James R. Damewood, JR

Senior Director of Occupational Toxicology and Industrial Hygiene

Executive Summary:

Board certified (DABT) toxicologist and Ph.D. chemist with broad experience and significant track record of accomplishment in the pharmaceutical and chemical industries in both senior scientist and managerial positions.

Education:

Postdoctoral Research Fellow, Chemistry, University of Wisconsin, Madison, WI

Ph.D., Chemistry, Princeton University, Princeton, NJ Hugh Stott Taylor Fellow; Halcon International Fellow

MA, Chemistry, Princeton University, Princeton, NJ

BA, Chemistry, University of Maryland Baltimore County, Baltimore, MD (UMBC), Magna Cum Laude. UMBC Student Scholars Prize; UMBC Alumni Service Award 2001

Work History:

2018 - Present **Senior Director of Occupational Toxicology and Industrial Hygiene,** Affygility Solutions

- Manager for Toxicology Section.
- Providing potent compound safety, occupational toxicology and industrial hygiene services to pharmaceutical, biotechnology and medical device companies world-wide.

2017 - 2018 **Research Manager, Principal Research Toxicologist,** Corteva Agriscience™, Agricultural Division of DowDuPont™, Haskell Global Center for Health Sciences

- Research Manager for the Metabolism, Toxicokinetic, and Analytical Section of the Haskell Global Center for Health Sciences, Corteva AgriscienceTM, Agricultural Division of DowDuPontTM.
- Progressing a wide spectrum of investigational sciences, including in vitro and in vivo metabolism, toxicokinetics, analytical sciences, computational toxicology, gene expression profiling, mechanism and mode of action studies, and the development and application of novel in vitro tests and in silico methods that show translational relationships with in vivo systems.

2011 - 2018 **Business Liaison, Principal Research Toxicologist (Senior Research Toxicologist 2011-2012),** Haskell Global Centers for Health and Environmental Sciences, E.I. DuPont de Nemours & Co., Wilmington, DE

- Responsible for supporting business efforts to develop products that are safe for humans and the environment. Consultation on issues of safety/toxicology and coordination of Haskell Global Centers activities in support of business regulatory and product stewardship activities.
- Provided safety/toxicology and product stewardship support to ~60 ongoing Central Research and Development projects extending across all research areas of the company world-wide.

2005 - 2010 **Principal Scientist II, Lead Optimization Chemistry,** ASTRAZENECA, Wilmington, DE

- Local and global liaison between Chemistry and Preclinical Toxicology (Safety Assessment) as a Chemical Toxicology Specialist. Collaboratively developed new scientific approaches to the evaluation of seizure liability, established connections between phospholipidosis and histopathological findings, and developed predictive in silico models in critical areas of importance to drug safety.

2000 – 2005 **Associate Director, Chemistry;** Section Head, Computational Chemistry & Informatics, ASTRAZENECA, Wilmington, DE

1998 – 2000 **Senior Group Leader,** Molecular Modeling and Structural Biology, ASTRAZENECA, Wilmington, DE

1996 – 1998 **Principal Chemist,** ASTRAZENECA, Wilmington, DE

1990 – 1996 **Senior Research Chemist,** ASTRAZENECA, Wilmington, DE

1984 – 1990 **Assistant Professor of Physical Organic Chemistry, Department of Chemistry and Biochemistry (1984- 1990) Adjunct Professor (1990-1991).** Cottrell Foundation Research Award, Dreyfus Research Grant. UNIVERSITY OF DELAWARE, Newark, DE.

Certifications, Professional Activities, and Affiliations:

Diplomate, American Board of Toxicology (DABT)

Certified Six Sigma Green Belt

Scientific Advisory Board, Science and Mathematics Division / Chemistry, Stevenson University, Stevenson MD, 2004 - present

National Institutes of Health Center for Scientific Review, Member, Medicinal Chemistry Study Section (MCHA), July 1, 1997 - June 30, 2001 Ad Hoc Member, Medicinal Chemistry Study Section (MCHA) June, 1996; October, 1995; August, 1995; June 2002. External Reviewer (MCHA) February 2002.

