Synchrotron data in the CSD

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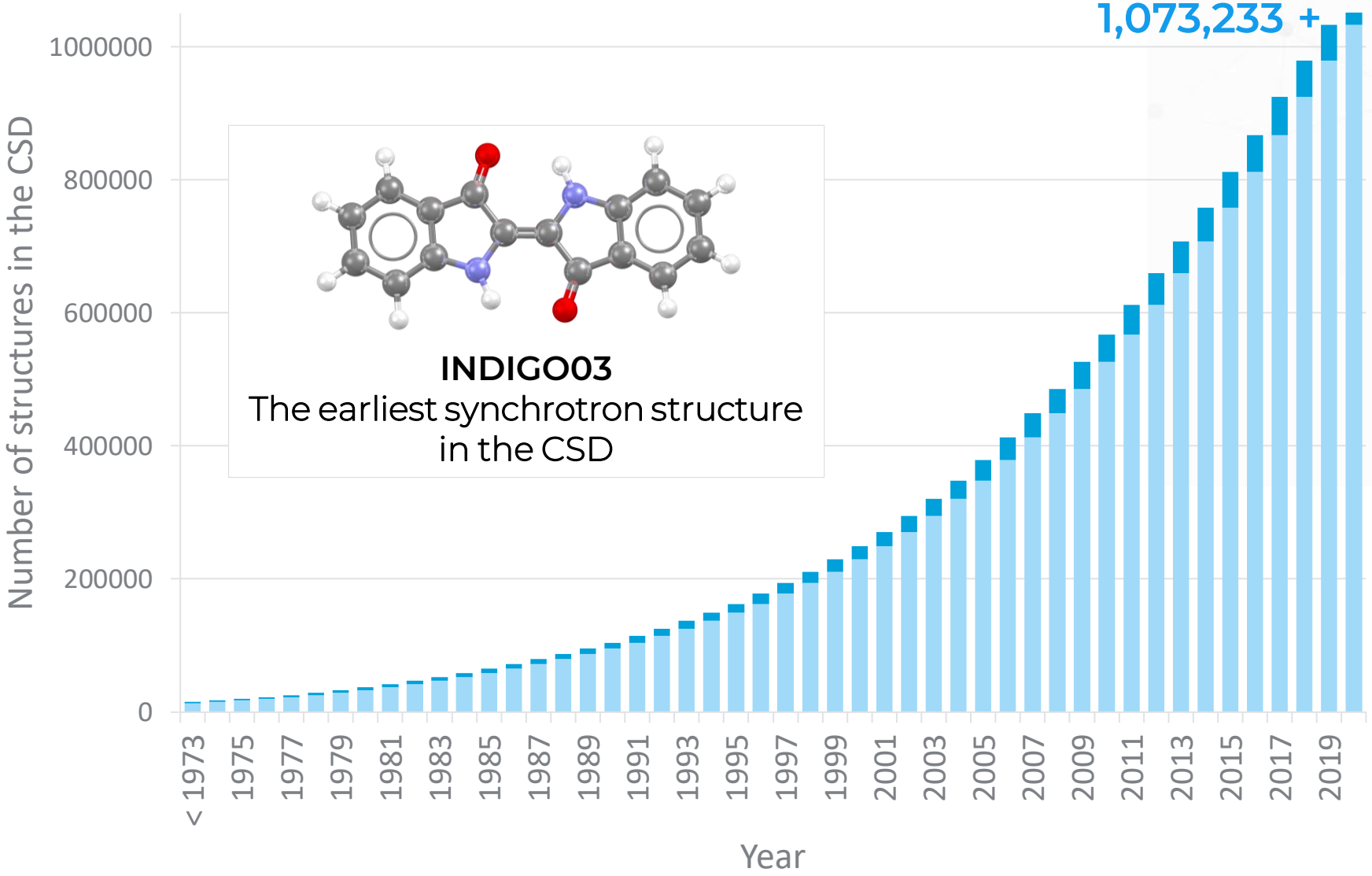
advancing structural science

The Cambridge Structural Database (CSD)



INDIGO03
The earliest synchrotron structure in the CSD

The CSD is a database of small molecule organic and metal-organic crystal structures.

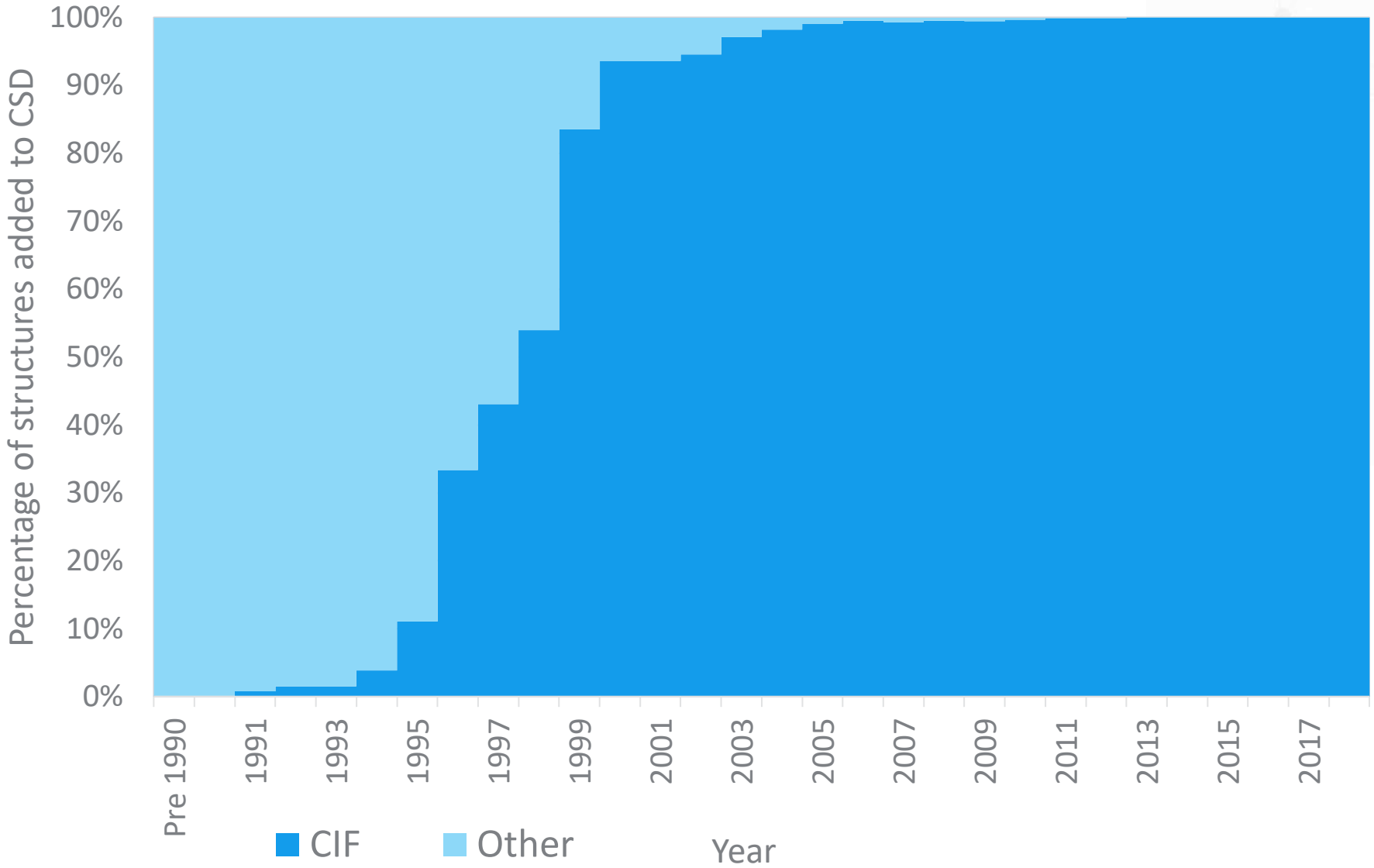
Every entry enriched and annotated by experts.

