



CCDC

advancing structural science

The Cambridge Structural Database

ECS7 2022

14 July 2022



Ilaria Gimondi

Education and
Outreach Officer



Suzanna Ward

Head of Data and
Community

igimondi@ccdc.cam.ac.uk

ward@ccdc.cam.ac.uk

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

International repository of 3D curated structures

Collaborative research and knowledge-based services

Scientific software

Education and Outreach

CCDC

Structural databases



PDB
>190,000
polypeptides,
nucleotides
& saccharides



CSD
>1.1 million
organic and
metal-organic

ICSD
>260,000
(no C-H and C-C
bonds)
Elements,
minerals,
metals

ICDD
Powder
diffraction
files

 **FIZ Karlsruhe**
Leibniz Institute for Information Infrastructure



CCDC

The vision of the CSD



- 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

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

The vision

BERNAL'S VISION: FROM DATA TO INSIGHT

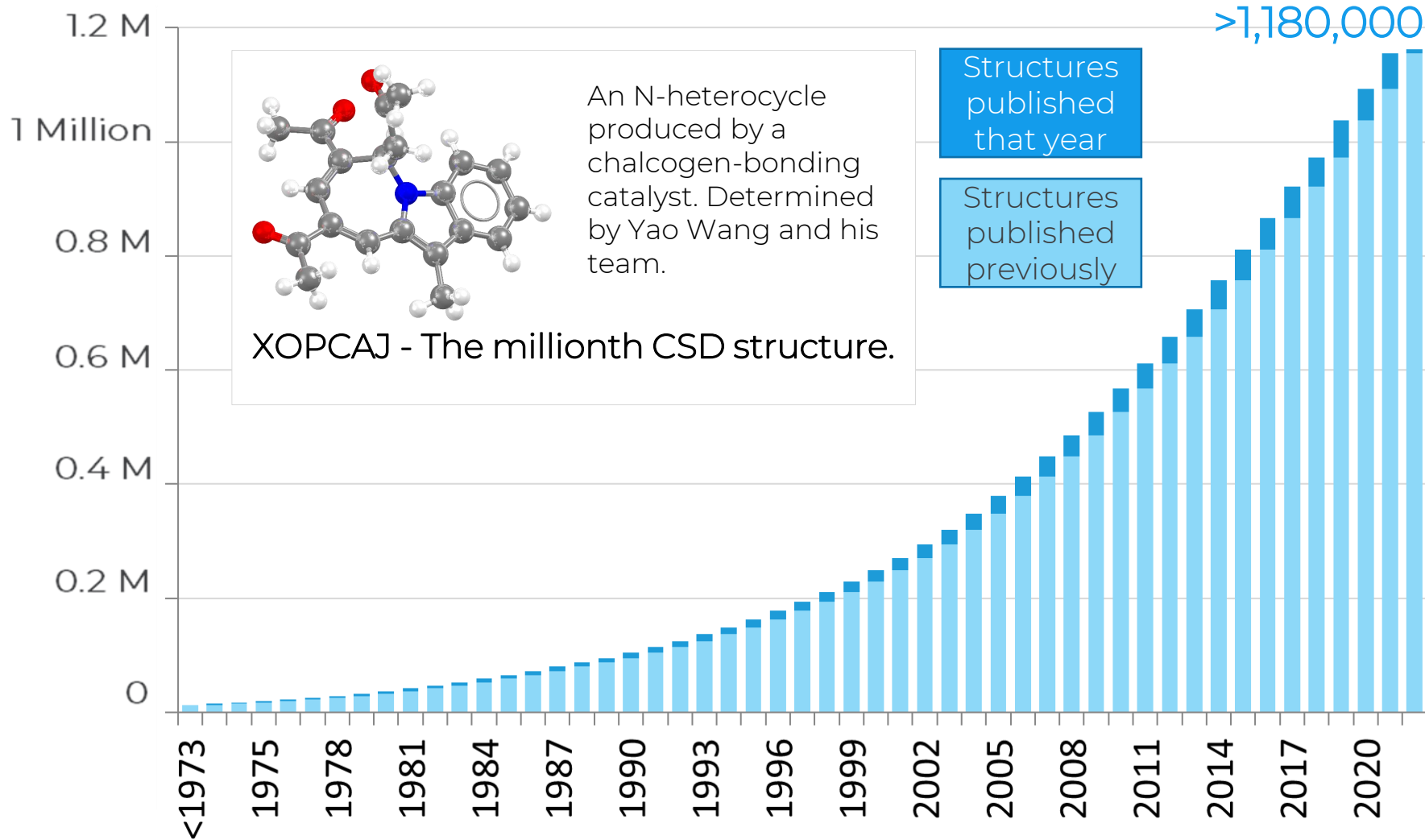
by Dr Olga Kennard OBE FRS

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)

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



Inside the Cambridge Structural Database

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

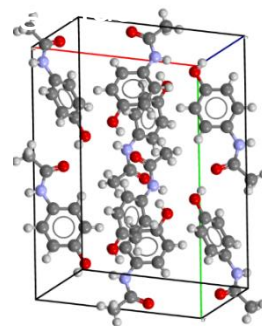
Organic
43%

Metal-Organic
57%

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

Organic

- Drugs
- Agrochemicals
- Pigments
- Explosives
- Protein ligands



Additional data

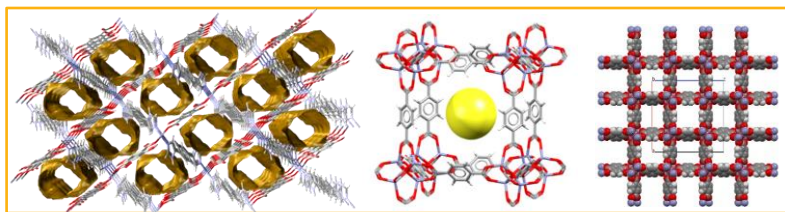
- 11,525 polymorph families
- 171,683 melting points
- 909,992 crystal colours
- 778,663 crystal shapes
- 24,916 bioactivity details
- 11,387 natural source data
- > 250,000 oxidation states

Not Polymeric
89%

Polymeric: 11%

Metal-Organic

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

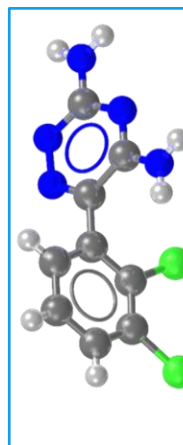


Single
Component
56%

Multi
Component
44%

Links and subsets

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

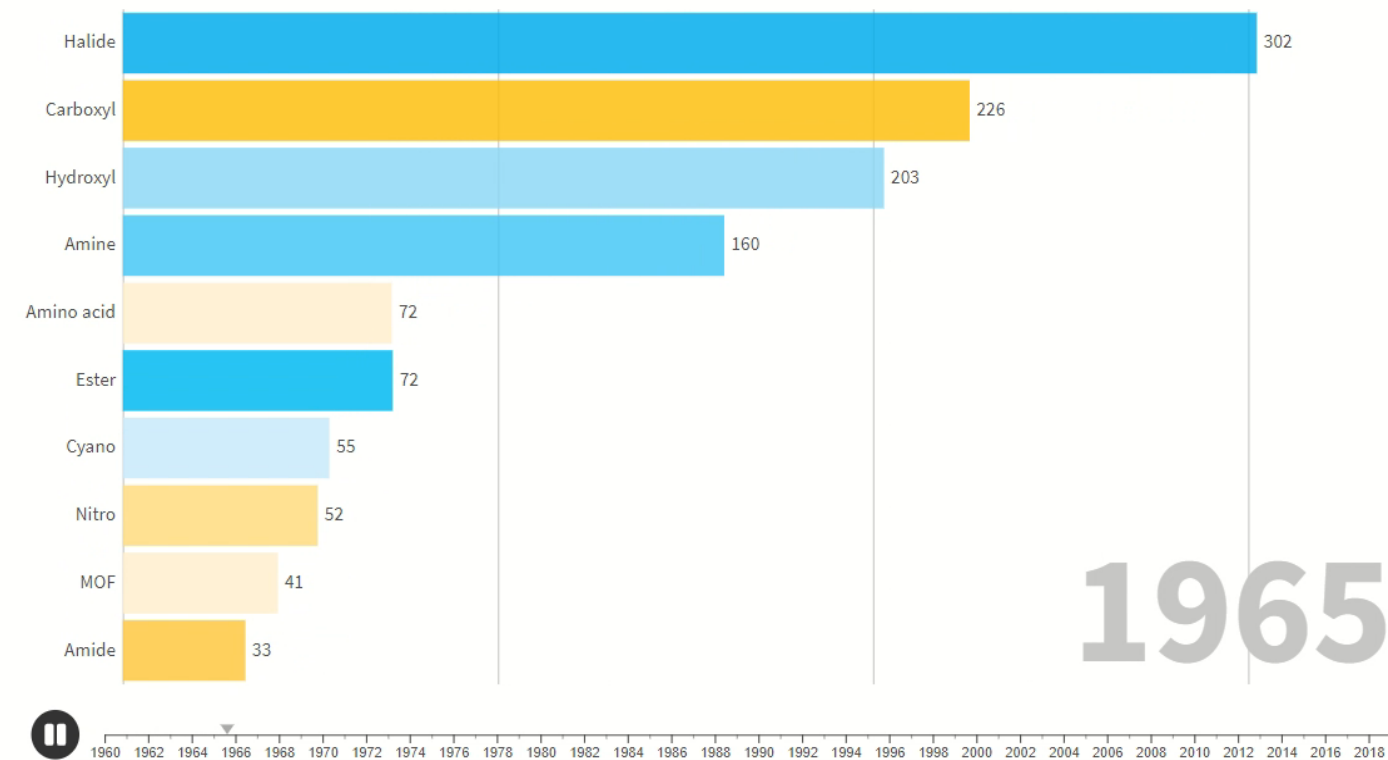


Exploring the CSD


- > 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

Chemistry in the CSD

Number of structures containing certain chemical groups



A trusted and linked repository



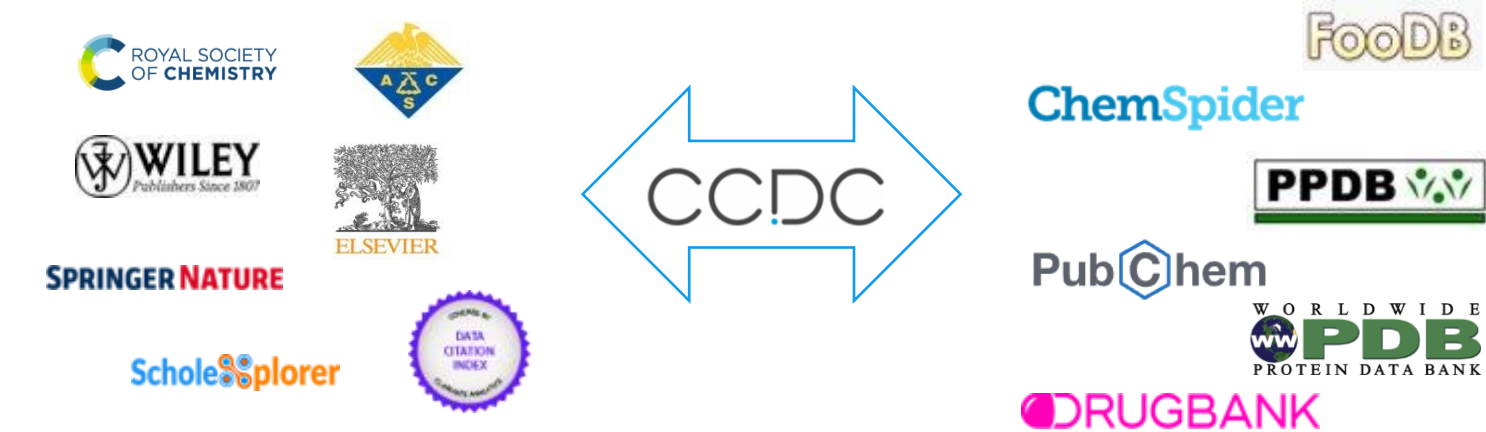
IUPAC InChIs for Chemical Structures

InChI TRUST

DataCite DOIs for Digital Objects
FIND, ACCESS, AND REUSE DATA

Crossref

ORCID ORCID iDs for Researchers



ROYAL SOCIETY OF CHEMISTRY

WILEY Publishers Since 1807

SPRINGER NATURE

Scholesplorer

ELSEVIER

CCDC

ChemSpider

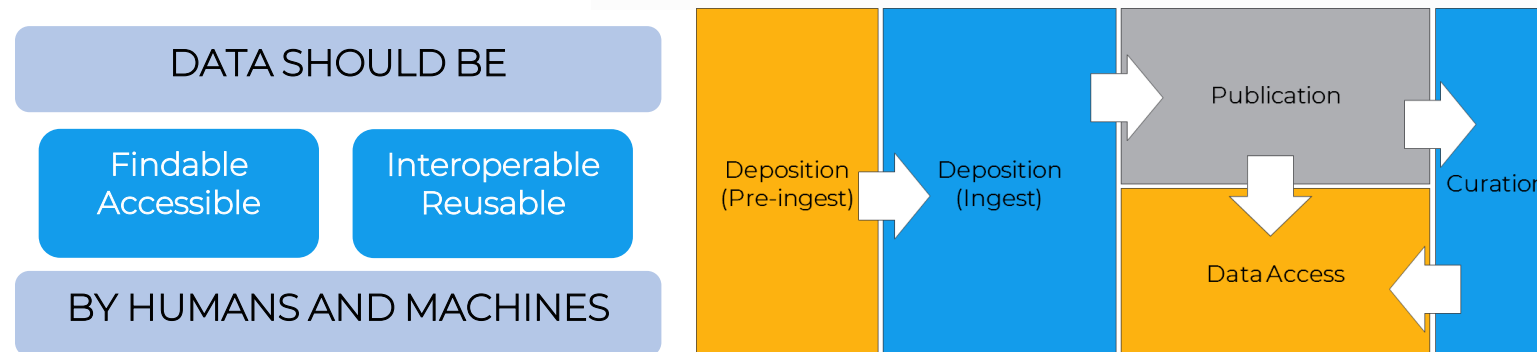
FoodDB

PPDB

PubChem

WORLDWIDE PDB PROTEIN DATA BANK

DRUGBANK

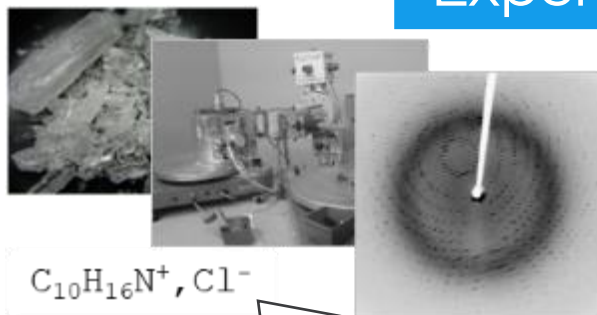


Wilkinson, M. D. et al. The FAIR Guiding Principles for scientific data management and stewardship. *Sci. Data* 3:160018 DOI: 10.1038/sdata.2016.18 (2016)

CCDC

From experiment to knowledge

Experiment



```
_diffn_ambient_temperature 90(2)
_diffn_radiation_type MoK $\alpha$ 
_diffn_radiation_wavelength 0.71073
_diffn_radiation_monochromator graphite
_diffn_measurement_device_type 'Bruker APEX CCD area-detector'
_diffn_measurement_method '\u03c8 and \u03c6'
_diffn_detector_area_resol_mean 512
_diffn_reflns_number 6892

loop_
  _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_occupancy
  _atom_site_calc_flag
  _atom_site_refinement_flags
  _atom_site_symmetry_multiplicity
  _atom_site_disorder_assembly
  _atom_site_disorder_group
Cl C11 0.23185(8) 0.78905(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 0.6996(4) 0.7867(6) 0.4367(2) 0.0224(5) Uani d U 1 1 . . .
C C2 0.7510(5) 0.8922(5) 0.7089(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 . . .
C C4 0.8700(4) 0.5637(4) 0.7481(3) 0.0236(6) Uani d U 1 1 . . .
```

[RSC Publishing | Journals](#)
June 2011, Volume 18, Issue 6, pp 659-666 | [View](#)

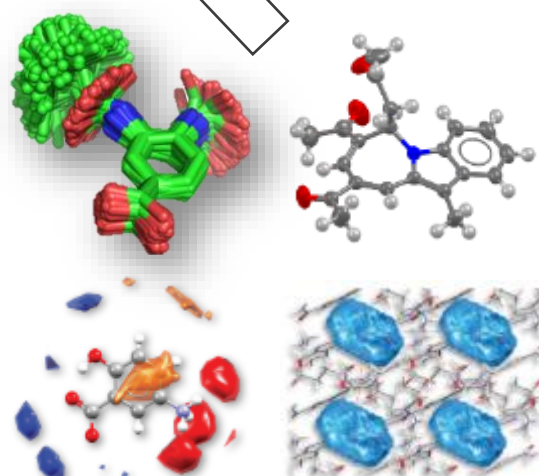
Ritonavir: An Extraordinary Example of Conformational Polymorphism

Authors: [John Kester](#), [Stephen Spickett](#), [Wojciech Morys](#), [John Quick](#), [Walter Dalko](#), [William Hester](#), [John Merson](#)

Article | 2 | 528 | 657
[Basic](#) [Feedback](#) [Metrics](#)

Abstract

Purpose. In the summer of 1998, Novartis semi-solid capsules supplied 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.



CCDC

Knowledge

Database	Database Number
# 103493	781670
# 103494	781670
# 103495	781670
# 103496	781670

The image shows a screenshot of the CCDC website. It features a 3D ball-and-stick model of a molecule, a chemical structure diagram, and various interactive buttons like 'Ligand', 'View', and 'Open'. The interface is clean and professional, typical of a scientific database.

Article of Ritonavir

Database Number: 781670

Date Created: 11/06/2010 11:00:00 AM

Author(s): John Kester, Stephen Spickett, Wojciech Morys, John Quick, Walter Dalko, William Hester, John Merson

Keywords: Ritonavir; Hydrogen Bonding; Conformational Polymorphism

Searchable: 01/12/2010

Available at: [http://www.ccdc.cam.ac.uk](#)

CCDC

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

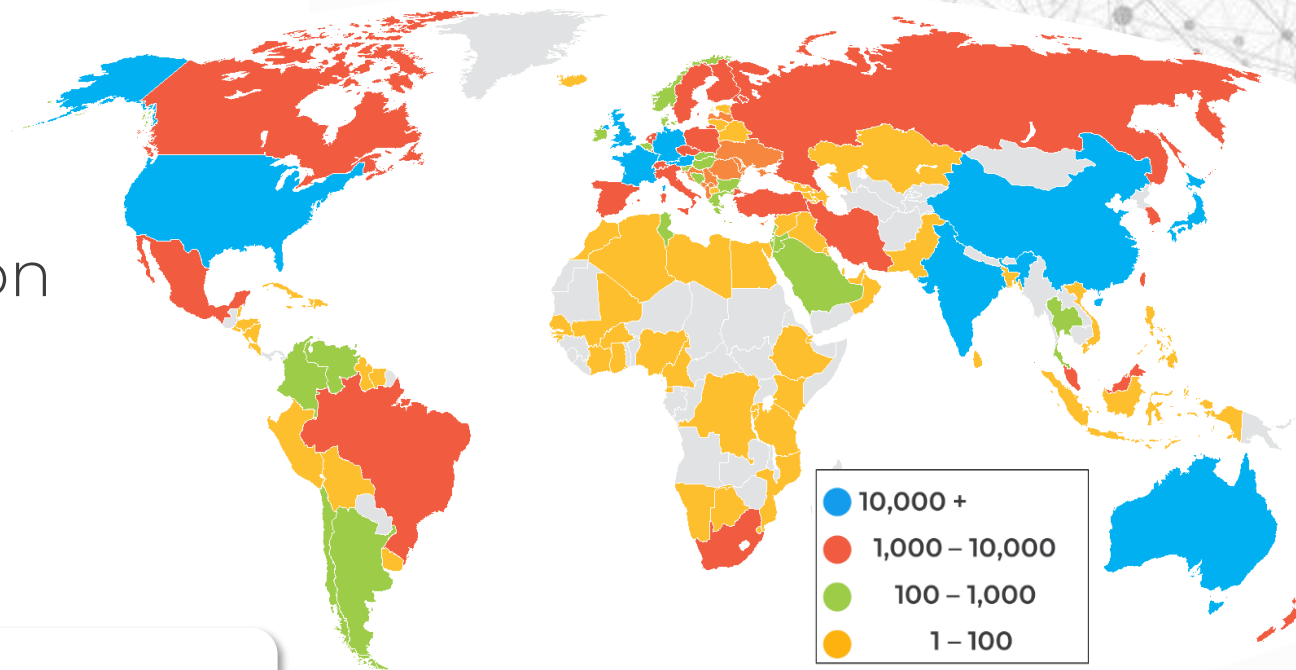


Raise your hand up if you have

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.

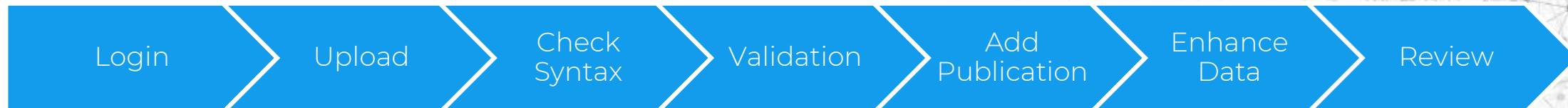


Submitting X-ray Crystallographic Data

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.

CCDC

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

Deposition

1 Login → 2 Upload → 3 Check Syntax → 4 Validation → 5 Add Publication → 6 Enhance Data → 7 Review → 8 Submit

CIF deposition Check Syntax

First name(s)

Last name(s)

Your email address

Your ORCID ID

Additional email addresses

Institution (e.g. University/Company)

Deposition number(s) for revision

CIF/HKL/RES/FCF/Word/ZIP files

Check Syntax

The files highlighted in red have syntax errors. Please click on any red file before proceeding to validation. For more information, see the help page.

Pick file to edit

structure01.cif

structure02.cif

Validation

View reports on the consistency and integrity of your structures

Structure

IUCr checkCIF

Unit cell check

structure01.cif

data_1

View Report

Enter Response

View Hits

structure02.cif

data_sa2906c

View Report

Enter Response

View Hits

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 _diffn_reflns_theta_full value (too) Low 13.50 Degree

PLAT029 _diffn_measured_fraction_theta_full value Low .. 0.677 Note

Level B

PLAT415 Short Inter D-H...H-X H1 ... H623 .. 2.00 Ang.

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

View group symbols key

CSD Communications

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

ISSN 2631-9888



If you do not intend to publish your data in the sciences through the Cambridge Structural Database (CSD) please click the 'Publish in a Database' button below to publish your data through the CSD as a [CSD Communication](#). Inorganic data will be published in the [CSD Inorganic](#) database.

[Publish in a Database](#)

Archive

The *CSD Communications* archive contains all of the data published (CSD) by the Cambridge Crystallographic Data Centre (CCDC) as *Communications*. Select a year to view all *CSD Communications*.

