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Fanwood, NJ 07023
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Education

Biochemistry, Ph.D

December 2001

Department of Biochemistry and Molecular Biology, Michigan State University, East Lansing, MI.

Thesis Title: *Computational Techniques for Modeling Protein-Ligand Interactions and their Application to Serine Proteases and Asparaginyl-tRNA Synthetase*

Research Advisor: Dr. Leslie A. Kuhn

Focus: Computational methods for protein structural analysis, computational ligand screening, molecular modeling, algorithm development, protein-water interactions.

Biochemistry, B.S.

May 1996

Department of Biochemistry, Michigan State University, East Lansing, MI.

Also a member of the Honors College

Professional Experience

Senior Scientist, Drug Discovery Applications

April 2004 – October 2008

Schrödinger, Inc.,

New York, NY

Responsible for working with outside research groups in academic institutions, biotechnology companies, and pharmaceutical companies to apply the scientifically leading Schrödinger suite of drug discovery software to drug development projects, including lead identification and lead optimization. Involved use of virtual screening, pharmacophore search, QSAR, and cheminformatics methods. Deeply involved in internal drug discovery and software validation projects involving a large amount of structural and published activity data collation as well as identifying a large number of new protein targets to greatly expand our validation suite. Extensive use of the Schrödinger Python application environment for both small scale and large scale script development, including projects customized for specific Schrödinger customers.

Postdoctoral Research Associate

January 2002 – March 2004

AG Klebe, Institute for Pharmaceutical Chemistry, University of Marburg

Marburg, Germany

Worked in a varied academic pharmaceutical research group predominantly on developing improved scoring functions for structure-based docking applications. This involved extensive scientific research as well as programming to implement these techniques. Involved in advising more junior members of the research group on their projects.

Graduate Research Assistant

August 1996 – January 2002

Department of Biochemistry and Molecular Biology, Michigan State University

East Lansing, MI

Conducted studies into methods for computational ligand screening including the use of ligand flexibility, protein side-chain flexibility, and water molecule interactions as the SLIDE docking algorithm. Developed techniques for analysis of conserved water sites in protein structures and studied such in thrombin and trypsin structures. Developed techniques for prediction of water molecule displacement upon ligand binding involving evolutionary computational techniques.

Technical Competencies

- Extensive knowledge of the Schrödinger suite (Maestro, Glide, MacroModel, Phase, Prime, Canvas) of molecular modeling and computational chemistry software.
- Additional experience with Accelrys (InsightII), Tripos, and MOE software packages.
- Extensive knowledge of the Python programming language including GUI (TKinter) programming as well as knowledge of C/C++, Perl, and shell scripting languages.
- Knowledge of HTML, PHP, and MySQL web development environments.
- Extensive knowledge of Windows, Linux, and Unix environments.