

CSD Tutorial

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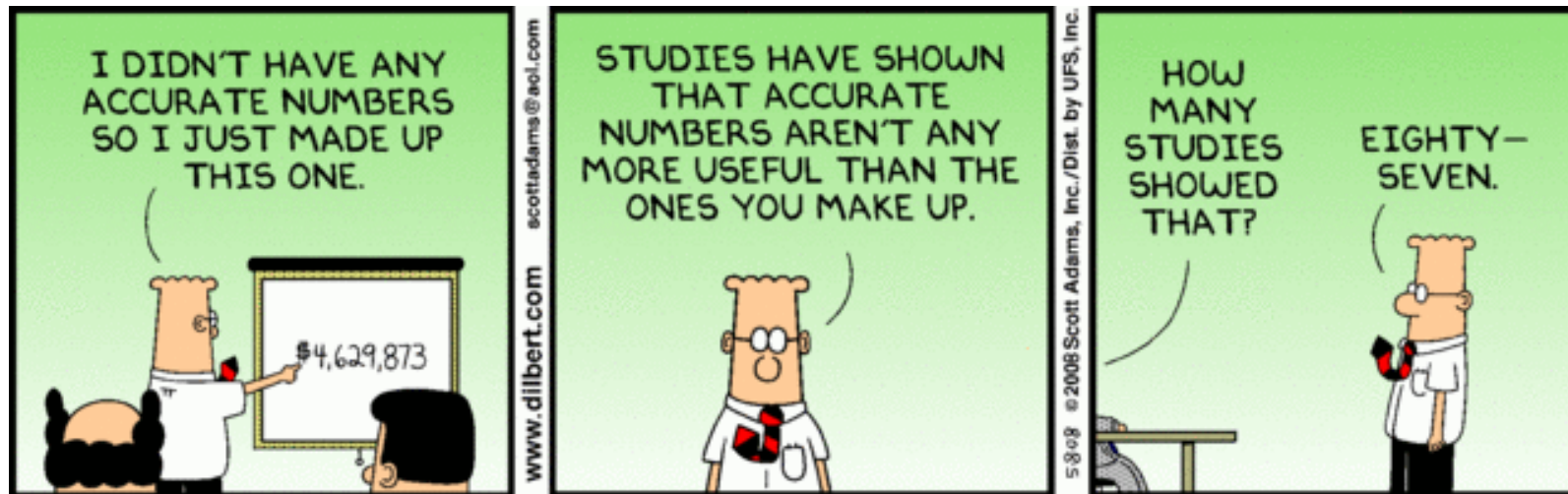
The Cambridge Crystallographic Data Centre

What is a crystallographic database?

- A structured collection of data about crystals and crystal structures
- Typically containing information on:
 - Chemical composition, position of atoms, unit cell dimensions, space group, experimental parameters and bibliographic details
 - Plus more information about structures if relevant to the scientific area
- What makes crystallography special?
 - Standard agreed file format
 - *Every* published structure is added to the appropriate database
 - Established *curated* databases rather than just collections of data
- A database implies some level of quality control and some level of processing & validation to the structures
 - Allowing you to learn from the data without having to re-process it

Importance of data quality

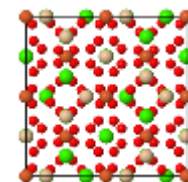
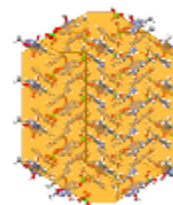
- The ability of a database search to answer a question is limited by the quality of the data



- Not just the quality of the diffraction experiment & the refinement, but also the CIF & data included!

Before we start....

- What kind of crystallography are you interested in?
 - Organic or metal-organic
 - Inorganic
 - Protein
- Who had heard of the CSD?
- Who has searched the CSD online?
- Who has used desktop software such as Mercury, Conquest or Mogul to look at the CSD?
- Who has determined their own crystal structure?
- Who has used our deposition service?
- Who has got their own structure in the CSD?



What do you need for today?

- Who still needs the CSD installed on their laptop?
- Who still needs the workshop materials and example files?

How you can access our tools?

- www.ccdc.cam.ac.uk

The image shows a screenshot of the CCDC (Cambridge Crystallographic Data Centre) website. The top navigation bar includes links for Community, Research & Consultancy, Solutions, News & Events, Support & Resources, and About Us. A dropdown menu is open under 'Solutions', listing options: Solutions, CSD, CSD-Community, CSD-Entorp, CSD-System, CSD Discovery, CSD-Materials, and Partner Software. The 'CSD-Community' option is highlighted. Below the navigation bar, there is a banner for 'ACS FALL 2019 MEETING' and a section titled 'World-leading experts in structural chemistry data, software and knowledge for materials science'. A second, semi-transparent window is overlaid on the right side of the page, titled 'CSD-Community'. This window contains a list of tools and services offered by CCDC, each with an icon and a brief description.

CCDC

Search Register Sign In

Community Research & Consultancy Solutions News & Events Support & Resources About Us









ACS FALL 2019 MEETING
August 25-29. Meet with 1334.

World-leading experts in structural chemistry data, software and knowledge for materials science

Big data leads the way for structural chemistry
The Cambridge Structural Database reaches 1,000,000 structures

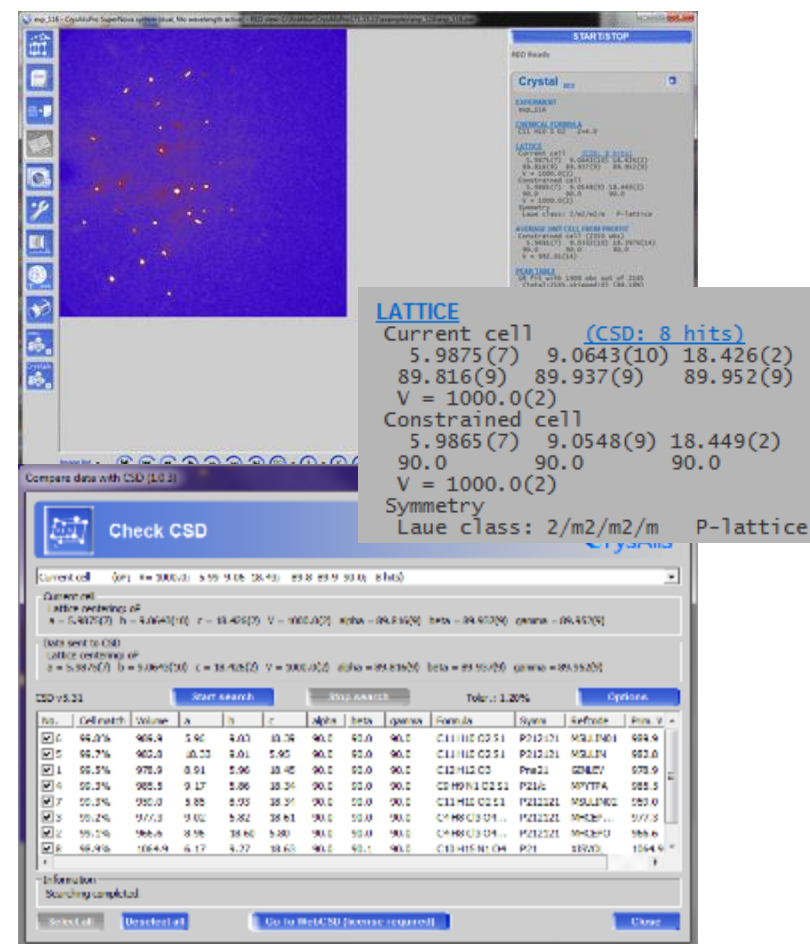
CSD-Community

The CCDC offers a selection of products and services free of charge for the benefit of the scientific community. The services detailed below cover a wide range of crystallographic tools - from data collection, validation and visualisation to teaching, research and analysis.

 Mercury Crystal Structure Visualisation and Exploration Made Easy. Advanced features in Mercury are available with a CSD-System in the full Mercury software.	 CellCheckCSD A command-line tool for performing crystal structure reduced cell checks against the CSD
 enCIFer CIF checking, editing and visualisation software from the CCDC	 CSD Educational Collection Free 750+ structure subset of the CSD for teaching purposes
 CSDSymmetry The most complete collation of observed molecular and crystallographic symmetry properties to date	 Access Structures View and retrieve structures in the Cambridge Structural Database
 Deposit Structures Upload your data to the CCDC for inclusion in the Cambridge Structural Database	 My Structures View, retrieve, edit and update your deposited data and share your structures with co-workers pre-publication

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



Data Deposition

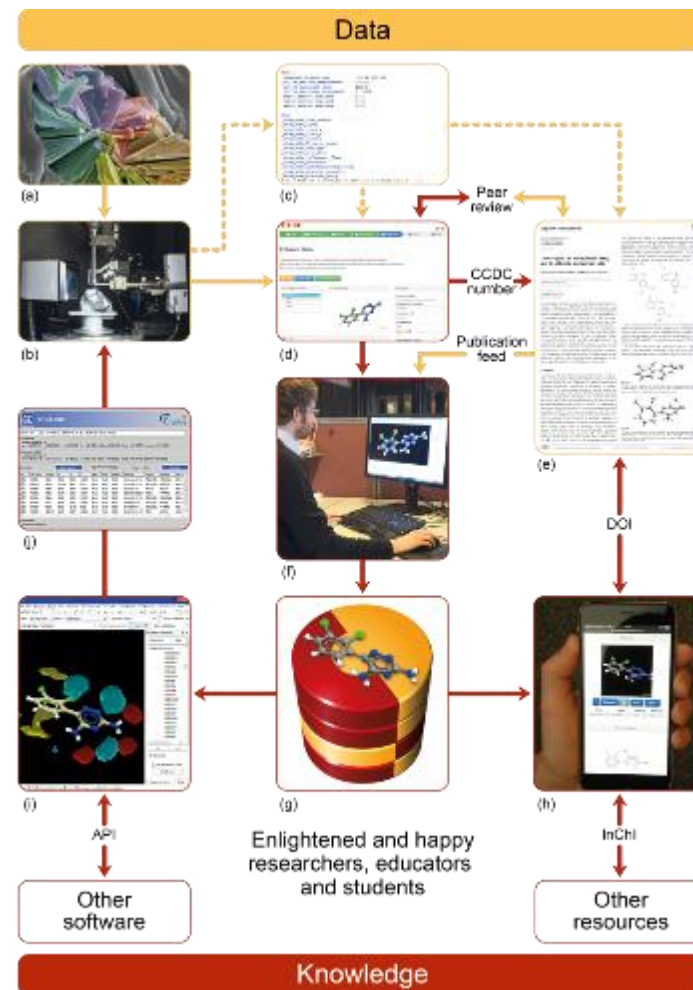
Deposition

- Data deposited pre-publication
 - When you know most about your structure
 - Enables links to data sets at the point of publication
 - Tailored deposition service

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.



Instructional videos


Home / Community / Educational Resources

Educational Resources


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

The CCDC and our colleagues continually produce educational materials for use in classroom and computer lab settings, or as independent study modules. Many of these materials make use of the Teaching Subset - a freely available set of over 750 structures that can be investigated with the free version of our Mercury visualisation and analysis program. Of course, all of our nearly 1 million entries are available for free through our [Cambridge Structural Database portal](#).


If you are an educator looking for resources, or if you would like to share them with the community, please contact us.



Information on the Teaching Subset



View short How-To videos from our YouTube Channel



How-To Video Guides CSD-Enterprise

View short How-To videos from our YouTube Channel

CSD Community

Deposit Structures



CSD Community

Updating Publication Information



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

Demo Files

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

Downloads

Legacy Downloads ☐

CSD-Community

CSD Symmetry

CSD Educational Collection

Example CIF 1 for CSD Deposit with Syntax Error	Details	Download
Example CIF 2 for CSD Deposit without Syntax Error	Details	Download
CSD Educational Collection refcode list	Details	Download
CSD Educational Collection CIFs	Details	Download

CellCheckCSD

Mercury (incorporating enCIFer)

Deposition Tutorial

- <https://www.ccdc.cam.ac.uk/deposit/>

Structure Deposition Workshop

Version 1.0 – January 2019


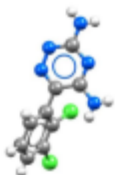


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- Further exercises.....

Example 1. Depositing CIF files

In the following example, you will learn how to register for a free account for the CCDC website. This will allow you to deposit data more easily, access and share your data using the MyStructures service. You will then look at depositing crystal data with the CCDC in the CIF file format. To do this, you will use the joint CCDC and R2 Karlsruhe web deposition service.

Obtaining example CIF files

In this example, you will use two example CIF files; one with correct syntax, and one where there are some syntax errors which need to be corrected during the deposition process. These files can be obtained from the CCDC website.

1. Open a web browser and navigate to <https://www.ccdc.cam.ac.uk/support-and-resources/downloads/>
2. Under CSD-Community, click on CSD Educational Collection and click Download beside Example CIF 2 for CSD Deposit with Syntax Error.
3. Click Agree & Download and save the "example_1.cif" file.
4. Repeat steps 2 and 3 for Example CIF 2 for CSD Deposit without Syntax Error to download the "example_2.cif" file. Remember the location where you save these files.

CIF deposition and validation service

Use this service to deposit your CIF files online and receive a CCDC CIF file number. You can also use this service to check the syntax of your CIF files before depositing them.

Sign in with your CCDC account

Obtain an invitation

Personal details

Upload CIF file

CheckCIF reports

Enhance your data

Review and submit

MyStructures

CCDC logo

Downloads

CSD-Community

Search for keywords

CSD-Community

Example CIF 1 for deposit with Syntax Error

Example CIF 2 for deposit with Syntax Error

Example CIF 3 for deposit without Syntax Error

Example CIF 4 for deposit without Syntax Error

Example CIF 5 for deposit without Syntax Error

Example CIF 6 for deposit without Syntax Error

Example CIF 7 for deposit without Syntax Error

Example CIF 8 for deposit without Syntax Error

Example CIF 9 for deposit without Syntax Error

Example CIF 10 for deposit without Syntax Error

Example CIF 11 for deposit without Syntax Error

Example CIF 12 for deposit without Syntax Error

Example CIF 13 for deposit without Syntax Error

Example CIF 14 for deposit without Syntax Error

Example CIF 15 for deposit without Syntax Error

Example CIF 16 for deposit without Syntax Error

Example CIF 17 for deposit without Syntax Error

Example CIF 18 for deposit without Syntax Error

Example CIF 19 for deposit without Syntax Error

Example CIF 20 for deposit without Syntax Error

Example CIF 21 for deposit without Syntax Error

Example CIF 22 for deposit without Syntax Error

Example CIF 23 for deposit without Syntax Error

Example CIF 24 for deposit without Syntax Error

Example CIF 25 for deposit without Syntax Error

Example CIF 26 for deposit without Syntax Error

Example CIF 27 for deposit without Syntax Error

Example CIF 28 for deposit without Syntax Error

Example CIF 29 for deposit without Syntax Error

Example CIF 30 for deposit without Syntax Error

Example CIF 31 for deposit without Syntax Error

Example CIF 32 for deposit without Syntax Error

Example CIF 33 for deposit without Syntax Error

Example CIF 34 for deposit without Syntax Error

Example CIF 35 for deposit without Syntax Error

Example CIF 36 for deposit without Syntax Error

Example CIF 37 for deposit without Syntax Error

Example CIF 38 for deposit without Syntax Error

Example CIF 39 for deposit without Syntax Error

Example CIF 40 for deposit without Syntax Error

Example CIF 41 for deposit without Syntax Error

Example CIF 42 for deposit without Syntax Error

Example CIF 43 for deposit without Syntax Error

Example CIF 44 for deposit without Syntax Error

Example CIF 45 for deposit without Syntax Error

Example CIF 46 for deposit without Syntax Error

Example CIF 47 for deposit without Syntax Error

Example CIF 48 for deposit without Syntax Error

Example CIF 49 for deposit without Syntax Error

Example CIF 50 for deposit without Syntax Error

Example CIF 51 for deposit without Syntax Error

Example CIF 52 for deposit without Syntax Error

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Example CIF 62 for deposit without Syntax Error

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Example CIF 91 for deposit without Syntax Error

Example CIF 92 for deposit without Syntax Error

Example CIF 93 for deposit without Syntax Error

Example CIF 94 for deposit without Syntax Error

Example CIF 95 for deposit without Syntax Error

Example CIF 96 for deposit without Syntax Error

Example CIF 97 for deposit without Syntax Error

Example CIF 98 for deposit without Syntax Error

Example CIF 99 for deposit without Syntax Error

Example CIF 100 for deposit without Syntax Error

Dataset identifiers

Deposition Numbers - Message (HTML)

File Message Insert Options Format Text Review Help Tell me what you want to do

From deposit_reply@ccdc.cam.ac.uk

To... Depositor

Cc...

Subject Deposition Numbers

Dear Depositor,

Thank you for depositing your crystal structure(s) at the Cambridge Crystallographic Data Centre. The data have been assigned to the following deposition numbers.

CCDC XXXXXXXX-XXXXXXYY

Summary of Data CCDC XXXXXXXX

Formula: C_x H_y O_z

Unit Cell Parameters: a XXXX b XXXX c XXXX Space Group

Summary of Data CCDC XXXXXXXX

Identifier sent after deposition so it can be included in a manuscript

[illegible]

What if I want to revise my data?

