CSD product datasheet 2022

Academic users

	CSD-Community	CSD-Enterprise
Data		
CSD deposited and curated data	✓[1]	✓
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		✓
Analyse		
Plotting and charting		✓
Descriptive statistics		✓
Interactive visualisation		✓
Filtering and categorisation		✓
Reporting		✓
Integrations		
CSD Pipeline Pilot Component Collection		✓
CSD KNIME Component Collection		✓

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Academic users

advancing structural science

	CSD-Community	CSD-Enterprise
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		✓
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		✓

[1] Essential curated information for each entry is freely available through Access Structures on the CCDC website. More enhanced curated information is available through CSD-Core, CSD-Discovery, CSD-Materials and CSD-Enterprise