What’s new?

**CSD-Discovery – Discover new molecules**

For pharmaceutical and agrochemical researchers, CSD-Discovery provides in one place all the tools you need for discovering new molecules.

Last year, we introduced a new application to CCDC’s portfolio: CSD-CrossMiner. During 2018, we’ve improved and enhanced this software to make it more memory efficient when storing large numbers of hits.

This year we’ve focussed on improving programmatic access to CSD-CrossMiner through our CSD Python API. The new release allows users to automate pharmacophore searches in their own workflow using these methods.

We’ve added a simple but much requested feature in the latest version. One common request for CSD-CrossMiner is to be able to filter down results to remove classes of hits. It’s now possible to express ‘non-3D’ filters on substructures in hit results, so users can restrict hits to remove or only include compounds that contain a particular substructure.

2018 also saw delivery of new CSD Python API methodologies for non-sequence-based cavity searching. The CSD Python API now contains 3 different approaches for cavity & pocket searching in proteins which allow a trade-off between very high speed and very high accuracy.

www.ccdc.cam.ac.uk