- You can revise your deposited data prior to publication

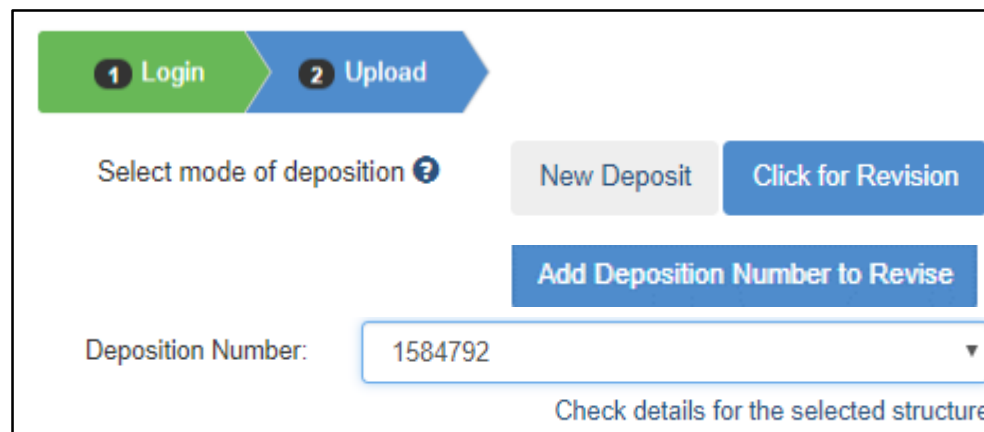
- During deposition:

1. **If logged in:**

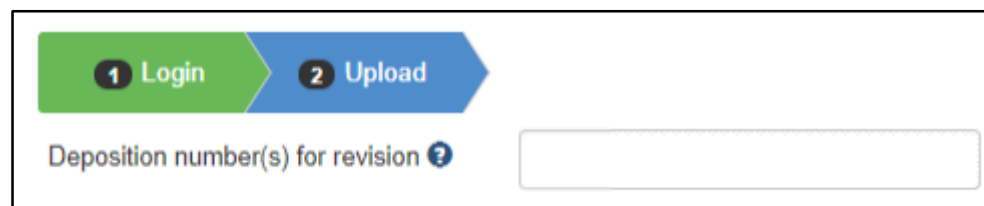
- a) 'Click for Revision'
- b) 'Add Deposition Number to Revise'
- c) Select Deposition Number you wish to revise

2. **If not logged in:**

- a) Add Deposition Number to 'Deposition Number(s) for revision box'



The screenshot shows the 'Upload' step of a two-step process (1 Login, 2 Upload). Below the progress bar, there is a 'Select mode of deposition' label with a help icon. To the right are two buttons: 'New Deposit' (grey) and 'Click for Revision' (blue). Below these is a blue button labeled 'Add Deposition Number to Revise'. Further down, there is a 'Deposition Number:' label followed by a dropdown menu showing '1584792'. At the bottom right, there is a link that says 'Check details for the selected structure'.



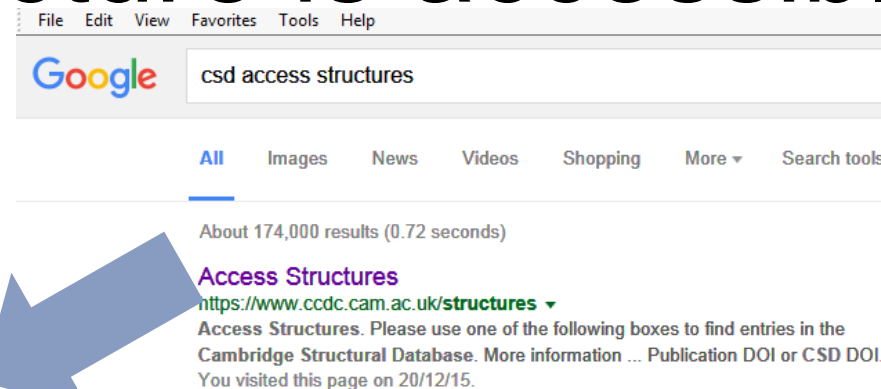
The screenshot shows the 'Upload' step of a two-step process (1 Login, 2 Upload). Below the progress bar, there is a label 'Deposition number(s) for revision' with a help icon, followed by an empty text input box.

- Revised dataset will be assigned the same Deposition Number
- Old revisions are stored but not visible

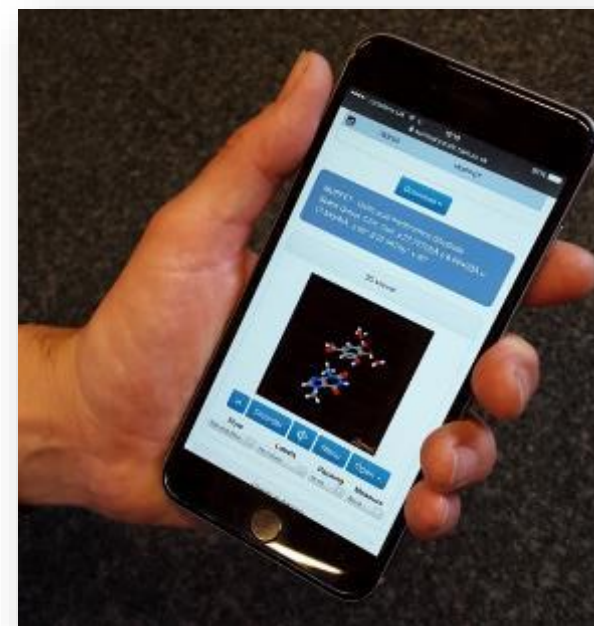
Data Access

Every individual structure is accessible.....

- Google CSD Access Structures
- Got to CCDC website
- Search and view

A screenshot of the CCDC Access Structures search interface. It features a search bar labeled 'Identifier(s)' with a placeholder text 'CCDC Number(s), CSD Number(s), CSD Refcode(s) or ICSD Number(s)'. Below the search bar, there are several input fields: 'DOI' (with a placeholder 'Example: publications.CCDC.CC.ac.uk/CCDC-DOI'), 'Refcode' (with a placeholder 'ICSD-1234'), 'Journal' (with a placeholder 'A. J. Chem. Soc., Perkin Trans. 2, 1970, 1234'), 'Full-text available' (with a dropdown menu set to 'Yes'), and 'CSD Refcode' (with a dropdown menu set to 'Yes'). There is also a 'Search' button at the bottom.

- Some of my favourite CSD Refcodes:
 - KITTEN, DISNEY, TURKEY, BADBOY, ITALIA
- Tell us yours!



Accessing data from general resources

The image displays two web interfaces for accessing chemical data. On the left is the ChemSpider interface, showing a 3D ball-and-stick model of a molecule and its chemical diagram. On the right is the PubChem interface, showing a list of crystal structures for compound 1983. A large blue arrow points from the PubChem 'Crystal Structures' section to the ChemSpider interface.

ChemSpider Interface:

- Names and identifiers: <http://dx.doi.org/10.5517/cc4zfp6>
- Comments: Structure CCDC 148418 from the Cambridge Structural Database reported in RSC article <http://dx.doi.org/10.1039/b000825g>
- Unit cell: $a=14.4429(5)\text{\AA}$, $b=8.0609(3)\text{\AA}$, $c=24.3908(7)\text{\AA}$, $\alpha=90.00^\circ$, $\beta=99.510(2)^\circ$, $\gamma=90.00^\circ$, $T=123(2)\text{K}$, space group $P2_1/n$, $Z=4$
- Submitted by: [antonywilliams](#)

PubChem Interface:

4.3 Crystal Structures

Crystal Structures: 1 of 31 (CCDC Number)	
CCDC Number	129925
Crystal Structure Data	DOI:10.5517/cc4c54t

Thumbnail:

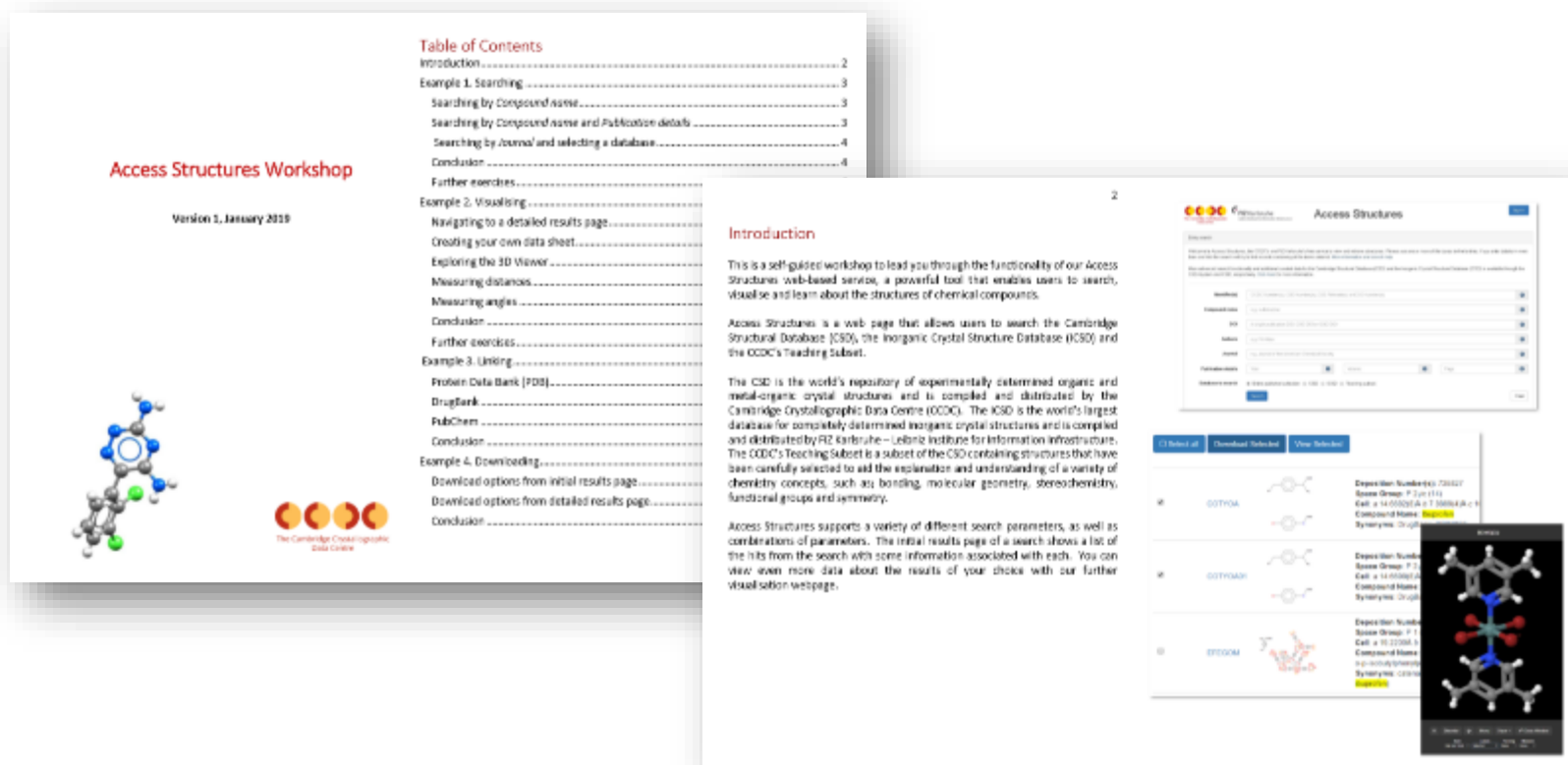
Associated Article: [DOI:10.1107/S0108270197018386](https://doi.org/10.1107/S0108270197018386)

* from The Cambridge Structural Database

<https://pubchem.ncbi.nlm.nih.gov/compound/1983#section=Crystal-Structures>

Access Structures Tutorial

- <http://www.ccdc.cam.ac.uk/structures>



The image displays two overlapping pages from the Access Structures tutorial. The left page is the 'Access Structures Workshop' (Version 1, January 2019), which includes a 'Table of Contents' and a '3D Viewer' interface. The right page is the 'Introduction' page, which provides an overview of the service and its search capabilities. Both pages feature the Cambridge Crystallographic Data Centre logo and a 3D molecular model.

Access Structures Workshop
Version 1, January 2019

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Introduction

This is a self-guided workshop to lead you through the functionality of our Access Structures web-based service, a powerful tool that enables users to search, visualise and learn about the structures of chemical compounds.

Access Structures is a web page that allows users to search the Cambridge Structural Database (CSD), the Inorganic Crystal Structure Database (ICSD) and the CCDC's Teaching Subset.

The CSD is the world's repository of experimentally determined organic and metal-organic crystal structures and is compiled and distributed by the Cambridge Crystallographic Data Centre (CCDC). The ICSD is the world's largest database for completely determined inorganic crystal structures and is compiled and distributed by RZ Karlsruhe – Leibniz Institute for Information Infrastructure. The CCDC's Teaching Subset is a subset of the CSD containing structures that have been carefully selected to aid the explanation and understanding of a variety of chemistry concepts, such as: bonding, molecular geometry, stereochemistry, functional groups and symmetry.

Access Structures supports a variety of different search parameters, as well as combinations of parameters. The initial results page of a search shows a list of the hits from the search with some information associated with each. You can view even more data about the results of your choice with our further visualisation webpage.

WebCSD

Simple SearchStructure SearchUnit Cell Search

Unit Cell Searching

Lattice centringPrimitive (P)

a

e.g. 10.0

b

e.g. 10.0

c

e.g. 10.0

Search

Simple SearchStructure SearchUnit Cell Search

Simple text and numeric searching

Welcome to WebCSD. This service now includes the ability to search by structure. Please use one or more of the boxes to find entries and search help

Identifier(s)

CCDC Number(s), CSD Number(s)

Compound name

e.g. sulfadiazine

DOI

A single publication DOI, CSD Number(s)

Authors

e.g. F.H.Allen

Journal

e.g. Journal of the American Chemical Society

Publication details

Year

?

Volume

Database to search

☒ Entire published collection ☐ CSD ☐ ICSD ☐ Teaching subset

+ Add New Search Field

Search

Simple SearchStructure SearchUnit Cell Search

Chemical structure searching

Please draw your diagram or add a SMARTS string in the 'advanced' section below.

EI

C

N

O

S

H

F

Cl

Br

X

I

+

-

?

c1ccc(cc1)-c2ccc3c(c2)ncnc3

dotmatics

Match condition: ☐ Exact ☒ Substructure ☐ Similarity

SearchClear

Advanced

Help

Keyboard shortcuts

- Copy: Ctrl-C
- Delete: Ctrl-X
- Paste: Ctrl-V
- Undo: Ctrl-Z
- Redo: Ctrl-Y
- Select all: Ctrl-A

Query features

Query features describe how an atom or bond should behave in substructure searches. To add a feature:

- Right click on atom or bond
- Hover over 'query features' (atom only)
- Hover over a feature type (e.g. H-count, type)
- Select one of the options

More Information

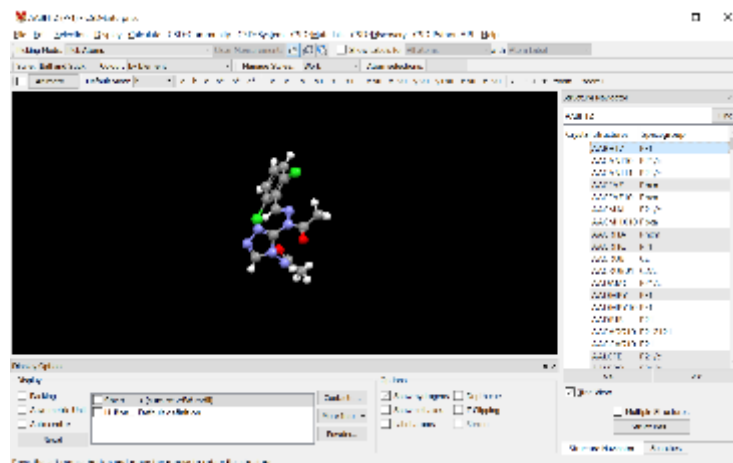
Educational resources – A teaching DB

The screenshot shows the CCDC website's 'Educational Resources' section. At the top, there's a navigation bar with links like 'Community', 'Research & Consultancy', 'Solutions', 'News & Events', 'Support & Resources', and 'The CCDC'. Below this, a breadcrumb trail reads 'Home / Community / Educational Resources'. The main heading is 'Educational Resources'. The text explains that the CCDC database contains over 800,000 real crystal structures and offers a 'Teaching Subset' of over 750 structures for free use. It also mentions a 'Mercury' visualization program. A call to action invites educators to contact education@ccdc.cam.ac.uk for supplementary materials. Below the text are five interactive tiles: 'Information on the Teaching Subset' (with a molecular model), 'Access a series of teaching modules developed by our collaborators' (with a molecular model), 'Download a series of self-guided workshop materials for CCDC tools and features' (with a book icon), 'View short How-To videos from our YouTube Channel' (with a video player icon), and 'The Periodic Table in Crystal Structures' (with a periodic table icon).

This screenshot shows the 'Access Structures' page on the CCDC website. It features a header with the CCDC logo and navigation links. The main heading is 'Az-Introduction to "Access Structures"'. The text explains that the full CSD database contains over 800,000 real crystal structures and that individual structures can be viewed and manipulated for free using the 'Access Structures' option. A 'Getting Started' section provides two methods to find a structure: 1. Using the CSD 'Access Structures' function on a computer or tablet, and 2. Finding the 'Access Structures' page using a search engine. A 'Basics' section explains how to view a particular structure by typing its refcode (e.g., 'CAFINE') into the 'CSD refcode' box. It also describes the 'Style' drop-down menu for changing the display and the 'Labels' drop-down menu for labeling atoms. A 'Packing' section explains how to view the unit cell and bulk structure. A 'TOP TIP' box advises users to look at the larger crystal structure (e.g., the unit cell) and the bulk structure (e.g., the 3x3x3 unit cells) to avoid confusion. The page includes a molecular model of caffeine and a chemical structure diagram.

