



Cambridge Crystallographic Data Centre Accelerates Drug Development

The Cambridge Crystallographic Data Centre (CCDC) is a nonprofit organization that collates and organizes the Cambridge Structural Database (CSD)—a catalog of over 1.1 million enhanced small molecule structures. The CCDC wants to enable drug discovery scientists to understand hydrogen bonding within protein-ligand complexes to help with drug design. The CCDC worked with AWS and Intel to produce a public-facing database of protein structures with intelligently derived and computationally optimized atomic positions for hydrogen atoms. The CCDC runs its curation workflows on Amazon EC2 and uses Intel® Xeon® Scalable processors to refine its structural database. The Intel-AWS pairing significantly decreased optimization time and made it possible to share the enhanced version of the CSD with the public.

“With the power of Intel and AWS, we’ve essentially eliminated that process, presenting researchers with predictions of protonation states in important protein structures, saving hundreds of thousands of hours of life sciences research time across the globe.”

**Jason Cole, Senior
Research Fellow, CCDC**

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