GLEN EUGENE KELLOGG

Department of Medicinal Chemistry
School of Pharmacy
Medical College of Virginia
Virginia Commonwealth University
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I. BIOGRAPHICAL

A. Personal

Born November 2, 1957, Syracuse, New York
Graduated high school, Albuquerque, New Mexico
Married, two children (twins: Sean and Erik, born April 16, 1993)

B. Education

B.S., University of New Mexico, Albuquerque, December 1979

Ph.D., University of Arizona, Tucson, August 1985

Thesis: Electronic Factors of C-H and C=C Bond Activation: Experimental Information from UV and X-ray Photoelectron Spectroscopies.

Director: Professor Dennis L. Lichtenberger

C. Professional Experience

2024-present	Emeritus Professor, Department of Medicinal Chemistry, Virginia Commonwealth University
Spring 2020:	Visiting Professor, Dipartimento di Scienza e Tecnologia del Farmaco, degli Studi di Torino, Italy.
2018-2023:	Associate Chair, Department of Medicinal Chemistry, Virginia Commonwealth University
2014-2023:	Professor, Department of Medicinal Chemistry & Institute for Structural Biology and Drug Discovery, VCU.
2005-2018:	Assistant Chair, Department of Medicinal Chemistry, Virginia Commonwealth University

1999-2023:	Director of Modeling Core for Structural Biology, VCU Massey Cancer Center.
1999-2014:	Associate Professor, Department of Medicinal Chemistry & Institute for Structural Biology and Drug Discovery, VCU.
1994-1999:	Assistant Professor, Department of Medicinal Chemistry, VCU, Director of Departmental Molecular Modeling Facilities.
1991-2002:	Affiliate Assistant/Associate Professor, Department of Biomedical Engineering (BME), VCU.
1989-1994:	Instructor, Department of Medicinal Chemistry, VCU.
1989, 1993:	Visiting Professor, Randolph-Macon College, Ashland, Virginia
1986-1988:	Postdoctoral Research Associate with Professor Tobin J. Marks, Northwestern University, Evanston, Illinois.
1981-1985:	Graduate Research Assistant, University of Arizona (UA).
1976-1980:	Staff Scientist (final position), University of New Mexico Engineering Research Institute: field/laboratory materials evaluation and computer modeling

D. Teaching Experience

Lecturer for Medicinal Chemistry for Nurse Anesthesia; Course Coordinator/Lecturer for undergraduate Medicinal Chemistry & Drug Design course; Lecture/Laboratory Instructor for graduate-level Molecular Modeling Survey; Lecturer for Bioinformatics and Computational Genomics course; Lecturer for Principles of Pharmacy; Lecturer for Medicinal Chemistry II; Laboratory Instructor for Pharmaceutical Analysis (Skills Lab III); Lecturer for Pharmaceutical Science Survey: From Bench to Shelf; Course Coordinator/Instructor for graduate-level Advanced Molecular Modeling; Course Coordinator/Instructor for graduate-level Topics in Medicinal Chemistry; Course Coordinator/Lecturer for Pharmaceutical Analysis; Lecturer for Advanced Medicinal Chemistry.

E. Student Thesis and Dissertation Committees

Thomas D. Abraham, M.S. (Mathematical Sciences), "Aggregation and Generalization in the E/R and Bubble Diagrams", April 23, 1993.

Rajkamari Jashnani, Ph.D. (Pharmacy and Pharmaceutics), "Effect of Salt Selection and Environmental Conditions on Dry Powder Aerosol Generation", June 24, 1994.

Vrinda R. Nayak, Ph.D. (Medicinal Chemistry), "N-Glycosylation of Amobarbital and Related Barbiturates in Humans and Mice", April 7, 1995.

Jiageng Niu, Ph.D. (Chemical Physics), “The Nature of the Interaction of Metal Atoms and Clusters with Hydrogen Molecules and Helium Atoms”, July 17, 1995.

Telih Boyiri, Ph.D. (Medicinal Chemistry), “Design and Synthesis of Potential Antisickling Agents”, July 28, 1995.

David T. Wei, M.S. (Biomedical Engineering)*, HINT: Using Hydropathic Interactions to Understand Binding Properties of Biomolecules”, November 21, 1996.

Peter Meiller, M.S. (Mathematical Sciences), "Fourier Transform Data Compaction Techniques in Molecular Conformation Space: Reducing Storage Requirements for 3D Data Bases", December 3, 1996.

David M. Barrett, M.S. (Biomedical Engineering), “Evaluation of the Adjuvant Activity of the Silicone Components of Medical Devices”, May 29, 1997.

Ijeoma Nnamani, Ph.D. (Medicinal Chemistry), “Synthesis and Testing of Potential Antisickling Agents”, July 15, 1997.

Cy Anderson, Ph.D. (Biomedical Engineering), “Receptor-Ligand Interactions: Investigations in Modeling Applied Alignments and Overlay Optimization”, June 26, 1998.

Nimit Chomnawang, M.S. (Biomedical Engineering)*, “Visualization of Light Propagation in the Cornea and Sclera”, January 13, 1999.

John Stewart, Ph.D. (Biomedical Engineering), “Automated Aneurysm Detection in Unread Magnetic Resonance Angiography (MRA) Studies Using Computational Differential Geometry”, March 4, 1999.

John Cox, Ph.D. (Chemistry), “Interactions between Multinuclear Platinum Complexes and DNA With a Focus on Ligands, Linker Groups, and Kinetics: A Molecular Modeling and [^{1}H, ^{15}N] NMR Study”, March 28, 2000.

Adnan A. Kadi, M.S. (Medicinal Chemistry), “Studies on the Metabolism of Phenobarbital: A New Metabolite?”, August 14, 2000.

Karen M. Carter, M.S. (Medicinal Chemistry), “Impurities in Illicit Metamphetamine: Studies with Chloroephedrine and 1,2-Dimethyl-3-phenylaziridine”, August 15, 2000.

Tadasha Culbeath, M.S. (Biomedical Engineering), “Computer Manipulation of Human Dentin Phosphoprotein Molecular Models to Elucidate Preferred Structural Conformations”, September 13, 2000.

James Burnett, Ph.D. (Medicinal Chemistry)*, “Modifying Hemoglobin Structure

and Function: A Computational Method for Estimating Changes in Free Energies of Biomolecular Associations Upon Mutation; and the Synthesis, Biological Testing, and Structural Analysis of Fluorinated Derivatives of Allosteric Modifiers", December 9, 2000.

Xin He, Ph.D. (Medicinal Chemistry), "Discovery of Novel Inhibitors of β-Ketoacyl-acyl Carrier Protein Synthase III (FabH)", April 18, 2002.

Michael Oehlsen, Ph.D. (Chemistry), "Model Studies on the Metabolism of Anticancer Active Polynuclear Platinum Complexes", April 10, 2003.

Derek J. Cashman, Ph.D. (Medicinal Chemistry)*, "A Computational Model for Targeting Nucleic Acids: Estimating Changes in Free Energy of Drugs in Complex with RNA and Variable Sequences of DNA", November 20, 2003.

Adnan Kadi, Ph.D. (Medicinal Chemistry), "Liquid Chromatography - Mass Spectrometry in the Characterization of Select Phenobarbital Metabolites", December 2, 2003.

Brian Vest, M.S. (Chemistry), "Ab-initio Study of the Base-Catalyzed Oxidation of 3,5-di-tert-butylorthoquinone in Hydrogen Peroxide Solution", July 7, 2004.

Elliot H. Sanders, Ph.D. (Chemical Engineering), "Electrostatic Processing of Polymers and Polymer Composites", August 5, 2004.

Sharangdhar Phatak, M.S. (Biomedical Engineering)*, ZAP, "A Technologically Advanced Solution for the Poisson-Boltzmann Equation: Case Studies in QSAR and Drug Design", November 29, 2004.

Deliang Chen, Ph.D. (Medicinal Chemistry)*, "New Computational Tools to Study the Role of Water in Ligand Binding and to Optimize Selectivity", December 3, 2004.

Sunil Iyer, Ph.D. (Pharmaceutics), "A 'Biorelevant' Approach to Accelerated Drug Release Testing and In Vitro-In Vivo Correlation of a Long-Acting Naltrexone Implant", July 31, 2006.

Atilio Anzellotti, Ph.D. (Chemistry), "Study of Covalent and Non-Covalent Interactions in Ternary Systems Involving: Metal/DNA-RNA/Protein, Where Metal = Pt(II), Pd(II)", March 13, 2007.

Sarbjot Sachdeva, Ph.D. (Medicinal Chemistry), "Interactions of mtFabH with its Substrates and Inhibitors Reveal Novel Mechanistic Insights", November 14, 2007.

Arjun Raghuraman, Ph.D. (Medicinal Chemistry), "Designing Non-saccharide Heparin/Heparan Sulfate Mimics", April 20, 2008.

Nagesh Pulicherla, Ph.D. (Medicinal Chemistry), "Characterization of Yeast 18S rRNA Dimethyltransferase, Dim1p", May 2, 2008.

Donna L. McGovern, Ph.D. (Medicinal Chemistry), “Salvinorin A: Fragment Synthesis and Modeling Studies”, April 23, 2009.

Jitesh R. Shah, Ph.D. (Medicinal Chemistry), “Design and Synthesis of Molecular Probes for the Study of 5-HT2A and H1 Receptors”, May 26, 2009.

Ashwini Goswami, M.S. (Medicinal Chemistry), “Development of PPAR-γ Receptor Agonists as Therapeutic Agents for Diabetes”, May 27, 2009.

Ashtosh Tripathi, Ph.D. (Medicinal Chemistry)*†, Development of HINT Based Computational Tools for Drug Design: Applications in the Design and Development of Novel Anti-Cancer Agents”, July 15, 2009.

Jenson Verghese, M.S. (Medicinal Chemistry), “Synthesis and Biochemical Studies on Sulfated Monomers of Low Molecular Weight Lignins”, July 16, 2009.

Chandravel Krishnasamy, Ph.D. (Medicinal Chemistry), “Molecular Modeling Studies of Heparin and Heparin Mimetics Binding to Coagulation Proteins”, August 3, 2009.

Kendra M. Haney, M.S. (Medicinal Chemistry), “Synthesis and Biological Evaluation of Anibamine, a Natural Product CCR5 Anatagonist, and its Analogs as Novel Anti-Prostate Cancer Agents”, November 23, 2009.

Amit Gandhi, Ph.D. (Medicinal Chemistry), “Vitamin B6 Metabolism and Regulation of Pyridoxal Kinase”, December 7, 2009.

Aaron B. Bate, M.S. (Chemistry), “Noncovalent Interaction of Platinum Planar Amine Compounds with Tryptophan: As a Strategy to Interfere with P53-MDM2 Interactions and Targeting Retroviral Zn Finger-DNA Interaction (HIV NCP7)”, December 9, 2009.

Scott A. Lawrence, Ph.D. (Pharmacology), “The Mechanism of Mitochondrial Folate Transport by the Mitochondrial Folate Transporter”, April 29, 2010.

Prajakta Badri, Ph.D. (Pharmaceutics), “Prediction of Human Systemic, Biologically Relevant Pharmacokinetic (PK) Properties Based on Quantitative Structure Pharmacokinetic Relationships (QSPKR) and Interspecies Scaling (PK-AS)”, July 27, 2010.

