

# ConQuest to Mercury: From Searching to Data Analysis

CCDC Virtual Workshop

October 2024

Guest Speaker:



**Catherine Esterhuysen**

Professor of Physical  
Chemistry

Stellenbosch University



# Learning outcomes for today

- How to construct a [CSD search](#) using [ConQuest](#).
- How to [define 3D parameters](#) in ConQuest searching.
- How to [export ConQuest results](#) to Mercury
- How to [analyse results](#) using the [Data Analysis module](#).
- [Tips and tricks](#) for [effective searching](#) in ConQuest .
- How this functionality has been used by [global researchers](#) through the [exploration of recent case studies](#).

# Agenda

- Introduction to the CSD
- *Show One*: Research exploring Hydrogen and Halogen bonding
- *Show One*: Introduction and demonstration of ConQuest and Mercury
- *Try One*: Hands-on examples
- *Explore More*: More advanced tips and tricks and case-studies
- *Explore More*: Quiz and Summary
- *Extra time*: More time for hands on and Q&A



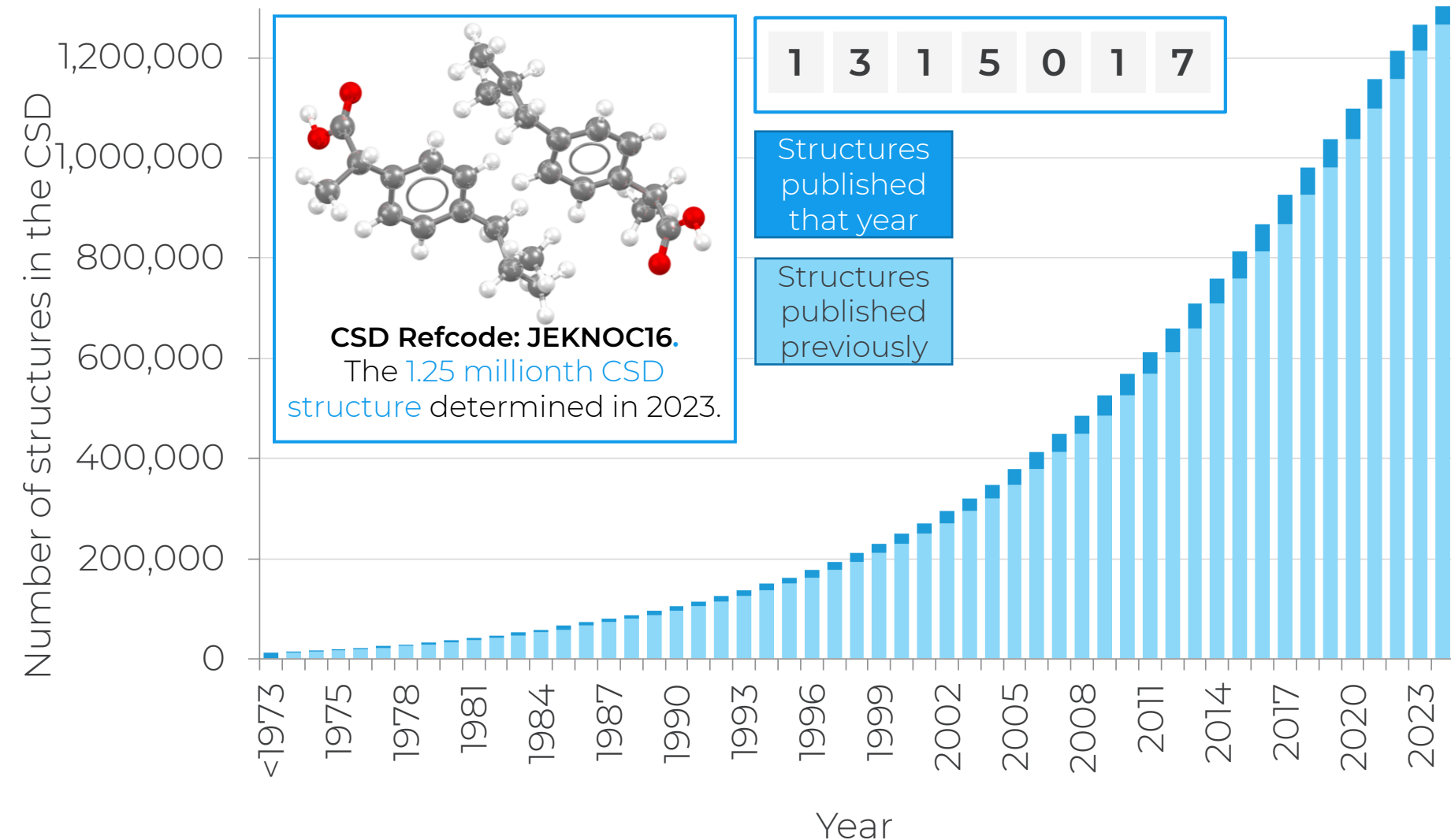
We will make the recording available to you in the next few days.



After the session you can earn a completion certificate for today by taking the test.

CCDC

# The Cambridge Structural Database



- Every published structure
  - Inc. ASAP & early view
  - *CSD Communications*
  - Patents
  - University repositories
  - Thesis
- Every entry enriched and annotated by experts
- Discoverability of data and knowledge
- Sustainable for over 59 years
- A trusted CoreTrustSeal repository



Certified as Trustworthy  
by CoreTrustSeal

# Inside the Cambridge Structural Database

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

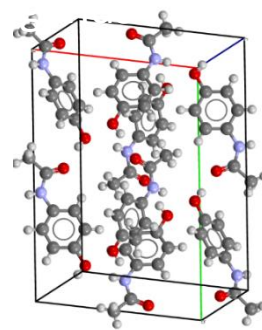
Organic  
45%

Metal-Organic  
55%

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

## Organic

- Drugs
- Agrochemicals
- Pigments
- Explosives
- Protein ligands



## Additional data

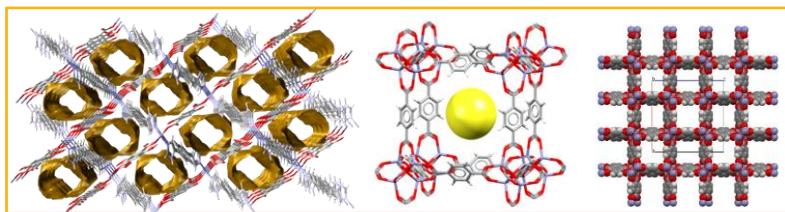
- 13,478 polymorph families
- 174,987 melting points
- 1,075,904 crystal colours
- 951,746 crystal shapes
- 30,275 bioactivity details
- 13,641 natural source data
- > 350,000 oxidation states

Not Polymeric  
89%

Polymeric: 11%

## Metal-Organic

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

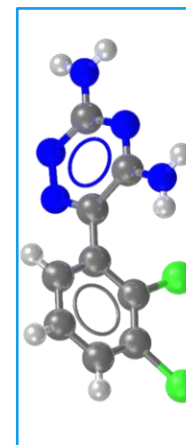


Single  
Component  
58%

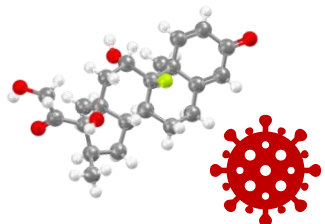
Multi  
Component  
42%

## Links and subsets

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



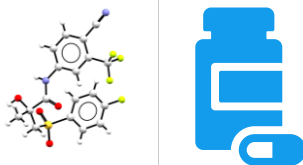
COVID-19



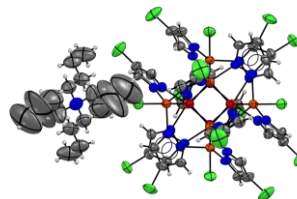
Pesticides



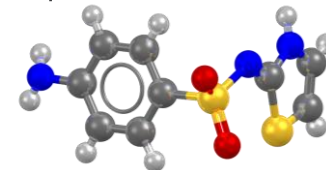
Drugs



ADPs



Best  
representative



Teaching

## CSD Subsets

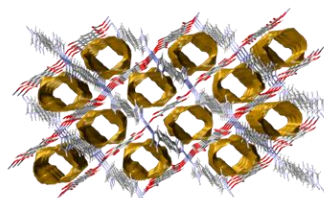
*Groups of structures that may be more difficult to find in CSD from searching alone*

- Easy access to the most relevant structures.
- Using our in-house and external expertise.
- Convenient starting point for research and analysis.

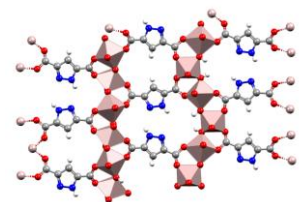
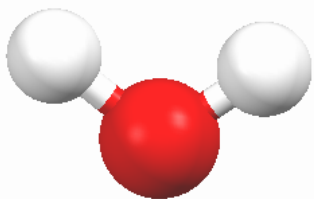
MOF  
Dimensionality

- 1D
- 2D
- 3D

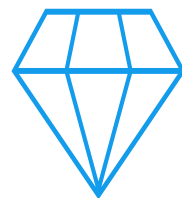
MOFs



Hydrates

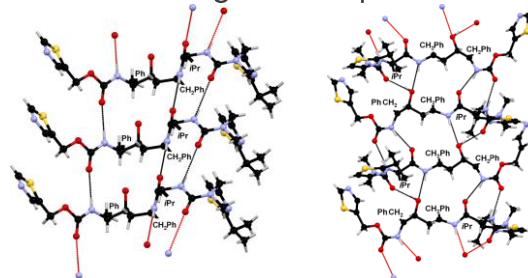


Electron  
Diffraction

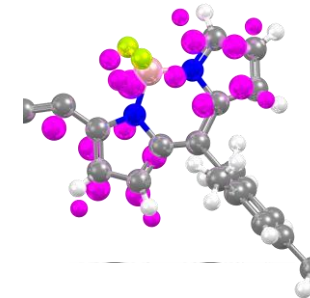


High  
Pressure

Polymorphs



Disorder



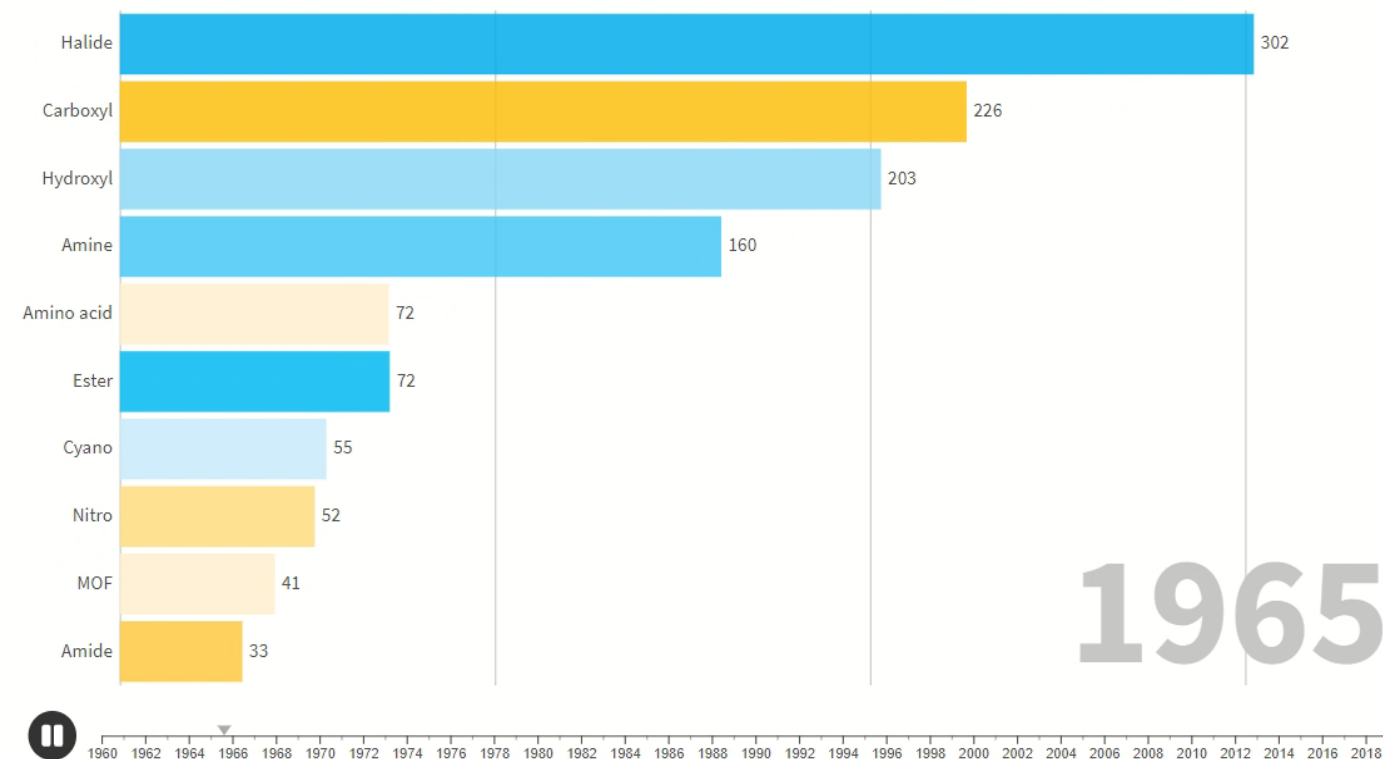


# Exploring the CSD

- > 1 million structures
  - > 94M 3D coordinates
- > 28 million bond lengths
  - > 2M unique distributions
- > 40 million valence angles
  - > 3M unique distributions
- > 14 million torsion angles
  - > 800K unique distributions
- > 2 million rings
  - > 400K unique distributions
- > 2 million hydrogen bonds
  - > 30 million Isostar contacts

## Chemistry in the CSD

Number of structures containing certain chemical groups



# The CSD Portfolio

CSDEnterprise.