Every published structure:

- Inc. ASAP & early view
- *CSD Communications*
- Patents
- University repositories

CCDC

The Cambridge Structural Database (CSD)



Data can be deposited to CCDC through an online deposition platform or via email.

Pre-CIF, entries were created by typing data from tables in papers.

When CIF is not available, CCDC manually creates a CIF from the accessible information.

365 structures (< 0.6%) added to the CSD with a manually created CIF in 2019.

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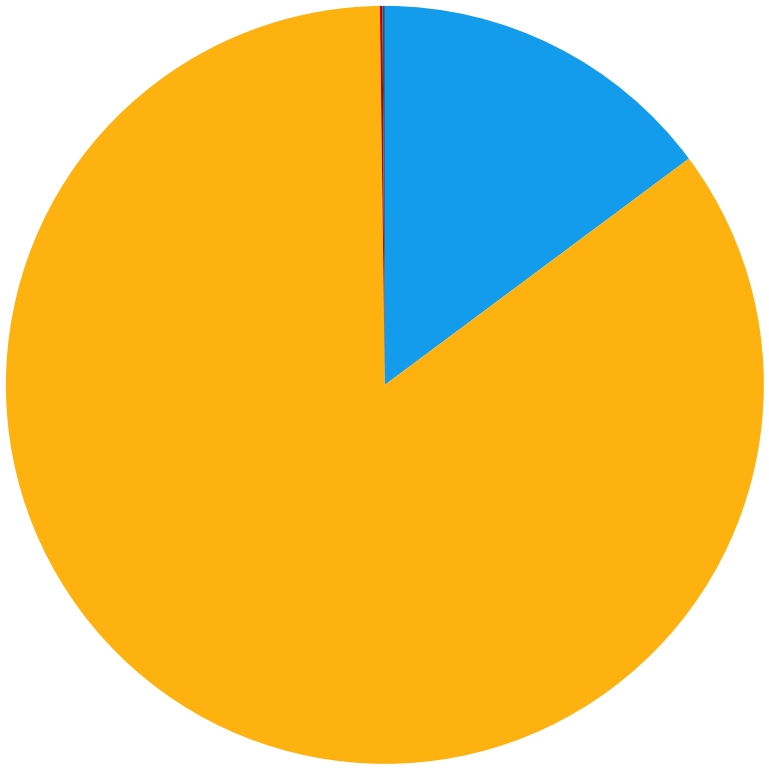
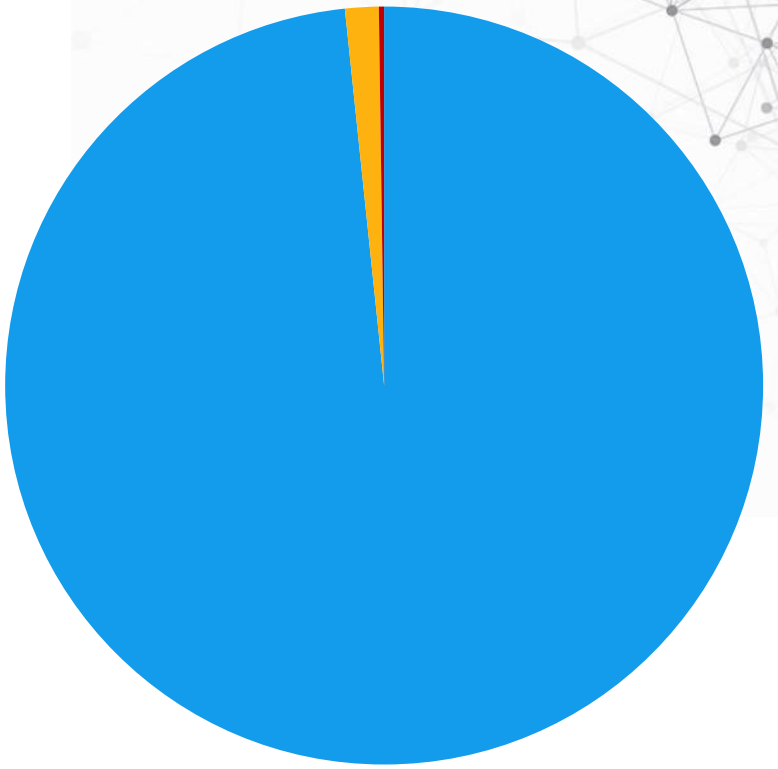
Synchrotron data in the PDB vs CSD

