

JAMES R. DAMEWOOD, JR. PH.D., DABT, ERT

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SUMMARY

Toxicologist, Chemist, Computational Chemist with broad experience and significant track record of accomplishment in the pharmaceutical, agrochemical and chemical industries in both senior scientist and managerial positions. Member and leader of numerous high performing multidisciplinary project teams. Adviser and consultant in multiple and diverse business areas, with a focus on designing and delivering products that are both regulatory compliant and safe for humans and the environment. Excellent organizational skills, presentation skills, and analytical abilities with a strong results orientation.

PROFESSIONAL EXPERIENCE

Chemical Toxicology Consulting, LLC.

2022 - present

Principal

- Supporting client toxicology requirements in multiple areas.
Affyigility Solutions (Sr. Toxicology Advisor): support of pharmaceutical and pharmaceutical manufacturing activities in multiple client companies.
Delrin (formerly a DuPont company): including coordinating and interpreting GLP and non-GLP toxicology and bio-compatibility studies.
- Notable non-proprietary activities:
Formaldehyde Panel Member, American Chemistry Council
American Chemical Society, Committee on Science

Janssen Pharmaceuticals (Johnson & Johnson Family of Companies)

2020 - 2022

Global Senior Director, Predictive & Computational Toxicology

- Supporting cellular health assessment (e.g., mitochondrial toxicity, cytotoxicity, oxidative stress, etc.), toxicogenomics, expression profiling, target liability assessment, phototoxicity, computational toxicology, *in silico* predictive toxicology.
- Guiding the implementation and/or development of *in vitro* experimental and *in silico* computational approaches that address key toxicology problems faced by discovery projects.
- Partnering with the design function to de-risk project team delivery and assist with toxicology problem solving in the therapeutic areas.
- Partnering with phenotypic profiling from the perspective of toxicology.
- Serving as a liaison between toxicology and the medicinal chemistry function. Rapidly identify realized or potential toxicology challenges in discovery programs.
- Influencing, educating, and supporting medicinal chemistry with toxicology approaches that can help resolve compound liabilities.

Affyigility Solutions

2018 - 2020

Senior Director of Toxicology

- Leading toxicology support of pharmaceutical research, development and manufacturing.
- Working with companies in over 60 countries to provide toxicology consulting during both discovery and development phases. Providing potent compound safety assessments, excipient level justifications, contamination assessments, health-based exposure level assessments, occupational exposure limits for active pharmaceutical ingredients, acceptable daily exposure levels and permitted daily exposure levels.

- Mentoring and developing staff in areas critical to toxicology support for pharmaceutical research and development.
- *CPhI Pharma Award Recipient 2020 – Recognizing Excellence in Pharma: Affygility, Regulatory Procedures and Compliance*

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

Metabolism, Toxicokinetics, and Analytical Section

- Research Manager for the Metabolism, Toxicokinetic, and Analytical Section of the Haskell Global Center for Health Sciences, Corteva Agriscience™, Agricultural Division of DowDuPont™.
- 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.
- Coordination of GLP and non-GLP toxicology studies.

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

- 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. Business units supported include: Packaging and Industrial Polymers, Polymer Products, Central Research & Development (company-wide research), Science & Innovation, Crop Protection, Performance Coatings, and Electronics & Communication.
- Collaboratively established product stewardship within the Central Research & Development organization, including approaches customized to the early research environment, bringing considerations of safety/toxicology/regulatory/public perception to the early research environment. Cooperatively developed the international CR&D product stewardship network.
- Provide safety/toxicology and product stewardship support to ~60 ongoing Central Research and Development projects extending across all research areas of the company.
- Provide training in hazard, exposure, public perception and product stewardship globally within the DuPont Central Research & Development organization (US, India, China, Brazil, Canada), training over 600 senior and associate scientists.
- Serves as a member of the Haskell Acceptable Exposure Limit (AEL) committee to establish occupational exposure limits for chemicals of interest to DuPont.
- Establishing member of the DuPont GRAS (generally recognized as safe) Advisory Team that internally reviews and supports all proposed GRAS determinations for new food materials.
- Provides training and mentorship to less experienced Business Liaison colleagues in multiple business areas and lead three recruiting campaigns for Business Liaisons.
- Provides strategy and practical input into the development of predictive toxicology and Tox21 at Haskell Global Centers.
- Member of food additive, food contact, polymer advocacy and chemical awareness team within DuPont.
- Coordination of GLP and non-GLP toxicology studies.