Swati Agrawal, Ph.D. (Pharmaceutics), “Investigation and Optimization of a Solvent / Anti-Solvent Crystallization Process for the Production of Inhalation Particles”, July 29, 2010.

Aurijit Sarkar, Ph.D. (Medicinal Chemistry)*†‡, “Development and Applications of the HINT Force Field in Prediction of Antibiotic Efflux and Virtual Screening for Antivirals”, August 18, 2010.

Mostafa H. Ahmed, M.S. (Medicinal Chemistry)*, “Water Molecules: A Closer Look at Their Behavior at Protein-Protein Interfaces and Their Contributions to

the Docked Model of Pyridoxal Kinase – Serine Hydroxymethyltransferase Complex", August 15, 2011.

Preetpal Sidhu, Ph.D. (Medicinal Chemistry), "Designing Allosteric Inhibitors of Thrombin", November 7, 2011.

Matthew R. Baker, Ph.D. (Medicinal Chemistry), "Synthesis, Screening and Cocrystallization of Adenosine Based Inhibitors with Methyltransferases, ErmC' and KsgA", November 17, 2011.

Rami A. Al-Horani, Ph.D. (Medicinal Chemistry), "Designing Direct and Indirect Factor Xa Inhibitors", May 7, 2012.

Amit Somani, Ph.D. (Pharmacotherapy and Outcomes Science), "In Vitro In Vivo Methods and Pharmacokinetic Models for Subcutaneously Administered Peptide Drug Products", July 31, 2012.

Aditi A. Mulgaonkar, Ph.D. (Pharmaceutics), "Assessment of the Role of Solute Carrier Drug Transporters in the Systemic Disposition of Fluoroquinolines: An *In Vitro-In Vivo* Comparison", August 1, 2012.

Rahul Mahajan, Ph.D. (Physiology and Biophysics), "G$\beta\gamma$ Acts at an Inter-Subunit Cleft to Activate GIRK1 Channel", October 9, 2012.

Orgil Elbegdorj, Ph.D. (Medicinal Chemistry), "Design, Syntheses, and Biological Evaluation of 14-N-Substituted Naltrexone Derivatives as Opioid Receptor Ligands", January 29, 2013.

Atul Jain, Ph.D. (Medicinal Chemistry), "Positive Allosteric Modulators of Alpha4 Beta2 Neuronal Nicotinic Acetylcholine Receptors: Synthesis and In Vitro Studies", February 12, 2013.

May H. Abdel Aziz, Ph.D. (Medicinal Chemistry), "Kinetic and Thermodynamic Studies of Thrombin Inhibitors", February 28, 2013.

Christopher K. Arnatt, Ph.D. (Medicinal Chemistry), "Development of Antagonists Targeting Chemokine Receptor CCR5 and the Chemokine Receptor CCR5 – Mu Opioid Receptor Heterodimer", April 12, 2013.

Hardik I. Parikh, Ph.D. (Medicinal Chemistry)*§, "Understanding Molecular Interactions: Application of HINT-Based Tools in the Structural Modeling of Novel Anticancer and Antiviral Targets, and in Protein-Protein Docking", April 25, 2013.

Mesay Habtemariam, M.S. (Bioinformatics)*, "Bioinformatics Approach to Probe Protein-Protein Interactions: Understanding the Role of Interfacial Solvent in the Binding Sites of Protein-Protein Complexes; Network-Based Predictions and Analysis of Human Immunodeficiency Virus Proteins", April 29, 2013.

Chenxiao Da, Ph.D. (Medicinal Chemistry)*, "The Development and Applications of the HINT Scoring Function: Exploring Colchicine-Site Anticancer Agents and

Tautomerism", May 2, 2013.

A. Gerard Daniel, Ph.D. (Chemistry), "Zinc Environment in Proteins: The Flexible and Reactive Core of HIV-1 NCp7 and The Inhibitory Site of Caspase-3", December 2, 2013.

Jenson Verghese, Ph.D. (Medicinal Chemistry), "Investigations of Novel Mechanisms of Action for Anti-Bacterial and Anti-Cancer Agent Development", May 1, 2014.

Saheem Zaidi, Ph.D. (Medicinal Chemistry)*, "Understanding Ligand Binding, Selectivity, and Functions on the G Protein-Coupled Receptors: A Molecular Modeling Approach", May 6, 2014.

Gopichand Gottipati, Ph.D. (Pharmaceutics), "Prediction of Human Systemic, Biologically Relevant Pharmacokinetic (PK) Properties Using Quantitative Structure Pharmacokinetic Relationships (QSPKR) and Interspecies Pharmacokinetic Allometric Scaling (PK-AS) Approaches for Four Different Pharmacological Classes of Compounds", July 22, 2014.

Ahmad J. Obaidullah, M.S. (Medicinal Chemistry)*, "A Route to Discover Small Molecule Inhibitors of PsaA, a Potential Target for *Streptococcus Pneumoniae*", July 23, 2014.

Mostafa H. Ahmed, Ph.D. (Medicinal Chemistry)*, "Hydropathic Interactions and Protein Structure: Utilizing the HINT Force Field in Structure Prediction and Protein-Protein Docking", October 1, 2014.

Jeremy Chojnacki, Ph.D. (Medicinal Chemistry)*†, "Novel Compounds as Potential Alzheimer's Disease Therapeutics and Inhibitors of the Nlrp3 Inflammasome", December 2, 2014.

Robert Coover, Ph.D. (Medicinal Chemistry), "Development of Irreversible Substrate Competitive Probes for PKA Activity", June 4, 2015.

Osama Al Wassil, Ph.D. (Medicinal Chemistry), "Elaboration and Design of α7 nAChR Negative Allosteric Modulators", June 23, 2015.

Victoria N. Stone, Ph.D. (Microbiology), "A Novel Antrimicrobial Drug Discovery Approach in the Periodontal Pathogen *Porphryomonas gingivalis*", October 23, 2015.

Supriya A. Gaitonde, Ph.D. (Medicinal Chemistry), "A Study of the Action of Risperidone at 5-HT2A Receptors", April 20, 2016.

Sudha Korwar, Ph.D. (Medicinal Chemistry), "Design and Structure-Activity Relationship of Small Molecule C-terminal Binding Protein (CtBP) Inhibitors and Investigation of the Scope of Palladium Multi-Walled Carbon Nanotubes (Pd-MWCNT) Catalyst in C–H Activation Reactions", April 22, 2016.

Yunfei Mao, Ph.D. (Medicinal Chemistry), “Substrate Recognition and Mechanistic Studies on Protein N-Terminal Methyltransferase 1”, June 30, 2016.

Kavita Ananthanarayan Iyer, Ph.D. (Medicinal Chemistry), “Exploring the Concept of Human OCT3 Inhibitors as a Novel Class of Antidepressants”, November 18, 2016.

Amrita Dileep Sule, Ph.D. (Molecular Biology and Genetics), “ATM Mediated Phosphorylation on PP2A-Aα Subunit Regulates the DNA Damage Response, Cell Growth and Quality of Double Strand Break Repair Via Cellular Shuttling”, November 21, 2016.

Hebing Liu, Ph.D. (Pharmaceutics), “Three Dimensional Homology Modeling of Organic Cation Transporter 3 to Identify Structural Elements Mediating Transporter-Substrate Interactions”, May 3, 2017.

Samuel Obeng, Ph.D. (Medicinal Chemistry), “Design, Synthesis, and Biological Screening of Selective Mu Opioid Receptor Ligands as Potential Treatments for Opioid Addiction”, May 4, 2017.

Urjita H. Shah, Ph.D. (Medicinal Chemistry), “A Roadmap for Development of Novel Antipsychotic Agents Based on a Risperidone Scaffold”, May 5, 2017.

Daniel K. Afosah, Ph.D. (Medicinal Chemistry), “Study of Molecular Interactions of Glycosaminoglycans and Glycosaminoglycan Mimetics with Their Protein Targets”, June 1, 2017.

Ahmad J. Obaidullah, Ph.D. (Medicinal Chemistry)*, “Using Hydropathic Molecular Modeling Tools to Enhance Understanding of Protein-Ligand Interactions in Biological Systems”, November 16, 2017.

Abigail Leigh Glascock, Ph.D. (Integrated Life Sciences), “Evolution and Niche Specialization of Microbial Taxa in Vaginal Infection and Pregnancy”, March 12, 2018.

Alhumaidi Bader Alabbas, Ph.D. (Medicinal Chemistry), “Glycosaminoglycan Ligases in the Production of Oligosaccharides”, March 30, 2018.

Jacob Fulp, Ph.D. (Medicinal Chemistry), “The Development of Novel Inhibitors of the NLRP3 Inflammasome”, May 1, 2018.

Malaika Argade, Ph.D. (Integrated Life Sciences), “Galantamine’s Deconstruction in the Quest of a PAM Pharmacophore”, May 7, 2018.

Abhishek Kulkarni, M.S. (Medicinal Chemistry), “Design, Synthesis and Pharmacological Characterization of Potential Mu Opioid Receptor Selective Ligands”, April 25, 2019.

Bethany A. Reineke, Ph.D. (Medicinal Chemistry), “Development of Bivalent Ligands Targeting the Putative Mu Opioid Receptor and Chemokine Receptor

CXCR4 Heterodimer, April 29, 2019.

Shravan Morla, Ph.D. (Medicinal Chemistry), “Glycosaminoglycan Mimetics for the Treatment of Cancer and Lung Inflammation”, May 3, 2019.

Rachel A. Davies, Ph.D. (Medicinal Chemistry), “Structure Activity Relationship Studies of Synthetic Cathinones and Related Agents”, May 9, 2019.

Nicole M. Luzi, Ph.D. (Medicinal Chemistry), “An Enzymology and Inhibition Study of a cAMP-Dependent Protein Kinase Mutant Linked to ACTH-Independent Cushing’s Syndrome”, September 9, 2019.

Eric Ginsburg, Ph.D. (Chemistry), “Heperan Sulfate. A New Ligand for Coordination Compounds”, March 30, 2020.

Mengchu Li, Ph.D. (Medicinal Chemistry), “Systematic Structural-Activity Relationship Studies of Nalfurafine”, March 5, 2021.

Jakob C. Green, Ph.D. (Medicinal Chemistry), “Mechanistic Insights of Mitochondrial Reactive Oxygen Species and Neuroinflammation in Alzheimer’s Disease Models”, May 6, 2021.

Anfal Sarihan Aljahdali, Ph.D. (Medicinal Chemistry), “Diphosphoglycerate Mutase: A Potential Target for Sickle Cell Disease”, May 7, 2021.

Claudio Catalano, Ph.D. (Medicinal Chemistry)*†, “Cryogen electron-microscopy (Cryo-EM) analysis of MscS, YnaI, Connexin 26 and Bioinformatic Analysis of Cysteine and Serine in Experimental Protein Structures”, July 30, 2021.

Prithvi Hemanth, Ph.D. (Medicinal Chemistry), “Pharmacophoric Evaluation of 5-HT_{2A} and 5-HT_{2B} Serotonin Receptors”, August 10, 2021.

Mary E. (Shoup) Zoepfl, Ph.D. (Chemistry), “Antiviral Effects of Metalloshielding: Differential Antiviral Activity of Polynuclear Platinum and Cobalt Compounds”, April 19, 2022.

Noah B. Herrington, Ph.D. (Medicinal Chemistry)*§, “Structure-Based Drug Discovery and Development of Protein Structure Prediction Tools Using and Empirical Force Field”, August 3, 2022.