CSDCore.



ConQuest

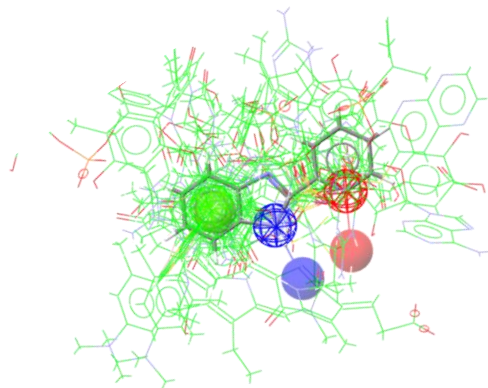


Mercury



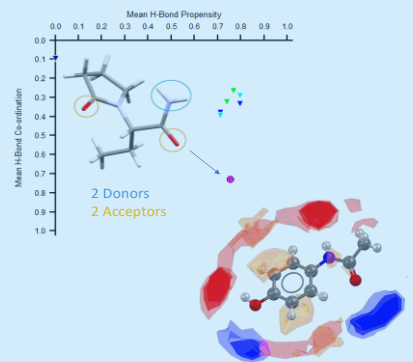
CSDDiscovery.

*Design of new molecules*



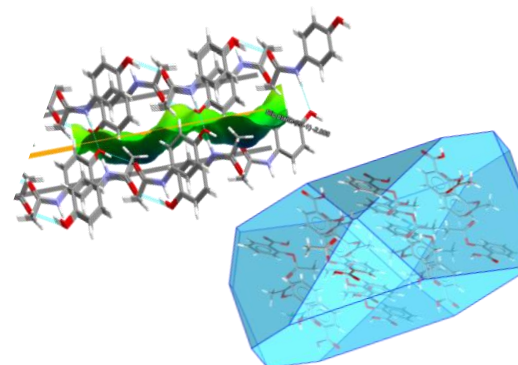
CSDMaterials.

*Assessment of solid form stability and properties*



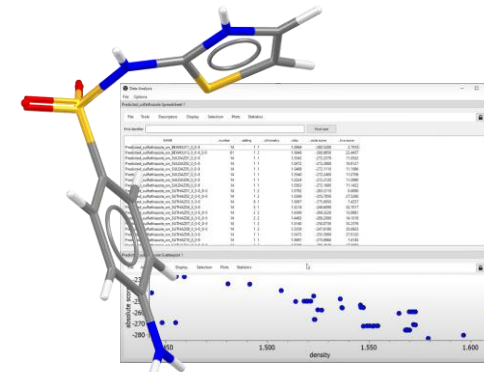
CSDParticle.

*Anticipate particle properties and behaviour*



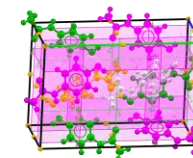
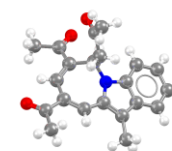
CSDTheory.

*Generate solid form landscapes*



CSDCommunity.

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



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

CCDC



# Agenda



We will make the recording available to you in the next few days.

- Introduction to the CSD
- *Show One:* Research exploring Hydrogen and Halogen bonding
- *Show One:* Introduction and demonstration of ConQuest and Mercury
- *Try One:* Hands-on examples
- *Explore More:* More advanced tips and tricks and case-studies
- *Explore More:* Quiz and Summary
- *Extra time:* More time for hands on and Q&A

# Agenda

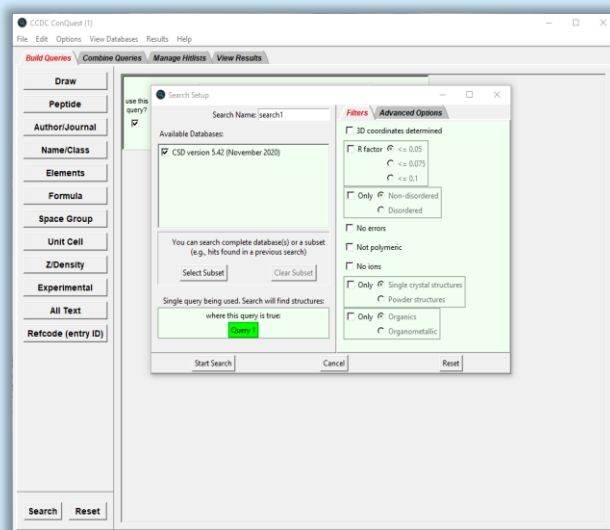


We will make the recording available to you in the next few days.

- Introduction to the CSD
- *Show One*: Research exploring Hydrogen and Halogen bonding
- *Show One*: Introduction and demonstration of ConQuest and Mercury
- *Try One*: Hands-on examples
- *Explore More*: More advanced tips and tricks and case-studies
- *Explore More*: Quiz and Summary
- *Extra time*: More time for hands on and Q&A

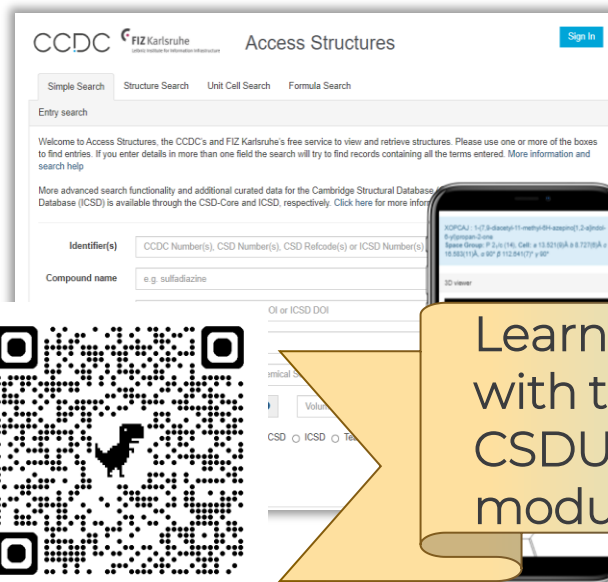
# Structure searching

## Desktop



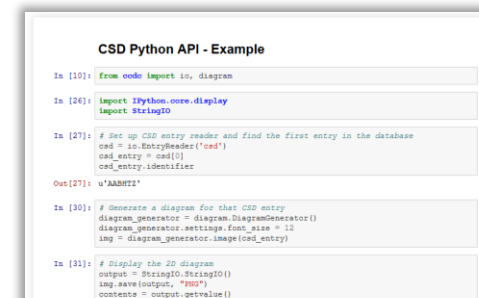
ConQuest

## Web Browser



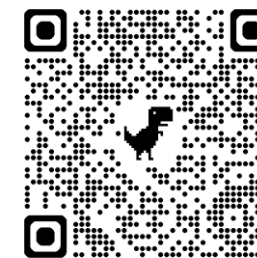
WebCSD /  
Access Structures

## Programmatic



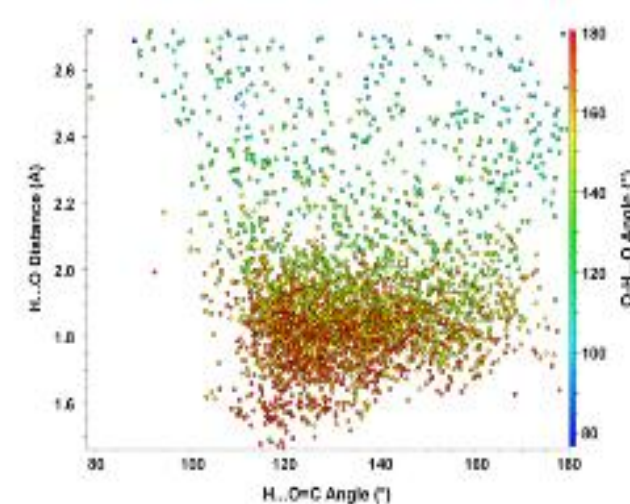
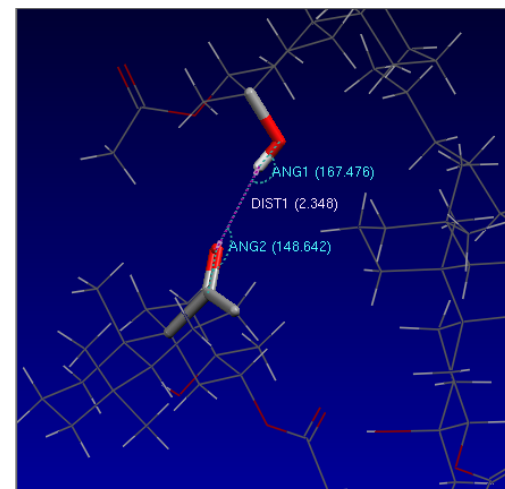
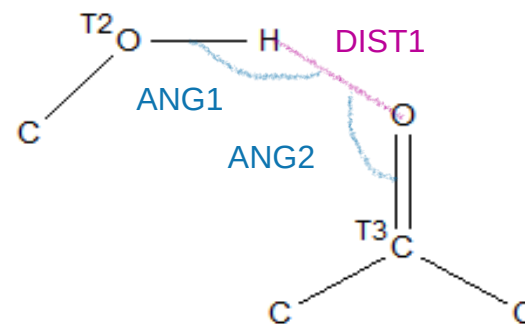
CSD Python API

Learn on demand  
with the  
CSDU  
modules!



# What is ConQuest?

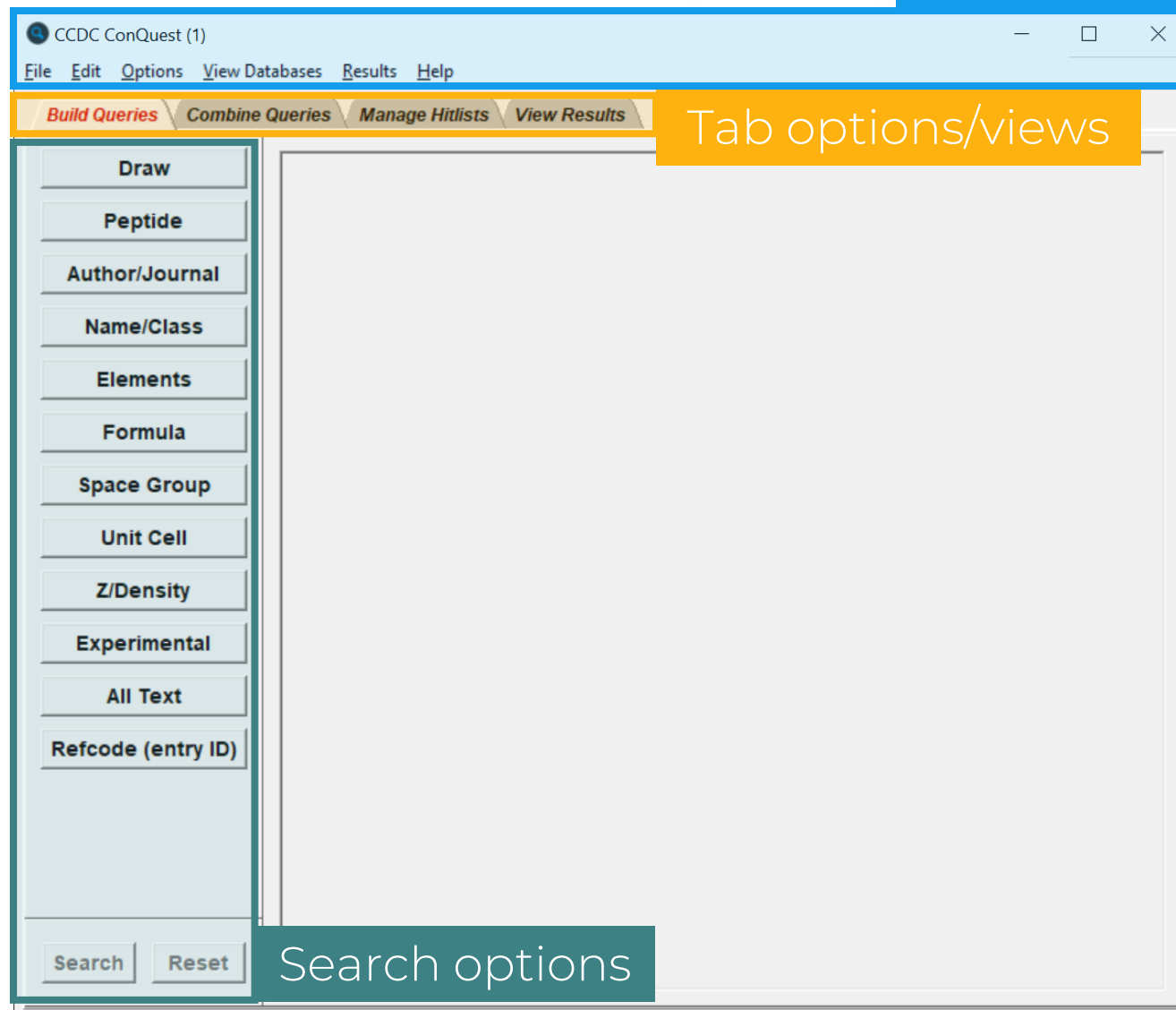
- Enables [search](#) and retrieval of information from the CSD
- Provides full range of [text / numeric](#) database search options
- More complex search functionality includes:
  - [Chemical structure](#) searching
  - [3D Geometrical](#) searching
  - Intermolecular non-bonded [contact searching](#)



