Visualisation and analysis in Mercury – Intermediate level

CCDC Virtual Workshop Spring 2021 – Session 1

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April 2021

CCDC
advancing structural science

Learning outcomes for today

- Learn how to use advanced Mercury features to analyse structures
- Familiarise yourself with functionalities from the Calculate menu
  - Enabling you to explore structures in more depth
  - Including contacts, planes and centroids
- Familiarise yourself with functionalities from the Display menu
  - including displaying the symmetry elements and voids within a structure

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Inside the Cambridge Structural Database

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

Organic
43%

Metal-Organic
57%

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

Not Polymeric
89%

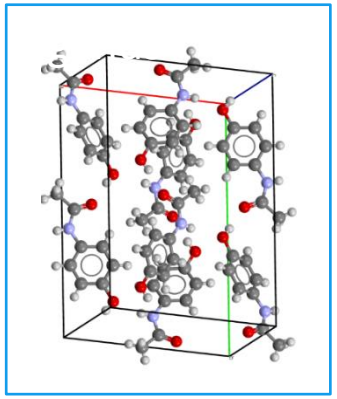
Polymeric: 11%

Single Component
56%

Multi Component
44%

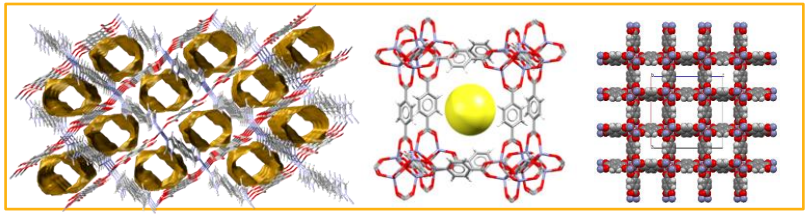
Organic

- Drugs
- Agrochemicals
- Pigments
- Explosives
- Protein ligands



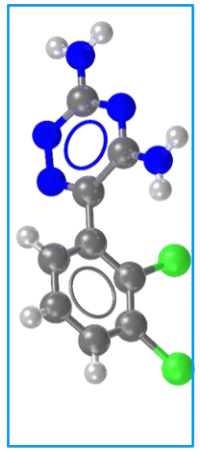
Metal-Organic

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



Additional data

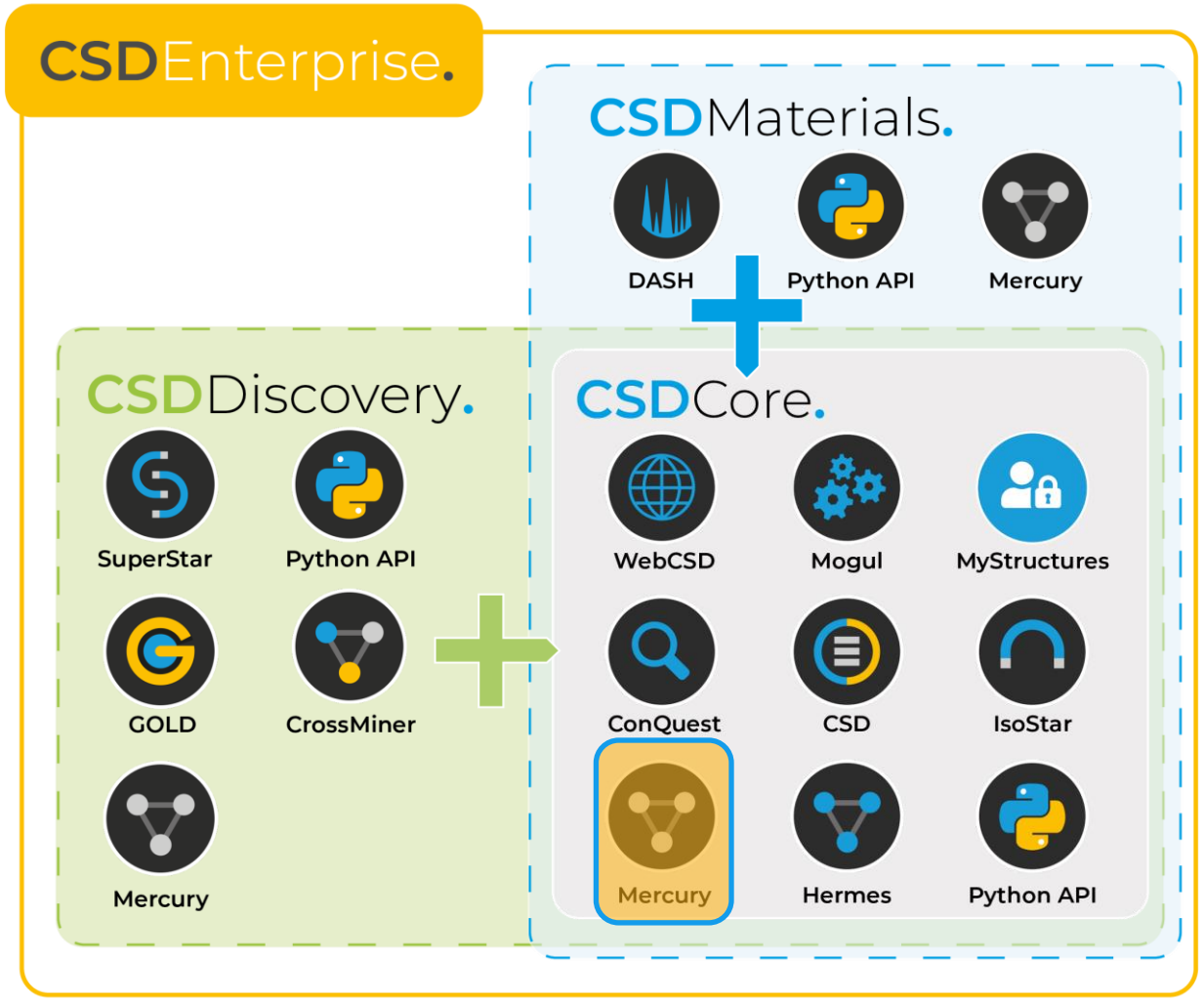
- 11,525 polymorph families
- 171,683 melting points
- 909,992 crystal colours
- 778,663 crystal shapes
- 24,916 bioactivity details
- 11,387 natural source data
- > 250,000 oxidation states



Links and subsets

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

The CSD Portfolio



Professional Services

Research & Knowledge partnerships

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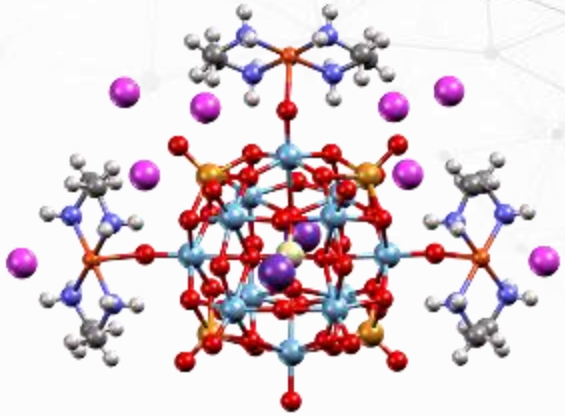
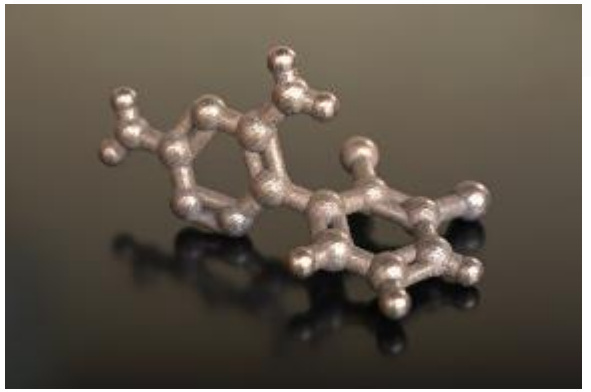
Mercury – Structure visualisation

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





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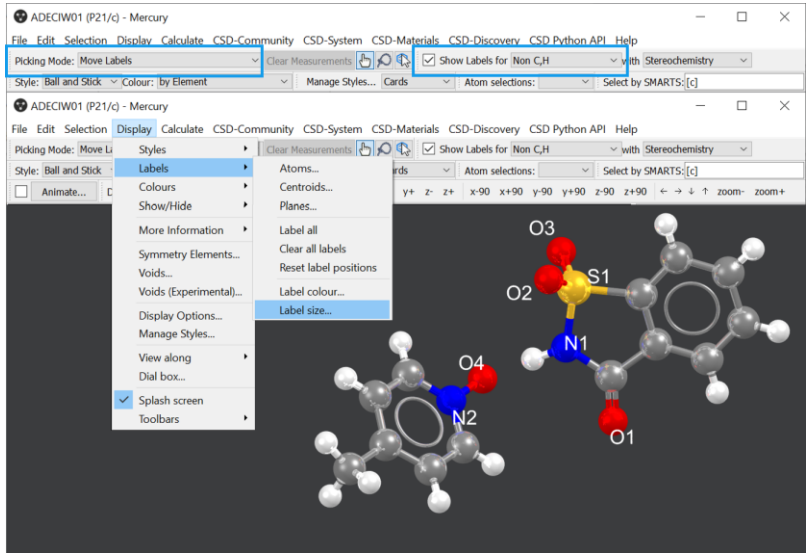
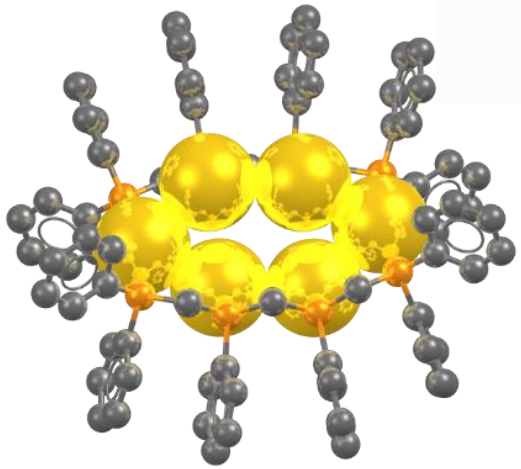
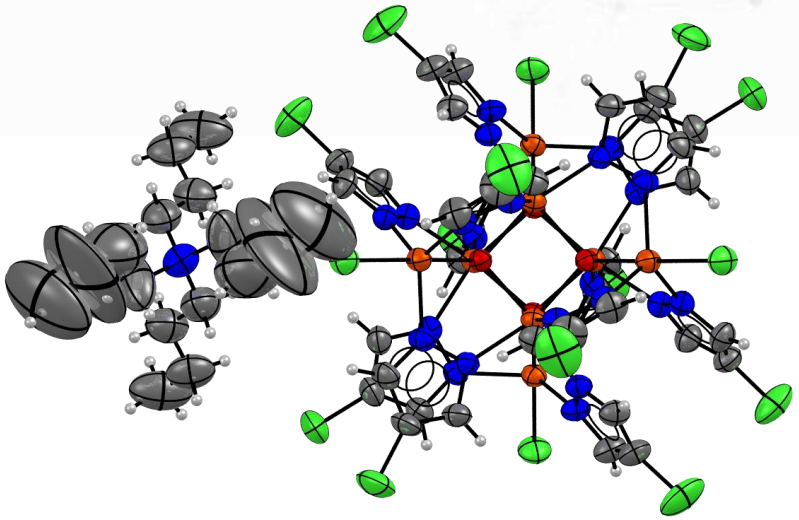
Structure visualisation – Beginners session

What have we already learnt?

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







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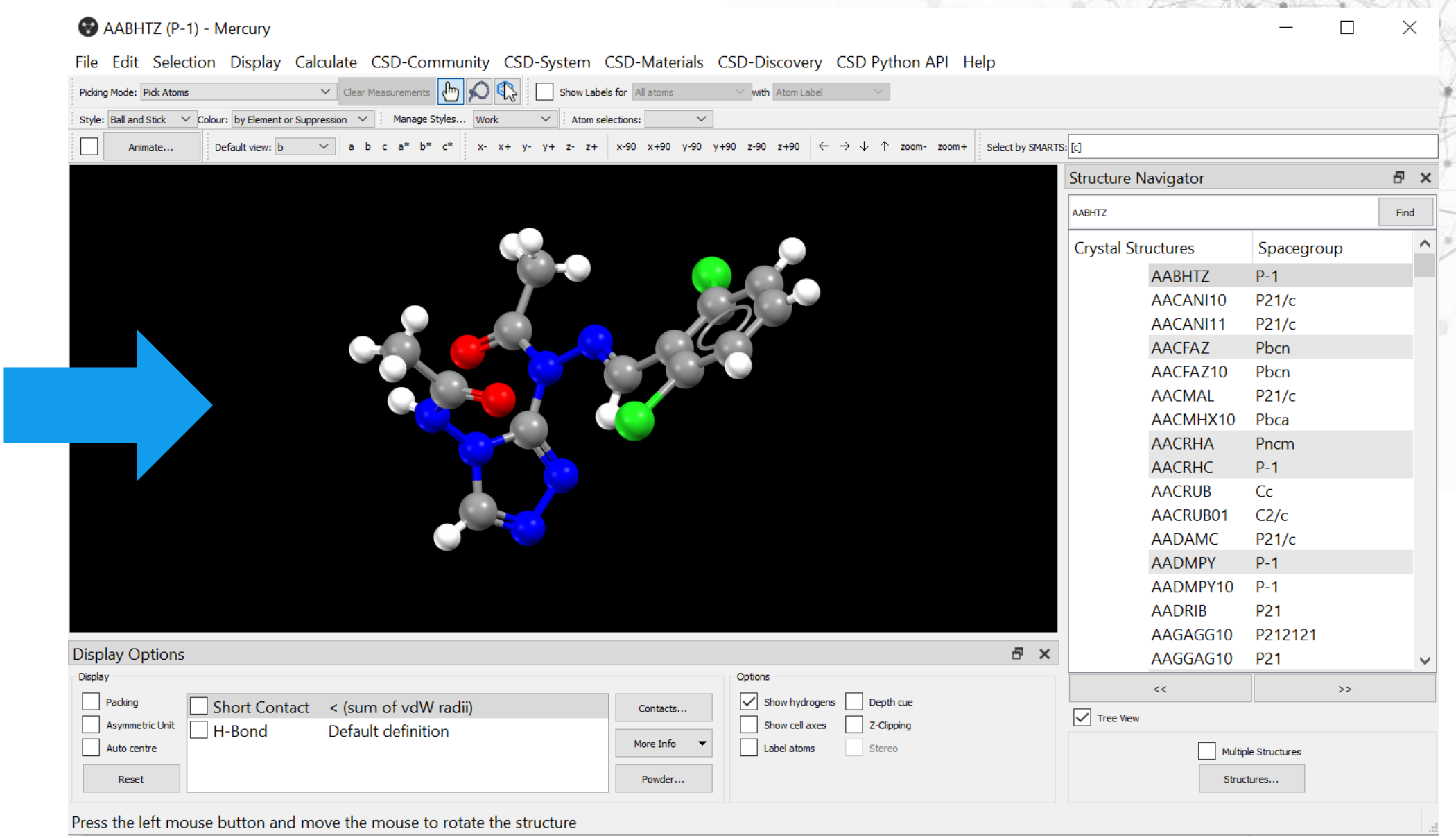
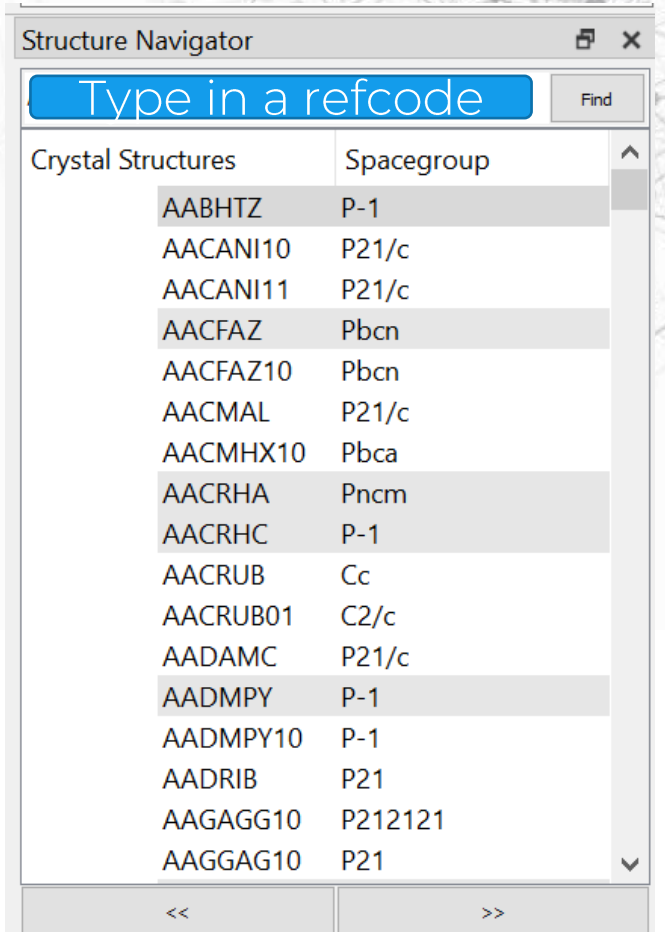
Show One: Mercury Demo



A reminder: The basics

- Left mouse button and move – allows you to rotate structure
- Middle Mouse button and move – allows you to move structure
- Right mouse button and move – allows you to zoom in and out of structure
- Structure Navigator – Allows you to view any structure in the CSD



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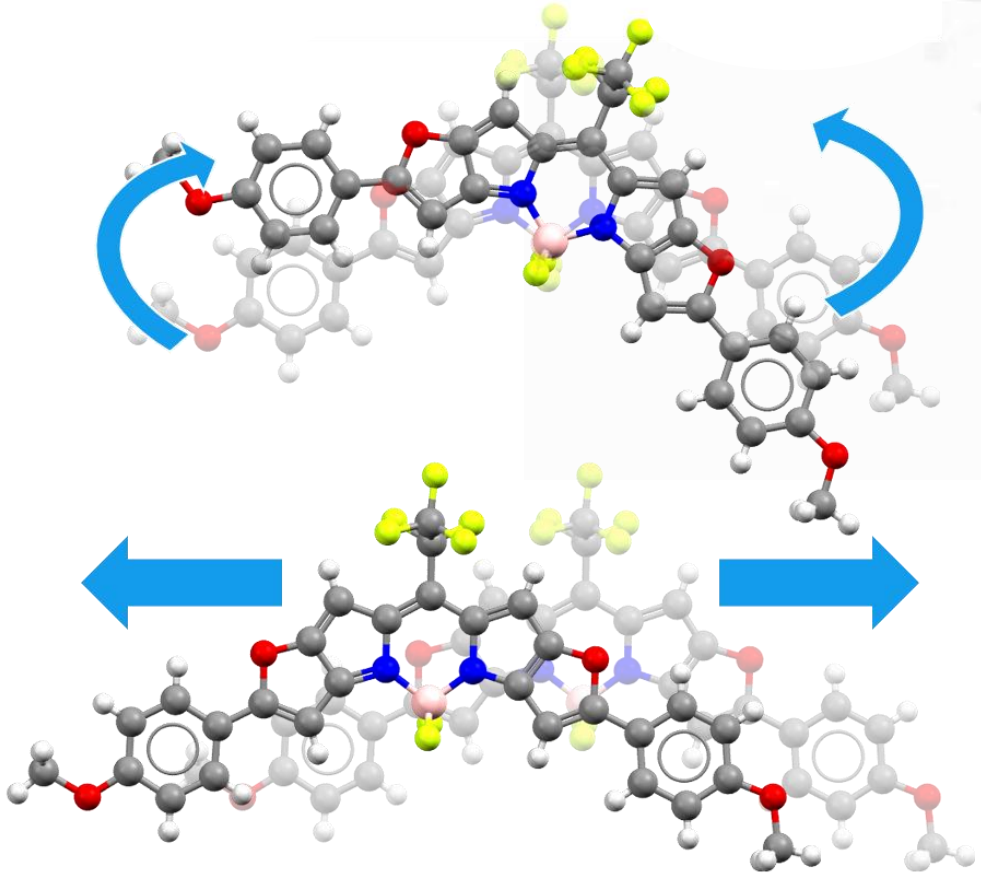
A reminder: The basics

With the keyboard:



CSD Refcode: GIMXUY

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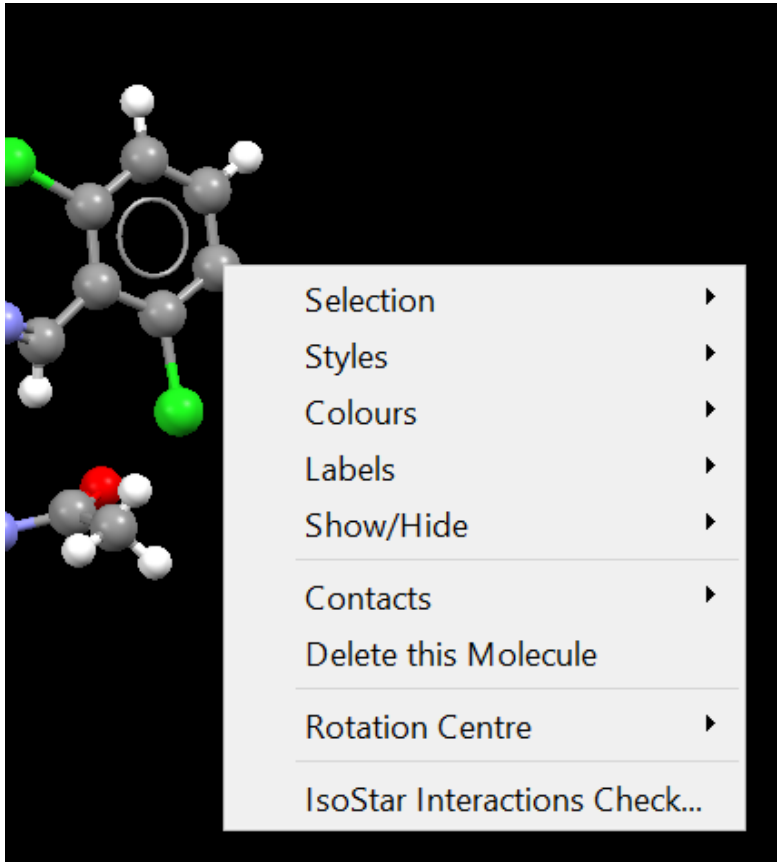
A reminder: Right mouse click

Near a molecule



Away from a molecule

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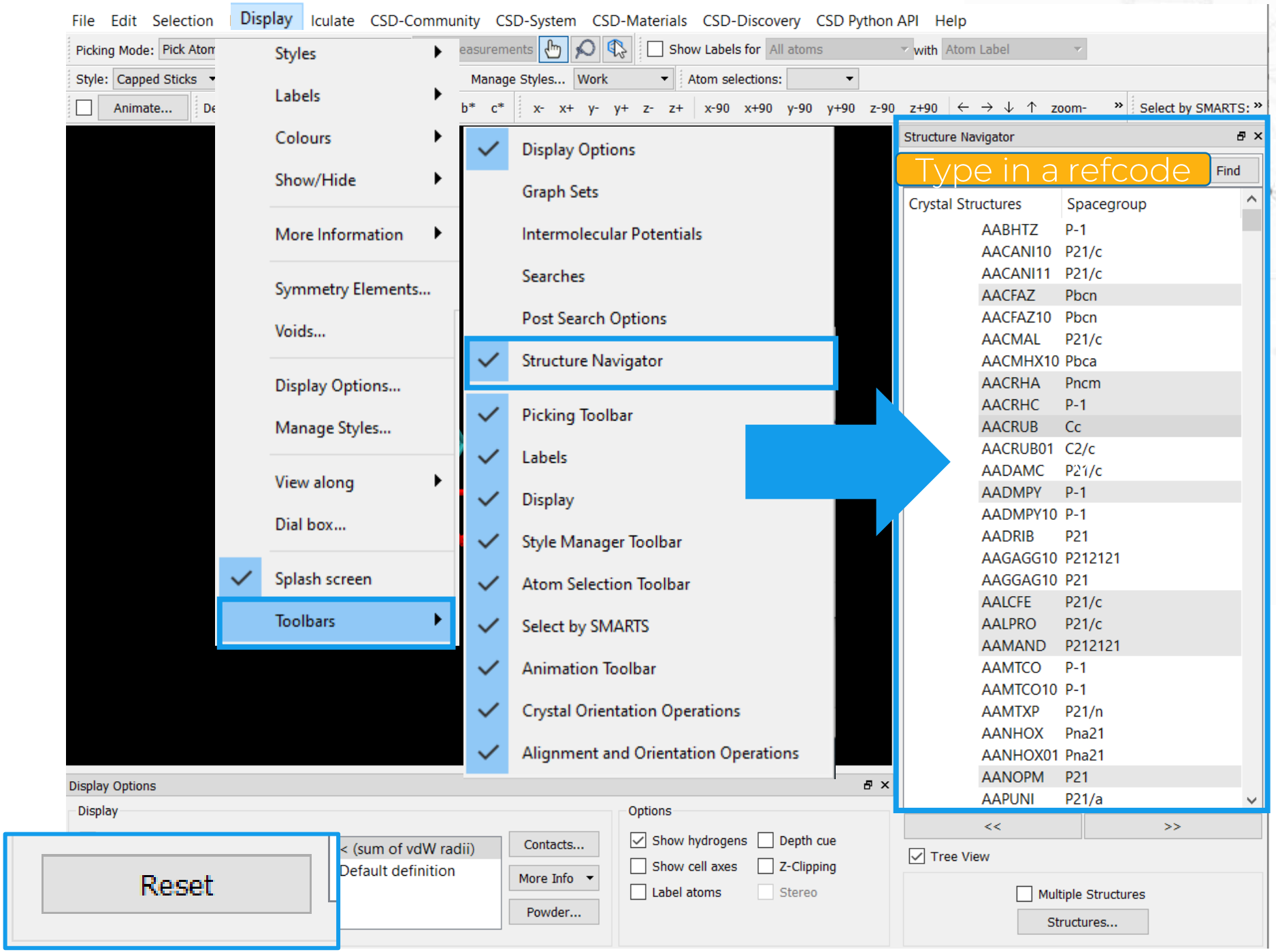

