# Searching the CSD using ConQuest

## CCDC Virtual Workshop 2020 – Session 1

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advancing structural science

# Learning outcomes for today

- How to search over a million published crystal structures using our desktop software
- How to refine your results to structures in targeted subsets allowing you to explore drugs, pesticides and MOFs in more detail

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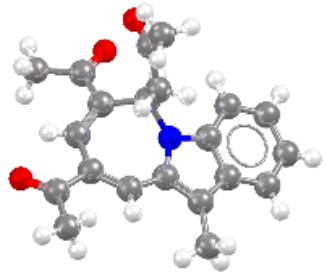
# CSD Refcodes



CSD Refcode - XOPCAJ

What is XOPCAJ?

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

## Refcode families

- The same substances are assigned the *same* 6 letter code plus an additional 2 numbers
  - Polymorphs
  - New determinations or re-refinements of the same substance
  - Determinations at different temperatures/pressures
- Stereoisomers or different solvates, co-crystals, etc are assigned *different* refcode families

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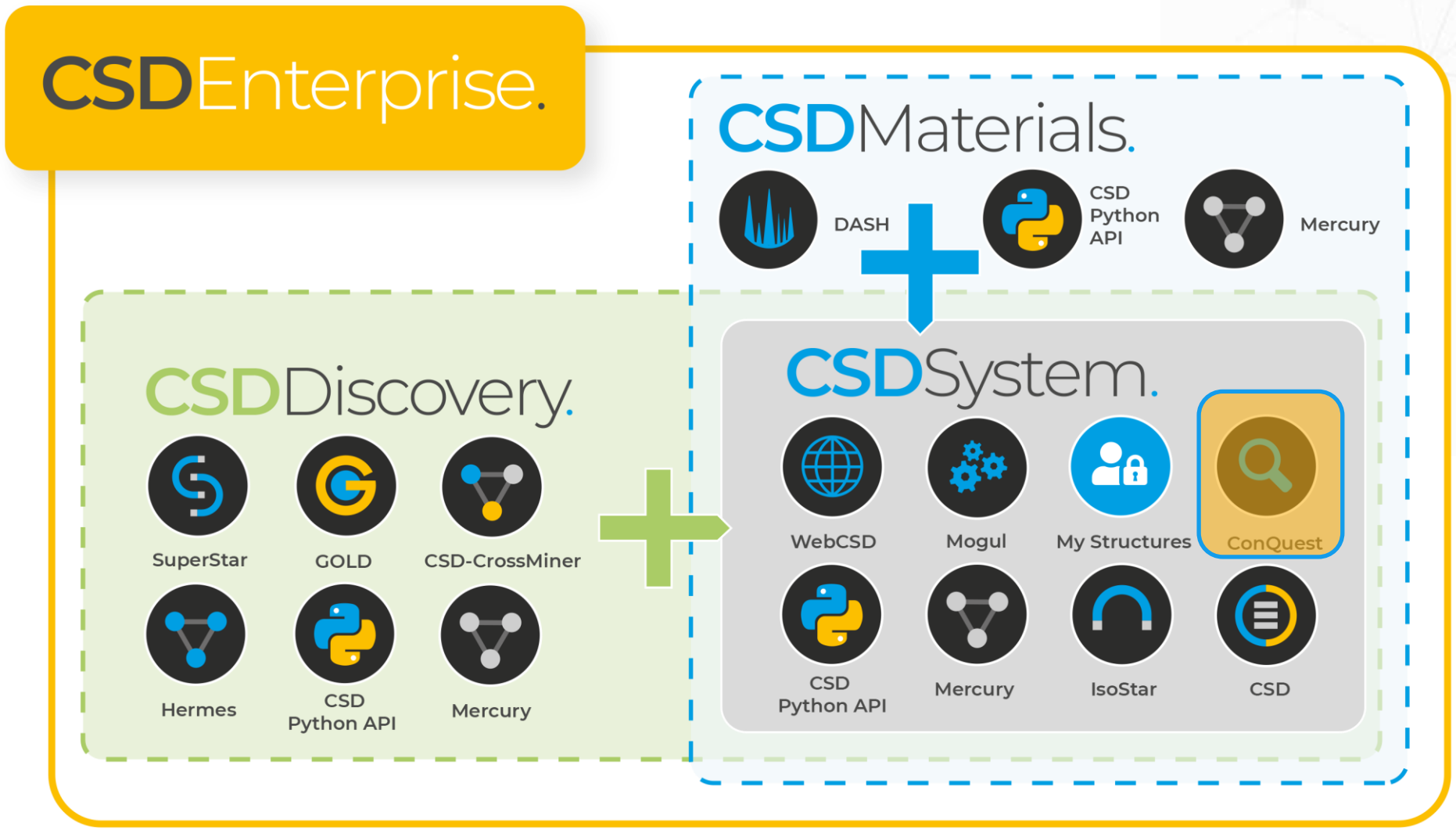
# The CSD software



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# CSD-System – What does it enable?

- It makes it easy to answer very specific structure questions on your desktop using highly flexible 3D searching of the CSD
- Quickly identify the most relevant structures across the CSD based on a wide range of properties including chemical constraints such as cyclicity
- Use interaction and structure-property knowledge gained to drive design decisions

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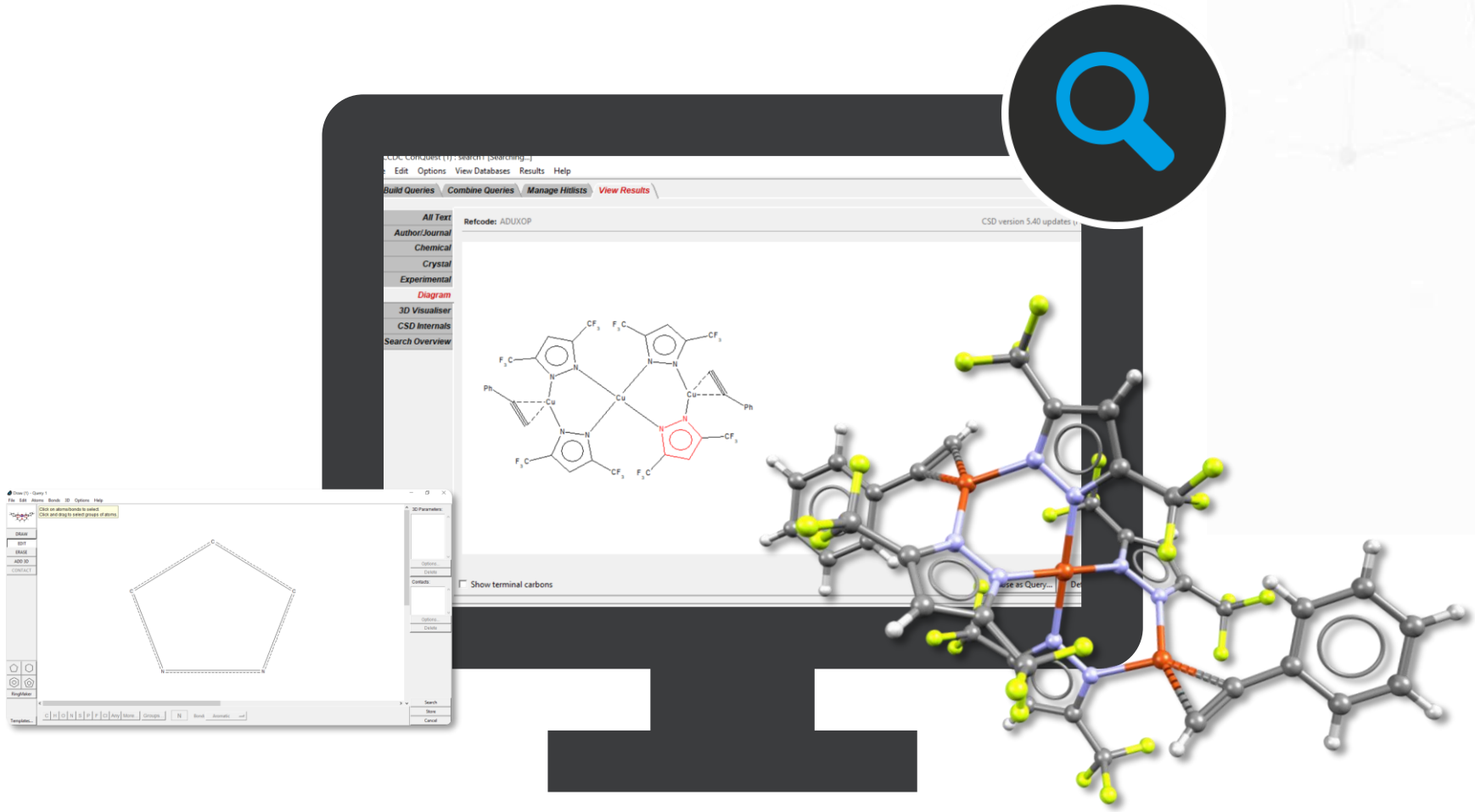
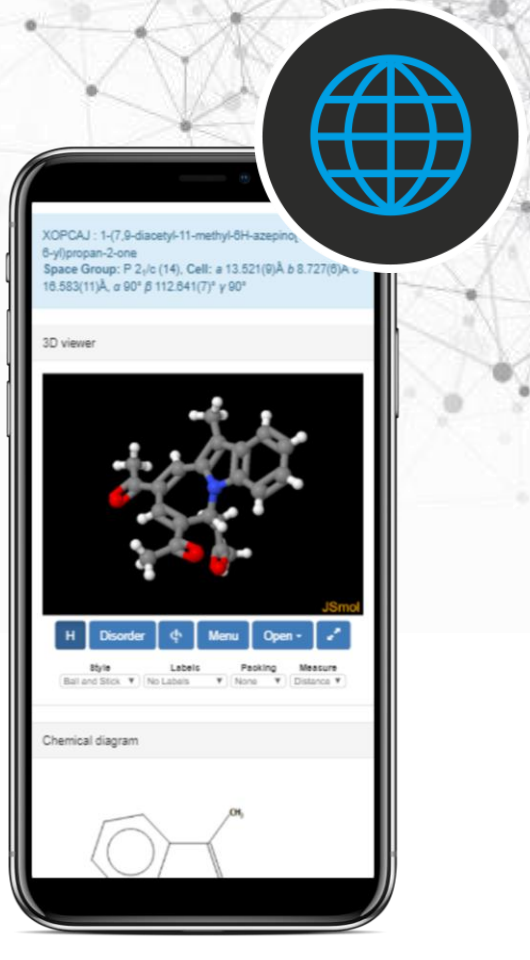
# CSD-System: Search



