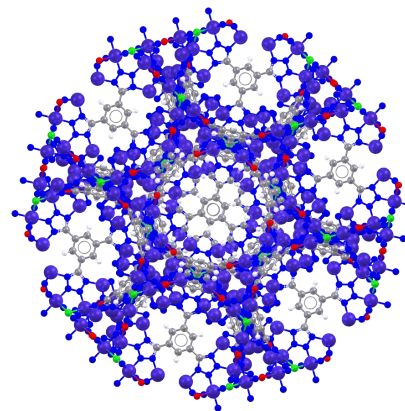




Advanced Functionality for Visualization and Analysis of Structures in Mercury

CCDC Virtual Workshop

30th April 2024

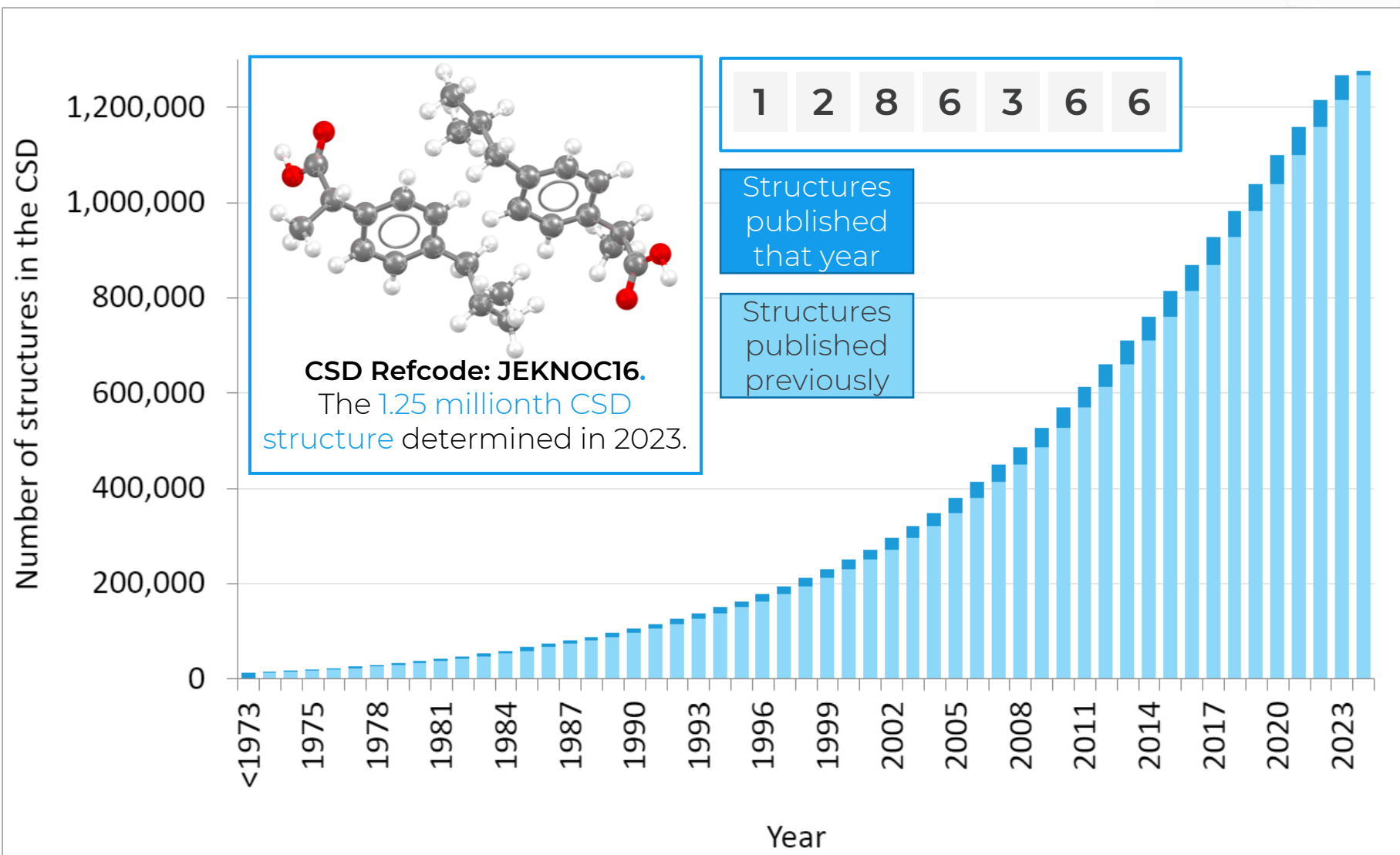


CCDC
advancing structural science

Learning outcomes for today

- Understand more about the [advanced functionality in Mercury](#) and how it can be used to visualise, analyse and compare solid forms effectively, including guidance on:
 - Applications of the new [disorder visualization](#) feature.
 - [Edit](#) structures, [select](#), hide or delete parts of the structure and create your own [style](#)!
 - Structure and molecule overlay, for [comparing crystal structures](#) packing and molecular conformations and stereochemistry.
 - [Visualize a slice](#) of the crystal packing along BFDH planes.
 - [Conformer generator](#) for generating plausible conformers of compounds of interest.
 - [Programmatic access](#) through CSD Python API menu - no need for coding with the pre-loaded functionality!
- Learn [tips and tricks](#) for using a range of tools effectively to [save you time](#) and help you [advance your research](#)
- [Gain confidence](#) in the functionality used today so you can [apply the techniques on your own systems/structures](#).

The Cambridge Structural Database



- 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 58 years
- A trusted CoreTrustSeal repository



Certified as Trustworthy
by CoreTrustSeal

Inside the Cambridge Structural Database

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

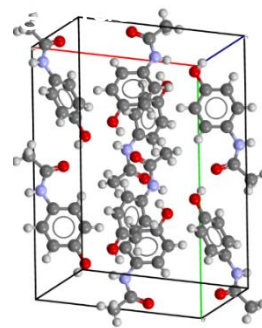
Organic
45%

Metal-Organic
55%

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

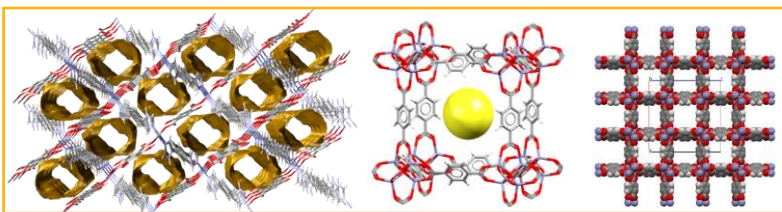
- 13,478 polymorph families
- 174,987 melting points
- 1,075,904 crystal colours
- 951,746 crystal shapes
- 30,275 bioactivity details
- 13,641 natural source data
- > 350,000 oxidation states

Not Polymeric
89%

Polymeric: 11%

Metal-Organic

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

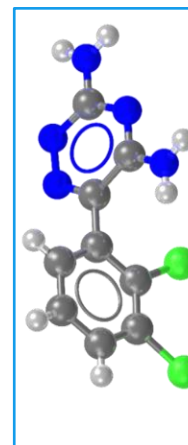


Single
Component
58%

Multi
Component
42%

Links and subsets

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



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

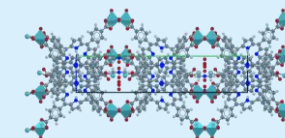
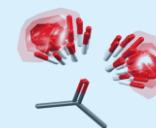


We clearly recognised even in those early days, that data banks have three principal functions. Firstly they must gather together existing knowledge and make it readily available to the scientific community. Secondly they can be used to reduce a large number of observations to a small set of constants 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)

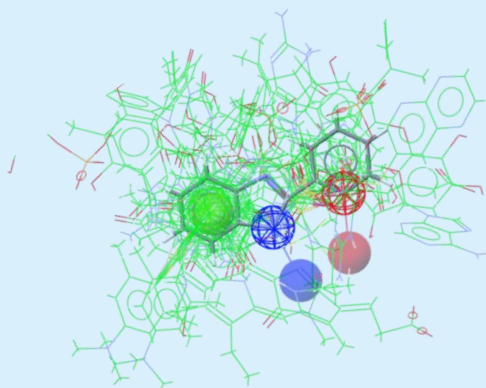
The CSD Portfolio today



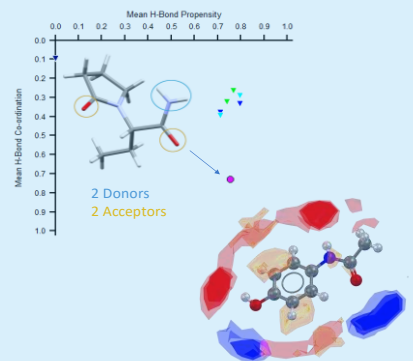
CSDCore. Search, visualise, analyse and communicate structural data
Insights into molecular and crystal shape and interactions



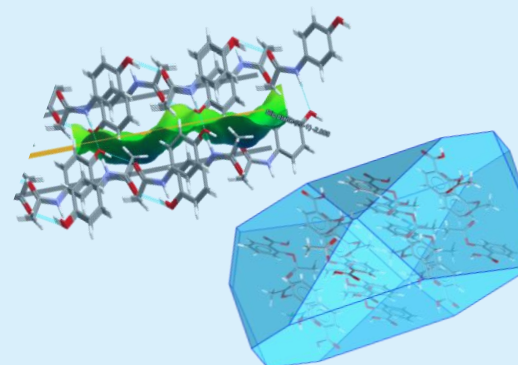
CSDDiscovery.
Design of new molecules



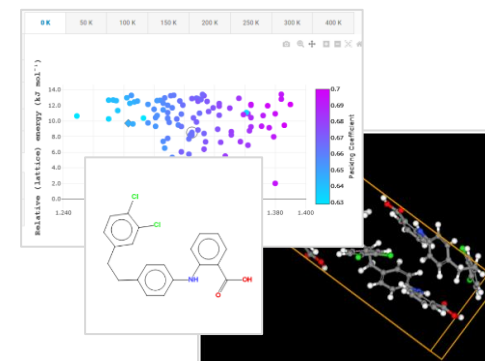
CSDMaterials.
Assessment of solid form stability and properties



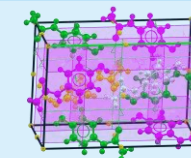
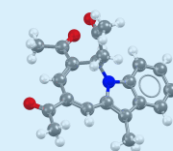
CSDParticle.
Anticipate particle properties and behaviour



CSDTheory.
Insights from predicted structure landscapes



CSDCommunity. Deposit, publish, access and visualise structural data
Free functionality to share and learn from structures



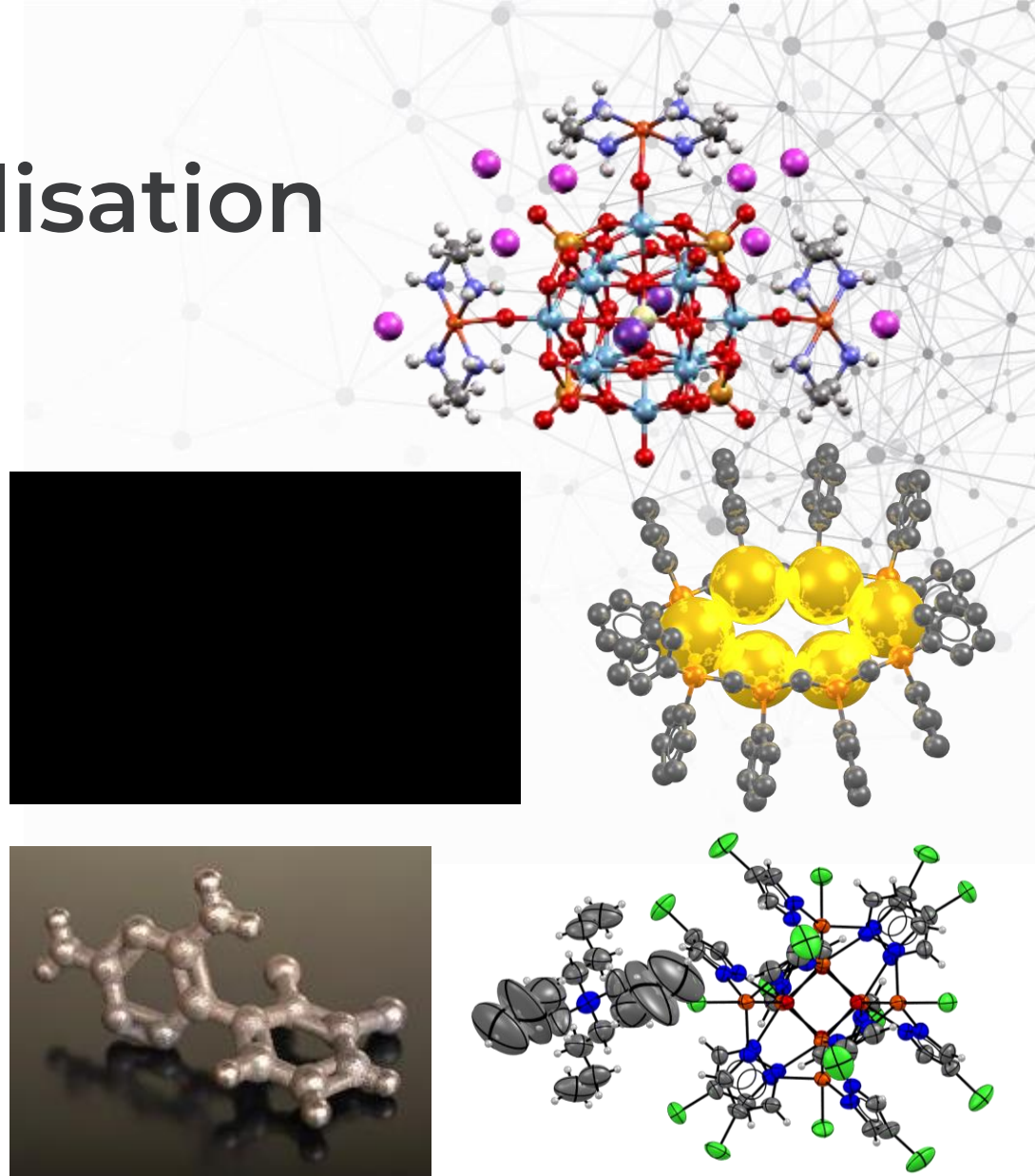
Medicinal & Computational Chemists ♦ Crystallographers & Structural Biologists ♦ Solid Form & Crystallisation Scientists ♦ Functional Materials Scientists ♦ Educators ♦ Industry and Academia

CCDC

Mercury – Structure visualisation

With Mercury you can:

- Explore [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

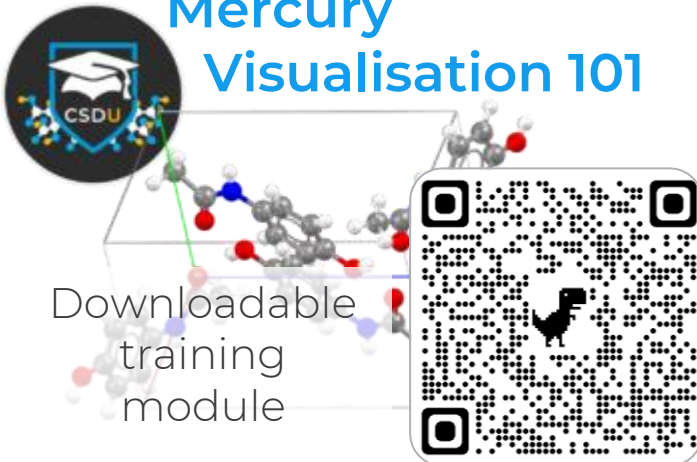


Structure visualisation – Basics

What have we learnt in previous workshops and resources?

- The basics of the Mercury **interface**.
- Basic options to **visualise** small molecule crystal structures.
- Analysis and visualisation of **Hydrogen bonds**.
- Visualisation of the **packing and basic symmetry**.
- Creation of **high-resolution** publication ready **images**.

Mercury
Visualisation 101

A graphic for the 'Mercury Visualisation 101' resource. It features a circular logo on the left with a graduation cap and the text 'CSDU'. To the right is a 3D ball-and-stick model of a crystal structure. Further right is a large QR code. The text 'Downloadable training module' is positioned between the logo and the QR code.

Downloadable training module

Introduction

Mercury is the visualisation and analysis software of the Cambridge Structural Database (CSD). Mercury is used in investigating and analysing crystal structures with features that allow a user to generate packing diagrams, display and assess the strength of intermolecular interaction networks, calculate and display voids, create 3D theoretical crystal morphologies and more (features availability subject to appropriate licence). With Mercury you can visualise 3D structures from the CSD as well as your own. You can also produce high-quality publication-ready images, frames for videos, and 3D print files.

Before beginning this workshop, ensure that you have installed Mercury. Please contact your site administrator or workshop host for further information.

Learning Outcomes

In this workshop we will learn about analysis tools in Mercury, specifically we will learn how to:

- Measure distances, angles and torsions.
- Calculate and display centroids and planes.

This workshop will take approximately 25 minutes to be completed.

Note: The exercises.

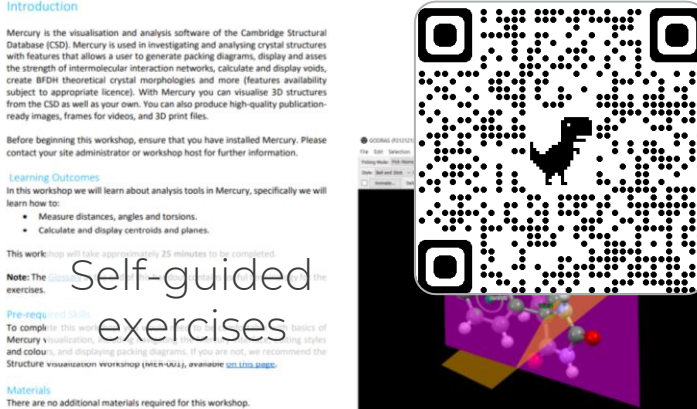

Pre-requisites

To complete this workshop, you should have a basic understanding of Mercury visualisation, including packing diagrams, and display styles and colour. If you are not, we recommend the Structure Visualisation Workshop (MERC-VIS), available on the CSD website.