A reminder:

- Recovering Toolbars
- Resetting view

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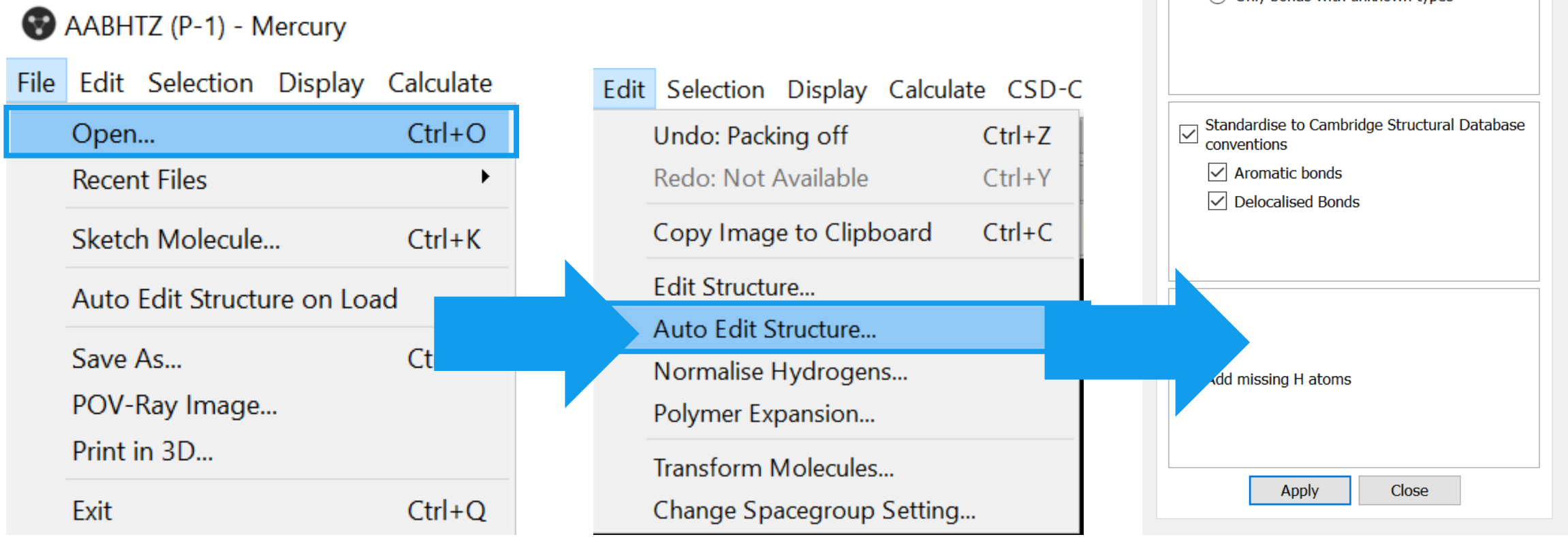
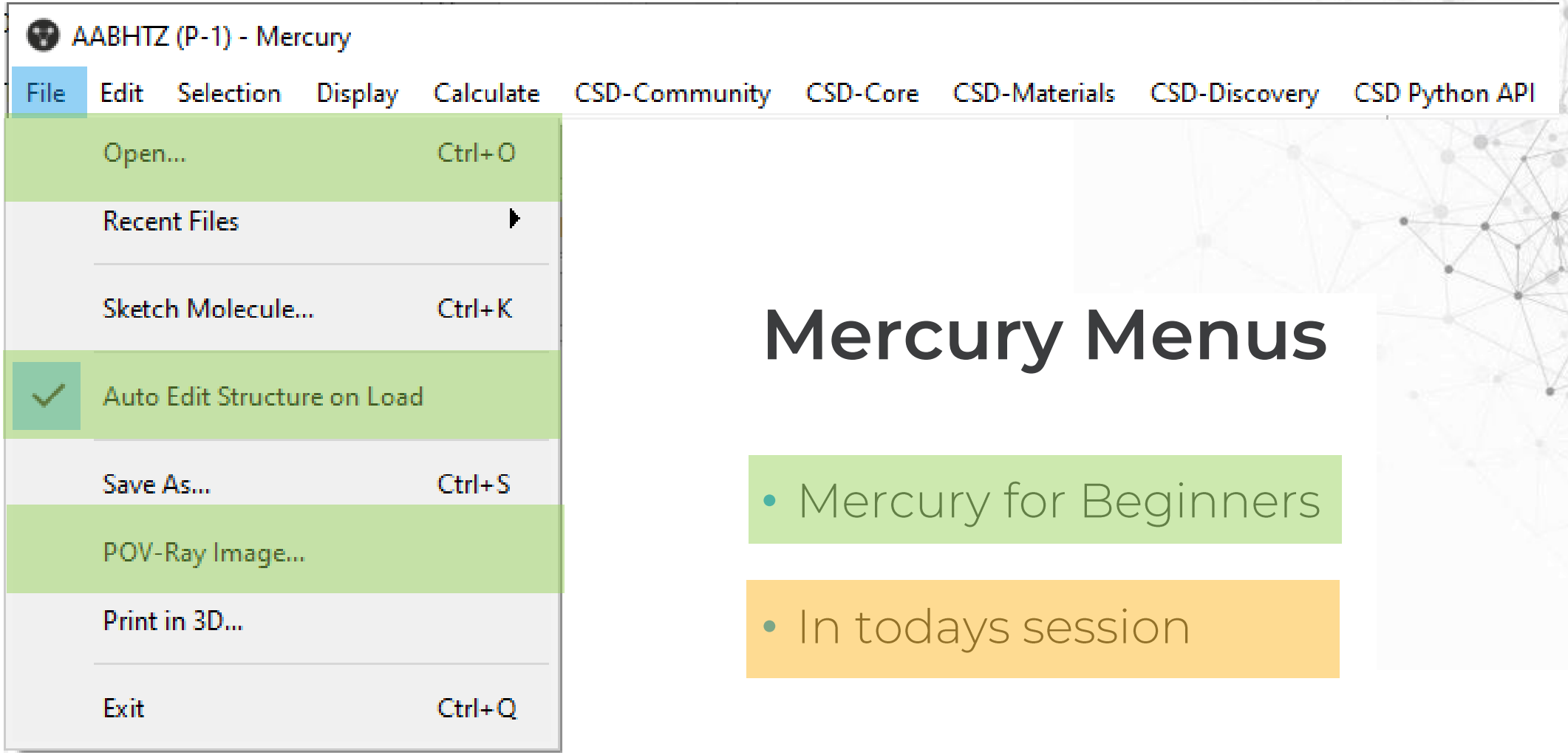
A reminder: Using your own file

- 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





Mercury Menus

- Mercury for Beginners
- In todays session

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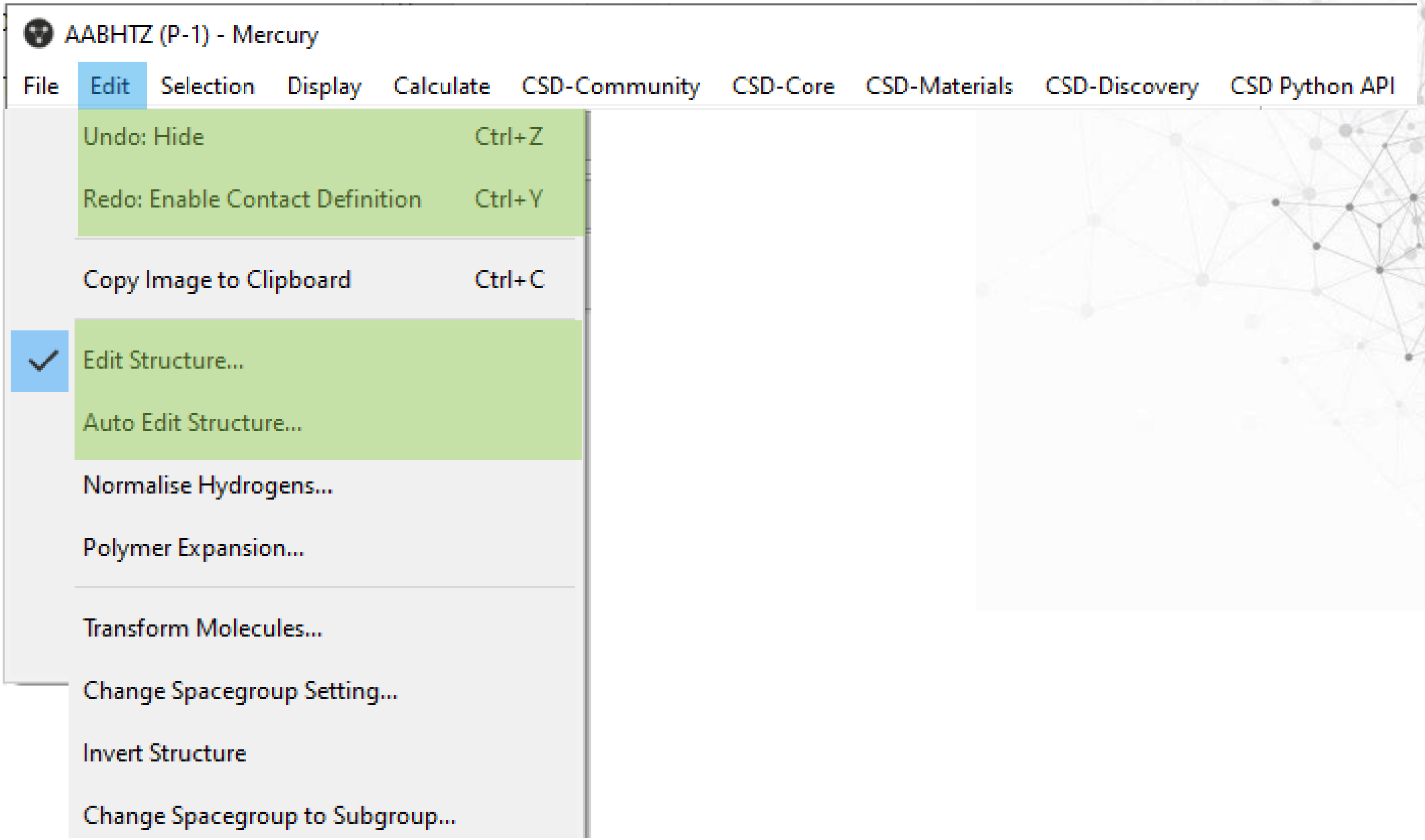
AABHTZ (P-1) - Mercury
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CSD-Discovery
CSD Python API
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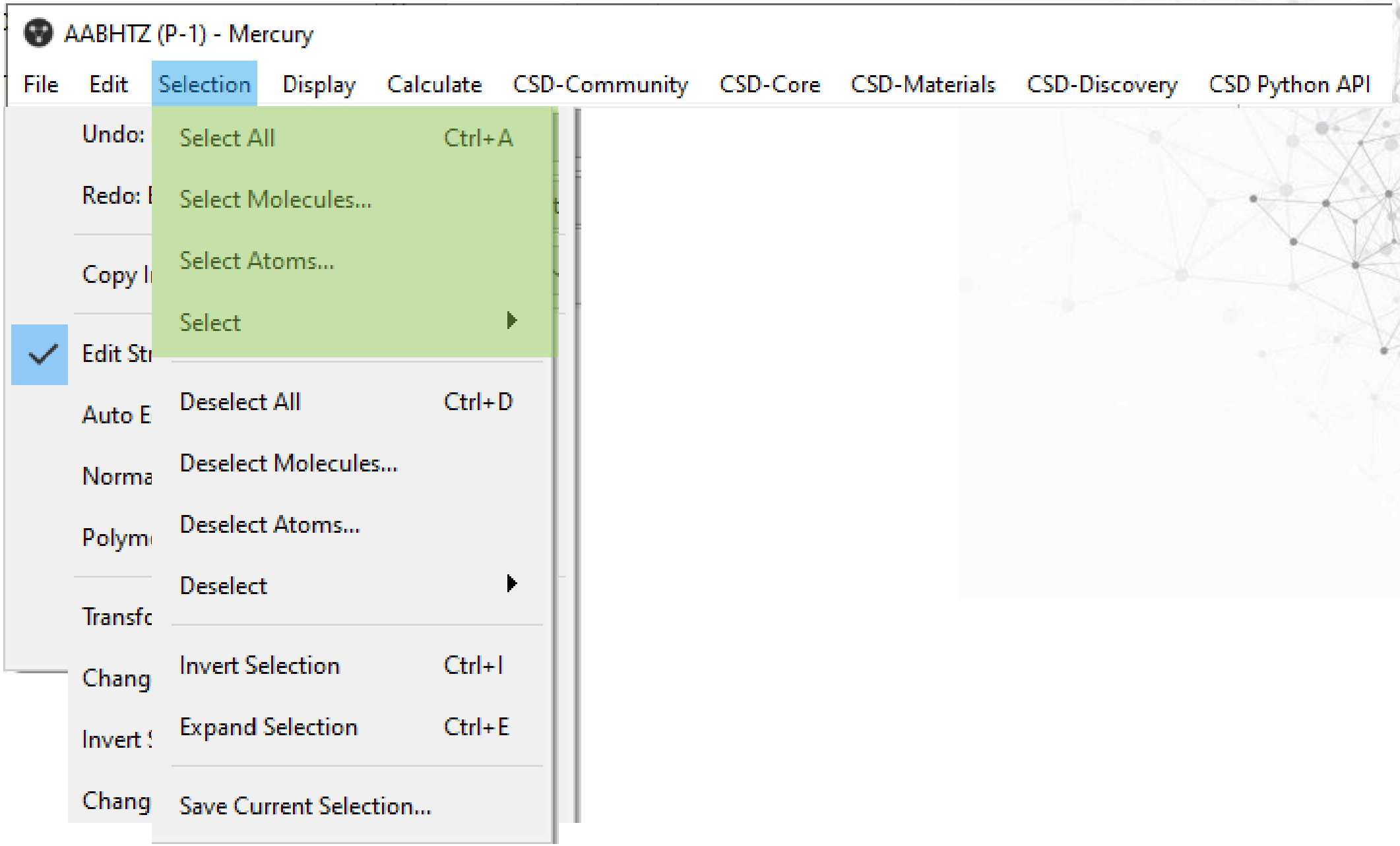
Auto Edit Structure...
Normalise Hydrogens...
Polymer Expansion...
Transform Molecules...
Change Spacegroup Setting...
Invert Structure
Change Spacegroup to Subgroup...