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

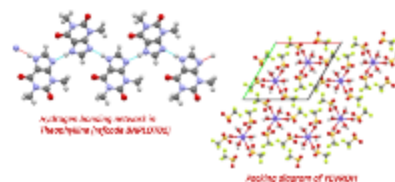
Educational resources and tutorials



Example 1. Generating Structure Views

To communicate science effectively, researchers must be able to provide clear images of structural models for inclusion in manuscripts and presentations. The program Mercury contains many features which can assist in the production of high-quality, high-resolution graphics of molecules.

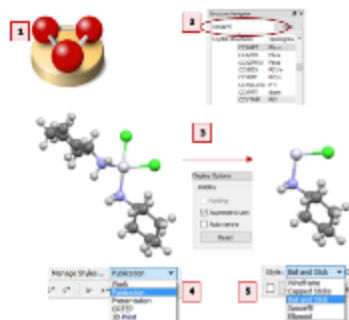
This example shows you how to build structural views such as packing diagrams, void space, and intermolecular interactions, which can then be output in a range of formats for use in various communications. For these purposes we will be using **Mercury** in the Teaching Subsets, however, the following methods can be applied to any entry in the CSD, or any of your own structure files.



Generating a Simple Molecular View

In this section, you will learn how to manipulate style options in order to generate a simple molecular view.

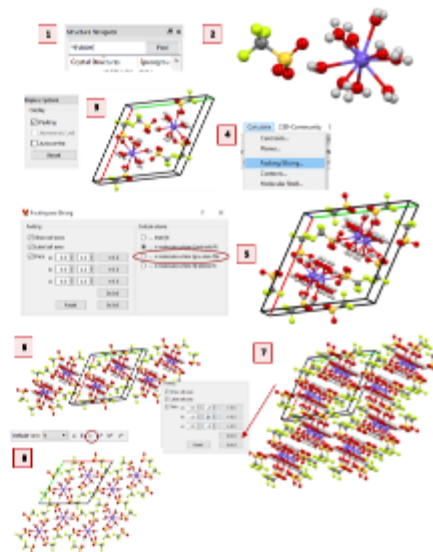
1. Open Mercury by clicking the icon, or launching from the start menu.
2. In the Structure Navigator window, type the refcode CCMPT, to bring up the structure of a diaphan molecule.
3. The whole molecule should be displayed in the viewing window. In the Display Options toolbar, tick the box for Asymmetric Unit and you will see half of the molecule disappear. Untick the box to bring back the whole molecule.
4. To generate the view in Step 3 above, choose Publication from the Mercury Styles dropdown menu. Experiment by choosing other styles from this menu.
5. To change the style of the atoms and bonds in the structure, but to keep the white background, use the Styles dropdown box. Experiment with this by choosing some other options. Return to 'Ball and Stick' when you are done.



Generating a Packing Diagram

In this section, you will learn how to generate a packing diagram of a structure.

1. In Mercury, type the refcode YBWHH in the Structure Navigator toolbar.
2. This will display the metal-organic salt compound, non-aqueous-sulfonate, which crystallizes in the space group P6₃/m. Tick and untick the Asymmetric Unit box to see what atoms are generated by symmetry (Step 3 above).
3. Tick the Packing box in the Display Options toolbar to generate a packing diagram.
4. To change the settings of the packing diagram, choose Go/View > Packing/Sliding from the top menu. This will launch the Packing and Sliding dialog box.
5. The top half of this window contains the packing preferences. Click the radio button next to 'in molecules where any atom fits' and see how this changes the packing diagram in the Mercury window. Notice how two more metal-hydrate complexes appear in the center of the view and triflate anions appear at the edges.
6. To change the range of the packing diagram along any individual axis, click the +0.5 buttons by the corresponding axis. Or type a specific range in the text boxes. This example is -1.0 - 2.0 along the b axis.
7. Alternatively, click the 2x2x2 or 3x3x3 buttons to make an expanded packing diagram along all three axes at once.
8. To orient the view along the crystallographic axes, click the a, b, or c button just above the viewing window.
9. When you are done, click the Close button at the bottom of the Packing and Sliding dialog box to exit.

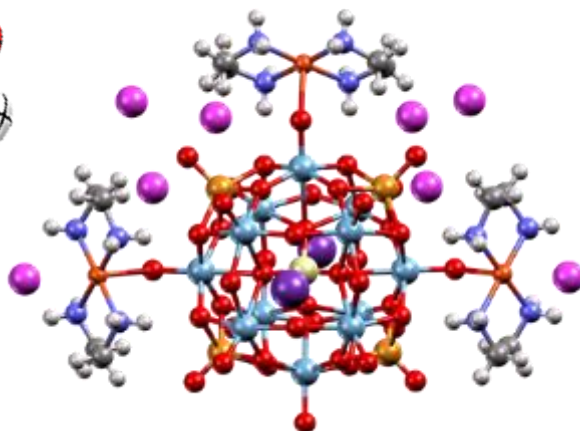
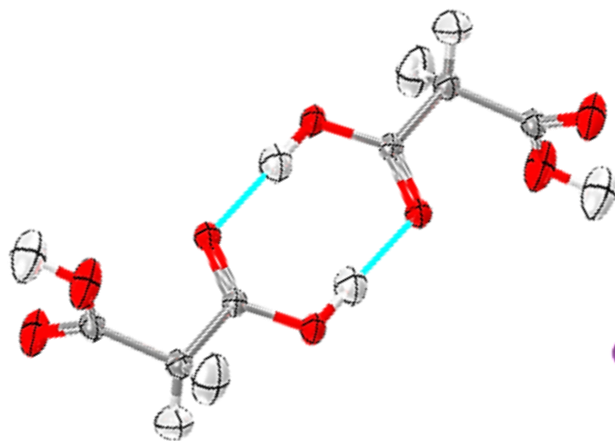
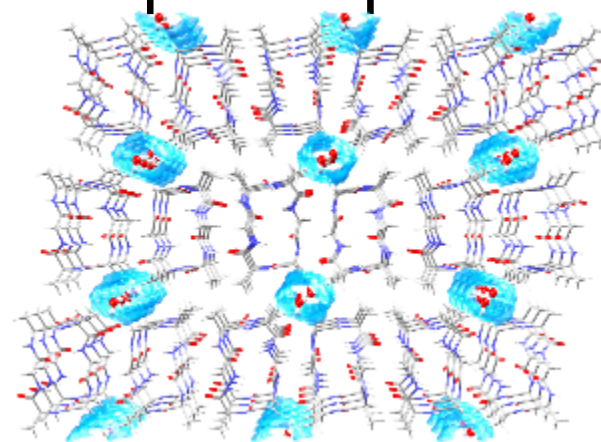


Exploring Mercury

Visualisation

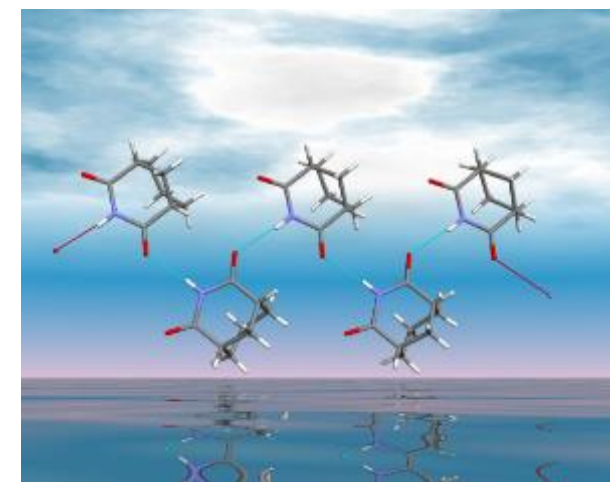
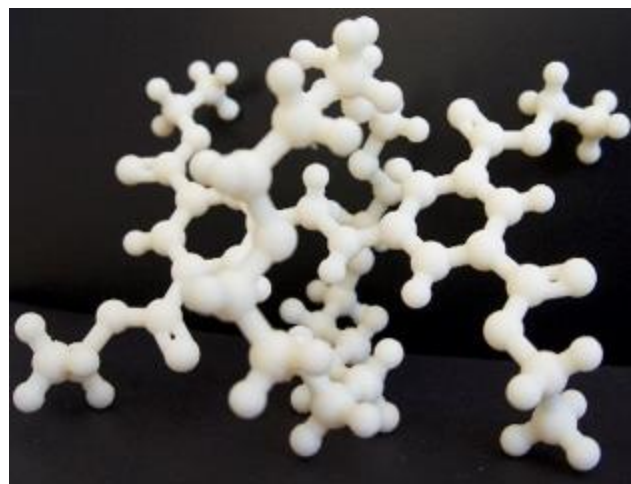
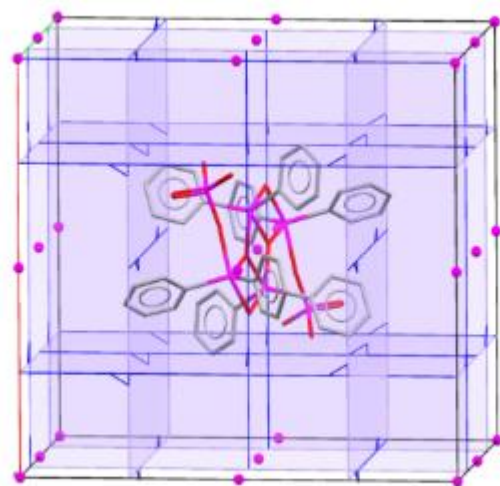
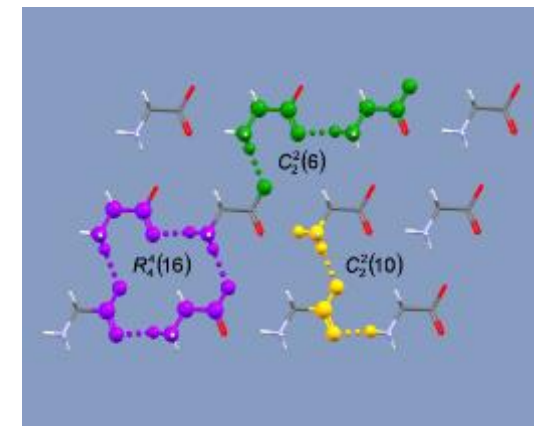
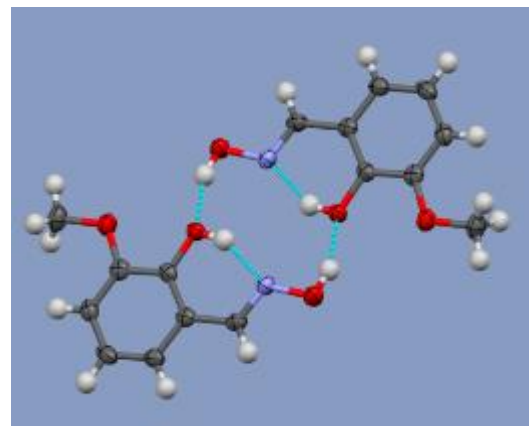
Scientific communication

- The right representation can convey complex topics easily

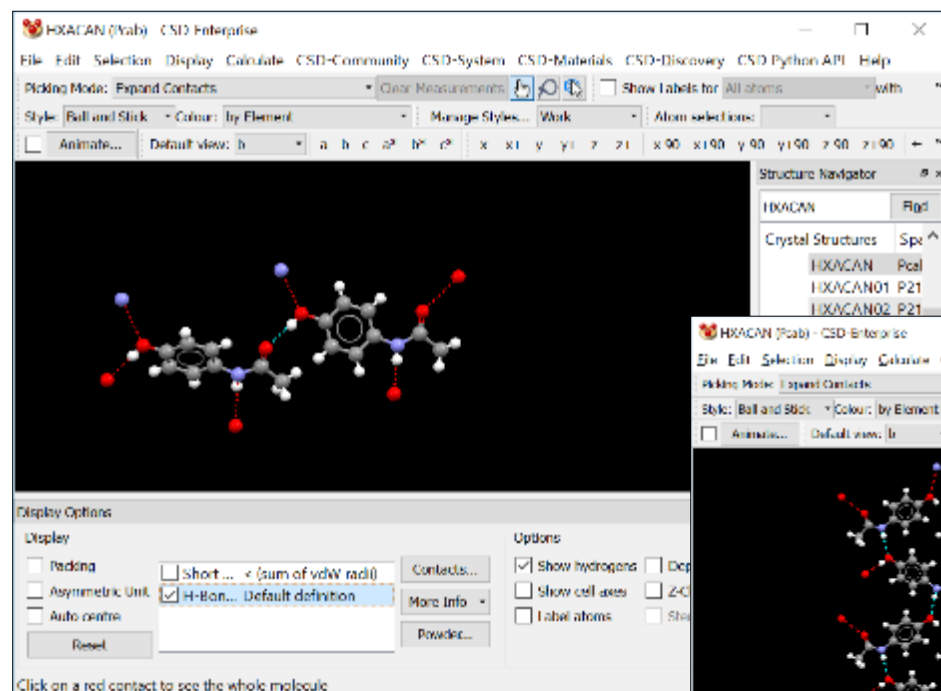


Structure visualisation

- Symmetry elements
- Displacement ellipsoids etc.
- POV-Ray
- 3D printing
- Graph sets
- Movies



Hydrogen bonds



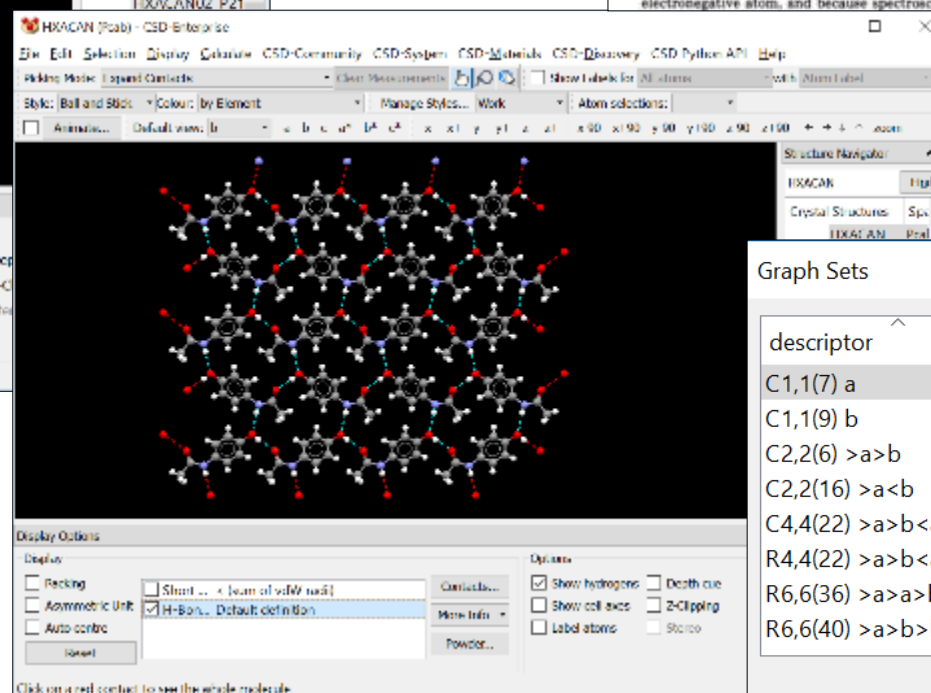
Encoding and Decoding Hydrogen-Bond Patterns of Organic Compounds

MARGARET C. ETTER

Department of Chemistry, University of Minnesota, Minneapolis, Minnesota 55455

Received June 20, 1989 (Revised Manuscript Received January 31, 1990)

Are hydrogen-bond patterns predictable? Benzoic acids form cyclic dimers. Salicylic acid has an intramolecular hydrogen bond. These hydrogen-bond patterns seem obvious because they satisfy the chemical criteria of pairing a somewhat acidic hydrogen with an electronegative atom, and because spectroscopic and