Materials

There are no additional materials required for this workshop.

Self-guided exercises

A graphic for the 'Self-guided exercises' resource. It includes a text box on the left with an introduction, learning outcomes, and prerequisites. To the right is a large QR code. Below the QR code is a small 3D model of a crystal structure.A graphic for the 'Short how-to videos' resource. It features a 3D ball-and-stick model of a crystal structure on the left. To the right is a large QR code. The text 'Short how-to videos' is overlaid on the model.

Short how-to videos

How to define and visualize hydrogen bonds in Mercury - video...

Mercury Overview

More advanced
functionality to analyse
and learn from structures



Display
options to
visualise and
navigate
structures



AABHTZ (P-1) - Mercury

File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Theory CSD-Particle 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

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) ☐ H-Bond Default definition

☐ Asymmetric Unit ☐ Auto centre

Reset

Options

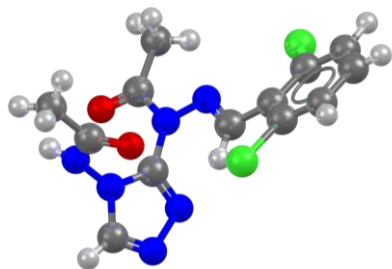
☒ Show hydrogens ☐ Depth cue ☐ Show cell axes ☐ Z-Clipping ☐ Label atoms ☐ Stereo

Contacts... More Info Powder...

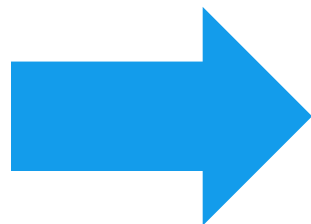
Explore over 1.25 million curated structures

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

CSD Refcodes



CSD Refcode -
AABTHZ



What is AABHTZ?

- 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

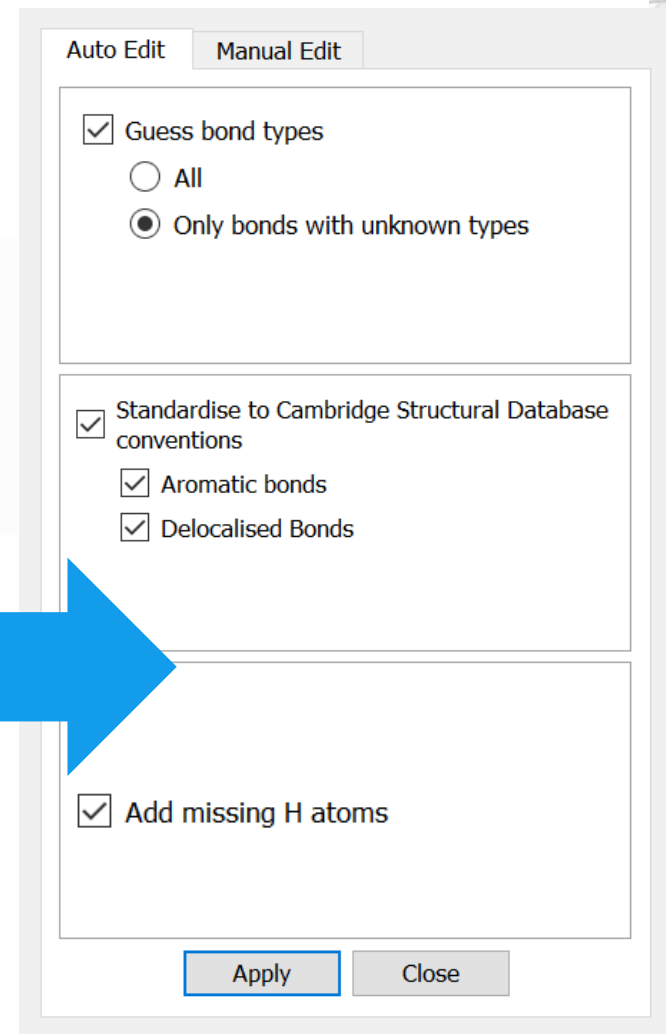
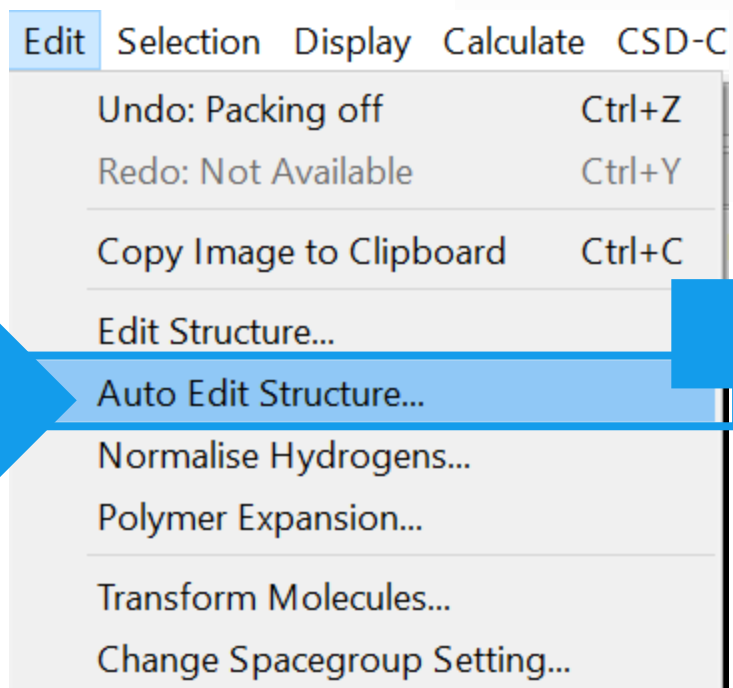
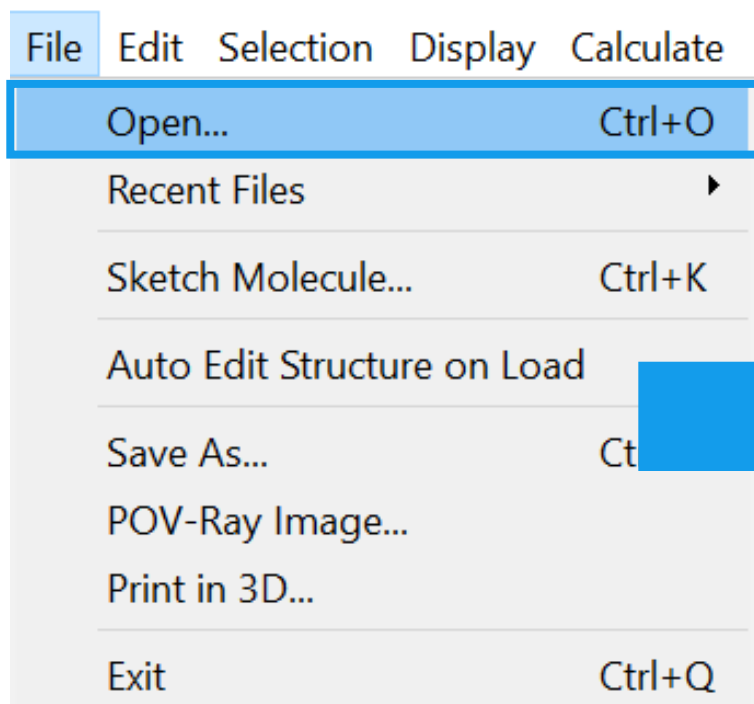
Some of my favourite refcodes are: KITTEN, BATMAN, DISNEY, GAUTAM, GLYCIN

Import and assign
bond types and
missing hydrogens
(optional)

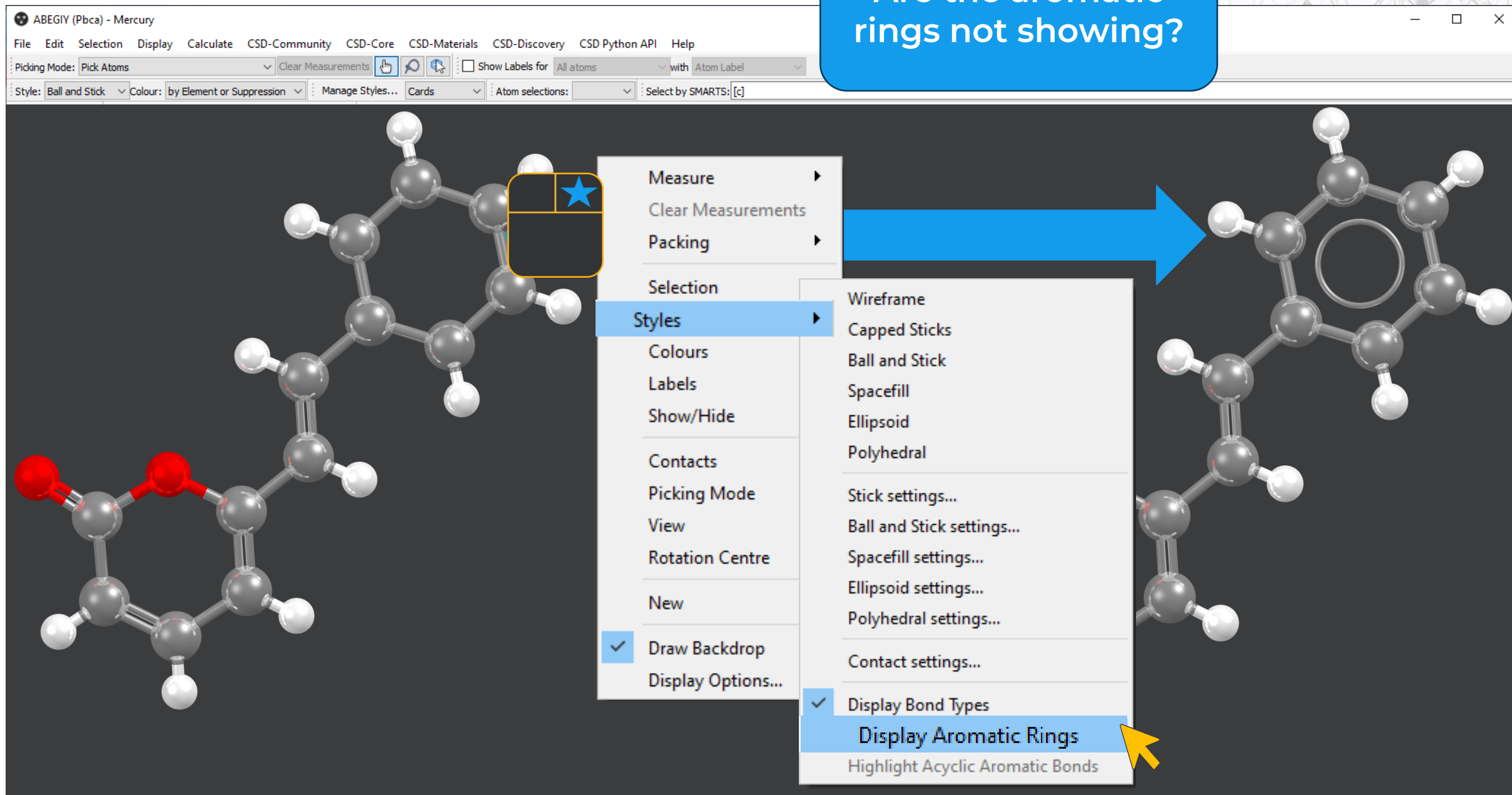
Visualise your own structures

- 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

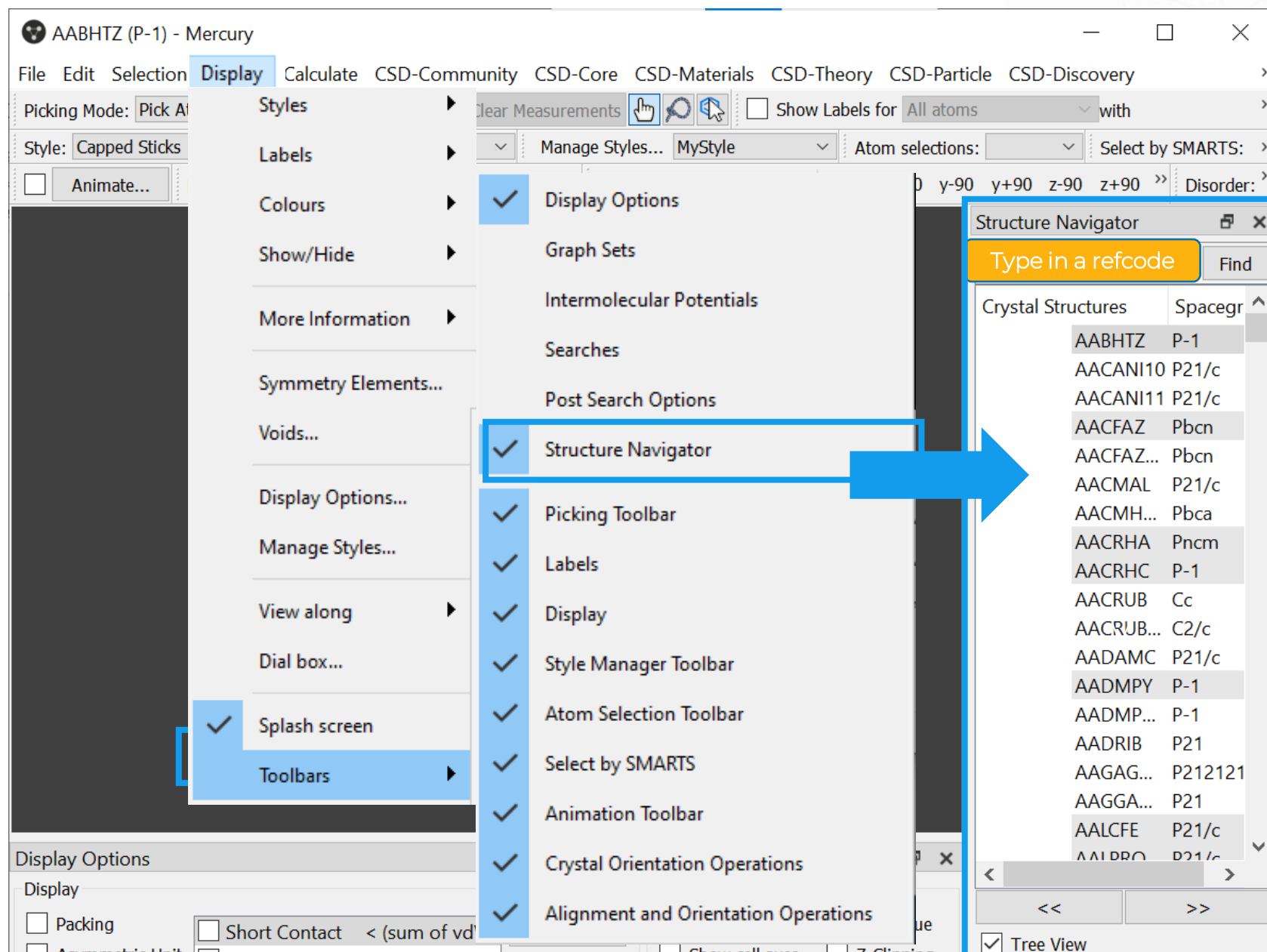
AABHTZ (P-1) - Mercury



Are the aromatic rings not showing?

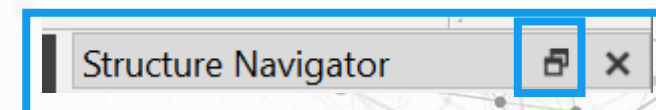


Lost toolbars?



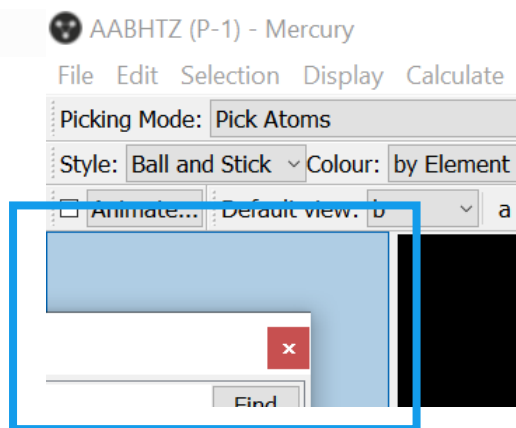
Extra Tip

Click on the resize icon or drag the top to pop the toolbar out.



Extra Tip

To pop the toolbar back in drag it to the area you want it.



Improve visualization with lots of display options!

