CCDC

advancing structural science

The Cambridge Structural Database

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ECS7 2022

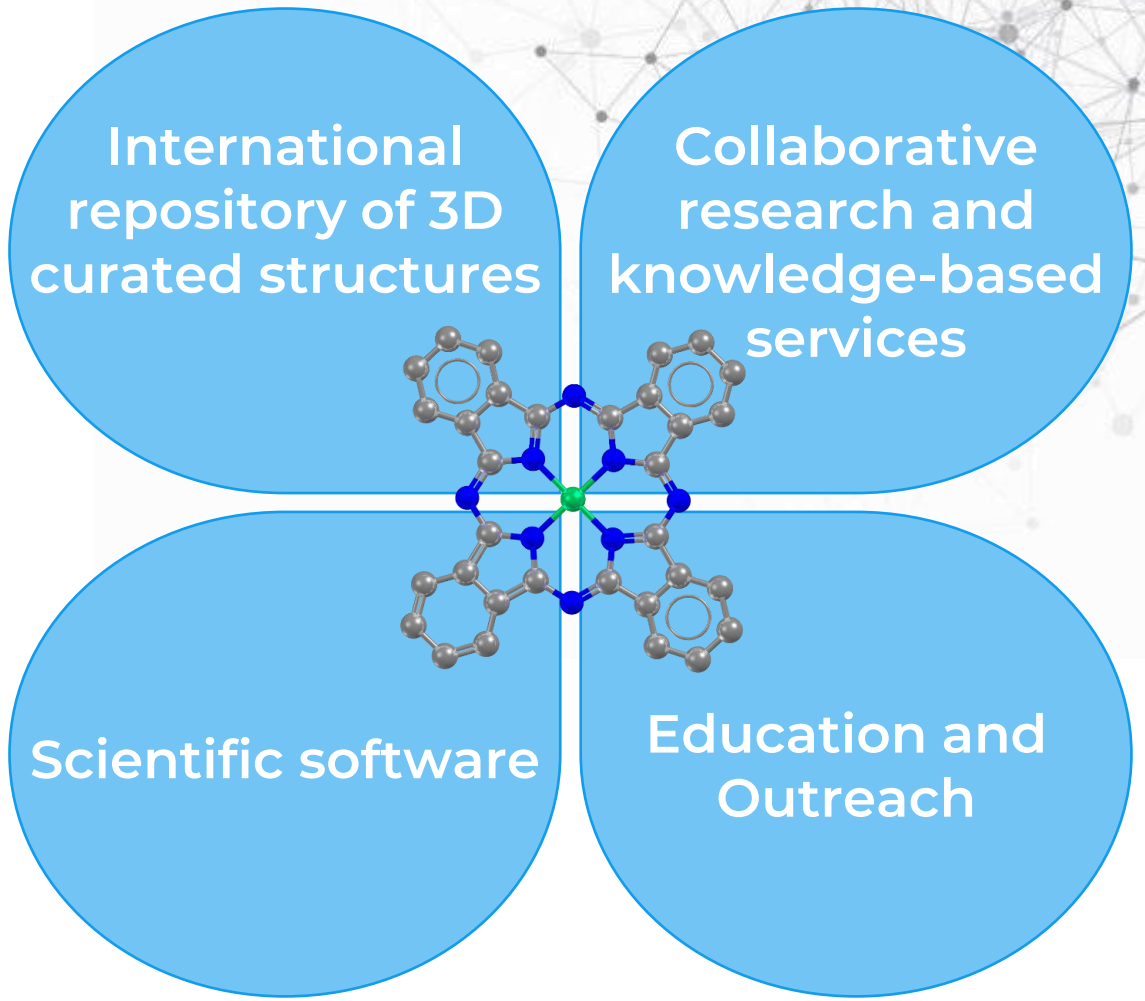
14 July 2022

CCDC

advancing structural science

What we do at the CCDC

Charitable Objective: Advancement of chemistry and crystallography for the public benefit through providing high quality information services and software



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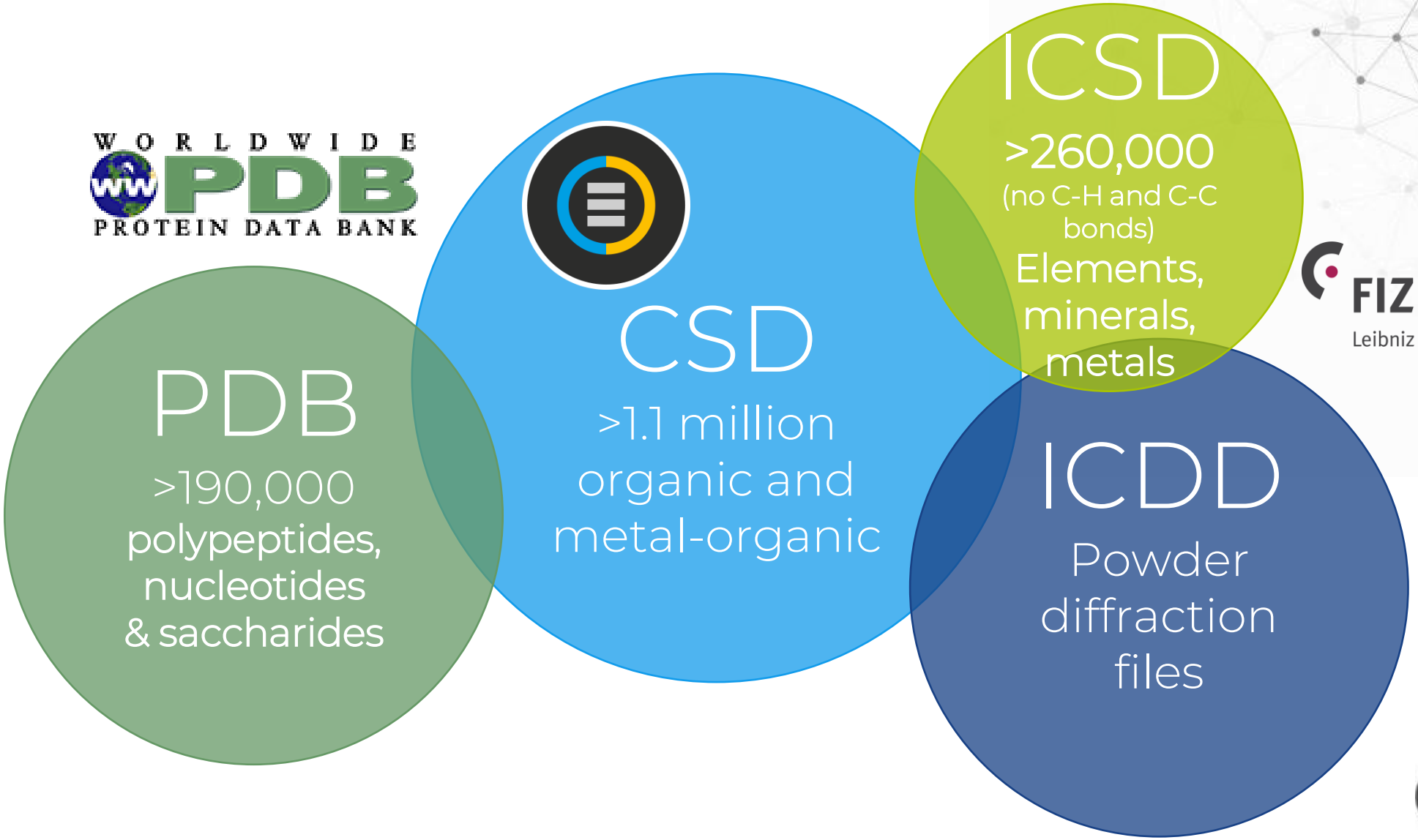
Structural databases



WORLDWIDE PDB PROTEIN DATA BANK

FIZ Karlsruhe
Leibniz Institute for Information Infrastructure

ICDD®

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The vision of the CSD

J.D. Bernal and research group including Olga Kennard at Stonehenge in 1948

- Established in 1965 by Dr Olga Kennard
- She and J.D. Bernal had a vision that a collective use of data would lead to new knowledge and generate insights

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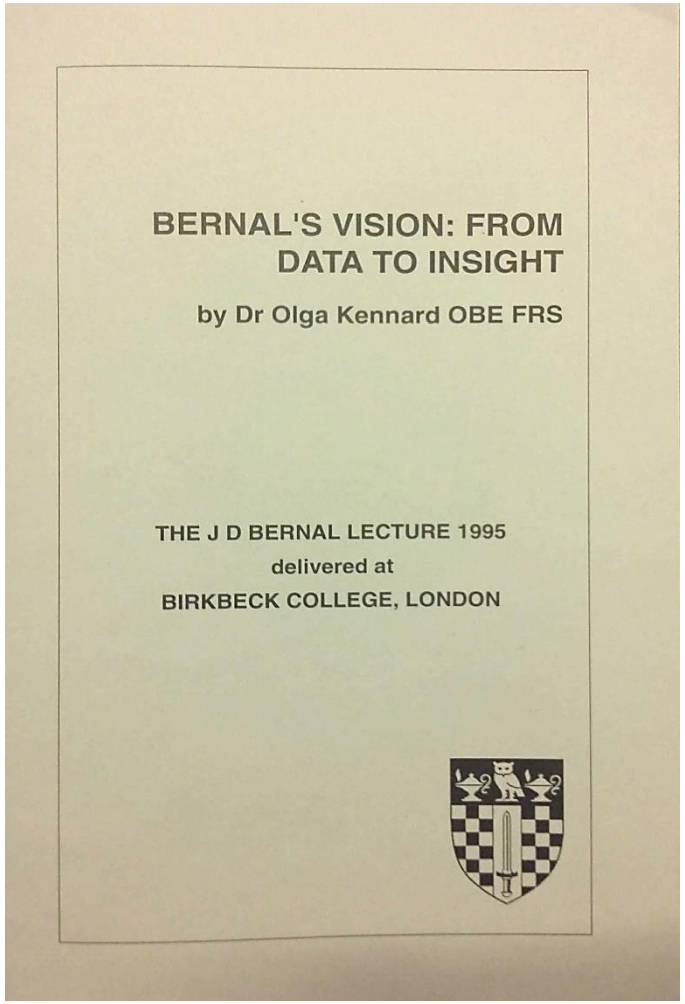
The vision



BERNAL'S VISION: FROM DATA TO INSIGHT

by Dr Olga Kennard OBE FRS

THE J D BERNAL LECTURE 1995
delivered at
BIRKBECK COLLEGE, LONDON

We clearly recognised even in those early days, that data banks have three principal functions. Firstly they must gather together existing knowledge and make it readily available to the scientific community. Secondly they can be used to reduce a large number of observations to a small set of constants and rules, and in this way transform a data base to a knowledge base. Such a knowledge base may obviate the need for further individual experiments in specific areas. Thirdly, they facilitate the comparison and collective analysis of individual results to gain insight into new or as yet unexplained phenomena. These ideas have been at the heart of the work of the Cambridge Crystallographic Data Centre and the driving force for improving methods of data collection, storage and dissemination. Most importantly they influenced development of computer programs and methodologies which are needed for the analysis and transformation of the accumulated information. (5)

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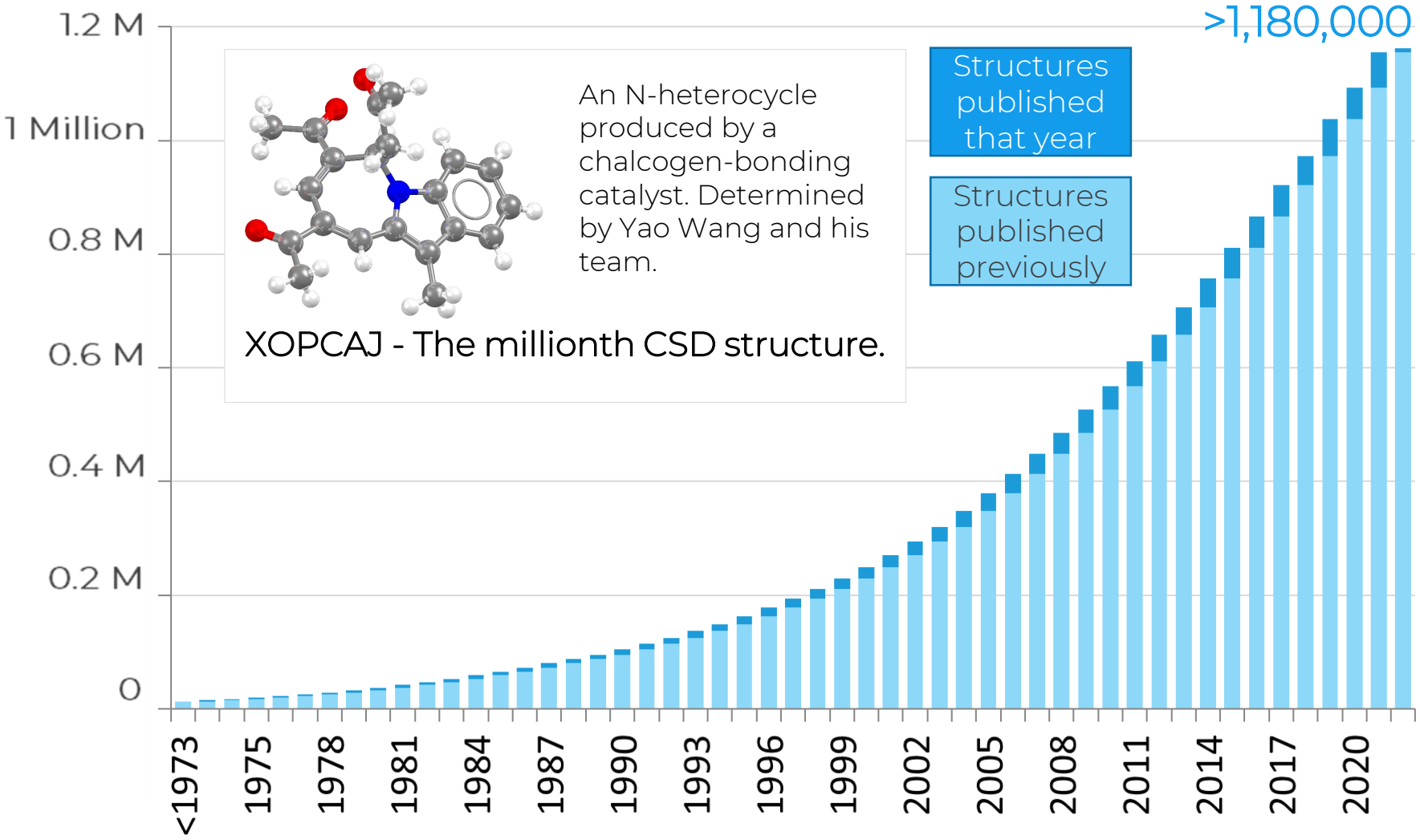
The Cambridge Structural Database (CSD)



- Every published structure
  - Inc. ASAP & early view
  - CSD Communications
  - Patents
  - University repositories
  - Thesis
- Every entry enriched and annotated by experts
- Discoverability of data and knowledge
- Sustainable for over 55 years
- A trusted CoreTrustSeal repository

CORE TRUST SEAL

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Inside the Cambridge Structural Database

The CSD is a database of all the published organic and metal-organic experimental crystal structures

Organic
43%

Metal-Organic
57%

At least one transition metal, lanthanide, actinide or any of Al, Ga, In, Tl, Ge, Sn, Pb, Sb, Bi, Po

Not Polymeric
89%

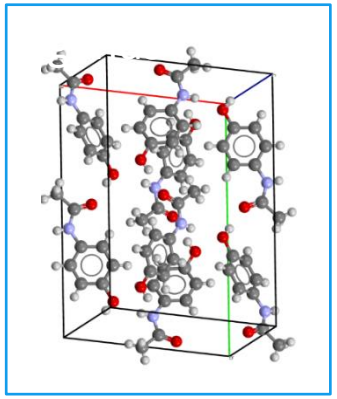
Polymeric: 11%

Single Component
56%

Multi Component
44%

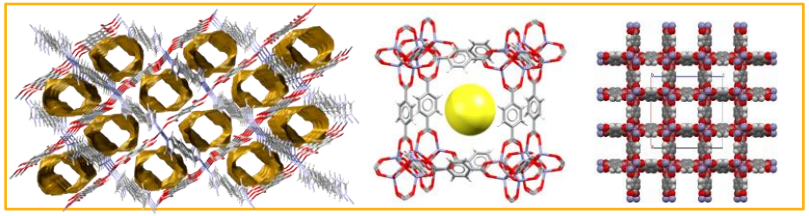
Organic

- Drugs
- Agrochemicals
- Pigments
- Explosives
- Protein ligands



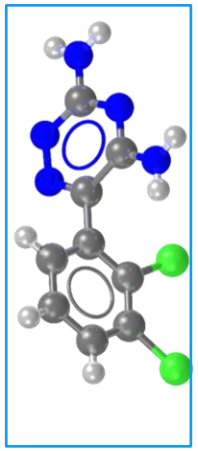
Metal-Organic

- Metal Organic Frameworks
- Models for new catalysts
- Porous frameworks for gas storage
- Fundamental chemical bonding



Additional data

- 11,525 polymorph families
- 171,683 melting points
- 909,992 crystal colours
- 778,663 crystal shapes
- 24,916 bioactivity details
- 11,387 natural source data
- > 250,000 oxidation states

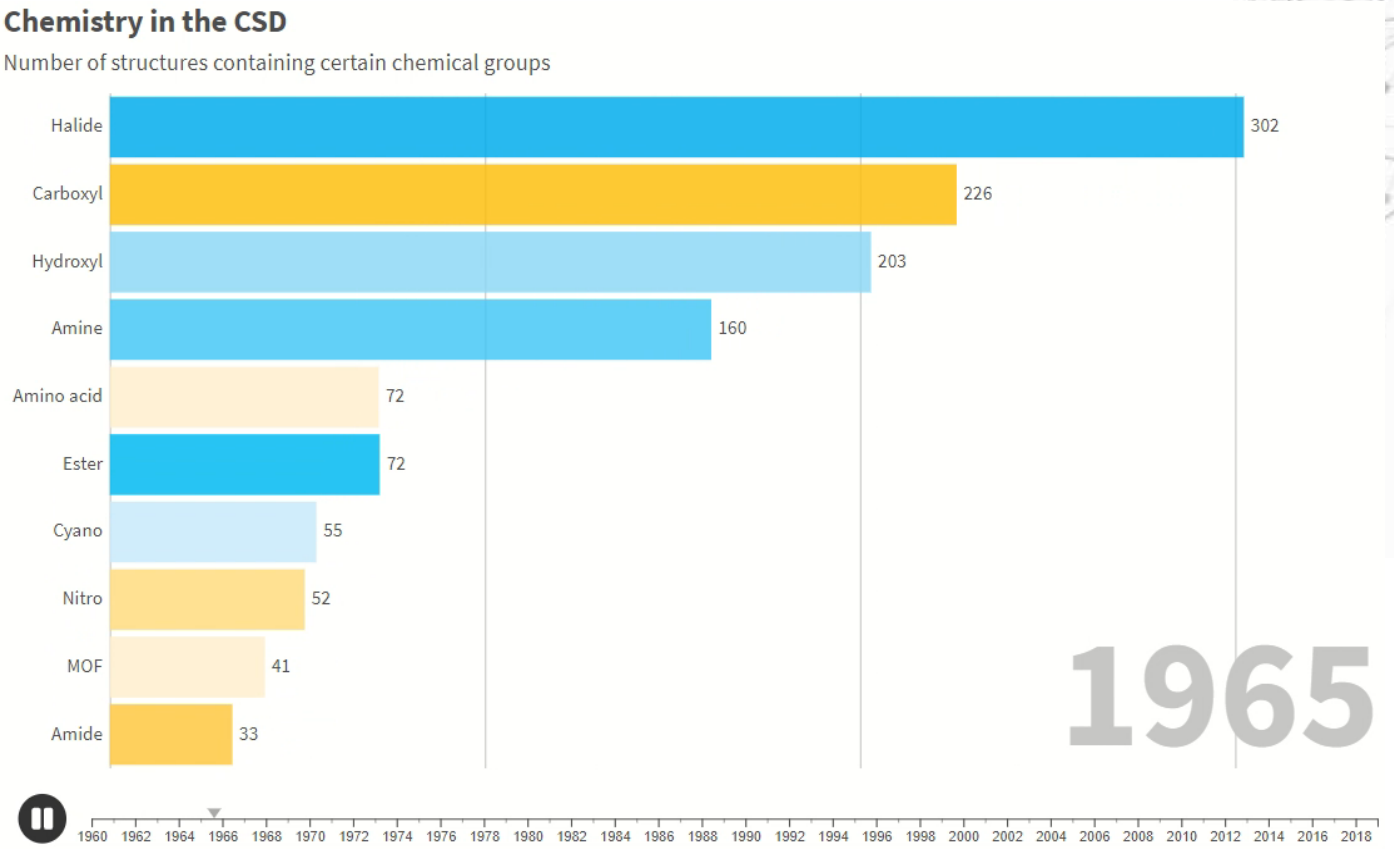


Links and subsets

- DrugBank
- Druglike
- MOFs
- PDB ligands
- PubChem
- ChemSpider
- Pesticide PDB

Exploring the CSD

- > 1 million structures
  - >94M 3D coordinates
- > 28 million bond lengths
  - >2M unique distributions
- > 40 million valence angles
  - >3M unique distributions
- > 14 million torsion angles
  - >800K unique distributions
- > 2 million rings
  - >400K unique distributions



Images and graphics created using the CSD Python API and Flourish

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A trusted and linked repository

InChIs for Chemical Structures

DOIs for Digital Objects

ORCID iDs for Researchers

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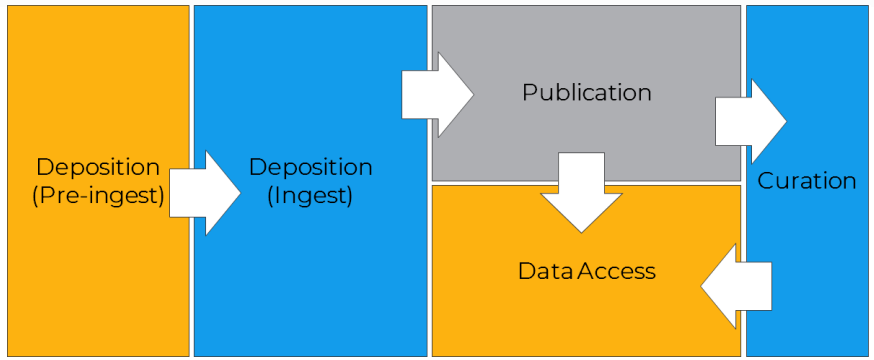
DATA SHOULD BE

Findable
Accessible
Interoperable
Reusable

BY HUMANS AND MACHINES



Wilkinson, M. D. et al. The FAIR Guiding Principles for scientific data management and stewardship. *Sci. Data* 3:160018 DOI: 10.1038/sdata.2016.18 (2016)

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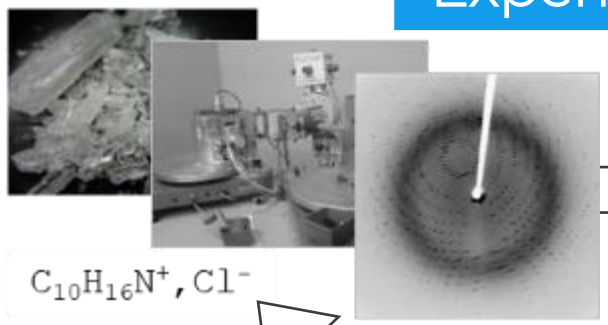
From experiment to knowledge

Experiment



$C_{10}H_{16}N^+,Cl^-$

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_diffrn_measurement_method       '\w and \o'
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_diffrn_refins_number            5892

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_atom_site_type_symbol
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_calc_flag
_atom_site_refinement_flags
_atom_site_occupancy
_atom_site_symmetry_multiplicity
_atom_site_disorder_assembly
_atom_site_disorder_group
Cl Cl1 0.23185(8) 0.78305(9) 0.55574(6) 0.02213(16) Uani d . 1 1 . .
N N1 0.8031(3) 0.6811(3) 0.5363(2) 0.0172(4) Uani d U 1 1 . .
C C1 0.6896(4) 0.7867(6) 0.4357(2) 0.0224(5) Uani d U 1 1 . .
C C2 0.7510(5) 0.8922(5) 0.7083(3) 0.0256(6) Uani d U 1 1 . .
C C3 0.7409(4) 0.6944(4) 0.6644(3) 0.0187(5) Uani d U 1 1 . .
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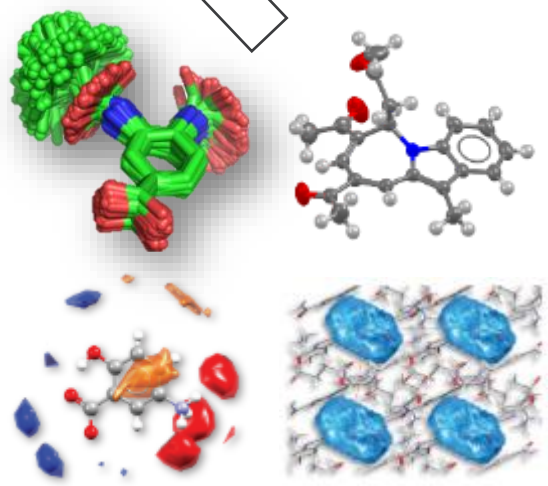
Ritonavir: An Extraordinary Example of Conformational Polymorphism

Abstract

Purpose. In the summer of 1998, Norvir semi-solid capsules supplies were threatened as a result of a new much less soluble crystal form of ritonavir. This report provides characterization of the two polymorphs and the structures and hydrogen bonding network for each form.



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Knowledge

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About you

Have you done any of the following before?

- Searched the CSD using ConQuest
- Searched the CSD using Access Structures or WebCSD
- Visualised or explored crystal structures with Mercury
- Collected and / or refined your own crystal structure
- Deposited a structure with the CCDC

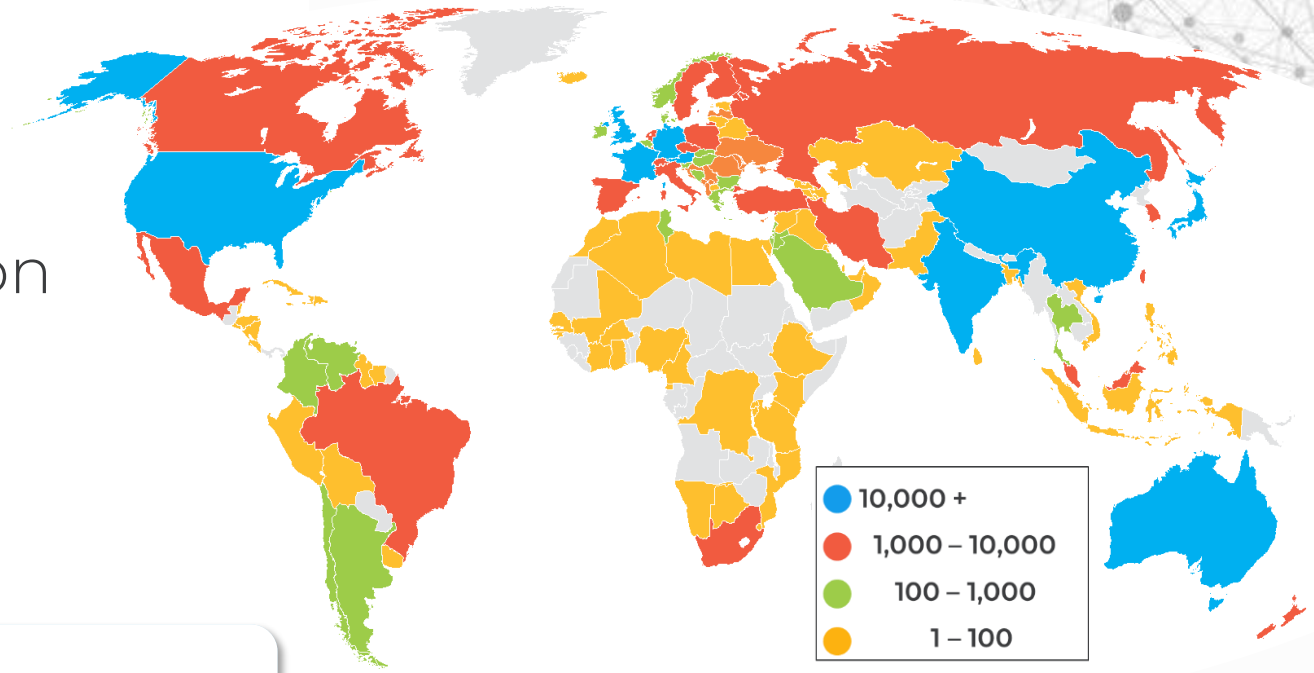
Raise your hand up if you have

CCDC

Deposition

- Data deposited pre-publication
  - Enables links to data sets at the point of publication
  - Tailored deposition service

Countries contributing data



Small molecule single crystal data

Authors should present their crystal data in a CIF (Crystallographic Information File) format and deposit any organic or organometallic structural information with the Cambridge Crystallographic Data Centre (CCDC) before they submit their manuscript to us. Data will be held in the CCDC's confidential archive until publication of the article, when data for organic and organometallic compounds will be entered into the Cambridge Structural Database. Authors are encouraged to deposit inorganic crystal structures with the ICSD, hosted by FIZ Karlsruhe.

During submission of a manuscript to the Royal Society of Chemistry using our online submission system, authors will be asked to provide CCDC reference numbers; CIFs should not be submitted with the manuscript (these should have already been deposited with the CCDC/ICSD, see above). Any revised CIFs obtained subsequently should be deposited directly with the CCDC before the revised manuscript is submitted to us. CCDC or ICSD numbers should be included in the manuscript prior to submission.

ACS Publications
Most Trusted. Most Cited. Most Read.

Search text, DOI, authors, etc.

Submitting X-ray Crystallographic Data

Authors are required to submit Crystallographic Information Files (CIFs), structure factor tables, and CheckCIF reports for all new, unpublished organic, metal-organic, and inorganic structures to the Cambridge Crystallographic Data Centre (CCDC) **prior to manuscript submission**. Note that CIFs may be used for reviewing purposes, and significant delays in the peer review process can occur if CIFs are not submitted in advance.

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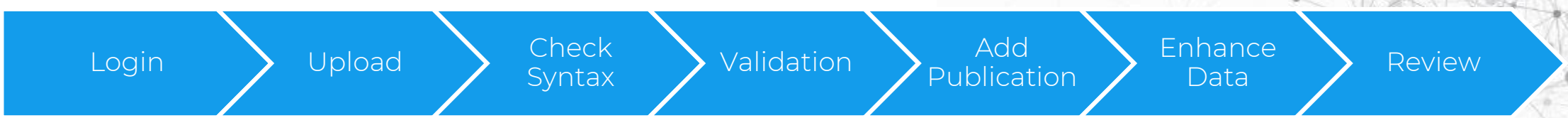
Deposition workflow

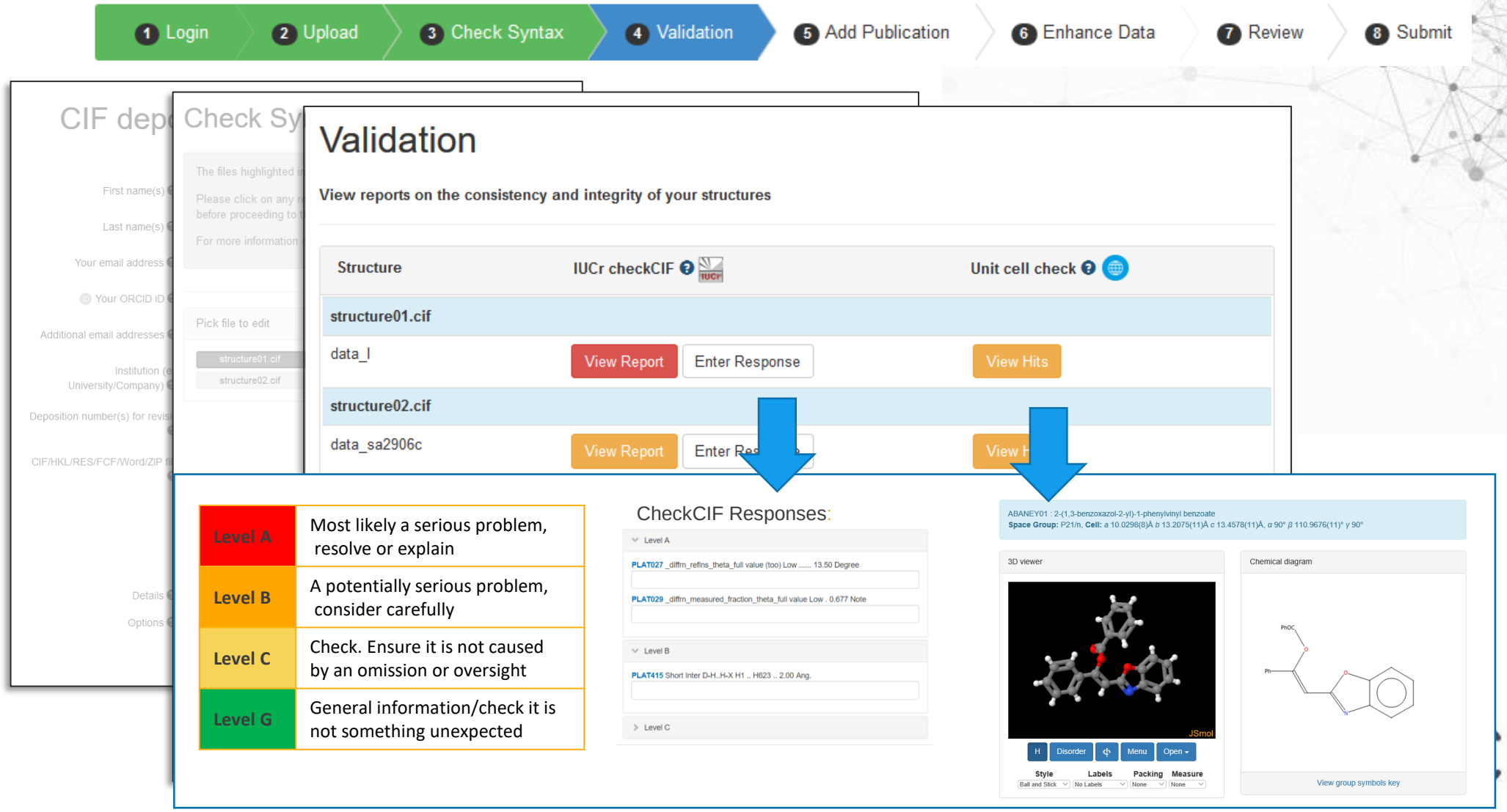


- Our deposition service aims to make it easy for you to:
  - Follow community recommendations
  - Provide reliable data and metadata
  - Deposit all organic, inorganic and metal-organic data

- Components include:
  - Identification of contributors
  - Use of standard formats & syntax checking
  - Generation of validation report
  - Capture of publication, experimental and chemical metadata
  - Additional enrichment of data by CCDC or FIZ
  - Ability to publish directly in the CSD or ICSD

CCDC

Deposition


1 Login
2 Upload
3 Check Syntax
4 Validation
5 Add Publication
6 Enhance Data
7 Review
8 Submit
Validation
View reports on the consistency and integrity of your structures
Structure
IUCr checkCIF
Unit cell check
structure01.cif
data_l
View Report
Enter Response
View Hits
structure02.cif
data_sa2906c
View Report
Level A
Most likely a serious problem, resolve or explain
Level B
A potentially serious problem, consider carefully
Level C
Check. Ensure it is not caused by an omission or oversight
Level G
General information/check it is not something unexpected
CheckCIF Responses:
Level A
PLAT027 _diffrn_refins_theta_full value (too) Low ..... 13.50 Degree
PLAT029 _diffrn_measured_fraction_theta_full value Low . 0.677 Note
Level B
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Level C
ABANEY01 : 2-(1,3-benzoxazol-2-yl)-1-phenylvinyl benzoate
Space Group: P21/n, Cell: a 10.0298(8)Å b 13.2075(11)Å c 13.4578(11)Å, α 90° β 110.9676(11)° γ 90°
3D viewer
Chemical diagram
JSmol
H
Disorder
Menu
Open
Style
Labels
Packing
Measure
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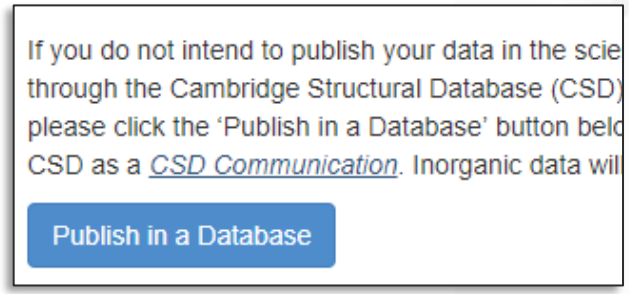
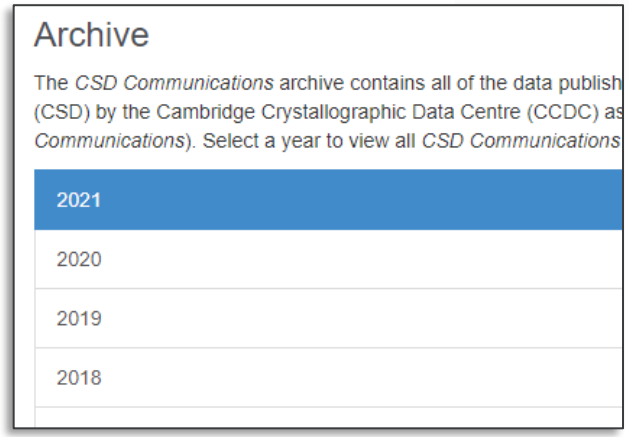
View group symbols key