CCDC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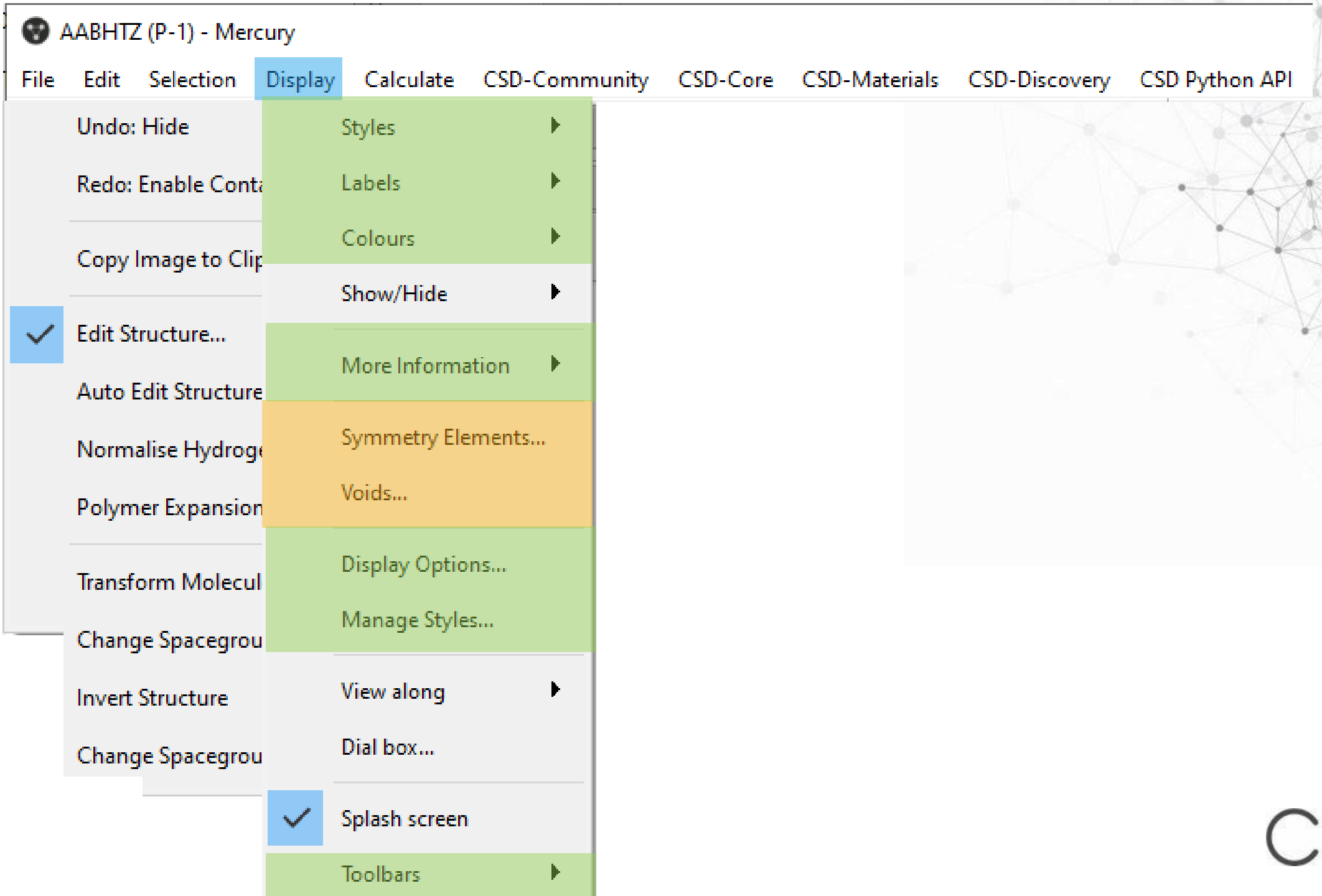
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Splash screen
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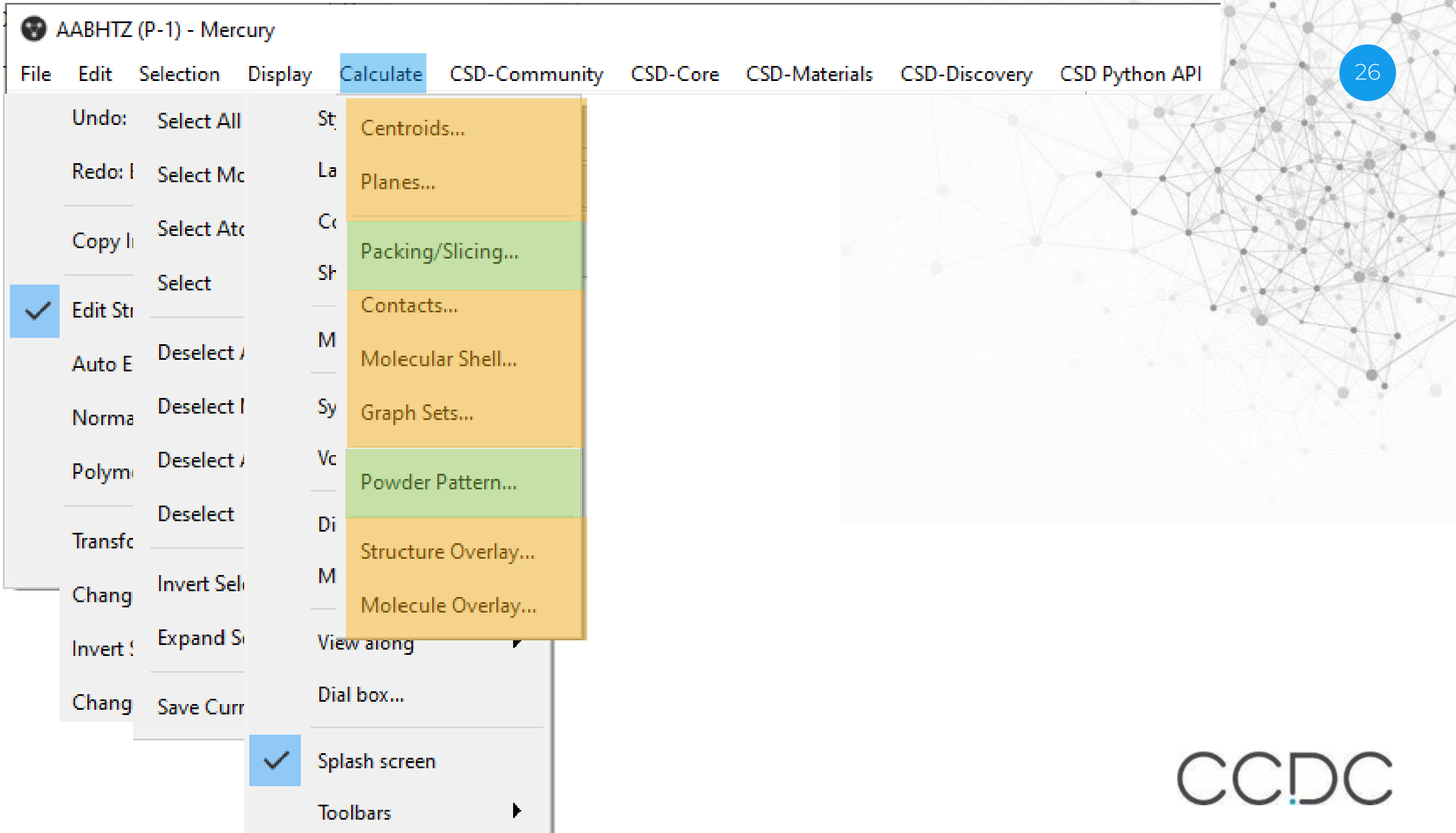
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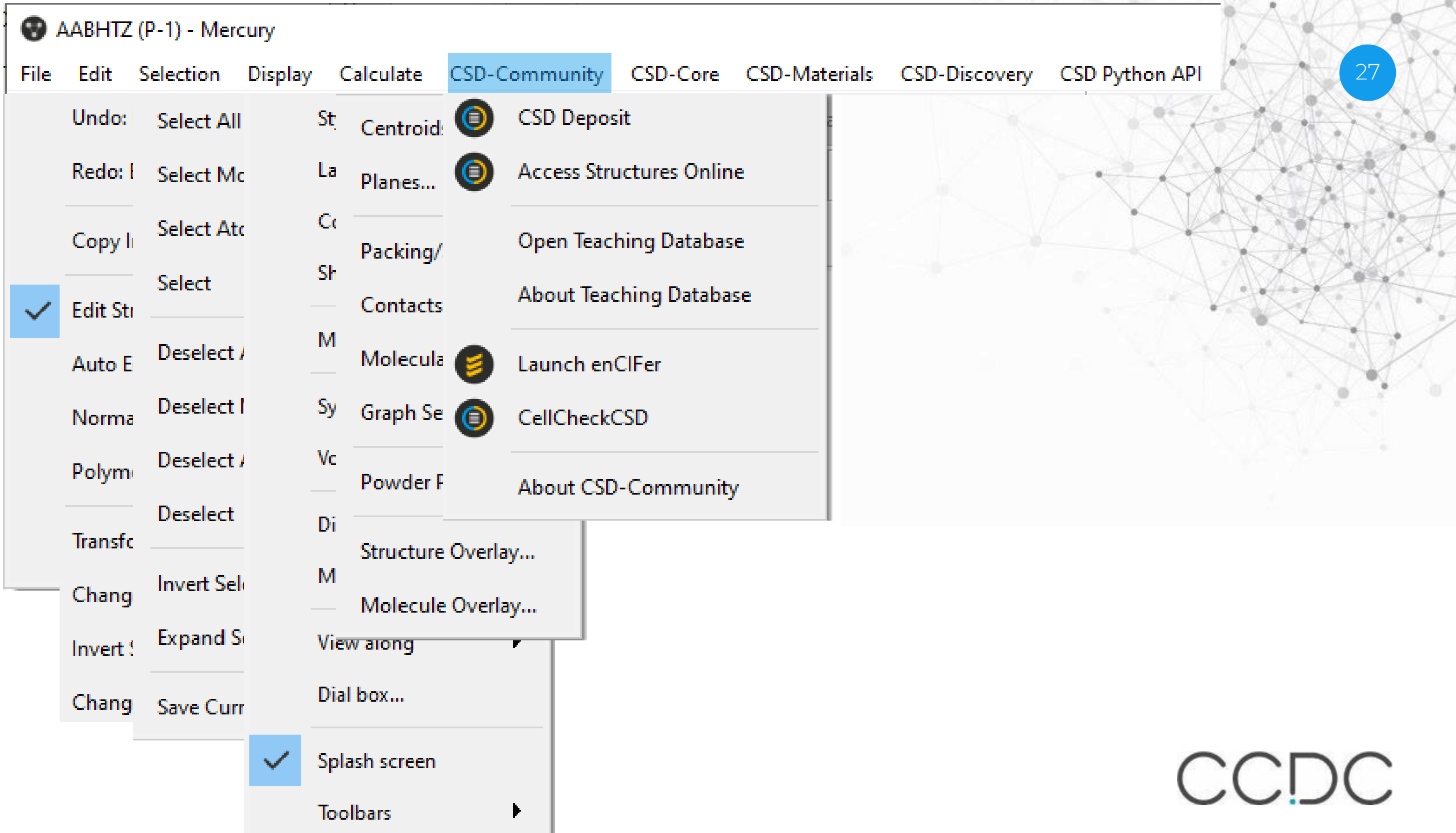
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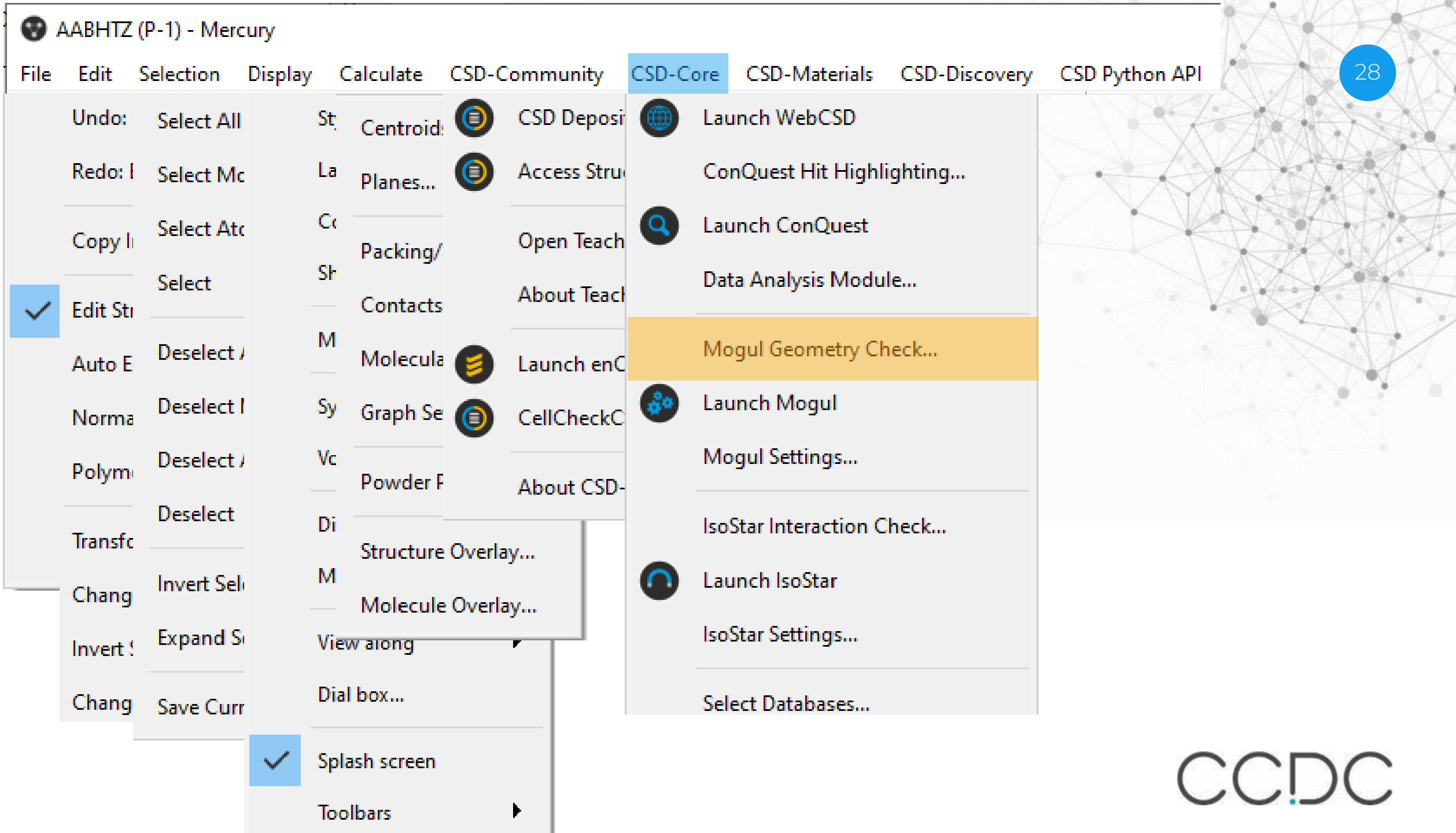
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Molecule Overlay...
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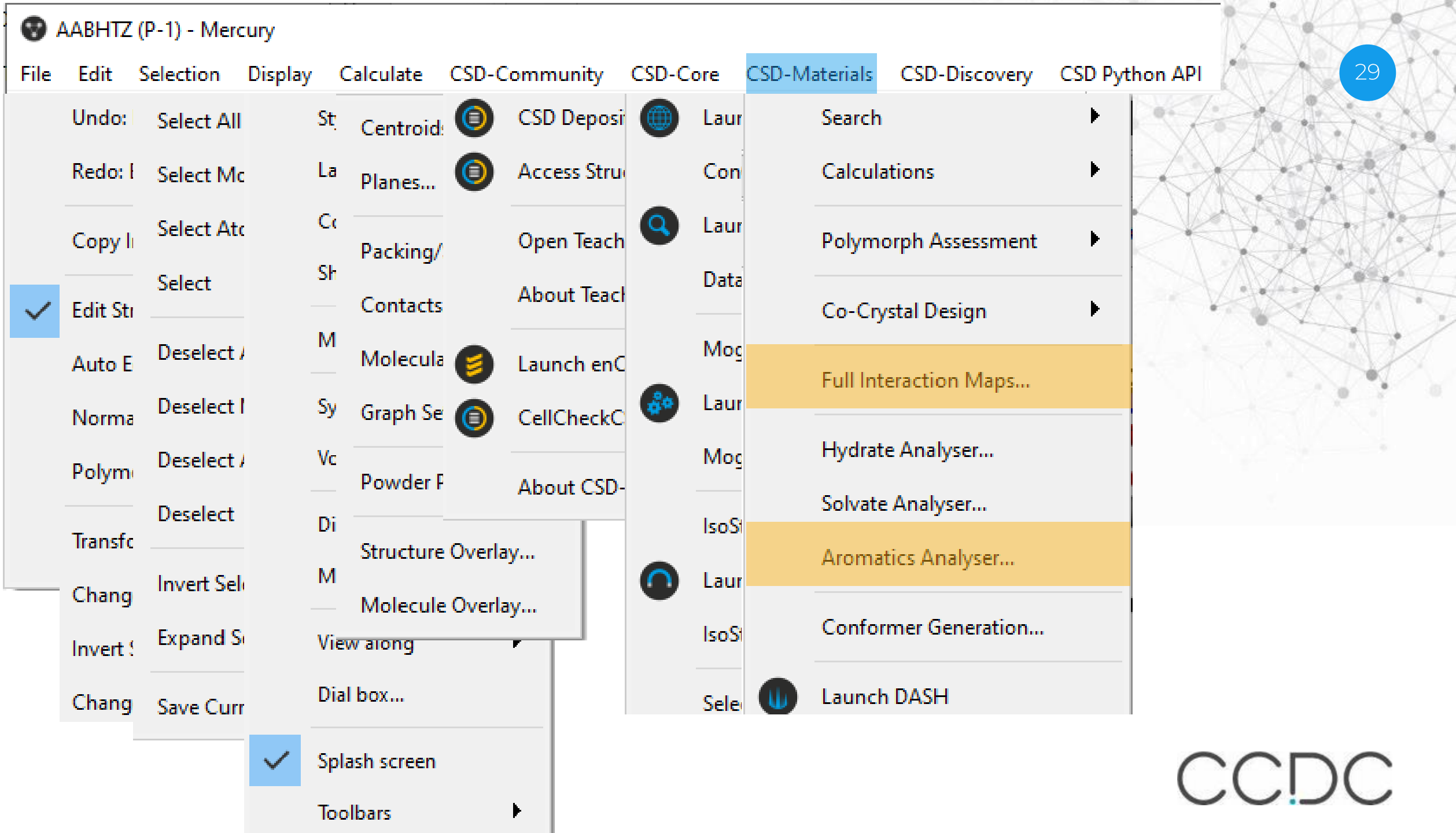
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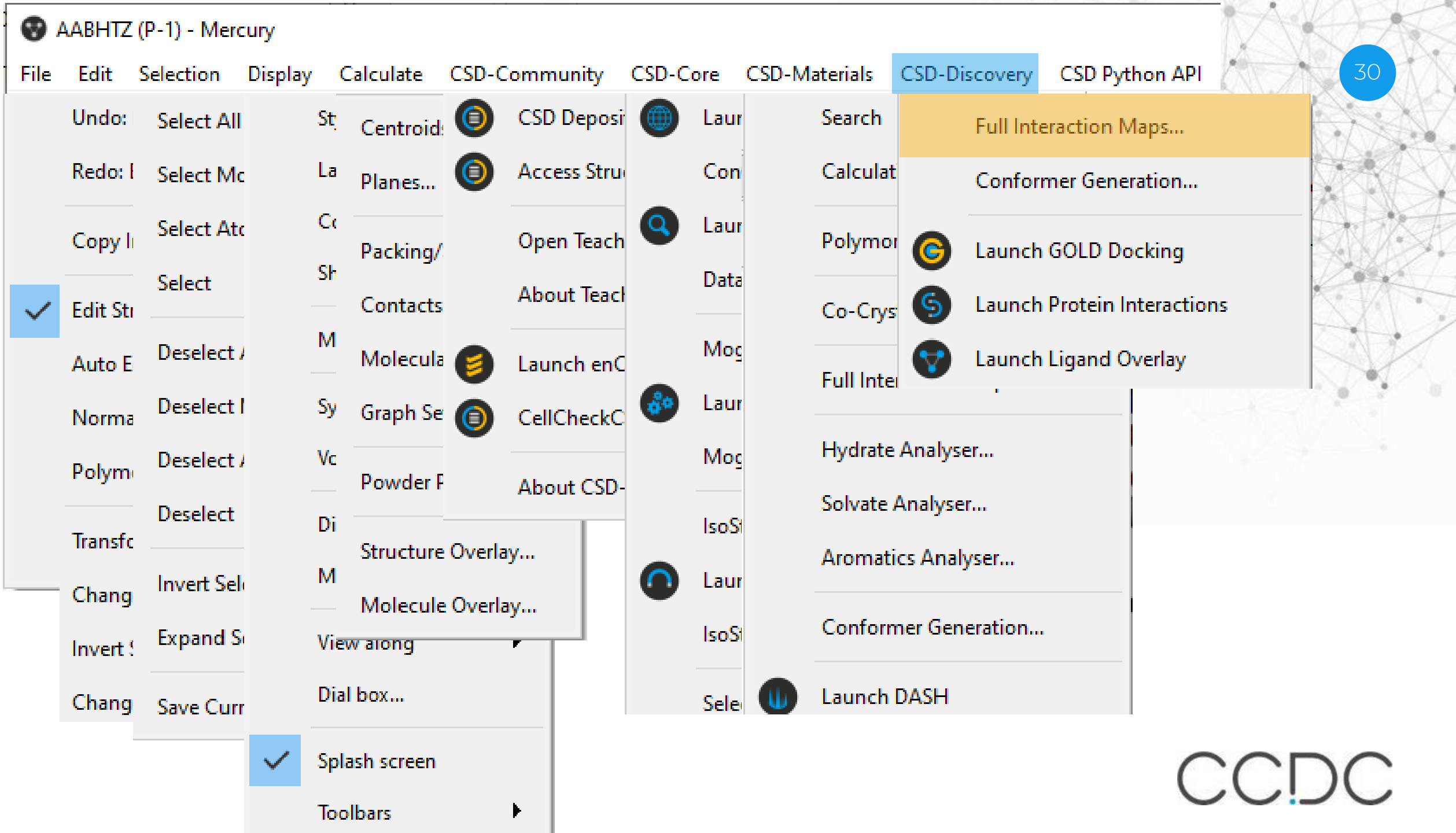
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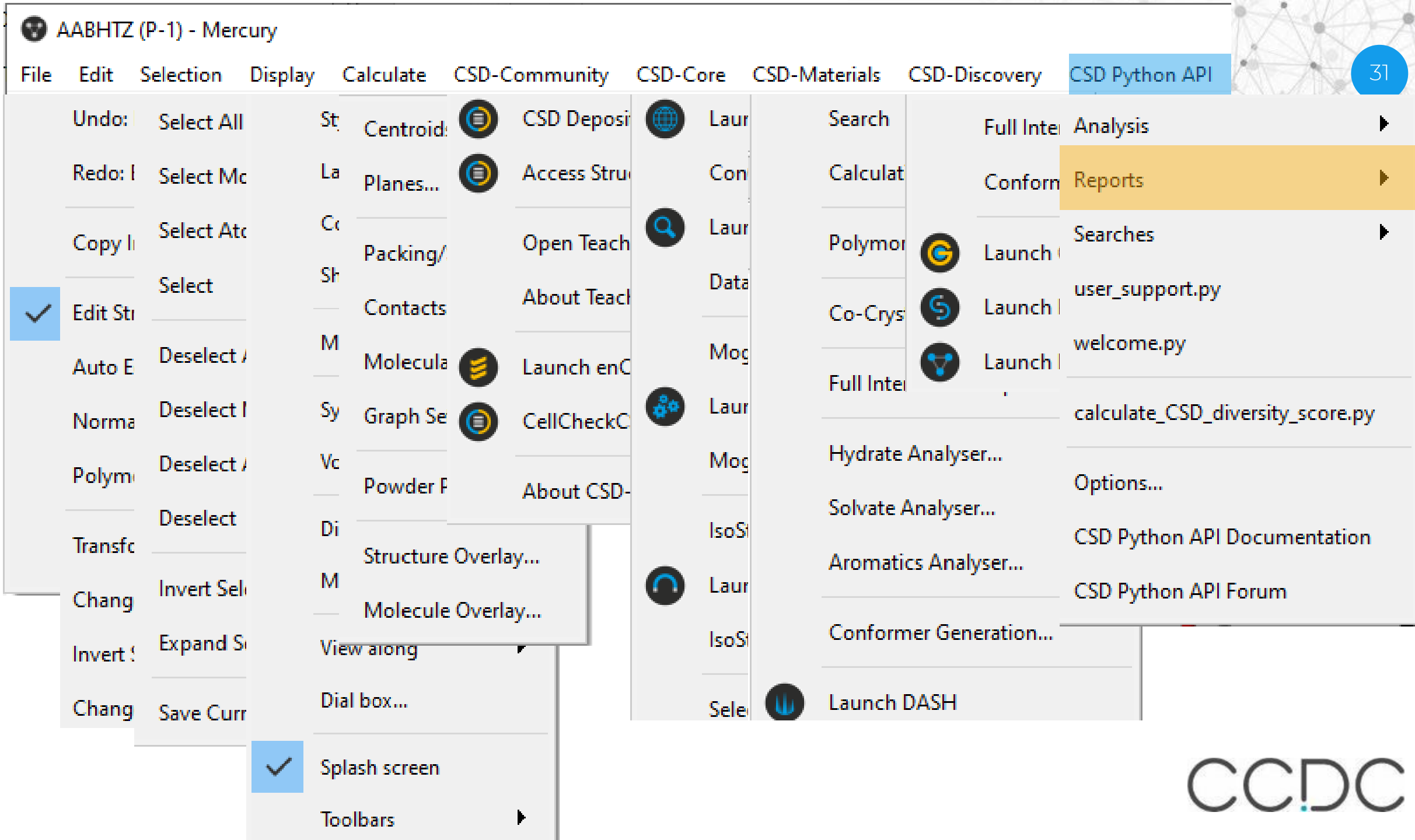
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CSD Python API Documentation
CSD Python API Forum

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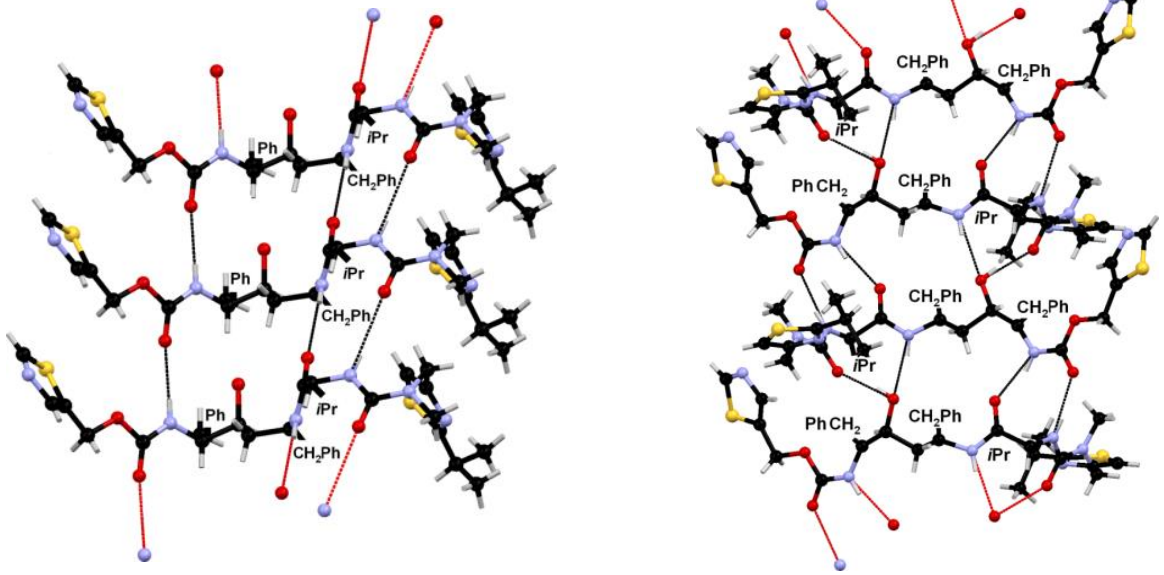
Calculate - Exploring contacts

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

A real-life example...

Can structural knowledge mitigate risk?

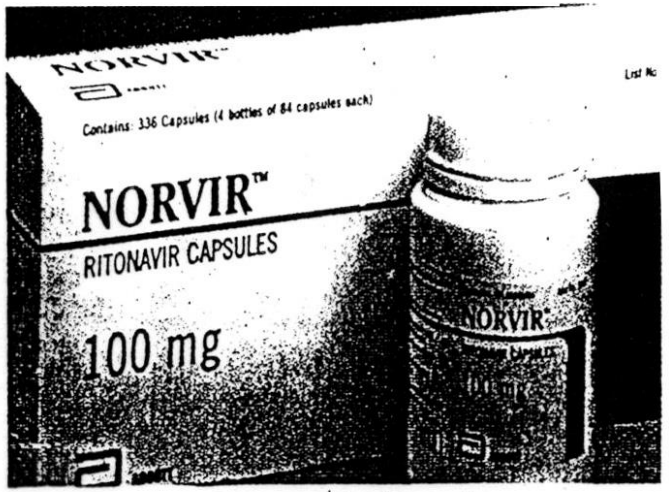


Different interactions

Different solubility
Different stability

Manufacturing problems hit Abbott's HIV drug ritonavir

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



Capsules unlikely to be available from mid-August

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

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

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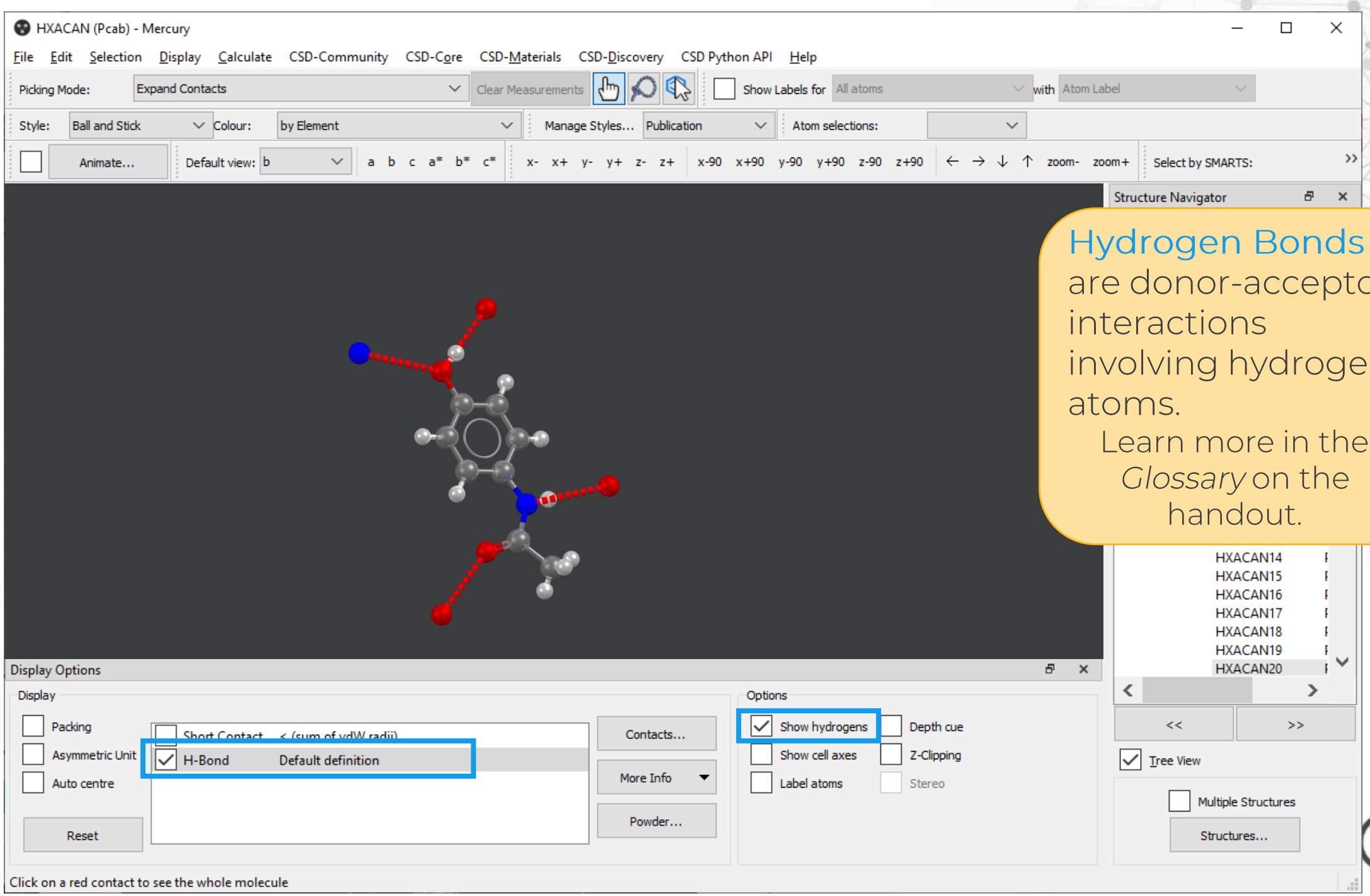
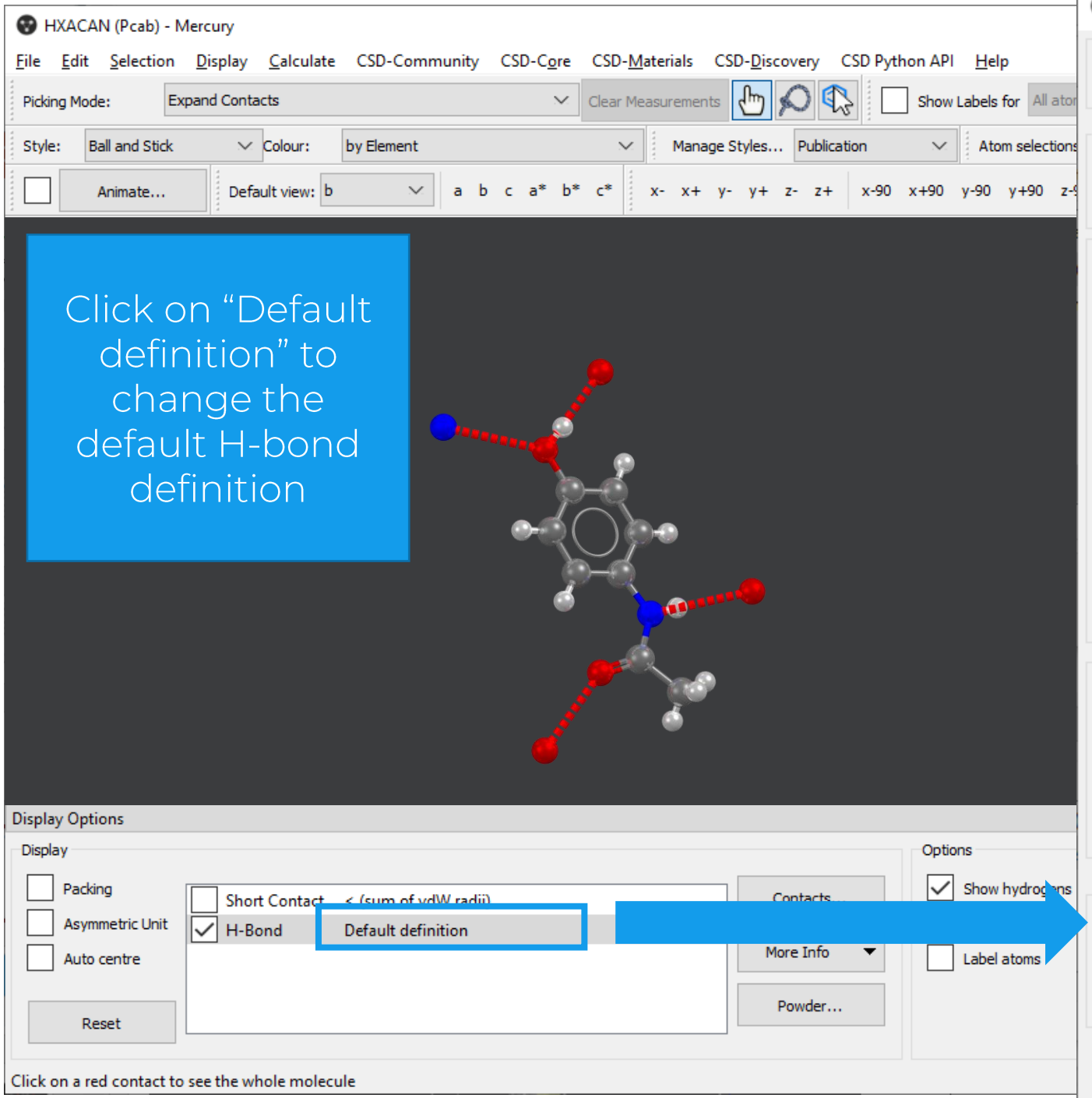


Hydrogen Bonds are donor-acceptor interactions involving hydrogen atoms.