New York Academy of Sciences, 1980; World Association of Theoretically Oriented Chemists (Life Member), 1988; Drug Information Association, 1993; International Union of Pure and Applied Chemistry; Phi Kappa Phi, 1978; Sigma Xi, 1978; AAAS; American Chemical Society (Chair of DE section Awards Committee 1986 and 1987); Full member, Society of Toxicology.

Certifications, Professional Activities, and Affiliations:

Practical Primer on Pesticides, Keller and Heckman (2017)

Food Packaging Law, Keller and Heckman (2016)

Practical Food Law, Keller and Heckman (2015)

Mid America Toxicology Course (2009)

Pharmaceutical Toxicology (PERI, 2008)

Premarketing Clinical Drug Safety and Risk Assessment (PERI, 2008)

Publications:

1. The Effect of Solvent on Intramolecular General Base Catalysis in the Hydrolysis of α, β-Unsaturated Schiff Bases, R. M. Pollack, R. H. Kayser, J. R. Damewood, Jr., J. Am. Chem. Soc. **99**, 8232 (1977).
2. An Ab Initio Investigation of Rotation and Inversion Barriers in Formylphosphine, J. R. Damewood, Jr., K. Mislow, Monatsh. Chem. **111**, 213 (1980).
3. Molecular Structure of 1,8-Bis(trimethylelement)naphthalenes, J. F. Blount, F. Cozzi, J. R. Damewood, Jr., L. D. Iroff, U. Sjöstrand, K. Mislow, J. Am. Chem. Soc., **102**, 99 (1980).
4. Enantiomerization Trends in 1,8 Bis(trimethylelement)-naphthalenes, W. D. Hounshell, F.A. L. Anet, F. Cozzi, J. R. Damewood, Jr., C. A. Johnson, U. Sjöstrand, K. Mislow, J. Am. Chem. Soc., **102**, 5941 (1980).
5. Static and Dynamic Stereochemistry of Hexaethylbenzene and of its Tricarbonylchromium, Tricarbonylmolybdenum and Dicarbonyl(triphenylphosphine)-chromium Complexes, D. J. Iverson, G. Hunter, J. F. Blount, J. R. Damewood, Jr., K. Mislow, J. Am. Chem. Soc., **103**, 6073 (1981).
6. Crystal and Molecular Structure of Diphenylmethane, J. C. Barnes, J. D. Paton, J. R. Damewood, Jr., K. Mislow, J. Org. Chem., **46**, 4975 (1981).