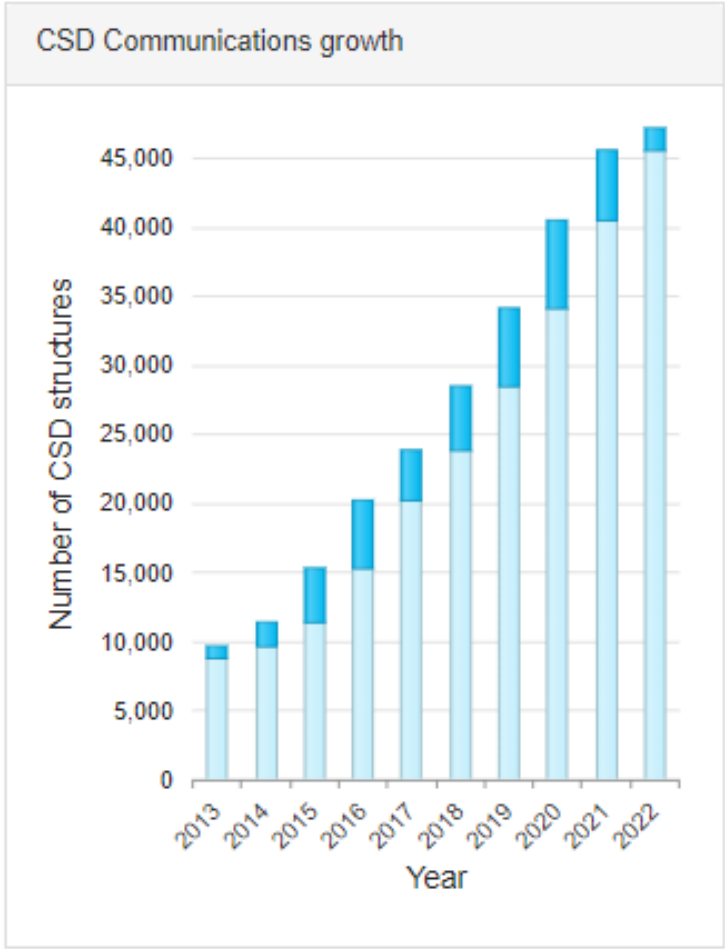
CSD Communications

ISSN 2631-9888

Small molecule crystal structure data published just through the Cambridge Structural Database without a journal article







https://www.ccdc.cam.ac.uk/Community/csd-communications/

Once deposited your data is curated

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_atom_site_type_symbol
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_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
_atom_site_symmetry_multiplicity
_atom_site_calc_flag
_atom_site_refinement_flags
_atom_site_disorder_assembly
_atom_site_disorder_group
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S1 S 0.5321(3) 0.8260(6) 0.9322(3) 0.0327(11) Uani 0.50 1 d PDU A 1
C2 C 0.5529(4) 0.8802(9) 0.8184(9) 0.029(4) Uani 0.50 1 d PDU A 1
C3 C 0.5286(7) 0.8174(18) 0.7440(7) 0.031(4) Uani 0.50 1 d PDU A 1
H3A H 0.5350 0.8343 0.6771 0.037 Uiso 0.50 1 calc PR A 1
C4 C 0.4918(8) 0.7220(19) 0.7783(8) 0.027(4) Uani 0.50 1 d PDU A 1
C5 C 0.4900(6) 0.7171(14) 0.8779(9) 0.029(4) Uani 0.50 1 d PDU A 1
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S2 S 0.38755(19) 0.6658(5) 0.9578(5) 0.0400(10) Uani 0.50 1 d PDU A 1
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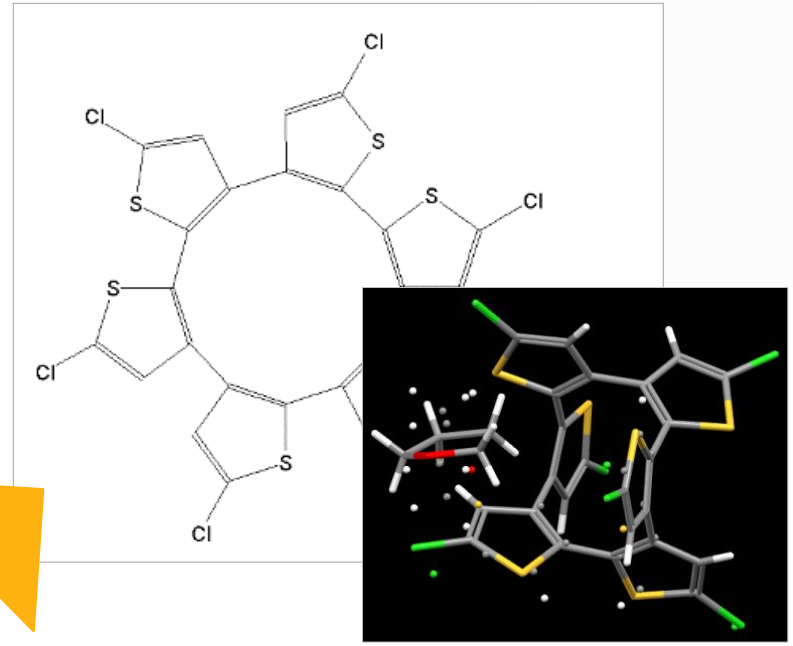
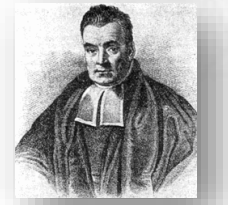
Chemistry assignment makes data findable, interoperable and reusable

An automated probabilistic approach using data in the CSD





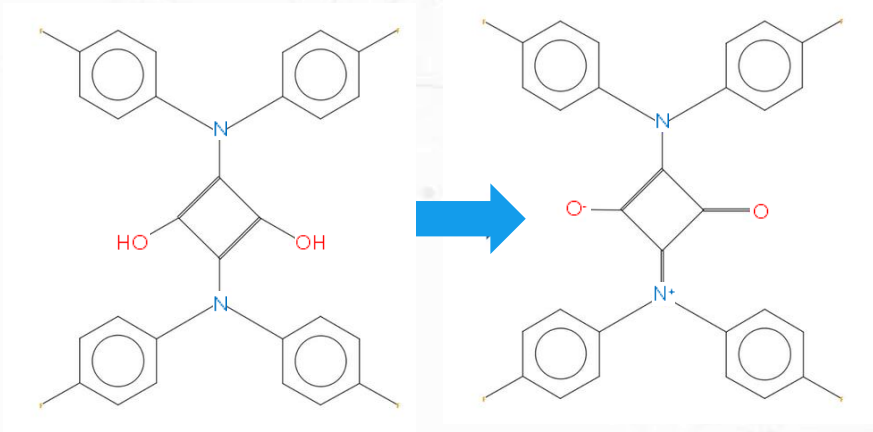
$$P(A|B) = \frac{P(B|A)\,P(A)}{P(B)}.$$

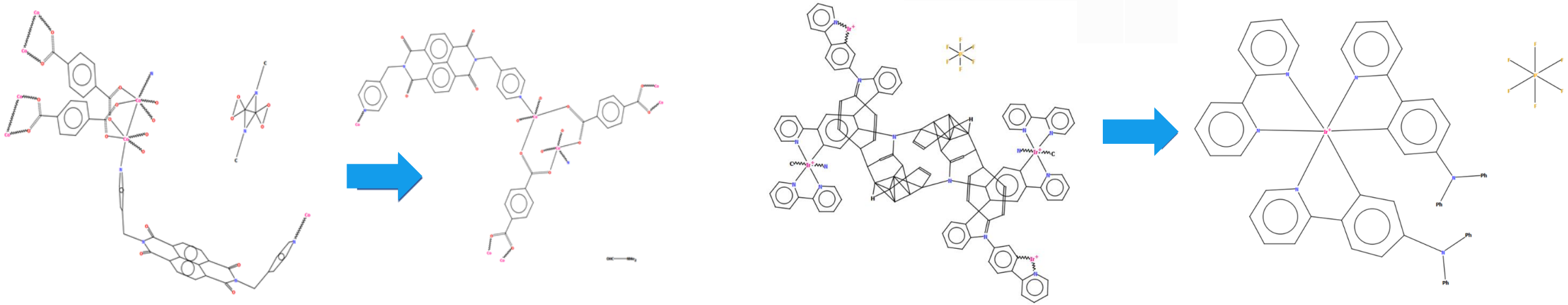
I.J.Bruno, G.P.Shields, R.Taylor, *Acta Cryst.* (2011). B67, 333-349 DOI: 10.1107/S0108768111024608

CCDC

Using experts to ensure quality

- Each entry looked at by expert Scientific Editors
- Automation focuses editorial efforts
- Manual validation of automated chemical interpretations improves automated methods



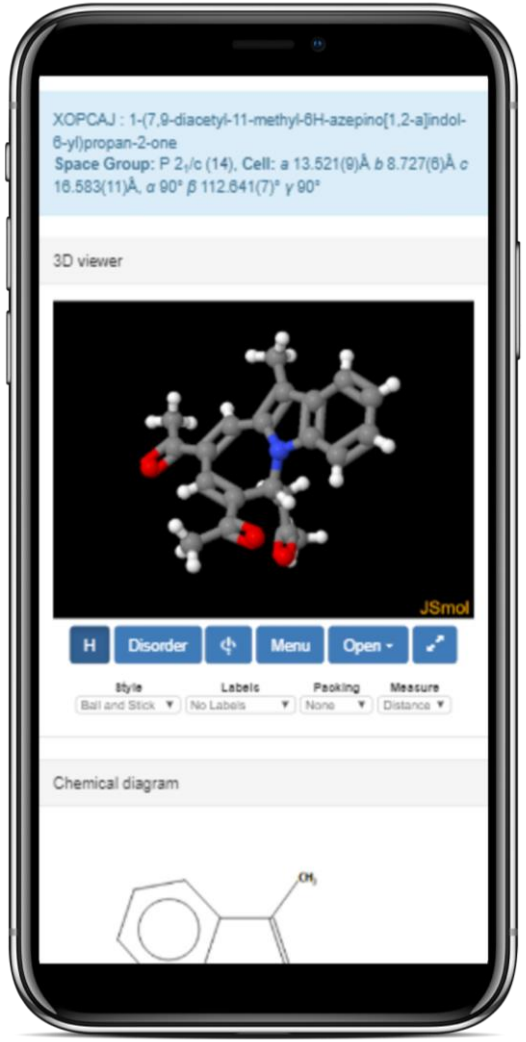


https://www.ccdc.cam.ac.uk/Community/blog/CSD-data-curation-the-human-touch/

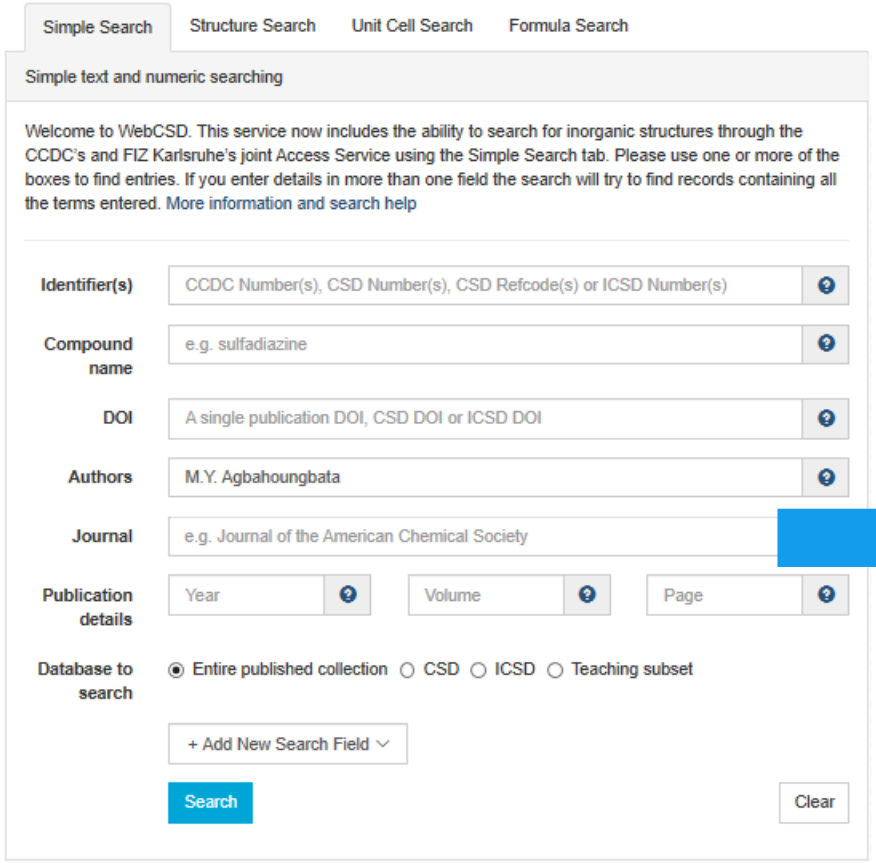
CCDC

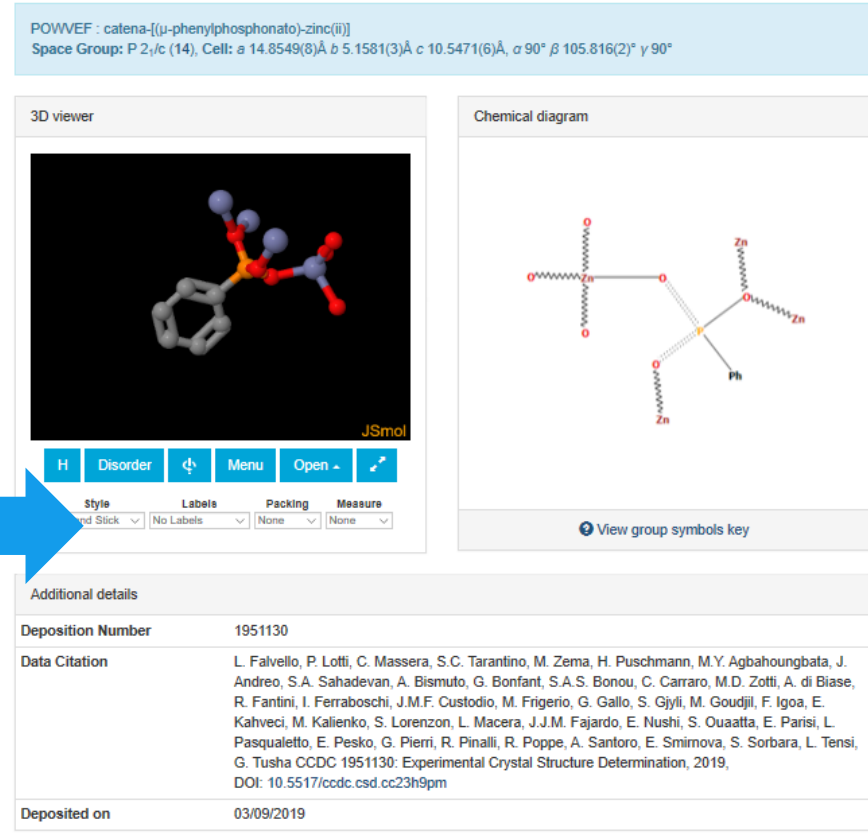
Access Structures

www.ccdc.cam.ac.uk/structures



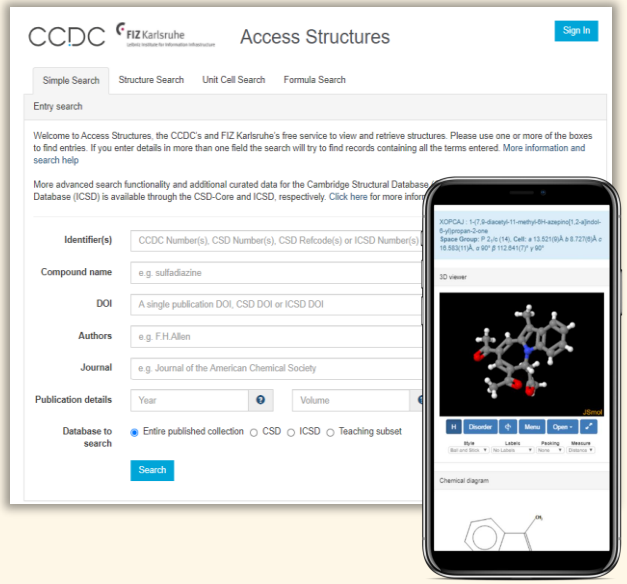
- Access Structures allows you to search CSD and ICSD
- Every individual dataset is free to view and download





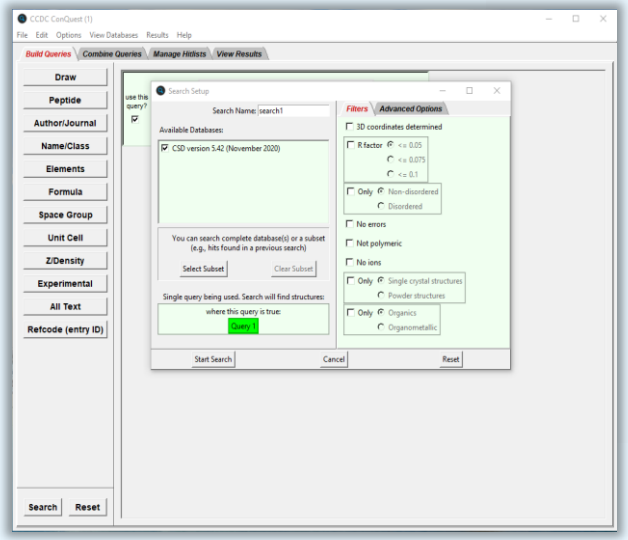
Finding structures

Web Browser



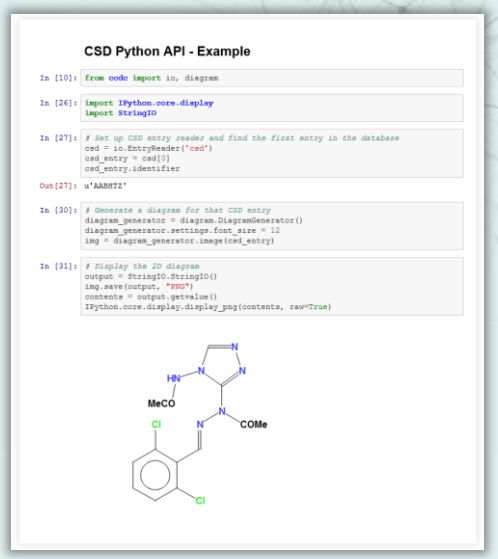
Access Structures / WebCSD

Desktop



ConQuest

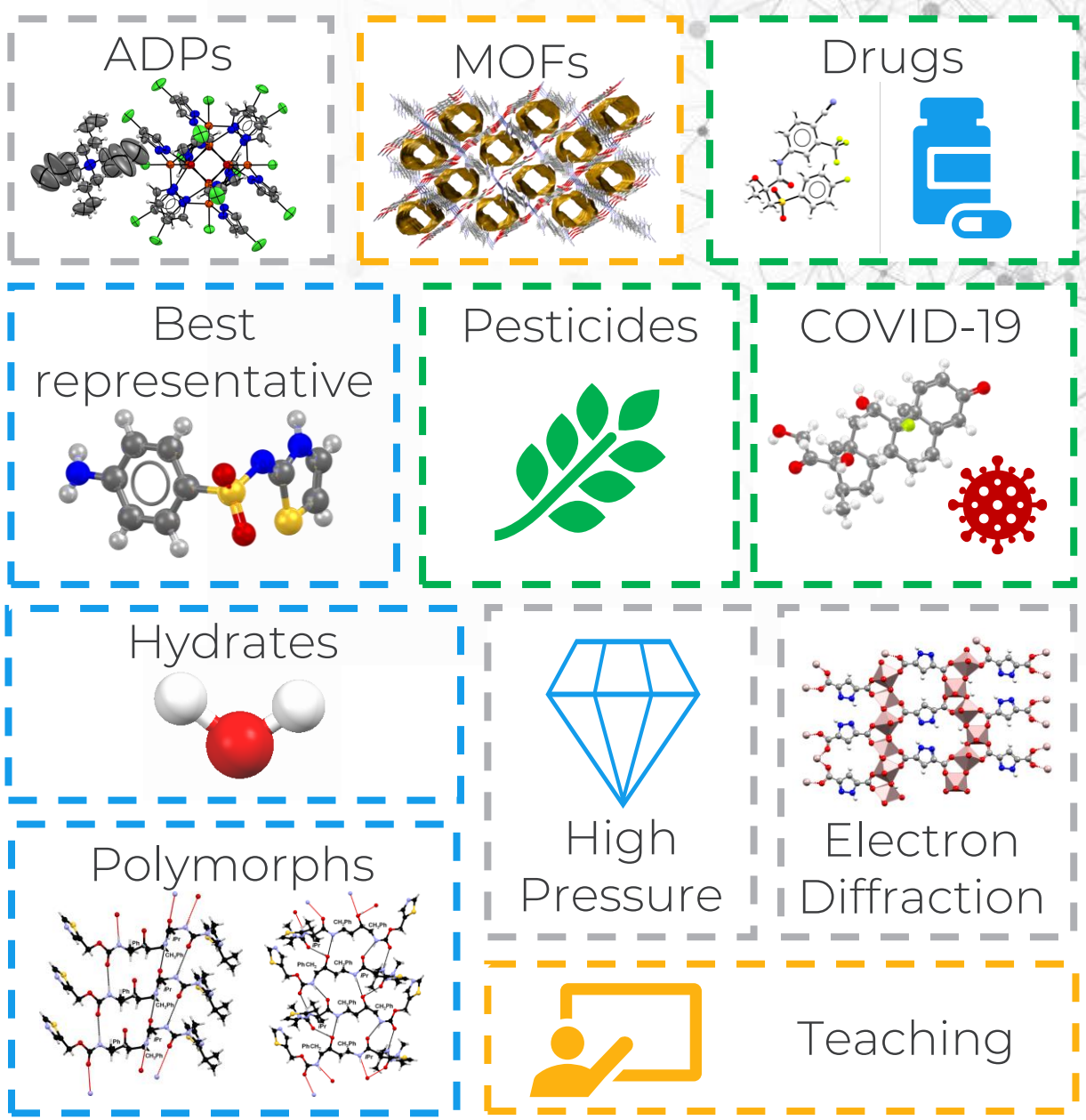
Programmatic



CSD Python API

Targeted collections

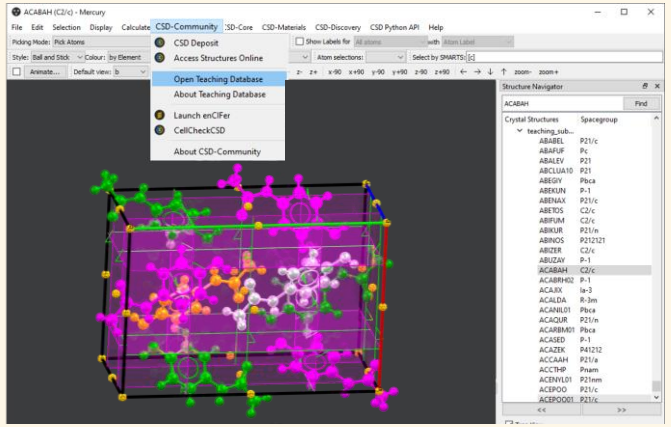
- Easy access to the most relevant structures
- Benefit from our in-house and external expertise
- Convenient starting point for analysis using CSD or 3rd party tools
- A basis for your research and crystal engineering



https://www.ccdc.cam.ac.uk/Community/blog/how-to-use-the-new-electron-diffraction-polymorphs-hydrates-and-high-pressure-CSD-subsets/

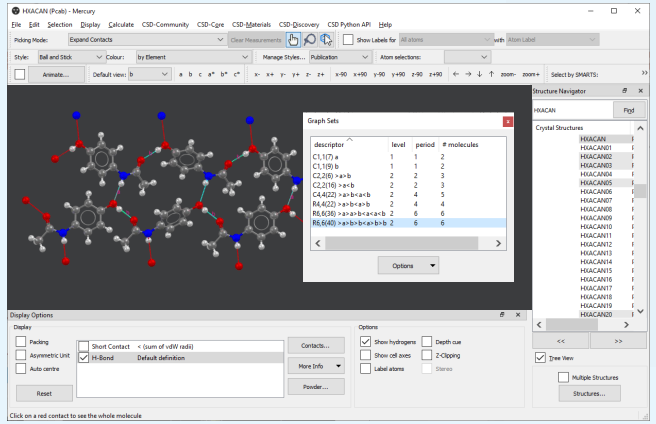
Visualising and exploring structures

The basics



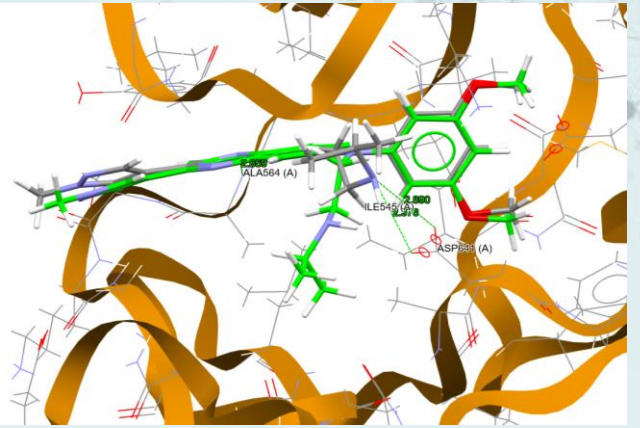
Free Mercury

Advanced



Full Mercury

Macromolecules



Hermes

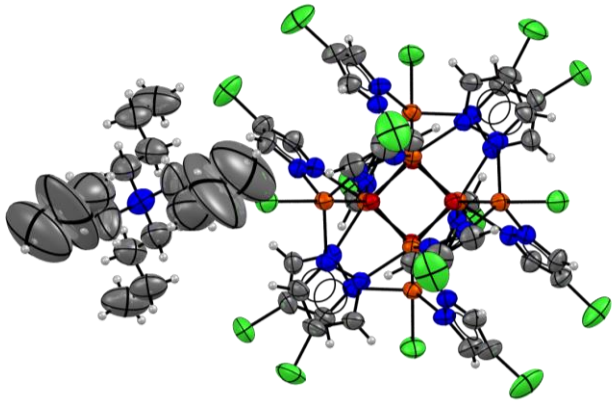
CCDC

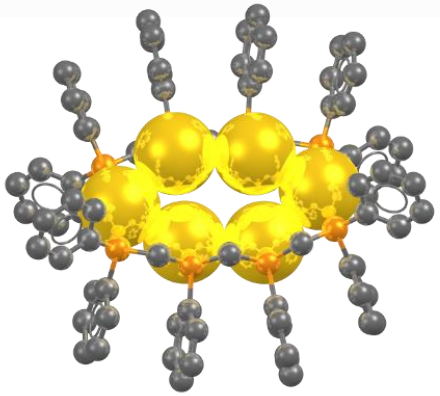
Why use Mercury to visualise str

Find out more in the CSD session today

We can use Mercury to explore over 1.1 million structures

- It is designed for visualisation and analysis of crystal structures – *ad hoc* set of styles, colours and features.
- To gain new insights on your structures using knowledge in the CSD
- To create high-resolution images, high-resolution videos, and 3D print files for publications, presentations, reports, thesis and videos

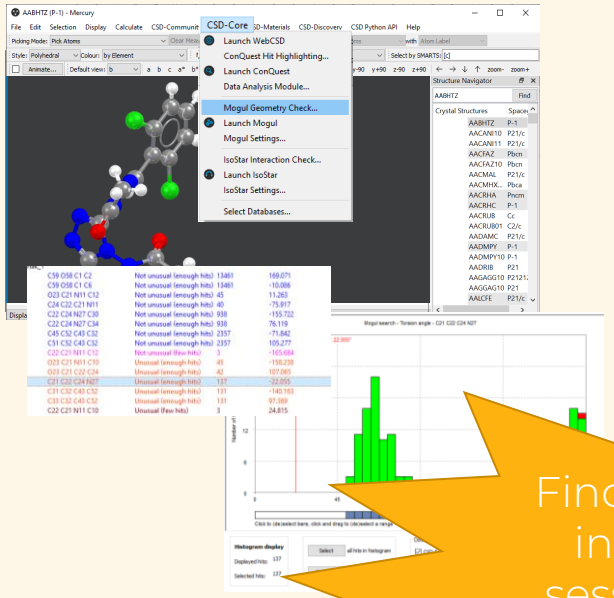




CCDC

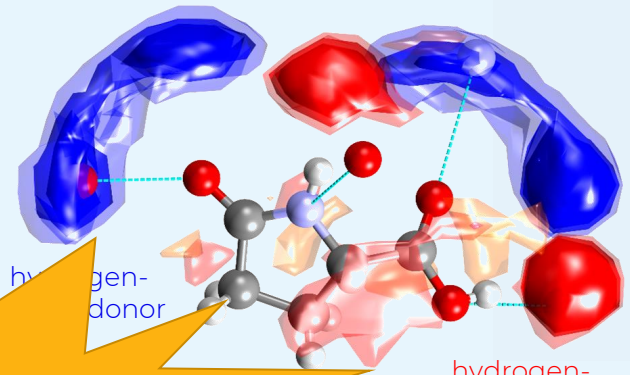
Analysing structures

Geometries



Mogul

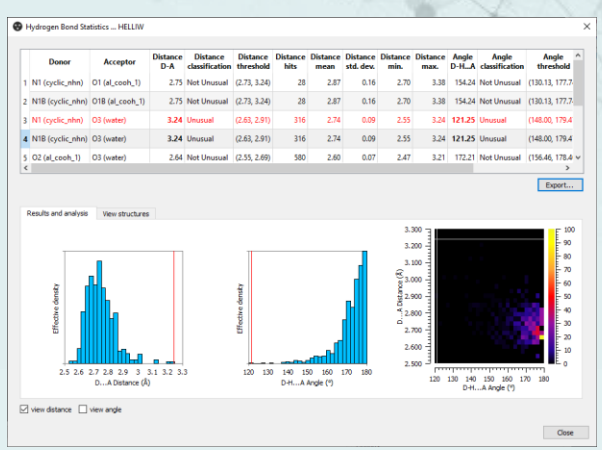
Interactions



Isostar and FIMs

Find out more in the CSD session today

Advanced

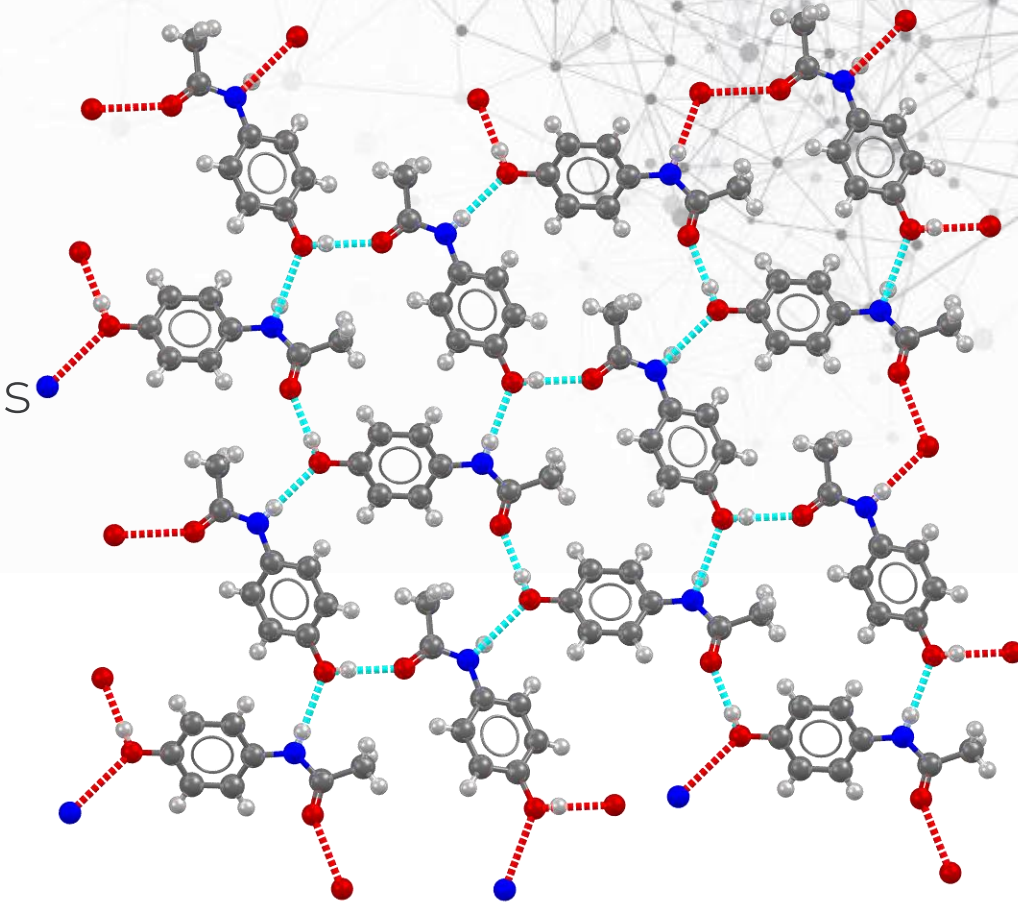


CSD Materials

CCDC

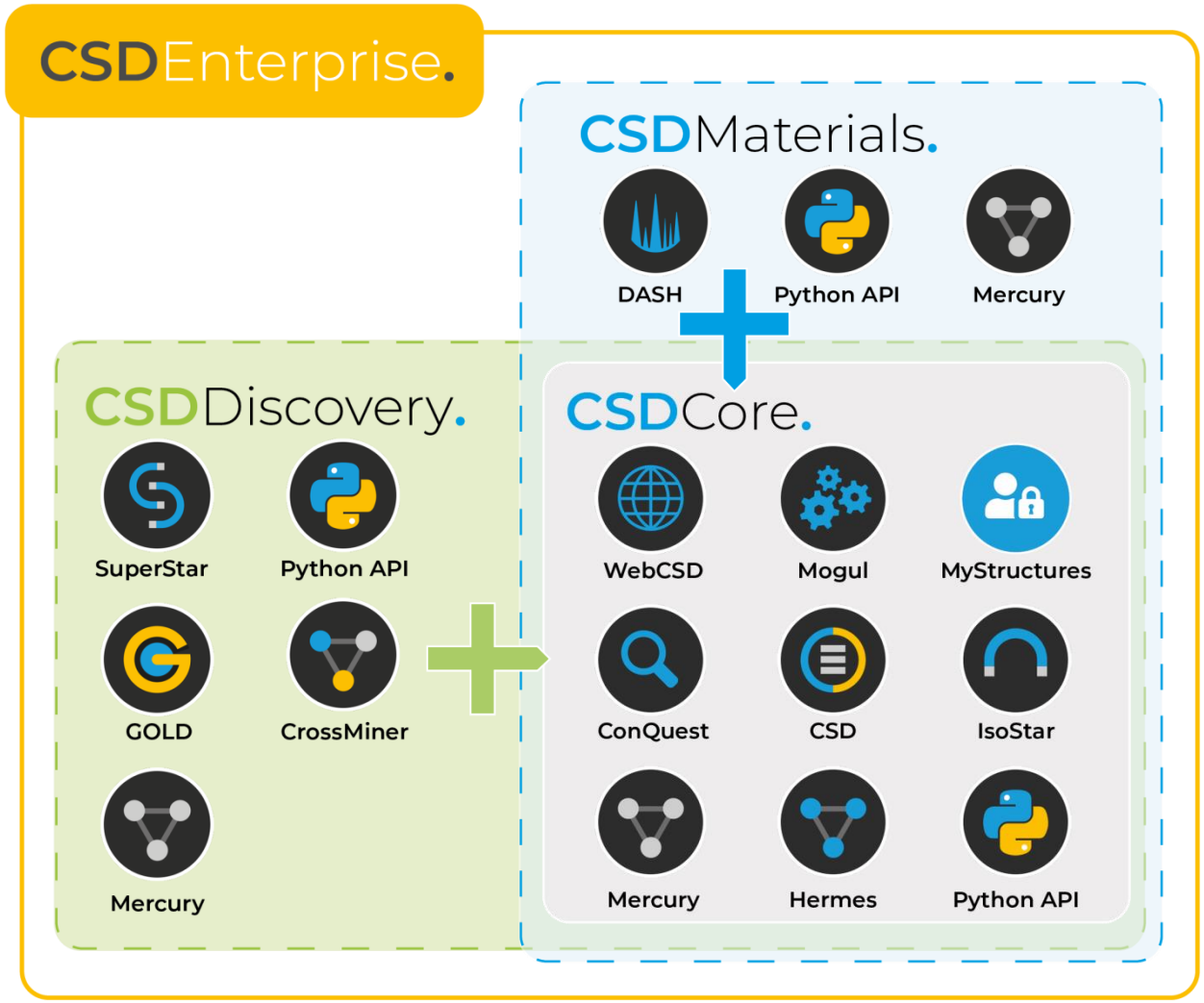
Why analyse structural data?

- To explore over 1.1 million structures and see in 3D how molecules pack and the different intermolecular interactions inside the structures
- By understanding intermolecular interactions and crystal packing it can help us to design new solids with desired physical and chemical properties
  - This is known as crystal engineering
- This can be particularly helpful when exploring different polymorphic forms and can help us to better understand crystal stability



CCDC

The CSD software



Professional Services

Research & Knowledge partnerships

CSDCommunity.

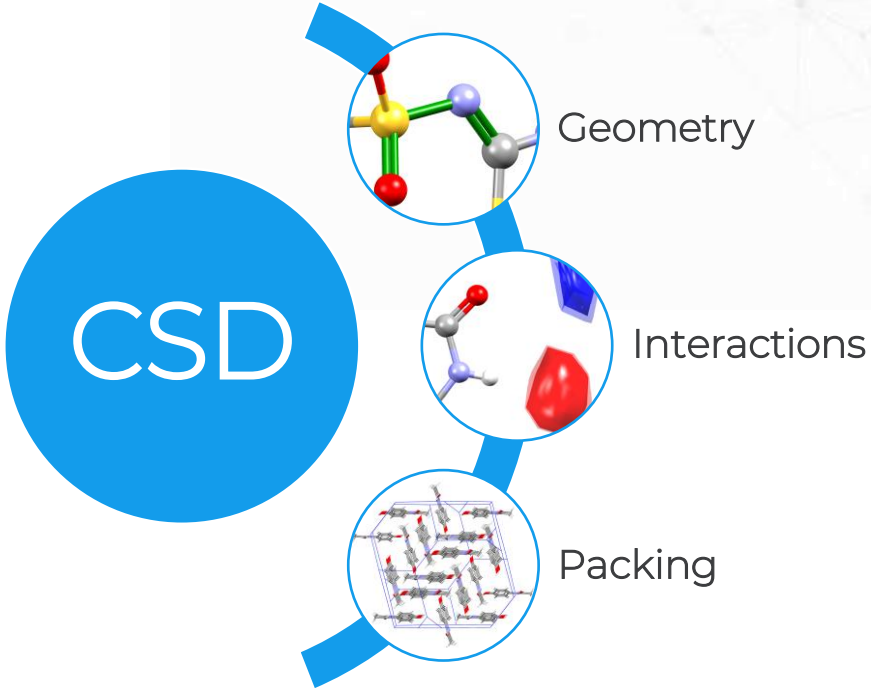
Mercury
enCIFer
Symmetry
Deposit
CellCheck
Educational
Access
MyStructures

CCDC

The CCDC Portfolio

- The CSD is at the heart of the CCDC Portfolio and provides the accurate structural data from which key insights can be extracted.

  - Over 1 million crystal structures.
  - Many millions of geometric parameters.
  - Many millions of interactions.
  - Over 10,000 polymorph families.

