

DAVID J. WILD, Ph.D. *Academic Curriculum Vitae*



David John Wild
2706 Brigs Bend
Bloomington, IN 47401, U.S.A.
Tel (734) 709-0753
Email david @ wild-ideas.org

Born March 4th 1970, British
Green Card holder, Married

Summary

Ph.D. in Chemoinformatics, B.Sc. in Computing Science
14 years research experience in chemoinformatics
Active chemoinformatics research group at Indiana University
Director of small consulting company

Academic qualifications

- 1988 – 1991 B.Sc. (Hons) Class II-1 in Computing Science, Aston University, U.K.
1991 – 1994 Ph.D. in Chemoinformatics, Dept. Information Studies, Sheffield University, U.K.

Academic & professional positions held

- 1994 - 1997 Postdoctoral Research Associate, Dept. Information Studies, Sheffield University, U.K.
1998 – 2000 Postdoctoral Research Fellow, Pfizer Global R&D, Ann Arbor, Michigan, U.S.A.
2000 - 2002 Senior Scientist, Pfizer Global R&D, Ann Arbor, Michigan, U.S.A.
2002 - 2005 Adjunct Assistant Professor of Pharmaceutical Engineering, University of Michigan, Ann Arbor, MI., U.S.A.
2002 - Mar. 2004 - Director of Wild Ideas Consulting, a scientific computing consulting and research company.
Visiting Assistant Professor of Informatics, Indiana University, Bloomington, IN., U.S.A.

Research

- 1991-1994 Doctoral work included the development of massively parallel algorithms for rapid similarity searching of three dimensional chemical structure databases, and field-based similarity techniques for overlaying molecular electrostatic potential, steric and hydrophobic fields.
- 1994-1997 At the University of Sheffield, funded by the BBSRC to develop *FBSS*, a genetic-algorithm based program for the alignment and similarity analysis of three dimensional chemical structures. The program has been the focus of several publications and is still being used and developed at Sheffield and at pharmaceutical companies. During this period also acted as a supervisor to research students.
- 1998-2002 At Pfizer Global Research & Development, led multi-million dollar research collaborations with Tripos, Inc. and Bioreason, Inc. for the development of High Throughput Screening data analysis tools. Developed and published novel in-house techniques for the analysis of High Throughput Screening data, and published three papers in academic journals on research done. Led a small scientific computing research & development group.
- 2004- Established a brand new chemical informatics research group at Indiana University School of Informatics, based on both IUPUI and IUB campuses and focused on techniques and strategies for handling large volumes and diverse sources of chemical and related information. Ongoing projects include the design of informatics systems in the “lab of the future” (in collaboration with Eli Lilly), usability studies of chemoinformatics tools, integration of chemical and biological data sources for Alzheimers disease research (collaboration with IO-Informatics and others), and high performance computing for clustering huge chemical datasets. The group currently has nine active members (including four faculty). Four publications resulting from the work in the group are in preparation or submission (see reference section for submitted papers).
- 2005 Significant contributor to NIH *Exploratory Center for Cheminformatics Research* grant proposal (led by Geoffrey Fox)

Teaching

- 1994-1998 Taught introductory Information Studies graduate classes and laboratory sessions at the University of Sheffield, UK.
- 2002-2005 Taught winter semester *Introduction to Chemoinformatics* graduate class at the University of Michigan, as part of the Pharmaceutical Engineering program, including full-time and industry part-time students.
- 2004- Established a new chemical informatics curriculum at Indiana University School of Informatics, including redesigning and teaching fall semester *Chemical Information Technology* class (I571) and creating and teaching the new winter semester *Programming for Chemical Informatics* (I590) class. The curriculum has been developed such that it can be taught at multiple locations, with classes currently carried out concurrently at IUPUI and IUB. Progressed the use of distance learning technologies for chemical informatics teaching at Indiana University (presented at 2005 International Conference on Chemical Structures). From fall 2005, the classes are being made available to all US-resident students and professionals through distance learning technologies. From fall 2006, we also plan on offering the class to all CIC “big ten” university students through *CourseShare*.
- 2005- Established collaboration between Indiana University and Eli Lilly for the development of industry-focused chemoinformatics teaching modules. These will provide a basis for future distance learning modules targeted to off-site and industry students.

Service

- 2001- Reviewer for the *Journal of Chemical Information and Modeling* and the *Journal of Computer-Aided Molecular Design*
- 2003 Panel member for the AAAS Science Next Wave event at the University of Michigan, helping young research students develop their careers and interviewing skills
- 2003 Founded the *chemoinf* chemoinformatics email discussion list (currently 148 members) and the associated portal *chemoinf.com*
- 2004- Member of the Indiana University School of Informatics Corporate Partners Task Force. Have worked to strengthen links between the School of Informatics and industry, including Eli Lilly in Indianapolis, and Pfizer in Ann Arbor.