7. Crystal and Molecular Structure of Dicarbonyl(hexaethylbenzene)-(triethylphosphine)chromium(0), G. Hunter, J. F. Blount, J. R. Damewood, Jr., D. J. Iverson, K. Mislow, Organometallics, **1**, 448 (1982).
8. Structure Calculations for Silane Polymers, J. R. Damewood, Jr., R. West, Macromolecules, **18**, 159 (1985).
9. Organosilane High Polymers: Thermochromic Behavior, P. Trefonas III, J. R. Damewood,Jr., R. West, R. D. Miller, Organometallics, **4**, 1318 (1985).
10. X-Ray Crystal Structure and Conformational Analysis of Tetradecamethylcycloheptasilane, F. Shafiee, J. R. Damewood, Jr., K. J. Haller, R. West, J. Am. Chem. Soc., **107**, 6950 (1985).
11. Conformational Analysis of Poly(di-n-hexyl)silylene, J. R. Damewood, Jr., Macromolecules, **18**, 1793 (1985).
12. Using the Terms Homochiral and Heterochiral, J. R. Damewood, Jr., Chemical and Engineering News, November 4, 1985, p. 5.
13. Pyramidal Inversion and Electron Delocalization in the Silacyclopentadienyl Anion, J. R. Damewood, Jr., J. Org. Chem., **51**, 5028 (1986).
14. Conformational Analysis of Hexadecamethylcyclooctasilane, J. R. Damewood, Jr. and R. Gambogi, Tetrahedron, **42**, 6411 (1986).
15. The Hydration of Polar Organic Molecules: The Interaction of Acetonitrile with Water, J. R. Damewood, Jr. and R. A. Kumpf, J. Phys. Chem., **91**, 3449 (1987).
16. Molecular Mechanics Studies of Molecular Recognition, J. R. Damewood, Jr., Chemical Design Automation News, November 1987.
17. A Molecular Mechanics Study of Neutral Molecule Complexation with Crown Ethers, J. R. Damewood, Jr., W. P. Anderson, J. J. Urban, Computational Chem., **9**, 111 (1988).
18. Isomer-Dependent Complexation of Malononitrile by Dicyclohexyl 18-Crown-6, J. R. Damewood, Jr., J. J. Urban, T. C. Williamson, A. L. Rheingold, J. Org. Chem., **53**, 167 (1988).
19. Pyramidal Inversion in Silyl Anions, J. R. Damewood, Jr., C. M. Hadad, J. Phys. Chem., **92**, 33 (1988).
20. An MO Approach to Substituent Effects in Amine-CO2 Interactions, A. K. Chakraborty, G. Astarita, K. B. Bischoff, J. R. Damewood, Jr., J. Am. Chem. Soc., **110**, 6947 (1988).
21. Do Nitromethane and Malononitrile form C-H...O Hydrogen Bonds? Implications for Molecular Recognition by Crown Ethers, J. R. Damewood, Jr., R. A. Kumpf, J. Chem. Soc., Chem. Commun. 621 (1988).
22. Molecular Mechanics Calculation of Intermolecular Potential Energy Surfaces for the Hydration of Formaldehyde, W. C. F. Mühlbauer, J. R. Damewood, Jr., J. Phys. Chem. **92**, 3693 (1988).
23. Interrelationships Among Heats of Formation and Molecular Mechanics Steric Energies, J. F. Liebman, C. Hadad, J. R. Damewood, Jr., Tetrahedron, **45**, 1623 (1989).
24. Interaction of Formaldehyde with Water, R. A. Kumpf, J. R. Damewood, Jr., J. Phys. Chem., **93**, 4478 (1989).

25. Conformational Energies and Unperturbed Chain Dimensions of Poly(phenylmethylsilylene) and the Parent Poly(silastyrene), W. J. Welsh, J. R. Damewood, Jr., R. West, Macromolecules, **22**, 2947 (1989).