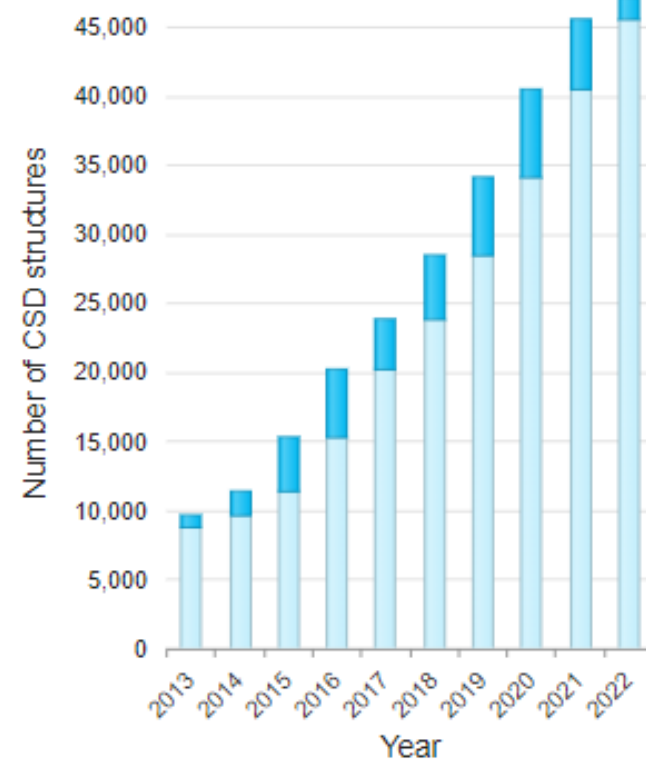
2021

2020

2019

2018

CSD Communications growth



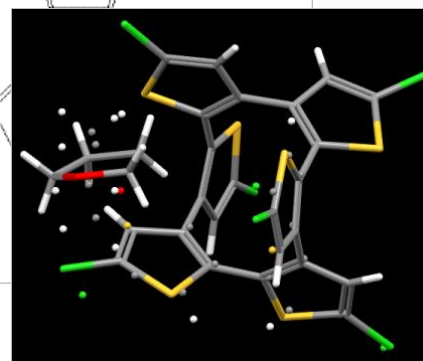
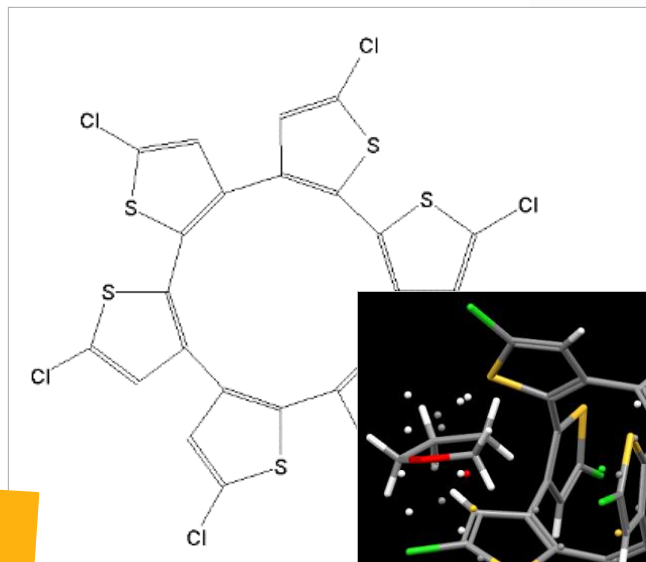
<https://www.ccdc.cam.ac.uk/Community/csd-communications/>

Once deposited your data is curated

An automated probabilistic approach using data in the CSD

```
loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _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
C11 Cl 0.5993(2) 1.0007(7) 0.8131(17) 0.044(3) Uani 0.50 1 d PDU A 1
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
C12 Cl 0.3202(2) 0.4982(6) 1.0830(5) 0.0586(15) Uani 0.50 1 d PDU A 1
S2 S 0.38755(19) 0.6658(5) 0.9578(5) 0.0400(10) Uani 0.50 1 d PDU A 1
```

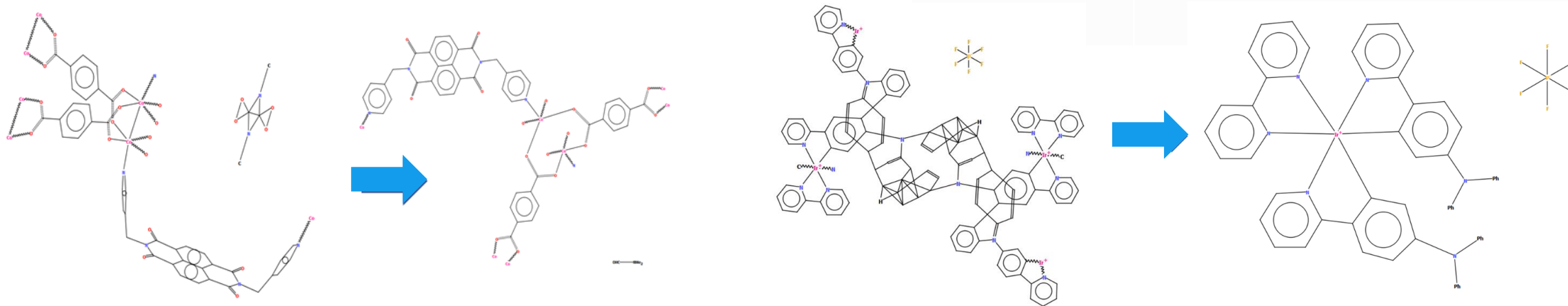
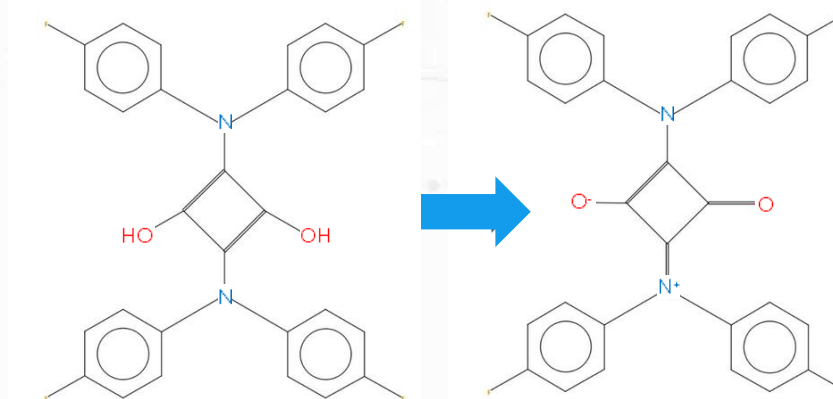
Chemistry assignment makes data findable, interoperable and reusable



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

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



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



Simple Search Structure Search Unit Cell Search Formula Search

Simple text and numeric searching

Welcome to WebCSD. This service now includes the ability to search for inorganic structures through the CCDC's and FIZ Karlsruhe's joint Access Service using the Simple Search tab. Please use one or more of the boxes to find entries. If you enter details in more than one field the search will try to find records containing all the terms entered. More information and search help

Identifier(s)

Compound name

DOI

Authors

Journal

Publication details: Year , Volume , Page

Database to search: Entire published collection CSD ICSD Teaching subset

POWVEF : catena-[(μ -phenylphosphonato)-zinc(II)]
Space Group: P 2₁/c (14), Cell: a 14.8549(8)Å b 5.1581(3)Å c 10.5471(6)Å, α 90° β 105.816(2)° γ 90°

3D viewer

Chemical diagram

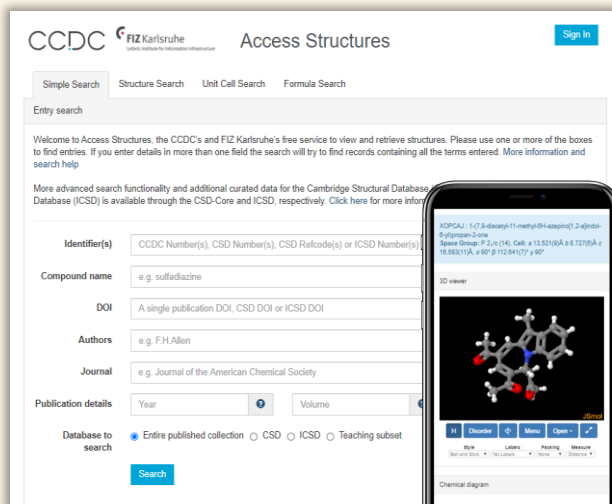
View group symbols key

Additional details

Deposition Number	1951130
Data Citation	L. Falvello, P. Lotti, C. Massera, S.C. Tarantino, M. Zema, H. Puschmann, M.Y. Agbahoungbata, J. Andreo, S.A. Sahadevan, A. Bismuto, G. Bonfant, S.A.S. Bonou, C. Carraro, M.D. Zotti, A. di Biase, R. Fantini, I. Ferraboschi, J.M.F. Custodio, M. Frigerio, G. Gallo, S. Gjyli, M. Goudjil, F. Igoa, E. Kahveci, M. Kalienko, S. Lorenzon, L. Macera, J.J.M. Fajardo, E. Nushi, S. Ouatta, E. Parisi, L. Pasqualeto, E. Pesko, G. Pierri, R. Pinalli, R. Poppe, A. Santoro, E. Smirnova, S. Sorbara, L. Tensi, G. Tusha CCDC 1951130: Experimental Crystal Structure Determination, 2019, DOI: 10.5517/ccdc.csd.cc23h9pm
Deposited on	03/09/2019

Finding structures

Web Browser



CCDC ^{FIZ Karlsruhe} Access Structures Sign In

Simple Search Structure Search Unit Cell Search Formula Search

Entry search

Welcome to Access Structures, the CCDC's and FIZ Karlsruhe's free service to view and retrieve structures. Please use one or more of the boxes to find entries. If you enter details in more than one field the search will try to find records containing all the terms entered. More information and search help

More advanced search functionality and additional curated data for the Cambridge Structural Database (ICSD) is available through the CSD-Core and ICSD. Click here for more information

Identifier(s)

Compound name

DOI

Authors

Journal

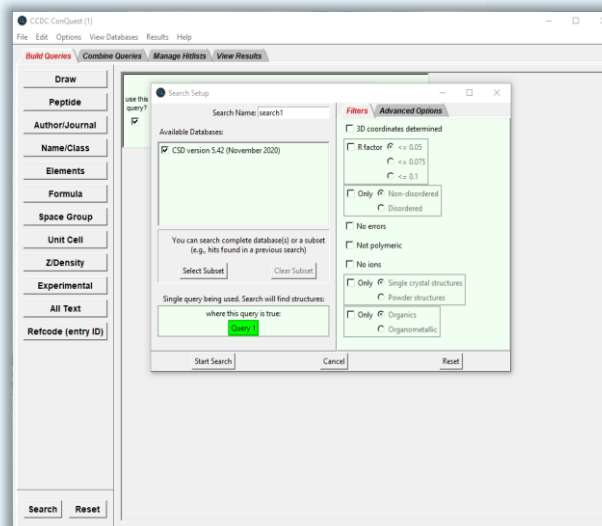
Publication details Year Volume

Database to search Entire published collection CSD ICSD Teaching subset



Access Structures /
WebCSD

Desktop



CCDC ConQuest (1)

Build Queries Combine Queries Manage Histories View Results

Draw

Peptide

Author/Journal

Name/Class

Elements

Formula

Space Group

Unit Cell

Z-Density

Experimental

All Text

Refcode (entry ID)

Search Setup

Search Name: search1

Available Databases

CSD version 5.42 (November 2020)

Filters

Advanced Options

3D coordinates determined

R factor ≤ 0.05

≤ 0.075

≤ 0.1

Only Non-disordered

Disordered

No errors

Not polymeric

No ions

Only Single crystal structures

Powder structures

Only Organics

Organometallic

You can search complete database(s) or a subset (e.g. hits found in a previous search)

Select Subset Clear Subset

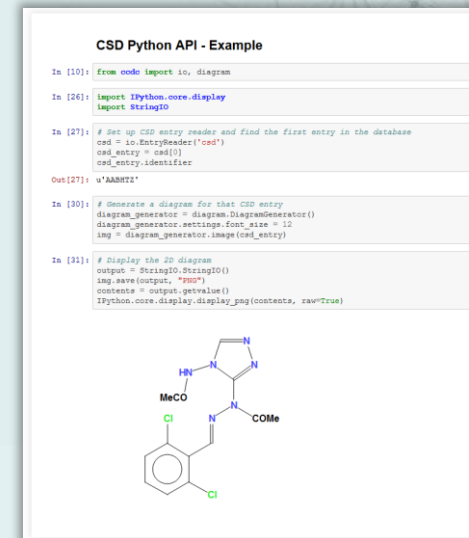
Single query being used. Search will find structures where this query is true:

Query



ConQuest

Programmatic



CSD Python API - Example

```
In [10]: from ccdc import io, diagram
In [26]: import IPython.core.display
import IPython
In [27]: # Set up CSD entry reader and find the first entry in the database
csd = io.EntryReader('csd')
csd_entry = csd()
csd_entry.identifier
Out [27]: 'AABHTA'
In [30]: # Generate a diagram for that CSD entry
diagram_generator = diagram.DiagramGenerator()
diagram_generator.settings.font_size = 12
img = diagram_generator.image(csd_entry)
In [31]: # Display the 3D diagram
output = IPython.display.HTML()
img.save(output, "PNG")
content = output.getvalue()
IPython.core.display.display_png(content, raw=True)
```

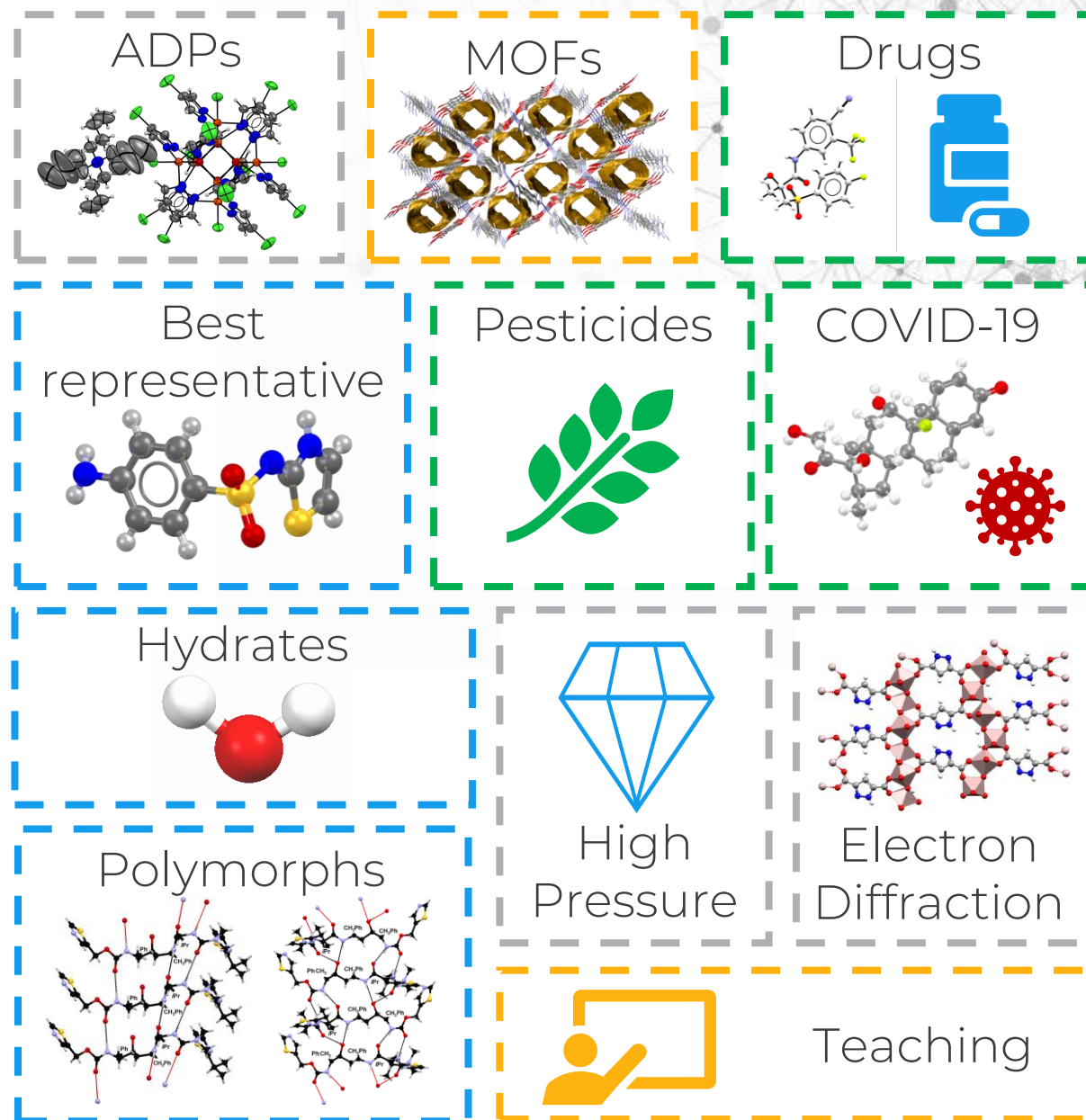
Cc1ccc(Cl)c(Cl)c1CN1C=NC2=NC=NC=C12

CSD Python API

Targeted collections

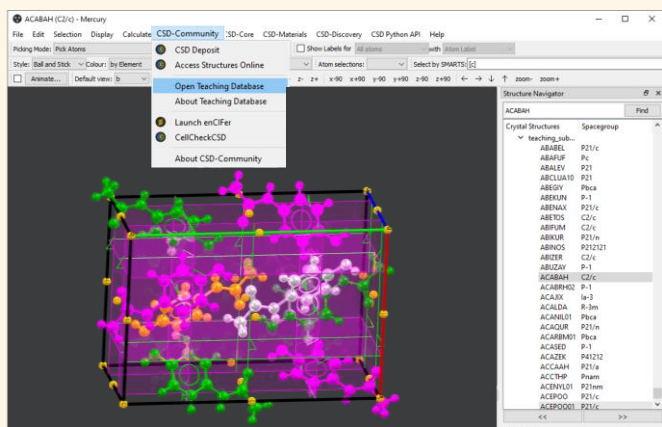
- Easy access to the most relevant structures
- Benefit from our in-house and external expertise
- Convenient starting point for analysis using CSD or 3rd party tools
- A basis for your research and crystal engineering

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



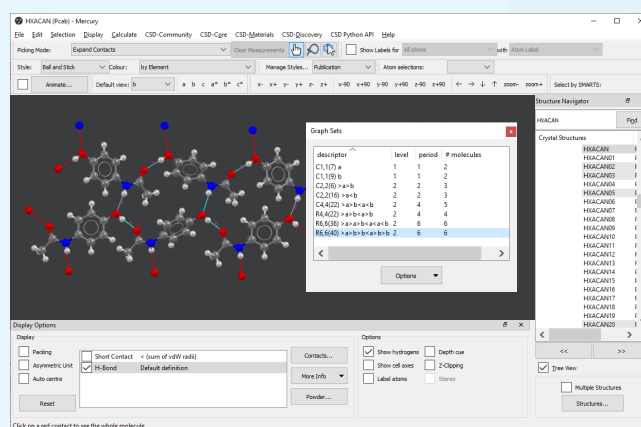
Visualising and exploring structures

The basics



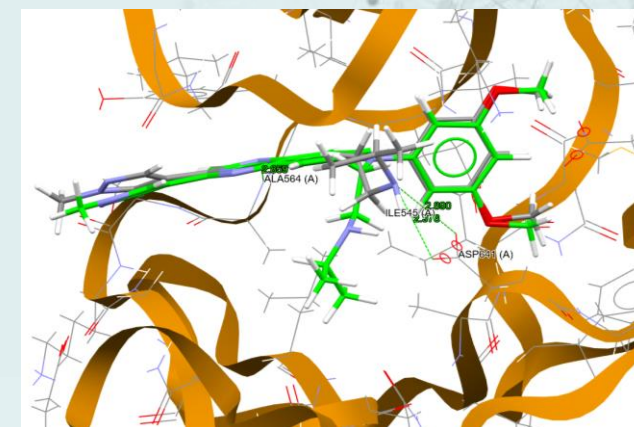
Free Mercury

Advanced



Full Mercury

Macromolecules



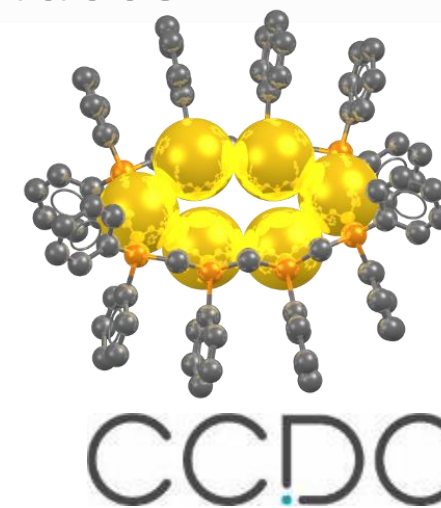
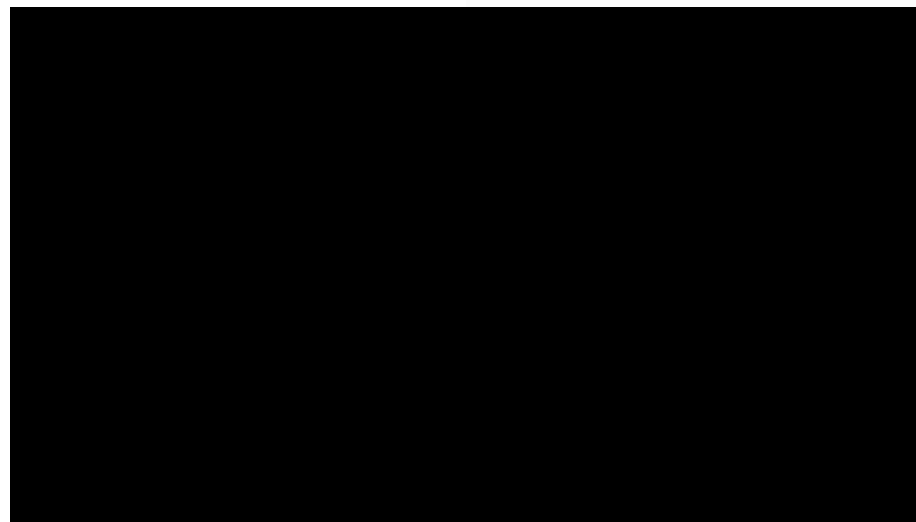
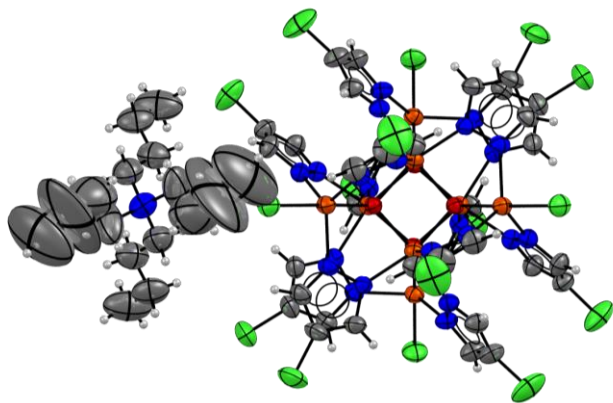
Hermes

Why use Mercury to visualise structures

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



Analysing structures

Geometries

The screenshot shows the CSD-CommuniX software interface. The 'Mogul' menu is open, listing options like 'Launch WebCSD', 'ConQuest Hit Highlighting...', 'Launch ConQuest Data Analysis Module...', 'Mogul Geometry Check...', 'Launch Mogul', 'Mogul Settings...', 'IsoStar Interaction Check...', 'Launch IsoStar', 'IsoStar Settings...', and 'Select Databases...'. Below the menu, a table displays hydrogen bond statistics for various donor-acceptor pairs.

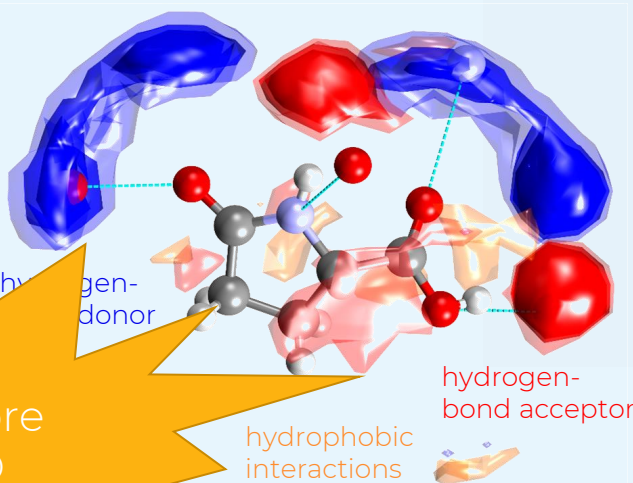
Donor	Acceptor	Distance	Distance D-A classification	Distance threshold	Distance mean	Distance std.dev.	Distance min.	Distance max.	Angle D-H...A classification	Angle threshold		
1 N1 (cyclic_nhn)	O1 (al_cooH_1)	2.75	Not Unusual	(2.73, 3.24)	28	2.87	0.16	2.70	3.38	154.24	Not Unusual	(130.13, 177.7)
2 N1B (cyclic_nhn)	O1B (al_cooH_1)	2.75	Not Unusual	(2.73, 3.24)	28	2.87	0.16	2.70	3.38	154.24	Not Unusual	(130.13, 177.7)
3 N1 (cyclic_nhn)	O3 (water)	3.24	Unusual	(2.63, 2.91)	316	2.74	0.09	2.55	3.24	121.25	Unusual	(148.00, 179.4)
4 N1B (cyclic_nhn)	O3 (water)	3.24	Unusual	(2.63, 2.91)	316	2.74	0.09	2.55	3.24	121.25	Unusual	(148.00, 179.4)
5 O2 (al_cooH_1)	O3 (water)	2.64	Not Unusual	(2.55, 2.68)	580	2.60	0.07	2.47	3.21	172.21	Not Unusual	(156.46, 178.4)



Mogul

Find out more in the CSD session today

Interactions



Isostar and FIMs

Advanced

The 'Hydrogen Bond Statistics - HELLIW' dialog box displays a table of hydrogen bond statistics and three histograms. The table lists donor-acceptor pairs, distances, and angles. The histograms show the distribution of effective density for D...A distance, D-H...A angle, and D-H...A angle.

Donor	Acceptor	Distance	Distance D-A classification	Distance threshold	Distance mean	Distance std.dev.	Distance min.	Distance max.	Angle D-H...A classification	Angle threshold		
1 N1 (cyclic_nhn)	O1 (al_cooH_1)	2.75	Not Unusual	(2.73, 3.24)	28	2.87	0.16	2.70	3.38	154.24	Not Unusual	(130.13, 177.7)
2 N1B (cyclic_nhn)	O1B (al_cooH_1)	2.75	Not Unusual	(2.73, 3.24)	28	2.87	0.16	2.70	3.38	154.24	Not Unusual	(130.13, 177.7)
3 N1 (cyclic_nhn)	O3 (water)	3.24	Unusual	(2.63, 2.91)	316	2.74	0.09	2.55	3.24	121.25	Unusual	(148.00, 179.4)
4 N1B (cyclic_nhn)	O3 (water)	3.24	Unusual	(2.63, 2.91)	316	2.74	0.09	2.55	3.24	121.25	Unusual	(148.00, 179.4)
5 O2 (al_cooH_1)	O3 (water)	2.64	Not Unusual	(2.55, 2.68)	580	2.60	0.07	2.47	3.21	172.21	Not Unusual	(156.46, 178.4)

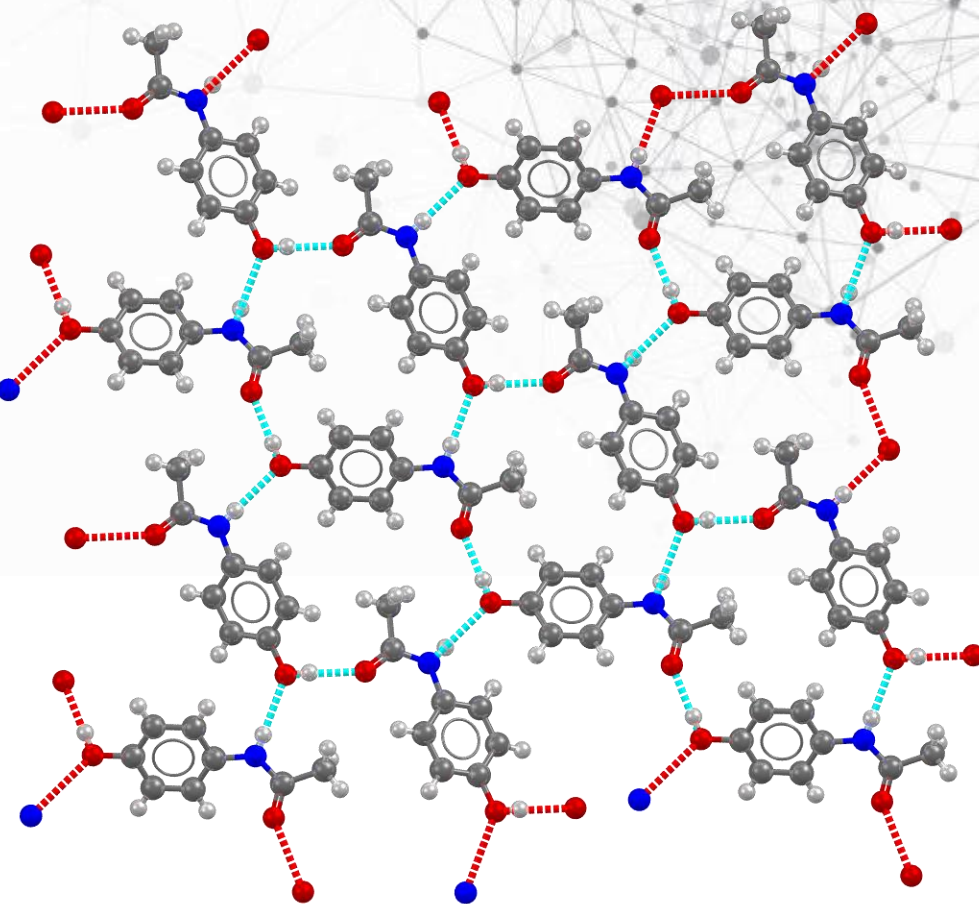
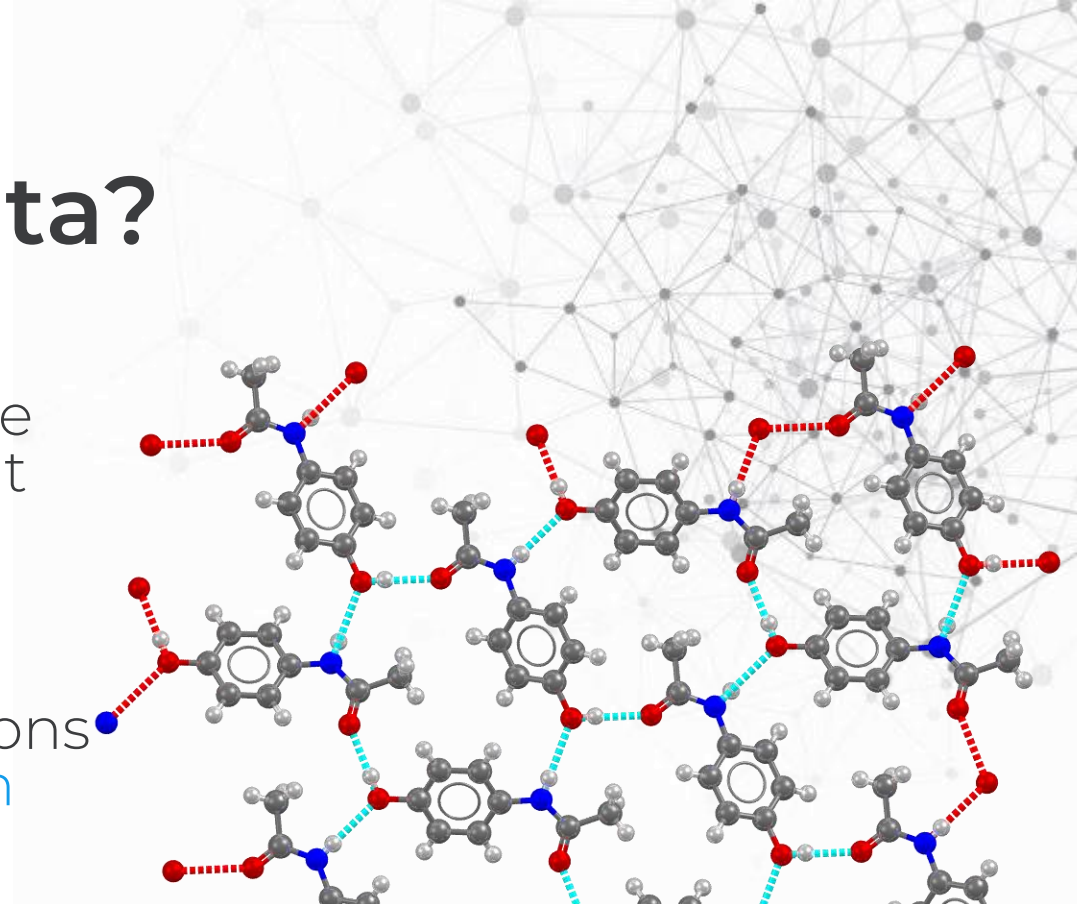