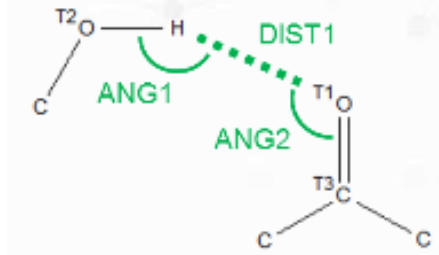



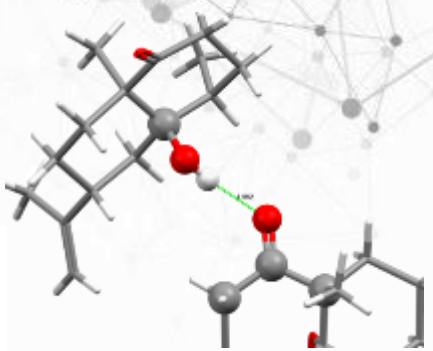

On your desktop: ConQuest

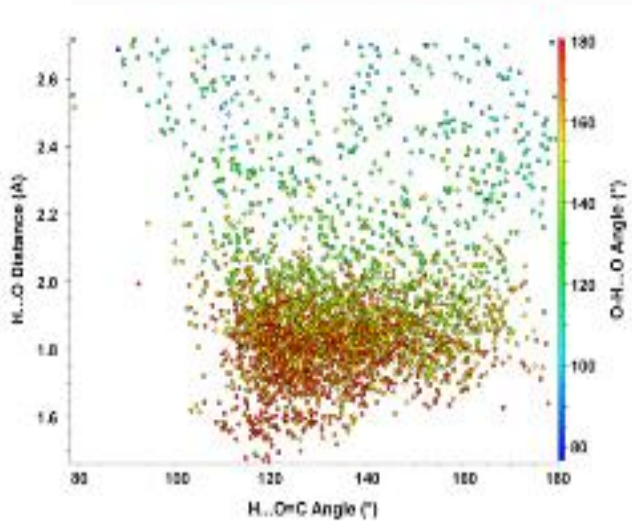
On a browser: WebCSD

# 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



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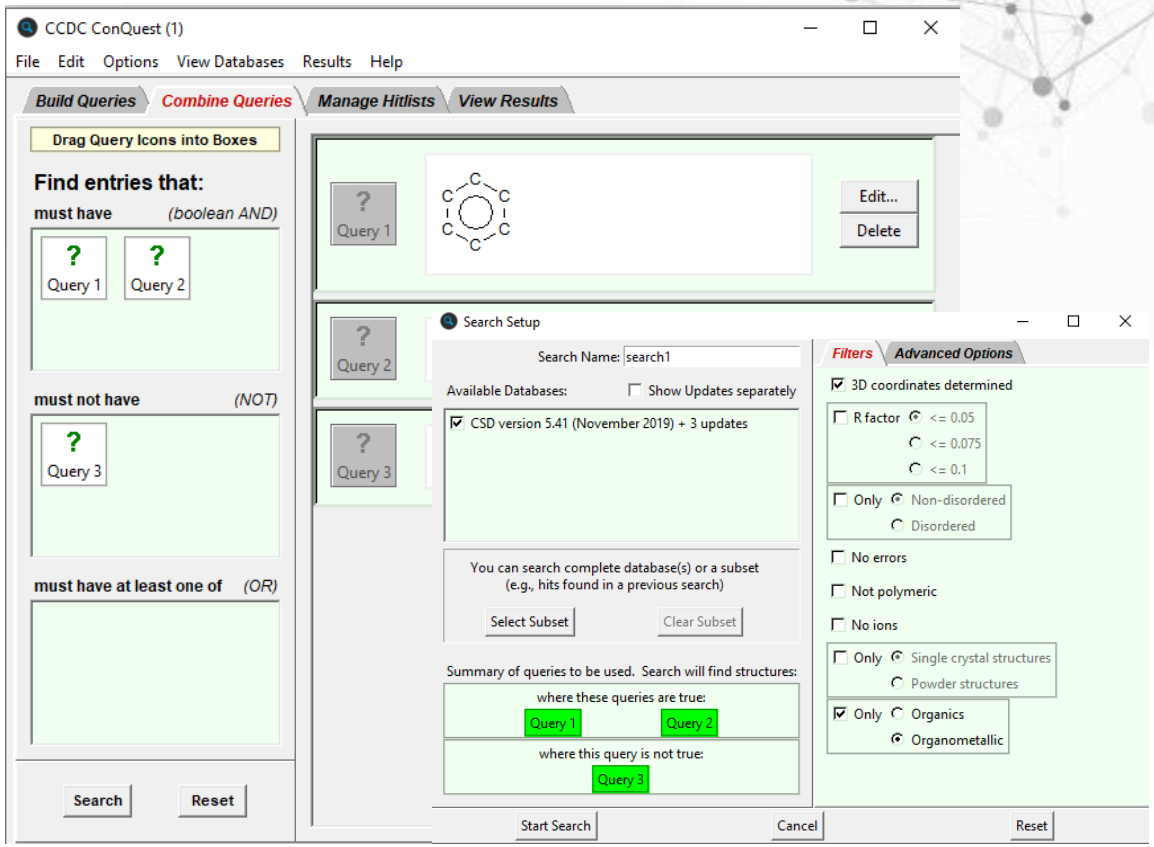
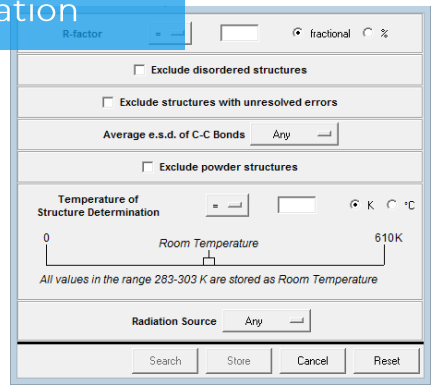
# ConQuest

- Large range of filtering options based on experimental or chemical considerations (*e.g. R*-factor, temperature, only organics)
- Combine searches using various Boolean options and manage hitlists post-search
- Export results to Mercury for visualisation and advanced numerical analysis & plotting

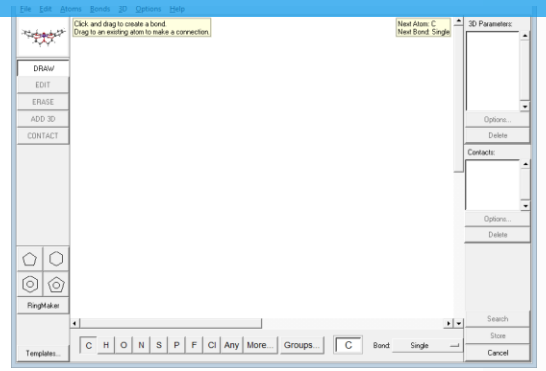


# ConQuest features

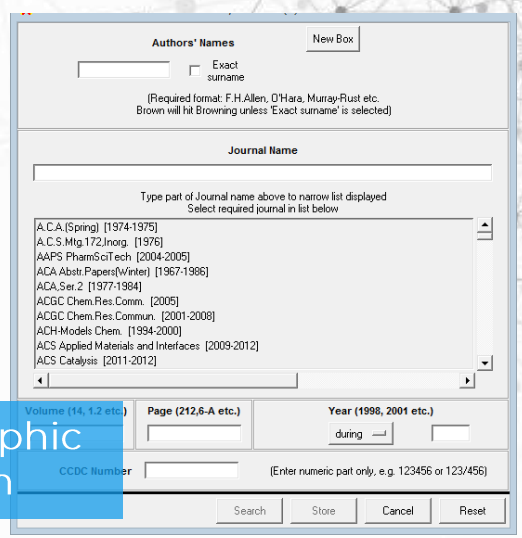
Search for information relating to the structure determination

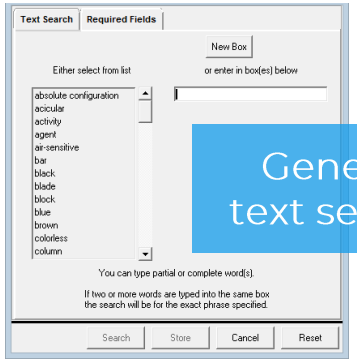



Structure sketcher, enabling set-up of basic substructure searches and complex 3D queries