ASTRAZENECA, Wilmington, DE

1990-2010

Principal Scientist II, Lead Optimization Chemistry (2005-2010)

- 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. Developed and delivered educational materials to global Chemistry colleagues on safety issues such as genetic toxicity, seizure, and aromatic hydrocarbon receptor (AhR) activity.
- Designed, developed and applied a novel, ligand - based *de novo* design approach and used the approach to design the first potent, orally available, nonbasic 5HT_{1b} antagonist. *Recipient of 2008 AstraZeneca Breakthrough Award*.
- Originated and negotiated a no-cost collaboration with Tripos, Inc. that resulted in the commercialization of our novel *de novo* design approach (above) into the product MUSE. This resulted in substantial capability enhancements and cost savings to AstraZeneca.
- Established structure activity relationships and predictive *in silico* models for aromatic hydrocarbon receptor activation in a critical CNS project. Helped to lead project team to design compounds that were not active at the aromatic hydrocarbon receptor. *Recipient of 2009 AstraZeneca Breakthrough Award*.
- Delivered computational and chemical perspective to the multidisciplinary Cardiac Safety Working Group. This group established agreed guidelines to help avoid QT prolongation issues.
- Pioneered exploiting information in the Adverse Event Reporting System (AERS) database to help identify areas of potential safety concern for emerging drug candidates.
- Designed and collaboratively developed DASHBOARD, a global project progression and evaluation application that increased the transparency of optimization efforts, data availability, compound tracking and turn-around times for project assays while also assisting with the challenging problem of maintaining project focus on multi-parameter optimization.
- Chaired the Structure-Based Pan mGluR Modulation Group, a multidisciplinary and multicompany collaboration that provided the first evidence that AstraZeneca compounds bind to a distinct modulatory site in mGluR2. Site specific mutants were used to clarify project structure activity relationships.

Associate Director, Chemistry; Section Head, Computational Chemistry & Informatics (2000 – 2005)

- Re-staffed the Section to 7 Ph.D.'s (from 2) after merger, and managed group activities. Group obtained global recognition with two Science and Technology Achievement awards.
- Established computational chemists as full members of discovery project teams.
- Lead the multidisciplinary development of CHEMSTRUC, a unique and powerful capability that mines chemical structure information in patents and literature into a globally distributed relational database. *First place 2005 R&D Challenge Award* (single award throughout global AstraZeneca).
- Established and chaired the Structural Biology Working group, a multidisciplinary group that prioritized Wilmington structural biology possibilities and served as the liaison group with the Swedish structural biology group. The approach of this group was used as a global model.
- Established the Wilmington research demand management process for Information Technology support. Lead the Discovery Informatics Steering Group prioritizing discovery needs and helping to establish priorities for ca 25 information technology staff.

ZENECA, Wilmington, DE

1990-2000

(Formerly ICI Americas), Physical Sciences

Senior Group Leader, Molecular Modeling and Structural Biology (1998-2000)

- Managed the research of 8 staff (7 Ph.D.) in computational chemistry, protein biochemistry, X-ray crystallography, and protein NMR delivering and utilizing protein structures in molecular design.
- Delivered computational chemistry support to project teams. Significant advances in computational chemistry and informatics in the areas of HTS analysis, compound collection enhancement and informatics analysis (R&D Directors Award received in group for a globally distributed decision support tool, PANDORA).
- Initiated large-scale education and support of Medicinal Chemists in the science and application of computational and molecular modeling methods.

Principal Chemist (1996-1998)

- Organized and lead the US High Throughput Screening Hits Evaluation Team that increased the quality of HTS analysis while also increasing the efficiency of analysis time from a typical ca 6 months to ca 2 weeks.
- Chaired the Working Party for Data Integrity, a multidisciplinary team that established corporate data integrity guidelines that remain in use today as the basis for corporate data stores.
- Lead the computational chemistry aspects of the global compound collection enhancement initiative resulting in the addition of purchased and synthesized (including combinatorial chemistry) compounds to the company compound library.