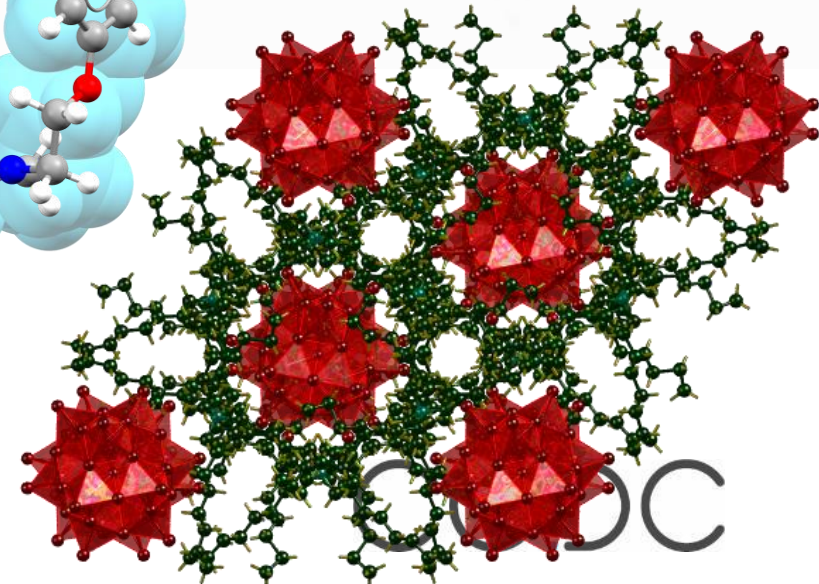
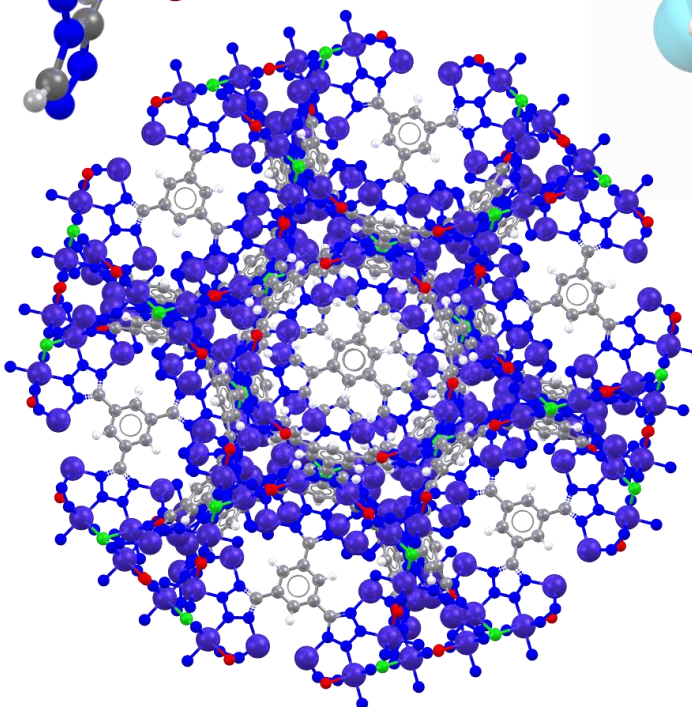
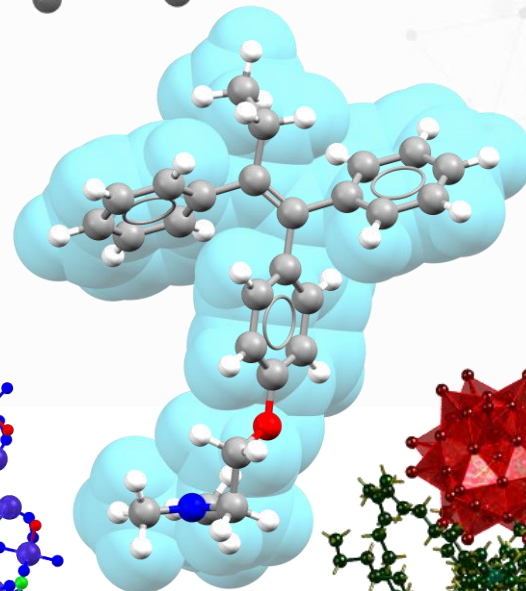
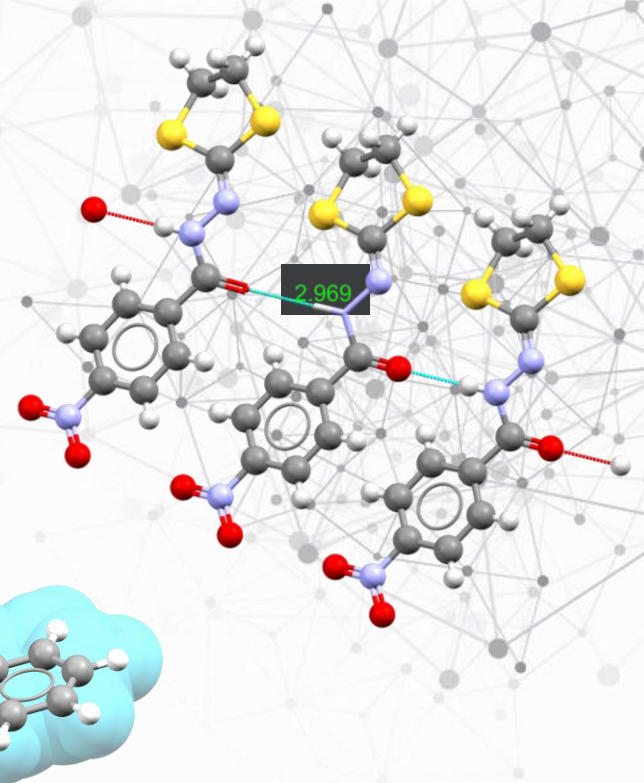
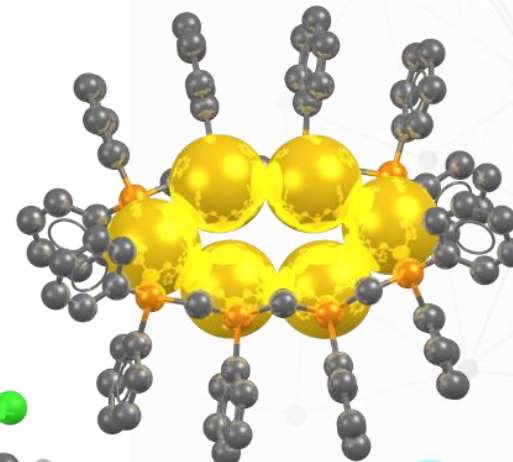
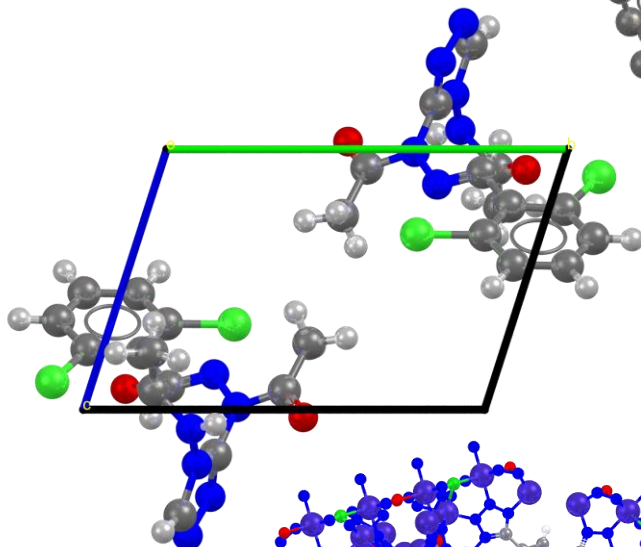
Display

Styles	Wireframe
Labels	Stick
Colours	Ball and stick
Show/Hide	Spacefill
More Information	Ellipsoid
Symmetry Elements...	Polyhedral
Voids...	Stick settings...
Display Options...	Ball and Stick settings...
Manage Styles...	Spacefill settings...
View along	Ellipsoid settings...
Dial box...	Polyhedral settings...
✓ Splash screen	Contact settings...
Toolbars	Measurement settings...
	Selected

Calculate

Centroids...
Planes...
Packing/Slicing...
Contacts...
Molecular Shell...
Graph Sets...
Powder Pattern...
Structure Overlay...
Molecule Overlay...

Colour:	by Element or Suppression
view:	by Element
	by Symmetry equivalence
	by Atomic displacement
	by Symmetry operation
	by Gasteiger charge
	by Partial charge
	by Element or Suppression



Working with colleagues and want consistent look of your publication images?

Step 1: Create your personalised style

1 Manage Styles...

2 Apply, Edit..., Copy...

3 Style name: Research Project

4

5

	Style	Colour
Atoms: Non Hydrogen	Polyhedral	By Element
Atoms: Hydrogen	Polyhedral	By Element
Bonds	Polyhedral	By Connected Atoms
Contacts: Hanging	Stick	Red
Contacts: Expanded	Stick	Cyan
Cell Edges	Stick	Black
Centroids	Solid	Red
Planes	Solid	Red

Display Options... Change background, depth cue, labels, lighting, etc.

Element Colours... Change colours of common elements

Symmetry Equiv. Colours... Change Symmetry Equivalence colours

Stick Settings... Change stick display options

Ball & Stick Settings... Change ball and stick display options

Spacefill Settings... Change spacefill display options

Ellipsoid Settings... Change ellipsoid display options

Polyhedral Settings... Change polyhedral display options

Contact Settings... Change contact display options

Measurement Settings... Measurement options

Defaults

Apply

Step 2: Save it and share it with your collaborators

ABUJIG (R-3c) - Mercury

File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials

Picking Mode: Pick Atoms

Style: Polyhedral Colour: by element

Manage Styles... MyStyle

Animate... Default view: b

Style Manager

- Work
- Publication
- Presentation
- ORTEP
- 3D Print
- Work-2
- MyStyle
- October
- December
- Research Project

Apply Edit... Copy... New... Open... Save As... Rename... Delete Close

Save As

Images_structures

Organise New folder

This PC 3D Objects Desktop

File name: Research Project

Save as type: Mercury Styles (*.msd)

Hide Folders Save Cancel

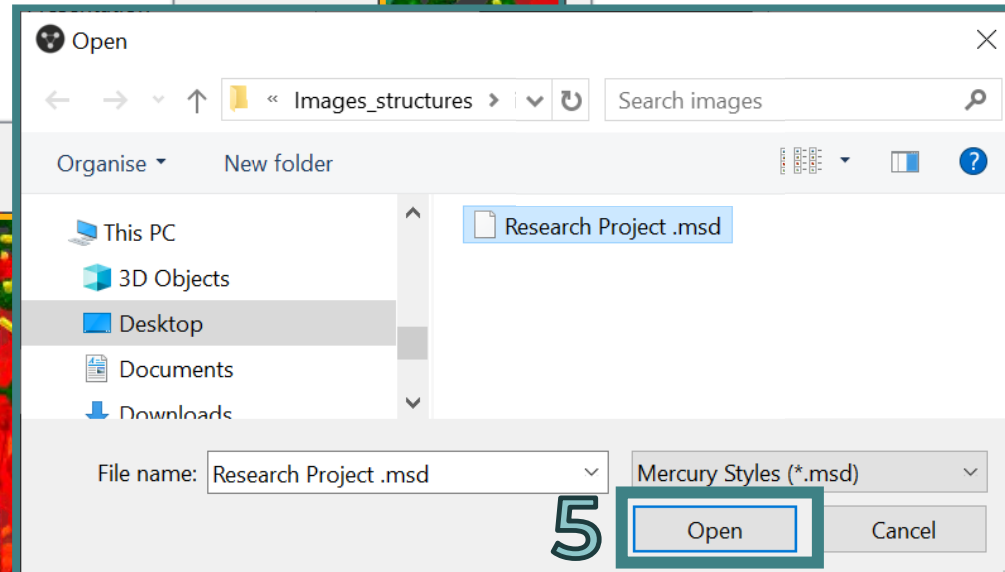
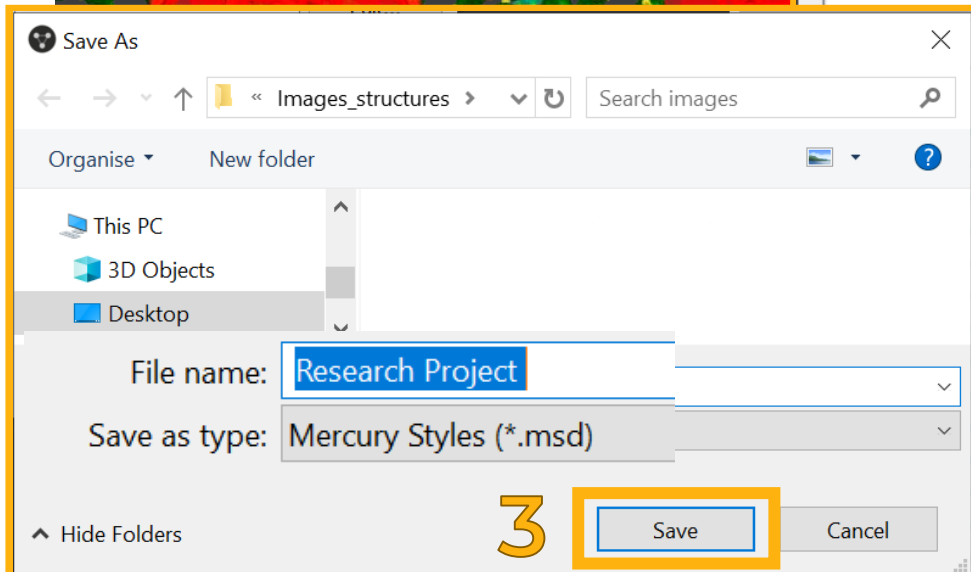
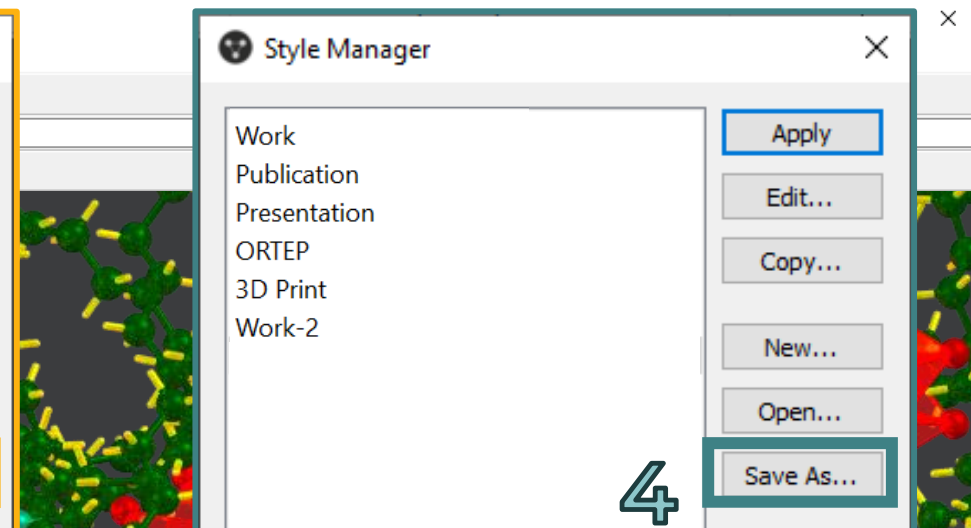
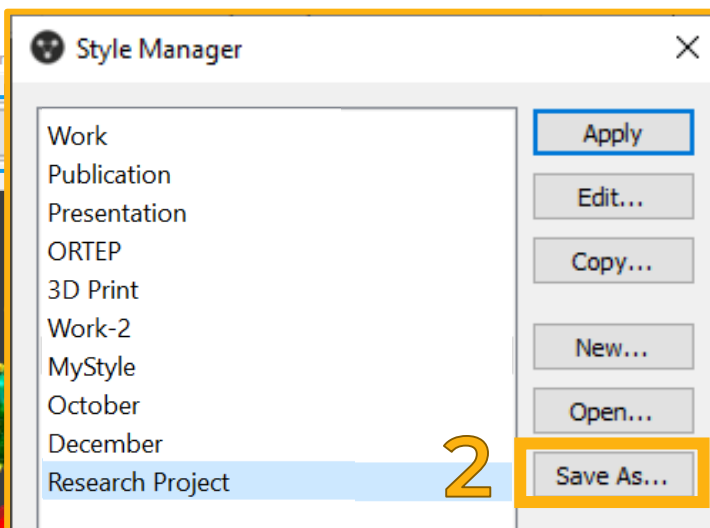
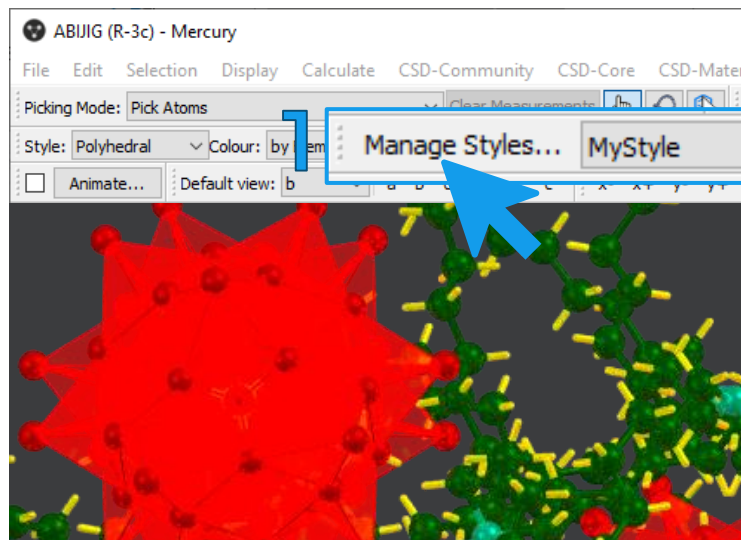
1

2

3

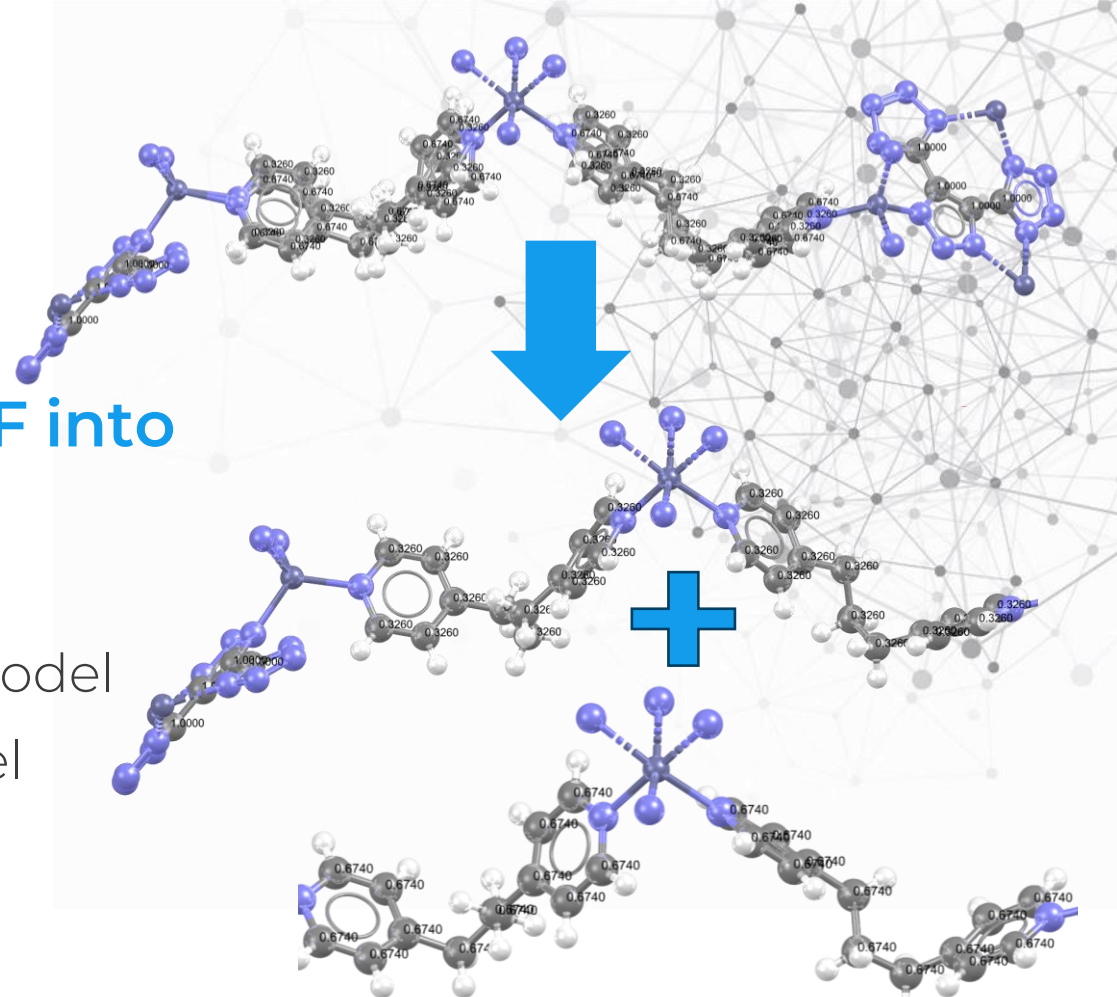
Step 2: Save it and share it with your collaborators

Step 3: Your collaborators can then open and save your new style.