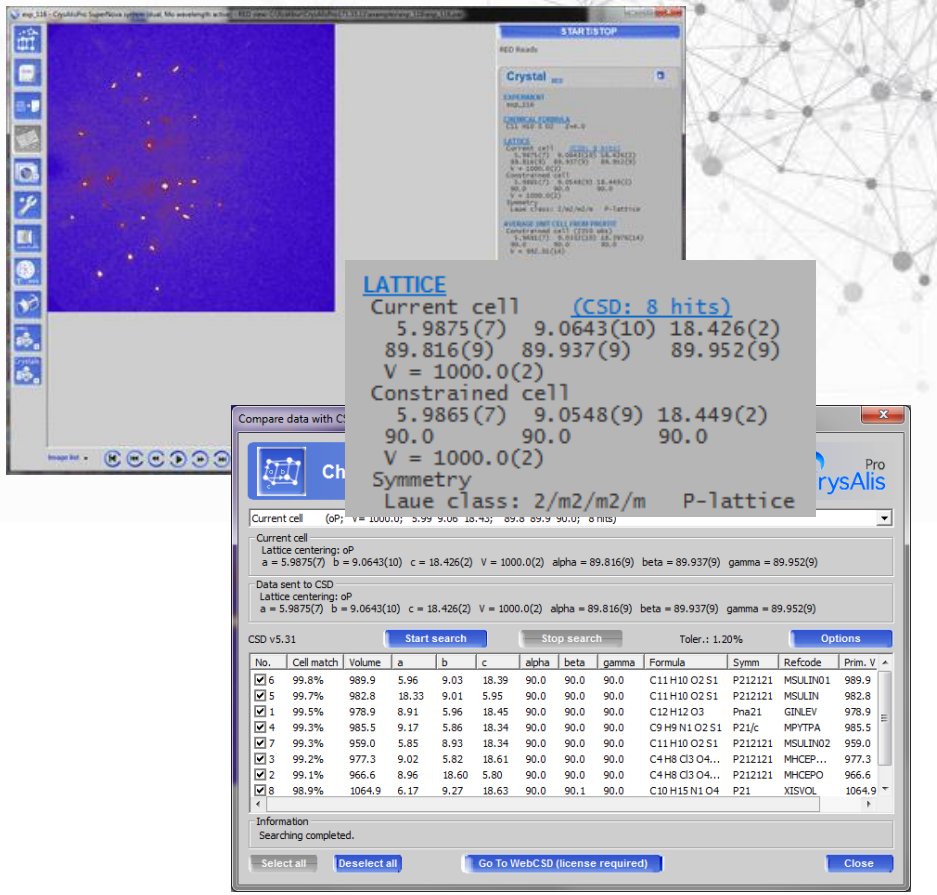


https://pubs.acs.org/doi/abs/10.1021/acs.chemrev.9b00155

CCDC

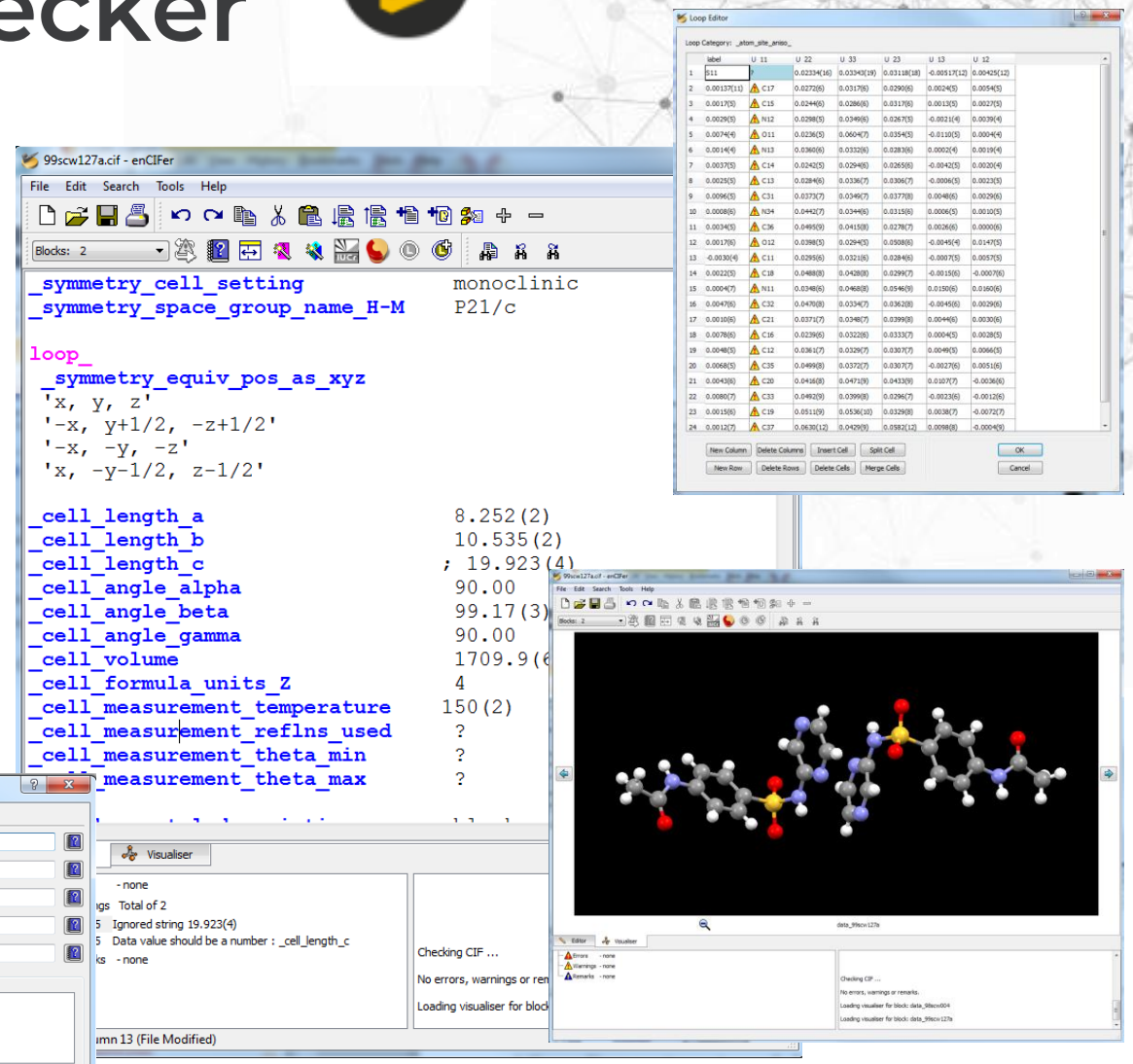
CSD-Community - CellCheckCSD

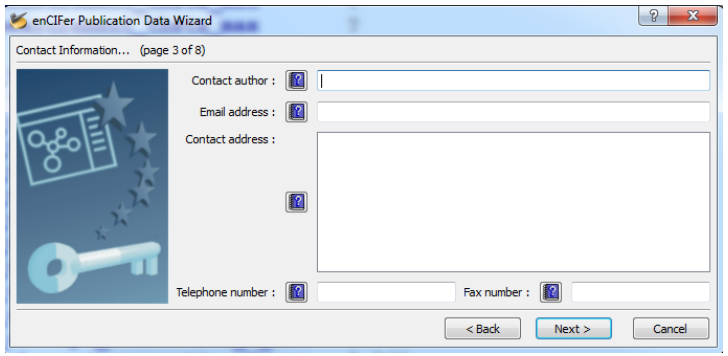
- Freely available through CSD-Community
- An automated tool for checking unit cells against the CSD during data collection
- Used to:
  - Match existing cell dimensions
  - Check sample is novel
  - Check crystal is not starting material or a by-product
  - Ensure diffractometer time used effectively
- Usually downloaded from instrument manufacturer

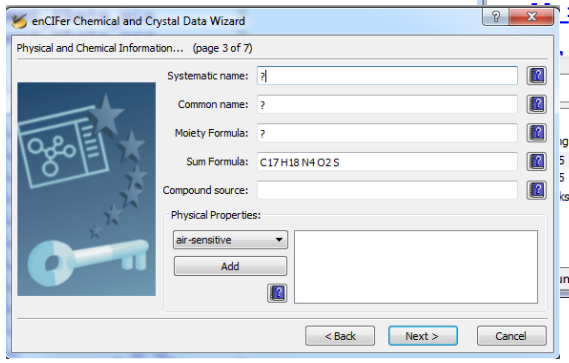


EnCIFer – CIF syntax checker

- Enables validation and preparation of CIFs for deposition with journals & databases
- Allows CIF editing without corrupting syntax
- Data entry wizards enables addition of:
  - Publication details
  - chemical, physical & crystallographic properties
- Visualises structures in a CIF
- Links to CCDC Deposition



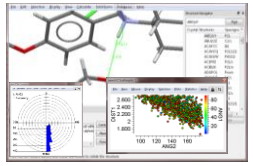




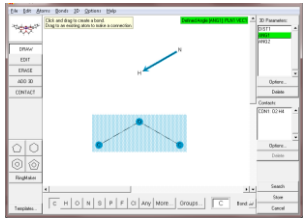
http://www.ccdc.cam.ac.uk/free_services/encifer/

CSD-Core overview

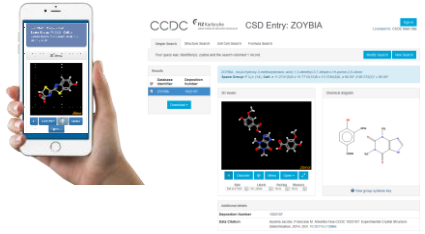
Mercury: Visualisation & numerical analysis



ConQuest: Advanced 3D searching & data generation

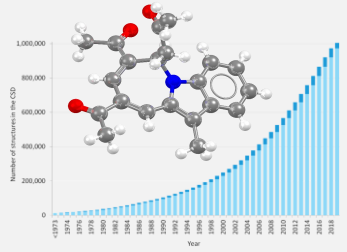


WebCSD: Online search & entry level interface



Hermes: Visualisation of macromolecules

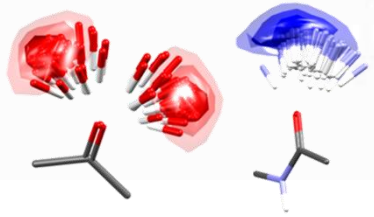
Cambridge Structural Database



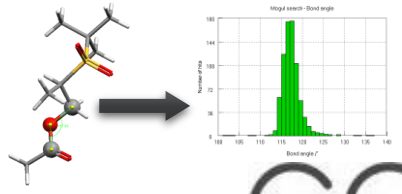
CSD-Editor: Create in-house database

CSD Python API: Access to data & all functionality

IsoStar: Intermolecular interaction analysis



Mogul: Molecular geometry analysis

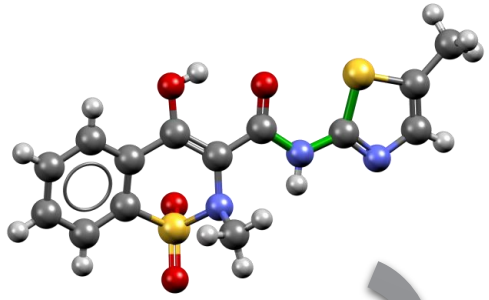


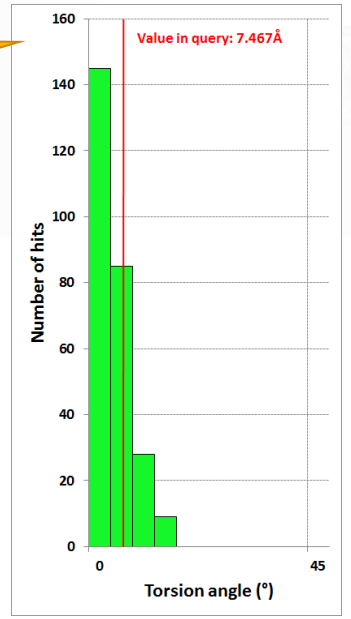
CCDC

Mogul: Molecular geometry

Mogul:

- Mines millions of chemically classified bond lengths, angles, torsion angles and ring conformations in the CSD.
- Provides precise information on favourable molecular geometries.
- Runs in a few to ten seconds.
- Used by wwPDB for ligand validation.





Find out more in the CSD session today

Applications:

- Validation of:
  - molecular geometries.
  - docking solution.
- Generation of low energy conformations.
- Selection of linking groups.
- Rationalisation of inactivity.

Bruno I., *et al. J. Chem. Inf. Comput. Sci.* 2004, 44, 2133-2144. DOI: 10.1021/ci049780b

CCDC

IsoStar: Intermolecular interactions

Isostar:

- Experimental data from CSD and PDB protein-ligand complexes
- Interaction distributions displayed as scatterplots or contour surfaces
- Knowledge base used to generate Full Interaction

Applications:

- How do particular groups typically interac CSD?

(e.g. do hydrogen-bonds to ether oxygen lie alone lone pairs?)

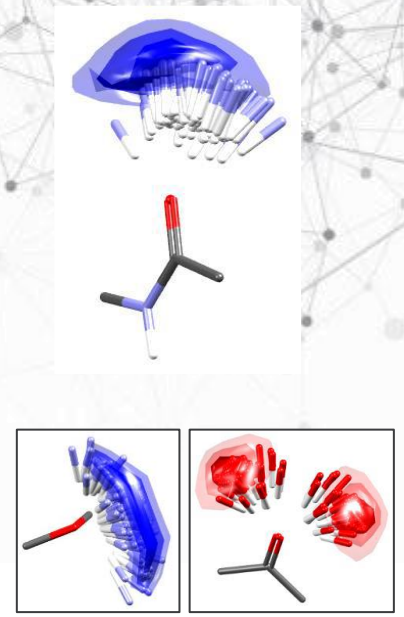
- How do particular ligand groups interact with particular protein residues?

(e.g. from a drug design perspective, how can we bind to a tryptophan?)

- What particular group can be a bioisostere for another particular group?

(e.g. do thiazole and oxazole form similar H-bond interactions?)

Find out more in the CSD session today



I. J. Bruno, *et al. J. Comput.-Aided Mol. Des.* 1997, 11, 525-537. DOI: 10.1023/A:1007934413448.

CCDC

CSD-Materials Overview

Co-crystals: explore potential co-formers with molecular complementarity

CSD Python API: Access to data & all functionality

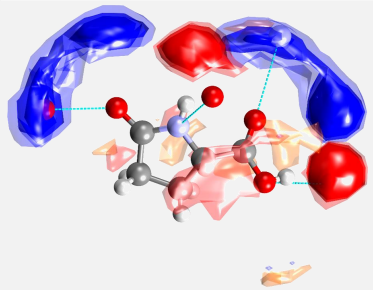
Full Interaction Maps: discover preferred intra- and inter- molecular interactions.

Crystal Morphology: calculate and display BFDH morphologies.

Solvate Analyser: explore and analyse even complex solvates.

Hydrate Analyser: understand the effects of hydration on your solid form.

CSD-Materials



Understand your solid form.

Insights from CSD – experimentally derived.

Crystal Packing: packing feature, similarity and motif searches and H-bond propensity analysis.

Multi-component screening: based on molecular complementarity.

Hydrogen Bond Statistics: assess how (un)usual observed H-bonds are to assess stability

Conformer Generator: explore molecular geometry with validation from the CSD.

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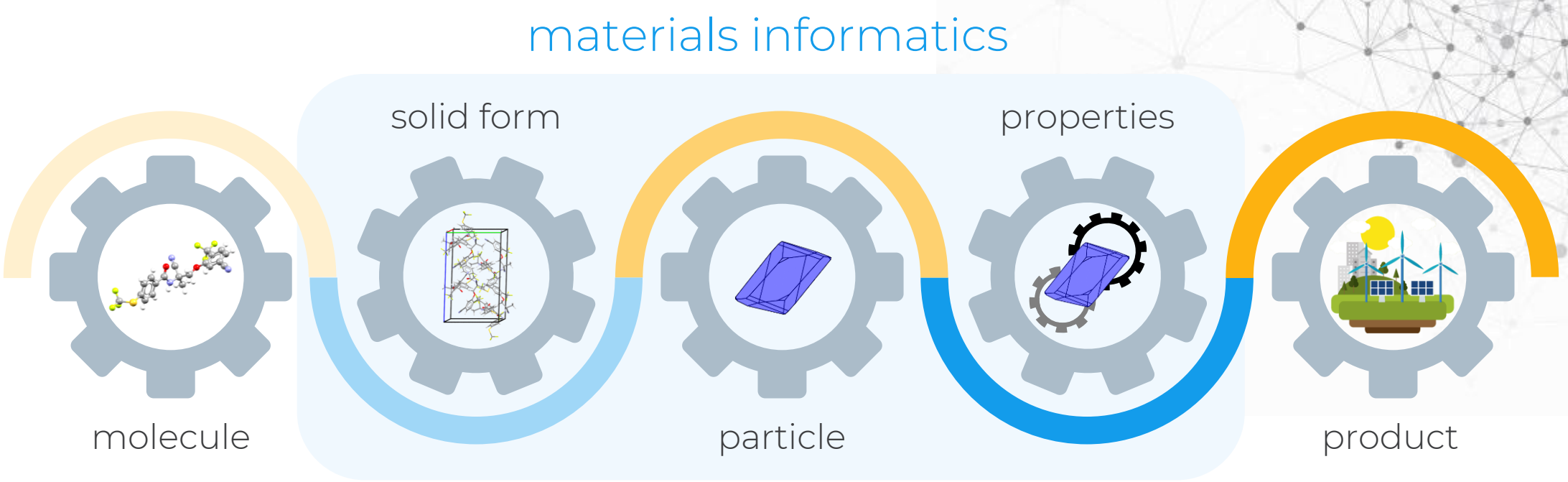
Data inspired materials design



- Structural knowledge used to inform key decisions.
- Integrated digital workflows to guide development and identify risks.

CCDC

CSD-Discovery overview

GOLD: Protein-ligand docking and virtual screening

CSD-CrossMiner: Interrogate the CSD and the PDB for common interaction patterns

Ligand-based **virtual screening** workflow to find new hits.

CSD-Conformer Generator: Generation of molecular conformations.

CSD-Ligand Overlay: Flexible alignment of ligands.

CSD Python API: Create CSD-driven analyses and workflows.

Script-based interfaces to the **Field-Based Ligand Screener**; protein **cavity and sub-pocket search** and comparison; **protein-ligand substructure & interaction pattern mining.**

SuperStar: Analyse, predict and understand protein and ligand interactions

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A wealth of structures, stories and possibilities

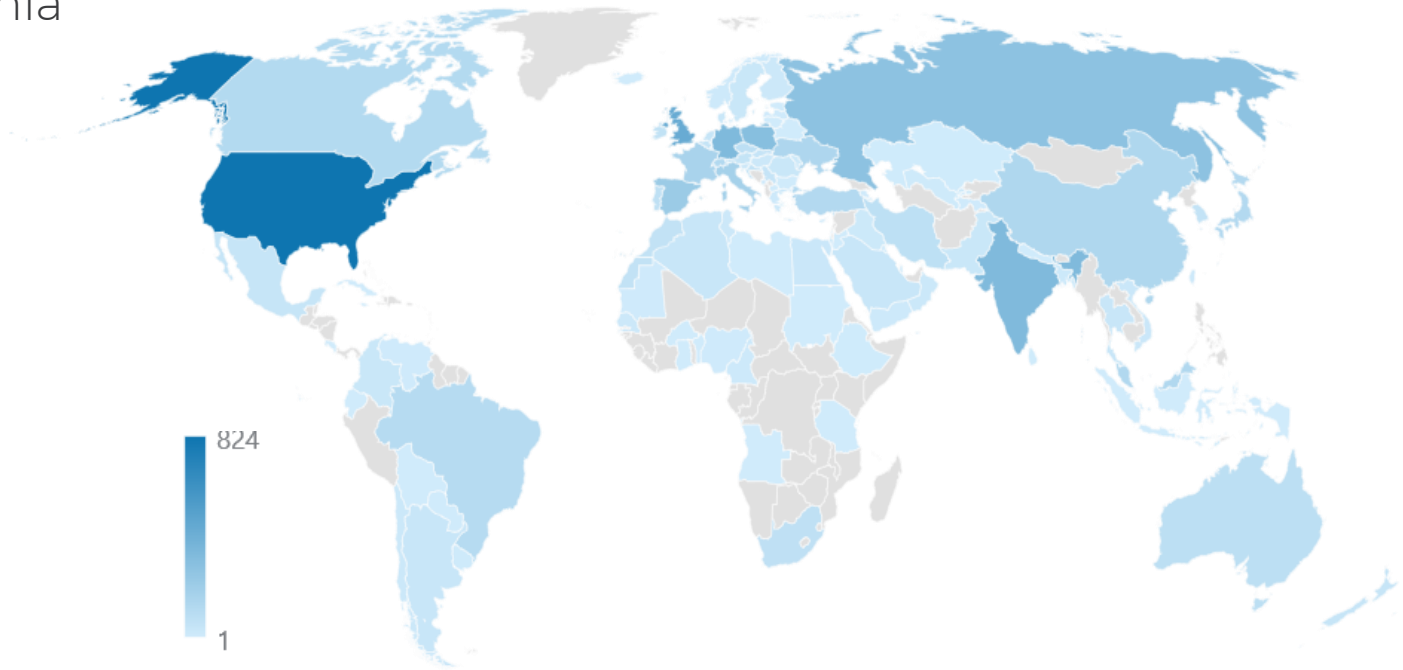
CSD one million special issue

- 33 articles from industry and academia

1 million structures.
stories.
possibilities.

Cambridge Structural Database, CSD

CCDC
advancing structural science



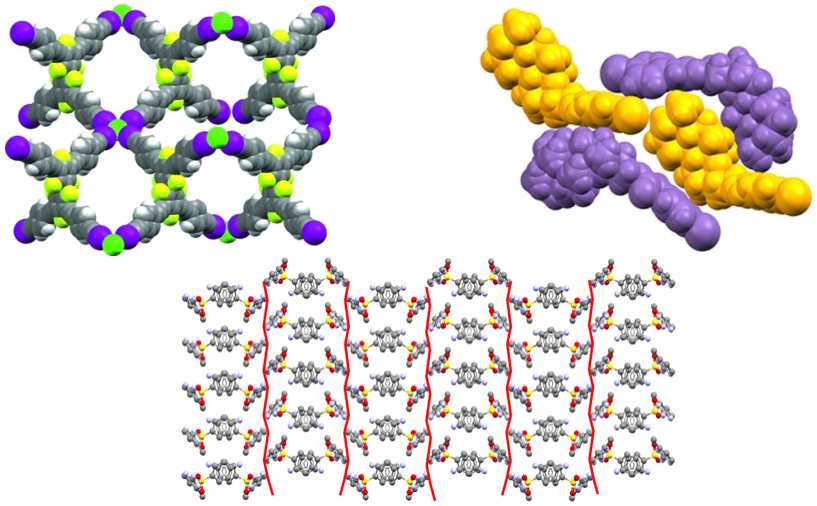
The CSD - A wealth of knowledge gained from a million structures. *CrystEngComm*, 2020,22, 7131-77502
The CSD. C.R.Groom, I.J.Bruno, M.P.Lightfoot and S.C.Ward, *Acta Cryst.* (2016). B72, 171-179 DOI: 10.1107/S2052520616003954

CCDC

The whole is greater than the sum of its parts

CSD Insights

- Molecular geometries
- Molecular interactions
- Molecular assemblies



CSD Applications

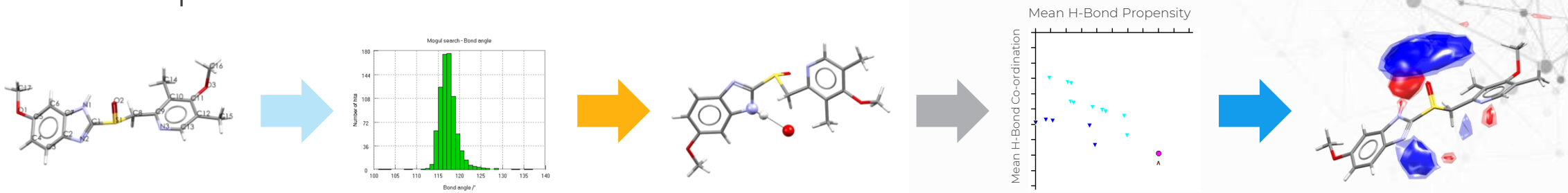
- Teaching
- Drug Design
- Materials Design
- Structure Solution
- Energetic materials
- Paints, Pigments and Dyes
- Organic Semiconductors
- Nonlinear Optical Materials
- Catalysts
- Gas Storage and Separation
- Crystal Engineering

https://doi.org/10.1021/acs.chemrev.9b00155

CCDC

Using the CSD to develop new drugs

- By combining experimental and informatics results, scientists can have greater confidence in progressing a solid form in development



Read in CIF | Geometry check | H bond pairing / coordination | H bond propensity | Packing analysis

- CCDC, in having extensively worked with some of our closest pharma partners, has seen first-hand the systems in current development pipelines and the problems faced on a daily basis

N. Feeder *et al.*, *Pharm Pharmacology*, 2015, *67*, 857-868 DOI: 10.1111/jphp.12394

CCDC

More to explore...

www.ccdc.cam.ac.uk/Community/educationalresources/

CCDC

Community

- Community
- Blog
- Deposit a Structure
- Access Structures
- CSD-Community
- International Year of the Periodic Table
- Awards and Sponsorship
- FAIRE Programme
- Collaborators and Partnerships
- Initiatives
- Training and Educational Resources
- CSD Communications

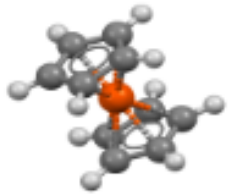
To keep up to date with the latest news from education and outreach at the CCDC sign up for the Education and Outreach Newsletter **here**.

Software Training

Self-guided workshops

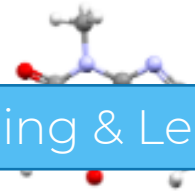
CSD session at 15:30

On-demand modules with completion certificate

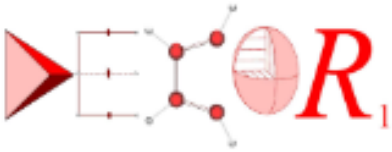


Information on the Teaching Subset

Teaching & Learning

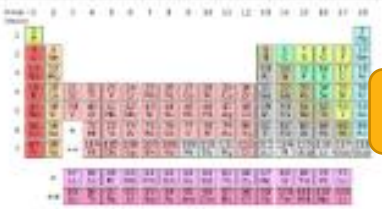


Access a series of teaching modules for use in the classroom



DECOR: Educational Resources for Teaching Crystallography

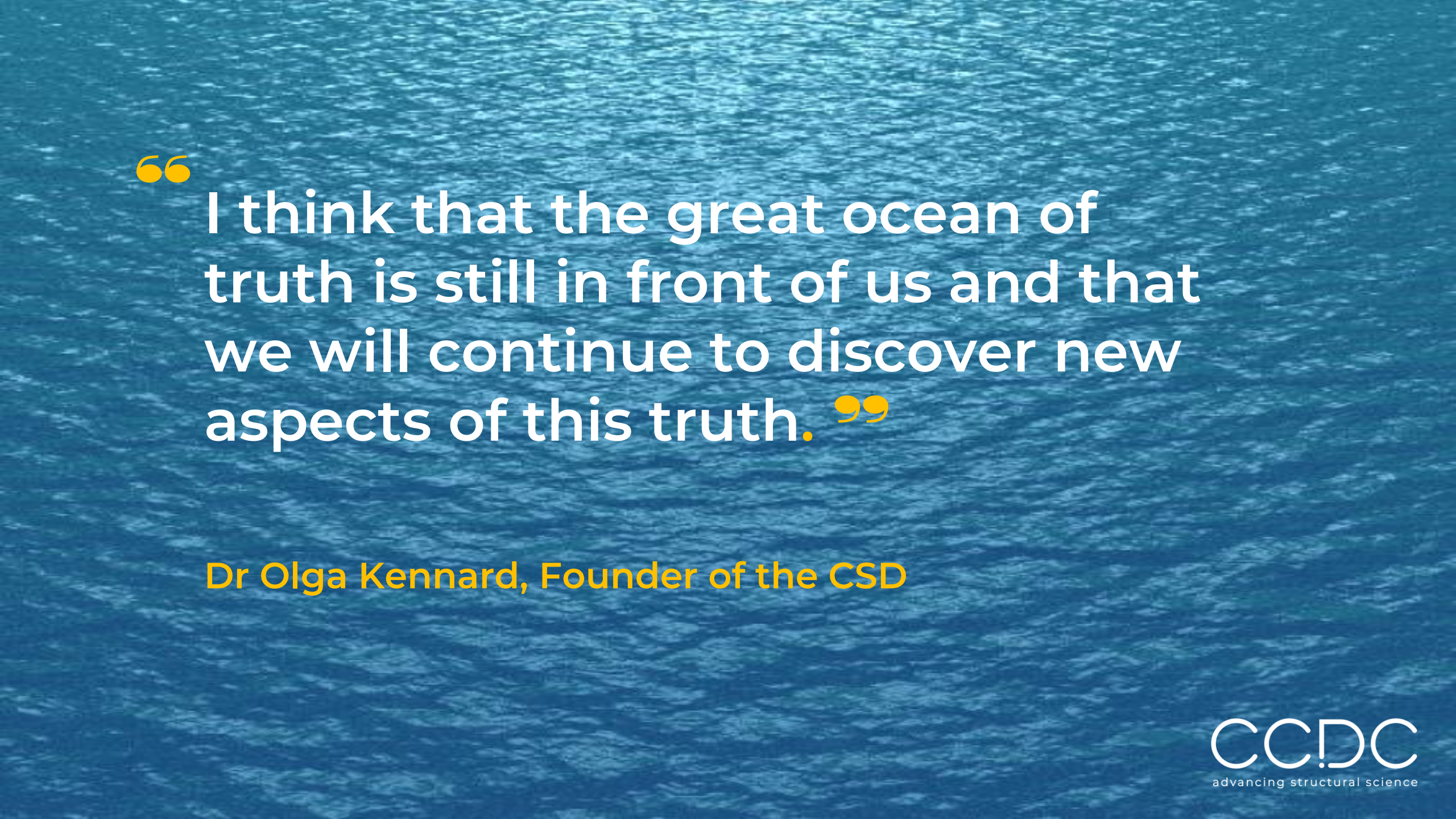
Access fun science activities for kids through the CCDC Home learning page



Explore the Periodic Table through Crystal Structures

Outreach

Bound! a Protein-Drug matching card game


“I think that the great ocean of truth is still in front of us and that we will continue to discover new aspects of this truth.”
Dr Olga Kennard, Founder of the CSD
CCDC
advancing structural science

CSD-NICZUX

The Cambridge Structural Database - Learning from one million crystal structures

Ilaria Gimondi

Education and Outreach Officer

Suzanna Ward

Head of Data and Community

igimondi@ccdc.cam.ac.uk
ward@ccdc.cam.ac.uk

Agenda

- Introduction to the CSD
- Visualizing structures in the CSD
  - Slides and follow-along demo
- Analysing the geometry of structures using Mogul
  - Slides and follow-on along demo
- Analysing intermolecular interactions using FIMs
- Wrap up, quiz and summary

CCDC

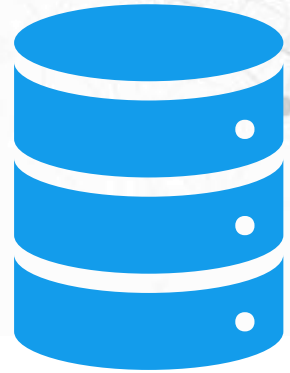
Learning outcomes for today

- How to visualise and explore over a million crystal structures
  - What the Cambridge Structural Database is and how it can be used in your research
  - How to visualise structures using Mercury
  - How to explore the packing, symmetry and hydrogen bonded networks of structures
- How to analyse the geometries of structures using Mogul
  - Familiarise yourself with the basics of Mogul
  - How to get more insights into your crystal structures and interpret results obtained from Mogul
  - How to use Mogul for CSD structures and new structure determinations
- How to analyse the interactions within a crystal structure
  - Familiarise yourself with how Full Interaction Maps are generated and how to create them
  - How to interpret results obtained from FIMs
  - Why looking at interactions are important and how FIMs can be used in your research

CCDC

What is a crystallographic database?

- They usually include:
  - Bibliographic data
  - Crystallographic, chemical and experimental information
  - Atomic coordinates



- What makes a crystallographic data special?
  - Standard agreed file format
  - Every published structure is added to the appropriate database
  - There are established curated databases rather than just collections of data with some level of quality control through processing & validation
  - They enable you to learn from the wealth of data they contain

CCDC

What can you do with a database?

- Most importantly, when used effectively you can derive **structural insight** from a database
- They provide insights and context around:
  - Cell dimensions and space groups
  - Intramolecular geometry & Intermolecular interactions
  - Metal coordination geometry
  - Supramolecular packing

Data: "a tomato is a fruit"

Insight: "based on all the fruit salads observed, perhaps you shouldn't put a tomato in a fruit salad!"

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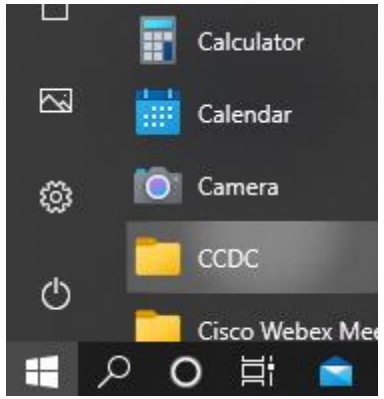
About you

1. Have you done any of the following before?
   - Analysed molecular geometries using Mogul
   - Analysed interactions using Full Interaction Maps

2. Do you have the CSD portfolio installed?
   - Yes I have the full CSD
   - Yes - but I have not activated my license
   - Yes - but only the Teaching Subset and free Mercury
   - No



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Agenda

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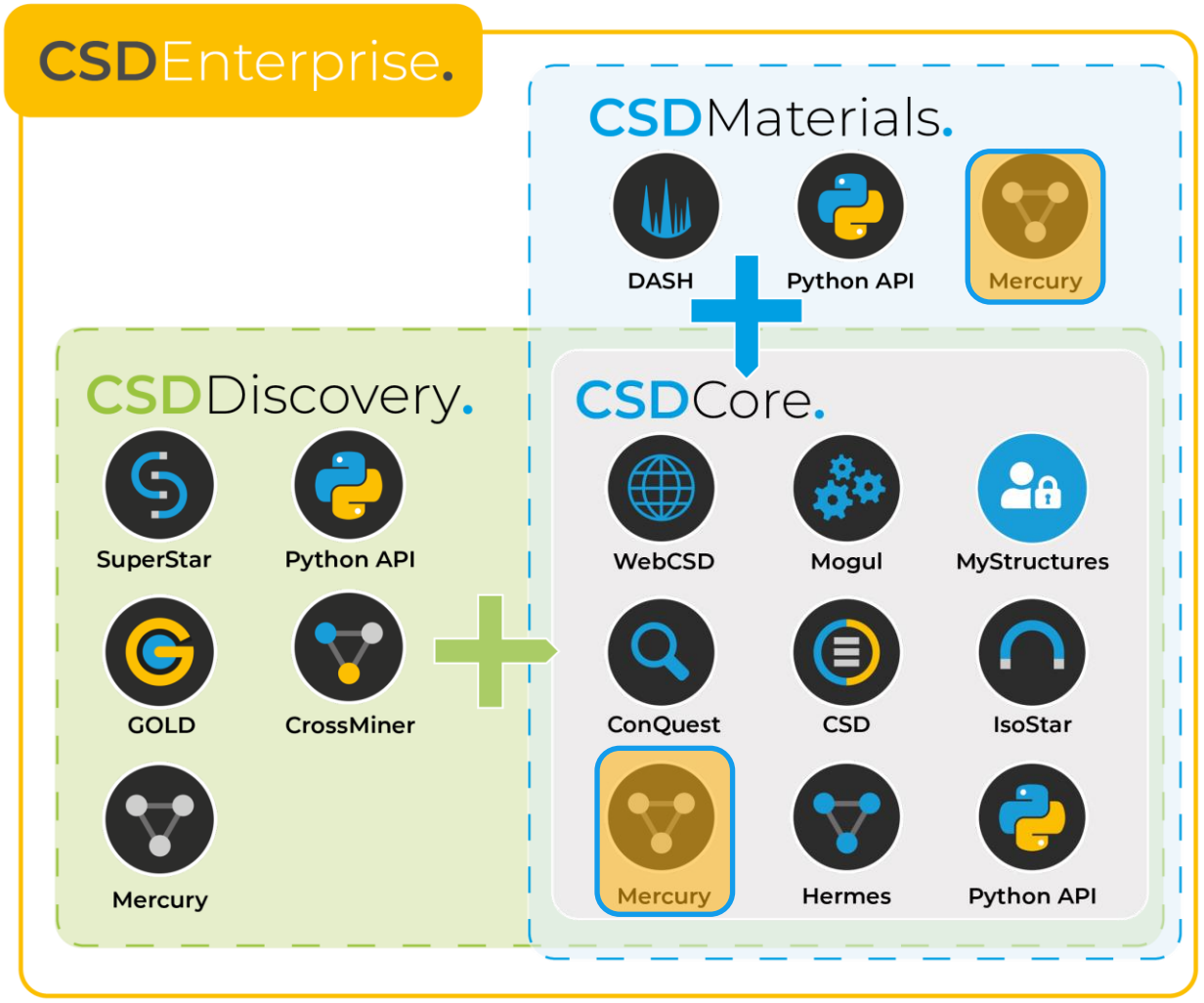
CCDC

The CSD Portfolio



Professional Services

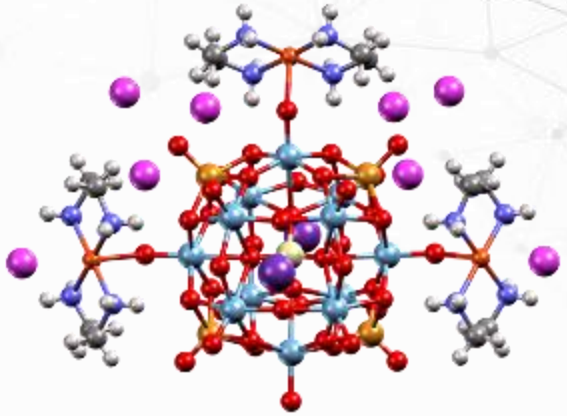
Research & Knowledge partnerships

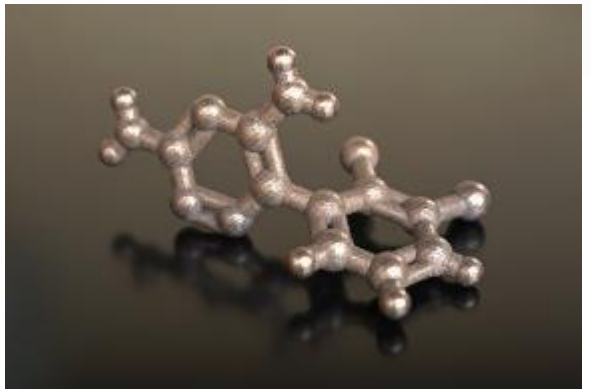
CCDC

Mercury – Structure visualisation

With Mercury you can:

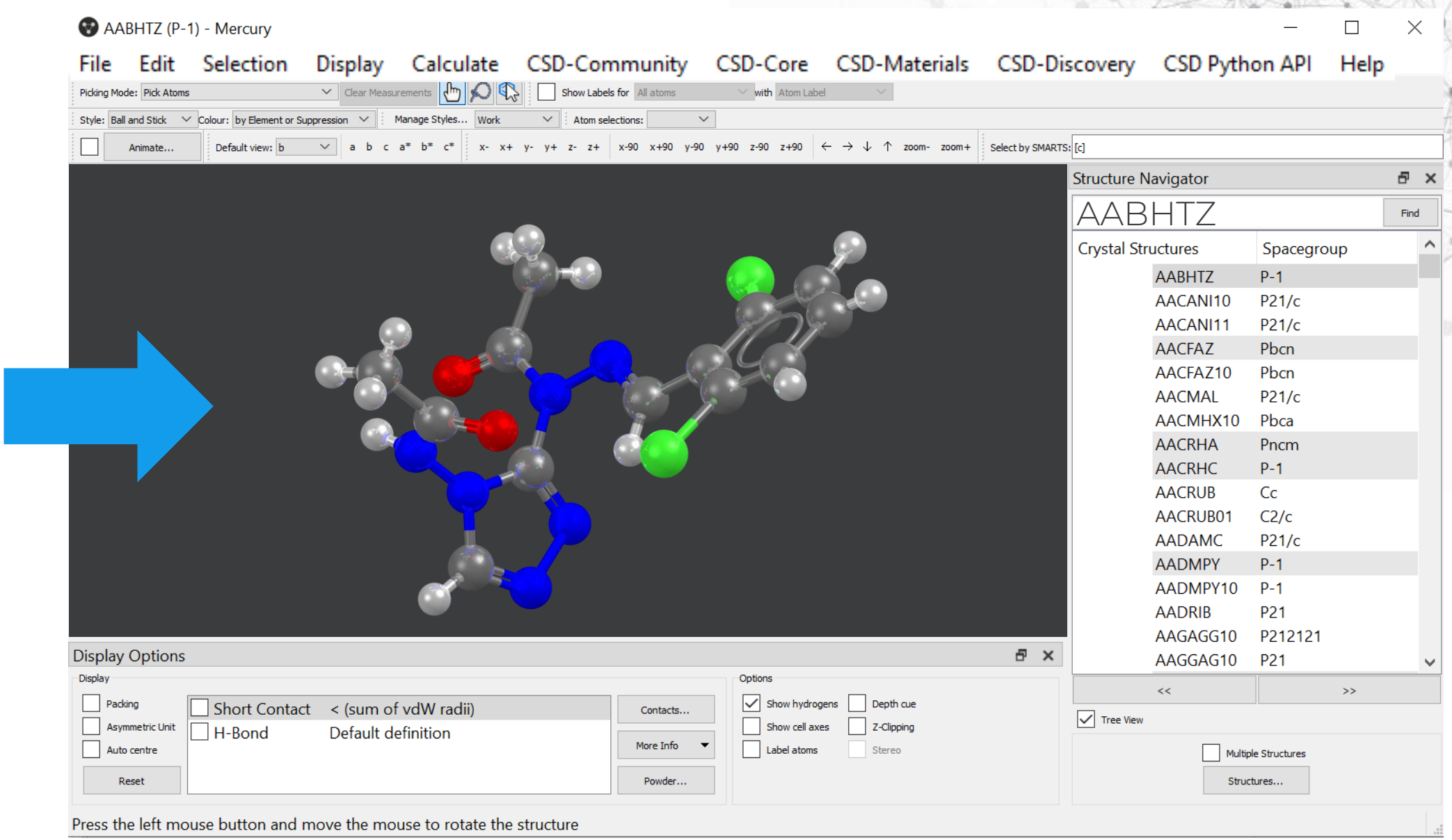
- Explore over 1 million crystal structures, molecular conformations, crystallographic planes and simulated morphologies
- Generate high quality structural images for effective scientific communication
- Output model files for 3D printing
- Analyse geometries, interactions and the packing inside structures