PDB



Lab X-ray Synchrotron Neutron Electron

CSD



Lab X-ray Synchrotron Neutron Electron

1 PDB Statistics from Biosync (http://biosync.sbkb.org/) and PDB website, accessed 25/06/2020
Diffraction data only.

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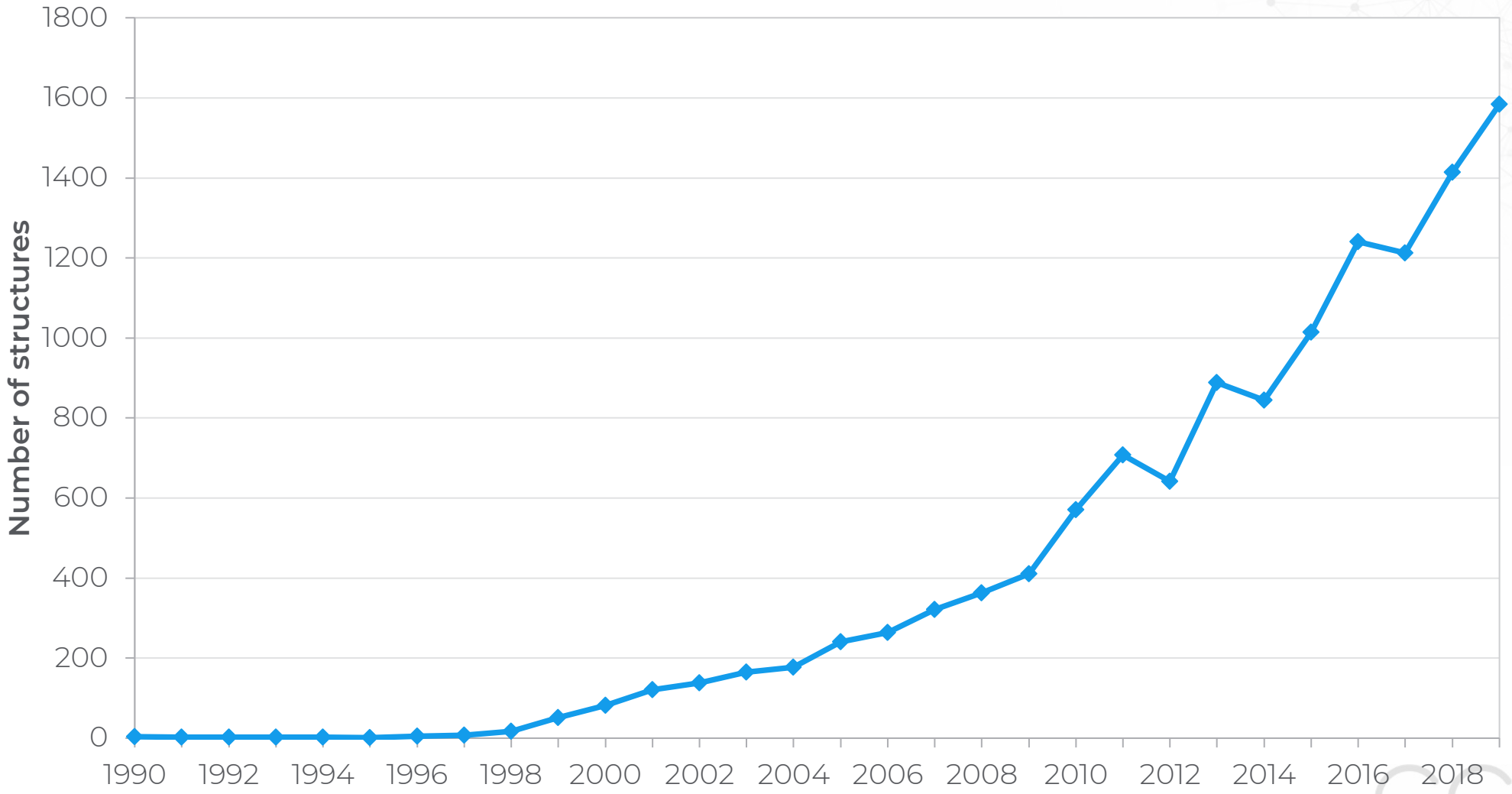
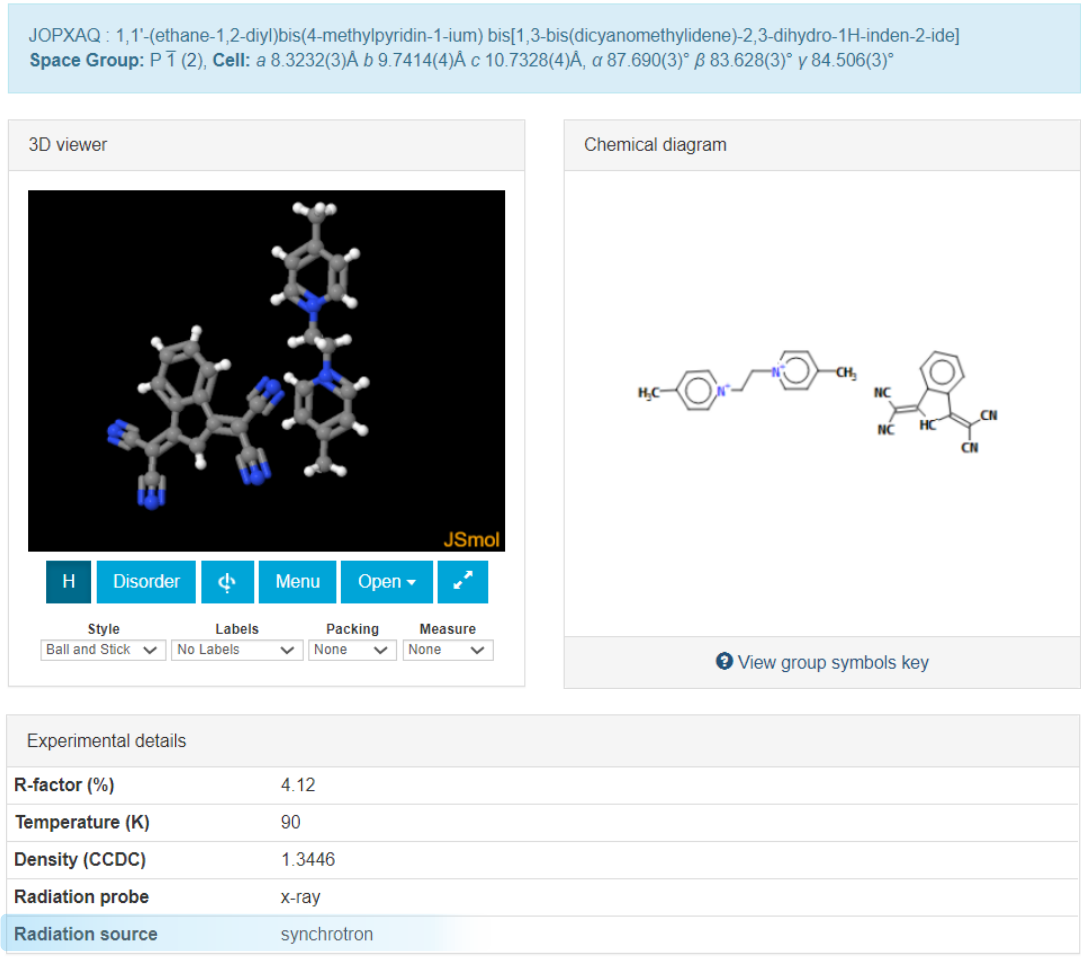
Synchrotron data in the CSD