Other Information

- Professional I am a regular presenter at academic conferences including the American Chemical Society, the International Conference on Chemical Structures, and the Daylight User Group meeting. I am a member of the American Chemical Society.
- Programming Fluent in C, Perl, HTML, Unix/Linux programming. Some experience in C++, Visual Basic / VBA and Java. Experienced in Web application development, software and interface design, HCI techniques, parallel computer programming on a variety of machines, SYBYL, Daylight & BCI toolkits & other computational chemistry development environments.
- Work Status I am a British Citizen, and a U.S. Green Card holder.
- Churches My wife and I have held a variety of church leadership roles at several churches, including leading groups of 10-100 people, event organisation, counselling, working with people from difficult backgrounds, outreach projects, and music.
- Miscellaneous I'm interested in graphic and information design, theology (particularly science & Christianity), nature, radio communications, outdoor adventure, and play a number of musical instruments. I also volunteer in wildlife rehabilitation and emergency management.

Peer-reviewed publications (chronological order)

Artymiuk, P.J., Bath, P.A., Grindley, H.M., Pepperrell, C.A., Poirrette, A.R., Rice, D.W., Thorner, D.A., Wild, D.J., Willett, P., Similarity Searching in Databases of Three-Dimensional Molecules and Macromolecules, *Journal of Chemical Information and Computer Sciences*, 1992, 32, 617-630.

Wild, D.J., Willett, P. Similarity Searching in Files of Three-Dimensional Chemical Structures. Implementation of Atom Mapping on the Distributed Array Processor DAP-610, the MasPar MP-1104, and the Connection Machine CM-200. *Journal of Chemical Information and Computer Sciences*, 1994, 34, 224-231.

Wild, D.J., Willett, P. Similarity Searching in Files of Three-Dimensional Chemical Structures: Alignment of Molecular Electrostatic Potential Field with a Genetic Algorithm, *Journal of Chemical Information and Computer Sciences.*, 1996, 36, 159-167.

Thorner, D.A., Wild, D.J., Willett, P., Wright, P.M. Similarity Searching in Files of Three-Dimensional Chemical Structures: Flexible Field-Based Searching of Molecular Electrostatic Potentials, *Journal of Chemical Information and Computer Sciences*, 1996, 36, 900-908.

Wild, D.J., Willett, P. Field-Based Similarity Searching in Databases of Three-Dimensional Chemical Structures, in Collier, H. (ed), *Proceedings of the 1997 International Chemical Information Conference*, Tetbury:Infonortics, 1997

Thorner, D.A., Wild, D.J., Willett, P., Wright, P.M. Calculation of Structural Similarity by the Alignment of Molecular Electrostatic Potentials, *Perspectives in Drug Discovery and Design*, 1998, 9/10/11, 301-320

Gillett, V.J., Wild, D.J., Willett, P., Bradshaw, J., Similarity and Dissimilarity Methods for Processing Chemical Structure Databases, *The Computer Journal*, 1998, 41, 547-558

Drayton, S.K., Edwards, K., Jewell, N., Turner, D.B., Wild, D.J., Willett, P., Wright, P. M., Simmons, K., Similarity Searching in Files of Three-Dimensional Chemical Structures: Identification Of Bioactive Molecules, *Internet Journal of Chemistry* (www.ijc.com); 1, 1998

Wild, D.J., Blankley, C.J. VisualiSAR: A Web-Based Application for Clustering, Structure Browsing and SAR Study, *Journal of Molecular Graphics and Modelling*, 1999, 17, 85-89.

Wild, D.J., Blankley, C.J. Comparison of 2D Fingerprint Types and Hierarchy Level Selection Methods for Structural Grouping using Wards Clustering, *Journal of Chemical Information and Computer Sciences.*, 2000, 40, 155-162.

Bohl, M., Dunbar, J., Gifford, E.M., Heritage, T., Wild, D.J., Willett, P., Wilton, D.J. Scaffold Searching: Automated Identification of Similar Ring Systems for the Design of Combinatorial Libraries. *Quantitative Structure-Activity Relationships*, 2002, 21, 6.

Wild, D.J. Strategies for Using Information Effectively in Early-stage Drug Discovery, in Ekins, S. (ed), *Computer Applications in Pharmaceutical Research and Development*. Book submitted November 2005.

Wild, D.J., Wiggins, G.D., The use of Distance Education in Chemoinformatics Teaching and Research, *Journal of Chemical Information and Modeling*, Submitted July 2005.