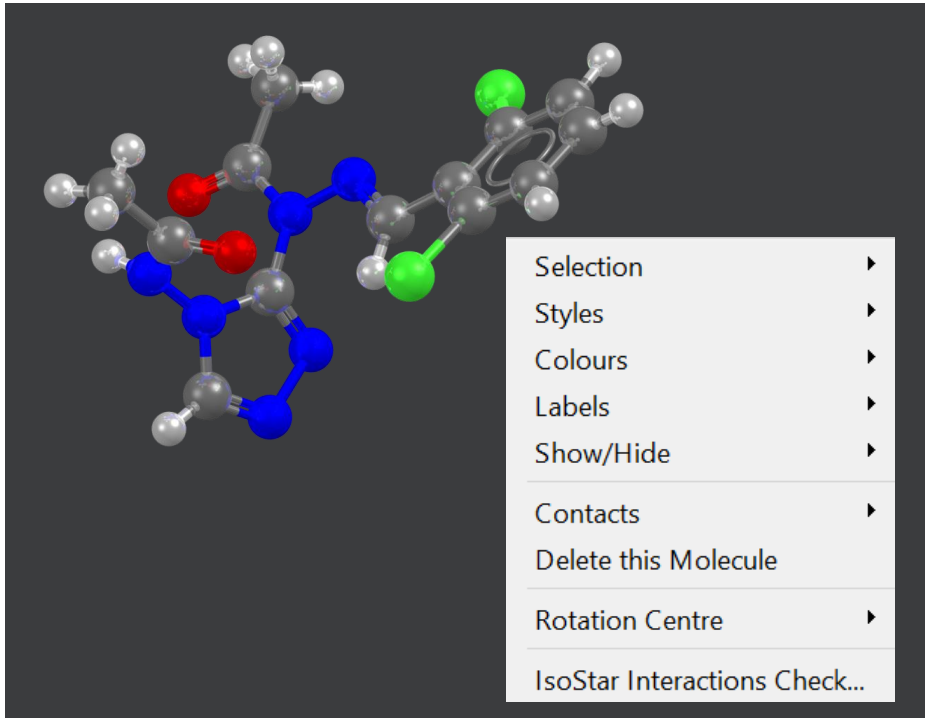
CCDC

The basics of Mercury

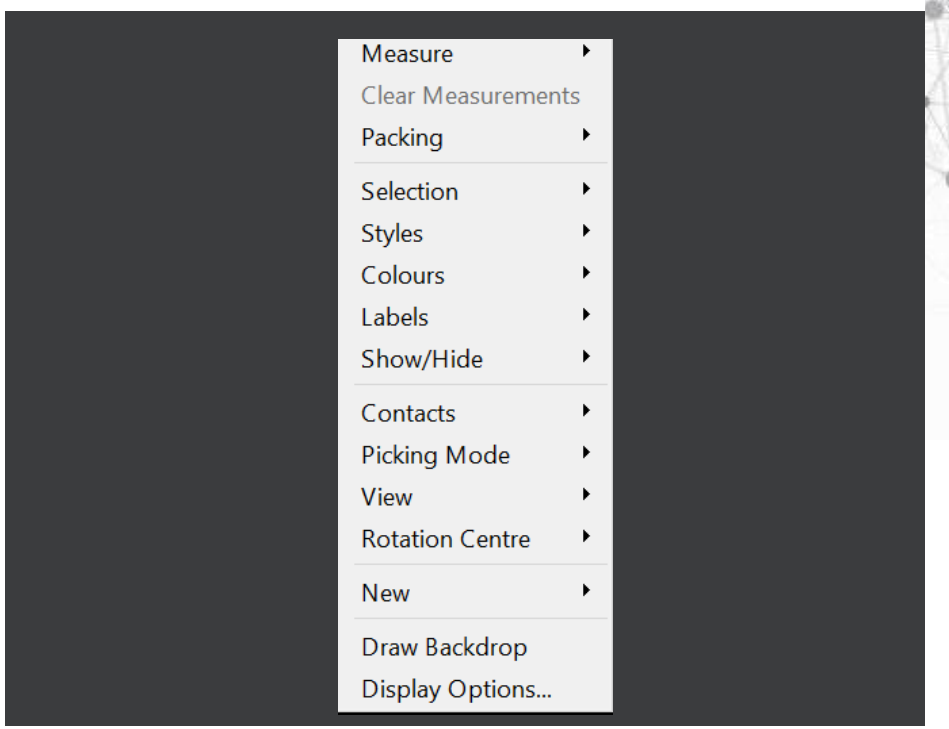


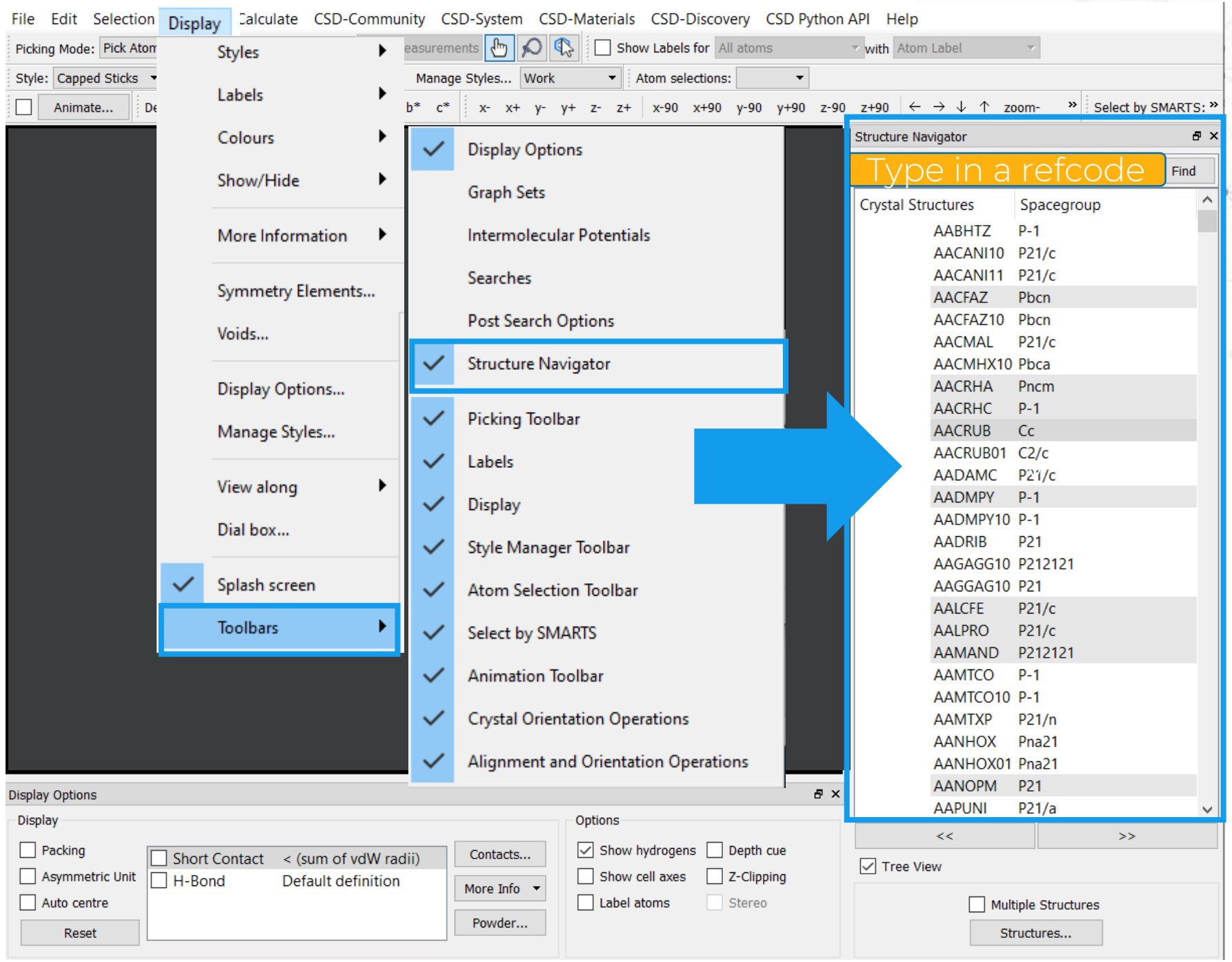
Right mouse click

Near a molecule



Away from a molecule



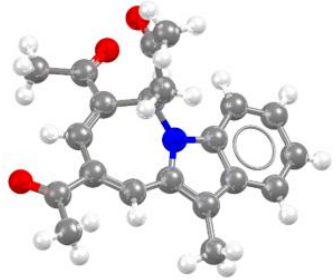


Handy tips:

- Recovering Toolbars
- Resetting view

CCDC

CSD Refcodes



CSD Refcode - XOPCAJ

What is XOPCAJ?

- A CSD Refcode
- A database reference code
- Containing 6-8 characters
- Used to identify entries in the CSD

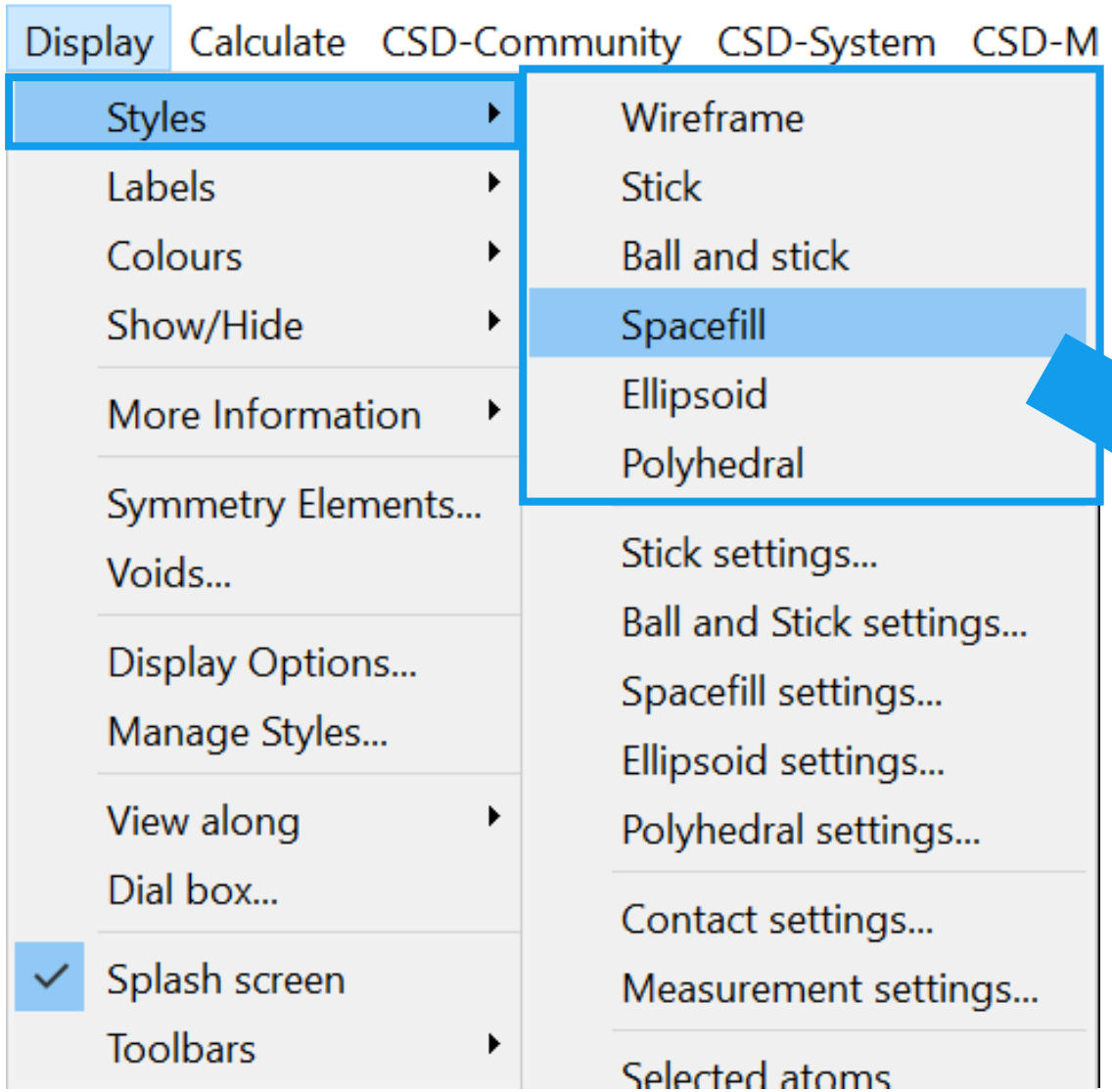
Refcode families

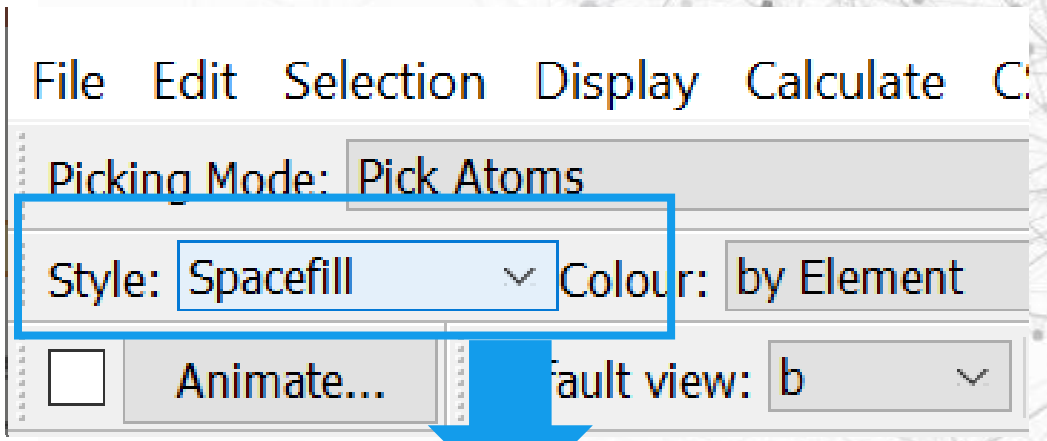
- The same substances are assigned the *same* 6 letter code plus an additional 2 numbers
  - Polymorphs
  - New determinations or re-refinements of the same substance
  - Determinations at different temperatures/pressures
- Stereoisomers or different solvates, co-crystals, etc are assigned *different* refcode families

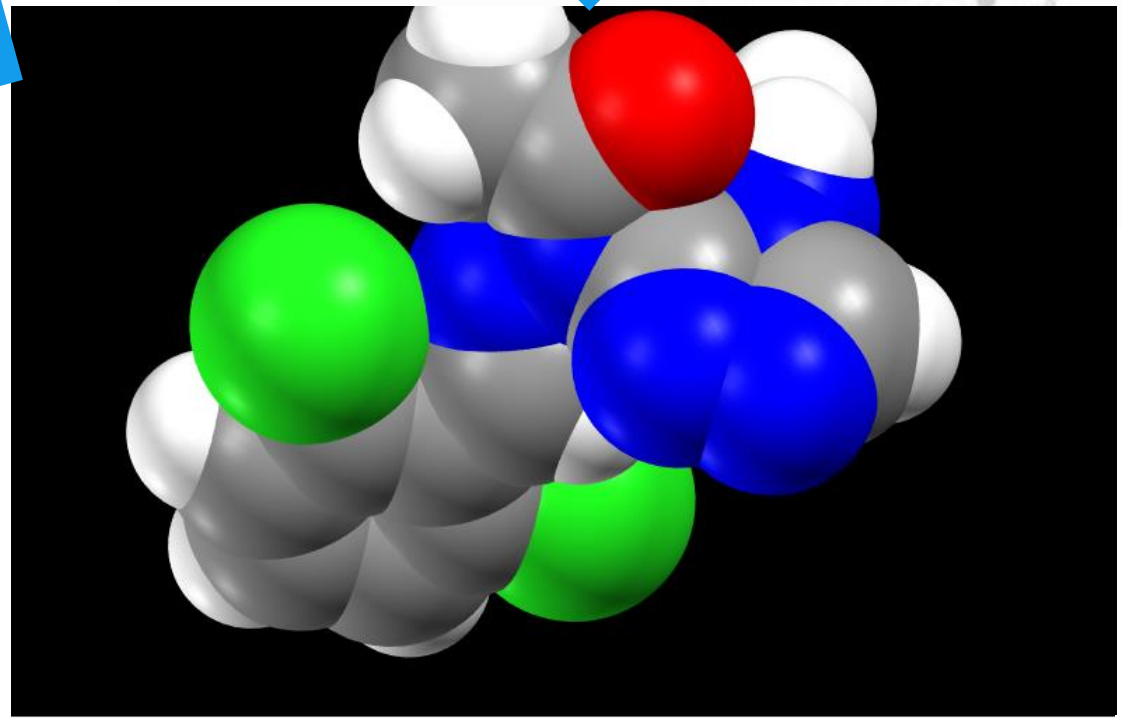
Some of my favourite refcodes are: KITTEN, BATMAN, DISNEY, GAUTAM, GLYCIN

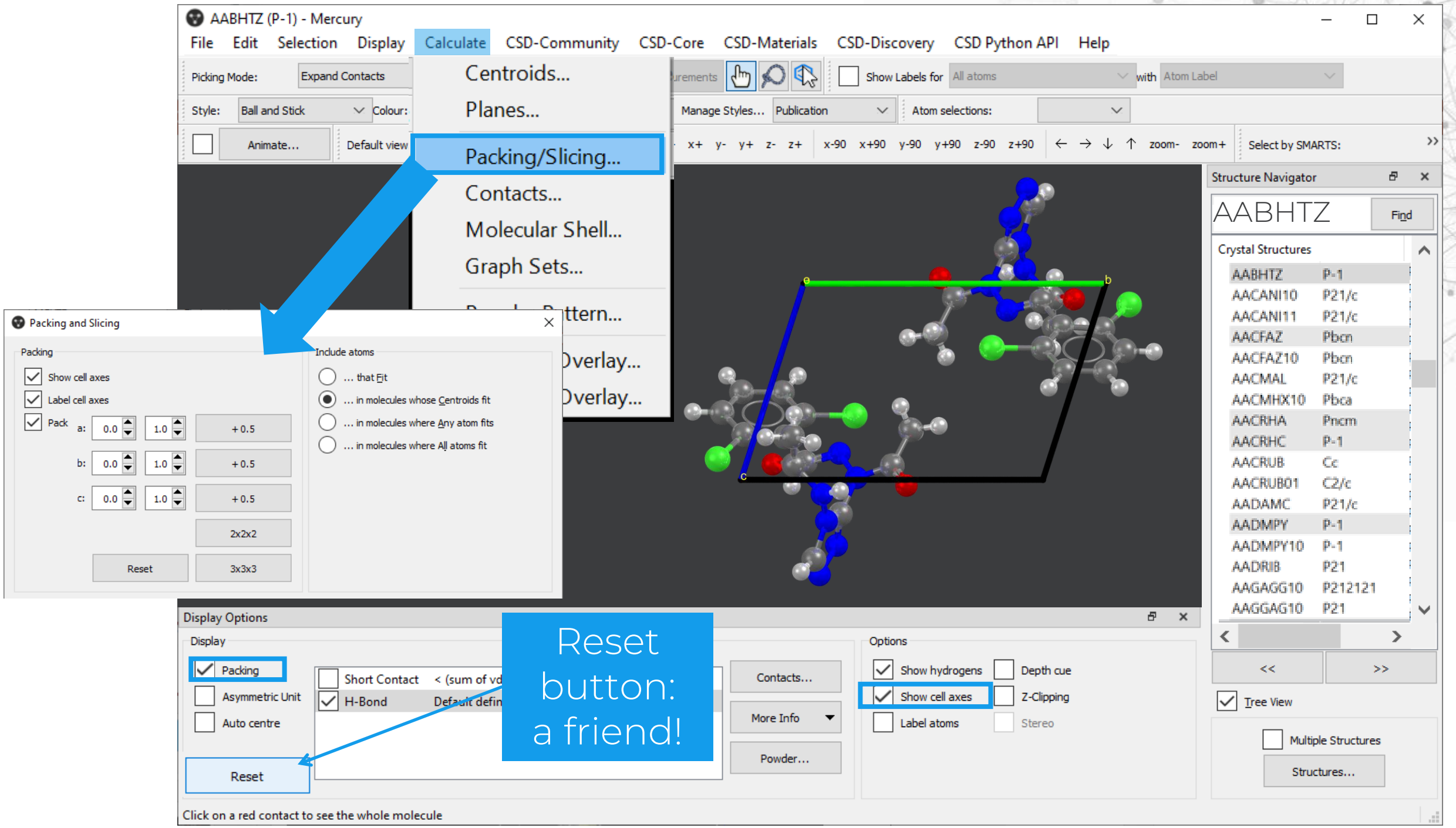
CCDC

Changing display - Style



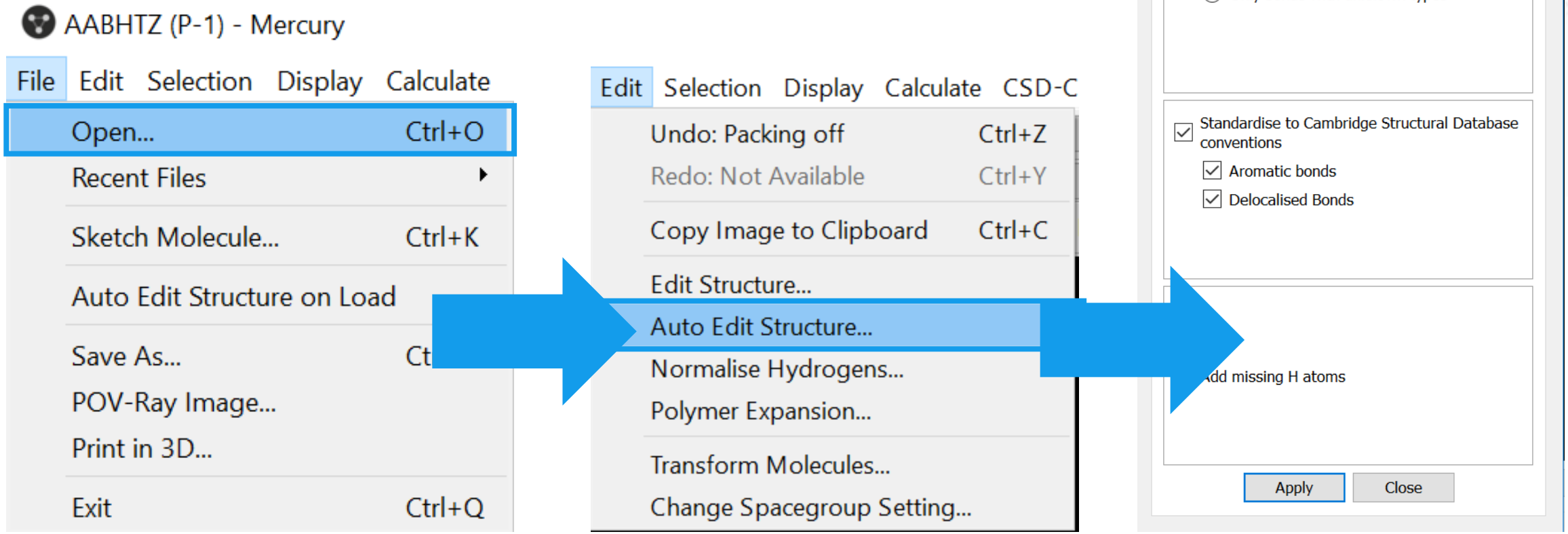




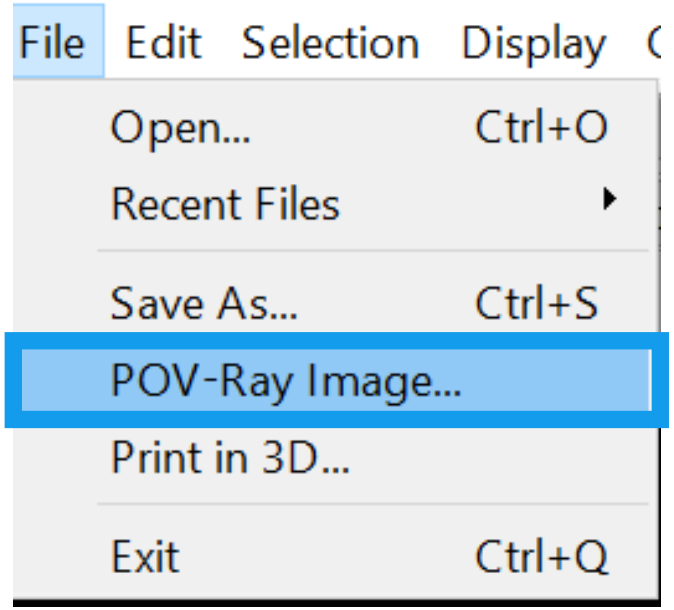

AABHTZ (P-1) - Mercury
File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Discovery CSD Python API Help
Centroids...
Planes...
Packing/Slicing...
Contacts...
Molecular Shell...
Graph Sets...
Overlay...
Overlay...
Packing and Slicing
Packing
Show cell axes
Label cell axes
Pack
Include atoms
... that Fit
... in molecules whose Centroids fit
... in molecules where Any atom fits
... in molecules where All atoms fit
+0.5
2x2x2
3x3x3
Reset
Structure Navigator
AABHTZ
Find
Crystal Structures
Display Options
Display
Packing
Asymmetric Unit
Auto centre
Short Contact
H-Bond
Contacts...
More Info
Powder...
Options
Show hydrogens
Depth cue
Show cell axes
Z-Clipping
Label atoms
Stereo
Tree View
Multiple Structures
Structures...
Reset button: a friend!
Click on a red contact to see the whole molecule

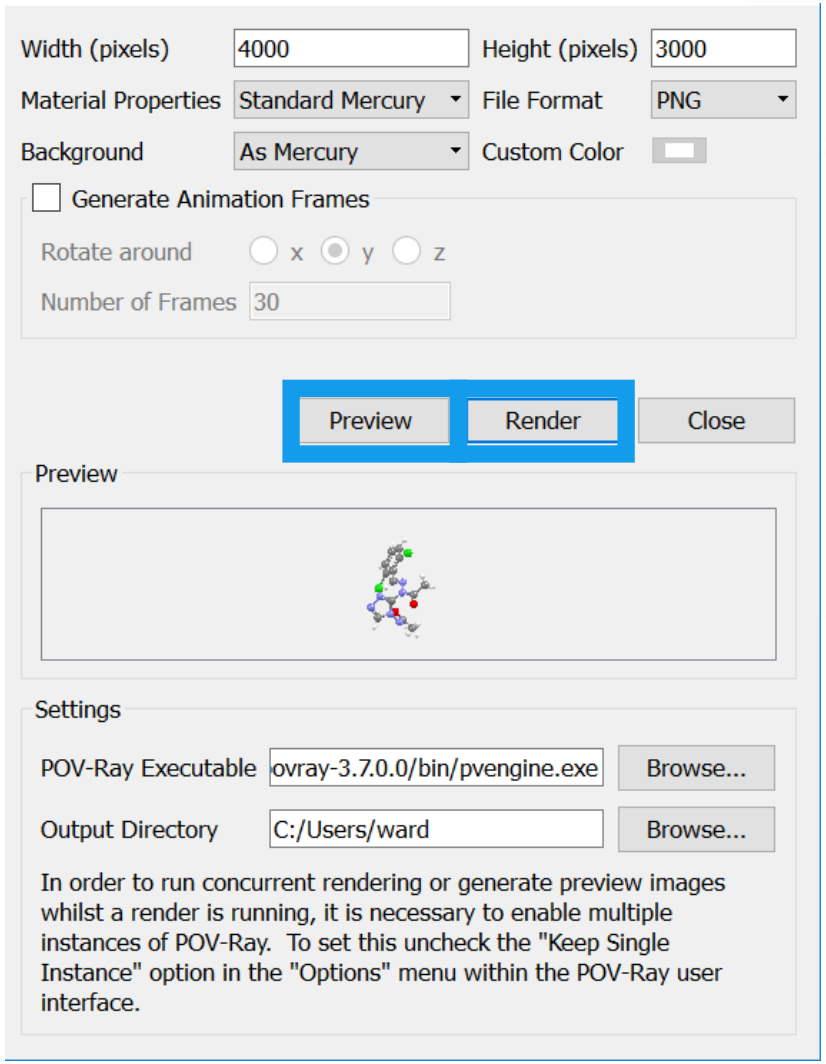
Using your own file

- File > Open – to open one of your own files for example a CIF
- Edit > Auto Edit Structure to assign bond types
- File > Auto Edit Structure on Load to automate



Generating high quality images





File > POV-Ray Image

Change Resolution

- Width = 4000
- Height = 3000

Change ‘Material Properties’ to ‘Metallic’

Set ‘Background’ to ‘Transparent’

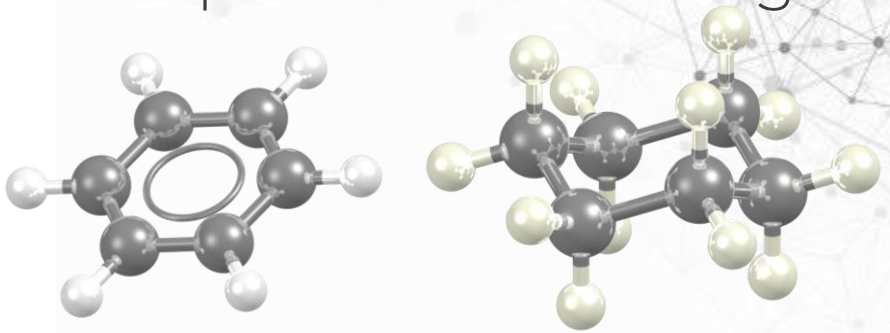
Press ‘Preview’

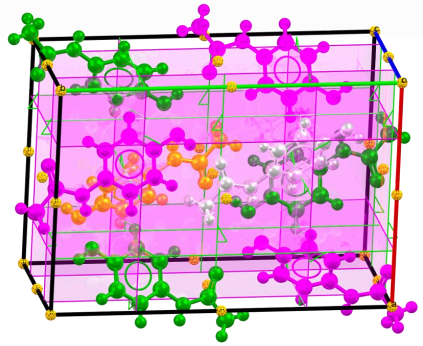
CCDC

From visualization to deeper understanding

By exploring 3D structures, we can gain a deeper understanding of:

- Chemistry
  - The geometry of molecules
  - The geometry around metals
- Solid forms
  - How molecules pack together
  - What voids and channels exist within a structure
  - What interactions help to stabilise the structure
  - How structures including polymorphic structures compare
  - The symmetry within a structure and different space groups

