Using the CSD to augment your research

By using ConQuest

February 2021

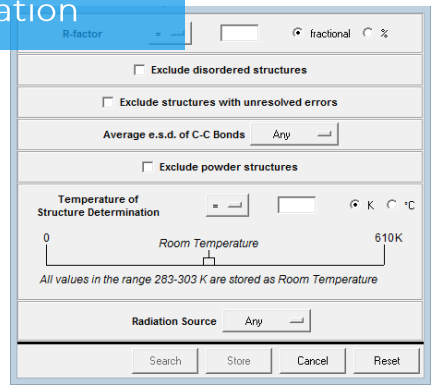
NCS Crystallography for beginners

ncs | UK National Crystallography Service

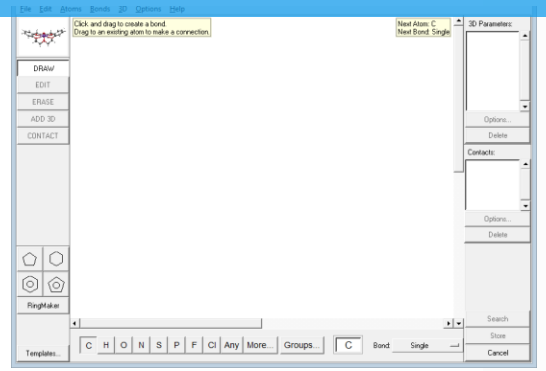
CCDC
advancing structural science

ConQuest features

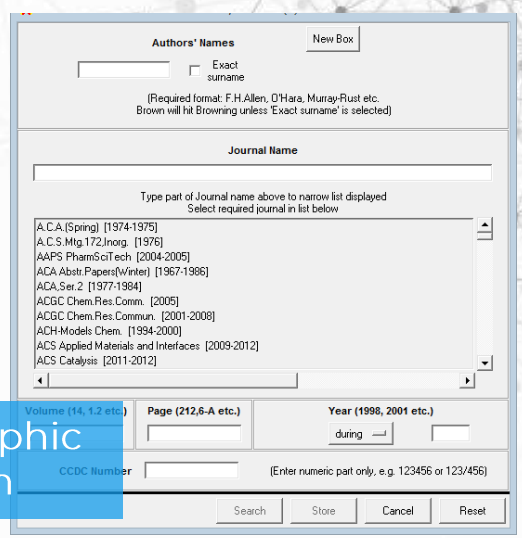
Search for information relating to the structure determination

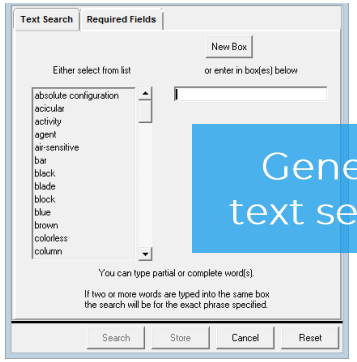


Structure sketcher, enabling set-up of basic substructure searches and complex 3D queries