CSD Materials

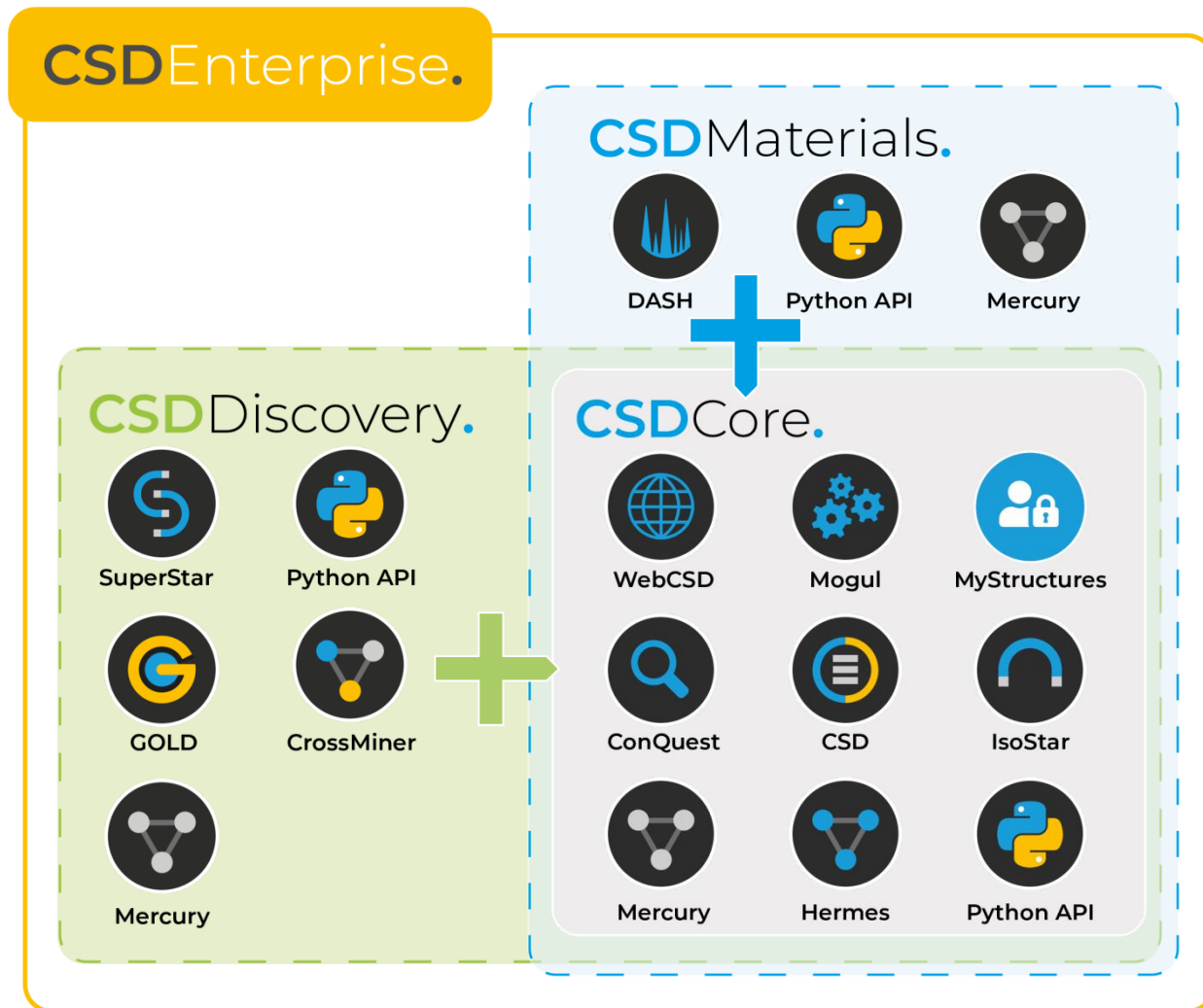


Why analyse structural data?

- 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**



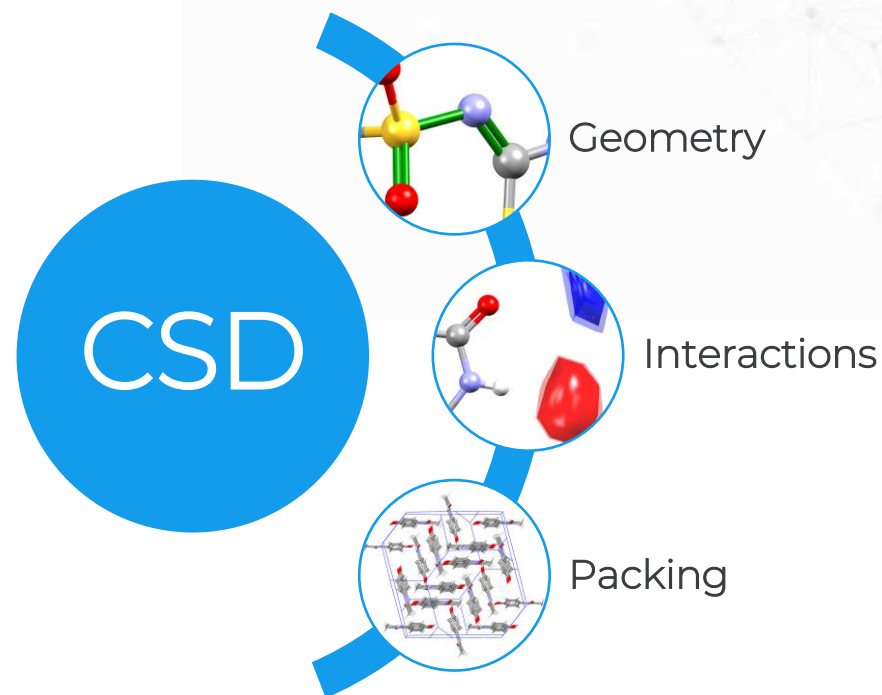
The CSD software



The CCDC Portfolio

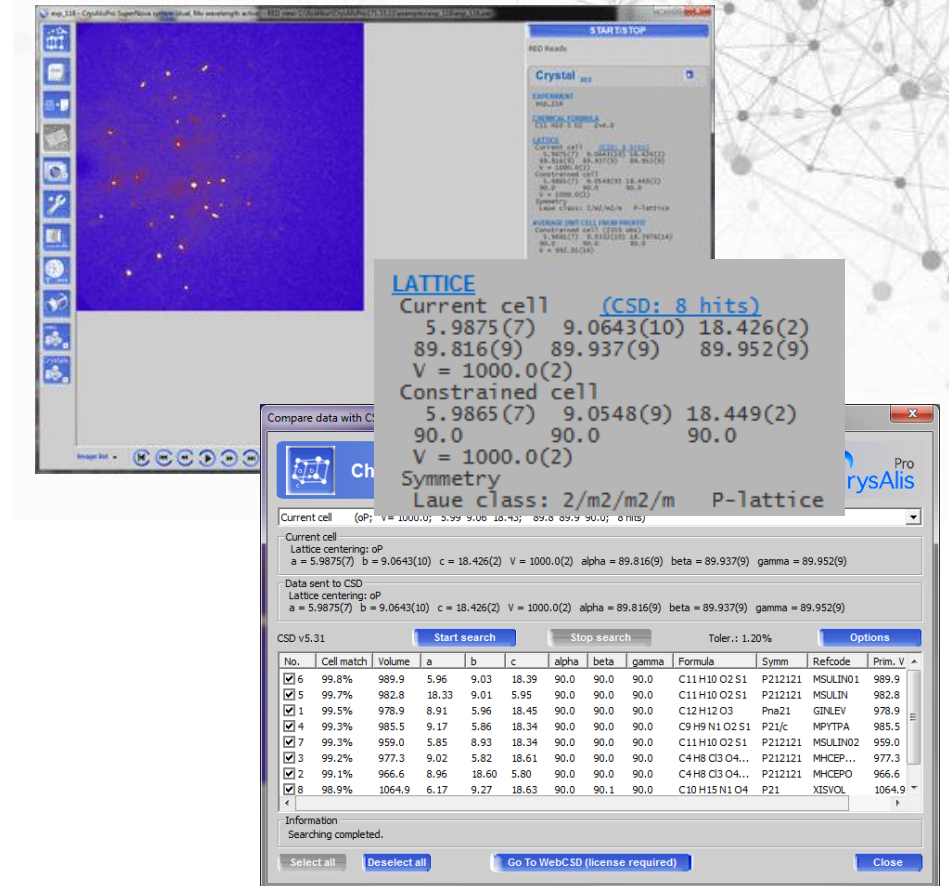
- The CSD is at the heart of the CCDC Portfolio and provides the **accurate** structural data from which key **insights** can be extracted.

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



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



The screenshot displays the EnCIFer software interface. The main window shows a CIF file named '99scw127a.cif' being edited. The text in the editor includes:

```
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M P21/c

loop_
_symmetry_equiv_pos_as_xyz
'x, y, z'
'-x, y+1/2, -z+1/2'
'-x, -y, -z'
'x, -y-1/2, z-1/2'

_cell_length_a                  8.252(2)
_cell_length_b                  10.535(2)
_cell_length_c                  19.923(4)
_cell_angle_alpha               90.00
_cell_angle_beta                99.17(3)
_cell_angle_gamma               90.00
_cell_volume                     1709.9(6)
_cell_formula_units_Z           4
_cell_measurement_temperature   150(2)
_cell_measurement_reflns_used   ?
_cell_measurement_theta_min     ?
_cell_measurement_theta_max     ?
```

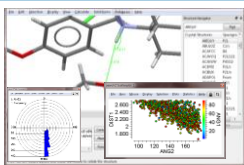
Below the editor, a 'Visualiser' window shows a 3D ball-and-stick model of the crystal structure. The status bar at the bottom indicates 'Checking CIF ...' and 'No errors, warnings or errors'. A message box also states 'Loading visualiser for block_data_99scw127a'.

The image shows two wizard windows from the EnCIFer software. The left window is the 'enCIFer Publication Data Wizard' (page 3 of 8), which prompts for contact information such as 'Contact author', 'Email address', 'Contact address', 'Telephone number', and 'Fax number'. The right window is the 'enCIFer Chemical and Crystal Data Wizard' (page 3 of 7), which prompts for physical and chemical information, including 'Systematic name', 'Common name', 'Moiety Formula', 'Sum Formula' (shown as C17H18N4O2S), 'Compound source', and 'Physical Properties' (with 'air-sensitive' selected).

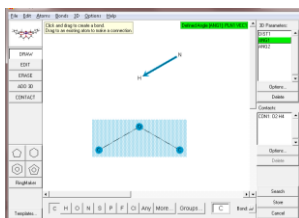
CSD-Core overview



Mercury: Visualisation & numerical analysis



ConQuest: Advanced 3D searching & data generation



WebCSD: Online search & entry level interface



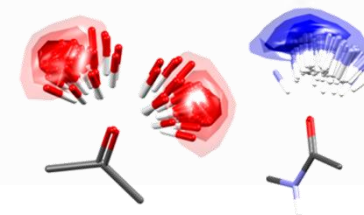
Hermes: Visualisation of macromolecules



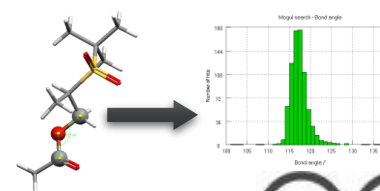
CSD Python API: Access to data & all functionality



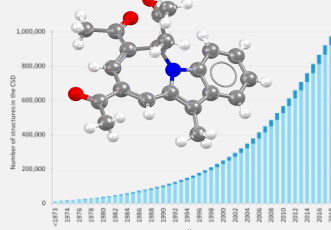
IsoStar: Intermolecular interaction analysis



Mogul: Molecular geometry analysis



Cambridge Structural Database



CSD-Editor: Create in-house database

CCDC

Mogul: Molecular geometry

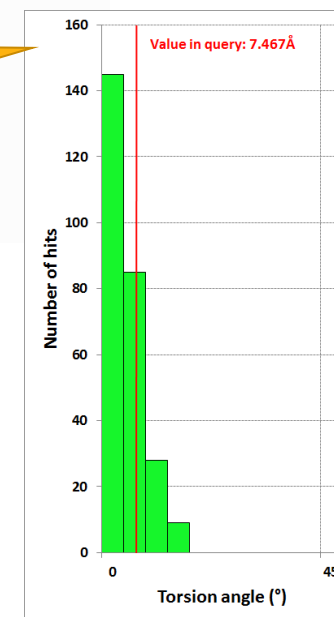
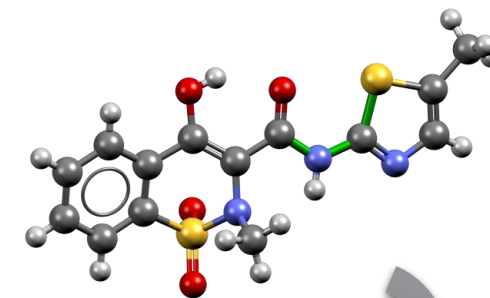
Mogul:

- 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.

Applications:

- [Validation](#) of:
 - molecular geometries.
 - docking solution.
- [Generation](#) of low energy conformations.
- [Selection](#) of linking groups.
- [Rationalisation](#) of inactivity.

Find out more
in the CSD
session today



IsoStar: Intermolecular interactions

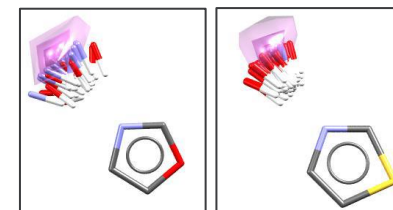
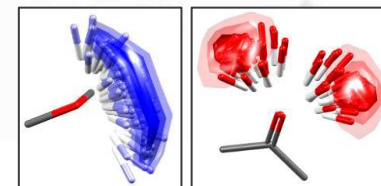
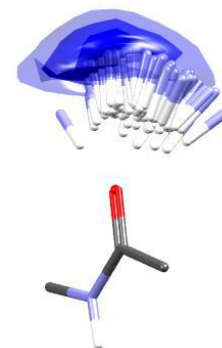
Isostar:

- 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 interact? (e.g. do hydrogen-bonds to ether oxygen lie along 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



CSD-Materials Overview

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

CSD Python API: Access to data & all functionality



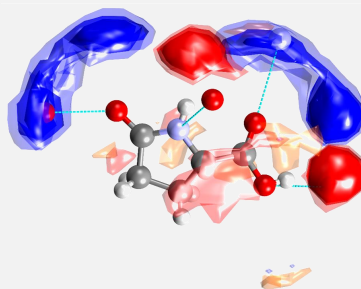
Full Interaction Maps: discover preferred intra- and inter- molecular interactions.

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.

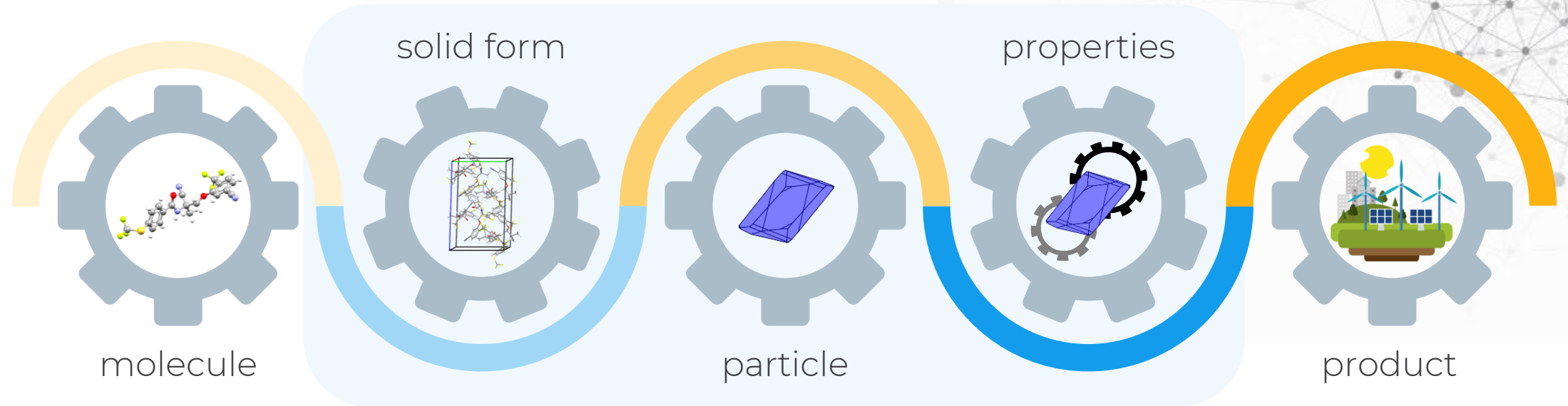
Multi-component screening: based on molecular complementarity.

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

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

Data inspired materials design

materials informatics



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

CSD-Discovery overview

CSD-Discovery.



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

A wealth of structures, stories and possibilities

CSD one million special issue

- 33 articles from industry and academia

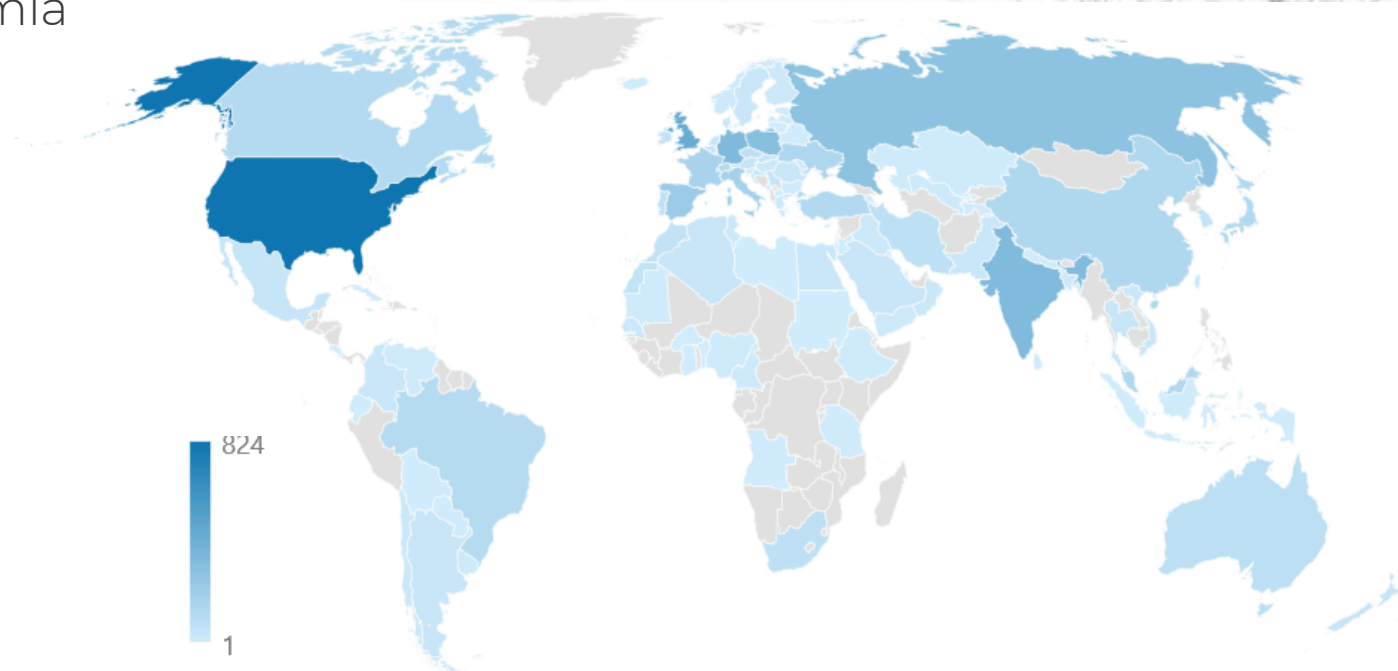
**1 million structures.
stories.
possibilities.**



Cambridge Structural
Database, CSD



CCDC
advancing structural science



The CSD - A wealth of knowledge gained from a million structures. *CrystEngComm*, 2020,22, 7131-77502

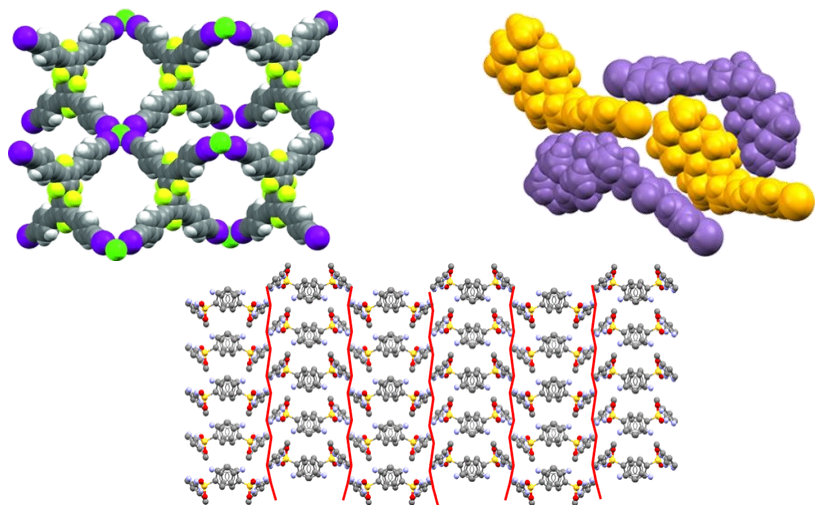
The CSD. C.R.Groom, I.J.Bruno, M.P.Lightfoot and S.C.Ward, *Acta Cryst.* (2016). B72, 171-179 DOI: 10.1107/S2052520616003954

CCDC

The whole is greater than the sum of its parts

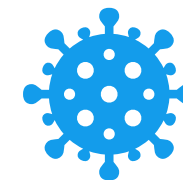
CSD Insights

- Molecular geometries
- Molecular interactions
- Molecular assemblies



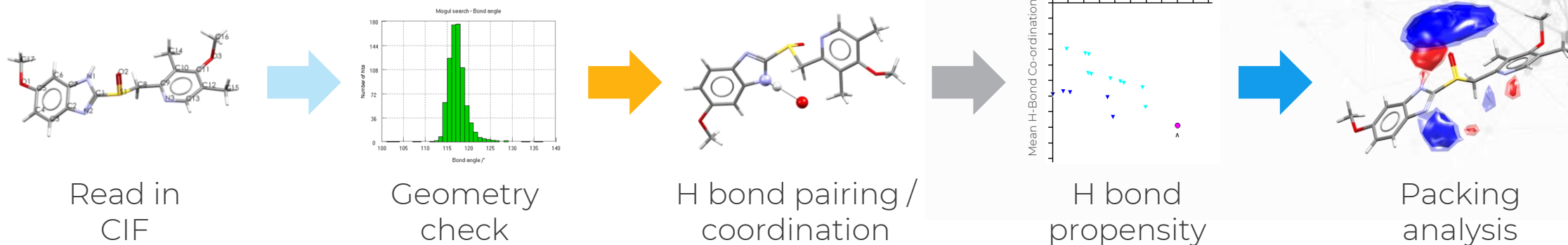
CSD Applications

- 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



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

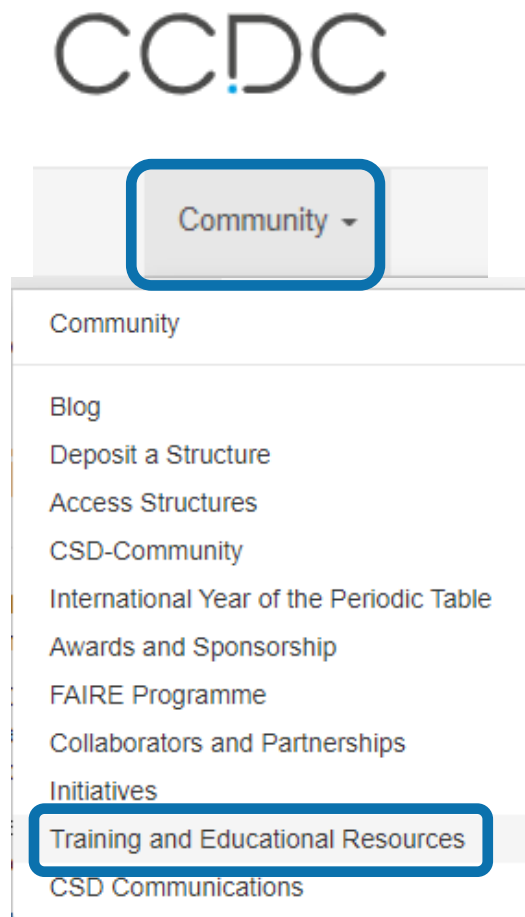


- CCDC, in having extensively worked with some of our closest pharma partners, has seen first-hand the systems in current development pipelines and the problems faced on a daily basis

More to explore...