26. The Interaction of CO2 and Water: A Combined Ab Initio and SOLDRI Molecular Mechanics Study, J. R. Damewood, Jr., R. A. Kumpf, W. C. F. Mühlbauer, J. Phys. Chem., **93**, 7640 (1989).
27. Parameterization of Molecular Mechanics Calculations for the Accurate Description of Hydrogen Bonding Interactions, J. R. Damewood, Jr., R. A. Kumpf, W. C. F. Mühlbauer, J. J. Urban, J. E. Eksterowicz, J. Phys. Chem., **94**, 6619 (1990).
28. Accurate Free Energy Perturbation Calculation of the Hydration Free Energies of Fe+2 and Fe+3, J. J. Urban, J. R. Damewood, Jr., J. Chem. Soc., Chem. Commun., 1636 (1990).
29. The Design of Orally Active, Nonpeptidic Inhibitors of Human Leukocyte Elastase, F. J. Brown, D. W. Andisik, P. R. Bernstein, C. B. Bryant, C. Ceccarelli, J. R. Damewood, Jr., P. D. Edwards, R. A. Earley, S. Feeney, R. C. Green, B. Gomes, B. J. Kosmider, R. D. Krell, A. Shaw, G. B. Steelman, R. M. Thomas, E. P. Vacek, C. A. Veale, P. A. Tuthill, P. Warner, J. C. Williams, D. J. Wolanin, S. A.Woolson, J. Med. Chem., **37**, 1259 (1994).
30. Nonpeptidic Inhibitors of Human Leukocyte Elastase. 2. Design, Synthesis, and In Vitro Activity for a Series of 3-Amino-6-Arylpyridin-2-one-Containing Trifluoromethyl Ketones, J. R. Damewood, Jr., P. D. Edwards, S. Feeney, B. Gomes, G. B. Steelman, P. A. Tuthill, J. C. Williams, P. Warner, S. Woolson, D. J. Wolanin, C. A. Veale. J. Med. Chem., **37**, 3303 (1994).
31. Nonpeptidic Inhibitors of Human Leukocyte Elastase. 3. Design, Synthesis, X-ray Crystallographic Analysis, and Structure-Activity Relationships for a Series of Orally Active 3-Amino-6- Phenylpyridin-2-ones, P.R. Bernstein, D. Andisik, P. Bradley, C. B. Bryant, C. Ceccarelli, J. R. Damewood, Jr., R. Earley, S. Feeney, B. C. Gomes, B. J. Kosmider, G. B. Steelman, R. M. Thomas, E. P. Vacek, C. A. Veale, J. C. Williams, D. J. Wolanin, S. A. Woolson. J. Med. Chem., **37**, 3313 (1994).
32. Non-Peptidic Inhibitors of Human Leukocyte Elastase 4: Design, Synthesis, and In Vitro and In Vivo Activity of a Series of E-Carbolinone-Containing Trifluoromethyl Ketoness. C. A. Veale, J. R. Damewood, Jr., G. B. Steelman, C. Bryant, B. Gomes, J. Williams. J. Med. Chem., **38**, 86 (1995).
33. Non-peptidic Inhibitors of Human Leukocyte Elastase. 5. Design, Synthesis, and X-ray Crystallography of a Series of Orally Active 5-Aminopyrimidin-6-one-Containing Trifluoromethyl Ketones. C. A. Veale, P.R. Bernstein, C. B. Bryant, C. Ceccarelli, J. R. Damewood, Jr., R. Earley, S. Feeney, B. C. Gomes, B. J. Kosmider, G. B. Steelman, R. M. Thomas, E. P. Vacek, J. C. Williams, D. J. Wolanin, S. A. Woolson. J. Med. Chem., **38**, 98 (1995).
34. Synthesis and Biological Activity of a Series of 4-Aryl Substituted Benz[b]azepines: Antagonists at the Strychnine Insensitive Glycine Site. P. F. Jackson, T. W. Davenport, L. Garcia, J. A. McKinney, M. G. Melville, G. G. Harris, M. J. Chapdelaine, J. R. Damewood, L. M. Pullan, J. M. Goldstein. Bioorg. Med., **5**, 3097 (1995).