Visualizing disorder

- New functionality when you **load a CIF into Mercury:**
 - Visualise the different **disorder models**
 - Visualize the **contacts** for each disorder model
 - Visualize the **voids** for each disorder model
 - Available from **July 2023** onwards
- More disorder work planned.



File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Theory CSD-Particle 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 Manage Styles... Work 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+

Disorder: A● All

● $x > 0.6$
● $0.6 > x > 0.4$
● $x < 0.4$

Change disordered atoms colours

The screenshot shows the Mercury software interface with the 'Display' menu open. The 'Colours' option is selected, leading to the 'Element Colour Options' dialog box. The dialog box displays a periodic table where elements are color-coded. A blue arrow points from the 'Element colours...' option in the 'Display' menu to the dialog box. Another blue arrow points from the 'Unknown' label in the dialog box to the 'Unknown' label in the 'Colours' dropdown menu of the 'Display' menu.

Mercury (P21/c) - Mercury

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

Picking Mode: Pick Atoms Colour: by Element or Suppression Show Labels for All a

Style: Ball and Stick Colour: by Element or Suppression Manage Styles... Cards Atom selections:

PIYDEI (P21/c) - Mercury

File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Discovery

Picking Mode: Pick Atoms Measurements Show Labels for All a

Style: Ball and Stick Manage Styles... Cards Atom selections:

Colours

- Atoms...
- Bonds...
- Centroids...
- Planes...
- Contacts...
- Element colours...
- Symmetry Equivalence colours...
- Labels...
- Background settings...

Element Colour Options

Unknown

Unknown

Defaults Close

View multiple structures

Structure Navigator

Find

Crystal Structures Spacegroup

HXACAN	Pcab
HXACAN01	P21/a
HXACAN02	P21/c
HXACAN03	P21/n
HXACAN04	P21/n
HXACAN05	P21/a
HXACAN06	P21/a
HXACAN07	P21/n
HXACAN08	Pbca
HXACAN09	P21/n
HXACAN10	P21/n
HXACAN11	P21/n
HXACAN12	P21/n

<< >>

☒ Tree View

☒ Multiple Structures

Structures...

Tick *Multiple Structures* to display more than one structure. Untick *Multiple structures* to display one structure.

Note: you will need to move to another structure in the Structure Navigator for it to take effect.

Multiple Structures

Actions, e.g. packing, will be applied to Active structure(s) only

Rotation is around

☒ Global rotation centre ☐ Local rotation centres

Delete All ☒ All ☒ All ☒ All

	Structure	Visible	Active	Movable	Colour
1 Delete	HXACAN	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	by Element
2 Delete	HXACAN01	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	by Element

☐ Move the structure that is nearest the mouse cursor

by Element

by Symmetry

by Atomic Displacement

☐ White

☐ Light Grey

☐ Grey

☐ Dark Grey

☐ Black

☐ Pink

☐ Red

☐ Orange

☐ Yellow

☐ Light Green

☐ Green

☐ Light Blue

☐ Cyan

☐ Blue

☐ Purple

☐ Violet

☐ Magenta

Custom...

Custom Carbon...

Centroids...

Planes...

Packing/Slicing...

Contacts...

Molecular Shell...

Graph Sets...

Powder Pattern...

Structure Overlay...

Molecule Overlay...

☒ Show Labels for Stereocentres

with Stereochemistry

es... SANZI STYLE TEST

Atom selections:

Select by SMARTS: [c]

x+ y- y+

Automatic Molecule Overlay

zoom+

Options

Select **two molecules** (by selecting at least one atom in each) then press **Overlay**. The molecules must have at least three atoms, and the same number of atoms. After overlay is complete, you must select **Reset** before repeating the overlay or selecting different molecules.

Overlay

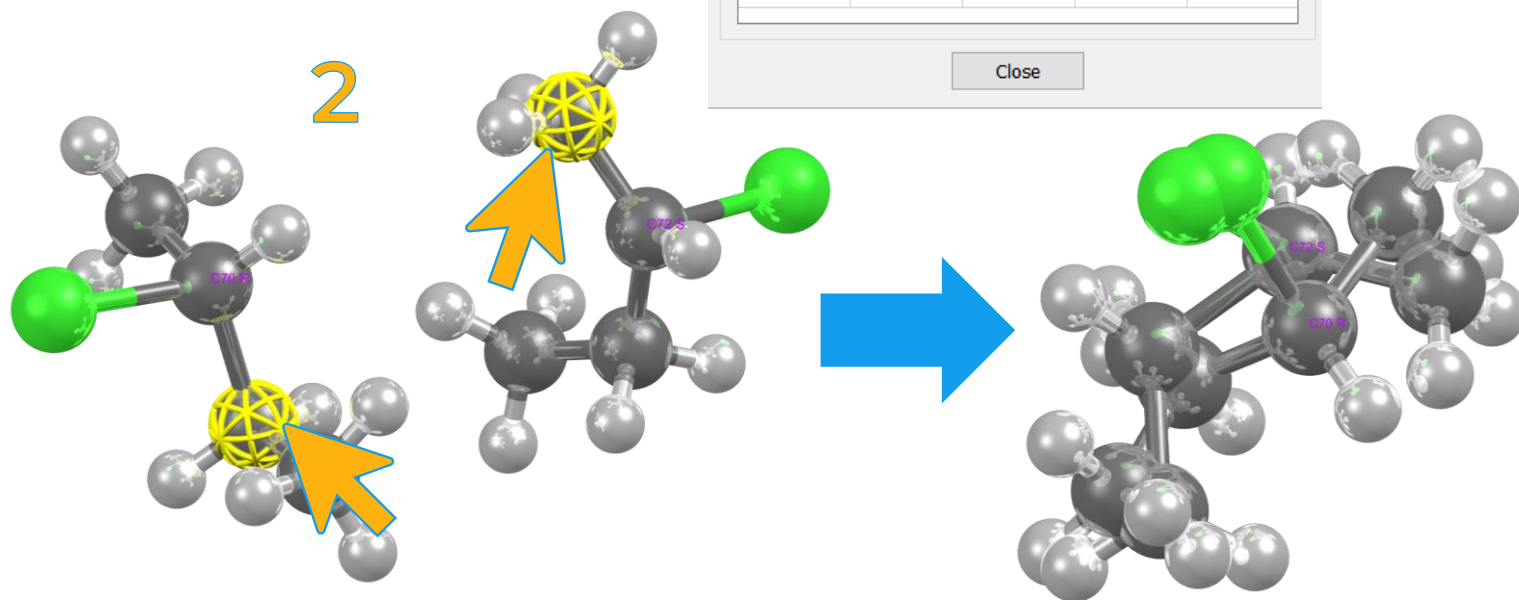
Results

Flexibility	Inversion	RMSD	Max. D	Display
-	-			<input checked="" type="radio"/>
-	X			<input type="radio"/>
X	-			<input type="radio"/>
X	X			<input type="radio"/>
Original	Geometry	----	----	<input type="radio"/>

Close

1

2



Molecule Overlay

When to use:

- To compare the chirality of stereochemistry of molecules.
- To compare conformers.

What it does:

- Uses inversion and flexibility to calculate overlays.

What you can use it on:

- 2 molecules in different structures
- Or 2 molecules in a single structure.
- On identical or non-identical molecules.

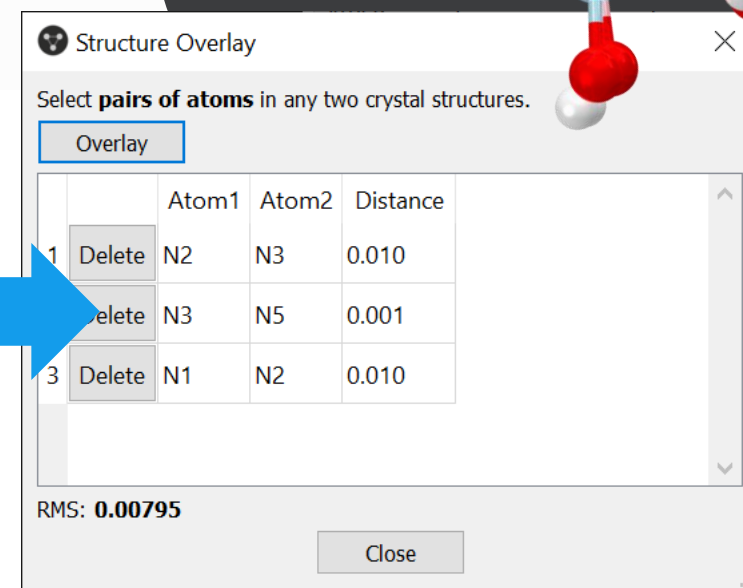
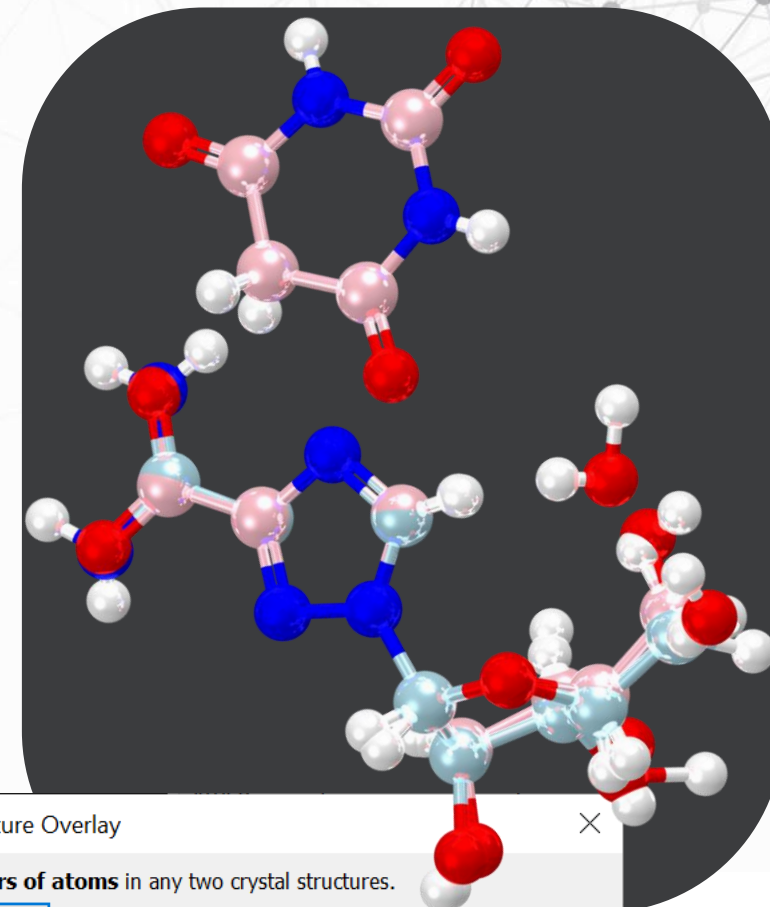
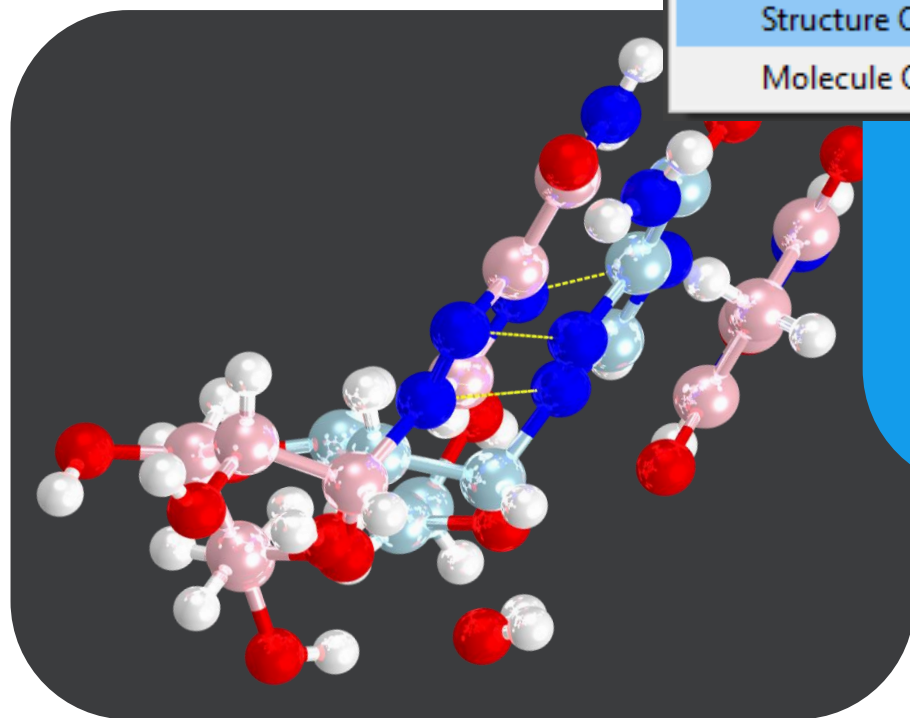
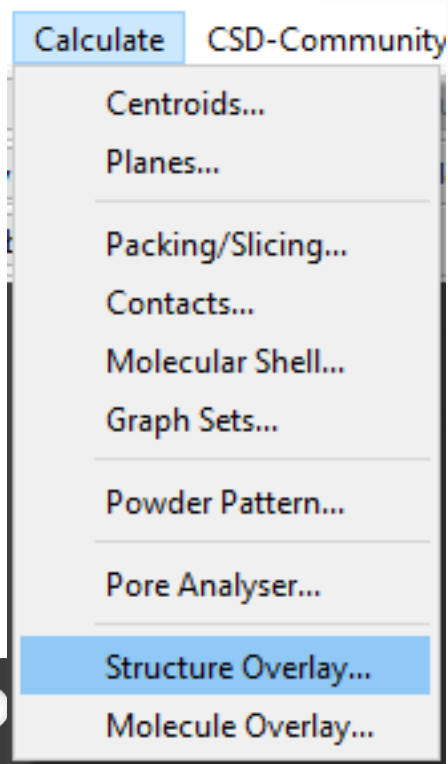
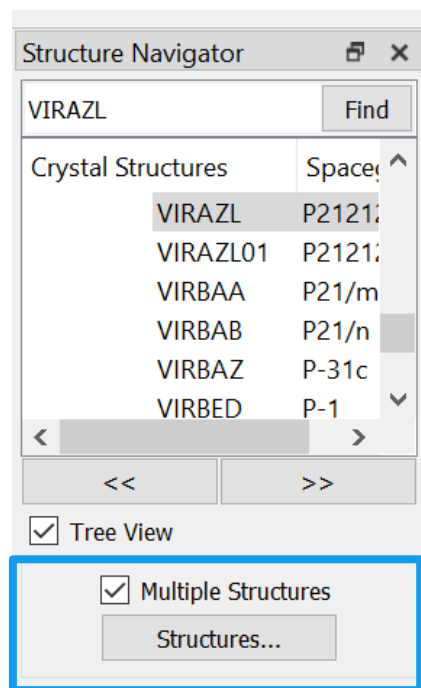
Tip