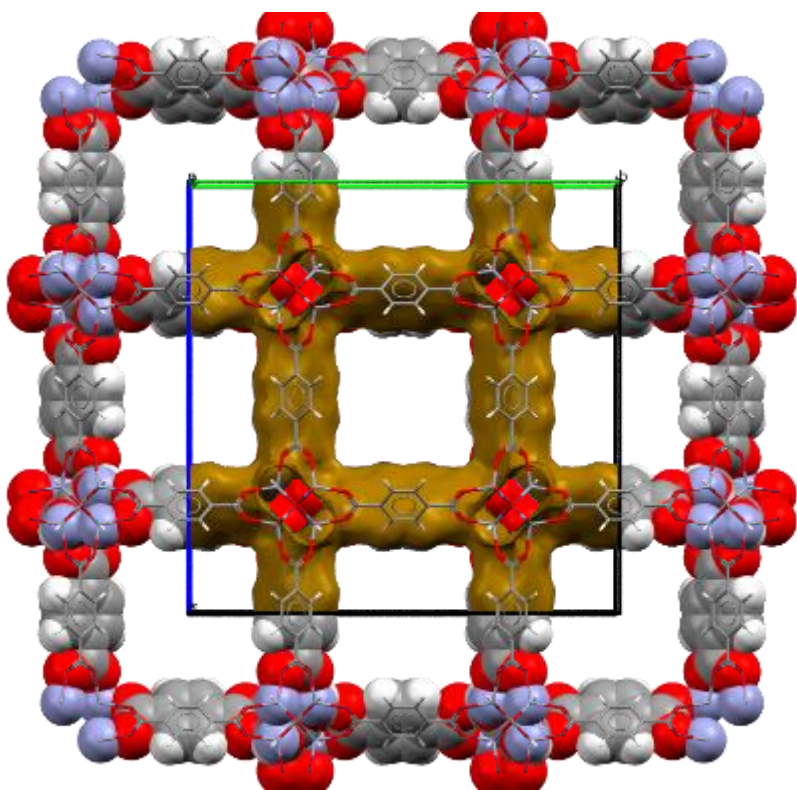


Graph Sets

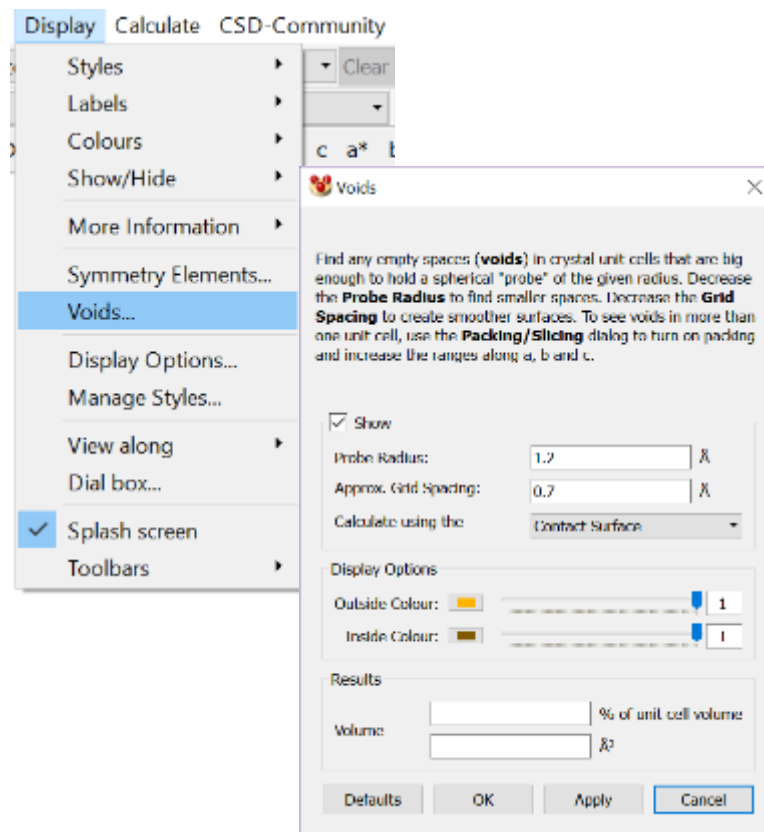
descriptor	level	period	# molecules
C1,1(7) a	1	1	2
C1,1(9) b	1	1	2
C2,2(6) >a>b	2	2	3
C2,2(16) >a<b	2	2	3
C4,4(22) >a>b<a<b	2	4	5
R4,4(22) >a>b<a>b	2	4	4
R6,6(36) >a>a>b<a<a<b	2	6	6
R6,6(40) >a>b>b<a>b>b	2	6	6

Options

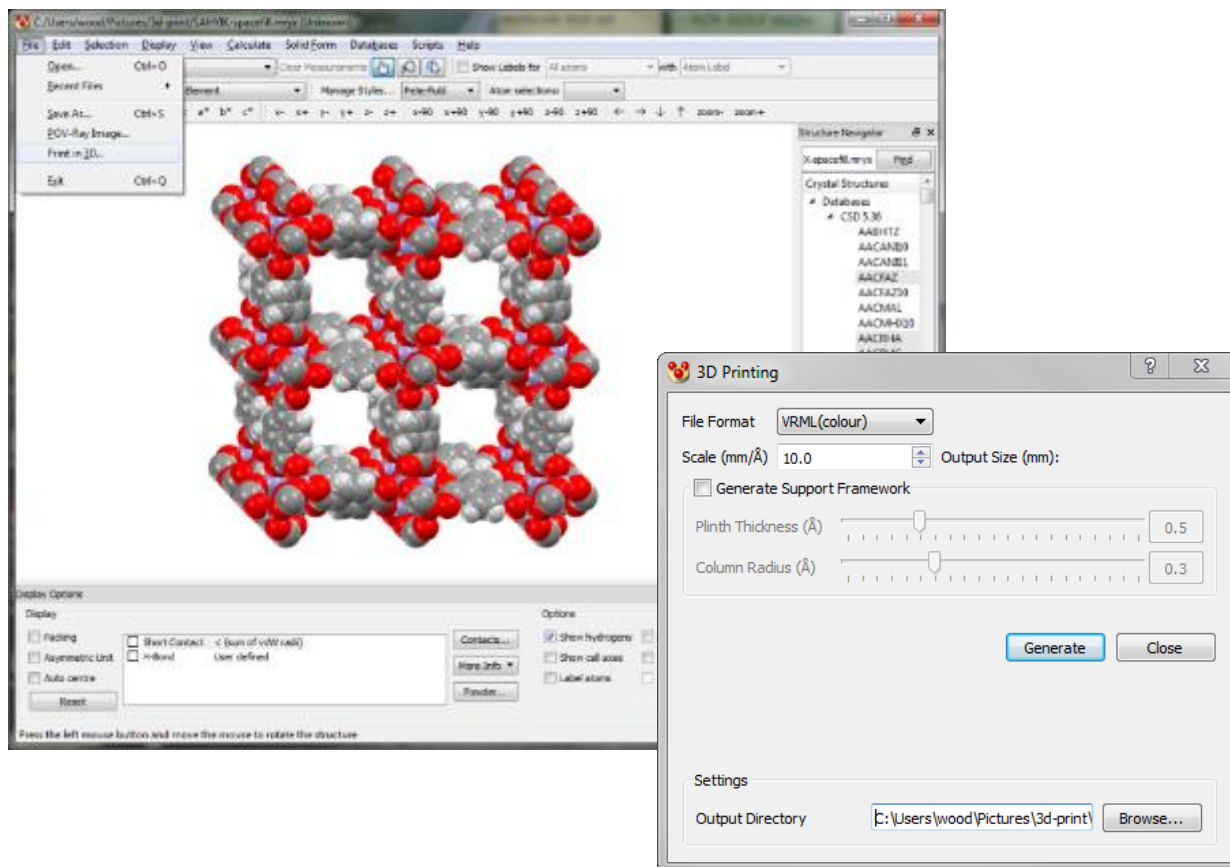
Empty space visualisation



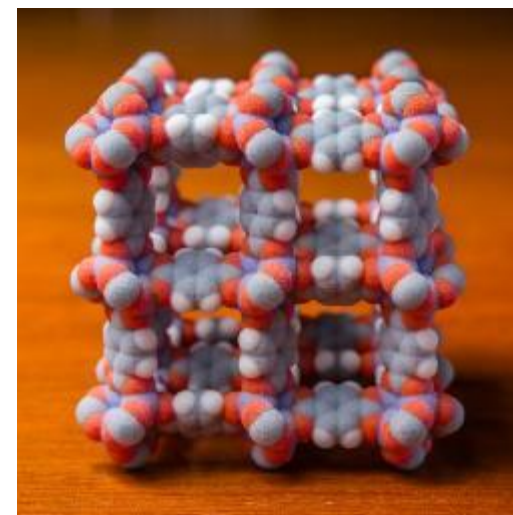
SAHYIK – MOF5



3D printing

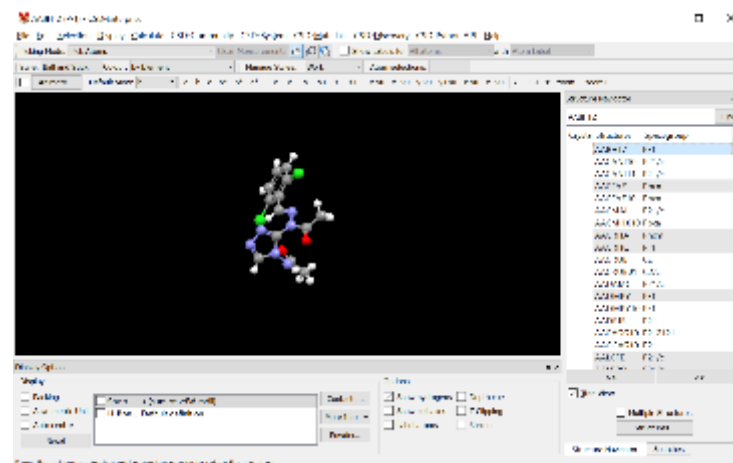


**Simple interface to
set up file
production + 3D
print style**



Example 1

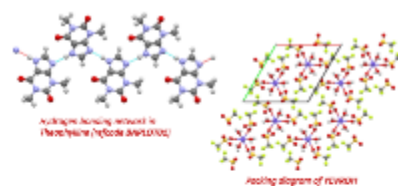
- Simple molecular views
- Generating packing diagrams
- Displaying intermolecular contacts
- Generating graph sets



Example 1. Generating Structure Views

[6,000/30] communicate science effectively, researchers must be able to provide clear images of structural models for inclusion in manuscripts and presentations. The program Mercury contains many features which can assist in the production of high-quality, high-resolution graphics of molecules.

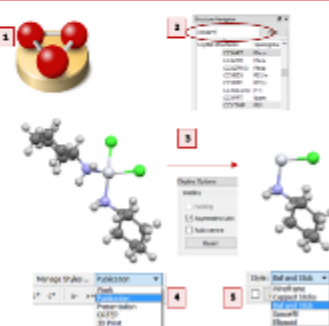
This example shows you how to build structural views such as packing diagrams, void space, and intermolecular interactions, which can then be output in a range of formats for use in various communications. For these [examples](#) we will be using entries in the Teaching Suite, however, the following methods can be applied to any entry in the CSD, or any of your own structure files.



Generating a Simple Molecular View

In this section, you will learn how to manipulate style options in order to generate simple molecular views.

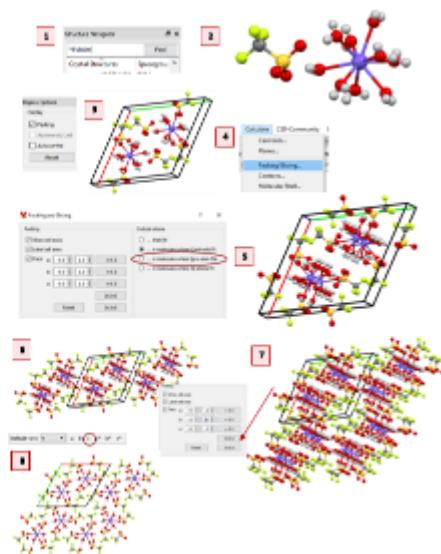
1. Open Mercury by clicking the icon, or launching from the start menu.
2. In the Structure Navigator window, type the refcode CCNPPT, to bring up the structure of a disphenyl derivative.
3. The whole molecule should be displayed in the viewing window. In the Display Options toolbar, tick the line for Asymmetric Unit and you will see half of the molecule disappear. Untick the box to bring back the whole molecule.
4. To generate the view in Step 3 above, choose Publication from the Mercury Style dropdown menu. Experiment by choosing other styles from this menu.
5. To change the style of the atoms and bonds in the structure, but to keep the white background, use the Styles dropdown box. Experiment with this by choosing some other options. Return to 'Ball and Stick' when you are done.



Generating a Packing Diagram

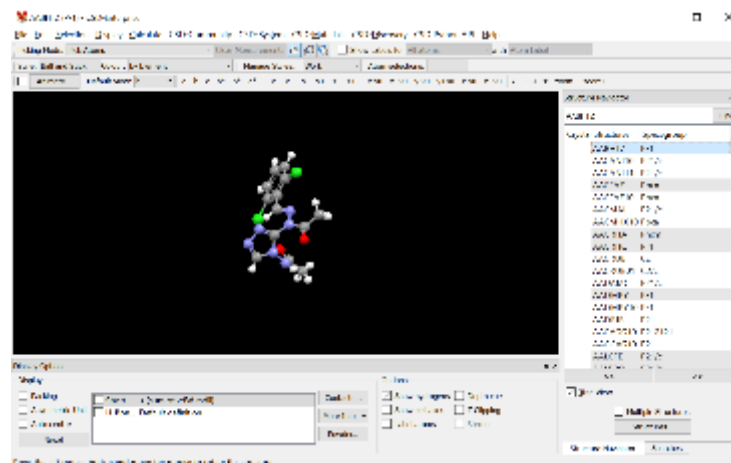
In this section, you will learn how to generate a packing diagram of a structure.

1. In Mercury, type the refcode YBWHOH in the Structure Navigator toolbar.
2. This will display the metal-organic salt compound, nona-aqua-cadmium(II) bis(trifluoromethanesulfonate) which crystallizes in the space group $P6_3/m$. Tick and untick the Asymmetric Unit box to see what atoms are generated by symmetry (Step 3 above).
3. Tick the Packing box in the Display Options toolbar to generate a packing diagram.
4. To change the settings of the packing diagram, choose Go to > Packing/Sliding from the top menu. This will launch the Packing and Sliding dialog box.
5. The top half of this window contains the packing preferences. Click the radio button next to "...in molecules where any atoms fit" and see how this changes the packing diagram in the Mercury window. Notice how two more metal-hydrate complexes appear in the center of the view and triflate anions appear at the edges.
6. To change the range of the packing diagram along any individual axis, click the +0.5 buttons by the corresponding axis. Or type a specific range in the text boxes. This example is -1.0 - 2.0 along the b axis.
7. Alternatively, click the 2x2x2 or 3x3x3 buttons to make an expanded packing diagram along all three axes at once.
8. To orient the view along the crystallographic axis, click the c button (just above the viewing window).
9. When you are done, click the Close button at the bottom of the Packing and Sliding dialog box to exit.



Example 2

- High resolution images
- Generating rotating images
- Generating a 3D print model file



Example 1. Generating Images and 3D Print Files

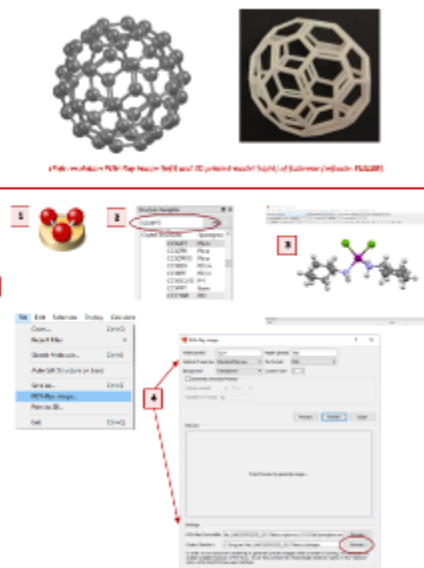
There are many ways to visualise the structure views created in Mercury, including high-resolution static views, animated rotating images, and 3D printed models. Each of these formats has its place in manuscripts, lecture presentations, websites, and tactile class-room displays.

The following exercises will show you how to generate high-resolution graphics files, the files needed to produce an animated rotating GIF, and files that can be sent to a 3D printer to produce a structural model directly from Mercury.

High-resolution images

POV-Ray, or Persistence of Vision [Raytracer](#), is a program which can be used to create very high-resolution and stylistic images. This example is not a definitive guide to POV-Ray, but will show you how to create a high-resolution image via the POV-Ray plug-in in Mercury.

1. Open Mercury by clicking the icon, or launching from the start menu.
2. In the Structure Navigator window, type the refcode CCRAPT, to bring up the structure of a cationic derivative.
3. Change colours and styles as in previous examples to obtain your desired view. Make sure the image appears in Mercury exactly how you want it to appear in your manuscript or presentation. Here the colours of the Pt and O atoms have been changed, and the molecule rotated to a new orientation.
4. From the top menu, choose File > POV-Ray Image... to launch the POV-Ray Image dialog box. The upper section of this window includes information on the resolution and style of the POV-Ray generated image. The bottom section includes a path to the POV-Ray executable and an Output directory. You should not need to change the POV-Ray executable location, but you may want to change the Output Directory location. Click Browse... to do this.

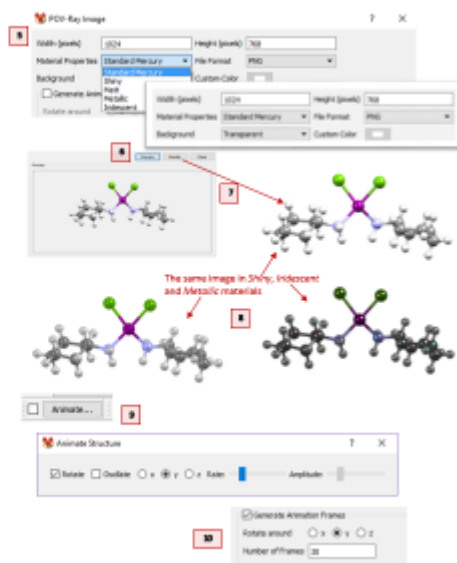


5. Change the Material Properties to the desired setting by clicking in the dropdown box and clicking the appropriate type. Select Transparent from the Background dropdown menu. Leave all other default values the same.
6. For complicated or large images, or on slow computers, POV-Ray may take a while to create the image file. Click Preview to check what the image will look like before rendering the full-size file. The POV-Ray window will briefly appear as the rendering proceeds.
7. When you are satisfied with the output, click Render to create the file. You can find the .ppg file in the output directory shown in the bottom of the window.
8. Using different Material Properties creates different image styles. Try different materials to see the effects.

Generating Rotating Images.

For presentations or websites, you may want to display a rotating image of your molecule, to highlight stereochemistry, or other spatial effects that are not obvious in static images. This section will show you how to generate images that can be used to make animated (rotating) molecule graphics.