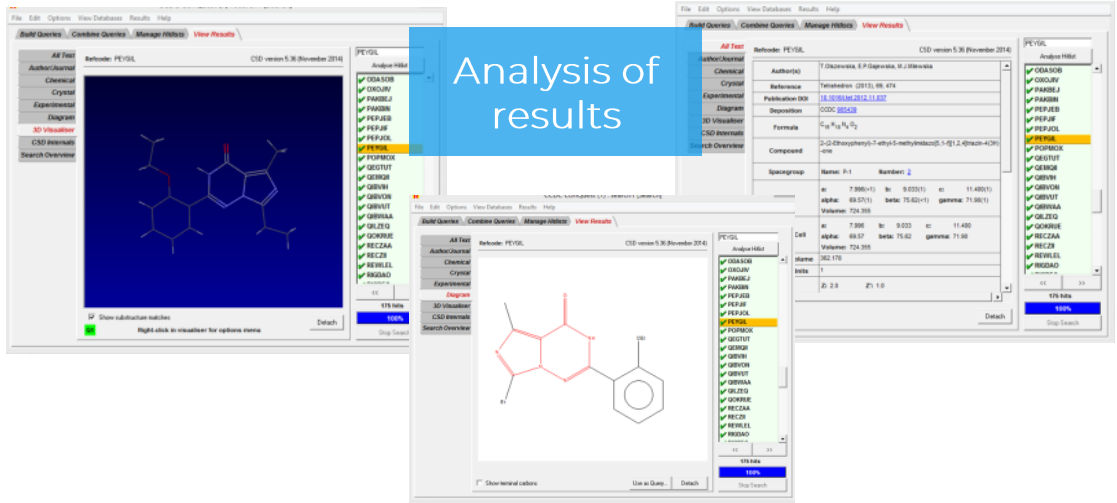
Bibliographic search



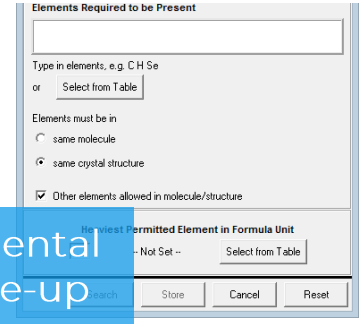


Generic text search

Analysis of results



Elemental make-up



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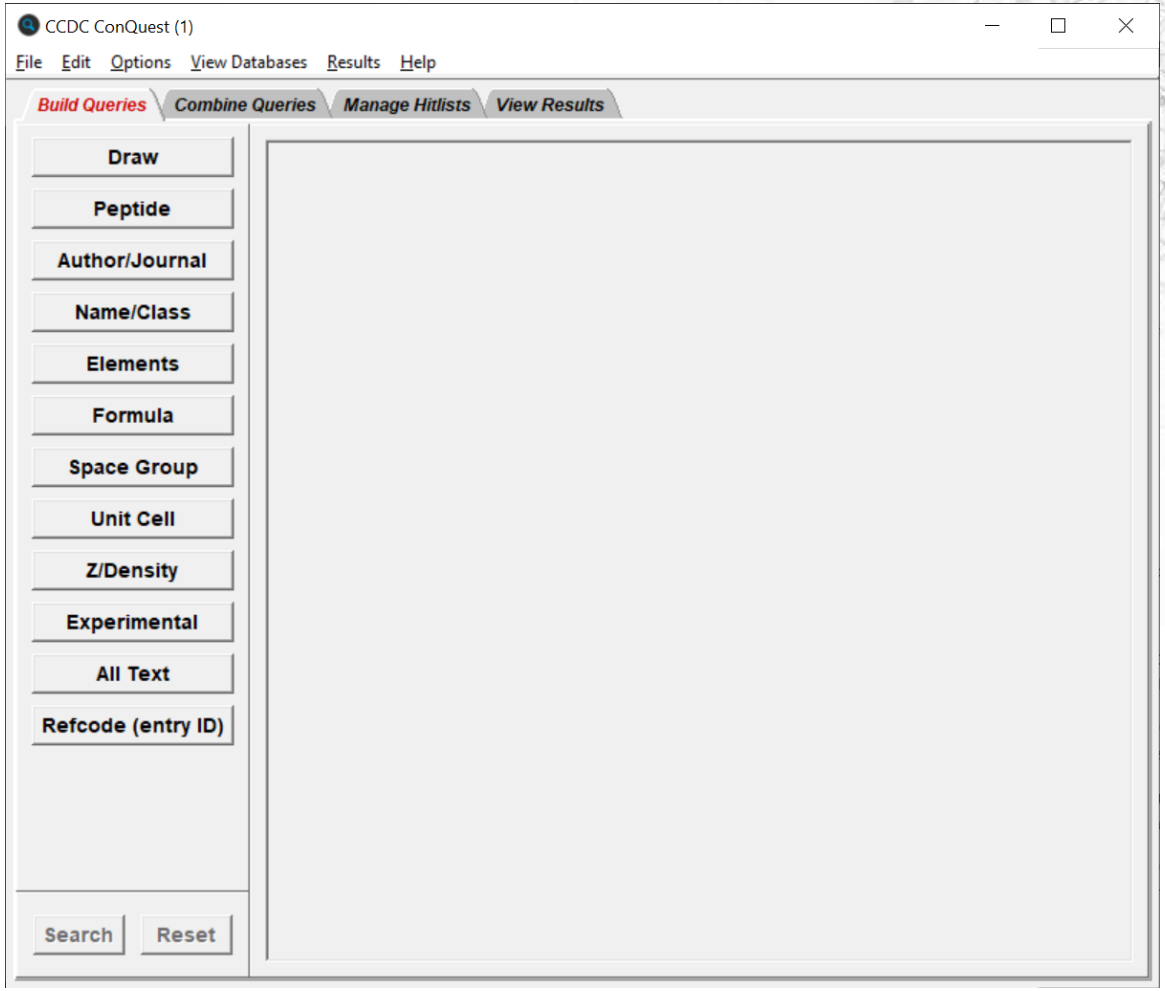
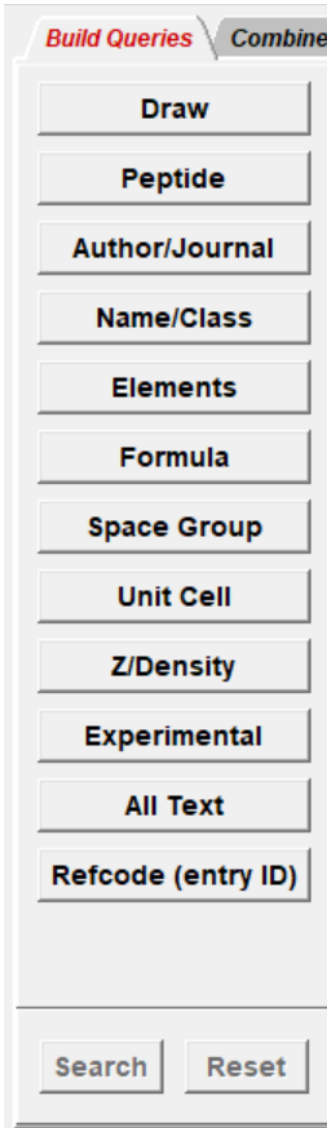
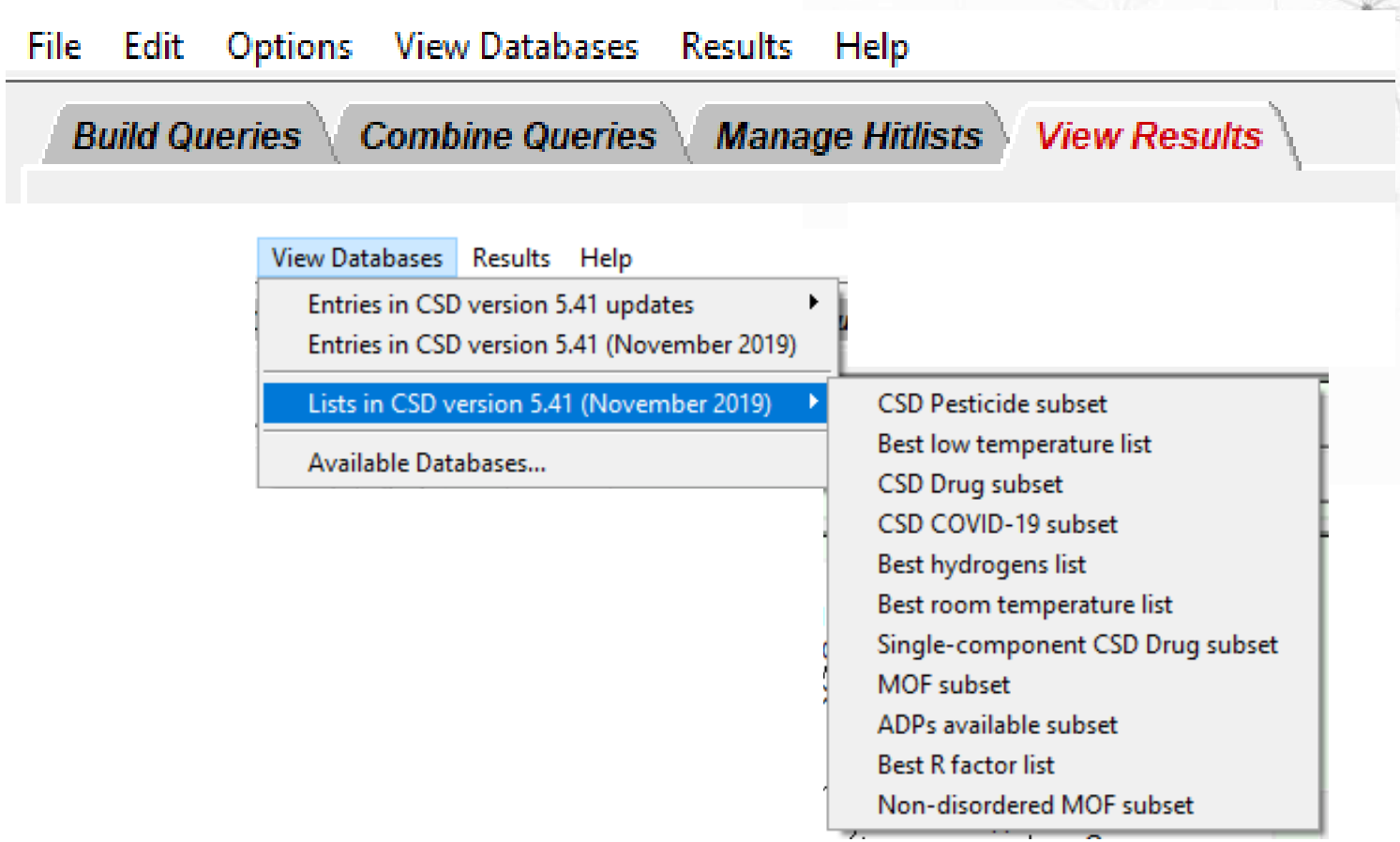
Show One: ConQuest – Opening and search options

