Charles H. Reynolds
Gfree Bio, LLC
Email: creynolds@gfreebio.com, www.gfreebio.com

Experience

2011-present Founder, Gfree Bio, LLC

- Gfree Bio develops and delivers modeling, informatics, and structure-based design capabilities for emerging biotech companies. Gfree Bio has employed its computational chemistry capabilities to advance many successful drug discovery programs for over 30 companies ranging from start-ups to publicly traded companies.
- Principal Investigator for NIH STTR program (2016-2017) at Gfree Bio to develop new methodology for refining protein-ligand cocrystal structures.
- Acting Chief Scientific Officer, PPI Mimics, LLC (2013-2015), and Principal Investigator for two successful NIH STTR Phase I applications.
- Other collaborations include: NIH SBIR The Wistar Institute; multiple NIH SBIRs Phelix Therapeutics; NIH STTR Fox Chase Chemical Diversity and Drexel College of Medicine.

2009-present Director (Industry Advisory Board) QuantumBio Inc.

- Provided scientific and business development advice to senior management.

2010-2011 Senior Director and Head of Discovery Technologies, Ansaris

- Responsible for scientific computing, proprietary discovery technology, structural biology, and IT. Member of senior management team with significant business development responsibilities.

- Initiated a major update of core computational fragment-based drug design platform. Refocused technology to target small molecule ligands for protein-protein interactions. Updated and improved software (speed, efficiency, user-interface).

- Leadership role in identification and prosecution of an internal target that led to a significant pharma partnering opportunity.

- Executive management of major research collaboration with Novartis.

2000-2010 Research Fellow, Johnson & Johnson Pharmaceutical R&D

- Responsibilities included managing modeling and informatics research teams at the Spring House, PA and La Jolla, CA sites. Managed significant hardware and software budgets across multiple US sites.

- Teams under my direction provided critical support for progression of tens of compounds to early development, three compounds to first in human, and one Phase-II candidate. Contributed to carisbamate NDA and European registration for Dacogen®.

- Led development of new discovery methodology at J&J including: informatics tools for fragment-based design, novel protocols for improved crystal-structure refinement, linear interaction energy approaches for ligand optimization, a similarity-based tool for scoring reagents for "drug-likeness," application of linear-scaling quantum calculations to analysis of protein structures, and structure-based ADME-Tox. The latter effort includes a published multi-state homology model for the hERG channel that was employed successfully in multiple discovery programs and was honored in 2008 as a most cited article by Elsevier.

- Migrated J&J Computer-Aided Drug Discovery (CADD) groups to linux-based clusters and workstations, and consolidated CADD software licenses across sites. This effort resulted in a significant improvement in computational capabilities while reducing the overall cost of high-performance computing.

- Member of the New Targets Evaluation Committee for drug discovery. Organized a series of global J&J CADD and structural-biology meetings. Initiated external research collaborations at Penn State, Yale, and the University of Florida. Coordinated J&J's first structural-biology collaboration with DeCode Biostructures (now Emerald).

1995-2000 Research Fellow, **1984-1994** Senior Scientist, Rohm and Haas (DowDuPont)

- Co-inventor of a new class of ergosterol biosynthesis inhibitor antifungals. Awarded the highest scientific award in the company (Otto Haas Award).

- Led an interdisciplinary team of a dozen scientists tasked with developing new drug therapies and diagnostic aids. This project resulted in a novel nanoparticle-based targeted contrast agent for MR imaging. Roles included developing the concept and selling it to R&D management, leading the team, establishing a collaboration with the University of Pennsylvania Medical School, and developing a market analysis in collaboration with Argonex (a biotechnology company that is now part of Millipore).

2019-present Editorial Advisory Board, Journal Chemical Information and Modeling

2014-present Editorial Advisory Board, ACS Medicinal Chemistry Letters

2013 J.T. Oden Visiting Faculty Fellow, ICES, The University of Texas at Austin

2010-present Adjunct Professor, Pennsylvania Drug Discovery Institute

2008-2018 Member, American Chemical Society Publications Committee

2007-present NIH study sections, BDMA, BCMB, IMST-10, IMST-11, NCI ZCA1

2006-2011 Scientific Advisory Board, Keystone Symposia

2006-2009 Councilor, American Chemical Society

1998-2006 Editorial Advisory Board, Journal of Molecular Graphics and Modeling

1998 Joint postdoctoral research supervisor, University of North Carolina at Chapel Hill

1996-1998 Joint graduate research supervisor, The Pennsylvania State University

1990 Adjunct Professor, The University of Pennsylvania

Additional Experience and Leadership Activities.