9. To see how the rotation will look, click the **Animate...** button in the Mercury window. Tick the box next to **Rotate** and select the radio button for the 'y' axis. This will start the molecule rotating in the Mercury viewer. Select different axes (one at a time) and note how the molecule rotates.
10. Once you have decided on the orientation of your molecule and the axis of rotation, return to the **POV-Ray Image** dialog box. Tick box next to "Generate Animation Frames." Now specify the axis of rotation (x, y, or z) and the "Number of Frames" to generate. The structure will always rotate through 360 degrees, so the higher number of frames, the higher the "resolution" of the rotating image. The default value of 30 is typically a good compromise between file size and resolution. Click **Render** to generate the 30 images.

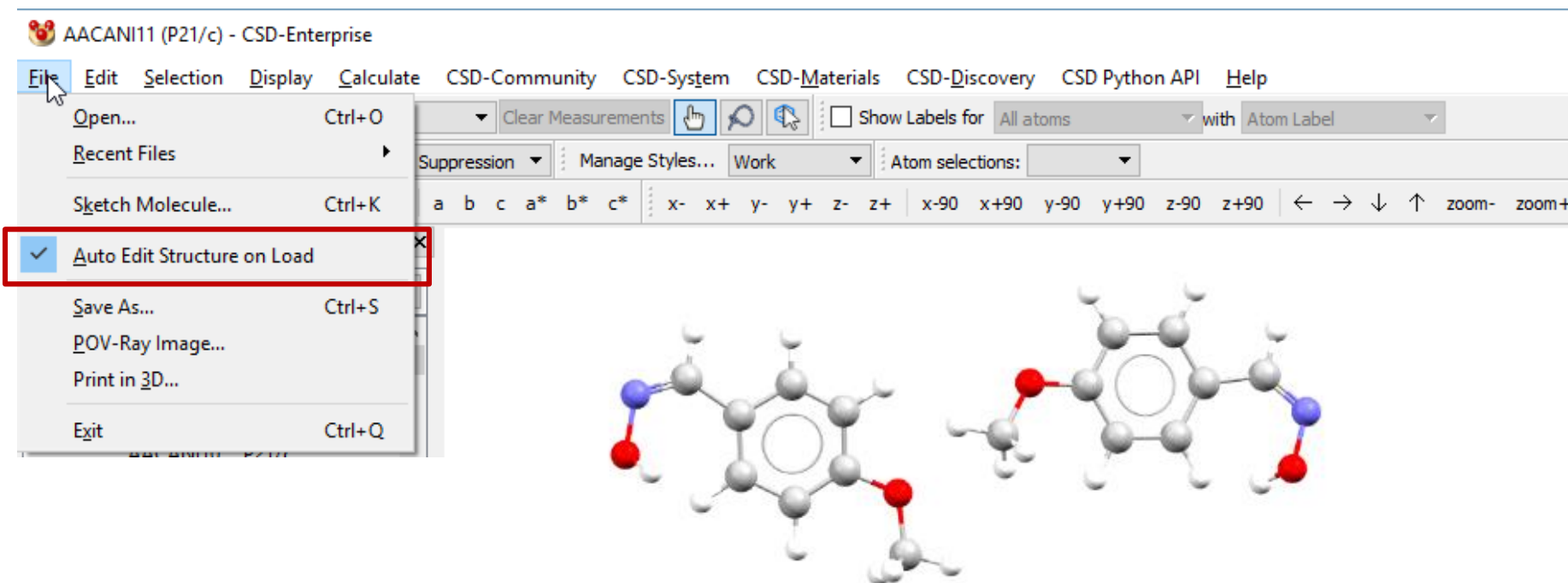


Exploring Mercury

Tips and Tricks

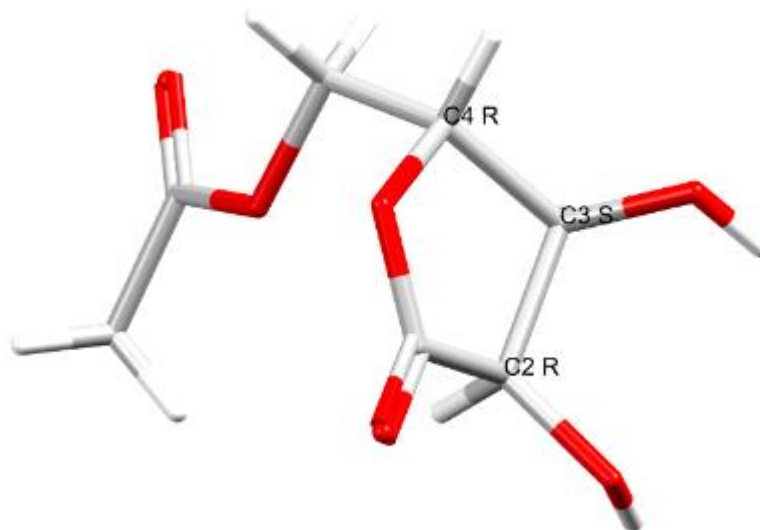
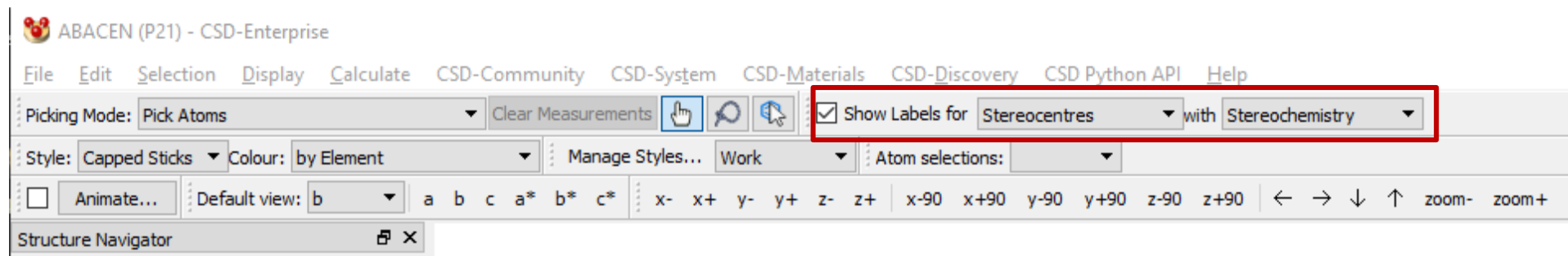
It's the simple things

- Do you load .cif files into Mercury a lot?



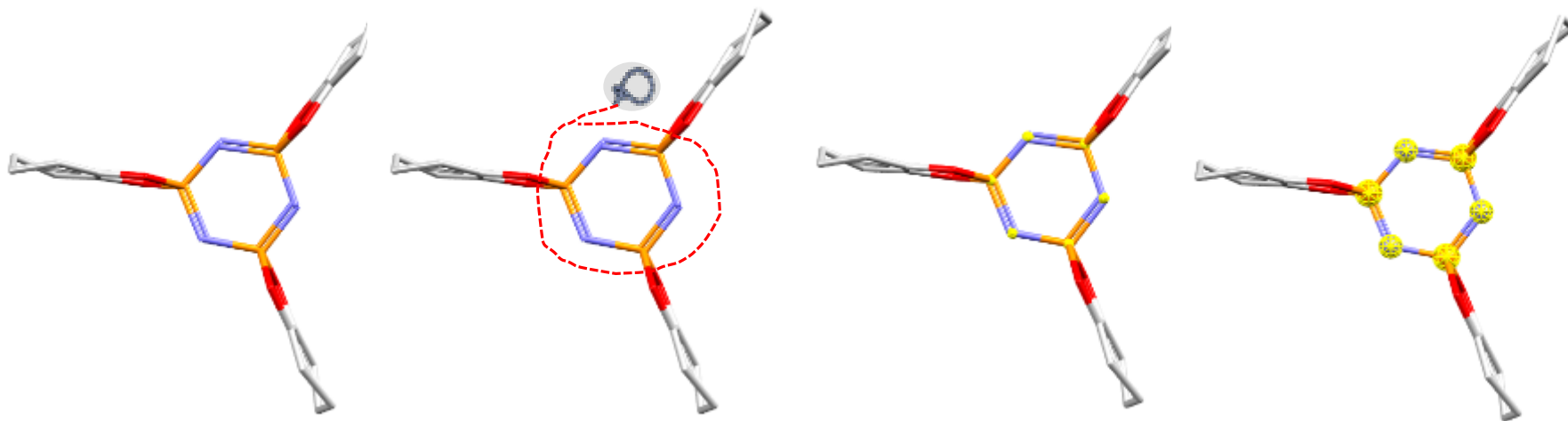
It's the simple things

- Do you look at chiral molecules a lot?



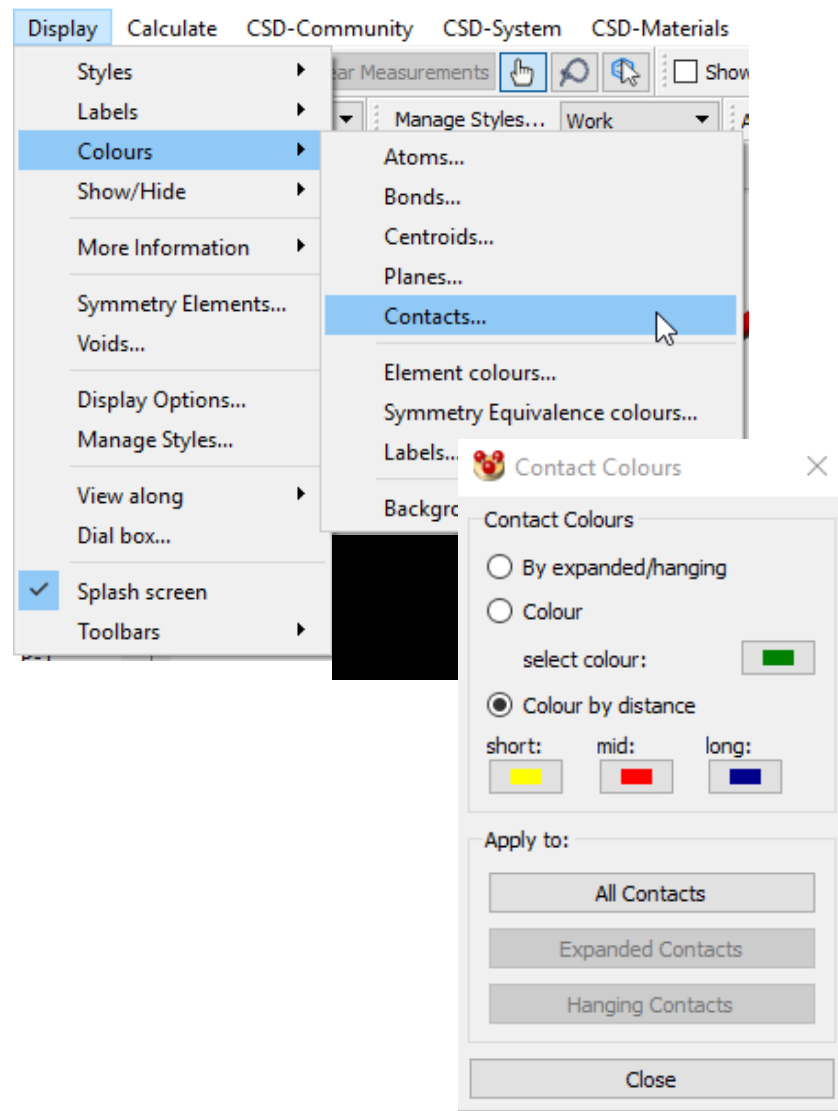
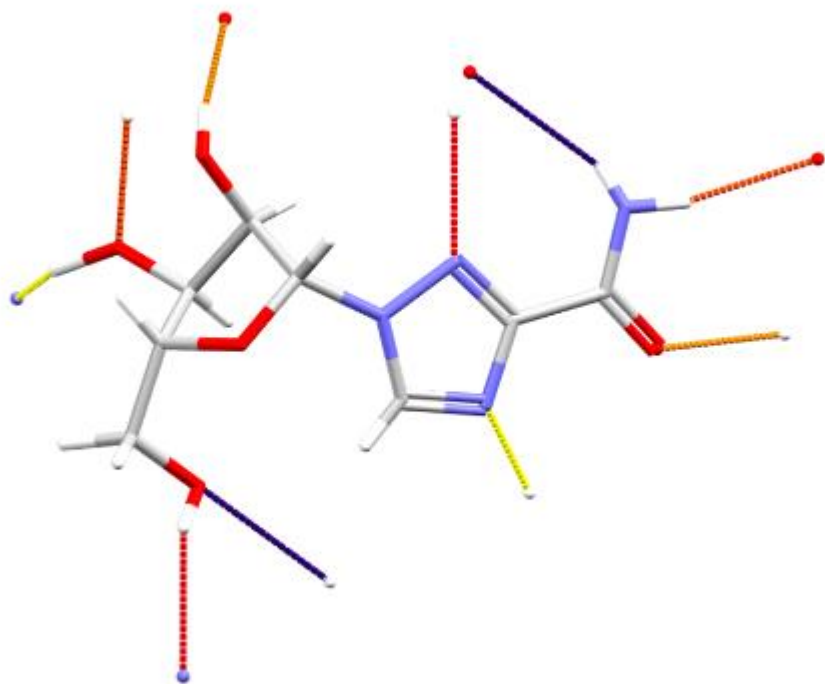
It's the simple things

- Do you select parts of molecules often (to change display styles for example?)
- Alt-Left Mouse button invokes lasso selection



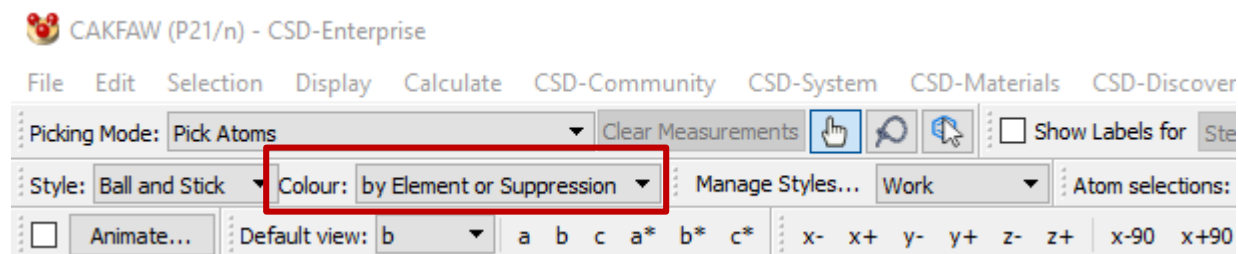
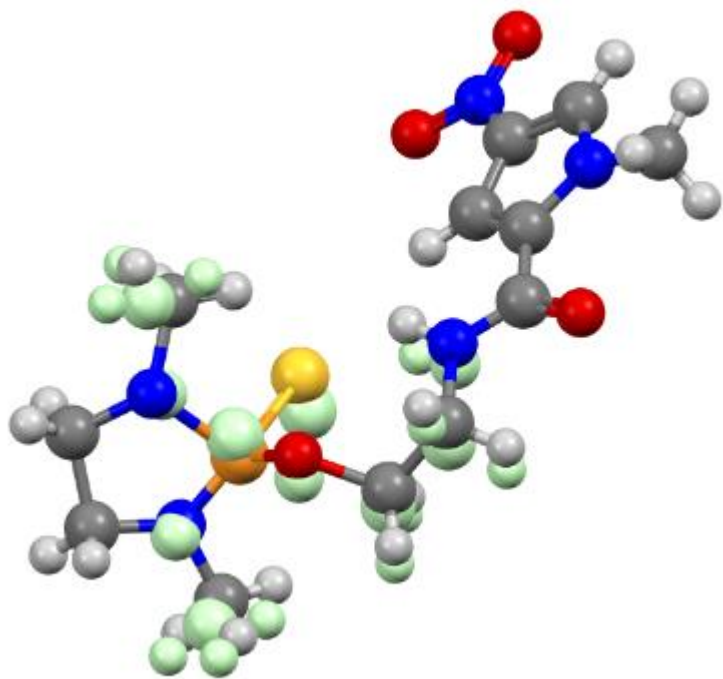
It's the simple things

- Do you look at hydrogen bonds a lot?
- Colour by distance

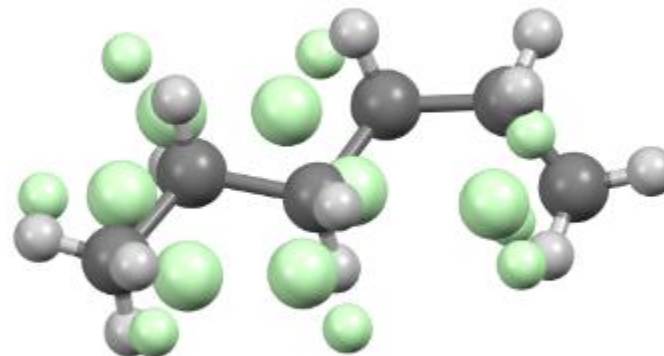


It's the simple things

- Disordered structures?