# ConQuest: Opening and search options

File menus

Tab options/views



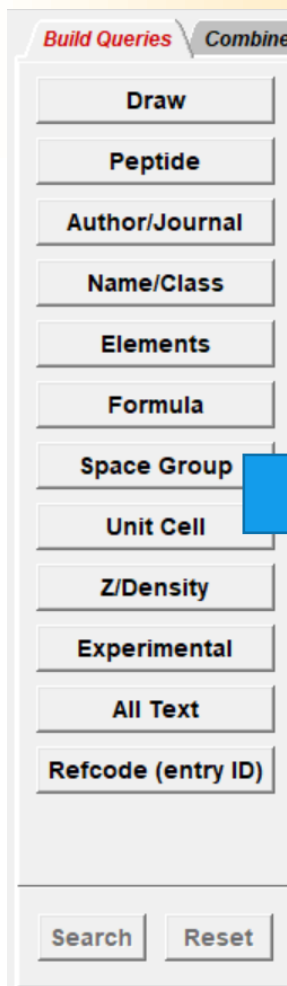
Search options

# How to search in ConQuest

1. Build a Query:  
what do you want to find?

2. Click search and select  
filters: do you need to  
restrict your search?

3. Visualise and analyse  
results: what can you learn  
from this data?



Build Queries Combine

Draw

Peptide

Author/Journal

Name/Class

Elements

Formula

Space Group

Unit Cell

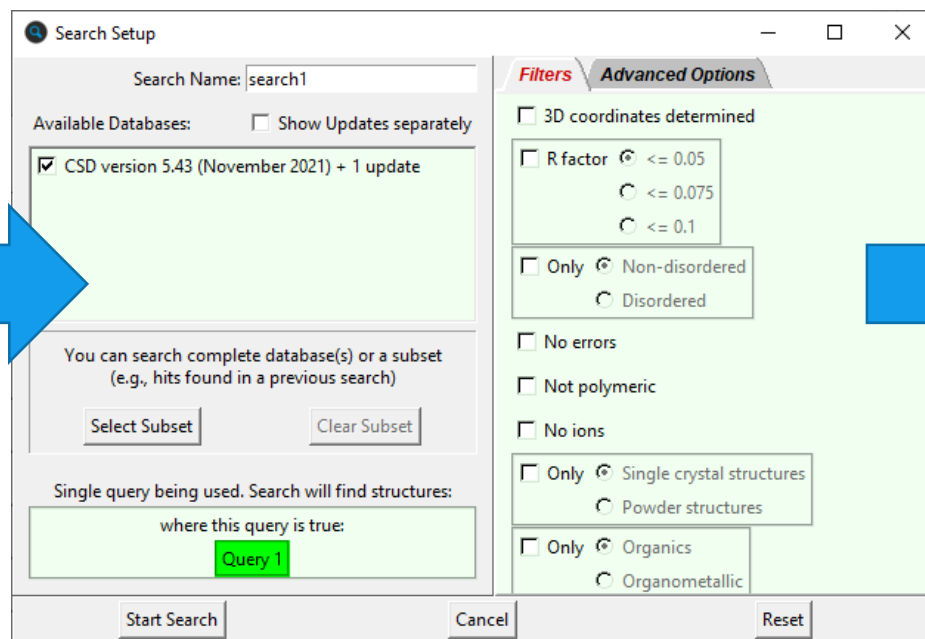
Z/Density

Experimental

All Text

Refcode (entry ID)

Search Reset



Search Setup

Search Name: search1

Available Databases: ☐ Show Updates separately

☒ CSD version 5.43 (November 2021) + 1 update

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

Select Subset Clear Subset

Single query being used. Search will find structures:  
where this query is true:  
Query 1

Start Search Cancel Reset

Filters Advanced Options

☐ 3D coordinates determined

☐ R factor  $\leq 0.05$   
 $\leq 0.075$   
 $\leq 0.1$

☐ Only ☒ Non-disordered  
☐ Disordered

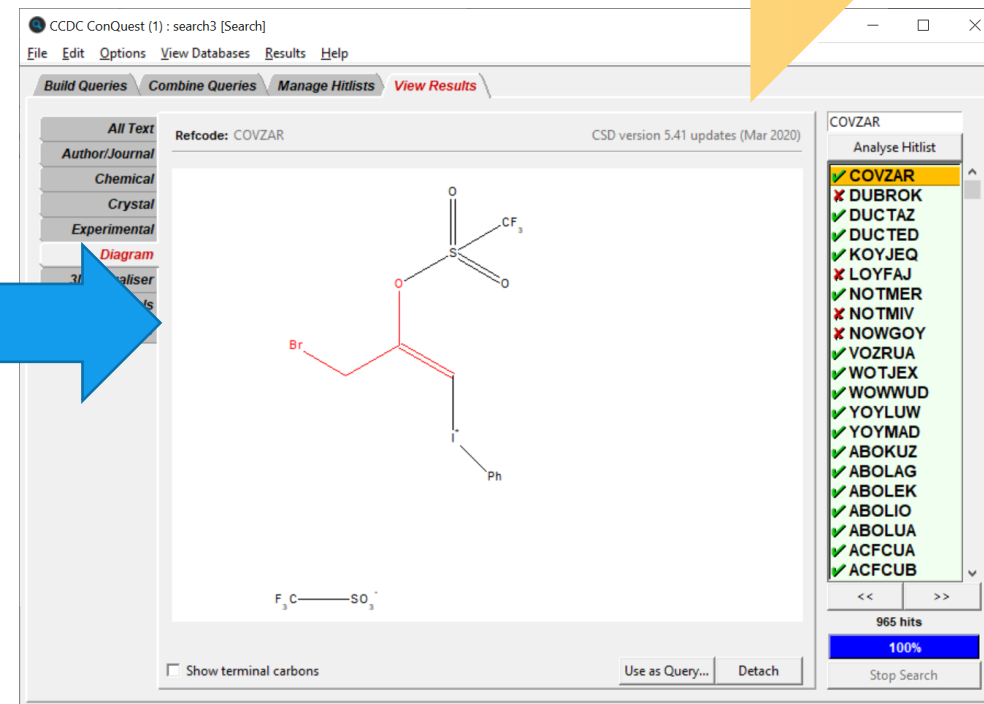
☐ No errors

☐ Not polymeric

☐ No ions

☐ Only ☒ Single crystal structures  
☐ Powder structures

☐ Only ☒ Organics  
☐ Organometallic



CCDC ConQuest (1) : search3 [Search]

File Edit Options View Databases Results Help

Build Queries Combine Queries Manage Hitlists View Results

All Text Author/Journal Chemical Crystal Experimental Diagram

Refcode: COVZAR CSD version 5.41 updates (Mar 2020)

COVZAR

Analyse Hitlist

- ✓ COVZAR
- ✓ DUBROK
- ✓ DUCTAZ
- ✓ DUCTED
- ✓ KOYJEQ
- ✗ LOYFAJ
- ✓ NOTMER
- ✗ NOTMIV
- ✗ NOWGOY
- ✓ VOZRUA
- ✓ WOTJEX
- ✓ WOWWUD
- ✓ YOYLW
- ✓ YOYMAD
- ✓ ABOKUZ
- ✓ ABOLAG
- ✓ ABOLEK
- ✓ ABOLIO
- ✓ ABOLUA
- ✓ ACFCUA
- ✓ ACFCUB

965 hits 100% Stop Search

Chemical structure diagram showing a brominated organic molecule and a triflate anion ( $\text{F}_3\text{C}-\text{SO}_3^-$ ).

Show terminal carbons Use as Query... Detach



# Draw

**Build Queries** **Combine**

**Draw**

Peptide

Author/Journal

Name/Class

Elements

Formula

Space Group

Unit Cell

Z/Density

Experimental

All Text

Refcode (entry ID)

Draw (1) - New

File Edit Atoms Bonds 3D Options Help

Element  
Add Group  
Expand Chemical Groups  
Hydrogens  
Charge  
Number of Bonded Atoms  
Cyclicity  
All Atoms in Same Molecule

Drawing Options...  
Snap to Grid  
Save Window Size  
Limit Window Size  
Auto-Generate H  
Balloon Help

Next Atom: C  
Next Bond: Single

3D Parameters:

Options...  
Delete

Contacts:

Options...  
Delete

Search  
Store  
Cancel

Draw

EDIT

ERASE

ADD 3D

CONTACT

Ring template selector or builder

List of templates for challenging structures e.g. adamantane

RingMaker

Templates...

C H O N S P F Cl Any More... Groups... C

Bond: Single

Additional menu options to explore

Define atoms, bonds or molecules to be searched

Define lengths, angles, torsions or geometric objects e.g. planes or centroids as parameters to be searched

Ring template selector or builder

List of templates for challenging structures e.g. adamantane

Select specific or general atom types/functional groups

Select bond type

# ConQuest – Draw/Structure search

The screenshot displays the ConQuest software interface for drawing and searching chemical structures. The main window is titled "Draw (1) - New" and contains a menu bar (File, Edit, Atoms, Bonds, 3D, Options, Help) and a toolbar with icons for drawing, editing, and erasing. A sidebar on the left lists various search criteria: Draw, Peptide, Author/Journal, Name/Class, Elements, Formula, Space Group, Unit Cell, Z/Density, Experimental, All Text, and Refcode (entry ID). The central workspace shows a chemical structure of a six-membered ring with a nitrogen atom (N) and a red atom (M) attached. A context menu is open over the structure, listing options: Element, Add Group, Hydrogens, Charge, Number of Bonded Atoms (selected), Cyclicity, and Delete Atom. A sub-menu for "Number of Bonded Atoms" is also visible, showing options 1 through 8, with "Unspecified" selected. To the right, a "3D Parameters" panel is shown. Below the main window, an "Other Atom Type" dialog box is open, displaying a periodic table with various elements highlighted. A blue arrow points from the "Other Elements..." option in the context menu to the "Other Atom Type" dialog. At the bottom, a "Bond" dropdown menu is set to "Single".



Left click in space to add an atom



Left click and drag from an atom to attach an atom



Right click on an atom or bond to edit or add extra properties to it

# Results

Query highlighted

Analyse hitlist

Different ways to view the results

Link to the publication

Link to deposited CIF file

Link to the International Tables

A hit list of structures by Refcode

Total number of search results

CCDC ConQuest (1) : search1 [Search]

File Edit Options View Databases Results Help

Build Queries Combine Queries Manage Hitlists View Results

Refcode: AVETAW CSD version 5.43 (November 2021)

|                  |                                                                                                     |
|------------------|-----------------------------------------------------------------------------------------------------|
| Author(s)        | M. Bolocchi, M. Bonizzoni, L. Fabbrizzi, F. Foti, M. Licchelli, A. Taglietti, M. Zema               |
| Reference        | Dalton Trans. (2004), , 653                                                                         |
| Publication DOI  | <a href="https://doi.org/10.1039/b312980b">10.1039/b312980b</a>                                     |
| Deposition       | <a href="#">CCDC 221987</a>                                                                         |
| Formula          | $C_{10}H_{24}N_4Ni^{2+} \cdot 2(ClO_4^-)$                                                           |
| Compound         | (3-(4-(3-Aminopropyl)piperazin-1-yl)propylamine)-nickel(ii) diperchlorate                           |
| Spacegroup       | Name: P6ca Number: <a href="#">61</a>                                                               |
| Cell             | a: 14.426(2) b: 15.390(2) c: 16.171(2)<br>alpha: 90.00 beta: 90.00 gamma: 90.00<br>Volume: 3590.306 |
| Reduced Cell     | a: 14.426 b: 15.390 c: 16.171<br>alpha: 90.00 beta: 90.00<br>Volume: 3590.306                       |
| Molecular Volume | 448.788                                                                                             |
| Chemical Units   | 2                                                                                                   |
| Z, Z'            | Z: 8.0 Z': 1.0                                                                                      |

Detach

AVETAW

Analyse Hitlist

- ✓ AVETAW
- ✓ AVETEA
- ✓ BAQFOO
- ✓ BETHEO02
- ✓ BOGKOX
- ✓ DUCWAA
- ✓ DUCWOO
- ✓ EBELON
- ✓ EBELUT
- ✓ FASQOI
- ✓ FASQUO
- ✓ GOLLUR
- ✓ HIGGAG
- ✓ HUDBEO
- ✓ IBIYOH
- ✓ IBIYUN
- ✓ IBIZAU
- ✓ IBIZEY
- ✓ IWAKEW
- ✓ IWAKIA
- ✓ KELZOQ