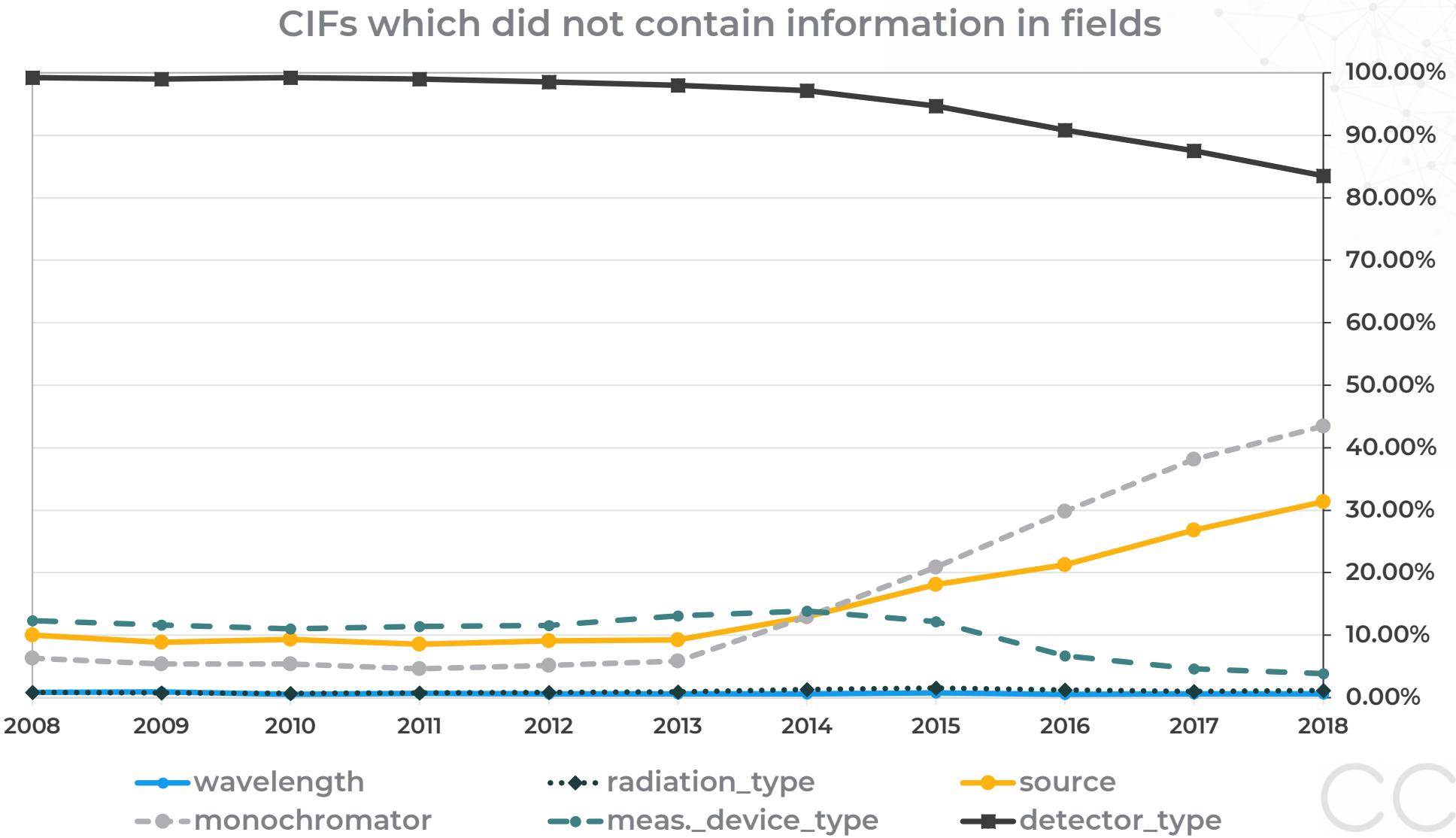


Identification of synchrotron data

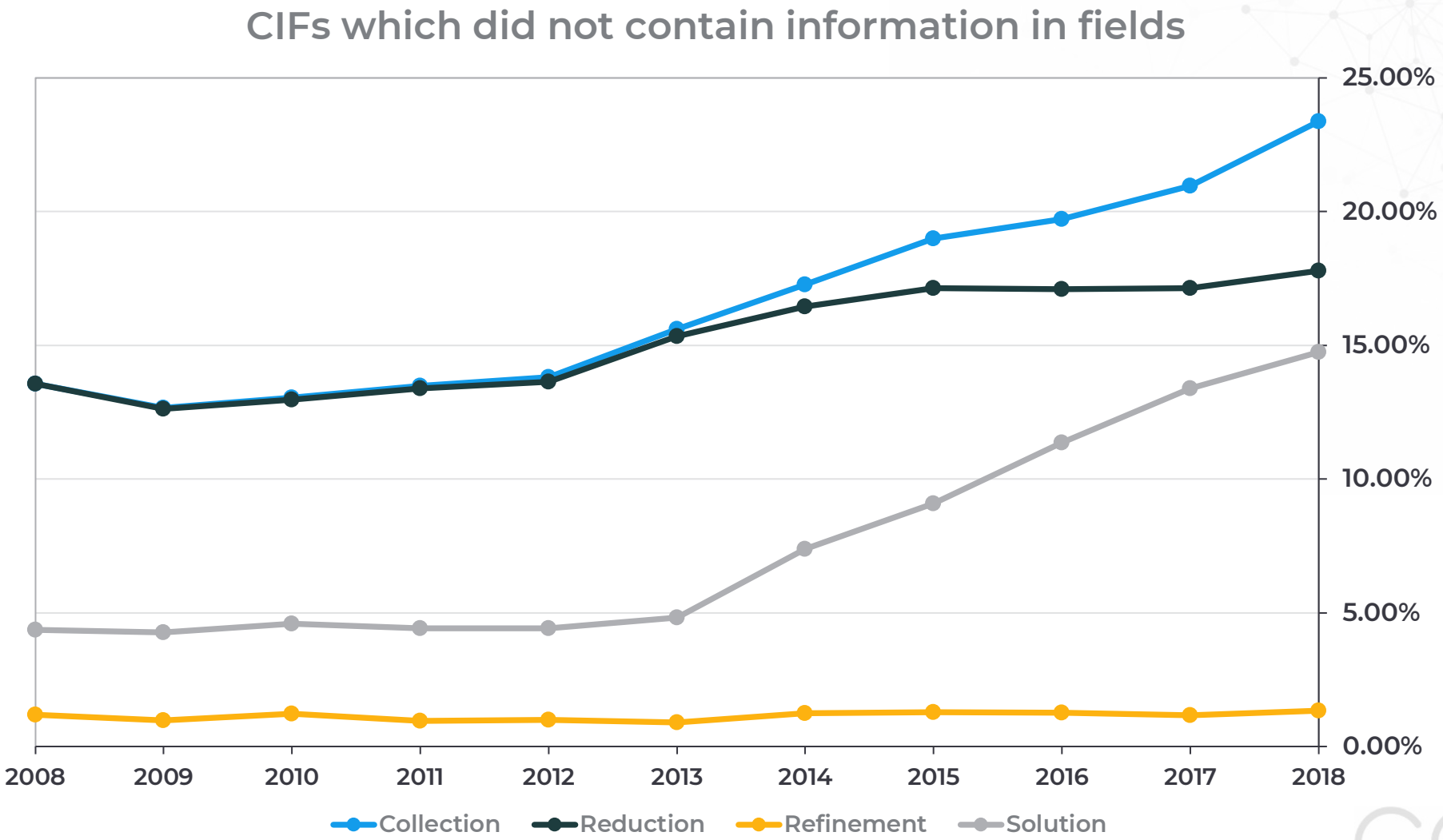
- Structures are flagged with ‘synchrotron’ in the CSD.
- These structures are identified during the data curation process either automatically by the curation software, which checks a select number of CIF fields, or manually labelled by an Editor.