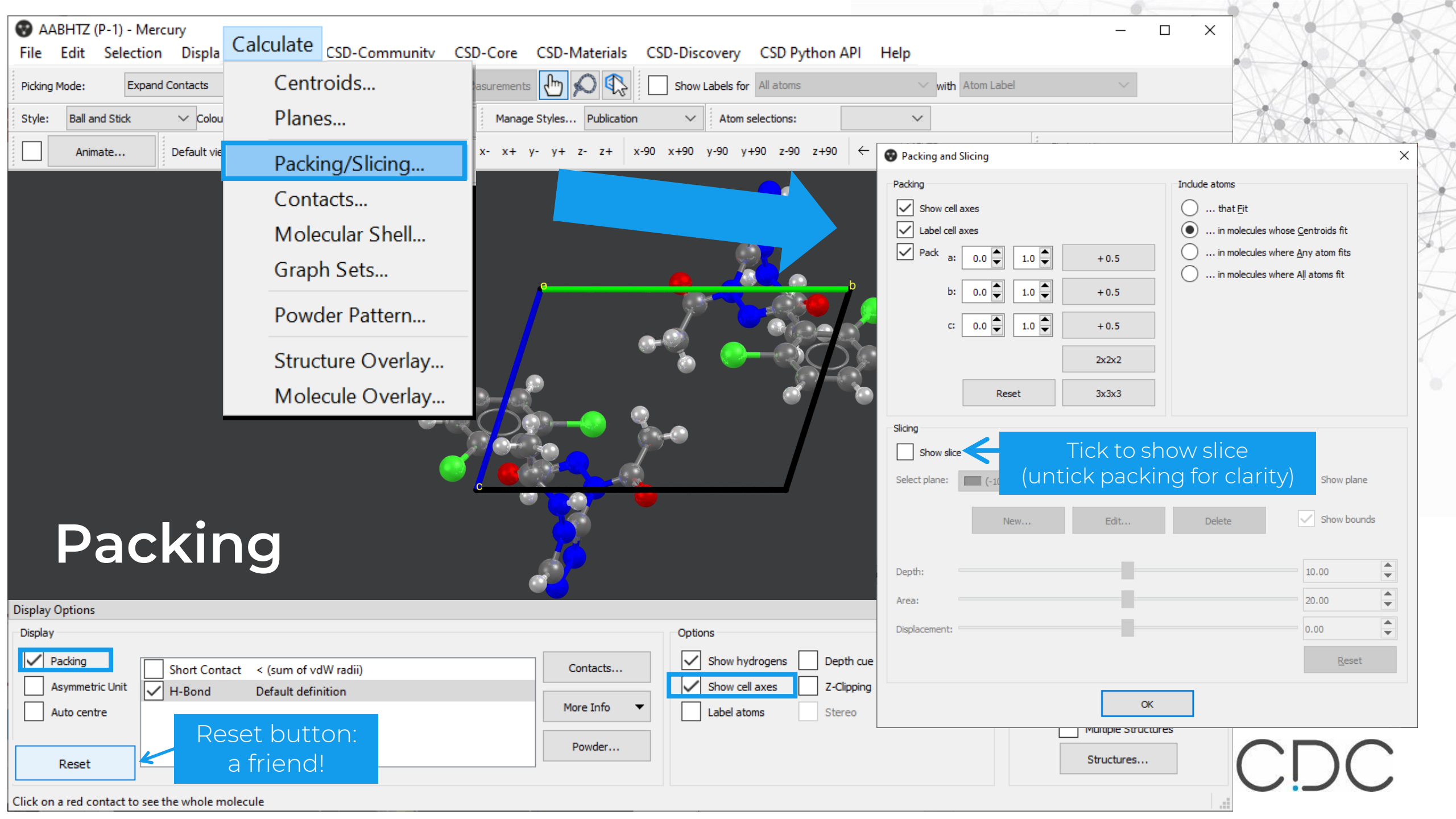
- If the reported RMSD for the overlay is quite low, but the Max. D value is large, it may be an indication that the molecules are quite similar, except for a localised area.
- For example, a comparison of cis and trans geometries may result in a low RMSD but high Max. D.

Structure Overlay

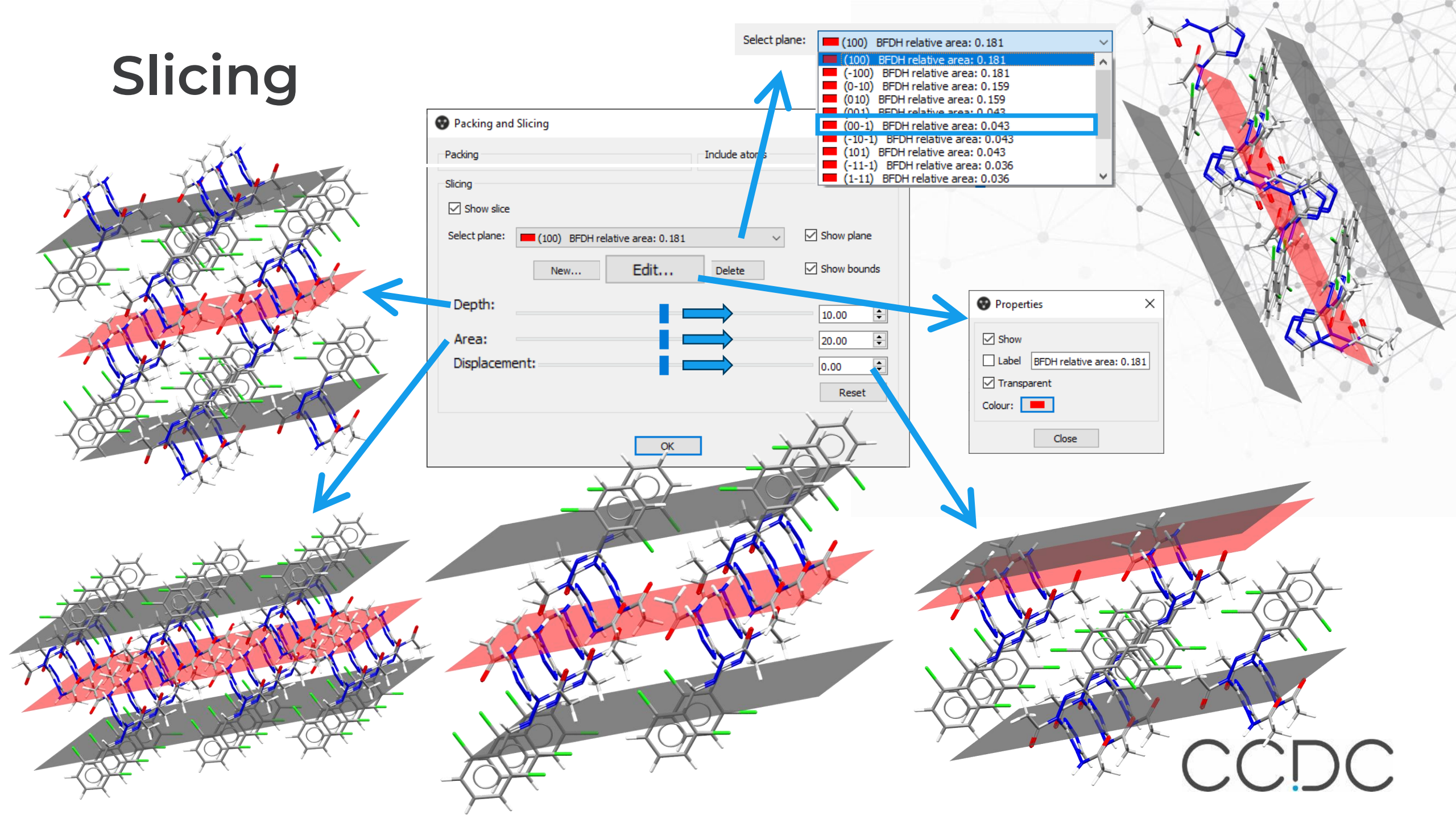
Tick Multiple structures to load more than one structure

CSD Refcodes: VIRAZL, FOQROU (light blue – pink)

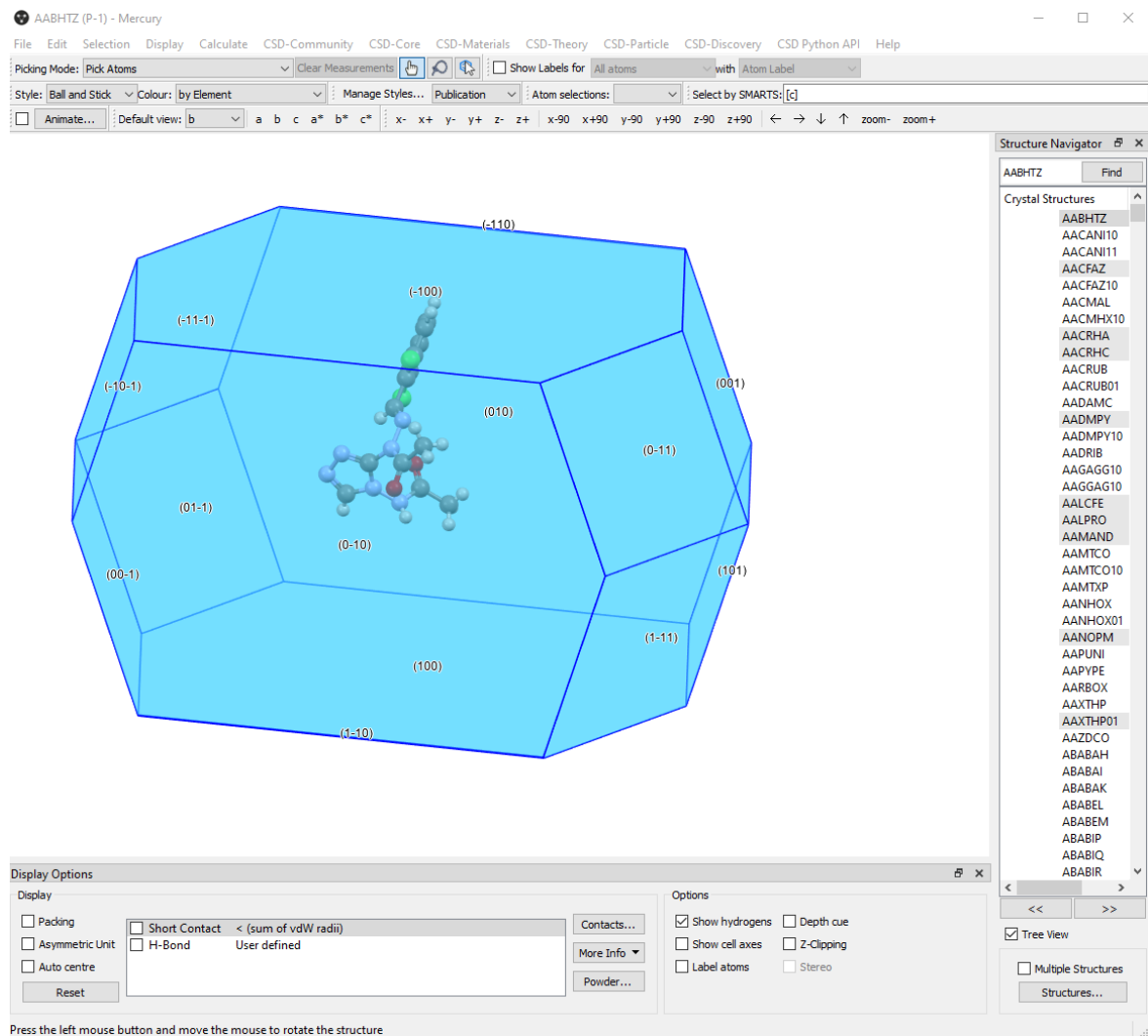




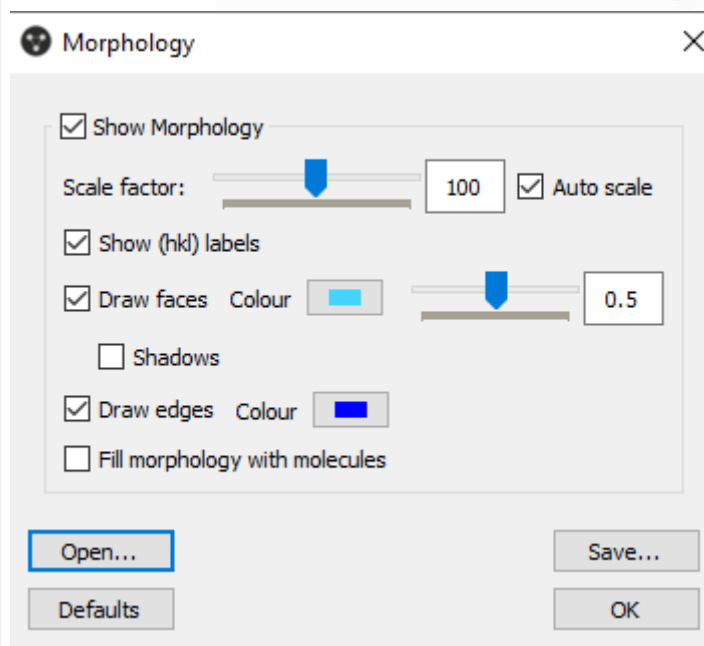
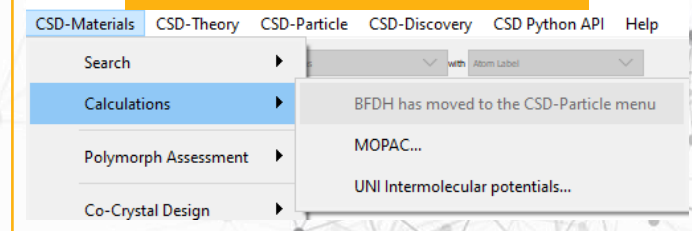
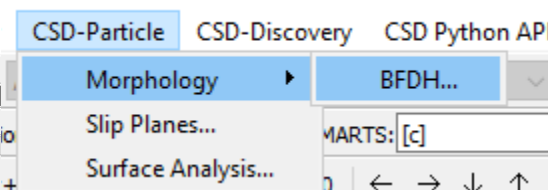
Slicing



A reminder: BFDH Morphology

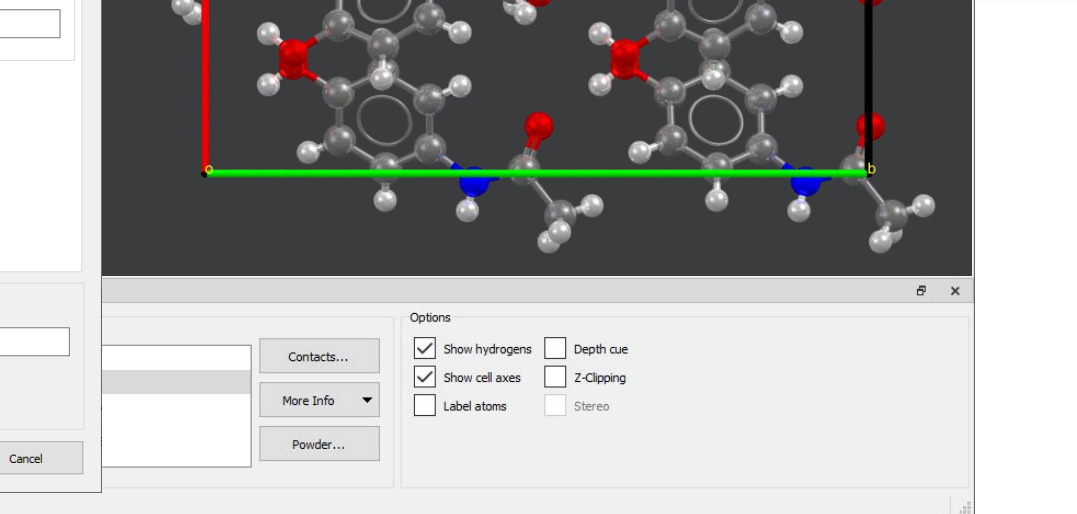


BFDH has moved



Display Options

Save and Load



Calculating planes

HXACAN (Pcab) - Mercury

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

Picking Mode: Lasso Atoms

Style: Ball and Stick

Clear Measurements Show Labels for All atoms with Atom Label

Manage Styles... Publication Atom selections:

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

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

Planes

Pick an object from the list below, or in the graphics window, or right-click on a list item

New Plane... Edit... Delete

Close

Plane Properties

Mean plane bkl

Select at least three atoms to calculate least squares plane:

Pick atom to select:

☐ Picked atom
☐ Picked molecule
☒ Ring

Select:

All
Non-hydrogen
Hydrogen

☒ Show
☒ Label mean:
☒ Transparent
Colour: yellow

OK Cancel

Plane Properties

Mean plane bkl

Create Miller plane:

Miller indices

h: k: l:

☒ Show
☒ Label (000)
☒ Transparent
Colour: yellow

OK Cancel

Options

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

Contacts...
More Info
Powder...