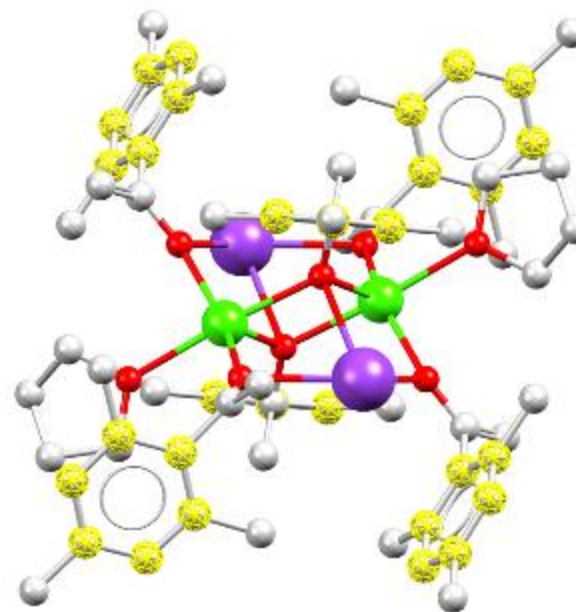
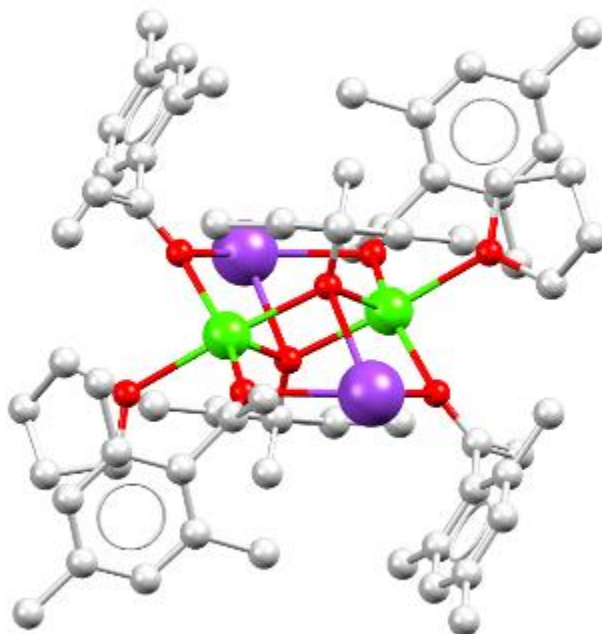
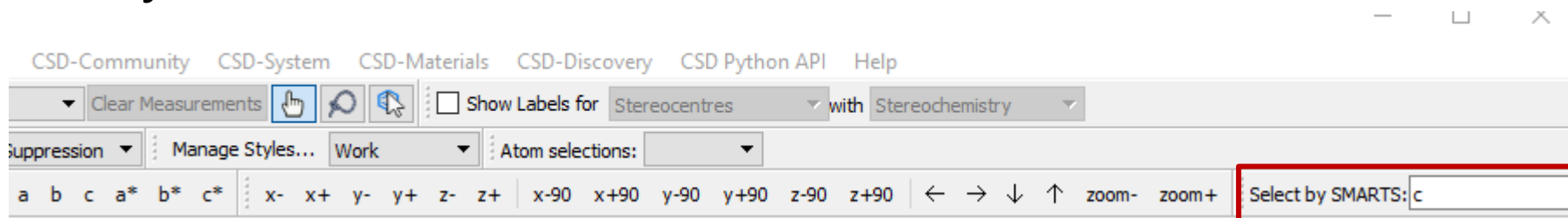


“Suppression” is our term for disordered atoms



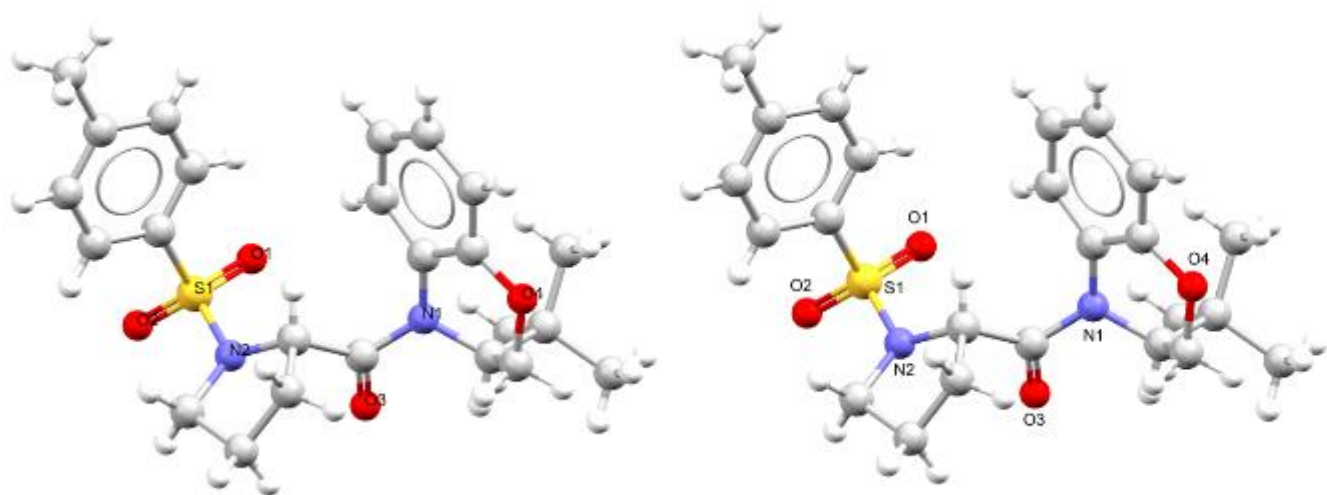
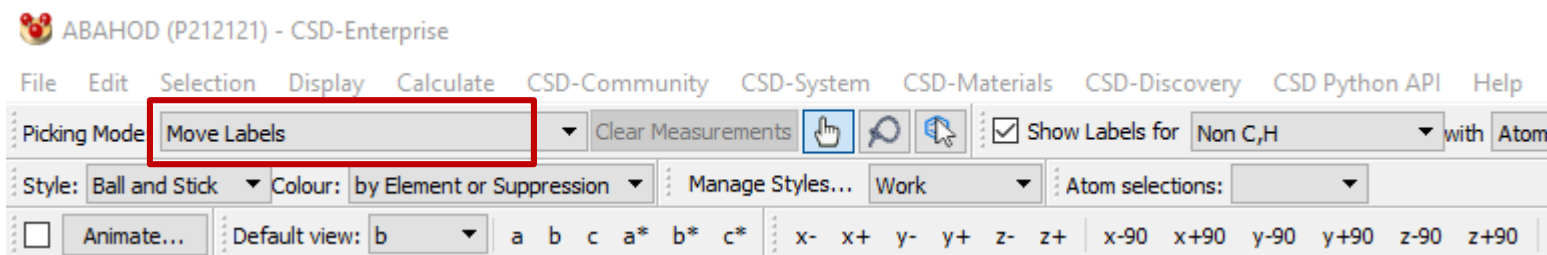
It's the simple things

- Select by SMARTS



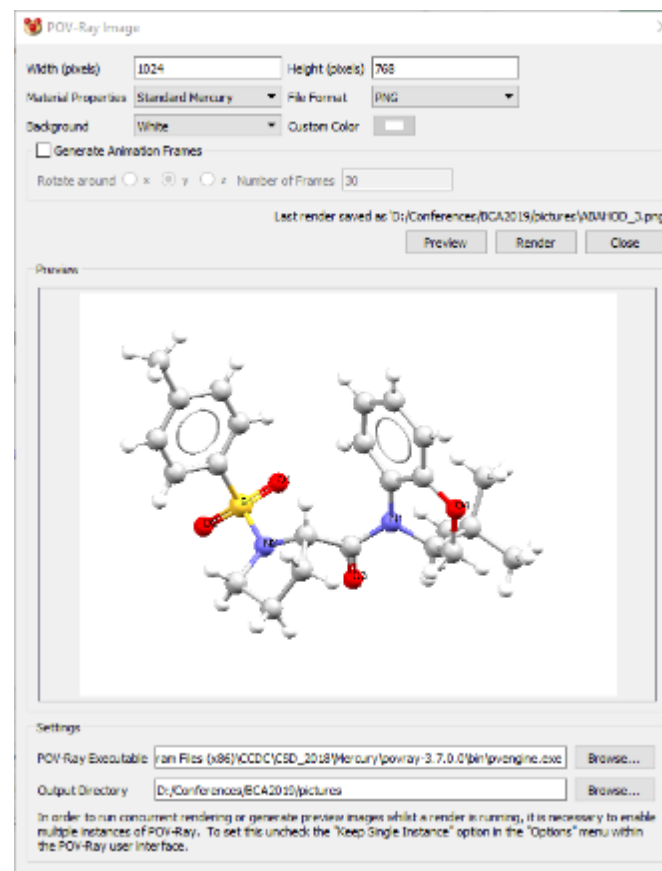
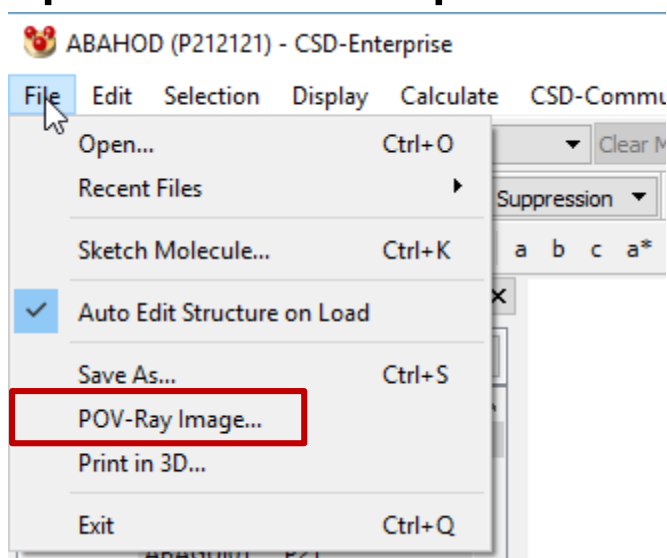
It's the simple things

- Make pictures for publications or slides?



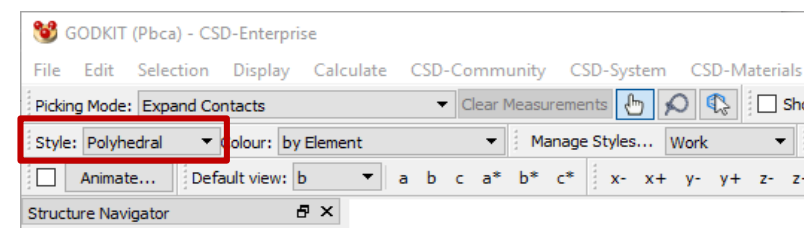
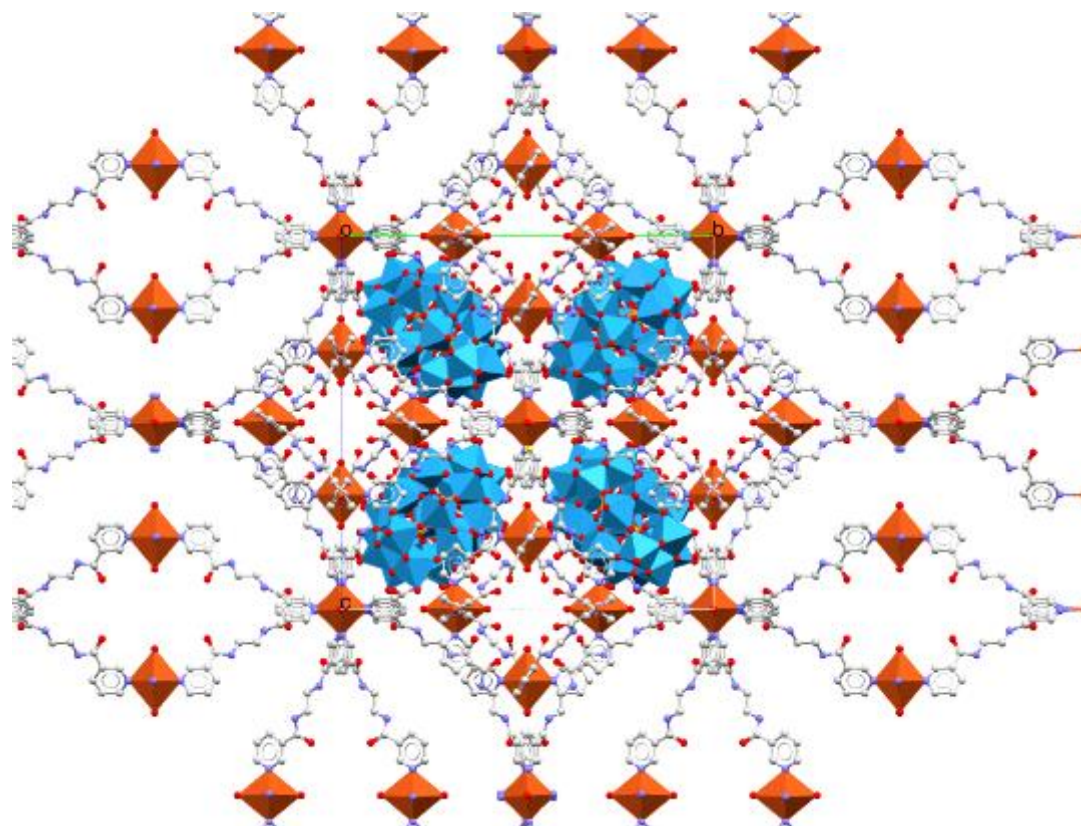
It's the simple things

- Make pictures for publications or slides?



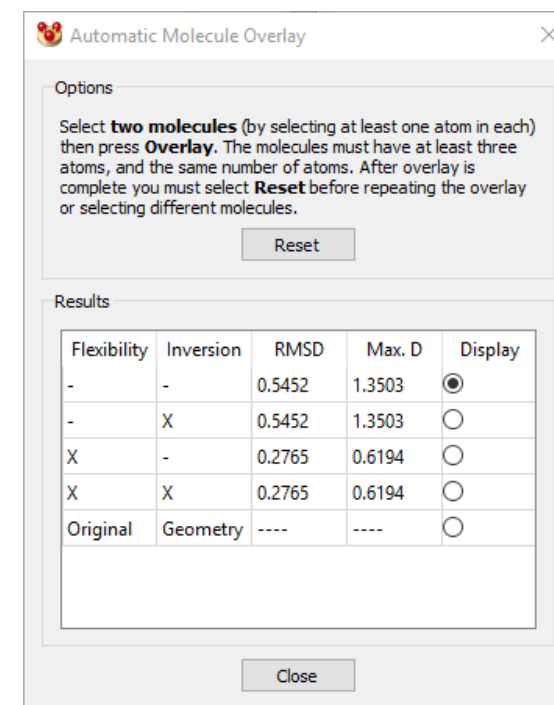
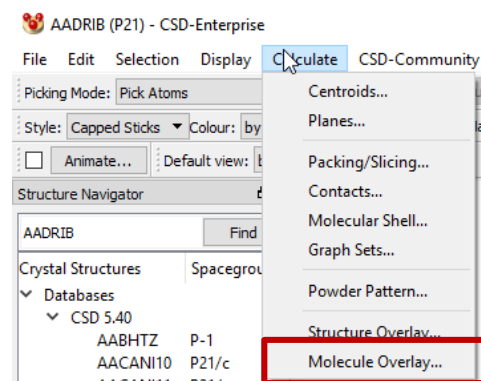
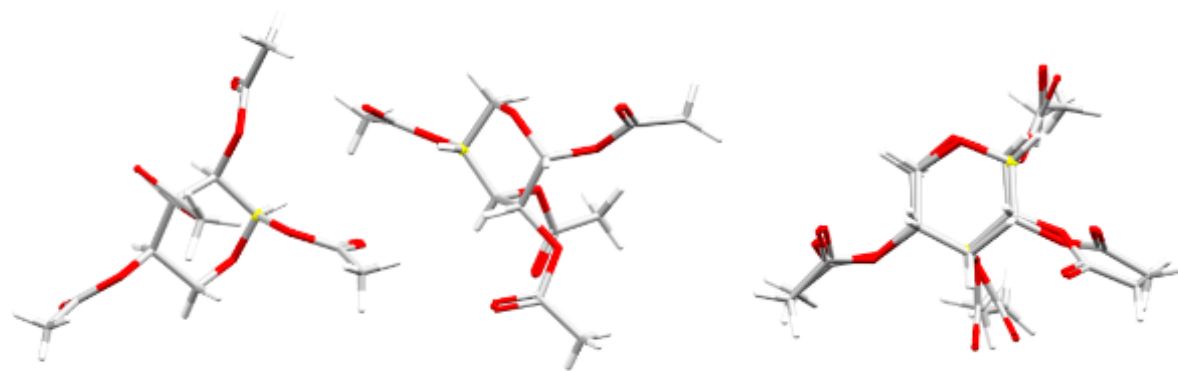
It's the simple things

- Work with coordination metals?



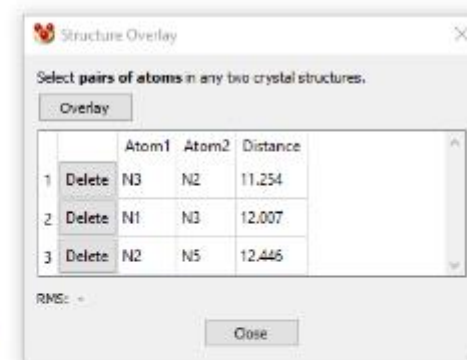
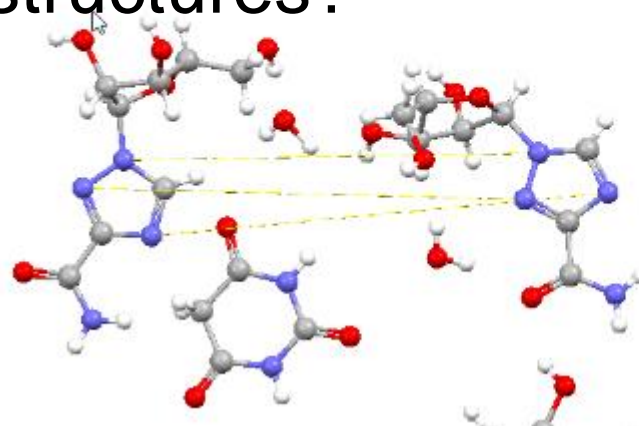
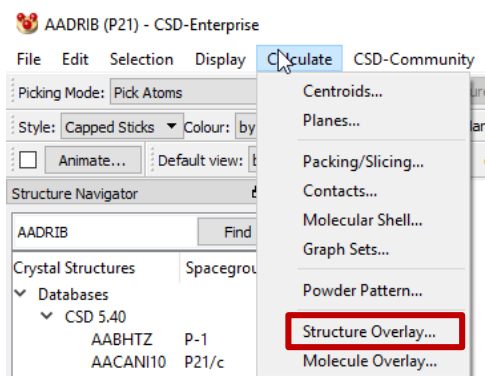
And a little more involved

- Molecule Overlay
- 2 molecules in the asymmetric unit and want to compare their conformations?

