HERSCHEL J. R. WEINTRAUB, PH.D.
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TECHNICAL EXPERIENCE

Extensive experience in Chemical Informatics, Drug Discovery, Computational Chemistry, and related areas. Expertise in Pharmaceutical and Biotech R&D management, and R&D IT management. Built and managed teams of 3 to 40+ individuals and managers. Experience in working closely with Pharmaceutical and Biotech R&D Scientists, Project Team Leaders, IT professionals, R&D, and C-level management. Experience in Pharmacy and Life Science education as full-time as well as adjunct faculty. *Ad-hoc* reviewer for the NIH in areas related to computational chemistry and drug discovery. Additional experience in data integration, enterprise annotation, and user interface requirements.

PROFESSIONAL EXPERIENCE

CADD*informatics* **2001-**
Consulting Practice, incorporated in 1986
Informatics and Computational Drug Discovery Consultant to the Pharmaceutical and Biotech Industries.

- Computational Chemistry / Proteomics / Molecular Modeling / Library Design
- Knowledge Management
- Data Integration
- High Performance Computing in Pharma/Biotech R&D
- Strategic Planning
- Electronic Laboratory Notebooks, Chemical Registration Systems, Biological Assay Management Systems
- Project Management

IBM Life Sciences **2002-2005**
Principal, IBM Life Sciences
Domain (Pharma/Biotech R&D Informatics) and pre-sales consulting in areas of data integration, enterprise R&D transformation, chemical informatics, imaging, annotation, and others.

- Thought Leadership in development of new applications in Pharma/Biotech R&D domain
- Pharma and Biotech R&D infrastructure consulting including Data Integration and Knowledge Management
- Thought Leadership in Chemical Informatics
- High Performance Computing domain expertise in Pharma & Biotech

Genentech, Inc., South San Francisco, California **1999-2001**
Director, Scientific Computing

- Lead and directed the Scientific Computing Department, providing support for Research, Development, and Regulatory Affairs. Responsible for the Scientific Library and Graphics units.
- Responsible for budget of $6+ million and staff of ~40.

Helios Pharmaceuticals, Louisville, Kentucky
(Start-up company. No longer in business.)
Vice President, Computational Chemistry and Informatics

- Conducted executive presentations of computational approaches used in library design and validation to potential corporate partners.
- Responsible for development and implementation of chemical structure database, compound library design tools, compound tracking, and diversity assessment initiatives.
- Established department in small biotech start-up. Responsibilities included recruitment and management of staff to implement IT infrastructure (servers, network, desktop computers, etc.).
- Designed and implemented a "user-friendly" integrated informatics system for pharmaceutical discovery.

R.W. Johnson Pharmaceutical Research Institute, Raritan, New Jersey
(A Johnson & Johnson Company)

Assistant Director, Discovery Research, Computer Assisted Drug Discovery
Assistant Director, Medicinal Chemistry

- Expanded multi-site computational chemistry team from two members to eight.
- Lead team that discovered first “small molecule” inhibitor of a protein-protein interaction (erythropoetin-erythropoetin receptor) and successfully integrated molecular modeling technologies into therapeutic teams, making significant contributions toward advancing several compounds into development.
- Served on an interdisciplinary team that visited several biotech companies to identify potentially beneficial technologies. The areas investigated included combinatorial chemistry, data handling, computational chemistry, and development of non-peptide "drugs" from protein or peptide leads (primarily in the area of hematopoiesis).
- Acquired eight processor “low cost” Cray supercomputer and negotiated savings of nearly 50%.

Marion Merrell Dow Research Institute (now **Sanofi-Aventis**)**,** Cincinnati, Ohio
Department Head, Global Theoretical Chemistry and Scientific Supercomputing
Group Leader, Chemical Sciences

- Evaluated and acquired a Cray supercomputer (the third in the pharmaceutical industry) resulting in improved research efficiency. Company received a major industry award for innovation in MIS in two consecutive years.
- Established computational chemistry group. Provided leadership and support to multi-national research organization in the US, France, and Italy.
- Established close working relationships with research computing group to facilitate highly productive interactions. At that time, such interaction was atypical in the pharmaceutical industry.
- Identified and worked with therapeutic teams for the acquisition of x-ray structures of target enzymes from academic laboratories.

Abbott Laboratories, Abbott Park, Illinois
Senior Theoretical Chemist

Eli Lilly and Company, Indianapolis, Indiana
Senior Physical Chemist

Purdue University, School of Pharmacy, West Lafayette, Indiana
Assistant Professor, Medicinal Chemistry
Director, Computer-Based Education

- Directed one of the first "computer-based education" laboratories, using computer technology developed at the University of Illinois (the "PLATO" system) and courseware developed at Purdue and other institutions.

Selected Consulting Clients (CADD*informatics*)

Anacor AstraZeneca, Wilmington, Delaware; **Dupont Central Research**, Wilmington, Delaware; **Neurogen**, Branford, Connecticut; **Trega Biosciences** (**Lion Biosciences)**, San Diego, California; **IMClone**, New York, NY; **Abbott Laboratories**, Abbott Park, Illinois; **Lilly Research Laboratories**, Indianapolis, Indiana; **CompuDrug**, Wien, Austria; **Becton Dickinson**, Research Triangle Park, North Carolina; **TransTech Pharma**, High Point, North Carolina; **Union Carbide**, Research Triangle Park, North Carolina; **Pain Therapeutics**, San Mateo, California; **Norwich Pharmacal** (Proctor & Gamble Pharmaceuticals), Norwich, New York.