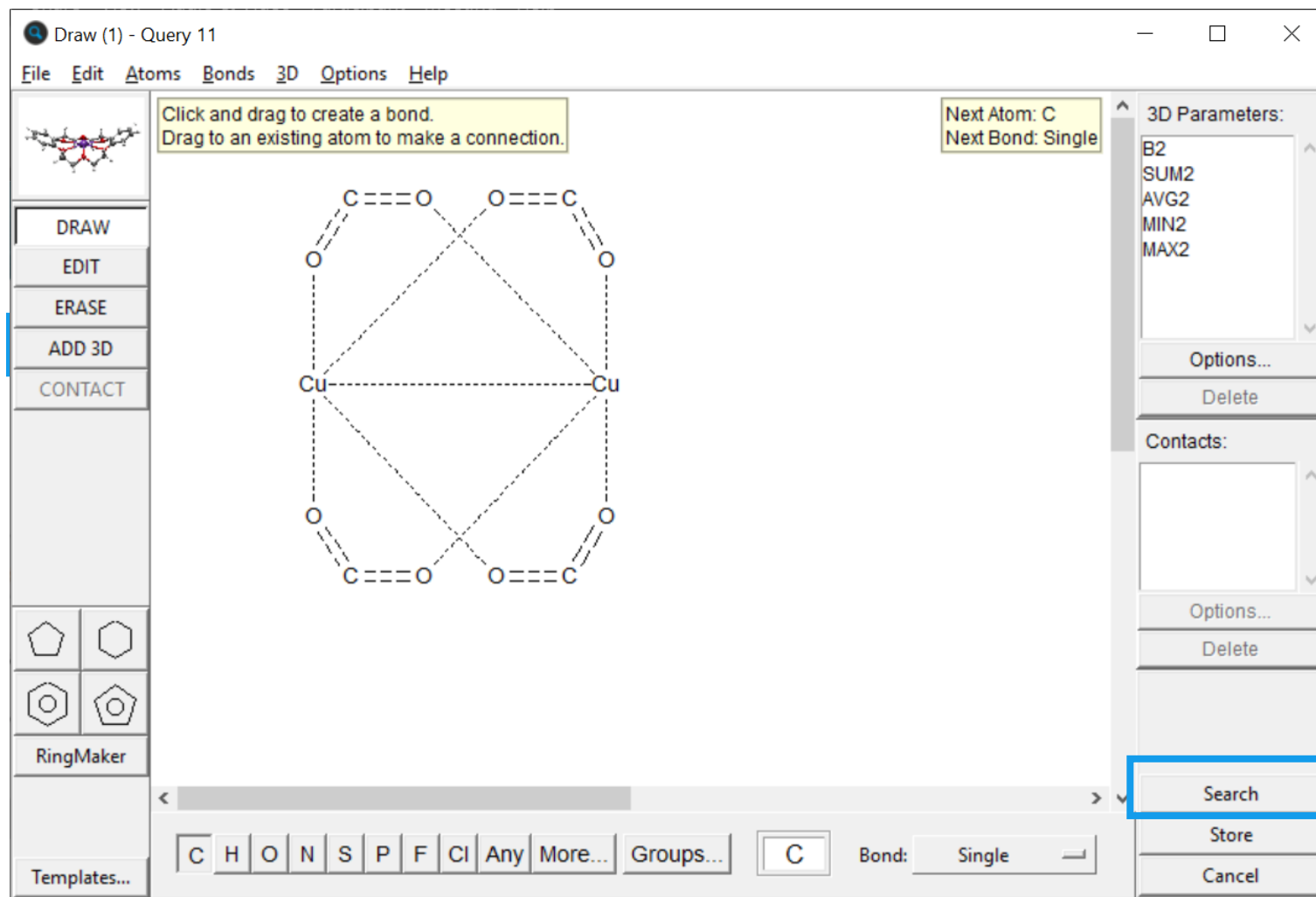
<< >>

50 hits

100%

Stop Search

# 3D searching



1. Draw your substructure
2. Click Add 3D
3. Select parts of the structure you are interested in
4. Define the parameters you want to analyse
5. Search or store your query
6. View the results
7. Analyse the hit list

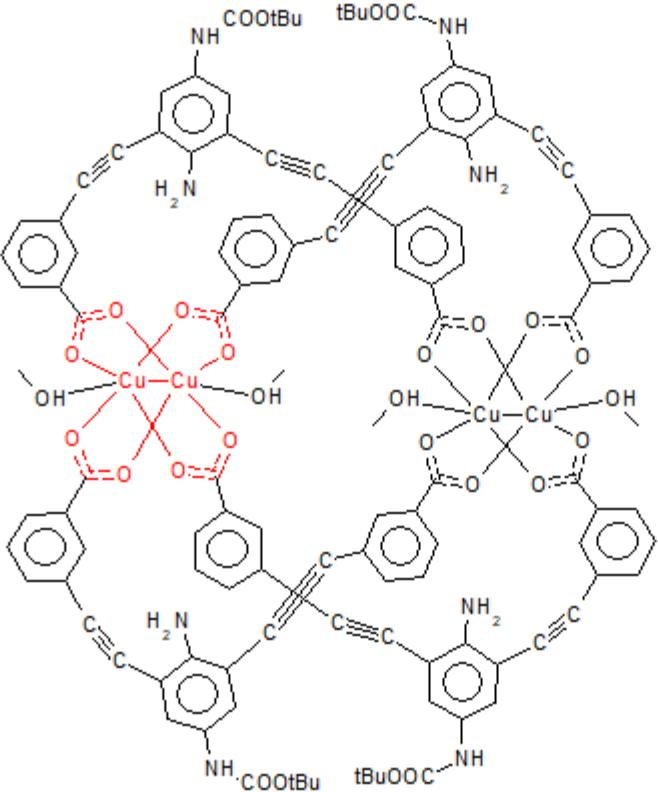
CCDC ConQuest (1) : search11 [Search]

File Edit Options View Databases Results Help

Build Queries Combine Queries Manage Hitlists View Results

All Text  
Author/Journal  
Chemical  
Crystal  
Experimental  
Diagram  
3D Visualiser  
CSD Internals  
Search Overview

Refcode: JUZTOQ CSD version 5.42 updates (Feb 2021)



Parameters

|      |       |
|------|-------|
| B2   | 2.603 |
| SUM2 | 2.603 |
| AVG2 | 2.603 |
| MIN2 | 2.603 |
| MAX2 | 2.603 |

Multiple Hits: Show 1 of 2 ☒ Show Parameters

☐ Show terminal carbons Use as Query... Detach

Search highlighted in 2D

Parameters displayed

JUZTOQ  
Analyse Hitlist

Visualise Structures

Analyse Data

Select All

Deselect All

Invert Selection

Analyse in Mercury

Select the items you wish to include from the choices below

File type: Mercury data file ( .c2m )

☒ Include Defined Parameters

Crystal data

☐ R-factor

☐ Space Gp. Symbol

☐ Space Gp. Number

☐ No. of Coordinates

☐ Z Value

☐ Z Prime

☐ Study Temp.

☐ Calc. Density

Cell data

☐ a

☐ b

☐ c

☐ Alpha

☐ Beta

☐ Gamma

☐ Cell Volume

☐ Reduced Cell a

☐ Reduced Cell b

☐ Reduced Cell c

☐ Reduced Cell Volume

☐ Reduced Cell Alpha

☐ Reduced Cell Beta

☐ Reduced Cell Gamma

Other

☐ Publication Year

☐ Unique Chemical Units

☐ Multiplier Sum

☐ Compound Name

829 h

0%

Reset

Cancel

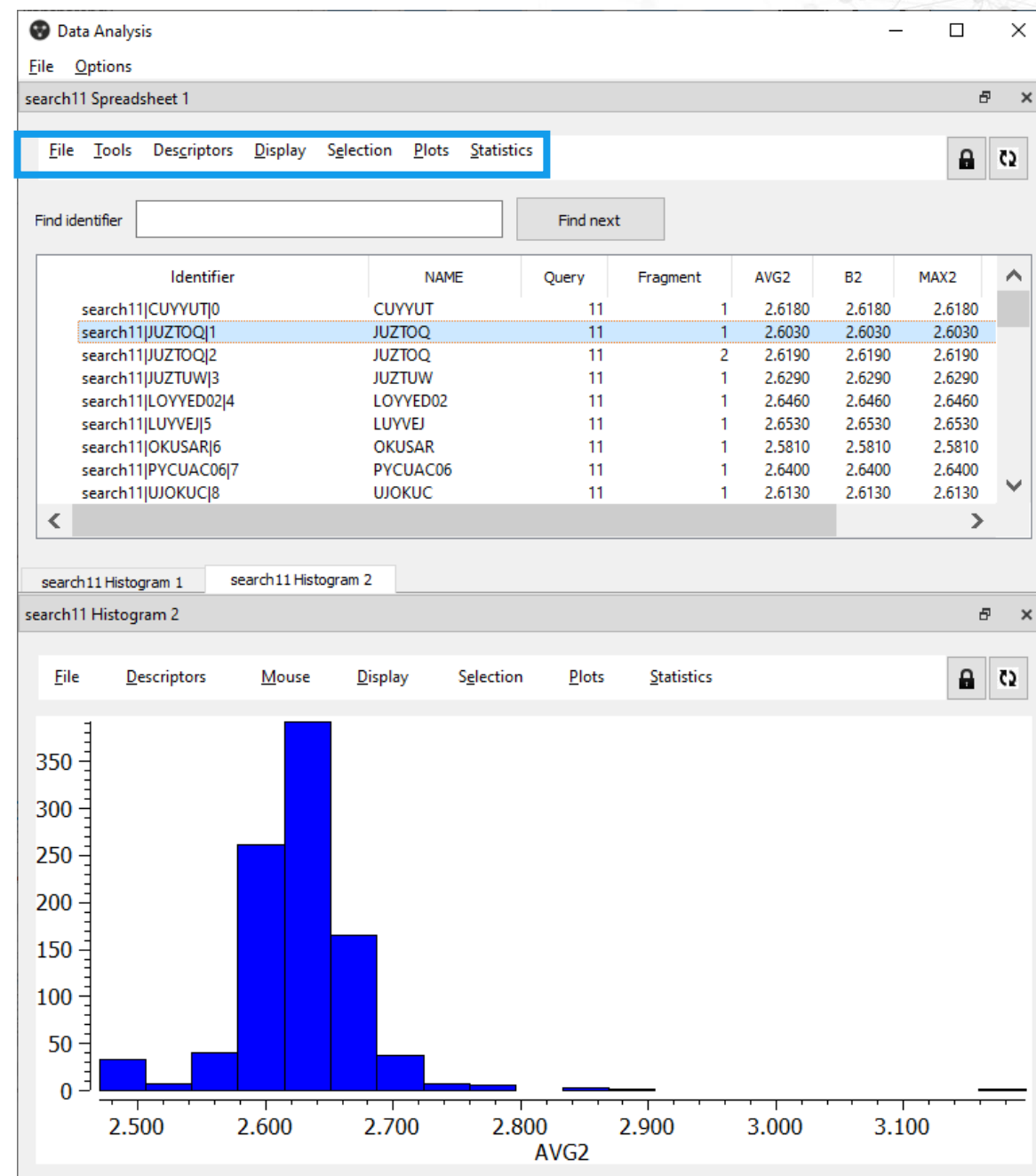
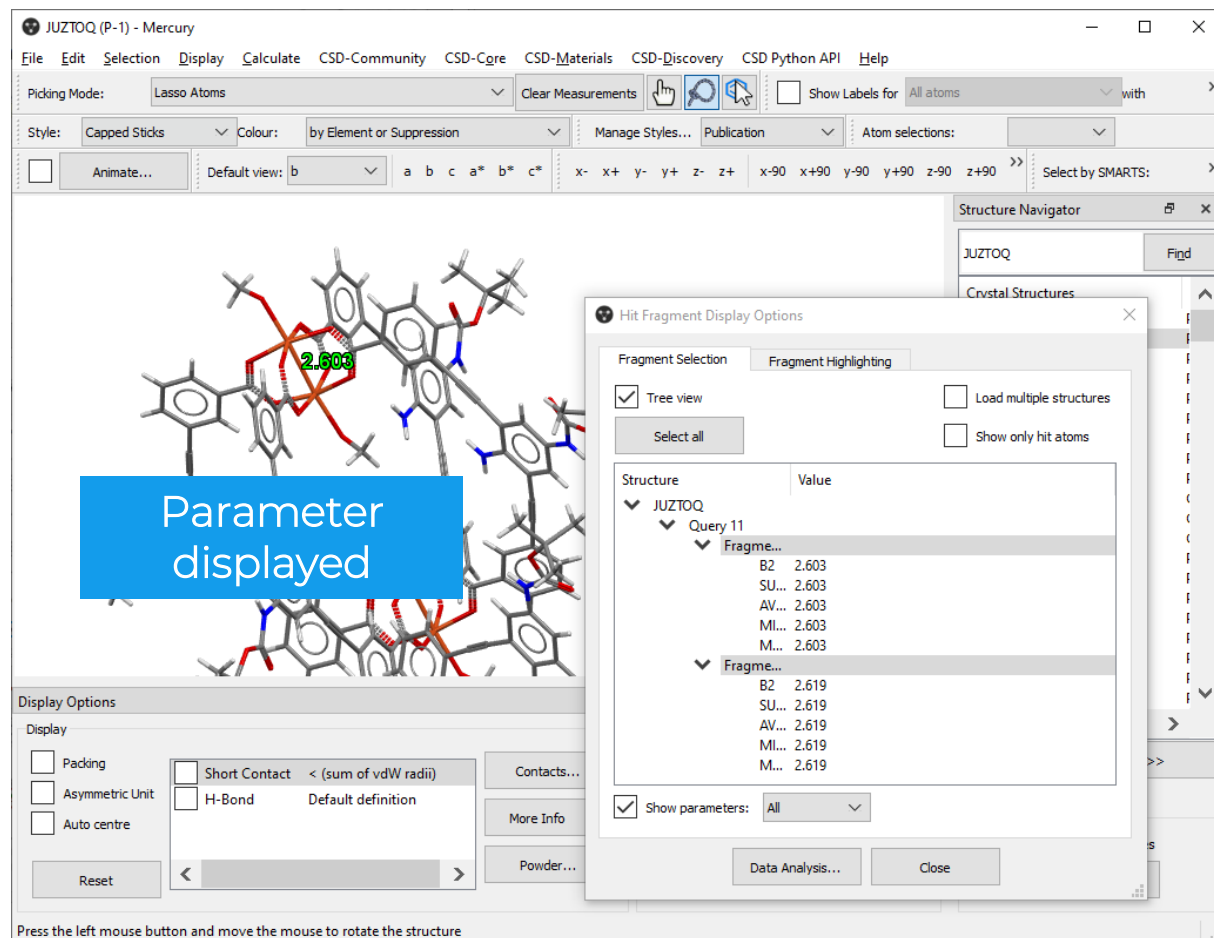
Analyse in Mercury