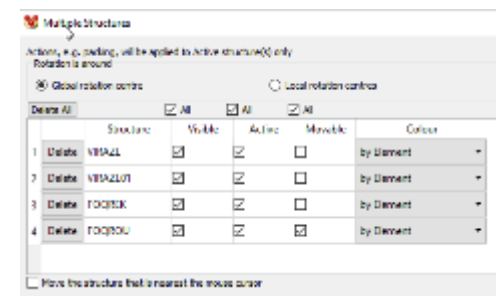


And a little more involved

- Overlaying more than 2 structures?



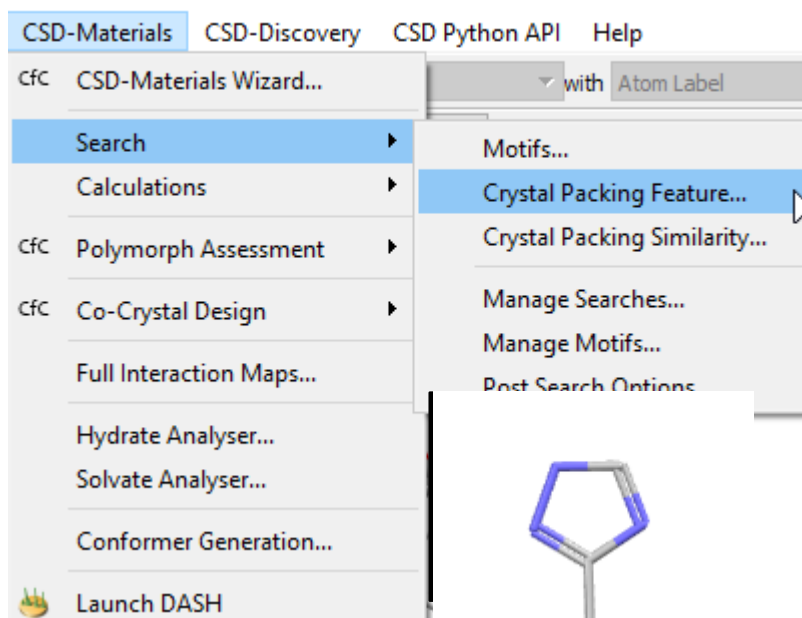
Last molecule selected is the one that moves



Multiple structures dialog allows you to “freeze” and hide the overlaid molecules

And a little more involved

- Want to overlay molecules from different structures? (and you don't want to use structure overlay)

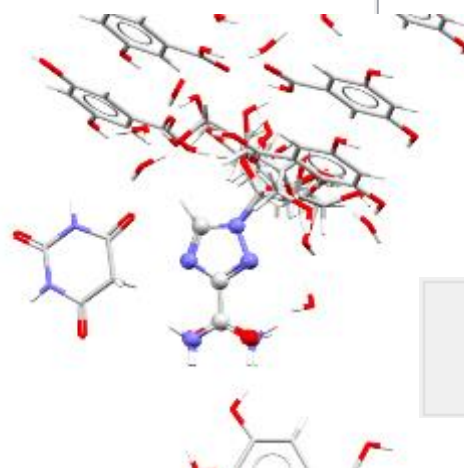


Select substructure

Packing Feature_feature4_search Options

5 hits out of 5 possible (100%) RMS

FOQREK	1.132
FOQRIO	1.118
FOQROU	1.127
VIRAZL	0
VIRAZL01	0.097

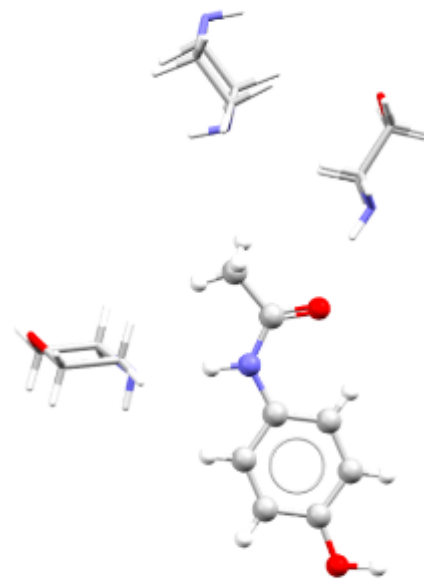
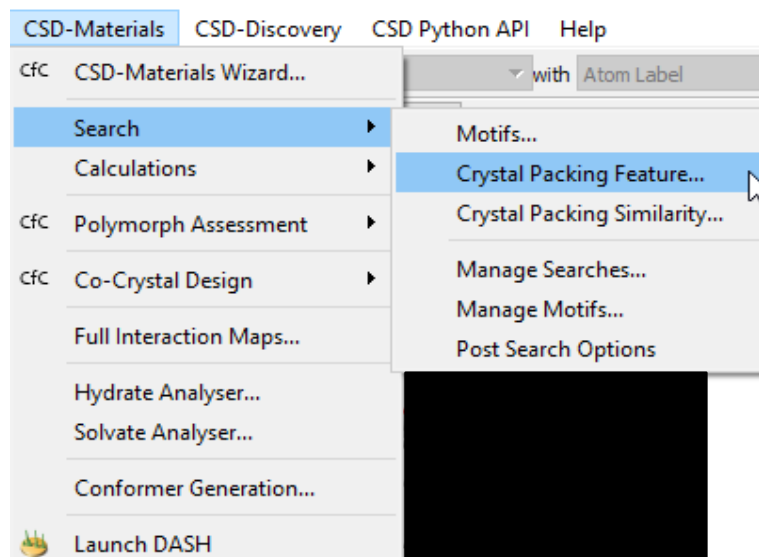


☒ Multiple Structures

Structures...

And a little more involved

- Do you want to find all crystal structures containing a particular molecule?
 - Solid form landscape of paracetamol, ethanol solvates, anything with a common substructure, not just packing features...



The screenshot shows the 'Packing Feature_feature6_search' results window. It displays a list of 85 hits, each with a name and an RMS value. The results are sorted by RMS value in descending order.

Hit	RMS
AHEPUY	0.367
AMUBAM	0.363
COKCEL	0.302
COTYOA02	0.297
COTYOA03	0.835
COTZAN02	0.193
COTZAN03	0.234
COTZAN04	0.291
COTZAN06	0.228
CUQKAC	0.545
HUMJEE	0.394
HXACAN	0
HXACAN01	0.207
HXACAN04	0.185
HXACAN06	0.211
HXACAN07	0.187
HXACAN08	0.079
HXACAN09	0.219
HXACAN10	0.195
HXACAN11	0.208
HXACAN12	0.241
HXACAN13	0.215
HXACAN14	0.215
HXACAN15	0.207
HXACAN16	0.2
HXACAN17	0.198
HXACAN18	0.196
HXACAN19	0.166
HXACAN21	0.082
HXACAN22	0.083
HXACAN23	0.092
HXACAN24	0.133
HXACAN25	0.060

And a little more involved

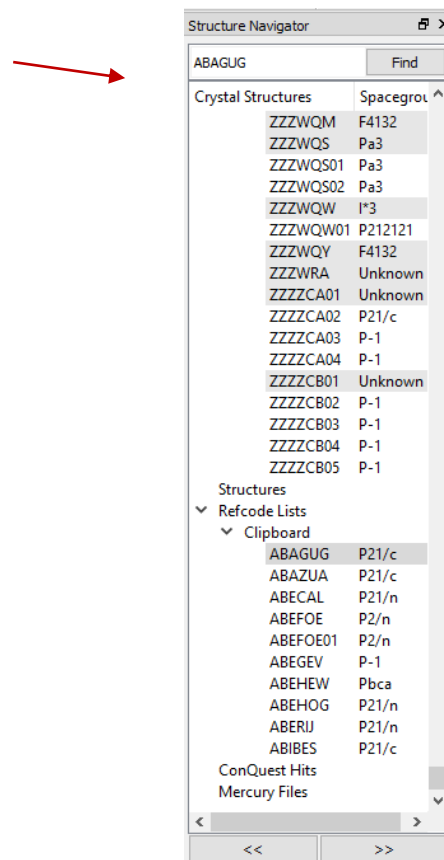
- Do you build subsets of structures based on a particular property? Cut and paste from Excel....

	A	B	C	G	H	I	J	K	L	M	N	O	P	R	S	T
7	Refcode	spacegr	zprime	mol_co	molecu	active_r	laxis	maxis	saxis	lm_rati	ls_ratic	ms_rati	shape_	Atoms	Aromat	Ring_A
54	ABAGUG	P21/c	0.5	1269.882	1269.882	1269.882	20.021	16.593	15.394	1.207	1.301	1.078	0.054	180	6	36
134	ABAZUA	P21/c	1	556.5447	556.5447	556.5447	19.086	12.307	11.725	1.551	1.628	1.05	0.055	80	6	36
148	ABECAL	P21/n	1	354.4418	354.4418	354.4418	20.035	9.386	3.592	2.135	5.577	2.613	0.13	46	6	35
166	ABEFOE	P2/n	0.5	618.7596	618.7596	618.7596	13.965	12.457	9.76	1.121	1.431	1.276	0.091	82	6	36
167	ABEFOE01	P2/n	0.5	618.7596	618.7596	618.7596	13.965	12.457	9.76	1.121	1.431	1.276	0.091	82	6	36
175	ABEGEV	P-1	1	620.7754	620.7754	620.7754	14.918	13.838	13.373	1.078	1.116	1.035	0.069	84	6	36
186	ABEHEW	Pbca	1	744.746	744.746	744.746	16.992	15.583	10.971	1.09	1.549	1.42	0.084	95	6	36
191	ABEHOG	P21/n	1	700.6936	700.6936	700.6936	15.065	14.07	10.708	1.071	1.407	1.314	0.087	88	6	36
283	ABERIJ	P21/n	1	694.7266	694.7266	694.7266	15.2	15.144	10.921	1.004	1.392	1.387	0.091	86	6	36
308	ABIBES	P21/c	1	492.756	492.756	492.756	14.536	12.656	9.635	1.148	1.509	1.314	0.09	64	6	36

Property in this column is the number of aromatic rings in molecule. Chosen structures with 6 aromatic rings.

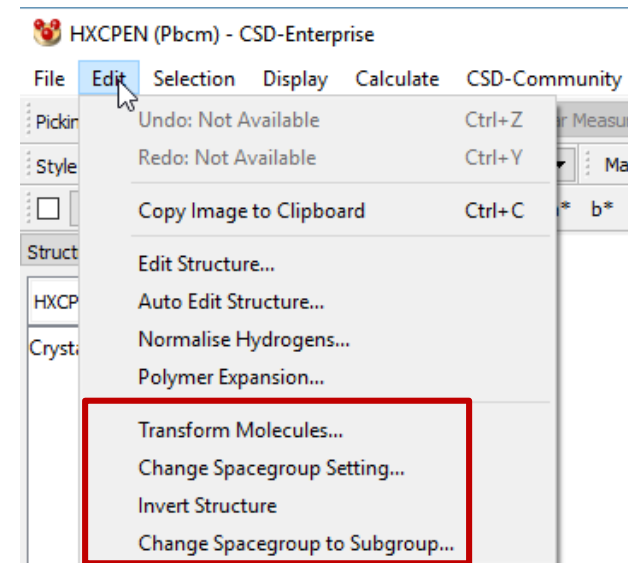
And a little more involved

- Do you build subsets of structures based on a particular property? Cut and paste from Excel....into Mercury



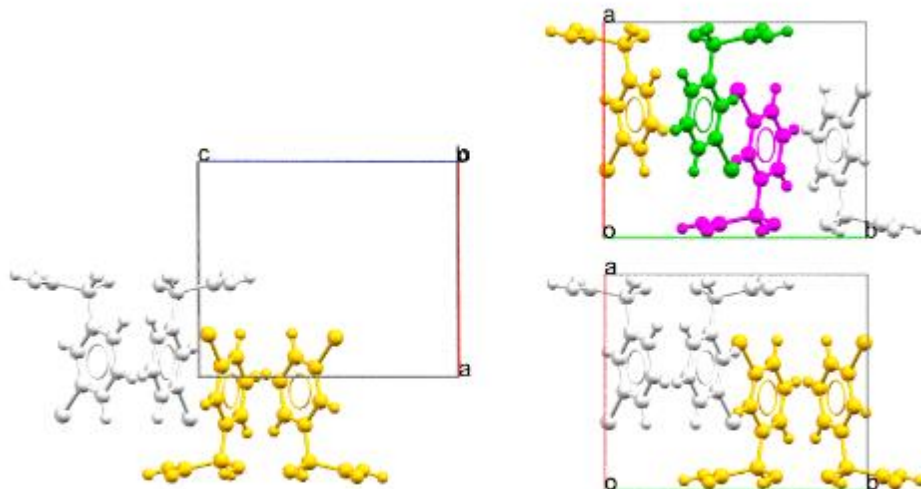
And a little more involved

- Editing a structure
 - Invert a structure/ Invert a molecule
 - Removing symmetry by choosing a subgroup
 - Changing the space group setting: P21/n to P21/c



And a little more involved

- Do you explore structural changes due to phase transitions?
- FIZPEL/ FIZPEL01



P-1
Low temp

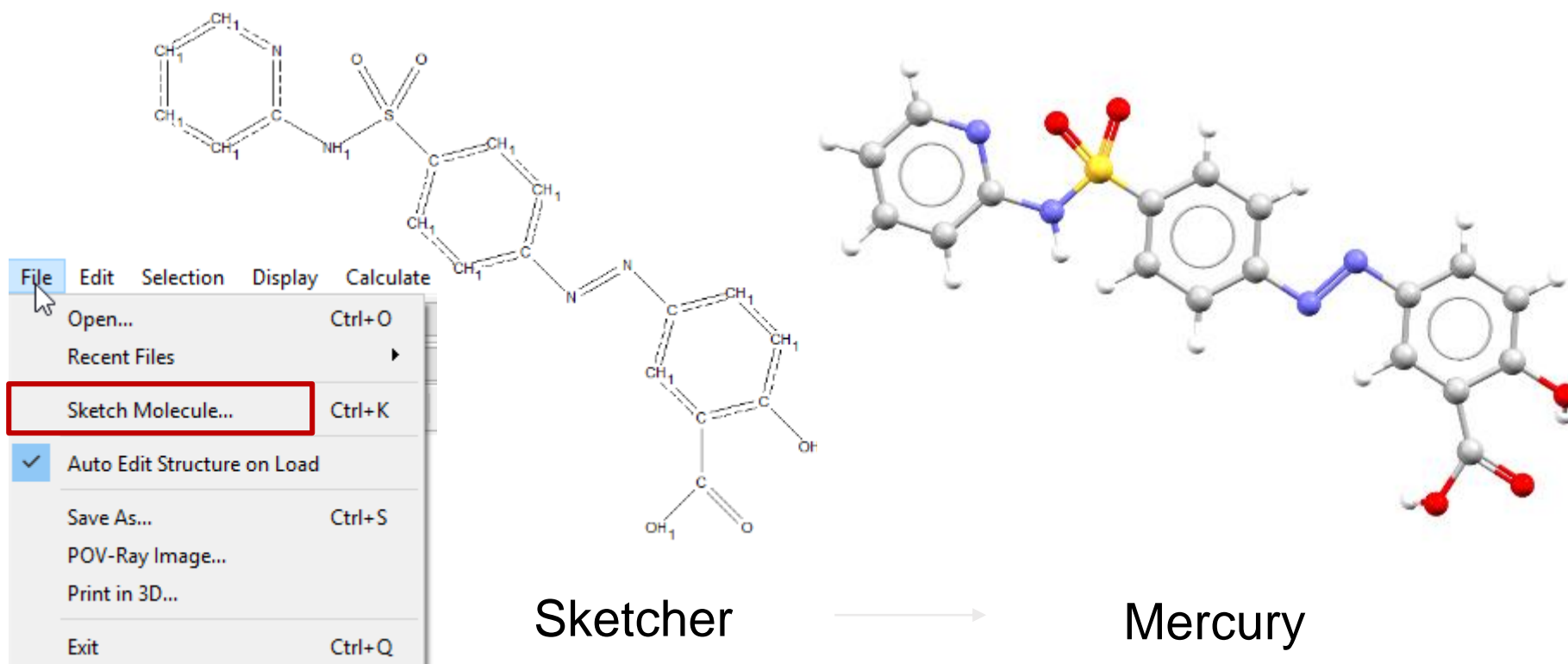
P2₁/c
Room Temp

Mirror symmetry
relationship
formalised in P21/c

Transformed to subgroup P-1

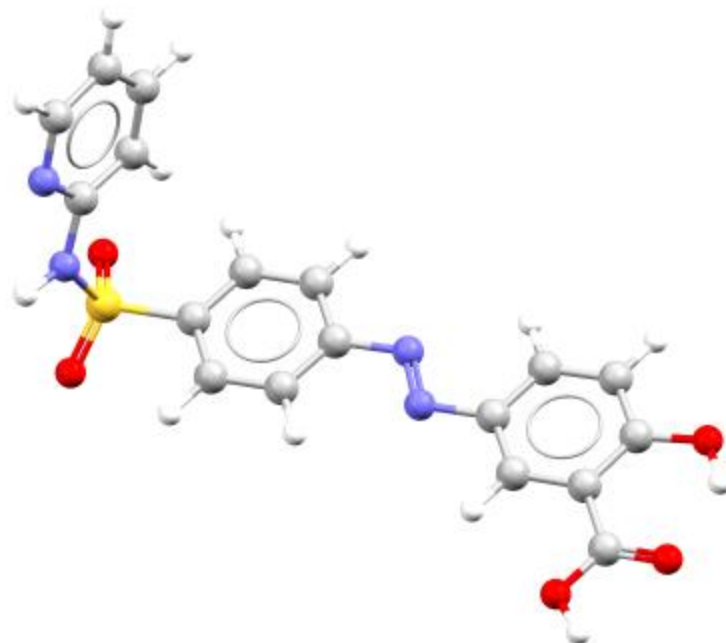
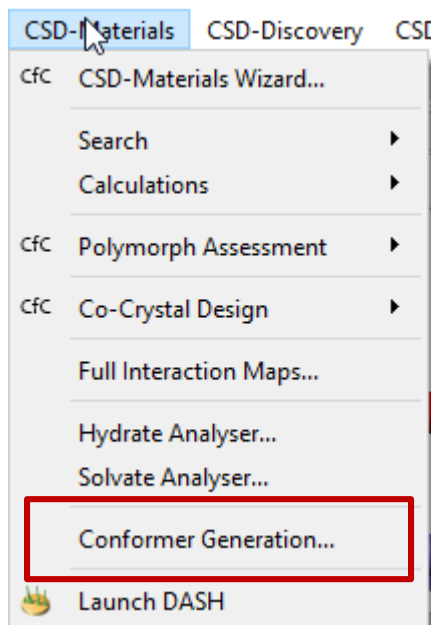
And a little more involved

