Discover new molecules

CSD-Discovery

For discovery chemists, the components in CSD-Discovery provide the means to:

- Interrogate protein ligand complexes
- Dock small molecules, generate probable molecular conformations
- Search for likely overlays of active ligands
- Propose scaffold hops or isosteric replacements
- Produce easy integrations into internal systems

Bringing together the Protein Data Bank (PDB) and Cambridge Structural Database (CSD) and much more.

**Generation of Molecular Conformations**
Rapidly and effectively generate plausible molecular conformations, using the wealth of information available in the Cambridge Structural Database, to benefit ligand-based molecular screening and pharmacophore prediction.

**Protein-Ligand Docking**
Dock small molecules into proteins flexibly; optionally sampling protein flexibility and solvent location during docking using the world-renowned docking package, GOLD, to provide fast and accurate binding mode prediction in lead discovery and lead optimisation.

**Flexible Alignment of Ligands**
Align ligands using generated conformations to build realistic pharmacophore hypotheses for use in field-based virtual ligand screening or scaffold hopping.

**Script-based Interfaces**
Create tailored Python scripts using the whole spectrum of CSD functionality to answer your targeted research functionality questions. Integrate access to CSD-Discovery workflows seamlessly with 3rd party software.

**Searching for Scaffold Hops and Pharmacophoric Patterns**
Mine both the CSD and the PDB using pharmacophores or substructure searching interactively to find repeated patterns of interactions or possible suggestions for potential scaffold hops using CSD-CrossMiner. Such information can lead to credible and non-obvious ideas and directions for lead development.