100%

Stop Search

CCDC

# Data analysis





# Mercury Overview

More advanced  
functionality to analyse  
and learn from structures

AABHTZ (P-1) - Mercury

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

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

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

Animate... Default view: b a b c a\* b\* c\* x- x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-90 z+90 ← → ↓ ↑ zoom- zoom+

Structure Navigator

AABHTZ

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

Display  
options to  
visualise and  
navigate  
structures

Explore over  
1.25 million  
curated  
structures

Display Options

Display

- ☐ Packing
- ☐ Asymmetric Unit
- ☐ Auto centre

☐ Short Contact < (sum of vdW radii)

☐ H-Bond Default definition

Reset

Contacts...

More Info

Powder...

Options

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

☒ Tree View

☐ Multiple Structures

Structures...

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



## Mercury Visualisation 101

Downloadable  
training  
module



## Self-guided exercises

# Show One: Demo of ConQuest and Mercury

- In this demo we will use ConQuest and Mercury to follow one of Catherine's investigations in *Cryst. Growth Des.* 2024, 24, 2, 859–870.
- Construct a 3D search on ConQuest.
- Export results to Mercury.
- Use the Data Analysis tool to explore Hydrogen Bonded  $R^2_2(8)$  Rings.

We will make the recording available to you in the next few days.



# Try One: hands-on exercise

We will make the recording available to you in the next few days.

## It's your turn!

- Try the [example](#) from the handout.
- Your tutors are on hand to help you!
- To ask questions during this time type a message in the chat box.

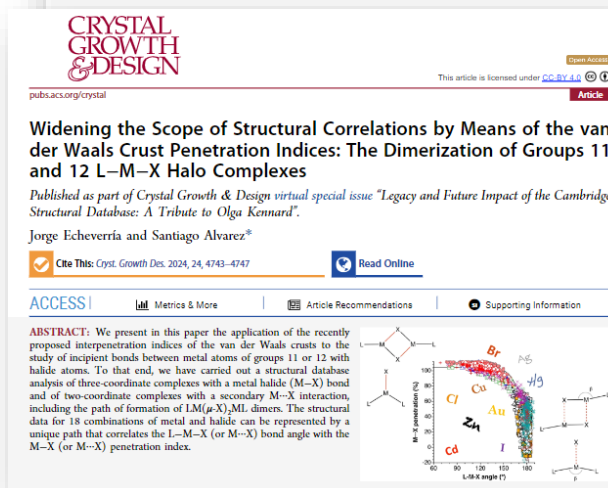
These exercises follow research in another recent article:

- J. Echeverría and S. Alvarez, *Cryst. Growth Des.*, 2024, 24, 4743–4747. DOI: 10.1021/acs.cgd.4c00335

<https://info.ccdc.cam.ac.uk/2024-autumn-virtual-workshop>

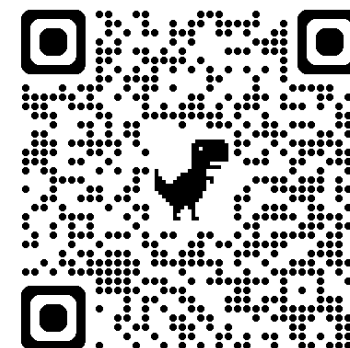
### Exploring Structure Correlations Using Mercury and ConQuest

Developed using  
2024.2 CSD Release



#### Table of Contents

|                                                                    |    |
|--------------------------------------------------------------------|----|
| Introduction.....                                                  | 2  |
| Learning Outcomes .....                                            | 2  |
| Pre-required Skills .....                                          | 2  |
| Materials.....                                                     | 2  |
| Example 1. The Dimerization of Group 11 L–M–X Halo complexes ..... | 3  |
| Part 1. Building search queries in ConQuest .....                  | 3  |
| Part 2. Data analysis in Mercury.....                              | 11 |
| Conclusion .....                                                   | 17 |
| Further exercises .....                                            | 17 |
| Summary.....                                                       | 18 |
| Next Steps.....                                                    | 18 |
| Glossary .....                                                     | 19 |
| Basics of Mercury Visualization .....                              | 20 |
| Review. ConQuest Interface .....                                   | 21 |
| Review. Draw Window.....                                           | 22 |
| ConQuest sketching conventions.....                                | 22 |



# Agenda

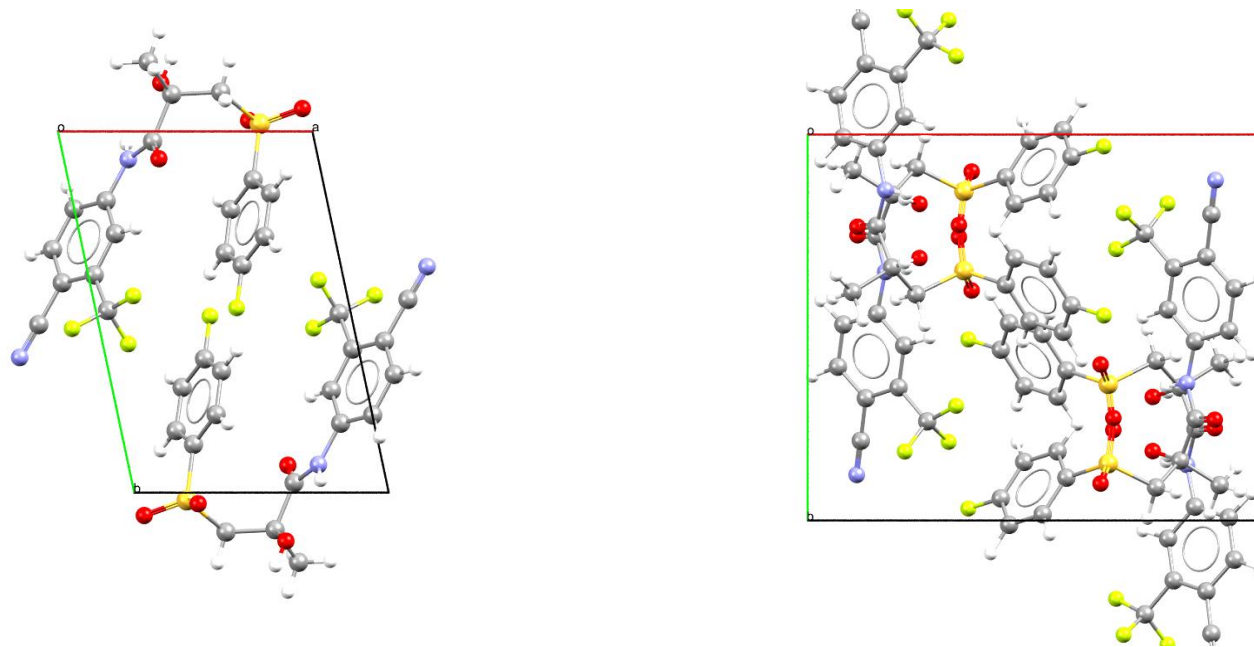


We will make the recording available to you in the next few days.

- Introduction to the CSD
- *Show One*: Research exploring Hydrogen and Halogen bonding
- *Show One*: Introduction and demonstration of ConQuest and Mercury
- *Try One*: Hands-on examples
- *Explore More*: More advanced tips and tricks and case-studies
- *Explore More*: Quiz and Summary
- *Extra time*: More time for hands on and Q&A

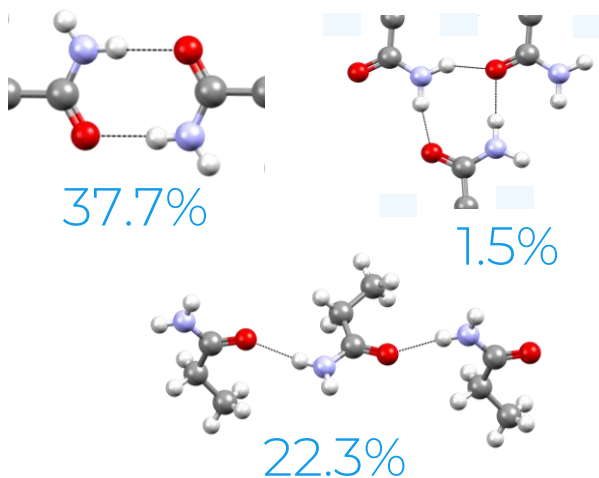
# Intermolecular interactions and packing

- To go further you can look at the [packing environment](#) of the molecules using a range of tools.
- Using the CSD for context (unusual hydrogen bond parameters for example) as well as enabling [comparison](#) of structures.