CIF completeness - Experimental



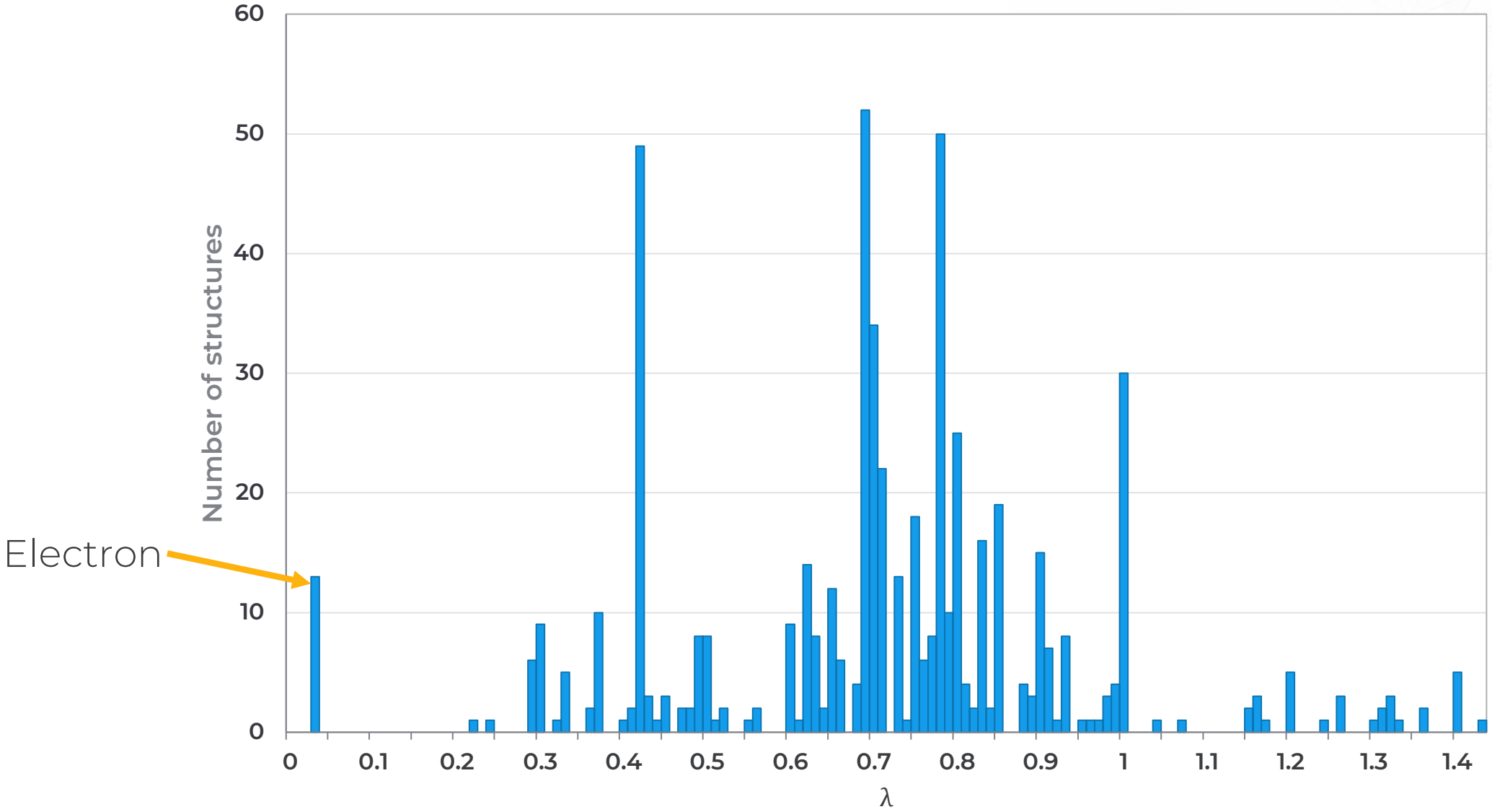
CIF completeness - Computational



CIF completeness – Outcomes

- Some structures were not identifiable from the CIF as it did not contain complete information.
  - 25 structures found by cross-referencing papers associated with the Australian Synchrotron and structures in the CSD.
  - ~ 600 structures report a ‘non-standard’ wavelength, yet contain no synchrotron identifying information.
