

## Lee Herman Consulting LLC

6 Mellon Rd.

Wellesley, MA 02482

781-608-8123

leehermanconsulting@comcast.net

### Core Competencies

- Drug discovery and project team support in oncology, inflammation, and metabolic disease therapeutic areas in collaboration with medicinal chemists, structural biologists, and others.
- Computational chemistry techniques such as docking, pharmacophore modeling, data mining (QSAR), virtual combinatorial library enumeration, virtual screening, HTS analysis and hit triage, homology modeling, clustering and diversity analysis, shape and similarity searching.
- Molecular modeling environments and programs (Pipeline Pilot (Scitegic), MOE (CCG), Glide (Schrodinger), ROCS and OMEGA (OpenEye), others).
- Compound property model building and prediction. Generation of ADME and physicochemical (e.g. solubility, absorption, serum binding, drug-likeness, GPCR agonism, kinase, hERG) models for use by project teams to help solve PK and ADME property liabilities associated with lead compounds.
- Development of computational tools and methods for molecular modeling, and software for enterprise-wide cheminformatics systems to assist the medicinal chemist collect, analyze, and visualize data, and predict properties of virtual compounds.
- Compound acquisition. Development of filtering tools, and the acquisition of compounds for corporate HTS collections. Chemists are much more likely to accept an HTS lead series for hit-to-lead follow-up when the hit comes from a well curated set of compounds, using medicinally sensible structural filters, physicochemical criteria, diversity metrics, and novel "drug-like" categorical models developed in collaboration with medicinal chemists.
- Implementation and maintenance of corporate and vendor screening and inventory databases, using Accord or Isis database technologies.
- Organic synthesis (traditional, combiChem, peptides). My formal training was in synthetic chemistry, so I speak the language.
- Selection, installation, and maintenance of resources (software and hardware) for molecular modeling, including expert tools and those appropriate for general use. Chemistry desktop support.

### Biography

#### Lee Herman, Ph.D.

Dr. Herman has more than 10 years of computational chemistry and cheminformatics experience in the pharmaceutical industry and 7 years of chemistry experience in hospitals and academic research institutions. As one of the first chemists at Millennium Pharmaceuticals, he was initially responsible for all of the cheminformatics and computational chemistry support as the company transitioned from genomics to drug discover. Later, he provided computational project support, continued to create web-based decision support tools, and continued to be liaison to the cheminformatics department as the primary representative of the medical chemists. Before Millennium, he developed new methods for the generation of combinatorial libraries at Perseptive Biosystems. Earlier, as a Harvard Fellow, he made use of his synthetic chemistry training at several major Boston area hospitals to develop novel radiopharmaceutical agents. Dr. Herman earned his PhD at Carleton University in Ottawa, Canada, where he trained in synthetic, computational, and natural products chemistry.