Learn more in the *Glossary* on the handout.


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
Style: Ball and Stick
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Manage Styles...
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Atom selections
Animate...
Default view: b
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Click on "Default definition" to change the default H-bond definition
Display Options
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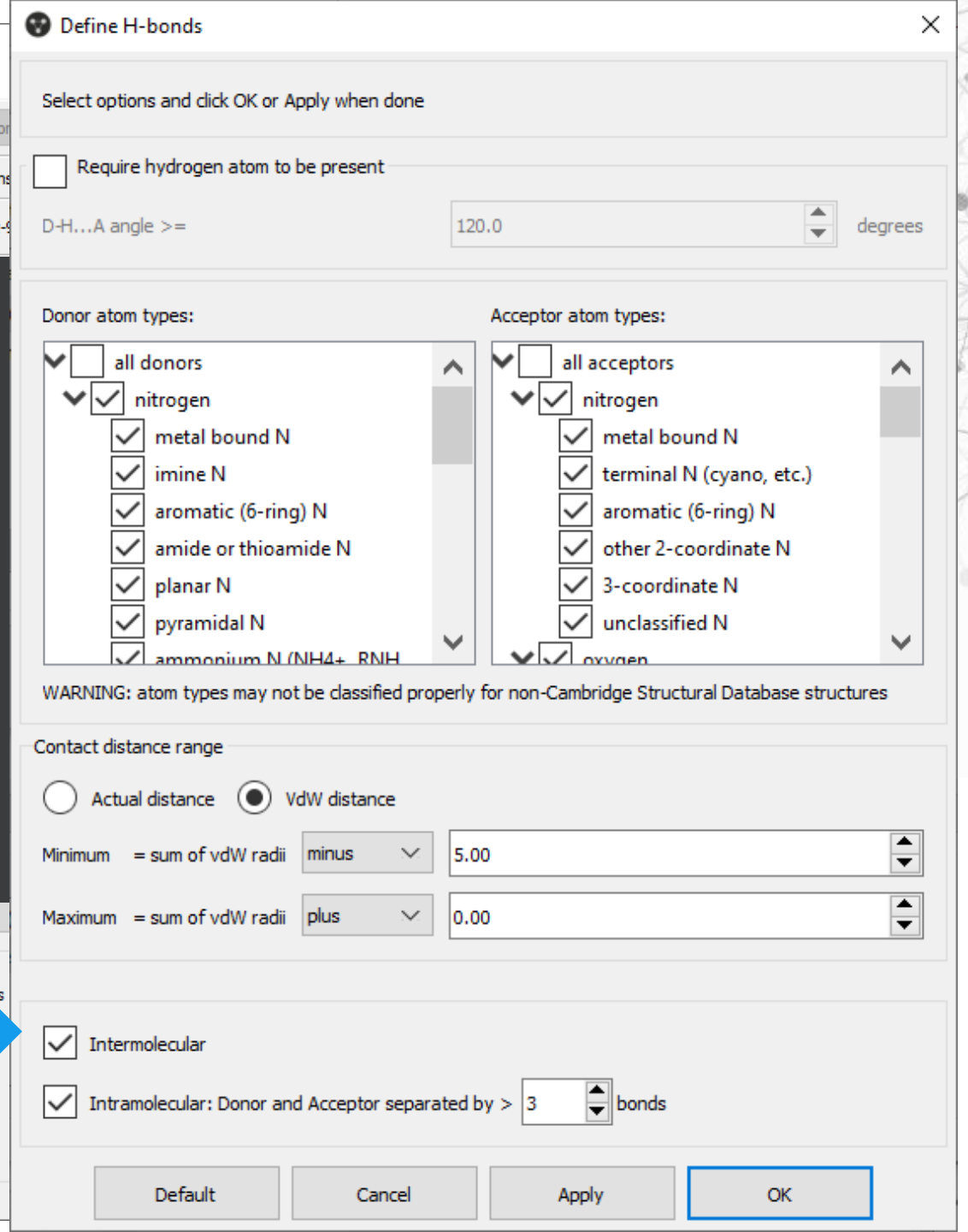
Show hydrogens
Label atoms
Click on a red contact to see the whole molecule


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
planar N
pyramidal 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
WARNING: atom types may not be classified properly for non-Cambridge Structural Database structures
Contact distance range
Actual distance
VdW distance
Minimum = sum of vdW radii
minus
5.00
Maximum = sum of vdW radii
plus
0.00
Intermolecular
Intramolecular: Donor and Acceptor separated by >
3
bonds
Default
Cancel
Apply
OK

HXACAN (Pcab) - Mercury

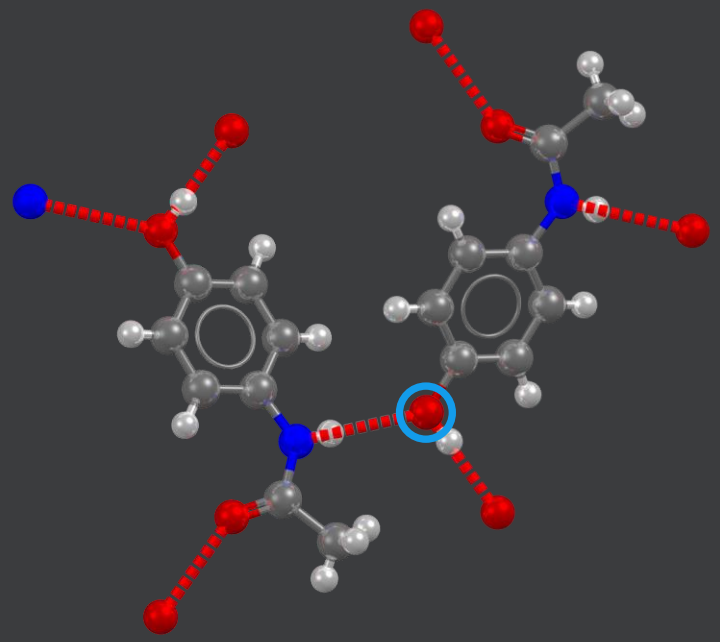
File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Discovery CSD Python API Help

Picking Mode: Expand Contacts | Clear Measurements | Show Labels for All atoms with Atom Label

Style: Ball and Stick | Colour: by Element | Manage Styles... Publication | Atom selections:

Animate... | Default view: b | a b c a* b* c* | x- x+ y- y+ z- z+ | x-90 x+90 y-90 y+90 z-90 z+90 | zoom- zoom+ | Select by SMARTS:

Left click on the atoms at the end of the dashed lines (known as hanging contacts) to expand the network



Selection
Styles
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Show/Hide
Contacts
Delete this Molecule
Rotation Centre
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Structure Navigator

HXACAN Find

Crystal Structures
HXACA
HXACA
HXACA
HXACA
HXACA

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

Expand All
Expand Contact
Expand Contacts from this Atom
Expand Contacts from this Molecule
Find Contacts from this Atom
Find Contacts from this Molecule
Delete Hanging Contacts
Delete Contact
Delete Contacts from this Atom
Delete Contacts from this Molecule
Delete this Molecule
Reset Contacts

Display Options

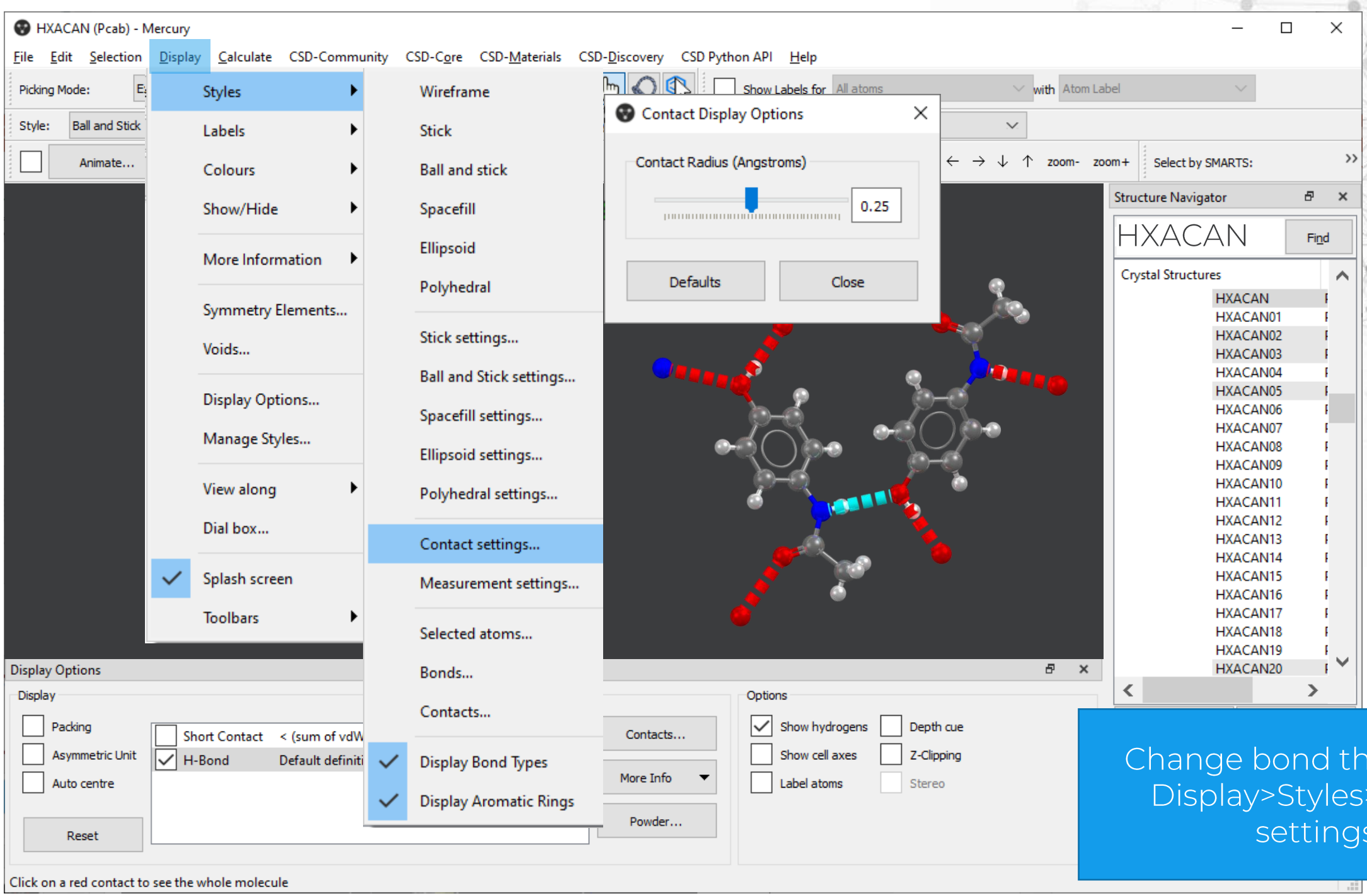
Display
Packing
Asymmetric Unit
Auto centre
Reset

Short Contact < (sum of vdW radii)
H-Bond Default definition

Contacts...
More Info
Powder...

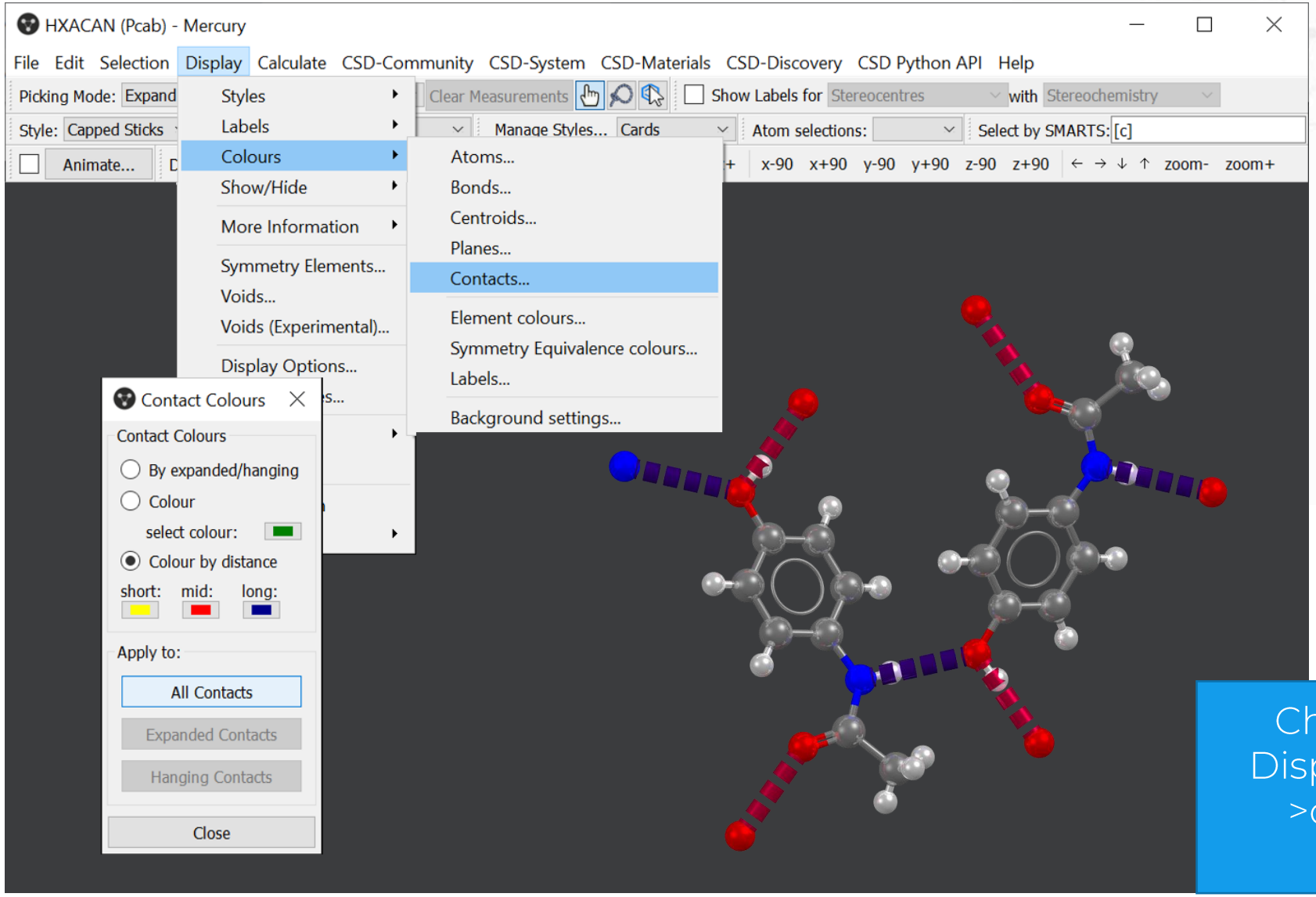
Options
Show hydrogens
Show cell axes
Label atoms
Depth cue
Z-Clipping
Stereo

Click on a red contact to see the whole molecule



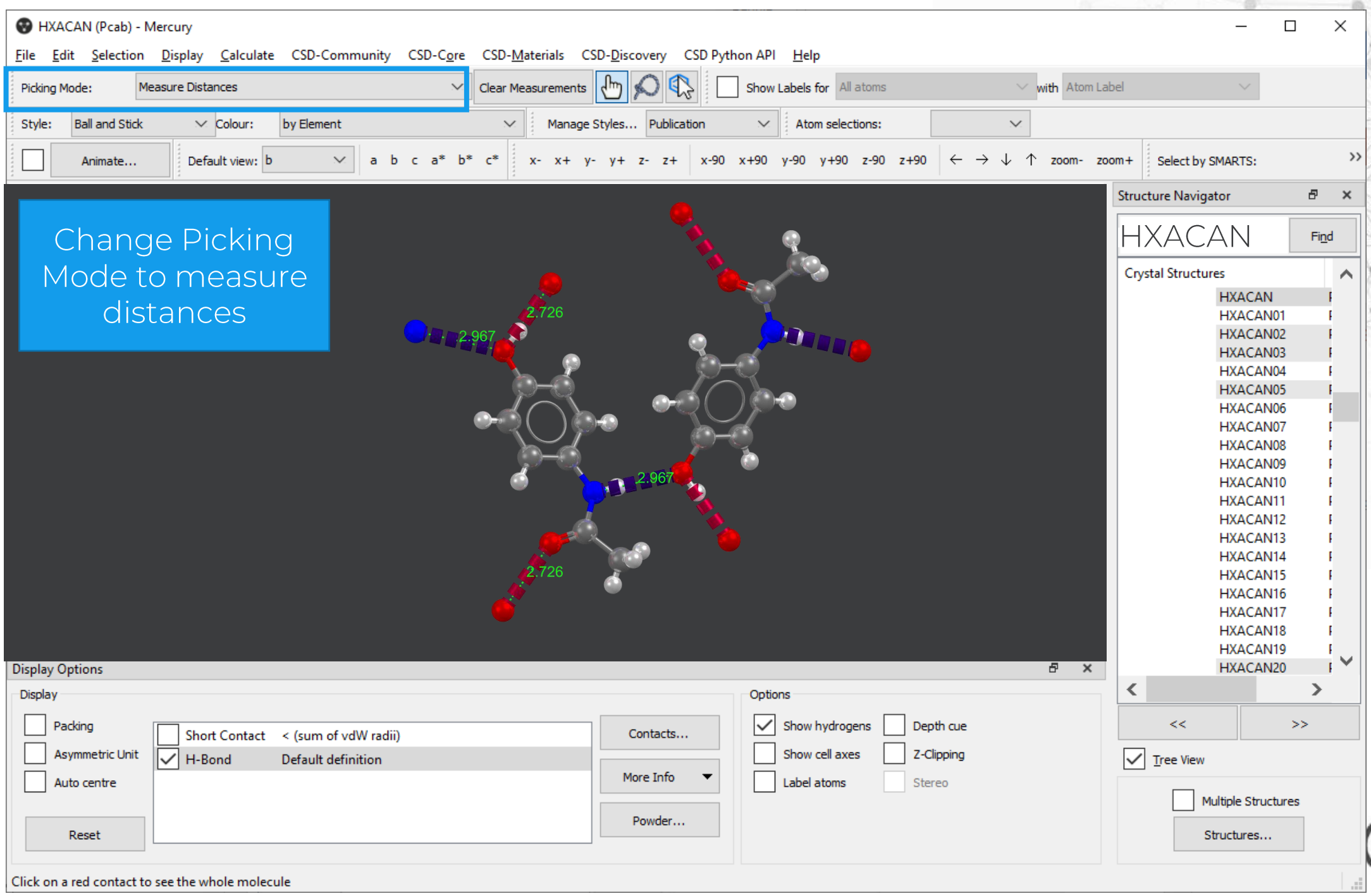
Change bond thickness by Display>Styles>Contact settings...

Colour H-bonds by distance



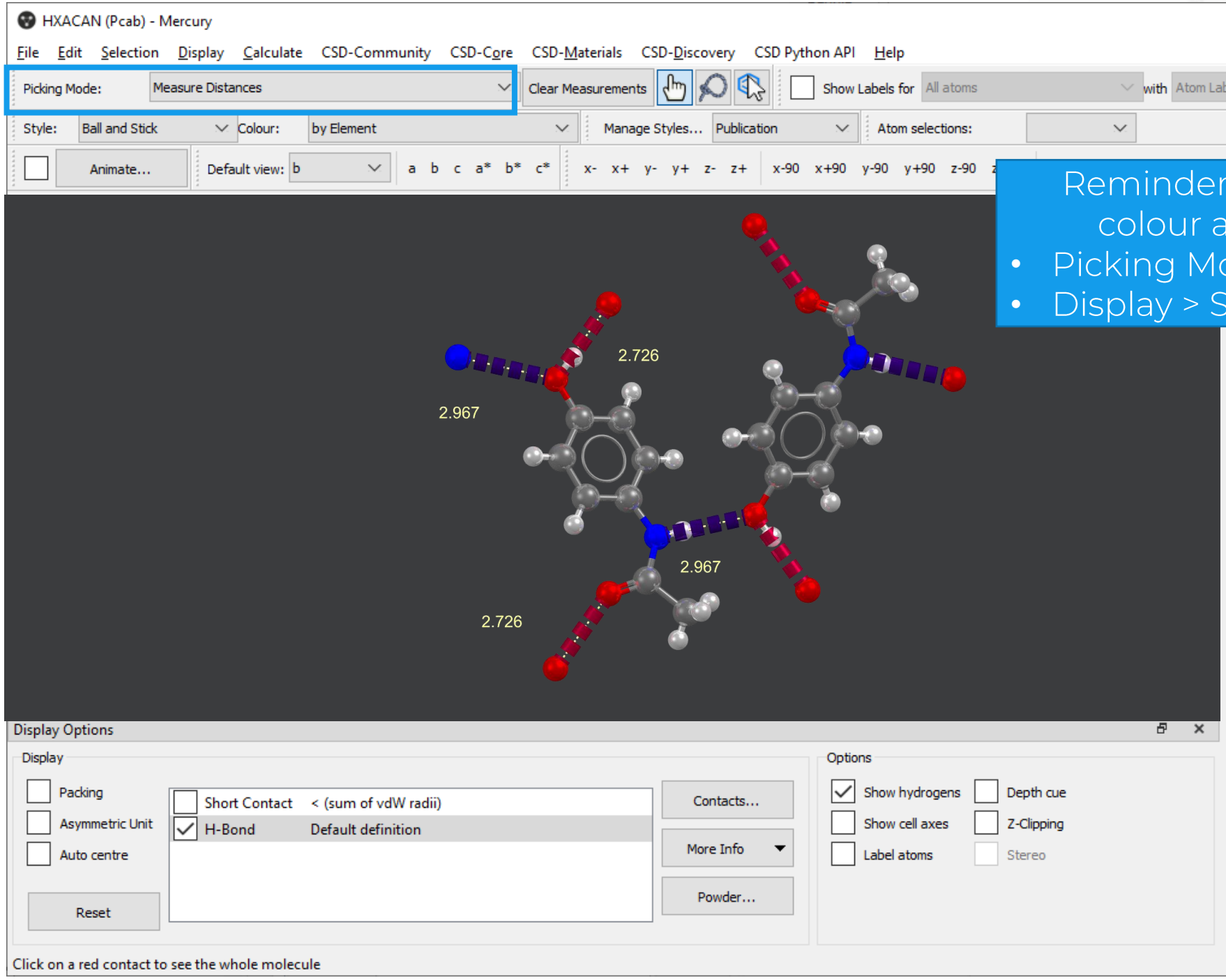
CSD Refcode: HXACAN

Change bond colours by Display>Colours>Contacts... >colour by distance>All contacts


HXACAN (Pcab) - Mercury
File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Discovery CSD Python API Help
Picking Mode: Measure Distances
Clear Measurements
Show Labels for All atoms with Atom Label
Style: Ball and Stick
Colour: by Element
Manage Styles... Publication
Atom selections:
Animate...
Default view: b
a b c a* b* c*
x- x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-90 z+90
zoom- zoom+
Select by SMARTS:
Change Picking Mode to measure distances
2.726
2.967
2.967
2.726
Structure Navigator
HXACAN
Find
Crystal Structures
HXACAN
HXACAN01
HXACAN02
HXACAN03
HXACAN04
HXACAN05
HXACAN06
HXACAN07
HXACAN08
HXACAN09
HXACAN10
HXACAN11
HXACAN12
HXACAN13
HXACAN14
HXACAN15
HXACAN16
HXACAN17
HXACAN18
HXACAN19
HXACAN20
<< >>
Tree View
Multiple Structures
Structures...
Display Options
Display
Packing
Asymmetric Unit
Auto centre
Reset
Short Contact < (sum of vdW radii)
H-Bond Default definition
Contacts...
More Info
Powder...
Options
Show hydrogens
Show cell axes
Label atoms
Depth cue
Z-Clipping
Stereo
Click on a red contact to see the whole molecule

Reminder – you can change position, colour and size of distance labels

- Picking Mode > Move Labels
- Display > Styles >Measurement settings



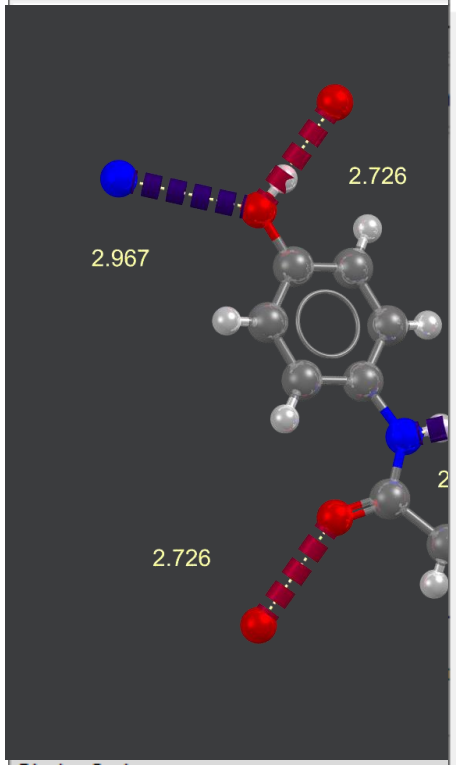
HXACAN (Pcab) - Mercury

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

Picking Mode: Measure Distances | 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



HXACAN

Current structure: HXACAN

Customise...