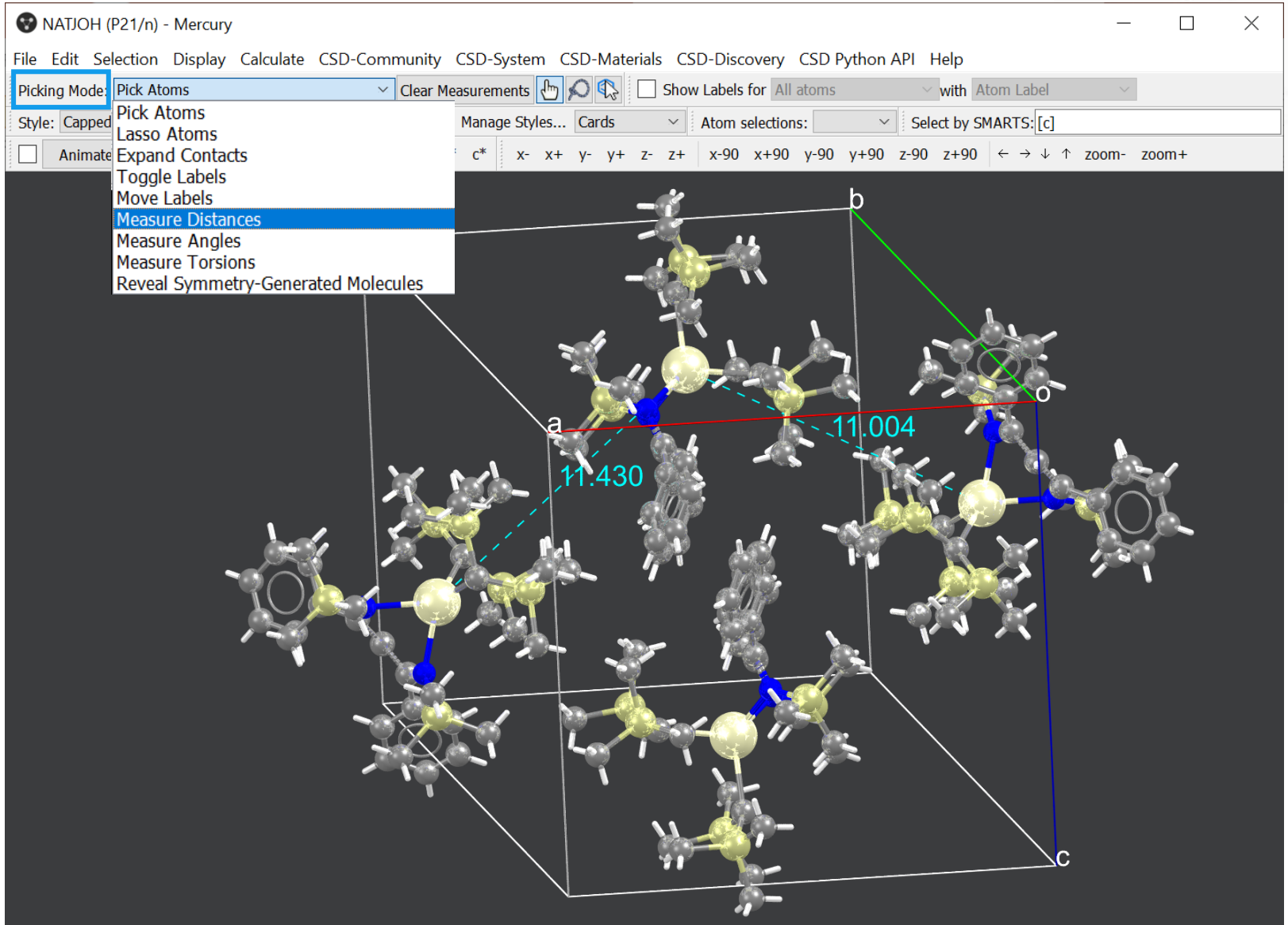


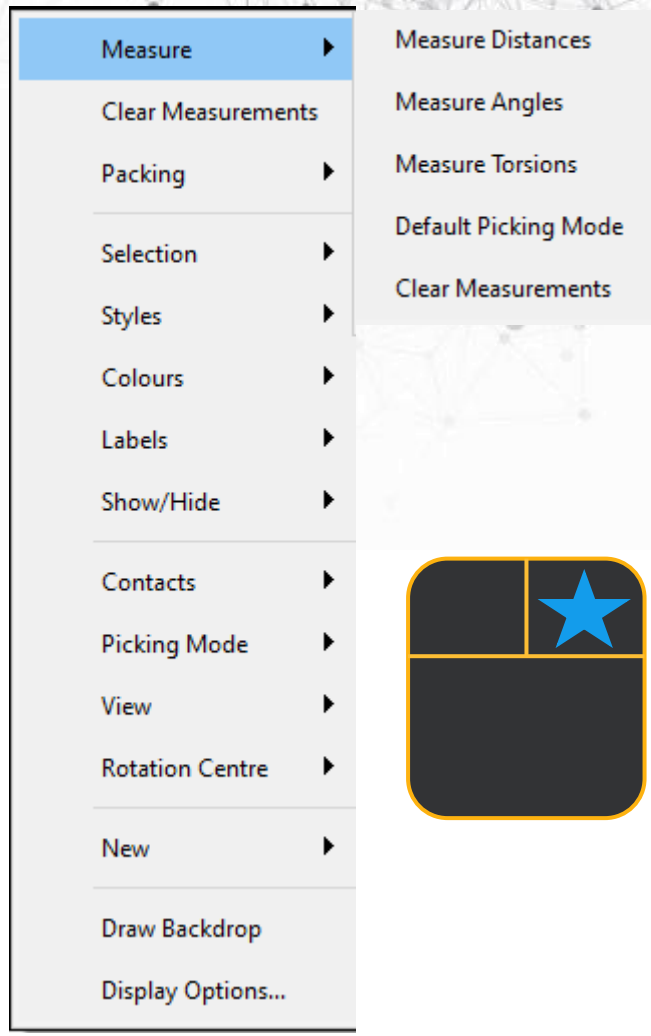


CCDC

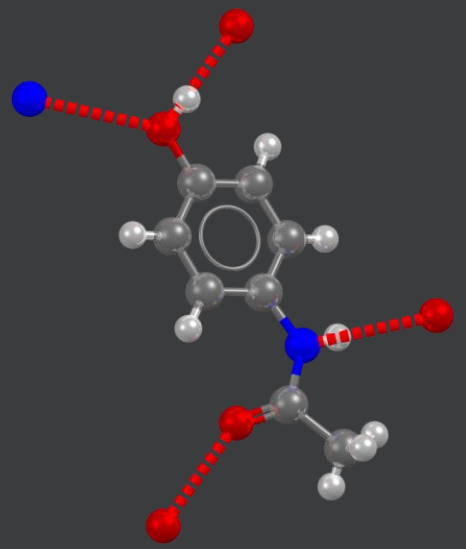
Measure distances

CSD Refcode:
NATJOH

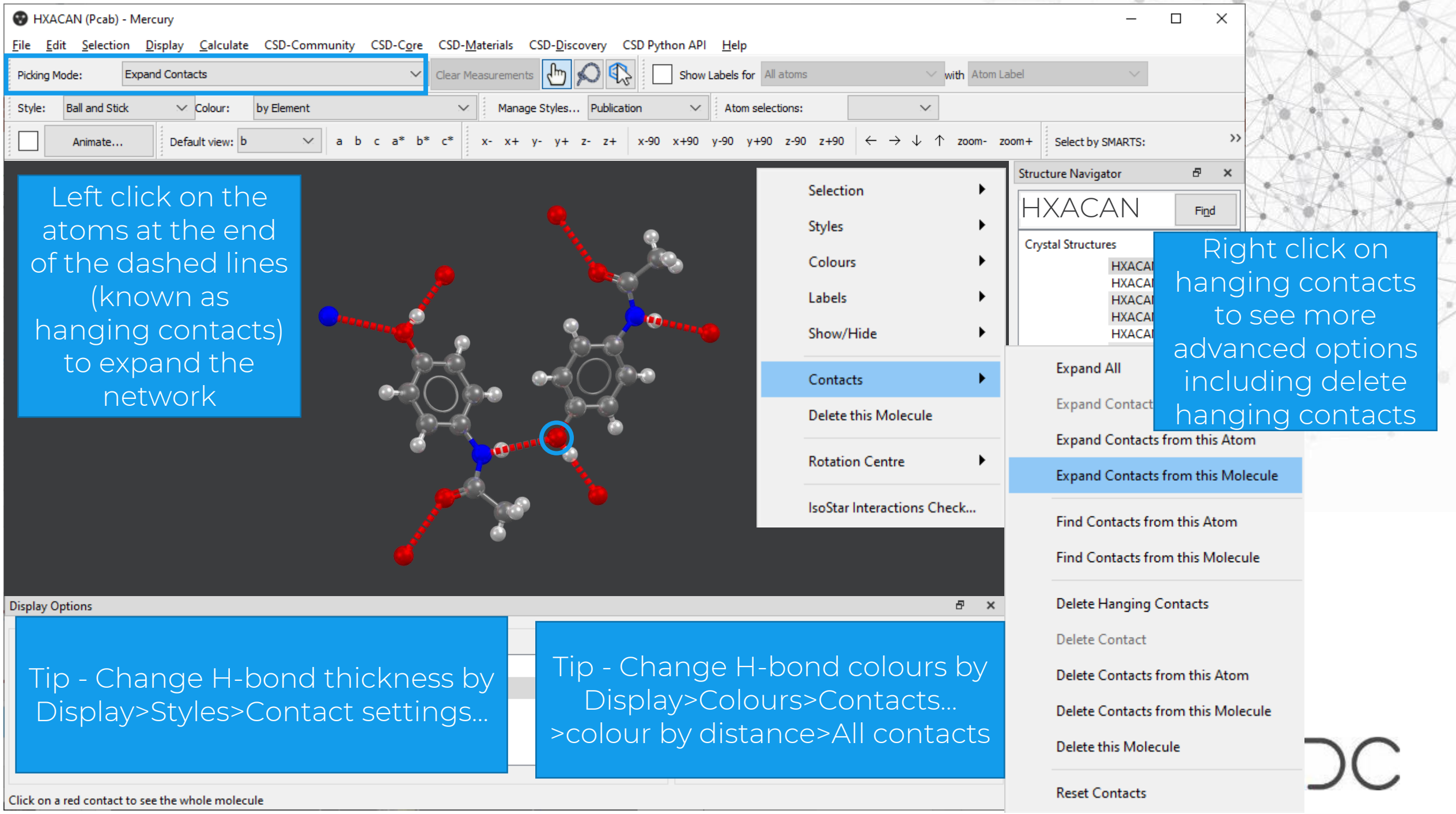




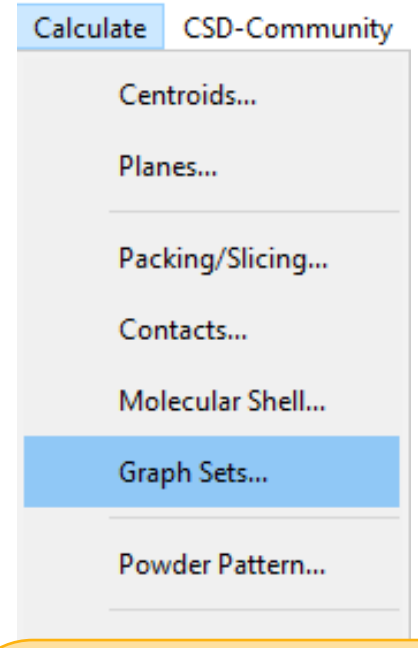
Visualising hydrogen bonds



Click on “Default definition” to change the default H-bond definition

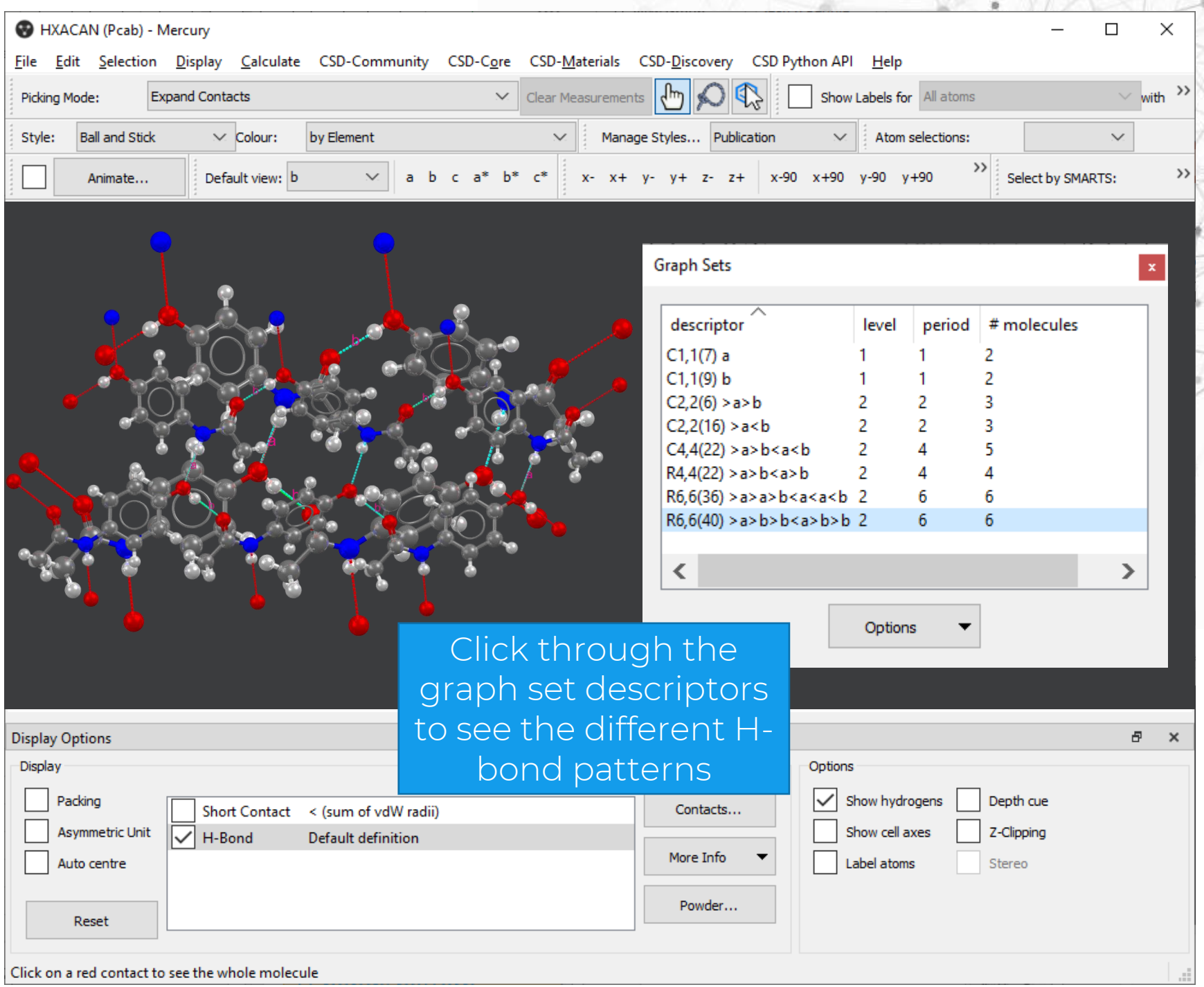

HXACAN (Pcab) - Mercury
File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Discovery CSD Python API Help
Picking Mode: Expand Contacts
Clear Measurements
Show Labels for All atoms with Atom Label
Style: Ball and Stick
Colour: by Element
Manage Styles... Publication
Atom selections:
Animate...
Default view: b
a b c a* b* c*
x- x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-90 z+90
zoom- zoom+
Select by SMARTS:
Left click on the atoms at the end of the dashed lines (known as hanging contacts) to expand the network
Selection
Styles
Colours
Labels
Show/Hide
Contacts
Delete this Molecule
Rotation Centre
IsoStar Interactions Check...
Structure Navigator
HXACAN
Find
Crystal Structures
Right click on hanging contacts to see more advanced options including delete hanging contacts
Expand All
Expand Contact
Expand Contacts from this Atom
Expand Contacts from this Molecule
Find Contacts from this Atom
Find Contacts from this Molecule
Delete Hanging Contacts
Delete Contact
Delete Contacts from this Atom
Delete Contacts from this Molecule
Delete this Molecule
Reset Contacts
Display Options
Tip - Change H-bond thickness by Display>Styles>Contact settings...
Tip - Change H-bond colours by Display>Colours>Contacts... >colour by distance>All contacts
Click on a red contact to see the whole molecule

Graph Sets

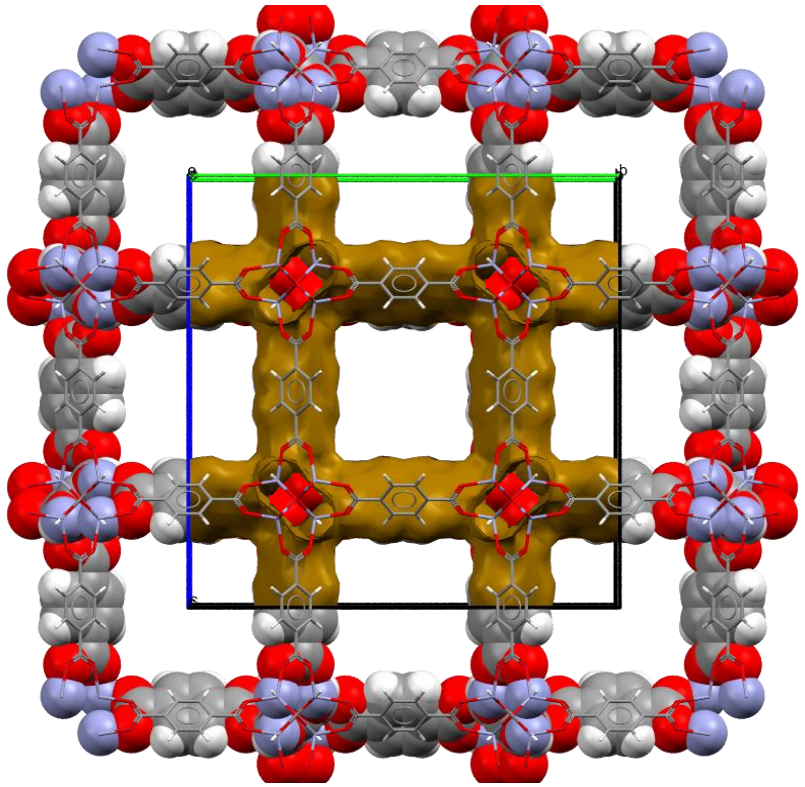


Graph Sets describe the H-bonds pattern.

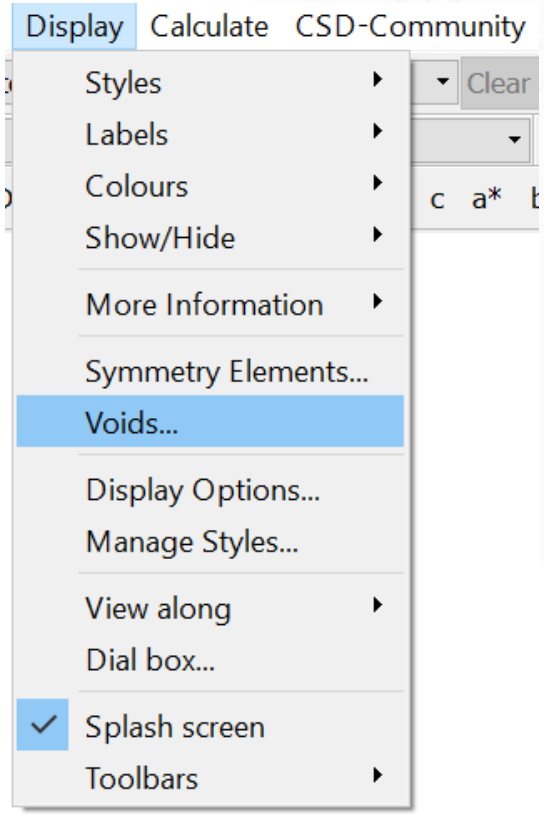
- M.C.Etter, *Acc. Chem. Res.*, 23, 120, 1990.
- J.Bernstein, R.E.Davis, L..Shimoni, N.-L. Chang, *Angew. Chem. Int. Ed.*, 34, 1555, 1995.
- W.D.S.Motherwell, G.P.Shields and F.H.Allen, *Acta. Cryst.* B56, 466, 2000.



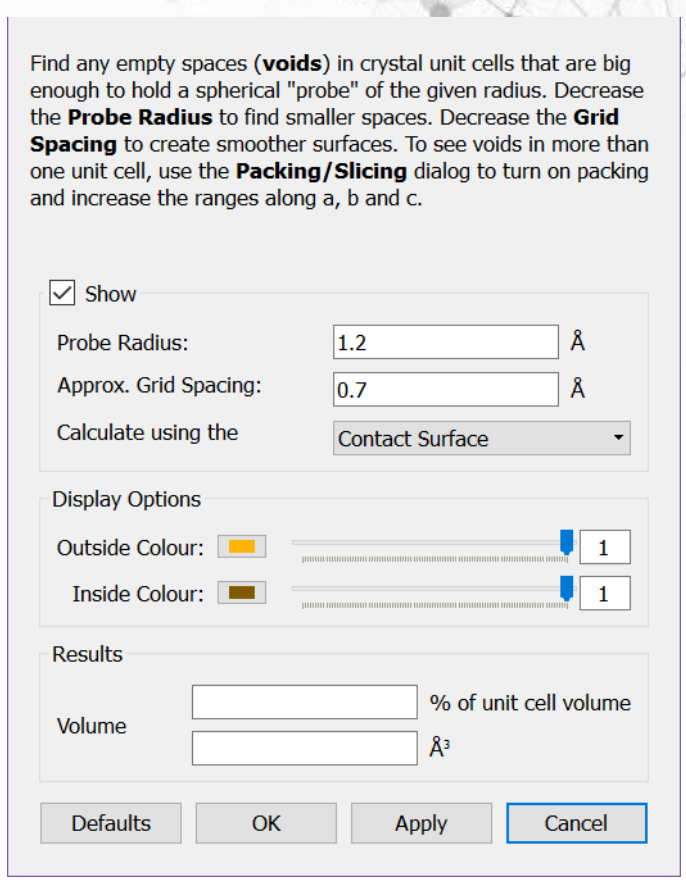
Empty space visualisation



CSD Refcode: SAHYIK (MOF5)

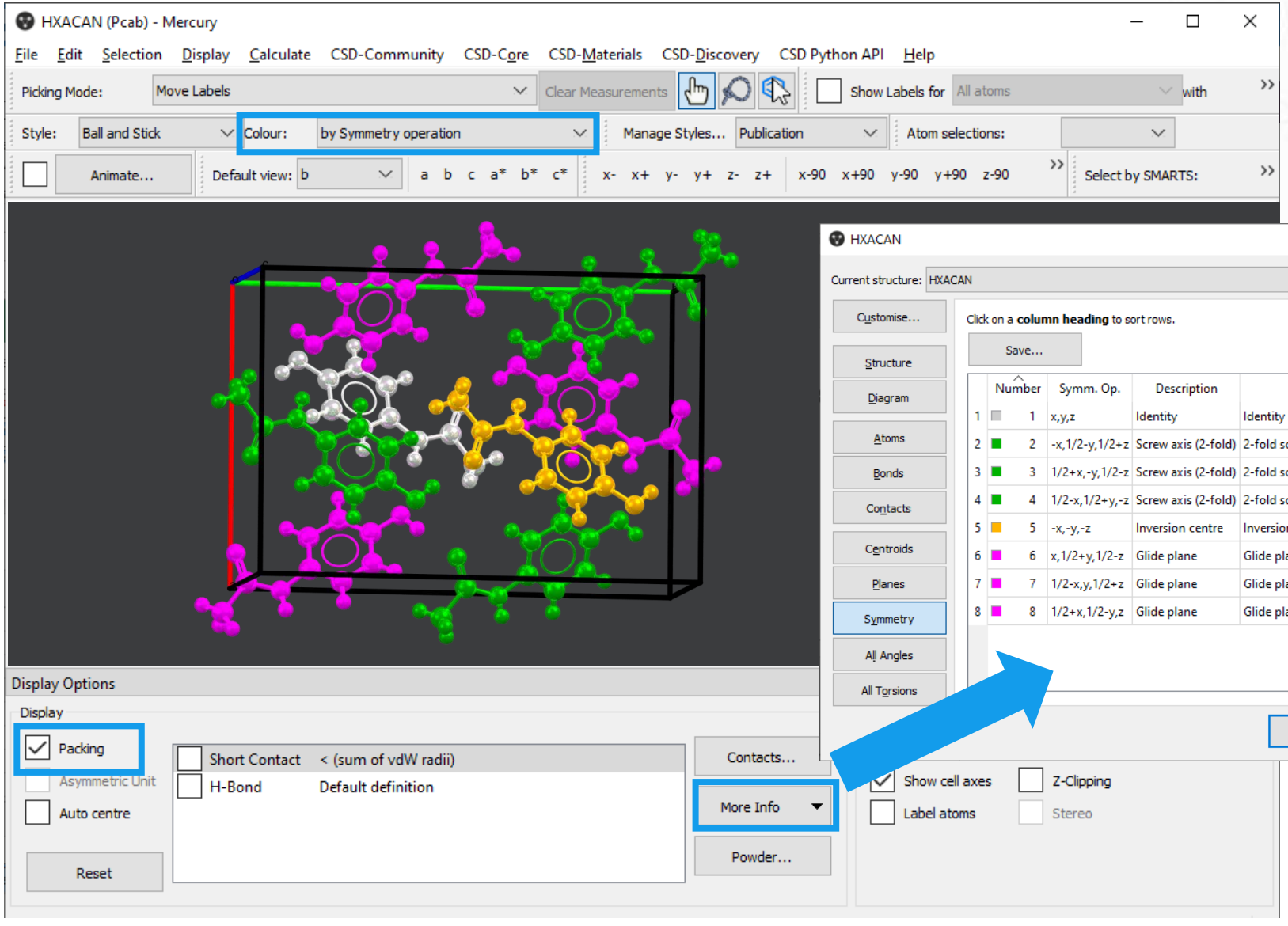


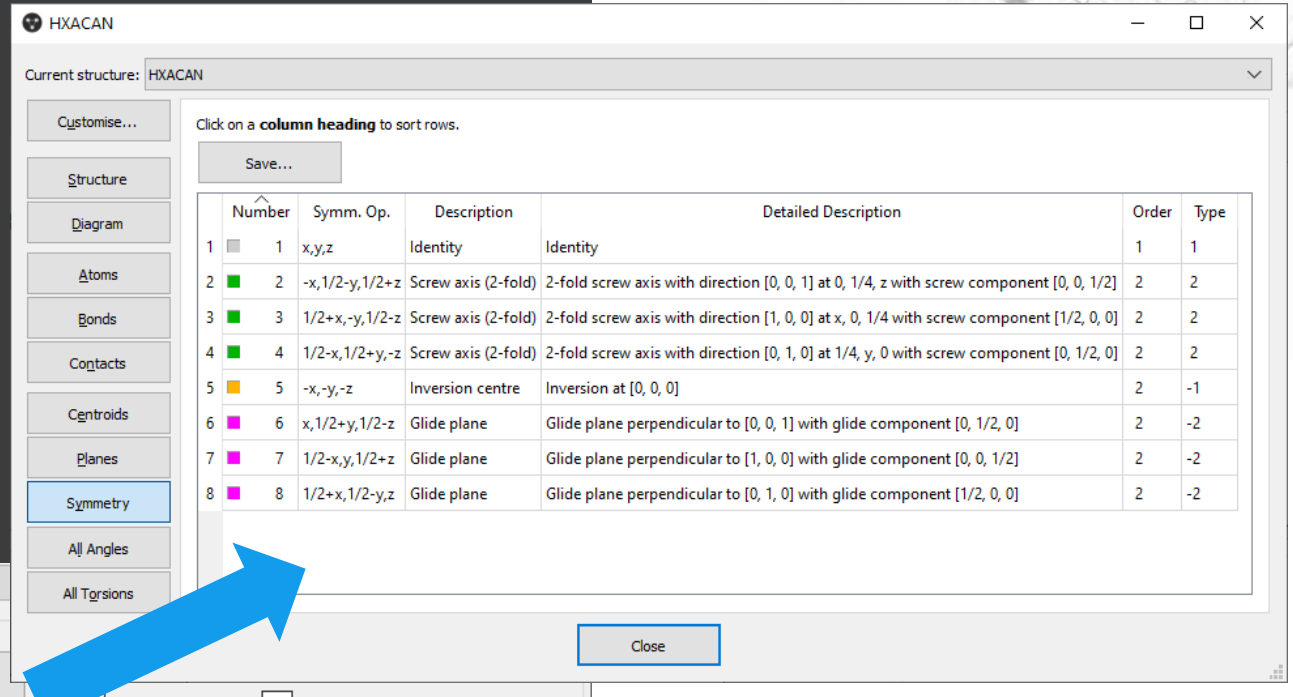
Analysing voids helps us better understand the nature of porous materials which can be used in sorption, in catalysis, separations and as sensors.



Exploring symmetry

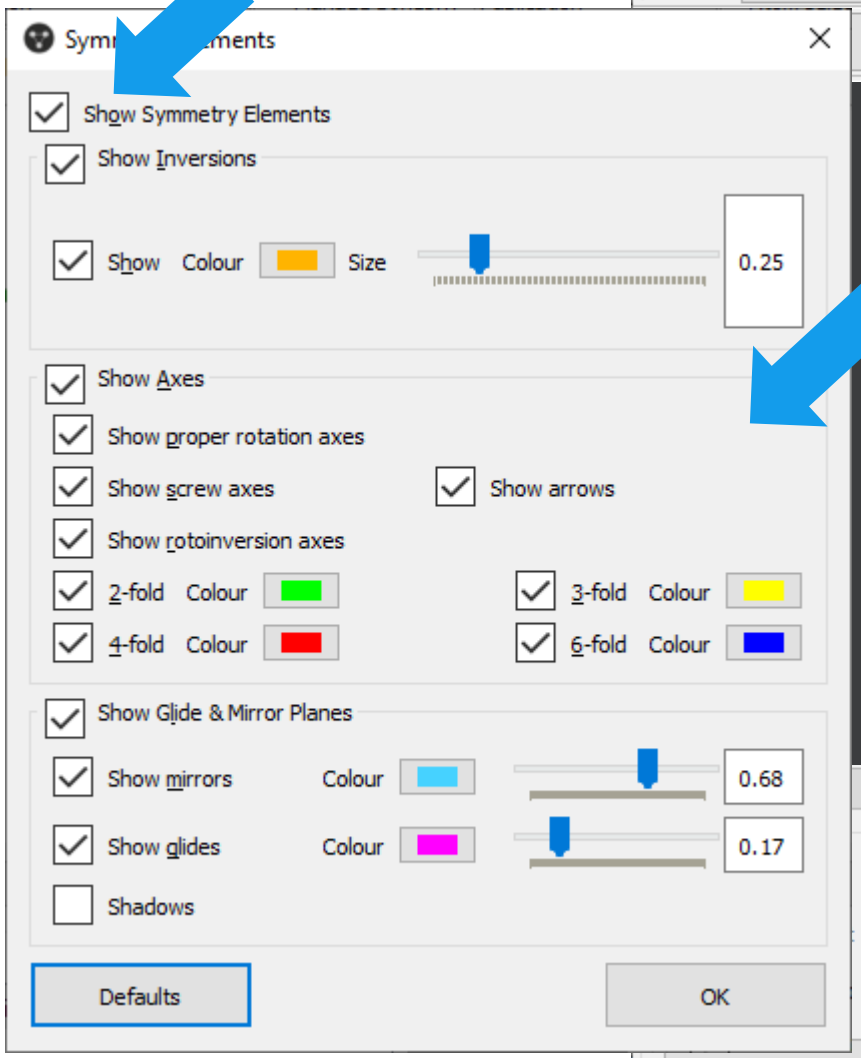
CSD Refcode:
HXACAN

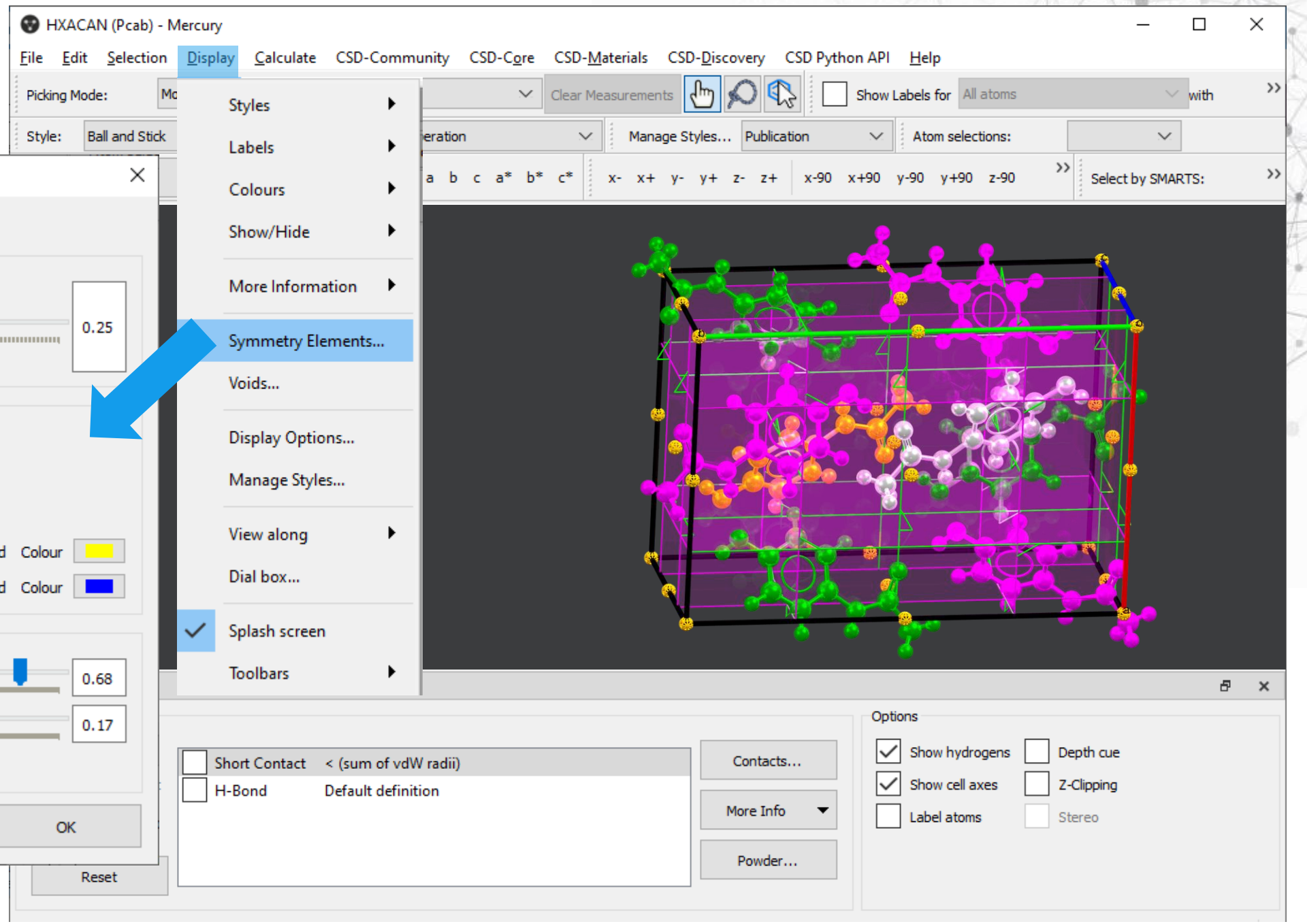




	Number	Symm. Op.	Description	Detailed Description	Order	Type
1	1	x,y,z	Identity	Identity	1	1
2	2	-x,1/2-y,1/2+z	Screw axis (2-fold)	2-fold screw axis with direction [0, 0, 1] at 0, 1/4, z with screw component [0, 0, 1/2]	2	2
3	3	1/2+x,-y,1/2-z	Screw axis (2-fold)	2-fold screw axis with direction [1, 0, 0] at x, 0, 1/4 with screw component [1/2, 0, 0]	2	2
4	4	1/2-x,1/2+y,-z	Screw axis (2-fold)	2-fold screw axis with direction [0, 1, 0] at 1/4, y, 0 with screw component [0, 1/2, 0]	2	2
5	5	-x,-y,-z	Inversion centre	Inversion at [0, 0, 0]	2	-1
6	6	x,1/2+y,1/2-z	Glide plane	Glide plane perpendicular to [0, 0, 1] with glide component [0, 1/2, 0]	2	-2
7	7	1/2-x,y,1/2+z	Glide plane	Glide plane perpendicular to [1, 0, 0] with glide component [0, 0, 1/2]	2	-2
8	8	1/2+x,1/2-y,z	Glide plane	Glide plane perpendicular to [0, 1, 0] with glide component [1/2, 0, 0]	2	-2

To show or remove symmetry elements



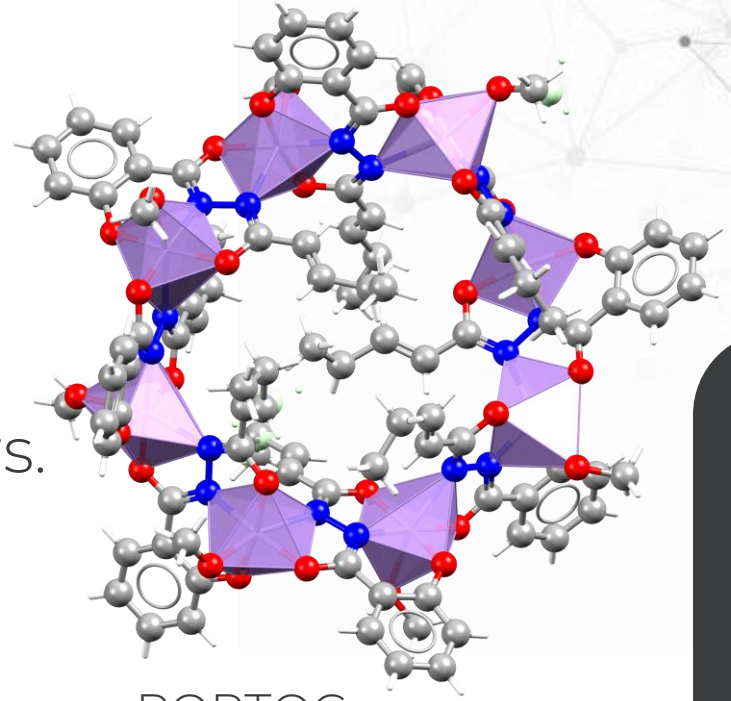


Follow along Mercury Demo

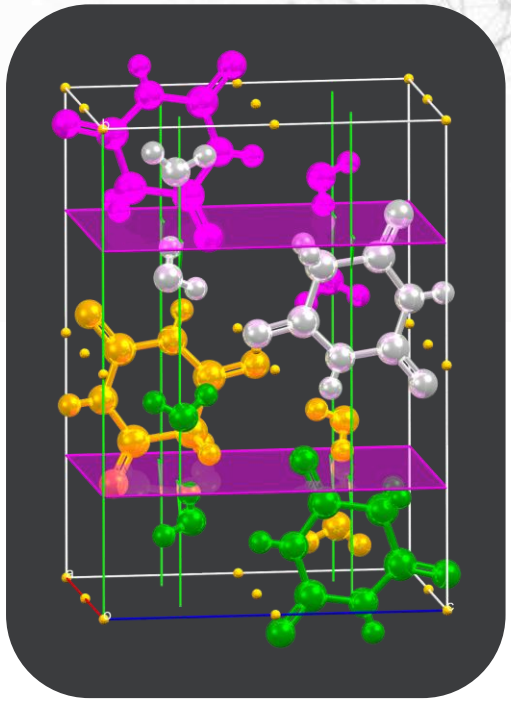
Visualisation options in Mercury

We will:

- Navigate the interface.
- Apply different styles and colours.
- Visualise packing.
- Visualise symmetry elements.



PORTOG



BARBAD09

CCDC

Agenda

- Introduction to the CSD
- Visualizing structures in the CSD
  - Slides and follow-along demo
- Analysing the geometry of structures using Mogul
  - Slides and follow-on along demo
- Analysing intermolecular interactions using FIMs
- Wrap up, quiz and summary

CCDC

Why analyse structural data?

- We can use Mercury to explore over 1.1 million structures and see in 3D how molecules pack together and the different intermolecular interactions inside the structures

- By understanding intermolecular interactions and crystal packing it can help us to design new solids with desired physical and chemical properties
  - ➢ Crystal engineering

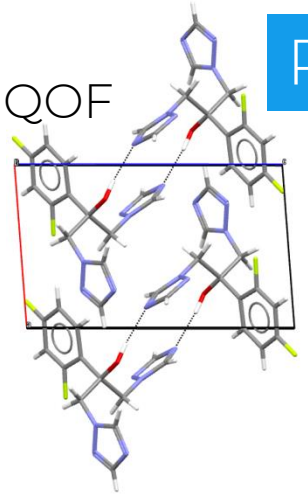
- This can be particularly helpful when exploring different polymorphic forms and can help us to better understand crystal stability

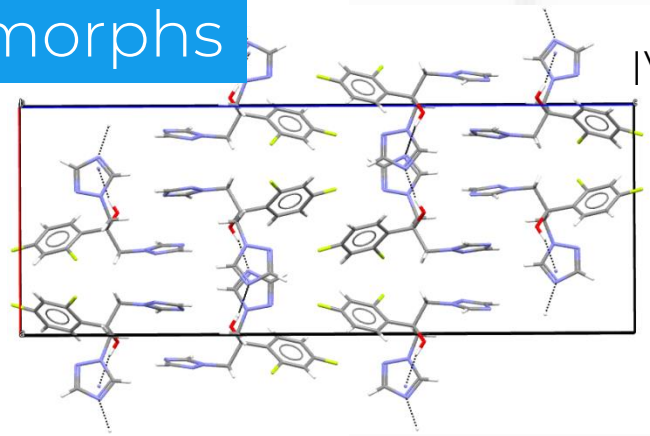
CCDC

A solid form landscape

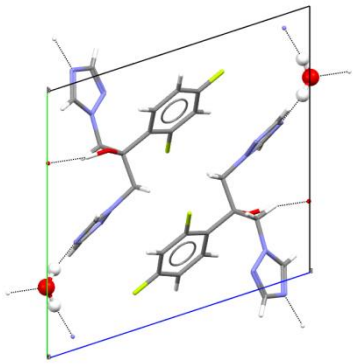
Polymorphs

IVUQOF





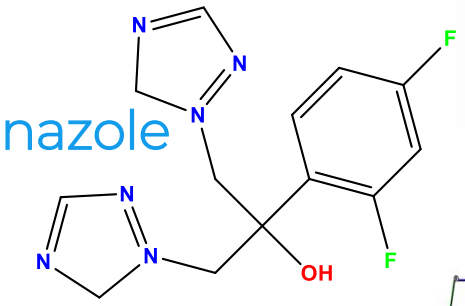
IVUQOF02

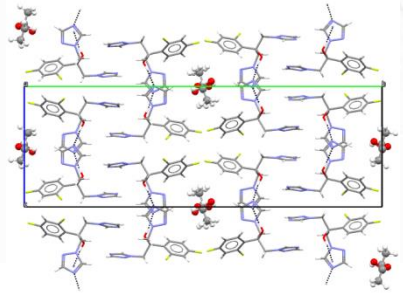


IVUQIZ

Hydrates

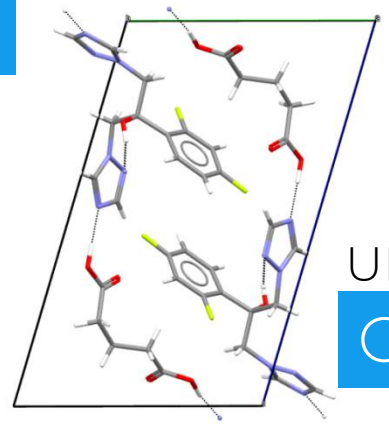
fluconazole





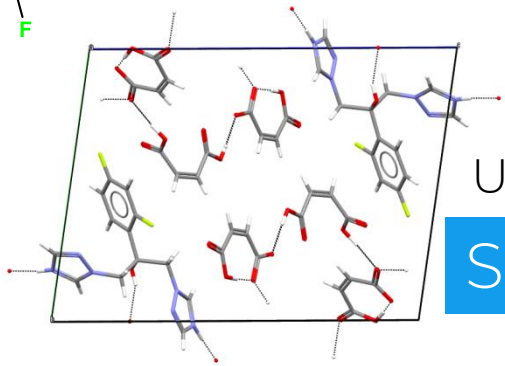
IVUQEV

Solvates



UPOQEW

Co-crystals



UPOQAS

Salts

CCDC

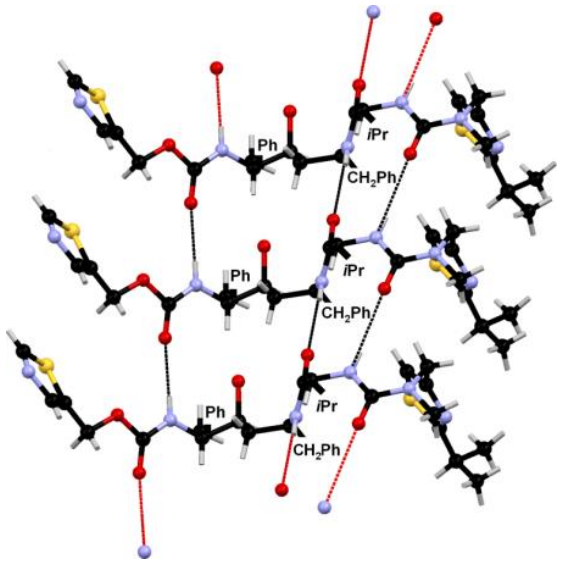
Exploring contacts and exploring chocolate

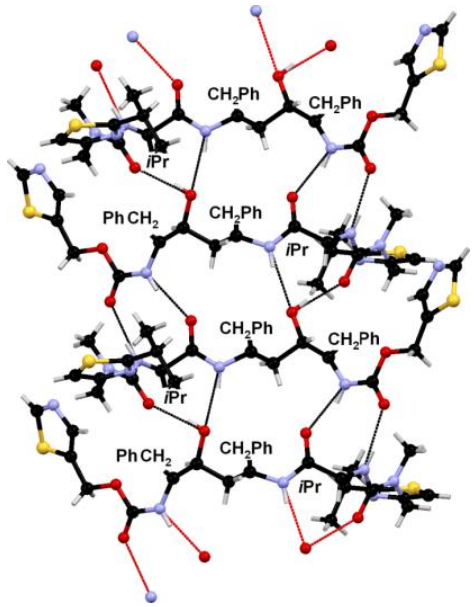
- Hydrogen bonds and short contacts can help to stabilise a crystal structure
- Different polymorphs with different bonding networks often exhibit different properties

CCDC

A real-life example.....

Can structural knowledge mitigate risk?