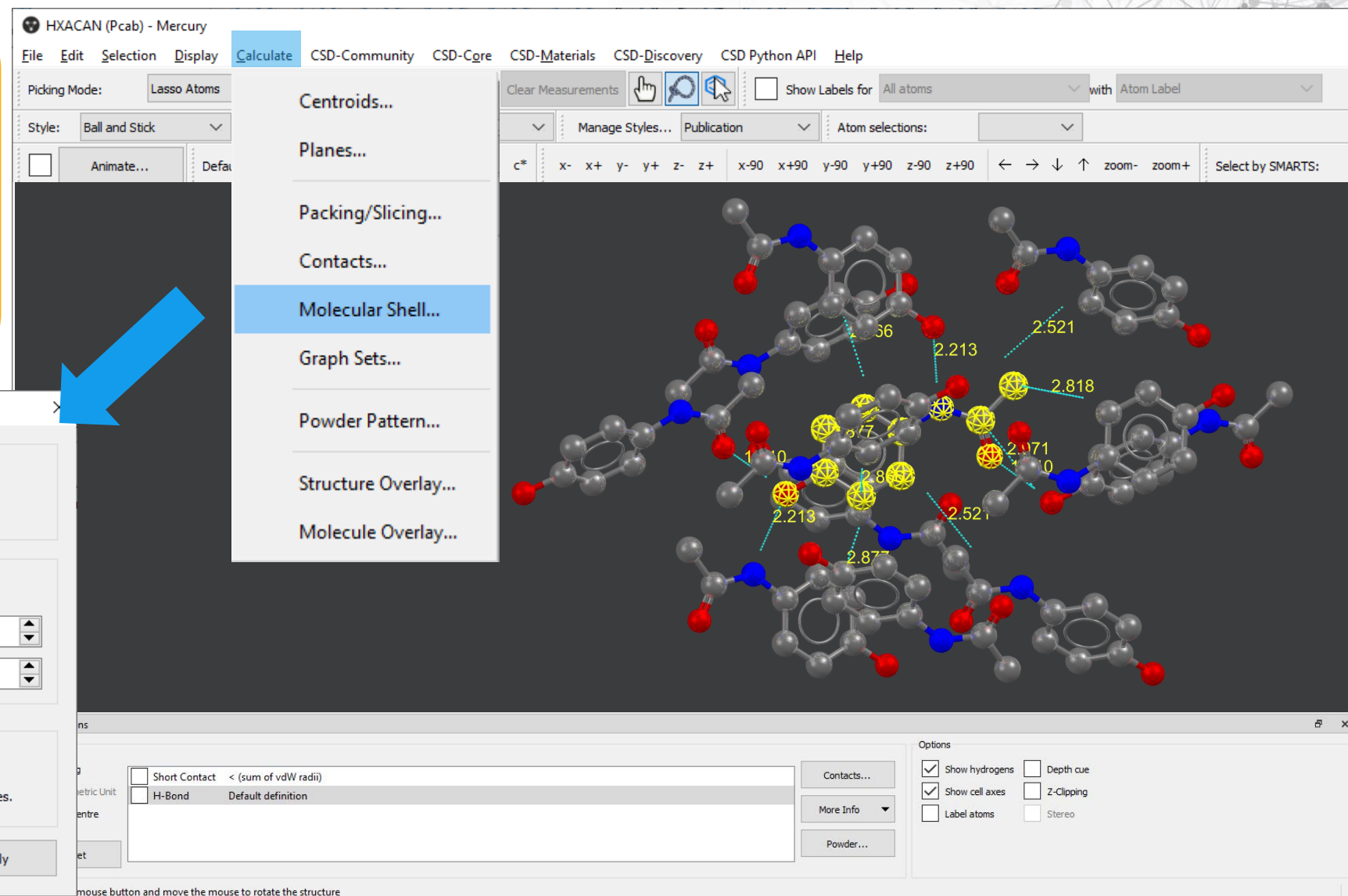
Tick "Transparent" to see through the plane

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

Exploring Molecular Shells

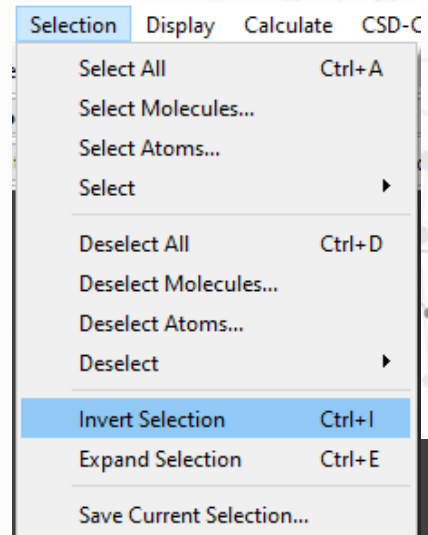
Molecular shells

contain atoms within a set distance from a selection (in some fields: “*coordination sphere*”).

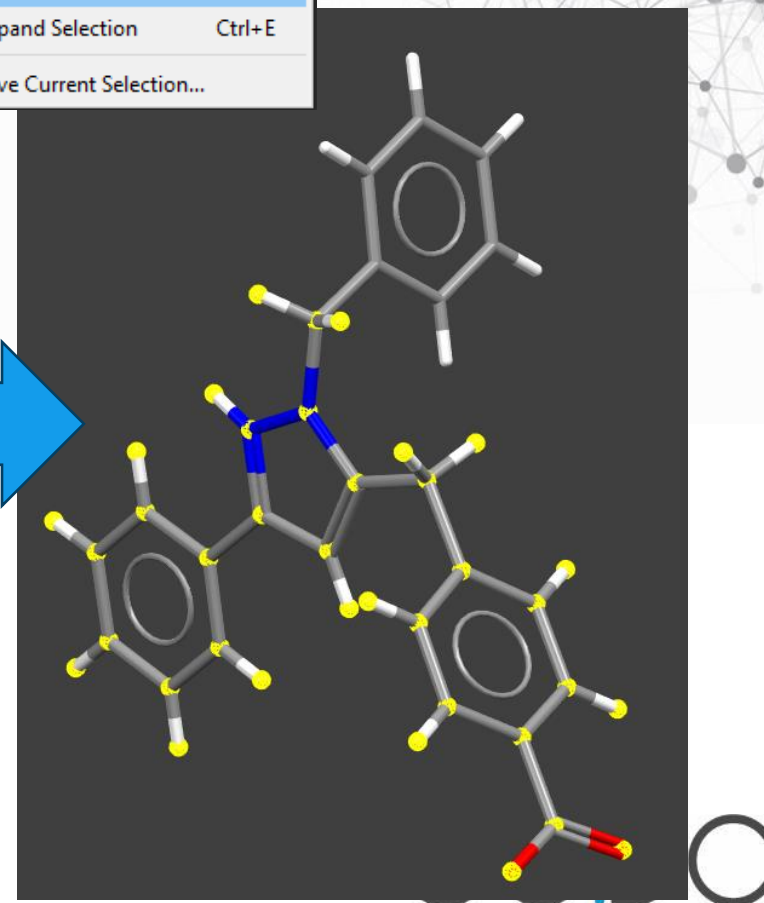
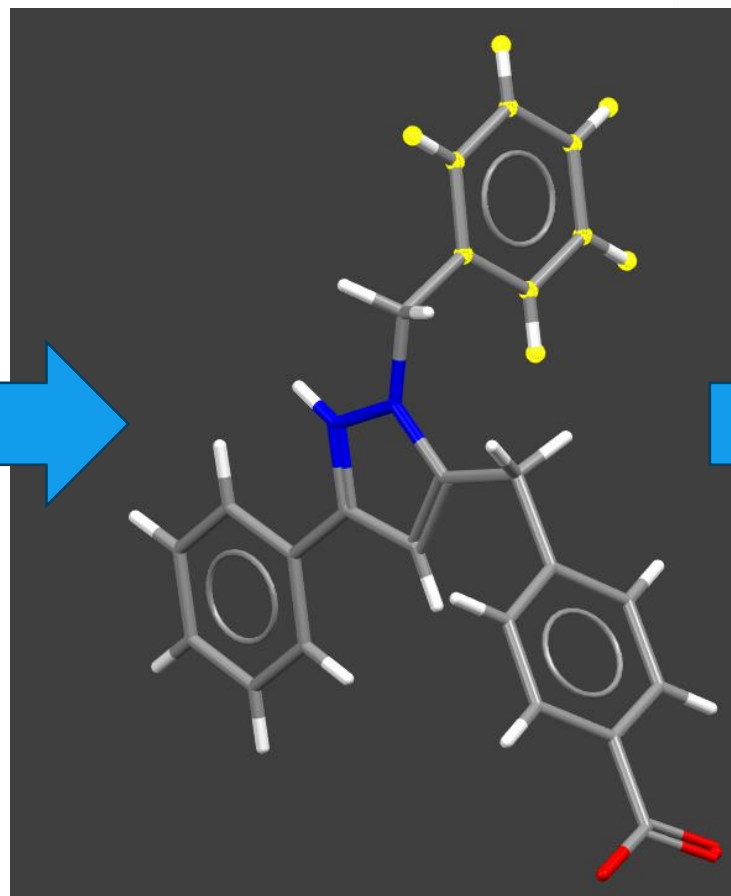
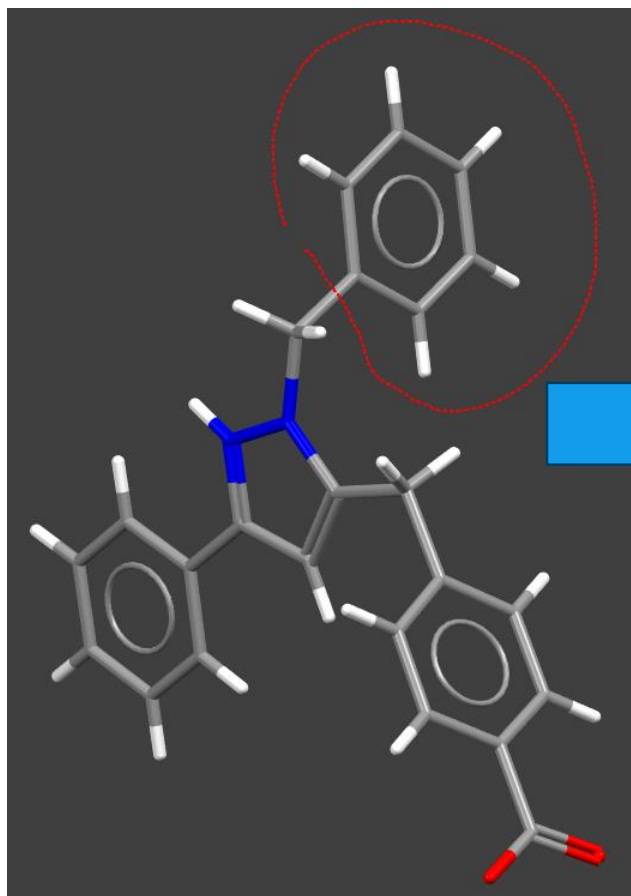


Select tips

Picking Mode: Lasso Atoms



CSD Refcode
FOQQOT

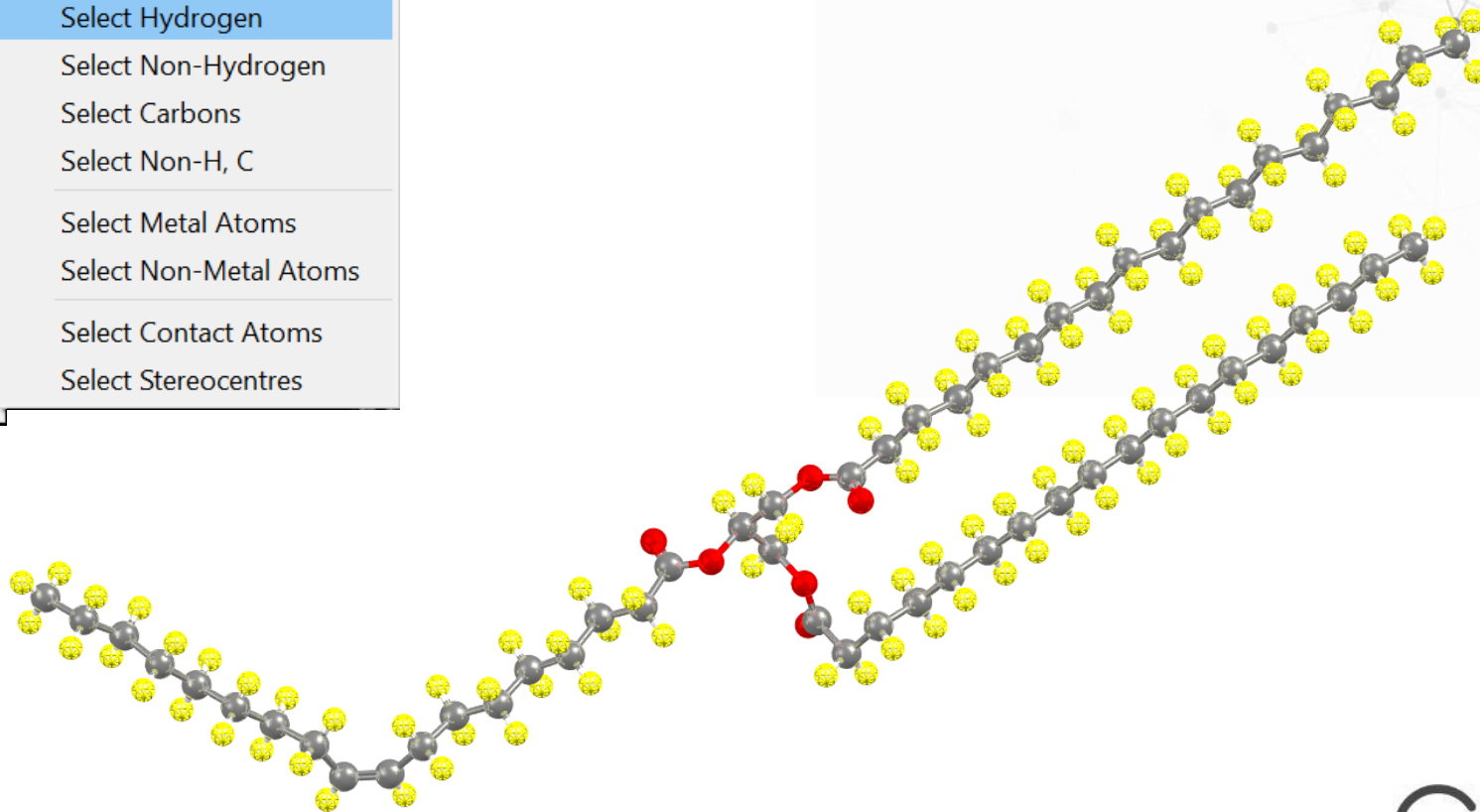


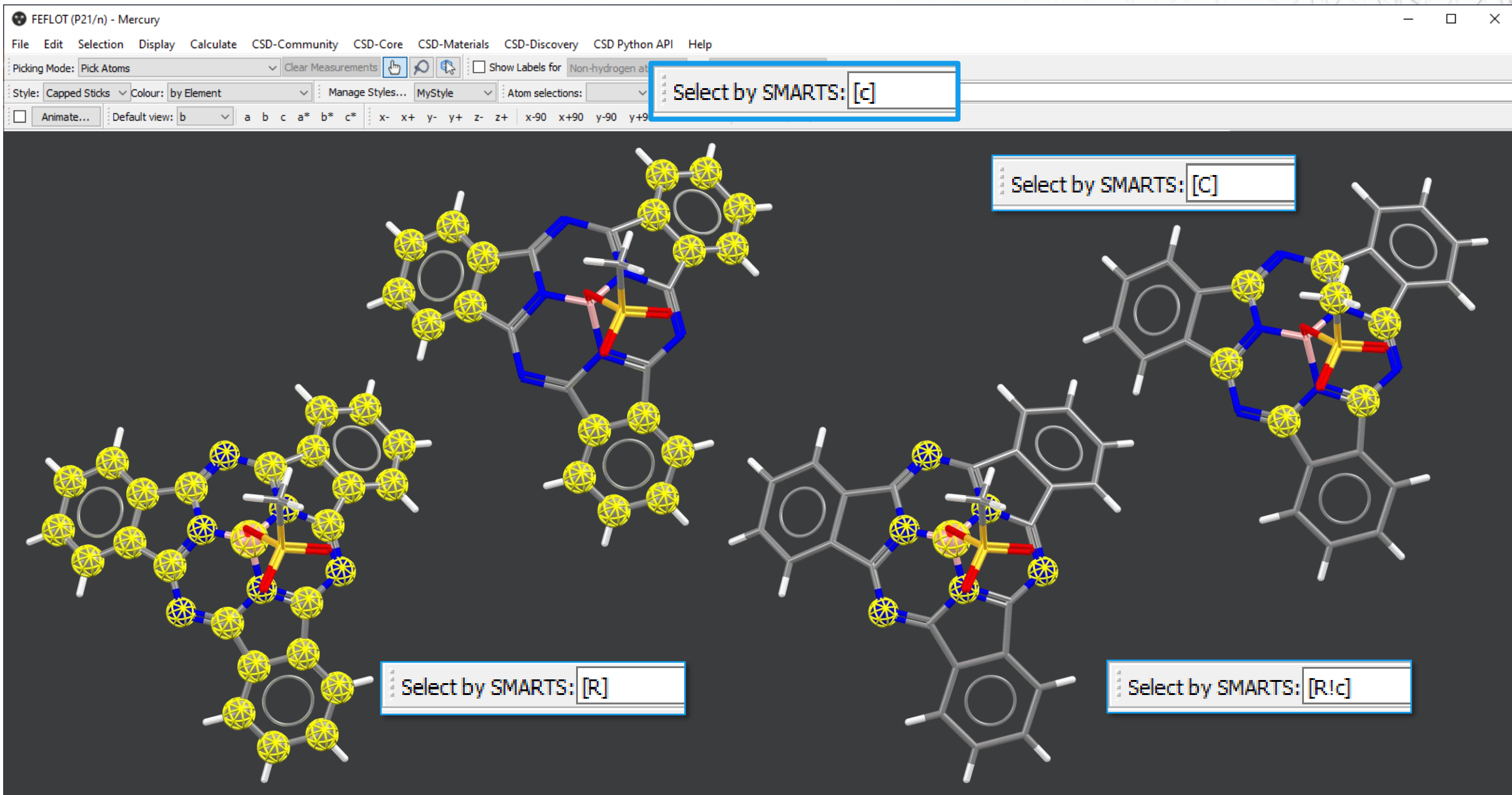
C

Select Tips

Selection

Select All	Ctrl+A	
Select Molecules...		
Select Atoms...		
Select		▶
Deselect All	Ctrl+D	
Deselect Molecules...		
Deselect Atoms...		
Deselect		▶
Invert Selection	Ctrl+I	
Expand Selection	Ctrl+E	
Save Current Selection...		
		Select Hydrogen
		Select Non-Hydrogen
		Select Carbons
		Select Non-H, C
		Select Metal Atoms
		Select Non-Metal Atoms
		Select Contact Atoms
		Select Stereocentres

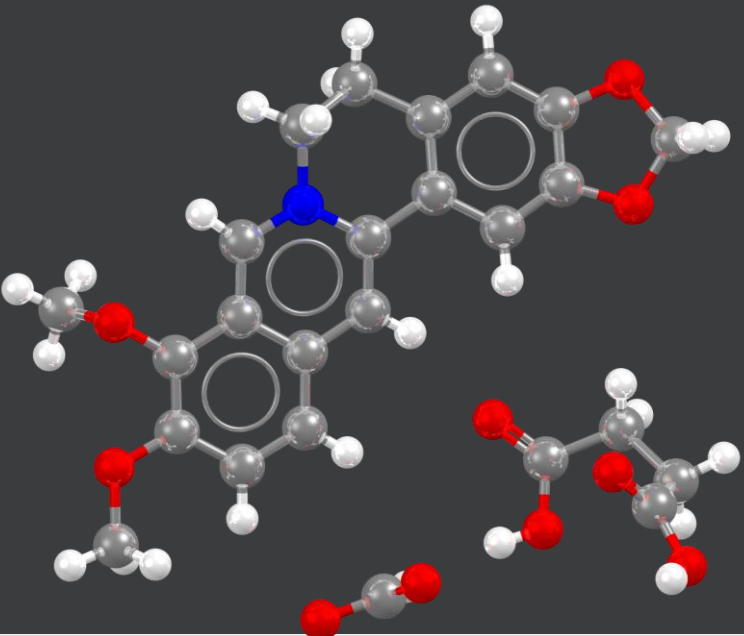




Missing information?