- Sketch a molecule and generate a conformation



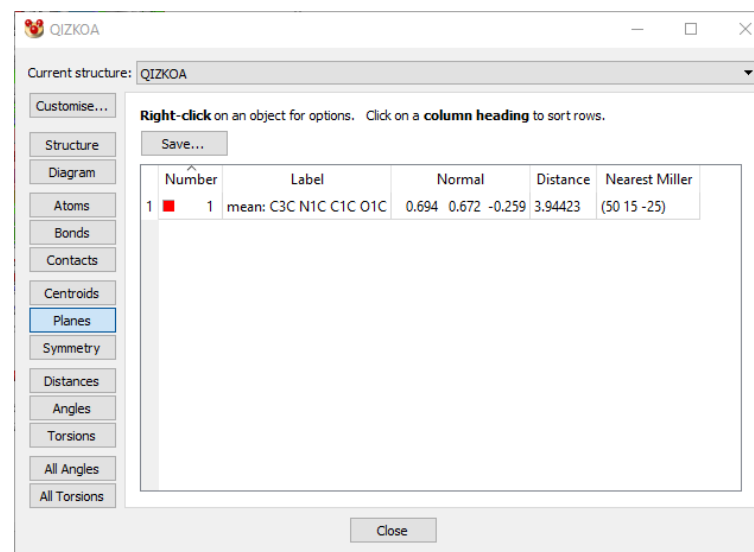
And a little more involved

- Sketch a molecule and generate a conformation....



Too many to mention:

- Custom view
- Powder pattern simulation
- Links to Isostar, GOLD, Mogul etc
- Motif searching and hydrogen bond propensity calculations
- More info dialog
 - Nearest Miller Plane
 - Selecting atoms from Atoms list
- MOPAC – point group symmetry



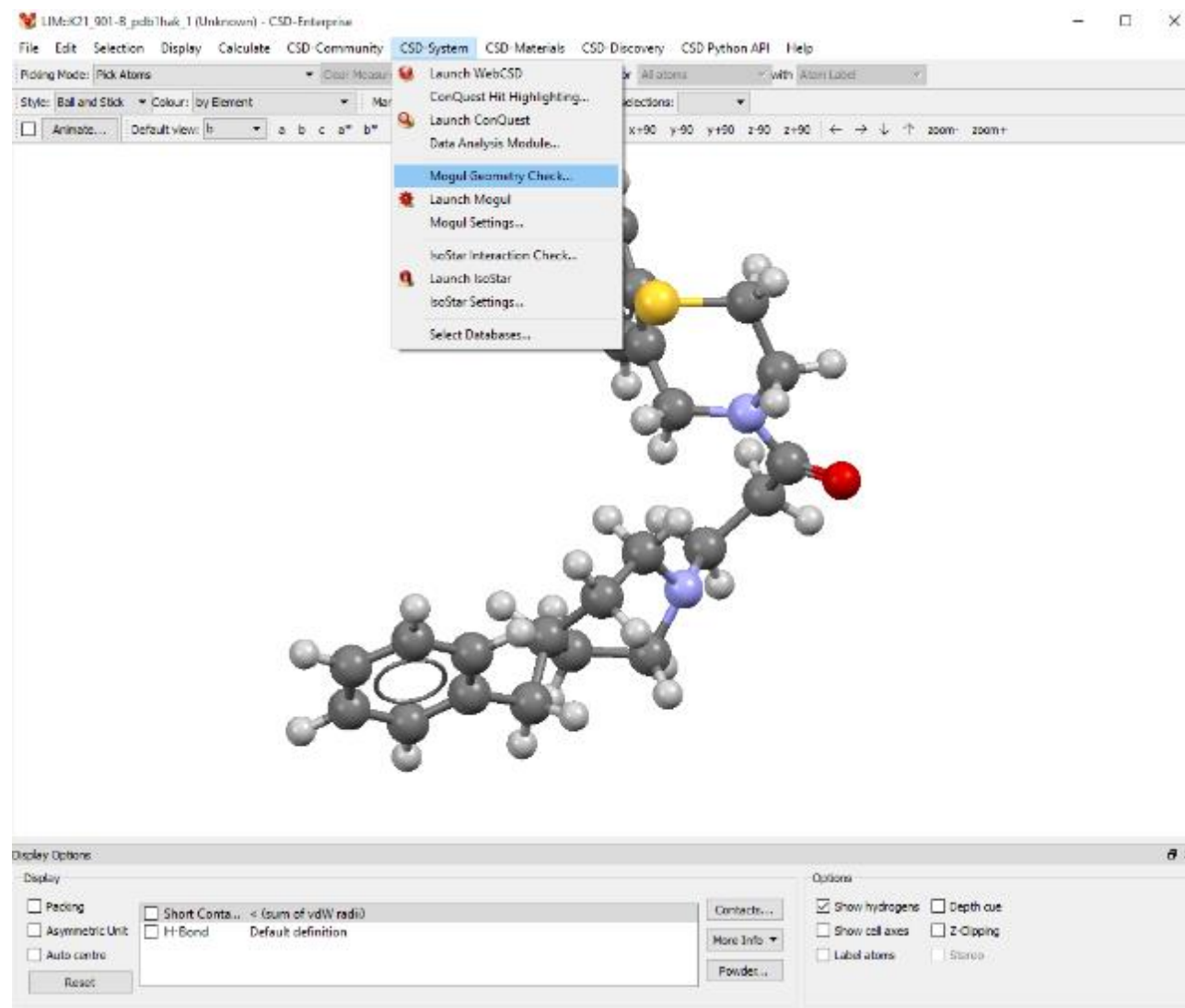
Mercury

Mogul, Full Interaction Maps, Crystal Packing

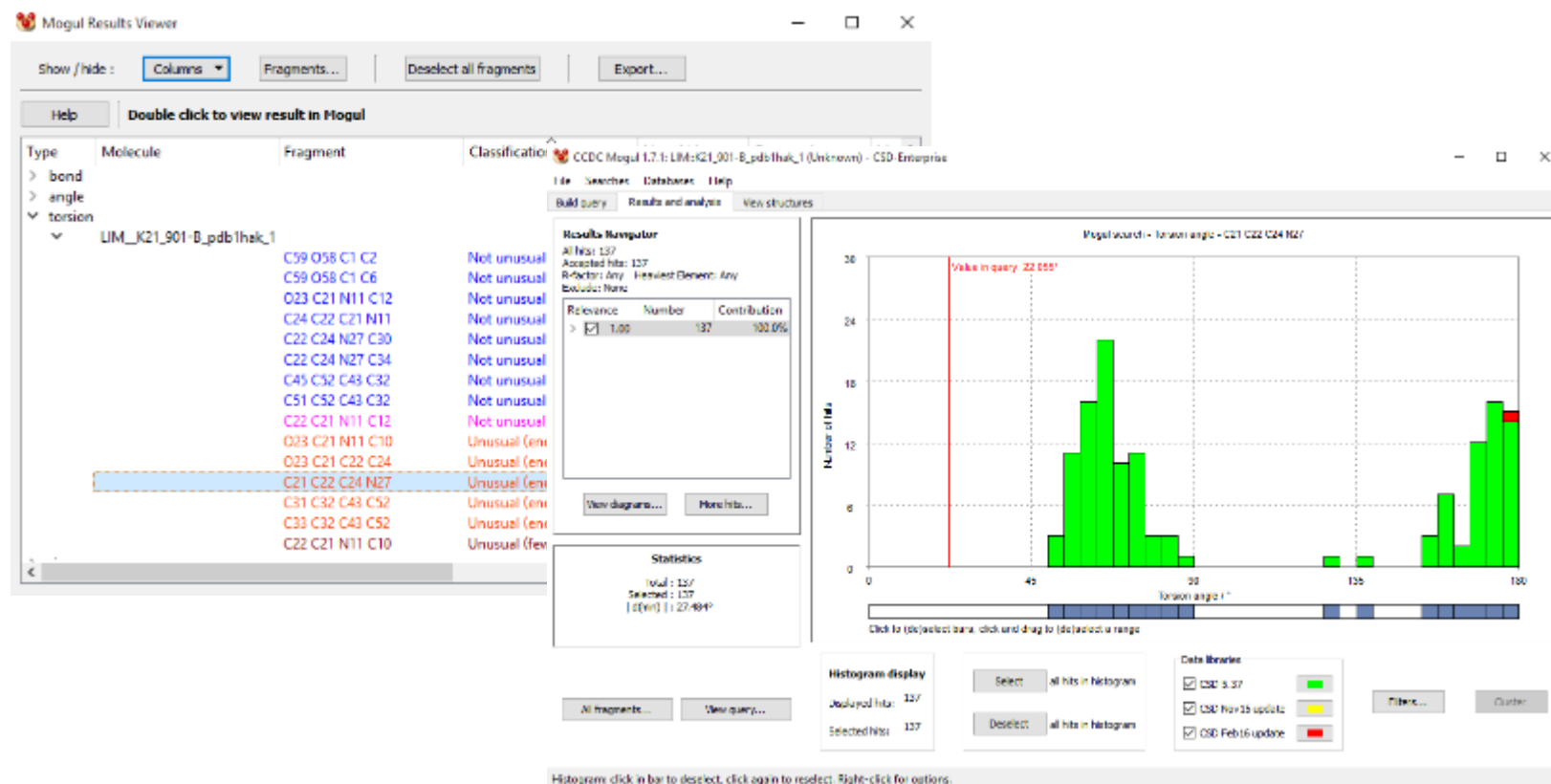
Mogul

- Incorporates **pre-computed libraries** of bond lengths, valence angles, torsion angles and ring conformations derived entirely from the CSD
- **Validate complete geometry**: retrieve distributions, and figures of merit for all bonds, angles, torsions and rings in the molecule
- **Fragment Generalisation**: If fragment specified is rare, Mogul will include CSD results from the most similar fragments
- **Hyperlinking to the CSD**: View CSD entries in specific areas of histogram
- **Integration with other software**: Instruction file permits other programs to interact with Mogul

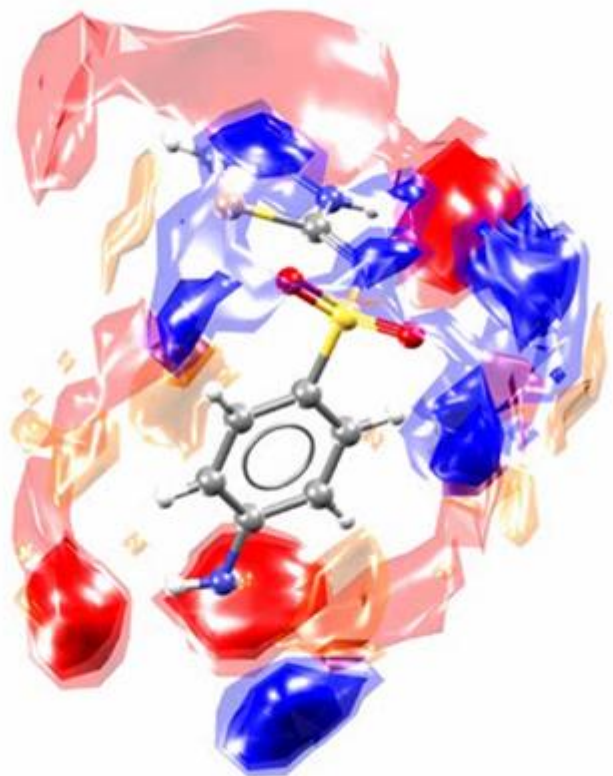
Mogul



Mogul



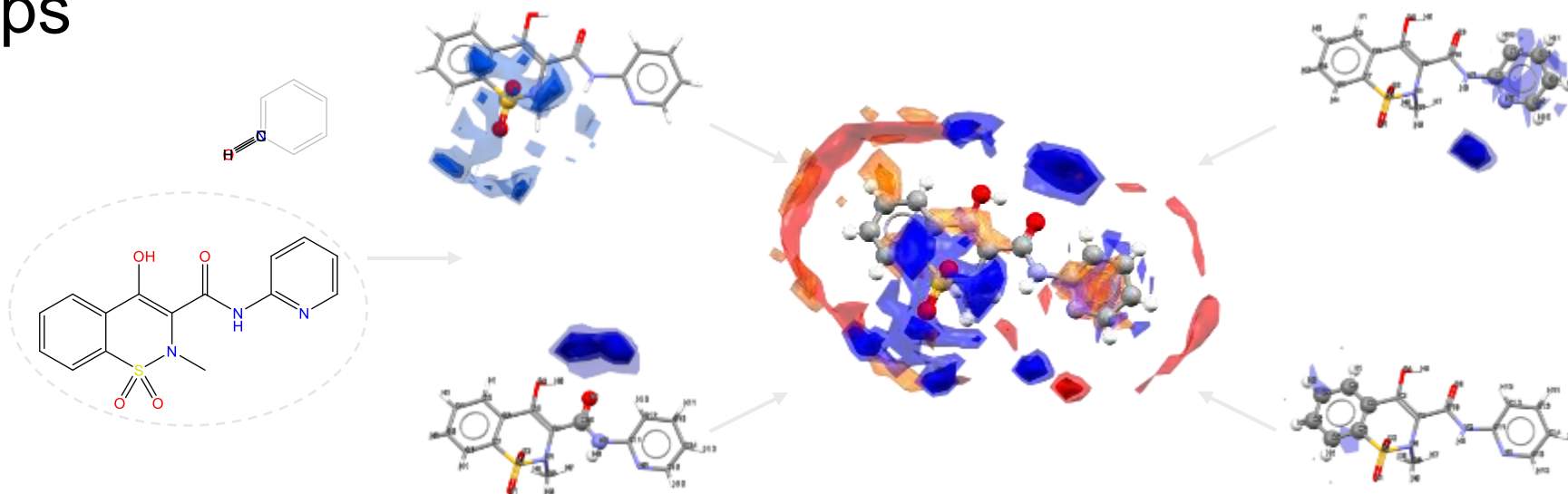
Full Interaction Mapping



- Provides your molecule's interaction preferences, in the context of the crystal structure, at the click of a button
- Based on validated experimental structural knowledge
- Interactions visualised simply in 3D within Mercury

Combining plots into Full Interaction Maps

- Molecule is broken down into fragments
- IsoStar maps for each fragment in the molecule & for multiple probe types are combined together to produce Full Interaction Maps



Further tutorials

- If you have time and are interested, we have some additional tutorials on assessing *intramolecular* conformations and analysing *intermolecular* interactions
 - Mogul
 - Full interaction maps
 - Packing features

Introduction

This tutorial will introduce you to the Full Interaction Maps and Mogul Geometry Check features included with Mercury under the CSD-Materials and CSD-System toolbars.

The Full Interaction Maps tool will generate a picture of the interaction landscape of your molecule from its three-dimensional coordinates. Using statistical distributions from the hundreds of thousands of structures included in the CSD, we can predict the most likely locations for a variety of functional groups. By comparing this distribution against a 3D packing diagram, we can determine whether a crystal structure fulfils the desired interactions of a particular conformation of a particular molecule. The Full Interaction Maps tool is instrumental in highlighting the potential for polymorphism of a given compound, assisting in the development of co-crystals, and understanding solid form stability.

Structural chemists can use the Mogul Geometry Check tool to validate the three-dimensional conformation of a particular molecule. The metric data from structures in the CSD can be used to show the most likely values a particular bond, angle, torsion or ring should adopt. The information obtained from a Mogul check can help identify inconsistencies within a crystal structure and can suggest values to be used for restraints during refinement. In addition, Mogul can also be run on 3D coordinates generated *in silico* as a validation of calculated structures.

The following exercises assume you have a working knowledge of the program Mercury, namely how to display and manipulate structures from a 3D coordinates file. There are many other features included with Mercury that are beyond the scope of this tutorial. For assistance with any aspect of Mercury, please ask your workshop instructor, or view the help guides included with the application.