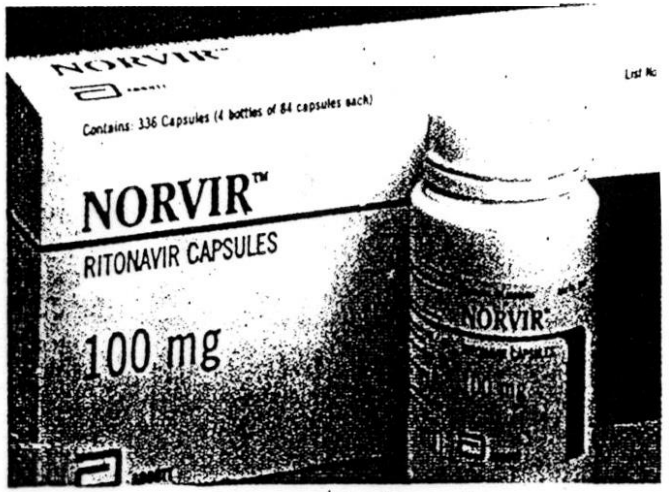


Different interactions

Different solubility
Different stability

Manufacturing problems hit Abbott's HIV drug ritonavir

Capsules of Abbott Laboratories' protease inhibitor Norvir (ritonavir) are likely to become unavailable by the middle of August. The company has a problem with the manufacture of the anti-HIV capsules which it cannot resolve at present.



Capsules unlikely to be available from mid-August

The problem relates to "undesirable" crystal formation. Abbott says that a series of ples from a number of marketed batches of capsules were examined and there was no

Bauer *et al. Pharm. Res.*, (2001) 859, DOI:10.1039/B910882C

Structural Informatics

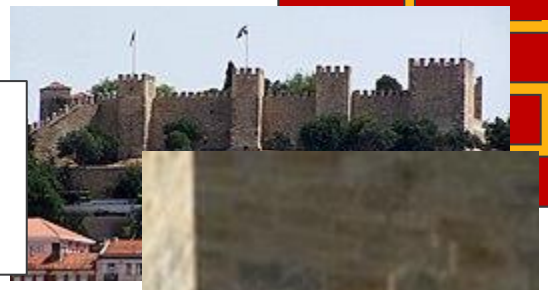
Which is the stable wall?

Belém Tower c. 1514

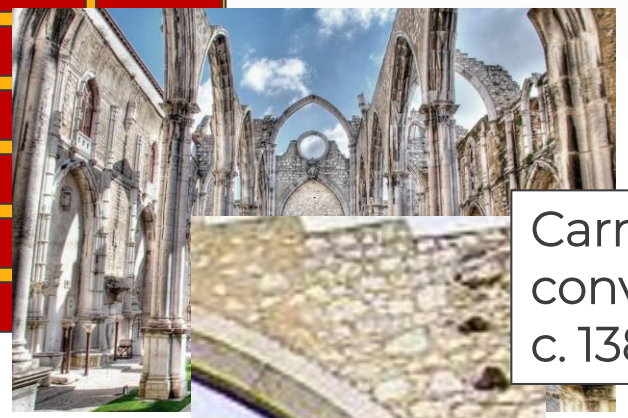
Águas Livres Aqueduct c.1731

A

B



Castelo de São Jorge

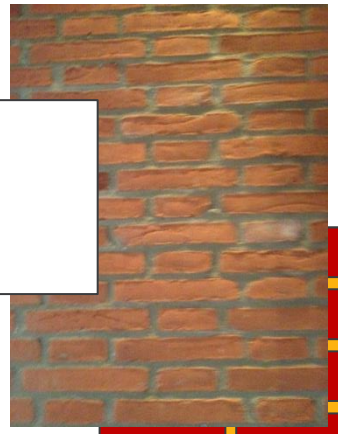


Carmo convent c. 1389

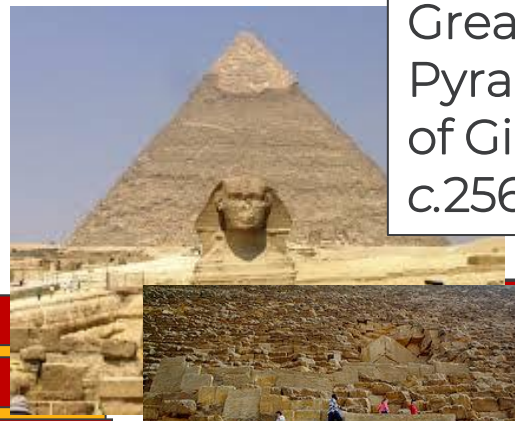
CCDC

Structural Informatics

Which is the stable wall?



The CCDC c.1992



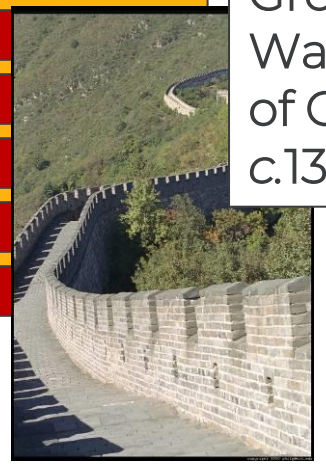
Great Pyramid of Giza c.2560 BC

Hadrian's Wall c.122

A

B

My House c.1967



Great Wall of China c.1368

The database of walls indicates that A is the frequently observed arrangement and therefore we can predict it is the most stable form

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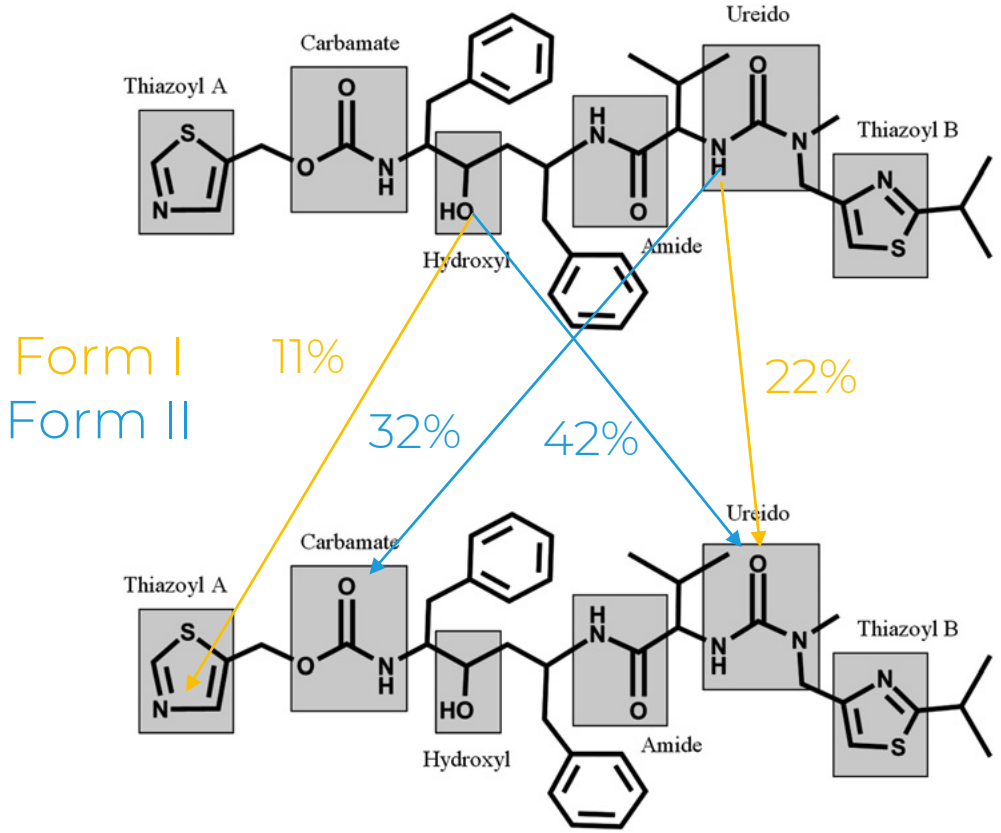
Predicting unlikely interactions

Predictive analytics is used to identify the likelihood of specific molecular interactions occurring from similar crystal structures



The integration of solid-form informatics into solid-form selection

Neil Feeder[a], Elna Pidcock[a], Anthony M. Reilly[a], Ghazala Sadiq[a], Cheryl L. Doherty[b], Kevin R. Back[b], Paul Meenan[c] and Robert Docherty[b]

One in half a million: a solid form informatics study of a pharmaceutical crystal structure

Peter T. A. Galek,*[a] Elna Pidcock,[a] Peter A. Wood,[a] Ian J. Bruno[a] and Colin R. Groom[a]

Navigating the Solid Form Landscape with Structural Informatics

Peter T. A. Galek, Elna Pidcock, Peter A. Wood, Neil Feeder, Frank H. Allen

Book Editor(s): Yuriy A. Abramov

Knowledge-based H-bond prediction to aid experimental polymorph screening

Peter T. A. Galek,*[ab] Frank H. Allen,[a] László Fábián[ab] and Neil Feeder[c]

Galek *et al*, *CrystEngComm*, (2009), 11, 2634 - 2639

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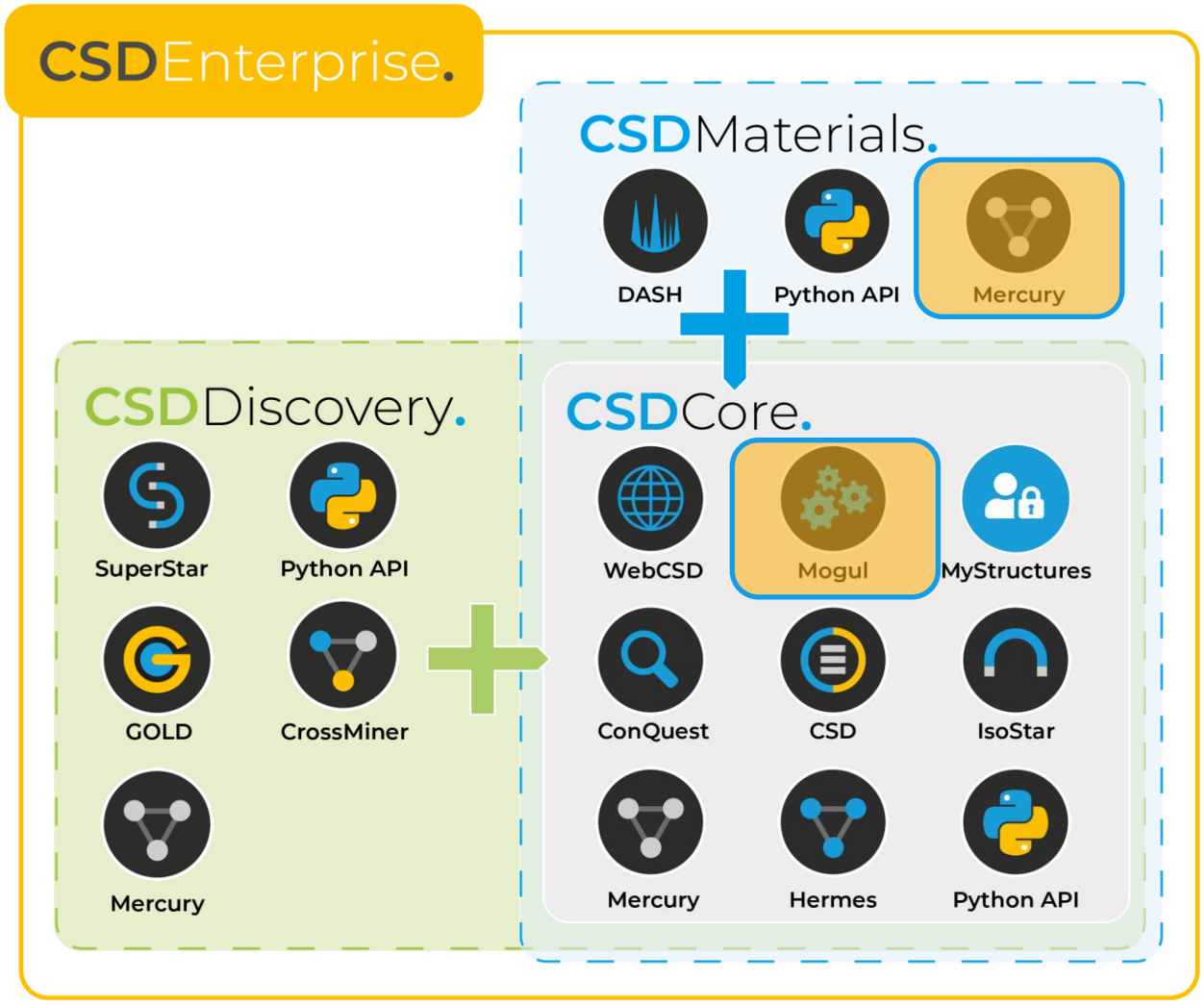
The CSD software



Professional Services

Research & Knowledge partnerships

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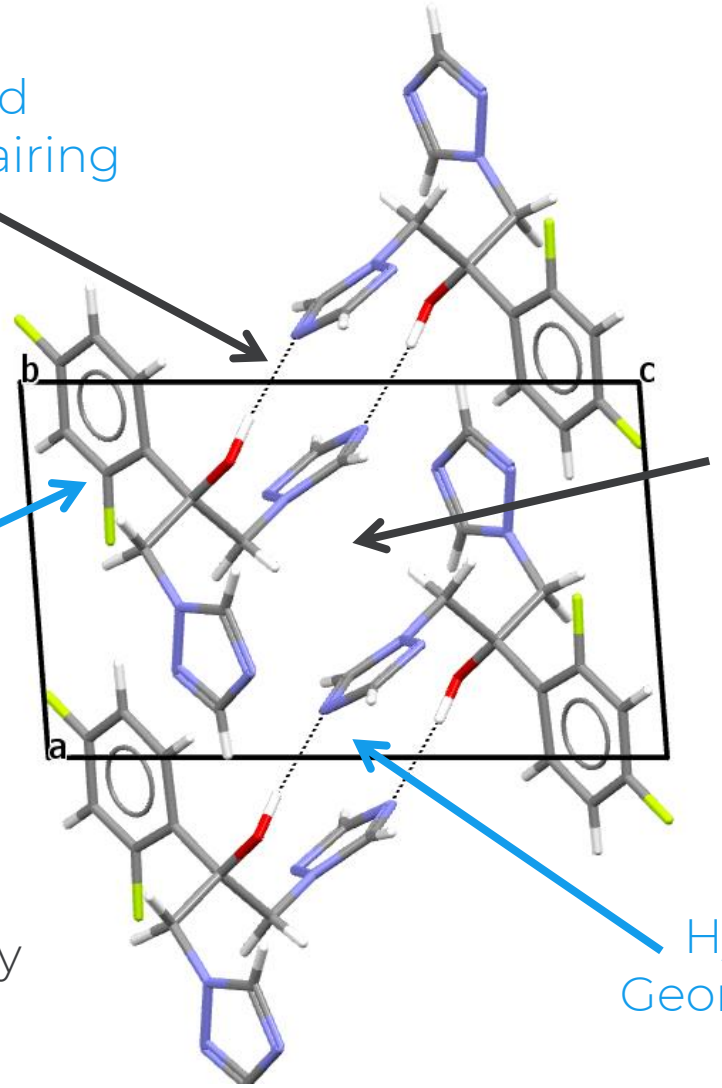
Characteristics that influence stability

Hydrogen Bond
Donor/Acceptor Pairing



'Non-Hydrogen Bond'
Intermolecular
Interactions

Molecular
Conformation

Hydrogen Bond
Geometry, Symmetry
and Motif

We can mine the CSD to identify these intra and intermolecular geometric preferences.

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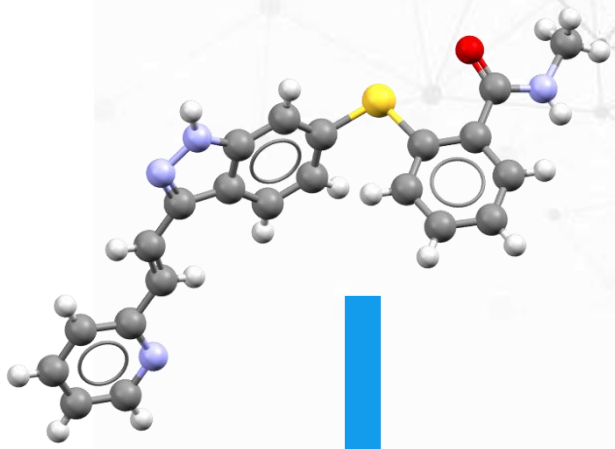
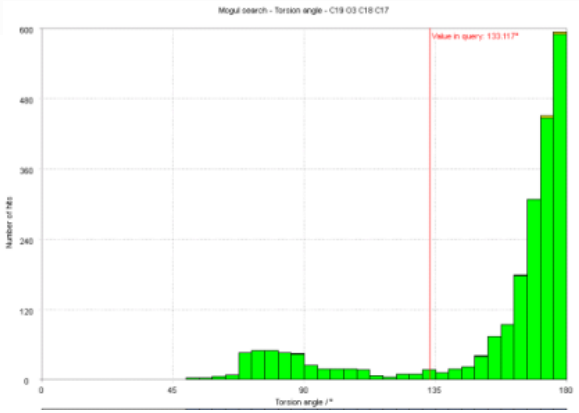
CSD-Core – Conformations

- Mogul provides precise information on preferred molecular geometries
- Validate molecular geometries rapidly using interactive plots & statistics
- Identify any unusual features of a given query structure
- Mine millions of chemically classified bond lengths, angles, torsion angles and ring conformations in the CSD





Bruno *et al., J. Chem. Inf. Comput. Sci.*, 44, 2133-2144, 2004

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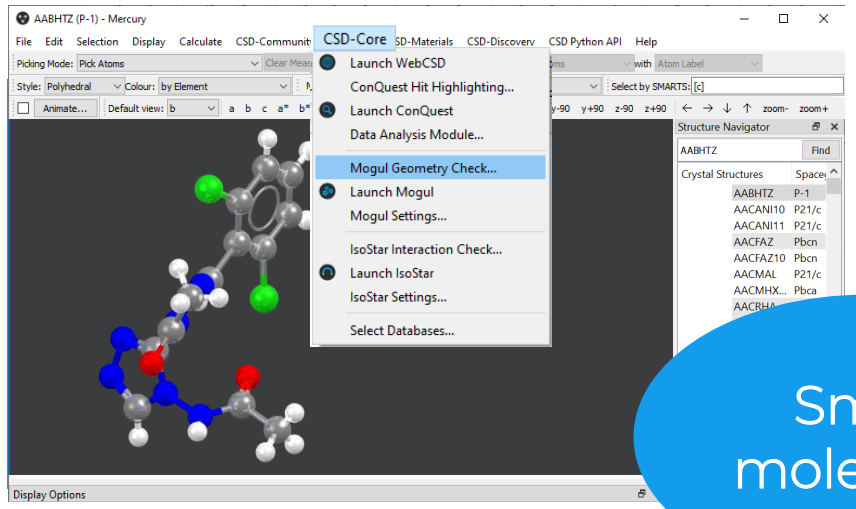
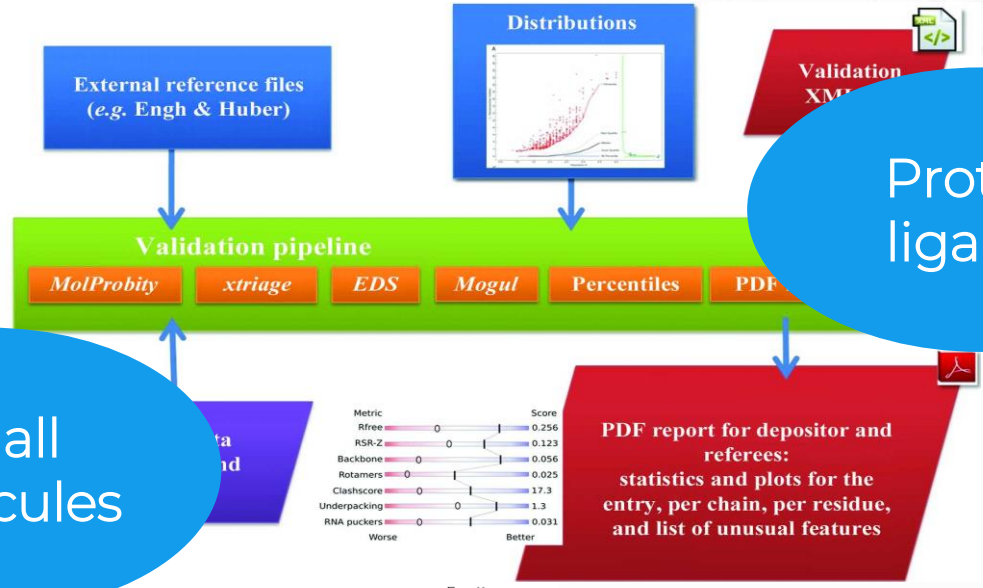
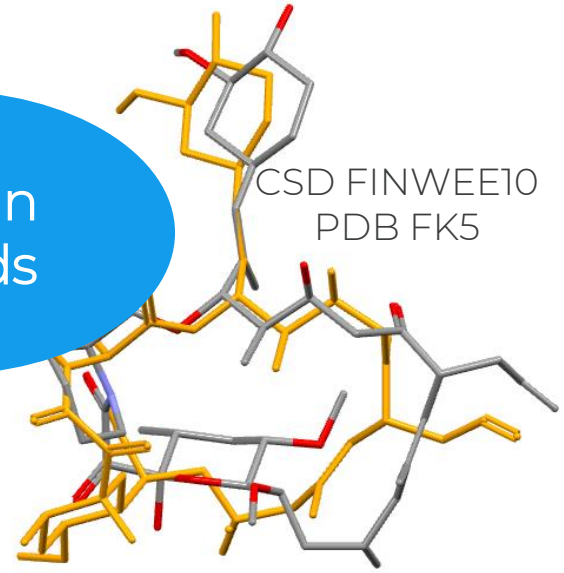
Using Mogul to check new structural data

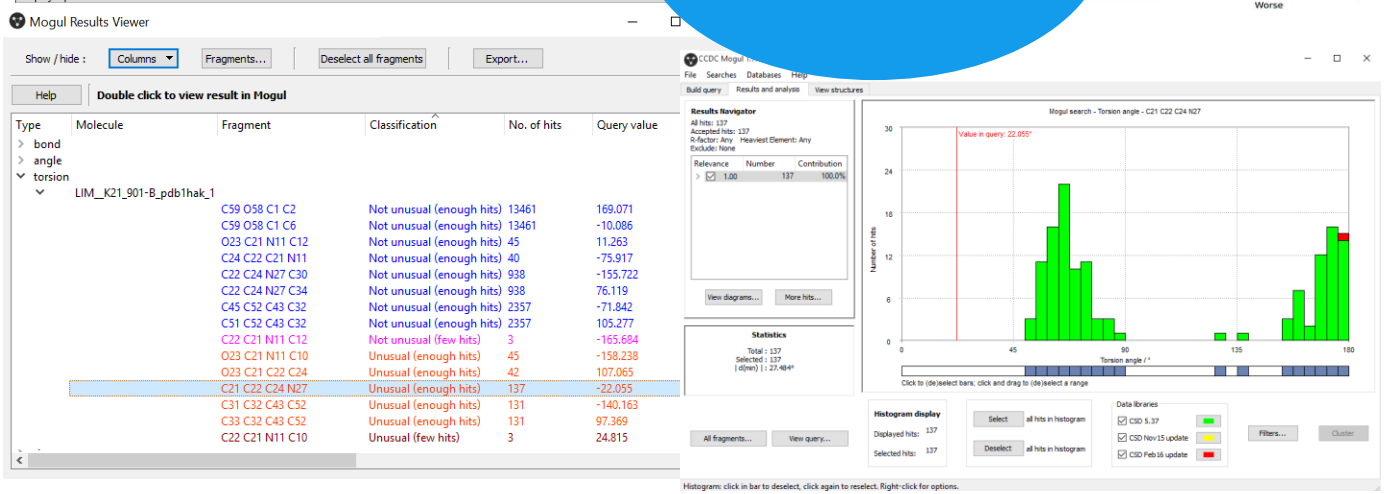


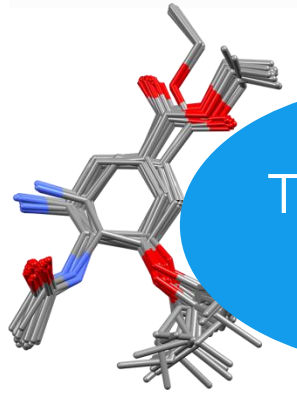


Small molecules

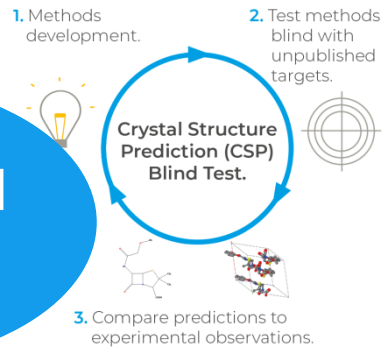
Protein ligands







Theoretical data



I.J.Bruno, G.P.Shields, R.Taylor, *Acta Cryst.* (2011). B67, 333-349 DOI: 10.1107/S0108768111024608

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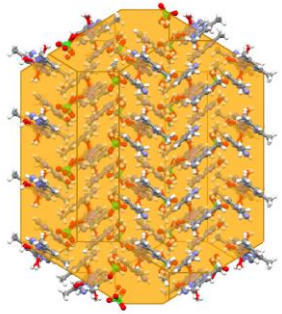
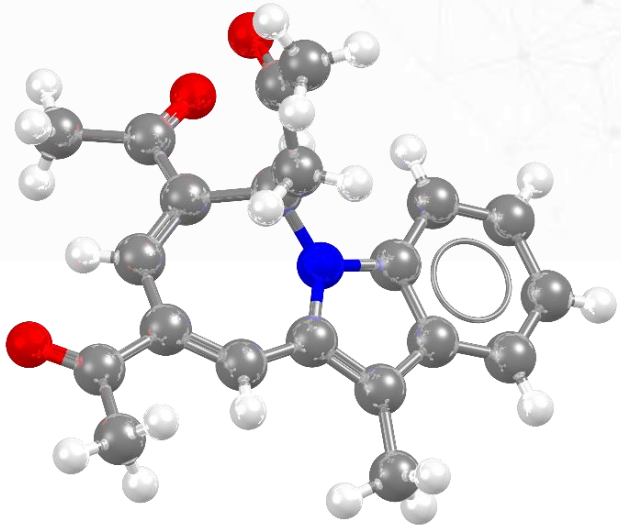
About you

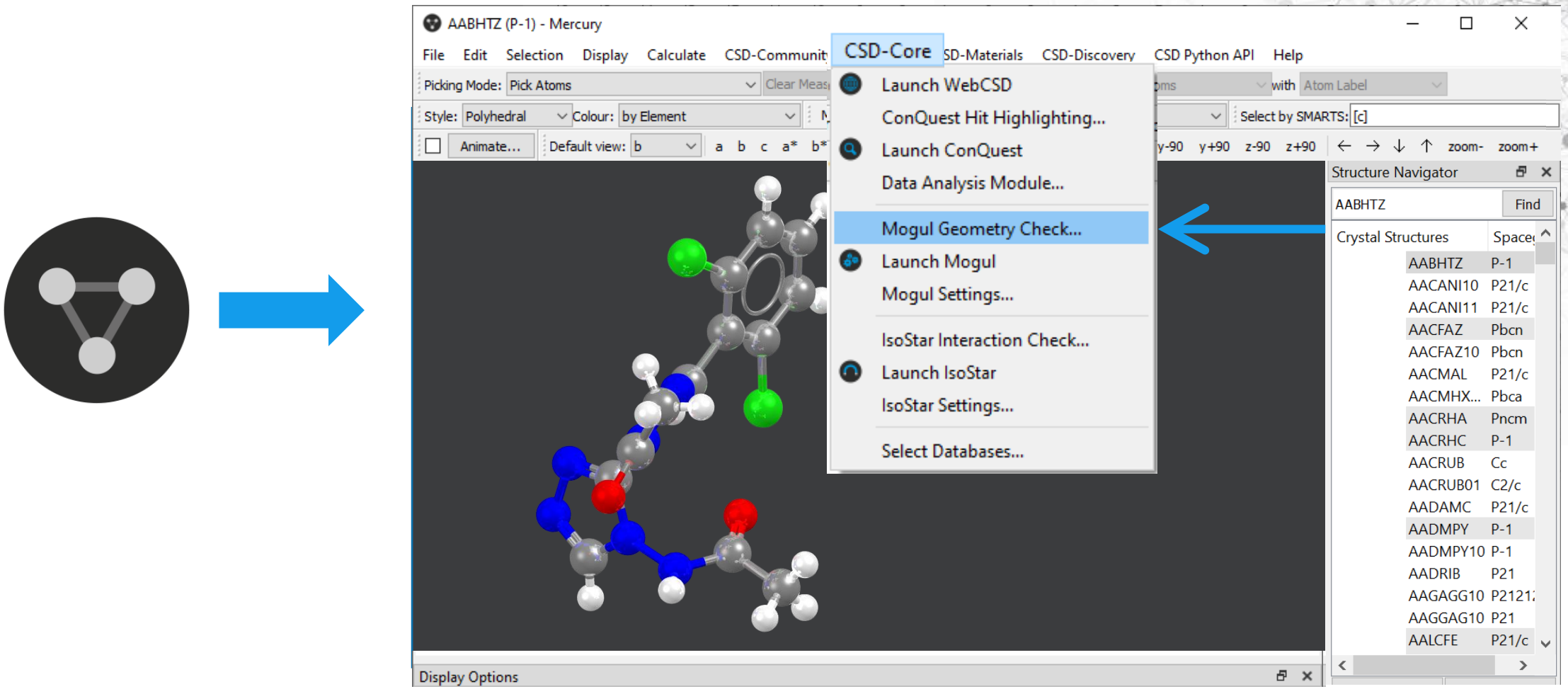
What would you like to analyse using Mogul?

- CSD/published structures
- Your own experimental structures
- Theoretical structures
- Protein ligands
- Other

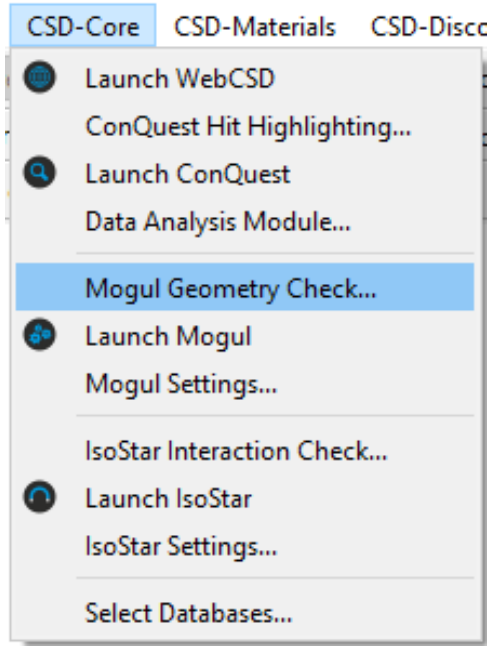


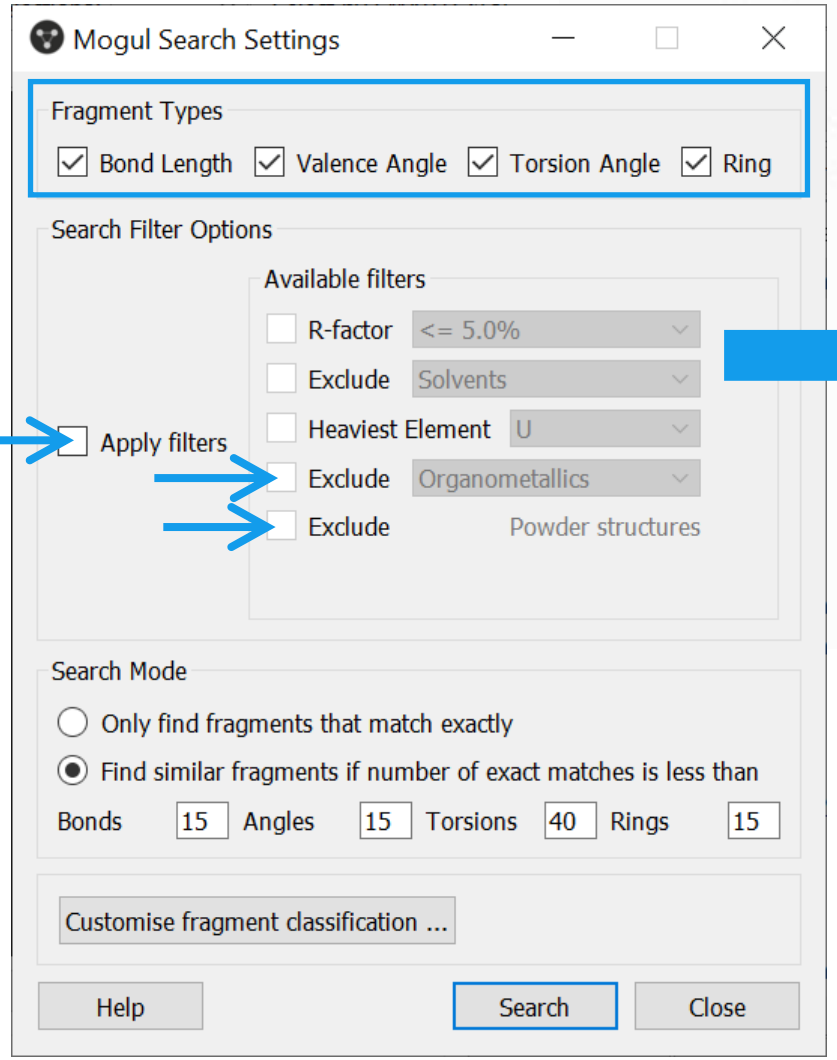


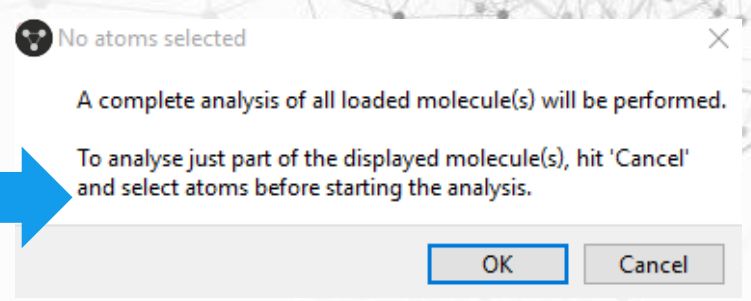
Mogul – Launch from Mercury

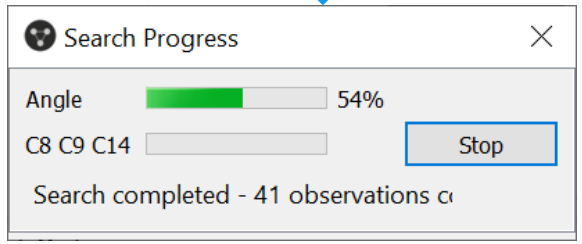


Mogul Geometry Check









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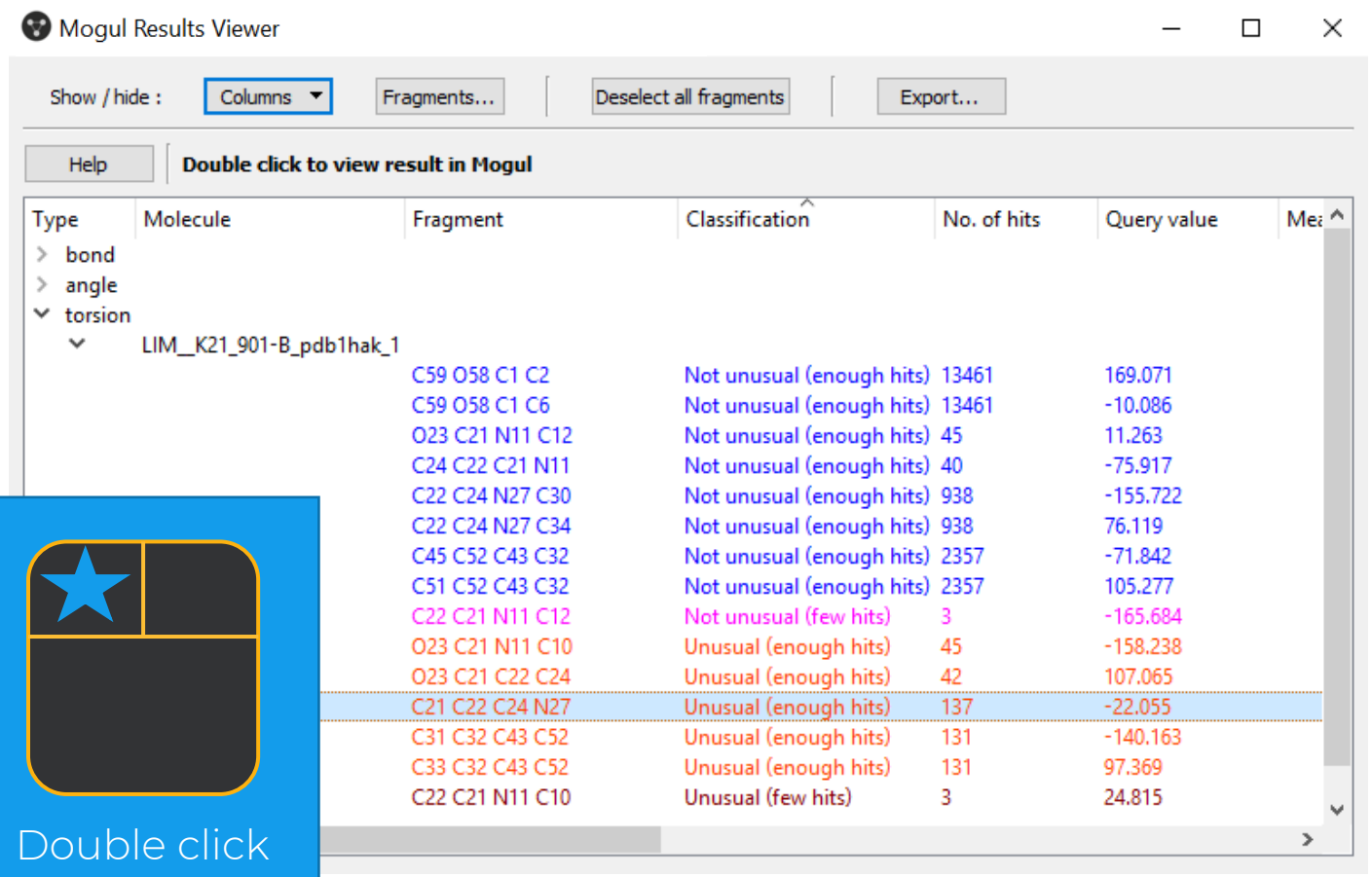
Mogul Geometry Check - Results

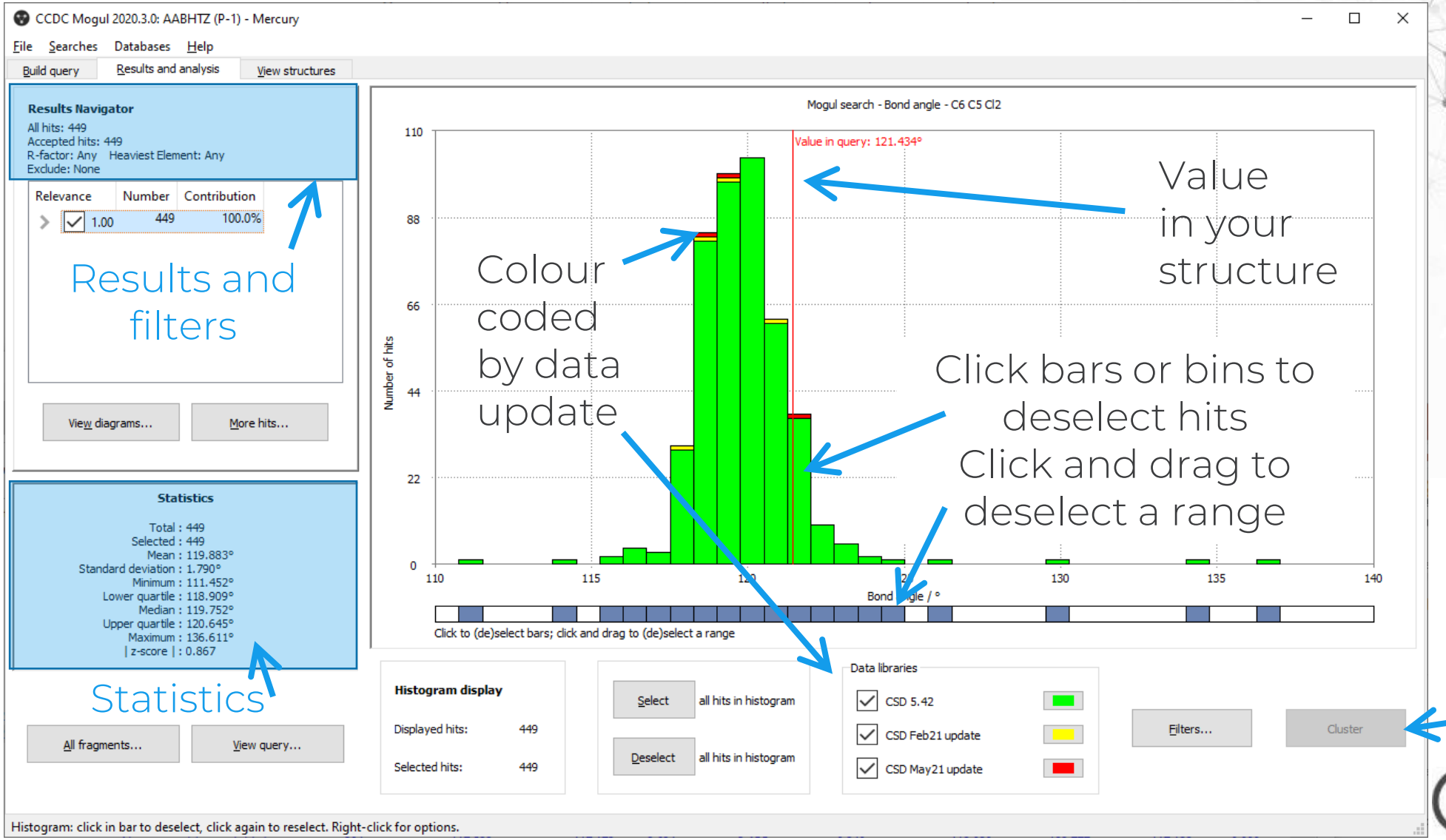


Double click on a row to view result in Mogul

Colour code:

- **Blue**: It is a **not unusual** value in the CSD and there are **enough data** in the CSD for comparison.
- **Pink**: It is a **not unusual** value in the CSD, but there are only **few data** in the CSD for comparison.
- **Orange**: It is an **unusual** value in the CSD and there are **enough data** in the CSD for comparison.
- **Brown**: It is an **unusual** value in the CSD, but there are only **few data** in the CSD for comparison.