Mohammed H. AL Mughram, Ph.D. (Medicinal Chemistry)*, “Protein Structure and Interaction: The Role of Aromatic Residues in Protein Structure and Interactions between Pyridoxine 5'-Phosphate Oxidase/Dopa Decarboxylase”, October 24, 2022.

Akua Kyereba Donkor, Ph.D. (Medicinal Chemistry), “X-Ray Crystallography: A Tool for Understanding Protein Function and Drug Discovery”, May 3, 2023.

Celsey Mackenna St. Onge, Ph.D. (Medicinal Chemistry), “Systematic Structure-Activity Relationship Study of Nalfurafine Towards Treatments for Substance Use

Disorders and Pain Management", June 14, 2023.

Samuel Holmes, Ph.D. (Medicinal Chemistry), "Characterizing 3-O-Sulfation-Induced Novel Compact Topologies on Heparin Sulfate and Their Interactions with Proteins", October 17, 2023.

Mohammed A. AlAwadh, Ph.D. (Medicinal Chemistry), "Developing Antiviral Drugs for COVID-19 and Hepatitis C: Targeting Key Viral Proteases", April 30, 2024.

Corentin E. Villot, Ph.D. (Chemistry), "Integrating Machine Learning and Electronic Structure Theory for Accurate and Transferable Prediction of Polarizability and Noncovalent Interactions", May 6, 2024.

Rachel Joshi, Ph.D. (Medicinal Chemistry)*

Savannah R. Biby, Ph.D. (Medicinal Chemistry)

Ahmed Ahmed Reda, Ph.D. (Medicinal Chemistry)

Charles Jones, PhD. (Medicinal Chemistry)

Tamim Chiba, Ph.D. (Medicinal Chemistry)

Rachael F. Flammia, Ph.D. (Medicinal Chemistry)

Shadid Uz Zaman, Ph.D. (Medicinal Chemistry)

*principal or co-principal advisor
†Department of Medicinal Chemistry J. Doyle Smith awardee
‡School of Pharmacy Charles T. Rector & Thomas W. Rorrer, Jr. Dean's awardee
§VCU Graduate Student Dissertation Fellowship awardee

F. Postdoctoral Associates and Visiting Scientists

2001-2002:	Micaela Fornabaio, Ph.D. Student, University of Parma, Italy
2003, 2005:	Pietro Cozzini, Professor, Department of Chemistry, University of Parma
2004-2007:	Micaela Fornabaio, Postdoctoral Associate (Ph.D., University of Parma)
2005-2007:	Yong Peng, Postdoctoral Associate (Ph.D., Michigan Technical University)
2006:	Francesca Spyrakis, Ph.D. Student, University of Parma, Italy
2006-2010:	Alexander Bayden, Postdoctoral Associate (Ph.D., University of Pittsburgh)

2007: Alessio Amadasi, Ph.D. Student, University of Parma, Italy

2007-2010: Vishal Koparde, Postdoctoral Associate (Ph.D., Vanderbilt University)

2013-2014 Hardik I. Parikh, Postdoctoral Associate (Ph.D., VCU)

2014-2015 Saheem A. Zaidi, Postdoctoral Associate (Ph.D., VCU)

2014-2015 Tarek S. Ibrahim, Visiting Professor, College of Pharmacy, Zagazig University, Egypt

2014-2018 Mostafa H. Ahmed, Postdoctoral Associate (Ph.D., VCU)

G. Industrial Consulting and Collaborations

1991-1992: Computer Aided Molecular Design, Abbott Laboratories

1991-present: Frederick Cancer Research Center, National Cancer Institute

1992-1993: DNX Corporation

1993-2013: eduSoft, LC (co-founder, President)

2004-2005: GlaxoSmithKline (King of Prussia, PA)

2005-2007: Mesa Analytics Consulting (Santa Fe, NM)

H. Service and Awards

National/International

2016: Scientific Committee, *In Silico*/*In Vitro* Approaches for Food Science: One Day Summer School, Parma, Italy, September, 2016.

2015: Inducted, Rho Chi, Pharmaceutical Sciences Honorary Fraternity (First VCU Faculty Inductee)

2013: Invited Discussion Leader: 2013 Gordon Research Conference on Computer-Aided Drug Discovery

2013-2015 Review Committee, Jeffress Trust Awards Program in Interdisciplinary Research

2013-2018: Editorial Board, *Journal of Biological Chemistry*, American Society for Biochemistry and Molecular Biology

2012: Organizing and Scientific Committee “From Structural Genomics to Drug Discovery: Nuclear Receptors: From

in silico modelling to *in vivo* experiments", September, 2012, Parma, Italy

2012: Editor, with P. Cozzini, "Computational Approaches to Nuclear Receptors", Royal Society of Chemistry Drug Discovery Series.

2011: Symposium Organizer, "Monty Kier – 45 Years of Computational Medicinal Chemistry", Southeast Regional Meeting of the American Chemical Society (SERMACS), October, 2011, Richmond, Virginia.

2010: Guest Editor, with P. Cozzini, F Spyrakis and A. Sarkar, Special Issue of *Current Topics in Medicinal Chemistry* "Applying Induced Fit in Drug Discovery: Square Pegs and Round Holes?"

2007-present: Editorial Board, *Medicinal Chemistry Research*, Springer

2007: Organizing and Scientific Committee "From Structural Genomics to Drug Discovery: Modeling the Flexibility", September, 2007, Parma, Italy

May-June 2004: Visiting Professor, Department of Biochemistry and Molecular Biology, University of Parma, Italy.

2003-present: Editorial Board, *Chemistry & Biodiversity*, Verlag Helvetica Chimica Acta

2002-present: Associate Member, Consorzio Interuniversitario Istituto Nazionale di Biostruttre e Biosistemi, Italy.

2002: Scientific Committee, Course "From Structural Genomics to Drug Discovery", Parma, Italy, September 27-28, 2002.

1999-2000: Organizing Committee and Treasurer, Symposium "Mathematical and Computational Aspects of Molecular Design", 2000 International Chemical Congress of Pacific Basin Societies, Honolulu Hawaii, December 14-19, 2000

2000: Symposium Organizer, "Computer-Aided Drug Discovery from Docking, Scoring and Virtual Screening", SE/SW Regional Meeting of the American Chemical Society, New Orleans, Louisiana, December 6-8, 2000.

1999: Guest Editor, Special Issue of *Medicinal Chemistry Research* "Ligand Docking and Scoring"

1997-1998: Organizing Committee, Webmaster, Abstract Committee, 26th National Medicinal Chemistry Symposium (Richmond, VA, June 1998)

1995: Invited Speaker: 1995 Gordon Research Conference on QSARs.

1993: Member Program Committee: MGS/ACA Workshop on Biomolecular Interactions (Albuquerque, NM, May 1993)

Virginia Commonwealth University

2020-2021: University Promotion and Tenure Task Force (Teaching)

2021-present Member, CCTR Endowment Fund Standing Scientific Review Committee

2019: Peer Promotion Committee, Prof. T. Ashton Cropp, Chemistry

2019: Peer Promotion Committee, Prof. Qinglian Liu, Physiology and Biophysics

2016 Member, Search Committee, Vice Provost for Life Sciences

2015: Peer Promotion Committee, Prof. Dana E. Selley, Pharmacology and Toxicology

2015-2016: Member, VCU Life Sciences Program Review Committee

2015: Peer Promotion Committee, Prof. Dana E. Selley, Pharmacology and Toxicology

2015: Member, Select Grievance Panel Hearing Board

2015: School of Pharmacy Nominee, VCU Distinguished Scholarship Award

2014: School of Pharmacy Nominee, VCU Distinguished Scholarship Award

2014: Peer Tenure Committee, Prof. Peter Uetz, Center for the Study of Biological Complexity

2008-2015: Higher Education Trust Fund Allocation Committee

2005-present: Center for High Performance Computing (CHiPC) Advisory Committee

2000-2003: Research Computing Advisory Committee

2000-2003: Internet 2 Advisory Committee

2000-2001: Infrastructure Workgroup, Student Computer Initiative Task Force

1999-2000: Alternate, Faculty Senate
2009-2010

1990-present: Modeling Consultant: Users Committee, Structural Biology Core Facility, Massey Cancer Center

School of Pharmacy, VCU

2022: Chair, Search Committee – Director, School of Pharmacy Information Technology (PharTech)

2021-2022: Co-chair, ACPE Accreditation Self Study Subcommittee: Finance and Facilities

2021: Peer Promotion Committee, Prof. David Dixon, Pharmacotherapy and Outcomes Science

2020-present: Information Technology Advisory Committee

2020-2023 Bachelor of Science in Pharmaceutical Sciences (BSPS) Working Group

2019: Peer Promotion and Tenure Committee, Prof. Mary Peace McRae, Pharmacotherapy and Outcomes Science

2018: Peer Promotion Committee, Prof. Evan Sisson, Pharmacotherapy and Outcomes Science

2015: Peer Promotion Committee, Prof. Michael Hindle, Pharmaceutics

2015: Peer Promotion Committee, Prof. Phillip Gerk, Pharmaceutics

2014-2018: Chair, Information Technology Advisory Committee

2014: Peer Promotion and Tenure Committee, Prof. Douglas Sweet, Pharmaceutics

2013-2014: ACPE Accreditation Self Study Subcommittee: Curriculum

2012-2014: Strategic Plan Update Committee

2011-2014: Strategic Plan Monitoring Committee

2011-2013: School of Pharmacy Parliamentarian

2010:	Peer Promotion and Tenure Committee, Prof. Masahiro Sakagami, Pharmaceutics
2010-2013:	School Promotions and Tenure Committee
2009-2013:	Outcomes and Assessment Committee
2006-2010:	Space Committee
2006-2007	ACPE Accreditation Self-Study Subcommittee: Mission and Facilities
2005-2006:	Teaching Excellence Award Committee
2005-2009:	Nominations Committee
2005-2007:	Promotion and Tenure Guidelines Committee
2000-2001:	ACPE Accreditation Self-Study Subcommittee: Students
1999-2000:	Sub-committee of Strategic Plan Initiative V: "Promote the national recognition of the school as a leader among the nation's major research schools/colleges of pharmacy"
1999-2003:	Dean's Award for Graduate Study Selection Committee
1995-2009:	Information Technology Advisory Committee, Chair (1999-2009)
1996, 2014:	School of Pharmacy Grievance Board
1994:	ACPE Self Study, Sub-committee for Organization and Administration & Goals and Objectives.