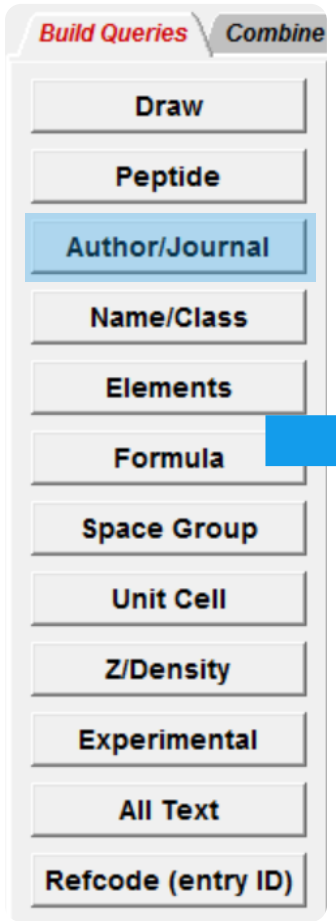


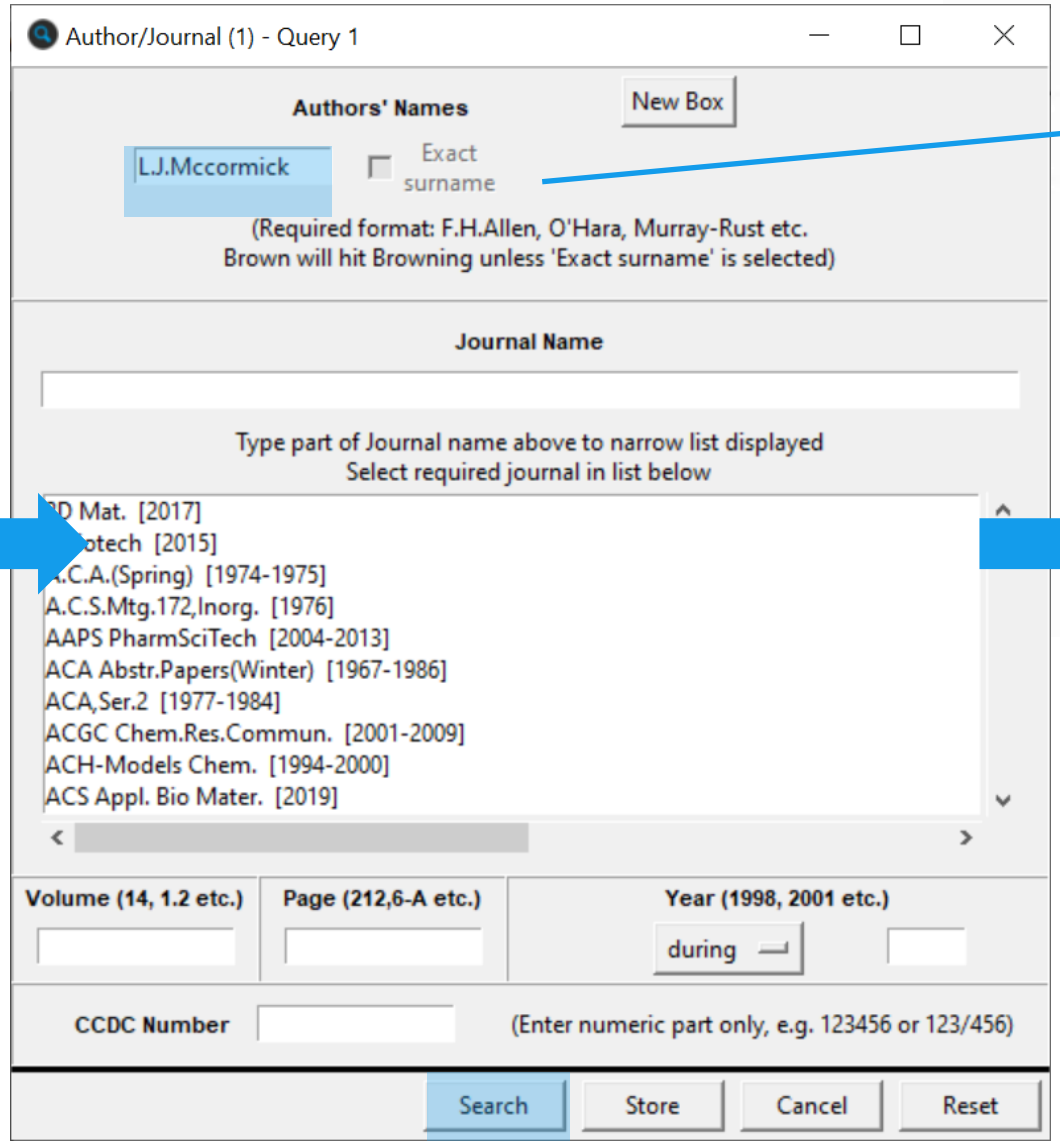
ConQuest – Searching and menu options



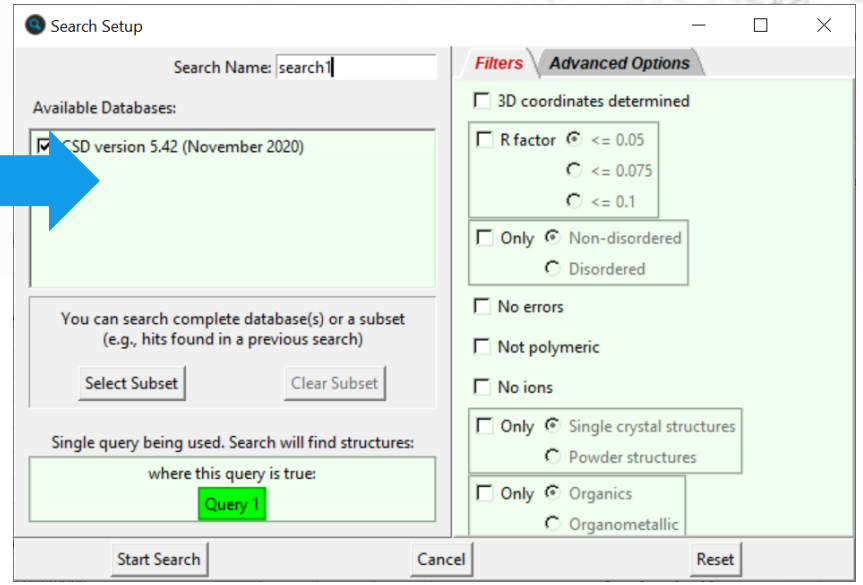


ConQuest – Author and journal search

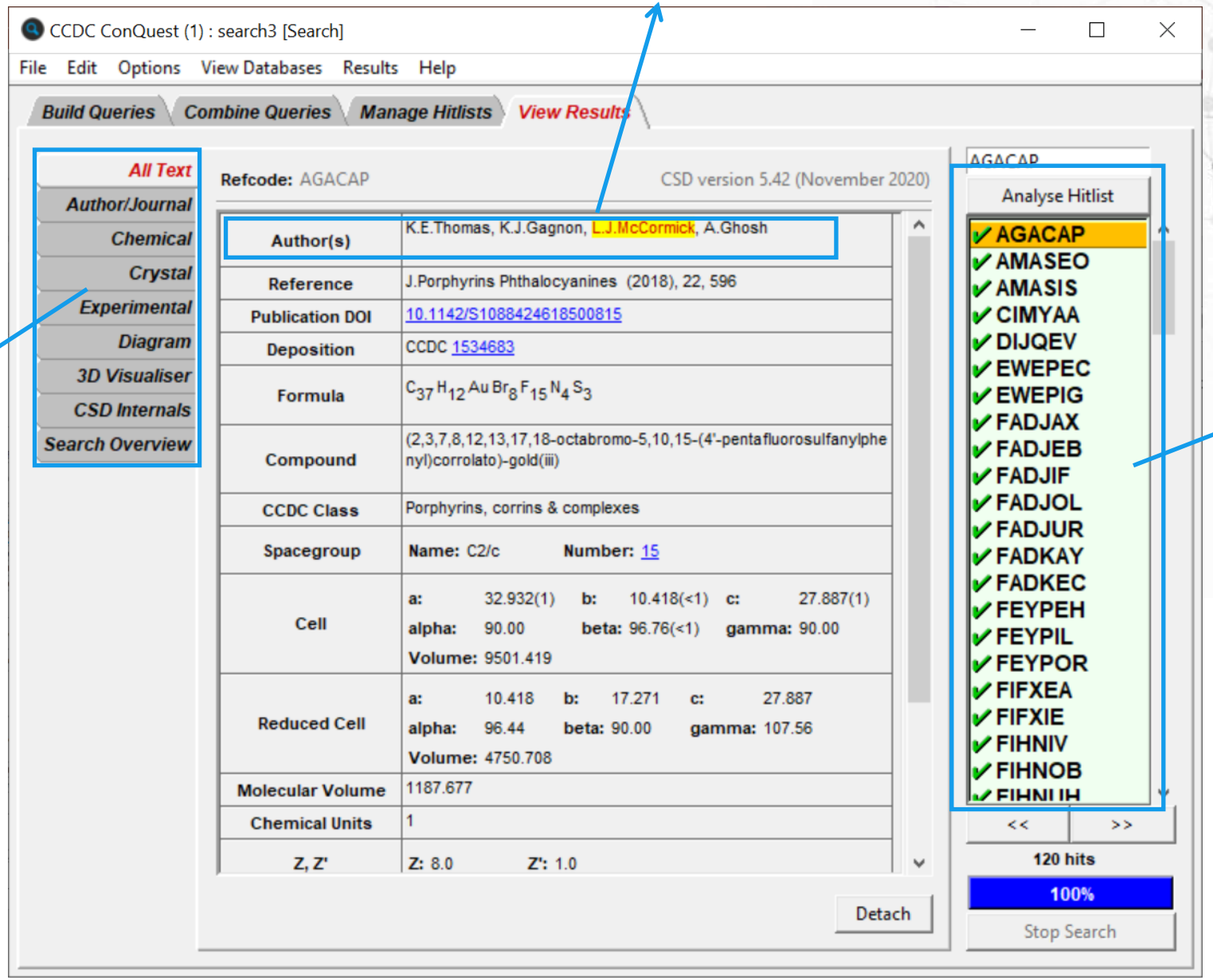




Author names should be initials followed by surname with no spaces e.g. S.J.Coles



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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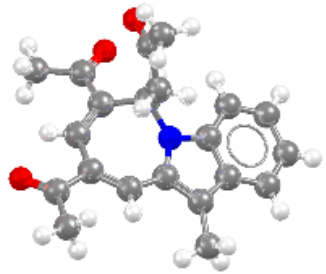
CSD Refcodes



