Kenneth M. Merz Jr.

Curriculum Vitae

(as of May 1, 2022)

Professional Address:

Department of Chemistry
Department of Biochemistry and Molecular Biology
Michigan State University
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Twitter: @kmerz1

Education:

University of California, San Francisco
September 1987 to February 1989
Supervisor: Peter Kollman (Deceased)
Research: Macromolecular Structure and Dynamics
Position: Post-doctoral Fellow

Cornell University
January 1986 to September 1987
Supervisor: Roald Hoffmann
Research: Applied Molecular Orbital Theory
Position: Post-doctoral Fellow

The University of Texas at Austin
June 1981 to December 1985
Supervisor: Michael J. S. Dewar (Deceased)
Research: Applied Electronic Structure Theory
Degree: Ph. D. in Organic Chemistry

Washington College
September 1977 to May 1981
Research: Synthesis of Polysaccharides.
Degree: B. S. in Chemistry

Professional Experience:

University Distinguished Professor, 2021-present

Editor-in-Chief, Journal of Chemical Information and Modeling, 2014-present

Joseph Zichis Chair in Chemistry, 2013-present

Director, Institute for Cyber Enabled Research (iCER), 2013-2019

Edmund H. Prominski Professor of Chemistry, 2011-2013

University of Florida Research Foundation (UFRF) Professor, 2011-2013

The University of Florida, Colonel Allan R. and Margaret G. Crow Term Professor, 2009-2011

The University of Florida, Professor of Chemistry and Member, Quantum Theory Project, 2005-present

The Pennsylvania State University, Professor of Chemistry, 1998-2005

Pharmacopeia, Inc. (now Ligand Pharmceuticals), Position: Senior Director of the ADMET R&D Group, 2000-2001

Pharmacopeia, Inc., (now Ligand Pharmceuticals) Position: Senior Director of the Center for Informatics and Drug Design (CIDD), 1998-2000

The Pennsylvania State University, Associate Professor of Chemistry, 1996-1998

The Pennsylvania State University, Assistant Professor of Chemistry, 1989-1996

Honors and Awards:

Chair-Elect Computers in Chemistry Division, American Chemical Society (ACS), 2011-2012

University of Florida Research Foundation (UFRF) Professor, 2011-2016

Alumni Citation, Washington College, 2011

Fellow of the American Chemical Society, 2010

Visiting Professor, Institute for Research in Biomedicine, Barcelona, Spain 2010

ACS Award for Computers in Chemical and Pharmaceutical Research 2010

Colonel Allan R. and Margaret G. Crow Term Professor 2009-11

Visiting Professor, École Polytechnique, Paris, France 2009

Visiting Professor, University of Florence, Florence, Italy 2008

Visiting Professor, ETH, Zurich, Switzerland 2007

Visiting Professor, University of Oviedo, Oviedo, Spain 2006

Fellow of the American Association for the Advancement of Science, 1999

Visiting Lecturer, Universite Louis Pasteur, Strasbourg 1998.

John Simon Guggenheim Fellowship, 1996-1997.

Visiting Lecturer, Universite Louis Pasteur, Strasbourg 1996-1997.

Office of Naval Research-Young Investigator, 1990-1993.

National Institutes of Health FIRST Award, 1991-1996.

Visiting Lecturer, University of Firenze, 1992.

Robert A. Welch Predoctoral Fellow, 1982 to 1985, The University of Texas at Austin.

Departmental Competitive Fellowships, Fall 1981, The University of Texas at Austin.

Robert A. Welch Summer Research Fellow, Summer 1981, The University of Texas at Austin.

Research Interests: Structure and ligand-based drug design – novel method development and applications to molecular design.

Computational mechanistic enzymology – exploration of enzyme structure and function to enable enzyme design.
Development of combined quantum mechanical/molecular mechanical methods (QM/MM) to explore chemical and biological reactivity.
Transition metal (TM) ion homeostasis – development and application of computational tools to explore TM ion transport in biology.
Application of machine learning/artificial intelligence methods to solve chemical and biological problems.
High-performance computing, data storage and networking to enable computational research.