OLOFUQ (P-1) - Mercury

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



Display Options

Display

☐ Packing ☐ Short Contact < (sum of vdW radii + 0.1Å)

☐ Asymmetric Unit ☐ H-Bond User defined

☐ Auto centre

Reset

Contacts... More Info ▼ Powder...

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

2 Customise...

3 Add >>

4 OK

Customise

Available Items (Right-click for options)

- Batch
- Remarks
- Chemical
 - Bioactivity
 - Conformer
 - Isomer
 - Source
 - Peptide Sequence
 - Classifiers
- Crystal
 - Color
 - Habit
 - Analogues

Selected Items (Right-click for options)

- Identifier
- Literature Reference
- Formula
- Compound Name
- Synonym
- Space Group
- Cell Lengths
- Cell Angles
- Cell Volume
- Z, Z'
- R-Factor (%)

Up Down

OK Cancel

Structure

Diagram

Atoms

Bonds

Contacts

Centroids

Planes

Symmetry

Distances

Angles

Torsions

All Angles

All Torsions

Literature Reference

ct.C:Cryst.Struct.Comm. (2003), **59**, o583, doi:[10.1107/S010827010301789X](https://doi.org/10.1107/S010827010301789X)

Formula

$C_{20}H_{18}N O_4^+, C H O_2^-, C_4H_6O_4$

Compound Name

9,10-Dimethoxy-2,3-methylendioxy-5,6-dihydrodibenzo(a,g)quinolizinium formate succinic acid

Synonym

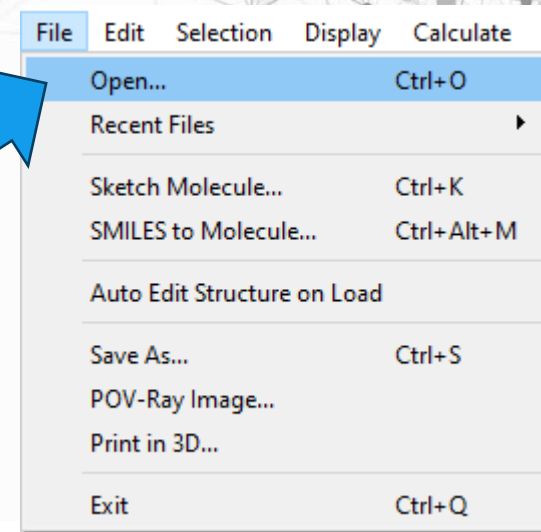
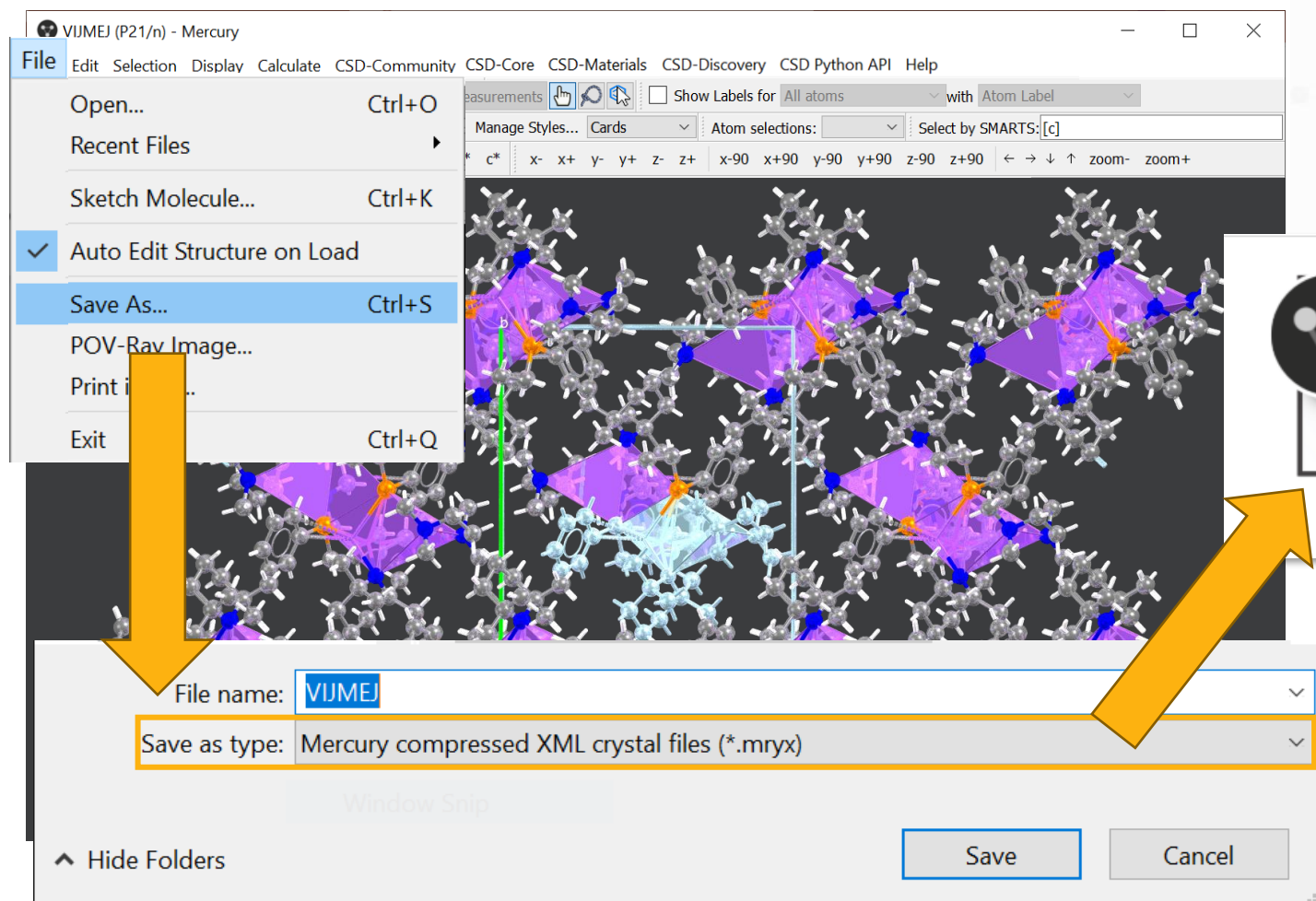
Berberine formate succinic acid; PDB Chemical Component code: BER

Bioactivity

berberine is an antimicrobial agent used for the treatment of eye infections, gastrointestinal disorders and other diseases

Close

Save your current display



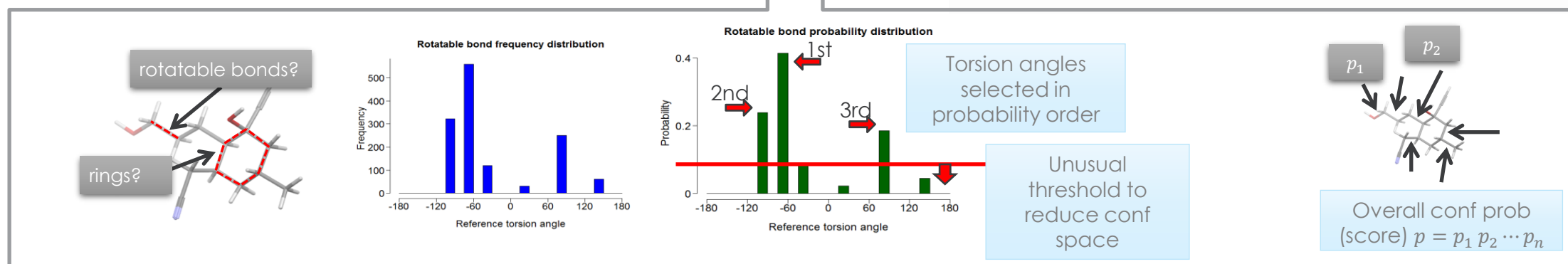
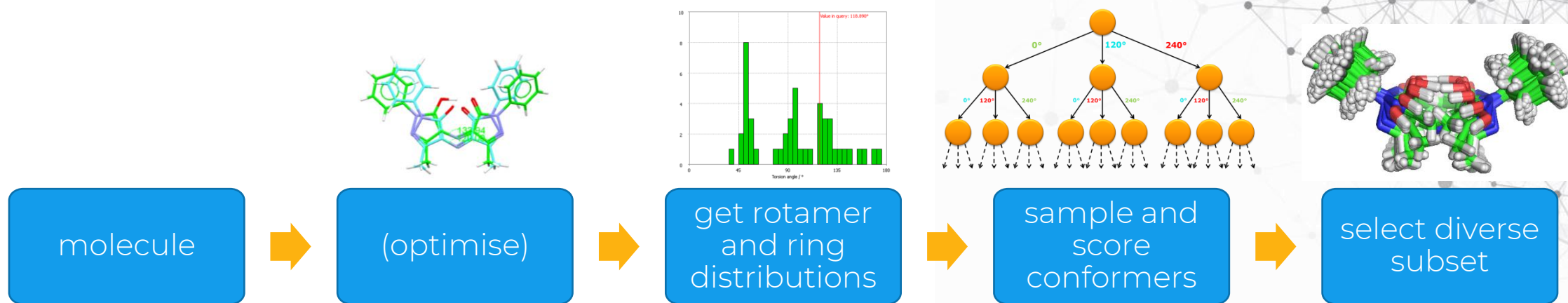
... and reopen it later!

CSD-Conformer Generator

Mogul can display distributions of important molecular geometries based on the bond lengths, angles, ring geometries, and torsions of the expertly curated structures in the CSD.

- Part of CSD-Discovery, CSD-Materials and CSD-Enterprise suites
- The starting point are [Mogul data libraries](#) with some changes and improvements to tailor them to conformer generation
- [2022.1](#) release of Conformer Generator version: [improved handling of flexible ring systems](#)
 - Using Mogul templates for isolated, fused, spiro-linked and bridged rings
 - If no template available, then generated on the fly with cyclic bond rotamer distributions
- [Fast](#) & [chemically plausible](#) conformations
- Initial optimisation step also useful to prepare compound libraries before virtual screening

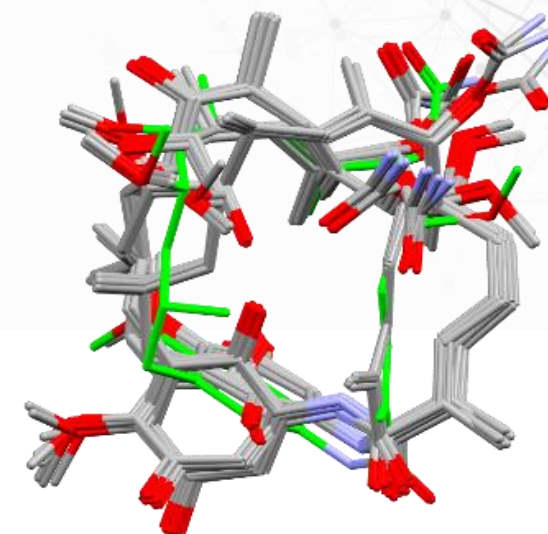
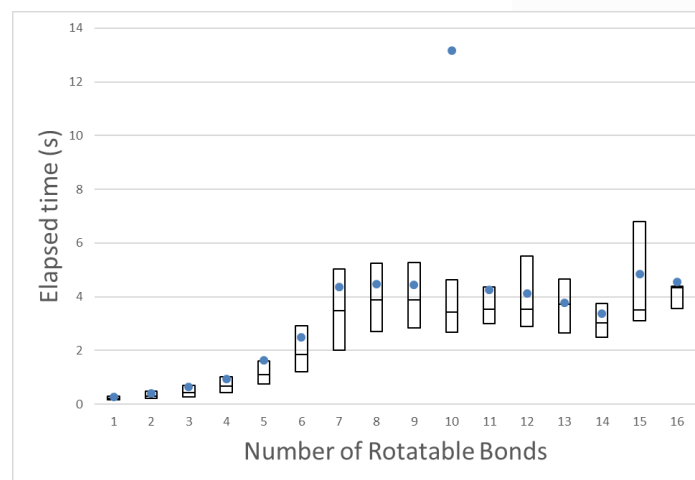
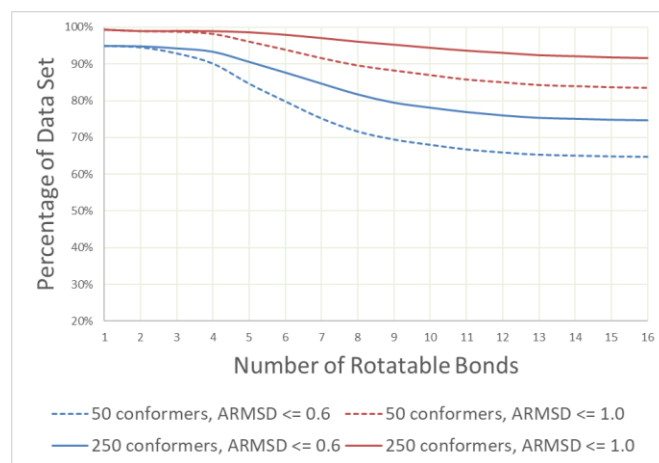
CSD-Conformer Generator: Methodology



CSD-Conformer Generator: Latest validation

- Performance evaluated against the Platinum* diverse data set → get fast & chemically plausible conformations

	Top n conformers			
	n	1	50	250
least ARMSD < 0.5 Å (%)	18	57	66	
least ARMSD < 1.0 Å (%)	39	84	92	
mean ARMSD			0.59	0.48



Geldanamycin, 19 atoms in ring (PDB 3C11): top 50 conformers, least ARMSED = 0.95 Å

No Coding? No problem!

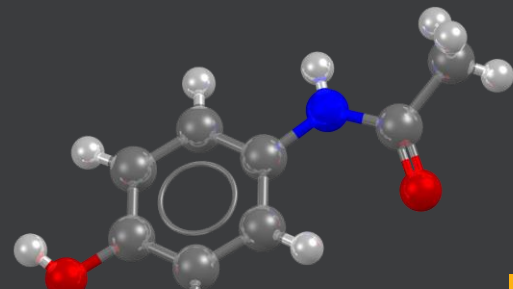
HXACAN (Pcab) - Mercury

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

Picking Mode: Lasso Atoms Clear Measurements

Style: Ball and Stick Colour: by Element Manage Styles...

Animate... Default view: b a b c a* b* c* x- x+ y- y+ z-



Analysis

Reports

Searches

user_support.py

welcome.py

calculate_CSD_diversity_score.py

Options...

CSD Python API Documentation

CSD Python API Forum

Display Options

Display

☒ Packing ☐ Short Contact < (sum of vdW radii)

☐ Asymmetric Unit ☐ H-Bond Default definition

☐ Auto centre

Reset

Contacts...

More Info

Powder...

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

Learn more in
our CSD
Python API
xxxxx!