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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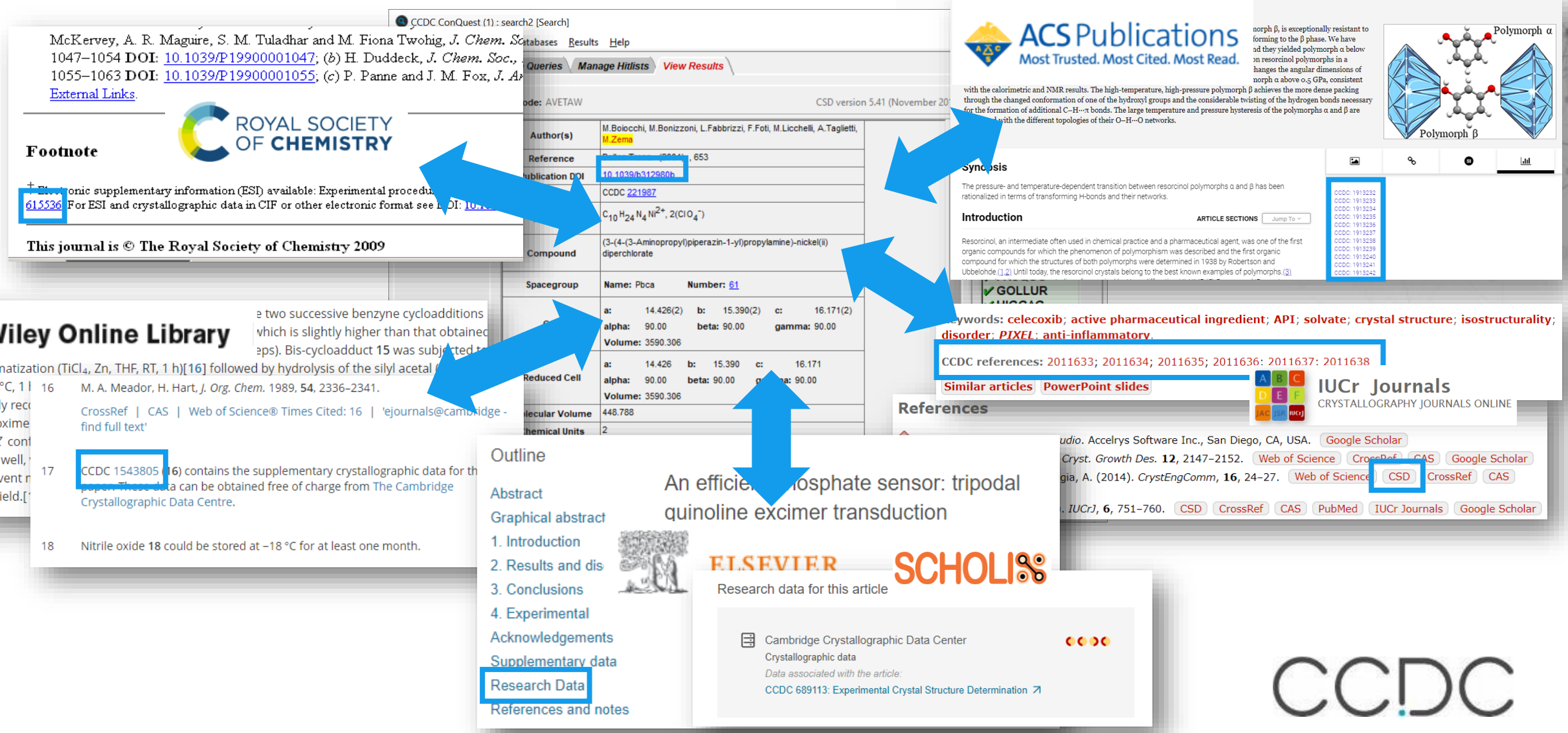
