



50 years of the
Cambridge Structural Database:
Origins, Influences & Directions

1 July – 3 July 2015
Downing College, University of Cambridge,
Regent Street, Cambridge, UK



I'd like to personally welcome each of you to this conference, marking the 50th anniversary of the Cambridge Structural Database.

The CSD should, of course, be seen as a community achievement. A shining example of data sharing and collaboration in science. But we should also recognise that it wouldn't exist without the vision, commitment and talent of many people associated with the Cambridge Crystallographic Data Centre. This includes our founders, our staff past and present, our Governors and Trustees, and those who run our National Affiliated Centres. This conference is our way of thanking you.

We will be celebrating and we shouldn't shy away from some self-congratulation, but we won't just be looking back at past success. We'll also be learning from things we might have done better. Most importantly, we'll be looking to the future. A future full of challenge and opportunity.

It's a great privilege to be associated with the CSD at this time. The superb line-up of speakers and range of backgrounds of the attendees only serve to demonstrate the regard in which the CSD is held and the far reaching impact it has.

I'd like to thank each of you for attending this conference, bringing your own expertise and individual perspective on this remarkable scientific resource. I can think of no better way of starting our next half century.

So, a very warm welcome to all of you, I look forward to a tremendous meeting.

Colin Groom
Executive Director



Program

JULY 1 – Origins & Development of the Cambridge Structural Database

12:00-13:30: Lunch & registration

13:30-14:00: Opening lecture by **Olga Kennard**

14:00-15:30: *50 Years of Sharing Structures (Chair: Colin Groom)*

Ian Bruno (CCDC) – “Sharing research data and knowledge – a fifty year perspective”

Helen Berman (PDB) – “The evolution of the Protein Data Bank”

Suzanna Ward (CCDC) – “A journey through the Cambridge Structural Database”

15:30-16:00: Tea break

16:00-17:30: *50 Years of Science & Software (Chair: Ian Bruno)*

Robin Taylor (CCDC) – “CSD research at the CCDC: A voyage through the years”

Angelo Gavezzotti (University of Milan) – “Twenty-five years of Cambridge Structural Database mining: Chemical bonds and chemical bonding”

Jason Cole (CCDC) – “The development of the CSD System: The challenges faced and the milestones achieved”

JULY 2 – Applications & Influences of the Cambridge Structural Database

- 09:00-10:30 *Molecular Recognition (Chair: Jason Cole)*
Martin Stahl (Roche) – “Mining the treasure trove: Interaction and conformation searching in structural databases”
Chris Hunter (University of Cambridge) – “Quantification of non-covalent interactions”
Gerhard Klebe (University of Marburg) – “From structure correlation in the CSD to the prediction of molecular recognition in protein-ligand complexes”
-
- 10:30-11:00 Coffee break
-
- 11:00-12:30 *Molecular Design (Chair: Beth Thomas)*
Klaus Müller (Roche) – “The CSD and Roche’s early entry into structure-based drug discovery”
Terry Stouch (Science for Solutions) – “The CSD: A fundamental resource for molecular modeling”
Alberto Gobbi (Genentech) – “We need Champagne, other drinks are not enough!”
-
- 12:30-14:00 Lunch & posters
-
- 14:00-15:30 *Solid Form Informatics (Chair: Shyam Vyas)*
Susan Reutzel-Edens (Eli Lilly and Company) – “Lessons learned in structure-based solid form design”
Joel Bernstein (Ben-Gurion University of the Negev & NYU Abu Dhabi) – “The CCDC and me”
Aurora Cruz-Cabeza (Roche) – “From desmotropy to conformational polymorphs”
-
- 15:30-16:00 Tea break
-
- 16:00-17:30 *Structural Chemistry (Chair: Pete Wood)*
Paul Raithby (University of Bath) – “The use of the CSD in understanding and designing solid-state organometallic reactions”
Greg Ferrence (Illinois State University) – “Permeating the Cambridge Structural Database into chemical education”
Nick Funnell (University of Oxford) – “Disorder and dimensionality”
Zéphirin Yav (University of Kinshasa) – “CSD use at the University of Kinshasa in D. R. Congo”
-

JULY 3 – Structural Knowledge in a Changing World

| | |
|-------------|--|
| 09:00-10:30 | <i>Structural Knowledge in a Changing World (Chair: Neil Feeder)</i> Chick Wilson (University of Bath) – “From structure to crystallisation and manufacturing: A journey from fundamentals to flow” Bob Docherty (Pfizer) – “Towards computational product and process design” |
| 10:30-11:00 | Coffee break |
| 11:00-12:30 | <i>The Next 50 Years (Chair: Suzanna Ward)</i> Christer Aakeröy (Kansas State University) – “What are we going to do with all this information?” Colin Groom (CCDC) – “The CSD at 50: How will structural science look in another 50 years?” |
| 12:30-12:45 | Closing remarks |
| 12:45-14:00 | Lunch & departure |



THE CAMBRIDGE
CRYSTALLOGRAPHIC
DATA CENTRE

www.ccdc.cam.ac.uk