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

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.](#)



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

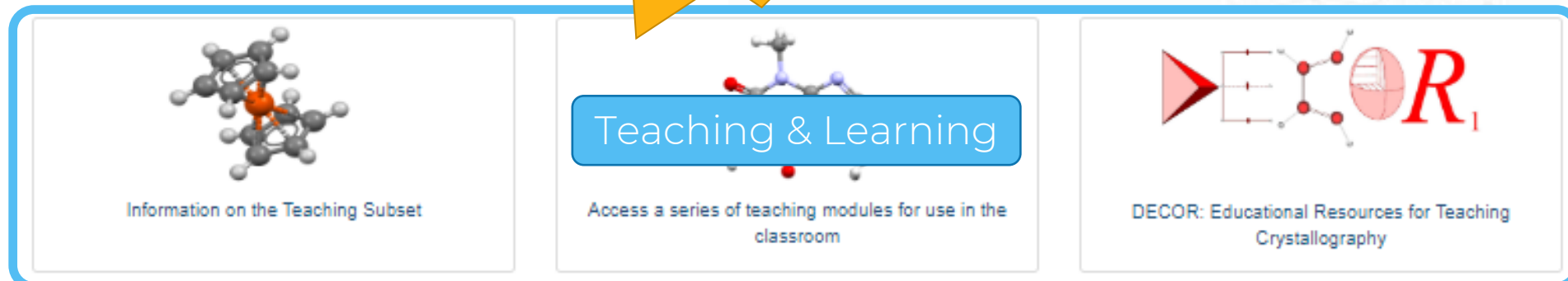


Software Training

Self-guided workshops

CSD session at 15:30

On-demand modules with completion certificate

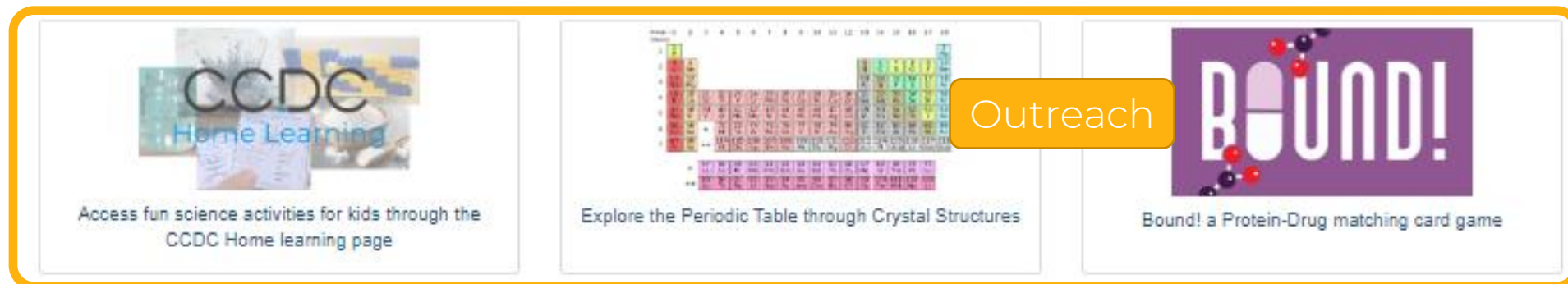


Information on the Teaching Subset

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

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



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

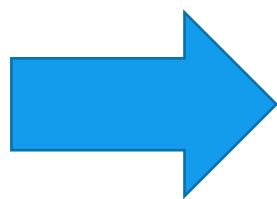
What is a crystallographic database?

- 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



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!”

About you

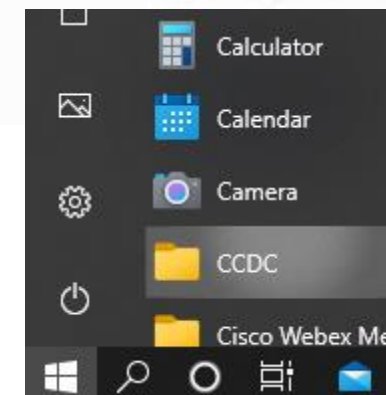
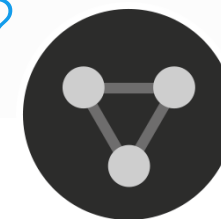


1. Have you done any of the following before?

- 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



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



The CSD Portfolio

CSD Enterprise.

CSD Materials.



DASH



Python API



Mercury

CSD Discovery.



SuperStar



Python API



GOLD



CrossMiner



Mercury

CSD Core.



WebCSD



Mogul



MyStructures



ConQuest



CSD



IsoStar



Mercury



Hermes

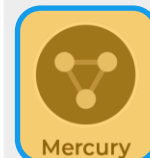


Python API

Professional Services

Research & Knowledge partnerships

CSD Community.



Mercury



enCIFer



Symmetry



Deposit



CellCheck



Educational



Access

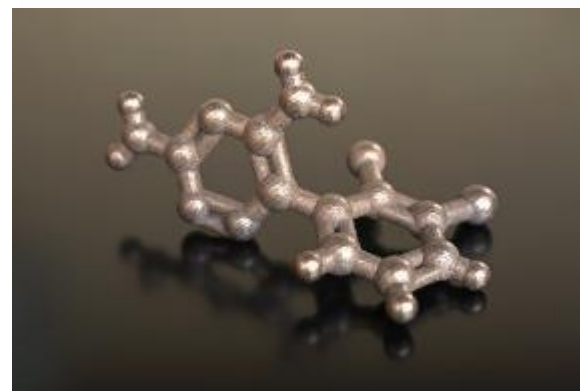
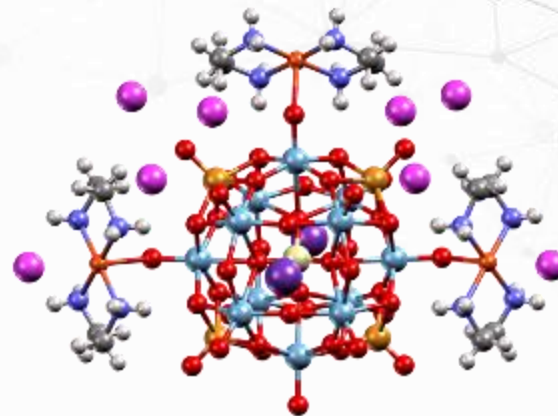


MyStructures

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



The basics of Mercury



AABHTZ (P-1) - Mercury

File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Discovery CSD Python API Help

Picking Mode: Pick Atoms Clear Measurements Show Labels for All atoms with Atom Label

Style: Ball and Stick Colour: by Element or Suppression Manage Styles... Work 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: [c]

Structure Navigator

AABHTZ Find

Crystal Structures	Spacegroup
AABHTZ	P-1
AACANI10	P21/c
AACANI11	P21/c
AACFAZ	Pbcn
AACFAZ10	Pbcn
AACMAL	P21/c
AACMHX10	Pbca
AACRHA	Pnmc
AACRHC	P-1
AACRUB	Cc
AACRUB01	C2/c
AADAMC	P21/c
AADMPY	P-1
AADMPY10	P-1
AADRIB	P21
AAGAGG10	P212121
AAGGAG10	P21

Display Options

Display

Packing Short Contact < (sum of vdW radii) Contacts...
 Asymmetric Unit H-Bond Default definition More Info
 Auto centre Reset Powder...

Options

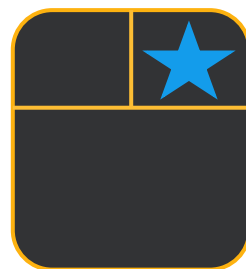
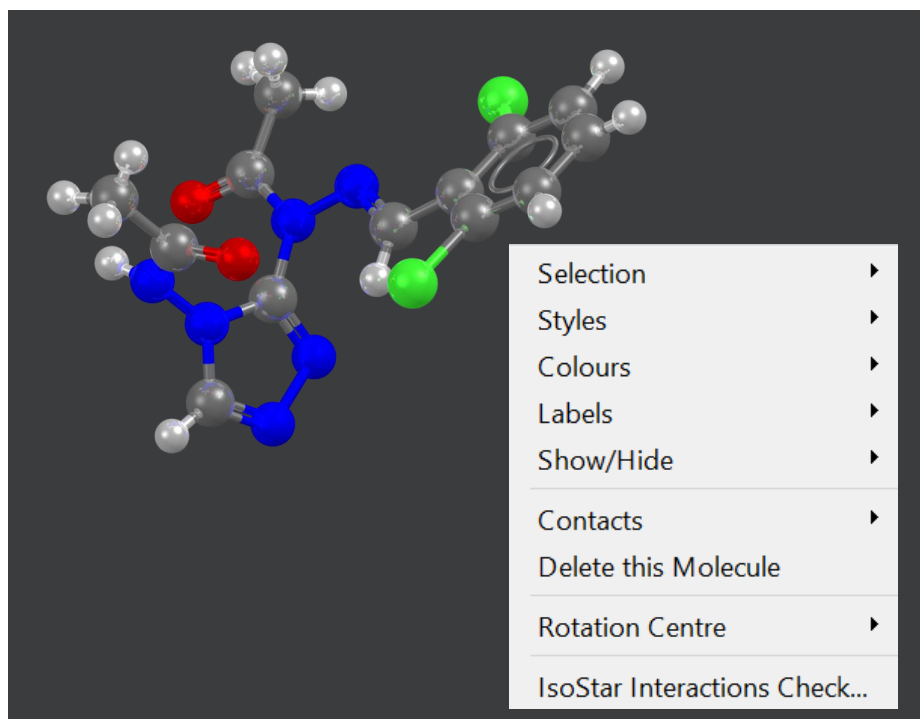
Show hydrogens Depth cue
 Show cell axes Z-Clipping
 Label atoms Stereo

Tree View Multiple Structures Structures...

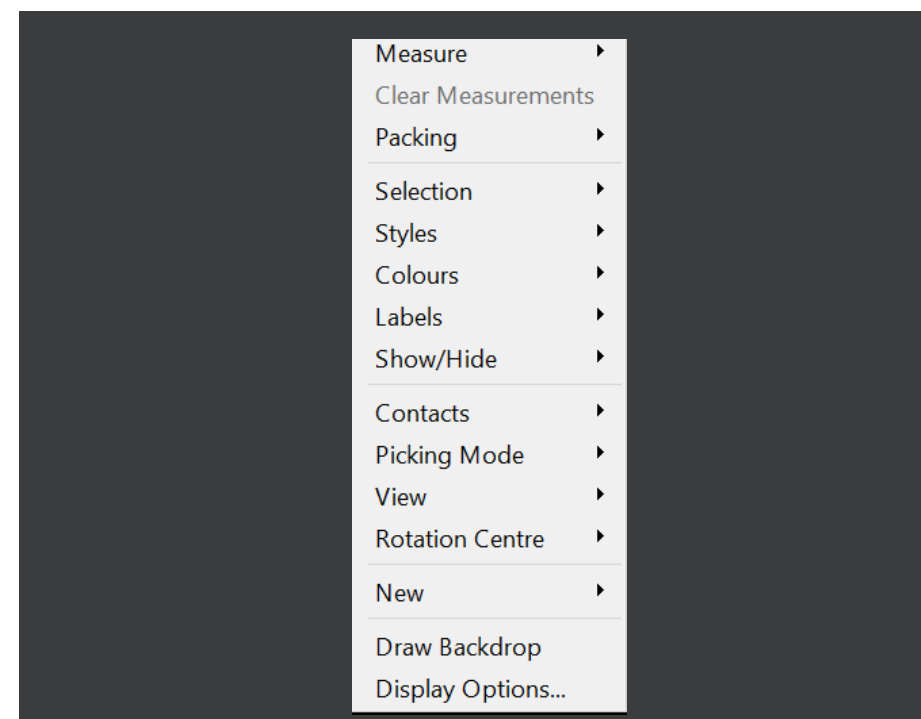
Press the left mouse button and move the mouse to rotate the structure

Right mouse click

Near a molecule






Away from a molecule







File Edit Selection **Display** Calculate CSD-Community CSD-System CSD-Materials CSD-Discovery CSD Python API Help

Picking Mode: Pick Atoms
Style: Capped Sticks
Animate... De

Measurements    Show Labels for All atoms with Atom Label

Manage Styles... Work Atom selections:

b* c* x- x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-90 z+90     zoom- >> Select by SMARTS: >>

Structure Navigator

Type in a refcode Find

Crystal Structures	Spacegroup
AABHTZ	P-1
AACANI10	P21/c
AACANI11	P21/c
AACFAZ	Pbcn
AACFAZ10	Pbcn
AACMAL	P21/c
AACMHX10	Pbca
AACRHA	Pncm
AACRHC	P-1
AACRUB	Cc
AACRUB01	C2/c
AADAMC	P21/c
AADMPY	P-1
AADMPY10	P-1
AADRIB	P21
AAGAGG10	P212121
AAGGAG10	P21
AALCFE	P21/c
AALPRO	P21/c
AAMAND	P212121
AAMTCO	P-1
AAMTCO10	P-1
AAMTXP	P21/n
AANHGX	Pna21
AANHGX01	Pna21
AANOPM	P21
AAPUNI	P21/a

Display Options

- Display Options
- Graph Sets
- Intermolecular Potentials
- Searches
- Post Search Options
- Structure Navigator
- Picking Toolbar
- Labels
- Display
- Style Manager Toolbar
- Atom Selection Toolbar
- Select by SMARTS
- Animation Toolbar
- Crystal Orientation Operations
- Alignment and Orientation Operations

Display Options

Display

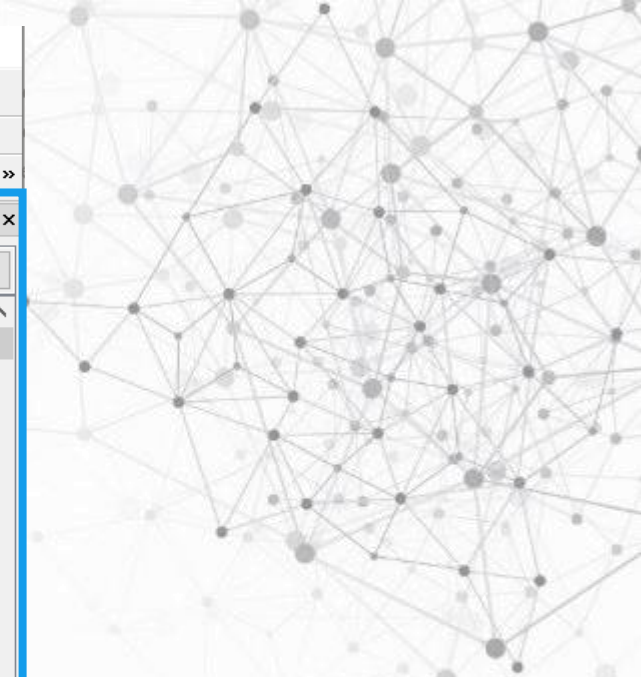
- Packing
- Asymmetric Unit
- Auto centre
- Short Contact < (sum of vdW radii)
- H-Bond Default definition

Options

- Show hydrogens
- Show cell axes
- Label atoms
- Depth cue
- Z-Clipping
- Stereo

Tree View

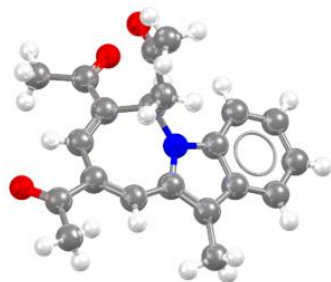
- Tree View
- Multiple Structures



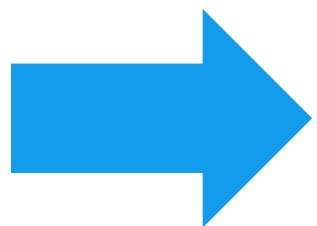
Handy tips:

- Recovering Toolbars
- Resetting view

CSD Refcodes



CSD Refcode -
XOPCAJ



What is XOPCAJ?

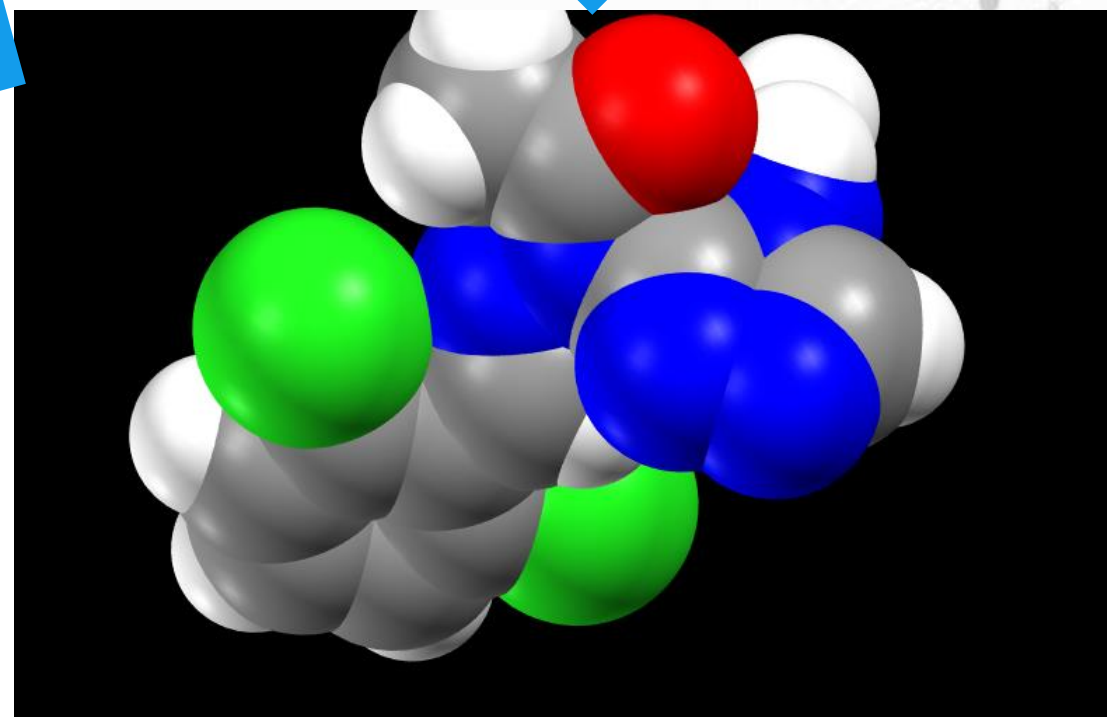
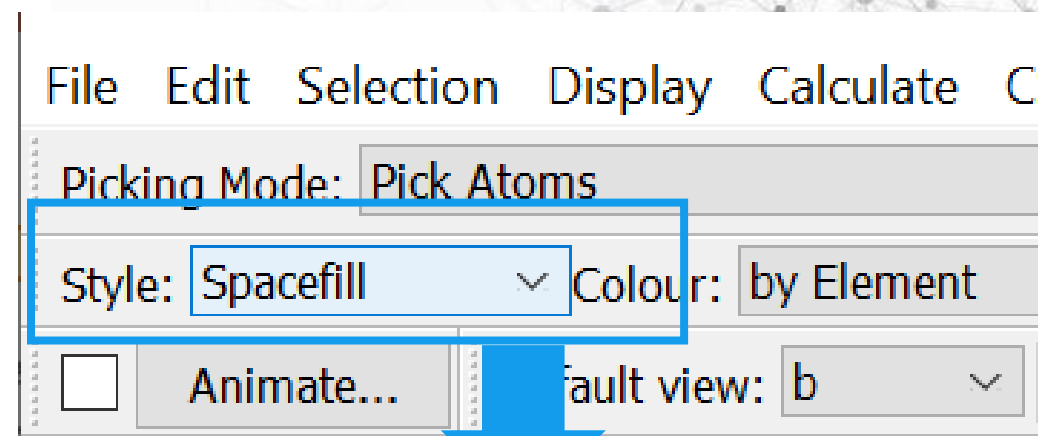
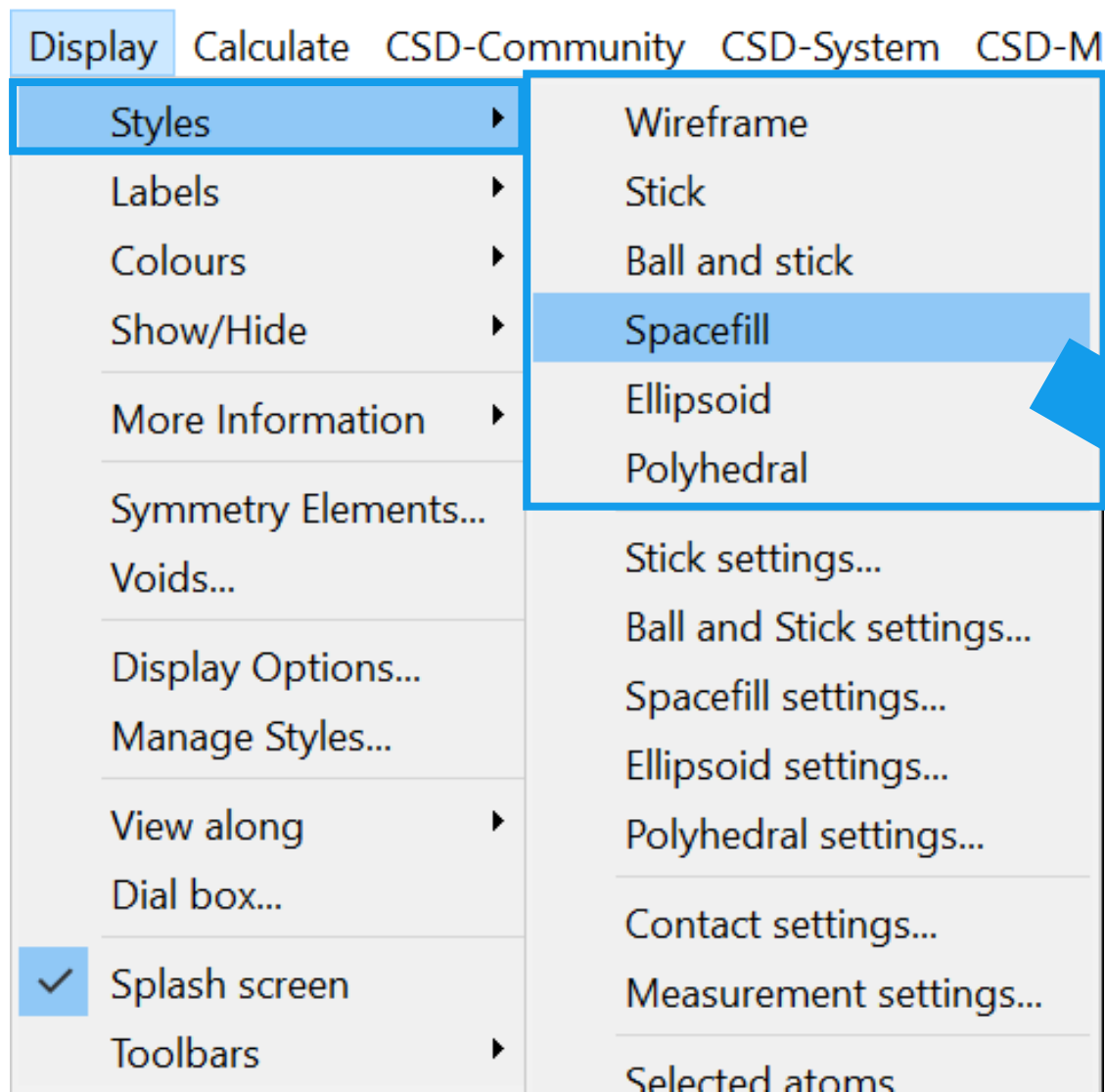
- A CSD Refcode
- A database reference code
- Containing 6-8 characters
- Used to identify entries in the CSD

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

Changing display - Style



AABHTZ (P-1) - Mercury

File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Discovery CSD Python API Help

Picking Mode: Expand Contacts

Style: Ball and Stick Colour:

Animate... Default view

Centroids...
Planes...
Packing/Slicing...
Contacts...
Molecular Shell...
Graph Sets...

Show Labels for All atoms with Atom Label

Manage Styles... Publication Atom selections:

x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-90 z+90 ← → ↓ ↑ zoom- zoom+ Select by SMARTS: >>

Structure Navigator

AABHTZ Find

Crystal Structures

AABHTZ	P-1
AACANI10	P21/c
AACANI11	P21/c
AACFAZ	Pbcn
AACFAZ10	Pbcn
AACMAL	P21/c
AACMHX10	Pbca
AACRHA	Pnccm
AACRHC	P-1
AACRUB	Cc
AACRUB01	C2/c
AADAMC	P21/c
AADMPY	P-1
AADMPY10	P-1
AADRIIB	P21
AAGAGG10	P212121
AAGGAG10	P21

Packing and Slicing

Packing

Show cell axes

Label cell axes

Pack

a: 0.0 1.0 +0.5

b: 0.0 1.0 +0.5

c: 0.0 1.0 +0.5

2x2x2

Reset

3x3x3

Include atoms

... that fit

... in molecules whose Centroids fit

... in molecules where Any atom fits

... in molecules where All atoms fit

Display Options

Display

Packing

Asymmetric Unit

Auto centre

Short Contact < (sum of vdW radii)

H-Bond Default definition

Reset

Options

Show hydrogens

Show cell axes

Label atoms

Depth cue

Z-Clipping

Stereo

Contacts...

More Info

Powder...