35. Peptide Mimetic Design with the Aid of Computational Chemistry. J. R. Damewood, Jr. Reviews in Computational Chemistry. K. B. Lipkowitz and D. B. Boyd, ed. VCH Publishers, Inc., New York, NY, p 1-79, 1996.
36. Orally Active Inhibitors of Human Leukocyte Elastase. C. A. Veale, P. R. Bernstein, C. M. Bohnert, F. J. Brown, C. Bryant, J. R. Damewood, Jr., R. Early, S. W. Feeney, P. D. Edwards, B. Gomes, J. M. Hulsizer, B. J. Kosmider, G. Moore, T. W. Salcedo, D. S. Silberstein, G. B. Steelman, M. Stein, A. Strimpler, R. M Thomas, E. P. Vacek, J. C. Williams, D. J. Wolanin, S. Woolson, J. Med. Chem., **40**, 3173 (1997).
37. Computer-Aided Design of Novel Inhibitors of Human Leukocyte Elastase. D. Andisik, P. Bernstein, F. Brown, C. Bryant, C. Ceccarelli, J. Damewood, P. Edwards, S. Feeney, B. Gomes, R. Green, B. Kosmider, A. Shaw, G. Steelman, R. Thomas, P. Tuthill, E. Vacek, C. Veale, P. Warner, J. Williams, D. Wolanin, S. Woolson Pharmacochemistry Library, **28**, 499-509 (1997).
38. Orally Active Trifluoromethyl Ketone Inhibitors of Human Neutrophil Elastase. C.A. Veale, P. R. Bernstein, C.M. Bohnert, F.J.Brown, C. Bryant, J. R. Damewood, Jr. Chemtracts, **11**, 546 – 549 (1998).
39. The Discovery of Non-Basic Atrial Natriuretic Peptide Clearance Receptor Antagonists: Part 1. C.A. Veale, V. C. Alford, D. Aharony, D. L. Banville, R. A. Bialecki, F. J. Brown, J. R. Damewood, C. L. Dantzman, P. D. Edwards, R. Jacobs, R. C. Mauger, M. M. Murphy, W. E. Palmer, K. K. Pine, W. L. Rumsey, L. E. Garcia-Davenport, A. Shaw, G. B. Steelman, J. M. Surian, E. P. Vacek, Bioorg. Med. Chem. Lett., **10**, 1949-1952 (2000).
40. Approaches to Seizure Risk Assessment in Preclinical Drug Discovery. A. Easter, M. E. Bell, J. R. Damewood, Jr., W. S. Redfern, J-P Valentin, M. J. Winter, C. Fonk, R. A. Bialecki, Drug Discovery Today, **14**, 876 - 884 (2009).
41. NovoFLAP: A Ligand-Based De Novo Design Approach for the Generation of Medicinally Relevant Ideas. J. R. Damewood, Jr., C. L. Lerman, B. B. Masek, J. Chem. Inf. Model., **50**, 1296-1303 (2010).
42. De Novo Design of a Picomolar Non-Basic 5HT1b Receptor Antagonist. D. A. Nugiel, J. Krumrine, D. C. Hill, J. R. Damewood, Jr., J. Med. Chem., **53**, 1876 – 1880 (2010).
43. Dibenzothiazepine Derivatives and Use Thereof. D. Brown, J. R. Damewood, Jr., P. Edwards, J. Hulsizer, J. C. Muir, E. M. Pierson, Jr., A. B. Shenvi, S. Wesolowski, D. Widzowski, M. Wood. WO/2009/154563.
44. Development and SAR of Functionally Selective Allosteric Modulators of GABA(A) Receptors C. Alhambra, C. Becker, A. Chang, J. R. Damewood, Jr., T. Daniels, B. T. Dembofsky, K. J. Herzog, C. L. Horchler, C. J. Ohnmacht, R. S. Schmiesing, A. Dudley, M. D. Ribadeneira, K. S. Knappenberger, C. Macaig, M. M. Stein, M. Chopra, X. F. Liu, E. Christian, J. L. Arriza, M. J. Chapdelaine, Bioorganic & Medicinal Chemistry, **19**, 2927-2938 (2011).
45. Phospholipogenic Pharmaceuticals are Associated with a Higher Incidence of Histological Findings than Nonphospholipogenic Pharmaceuticals in Preclinical Toxicology Studies L. Barone, S. Boyer, J. R. Damewood, Jr., J. Fikes, S. Mattis, G. Gipson, P. Ciaccio. Journal of Toxicology, **2012**, (2012). Article ID 308594.