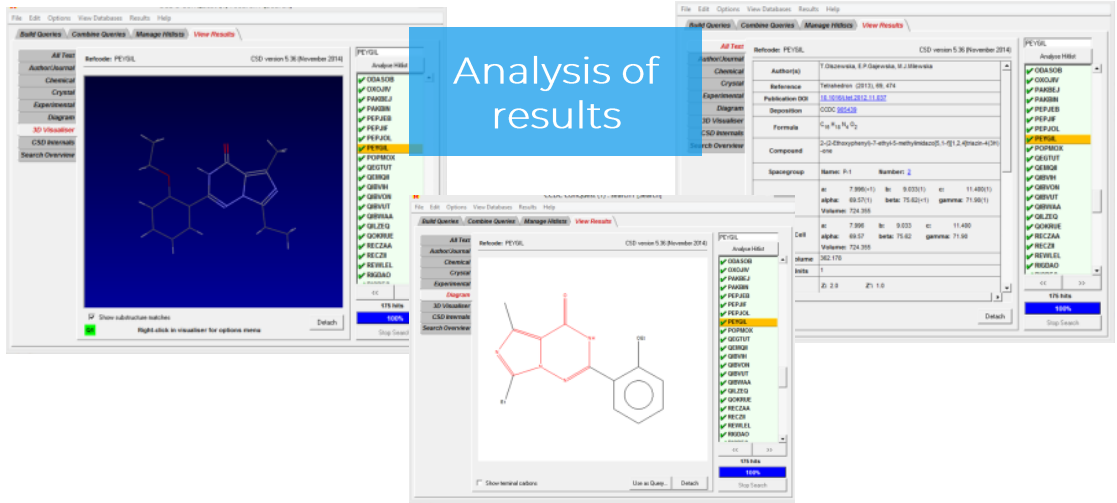

Bibliographic search



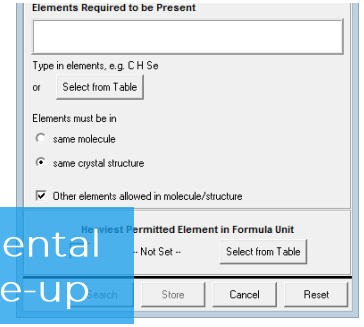




Generic text search

Analysis of results



Elemental make-up

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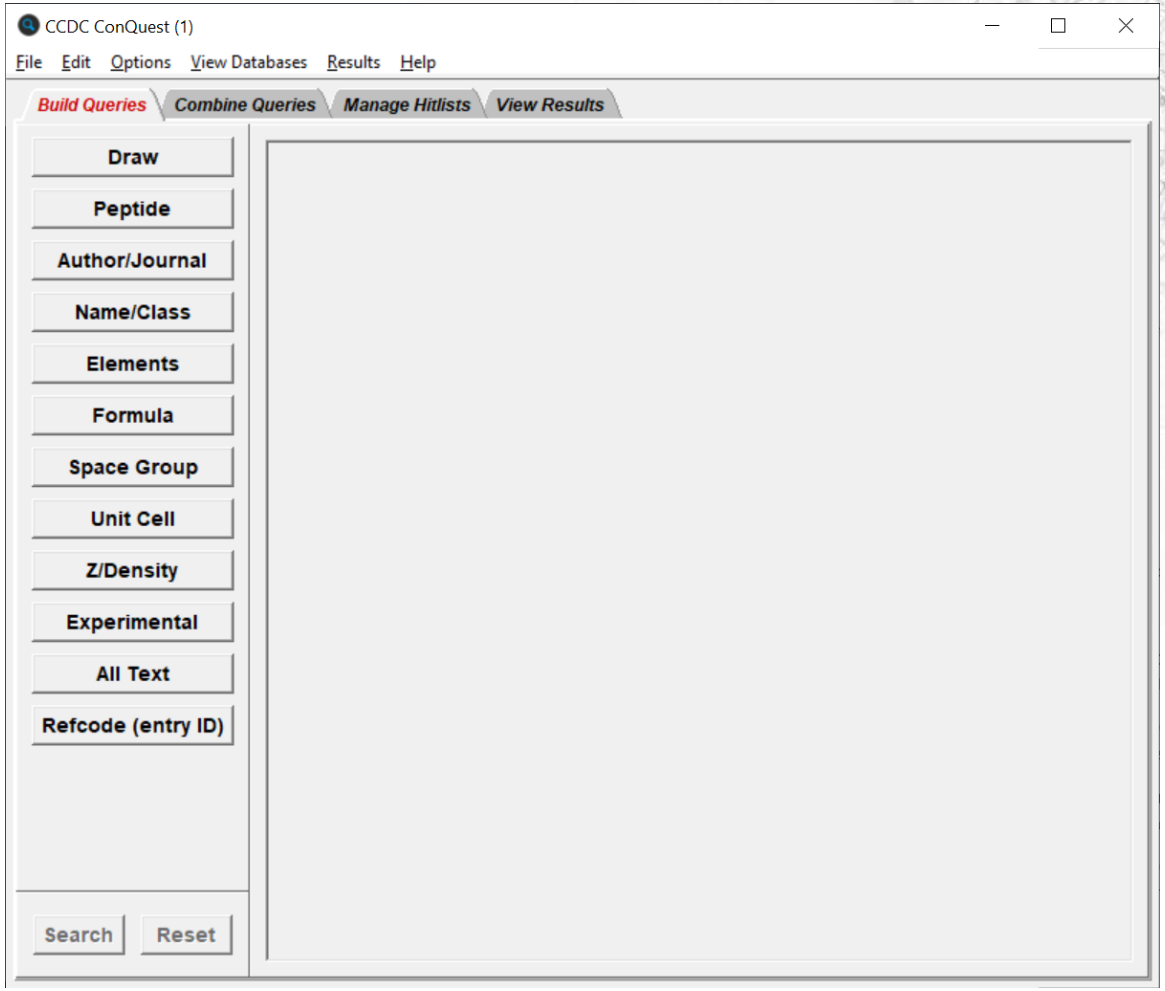
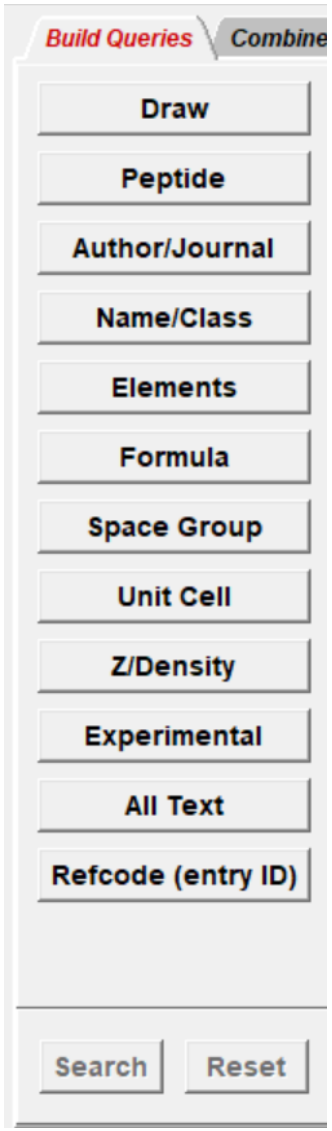
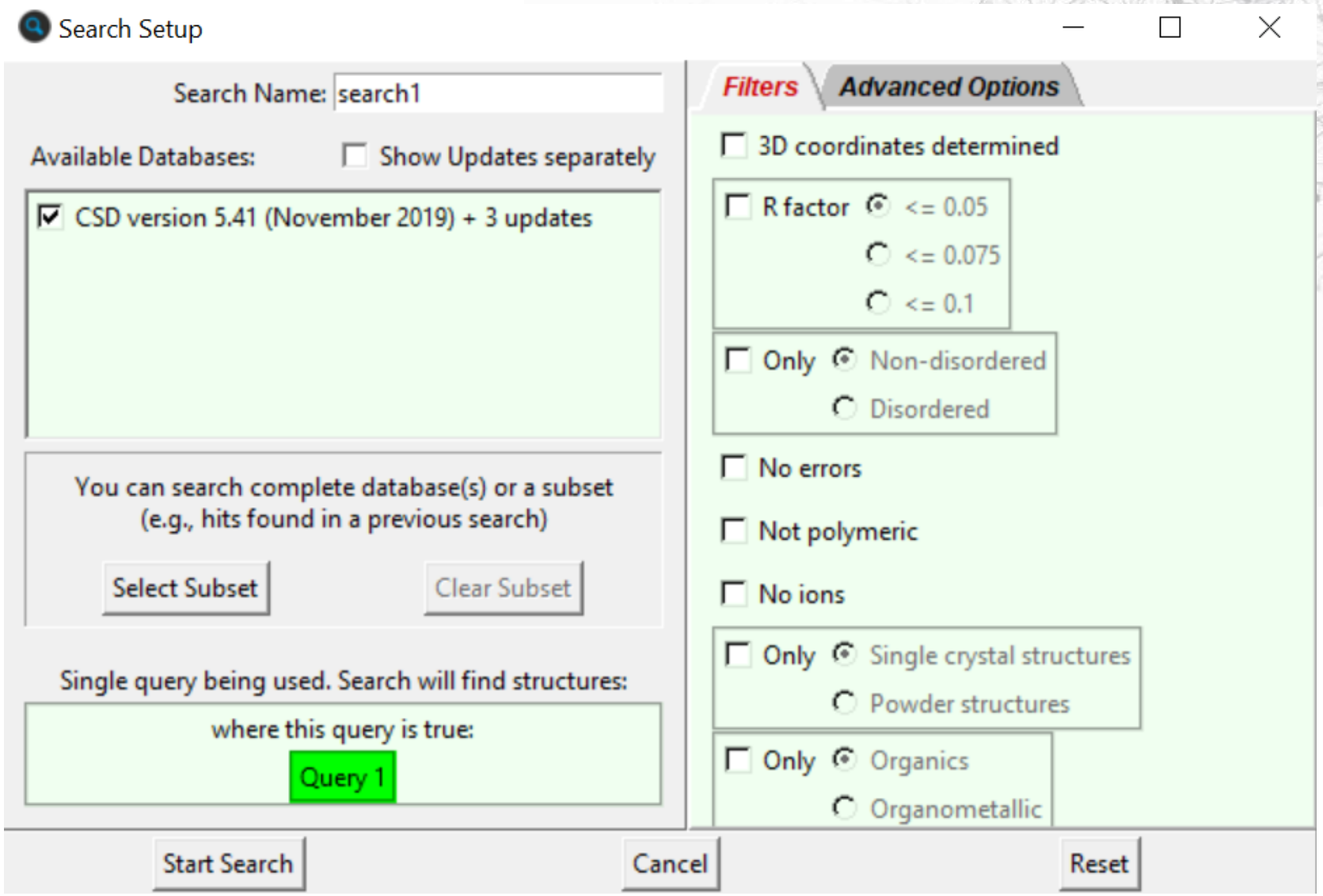
# *Show One*: ConQuest – Opening and search options