Senior Research Chemist (1990-1996)

- Computationally identified where inhibitors of Human Neutrophil Elastase, could be modified to rapidly overcome the problem of oral activity.
- Worked collaboratively with NMR spectroscopist to determine the 3D structure of ω -Conotoxin, the first protein structure determined in ICI.

UNIVERSITY OF DELAWARE, Newark, 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.

Affiliated Faculty, Department of Chemistry and Biochemistry

2018 - present

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**CERTIFICATIONS, PROFESSIONAL ACTIVITIES, AND AFFILIATIONS****Diplomate, American Board of Toxicology (DABT)****UK Register of Toxicologists, Royal Society of Biology (ERT)****Certified Six Sigma Green Belt**

Scientific Advisory Board, Science and Mathematics Division / Chemistry, Stevenson University, Stevenson MD, 2004 - 2017

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.

SELECTED PROFESSIONAL DEVELOPMENT

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 β -Carbolinone-Containing Trifluoromethyl Ketones. 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 5HT_{1b} 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. Horschler, 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 / 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. 1986 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 - Tallahassee, 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 Macrocyclic: 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 - Tallahassee, 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.
52. Occupational Toxicology Round Table (OTR) Co-chair "The Development and Application of Acceptable Daily Exposures and Permitted Daily Exposures", Sonoma, CA, October 2019.
53. 2022 Society of Toxicology, "AI/ML Models Based on Chemical and Phenotypic Descriptors Accurately Predict Mitochondrial Liabilities for Early De-Risking in Drug Discovery" Mesens, N; Van Dongen, C.; Le Van, T.; Kandula, M.; Herman, D.; Van Goethem, F.; Zoffmann, S.; Ceulemans, H.; Damewood, J.; Will, Y.; Zhang, L.; Peeters, P. San Diego, CA, March, 2022. 2022 Best SOT-CTSS Abstract Award.
54. 2022 Society of Toxicology, "AI/ML Models to Predict DILI Severity Using Chemical Properties and Predicted Off-Target Interactions" Rao, M.; Nassiri, V.; Geys, H.; Snoeys, J.; Mesens, N.; Van Goethem, F.; Irrechukwu, O.; Damewood, J.; Will, Y. San Diego, CA, March, 2022. 2022 Best SOT-CTSS Abstract Award.
55. 2022 Society of Toxicology, "Deriving Structural Alerts for the Qualitative Assessment of Mitochondrial Toxicity by Mining Data from a Glu/Gal Assay" Alhambra, C.; Mesens, N.; Damewood, J.; Will, Y. San Diego, CA, March, 2022.
56. Non-Clinical Statistics Conference NCS, "A fully *in silico* framework to predict Drug-induced liver injury in early stage of drug development" Rao, M.; Geys, H.; Irrechukwu, O.; Damewood, J.; Van Goethem, F.; Snoeys, J.; Will, Y. October 20, 2022.

ADDITIONAL INTERESTS

Gardening

Kenpo Karate (Third Degree Black Belt)

Euphonium Horn (Rehoboth Concert Band)

APPROVALS

COMPANY: AFFYGILITY SOLUTIONS LLC

ORIGINATOR: Jim Damewood DATE: 2026-05-14QUALITY Matt Basich DATE: 2026-05-14MANAGEMENT Jim Damewood DATE: 2026-05-14

EFFECTIVE DATE: 2026-05-14

CERTIFICATE *of* SIGNATURE

REF. NUMBER
VGFIG-XVGUB-KKHSN-UBFW

DOCUMENT COMPLETED BY ALL PARTIES ON
14 MAY 2026 17:37:06
UTC

SIGNER

DEAN CALHOUN

EMAIL
DCALHOUN@AFFYGILITY.COM


TIMESTAMP

SENT
14 MAY 2026 04:59:29

VIEWED
14 MAY 2026 05:15:02

SIGNED
14 MAY 2026 05:15:31

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IP ADDRESS
151.253.30.203

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TIMESTAMP

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