# CSD product datasheet 2022

CCDC
advancing structural science

| | CSD-Community | CSD-Core | CSD-Discovery | CSD-Materials | 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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| **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 | | | | ✓ | ✓ |
| **CCDC services** | | | | | |
| On-site training | | + | + | + | + |
| Custom script development | | + | + | + | + |
| In-house database building | | + | + | + | + |
| Solid form risk assessment | + | + | + | + | + |
| Co-crystal design | + | + | + | + | + |
| Virtual screening | + | + | + | + | + |

[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

+ Services are available – contact the CCDC for more information