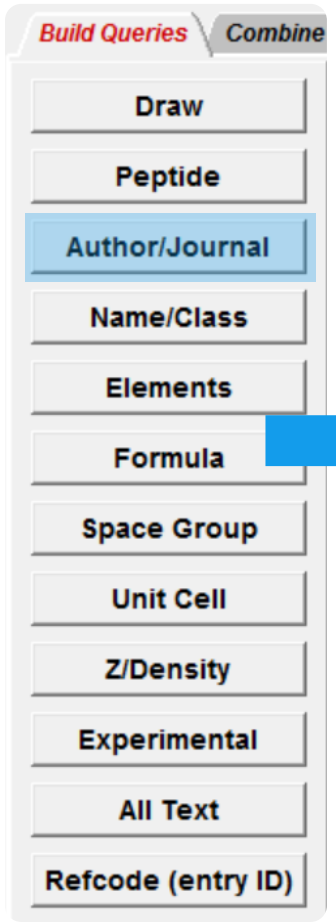


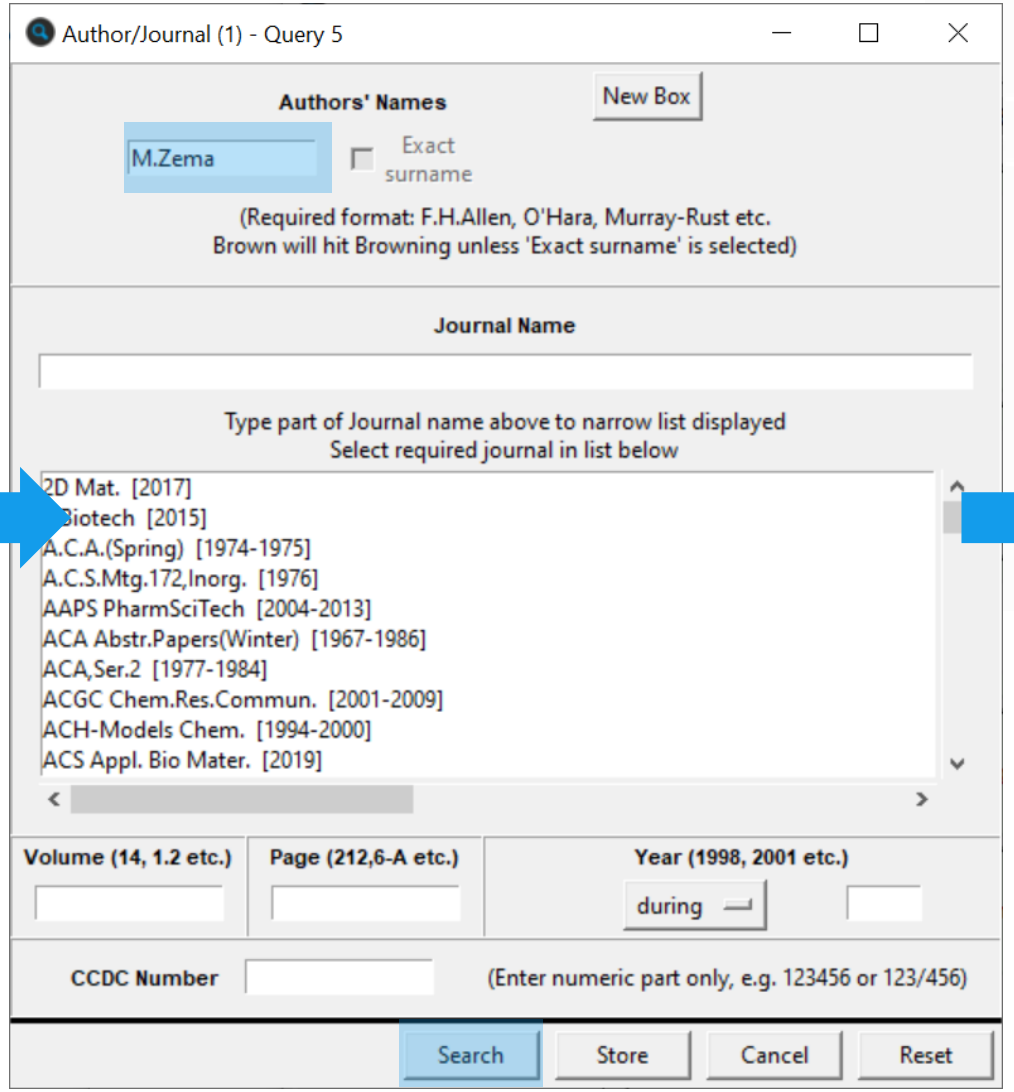
# ConQuest – Searching and filtering

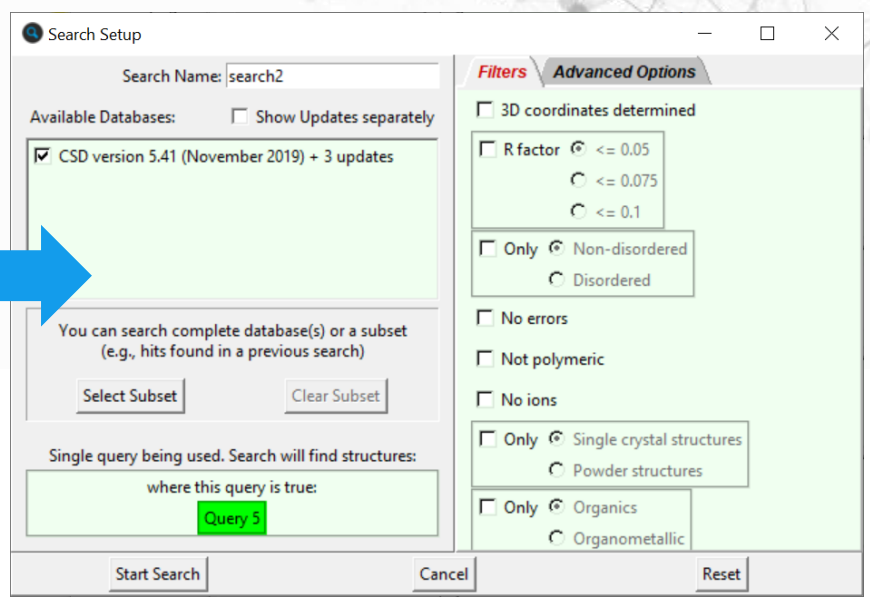


# ConQuest – Author and journal search

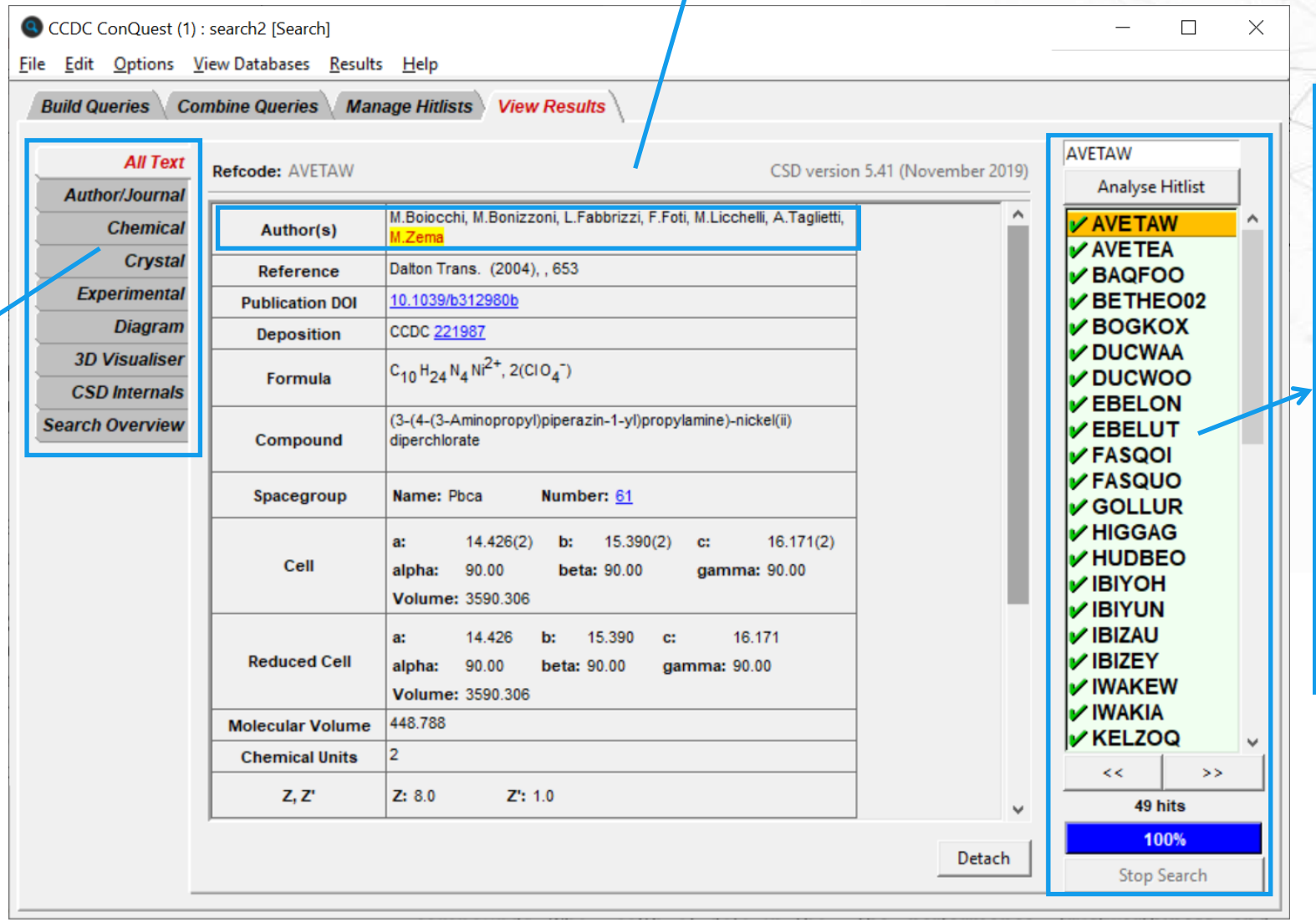


Query highlighted

Left clicking each tab will display different information




A hit list will be returned within the View Results tab of ConQuest. Left clicking on each REFCODE will toggle on and off that hit for future manipulation.

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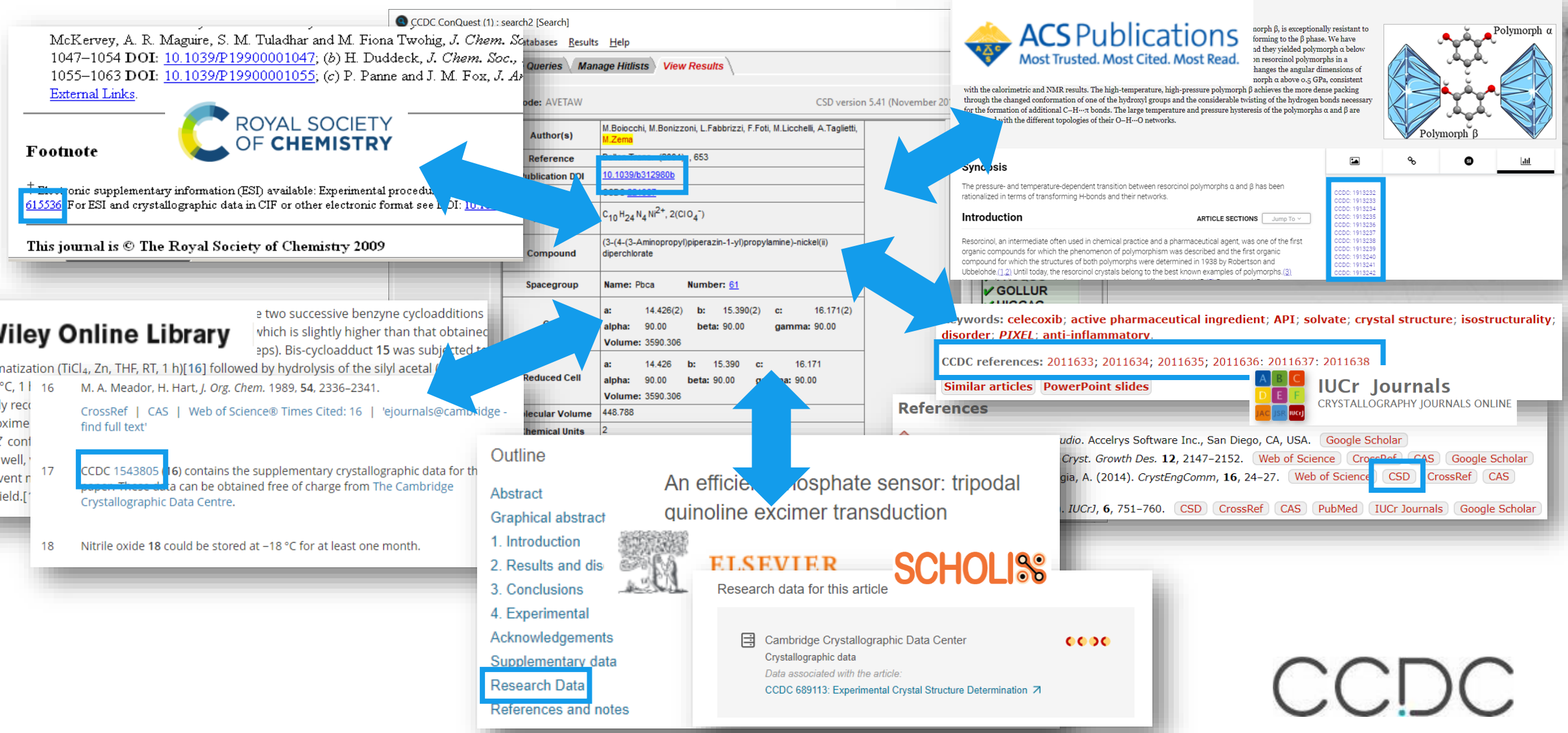
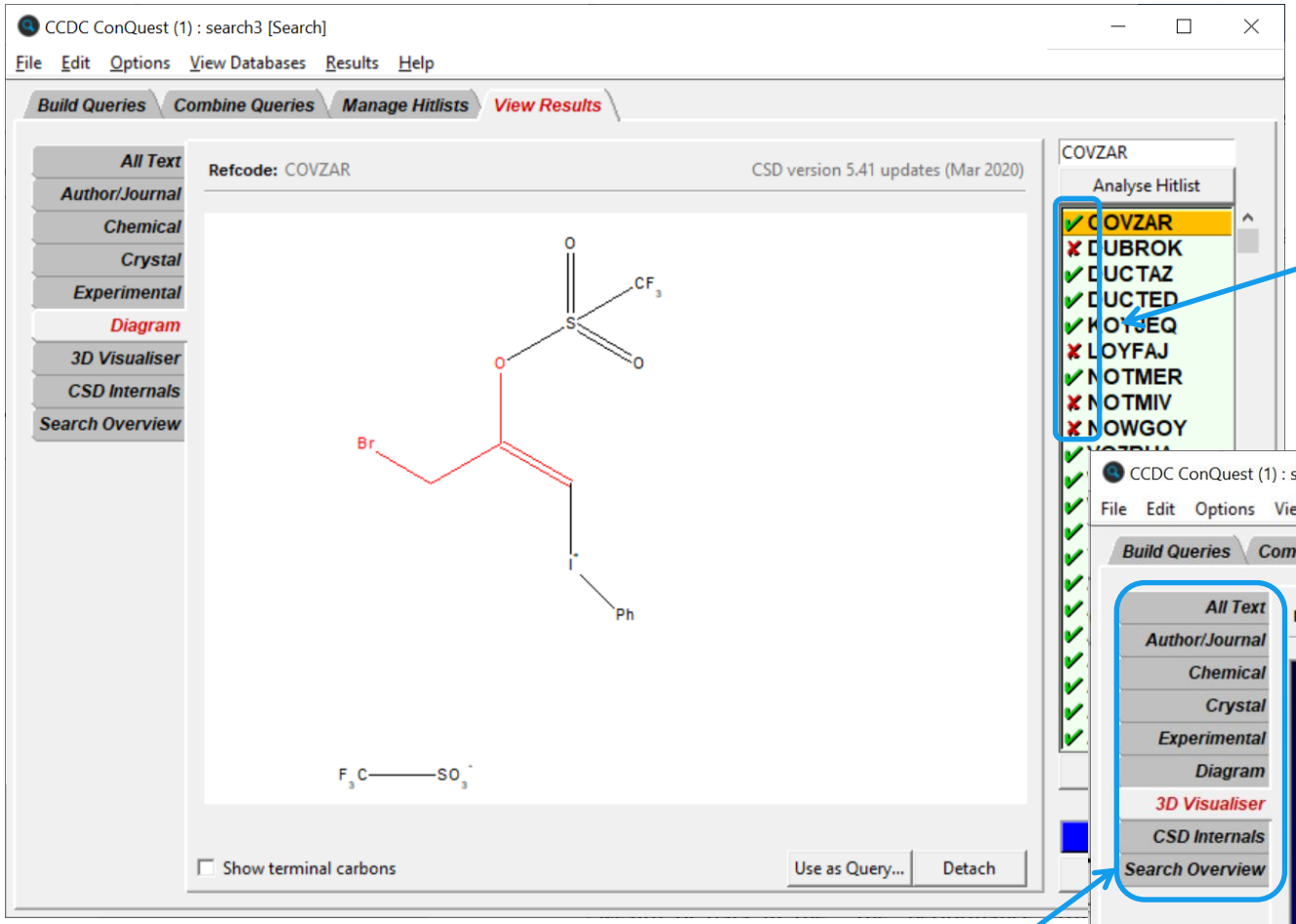
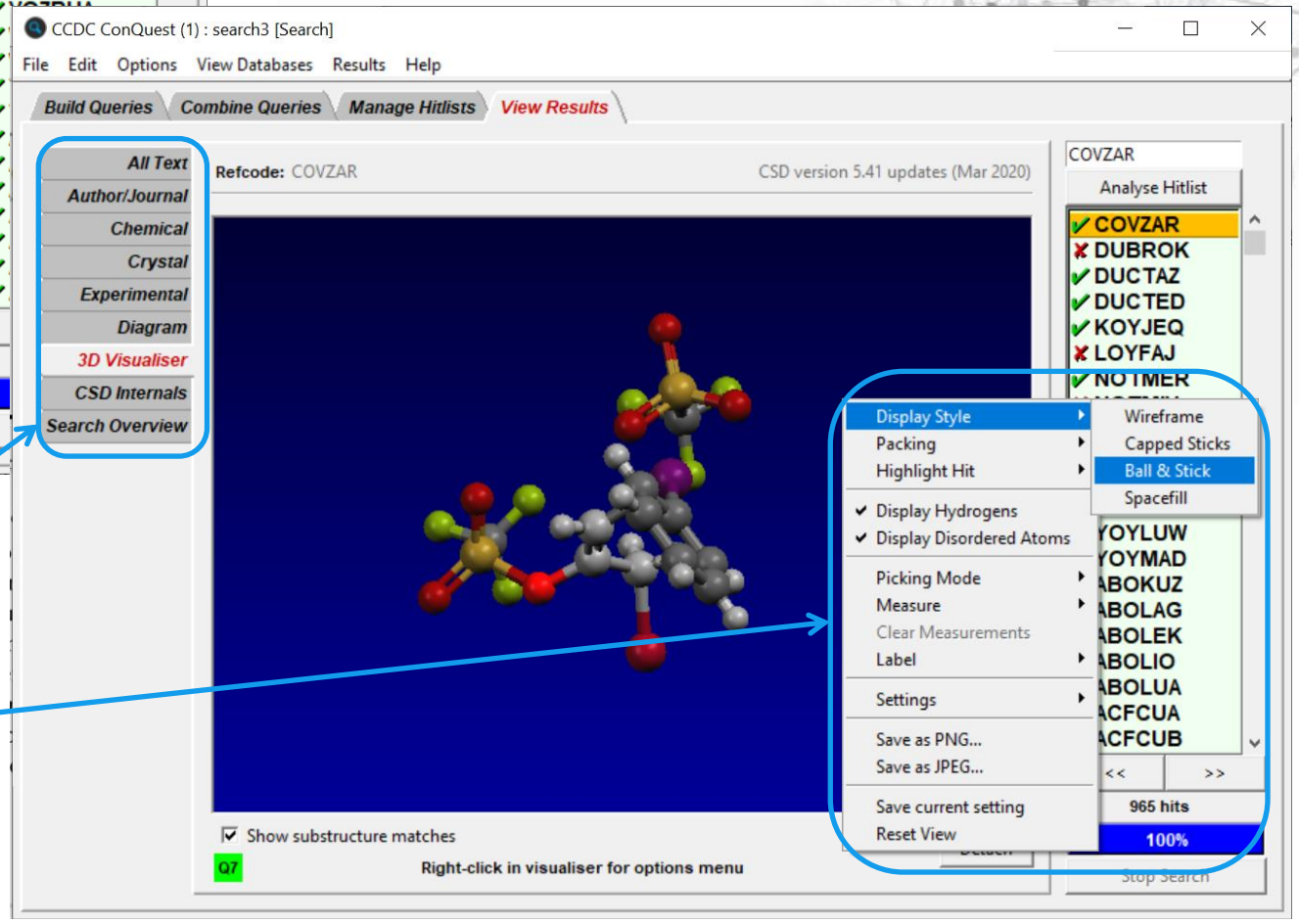
# From data to publication