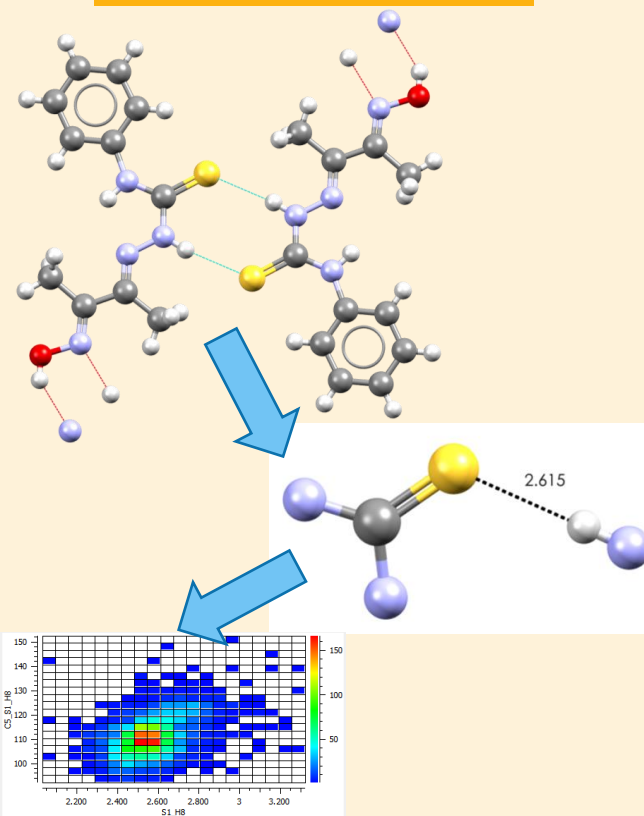
# Searching within Mercury

## Motifs

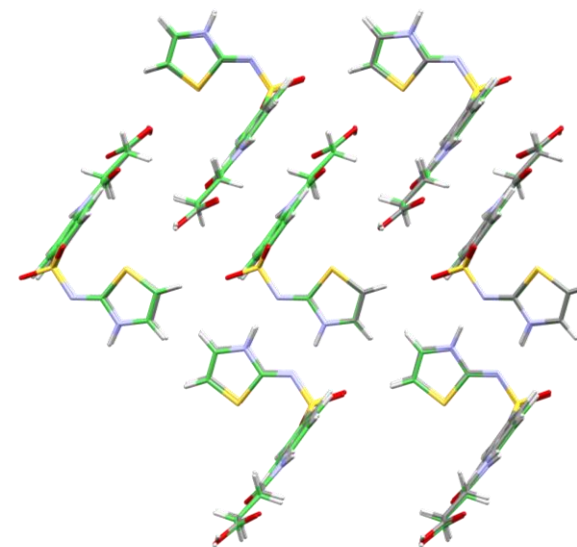


- H-bond motifs

## Crystal Packing Feature



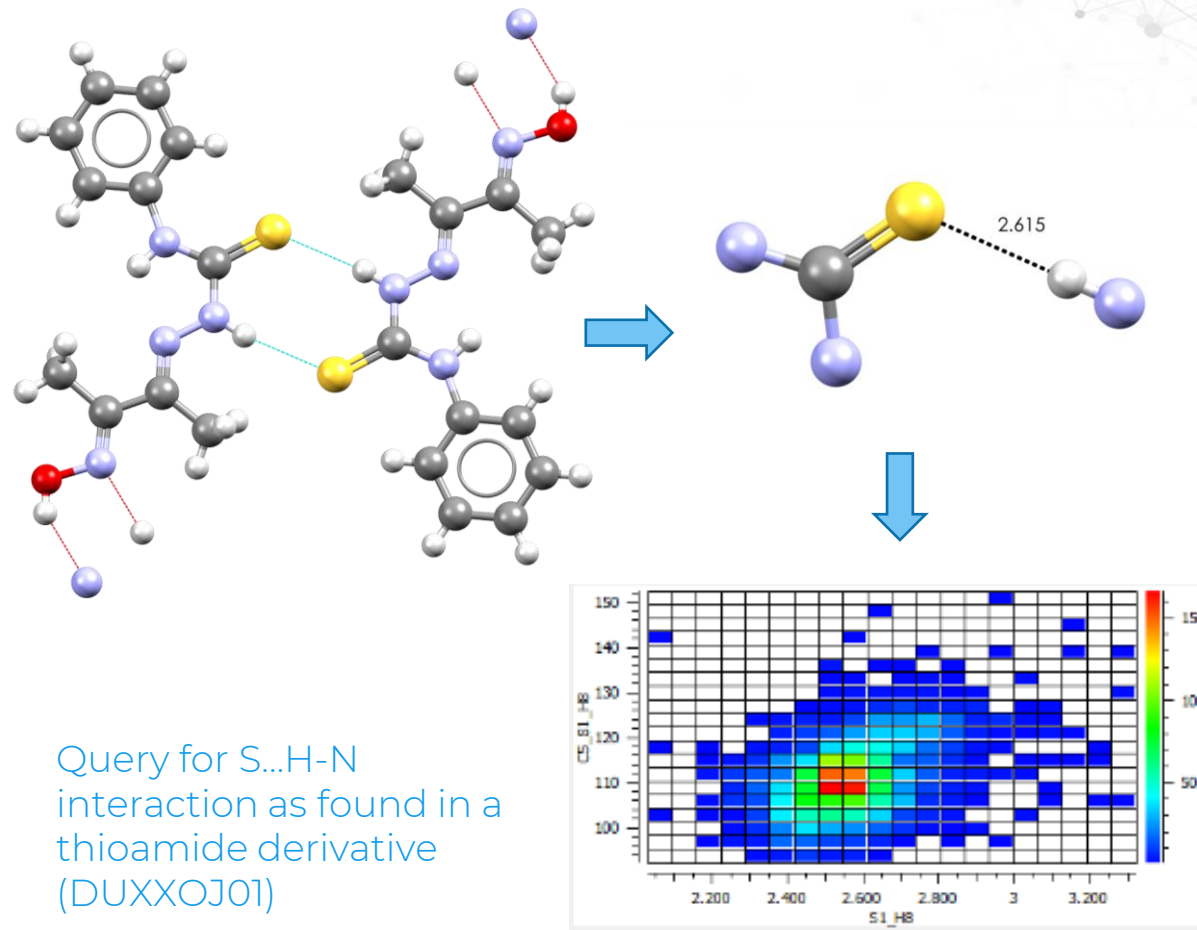
## Crystal Packing Similarity





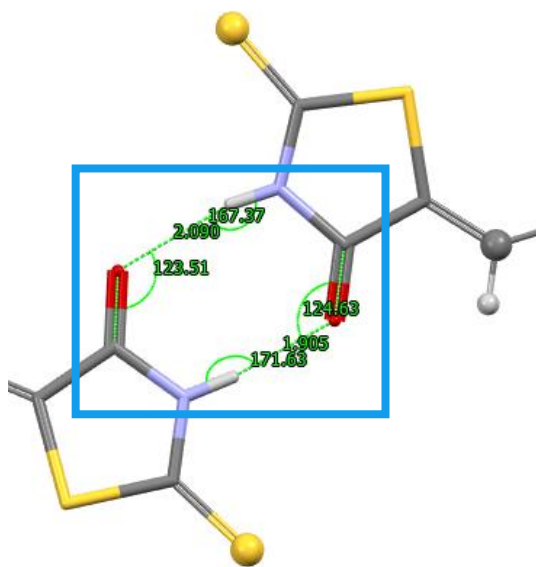
# Crystal Packing Feature Search

- Perform a **substructure search**
- Investigate **conformations** of **molecules** or bonded **fragments**.
- Search for:
  - non-covalent **interactions** such as  $\pi$ - $\pi$  or hydrogen bond interactions.
  - particular **spatial arrangements** of **functional groups**.
  - particular **spatial arrangements** of **molecules**.

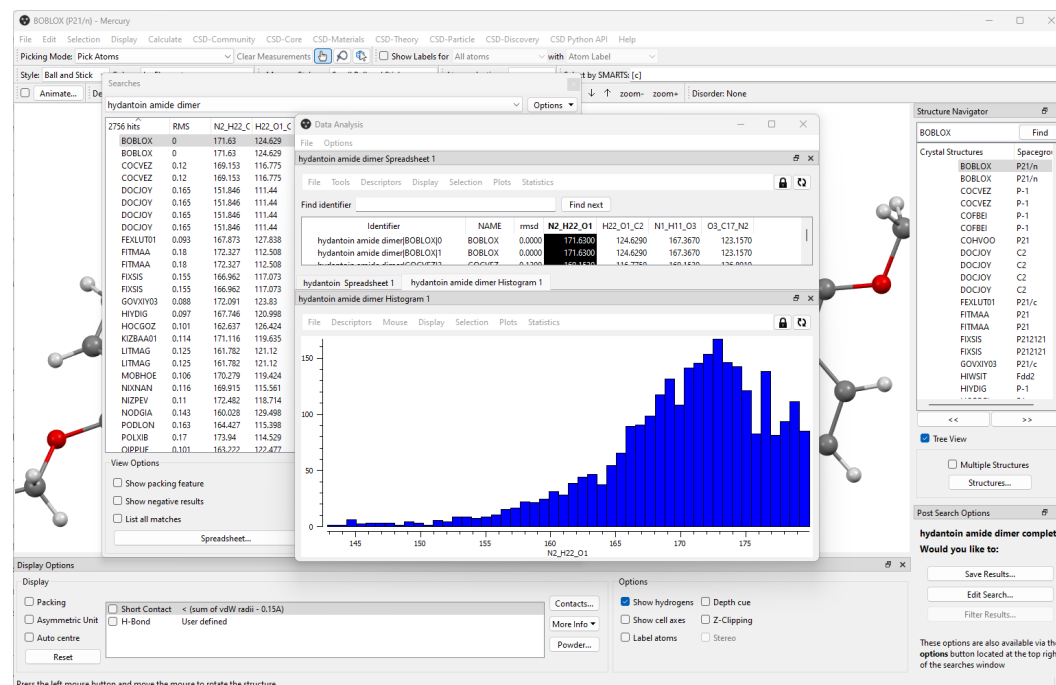


# Searching within Mercury: Crystal Packing Feature

- Pick a feature from the current structure in Mercury
- Search the whole CSD or within ConQuest hitlist



Packing  
Feature  
Search



# Crystal Packing Feature : Selecting a Feature

Core CSD-Materials CSD-Theory CSD-Particle CSD-Discovery CSD Python

Search  
Calculations  
Polymorph Assessment  
Co-Crystal Design  
Full Interaction Maps...  
Hydrogen Bond Statistics...  
Hydrate Analyser...  
Solvate Analyser...  
Aromatics Analyser...  
Conformer Generation...  
DASH has moved

Motifs...  
Crystal Packing Feature...  
Crystal Packing Similarity...  
Manage Searches...  
Manage Motifs...  
Post Search Options

Packing Feature Search Wizard

Use this wizard to search for a crystal packing feature

Load a crystal structure in the visualizer and then **select atoms** to select the spatial arrangement of atoms you wish to search for.

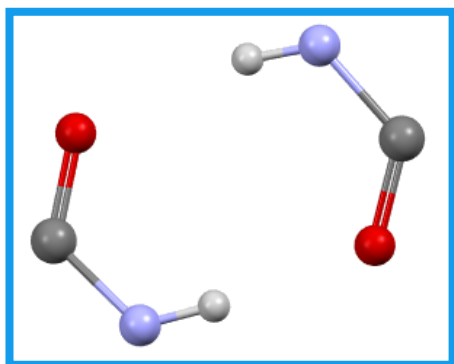
No atoms currently selected

Pick atoms from current structure

You have selected 8 atoms of 2 molecule(s) from BOBLOX

< Back Next > Cancel

# Crystal Packing Feature: Selecting Options



Picked fragment  
of structure

Packing Feature Search Wizard

**Allow variable atom and bond types**

Select the atoms and bonds you wish to vary and press 'Modify'. Or simply press 'Next'.

atoms bonds

| atom | residue | elements | hydrogens | bonds |
|------|---------|----------|-----------|-------|
| N1   | 2       | N        | 1         | 3     |
| O1   | 2       | O        | 0         | 1     |
| H11  | 2       | H        | 1         | 1     |
| C2   | 2       | C        | 0         | 3     |
| O3   | 1       | O        | 0         | 1     |
| H22  | 1       | H        | 1         | 1     |
| N2   | 1       | N        | 1         | 3     |
| C17  | 1       | C        | 0         | 3     |

Search Options

Modify

Reset

Add Constraint

- ☒ Number of hydrogens
- ☒ Number of bonds
- ☐ Charge
- ☐ Cyclicity

< Back Next > Cancel

Add constraints if  
required

Packing Feature Search Wizard

**Allow tolerances on the geometry of the packing feature**

Level of Geometric Similarity Required

☐ Very high ☐ High ☒ Medium ☐ Low ☐ Custom

Custom Tolerances

Distances must match those of selected feature to within + or - 30 %

Angles must match those of selected feature to within + or - 20 degrees

Match Options

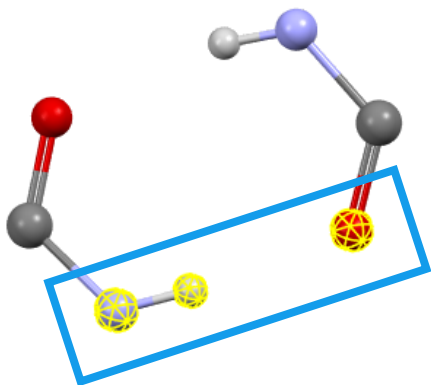
☐ All matched fragments must belong to same molecule

☐ Show distances ☐ Show angles

< Back Next > Cancel

Select search tolerance for  
RMSD calculations

# Crystal Packing Feature: Selecting Parameters



Select 3D parameters (like in ConQuest)

Packing Feature Search Wizard

### Select Parameters

Select atoms in the visualiser to select **distance**, **angle** or **torsion** parameters. Or simply press 'Next'.

**Current Selection:**

N2 H22 O1

Add Angle >

Parameter List

Delete

Rename

< Back Next > Cancel



Packing Feature Search Wizard

### Select Parameters

Select atoms in the visualiser to select **distance**, **angle** or **torsion** parameters. Or simply press 'Next'.

**Current Selection:**

Add >

Parameter List

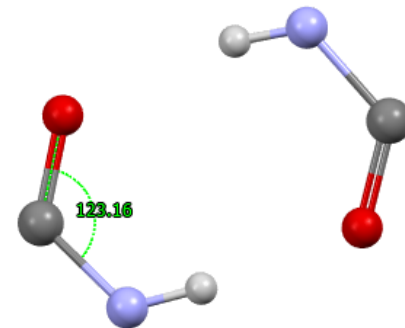
- N2\_H22\_O1
- H22\_O1\_C2
- N1\_H11\_O3
- O3\_C17\_N2