46. Development of Dietary Soluble Fibers by Enzymatic Synthesis and Assessment of their Digestibility in in vitro, Animal and Randomized Clinical Trial Models. O. Hasselwander, R. DiCosimo, Z. You, Q. Cheng, S. Rothman, S Suwannakham, Z. Baer, B. Roesch, K. Ruebling-Jass, J. P. Lai, R. Hurteau, M. Marquez, A. Kopatsis, A. Ouwehand, S. Forssten, P. Mukerji, J. M. Caverly-Rae, Y. P. Dragan, J.R.Damewood, Jr., K. Tiihonen, A. Ibarra. International Journal of Food Science and Nutrition, **2017**:1-16. doi: 10.1080/09637486.2017.1295027.

Invited Lectures and Presentations:

1. QCPE Workshop on the Practical Applications of Quantum Chemistry -Assistant Instructor, June 21- 26, 1981.
2. XVII Organosilicon Symposium - "Conformational Studies of Silane Polymers", June 3, 1983.
3. Shippensburg University-"Application of Molecular Mechanics Calculations to Problems in Organic Chemistry", October 18, 1985.
4. University of Maryland Baltimore County - "Studies in Molecular Stereochemistry", October 22, 1985.
5. XX Organosilicon Symposium - "Conformational Analysis of Hexadecamethyl-cyclooctasilane", April 18, 1986.
6. XX Organosilicon Symposium - "A Closer Look at the Silacyclopentadienyl Anion", April 18, 1986.
7. l986 Gordon Conference on Computational Chemistry - "Computational Studies of Molecular Recognition", August 18, 1986.
8. Bloomsburg University - "Studies in Molecular Recognition", November 3, 1986.
9. VIIIth International Symposium on Organosilicon Chemistry - "Silyl Anions: Inversion, Electronic and Geometric Structure", June 9 and 10, 1987 - (Symposium Fellow).
10. VIIIth International Conference on Computers in Chemical Research and Education, Beijing, China - "Molecular Mechanics Studies of Molecular Recognition", June 15-20, 1987 (Invited international presentation).
11. University of Delaware Department of Chemistry Colloquium-"Molecular Recognition and Molecule - Molecule Interactions", November 6, 1987.
12. New Jersey Institute of Technology - "The Use of Molecular Mechanics in the Study of Molecular Recognition and Molecule - Molecule Interactions", November 9, 1987.
13. SUNY Stony Brook - "Molecular Recognition and Molecule Molecule Interactions", November 19, 1987.
14. Villanova - "Molecular Recognition and Molecule - Molecule Interactions", February 9, 1988.
15. Conference on Molecular Mechanics and Molecular Dynamics - Tallahasse, Fl. "Calculation of Intermolecular Potential Energy Surfaces Using Modified Molecular Mechanics Techniques", April 4-8, 1988.
16. Army Research Office, Aberdeen Proving Grounds - "Studies in Molecular Recognition", April 13, 1988.

17. Mid Atlantic Regional Meeting (MARM) - American Chemical Society "The Hydration of Small Polar Organic Molecules" with R. Kumpf; "A Molecular Mechanics Study of Binding Energies of Dibenzo 18-Crown-6 and Acetonitrile and Nitromethane" with K. Kiick; "Molecular Mechanics Calculation of Intermolecular Potential Energy Surfaces: The Hydration of Formaldehyde" with W. Mühlbauer; "Synthesis of a Novel Macrocycle: Tunnelane" with T. Williamson; "Studies of Molecular Complexation with Crown Ether Derived Host Systems" with J. Urban; "Interaction of Methane and Water" with D. Kellogg.
18. Gordon Conference on Computational Chemistry - "Calculation of Intermolecular Potential Energy Surfaces Using Modified Molecular Mechanics Methods", July 4, 1988.
19. Sixth International Congress on Quantum Chemistry, Jerusalem, Israel-"Calculation of Intermolecular Potential Energy Surfaces by Ab Initio and Molecular Mechanics Methods", Jerusalem, Israel, August 21 - 25, 1988.
20. University of Wisconsin, Eau Claire - "Molecular Recognition and Molecule - Molecule Interactions", November 4, 1989.
21. The Johns Hopkins University - "Molecular Recognition and Molecule - Molecule Interactions", February 21, 1989.
22. 1989 Sanibel Symposium - "Molecular Mechanics Calculation of Intermolecular Potential Energy Surfaces: Hydrogen Bonded Systems", April 1 - 8, 1989.
23. IXth International Conference on Computers in Chemical Research and Education (ICCCRE) - Riva del Garda, Italy - "Molecular Mechanics Calculation of Intermolecular Potential Energy Surfaces: Hydrogen Bonded Systems", May 28 - June 2, 1989 (Invited international presentation).
24. Indiana University of Pennsylvania - "Computational Studies of Molecular Recognition and Molecule - Molecule Interactions", October 27, 1989.
25. United States Naval Academy - "Computational Studies of Molecular Recognition and Molecule - Molecule Interactions", November 17, 1989.
26. Numerical Simulation in Science Symposium - University of Delaware - "Free Energy Perturbation Simulations for Solutions", December 1, 1989.
27. Conference on Molecular Mechanics and Molecular Dynamics - Tallahasse, Fl. "Free Energy Perturbation Simulations for Solutions", April, 1990.
28. Chair, Physical Organic Session, National American Chemical Society Meeting,Washington, D.C., 1990.
29. University of Maryland, Baltimore County - Anniversary Symposium, Department of Chemistry and Biochemistry - "Designing Inhibitors for Human Neutrophil Elastase" April 3, 1992.
30. Gordon Research Conference - Enzymes, Coenzymes and Metabolic Pathways "Designing Inhibitors for Human Neutrophil Elastase," June 29-July 3, 1992.
31. 51st Pittsburgh Diffraction Conference - "Nonpeptidic Inhibitors of Human Neutrophil Elastase", with C. Ceccarelli, Philadelphia, PA, November 3-5, 1993.