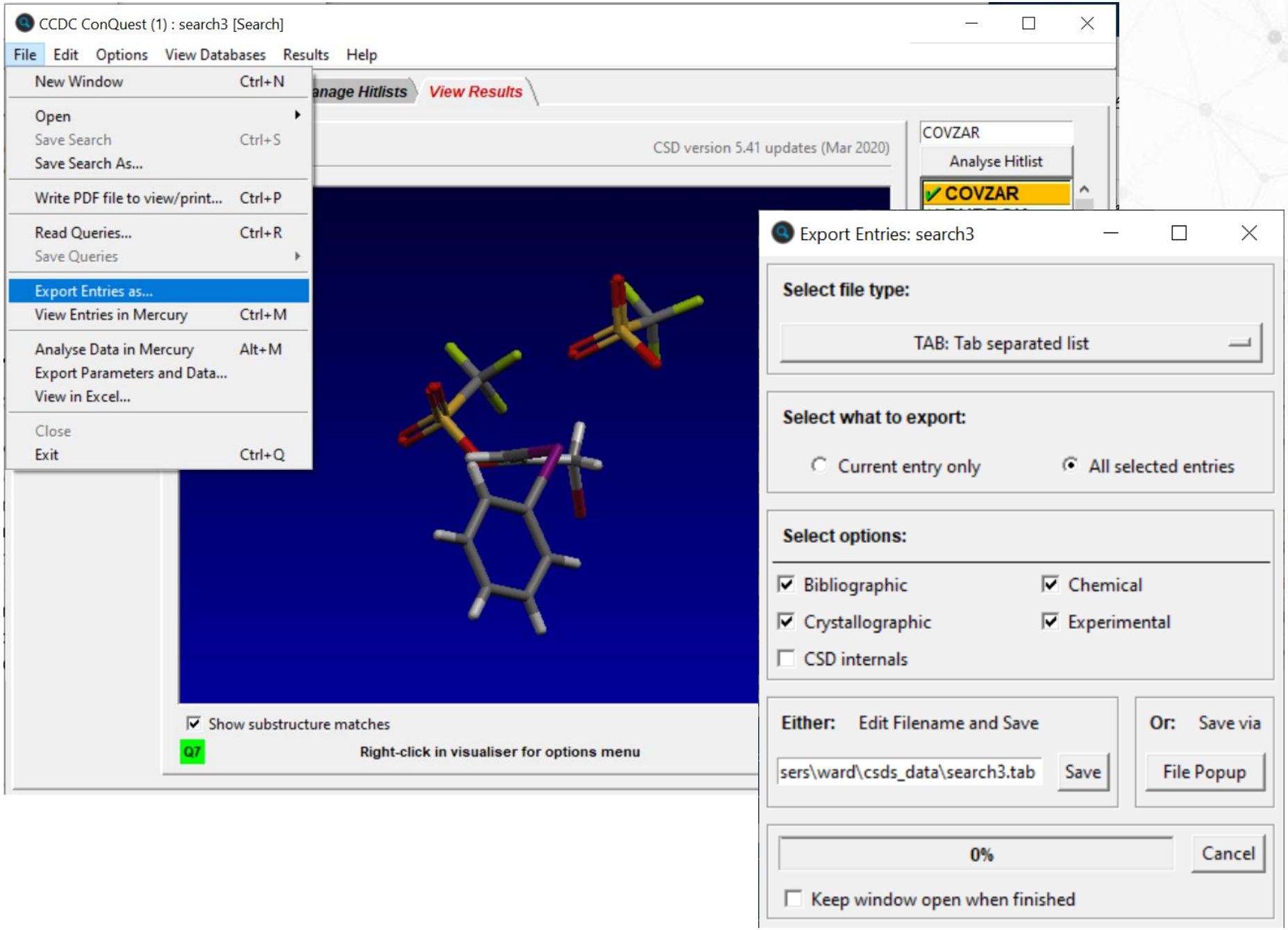
A hit list will be returned within the "results" tab of ConQuest.
Left clicking on each REFCODE will toggle on and off that hit for future manipulation.




Left clicking each tab will display different information

Right clicking on 3D visualiser enables you to change the display style




You can export results in a range of different formats to save data for future manipulation.

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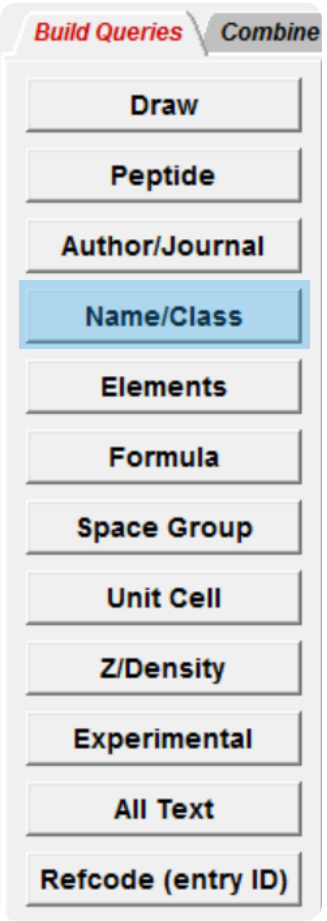
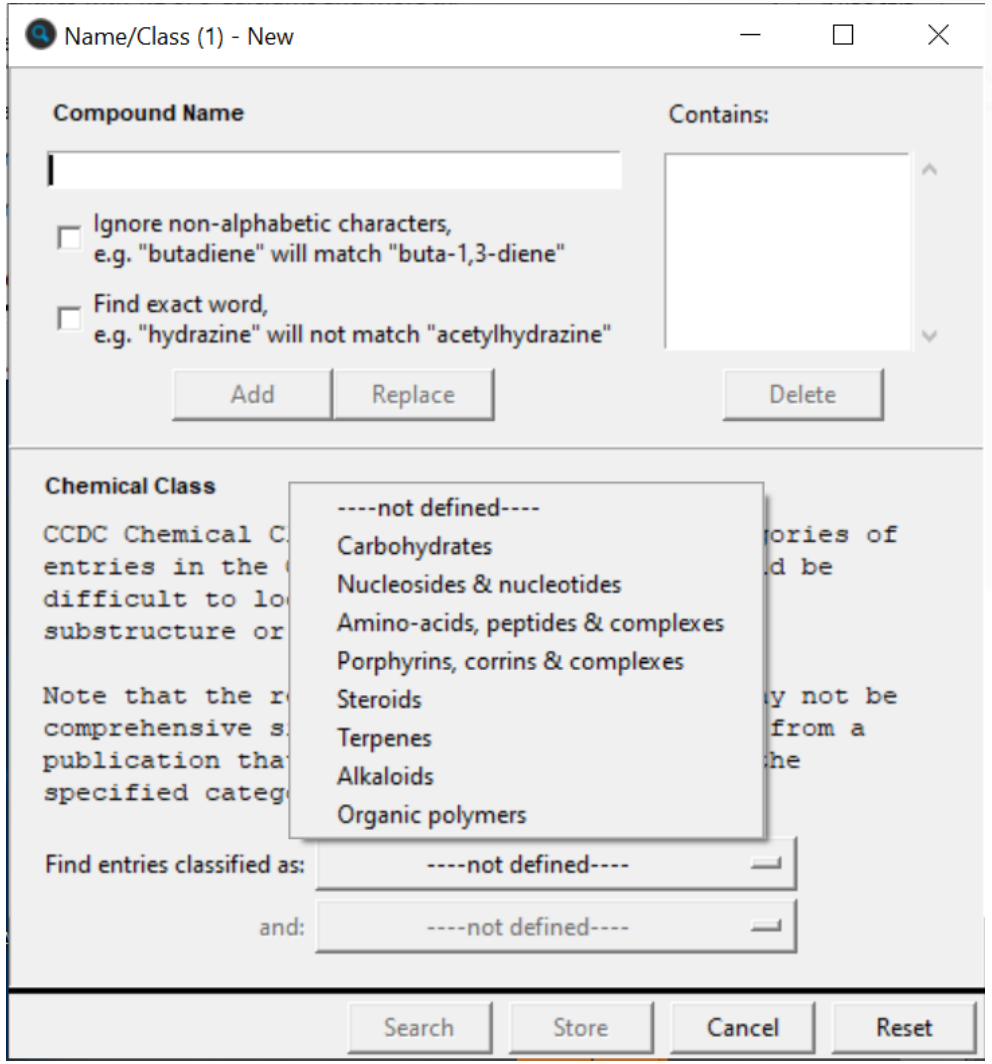
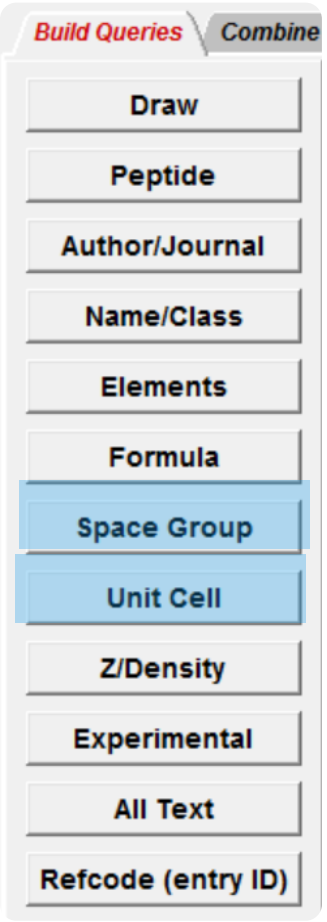
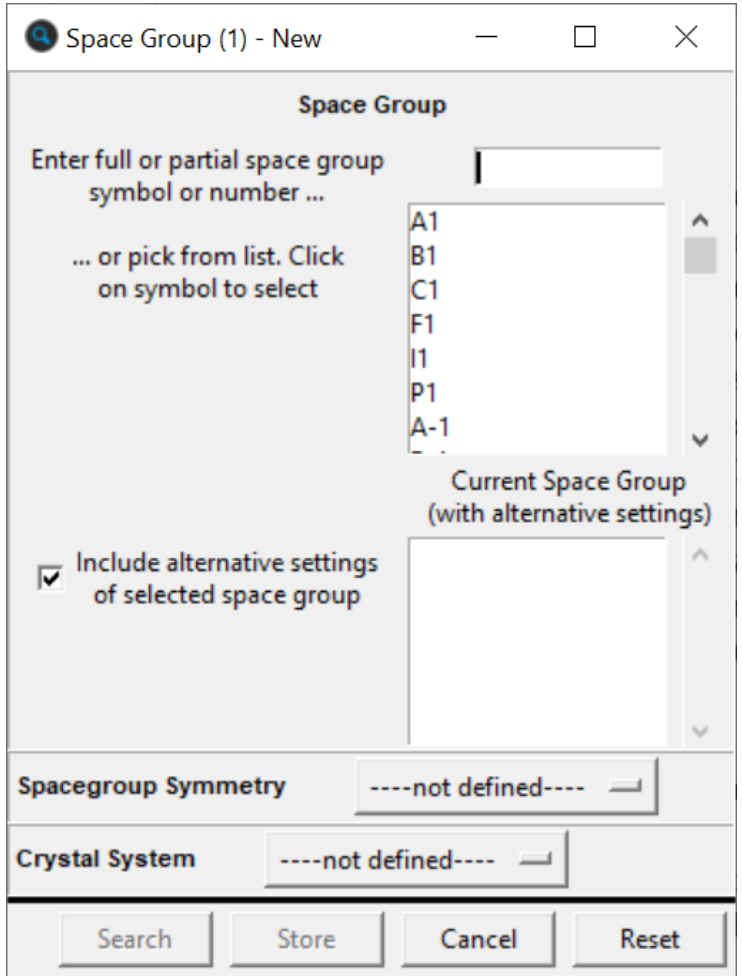
# ConQuest – Compound name search