EDUCATION

- Ph.D. Macromolecular Science, Case Western Reserve University, Cleveland, Ohio
- M.S. Macromolecular Science, Case Western Reserve University, Cleveland, Ohio
- B.S. Biomedical Engineering, Case Institute of Technology, Cleveland, Ohio
- Teaching-Research Postdoctoral Fellow, Department of Medicinal Chemistry and Pharmacognosy
  School of Pharmacy and Pharmacal Sciences, Purdue University, West Lafayette, Indiana
- USPHS-National Library of Medicine Fellow in Computer Science, University of Illinois

TECHNICAL SKILLS AND PROFESSIONAL TRAINING

Computational Chemistry Software (Schrodinger Suite, Sybyl, Biosym/MSI/Accelrys, ISIS [MDLI/Symyx], MOE, GRID, DOCK, Spartan), various QSAR Methods
Chemical Informatics Software (MDL MACCS, ISIS, Isentris, DeltaSoft ChemCart, CambridgeSoft, IDBS (ActivityBase), Accelrys (RS^3), Daylight.

Oracle (PL/SQL)

Project Management
Managing Multiple Projects
Time Management
Facilitating Successful Meetings
Effective Listening Skills

Fundamentals of Supervision
Managing Conflict and Confrontation
Managing Diversity
Partnering for Performance (Leadership)
IBM “Basic Blue” management training

ACADEMIC APPOINTMENTS

Adjunct Faculty, Grand Canyon University College of Nursing and Health Sciences, Phoenix, Arizona

Associate Faculty, Molecular Design Institute, University of California at San Francisco

Adjunct Professor of Medicinal Chemistry, Division of Pharmacology and Medicinal Chemistry, University of Cincinnati College of Pharmacy

MEMBERSHIP IN SCIENTIFIC AND PROFESSIONAL SOCIETIES

- International QSAR and Modeling Society (Board Member)
- Institute of Electrical and Electronics Engineers, including Computer Subgroup
- American Chemical Society, including Medicinal Chemistry, Computational Chemistry, and Chemical Information Subgroups

TEACHING, RESEARCH, SERVICE

- Taught two graduate-level and two undergraduate-level medicinal chemistry courses at Purdue and one graduate-level medicinal chemistry course at University of Cincinnati. Taught Introductory Chemistry and Statistics for Health Sciences courses at Grand Canyon University.
- Ph.D. Student Dissertation Advisor, (University of Cincinnati Medicinal Chemistry).
- Visiting Lectures in Drug Design Graduate Course, (University of Louisville).
- Awarded several NIH grants for conformational analysis related research while on Purdue faculty.
- Served on four faculty committees at Purdue, three as chair.

MAJOR AREAS OF RESEARCH INTEREST

- Drug Design by Theoretical Techniques
- Application of Computer Technology and Simulation to Drug Discovery and Medical Informatics
- Development of Theoretical Techniques for the Characterization of Molecular Systems
- Database Mining
- Development of "Chemist/Biologist/Scientist-friendly" informatics systems
- Integration of Informatics, Scientific Data, Combinatorial and Computational Chemistry, and HTS

MAJOR COMPUTER SOFTWARE DEVELOPED

Informatics System. Helios information system for chemical, biological, and computational data. Layered on MDL ISIS, Project Library/Central Library, Screen, and Oracle RDMS. This database was designed to capture structural and biological data from combinatorial chemistry and high-throughput screening facilitate flexible data retrieval.

COCOA and "**PlateViewer**." Team developed programs to view and optimize combinatorial chemistry synthesis and plate layout. Also provides a uniform "window" of structural, analytical, computational, and biological data.

INTERACT. A program to coordinate Abbott small molecule molecular display system and protein display system.

LIDDS. The Lilly Interactive Drug Design System, a "gateway" and data management system allowing access to the library of theoretical molecular design tools at Lilly Research Laboratories.

CAMSEQ. Software System for conformational studies of molecules in solution. This program is the basis of the CAMSEQ-II component of the NIH-EPA Chemical Information System as well as CHEMLAB, formerly marketed by Molecular Design Limited.

CAMSEQ/M. A microcomputer version of CAMSEQ.

Publications and Lectures

>30 Scientific Publications, >25 Contributed Papers, >100 Invited Lectures, 3 Patent Applications (IBM)

Other

- Board Member, International QSAR & Modeling Society (2000-2010)
- Focus Group Chair, Computational Drug Discovery, American Association of Pharmaceutical Sciences (2009-)
- Chairman, Gordon Conference on QSAR, Tilton, New Hampshire, August, 1997.
- Member, MACCS-3D Consortium (3D database searching technology).
- Organizer, "Innovations in Drug Design" Symposium, Marion Merrell Dow Research Institute, Cincinnati, Ohio.
- Organizer, Molecular Modeling Workshop, American Association of Colleges of Pharmacy Annual Meeting, Salt Lake City, Utah.
- Other Conferences and Symposia: Program co-organizer and session chair, IBC Conference on "Rational Drug Design," Coronado, California; Organizer and Chairman, Middle Atlantic Pharmacology Society Annual Meeting, Raritan, New Jersey; Program Chairman, Gordon Conference on QSAR, Tilton, New Hampshire, August, 1995; Program Co-Chairman and Co-Organizer, Molecular Modeling Symposium; Session Chairman, Gordon Conference on QSAR.
- Chairman, Tripos User's Group - US (Molecular Modeling Software).
- Chairman, Biosym User's Group - US (Protein Modeling Software).