Department of Medicinal Chemistry, VCU

2022:	Chair, Peer Promotion Committee, Prof. Malgorzata Dukat
2022:	Peer Promotion and Tenure Committee, Prof. Aaron May
2022:	Peer Promotion and Tenure Committee, Prof. Youzhong Guo
2019-2020:	Chair, Search Committee (hired J. Li)
2018-2019:	Chair, Search Committee (hired Y. Cen)
2018:	Chair, Peer Promotion Committee, Prof. Shijun Zhang
2015:	Peer Promotion Committee, Prof. Yan Zhang

2014: Chair, Peer Promotion and Tenure Committee, Prof. Keith Ellis

2014-2015: Chair, Search Committee (hired Y. Guo)

2013-2014: Chair, Search Committee (hired A. E. May)

2013: Chair, Peer Promotion and Tenure Committee, Prof. Shijun Zhang

2011-2012: Chair, Search Committee (hired R. Huang)

2009: Chair, Peer Promotion and Tenure Committee, Prof. Yan Zhang

2009-present Chair, Suite 200 Committee

2008-present: Executive Committee

2008-present: Graduate Operations Committee

2007-2008 Chair, Search Committee (hired K. C. Ellis)

1993-present: Computer Committee

Institute for Structural Biology, Drug Discovery and Development

2015-2016: Organizing Committee, The VCU 3D Summit 2016, A day of Drug Discovery and Development at VCU

Center for the Study of Biological Complexity, VCU

2014: Peer Promotion and Tenure Committee, Prof. Peter Uetz

2012 Chair, Peer Promotion Committee, Prof. J. Neel Scarsdale

2004-present Senior Fellow, CSBC

American Chemical Society

2001: Virginia Section: Industrial Innovation Award

1990-1992 Executive Committee

Outside

2022-2023: Christ Lutheran Church: Congregational Council

2014-2015:	Christ Lutheran Church: Vice President, Congregational Council
2005-2018	Richmond Kickers Youth Soccer, Volunteer
2004-present:	Christ Lutheran Church: Head Teller
2000:	Judge, Junior and Senior Chemistry, Metro Richmond Science Fair
1998:	Judge, Senior Chemistry, Metro Richmond Science Fair
1996-1997:	Christ Lutheran Church: Congregational Council
1996-2001:	Christ Lutheran Church, Finance Committee (Chair 1997-2001)
1996:	Hanover County Textbook Selection Committee (AP Chemistry)

I. Research Support

Sep 30, 1994	"Development of New Computer-Aided de Novo Drug Design Algorithms and Technology" submitted to A.D. Williams Fund, VCU, $10,000, funded February 1, 1995 to January 31, 1996
Mar 1, 1999	"A New Pharmacophoric Model for Doxorubicin-DNA Intercalation: Proposal for Experimental Verification and Design of New Active Agents" submitted to VCU American Cancer Society Fund, $8,525.
Jun 24, 2004	"New Hydropathy-Based Computer Tools for Drug Discovery", PI (22%), National Institutes of Health, 5R01GM071894, $1,325,975.
Mar 7, 2005	"Sub-award: Carolina Exploratory Center for Cheminformatics Research", sub-contract proposal for A. Tropsha (UNC-CH), PI (5%), National Institutes of Health, 1P20HG003898-01, $29,786, September 23, 2005 - July 31, 2007.
Sep 5, 2005	"Sub-award: Human parainfluenza virus: novel strategies for inhibiting viral entry", sub-contract proposal for A. Moscona (Cornell/Weill), PI, (0%), March of Dimes, $90,649, June 1, 2006 - May 31, 2009.
April 1, 2012	"Bioinformatics in 3D: Paradigm for biomacromolecular structure refinement and prediction", Virginia Commonwealth University, Presidential Research Incentive Program, $49,975, July 1, 2012 – December 31, 2013.

July 1, 2013 "Identification of small-molecule inhibitors of an endocarditis virulence factor", Todd O. Kitten, PI, (5%), Mid-Atlantic Affiliate - American Heart Association, $154,000, July 1, 2013 – June 30, 2015.

Feb 28, 2020 "Implementing a Novel Tool for Building More Native-Like Protein Structure Models", PI (10%), 1910 Genetics, Cambridge, MA, $70,000, February 28, 2020 – February 27, 2021.

Jan 1, 2021 "Inhibition of Sterol Carrier Protein-2 (SCP2) – a novel antidyslipidemic strategy", co-PI (5%) with Shobha Ghosh, Mid-Atlantic Affiliate - American Heart Association, $30,000, January 1, 2021 – December 31, 2023.

J. Peer Reviews

Journals:

1993: *Med. Chem. Res.* (6), *J. Mol. Graph.* (1)
1994: *Med. Chem. Res.* (3), *J. Pharm. Sci.* (1), *J. Mol. Graph.* (2), *J. Med. Chem.* (1)
1995: *Med. Chem. Res.* (2), *J. Mol. Graph.* (1)
1996: *Med. Chem. Res.* (2), *J. Med. Chem. (1), J. Comp. Chem. Inf. Sci.* (1), *J. Comp.-Aided Mol. Design* (1)
1997: *J. Comp.-Aided Mol. Design* (1), *Med. Chem. Res.* (1)
1998: *J. Med. Chem.* (2), *J. Comp. Chem. Inf. Sci.* (1), *Quant. Struct.-Act. Relat*. (1)
1999: *J. Med. Chem.* (1), *Pharm. Res.* (1), *Quant. Struct.-Act. Relat.* (1), *Med. Chem. Res.* (8)
2000: *J. Combinatorial Chem*. (1), *Quant. Struct.-Act. Relat*. (2)
2001: *J. Med. Chem.* (3), *Med. Chem. Res.* (2), *Quant. Struct.-Act. Relat*. (1), *J. Comp.-Aided Mol. Design* (1), *Bioorg. Med. Chem. Let.* (2), *J. Med. Res.* (1), *J. Comp. Chem. Inf. Sci.* (1)
2002: *Quant. Struct.-Act. Relat*. (1)*, Burger=s Medicinal Chemistry* (2), *J. Med. Chem.* (2), *Langmuir* (1), *J. Mol. Mod.* (1), *J. Controlled Rel.* (1), VCU Forbes Day (2)
2003: *Bioorg. Med. Chem. Let.* (1), VCU Forbes Day (2)*, J. Med. Chem.* (3), *Bioorg. Med. Chem.* (2), *J. Mol. Graphics Model.* (2)
2004: *J. Med. Chem*. (3), *J. Biomol. Struct. Dyn.* (2), *J. Chem. Inf. Comp. Sci.* (1), *Australian J. Chem.* (1), *Bioorg. Med. Chem.* (1), *QSAR Combinatorial Sci.* (1), *FEBS Lett.* (1), *J. Computer-Aided Mol. Design* (1)

2005: *J. Struct. Biol.* (1), *J. Med. Chem.* (3), *QSAR Combinatorial Sci.* (1), *J. Mol. Graph. Model.* (1), *J. Computer-Aided Mol. Design* (2),

2006: *J. Med. Chem.* (6), *QSAR Combinatorial Sci.* (2), *Chemosphere* (1), *J. Am. Chem. Soc*. (3), Eur. J. Med. Chem. (2), *Bioorg. Med. Chem. Lett.* (1), *Expert Opinion Drug Discov.* (1)

2007: *J. Med. Chem.* (2), *J. Computer-Aided Mol. Design* (2), *QSAR Combinatorial Sci.* (1), *Eur. J. Med. Chem.* (1), *Int. J. Mol. Sci.* (1), *Proteins: Struct. Func. Bioinf.* (3), *Drug Discov. Today* (1), *Bioorg. Med. Chem. Lett.* (1)

2008: *J. Med. Chem.* (3), *J. Computer-Aided Mol. Design* (1), *QSAR Combinatorial Sci.* (1), *Eur. J. Med. Chem.* (2), *J. Am. Chem. Soc.* (1), *Bioorg. Med. Chem. Lett.* (1), *Bioorg. Med. Chem.* (2), *J. Mol. Graph. Model.* (1)

2009: *J. Med. Chem.* (4), *J. Am. Chem. Soc.* (2), *Bioorg. Med. Chem.* (1), *Bioorg. Med. Chem. Lett.* (2), *J. Chinese Inst. Chem. Eng.* (1), *J. Computer-Aided Mol. Design* (1), *J. Comput. Chem*. (1), *Eur. J. Med. Chem.* (4), *Chem. Bio. Drug Design* (1), *J. Pharm. Res.* (2), *Med. Chem. Res.* (1), *Int. J. Phys. Sci.* (1), *J. Mol. Graph. Model.* (1)

2010: *J. Med. Chem.* (4), *J. Mol. Graph. Model.* (1), *J. Biomol. Struct. Dynamics* (1), *Proteins: Struct. Funct. Bioinf*. (2), *Int. J. Bioautomation* (1), *Mol. Bioinformat*. (1), *BMC Bioinf.* (1), *Bioorg. Med. Chem Lett.* (3), *ACS Med. Chem. Lett.* (2), *Curr. Topics Med. Chem*. (2), *Med. Chem. Res.* (1), *J. Chem. Inf. Model.* (1), *Chem. Biol. Drug Design* (1), *Curr. Pharm. Technology* (1), *BMC Struct. Biol.* (2), *Lett. Drug. Design Discov.* (2), *Eur. J. Med. Chem.* (1), *J. Chromatogr. B* (1)

2011: *Mol. Simulat.* (2), *Proteins: Struct. Funct. Bioinf*. (2), *Eur. J. Med. Chem.* (4), *J. Chem. Inf. Model.* (3), *J. Chromatogr. B* (1), *J. Am. Chem. Soc.* (2), *Med. Chem. Res.* (1), *J. Med. Chem.* (1), *Chem. Biol. Drug Design* (5), *Expert Opin. Drug Discov.* (1), *J. Biol. Chem.* (1)

2012: *Eur. J. Med. Chem.* (4), *J. Med. Chem.* (5), *Chem. Biol. Drug Design* (3), *BMC Struct. Biol*. (1), *J. Biol. Chem.* (2), *Eur. J. Pharmaceut. Sci.* (4), *Curr. Pharmaceut. Design* (1), *J. Computer-Aided Mol. Design* (1), *Toxicol. Lett.* (1), *Bioorg. Med. Chem Lett.* (1)

2013: *J. Med. Chem.* (2), *Eur. J. Pharmaceut. Sci.* (3), *Bioorg. Med. Chem.* (1), *Eur. J. Med. Chem.* (3), *Mol. Pharmaceut*. (1), *J. Phys. Chem.* (1), *J. Chem. Info. Model.* (2), *Int. J. Food Sci. Nutr.* (2), *Med. Chem. Res.* (2), *J. Biol. Chem.* (6), *Phys. Chem. Chem. Phys.* (2), *Med. Chem. Commun*. (2), *Bioorg. Med. Chem. Lett.* (2)

2014: *J. Biol. Chem*. (13), *Eur. J. Med. Chem*. (5), *SAR QSAR Environ. Res*. (1), *J. Chem. Inf. Model*. (4), *Proteins Struct. Funct. Bioinf.* (1), *J. Med. Chem*. (3), *Drug Discov. Today* (1), *J. Comput. Aided Mol. Design* (1), *Lett. Drug. Design Discov*. (1), *J. Phys. Chem*. (2), *J. Chromatogr. B* (1), *Comp. Biol. Chem*. (2), *Chem. Biol. Drug Design* (1)

2015: *J. Biol. Chem*. (5), *Eur. J. Med. Chem*. (4), *J. Chem. Inf. Model*. (1), *Proteins Struct. Funct. Bioinf.* (2), *J. Med. Chem*. (6), *J. Biomol. Struct. Dynam.* (2), *J. Comput. Chem.* (4), *J. Chromatogr. B* (1), *Med. Chem. Commun*. (1), *Med. Chem. Res*. (3), *Expert Opin. Drug Discov.* (1), *Bioorg. Med. Chem*. (1), *Sci. Advance* (1), *Bioorg. Med. Chem. Lett*. (1), *Antiviral Res*. (1), *J. Am. Chem. Soc.* (1), *Eur. J. Pharmaceut. Sci*. (1)