Mogul Geometry Check - Results



Histogram built with data from structures in the CSD

Cluster only available for rings

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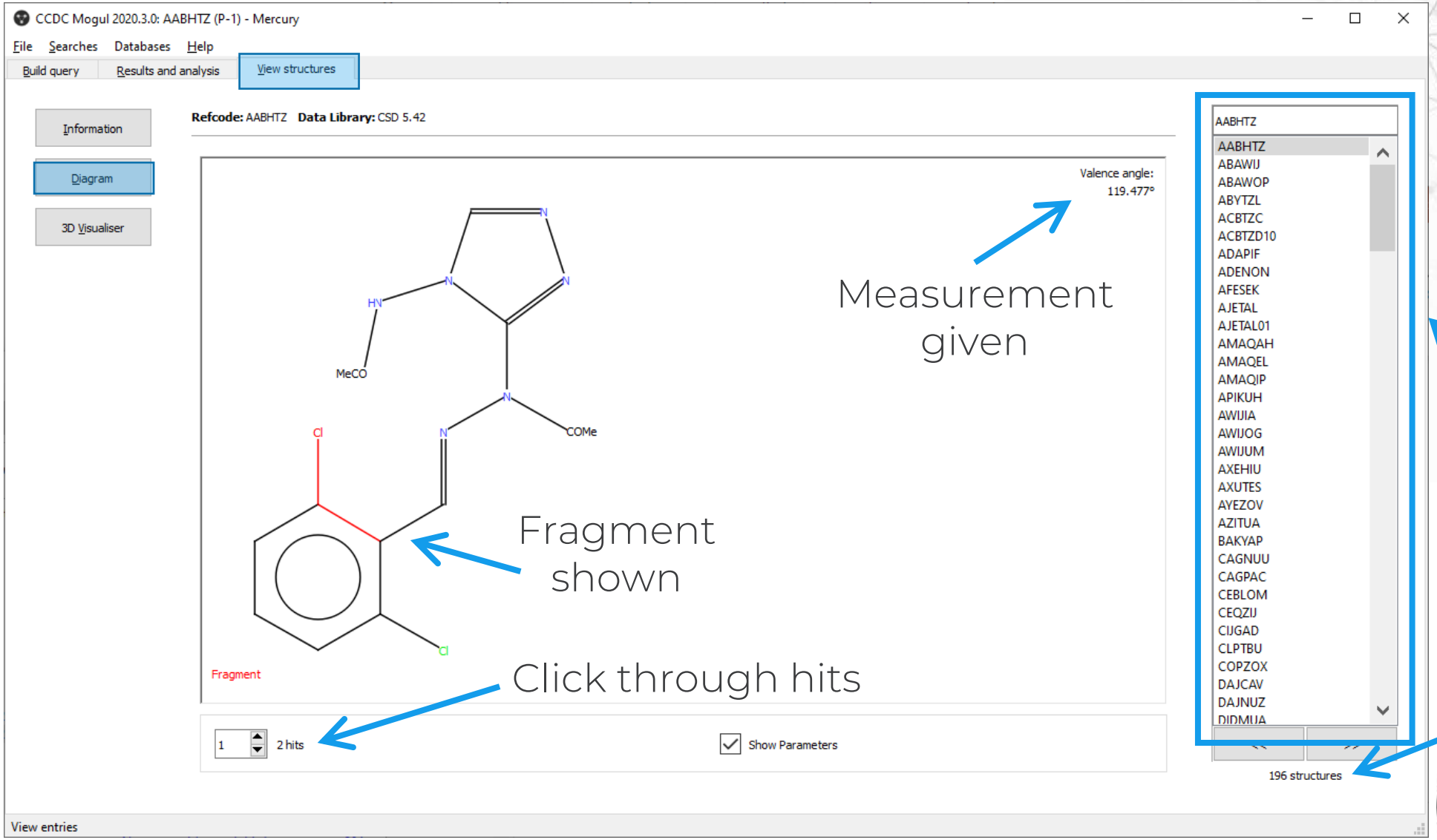
Mogul Geometry Check – View structures

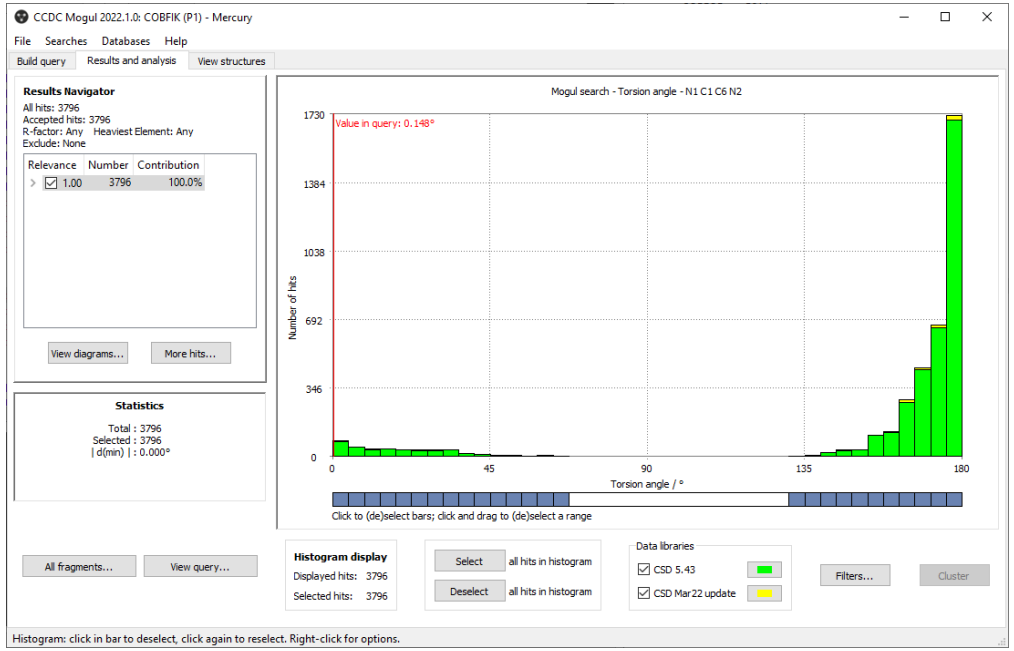


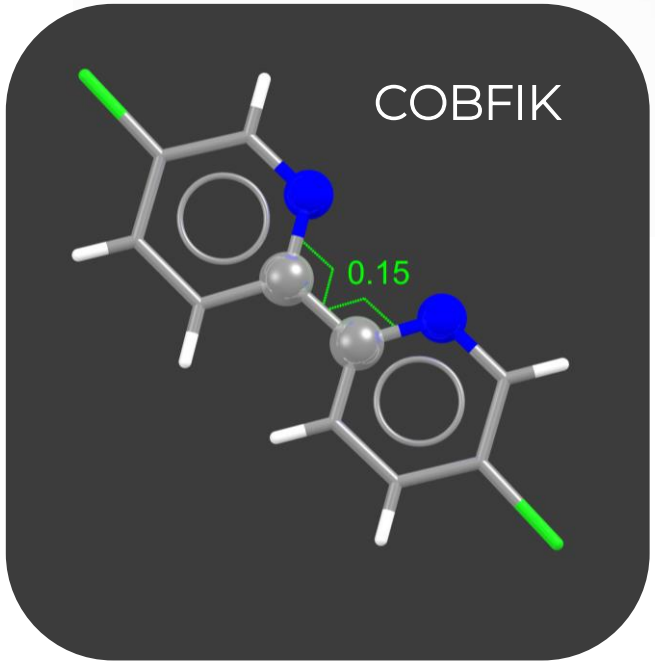
Follow along Mogul Demo

Example of a Mogul Geometry Check

We will:

- Run a Mogul Geometry Check from Mercury.
- Visualise and analyse the results.





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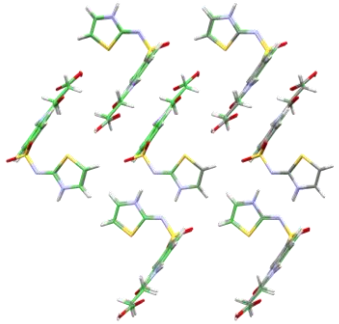
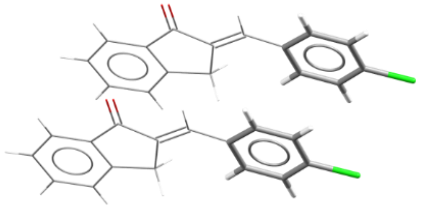
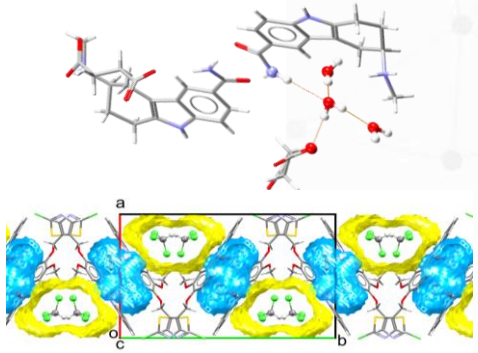
CSD-Materials overview



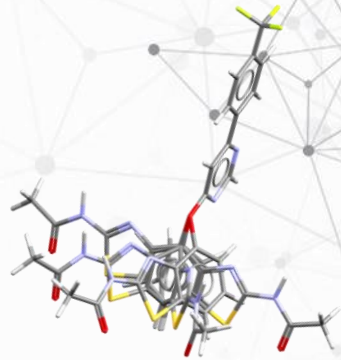
Crystal Packing Similarity



Motif Search & Packing Feature Search



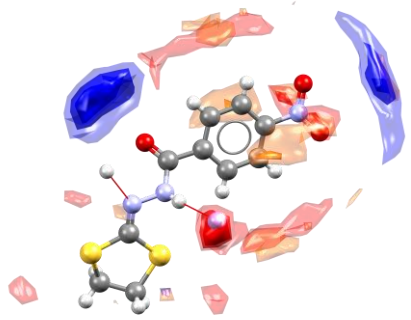
Hydrate Analyser & Solvate Analyser



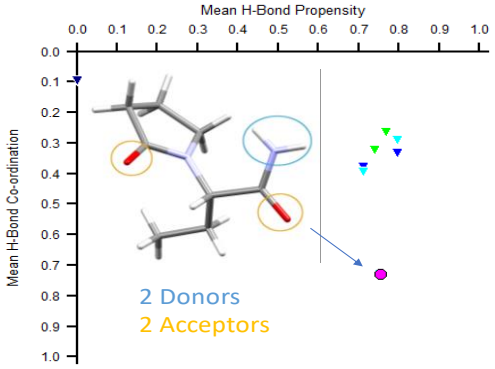
CSD Conformer Generator

Detailed Structural Analysis

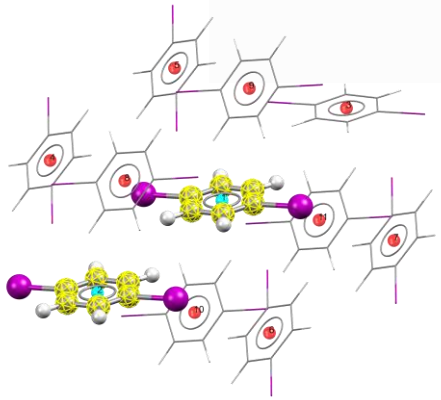
Solid Form Design



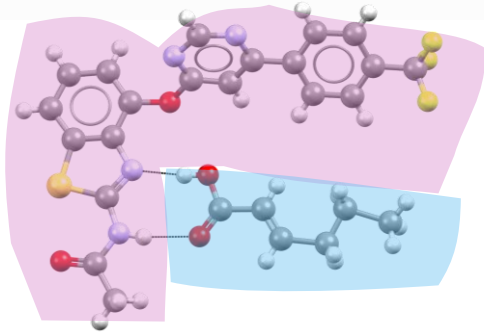
Full Interaction Maps



Hydrogen Bond Propensity



Aromatics Analyser



Molecular Complementarity

Solid Form Risk Assessment

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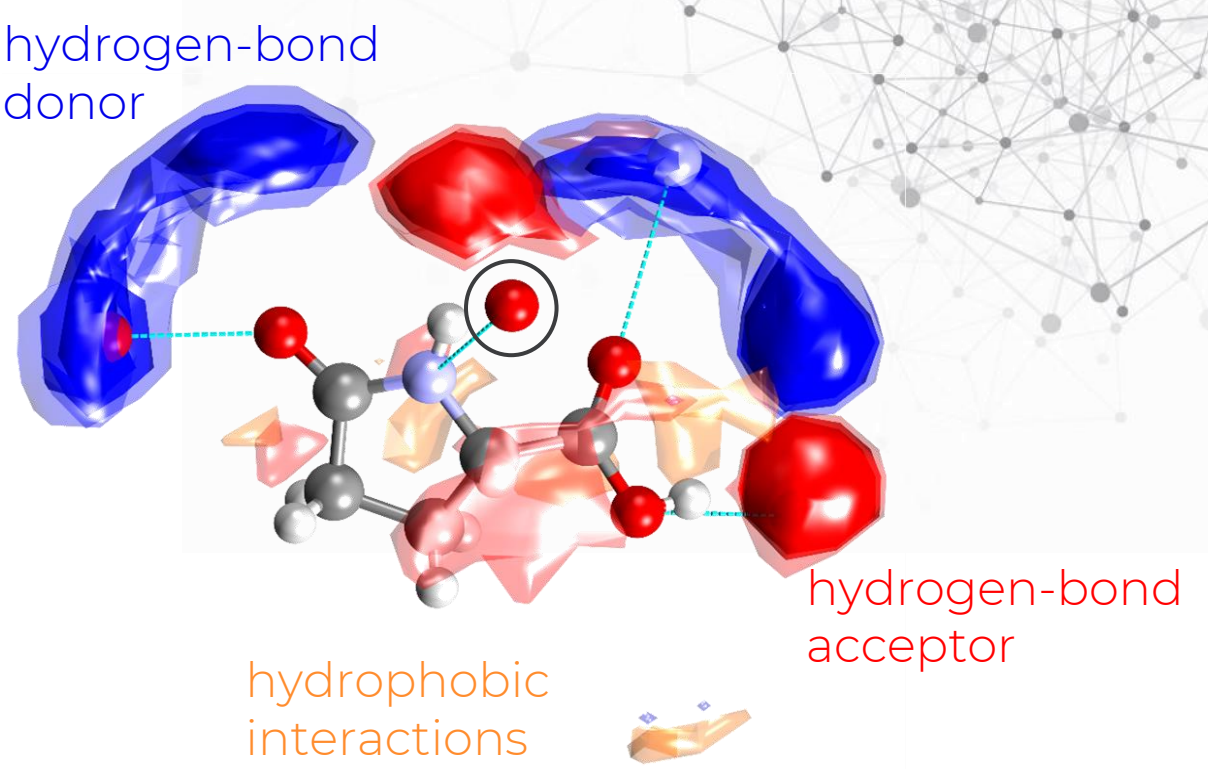
Full Interaction Maps (FIMs)

- Map interaction preferences around complete molecules in a crystal structure.
- Visualise observed atom-atom contacts with respect to likely geometries in 3D space.
- Identify interaction hot-spots around chemical groups.



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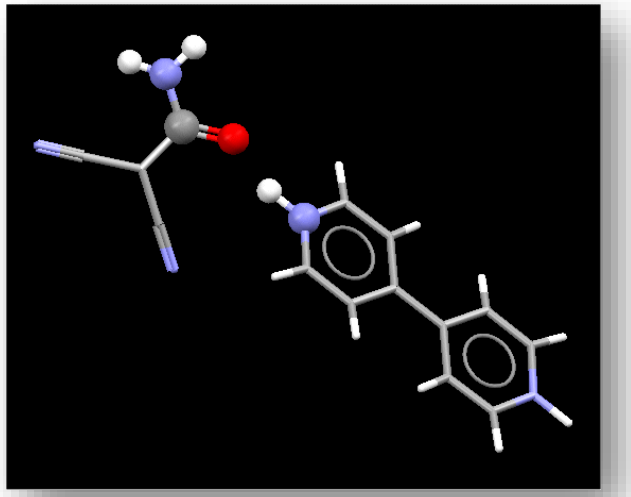
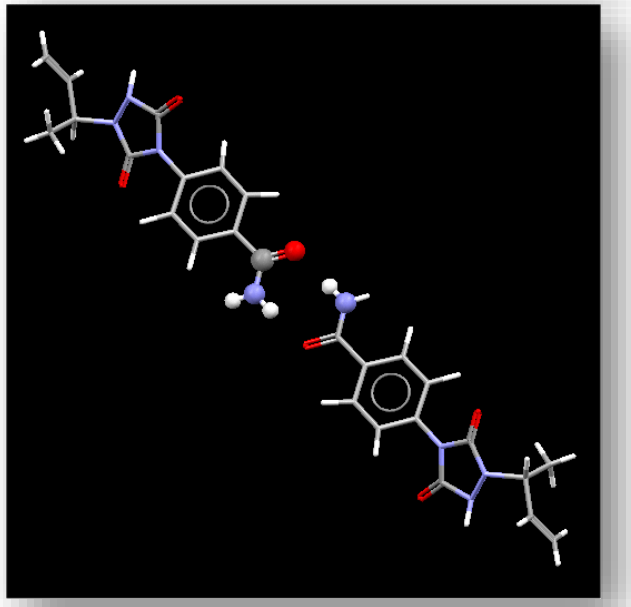
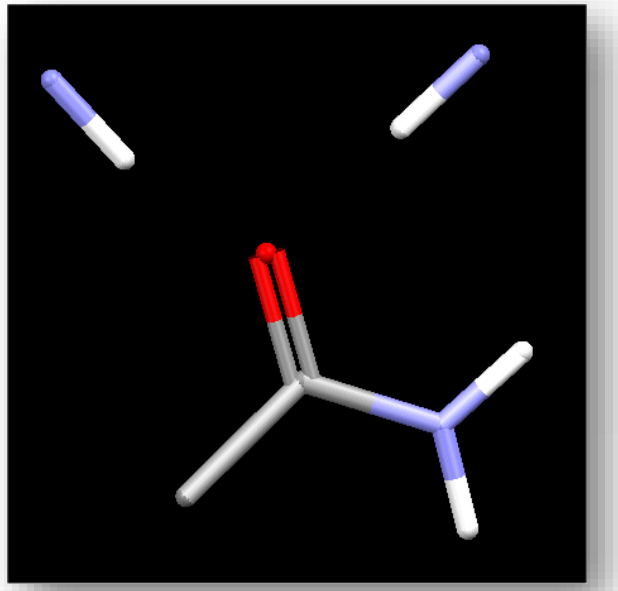
Understanding intermolecular interactions

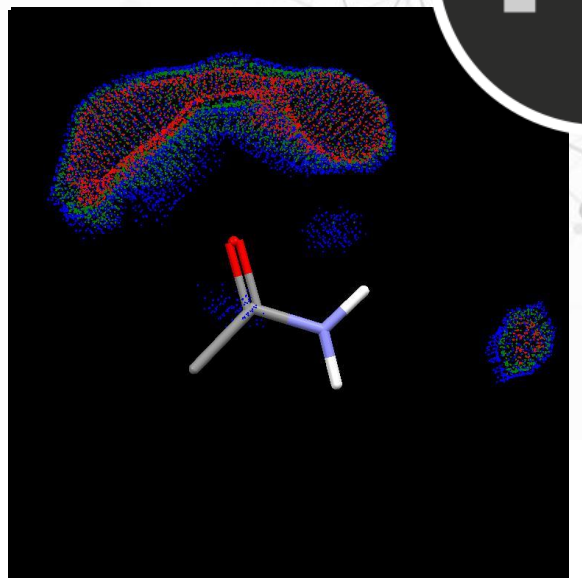




central group: -$CONH_2$

contact group: NH





Search for structures containing desired contact

Superimpose hits and display as scatterplots or contour plots

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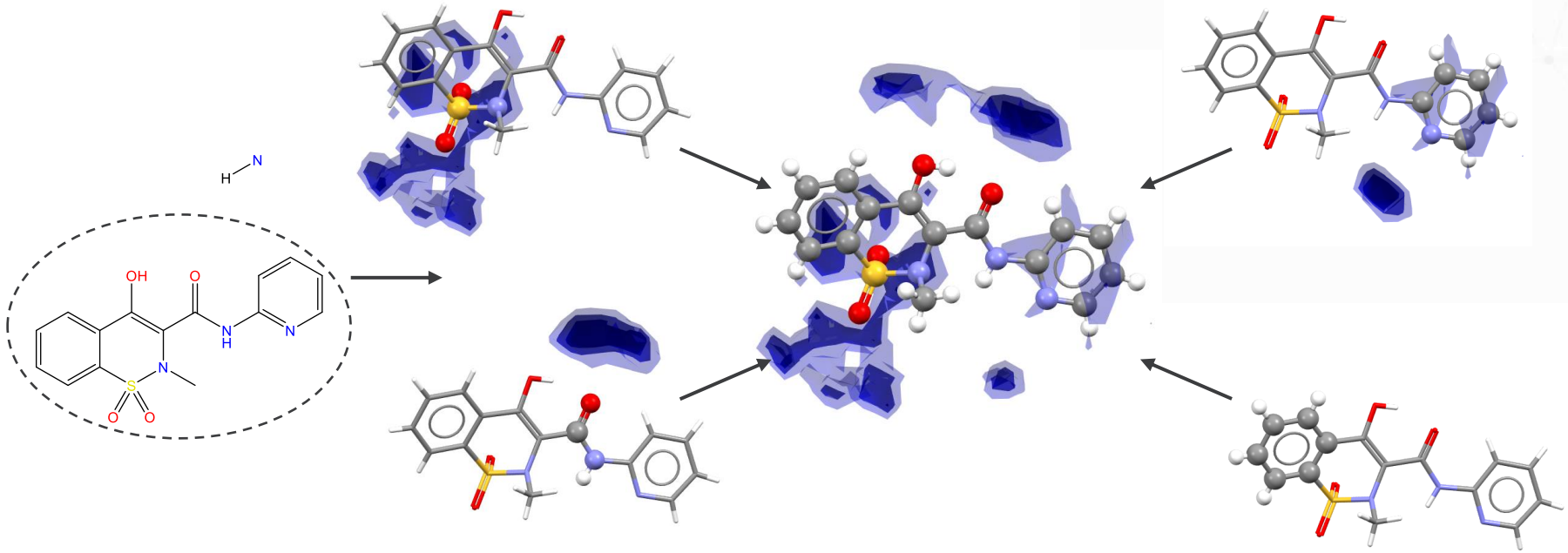
Combining plots into Full Interaction Maps

- Molecule is broken down into fragments
- IsoStar maps for each fragment are combined to give the Full Interaction Map



P. A. Wood *et al.*, *CrystEngComm* (2013), **15**, 65–72

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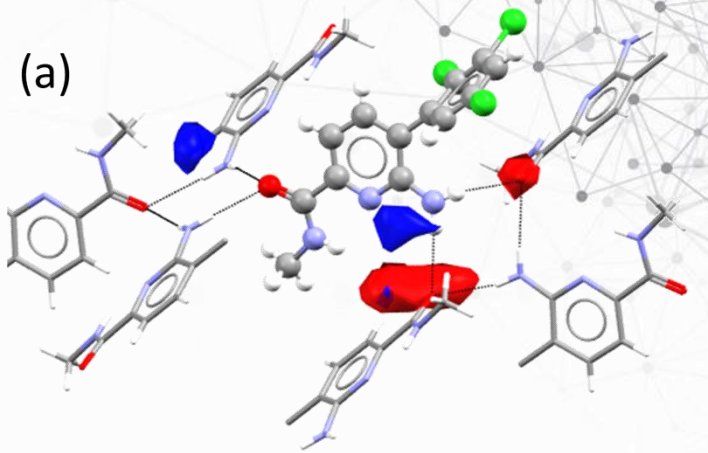
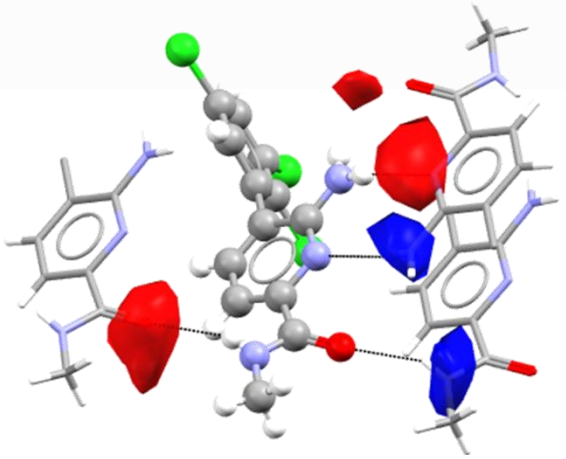
Predicting intermolecular interaction geometries

- “Early development candidate”
  - Two polymorphs, metastable (a) and stable (b)
  - Packing arrangement of stable form (b) satisfies Full Interaction Map particularly well
  - Packing arrangement of (a) does not





N. Feeder *et al.*, *J. Pharm. Pharmacol.* (2015), **67**(6), 857-868

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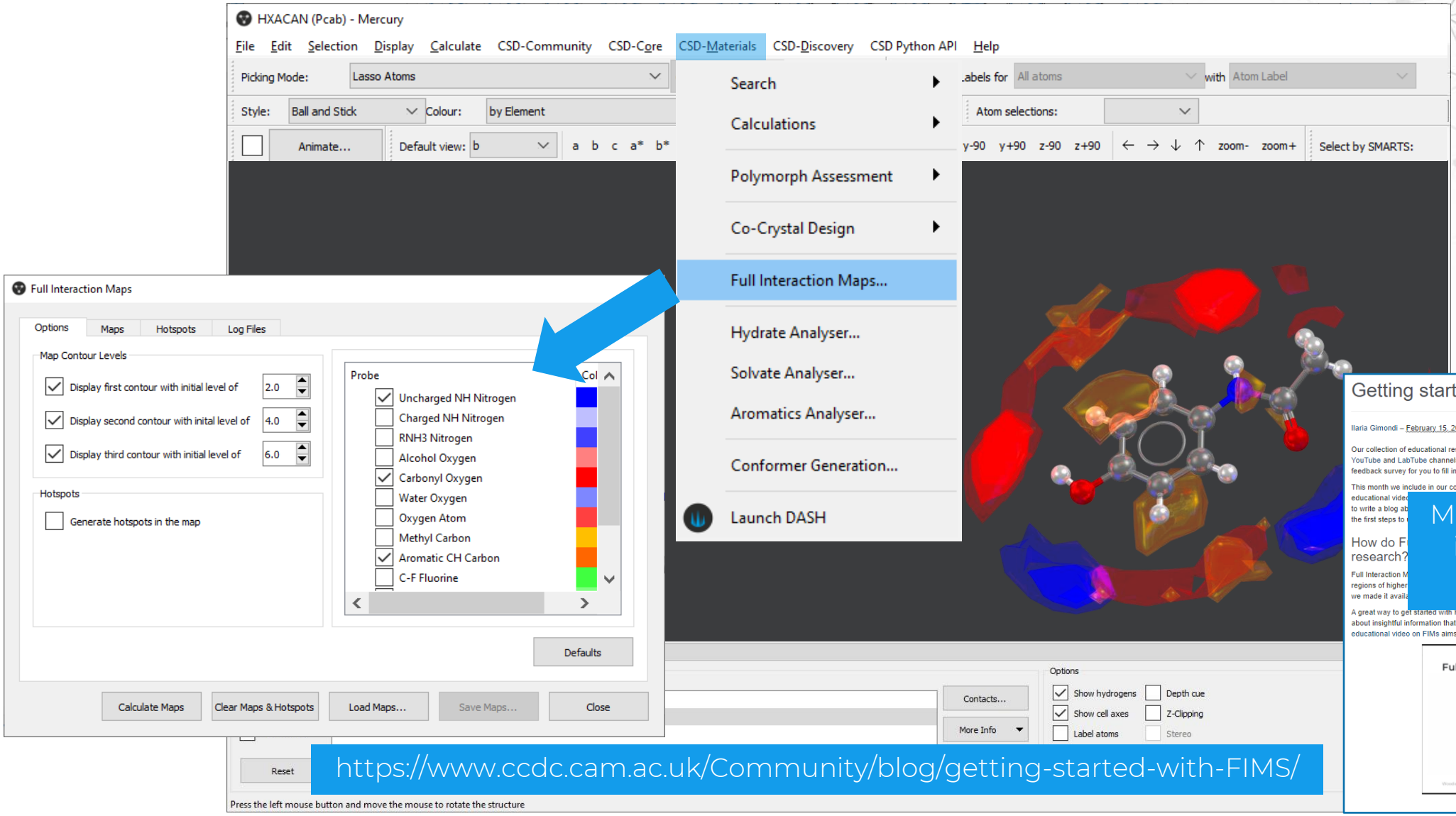
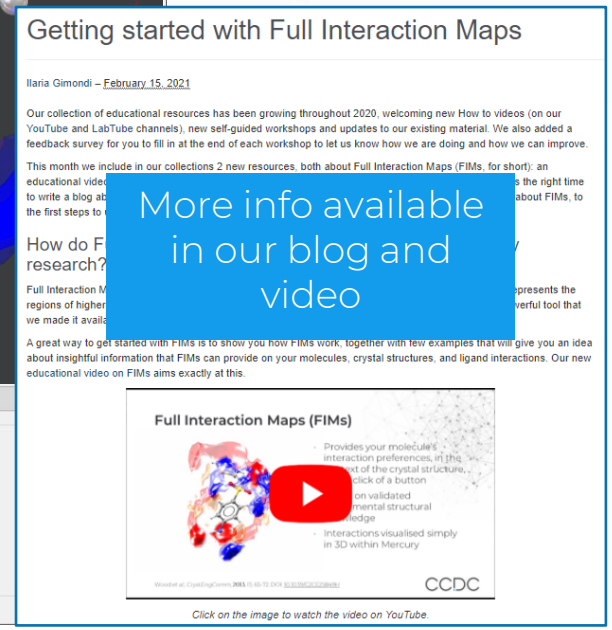
Creating a FIM

FIMs enable you to generate a 3D interaction map around a molecule representing regions of higher probability to find interactions with certain functional groups





More info available in our blog and video

https://www.ccdc.cam.ac.uk/Community/blog/getting-started-with-FIMS/

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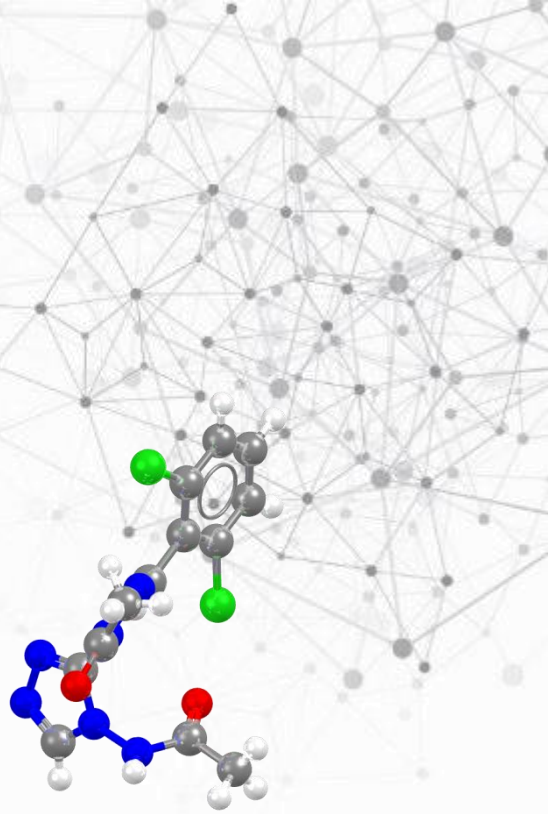
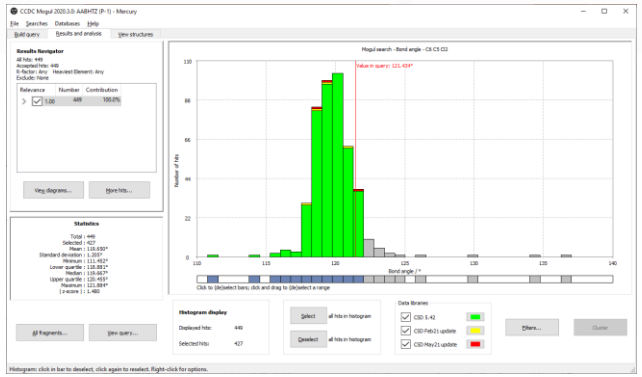
Explore More: Quiz



How to play!

- The questions will appear on the slide: pick and note down your answer within the time given!
- We will reveal and present the answer.
- Note down your score: one point for every right answer and zero for any wrong answer or not answered question.

Hint: keep Mercury and Mogul open alongside your notes from today.



1. When opening your own file in Mercury, how can you make sure that bond types, missing hydrogens and aromatic rings will be displayed?

A. Before loading the structure, go to File and tick Auto Edit Structure on Load, then load your structure and it will be automatically edited.

B. After loading the structure, go to Edit > Edit Structure, and manually apply the edits to bonds and hydrogens.

B. After loading the structure, go to Edit > Auto Edit Structure, tick the desired option on the menu and click Apply.

D. All the options are correct.

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2. From which menu can you access Mogul Geometry Check in Mercury?

A. CSD-Core

B. CSD-Materials

C. CSD-Discovery

D. All of the above

3. FIMs are built on the knowledge from the structures in the CSD, harnessed using another tool of the CSD Software: which one?

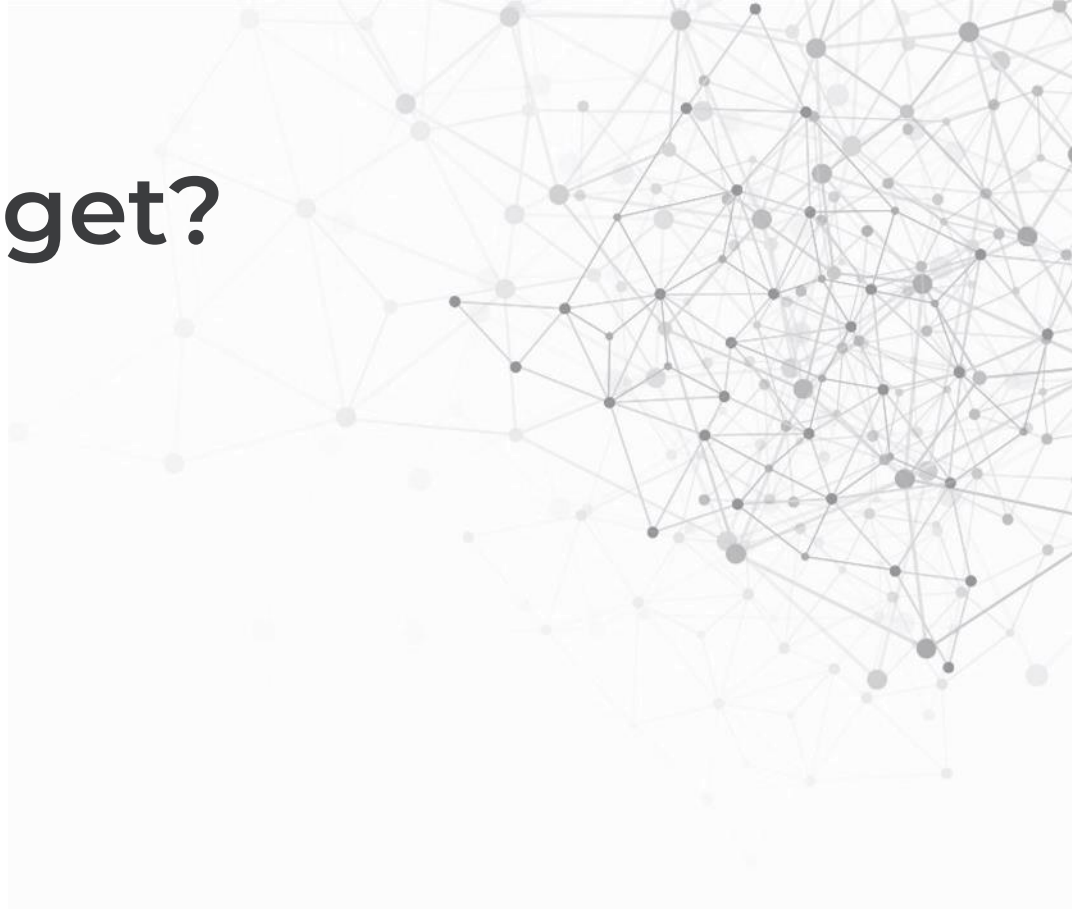
A. Mogul

B. Hermes

C. Isostar

D. None of the above

How many points did you get?



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What have we learnt?

- How to visualise and explore over a million crystal structures
  - What the Cambridge Structural Database is and how it can be used in your research
  - How to visualise structures using Mercury
  - How to explore the packing, symmetry and hydrogen bonded networks of structures
- How to analyse the geometries of structures using Mogul
  - Familiarity with the basics of Mogul
  - How to get more insights into your crystal structures and interpret results obtained from Mogul
  - How to use Mogul for CSD structures and new structure determinations
- How to analyse the interactions within a crystal structure
  - Knowledge of how Full Interaction Maps are generated and how to create them
  - How to interpret results obtained from FIMs
  - Why looking at interactions are important and how FIMs can be used in your research
- The value of using structural data in your research

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https://www.ccdc.cam.ac.uk/Community/educationalresources/

Want to explore more?