- Other inconsistencies found in a number of synchrotron CIFs e.g. radiation_type ‘synchrotron’ and _diffrn_source ‘sealed tube’/’rotating anode’

Structures with a non-standard wavelength



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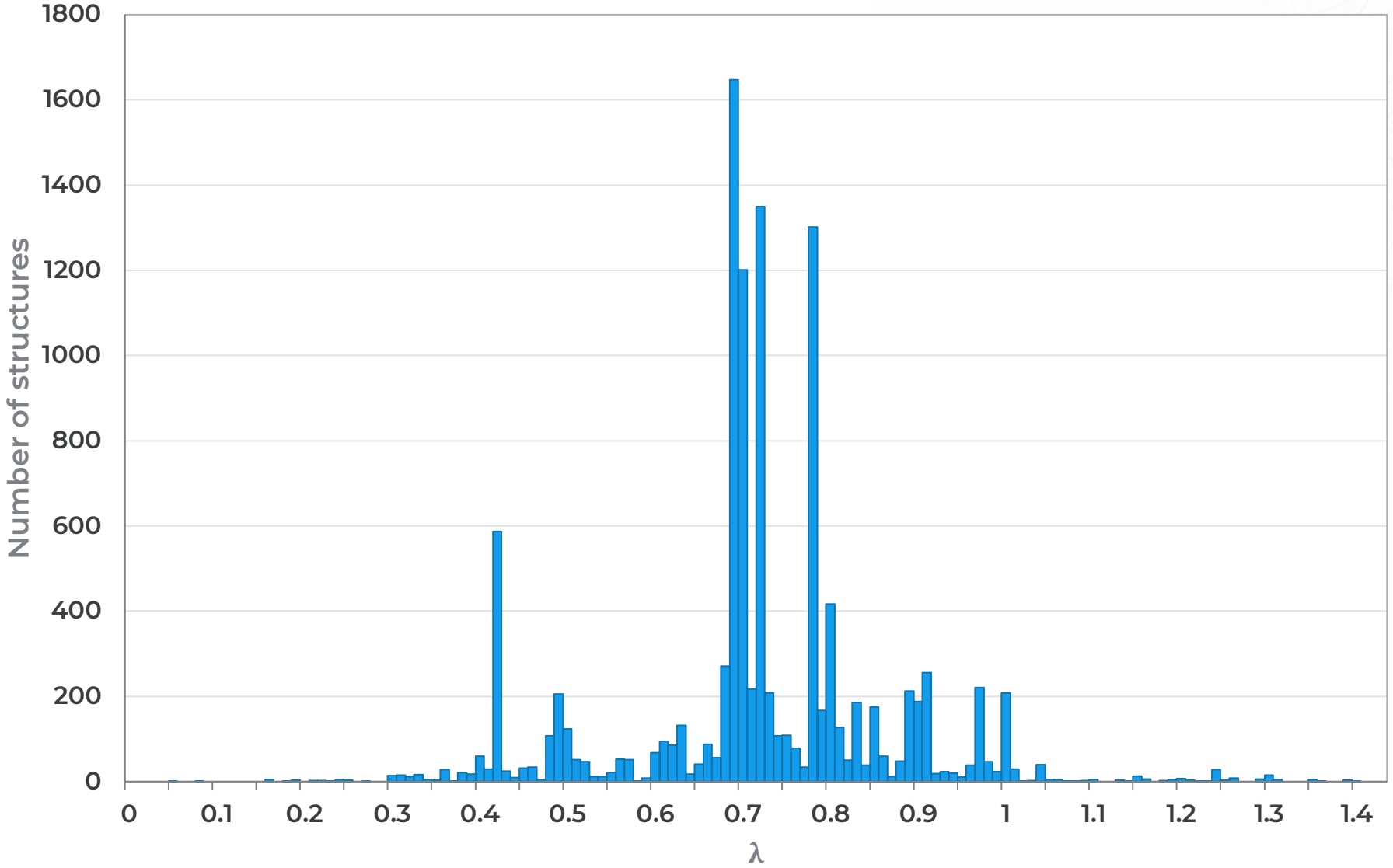
Wavelength of synchrotron structures



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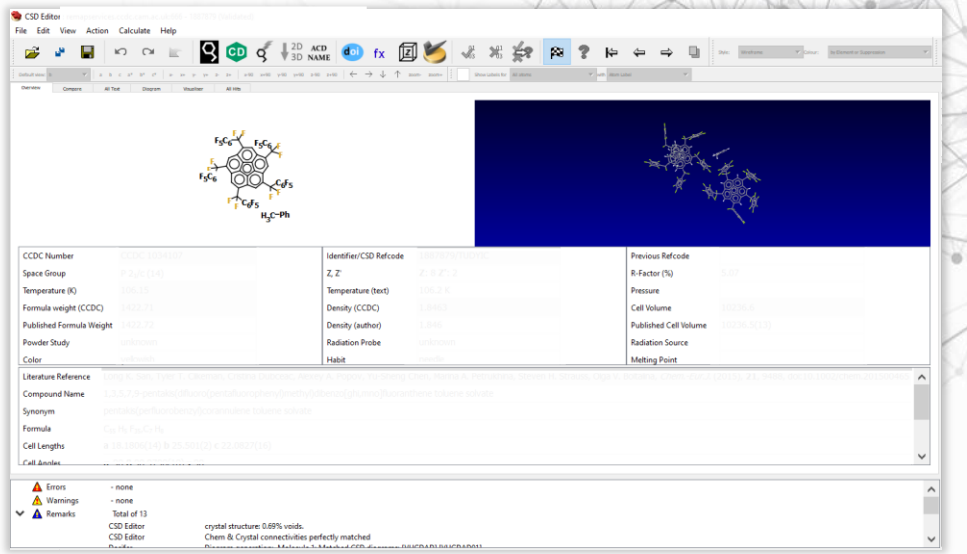
FAIR and FACT small molecule data