2016: *J. Med. Chem.* (3), *J. Biol. Chem.* (6), *Med. Chem. Res.* (1), *ACS Med. Chem. Lett.* (1), *Sci. Advance* (1), *Bioorg. Med. Chem. Lett.* (1), *RSC Advances* (1), *Molecules* (1)

2017: *J. Biol. Chem.* (3), *Med. Chem. Res.* (2), *ACS Med. Chem. Lett.* (3), *Biopolymers* (2), *Med. Chem. Res.* (2), *Molecules* (1), *Med. Chem. Comm.* (1), *Chem. Biol. Drug Design* (1), *J. Med. Chem.* (1), *J. Mol. Liquids* (1), *ACS Omega* (2)

2018: *J. Comput. Aid. Mol. Design* (2), *Phys. Chem. Chem. Phys.* (4), *J. Am. Chem. Soc.* (3), *J. Bio. Chem.* (8), *ChemMedChem* (1), *J. Chem. Info. Model.* (6), *Bioorg. Med. Chem. Lett.* (1), *Nucl. Recept. Res.* (1), *Chem. Bio. Drug Design* (1)

2019: *ACS Med. Chem. Lett.* (2), *Trends Food Sci.* (1), *J. Chem. Info. Model.* (2), *J. Phys. Chem.* (2), *BMC Bioinf.* (1), *J. Med. Chem.* (1), *IEEE/ACM Transact. Comput. Bio. Bioinf.* (1), *J. Bio. Chem.* (1)

2020: *J. Chem. Info. Model.* (3), *J. Comput. Aid. Mol. Design* (1)

2021: *Molecules* (2), *Front. Mol. Biosci.* (3), *Drug Discov. Today* (1), *Brief. Bioinfo.* (1), *Eur. J. Med. Chem.* (1), *Arab. J. Chem.* (1), *J. Comput. Aid. Mol. Design* (1)
2022: *J. Chem. Info. Model.* (2), *Med. Chem. Res.* (3), *Biomolecules* (1), *Comput. Struct. Biotech. J.* (1),
2023: *Biomolecules* (1), *PLoS ONE* (1), *J. Chem. Info. Model.* (2), *Front. Mol. Biosci.* (2), *Viruses* (1)

Books:
1996: for *J. Med. Chem.* (1)
1997: for *J. Med. Chem.* (1)
2004: for *J. Med. Chem*. (1)
2006 for *J. Med. Chem.* (1)
2009: for *J. Med. Chem.* (1)
2018: Epistructural Drug Design (proposal)

Proposals:
1994: NSF (1)
2000: Jeffress Foundation (1)
2002: ACS Petroleum Research Fund (1)
2003: ACS Petroleum Research Fund (1)
2005: Civilian Research Development Fund/Moldova (1), Science Foundation Ireland (2)
2007: Health Research Board Ireland (1), Virginia Alzheimer's and Related Diseases Research Award Fund (2)
2009: Science Foundation Ireland (1)
2010: Austrian Science Fund (1)
2011: Textbook proposal, Pearson Press (1), National Science Foundation CAREER award (1)
2013: LinkSCEEM & Cy-Tera High Performance Computing Production Access (Cyprus) (1), Qatar National Research Fund (1)
2014: Qatar National Research Fund (1)
2016: Jeffress Foundation (2)
2023: Israel Science Foundation (1)

Study Section:
1998-2016: NIH Small Business Section ZRG1 SSS-Z(1) Drug Development and Delivery
2004: NIH Computational Biology ZRG1 BST-D (01)
NIH SARS P01 review
2006: NIH Minority Institution Research Enhancement Program
2009: NIH Challenge Grants
2009-2010: NIH R13 Scientific Conference Grants
2010: NIH SARS P01 review

Site Visit:	2001:	NIH/NCI: University of Pittsburgh Program Project Grant
	2002:	NIH/NCI: University of California-Davis Program Project Grant
Extramural P&T:	2012:	Howard University
	2015:	Ohio State University
	2023:	University of Minnesota

K. Professional Affiliations

American Chemical Society
Division of Inorganic Chemistry
Virginia Section

II. PUBLICATIONS

A. Print

1. Electronic Structure and Bonding Characteristics of Cyclopentadienyl d Metal-Ligand Complexes. Core and Valence Ionization Study of CpM(CO)2 where M = Co and Rh and Cp = η^5-C_5H_5 and η^5-$C_5(CH_3)_5$. D.L. Lichtenberger, D.C. Calabro, and G.E. Kellogg, *Organometallics* **1984**, *3*, 1623-1630.
2. Ligand Additivity in the Valence Photoelectron Spectroscopy of Phosphine-Substituted Molybdenum Carbonyls. B.E. Bursten, D.J. Darensbourg, G.E. Kellogg, and D.L. Lichtenberger, *Inorg. Chem.* **1984**, *23*, 4361-4365.
3. Principles of Electronic Structure in Transition Metal Complexes. Additive Ligand Electronic Effects and Core-Valence Ionization Correlations for $Mo(CO)_{6-n}(PMe_3)_n$ where n = 0, 1, 2, 3. D.L. Lichtenberger, G.E. Kellogg, and G.H. Landis, *J. Chem. Phys.* **1985**, *83*, 2759-2768.
4. Electronic Structure Factors of Carbon-Hydrogen Bond Activation. The Photoelectron Spectroscopy of Cyclohexenylmanganese Tricarbonyl. D.L. Lichtenberger and G.E. Kellogg, *J. Am. Chem. Soc.* **1986**, *108*, 2560-2567.
5. Inexpensive and High-Precision Digital Power Supply and Counting Interface for UPS, XPS, and Auger Spectrometers. D.L. Lichtenberger, G.E. Kellogg, J.G. Kristofzski, D. Page, S. Turner, G. Klinger, and J. Lorenzen, *Rev. Sci. Instrum.* **1986**, *57*, 2366.
6. Localization Effects in the Auger Spectra of Ring Nitrogen Systems: Pyridine, Poly(2-vinyl)pyridine, Borazine, and Boron Nitride. R.R. Rye, J.A. Kelber, G.E. Kellogg, K.W. Nebesny, and D.L. Lichtenberger, *J. Chem. Phys.* **1987**, *86*, 4375-4383.
7. Experimental Quantum Chemistry. The Photoelectron Spectroscopy of Organotransition Metal Complexes. D.L. Lichtenberger and G.E. Kellogg, *Acc. Chem. Res.* **1987**, *20*, 379-387.

8. Photoelectron Spectroscopy: Experimental Characterization of Electronic Structure and Bonding in Organometallic Molecules. D.L. Lichtenberger, G.E. Kellogg, and L.S.K. Pang, in "Experimental Organometallic Chemistry: A Practicum in Synthesis and Characterization", A.L. Wayda and M.Y. Darensbourg, eds. A.C.S. Symposium Series, Volume 357, Washington, 1987, pp. 265-289.

9. Routes to Molecular Metals with Widely Variable Counterions and Band-Filling. Electrochemistry of a Conductive Organic Polymer with an Inorganic Backbone. T.J. Marks, J.G. Gaudiello, G.E. Kellogg, and S.M. Tetrick, in "Inorganic and Organometallic Polymers", M. Zeldin, K.J. Wynne, and H.R. Allcock, eds. A.C.S. Symposium Series, Volume 360, Washington, 1987, pp. 224-237.

10. Characterization of Metal Complex Positive Ions in the Gas Phase by Photoelectron Spectroscopy. D.L. Lichtenberger and G.E. Kellogg, in "Gas Phase Inorganic Chemistry", D.H. Russell, ed., Modern Inorganic Chemistry Series, Plenum, New York, 1989, pp. 245-277.

11. Electrochemistry of Cofacial Phthalocyanine Polymers: What Can We Learn About How Molecular Metal Collective Properties Respond to Wide Variations in Band Filling? G.E. Kellogg, J.G. Gaudiello, J.A. Schlueter, S.M. Tetrick, T.J. Marks, H.O. Marcy, W.J. McCarthy, and C.R. Kannewurf, in "Proceedings of the International Conference on Science and Technology of Synthetic Metals", *Synth. Metals* **1989**, *29*, F15-F24.

12. Relative Strengths of Early Transition Metal M-H and M-C Bonds in Substituted Niobocenes and Tantalocenes. Thermodynamic Trends and Electronic Factors of Olefin Insertion into a Metal-Hydride Bond. D.L. Lichtenberger, G.P. Darsey, G.E. Kellogg, R.D. Sanner, V.G. Young, Jr., and J.R. Clark, *J. Am. Chem. Soc.* **1989**, *111*, 5019-5028.

13. Molecular Metals with Widely Tunable Band Filling. Structure/Stoichiometry/ Counterion Relationships in the Electrochemistry of a Cofacially Joined Polymeric Phthalocyanine Metal. J.G. Gaudiello, G.E. Kellogg, S.M. Tetrick, and T.J. Marks, *J. Am. Chem. Soc.* **1989**, *111*, 5259-5271.

14. Molecular Metals with Widely Tunable Band Filling. Response of the Collective Properties of a Phthalocyanine Molecular Metal to Drastic Excursions in Partial Oxidation and Charge-Compensating Counterions. M. Almeida, J.G. Gaudiello, G.E. Kellogg, S.M. Tetrick, H.O. Marcy, W.J. McCarthy, J.C. Butler, C.R. Kannewurf, and T.J. Marks, *J. Am. Chem. Soc.* **1989**, *111*, 5271-5284.

15. Allosteric Modifiers of Hemoglobin. 2. Crystallographically Determined Binding Sites and Hydrophobic Binding/Interaction Analysis of Novel Hemoglobin Oxygen Effectors. F.C. Wireko, G.E. Kellogg, and D.J. Abraham, *J. Med. Chem.* **1991**, *34*, 758-767.

16. HINT - A New Method of Empirical Hydrophobic Field Calculation for CoMFA. G.E. Kellogg, S.F. Semus, and D.J. Abraham, *J. Computer-Aided Mol. Design* **1991**, *5*, 545-552.

17. New Tools for Modeling and Understanding Hydrophobicity and Hydrophobic Interactions. G.E. Kellogg, G.S. Joshi, and D.J. Abraham, *Med. Chem. Res.* **1992**, *1*, 444-453.

18. Polymeric Coordination Complexes Bridging Molecular Metals and Conductive Polymers. G.E. Kellogg and J.G. Gaudiello, in "Inorganic Materials", D.W. Bruce and D. O'Hare, eds., J. Wiley and Sons, Chichester, 1992, pp. 355-407.

19. KEY, LOCK, and LOCKSMITH. Complementary Hydrophobicity Map Predictions of Drug Structure from a Known Receptor/Receptor Structure from Known Drugs. G.E. Kellogg and D.J. Abraham, *J. Mol. Graph.* **1992**, *10*, 212-217.

20. Hydrophobic Fields. D.J. Abraham and G.E. Kellogg, in "3D QSAR in Drug Design, Theory, Methods and Applications", H. Kubinyi, ed., ESCOM Sciences Publishers BV, Leiden, 1993, pp. 506-522.

21. Effect of Distamycin on Chlorambucil-Induced Mutagenesis in pZ189: Evidence of a Role for Minor Groove Alkylation at Adenine N-3. P. Wang, G.B. Bauer, G.E. Kellogg, D.J. Abraham, and L.F. Povirk, *Mutagenesis* **1994**, *9*, 133-139.