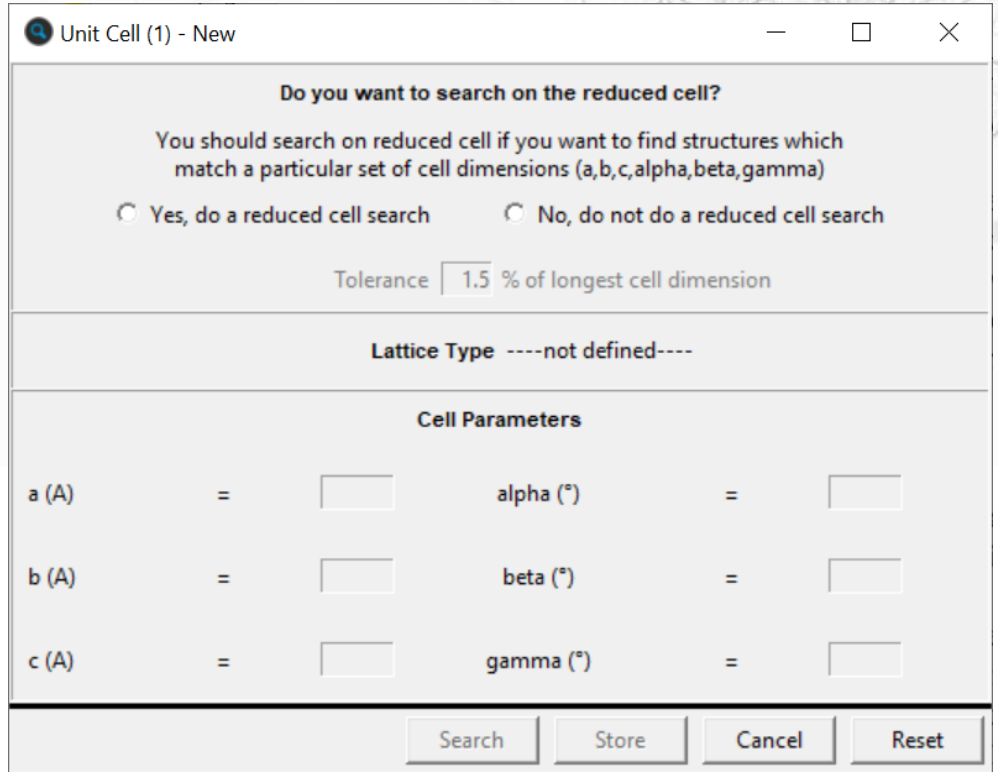


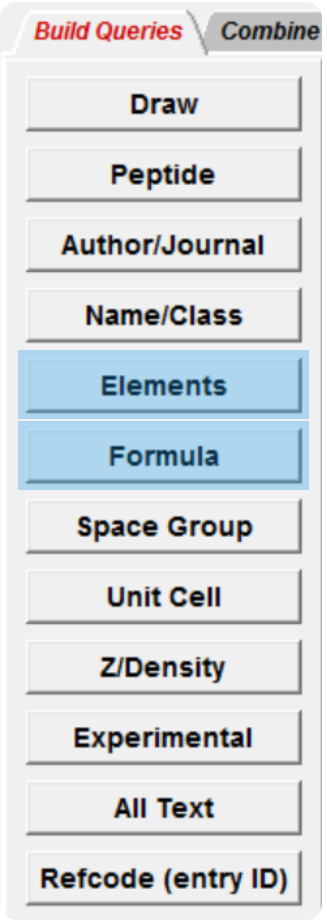
# ConQuest – Space Group and cell search