Structure
Diagram
Atoms
Bonds
Contacts
All Angles
All Torsions

Right-click on a contact for options. Click on a **column heading** to sort rows.

Save...

	Number	Atom1	Atom2	Length	Length-VdW	Symm. op. 1	Symm. op. 2	Expanded	Xorth1	Yorth1	Zorth1	Xorth2	Yorth2	Zorth2
1	1	O1	O2	2.726	-0.314	x,y,z	x,-1/2+y,1/2-z	No	3.1047	2.2725	1.9872	4.6854	0.0515	2.0050
2	2	O1	N1	2.967	-0.103	x,y,z	-1/2+x,1/2-y,z	No	3.1047	2.2725	1.9872	0.2137	1.6254	2.1528

To explore contacts more:
- More Info > Contact List

Close

Display Options

Display

Packing
Asymmetric Unit
Auto centre

Reset

Short Contact < (sum of vdW radii)
H-Bond Default definition

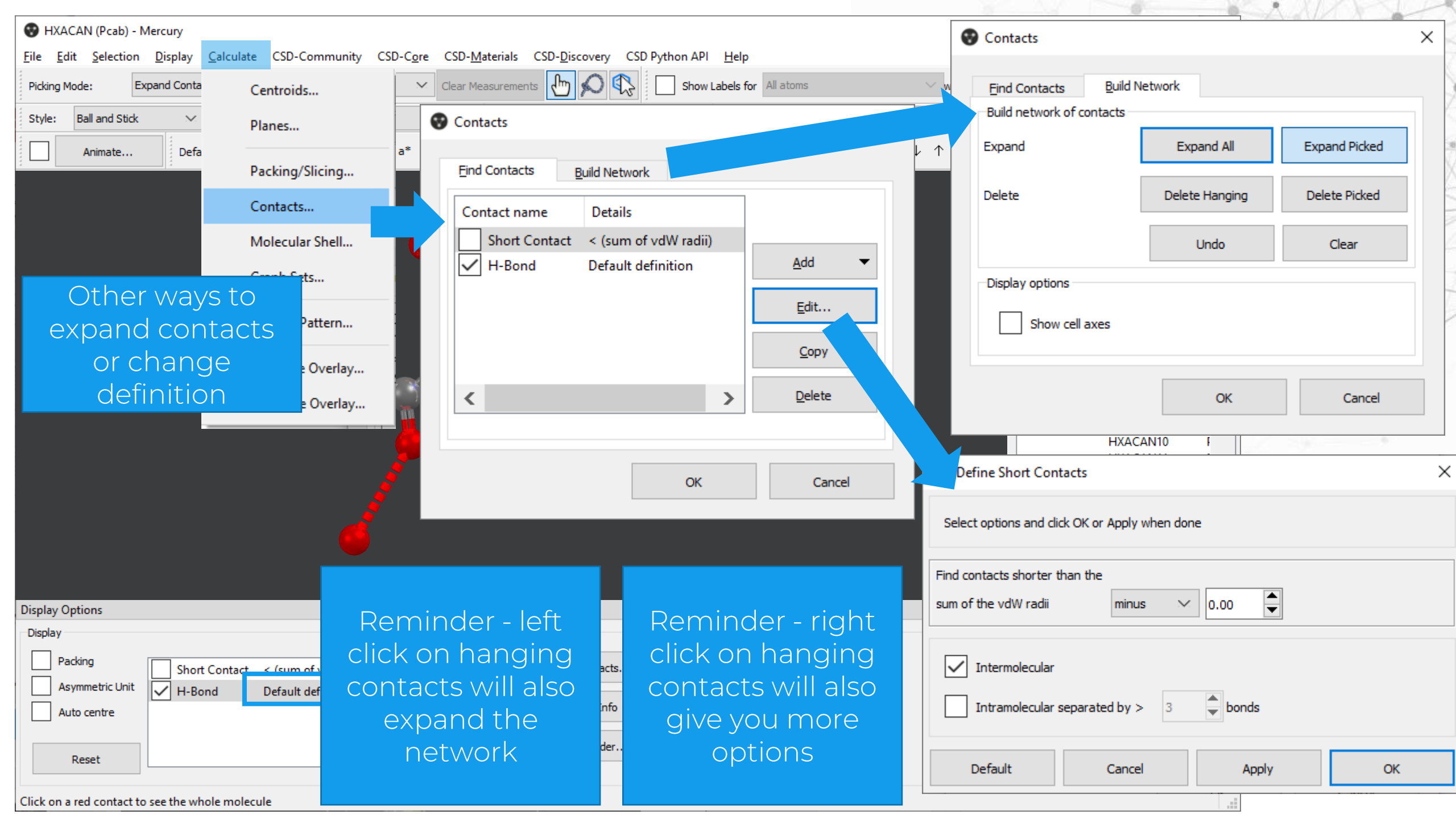
Co... ...
More Info
Powder...

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

<< >>
Tree View
Multiple Structures
Structures...

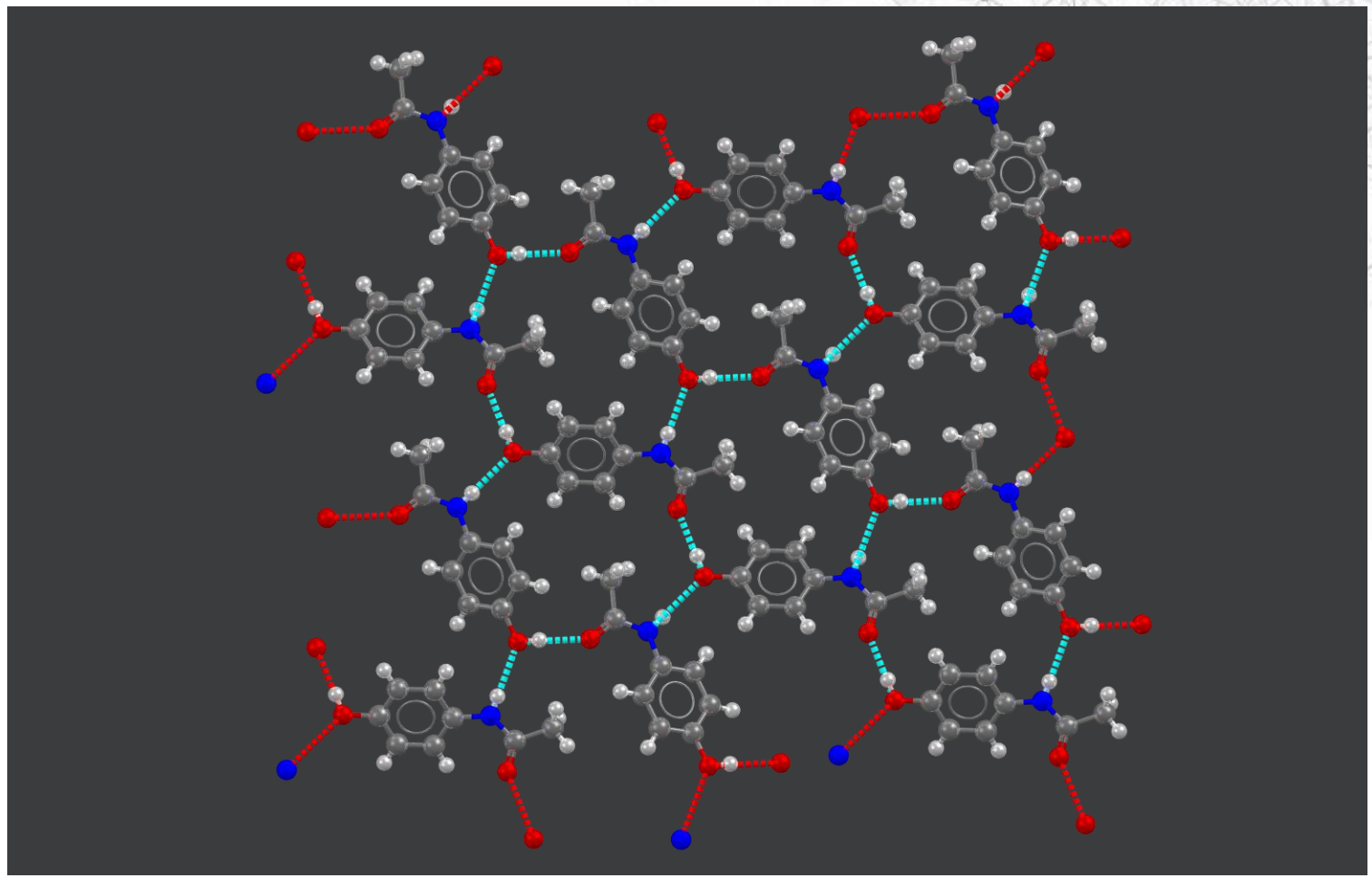
Click on a red contact to see the whole molecule

CDC


HXACAN (Pcab) - Mercury
File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Discovery CSD Python API Help
Centroids...
Planes...
Packing/Slicing...
Contacts...
Molecular Shell...
Contacts
Find Contacts
Build Network
Contact name
Details
Short Contact
< (sum of vdW radii)
H-Bond
Default definition
Add
Edit...
Copy
Delete
OK
Cancel
Contacts
Find Contacts
Build Network
Build network of contacts
Expand
Expand All
Expand Picked
Delete
Delete Hanging
Delete Picked
Undo
Clear
Display options
Show cell axes
OK
Cancel
Other ways to expand contacts or change definition
Define Short Contacts
Select options and click OK or Apply when done
Find contacts shorter than the
sum of the vdW radii
minus
0.00
Intermolecular
Intramolecular separated by >
3
bonds
Default
Cancel
Apply
OK
Display Options
Display
Packing
Asymmetric Unit
Auto centre
Reset
Short Contact
H-Bond
Default def
Click on a red contact to see the whole molecule
Reminder - left click on hanging contacts will also expand the network
Reminder - right click on hanging contacts will also give you more options

Building the H-bond network

You can continue to expand the H-bond network to explore the 1D,2D or 3D nature of the network

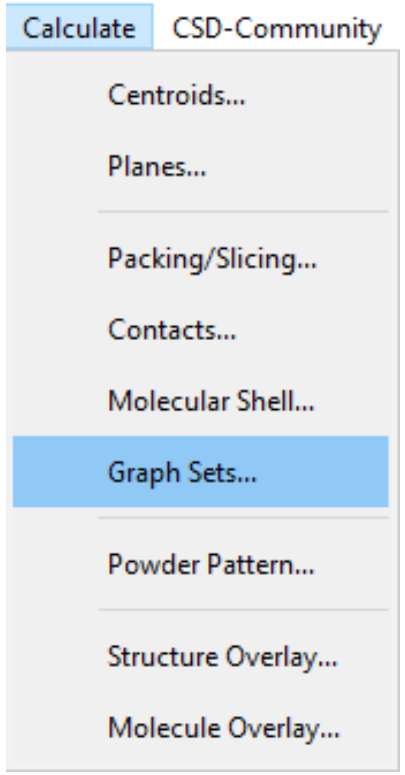


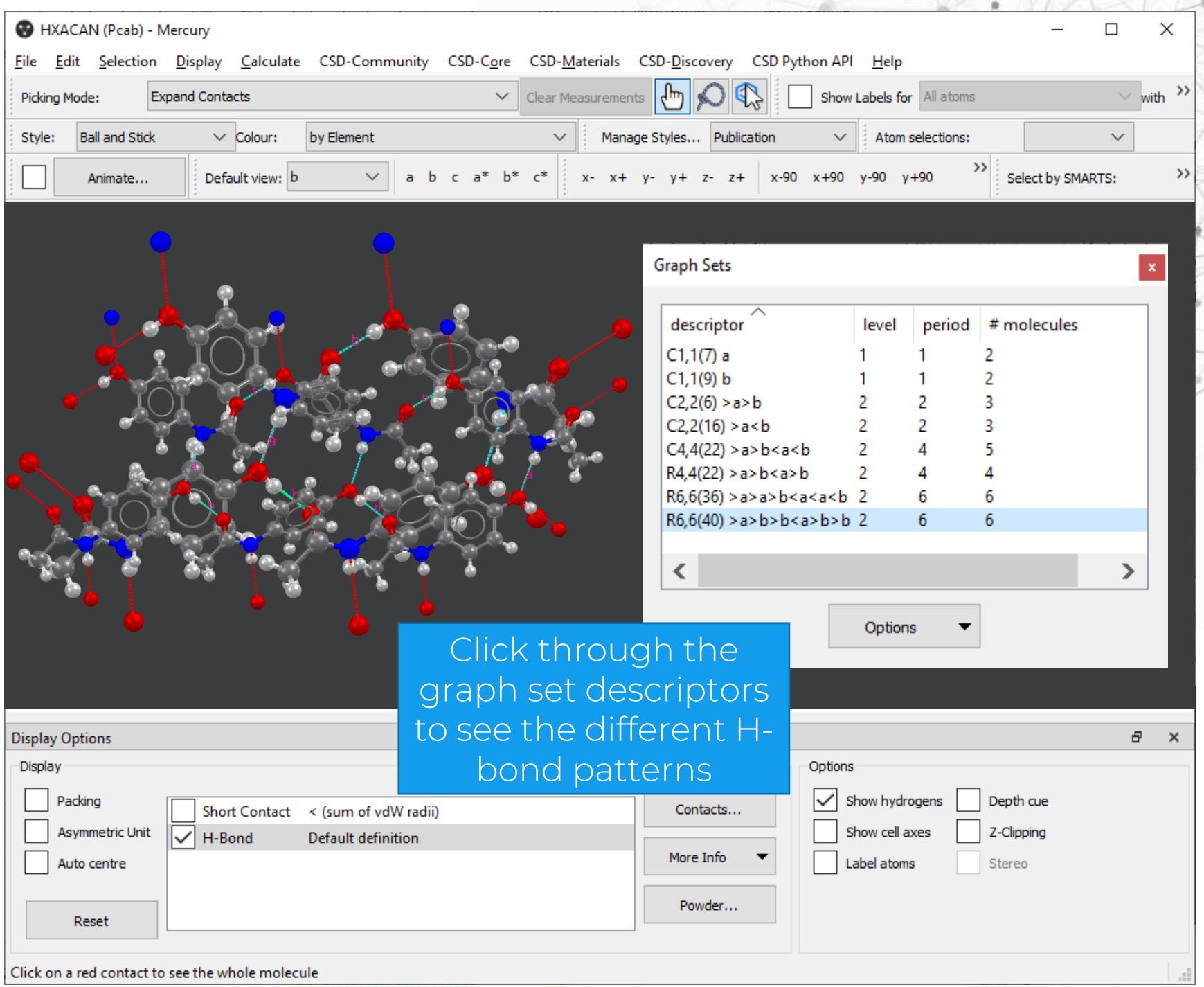
What type of network do you observe for HXACAN?

CSD Refcode: HXACAN

CCDC

Graph Sets





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

Graph Sets describe the **H-bonds pattern**.

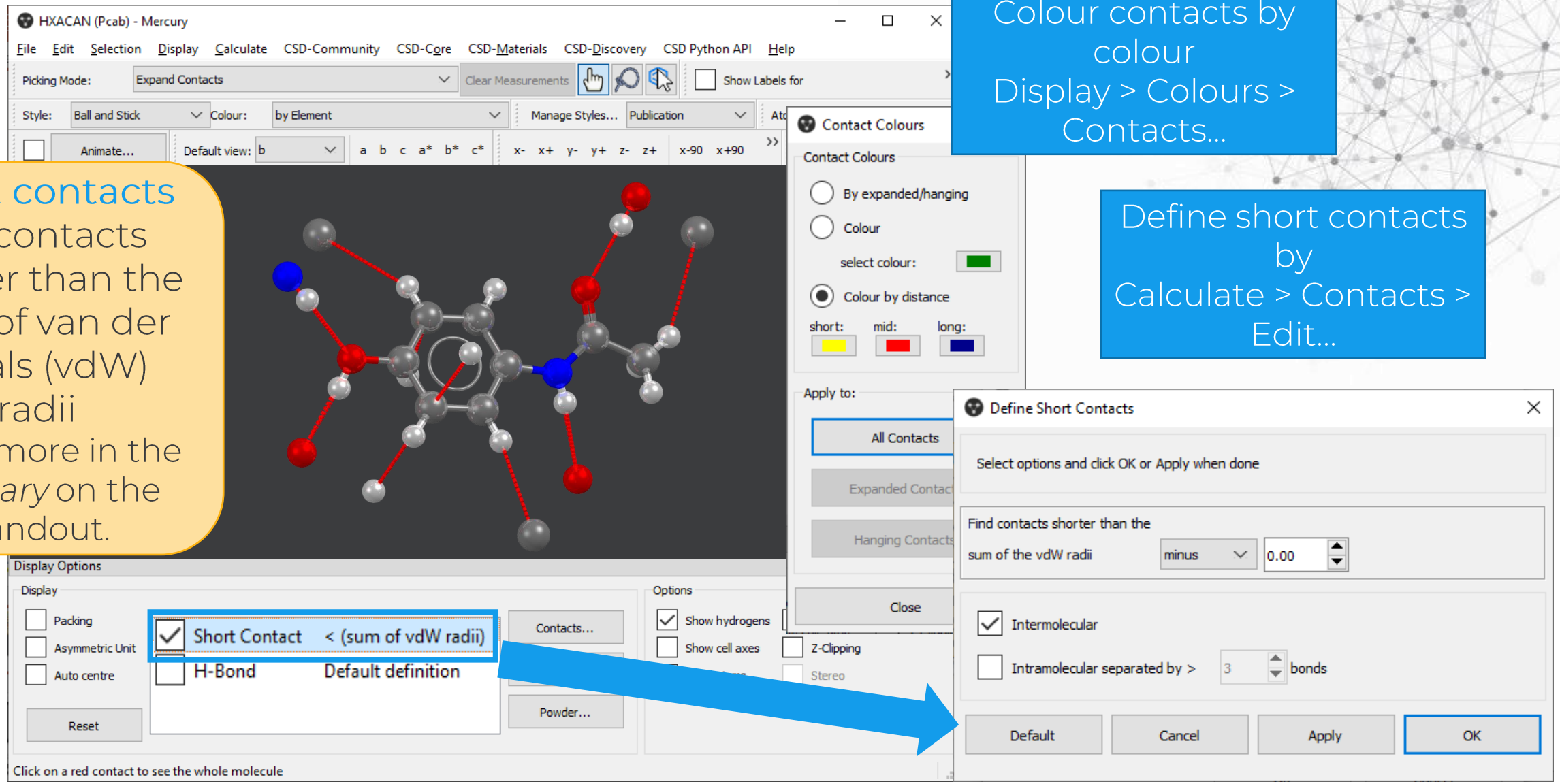
Learn more in the *Glossary* on the handout.

Finding short contacts

Short contacts are contacts shorter than the sum of van der Waals (vdW) radii
Learn more in the *Glossary* on the handout.

Colour contacts by colour
Display > Colours > Contacts...

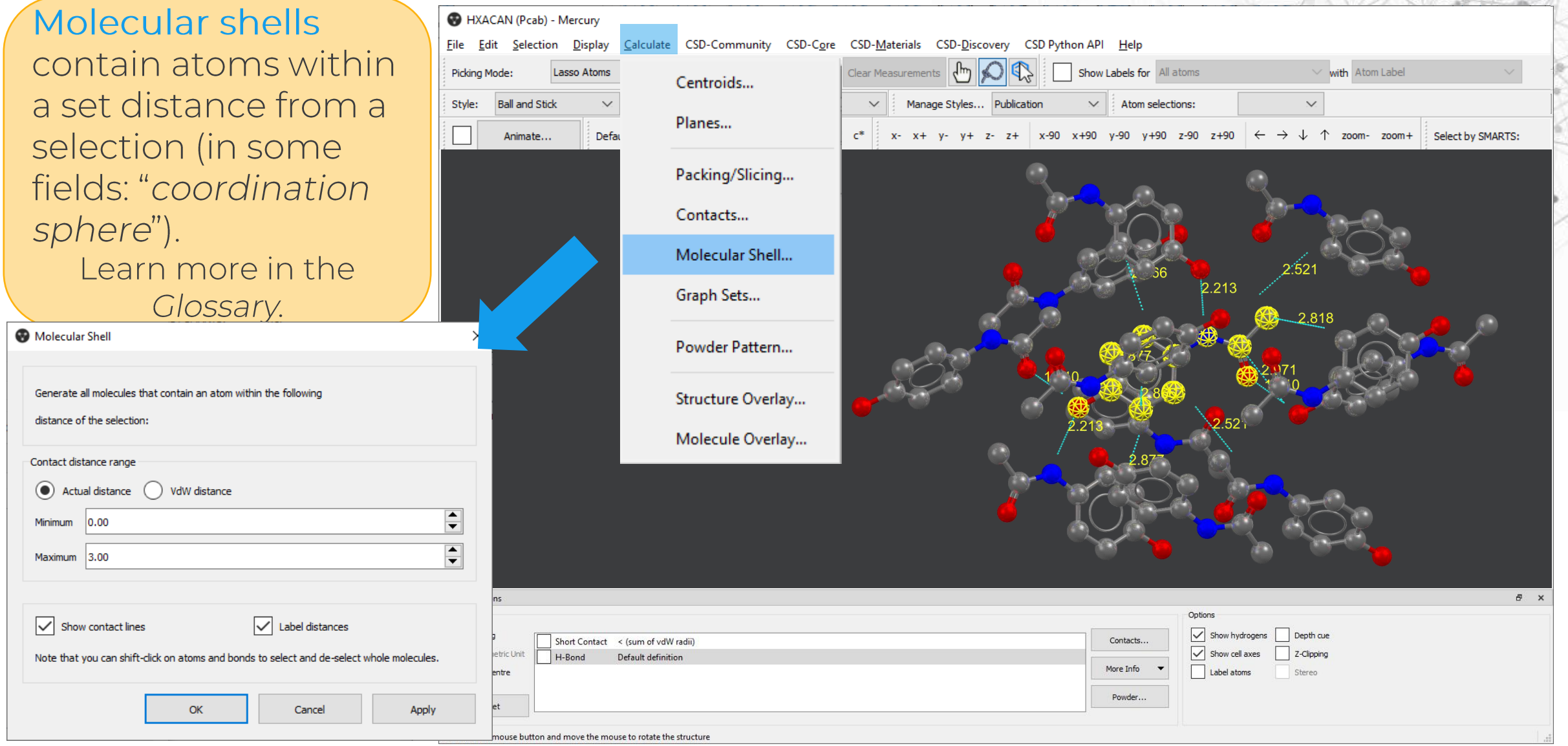
Define short contacts by
Calculate > Contacts > Edit...



