

SCOTT A. WILDMAN

Washington University School of Medicine
Biochemistry and Molecular Biophysics
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CURRENT POSITION:

Washington University School of Medicine, St. Louis, MO, (2008-present)
Research Assistant Professor, Biochemistry and Molecular Biophysics
Computational Drug Discovery: (MOE, OpenEye, AMBER) Protein-ligand interactions, structural implications of large protein families, approaches for structural modeling of kinase domains, ligand optimization techniques

EDUCATION:

University of Michigan, Ann Arbor, MI
Ph.D., Medicinal Chemistry (1997-2001)
Thesis: "Three-Dimensional Quantitative Structure-Activity Relationships Based on Atomic Property Descriptors"
Thesis Advisor: Gordon M. Crippen

State University of New York at Buffalo, Buffalo, NY
Medicinal Chemistry (1996-1997) GPA 3.9/4.0

Clarkson University, Potsdam, NY
Master of Science, Physical Chemistry (1994-1996, conferred May 1997) GPA 3.6/4.0
Thesis: "Accurate Relativistic Effective Core Potentials for Sixth-row p-block Elements"
Thesis Advisor: Phillip A. Christiansen
Bachelor of Science, Chemistry (1990-1994) GPA 3.1/4.0

INDUSTRIAL EXPERIENCE:

Pfizer Research Technology Center, Cambridge, MA, (2003-2008)
Principal Scientist, Molecular Informatics (2006-2008)
Senior Scientist, Molecular Informatics (2003-2006)
Computational Chemistry: (*Maestro, Jaguar, Phase, GOLD, Glide, ICM, MOE*)
Structure-based and ligand-based modeling for early-discovery therapeutic projects including HTS triage, protein construct design, virtual screening, homology modeling, fragment screening, docking and scoring, tautomer identification, compound and library design, and selectivity prediction
Small-molecule Superposition: Development and implementation of techniques
Protein-ligand Docking: Development of techniques to include prior structure knowledge
QSAR Modeling: Searching descriptor and algorithm space for optimal combinations
Project Leadership: Leadership of therapeutic projects toward specific targets and development of new technologies including coordination of multi-site projects
Colleague Supervision: Supervision of three colleagues

Pfizer Global Research and Development, Ann Arbor, MI, (2001-2003)

Scientist, Computer-Assisted Drug Discovery

Molecular Modeling: (*Sybyl, Unity, FlexS, CoMFA, HQSAR, Concord, Rachel, GOLD, MOE*) CADD modelling for therapeutic area projects including structure-based and ligand-based methods, similarity and diversity analysis, *de novo* design, ADME prediction, pharmacophore generation, 2-D and 3-D QSAR, database searching, and docking and scoring

Virtual Screening: (*FRED, MOE*) Development and implementation of techniques

Structural Bioinformatics: (*Sybyl, MOE, LOOK, Biopendium, Phylip, ClustalW*) Target analysis for exploratory projects involving homology modelling, sequence analysis, and protein construct design for NMR and crystallography

Warner Lambert Parke-Davis, Ann Arbor, MI, (1997),
Intern, Structure-Based Drug Design Chemistry (Synthesis)

GRADUATE EXPERIENCE:

University of Michigan, Ann Arbor, MI (1997-2001)

Molecular Modeling: (*Quanta96/97, MOE, DIANA*) Structure prediction of G-Protein Coupled Receptors

QSPR: (*MOE*) Calculation of molecular properties (partition coefficient, molecular refractivity) by atomic contributions

3-D QSAR: (*MOE*) Development of pharmacophore models and 3D QSAR methods at variable resolution incorporating minimal experimental data as intervals

Clarkson University, Potsdam, NY, (1993-1996),

Electronic Structure: (*Gaussian92, Columbus CI*) Relativistic and spin-orbit effects on molecules; Correction and generation of relativistic effective core potentials

Molecular Modeling: (*Spartan 3.0/4.0, Insight II, Quanta96/97*) Development of computational laboratory experiments for use in undergraduate courses

ADDITIONAL EXPERIENCE:

Board of Trustees, Fenway High School, Boston, MA (2007-2008)

Fenway High School is an alternative 9-12 program in the Boston public school system.

PUBLICATIONS:

Simone Sciabola, Robert V. Stanton, Sarah Wittkopp, Scott A. Wildman, Deborah Moshinsky, Shobha Potluri and Hualin Xi Predicting Kinase Selectivity Profiles Using Free-Wilson QSAR Analysis. *J. Chem. Inf. Model* **2008**, *48*, 1851-1867.

Scott A. Wildman and Robert V. Stanton Finding the best protocol for enzyme activity modeling. 234th ACS Meeting, Boston, MA, 2007.

Sarah Wittkopp, Julie E. Penzotti, Robert V. Stanton and Scott A. Wildman Knowledge-based docking for kinases with minimal bias. 234th ACS Meeting, Boston, MA, 2007.

Fauman, E. B., Guru, S. C., Johnson, A. R. and Wildman, S. A. Expression of Mutant TACE (tumor necrosis factor- α converting enzyme) Catalytic Domain. *PCT Int. Appl.*

WO2005080560A1, 2005.

Scott A. Wildman and Robert V. Stanton Using Atomic Property Values for the Selection of Small Molecule Superposition. 230th ACS Meeting, Washington DC, 2005.

Scott A. Wildman and Gordon M. Crippen Validation of DAPPER for 3D QSAR: Conformational Search and Chirality Metric. *J. Chem. Inf. Comput. Sci.* **2003**, *43*, 629-636.

Scott A. Wildman and Gordon M. Crippen Three-Dimensional Molecular Descriptors and a Novel QSAR Method. *J. Mol. Graphics Modell.* **2002**, *21*, 161-170.

Gordon M. Crippen and Scott A. Wildman *Quantitative Structure-Activity Relationships (QSAR): A Review of 3D QSAR in Combinatorial Library Design and Evaluation: Principles, Software Tools and Applications* Ghose, A. K.; Viswanadhan, V. N. Eds., Dekker, New York, 2001.

Scott A. Wildman and Gordon M. Crippen Evaluation of Ligand Overlap by Atomic Parameters. *J. Chem. Inf. Comput. Sci.* **2001**, *41*, 446-450.

Scott A. Wildman and Gordon M. Crippen Prediction of Physicochemical Properties by Atomic Contributions. *J. Chem. Inf. Comput. Sci.* **1999**, *39*, 868-873.

Scott A. Wildman, Gino A. DiLabio and Phillip A. Christiansen Accurate Relativistic Effective Potentials for Sixth-row Main Group Elements. *J. Chem. Phys.* **1997**, *107*, 9975-9979.