Molecular Geometry Report for HXACAN

Molecular Analysis

CCDC
advancing structural science

crystal_structure_report.py

molecular_geometry_report.py

quick_geometry_check.py

quick_packing_check.py

simple_report.py

H-bond Acceptors

Rotatable Bonds

Fraction N/O Atoms

Fraction Halogen Atoms

Bond Lengths

Atom 1	Atom 2
C2	C1
C3	C2
C3	O4
C5	O4
O6	C5
C6	C1
C6	C7
C1	N1
O1	O4
O2	C7
C7	N1

Bond Valence Angles

Atom 1	Atom 2	Atom 3
O6	C1	C2
C2	C1	N1
O6	C1	N1
C3	C2	C1
C2	C3	O4
C5	O4	C3
O1	O4	C5
O1	O4	C5
O6	C5	O4
C5	O6	C1
O2	C7	O6
C8	C7	N1
O2	C7	N1
C1	N1	C7

Crystal Structure Report for HXACAN

Crystal Structure Analysis

CCDC
advancing structural science

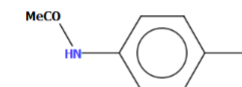


Figure 1. Diagram for HXACAN

Table 1. Selected Crystal Structure Information

Identifier	HXACAN
Formula	C8 H9 N1 O2
Space Group	Pcab
Cell Lengths (Å)	a 11.8050 b 17.1640 c 7.3930
Cell Angles (°)	α 90.00 β 90.00 γ 90.00
Cell Volume (Å ³)	1497.98
R-Factor	7.70

Volume and Packing Analysis

Table 2. Crystal Packing Information

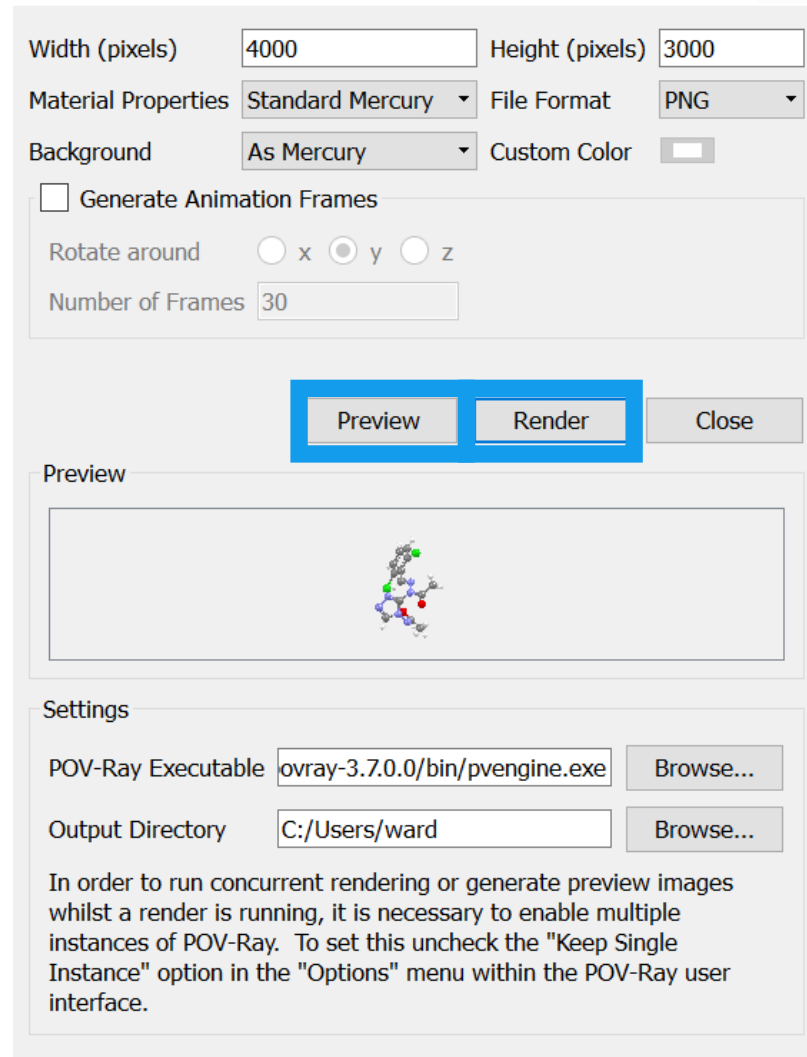
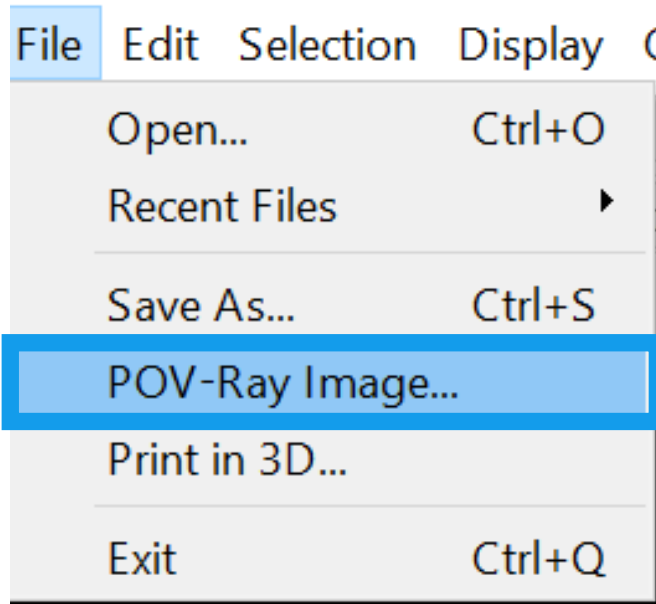
Estimated volume from 18 Å ³ rule	1584.0
Experimental volume	1497.977
Packing coefficient	0.69
CSD average packing coefficient for organic molecules	0.68(4)
Calculated void percentage	0.0
Calculated void volume	0.0

Fractional Atom Coordinates

Table 3. Atomic Coordinates

Atom	x	y	z
C1	0.446	0.339	0.291
C2	0.339	0.337	0.212
C3	0.279	0.268	0.207
C4	0.324	0.201	0.281

Generating high quality images



File > POV-Ray Image

Change Resolution

Width = 4000

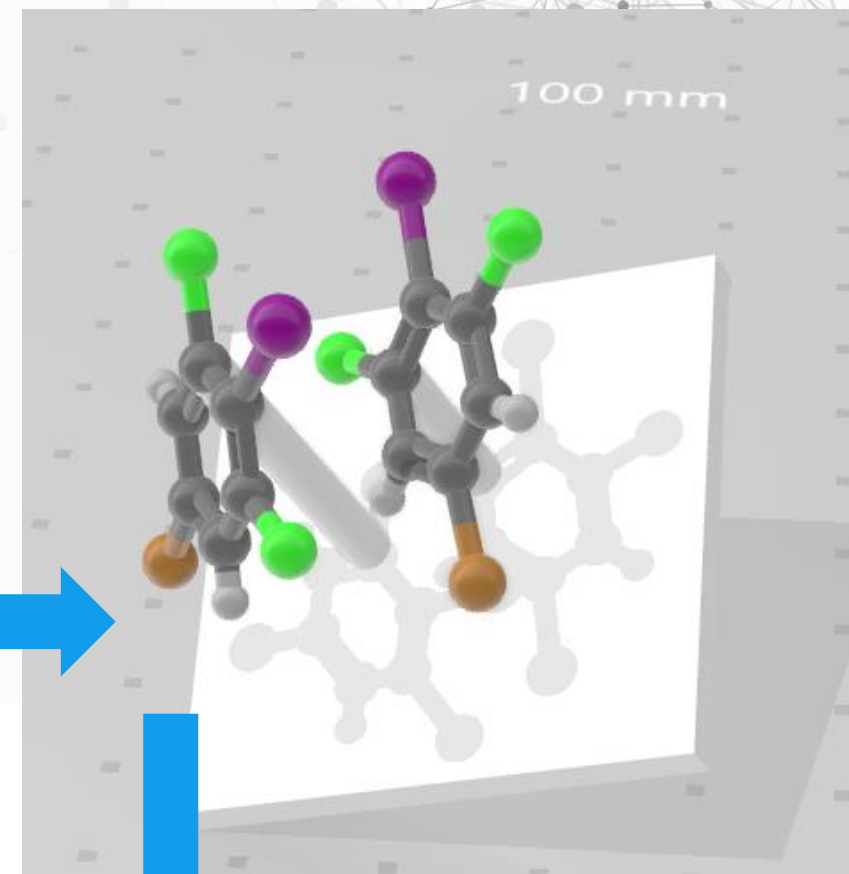
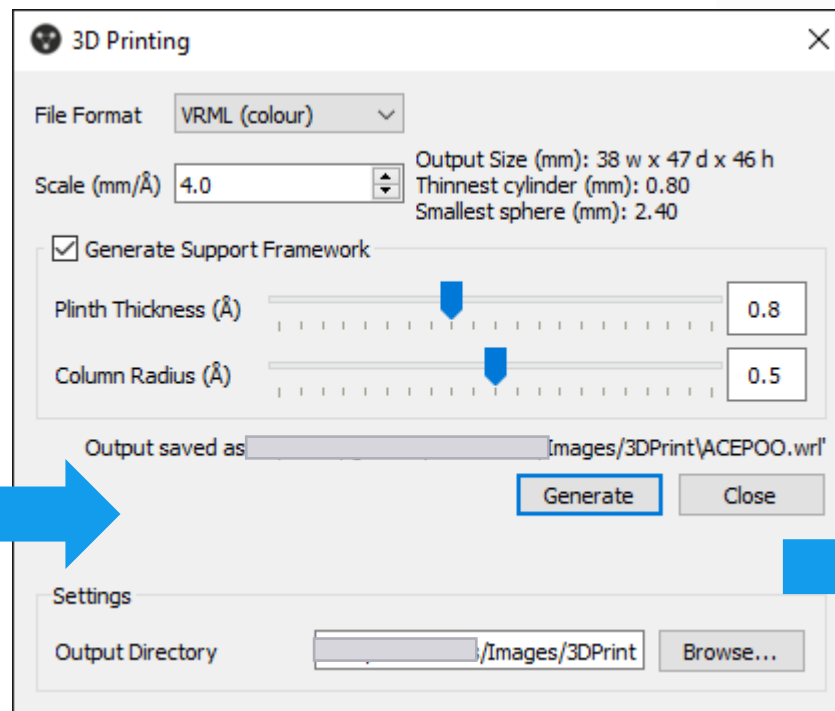
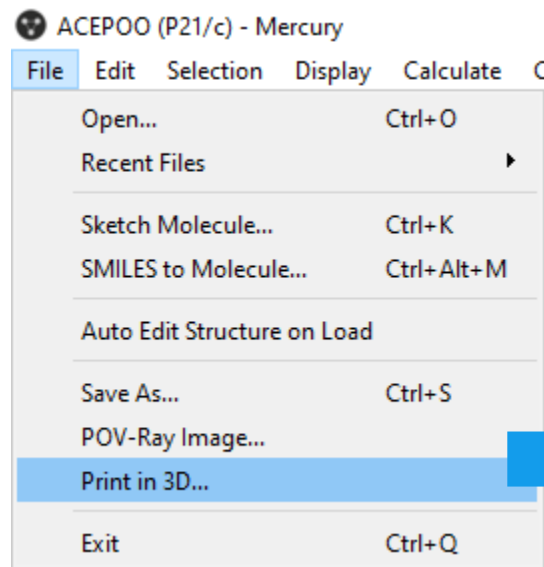
Height = 3000

Change 'Material Properties' to 'Metallic'

Set 'Background' to 'Transparent'

Press 'Preview'

3D printing



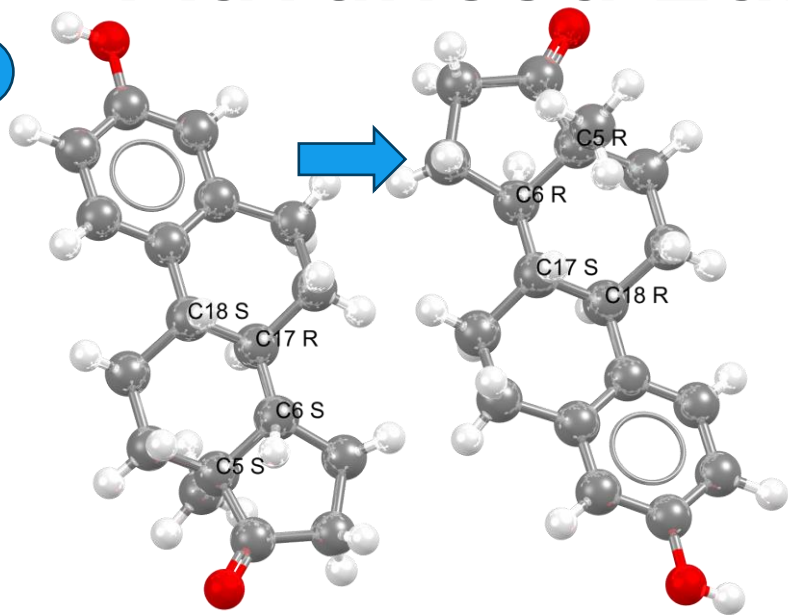
Print with your 3D printer
or at a 3D printing service!



Example of 3D printed structure of
CSD Refcode SAHYIK

Advanced Edit Features

3



4

Change Spacegroup to Subgroup

Entry:

Current Spacegroup: $P 2_1 2_1 2_1$ (19) setting 1

Available Subgroups:

- $P 1 1 2 1$ (4) setting 2 $[1/4, 0, 0]$
- $P 1 1 2 1$ (4) setting 2 $[1/4, 0, 0]$
- $P 2 1$ (4) setting 1 $[0, 0, 1/4]$
- $P 2 1 1 1$ (4) setting 3 $[0, 1/4, 0]$

OK Close Apply

Edit Selection Display Calculate CSD-Comm

Undo: Not Available Ctrl+Z
 Redo: Not Available Ctrl+Y
 Copy Image to Clipboard Ctrl+C
 Edit Structure...
 Auto Edit Structure...
 Edit Bond Distance Limits...
 Normalise Hydrogens...
 Polymer Expansion...

- 1 Transform Molecules...
- 2 Change Spacegroup Setting...
- 3 Invert Structure
- 4 Change Spacegroup to Subgroup...

1

Transform Molecules

Active Structure:

Symmetry Operators: Choose an operator below and click Transform to move all molecule(s), or click Copy to create a transformed copy of all molecule(s). Or select an atom in one or more molecules to apply the transformation to those particular molecules.

Crystal Symmetry Operators:
 $1/2-x, -y, 1/2+z$
 $-x, 1/2+y, 1/2-z$
 $1/2+x, 1/2-y, -z$

Unit Cell Translations: a b c

☒ Reset unit cell translations to zero automatically after copying or transforming

Transform Copy Close

2

Change Spacegroup Setting

Entry:

Space group Setting:

- 1: Hexagonal Axes (R-3)
- 1: Hexagonal Axes (R-3)
- 2: Rhombohedral Axes (R-3)

Standardise OK Cancel

Want to explore more?

On-demand training resources

Solutions **Community** Discover Consultancy

Access/Deposit Structures

CCDC for the Community

Education and Outreach

Events

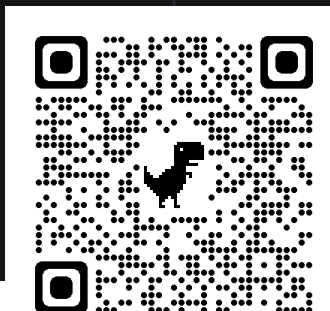
Free Products

Training and Learning

Free Online Courses

Self-Guided Workshops

Training and Support Videos



Surface Analysis with CSD-Particle

Start the CSDU module!

CSD-Particle

Tools to help you understand particle behaviour and anticipate manufacturing bottlenecks to guide formulation decisions.

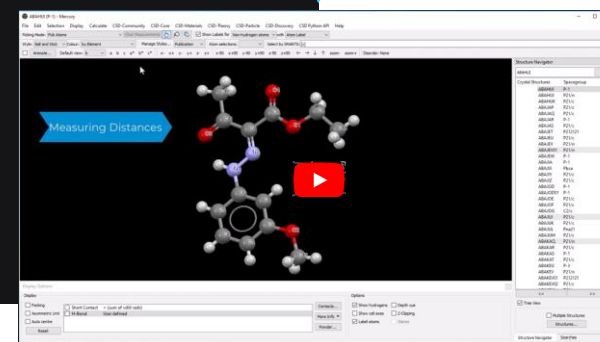
CSD-Particle Workshops

Investigation of Plastic and Elastic Properties with CSD-Particle Tools in Mercury (PAR-002)

Developed using 2023.3 CSD Mercury

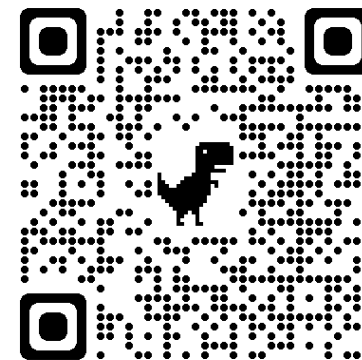
Table of Contents	2
Introduction	2
Learning Outcomes	2
Prerequisites	2
Materials	2
Example 1: Slip plane analysis to investigate elastic properties	3
Calculation of potential slip planes	3
Hydrogen bonds analysis	5
Exporting more potential slip planes	7
Conclusion	8
Example 2: Slip plane analysis to investigate plastic properties of polymorphs	9
Calculation of potential slip planes	9
Hydrogen bonds analysis	12
Conclusion	13
Summary	14
Next steps	14
Feedback	14
Feedback suggestions	14
Glossary	15

CCDC



CCDC

Free online training courses



With completion certificates!



CSDU

On-demand modules to learn how to use the CSD software at your own pace.



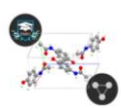
UWatch



UTry



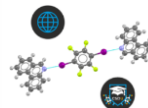
UTest



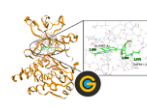
Mercury



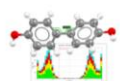
Python
API



WebCSD



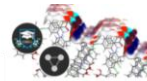
GOLD
Docking



Mogul

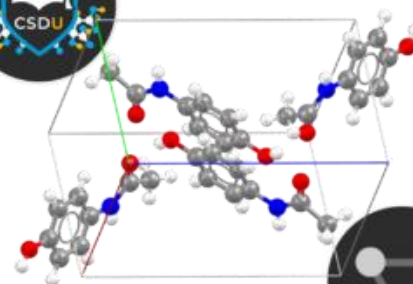


FIMs



Particle

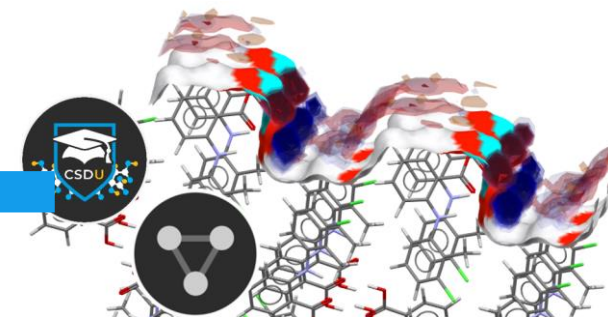
Visualization 101



Helping you to learn:

- The basics of **Mercury** software.
- How to **explore and pack** structures.
- How to create **high resolution images**.

Surface analysis



Helping you to learn:

- The basics of **CSD-Particle**.
- How to perform a **surface analysis**.
- How to visualise **likely interactions** with the **surface** using **Full Interaction Maps** (also a CSDU course!).

<https://www.ccdc.cam.ac.uk/community/training-and-learning/csdu-modules/>

Upcoming Virtual Workshops & Events

CCDC VIRTUAL WORKSHOP

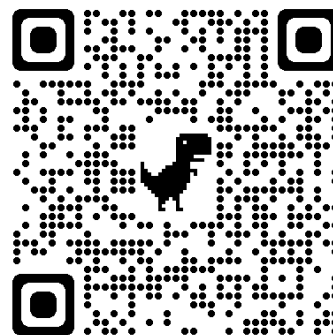
In-Depth
Comparison of
Polymorphic
Structures Using
Mercury




Tuesday, 14th May
10 am (BST)



REGISTER NOW




And more!!



CCDC Innovation in Discovery Science UGM 2024

Virtual
Thursday 9th May
9:30am-3:30pm BST



REGISTER TODAY

CCDC **discovery science** software users and non-users will collectively discuss the latest trends and advancements in the industry, including the rise of **AI and machine learning**.

Use cases will be presented and common challenges discussed.

<https://www.ccdc.cam.ac.uk/community/events/>

CCDC