Select Service:

Editor, Journal of Chemical Information and Modeling 2014-present. *Part of the American Chemical Society journal portfolio with over 1,000 submissions a year.*

Member and Chair Elect of the Multidisciplinary Program Planning Group (MPPG) of the ACS. *Professional organization of ~160,000 members.*

Thematic Chair for the 251st National ACS meeting in San Diego "Computers in Chemistry". *Professional organization of ~160,000 members / Meeting of over 10,000 attendees.*

Chair-Elect Computers in Chemistry Division, American Chemical Society (ACS), 2011-2012. *Professional organization ~160,000 members / Division of ~5,000 members.*

Member, College of the NIH CSR Reviewers 2010-2012.

Co-organizer of first Keystone Symposium on Computer-aided Drug Discovery 2008.

Co-organizer, ACS Prospectives Meeting, Advances in Structure-Based Drug Discovery 2007.

Standing member of the MSFA NIH Study Section2006-2009

ad hoc Reviewer for ZRG1 BCMB-Q NIH Study Section 2005.

Co-organizer, ACS Prospectives Meeting, Advances in Structure-Based Drug Discovery 2005.

ad hoc Reviewer for BMT NIH Study Section 2002-3.

Member Advisory Board for the NSF sponsored National Center for Supercomputer Applications 2002-04.

Member Peer Review Board for the NSF sponsored National Center for Supercomputer Applications 1997-2002.

ad hoc Reviewer for BBCA NIH Study Section 1997.

Member NSF sponsored MetaCenter Review Panel 1996-2002.

Member Peer Review Board for NSF sponsored Pittsburg Supercomputer Center and the National Center for Supercomputer Applications 1994-1997.

Reviewer for multiple major NIH and NSF project grants.

Member on and Chair of multiple Departmental (Graduate recruiting, Advisory, Faculty hiring, Department Head Search, Building) and University (Finance, Advisory, Internal Proposal Review) Committees at multiple institutions.

Completed Expert Witness Work and Testimony:

ViVV/GSK vs. Gilead (hired by attorneys for ViiV/GSK); expert report and deposition.

Technology Transfer:

"Molecular Docking Technique for Screening Combinatorial Libraries " D. J. Diller and K. M. Merz, Jr. US Patent No. 7,065,453.
"One-Dimensional Molecular Representation" S. L. Dixon, K. M. Merz, Jr. and M. Waldman US Patent No. 7,167,851.
"System and Method for Aqueous Solubility Prediction" A. Cheng and K. M. Merz, Jr. US Patent No. 6,957,151.
"Quantum Mechanics Based Method for Scoring Protein-Ligand Interactions" K. Raha and K. M. Merz, Jr. US Patent No. 7,904,283.
"Pharmacogenic Therapies Targetting Metal-Ion Transcriptional Regulation Machinery in Bacteria" K. M. Merz, Jr. and D. Chakravorty U.S. Patent No. 9,483,6009.
"Movable Type Method Applied to Protein-Ligand Binding" Z. Zheng and K. M. Merz Jr - US Patent No. 10,332,616.

Entrepreneurial Activities:

Founder and acting CSO of QuantumBio, Inc. 2001-2019
Co-Founder of Attmos, Inc. 2022

Editorial Board

Memberships:

Computational Biology and Chemistry (2008-2012)
International Journal of Quantum Chemistry (2005-2010)
Computational and Theoretical Nanoscience (CTN) (2003-2008)
Theoretical Chemistry Accounts (2002 – 2005)
Journal of Molecular Modeling (1997 - present)
Journal of Molecular Graphics and Modeling (1997-2011)

Societies:

Phi Kappa Phi
Sigma Xi
American Chemical Society
American Association for the Advancement of Science
New York Academy of Sciences
Biophysical Society
American Physical Society
Protein Society