22. The Effect of Physical Organic Properties on Hydrophobic Fields. D.J. Abraham and G.E. Kellogg, *J. Computer-Aided Mol. Design (Symposium Proceedings: 1993 Meeting of the Molecular Graphics Society)* **1994**, *8*, 41-49.

23. Cyclodextrin - Barbiturate Inclusion Complexes: A CoMFA/HINT 3-D QSAR Study. V.R. Nayak and G.E. Kellogg, *Med. Chem. Res.* **1994**, *3*, 491-502.

24. Evaluating Docked Complexes with the HINT Exponential Function and Empirical Atomic Hydrophobicities. E.C. Meng, I.D. Kuntz, D.J. Abraham, and G.E. Kellogg, *J. Computer-Aided Mol. Design* **1994**, *8*, 299-306.

25. All-Atom Models for the Non-nucleoside Binding Site of HIV-1 Reverse Transcriptase Complexed with Inhibitors: A 3D QSAR Approach. R. Gussio, N. Pattabiraman, D.W. Zaharevitz, G.E. Kellogg, I. Topol, W.G. Rice, C.A. Schaeffer, J.W. Erickson, and S.K. Burt, *J. Med. Chem.* **1996***, 39,* 1645-1650.

26. Differences in Hydropathic Properties of Ligand Binding at Four Independent Sites in Wheat Germ Agglutinin-Oligosaccharide Crystal Complexes. C.S. Wright and G.E. Kellogg, *J. Prot. Sci.*, **1996**, *5*, 1466-1476.

27. Polymeric Coordination Complexes Bridging Molecular Metals and Conductive Polymers. G.E. Kellogg and J.G. Gaudiello, in "Inorganic Materials, 2nd Edition", D.W. Bruce and D. O'Hare, eds., J. Wiley and Sons, Chichester, 1996, pp. 378-428.

28. The E-State Fields. Applications to 3D QSAR. G.E. Kellogg, L.B. Kier, P. Gaillard, and L.H. Hall, *J. Computer-Aided Mol. Design*, **1996**, *10*, 513-520.

29. C5aR Ligand Peptide 3D QSAR Study Performed with an Applied Linear Conformation. C. Anderson, G.E. Kellogg, and R.J. Freer, *J. Peptide Res.* **1997**, *49*, 476-483.

30. Hydropathic Analysis of the Noncovalent Interactions between Molecular Subunits of Structurally-Characterized Hemoglobins. D.J. Abraham, G.E. Kellogg, J.M. Holt, and G.K. Ackers, *J. Mol. Bio.* **1997**, *272*, 613-632.

31. Effects of Entropy on QSAR Equations for HIV-1 Protease: 1. Using Hydropathic Binding Descriptors. 2. Unrestrained Complex Structure Optimizations. G.E. Kellogg, D.T. Wei, and J.C. Meadows, *Med. Chem. Res.* **1997**, *7*, 259-270.

32. Finding Optimum Field Descriptors for 3D QSAR. G.E. Kellogg, *Med. Chem. Res.* **1997***, 7*, 417-427.

33. Utilization of a 3D QSAR Methodology for Data Mining the National Cancer Institute Repository of Small Molecules in Application to HIV-1 Reverse Transcriptase Inhibition. R. Gussio, N. Pattabiraman, G.E. Kellogg, D.W. Zaharevitz, *Methods* **1998**, *14*, 255-263.

34. Identification and Hydropathic Characterization of Structural Features Affecting Sequence Specificity for Doxorubicin Intercalation into DNA Double-Stranded Polynucleotides. G.E. Kellogg, J.N. Scarsdale, and F.A. Fornari, Jr., *Nucl. Acids Res.*, **1998**, *26*, 4721-4732.

35. Development of Empirical Biomolecular Interaction Models that Incorporate Hydrophobicity and Hydropathy. The HINT Paradigm. G.E. Kellogg and D.J. Abraham, *Analusis* **1999**, *27*, 19-22.

36. *Guest Editorial:* Ligand Docking and Scoring: New Techniques and Applications in Drug Discovery. G.E. Kellogg, *Med. Chem. Res.* **1999**, *9*, 439-444.

37. Discovery of Novel HIV-1 Reverse Transcriptase Inhibitors using a Combination of 3D Database Searching and 3D QSAR. D.W. Zaharevitz, R. Gussio, A. Wiegand, R. Jalluri, N. Pattabiraman, G.E. Kellogg, L.A. Pallansch, S.S. Yang and R.W. Buckheit, Jr., *Med. Chem. Res.* **1999**, 9, 551-564.

38. Ligand Docking and Scoring in DNA Oligonucleotides. Binding of Doxorubicin and Modeled Analogues to Optimize Sequence Specificity. G.E. Kellogg, D.J. Cashman and J.N. Scarsdale, *Med. Chem. Res.* **1999**, *9*, 592-603.

39. Computational Methodology for Estimating Changes in Free Energies of Biomolecular Association Upon Mutation. The Importance of Bound Water in Dimer-Tetramer Assembly of b37W Mutant Hemoglobins. J.C. Burnett, G.E. Kellogg and D.J. Abraham, *Biochemistry* **2000**, *39*, 1622-1633.

40. Structure-Based Design Modifications of the Paullone Molecular Scaffold for Cyclin-Dependent Kinase Inhibition. R. Gussio, D.W. Zaharevitz, C.F. McGrath, N. Pattabiraman, G.E. Kellogg, C. Schultz, A. Linke, C. Kunick, M. Loest, L. Meijer and E.A. Sausville, *Anti-Cancer Drug Des.* **2000**, *15*, 53-66.

41. Hydrophobicity. Is $LogP_{o/w}$ More than the Sum of Its Parts? G.E. Kellogg and D.J. Abraham, *Eur. J. Med. Chem.* **2000**, *35*, 651-661.

42. HINT Predictive Analysis of Binding Between Retinol Binding Protein and Hydrophobic Ligands. A. Marabotti, L. Balestreri, P. Cozzini, A. Mozzarelli, G.E. Kellogg and D.J. Abraham, *Bioorg. Med. Chem. Lett.* **2000**, *10*, 2129-2132.

43. Computationally Accessible Method for Estimating Free Energy Changes Resulting from Site Specific Mutations of Biomolecules. Systematic Modeling Building and Structural/Hydropathic Analysis of Deoxy and Oxy Hemoglobins. J.C. Burnett, P. Botti, D.J. Abraham and G.E. Kellogg, *Proteins: Str. Funct. Genet.* **2001**, *42*, 355-377.

44. Which Aminoglycoside Ring is Most Important for Binding? A Hydropathic Analysis of Gentamicin, Paromomycin and Analogs. D.J. Cashman, J.P. Rife and G.E. Kellogg, *Bioorg. Med. Chem. Lett.* **2001**, *11*, 119-122.

45. Very Empirical Treatment of Solvation and Entropy Effects. A Force Field Derived from LogP. G.E. Kellogg, J.C. Burnett and D.J. Abraham, Perspectives: *J. Computer-Aided. Mol. Design* **2001**, *15*, 381-393.

46. Simple, Intuitive Calculations of Free Energy of Binding for Protein-Ligand Complexes. 1. Models Without Explicit Constrained Water. P. Cozzini, M. Fornabaio, A. Marabotti, D.J. Abraham, G.E. Kellogg and A. Mozzarelli, *J. Med. Chem.* **2002**, *45*, 2469-2483.

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III. PRESENTATIONS

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90. Life, the Universe and Everything. Modeling Ligand Binding with an Empirical, Solvation-Based Free Energy Paradigm. G.E. Kellogg, M. Fornabaio, P. Cozzini, F. Spyrakis, A. Mozzarelli and D.J. Abraham, 2005 Gordon Conference on Computer Aided Drug Design, Tilton, New Hampshire, August, 2005.

91. Hydropathic Forcefield in 3D Database Searches and Computational Titration Applications. M. Fornabaio, F. Rastinejad, L.-Z. Mi, S. Kharalkar, M. Safo, M. Porotto, A. Moscona, D.J. Abraham and G.E. Kellogg, 2005 Gordon Conference on Computer Aided Drug Design, Tilton, New Hampshire, August, 2005.

92. A Non-Newtonian Approach for the Evaluation of Protein-DNA Binding Free Energy and Molecular Recognition. F. Spyrakis, P. Cozzini, A. Marabotti, G.E. Kellogg, D.J. Abraham and A. Mozzarelli, 2005 Gordon Conference on Computer Aided Drug Design, Tilton, New Hampshire, August, 2005.

93. Computational Titration Analysis of the pH Dependence of Human Parainfluenza Virus Hemagglutinin-Neuraminidase. M. Fornabaio, M. Porotto, A. Moscona and G.E. Kellogg, 230th A.C.S. National Meeting, Washington, D.C., August, 2005.

94. Analysis of the Interaction Between Proteins and DNA: Finding a Recognition Code. A. Marabotti, A. Facchiano, F. Spyrakis, P. Cozzini, G.E. Kellogg, D.J. Abraham and A. Mozzarelli, Biomolecular Simulation: From Prediction to Practice, 2005 International Meeting of the Molecular Graphics and Modelling Society, Dublin, Ireland, September, 2005.

95. Evaluating Docking Methods with a Hydropathic Scoring Function. M. Fornabaio, F. Spyrakis, C. Calò, A. Amadasi, A. Tripathi, P. Cozzini, A. Mozzarelli and G.E. Kellogg, 232nd A.C.S. National Meeting, San Francisco, California, September, 2006.

96. Screening for Non-nucleotide Based Inhibitors of Anthrax Edema Factor Using Molecular Docking. D.L. Chen, M. Misra, L.E. Sower, G. Menche, J.W. Peterson, G.E. Kellogg and

C.H. Schein, 62nd Southwest Regional Meeting of the American Chemical Society, Houston, Texas, October, 2006.

97. Inhibition of Hendra Virus Fusion. M. Porotto, L. Doctor, P. Carta, M. Fornabaio, O. Greengard, G.E. Kellogg and A. Moscona, 2006 NBC/NERCE Annual Meeting, Lake George, New York, October, 2006.

98. Computational Hydropathic Analysis of Polysubstituted Pyrrole Tubulin Inhibitors: A Docking Study. A. Tripathi, J.T. Gupton, S.L. Mooberry, D.A. Gewirtz and G.E. Kellogg, Summit on Systems Biology 2007: Integrative Basic, Clinical and Translational Research, Richmond, Virginia, June, 2007.

99. HINT, a "Natural" Forcefield for Virtual Screening. M. Fornabaio, P. Cozzini, A. Mozzarelli, D.J. Abraham and G.E. Kellogg, Summit on Systems Biology 2007: Integrative Basic, Clinical and Translational Research, Richmond, Virginia, June, 2007.

100. Design and Implementation of the Computational Titration Biomacromolecular Analysis as a Web-enabled Online Modeling Tool. A.S. Bayden, M. Fornabaio, A.R. Hess, J.N. Scarsdale and G.E. Kellogg, Summit on Systems Biology 2007: Integrative Basic, Clinical and Translational Research, Richmond, Virginia, June, 2007.

101. Towards the Identification of Novel Inhibitors for O-Acetilserine Sulfydrilase, a Potential Drug Target. A. Amadasi, E. Salsi, B. Campanini, P. Cozzini, G.E. Kellogg, P.F. Cook and A. Mozzarelli, Summit on Systems Biology 2007: Integrative Basic, Clinical and Translational Research, Richmond, Virginia, June, 2007.

