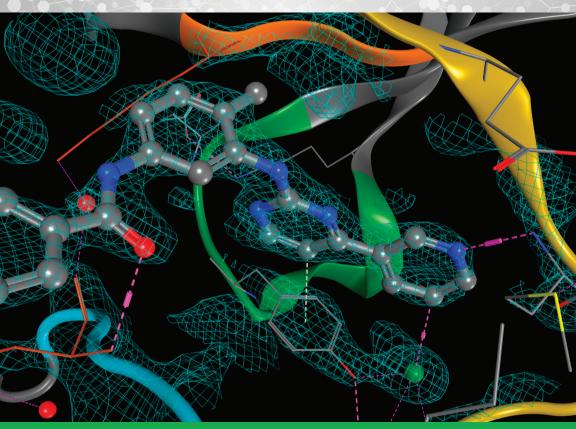
PSILO



Protein Structure Database and Visualization System

- Macromolecular Repository
- Data Visualization and Analysis
- Browser Interface for Search and Retrieval
- \circ 3D Ligand: Receptor and Pocket Similarity
- Protein Structure Alignment
- Data Standardization and Annotation
- Standard IT Infrastructure and Integration



PSILO[®] is a database system that provides a consolidated repository for macromolecular and protein-ligand structural information. It offers research organizations a means to systematically track, register and share both experimental and computational structural data. A web-browser interface facilitates the search, visualization and analysis of public and private structural data.

chemcomp.com

Macromolecular Repository

- Store Coordinate and Structure Factor Data
- Save Auxiliary Files alongside Original Data
- Fully RCSB-Compliant PDB, mmCIF, and XML Formats
- Bulk Import Script for Larger Datasets
- Web Interface for Individual Record Deposit

Data Visualization and Analysis

- Visualize Structures and Electron Densities
- Visualize Structures Aligned by Ligand, Pocket or Protein
- O 2D Ligand Interaction Diagrams Linked to the 3D Viewer
- Analyze, Plot, and Sort 3D Query Statistics
- BLAST Search Phylogenetic Tree, Interactive Alignment

Browser Interface for Search and Retrieval

- Google-Like Queries with Multiple Search Criteria
- \odot Standard Sketchers for Substructure and 3D Queries
- Download Hits as PDB, mmCIF, XML, MDB
- 2D and 3D Active Site Visualization
- Filter for Similar or Duplicate Records

3D Ligand: Receptor and Pocket Similarity

- 3D Pocket Similarity Search
- 3D Domain Motif Search
- Ligand:Receptor 3D Geometry Using Standard Sketchers
- Multi-Criteria Search, including Text, 2D Query
- Automatic Detection of Ligand-Independent Pockets

Protein Structure Superposition

- Optimized Structure Superposition
- Superpose on Pre-Defined Pocket Residues
- 3D Query Superposition
- Overlay Based on Protein Family Reference Alignment
- Rigid-Body Ligand Superposition

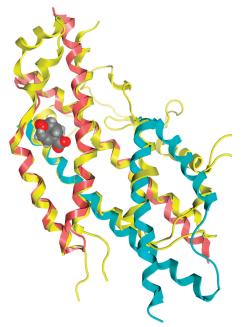
Automated Data Standardization and Annotation

- Bioinformatics Annotations (GO, SCOP, Etc.)
- Standard Orientations for Related Structures
- Mirroring of the RCSB for Weekly Updates
- Geometric Data Quality Assessment
- Maintenance of Popular Protein Families

Standard IT Infrastructure and Integration

- Simple to Maintain and Deploy IT Infrastructure
- Integrate with External/Internal Databases and Software
- Source Code Provided for Customization
- Group-Based Permission System
- Version Control

PSILO





NORTH AMERICA

Corporate Headquarters 1010 Sherbrooke Street W., Suite 910 Montreal, Quebec, Canada H3A 2R7 Tel.: +1 514 393 1055

EUROPE

United Kingdom St John's Innovation Centre Cowley Road, Cambridge CB4 OWS Tel.: +44 1223 422320

EUROPE Germany Kaiser-Wilhelm-Ring 11 50672 Köln

Tel.: +49 221 337790 0

ASIA Japan MOLSIS Chuo-ku, Tokyo 104-0032 Tel.: +81-3-3553-8030