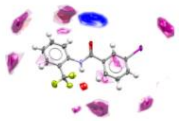
Training and Educational Resources

in the Cambridge Structural Database (CSD) extends far beyond a collection of crystal structures. Knowledge derived from these materials , and biology. Chemical and structural concepts are often difficult to grasp without real world, interactive examples for students to explore.

lly produce educational materials for use in classroom and computer lab settings, or as independent study modules. Many of these materials ely available set of over 750 structures that can be investigated with the free version of our Mercury visualisation and analysis program. Of entries are available for free through our Access Structures portal.

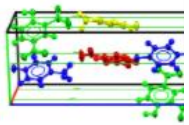
mentary teaching materials, find out more about the Teaching Database **here**. If you have developed your own modules using the CSD and r community, please contact us at education@ccdc.cam.ac.uk.

rom education and outreach at the CCDC, sign up for the Education and Outreach Newsletter **here**.



CSD-Materials

Tools to help you to understand your material's behaviours and refine its properties.

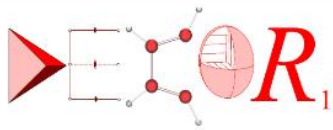


CSD-Core

Essential crystallographic and structural chemistry capabilities.

Information on the Teaching Subset

Access a series of teaching modules for use in the classroom



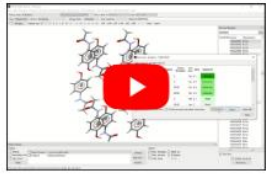
DECOR: Educational Resources for Teaching Crystallography

Register for E&O newsletter

On-demand modules with completion certificate

Self-guided workshops

Download a series of self-guided workshop materials for CCDC tools and features

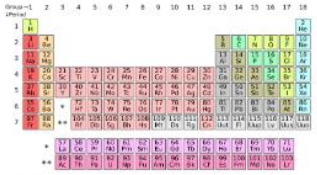


Watch software training and support videos

CSDU modules - Explore our on-demand training courses

YouTube and LabTube channels

Access fun science activities for kids through the CCDC Home learning page



Explore the Periodic Table through Crystal Structures

Bound! a Protein-Drug matching card game

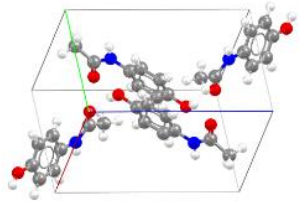
CCDC

CSDU

- On-demand modules to learn how to use the CSD Software at your own pace.
- Completion certificate after a final quiz!

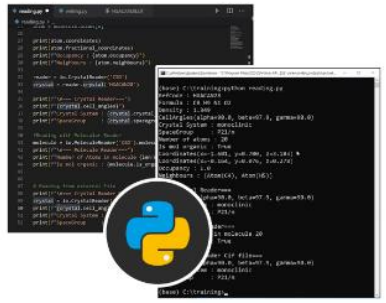
UWatch UTry UTest

Visualisation 101 - Visualising structural chemistry data with Mercury



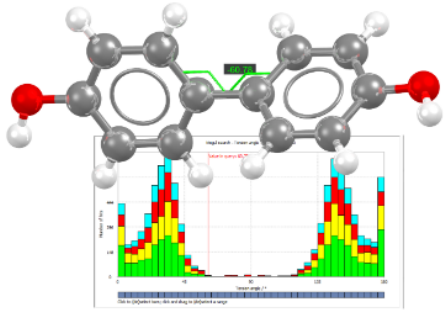
Begin module

Programmatic access to the CSD 101 – CSD Python API



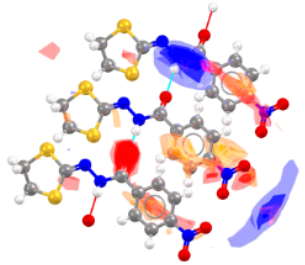
Begin module

Analysing molecular geometries 101 - basics of Mogul



Begin module

Analysing intermolecular interactions 101 - Full Interaction Maps



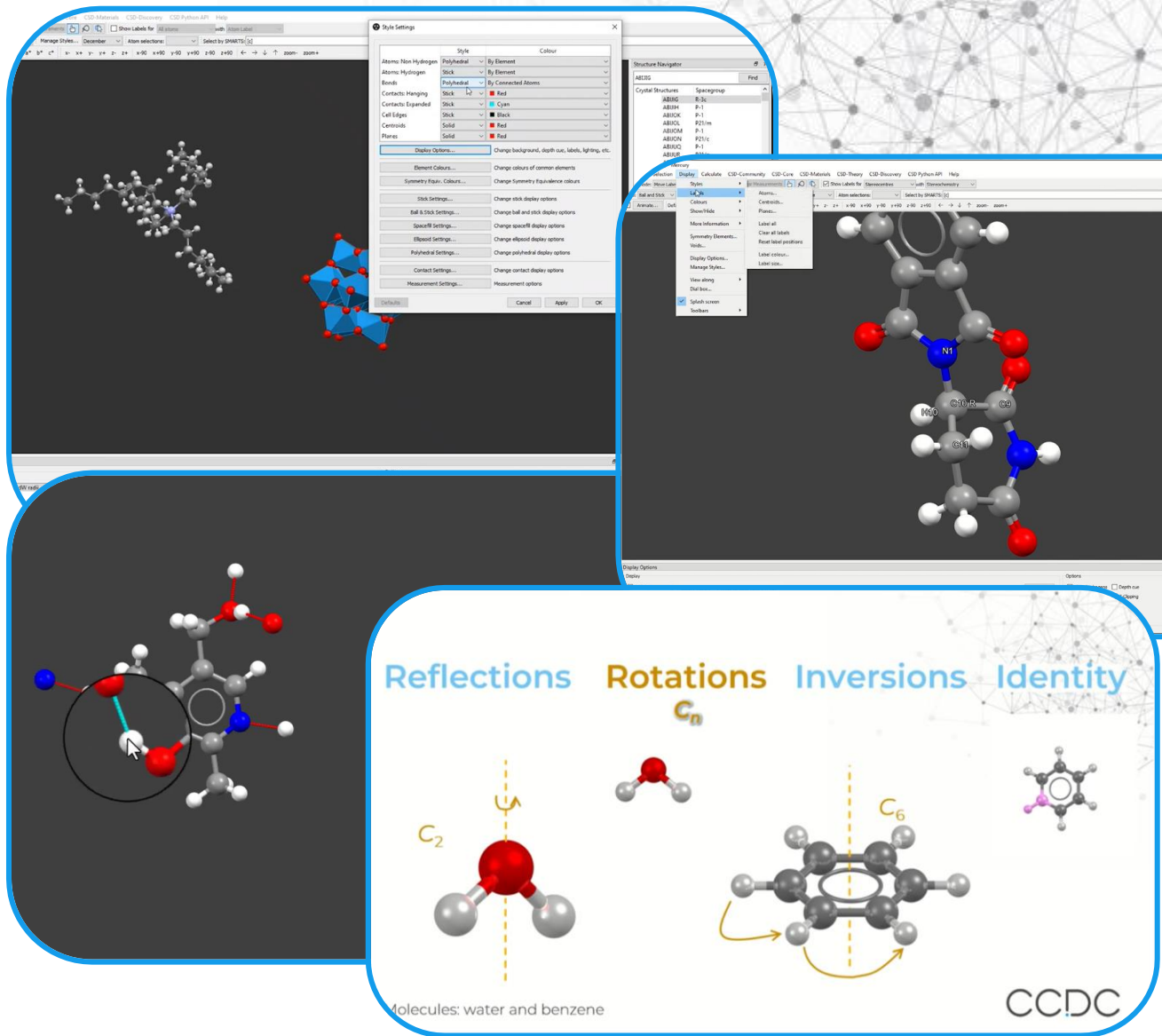
Begin module

https://www.ccdc.cam.ac.uk/Community/educationalresources/CSDU/

CCDC

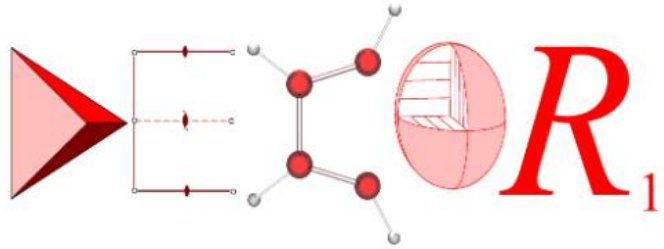
Videos highlights

- How-to: Create and share personalised styles in Mercury
- How-to: Labels in Mercury
- How-to: Basics of hydrogen bonds in Mercury
- Introduction to symmetry operators and point groups



The video names are links to the videos.

CIF resources you might find useful



These resources were originally developed by Mike Zdilla at Temple University under the DECOR initiative

Resources by Topic

Slides and web material to learn about CIFs.

CCDC
advancing structural science

Materials on crystallography (slides, videos, web pages, exercises, documents, ...) from lecturers in the communities shared publicly for other educators to use in their lectures and for students to practice, review, and explore new concepts.

https://www.ccdc.cam.ac.uk/Community/educationalresources/database-of-educational-crystallographic-online-resources/resources-by-topic/CIF/

A short guide to Crystallographic Information Files

A CIF or Crystallographic Information File is the standard format for storing crystallographic structural data. CIF information has a specific structure or format that needs to be followed to allow crystallographic programs to read the file.

CIFs are usually created automatically by the program used to process or refine crystallographic data; this means it is very unlikely that you will need to create a CIF from scratch (and we don't recommend editing CIFs by hand). However, being able to read and find information within a CIF is useful to help you be able to provide complete crystallographic information for your structures, as well as interrogate the data of others.

Access the CSD Data and Software

Until 31st July 2022

- You can explore CSD functionality using the workshop license!

After 31st July

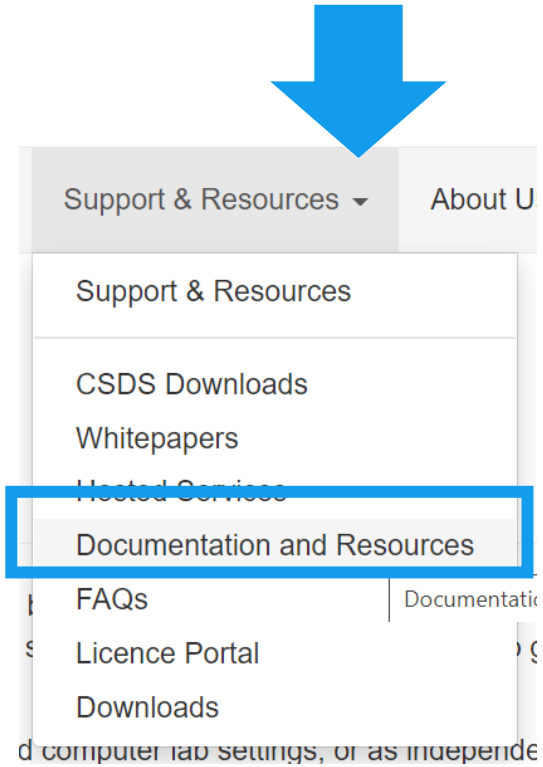
- If you wish to continue access at the end of the workshop license period, your institution probably already has access to the CSD.
- If your institution does not have a license or you do not manage to find the license contact, you can get in touch with admin@ccdc.cam.ac.uk, and they will be able to advise you.

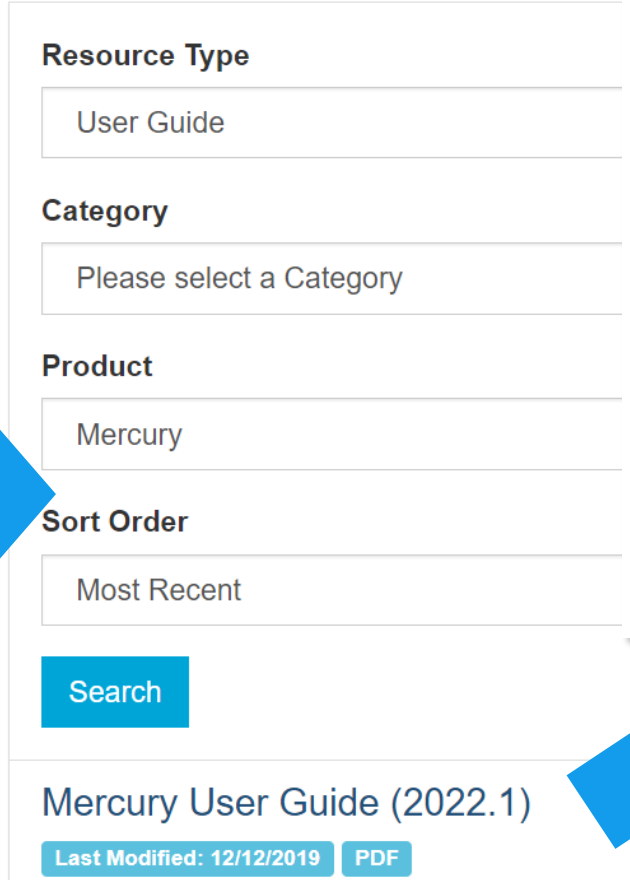
CCDC

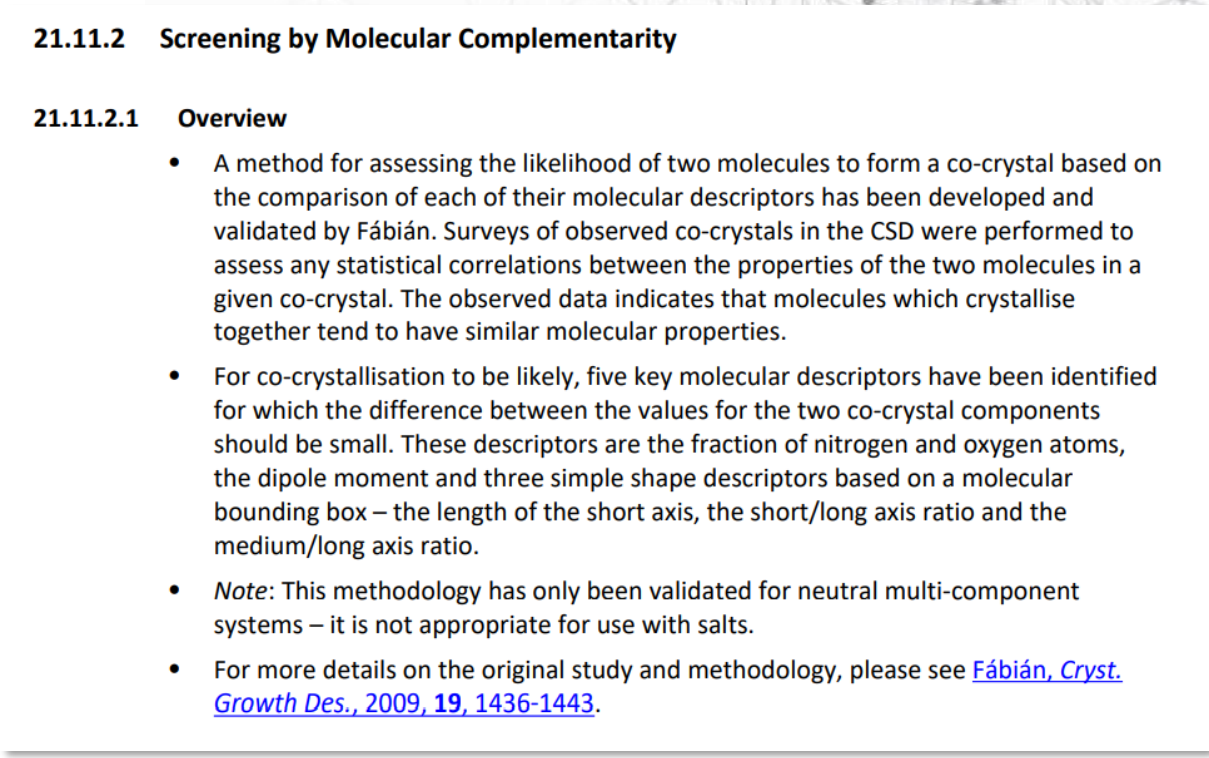
Documentation

How does this functionality work? How are the results obtained?

CCDC website







21.11.2 Screening by Molecular Complementarity

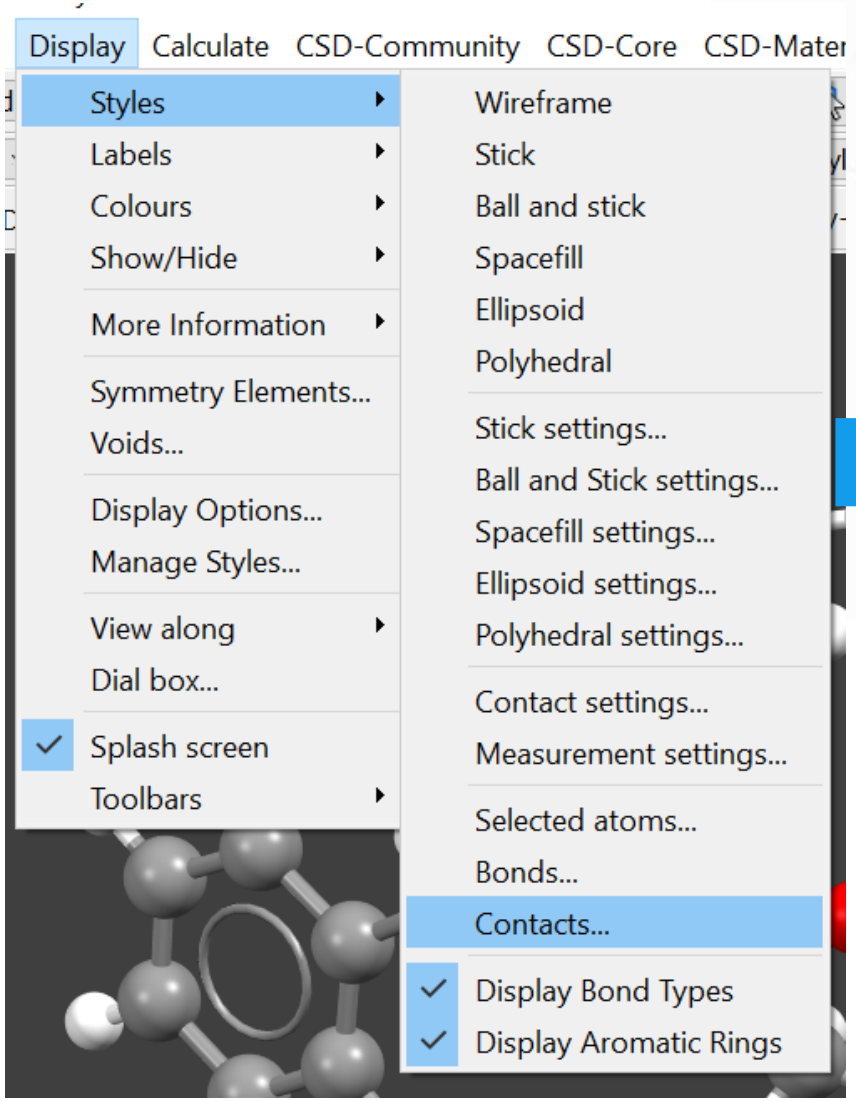
21.11.2.1 Overview

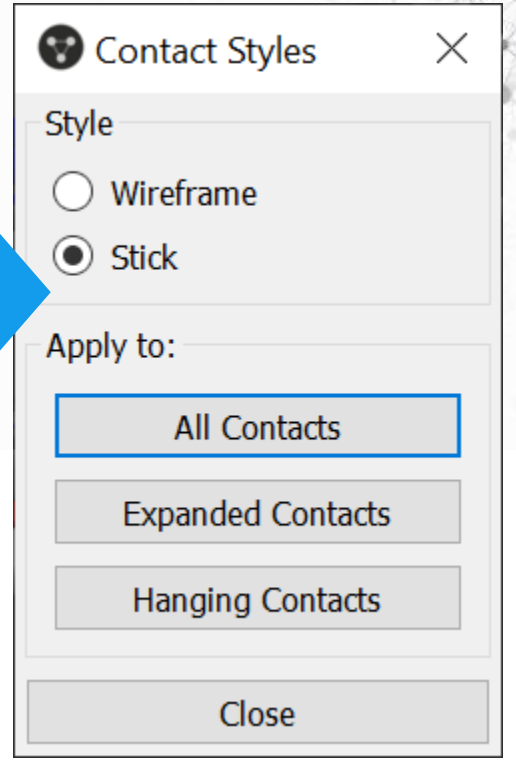
- A method for assessing the likelihood of two molecules to form a co-crystal based on the comparison of each of their molecular descriptors has been developed and validated by Fábián. Surveys of observed co-crystals in the CSD were performed to assess any statistical correlations between the properties of the two molecules in a given co-crystal. The observed data indicates that molecules which crystallise together tend to have similar molecular properties.
- For co-crystallisation to be likely, five key molecular descriptors have been identified for which the difference between the values for the two co-crystal components should be small. These descriptors are the fraction of nitrogen and oxygen atoms, the dipole moment and three simple shape descriptors based on a molecular bounding box – the length of the short axis, the short/long axis ratio and the medium/long axis ratio.
- *Note*: This methodology has only been validated for neutral multi-component systems – it is not appropriate for use with salts.
- For more details on the original study and methodology, please see Fábián, *Cryst. Growth Des.*, 2009, **19**, 1436-1443.

https://www.ccdc.cam.ac.uk/support-and-resources/ccdcresources/

Display contacts visualisation options in Mercury

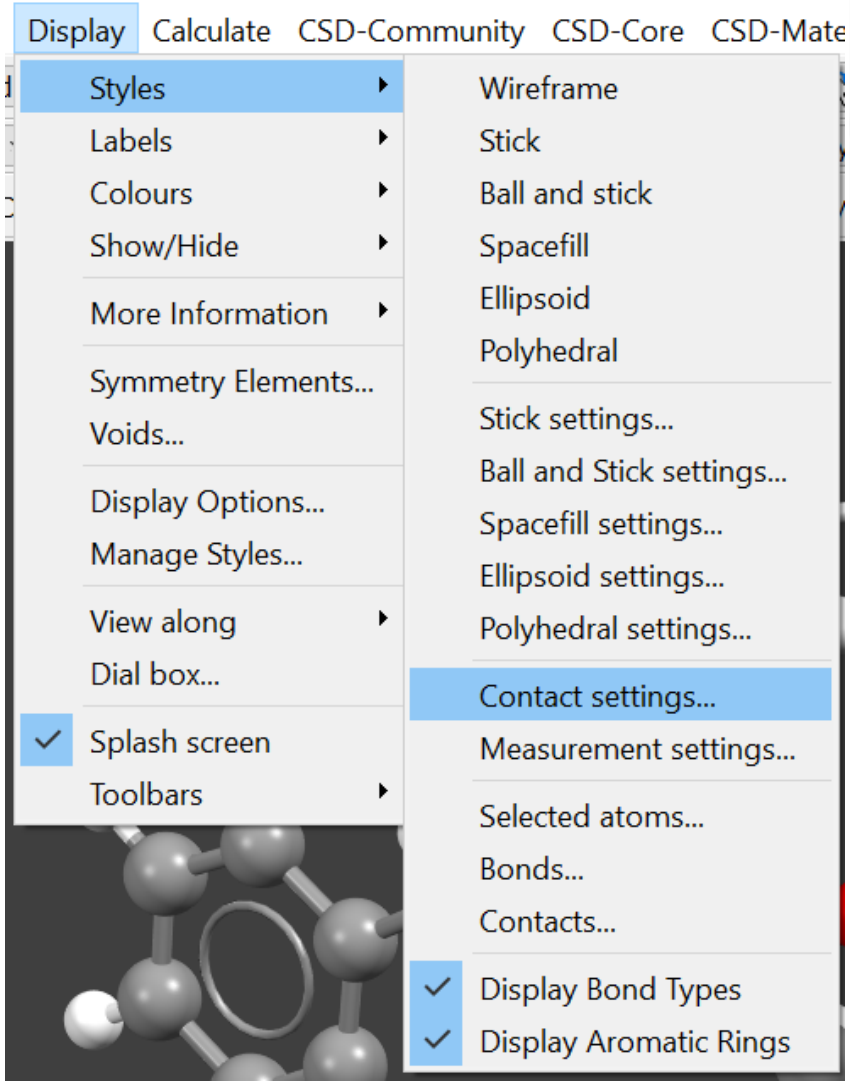
1. Set contacts style to sticks.

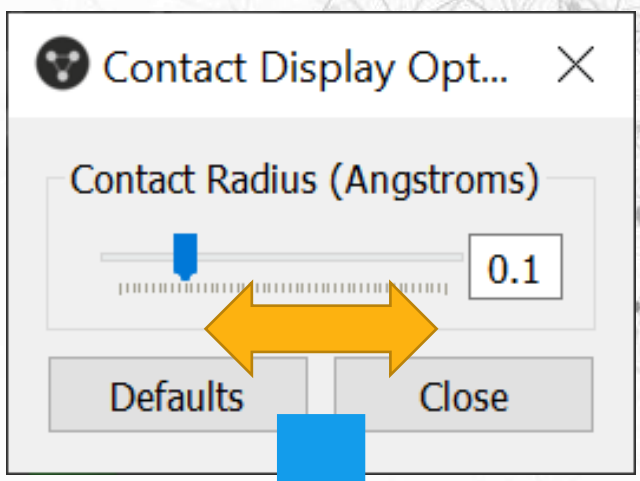


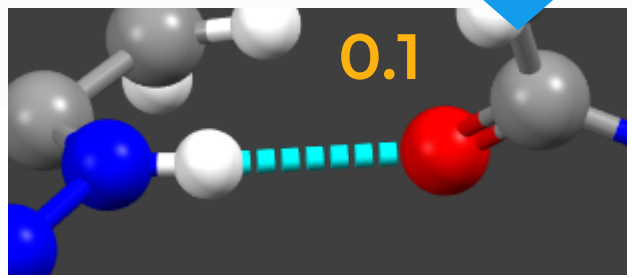


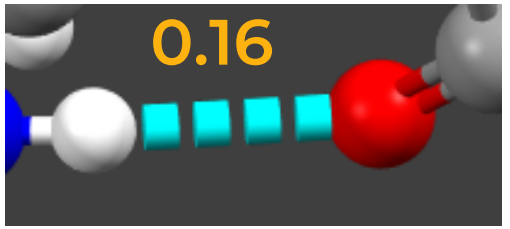
Display contacts visualisation options in Mercury

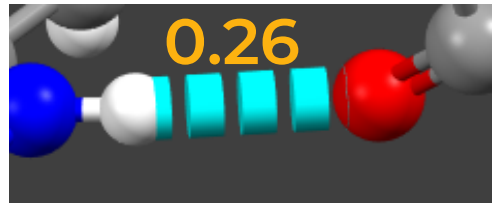
2. Change the thickness to change the number of segments you see in the contact line.





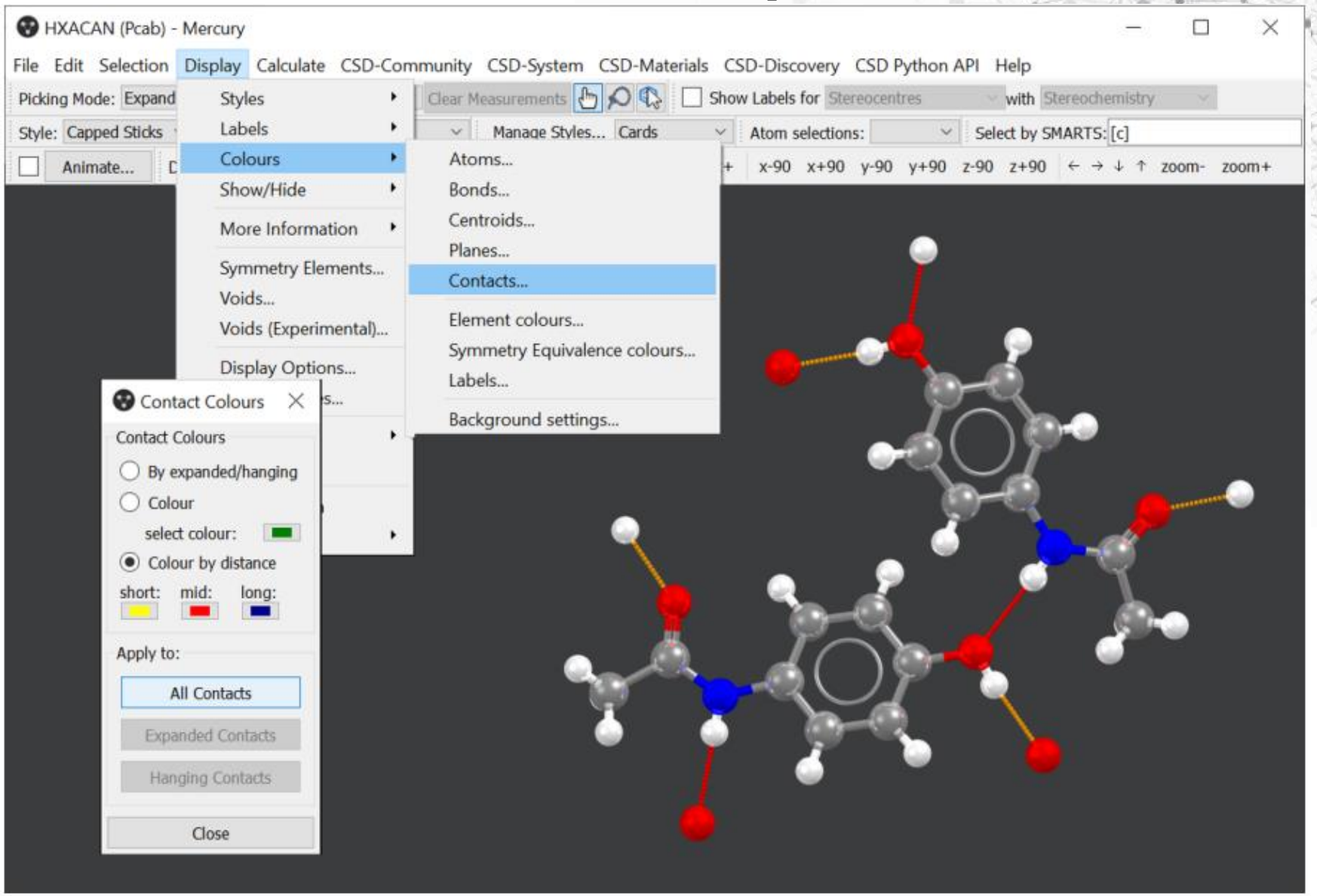




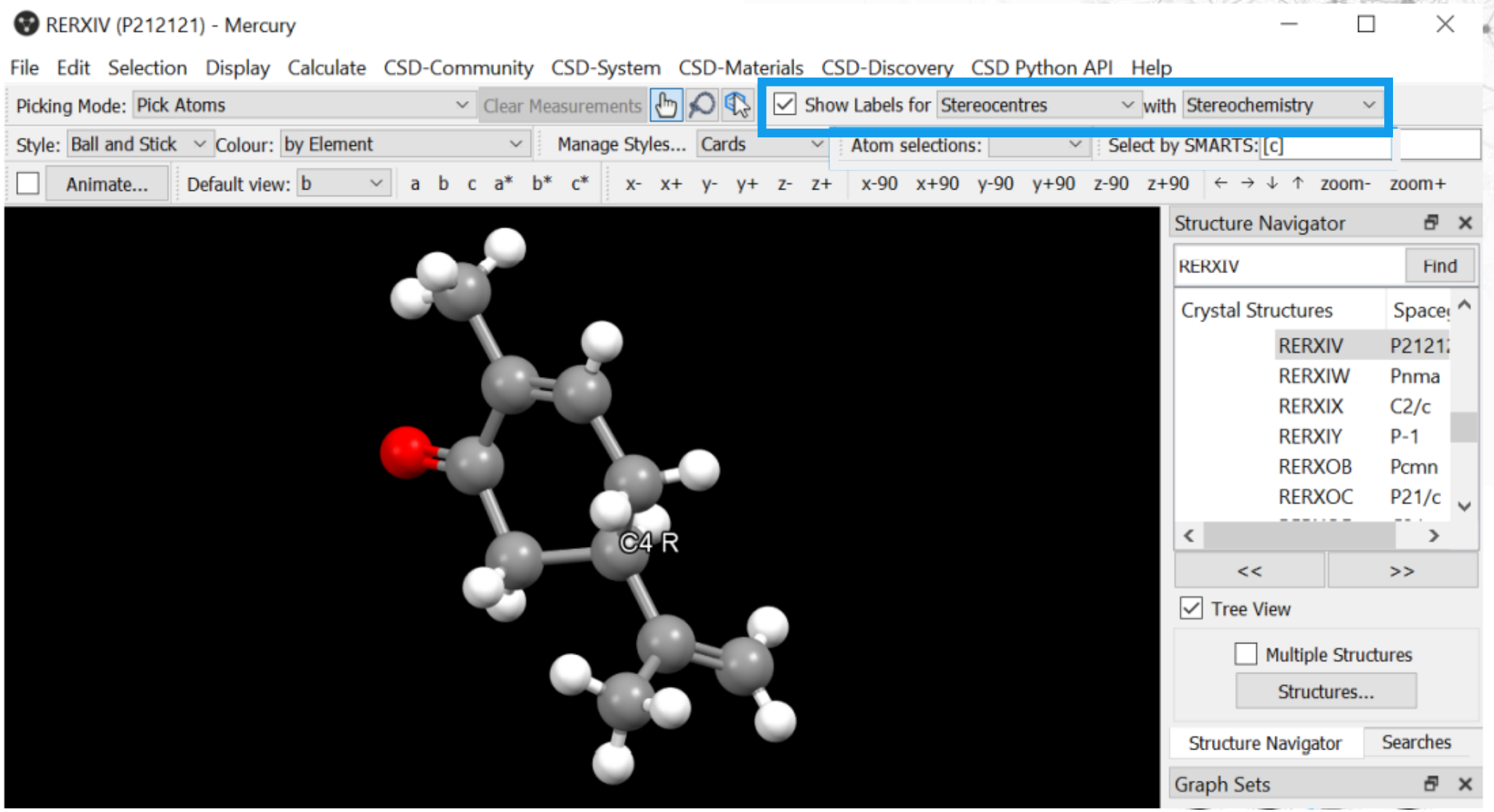


CCDC

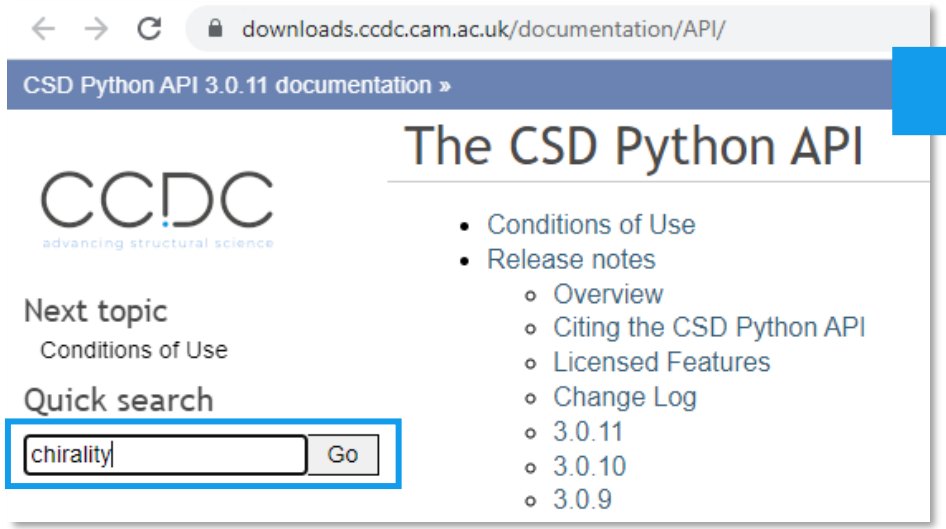
Display contacts visualisation options in Mercury

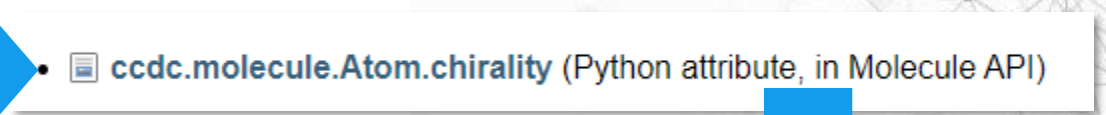


Label chiral molecules



Chirality in the CSD Python API





atomic_weight

The atomic weight of the atom.

bonds

The bonds which this atom forms

chain_label

The label of the chain in which the atom lies if available.

chirality

The R/S Chirality flag for this atom.

Returns one of '', 'R', 'S', 'Mixed', 'Error'.

coordinates

The x, y, z coordinates of the atoms in orthogonal space.

```
>>> atom = Atom(atomic_symbol='C', coordinates=(1.0, 2.0, 3.0))
>>> atom.coordinates
Coordinates(x=1.000, y=2.000, z=3.000)
```

The coordinates may be addressed by index or by key:

```
>>> atom.coordinates.x
1.0
>>> atom.coordinates[2]
3.0
```

Note that this function will return `None` if the atom does not have 3D coordinates.

```
>>> atom = Atom(atomic_symbol='C')
>>> print(atom.coordinates)
None
```

displacement_parameters

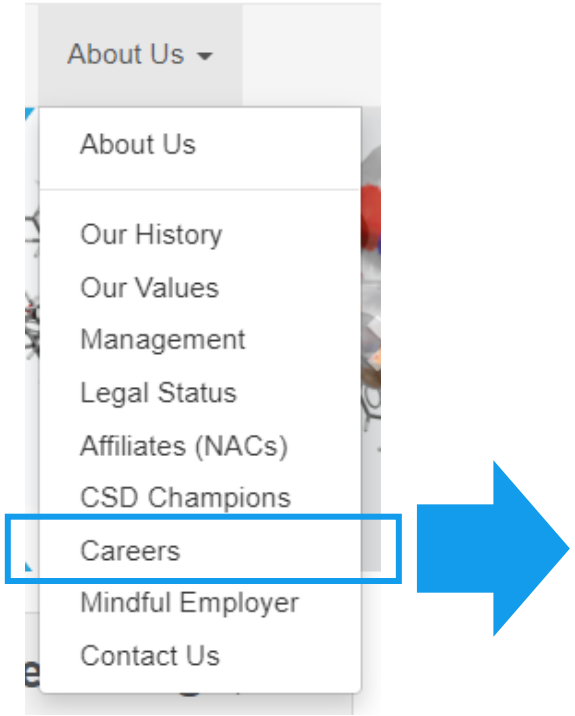
The displacement parameters of this atom.

Returns: `ccdc.molecule.Atom.DisplacementParameters` Or `None`

https://downloads.ccdc.cam.ac.uk/documentation/API/

Working at the CCDC

- You can see our open positions…



Our current vacancies

Jobs at CCDC UK

- Finance Manager (Part-time – 22.5 hours per week)
- HR Manager
- Marketing Executive
- Product Manager
- Research and Applications Scientist (CSP)
- Discovery Science Team Leader
- Cheminformatics Data Scientist
- Research and Applications Scientist
- Research and Applications Scientist - Computational and Data Sciences
- DevOps Engineer
- Junior Developer - Web and UI
- Junior Developer - Scientific/C++
- Senior Software Engineer / Software Manager

Jobs at CCDC US

- Customer Success Executive

CCDC PhD Studentships

Thank you for your interest in the CCDC. We don't have any open PhD studentships at this time, however, please check this webpage regularly as it will be updated as opportunities arise.

- … or send us an open application

CCDC