102. Biosynthetic Enzymes as Potential Drug Targets: O-Acetylserine Sulfhydrylase. E. Salsi, A. Amadasi, B. Campanini, P. Cozzini, G.E. Kellogg, P.F. Cook and A. Mozzarelli, European University Consortium for Advanced Pharmaceutical Education and Research: ULLA Summer School 2007, Leiden/Amsterdam, The Netherlands, June, 2007.

103. Investigating the Energetic Principles That Govern the Amino Acid-Nucleotide Base Recognition Process in Protein-DNA Complexes. F. Spyrakis, A. Marabotti, A. Facchiano, P. Cozzini, S. Alberti, G.E. Kellogg, D.J. Abraham and A. Mozzarelli, 2007 Gordon Conference on Computer Aided Drug Design, Tilton, New Hampshire, July, 2007.

104. The HINT Hydropathic Forcefield as the Engine in Virtual Screening Tools. M. Fornabaio, P. Cozzini, A. Mozzarelli, D.J. Abraham and G.E. Kellogg, 2007 Gordon Conference on Computer Aided Drug Design, Tilton, New Hampshire, July, 2007.

105. Polysubstituted Pyrroles as Tubulin Inhibitors – A Docking and Hydropathic Scoring Study. A. Tripathi, N.E. Vega, J.T. Gupton, S.L. Mooberry and G.E. Kellogg, VCU School of Pharmacy Research Day, Richmond, Virginia, October, 2007.

106. A New Class of Tubulin Inhibitors: Computational Hydropathic Analysis of Polysubstituted Pyrroles. A. Tripathi, N.E. Vega, J.T. Gupton, S.L. Mooberry and G.E. Kellogg, Twenty-Fourth Annual Daniel T. Watts Symposium, Virginia Commonwealth University, Richmond, Virginia, October, 2007.

107. Virtual Screening for Inhibitors of Human Parainfluenza Virus Type III. A. Sarkar, M. Fornabaio, A.S. Bayden, M. Porotto, L. Palermo, A. Moscona and G.E. Kellogg, VCU School of Pharmacy Research Day, Richmond, Virginia, October, 2007.

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110. Computational Hydropathic Analysis of Polysubstituted Pyrroles: A New Class of Tubulin Inhibitor. A. Tripathi, N.E. Vega, S.L. Mooberry, J.T. Gupton and G.E. Kellogg. 25th American Cancer Society Virginia Cancer Researchers Seminar, Virginia Commonwealth University, Richmond, November, 2007.

111. Computational Modeling and Biological Evaluation of Stilbene Analogs as Microtubule Inhibitors Having Anti-Leukemic Activity. A. Tripathi, D. Durrant, R.M. Lee, D. Simoni, and G.E. Kellogg. Massey Cancer Center, Cancer Research Retreat, Richmond, June, 2008.

112. Interaction between Serine Acetyltransferase and O-Acetyserine Sulfhydrylase: Kinetics and Design of Potential Bactericides. E. Salsi, A. Amadasi, A.S. Bayden, B. Campanini, S. Bettati, G.E. Kellogg, P. Cozzini, P.F. Cook and A. Mozzarelli. 22nd Symposium of The Protein Society, San Diego, California, July, 2008.

113. Applying Computational Titration to Selective Nitration of Tyrosines. A.S. Bayden, V.A. Yakovlev, G.E. Kellogg and R.B. Mikkelsen. 236th ACS National Meeting, Philadelphia, Pennsylvania, August, 2008.

114. Optimizing Models for Protein-Ligand Interactions Using a Hydrophobic Force Field, A. Sarkar, S. Zhang and G.E. Kellogg, 236th A.C.S. National Meeting, Philadelphia, Pennsylvania, August, 2008.

115. New Anti-Cancer Agents: De Novo Design from HINT Complementary Maps. A. Tripathi, G.E. Kellogg, J.T. Gupton and D.A. Gewirtz. 236th A.C.S. National Meeting, Philadelphia, Pennsylvania, August, 2008.

116. Modeling Interactions of Potential Antibiotic Targets OASS A and OASS B with Inhibitory Peptides. A.S. Bayden, G.E. Kellogg, A. Amadasi, P. Cook, E. Salsi, B. Campanini, F. Spyrakis, P. Cozzini and A. Mozzarelli. 25th Annual Daniel T. Watts Research Poster Symposium, Richmond, Virginia, October, 2008.

117. Computer Based De Novo Design of Novel Pyrrole Based Anti-Cancer Agents from HINT Complementary Maps. A. Tripathi, G.E. Kellogg, J.T. Gupton and D.A. Gewirtz. 2008 AAPS Annual Meeting and Exposition, Atlanta, Georgia, November, 2008.

118. Novel Applications of Python in Computational Chemistry Workflows. A.S. Bayden, J.N. Scarsdale, V.A. Yakolev, R.B. Mikkelsen and G.E. Kellogg. CUP X, Santa Fe, New Mexico, March, 2009.

119. Development and Application of HINT, Applied to Determining Protein-Ligand Interactions in *De Novo* Drug Design. J.A. Surface, A. Tripathi, G.E. Kellogg, A. Amadasi, F. Spyrakis, A. Mozzarelli, P. Cozzini, J.T. Gupton and D.A. Gewirtz, Summit on Systems Biology 2009, Richmond, Virginia, June, 2009.

120. In Search of Entropy, Site Flexibility, Water and Other Cool Stuff. G.E. Kellogg, A. Tripathi, A. Sarkar, J.A. Surface, A.S. Bayden, A. Amadasi, A. Mozzarelli, F. Spyrakis and P. Cozzini, 2009 Gordon Conference on Computer Aided Drug Design, Tilton, New Hampshire, July, 2009.

121. Identification of Inhibitors of O-acetylserine Sulfhydrylase via Virtual and Experimental Screening of a Biased Pentapeptide Library. F. Spyrakis, E. Salsi, A.S. Bayden, A. Amadasi, B. Campanini, S. Bettati, T. Dodatko, P. Cozzini, G.E. Kellogg, P.F Cook, S. L. Roderick and A. Mozzarelli, Therapeutic Applications of Computational Biology and Chemistry 2010, Hinxton, Cambridge, United Kingdom, March, 2010.

122. Hydropathic Interaction Networks. G.E. Kellogg, V.N. Koparde, P.D. Mosier and J.N. Scarsdale, The Interactome: From Atom-Atom Contacts to Networks in Systems Biology, Marburg, Germany, March, 2010.

123. Identification of Inhibitors for Bacterial O-acetylserine Sulfhydrylase-A and –B Isozymes via *in silico* Screening of a Biased Pentapeptide Library and *in vitro* Validation. E. Salsi, F. Spyrakis, A.S. Bayden, A. Amadasi, B. Campanini, S. Bettati, T. Dodatko, P. Cozzini, G.E. Kellogg, P.F Cook, S. L. Roderick and A. Mozzarelli, Proteine 2010, Parma, Italy, April, 2010.

124. Efflux Prediction by "Systems Hydropathy" Approach: An Innovative Use of Docking, Scoring & Statistical Methods. A. Sarkar, K. Anderson and G.E. Kellogg, Keystone Meeting on Computer-Aided Drug Design, Whistler, British Columbia, Canada, April, 2010.

125. Bridging Radicals and Other Factors Influencing Tyrosine Nitration. A.S. Bayden, V.A. Yakovlev, R.B. Mikkelsen and G.E. Kellogg, Chemical Insights into Biological Processes, Frederick, Maryland, August, 2010.

126. HINT (Hydropathic INTeractions): A "Natural" Force Field Linking Computational and Experimental Biochemists. A. Mozzarelli, F. Spyrakis, P. Cozzini and G.E. Kellogg, Workshop II: New Trends in Computational Chemistry for Industrial Applications, Barcelona, Spain, May, 2011.

127. Homology Models of C-C Chemokine Type-5 Receptors. Are Bound Waters Important in Binding Sites of Membrane Bound Receptors? S.A. Zaidi, P.D. Mosier, Y. Zhang and G.E. Kellogg, Annual Meeting of the Virginia Academy of Sciences, Richmond, Virginia, May, 2011.

128. Structure Based Predictive Models for Protein Post-Translational Modifications. M. Zhang, V.A. Yakovlev, R.B. Mikkelsen and G.E. Kellogg, Annual Meeting of the Virginia Academy of Sciences, Richmond, Virginia, May, 2011.

129. Incorporation of Tautomerism into Molecular Modeling: Progress in Developing Pyrrole-based Anti-tubulin Agents. C. Da, G.E. Kellogg, N. Telang and J. Gupton, Annual Meeting of the Virginia Academy of Sciences, Richmond, Virginia, May, 2011.

130. HINTs for Refining Low-Resolution Protein X-ray Structures. V.N. Koparde, G.E. Kellogg and J.N. Scarsdale, 2011 Annual Meeting of the American Crystallographic Association, New Orleans, Louisiana, May, 2011.

131. Comparing Homology Models of Chemokine Receptor CCR5 Built Using Different Templates and Exploration of Possible Role of Protein Bound Waters in Binding of its

Allosteric Antagonists. S.A. Zaidi, G. Li, Y. Zhang and G.E. Kellogg, VCU School of Pharmacy Research Day, Richmond, Virginia, October, 2011.

132. Docking and 3D-QSAR Studies on Pyrrole-Based Antitubulin Agents. C. Da, N. Telang, J.T. Gupton, S.L. Mooberry and G.E. Kellogg, VCU School of Pharmacy Research Day, Richmond, Virginia, October, 2011.

133. Structural Modeling of Human Cytomegalovirus UL98 Alkaline Nuclease. H.I. Parikh, A.L. Kuchta, M.A. McVoy and G.E. Kellogg, VCU School of Pharmacy Research Day, Richmond, Virginia, October, 2011.

134. New Synthetic Analogs of JG-03-14: A Colchicine Site Inhibitor of Microtubule Formation. N. Telang, C. Da, P. Barelli, X. Jia, J.T. Gupton, S.L. Mooberry and G.E. Kellogg, 2011 AAPS Annual Meeting and Exposition, Washington, D.C., October, 2011.

135. Molecular Modeling Studies on Pyrrole-Based Antitubulin Agents: Docking, 3D-QSAR and Incorporation of Tautomerism. C. Da, N. Telang, J.T. Gupton, S.L. Mooberry and G.E. Kellogg, 2011 Southeast Regional Meeting of the American Chemical Society, Richmond, Virginia, October, 2011.

136. Understanding Molecular Interactions: Applications of HINT in Different Aspects of Molecular Modeling. H.I. Parikh and G.E. Kellogg, 2011 Southeast Regional Meeting of the American Chemical Society, Richmond, Virginia, October, 2011.

137. Probing Pyrrole-Based Antitubulin Agents With Molecular Modeling. C. Da, N. Telang, J.T. Gupton, S.L. Mooberry and G.E. Kellogg, 2011 Massey Cancer Center Research Retreat, Richmond, Virginia, November, 2011.

138. Specificity of Heparin Interaction Arises from Subtle, But Distinct, Differences in Binding Site Topography. P.D. Mosier, C. Krishnasamy, G.E. Kellogg and U.R. Desai, 15th Annual San Diego Glycobiology Symposium, San Diego, California, March, 2012.

