee [C]	8/00-2009
	Tenure and Promotion Committee [C during one of three years]	2004-2007
<b>University</b>	Van Vleet Fellowship Committee	2/99
	Information Technology Task Force	1998-1999
	Fluency in Information Technology (FITness) Task Force	2000-2001
	College of Arts and Sciences Dean Search Committee	2001
	Standing Committee for Awarding Honorary Degrees	2005-2007
	IT Research Advisory Committee [C, 2008-2009]	2007-2009
	Willard R. Sparks Board of Visitors Eminent Faculty Award selection committee	2008-2010
	Chemical Hygiene Committee	2010-present
	Research Capacity Assessment Taskforce - Infrastructure Study Team	2012-2013
	Research Services Implementation Team	2013-2014
<b>Univ. Memphis Research Foundation</b>	Board Member	2009-present
<b>OTHER</b>		
Society/Organization/Journal	COMMITTEE/EDITORIAL BOARD/OFFICE (if Chair, add [C])	PERIOD
American Chemical Society	SE/SW Regional ACS Meeting – Program Chair	2010-2015
American Chemical Society	COMP Division – Symposium Organizer	2010
National Institutes of Health	Standing Review Panel Member: Molecular Structure Function D	2006-2011
National Institutes of Health	Standing Review Panel Member: International Collaborative Projects -1	2003-2006
American Chemical Society	SE/SW Regional ACS Meeting – Symposium Organizer “Bioactive Lipids”	2005
National Institutes of Health	International and Cooperative Projects Study Section (ICP, ICP-1)	2003-2005
American Chemical Society	CHED Division – Symposium Co-organizer “Alternative Assessments”	2002-2003
National Institutes of Health	International and Cooperative Projects Study Section (ICP), ad hoc member	2001
American Chemical Society	COMP Division – Symposium Organizer “Modeling Ligand Interactions with Membrane Proteins”	2001
American Chemical Society	Memphis Local Section Awards Committee [C]	2004-2006
American Chemical Society	Memphis Local Section [C]	2001
American Chemical Society	Memphis Local Section Chair-Elect	2000

American Chemical Society	Memphis Section Program Committee	1999
American Chemical Society	CHED Committee on Computers in Chemical Education	6/98-6/00
American Chemical Society	COMP Div.– Symposium Organizer “Using Computers to Facilitate Education”	3/99
American Chemical Society	COMP Division – Symposium Co-organizer “Rational Drug Design”	9/97
S. E. Theoretical Chem. Conf.	Planning Committee	1998-1999
J. Coll. Math. Sci. Teaching	Review Board	10/97-present
J. Chem. Educ.	Reviewer	
J. Med. Chem.	Reviewer	
Bioorg. Med. Chem. Letters	Reviewer	
J. Mol. Struct. THEOCHEM	Reviewer	
J. Mol. Graphics Modelling	Reviewer, Editorial Board Member	2004-present
J. Comput. Chem.	Reviewer	
J. Am. Chem. Soc.	Reviewer	
J. Comput-Aided Mol. Design	Reviewer	
Structural Chemistry	Reviewer	
Biochim. Biophys. Acta	Reviewer	
National Science Foundation	Reviewer	

## CONSULTING:

ORGANIZATION/COMPANY	PERIOD
Allen, Summers, Simpson, Lillie & Gresham, PLLC (Robert Green, partner)	1/14-2/14
Predix Pharmaceuticals	8/05-2007
Ceretek, Inc. (Science Advisory Board Member)	8/01-8/03
Exalpha Biologicals	2/01-2005
Wiley College Publishing	1/99-1/03
Brooks Cole College Publishing	1/00-1/03
The University of Mississippi	8/00-6/01