Delete

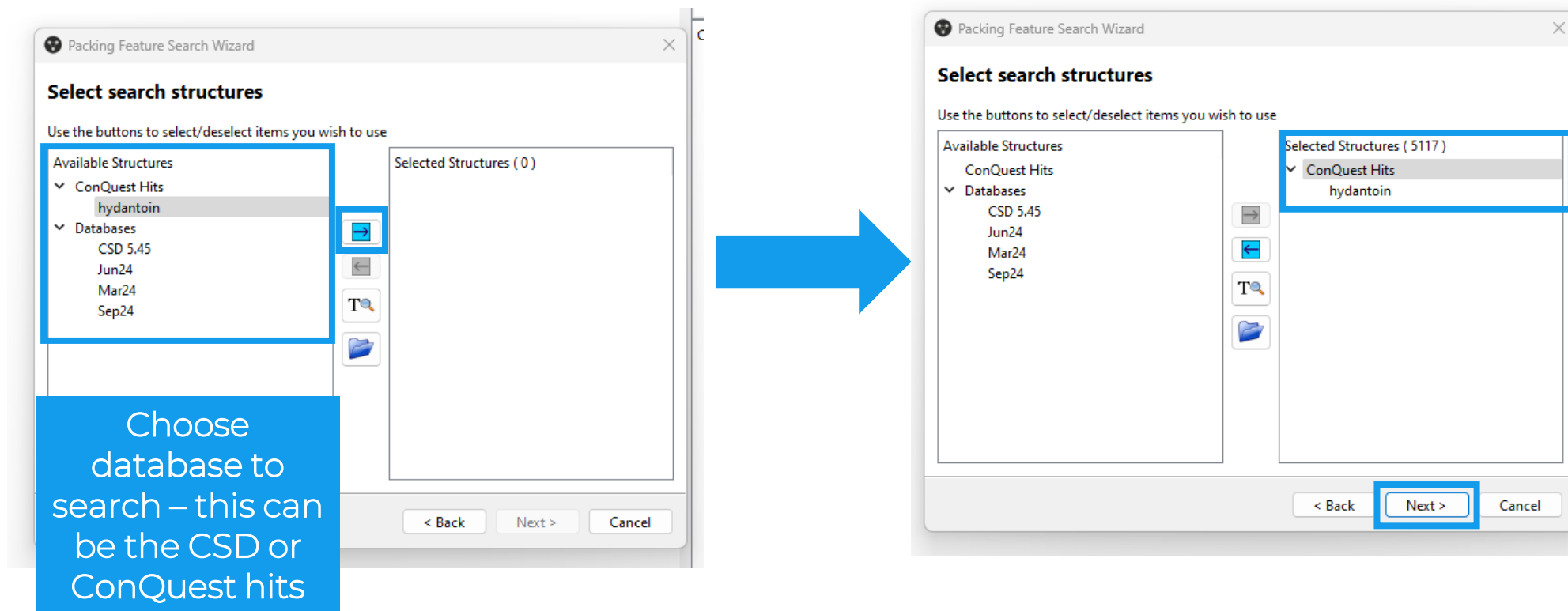
Rename

< Back Next > Cancel

Summary of selected 3D parameters



# Crystal Packing Feature: Selecting Search Structures





# Crystal Packing Feature: Launching Search

**Name the search and run it**

The screenshot shows the Mercury software interface with the 'Packing Feature Search Wizard' dialog box open. The dialog box has a title bar 'Packing Feature Search Wizard' and a close button. It contains two input fields: 'Packing feature name: amide dimer' and 'Search name: hydantoin amide dimer'. Below these fields are three buttons: '< Back', 'Start Search' (highlighted with a blue box), and 'Cancel'. The background shows the Mercury interface with a molecular structure and a list of crystal structures on the right. A blue box with the text 'Name the search and run it' is overlaid on the main window.

Mercury interface details:

- Menu bar: File, Edit, Selection, Display, Calculate, CSD-Community, CSD-Core, CSD-Materials, CSD-Theory, CSD-Particle, CSD-Discovery, CSD Python API, Help
- Toolbar: Picking Mode (Pick Atoms), Clear Measurements, Show Labels for (All atoms), with (Atom Label), Style (Ball and Stick), Colour (by Element), Manage Styles..., Small Ball and Stick, Atom selections, Select by SMARTS: [c], Animate..., Default view: b, a b c a\* b\* c\*, x- x+ y- y+ z- z+, x-90 x+90 y-90 y+90 z-90 z+90, Disorder: None
- Structure Navigator: BOBLOX, Find, Crystal Structures (list of structures including BOBLOX, COCVEZ, COFBEI, COHVOO, DOJCJOY, FEFLUT01, FITMAA, FIXSIS, GOVXIY03, HIWSIT, HIYDIG, HOBDDEL, HOBDDEL01, HOBDDEL01, HOBDIP, HOCGOZ, HOFNOJ, JOGPPE, KIZBAA01, LITMAG, LITMEK, LOBZIP, LOBZIP, LOBZIP)
- Display Options: Display (Packing, Asymmetric Unit, Auto centre), Short Contact (< (sum of vdW radii - 0.15A)), H-Bond (User defined), Contacts..., More Info..., Powder..., Reset
- Options: Show hydrogens (checked), Depth cue, Show cell axes, Z-Clipping, Label atoms, Stereo

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

# Crystal Packing Feature: Viewing Results

The screenshot displays the Mercury software interface with the BOBLOX (P21/n) search results for 'hydantoin amide dimer'. A blue callout box points to the 'Spreadsheet...' button in the 'View Options' panel, with the text 'Open spreadsheet of search results'.

**Search Results Table:**

|                | RMS     | N2_H22_C | H22_O1_C | N1_H11_C | O3_C17_N2 |
|----------------|---------|----------|----------|----------|-----------|
| BOBLOX 0       | 171.63  | 124.629  | 167.367  | 123.157  |           |
| BOBLOX 0       | 171.63  | 124.629  | 167.367  | 123.157  |           |
| COCVEZ 0.12    | 169.153 | 116.775  | 169.153  | 126.891  |           |
| COCVEZ 0.12    | 169.153 | 116.775  | 169.153  | 126.891  |           |
| DOCJOY 0.165   | 151.846 | 111.44   | 164.827  | 125.439  |           |
| DOCJOY 0.165   | 151.846 | 111.44   | 164.827  | 125.439  |           |
| DOCJOY 0.165   | 151.846 | 111.44   | 164.827  | 125.439  |           |
| DOCJOY 0.165   | 151.846 | 111.44   | 164.827  | 125.439  |           |
| DOCJOY 0.165   | 151.846 | 111.44   | 164.827  | 125.439  |           |
| FEFLUT01 0.093 | 167.873 | 127.838  | 167.873  | 123.083  |           |
| FITMAA 0.18    | 172.327 | 112.508  | 164.478  | 122.427  |           |
| FITMAA 0.18    | 172.327 | 112.508  | 164.478  | 122.427  |           |
| FIXSIS 0.155   | 166.962 | 117.073  | 165.162  | 127.071  |           |
| FIXSIS 0.155   | 166.962 | 117.073  | 165.162  | 127.071  |           |
| GOVXIY03 0.088 | 172.091 | 123.83   | 172.091  | 123.529  |           |
| HIYDIG 0.097   | 167.746 | 120.998  | 167.746  | 125.496  |           |
| HOCGOZ 0.101   | 162.637 | 126.424  | 162.637  | 125.294  |           |
| KIZBAA01 0.114 | 171.116 | 119.635  | 171.116  | 125.082  |           |
| LITMAG 0.125   | 161.782 | 121.12   | 161.782  | 130.994  |           |
| LITMAG 0.125   | 161.782 | 121.12   | 161.782  | 130.994  |           |
| MOBHOE 0.106   | 170.279 | 119.424  | 170.279  | 125.351  |           |
| NIXNAN 0.116   | 169.915 | 115.561  | 169.915  | 128.154  |           |
| NIZPEV 0.11    | 172.482 | 118.714  | 172.482  | 124.324  |           |
| NODGIA 0.143   | 160.028 | 129.498  | 160.028  | 124.985  |           |
| PODLON 0.163   | 164.427 | 115.398  | 164.427  | 124.833  |           |
| POLXIB 0.17    | 173.94  | 114.529  | 173.94   | 122.337  |           |
| CIPIUF 0.101   | 163.222 | 122.477  | 161.211  | 125.218  |           |

**View Options:**

- ☐ Show packing feature
- ☐ Show negative results
- ☐ List all matches
- [Spreadsheet...](#)

**Display Options:**

- ☐ Packing
- ☐ Asymmetric Unit
- ☐ Auto centre
- ☐ Short Contact < (sum of vdW radii - 0.15A)
- ☐ H-Bond User defined

**Options:**

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

**Structure Navigator:**

| Crystal Structures | Spacegroup |
|--------------------|------------|
| BOBLOX             | P21/n      |
| BOBLOX             | P21/n      |
| COCVEZ             | P-1        |
| COCVEZ             | P-1        |
| COFBEI             | P-1        |
| COFBEI             | P-1        |
| COHVOO             | P21        |
| DOCJOY             | C2         |
| DOCJOY             | C2         |
| DOCJOY             | C2         |
| DOCJOY             | C2         |
| FEFLUT01           | P21/c      |
| FITMAA             | P21        |
| FITMAA             | P21        |
| FIXSIS             | P212121    |
| FIXSIS             | P212121    |
| GOVXIY03           | P21/c      |
| HIWSIT             | Fdd2       |
| HIYDIG             | P-1        |

**Post Search Options:**

hydantoin amide dimer complete  
Would you like to:

- [Save Results...](#)
- [Edit Search...](#)
- [Filter Results...](#)

These options are also available via the options button located at the top right of the searches window

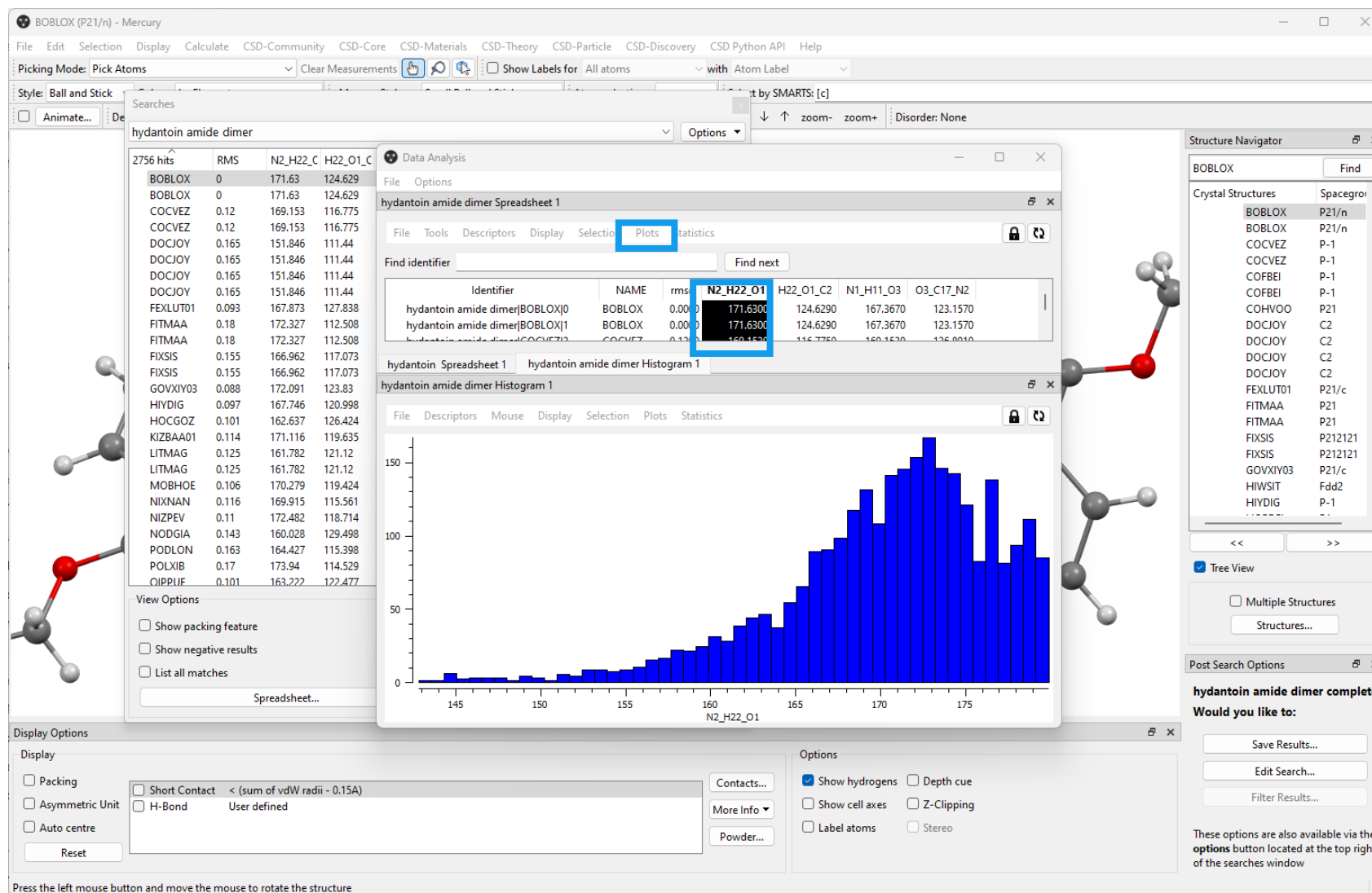
# Crystal Packing Feature: Viewing Spreadsheet

The screenshot displays the Mercury software interface with the 'Data Analysis' window open. The window shows a spreadsheet of search results for 'hydantoin amide dimer'. A blue arrow points to the 'H22\_O1\_C2' column header in the spreadsheet.