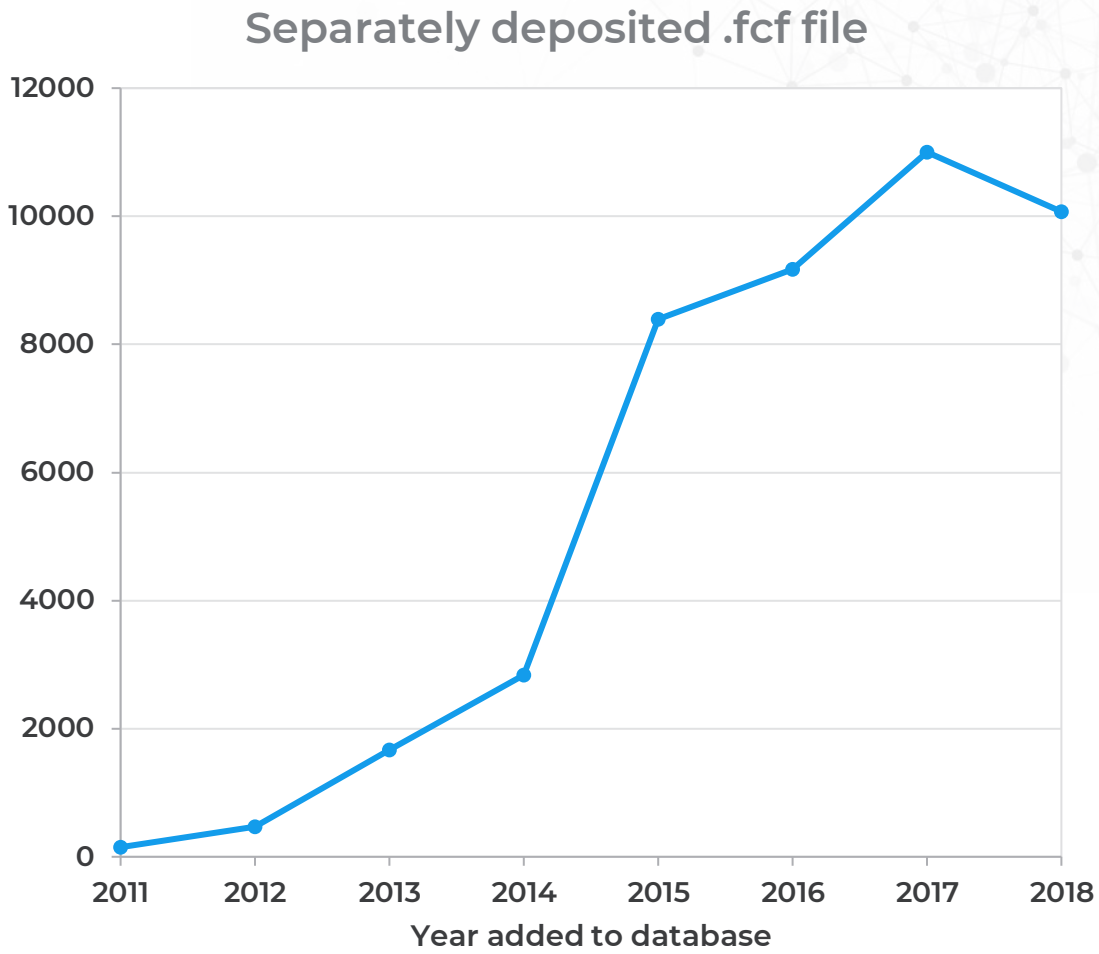
- Curation to ensure structures are labelled and presented consistently so are **findable** within the CSD.
- Option to download additional information associated with entry in WebCSD/Access Structures.



Helliwell, J. (2019). *Structural Dynamics*. 6, 054306., DOI:10.1063/1.5124439

Reflection intensities

- The deposition of structure factors is not explicitly required by CCDC.
- The number of separately deposited structure factor files is tending to increase.
- Many programs automatically include hkl, res and even structure factor information within the CIF.