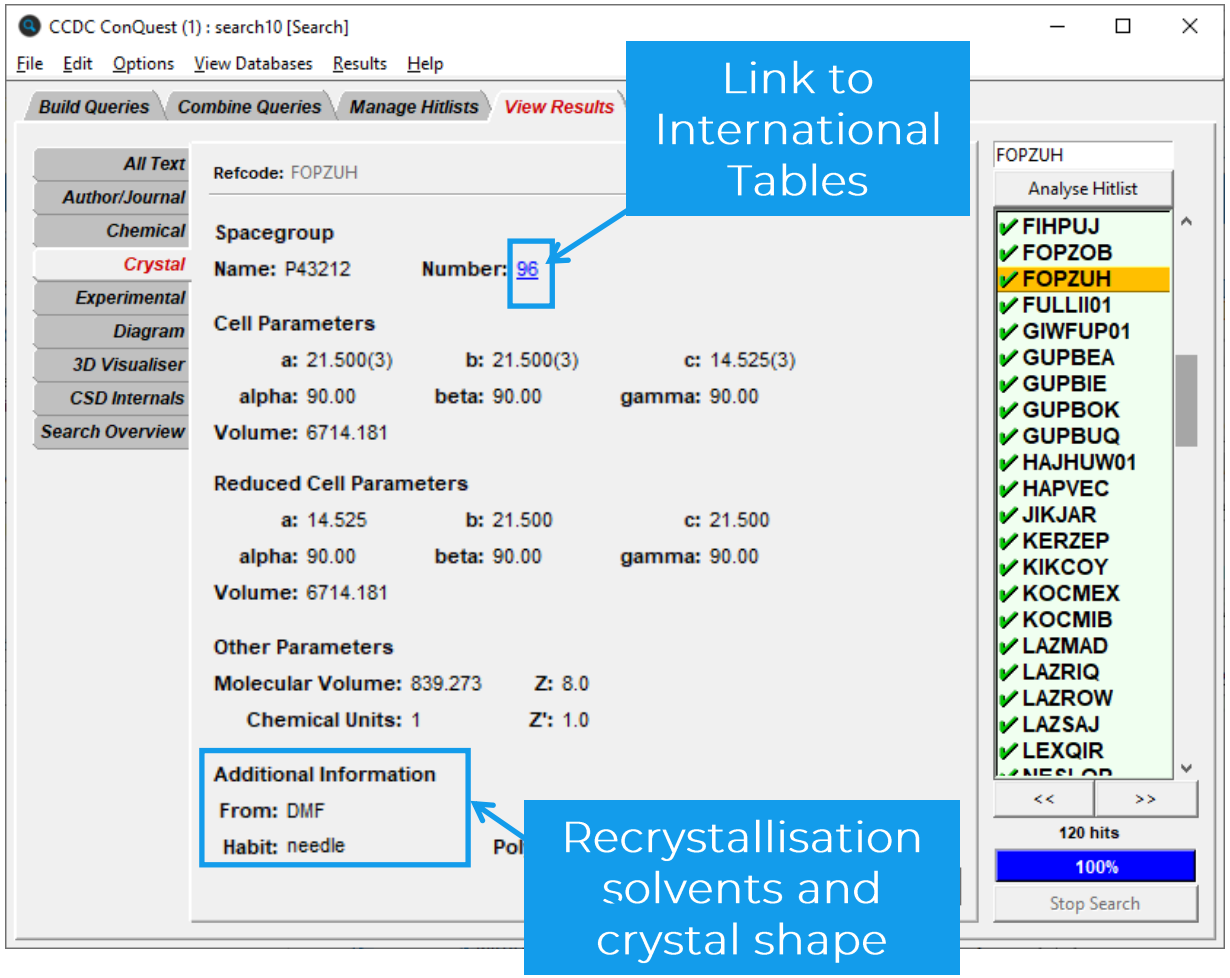
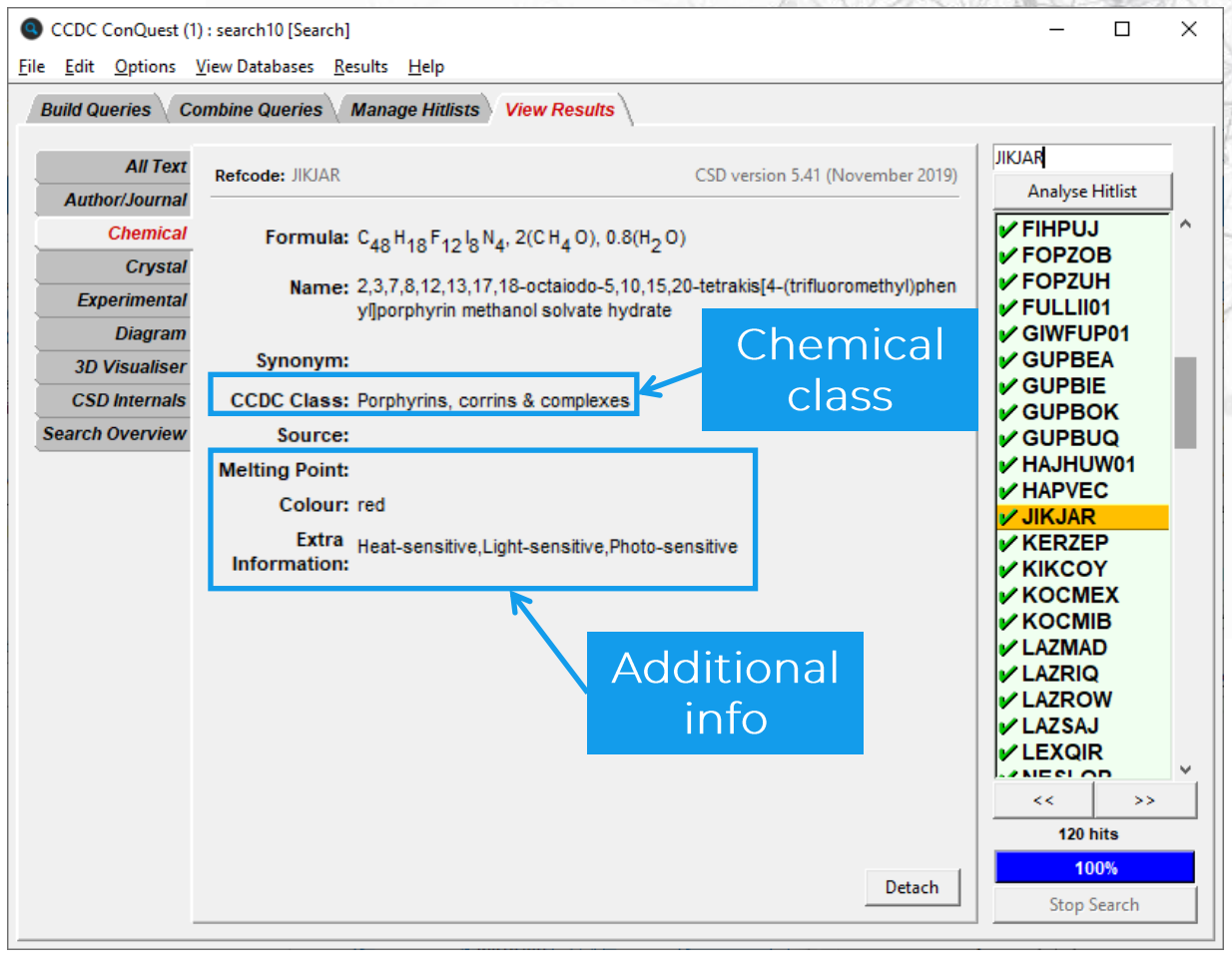
From data to publication and back