Exploring Molecular Shells

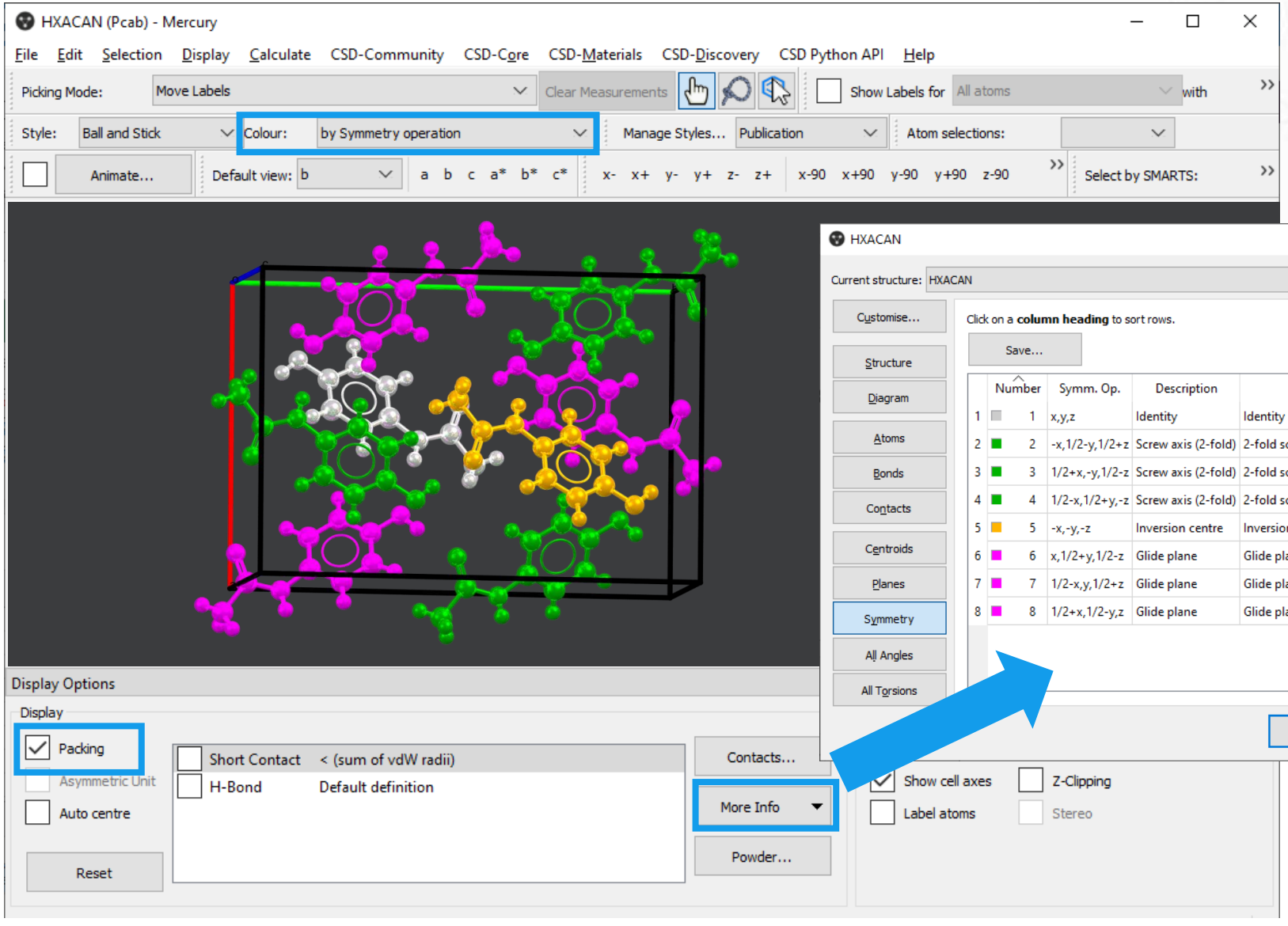
Molecular shells contain atoms within a set distance from a selection (in some fields: "*coordination sphere*").

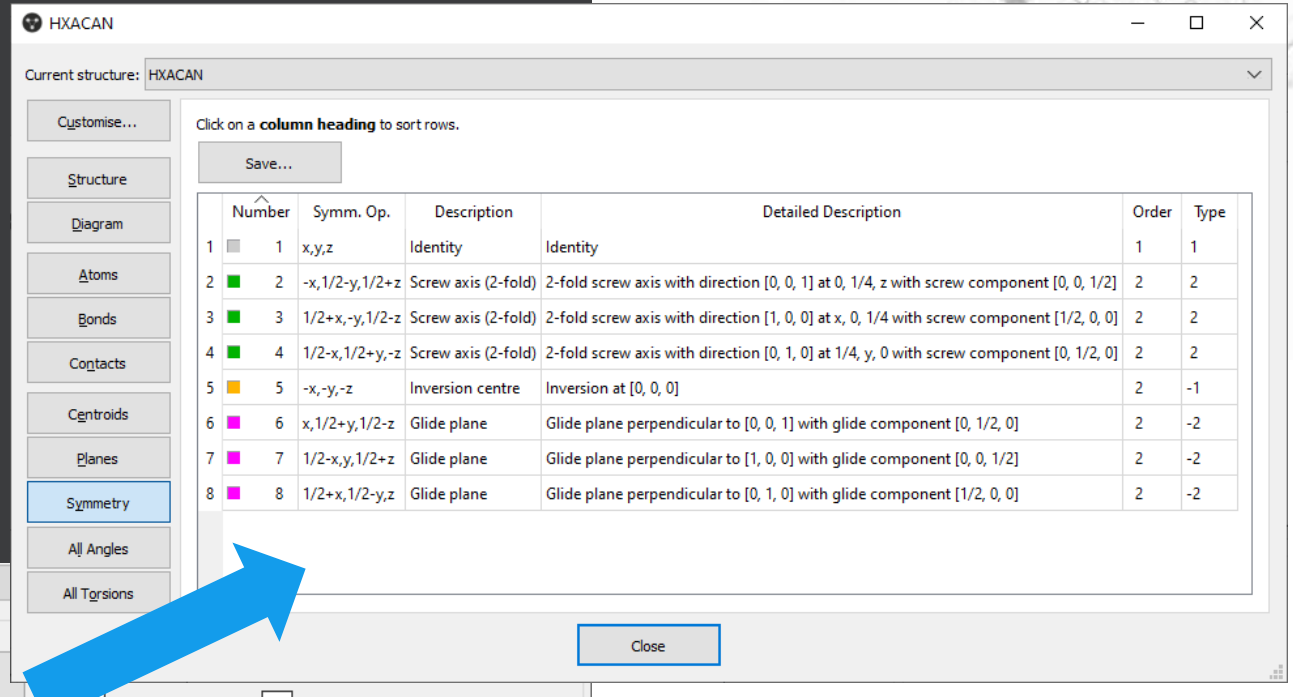
Learn more in the *Glossary*.



Exploring symmetry

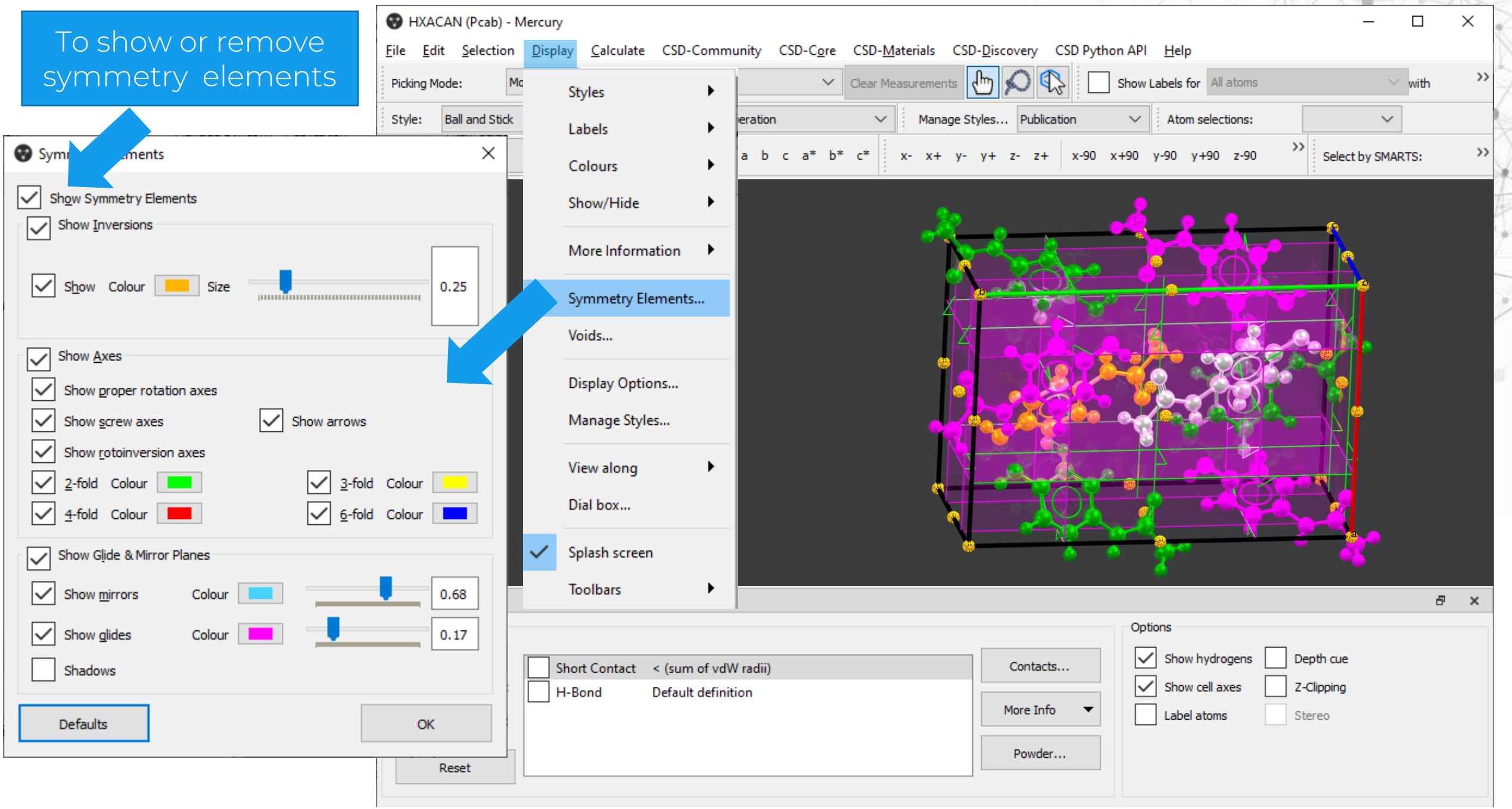
CSD Refcode:
HXACAN

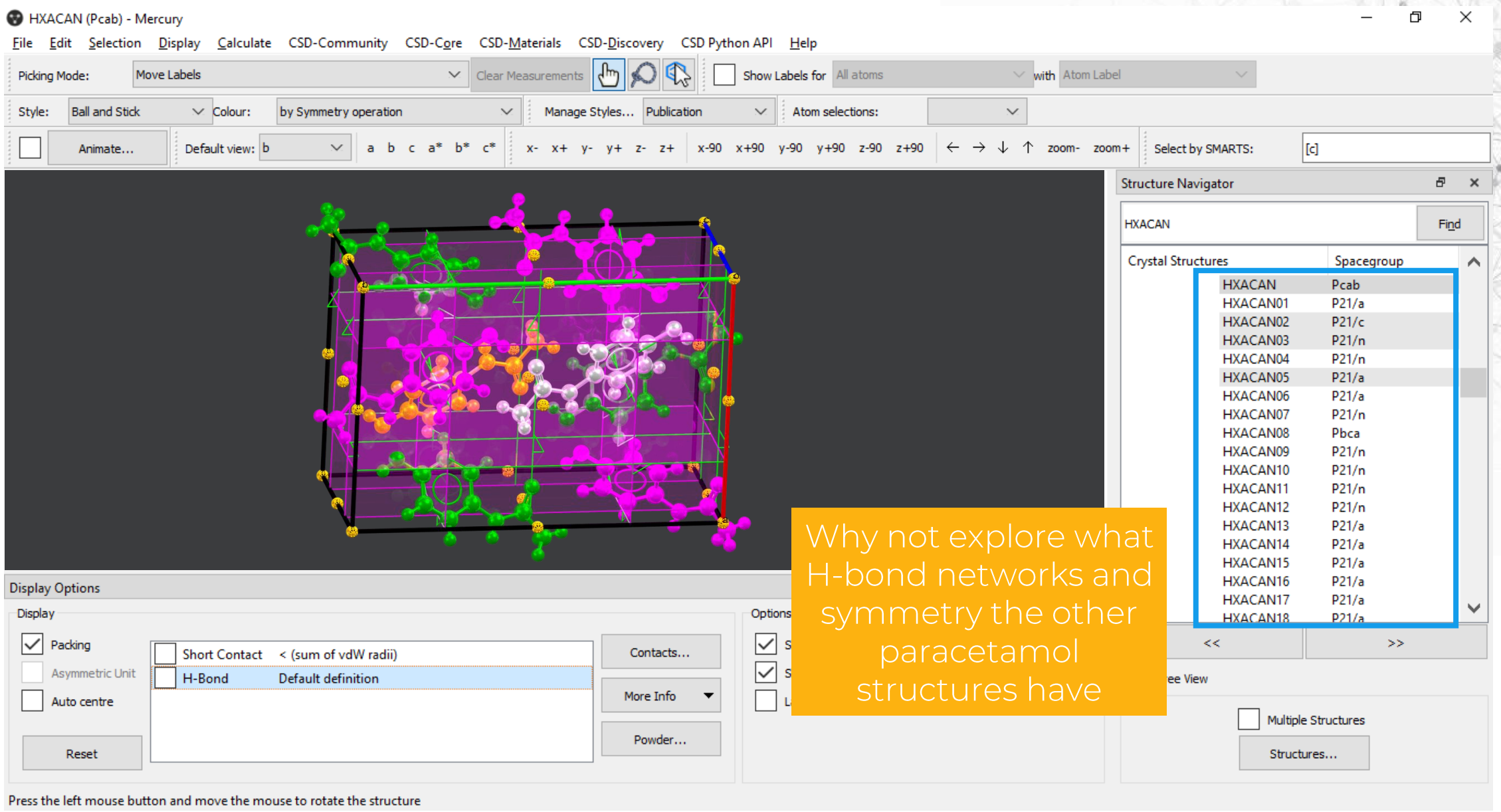




	Number	Symm. Op.	Description	Detailed Description	Order	Type
1	1	x,y,z	Identity	Identity	1	1
2	2	-x,1/2-y,1/2+z	Screw axis (2-fold)	2-fold screw axis with direction [0, 0, 1] at 0, 1/4, z with screw component [0, 0, 1/2]	2	2
3	3	1/2+x,-y,1/2-z	Screw axis (2-fold)	2-fold screw axis with direction [1,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

To show or remove symmetry elements

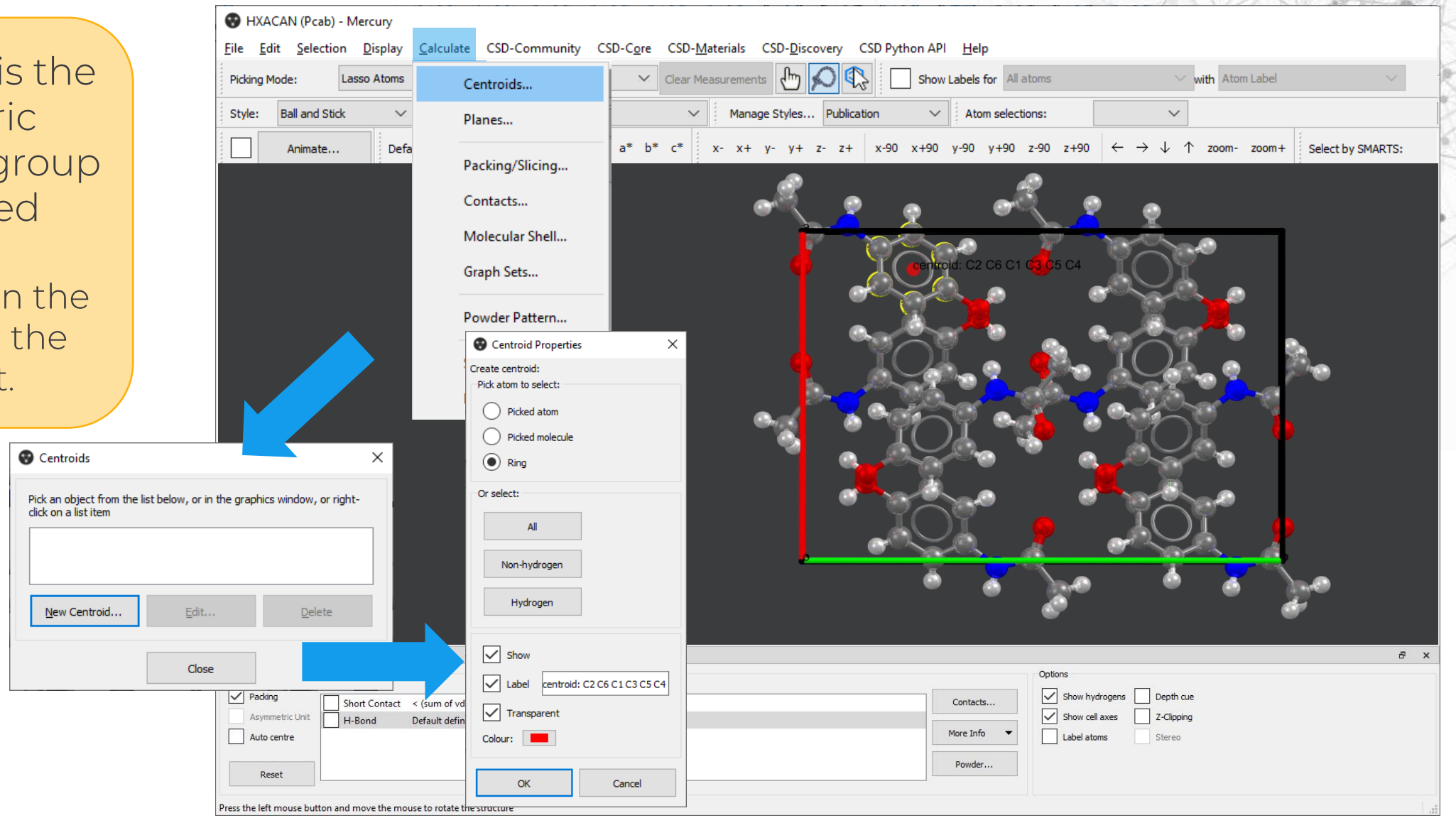




Why not explore what H-bond networks and symmetry the other paracetamol structures have

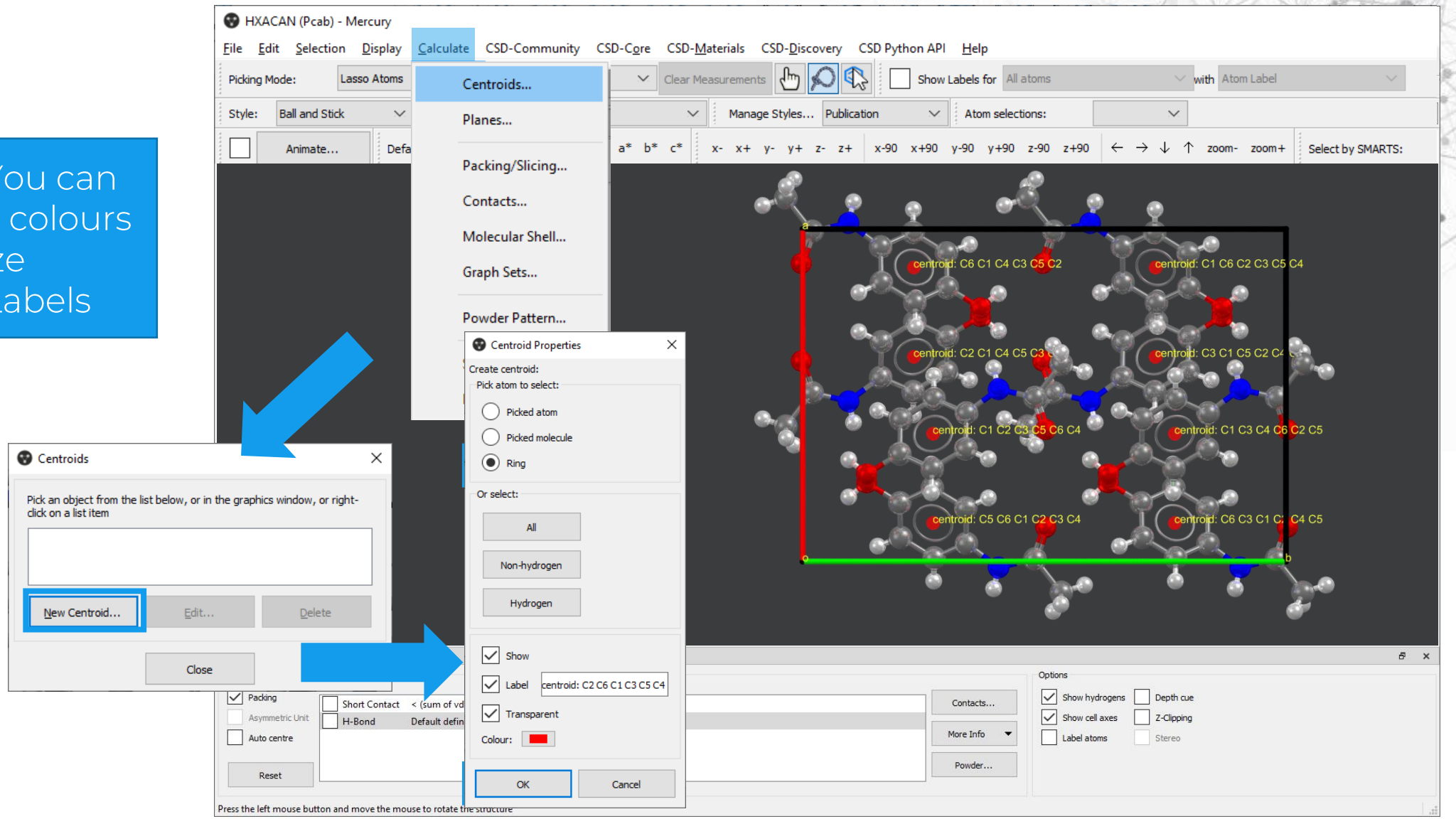
Calculating centroids

A centroid is the geometric centre of a group of selected atoms
Learn more in the *Glossary* on the handout.