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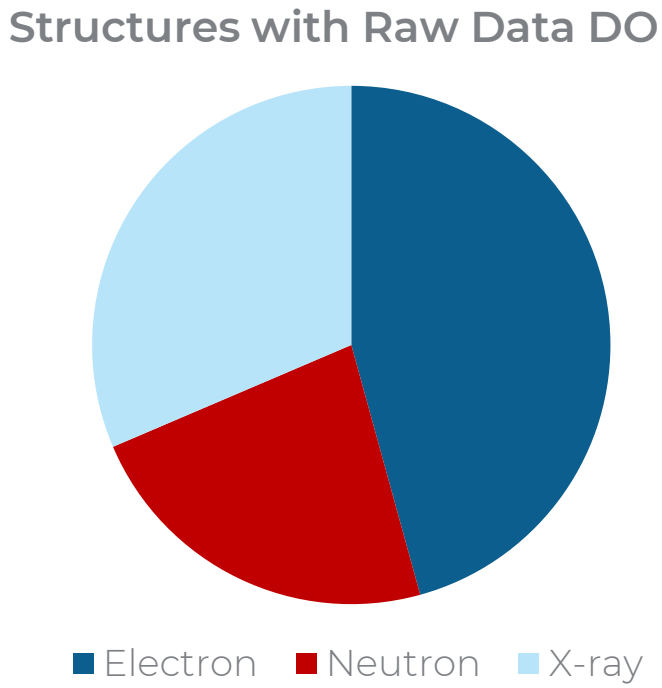
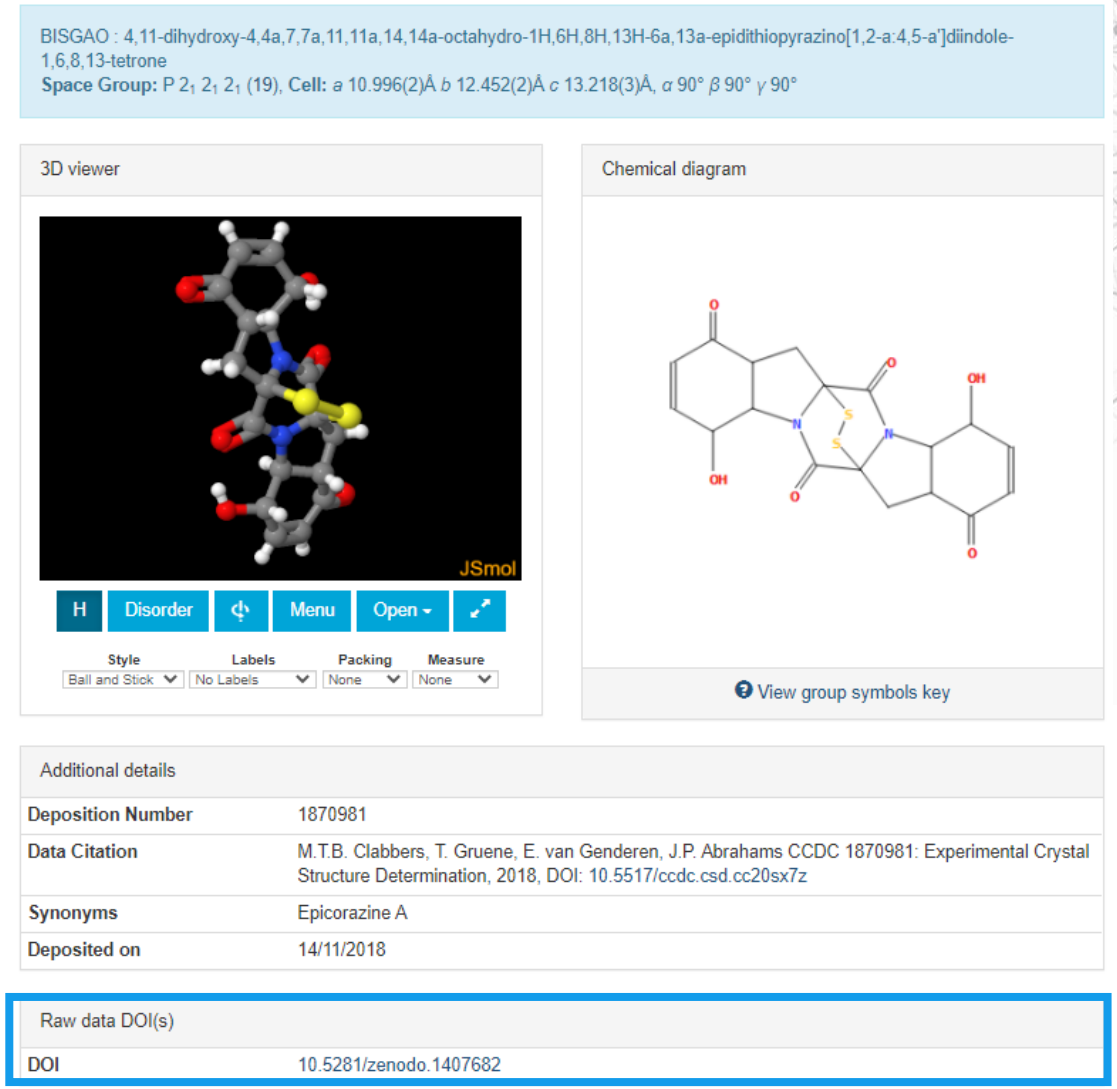
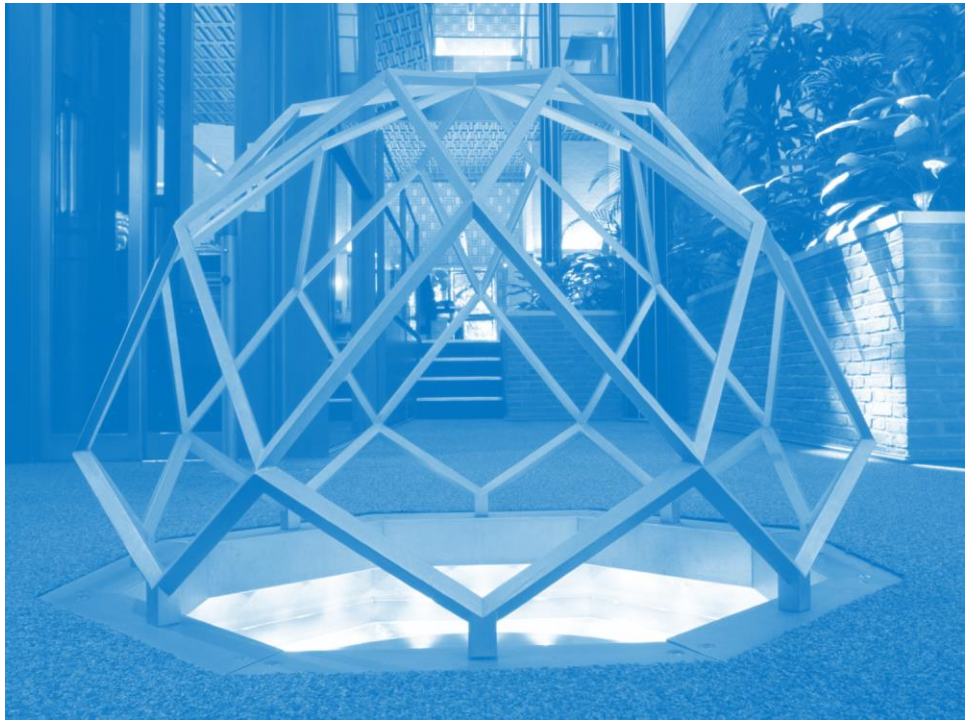
Raw Diffraction Data

- CCDC does not currently store raw diffraction data. However, a DOI for the raw data can be linked to the entry.
- 35 structures in CSD have raw data DOI.





Thank you for listening



Acknowledgements

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