CSD Product Datasheet 2025

Commercial users

Choose the right level of CSD software access for your work.

We also offer a range of services from proprietary database building, to solid form risk assessment, virtual screening, and co-crystal design. Contact us to talk about your needs.

Not sure? We're happy to help. Email admin@ccdc.cam.ac.uk

						Add-on packages	
	CSD Core	**CSD Discovery**	**CSD Materials**	**CSD Frameworks**	**CSD Enterprise**	**CSD Theory**	**CSD Particle**
Data							
CSD deposited and curated data	✓	✓	✓	✓	✓		
CSD teaching resources	✓	✓	✓	✓	✓		
Proprietary CSD extension	✓	✓	✓	✓	✓		
Access							
Retrieve via bibliographic info, DOI, CSD identifiers or compound name	✓	✓	✓	✓	✓		
Link from published articles and repositories	✓	✓	✓	✓	✓		
Publisher referee services	✓	✓	✓	✓	✓		
Search							
Search by chemical formula, cell parameters, 2D/3D substructure, similarity, and more...	✓	✓	✓	✓	✓		
Protein-ligand binding sites		✓			✓		
Visualize							
3D display and manipulation	✓	✓	✓	✓	✓		
High resolution graphics and movie generation	✓	✓	✓	✓	✓		
3D printing file output	✓	✓	✓	✓	✓		
PXRD pattern simulation	✓	✓	✓	✓	✓		
PXRD pattern comparison	✓	✓	✓	✓	✓		
Molecule and structure editing	✓	✓	✓	✓	✓		
2D diagram generation	✓	✓	✓	✓	✓		
Editing and Analysing							
Normalise Hydrogens	✓	✓	✓	✓	✓		
Transform Molecules	✓	✓	✓	✓	✓		
Invert Structure	✓	✓	✓	✓	✓		
Change symmetry, lattice centering, and unit cell	✓	✓	✓	✓	✓		
Sketch molecule		✓	✓	✓	✓		
SMILES to molecule		✓	✓	✓	✓		
Calculate void volume and properties	✓	✓	✓	✓	✓		
Pore analyser	✓	✓	✓	✓	✓		
Structure and molecule overlay	✓	✓	✓	✓	✓		

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	CSD Core	CSD Discovery	CSD Materials	CSD Frameworks	CSD Enterprise	CSD Theory	CSD Particle
Analyse							
Plotting and charting	✓	✓	✓	✓	✓		
Descriptive statistics	✓	✓	✓	✓	✓		
Interactive visualisation	✓	✓	✓	✓	✓		
Filtering and categorisation	✓	✓	✓	✓	✓		
Reporting	✓	✓	✓	✓	✓		
Integrations							
CSD Pipeline Pilot Component Collection	✓	✓	✓		✓		
CSD KNIME Component Collection	✓	✓	✓		✓		
Conformations							
Bond length assessment	✓	✓	✓		✓		
Valence angle assessment	✓	✓	✓		✓		
Torsion angle assessment	✓	✓	✓		✓		
Ring geometry assessment	✓	✓	✓		✓		
Conformer generation		✓	✓		✓		
Interactions							
Fragment interaction maps (IsoStar)	✓	✓	✓		✓		
Protein interaction maps (SuperStar)		✓			✓		
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		✓			✓		

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Solid Form Analysis							
Motif searching			✓	✓	✓		
Packing feature searching			✓	✓	✓		
Crystal packing similarity			✓	✓	✓		
Calculations			✓		✓		
Hydrogen bond propensity and coordination assessment			✓		✓		
Hydrate analysis			✓	✓	✓		
Solvate analysis			✓	✓	✓		
Aromatic analysis			✓		✓		
Co-crystal design			✓		✓		
Hydrogen bond statistics assessment			✓		✓		
Particle Analysis							
Predict particle facets							✓
Visualize surface chemistry and charge							✓
Identify slip planes							✓
Surface interactions analysis							✓
Full interaction maps on surface							✓
Determine H-bond dimensionality							✓
Visualize surface topology							✓
Quantify surface chemistry and topology							✓
Python API particle analysis							✓
Manage Crystal Structure Prediction (CSP) data							
Manage proprietary CSP data						✓	
View and analyse CSP results in a web-based interface						✓	
Generate CSP landscapes						✓	
Generate CSP landscape reports in 1 click						✓	
Store CSP data in a standardized way						✓	
Python API access to CSP data						✓	
Search for structures within Crystal Structure Prediction (CSP) landscapes, as well as searching for landscapes themselves						✓	
Predict solid forms using informatics, landscape generator						✓	