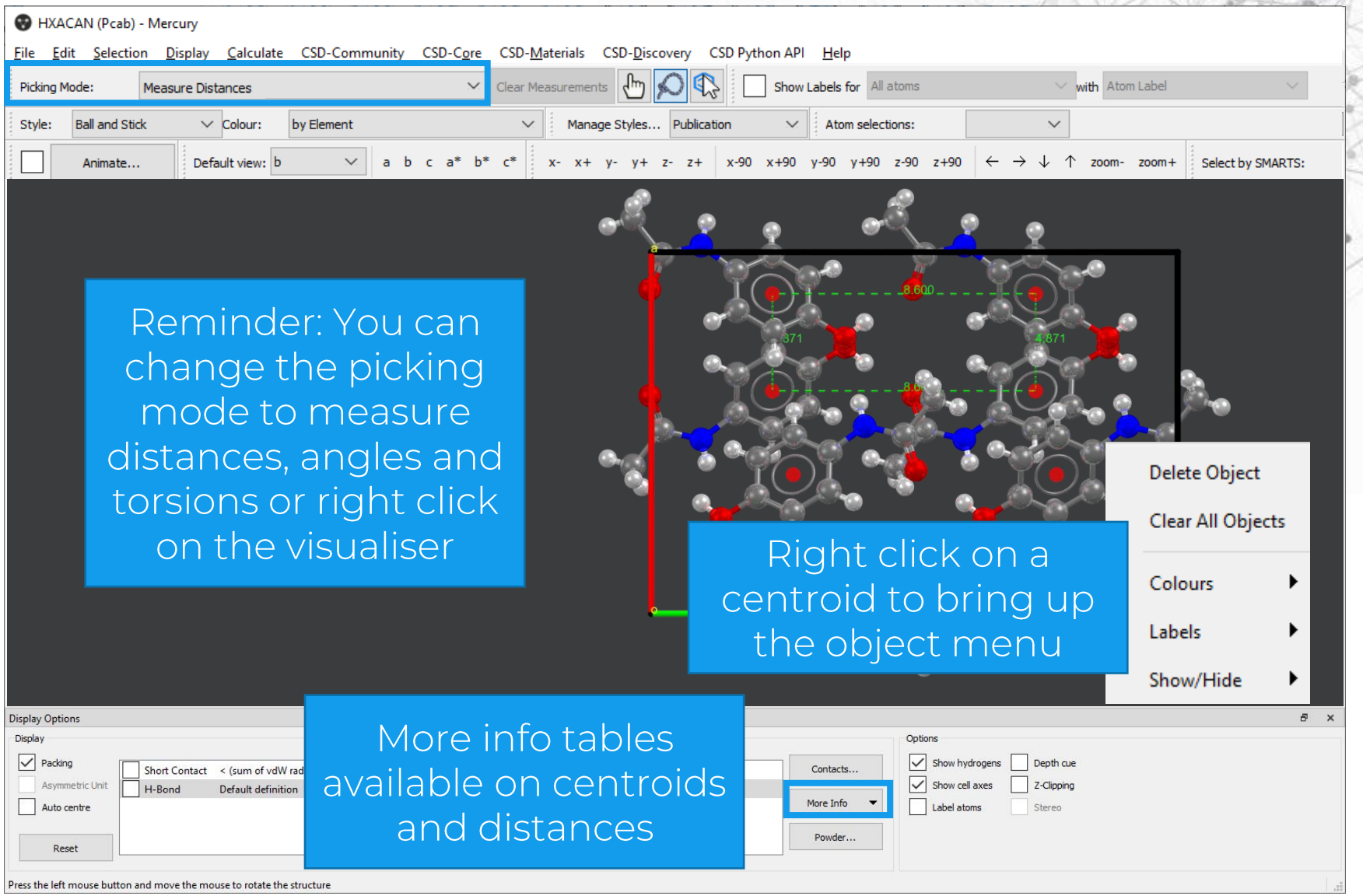
Calculating centroids

Reminder: You can change label colours and size
Display > Labels

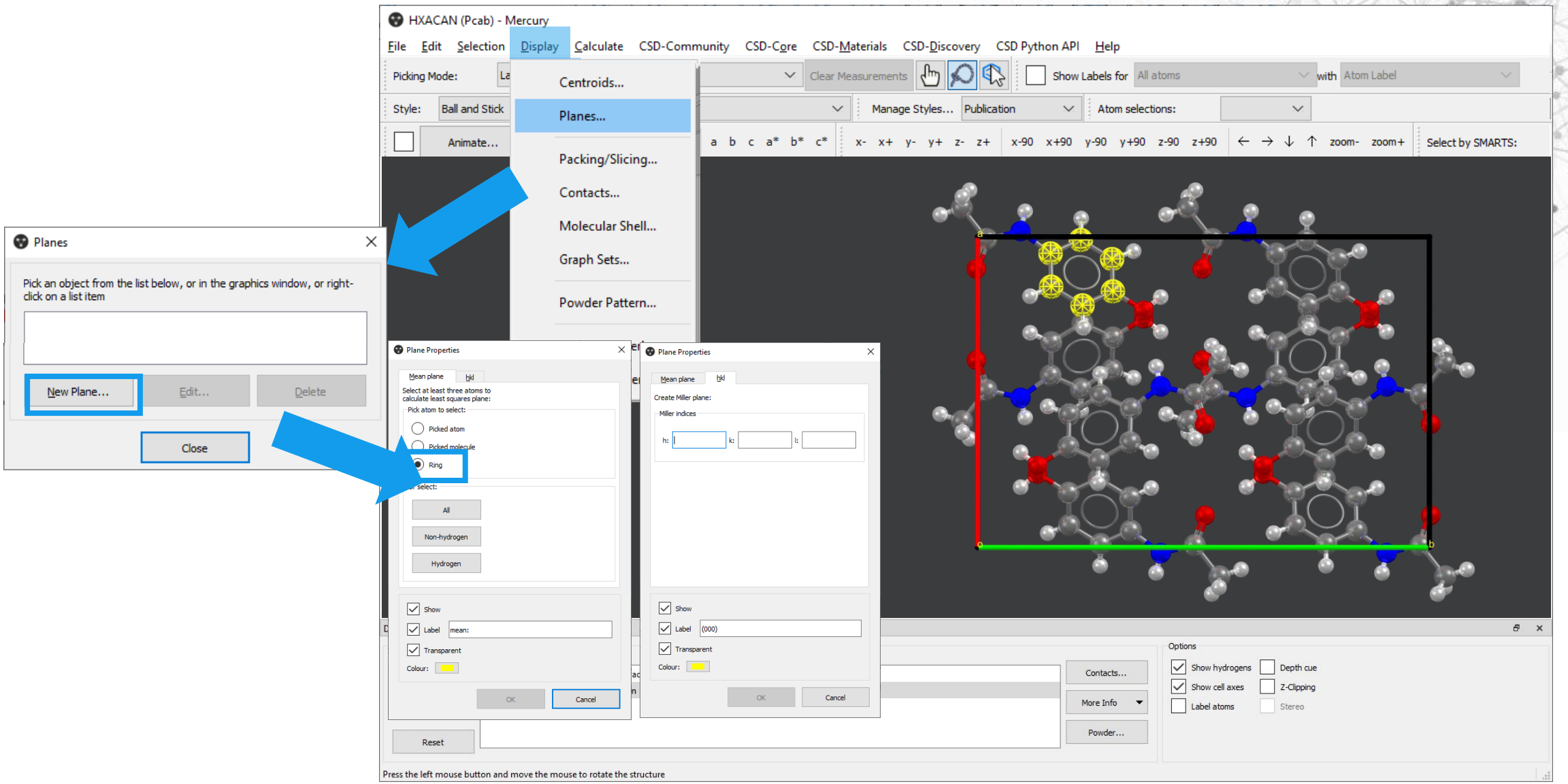


Measuring distances between centroids

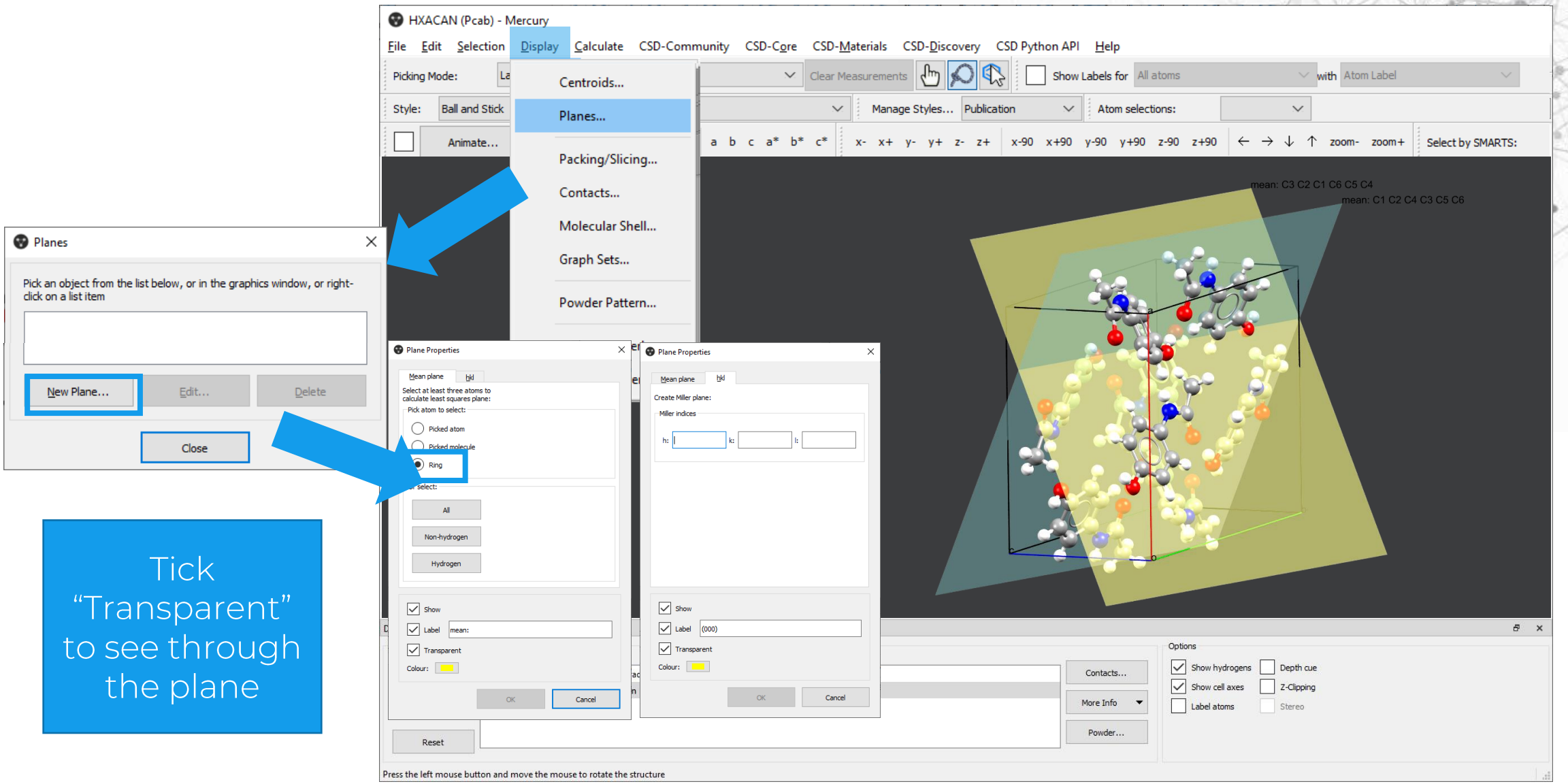
Why not explore how the distance and angles between the ring centroids differ in the other paracetamol structures



Calculating planes



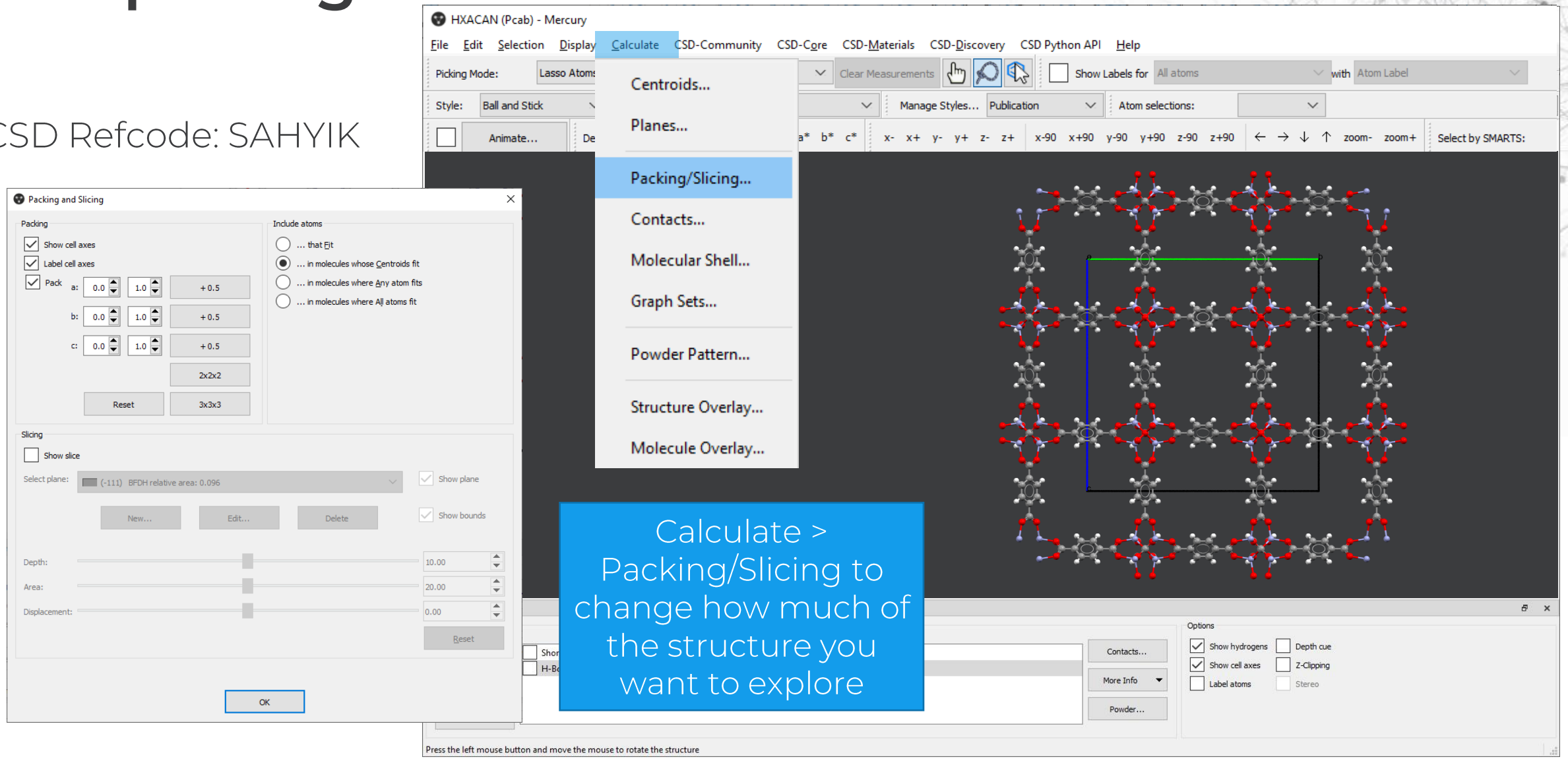
Calculating planes



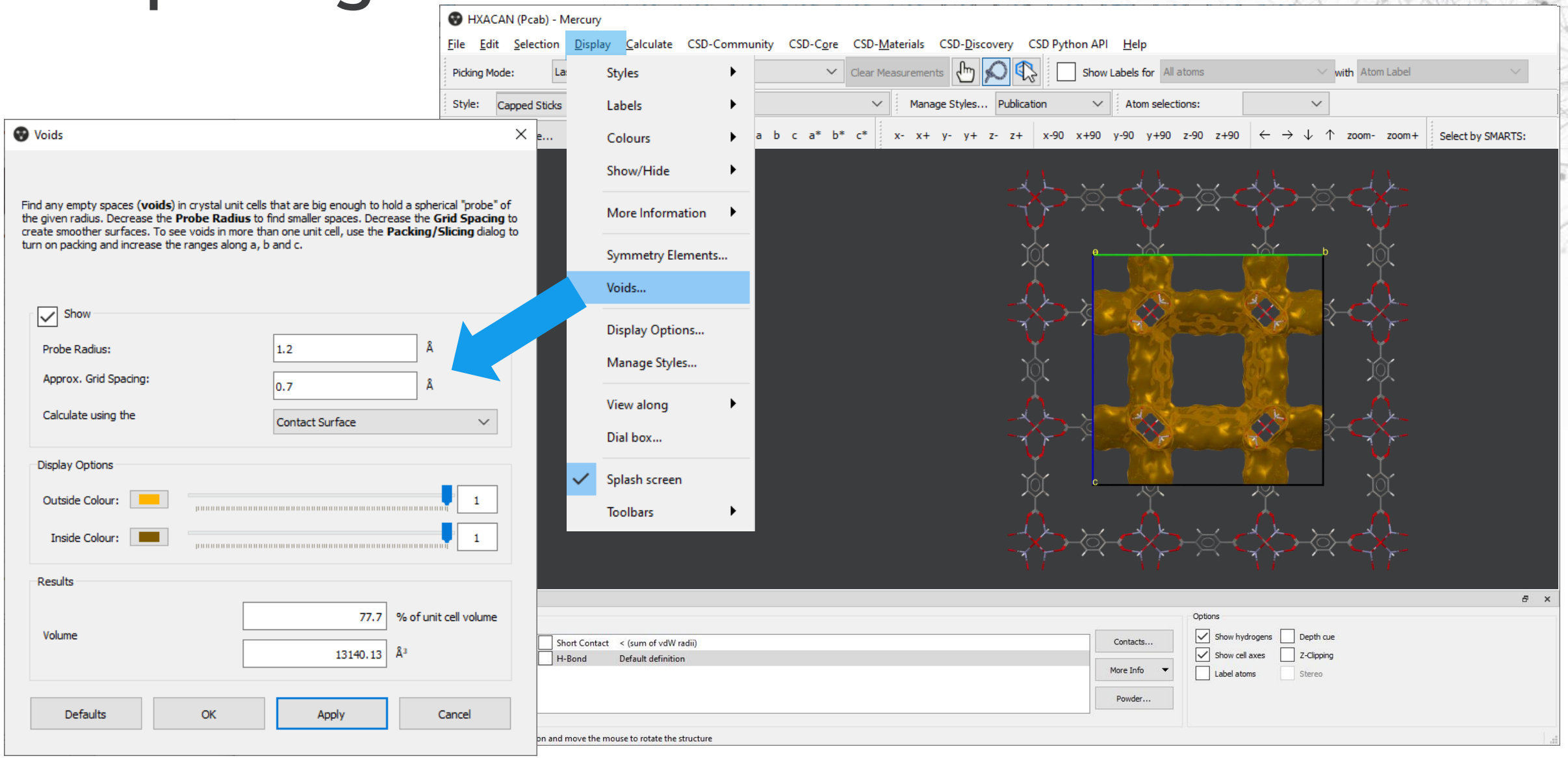
Tick "Transparent" to see through the plane

Exploring voids

CSD Refcode: SAHYIK



Exploring voids

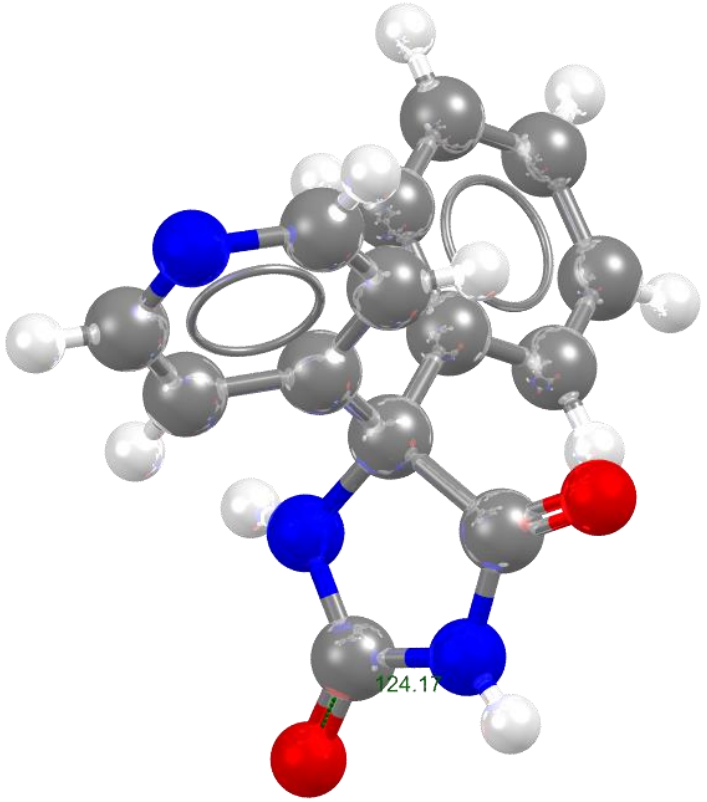


Explore More!

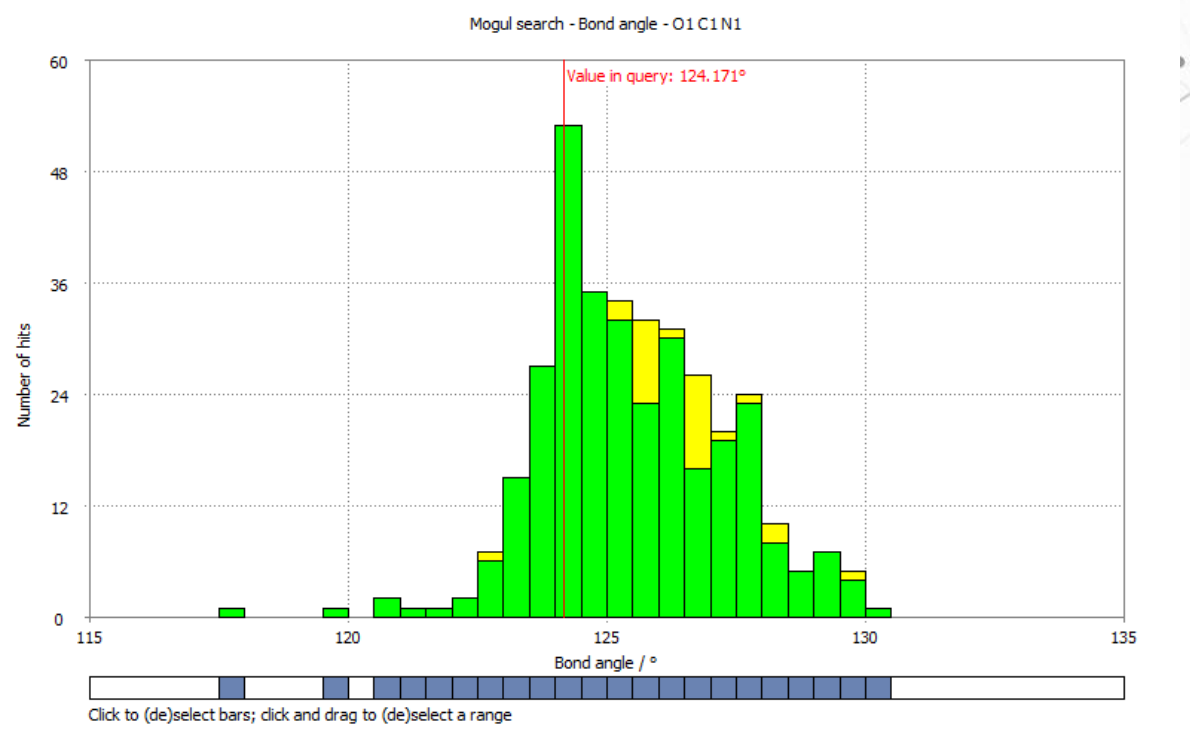
- So far we have explored the backbone of the Mercury analysis tools.
- You can also find a range of more advanced tools you can use to gain more insights into your structures.
- Lets explore a selection of these that either complement or are built on the ones discussed in this session.

CCDC

Measurements of bonds, angles, and torsions

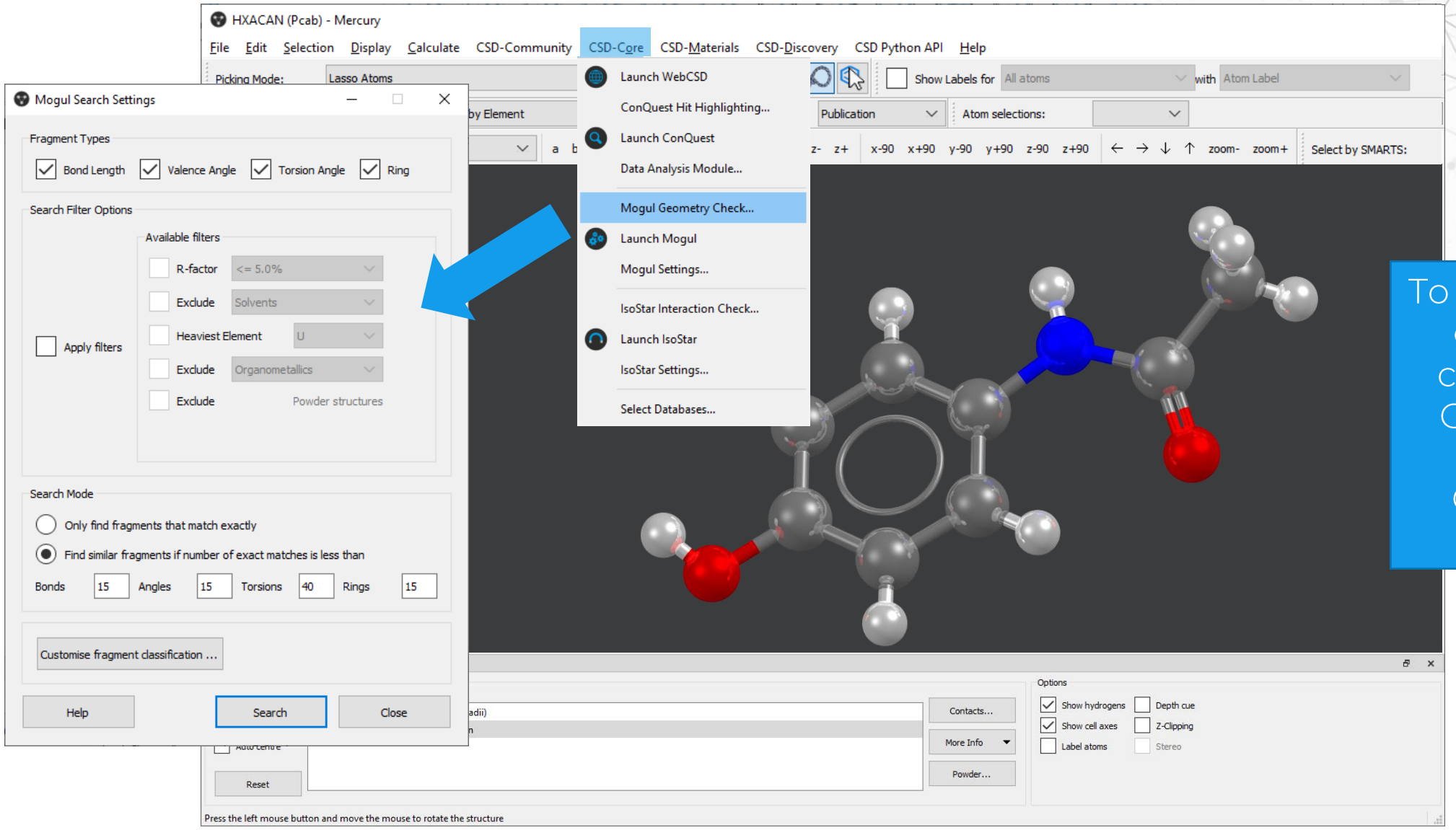


Mogul



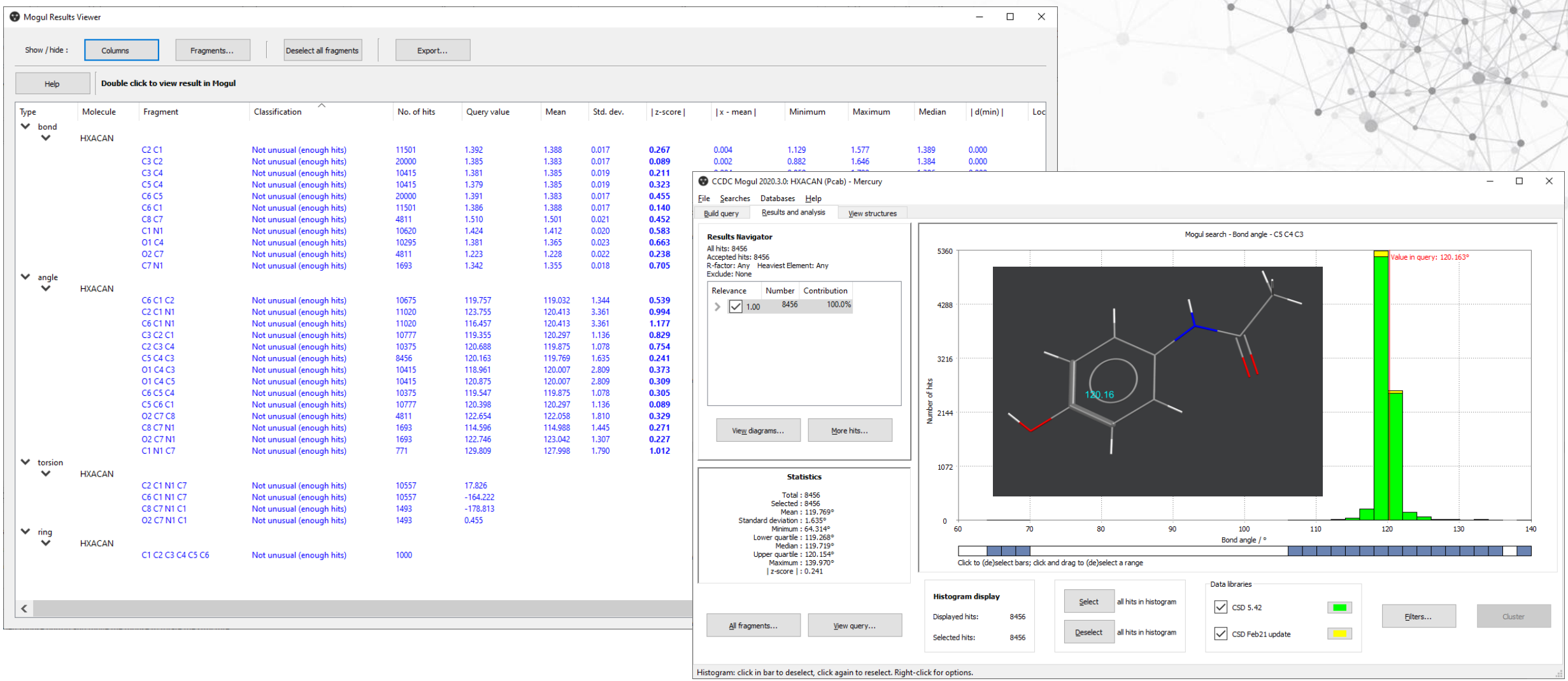
CCDC

Measurements of bonds, angles, and torsions



To run a Mogul geometry check go to CSD-Core > Mogul Geometry Check

Measurements of bonds, angles, and torsions



Creating reports

Molecular Geometry Report for HXACAN

CCDC advancing structural science

Molecular Analysis

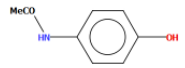


Figure 1. Diagram for HXACAN

Identifier
SMILES
Molecular Weight
Molecular Formula
Heavy Atoms
H-bond Donors
H-bond Acceptors
Rotatable Bonds
Fraction N,O Atoms
Fraction Halogen Atoms