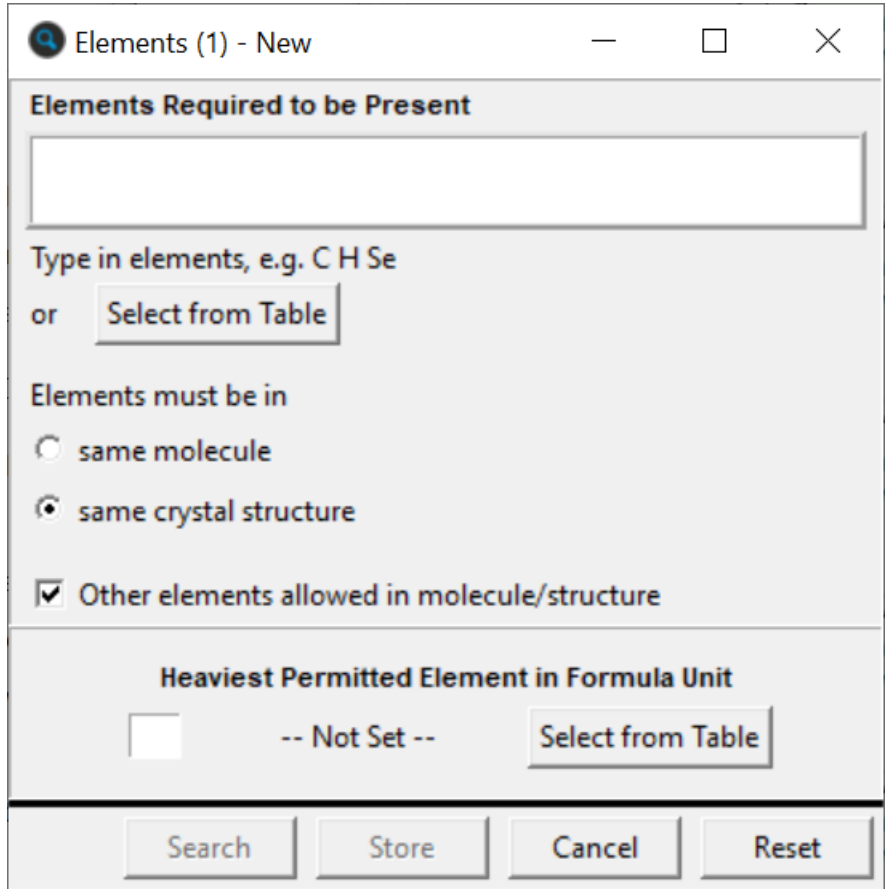


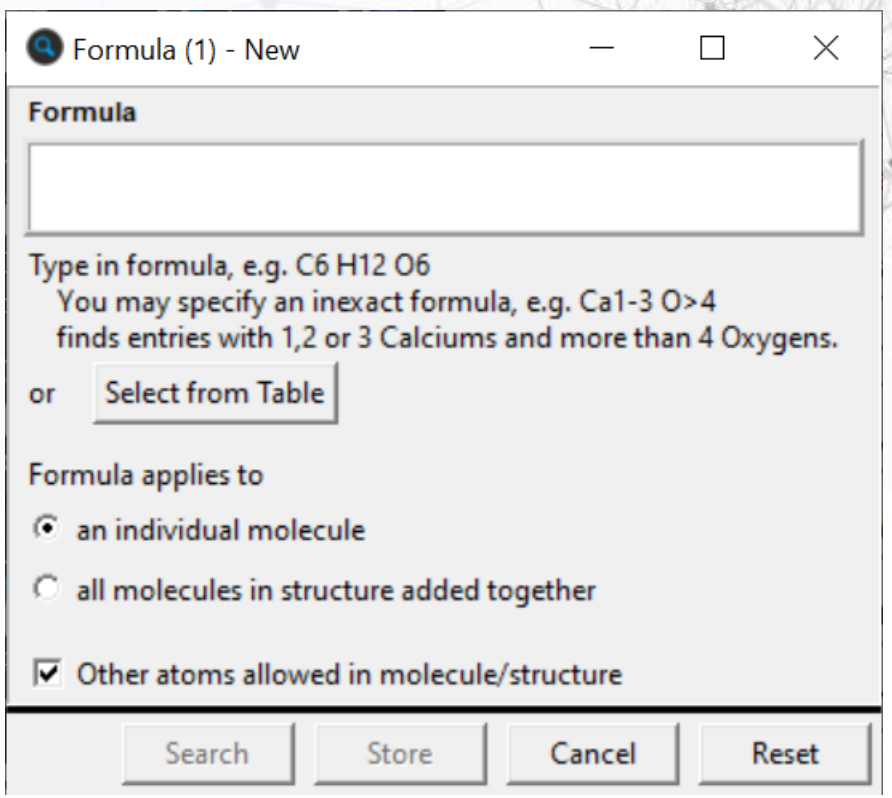



# ConQuest – Elements and formula search

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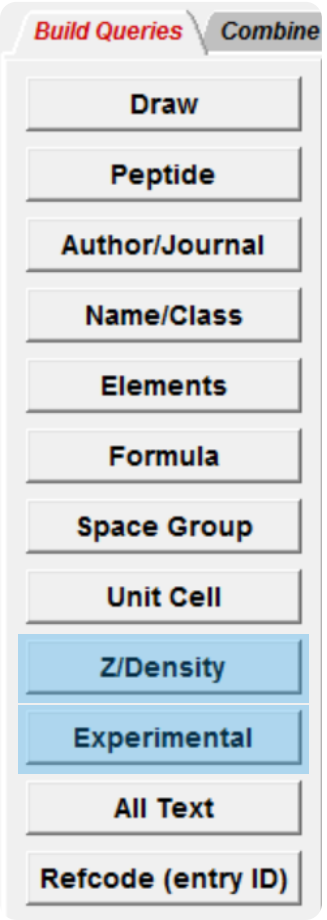
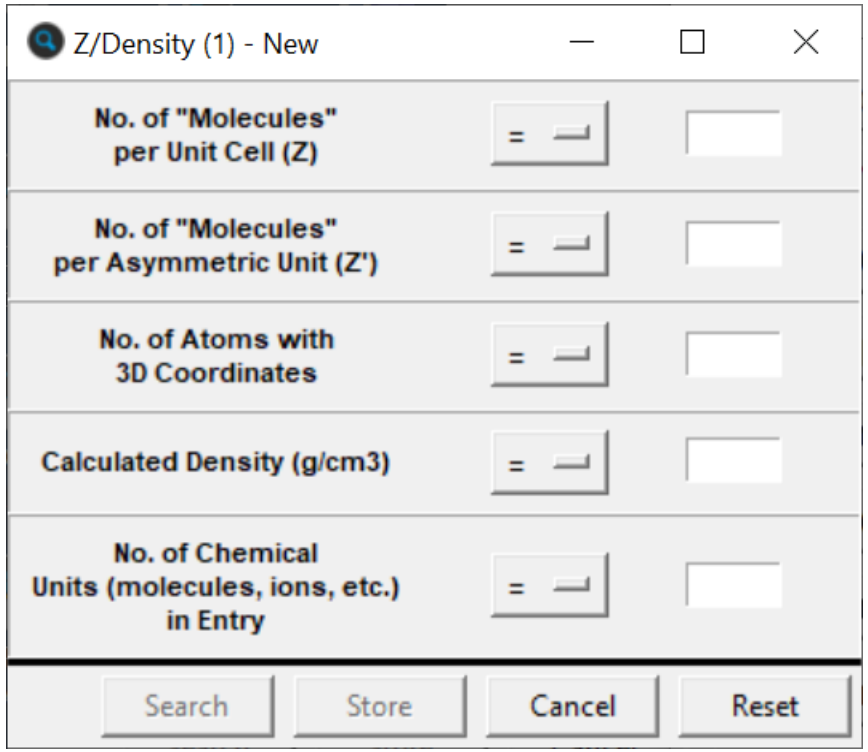
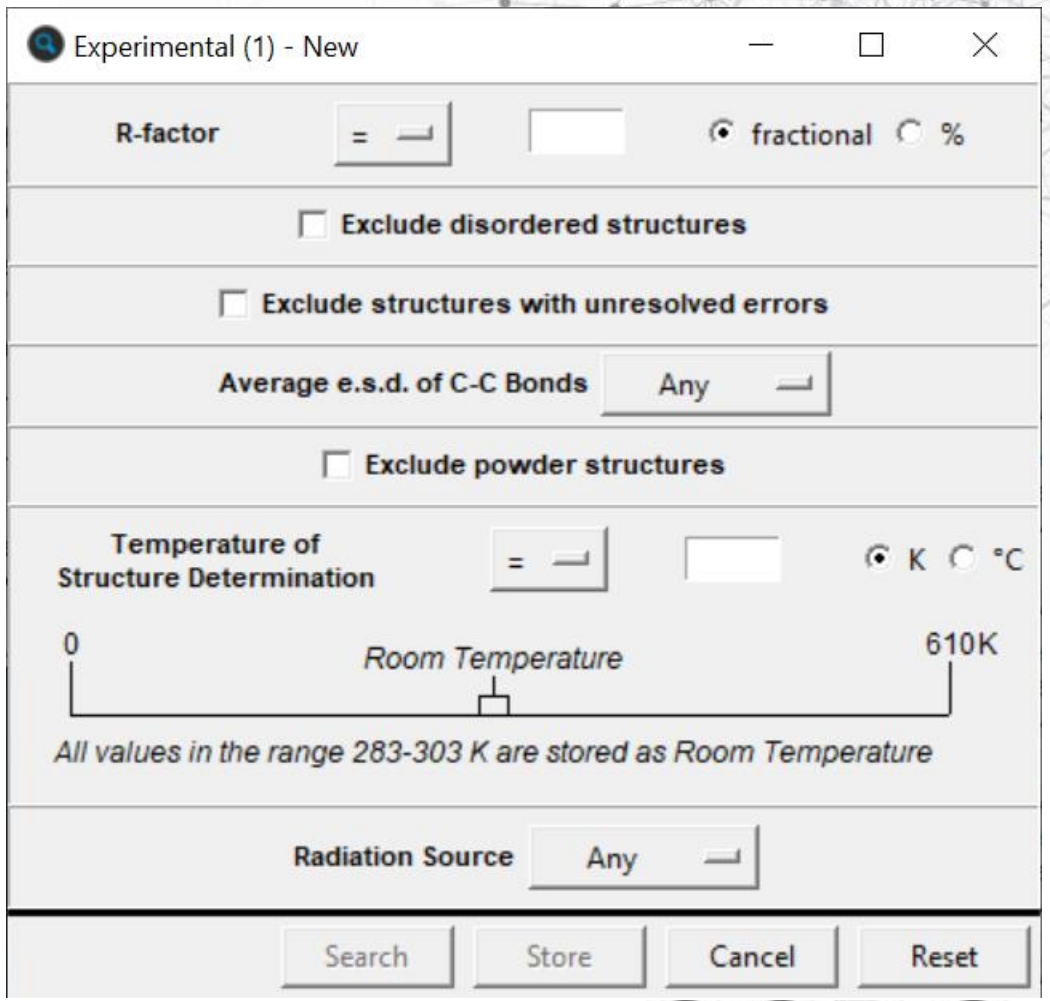
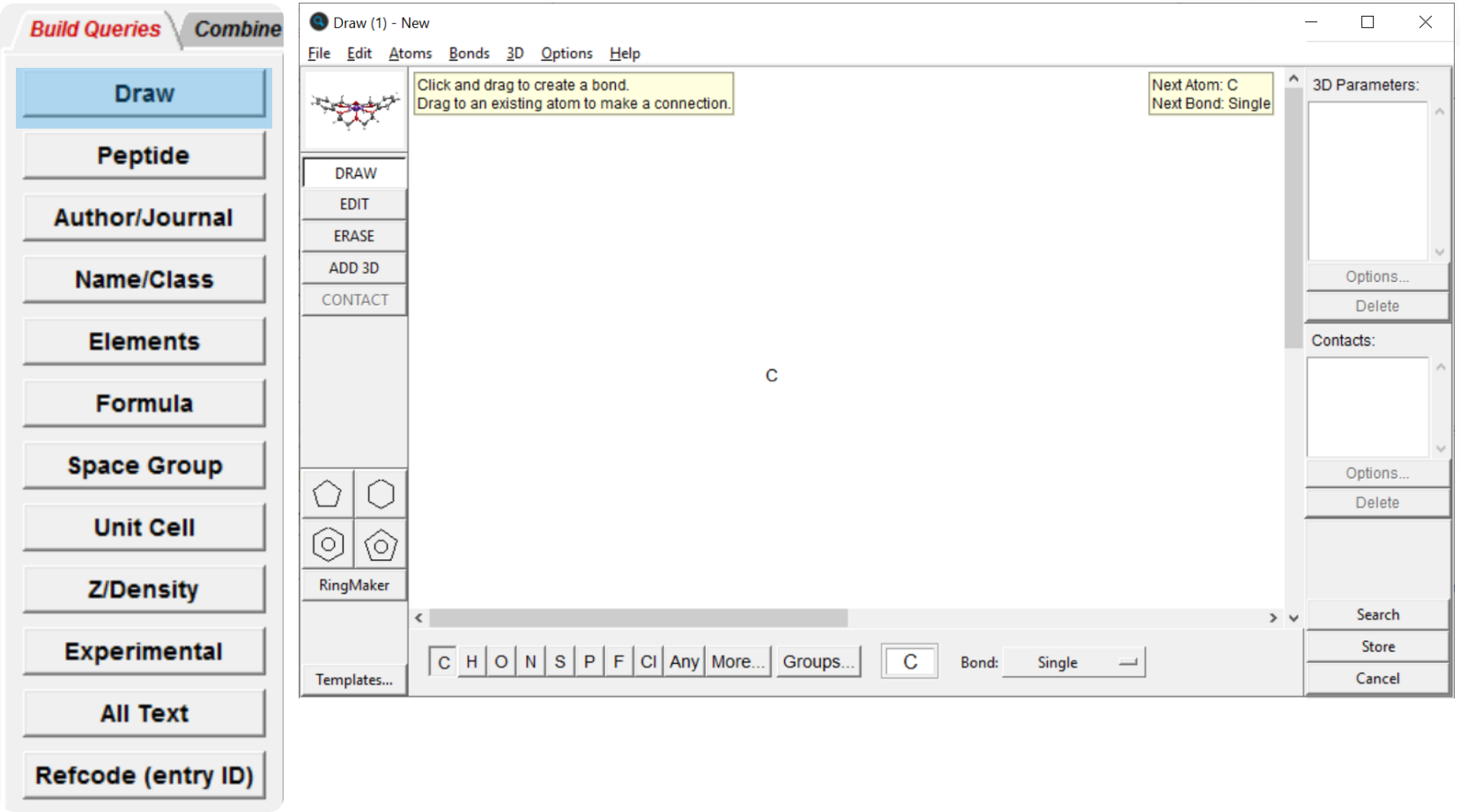
# ConQuest – Z/Density and experimental info search



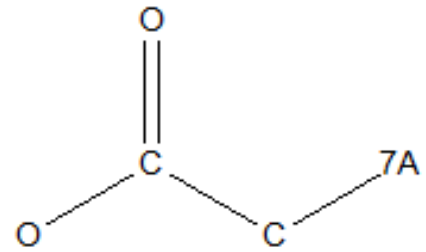



# ConQuest – Draw/Structure search




In the demo we will search for:




where 7A represents any halogen

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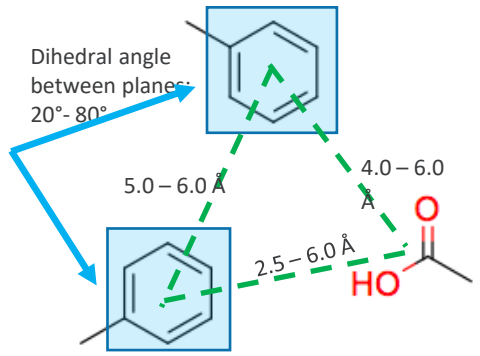
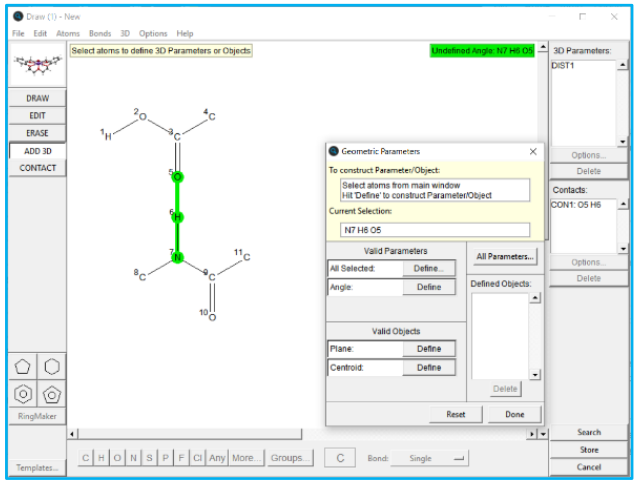
# What else can you explore in ConQuest?