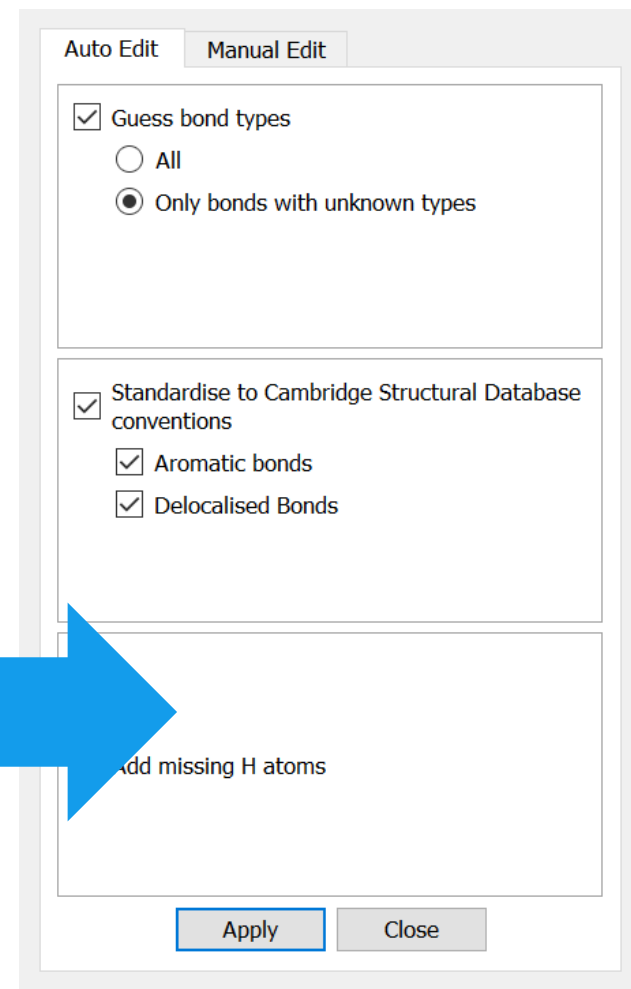
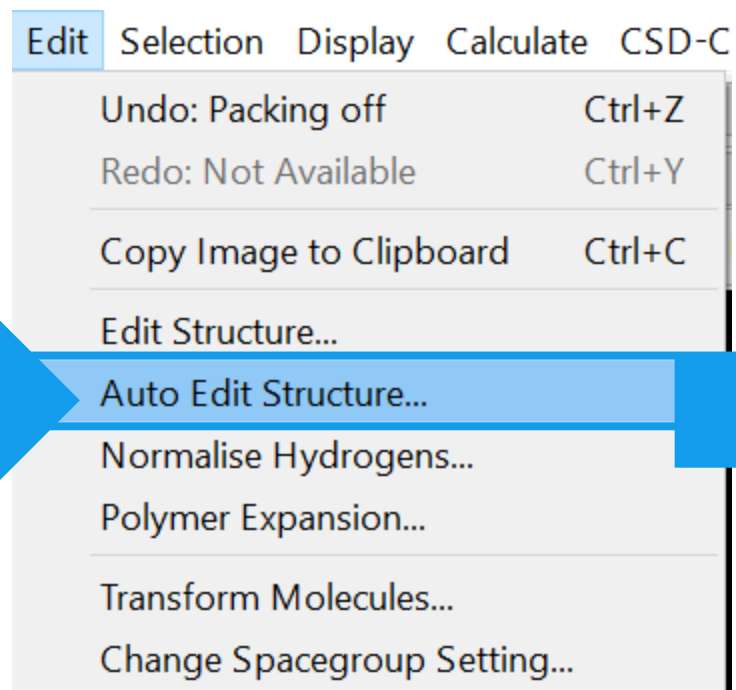
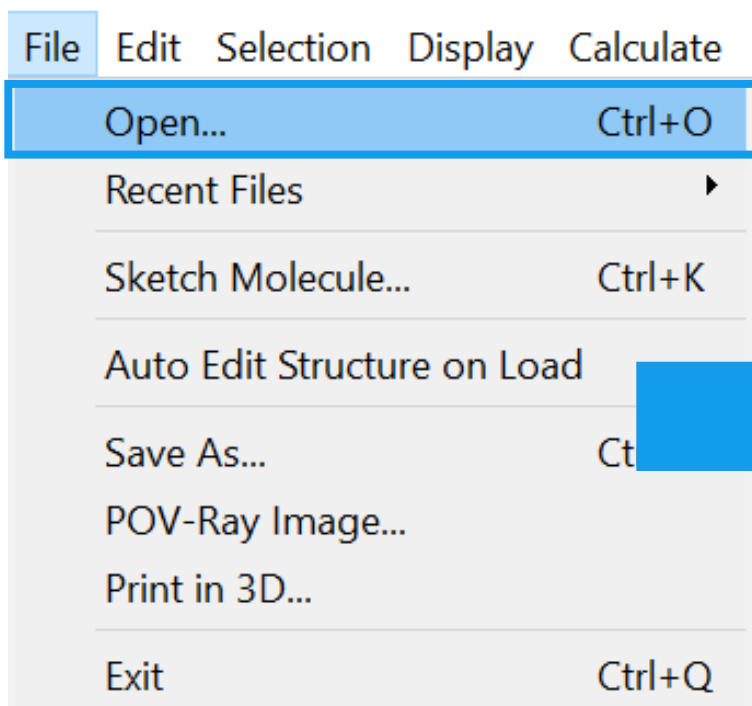
Reset button: a friend!

Click on a red contact to see the whole molecule

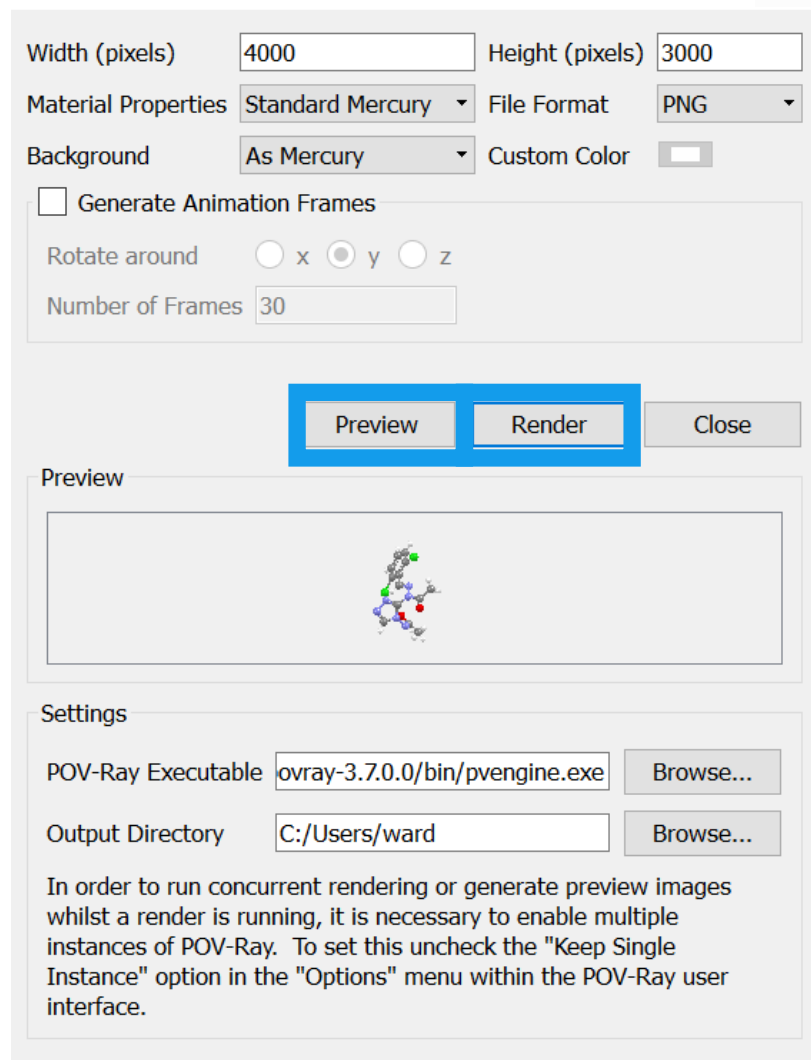
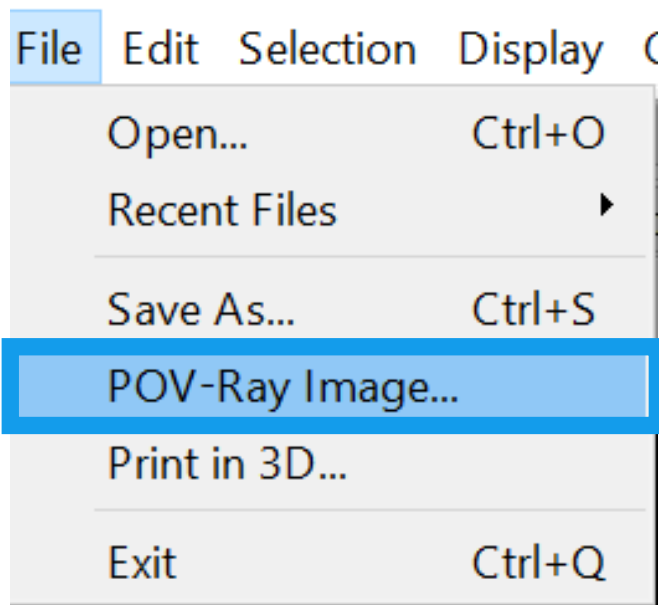
Using your own file

- 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

AABHTZ (P-1) - Mercury



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'

From visualization to deeper understanding

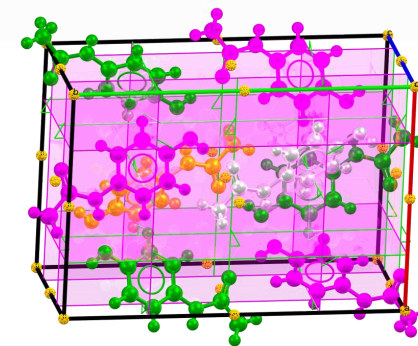
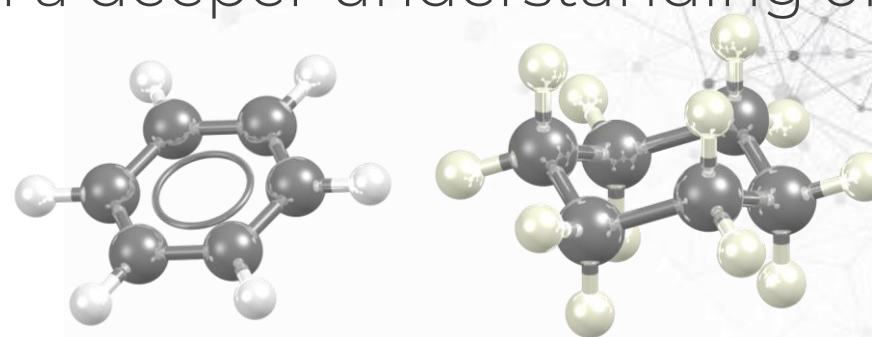
By exploring 3D structures, we can gain a deeper understanding of:

- Chemistry

- The geometry of molecules
- The geometry around metals

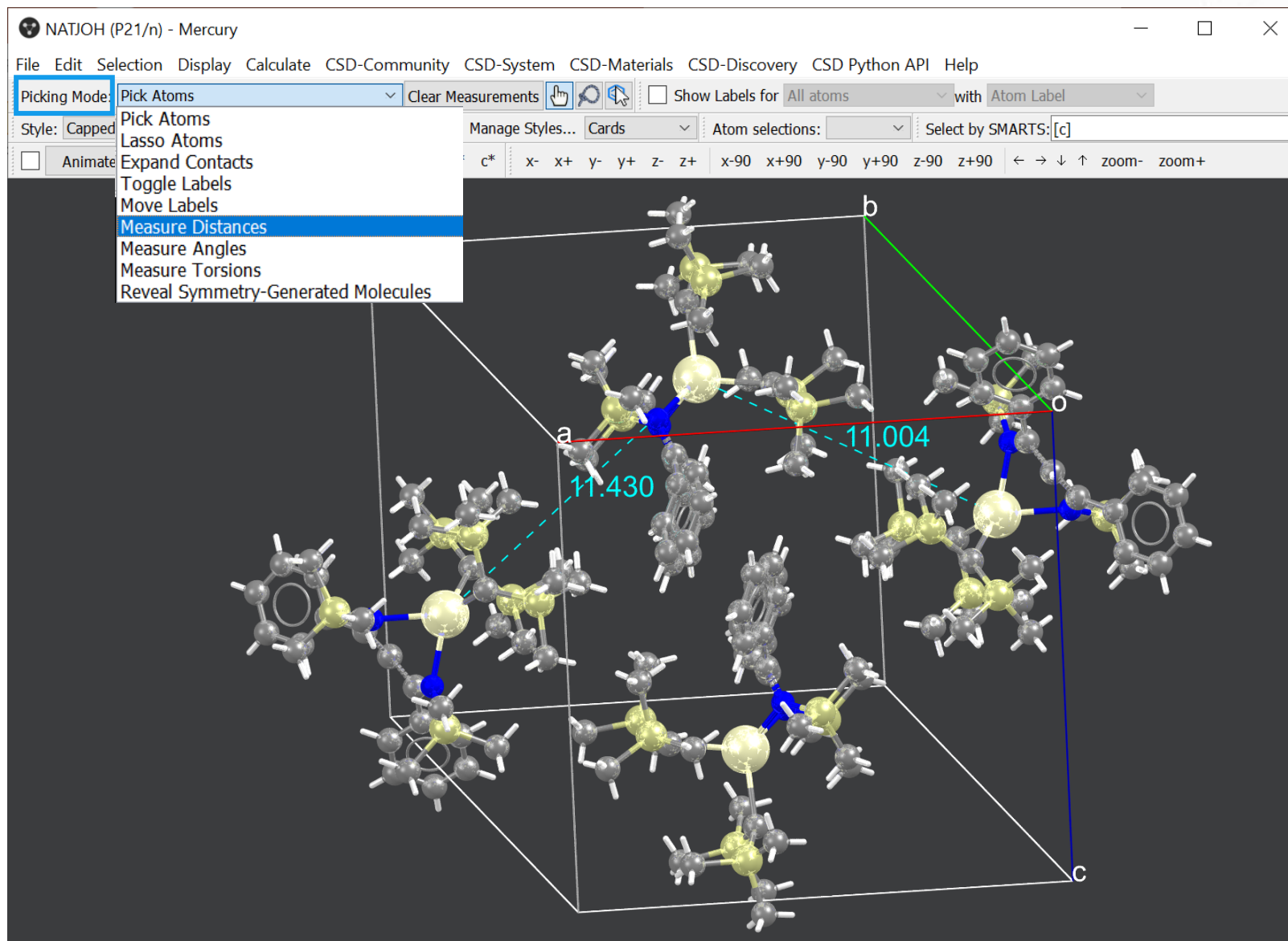
- Solid forms

- 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



Measure distances

CSD Refcode:
NATJOH



Measure

Measure Distances

Clear Measurements

Measure Angles

Packing

Measure Torsions

Selection

Default Picking Mode

Styles

Clear Measurements

Colours

Labels

Show/Hide

Contacts

Picking Mode

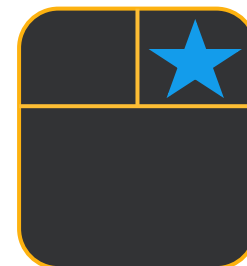
View

Rotation Centre

New

Draw Backdrop

Display Options...



HXACAN (Pcab) - Mercury

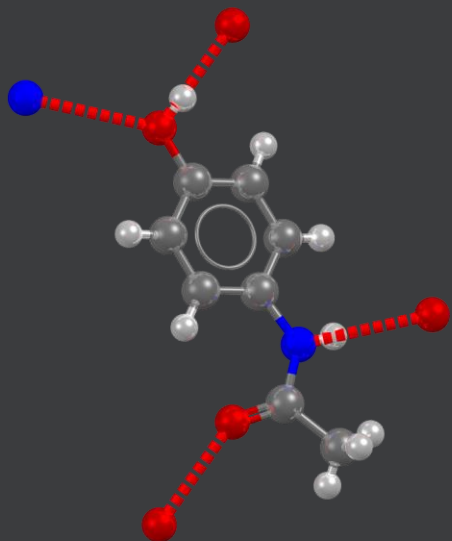
File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Discovery CSD Python API Help

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 Select by SMARTS:

Visualising hydrogen bonds



Structure Navigator

HXACAN Find

Crystal Structures

Define H-bonds

Select options and click OK or Apply when done

Require hydrogen atom to be present

D-H...A angle >= 120.0 degrees

Donor atom types:

- all donors
- nitrogen
 - metal bound N
 - imine N
 - aromatic (6-ring) N
 - amide or thioamide N

Acceptor atom types:

- all acceptors
- nitrogen
 - metal bound N
 - terminal N (cyano, etc.)
 - aromatic (6-ring) N
 - other 2-coordinate N
 - 3-coordinate N
 - unclassified N

Distance: 5.00

Separator separated by > 3 bonds

Default Cancel Apply OK

Click on "Default definition" to change the default H-bond definition

Display Options

Display

- Packing
- Asymmetric Unit
- Auto centre
- Short Contact < (sum of vdW radii)
- H-Bond Default definition

Options

- Show hydrogens
- Show cell axes
- Label atoms

Contacts... More Info Powder... Reset

Click on a red contact to see the whole molecule

HXACAN (Pcab) - Mercury

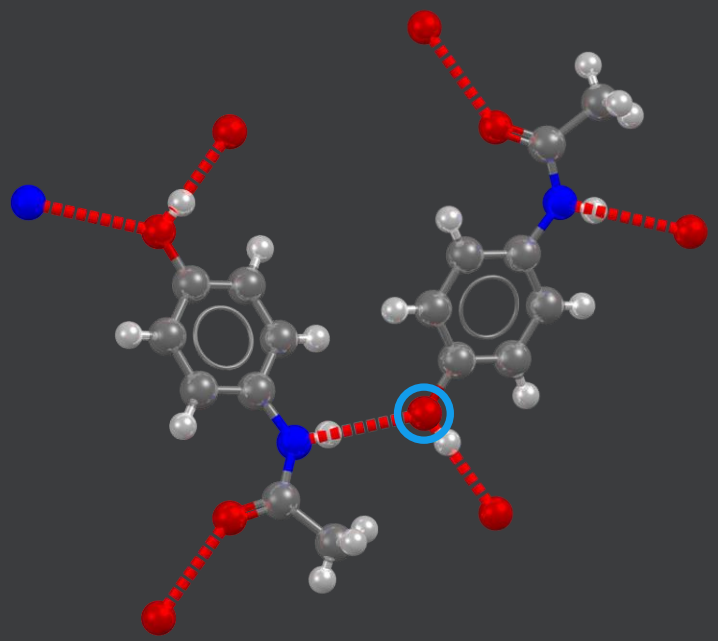
File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Discovery CSD Python API Help

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 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...

Right click on hanging contacts to see more advanced options including delete hanging contacts

Structure Navigator

HXACAN Find

Crystal Structures

- 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

Calculate CSD-Community

Centroids...

Planes...

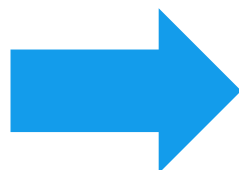
Packing/Slicing...

Contacts...

Molecular Shell...

Graph Sets...

Powder Pattern...



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.

HXACAN (Pcab) - Mercury

File Edit Selection Display Calculate CSD-Community CSD-Cgre CSD-Materials CSD-Discovery CSD Python API Help

Picking Mode: Expand Contacts Clear Measurements Show Labels for All atoms with >>

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 Select by SMARTS: >>

Graph Sets

descriptor ^	level	period	# molecules
C1,1(7) a	1	1	2
C1,1(9) b	1	1	2
C2,2(6) >a>b	2	2	3
C2,2(16) >a<b	2	2	3
C4,4(22) >a>b<a<b	2	4	5
R4,4(22) >a>b<a>b	2	4	4
R6,6(36) >a>a>b<a<a<b	2	6	6
R6,6(40) >a>b>b<a>b>b	2	6	6

Options

Display Options

Display

Packing Short Contact < (sum of vdW radii) Contacts...

Asymmetric Unit H-Bond Default definition More Info

Auto centre Reset Powder...

Options

Show hydrogens Depth cue

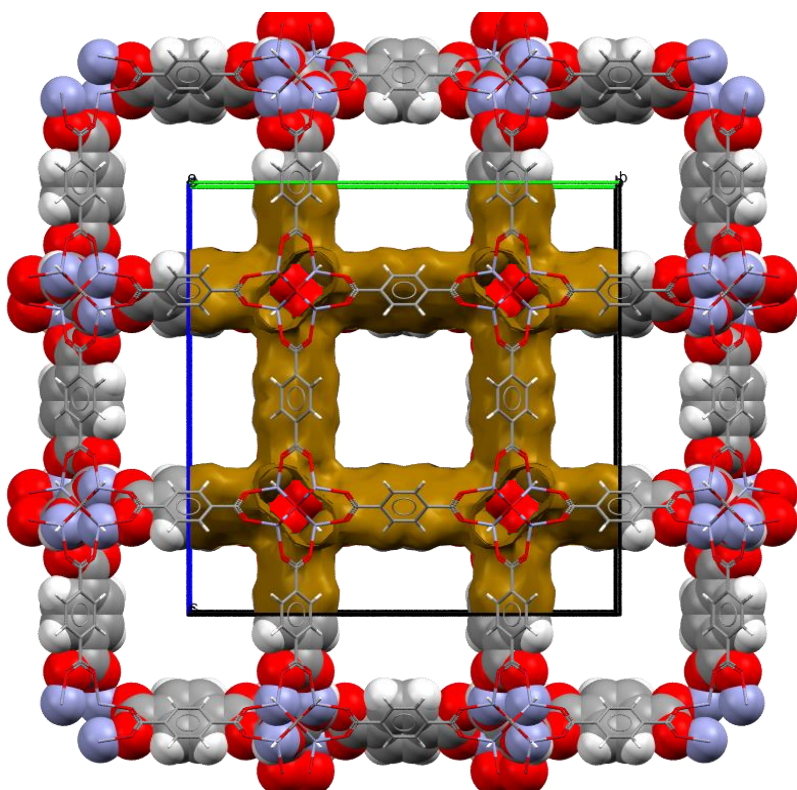
Show cell axes Z-Clipping

Label atoms Stereo

Click on a red contact to see the whole molecule

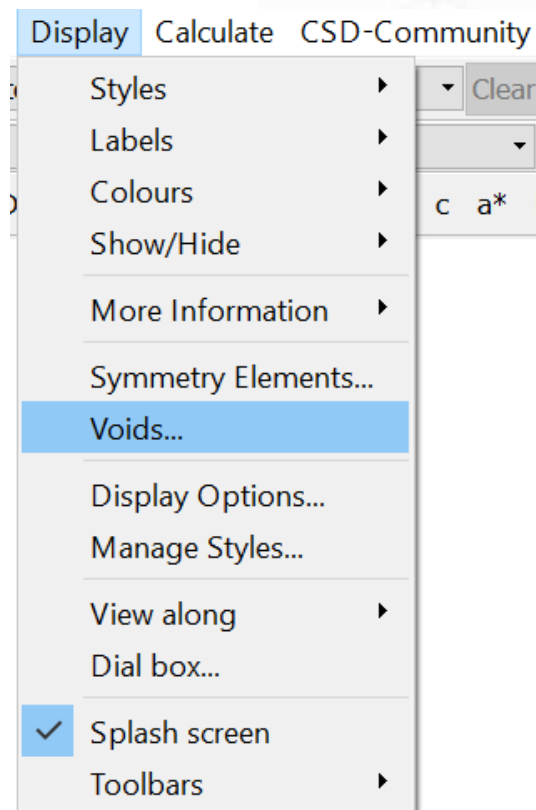
Click through the graph set descriptors to see the different H-bond patterns

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.



Find any empty spaces (**voids**) in crystal unit cells that are big enough to hold a spherical "probe" of the given radius. Decrease the **Probe Radius** to find smaller spaces. Decrease the **Grid Spacing** to create smoother surfaces. To see voids in more than one unit cell, use the **Packing/Slicing** dialog to turn on packing and increase the ranges along a, b and c.

Show

Probe Radius: Å

Approx. Grid Spacing: Å

Calculate using the

Display Options

Outside Colour:

Inside Colour:

Results

Volume % of unit cell volume

Å³

Defaults OK Apply Cancel

Exploring symmetry

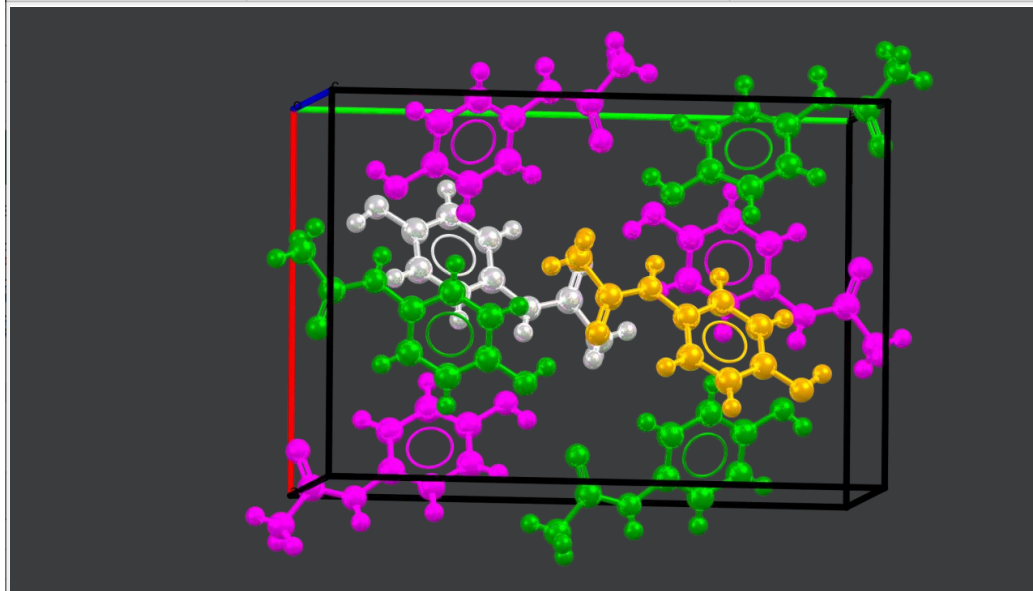
HXACAN (Pcab) - Mercury

File Edit Selection Display Calculate CSD-Community CSD-Cgre CSD-Materials CSD-Discovery CSD Python API Help

Picking Mode: Move Labels Clear Measurements Show Labels for All atoms with

Style: Ball and Stick Colour: by Symmetry operation 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 Select by SMARTS:



Display Options

Display

Packing

Asymmetric Unit

Auto centre

Reset

Short Contact < (sum of vdW radii)

H-Bond Default definition

Contacts...

More Info

Powder...

HXACAN

Current structure: HXACAN

Customise...

Structure

Diagram

Atoms

Bonds

Contacts

Centroids

Planes

Symmetry

All Angles

All Torsions

Click on a column heading to sort rows.

Save...

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

Close

CSD Refcode:
HXACAN

To show or remove symmetry elements

HXACAN (Pcab) - Mercury

File Edit Selection **Display** Calculate CSD-Community CSD-Core CSD-Materials CSD-Discovery CSD Python API Help

Picking Mode: Mo... Clear Measurements Show Labels for All atoms with >>

Style: Ball and Stick

Generation Manage Styles... Publication Atom selections: >>

a b c a* b* c* x- x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-90 >> Select by SMARTS: >>

Styles > Labels > Colours > Show/Hide > More Information > **Symmetry Elements...** Voids... Display Options... Manage Styles... View along > Dial box... Splash screen Toolbars >

Show Symmetry Elements
 Show Inversions
 Show Colour Size
 Show Axes
 Show proper rotation axes
 Show screw axes Show arrows
 Show rotoinversion axes
 2-fold Colour 3-fold Colour
 4-fold Colour 6-fold Colour
 Show Glide & Mirror Planes
 Show mirrors Colour
 Show glides Colour
 Shadows

Defaults OK

Short Contact < (sum of vdW radii) Contacts...
H-Bond Default definition More Info Powder...