CCDC ConQuest (1) : search10 [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: FOPZUH
Spacegroup
Name: P43212 Number: 96
Cell Parameters
a: 21.500(3) b: 21.500(3) c: 14.525(3)
alpha: 90.00 beta: 90.00 gamma: 90.00
Volume: 6714.181
Reduced Cell Parameters
a: 14.525 b: 21.500 c: 21.500
alpha: 90.00 beta: 90.00 gamma: 90.00
Volume: 6714.181
Other Parameters
Molecular Volume: 839.273 Z: 8.0
Chemical Units: 1 Z': 1.0
Additional Information
From: DMF
Habit: needle
FOPZUH
Analyse Hitlist
FIHPUJ
FOPZOB
FOPZUH
FULLII01
GIWFUP01
GUPBEA
GUPBIE
GUPBOK
GUPBUQ
HAJHUW01
HAPVEC
JIKJAR
KERZEP
KIKCOY
KOCMEX
KOCMIB
LAZMAD
LAZRIQ
LAZROW
LAZSAJ
LEXQIR
<< >>
120 hits
100%
Stop Search
Link to International Tables
Recrystallisation solvents and crystal shape


CCDC ConQuest (1) : search10 [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: JIKJAR
CSD version 5.41 (November 2019)
Formula: C48 H18 F12 I8 N4, 2(C H4 O), 0.8(H2 O)
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Synonym:
CCDC Class: Porphyrins, corrins & complexes