| Identifier                        | NAME     | rmsd   | N2_H22_O1 | H22_O1_C2 | N        | H11_O3   | O3_C17_N2 |
|-----------------------------------|----------|--------|-----------|-----------|----------|----------|-----------|
| hydantoin amide dimer[BOBLOX]0    | BOBLOX   | 0.0000 | 171.6300  | 124.6290  | 167.3670 | 123.1570 |           |
| hydantoin amide dimer[BOBLOX]1    | BOBLOX   | 0.0000 | 171.6300  | 124.6290  | 167.3670 | 123.1570 |           |
| hydantoin amide dimer[COCVEZ]2    | COCVEZ   | 0.1200 | 169.1530  | 116.7750  | 169.1530 | 126.8910 |           |
| hydantoin amide dimer[COCVEZ]3    | COCVEZ   | 0.1200 | 169.1530  | 116.7750  | 169.1530 | 126.8910 |           |
| hydantoin amide dimer[DOCJOY]4    | DOCJOY   | 0.1650 | 151.8460  | 111.4400  | 164.8270 | 125.4390 |           |
| hydantoin amide dimer[DOCJOY]5    | DOCJOY   | 0.1650 | 151.8460  | 111.4400  | 164.8270 | 125.4390 |           |
| hydantoin amide dimer[DOCJOY]6    | DOCJOY   | 0.1650 | 151.8460  | 111.4400  | 164.8270 | 125.4390 |           |
| hydantoin amide dimer[DOCJOY]7    | DOCJOY   | 0.1650 | 151.8460  | 111.4400  | 164.8270 | 125.4390 |           |
| hydantoin amide dimer[FEXLUT01]8  | FEXLUT01 | 0.0930 | 167.8730  | 127.8380  | 167.8730 | 127.8380 |           |
| hydantoin amide dimer[FITMAA]9    | FITMAA   | 0.1800 | 172.3270  | 112.5080  | 164.4780 | 122.4270 |           |
| hydantoin amide dimer[FITMAA]10   | FITMAA   | 0.1800 | 172.3270  | 112.5080  | 164.4780 | 122.4270 |           |
| hydantoin amide dimer[FIXSIS]11   | FIXSIS   | 0.1550 | 166.9620  | 117.0730  | 165.1620 | 127.0710 |           |
| hydantoin amide dimer[FIXSIS]12   | FIXSIS   | 0.1550 | 166.9620  | 117.0730  | 165.1620 | 127.0710 |           |
| hydantoin amide dimer[GOVXIY03]13 | GOVXIY03 | 0.0880 | 172.0910  | 123.8300  | 172.0910 | 123.5290 |           |
| hydantoin amide dimer[HYDIG]14    | HYDIG    | 0.0970 | 167.7460  | 120.9980  | 167.7460 | 125.4960 |           |
| hydantoin amide dimer[HOCGOZ]15   | HOCGOZ   | 0.1010 | 162.6370  | 126.4240  | 162.6370 | 125.2940 |           |
| hydantoin amide dimer[KIZBAA01]16 | KIZBAA01 | 0.1140 | 171.1160  | 119.6350  | 171.1160 | 125.0820 |           |
| hydantoin amide dimer[LITMAG]17   | LITMAG   | 0.1250 | 161.7820  | 121.1200  | 161.7820 | 130.9940 |           |
| hydantoin amide dimer[LITMAG]18   | LITMAG   | 0.1250 | 161.7820  | 121.1200  | 161.7820 | 130.9940 |           |
| hydantoin amide dimer[MOBHOE]19   | MOBHOE   | 0.1060 | 170.2790  | 110.4240  | 170.2790 | 125.3510 |           |

Click on a column in the spreadsheet to analyse results

# Crystal Packing Feature: Analysing Results



Plot graphs  
and conduct  
other  
analysis

# Try the feature!

- CSD-Materials self-guided workshops:  
<https://www.ccdc.cam.ac.uk/community/training-and-learning/workshop-materials/csd-materials-workshops/>
- “Motifs, Crystal Packing Feature and Crystal Packing Similarity Search”





# How are others using ConQuest and Mercury?

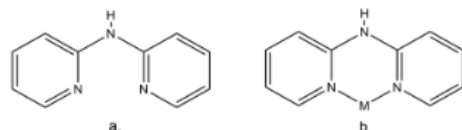
## Mercury in Action: A Geometry Analysis on Complexes With 2,2'-Dipyridylamine

Dr Tetteh investigated the geometry of first-row transition metal complexes with 2,2'-dipyridylamine and halogen ligands by searching the Cambridge Structural Database (CSD) with ConQuest and analysing the data with Mercury. Density Functional Theory (DFT) calculations were also performed to study the stability of the complexes.

The research is part of the Frank H. Allen International Research and Education (FAIRE) Programme, which supports academic researchers and educators from underrepresented communities with access to the wealth of information contained within the CSD.

### Why?

The ligand 2,2'-dipyridylamine (dpa, **Figure 1 a**) is widely used in coordination and organometallic chemistry for its ability to bind to a variety of metal centres and adopt different coordination modes, acting as a monodentate, bidentate, or bridging ligand. Among these, the bidentate coordination mode (**Figure 1 b**) is particularly stable thermodynamically, and hence it is frequently found in metal complexes.



Metal complexes that involve dpa are used as catalysts and other photophysical materials. The ligand is also used for MOFs design and as co-ligand for magnetic complexes. Despite its popularity, research still needs to be done to understand the chemistry of dpa and its behaviour when in crystal forms.

This work aimed to investigate first-row transition metal complexes with dpa and halogen ligands (F, Cl, Br, and I), and looked at rationalizing their geometry, electronic stability, and reactivity.



Samuel Tetteh, *Cryst. Growth Des.* 2024, 24, 1, 506–513.

## ConQuest in Action: Introducing Intramolecular $\pi$ -Interactions into Heteroleptic Complexes

Here we highlight how the use of ConQuest to search the Cambridge Structural Database (CSD) helped guiding the design and synthesis of new heteroleptic compounds – coordination complexes with more than one type of ligands. Read the full article and find out more about the CSD data, software, and services to advance structural science that were used in this work.

### Why?

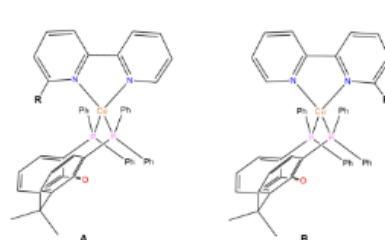
Heteroleptic copper(I) compounds can exhibit enhanced photoluminescence quantum yields (PLQY). This property is particularly interesting for applications in organic light emitting diodes (OLEDs) and light-emitting electrochemical cells (LECs).

In this work published in *CrystEngComm*, the scientists from the University of Basel reported the synthesis and characterization of six new heteroleptic copper(I) compounds. Beside performing solid-state photoluminescence studies, the team also analysed the crystal structures of the compounds and investigated the intramolecular interactions responsible for the enhanced emission.

### How?

Species with formula  $[\text{Cu}(\text{N}^*\text{N})(\text{P}^*\text{P})]^+$ , where  $\text{N}^*\text{N}$  = aromatic diimine and  $\text{P}^*\text{P}$  = chelating bis(phosphane) are known to be efficient LECs.

When the bis(phosphane) involved presents a wide bite angle (angle on a central atom between two bonds to a bidentate ligand), intramolecular  $\pi$ -stacking interactions can arise between the ligands, enhancing the emission and PLQY in these species. For this reason, the team chose to use *xantphos* and *POP* as  $\text{P}^*\text{P}$  ligands.



Catherine Housecroft, et al., *Cryst. Eng. Comm* 2023, 25, 3000–3012.



## CSD in Action: How Metal Ammine Complexes Interact With Aromatic Rings

Here we highlight a paper by Snežana D. Zarić and co-workers from the University of Belgrade.

In this work, the team analysed the Cambridge Structural Database (CSD) and used quantum chemical calculations to perform an in-depth study of the  $\text{NH}/\pi$  interactions between coordinated ammonia ( $\text{NH}_3$ ) and  $\text{C}_6$ -aromatic rings.

### Why?

$\text{NH}/\pi$  interactions are common in nature. They are found in proteins and related structures, and are involved in important mechanisms such as the transport of ammonia through the cell membrane.



Snežana D. Zarić et al. *Cryst. Growth Des.* 2024, 24, 4, 1705–1714.



# Want to explore more?

On-demand training resources

Solutions

Community

Discover

Consultancy

Access/Deposit Structures

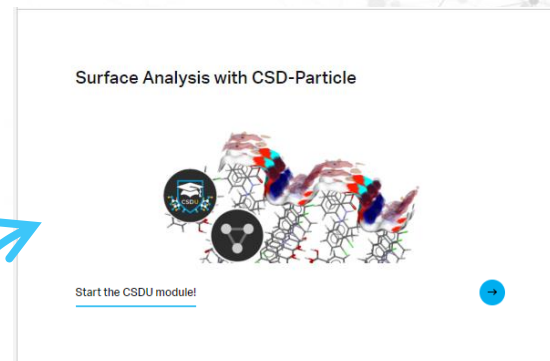
CCDC for the Community

Education and Outreach

Events

Free Products

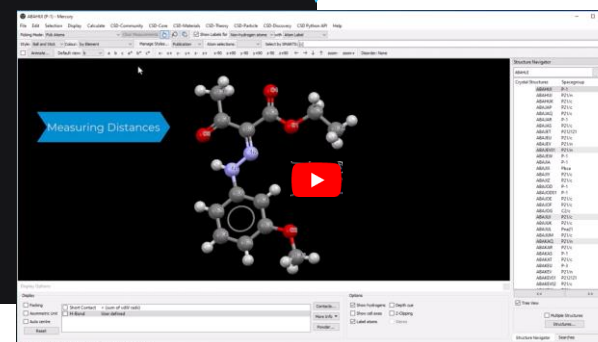
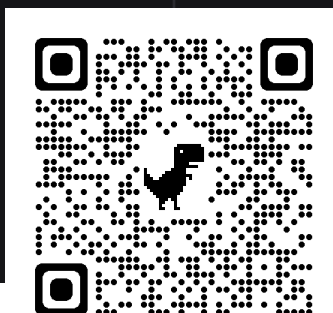
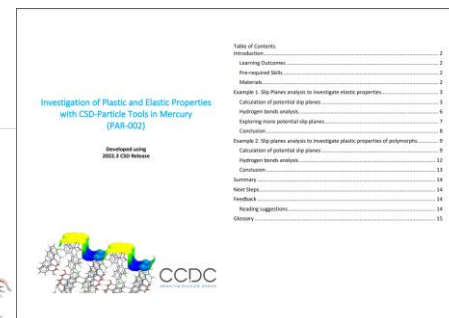
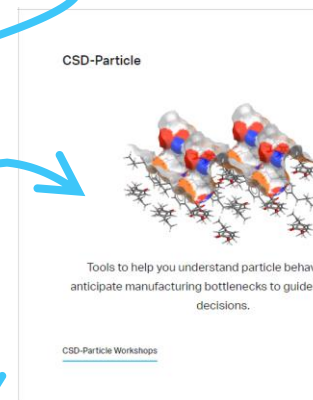
Training and Learning



Free Online Courses

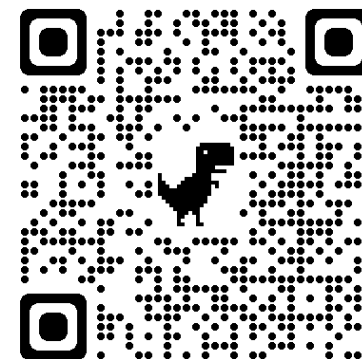
Self-Guided Workshops

Training and Support Videos



CCDC

# Free online training courses



With  
completion  
certificates!



## CSDU

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



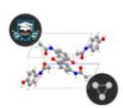
UWatch



UTry



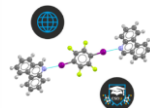
UTest



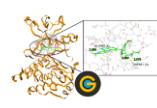
Mercury



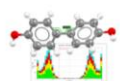
Python  
API



WebCSD



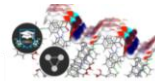
GOLD  
Docking



Mogul

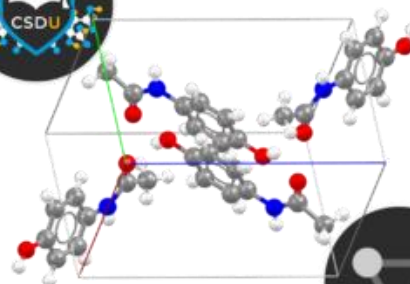


FIMs



Particle

## Visualization 101



Helping you to learn:

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

## CSD Python API



Helping you to learn:

- How **CSD entries** are **represented** in the API.
- How to **access CSD entries programmatically**.
- How to **read different file formats**.
- How to **run a search and output results**.

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

# More learning events

## CCDC Virtual Workshops

- **5<sup>th</sup> Nov CSD-CrossMiner**: Introducing interactive **pharmacophore searching** across the CSD and the PDB.

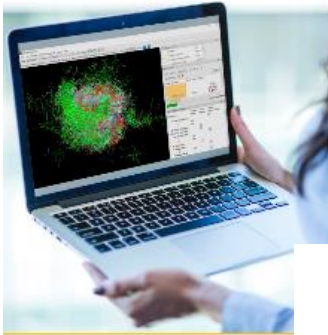
## CHEMAI Virtual Satellite Event

- **27<sup>th</sup> Nov** Unlocking **CSD data** for **Functional Materials innovation**.

## CCDC Webinars

- **Coming soon!** The CCDC also regularly host webinars alongside these workshops. Check out our website, social media or sign-up to our newsletter to stay up to date.

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



**CCDC**

**Virtual Workshop**  
Introduction to Pharmacophore Searching Using CSD-CrossMiner

**Special Guest Speaker**  
Dobromir Hranis  
PDB-CrossMiner Project Leader

Tuesday, 5th November  
10:30-12:15 (GMT)

**Registration is now open - just scan the QR code**



SCAN ME



**CHEMAI**  
Satellite Event

**CCDC**  
advancing structural science

**"Unlocking Data in the Cambridge Structural Database for Functional Materials Innovation"**

Online workshop to unlock your organization's potential by using the power of data and algorithms. Join for free.

Date: November 27, 2024  
Time: 15:00 - 16:30 CSET  
Speaker: Dr. Andrew Peel

**CCDC**