CSD Product Datasheet 2023

Commercial users

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Below you can find a table showing each of the software suites that are available, as well as our Add on Packages that can be purchased as an add on to any of our paid software suites.

					Add-on packages	
	CSD Core	CSD Discovery	CSD Materials	CSD Enterprise	CSD Theory	CSD Particle
Data						
CSD deposited and curated data	✓	✓	✓	✓		
CSD teaching resources	✓	✓	✓	✓		
Proprietary CSD extension	✓	✓	✓	✓		
Deposit						
Guided data deposition	✓	✓	✓	✓		
CIF syntax check	✓	✓	✓	✓		
Reduced cell check	✓	✓	✓	✓		
Data validation	✓	✓	✓	✓		
CSD DOI and curated CSD entry on publication	✓	✓	✓	✓		
Direct publication through *CSD Communications*	✓	✓	✓	✓		
Enhanced data discoverability	✓	✓	✓	✓		
Persistent, free storage of your data	✓	✓	✓	✓		
Deposition portal allowing you to access, edit and share your deposits	✓	✓	✓	✓		
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		✓		✓		
Visualise						
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	✓	✓	✓	✓		

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					Add-on packages	
	CSD Core	CSD Discovery	CSD Materials	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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	CSD Core	CSD Discovery	CSD Materials	CSD Enterprise	Add-on packages: CSD Theory	Add-on packages: CSD Particle
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					✓	
CCDC services						
On-site training	+	+	+	+	+	+
Custom script development	+	+	+	+	+	+
In-house database building	+	+	+	+	+	+
Solid form risk assessment	+	+	+	+	+	+
Co-crystal design	+	+	+	+	+	+
Virtual screening	+	+	+	+	+	+

+ Services are available on request and at charge– contact the CCDC for more information