Source:
Melting Point:
Colour: red
Extra Information: Heat-sensitive,Light-sensitive,Photo-sensitive
Detach
JIKJAR
Analyse Hitlist
FIHPUJ
FOPZOB
FOPZUH
FULLII01
GIWFUP01
GUPBEA
GUPBIE
GUPBOK
GUPBUQ
HAJHUW01
HAPVEC
JIKJAR
KERZEP
KIKCOY
KOCMEX
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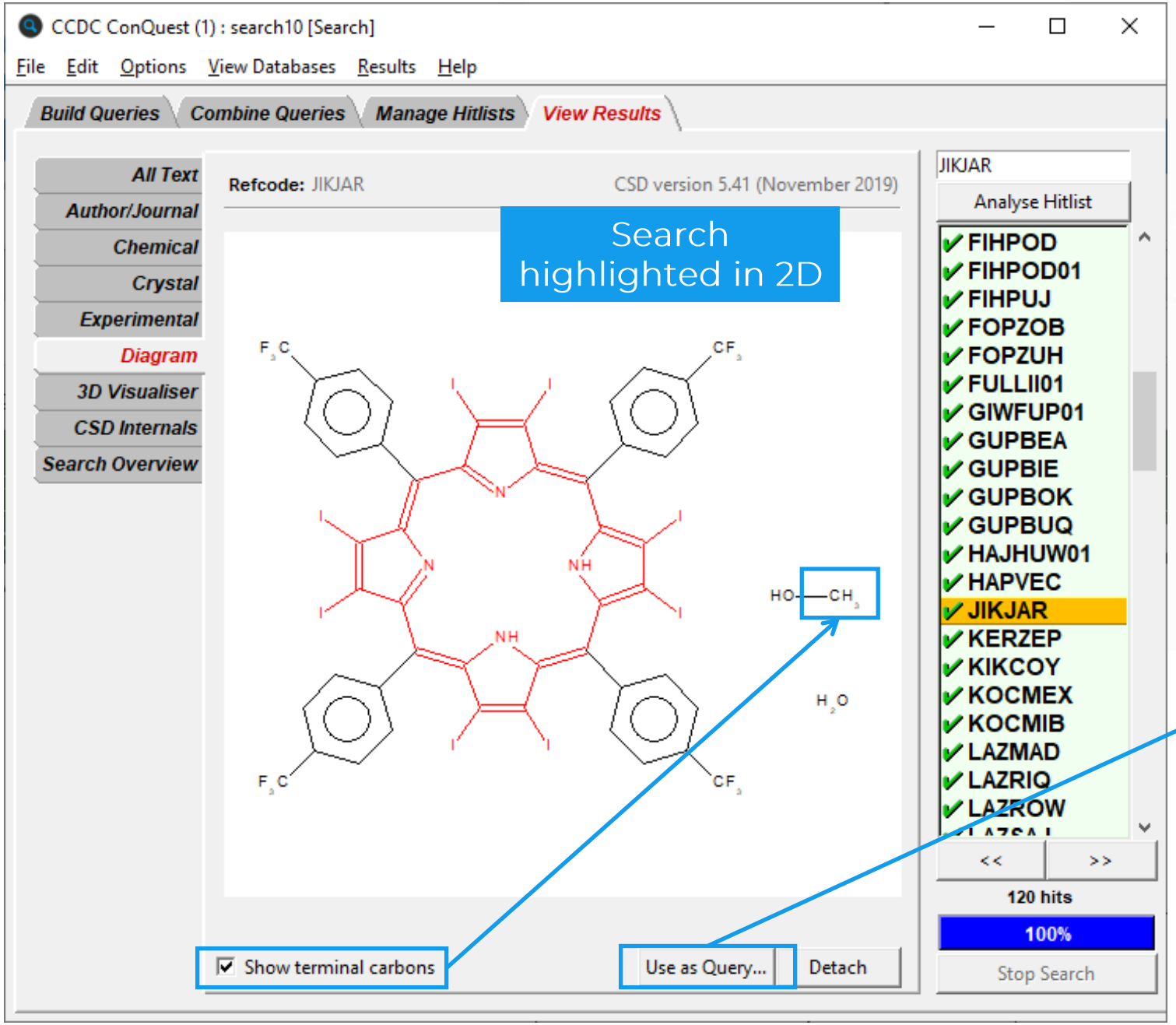
LAZMAD
LAZRIQ
LAZROW
LAZSAJ
LEXQIR
<< >>
120 hits
100%
Stop Search
Chemical class
Additional info


CCDC ConQuest (1) : search10 [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: JIKJAR
CSD version 5.41 (November 2019)
Search highlighted in 2D
Show terminal carbons
Use as Query...
Detach
JIKJAR
Analyse Hitlist
FIHPOD
FIHPOD01
FIHPUJ
FOPZOB
FOPZUH
FULLII01
GIWFUP01
GUPBEA
GUPBIE
GUPBOK
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HAJHUW01
HAPVEC
JIKJAR
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LAZRIQ
LAZROW
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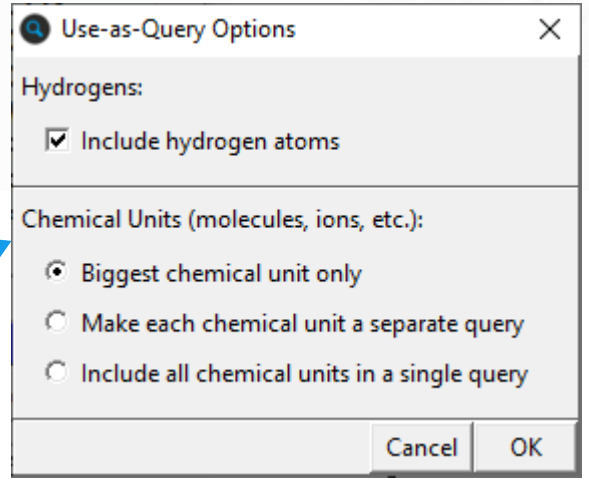
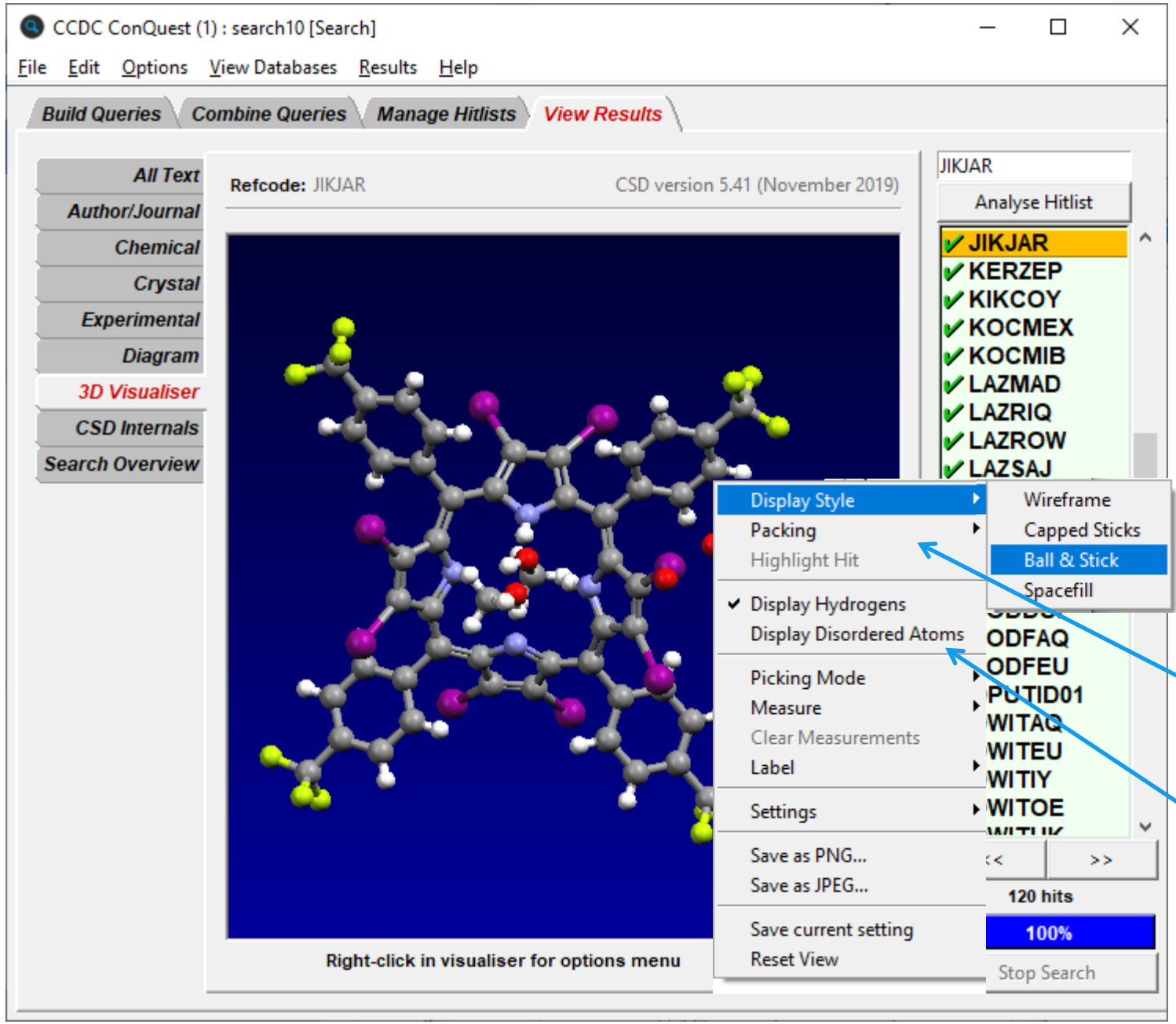
>>
120 hits
100%
Stop Search