## 3D Search

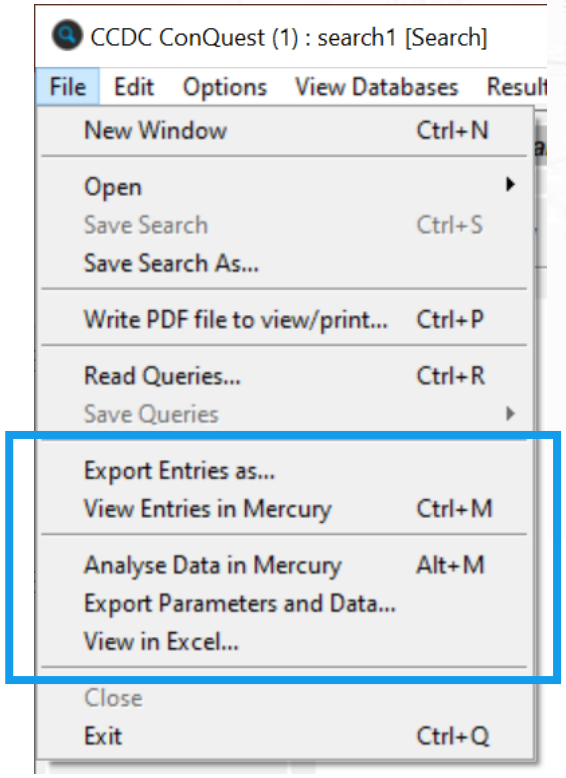


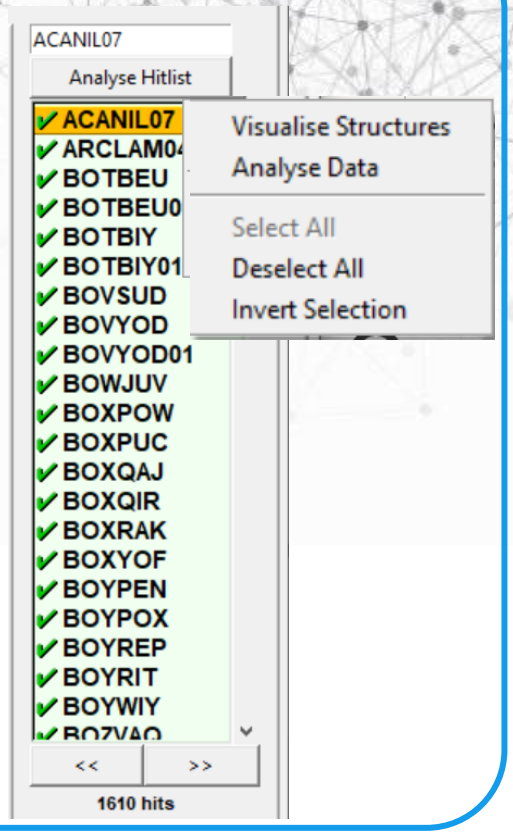

## Intermolecular Interactions



## Search In-House Databases

## Export & Analyse Data




... and more!

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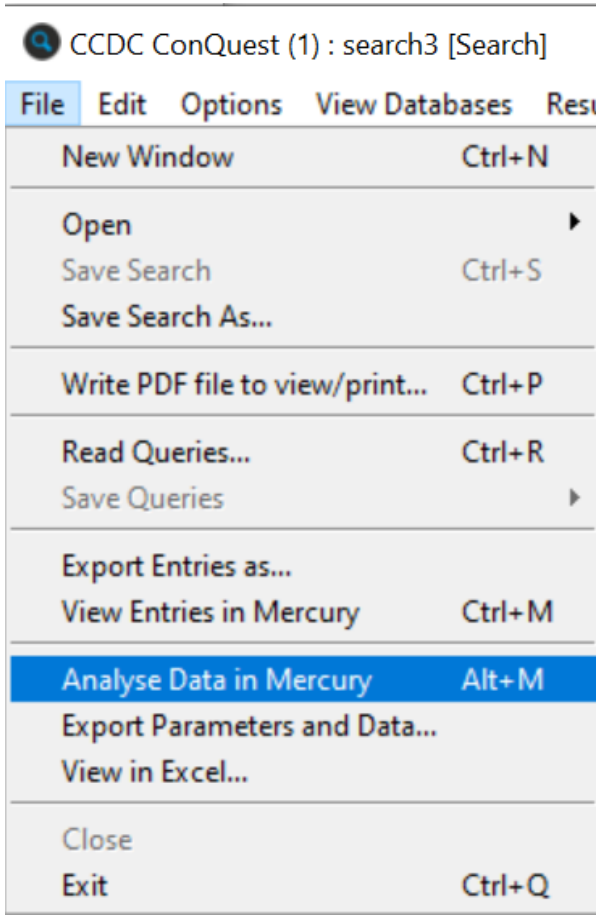
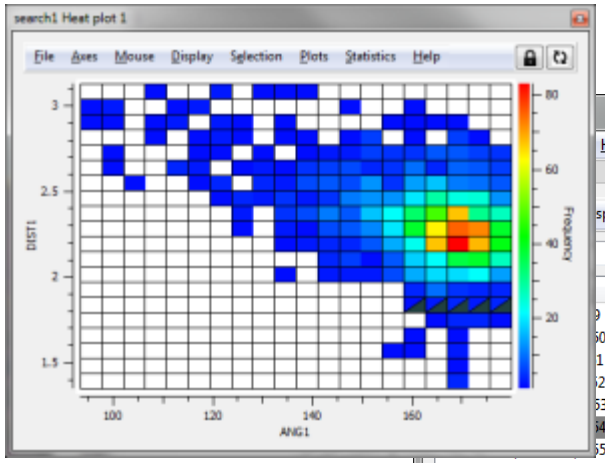
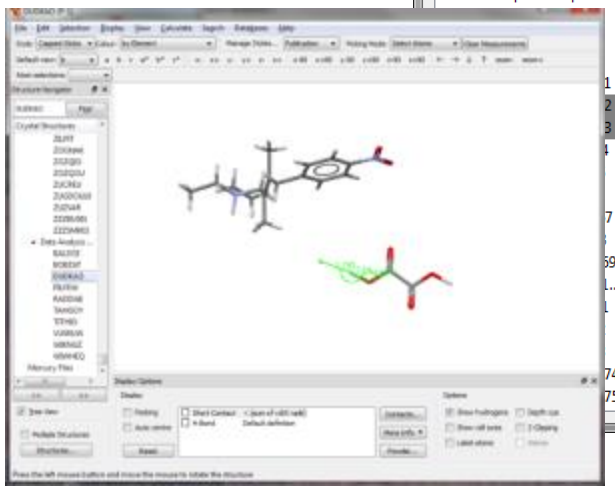
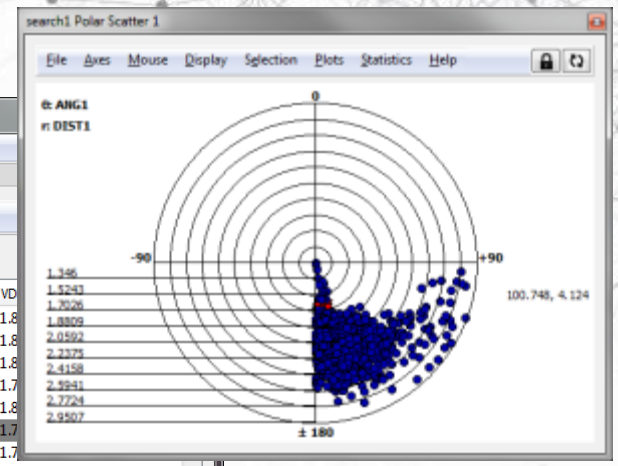
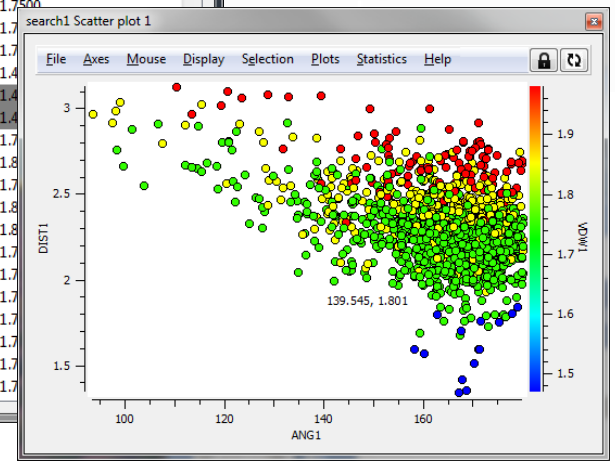
# Data analysis in Mercury

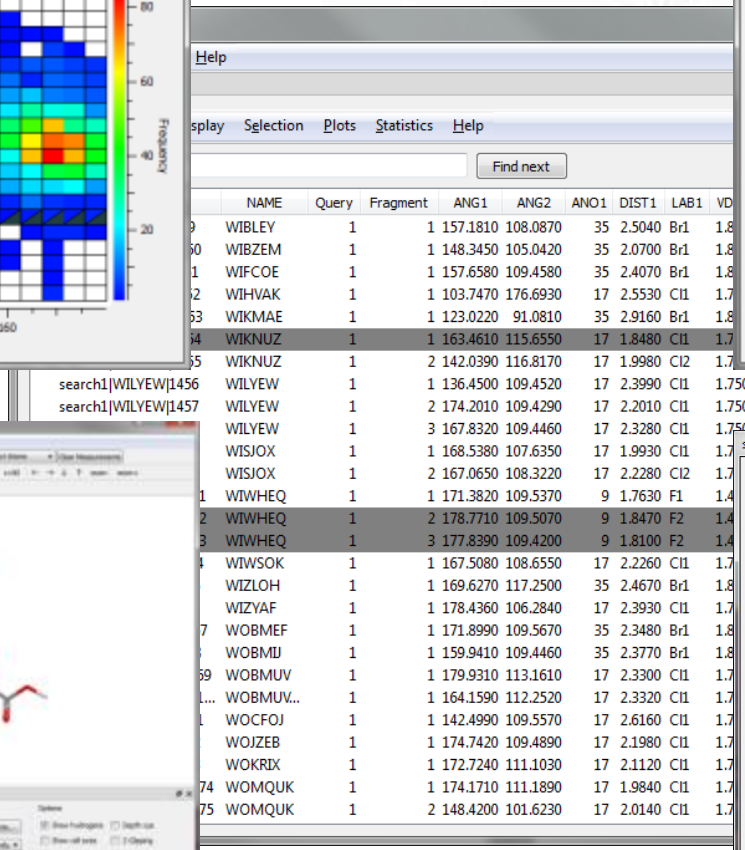


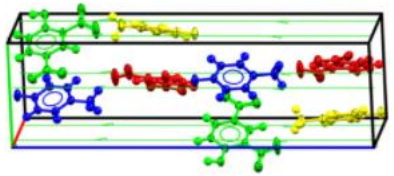





# Want to explore more?



**CSD-System**

Essential crystallographic and structural chemistry capabilities.

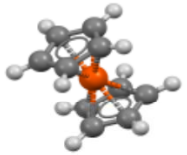
Self-guided workshops about ConQuest in https://www.ccdc.cam.ac.uk/Community/educationalresources/workshop-materials/csd-system-workshops/

## 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.

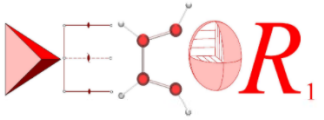
The CCDC and our colleagues continually produce educational materials for use in classroom and computer lab settings, or as independent study modules. Many of these materials make use of the Teaching Subset - a freely available set of over 750 structures that can be investigated with the free version of our Mercury visualisation and analysis program. Of course, our database of over one million entries are available for free through our Access Structures portal.

If you are an educator looking for supplementary teaching materials, find out more about the Teaching Database **here**. If you have developed your own modules using the CSD and would like to share them with the broader community, please contact us at education@ccdc.cam.ac.uk.



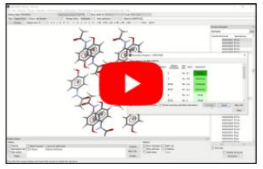
Information on the Teaching Subset

Access a series of teaching modules for use in the classroom

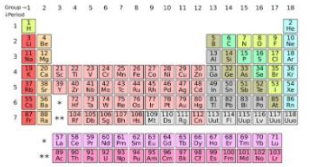



DECOR: Educational Resources for Teaching Crystallography


Download a series of self-guided workshop materials for CCDC tools and features



Watch software training and support videos



Explore the Periodic Table through Crystal Structures


Access fun science activities for kids through the CCDC Home learning page

YouTube and LabTube channels links from https://www.ccdc.cam.ac.uk/Community/educationalresources/ccdc-videos/