2015 National Academy of Sciences STTR program workshop; **2008** Co-organizer, first Keystone Symposium on computer-aided drug discovery; **2006-2009** Advisory Board for NSF sponsored science and math education initiative at Temple University (TU-SMART**); 2007** Co-organizer, ACS Prospectives Meeting, Advances in Structure-Based Drug Discovery; **2007** Inaugural Keck Foundation Lecture, St. Edward's University**; 2007** Lecturer, ACS computational chemistry short course**; 2005** Organizer, ACS Prospectives Meeting, Advances in Structure-Based Drug Discovery; **1999-2000** Rohm and Haas Technology Center Coordinator for Life Sciences; **1998-2000** Membership Committee, ACS Computers in Chemistry Division; **1999** Co-taught a computational chemistry short course (Jan Term) at Austin College; **1997** Chair, ACS Computers in Chemistry Division; **1991-1995** Treasurer, ACS Computers in Chemistry Division; **1989** Faculty, QCPE course.

Education

1984 Ph.D. in Theoretical Organic Chemistry, The University of Texas at Austin, Austin, Texas. Supervisor: Michael J.S. Dewar.

1979 B.A. in Chemistry, Austin College, Sherman, Texas. Honors in Chemistry.

Management Training

2013 Kauffman Institute Entrepreneur Training Program

2002 Johnson & Johnson Management Fundamentals

2001 Johnson & Johnson Manager and the Law

1993 First-Line Leadership

1992 The Leadership Challenge

Awards

2015 Gfree Bio selected as a Kauffman Foundation FastTrac success story

2012 Distinguished Alumni Award, Austin College

2010 Fellow of the American Chemical Society

2007 Standards of Leadership Award, Johnson & Johnson

2007 Platinum Encore Award, Johnson & Johnson (Dacogen registration in Europe)

2000 Johnson & Johnson Excellence in Science Award (four awarded company wide)

1987 Otto Haas Award, Rohm and Haas (highest award for scientific achievement).

1993 Marion Cox Award, Austin College; **1984** University of Texas Career Development Award; **1983** Robert A. Welch Foundation Pre-doctoral Fellowship, The University of Texas at Austin; **1978** P.S. Wharton Fellowship in chemistry, Austin College; **1978** National Science Foundation Undergraduate Research Scholarship, The University of Texas at Arlington; **1975-1979** Robert A. Welch Undergraduate Chemistry Scholarship.

Prior Expert Testimony

I have not provided expert testimony in connection with litigation in the past five years.

Publications

Author of over 100 papers, chapters, books, and patents

Publications

Agragiotis, D.K.; Holloway, M.K.; Johnson, S.A.; Reynolds, C.H; Stouch, T.R.; Tropsha, A.; Waller, C.L. Chemistry, information, and Frank: a tribute to Frank Brown, J. Computer-Aided Molecular Design, 2018, 32, 723-729. https://doi.org/10.1007/s10822-018-0135-9

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Yifang Huang, Eric D. Strobel, Chih Y. Ho, Charles H. Reynolds, Kelly A. Conway, Jennifer A. Piesvaux, Douglas E. Brenneman, George J. Yohrling, H. Moore Arnold, Daniel Rosenthal, Richard S. Alexander, Brett A. Tounge, Marc Mercken, Marc Vandermeeren, Michael H. Parker, Allen B. Reitz, Ellen W. Baxter, **Macrocyclic BACE inhibitors: Optimization of a micromolar hit to nanomolar leads**, Bioorganic & Medicinal Chemistry Letters, Volume 20, Issue 10, 15 May 2010, Pages 3158-3160.

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Zhang, Xiaohua; Gibbs, Alan C.; Reynolds, Charles H.; Peters, Martin B.; Westerhoff, Lance M. **Quantum Mechanical Pairwise Decomposition Analysis of Protein Kinase B Inhibitors: Validating a New Tool for Guiding Drug Discovery**. J. Chem. Inf. Model. (2010), 50, 651-661.

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Li, Jian; Reynolds, C. H. **A quantum mechanical approach to ligand binding: Calculation of ligand-protein binding affinities for stromelysin-1 (MMP-3) inhibitors**, Canadian Journal of Chemistry, (2009), 87, 1480-1484.

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Reynolds, Charles H.; Best, Scott A. **A fast molecular simulation to calculate lipophilicity.** CHEMTECH (1998), 28(11), 28-34.

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Reynolds, Charles H.; Shaber, Steven H. **Rational design of novel ergosterol biosynthesis inhibitor fungicides.** ACS Symposium Series (1995), 589(Computer-Aided Molecular Design), 171-82 2 Plates - pp. 230a-230b.

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Patents

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