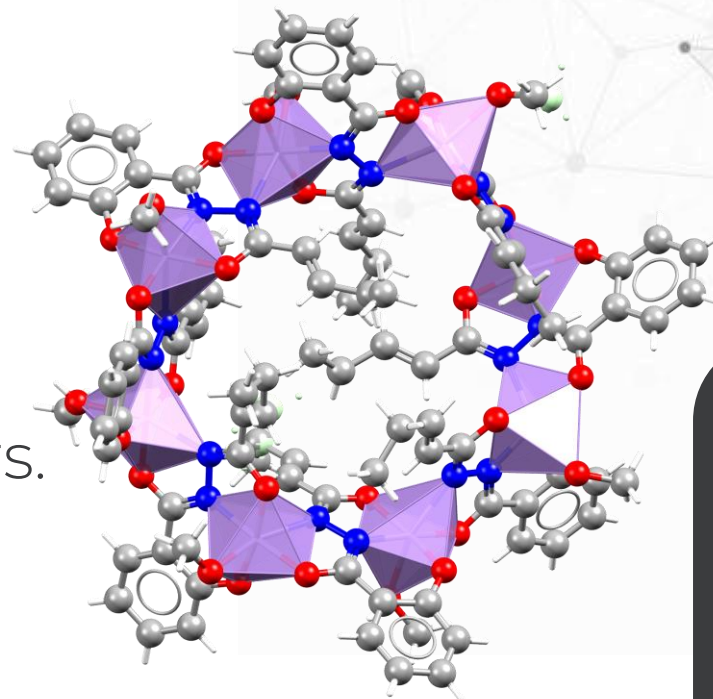
Options
 Show hydrogens Depth cue
 Show cell axes Z-Clipping
 Label atoms Stereo

Follow along Mercury Demo

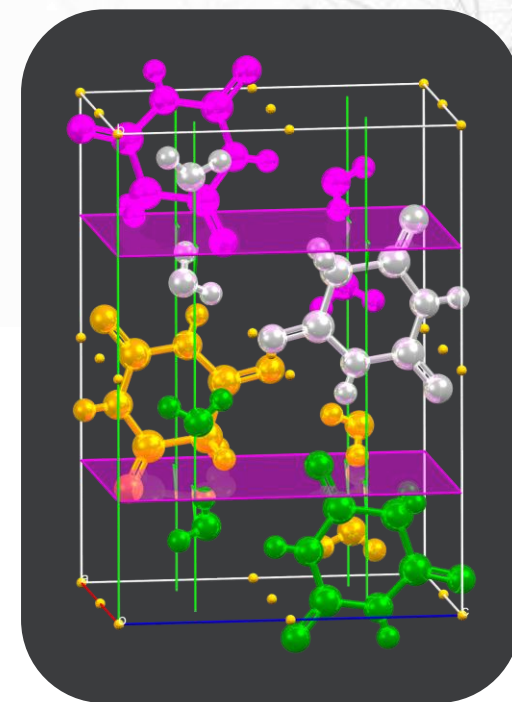
Visualisation options in Mercury

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



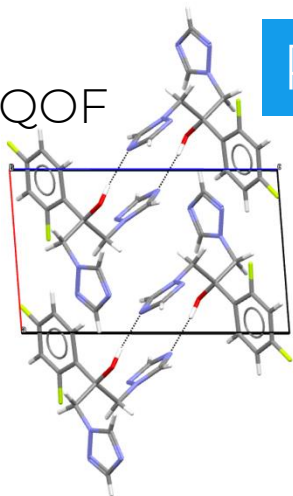
Why analyse structural data?

- 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](#)

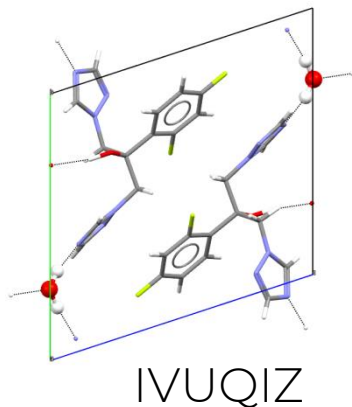
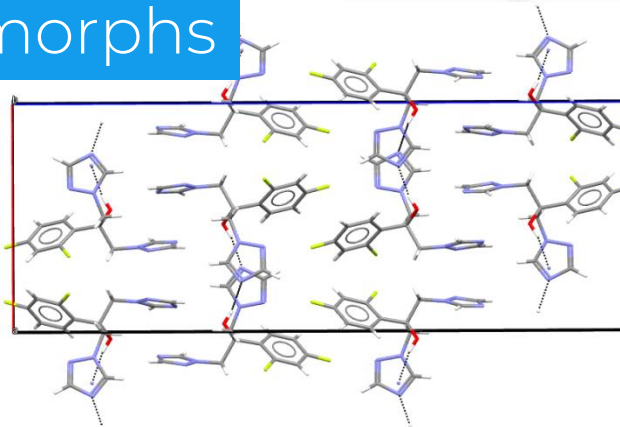
A solid form landscape

Polymorphs

IVUQOF

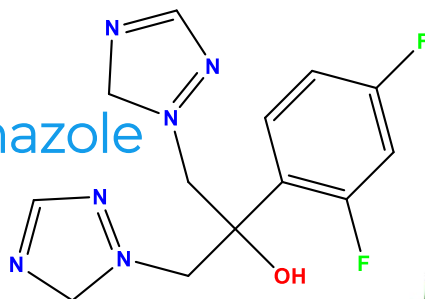


IVUQOF02

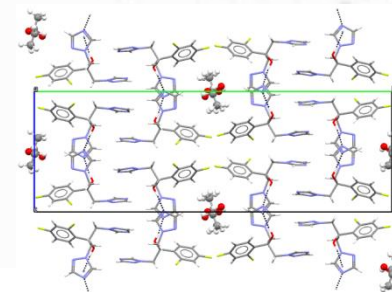


Hydrates

fluconazole



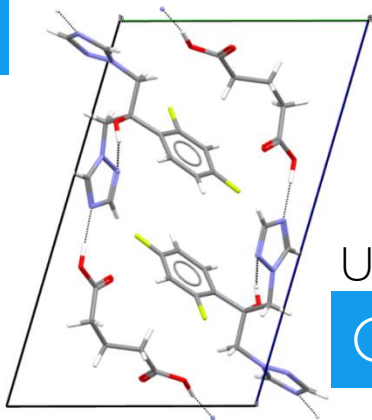
IVUQEV



Solvates

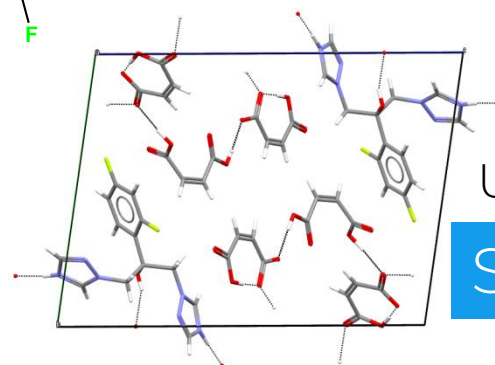
UPOQEW

Co-crystals



UPOQAS

Salts



CCDC

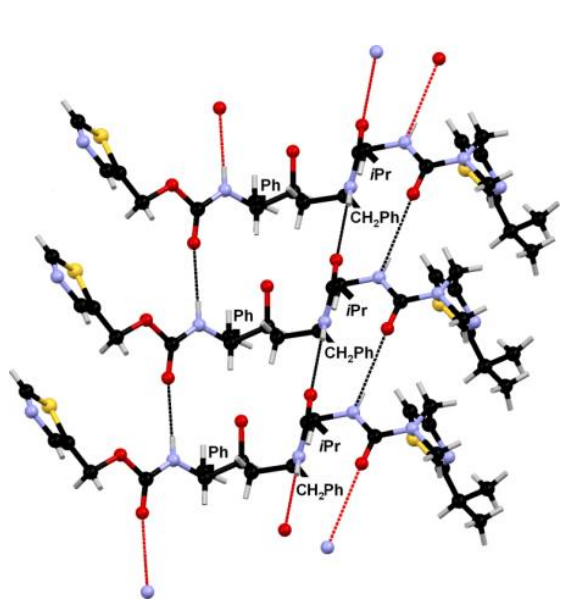
Exploring contacts and exploring chocolate

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

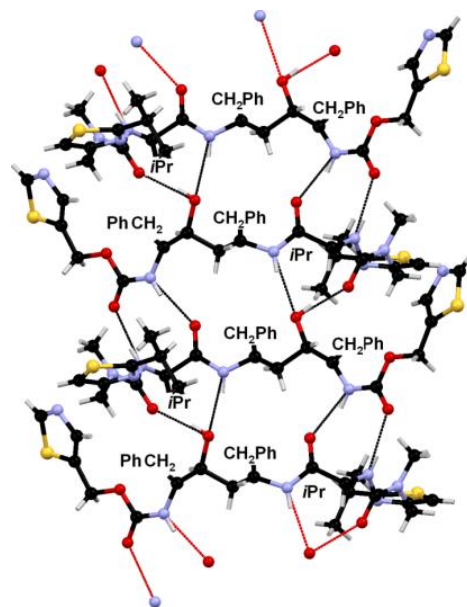


A real-life example....

Can structural knowledge mitigate risk?



Different interactions

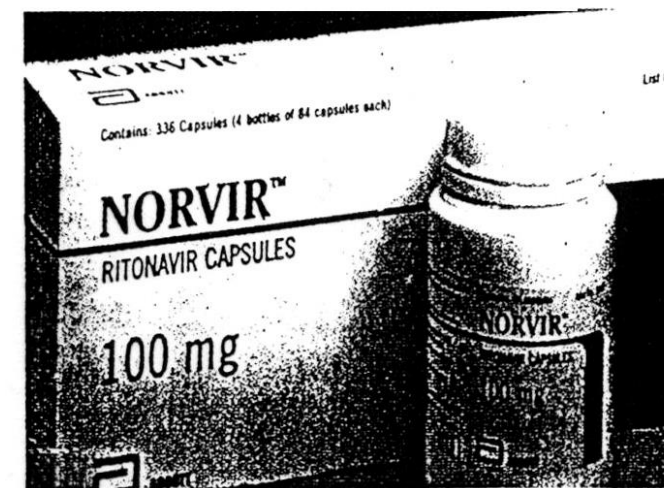


Different solubility
Different stability

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

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 capsules from a number of marketed batches of capsules were examined and there was no

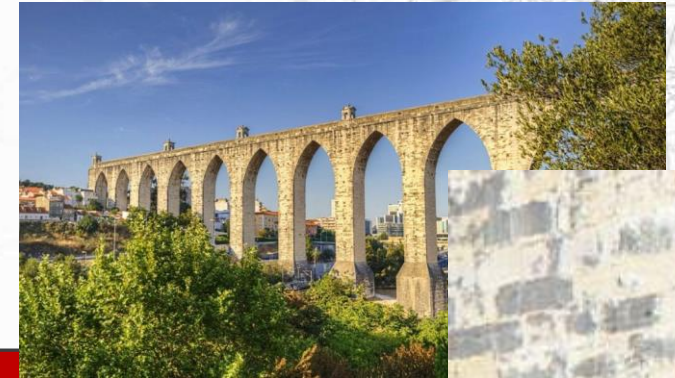
CCDC

Structural Informatics

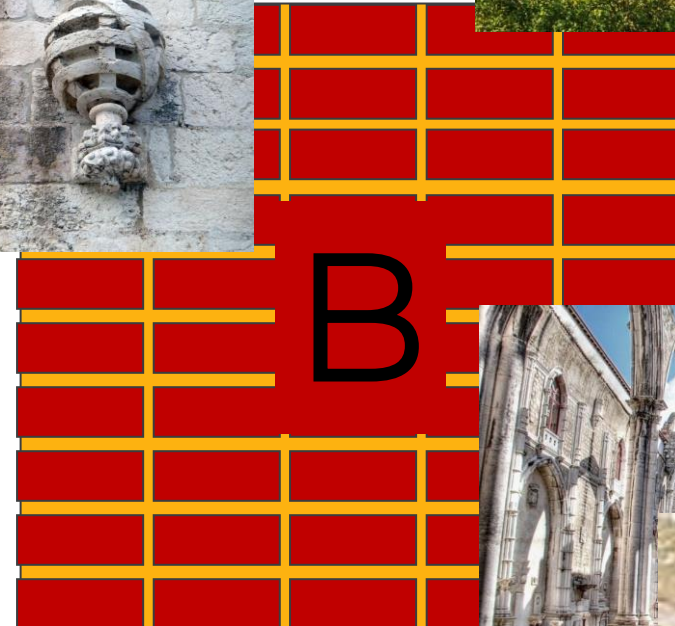
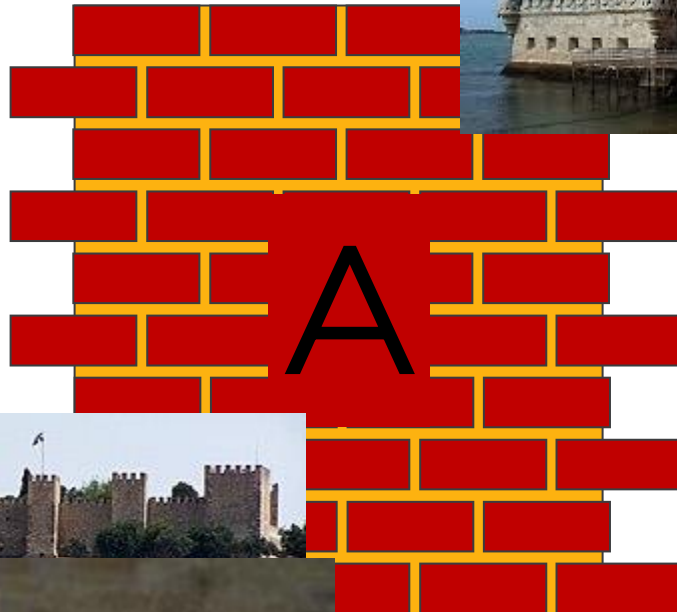
Which is the stable wall?



Belém Tower
c. 1514



Águas Livres
Aqueduct c.1731



Castelo de São Jorge

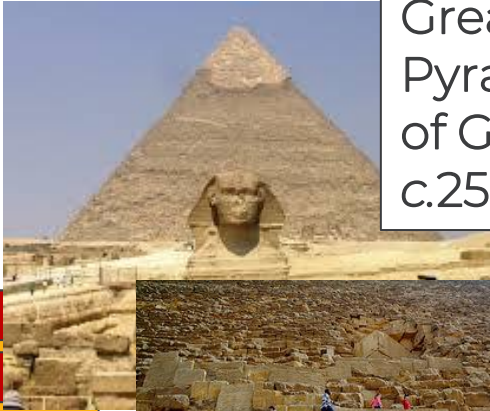


Carmo convent
c. 1389

Structural Informatics

Which is the stable wall?

The
CCDC
c.1992



Great
Pyramid
of Giza
c.2560 BC



Hadrian's Wall
c.122



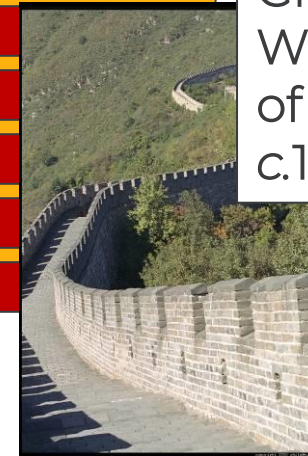
A

B

My
House
c.1967



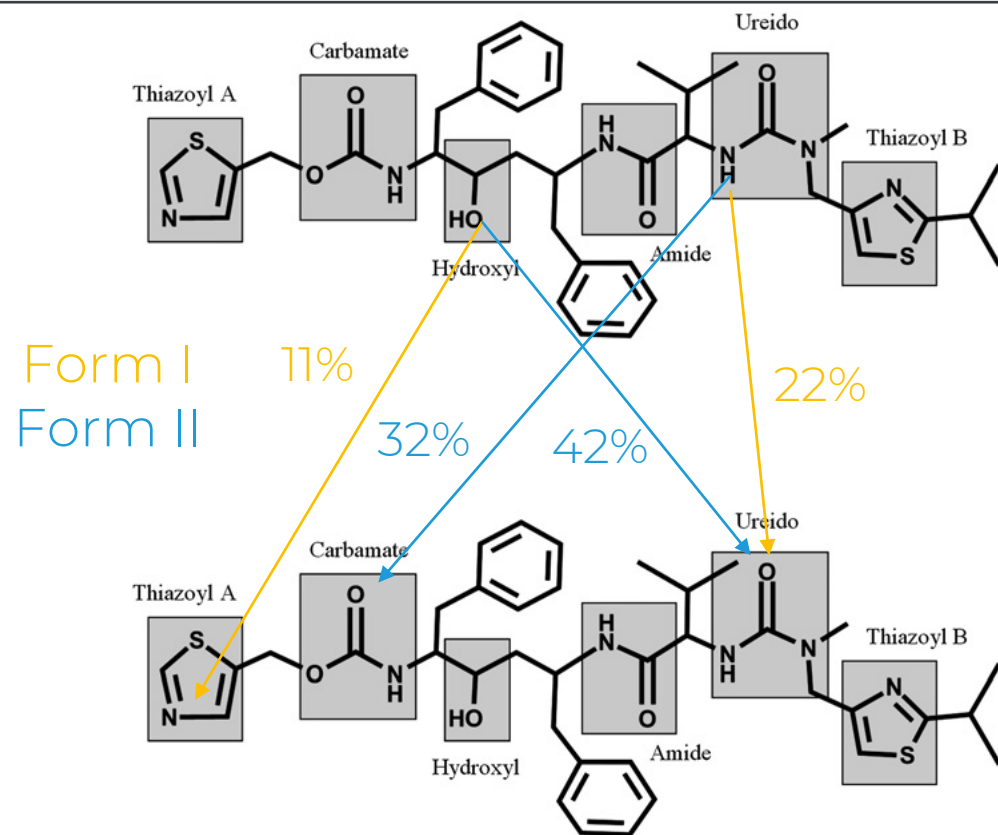
The database of walls indicates that A is the frequently observed arrangement and therefore we can predict it is the most stable form



Great
Wall
of China
c.1368

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

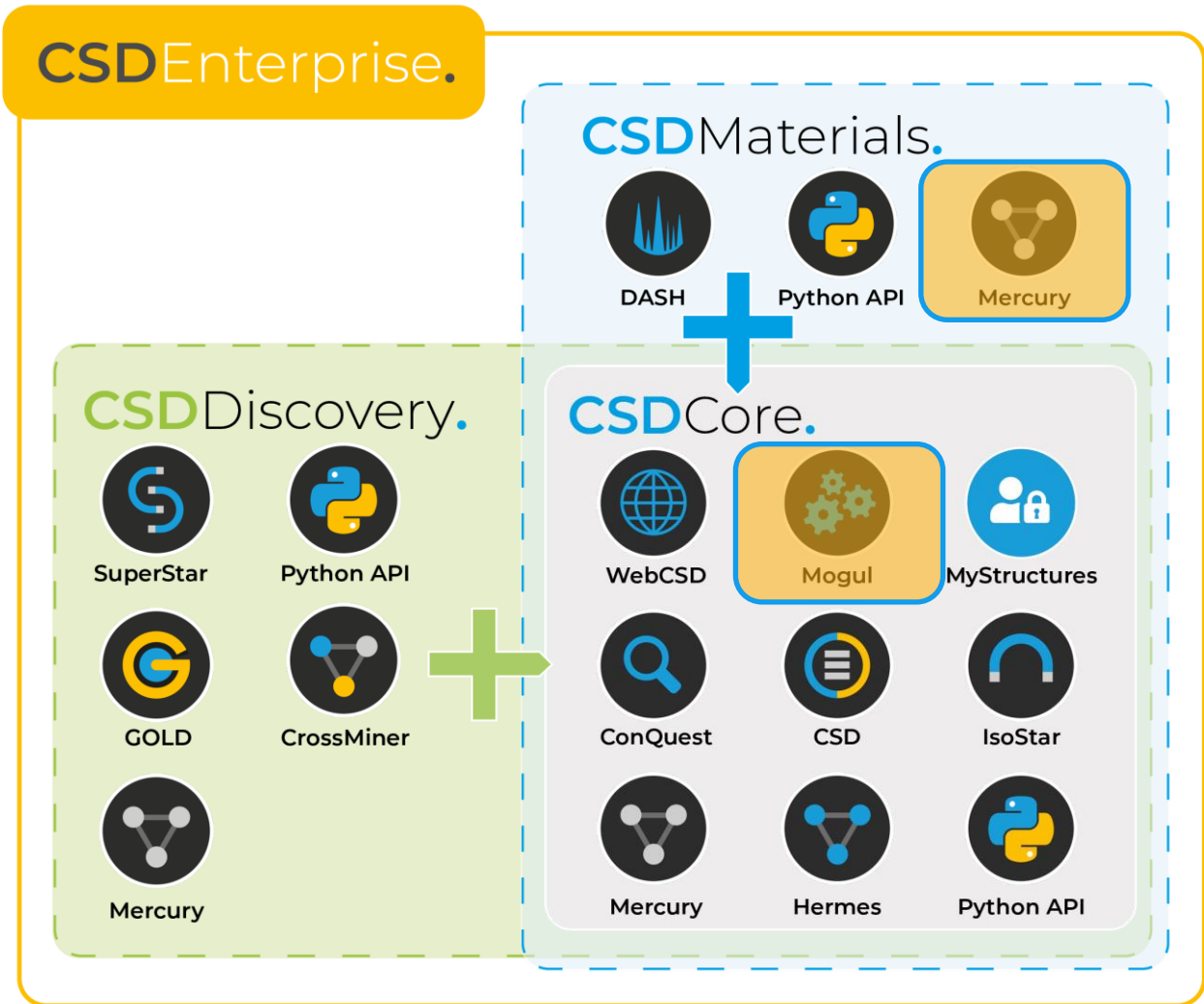
Peter T. A. Galek, Elna Pidcock, Peter A. Wood, Neil Feeder, Frank H. Allen

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 Fábrián](#)^{ab} and [Neil Feeder](#)^c

The CSD software



Characteristics that influence stability

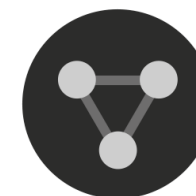
Hydrogen Bond Donor/Acceptor Pairing

Molecular Conformation

'Non-Hydrogen Bond' Intermolecular Interactions

Hydrogen Bond Geometry, Symmetry and Motif

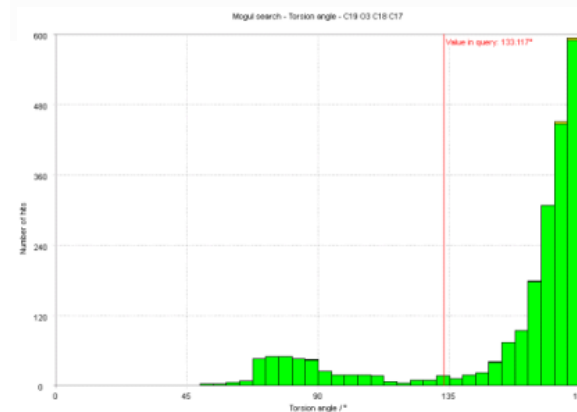
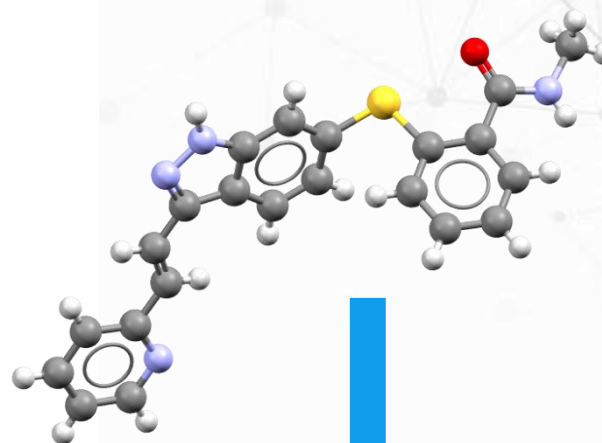
We can mine the CSD to identify these **intra** and intermolecular **geometric** preferences.



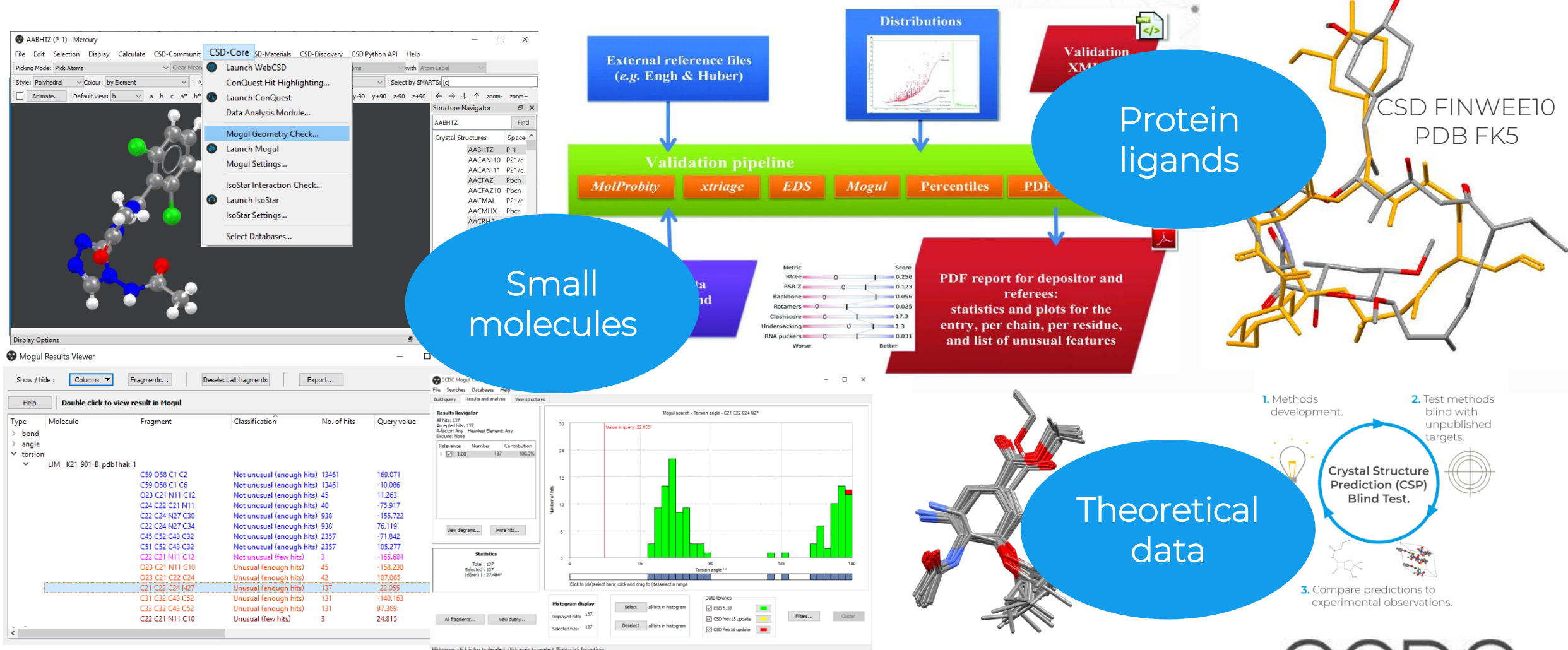
CCDC

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



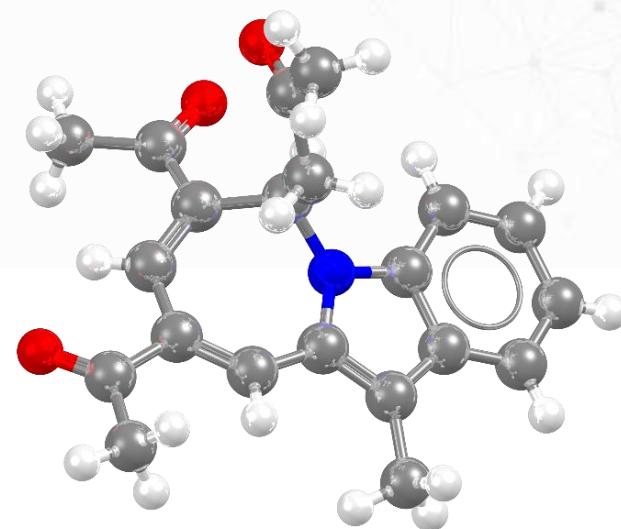
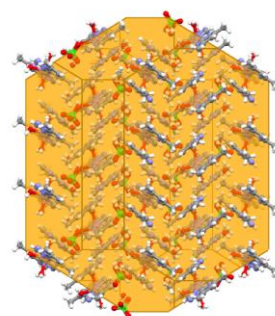
Using Mogul to check new structural data



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



The screenshot shows the Mercury software interface with the 'CSD-Core' menu open. The menu items are:

- Launch WebCSD
- ConQuest Hit Highlighting...
- Launch ConQuest
- Data Analysis Module...
- Mogul Geometry Check...**
- Launch Mogul
- Mogul Settings...
- IsoStar Interaction Check...
- Launch IsoStar
- IsoStar Settings...
- Select Databases...

