CCDC
advancing structural science

Discover New Pharmaceuticals and Agrochemicals

CSD-Discovery

- Discover new pharmaceuticals and agrochemicals
- 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

Combining the wealth of validated data form the Protein Data Bank (PDB) and the Cambridge Structural Database (CSD).

Over 300,000 PDB protein-ligand binding sites are included within CSD-CrossMiner and the Macromolecule Hub.

Generate Molecular Conformations for ligand-based molecular screening and pharmacophore prediction.

Protein-Ligand Docking to provide fast and accurate binding mode prediction in lead discovery and lead optimisation.

Align Ligands to build realistic pharmacophore hypotheses for use in field-based virtual ligand screening or scaffold hopping.

Script-Based Interfaces
Create tailored Python scripts for targeted research with 3rd party software integration.

Searching for Scaffold Hops and Pharmacophoric Patterns
Use pharmacophores or substructure searching to find repeated patterns of interactions or potential scaffold hops.

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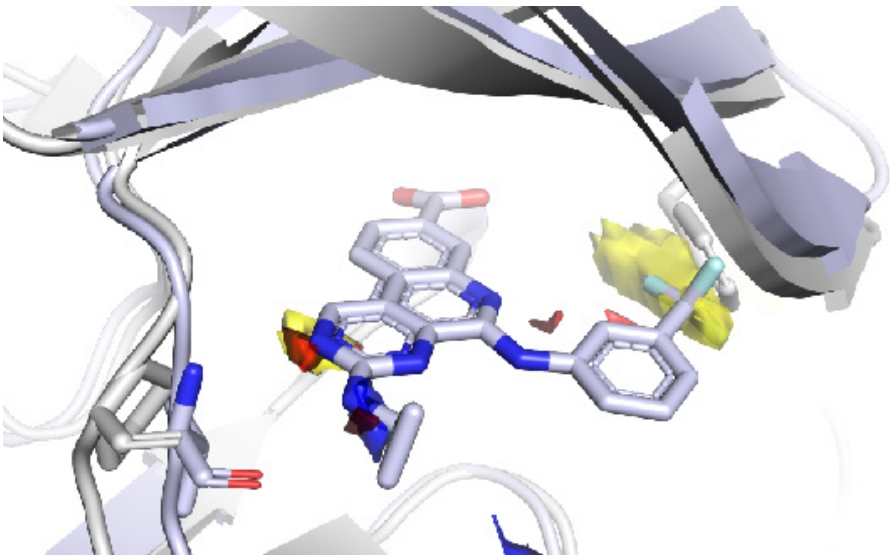
Optimise Your Pharmaceutical and Agrochemical Discovery

- Bond length assessment
- Valence angle assessment
- Torsion angle assessment
- Ring geometry assessment
- Conformer generation
- Fragment interaction maps
- Protein interaction maps
- Full interaction maps
- Ligand-based drug discovery
- Ligand overlay
- Field-based ligand screener
- Scaffold hopping
- Structure-based drug discovery
- Protein-ligand docking
- Ensemble docking
- Pose analysis
- Proprietary structures
- Cavity similarity searching
- Full access to the Cambridge Structural Database
- Search protein-ligand binding sites
- 3D display and manipulation
- High resolution graphics and movie generation
- Plotting and charting
- Descriptive statistics
- Interactive visualization
- Filtering and categorization

Learn More with the Ensemble Hotspot Mapping White Paper

Assess druggability and identify binding hotspots even in difficult targets

This free whitepaper explains how data-driven ensemble hotspot maps can be used to visually guide target validation and drug design. Use this approach to deeply understand selectivity and pocket druggability. Case studies using this approach from scale-up pharmatech ExScientia and a recent Nature publication are discussed, alongside full details of how the method works, and how to access it.
Download here: **https://info.ccdc.cam.ac.uk/whitepaper-selectivity-druggability-pharmaceutical-design**



Learn more at www.ccdc.cam.ac.uk