32. Computational Organic Chemistry Symposium, 207th National American Chemical Society Meeting, Featured Speaker - "Nonpeptidic Inhibitors of Human Neutrophil Elastase", San Diego, CA, March 14, 1994.
33. Chair, Physical Section, "Structure and Reactivity in Aqueous Solution - IV", 207th National American Chemical Society, San Diego, CA, March 15, 1994.
34. University of California San Francisco and Scripps Research Institute Structural Biology Symposium - "Nonpeptidic Inhibitors of Human Neutrophil Elastase", Cabo San Lucas, Mexico, May 1, 1995.
35. 210th National American Chemical Society Meeting, "4-Aryl Substituted Benz[b]azepines: Synthesis and Antagonist Activity at the Strychnine-Insensitive Glycine Receptor", Chicago, Ill, August, 1995, with T. W. Davenport, et al.
36. Random & Rational: Drug Discovery via Rational Design and Combinatorial Chemistry - "Nonpeptidic Inhibitors of Human Neutrophil Elastase", Princeton, NJ, September 11-12, 1995.
37. Rational Drug Design Conference on Computational Approaches to Analyze Protein-Ligand Interaction/Binding Affinities - "Peptidomimetic Design with the Aid of Computational Chemistry", Coronado, CA, December 11-12, 1995. (Video presentation).
38. Symposium Organizer and Chair, Computational Chemistry Assisted Drug Discovery, Symposium, 211th National American Chemical Society, New Orleans, LA, March 24-28, 1996.
39. Saint Louis ACS Award Symposium on Recent Advances in Computer-Aided Drug Design (CADD). Saint Louis, MO, April 24, 1998.
40. University of Delaware, Departmental Colloquium, “Computational Chemistry in Drug Discovery”, Newark, Delaware, December 5, 2001.
41. Molecular Medicine Marketplace: Target-Driven Chemistry, “The Changing Nature of Early Phase Discovery Chemistry in the Pharmaceutical Industry”, Santa Clara, CA, March 17, 2003.
42. University of Maryland Baltimore County, “Drug Discovery: An Example of Research at the Chemistry Biology Interface”, Baltimore, Maryland, March 15, 2006.
43. Université Paris V – René Descartes, Espace Lavoisier, Tripos European User Meeting, “What’s All the FLAP About?”, Paris, France, July 7, 2006.
44. 234th National American Chemical Society Meeting, Herman Skolnik Award Symposium for Robert Pearlman, “Flexible Ligand Alignment Protocols and Their Use in De Novo Design”, Boston, MA, August 20, 2007.
45. Tripos Science Summit, “Flexible Ligand Alignment Protocols and Their Use in De Novo Design”, Philadelphia, PA, October 9, 2008.
46. 9th Structure-Based Drug Design, “Designing Drugs Against Multiple Parameters: Multiparameter Ligand – Based De Novo Design”, Cambridge, MA, June 5, 2009.
47. Tripos Science Summit, “Efficient and Effective Navigation of Multiparameter Design Performance”, Philadelphia, PA, January 28, 2010.

48. Society Chemical Industry (SCI), Designing Safer Medicines in Discovery: Current and Emerging Opportunities to Reduce Attrition, "Avoiding Aromatic Hydrocarbon Receptor Liability in Drug Candidates", London, UK, March 17, 2011.
49. The Dell Lecture, "A Chemist's Perspective on Safety by Design", Stevenson University, Stevenson, MD, March 4, 2015.
50. 251st National American Chemical Society Meeting, Earle B. Barnes Award for Leadership in Chemical Management: Symposium in honor of Henry E. Bryndza, "Safety by design: Integration of safety/toxicology considerations into the early research process" San Diego, CA, March, 2016.
51. 256th National American Chemical Society Meeting, "Predictive Toxicology Approaches: Development, Challenges and Applications" Boston, MA, August, 2018.