The 'Structure Navigator' panel on the right displays a list of crystal structures:

Crystal Structures	Space
AABHTZ	P-1
AACANI10	P21/c
AACANI11	P21/c
AACFAZ	Pbcn
AACFAZ10	Pbcn
AACMAL	P21/c
AACMHX...	Pbca
AACRHA	Pncm
AACRHC	P-1
AACRUB	Cc
AACRUB01	C2/c
AADAMC	P21/c
AADMPY	P-1
AADMPY10	P-1
AADRIB	P21
AAGAGG10	P2121
AAGGAG10	P21
AALCFE	P21/c

Mogul Geometry Check

CSD-Core CSD-Materials CSD-Disc

- Launch WebCSD
- ConQuest Hit Highlighting...
- Launch ConQuest
- Data Analysis Module...
- Mogul Geometry Check...**
- Launch Mogul
- Mogul Settings...
- IsoStar Interaction Check...
- Launch IsoStar
- IsoStar Settings...
- Select Databases...



Mogul Search Settings

Fragment Types

Bond Length Valence Angle Torsion Angle Ring

Search Filter Options

Available filters

R-factor <= 5.0%

Exclude Solvents

Heaviest Element U

Exclude Organometallics

Exclude Powder structures

Apply filters

Search Mode

Only find fragments that match exactly

Find similar fragments if number of exact matches is less than

Bonds 15 Angles 15 Torsions 40 Rings 15

Customise fragment classification ...

Help Search Close



No atoms selected

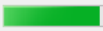
A complete analysis of all loaded molecule(s) will be performed.

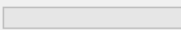
To analyse just part of the displayed molecule(s), hit 'Cancel' and select atoms before starting the analysis.

OK Cancel



Search Progress

Angle  54%

C8 C9 C14  Stop

Search completed - 41 observations

Mogul Geometry Check - Results

Mogul Results Viewer

Show / hide : Columns Fragments... Deselect all fragments Export...

Help Double click to view result in Mogul

Type	Molecule	Fragment	Classification	No. of hits	Query value	Mea
> bond						
> angle						
> torsion						
	LIM_K21_901-B_pdb1hak_1					
		C59 O58 C1 C2	Not unusual (enough hits)	13461	169.071	
		C59 O58 C1 C6	Not unusual (enough hits)	13461	-10.086	
		O23 C21 N11 C12	Not unusual (enough hits)	45	11.263	
		C24 C22 C21 N11	Not unusual (enough hits)	40	-75.917	
		C22 C24 N27 C30	Not unusual (enough hits)	938	-155.722	
		C22 C24 N27 C34	Not unusual (enough hits)	938	76.119	
		C45 C52 C43 C32	Not unusual (enough hits)	2357	-71.842	
		C51 C52 C43 C32	Not unusual (enough hits)	2357	105.277	
		C22 C21 N11 C12	Not unusual (few hits)	3	-165.684	
		O23 C21 N11 C10	Unusual (enough hits)	45	-158.238	
		O23 C21 C22 C24	Unusual (enough hits)	42	107.065	
		C21 C22 C24 N27	Unusual (enough hits)	137	-22.055	
		C31 C32 C43 C52	Unusual (enough hits)	131	-140.163	
		C33 C32 C43 C52	Unusual (enough hits)	131	97.369	
		C22 C21 N11 C10	Unusual (few hits)	3	24.815	

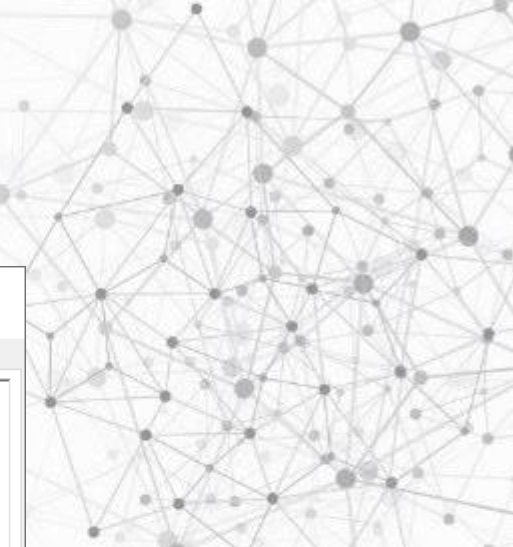
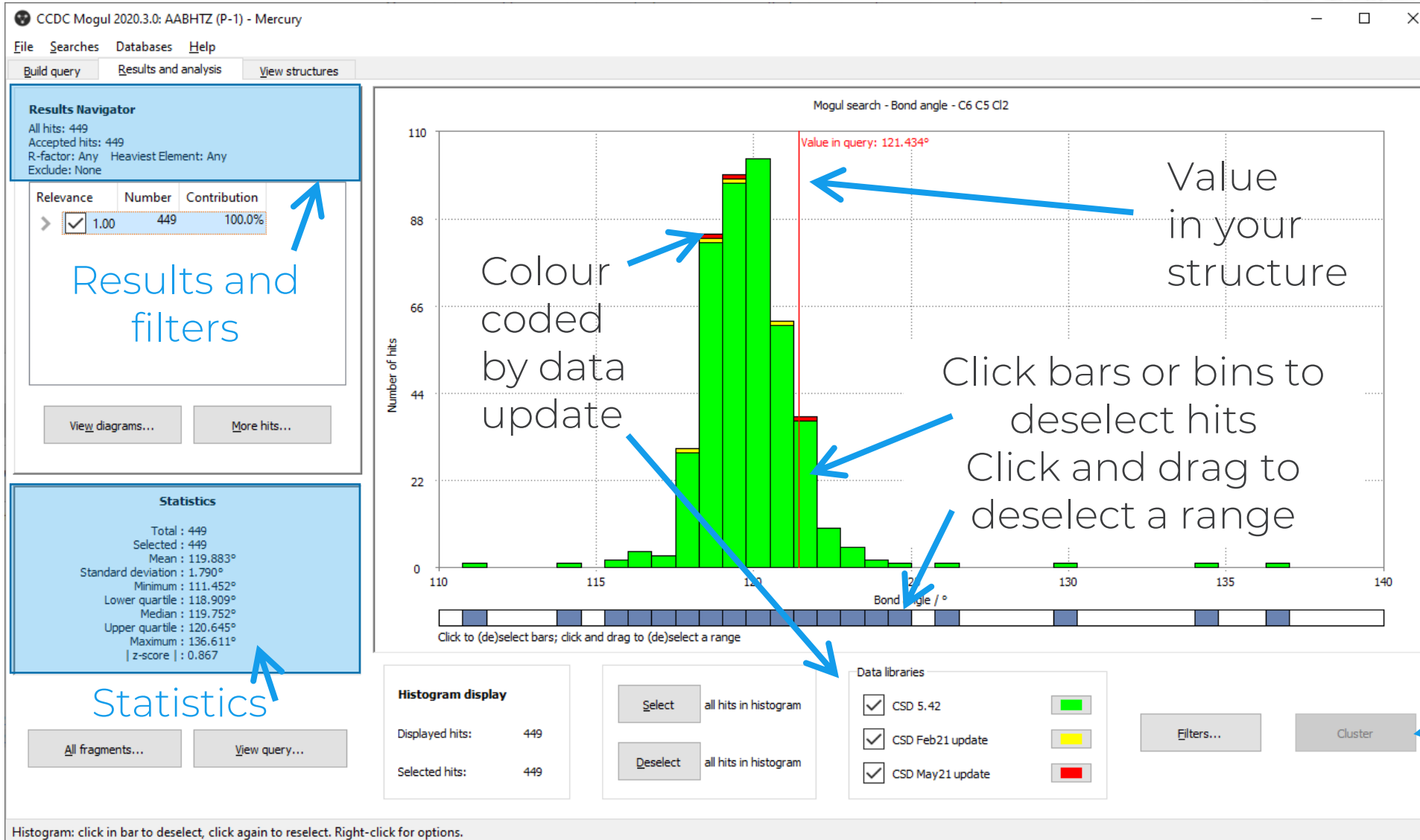


Double click
on a row to
view result in
Mogul

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

Mogul Geometry Check – View structures

The screenshot displays the CCDC Mogul 2020.3.0 interface. The main window shows a chemical structure of a fragment with a benzene ring, a chlorine atom, and a nitrogen-containing side chain. A valence angle of 119.477° is indicated. A list of 196 structures is shown on the right, with the first few refcodes visible. The interface includes a menu bar (File, Searches, Databases, Help), a toolbar (Build query, Results and analysis, View structures), and a sidebar (Information, Diagram, 3D visualiser). The refcode list is titled 'AABHTZ' and contains 196 entries. The number of hits is shown as 2.

CCDC Mogul 2020.3.0: AABHTZ (P-1) - Mercury

File Searches Databases Help

Build query Results and analysis View structures

Information

Diagram

3D visualiser

Refcode: AABHTZ Data Library: CSD 5.42

Valence angle: 119.477°

Measurement given

Fragment shown

Fragment

Click through hits

1 2 hits Show Parameters

AABHTZ

AABHTZ

ABAWIJ

ABAWOP

ABYTZL

ACBTZC

ACBTZD10

ADAPIF

ADENON

AFESEK

AJETAL

AJETAL01

AMAQAH

AMAQEL

AMAQIP

APIKUH

AWIJIA

AWIJOG

AWIJUM

AXEHIU

AXUTES

AYEZOV

AZITUA

BAKYAP

CAGNUU

CAGPAC

CEBL0M

CEQZIJ

CIJGAD

CLPTBU

COPZOX

DAJCAV

DAJNUZ

DIDMLIA

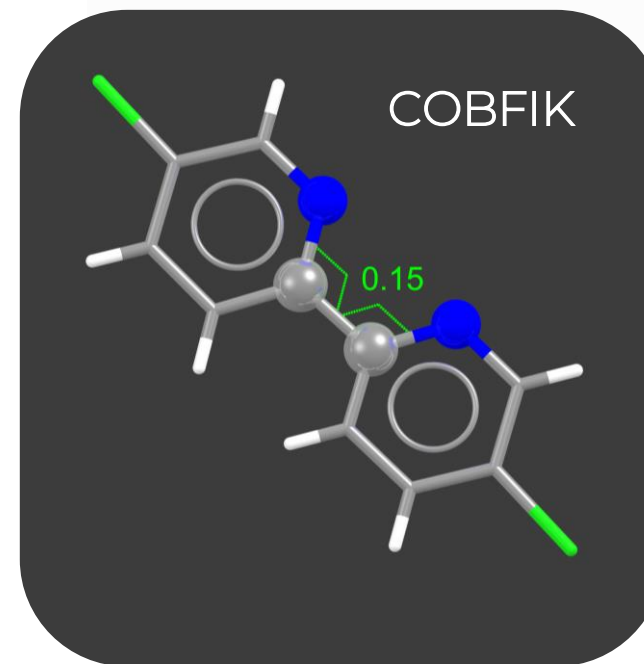
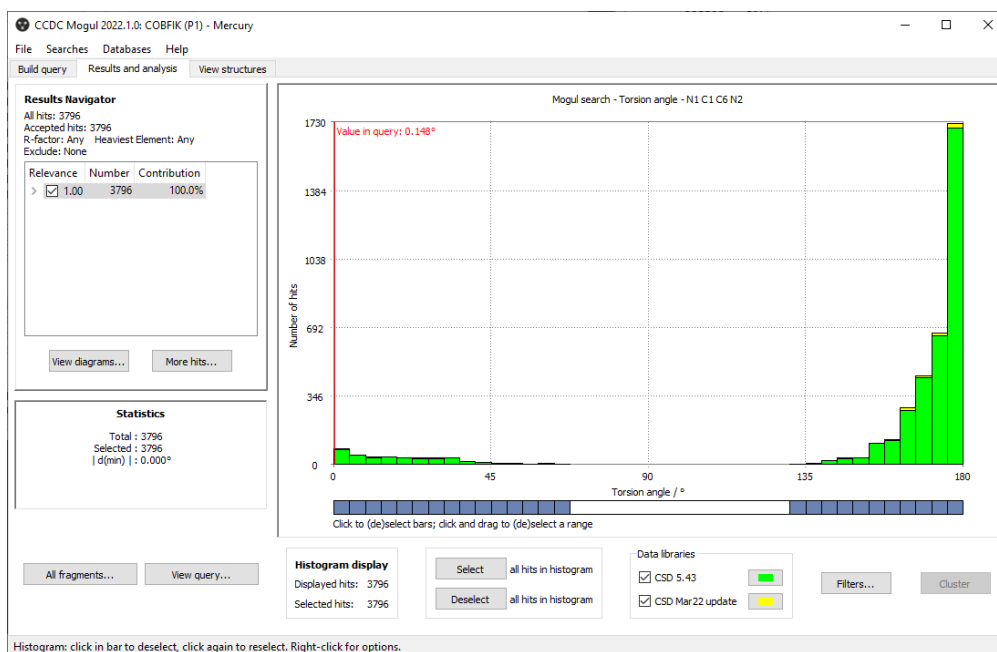
196 structures

Follow along Mogul Demo

Example of a Mogul Geometry Check

We will:

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

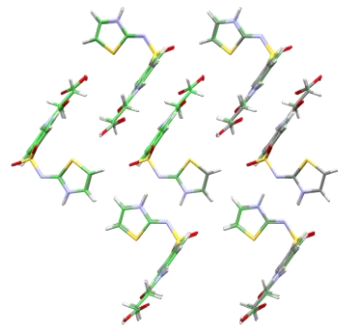


Agenda

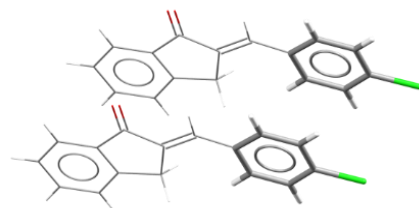
- Introduction to the CSD
- Visualizing structures in the CSD
 - Slides and follow-along demo
- Analysing the geometry of structures using Mogul
 - Slides and follow-on along demo
- [Analysing intermolecular interactions using FIMs](#)
- Wrap up, quiz and summary



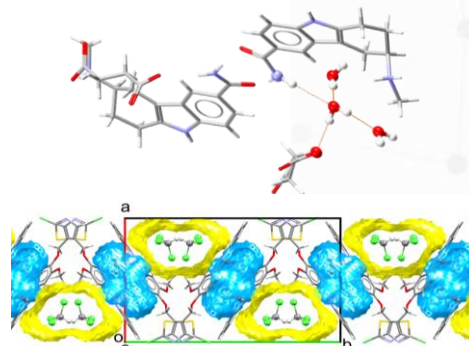
CSD-Materials overview



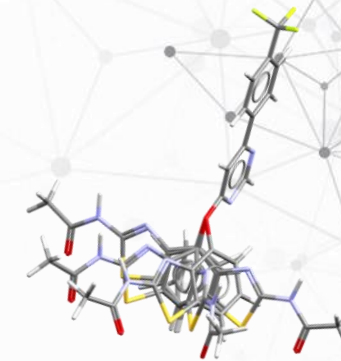
Crystal Packing Similarity



Motif Search & Packing Feature Search

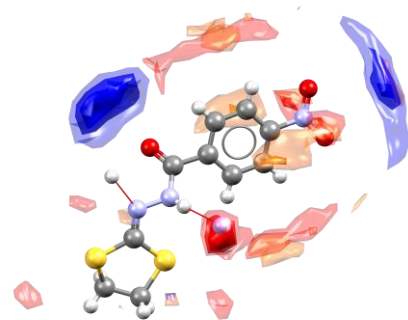


Hydrate Analyser & Solvate Analyser

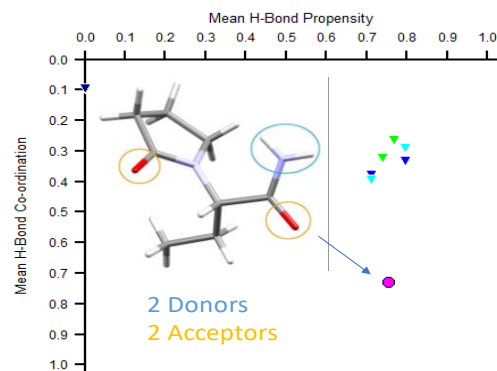


CSD Conformer Generator

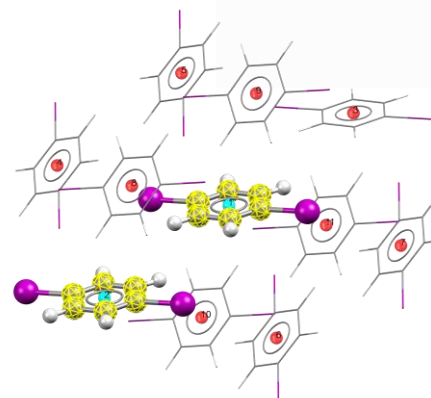
Detailed Structural Analysis



Full Interaction Maps

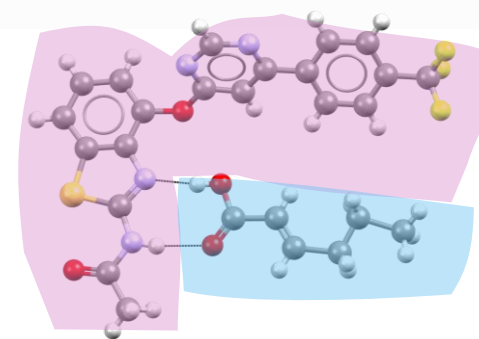


Hydrogen Bond Propensity



Aromatics Analyser

Solid Form Design

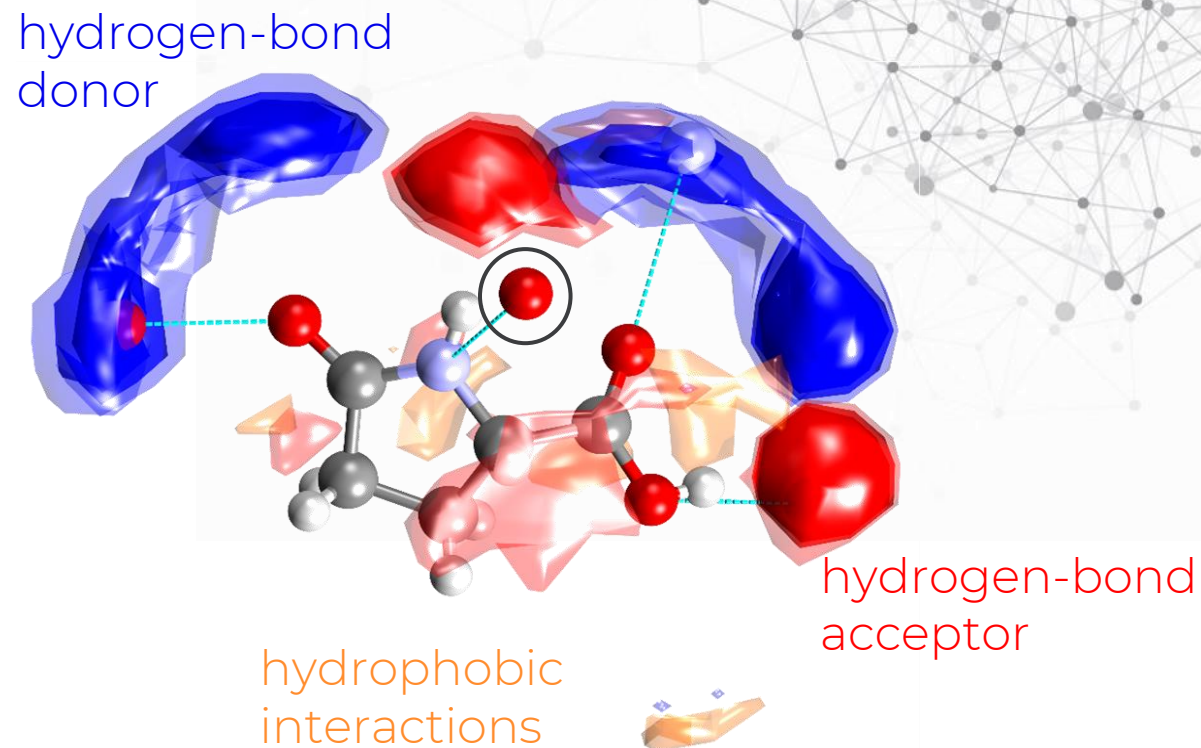


Molecular Complementarity

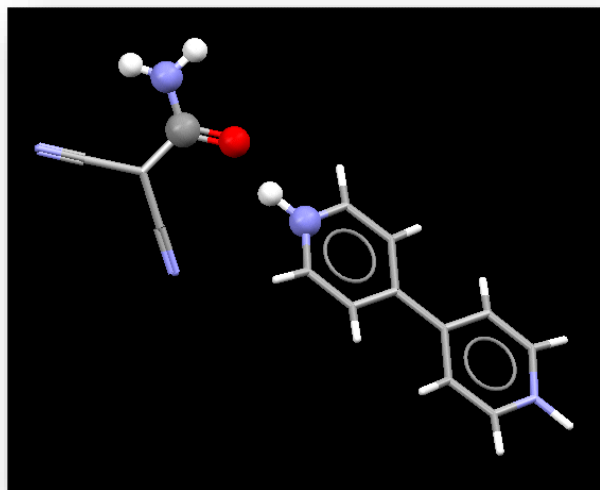
Solid Form Risk Assessment

Full Interaction Maps (FIMs)

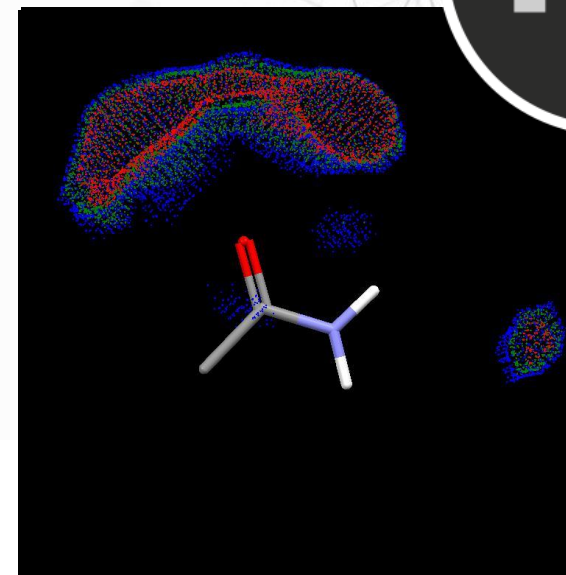
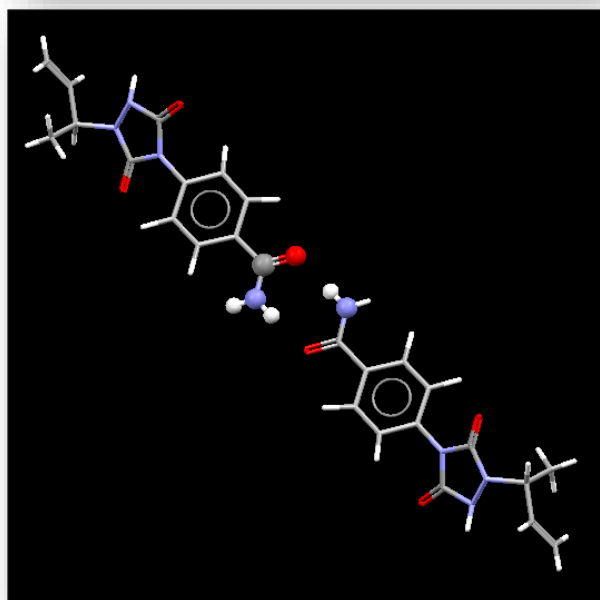
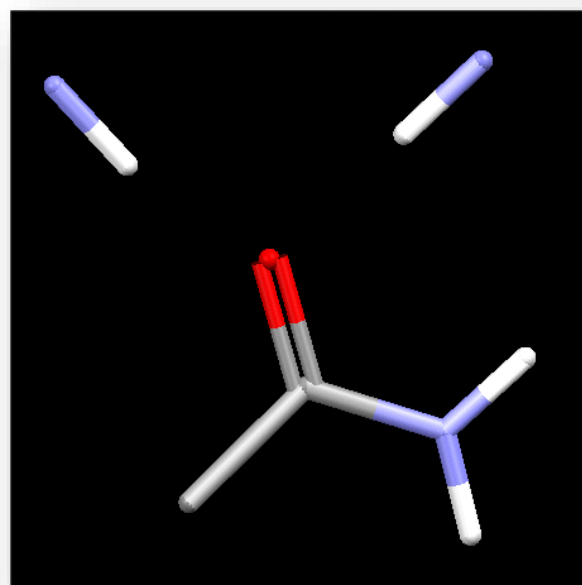
- Map interaction preferences around complete molecules in a crystal structure.
- Visualise observed atom-atom contacts with respect to likely geometries in 3D space.
- Identify interaction hot-spots around chemical groups.



