What’s new?

CSD-System – Harness knowledge-based science

In response to feedback from users and a desire to further develop our systems in the future in new directions, we have now finished rewriting our search engine in C++. The original search engine behind ConQuest was written in the 1970s and was tied to a specific database format (ASER). Since the development of Mercury, we’ve been writing new, reusable chemistry algorithms in C++ which have been slowly replacing the older parts of the CCDC code base and this has now fully replaced the old code.

The development of CSD searching since ’970

1970: 1st reference book to search
1978: 1st electronic structure search
1991: 1st graphical search interface
2018: Complete C++ search engine

The rewriting of ConQuest’s fundamental search engine means that:

- Many complex 2D substructure searches are now much faster
- Nearly all types of search are significantly faster than the previous version
- Element and formula searches are more effective
- Many text searches now give more accurate results, especially author searches which now properly handle international name conventions

During 2018, targeted improvements have also been made to WebCSD based on user feedback including:

- Ability to expand the 3D visualiser to full screen
- New formula searching option
- Additional templates for structure search