

PRESS RELEASE

Scientific Symposium and New Software for Crystallographers and Scientists Worldwide to Celebrate 50 Years of the Cambridge Structural Database

Cambridge, U.K and Piscataway, NJ, USA, 01 July 2015. The Cambridge Crystallographic Data Centre (CCDC) celebrates 50 years of the Cambridge Structural Database (CSD) with a Scientific Symposium and the launch of new software in the CSD-System suite. CSD-System provides full web-based access (WebCSD) to the world's most comprehensive collection of crystal structure data, plus 3D searching, new advanced visualisations, intermolecular interaction analysis, geometry analysis, and support for tailored application building through the new CSD Python API.

"The CSD is a remarkable example of community data sharing and collaboration in science that began 50 years ago and is of enormous importance today," commented Colin Groom, Executive Director of the CCDC. "We work with colleagues in industry and academia to address key challenges in chemistry, drug discovery, and materials science. Our software development enables everyone to unlock the immense value of crystal structure information in the CSD."

What's new for CSD-System visualisation?

- Fast and convenient generation of high quality graphics using POV-Ray rendering.
- Easy movie generation.
- One-click output of model files for 3D printing.

What's in the new CSD Python API?

- Access to the complete range of CSD functions, enabling users to embed crystallographic data analysis in tailored scripts.
- Ability to integrate crystal data and CSD functions into 3rd party software.
- Batch mode execution.

The new update for CSD-System will be available to download from the CCDC website from July 6th 2015. The CSD50 Scientific Symposium, "The Cambridge Structural Database at 50: Origins, Influences and Directions," takes place in Downing College, Cambridge, UK from July 1-3rd and features contributions from leading scientists, collaborators and CCDC researchers (www.ccdc.cam.ac.uk/CSD50). Everyone will be able to access recordings of presentations afterwards via the CCDC website and other online channels. The event will explore the central position of crystallography and structural chemistry in research today and will showcase the latest software developments from the CCDC.

About [The Cambridge Crystallographic Data Centre](http://www.ccdc.cam.ac.uk)

The Cambridge Crystallographic Data Centre is dedicated to the advancement of chemistry and crystallography for the public benefit. We support structural chemistry worldwide through collaborative research studies and by developing the Cambridge Structural Database (CSD), the world's only comprehensive, up-to-date, and fully-curated knowledge base of small molecule crystal structures.

The CSD was established 50 years ago as the world's first numerical database and now comprises over 775,000 entries. The CCDC enhances its value to research scientists by providing state-of-the-art structural analysis software and expert research services for receptor modelling, ligand design, docking, lead optimization, formulation studies and materials research. The CSD and associated software services are delivered to around 1,400 research sites worldwide, including academic institutions in 80 countries and all of the world's top pharmaceutical and chemical companies.

Originating in the Department of Chemistry at the University of Cambridge, the CCDC is now a UK Research Council Independent Research Organisation and a University of Cambridge Partner Institute, constituted as a registered charity. With 50 years of scientific expertise, the CCDC has demonstrated its strong track record in basic research through more than 750 peer-reviewed publications.

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