Understanding intermolecular interactions



central group: -CONH₂
contact group: NH

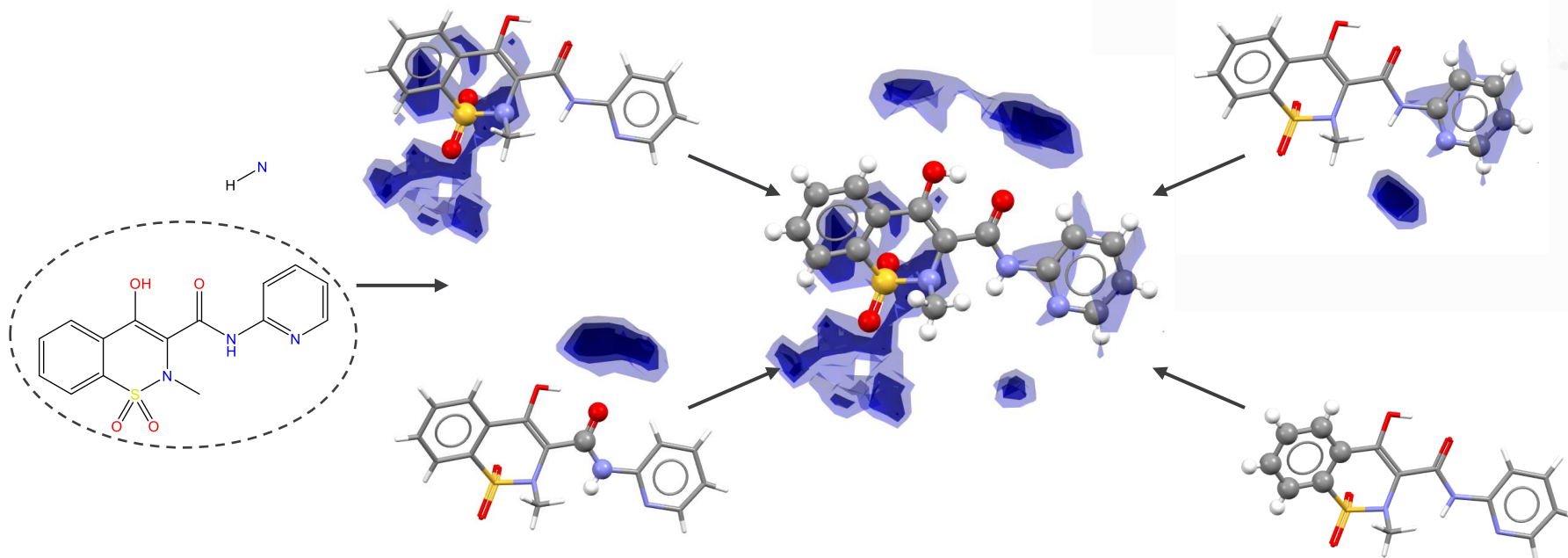


Search for structures containing desired contact

Superimpose hits and display as scatterplots or contour plots

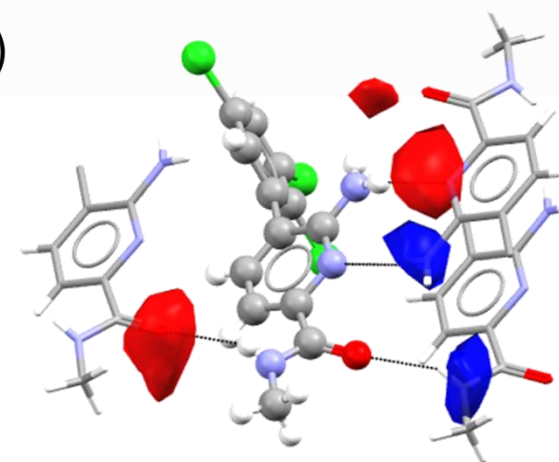
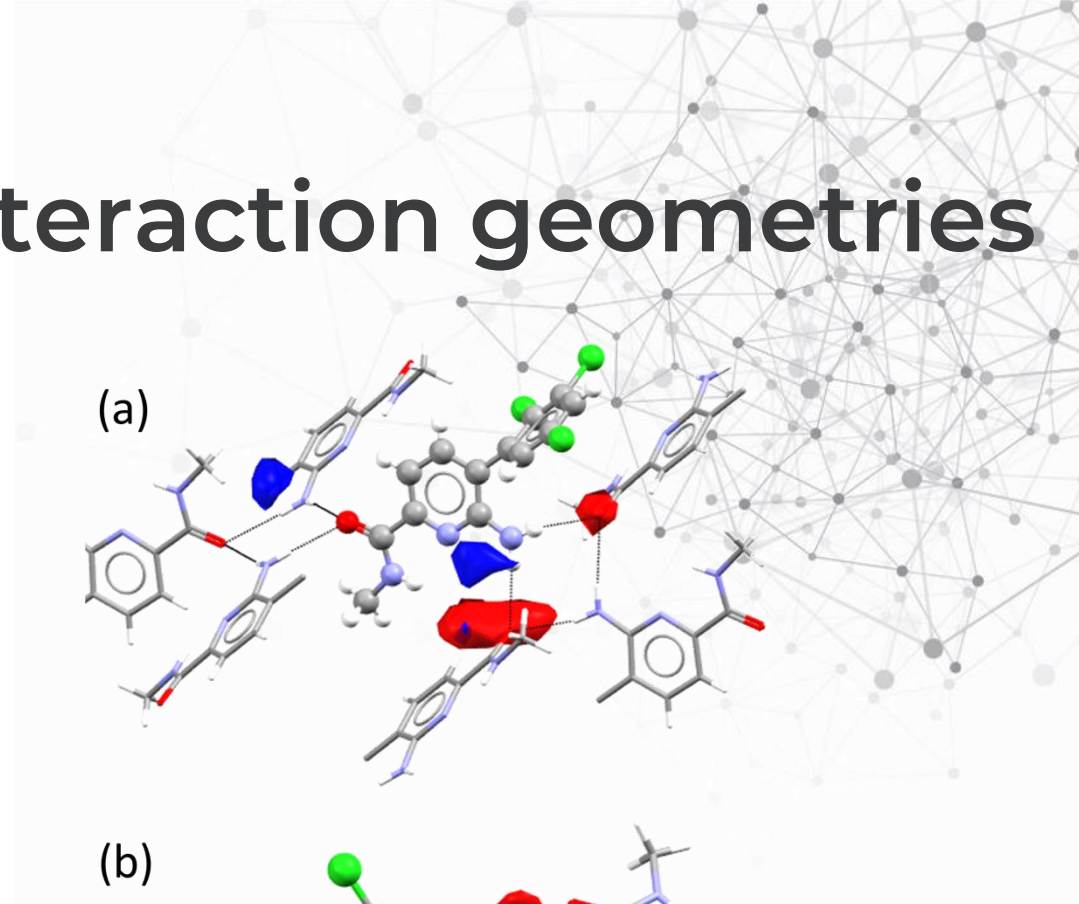
Combining plots into Full Interaction Maps

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



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



Creating a FIM

The screenshot shows the Mercury software interface. The 'CSD-Materials' menu is open, highlighting 'Full Interaction Maps...'. The 'Full Interaction Maps' dialog box is open, showing the 'Maps' tab. The 'Map Contour Levels' section has three checked options: 'Display first contour with initial level of 2.0', 'Display second contour with initial level of 4.0', and 'Display third contour with initial level of 6.0'. The 'Hotspots' section has 'Generate hotspots in the map' unchecked. The 'Probe' section has several checked options: 'Uncharged NH Nitrogen', 'Carbonyl Oxygen', 'Water Oxygen', 'Aromatic CH Carbon', and 'C-F Fluorine'. A color scale is visible next to the probe list. The 'Calculate Maps' button is highlighted. In the background, a 3D molecular model is shown with interaction maps overlaid in various colors (red, orange, yellow, green, blue).

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

Getting started with Full Interaction Maps

Ilaria Gimondi - February 15, 2021

Our collection of educational resources has been growing throughout 2020, welcoming new How to videos (on our YouTube and LabTube channels), new self-guided workshops and updates to our existing material. We also added a feedback survey for you to fill in at the end of each workshop to let us know how we are doing and how we can improve.

This month we include in our collections 2 new resources, both about Full Interaction Maps (FIMs, for short): an educational video to write a blog about the first steps to get started with FIMs, and a new How to video about FIMs, the right time to use them.

How do FIMs work? Full Interaction Maps (FIMs) are a powerful tool that represents the regions of higher probability to find interactions with certain functional groups. We made it available in our educational resources.

A great way to get started with FIMs is to show you how FIMs work, together with few examples that will give you an idea about insightful information that FIMs can provide on your molecules, crystal structures, and ligand interactions. Our new educational video on FIMs aims exactly at this.

Full Interaction Maps (FIMs)

Provides your molecule's interaction preferences, in the context of the crystal structure, with the click of a button. FIMs are validated against experimental structural data. Interactions visualised simply in 3D within Mercury.

CCDC

<https://www.ccdc.cam.ac.uk/Community/blog/getting-started-with-FIMs/>

Press the left mouse button and move the mouse to rotate the structure

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](#)

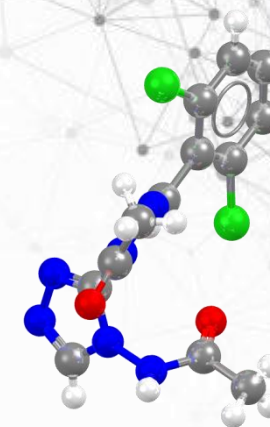


Explore More: Quiz

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.

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?



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](#)

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. We regularly produce educational materials for use in classroom and computer lab settings, or as independent study modules. Many of these materials are available in a freely available set of over 750 structures that can be investigated with the free version of our Mercury visualisation and analysis program. Of these materials, many entries are available for free through our Access Structures portal. For supplementary teaching materials, find out more about the Teaching Database [here](#). If you have developed your own modules using the CSD and want to share with the community, please contact us at education@ccdc.cam.ac.uk. For more information from 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

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

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

Register for E&O newsletter

On-demand modules with completion certificate

Self-guided workshops

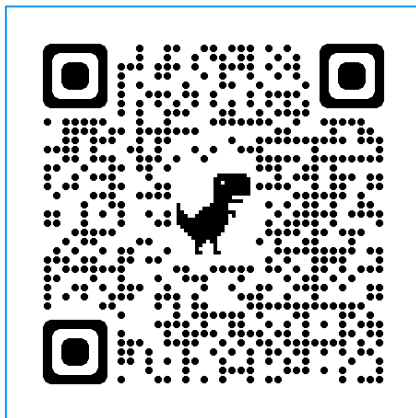
YouTube and LabTube channels





CSDU

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



UWatch

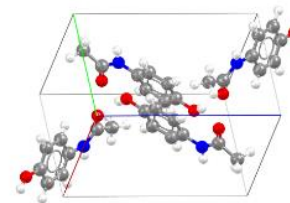


UTry



UTest

Visualisation 101 - Visualising structural chemistry data with Mercury



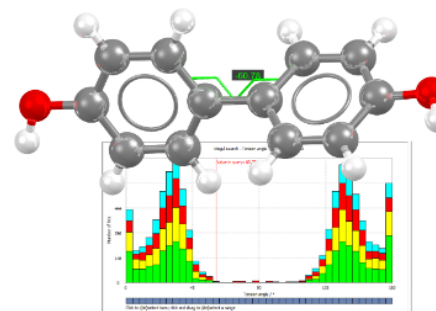
Begin module

Programmatic access to the CSD 101 – CSD Python API



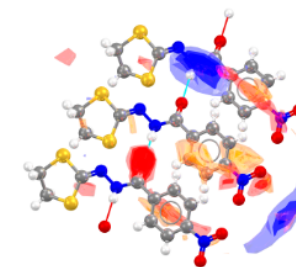
Begin module

Analysing molecular geometries 101 - basics of Mogul



Begin module

Analysing intermolecular interactions 101 - Full Interaction Maps



Begin module

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.

Reflections Rotations Inversions Identity

Molecules: water and benzene

CCDC

Access the CSD Data and Software

Until 31st July 2022

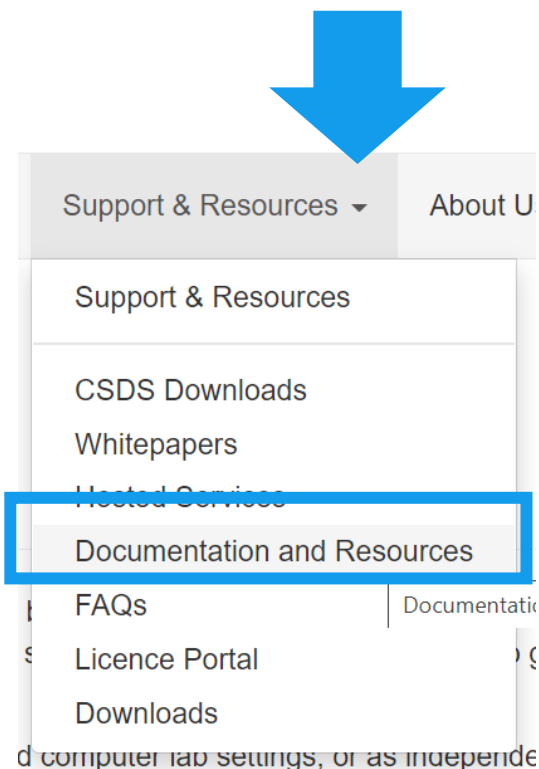
- You can explore CSD functionality using the [workshop license](#)!

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.

Documentation

CCDC website



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

Resource Type
User Guide

Category
Please select a Category

Product
Mercury

Sort Order
Most Recent

Search

Mercury User Guide (2022.1)
Last Modified: 12/12/2019 PDF

21.11.2 Screening by Molecular Complementarity

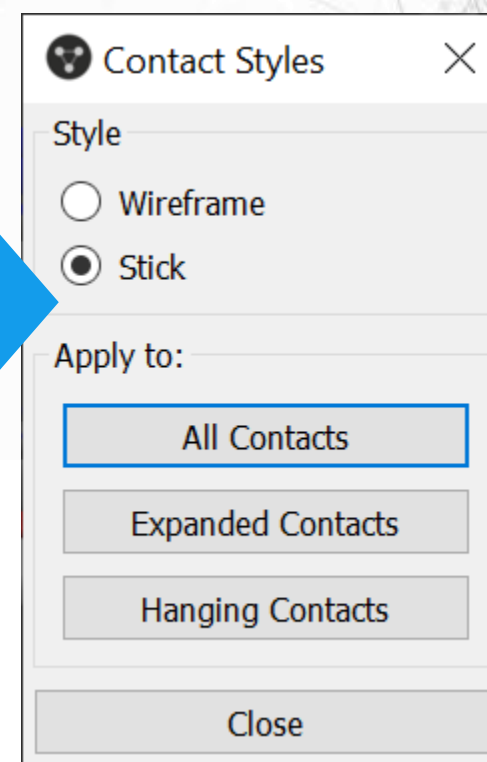
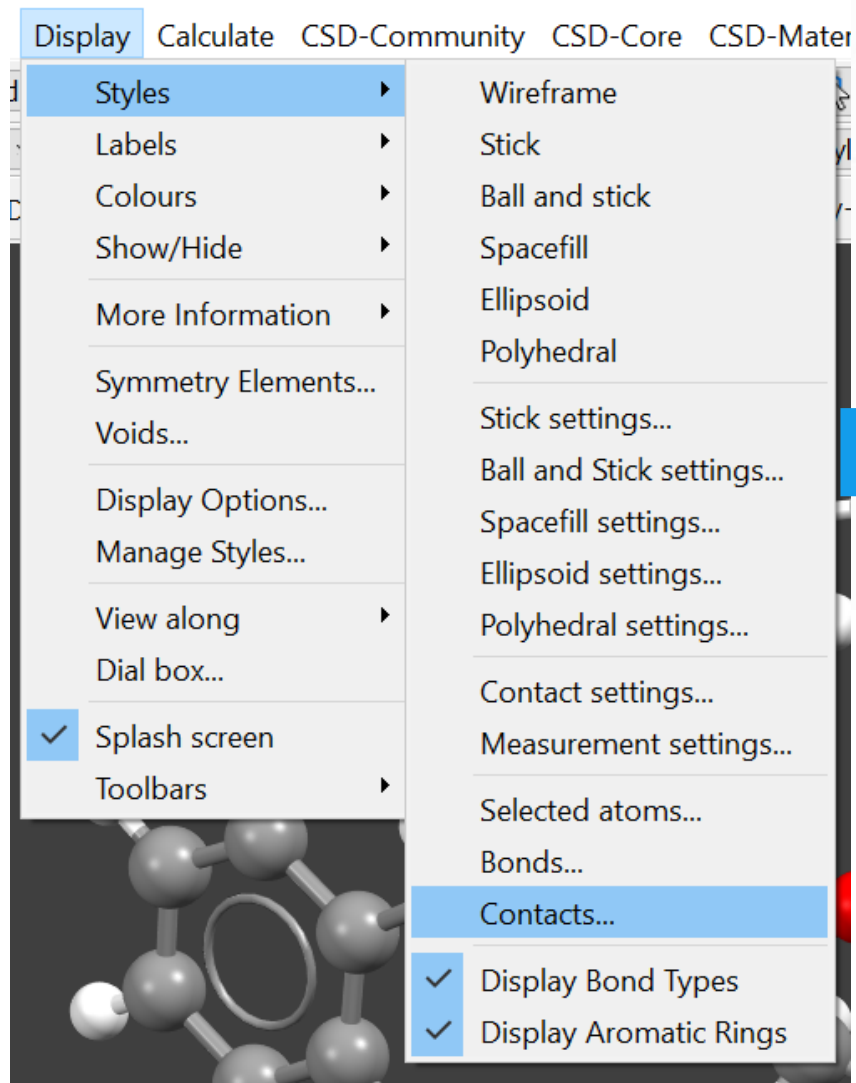
21.11.2.1 Overview

- 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 Fábíán. 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 [Fábíán, *Cryst. Growth Des.*, 2009, 19, 1436-1443.](#)

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

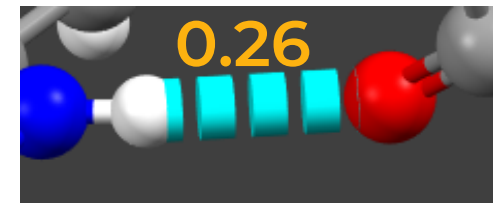
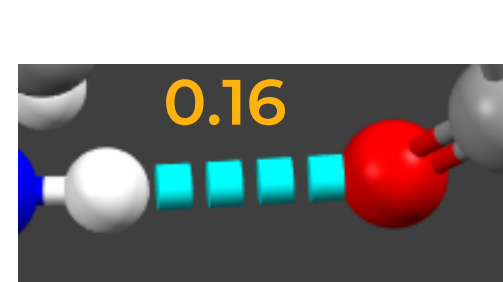
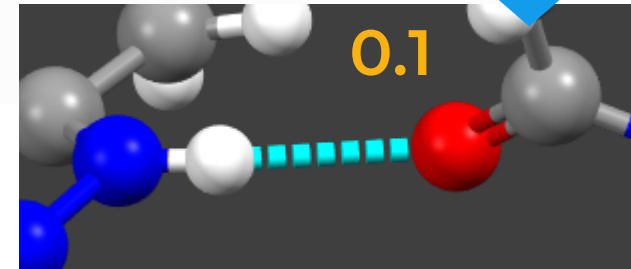
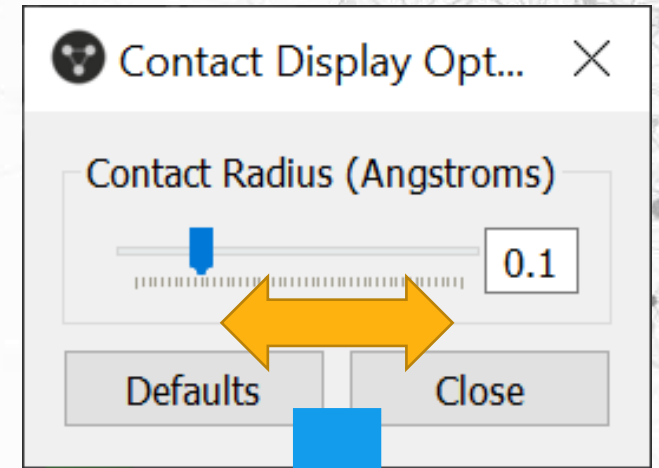
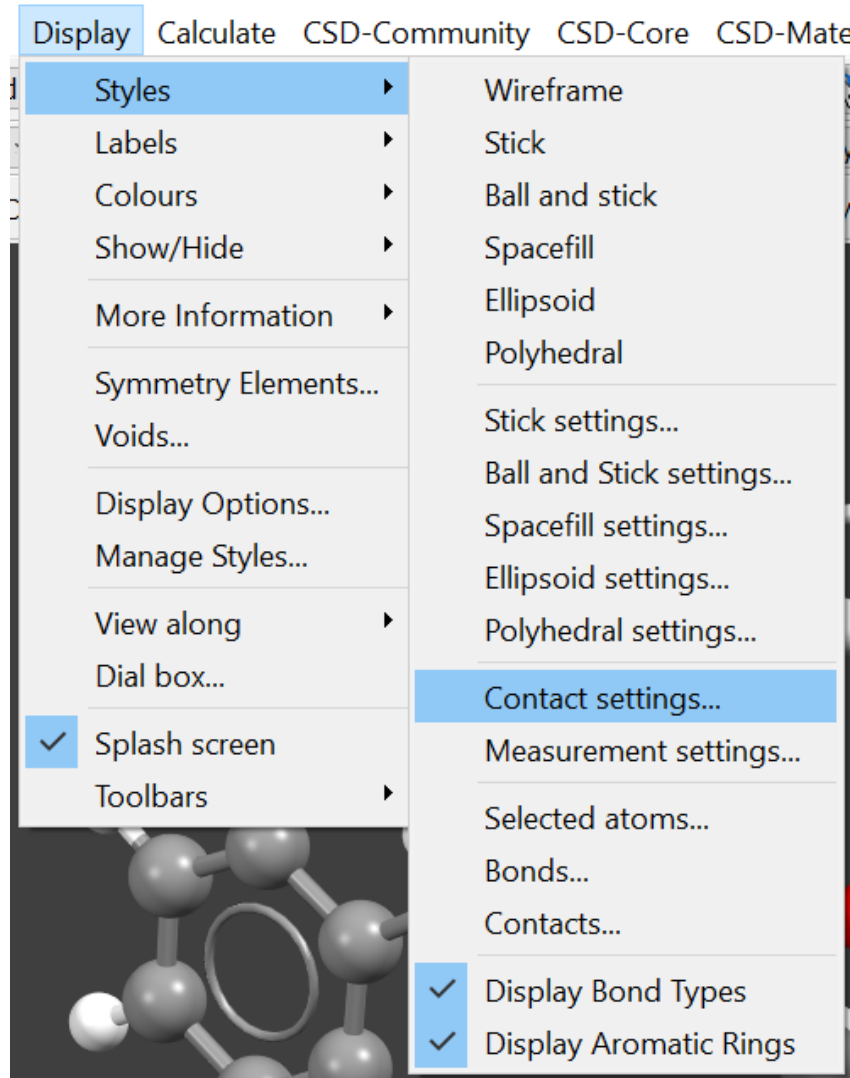
Display contacts visualisation options in Mercury

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.



Display contacts visualisation options in Mercury

The screenshot displays the Mercury software interface for the file 'HXACAN (Pcab) - Mercury'. The 'Display' menu is open, showing options for 'Colours', 'Show/Hide', 'More Information', 'Symmetry Elements...', 'Voids...', 'Voids (Experimental)...', and 'Display Options...'. The 'Colours' sub-menu is also open, listing 'Atoms...', 'Bonds...', 'Centroids...', 'Planes...', 'Contacts...', 'Element colours...', 'Symmetry Equivalence colours...', 'Labels...', and 'Background settings...'. The 'Contacts...' option is highlighted. In the foreground, the 'Contact Colours' dialog box is open, showing the following settings:

- Contact Colours
- By expanded/hanging
- Colour
- select colour:
- Colour by distance
- short: mid: long:
- Apply to:
-
-
-
-

The main window shows a 3D ball-and-stick model of a complex organic molecule with a central benzene ring. Several atoms are highlighted in red and blue, and dashed lines indicate intermolecular contacts. The interface includes a menu bar, a toolbar, and a status bar at the bottom with navigation controls like 'x-90', 'x+90', 'y-90', 'y+90', 'z-90', 'z+90', and 'zoom- zoom+'.

Label chiral molecules

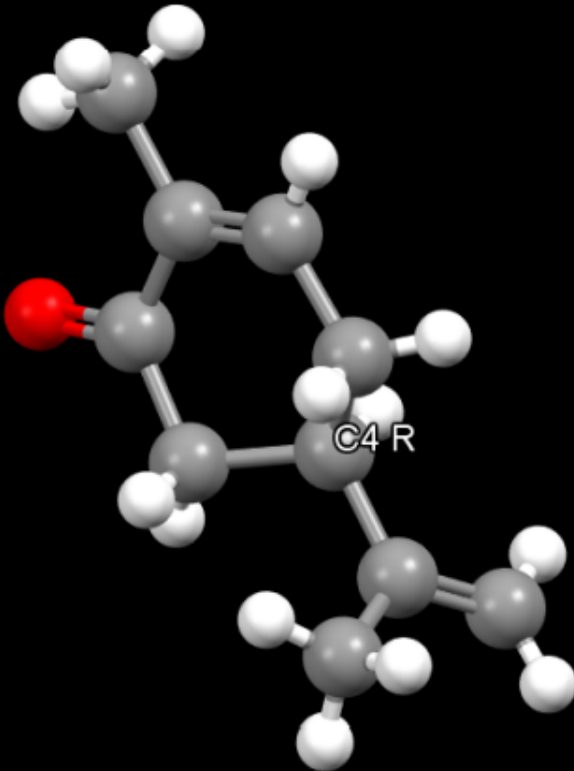
RERXIV (P212121) - Mercury

File Edit Selection Display Calculate CSD-Community CSD-System CSD-Materials CSD-Discovery CSD Python API Help

Picking Mode: Pick Atoms Clear Measurements Show Labels for Stereocentres with Stereochemistry

Style: Ball and Stick Colour: by Element Manage Styles... Cards Atom selections: Select by SMARTS:[C]

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+



Structure Navigator

Crystal Structures	Space
RERXIV	P2121
RERXIW	Pnma
RERXIX	C2/c
RERXIY	P-1
RERXOB	Pcmn
RERXOC	P21/c

Tree View

Multiple Structures

Structure Navigator Searches

Graph Sets

Chirality in the CSD Python API

← → ↻ downloads.ccdc.cam.ac.uk/documentation/API/

CSD Python API 3.0.11 documentation »

CCDC
advancing structural science

Next topic
Conditions of Use

Quick search

The CSD Python API

- Conditions of Use
- Release notes
 - Overview
 - Citing the CSD Python API
 - Licensed Features
 - Change Log
 - 3.0.11
 - 3.0.10
 - 3.0.9

• `ccdc.molecule.Atom.chirality` (Python attribute, in Molecule 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

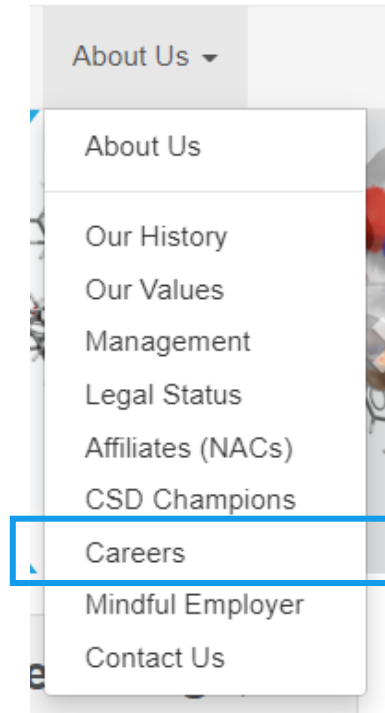
The displacement parameters of this atom.

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...
- ... or send us an open application



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.