139. Important But Ignored: Role of Water Molecules in Protein-Protein Docking. H.I. Parikh, M.H. Ahmed, M. Habtemariam, F. Spyrakis, P. Cozzini, J.N. Scarsdale and G.E. Kellogg, 243rd A.C.S. National Meeting, San Diego, California, March, 2012.

140. Bound Water at Protein-Protein Interfaces: Partners, Roles and Hydrophobic Bubbles as a Conserved Motif. M.H. Ahmed, F. Spyrakis, P. Cozzini, P.K. Tripathi, A. Mozzarelli, J.N. Scarsdale, M.A. Safo and G.E. Kellogg, 15th VCU Annual Graduate Student Research Symposium and Exhibit, Richmond, Virginia, April, 2012.

141. Development of Novel C-4 analogs of JG-03-14 as Antitubulin Agents. N.S. Telang, C. Da, J.T. Gupton; S.L. Mooberry and G.E. Kellogg, 244th A.C.S. National Meeting, Philadelphia, Pennsylvania, August, 2012.

142. Design and Implementation of a Scholarship Sequence in a PharmD Curriculum. L.B. Phipps, S.E. Harpe, P.W. Slattum, L.R. Moczygemba, G.E. Kellogg and J.-V.R Goode, AACP Annual Meeting: Pharmacy Education 2013, Chicago, Illinois. July, 2013.

143. Drug Discovery at Virginia Commonwealth University. U.R. Desai, K.C. Ellis, W.M. Holmes, R. Huang, G.E. Kellogg, D.L. Peterson and M.K. Safo, Academic Drug Discovery Consortium, Vanderbilt University, Nashville, Tennessee, October, 2013.

144. Design, Synthesis, Biological Evaluation and Molecular Modeling Studies on Novel C-4 Analogues of Pyrrole Based Antitubulin Agents. N.S. Telang, C. Da, J.T. Gupton; G.E.

Kellogg and S.L. Mooberry, 2013 AAPS Annual Meeting and Exposition, San Antonio, Texas, November, 2013.

145. Towards Isoform-Selectivity of Sphingosine Kinase Inhibitors: A Hydropathic INTeraction (HINT) Map Based Approach. H.I. Parikh, K. Liu, S. Zhang and G.E. Kellogg, VCU School of Pharmacy Research Day, Richmond, Virginia, November, 2013.

146. On Application of the 'Message–Address' Concept for Development of Selective mu Opioid Receptor Antagonists: A Molecular Modeling Approach. S.A. Zaidi, C.K. Arnatt, H. He, D.E. Selley, P.D. Mosier, G.E. Kellogg and Y. Zhang, VCU School of Pharmacy Research Day, Richmond, Virginia, November, 2013.

147. Targeting Cystalysin, A Virulence Factor Of Treponema Denticola-Supported Periodontitis. F. Spyrakis, B. Cellini, S. Bruno, P. Benedetti, E. Carosati, G. Cruciani, F. Micheli, A. Felici, P. Cozzini, G.E. Kellogg, C. Borri Voltattorni and A. Mozzarelli, Proteine2014, Padua, Italy, March, 2014.

148. Discovery of Small Molecule Inhibitors of PsaA, A Potential Target for *Streptococcus Pneumoniae*. A.J. Obaidullah, H.I. Parikah, T.O. Kitten and G.E. Kellogg, Annual Meeting of the Virginia Academy of Sciences, Richmond, Virginia, May, 2014.

149. A PP2A-ATM Protein Complex Regulates the DNA Damage Response and AKT Pro-Survival Signaling. A. Sule, M.H. Ahmed, G.E. Kellogg, K. Valerie, Massey Cancer Center Cancer Research Retreat, Richmond, Virginia, May, 2014.

150. The Anthraquinone Atanyl Blue PRL Inhibits the Cytomegalovirus Nuclease, UL98, and Blocks Viral Replication After Entry but Prior to Immediate Early Protein Expression. D.S. Parris, Z. Alam, Z. Al-Mahdi, Z. McKee, Y. Zhu, H.I. Parikh, G.E. Kellogg and M.A. McVoy, American Society for Virology 33rd Annual Meeting, Fort Collins, Colorado, June, 2014.

151. Deducing Opioid Receptor Activation: A Histidine Hurdle. S.A. Zaidi, G.E. Kellogg, Y. Zhang, B.L. Roth and P.D. Mosier, Computer-Aided Drug Design (CADD) Symposium, University of Maryland School of Pharmacy, Baltimore, Maryland, June, 2014.

152. Accurate Predictions of Molecular Interactions: A Prerequisite for Computational Drug Design/Discovery. H.I. Parikh and G.E. Kellogg, Computer-Aided Drug Design (CADD) Symposium, University of Maryland School of Pharmacy, Baltimore, Maryland, June, 2014.

153. How Well Can We Predict Efflux by ATP-Binding Cassette G2? R.D. Acharya, A. Sarkar and G.E. Kellogg, ASBMB-Virginia Undergraduate Affiliate Network Research Conference, Richmond, Virginia October, 2014.

154. Computational Strategies For The Discovery Of New Selective Inhibitors Towards Carbonic Anhydrase IX Isoform. L. De Luca, C. Catalano, R. Gitto, H.I. Parikh and G.E. Kellogg, Computationally Driven Drug Discovery Meeting 4th, Pomezia, Italy, February, 2015.

155. Insight into the Gs protein mediated 5-HT7 receptor signal transduction by molecular dynamics simulations. L. Basile, G. Alfonsino, M. Pappalardo, S. Guccione, S.A. Zaidi and G.E. Kellogg, XXIII National Meeting in Medicinal Chemistry, Italian Chemical Society, University of Salerno (Fisciano), Italy, September 2015.

156. G-protein Optimization via Molecular Dynamics simulations: Comparison of different models. L. Basile, G. Alfonsino, M. Pappalardo, S. Guccione, S.A. Zaidi and G.E. Kellogg, 10th AFMC International Medicinal Chemistry Symposium. Jeju, South Korea, October, 2015.

157. Discovery of Small Molecules Inhibitors of PsaA: A Potential Target for Streptococcus pneumonia. A.J. Obaidullah, M.H. Ahmed, T. Kitten and G.E. Kellogg, VCU School of Pharmacy Research and Career Day, Richmond, Virginia, October, 2016.

158. Pyrrole-based Antitubulin Agents at the Colchicine Site: SAR of C-5 Analogues in Explicitly Solvated Models. A.J. Obaidullah, C.C. Rohena, J.A. Sikorski, S.L. Mooberry, J.T. Gupton and G.E. Kellogg, 253rd American Chemical Society National Meeting, San Francisco, California, April, 2017.

159. Molecular Modeling Facility @ VCU Institute for Structural Biology, Drug Discovery and Development (ISB3D), P.D. Mosier, G.E. Kellogg and U.R Desai, Virginia Drug Discovery Rx Symposium, George Mason University, Fairfax, Virginia, June, 2018.

160. Shape 2.0: 3D Hydropathic Interaction Maps as a New Motif That Describes Protein Structure, G.E. Kellogg, M.H. Ahmed, C. Catalano, S.C. Portillo, M.K. Safo and J.N. Scarsdale, OpenEye CUP IX, Santa Fe, New Mexico, March, 2019.

161. Homology Modeling of Human Translocator Protein (TSPO), C. Catalano, W. Qiu, G.E. Kellogg, Y. Guo, Virginia Drug Discovery Rx Symposium, Roanoke, Virginia, May, 2019.

162. High-resolution Structure Determination of Mechanosensitive Channels with a Native Cell Membrane Nanoparticles System, C. Catalano, D. Ben-Hail, W. Qiu, G.E. Kellogg, A. des Georges and Y. Guo, International School of Crystallography, 54th Course: Cryo 3D Electron Microscopy, Erice, Sicily, Italy, June, 2019.

163. Structure Determination and Analysis of Borrelia burgdorferi Lactate Dehydrogenase, C. Catalano, C.W. Sze, G.E. Kellogg, C. Li, Y. Guo, VCU School of Pharmacy Research and Career Day, Richmond, Virginia, October, 2019.

164. HINTing at the Functional Diversification of the Lipid Binding Domains across Sec14-PITPs, A. Tripathi, A.J. Obaidullah, G.E. Kellogg, V.A. Bankaitis, Southeastern Regional Lipid Conference, Asheville, North Carolina, November, 2019.

165. Claudio Catalano, Research and Career Day, VCU School of Pharmacy, virtual, February, 2021.

166. Mohammed H. AL Mughram, Research and Career Day, VCU School of Pharmacy, virtual, February, 2021.

167. 3D Interaction Homology: Ionization State Optimization of Aspartate, Glutamate, and Histidine with Hydropathic Interaction Maps. N.B. Herrington and G.E. Kellogg, Research and Career Day, VCU School of Pharmacy, virtual, February, 2021.

168. 3D Interaction Homology: Ionization State Optimization of Aspartate, Glutamate and Histidine Residues with Hydropathic Interaction Maps. N.B. Herrington and G.E. Kellogg, 35th Annual Symposium of the Protein Society, virtual, July, 2021.

169. 3D Hydropathic Interaction Maps as a Novel Motif for Protein Structure Description: A Case Study of Phenylalanine, Tyrosine and Tryptophan Residues. M.H. AL Mughram and G.E. Kellogg, 35th Annual Symposium of the Protein Society, virtual, July, 2021.

170. A Novel eIF4A1 Inhibitor with Anti-Tumor Activity in Diffuse Large B-Cell Lymphoma. F. Kayastha, N.B. Herrington, B. Kapadia, A. Roychowdhury, G.E. Kellogg and R.B. Gartenhaus, Commonwealth of Virginia Cancer Research Conference, Richmond, Virginia, November, 2021.

168. 3D Interaction Homology: Combining Protein-Protein Interaction Maps for Constructing Protein Structure Prediction Tools. N.B. Herrington, C. Catalano, M.H. AL Mughram and G.E. Kellogg, 21st Annual OpenEye CUP Meeting, Santa Fe, New Mexico, March, 2022.

169. Novel Inhibitors of StAR-Related Lipid Transfer Protein 5 Inhibitors Target Plasma Membrane Lipid Raft Growth Signaling. S.M.H. Hajira, D. Rodriguez-Agudo, C. Sharon, R. Boothello, M.H. Ahmed, J. Faulx, G.E. Kellogg, G. Gil, W. Pandak, B.B. Patel, AACR Annual Meeting 2023, Orlando, Florida, April, 2023.

170. Discovery, development and characterization of potent and selective USP11 inhibitors. F. Kayastha, B. Kapadia, N.B. Herrington, A. Roychowdhury, G.E. Kellogg, R.B. Gartenhaus, AACR Annual Meeting 2023, Orlando, Florida, April, 2023.

C. Industrial

1. Monsanto (Ceregen), St. Louis. Missouri, March 1996.
2. GlaxoWellcome, Research Triangle Park, North Carolina, May 1996.
3. Wyeth-Ayerst Research, Princeton, New Jersey, June 1996.
4. Eli Lilly and Company, Indianapolis, Indiana, April 2001.
5. Glaxo-SmithKline, King of Prussia, Pennsylvania, January 2003.
6. AstraZeneca, Waltham, Massachusetts, August 2004.
7. DuPont Agrochemicals, Wilmington, Delaware, April, 2005.
8. AstraZeneca, Waltham, Massachusetts, June, 2008.