Bond Lengths

Atom 1	Atom 2	
C2	C1	1.392
C3	C2	1.385
C3	C4	1.381
C5	C4	1.379
C6	C5	1.391
C6	C1	1.386
C8	C7	1.51
C1	N1	1.424
O1	C4	1.381
O2	C7	1.223
C7	N1	1.342

Bond Valence Angles

Atom 1	Atom 2	Atom 3
C6	C1	C2
C2	C1	N1
C6	C1	N1
C3	C2	C1
C2	C3	C4
C5	C4	C3
O1	C4	C3
O1	C4	C5
C6	C5	C4
C5	C6	C1
O2	C7	C8
C8	C7	N1
O2	C7	N1
C1	N1	C7

Crystal Structure Report for HXACAN

CCDC advancing structural science

Crystal Structure Analysis

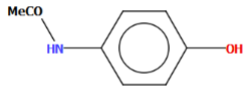


Figure 1. Diagram for HXACAN

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)	1497.98
R-Factor	7.70

Volume and Packing Analysis

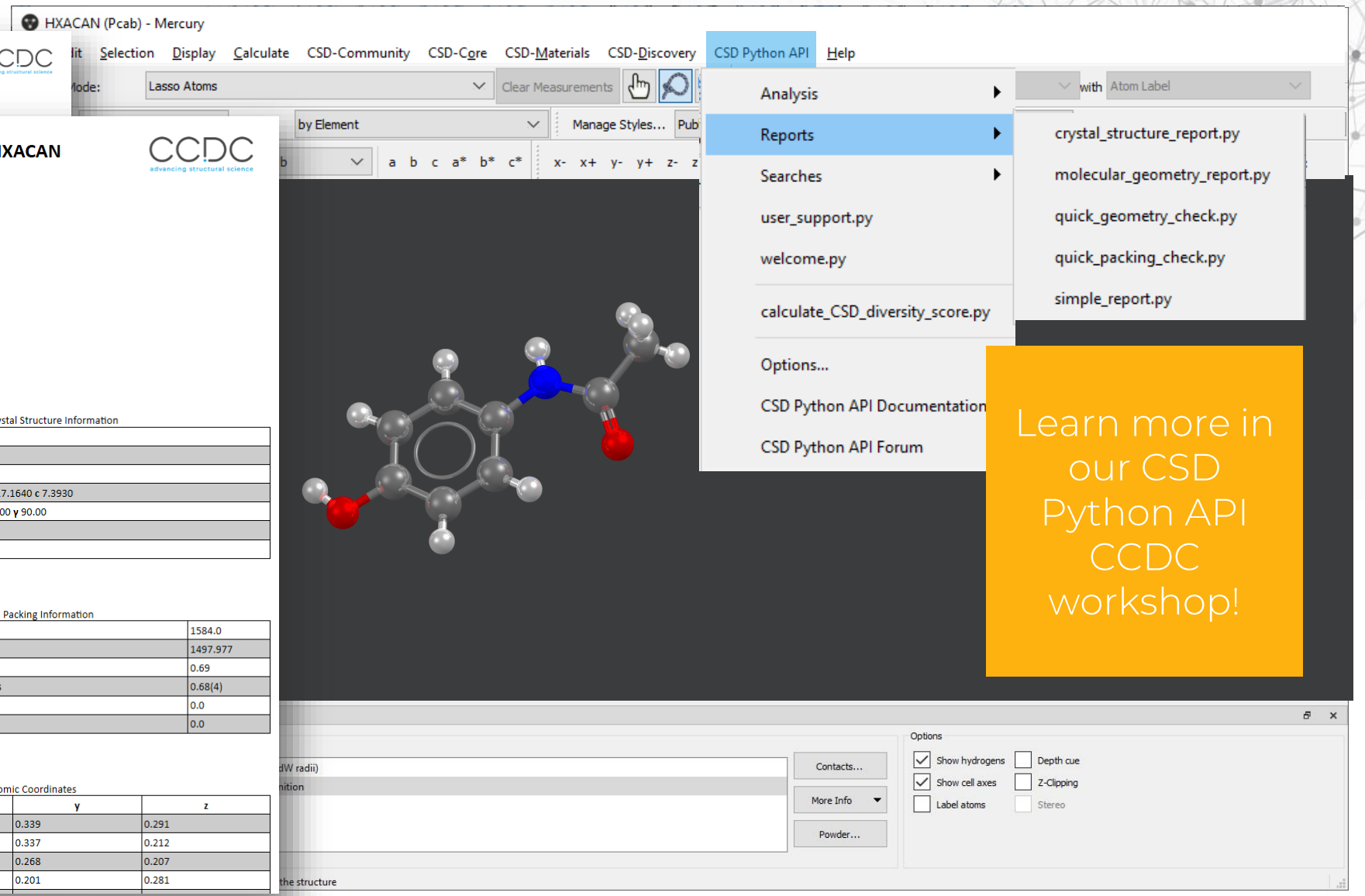
Table 2. Crystal Packing Information

Estimated volume from 18 Å³ 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

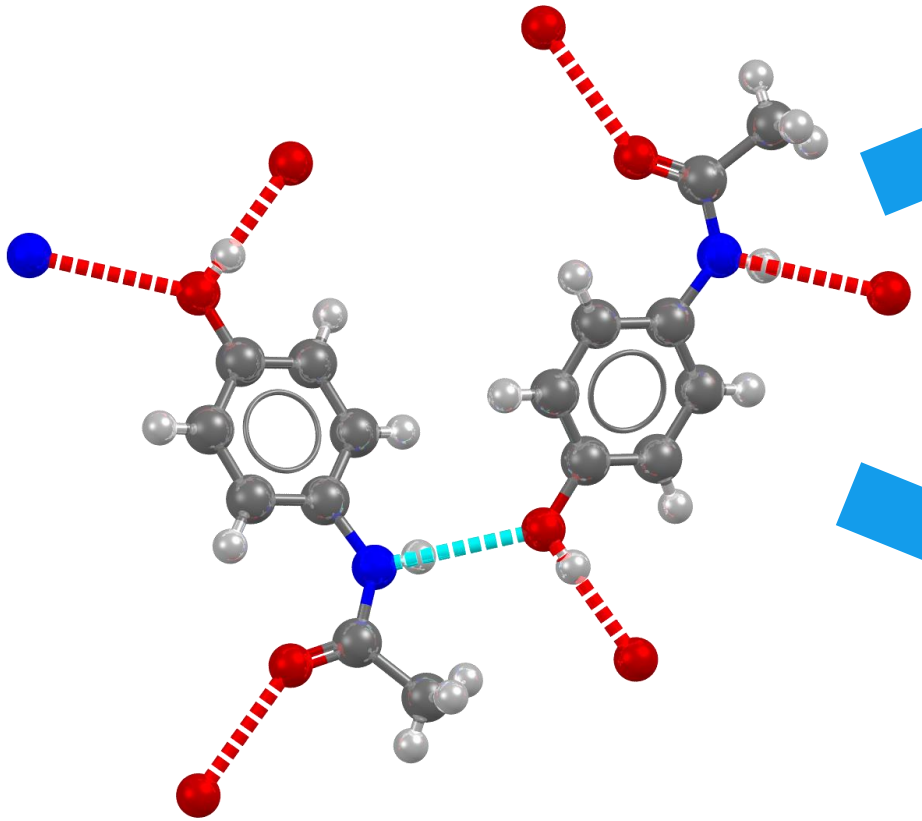
Table 3. Atomic Coordinates

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

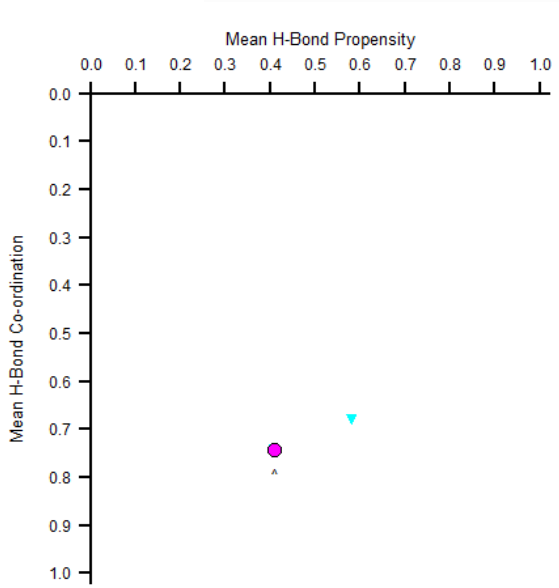


Learn more in our CSD Python API CCDC workshop!

Hydrogen Bonds



Full Interaction Maps (FIMs)

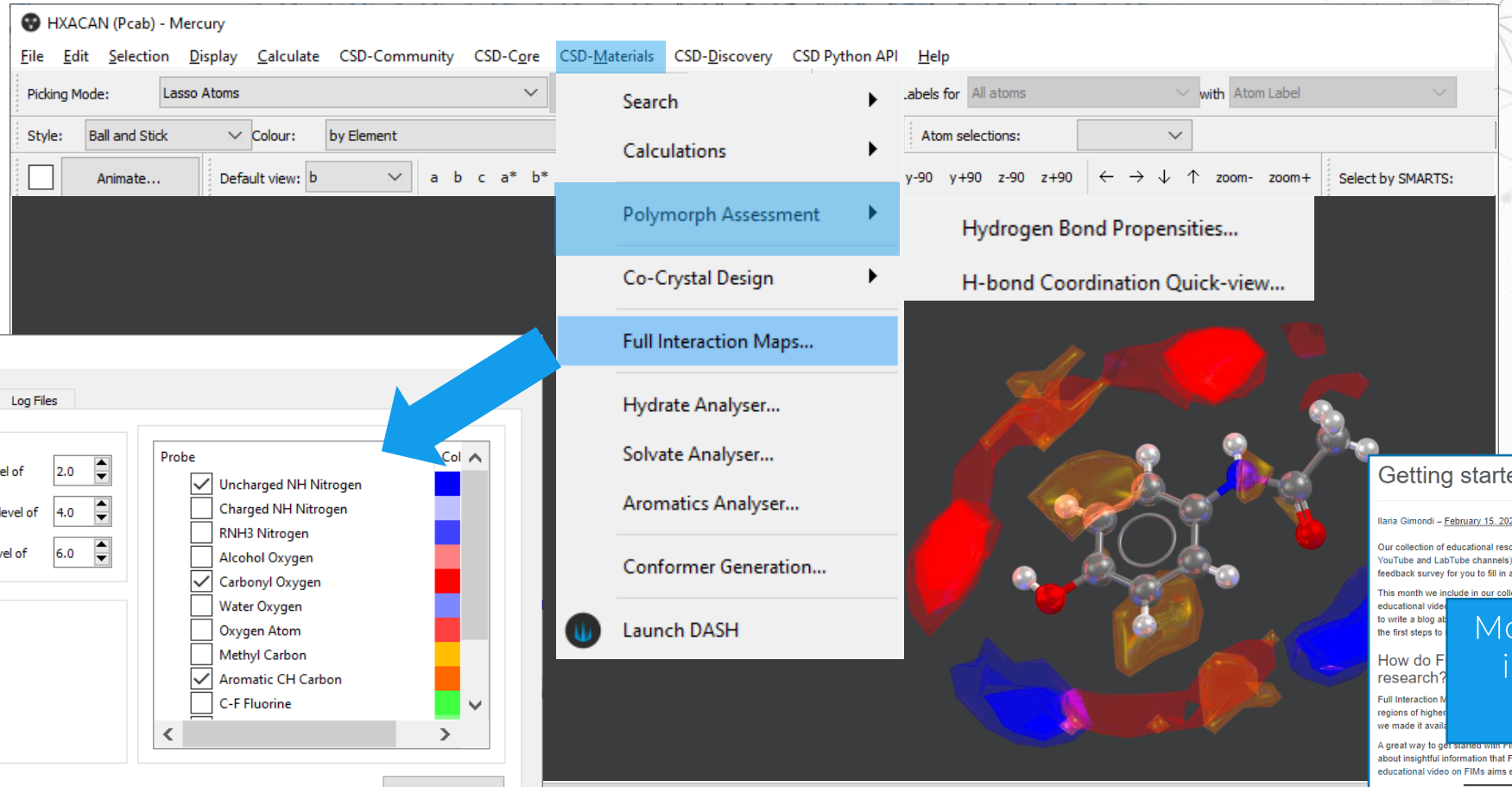


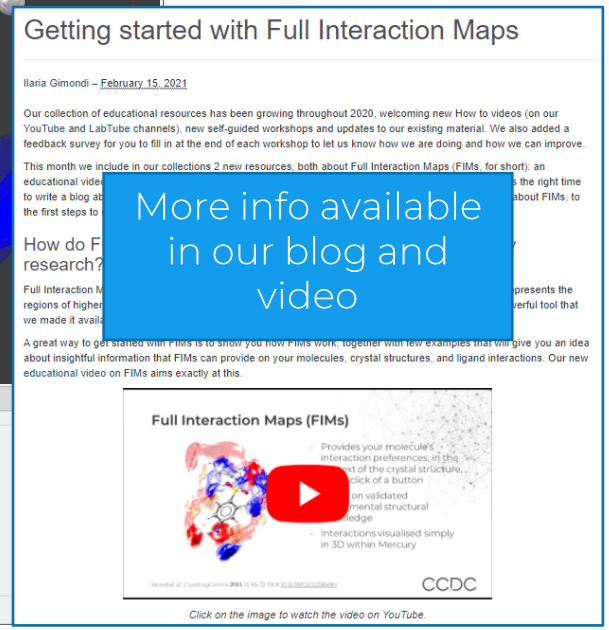
Hydrogen Bond Propensity (HBPs)

CCDC

Creating a FIMs and HBPs

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

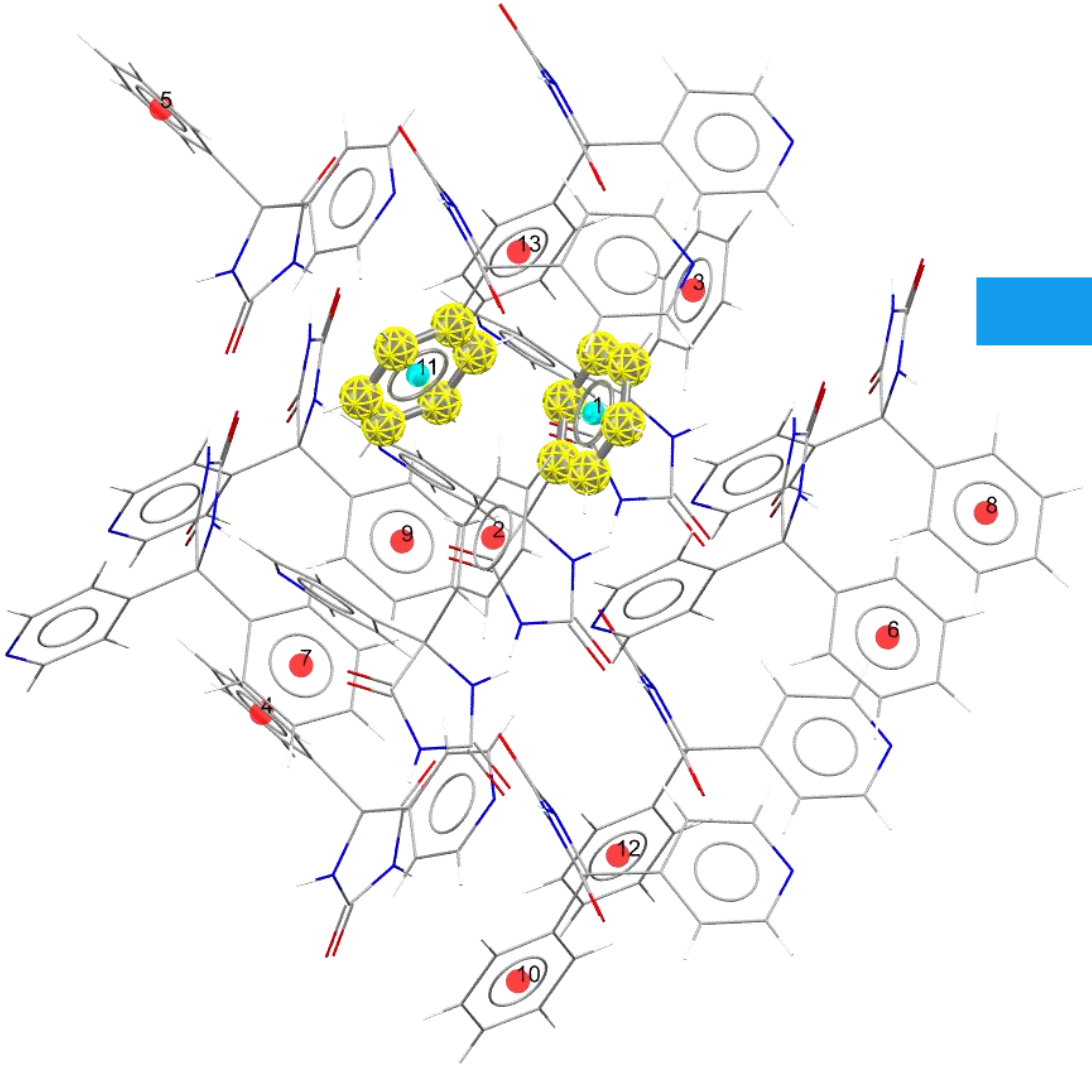




More info available in our blog and video

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

Centroids, orientations and interactions



Aromatics Analyser

Aromatics Analyser... GODRAS

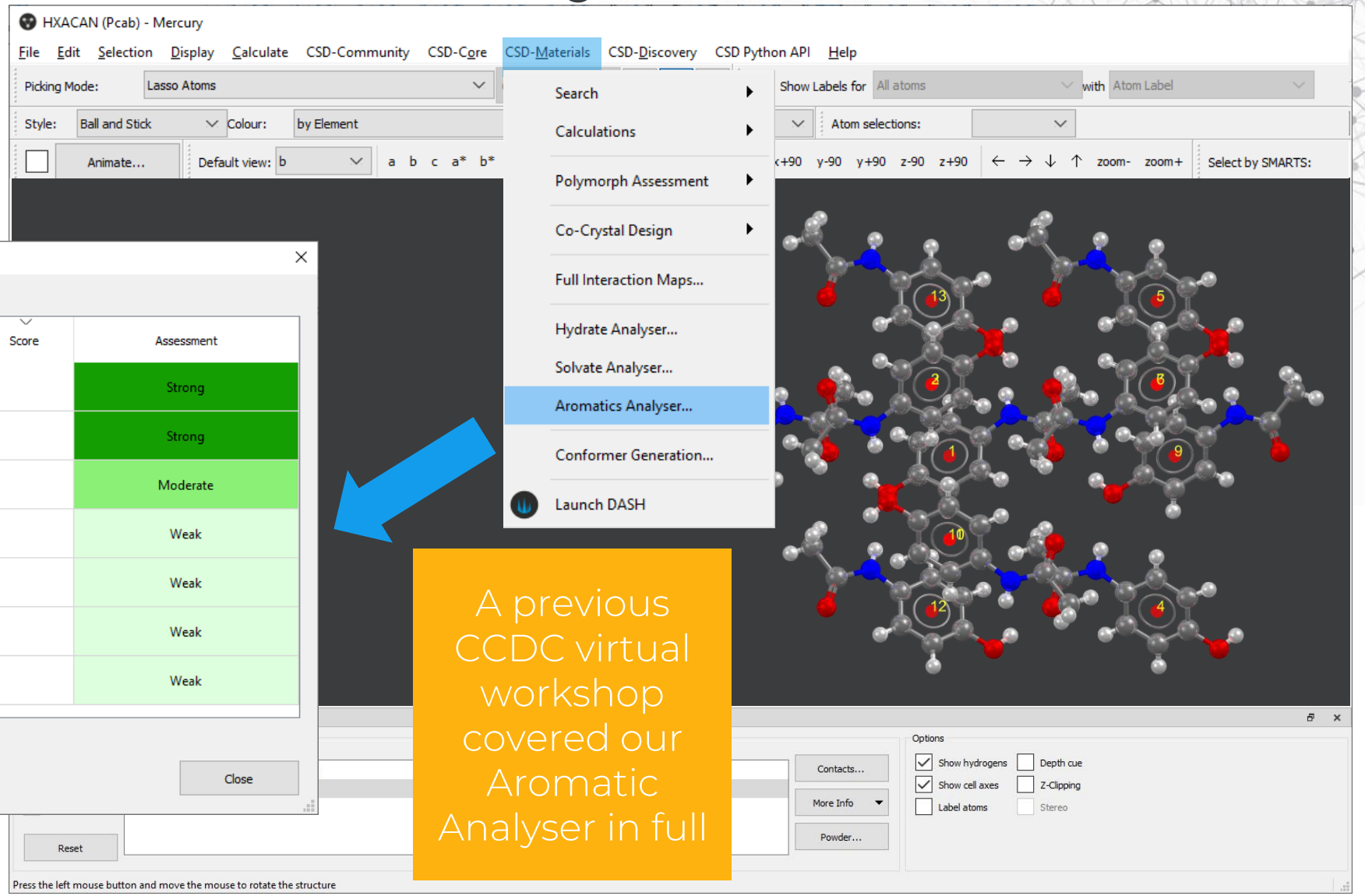
Select atoms in just **one** molecule

	Centroid1	Centroid2	Distance	Relative Orientation	Inter-molecular	Score	Assessment
1	1	11	4.91	67.32	Yes	8.9	Strong
2	1	13	4.91	67.32	Yes	8.9	Strong
3	1	2	7.27	0	Yes	1.5	Weak
4	1	3	7.27	0	Yes	1.5	Weak
5	1	6	8.07	77.39	Yes	0.8	Weak
6	1	7	8.07	77.39	Yes	0.8	Weak
7	1	8	9.16	77.39	Yes	0.4	Weak

☐ Include Intramolecular pairs ☐ Exclude symmetry equivalent interactions

Calculate | Export | Atom info | Close

Using the Aromatics Analyser



	Centroid1	Centroid2	Distance	Relative Orientation	Inter-molecular	Score	Assessment
1	1	2	4.65	58.43	Yes	8.9	Strong
2	1	10	4.87	50.79	Yes	8	Strong
3	1	12	5.94	26.95	Yes	5.9	Moderate
4	1	7	8.93	0	Yes	0.6	Weak
5	1	8	8.6	58.43	Yes	0.6	Weak
6	1	6	9.38	0	Yes	0.4	Weak
7	1	4	9.88	50.79	Yes	0.2	Weak