Use-as-Query Options
Hydrogens:
Include hydrogen atoms
Chemical Units (molecules, ions, etc.):
Biggest chemical unit only
Make each chemical unit a separate query
Include all chemical units in a single query
Cancel
OK

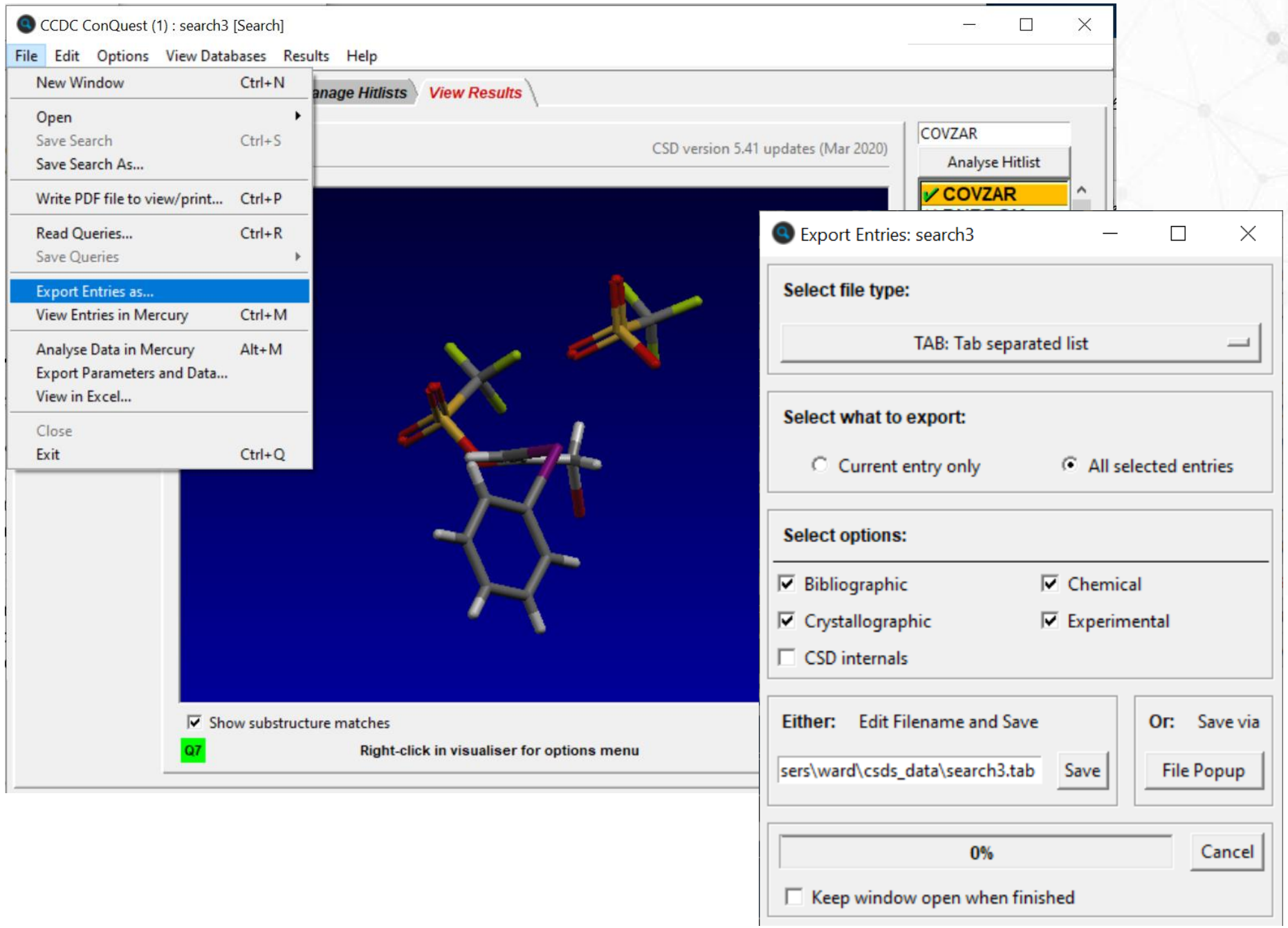


Left clicking each tab will display different information

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

Packing > Molecule or unit cell

Display or hide disordered atoms



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

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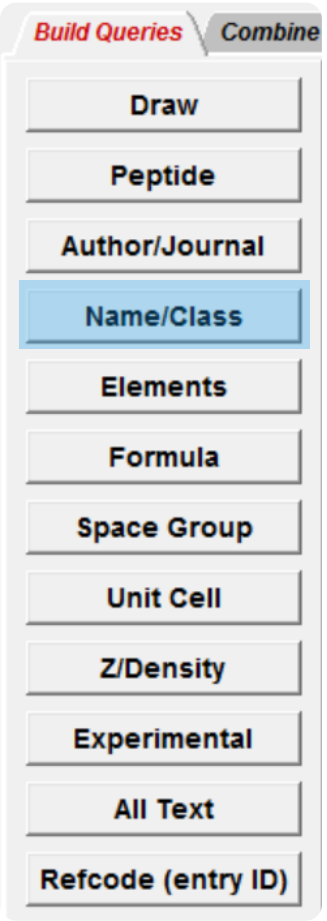
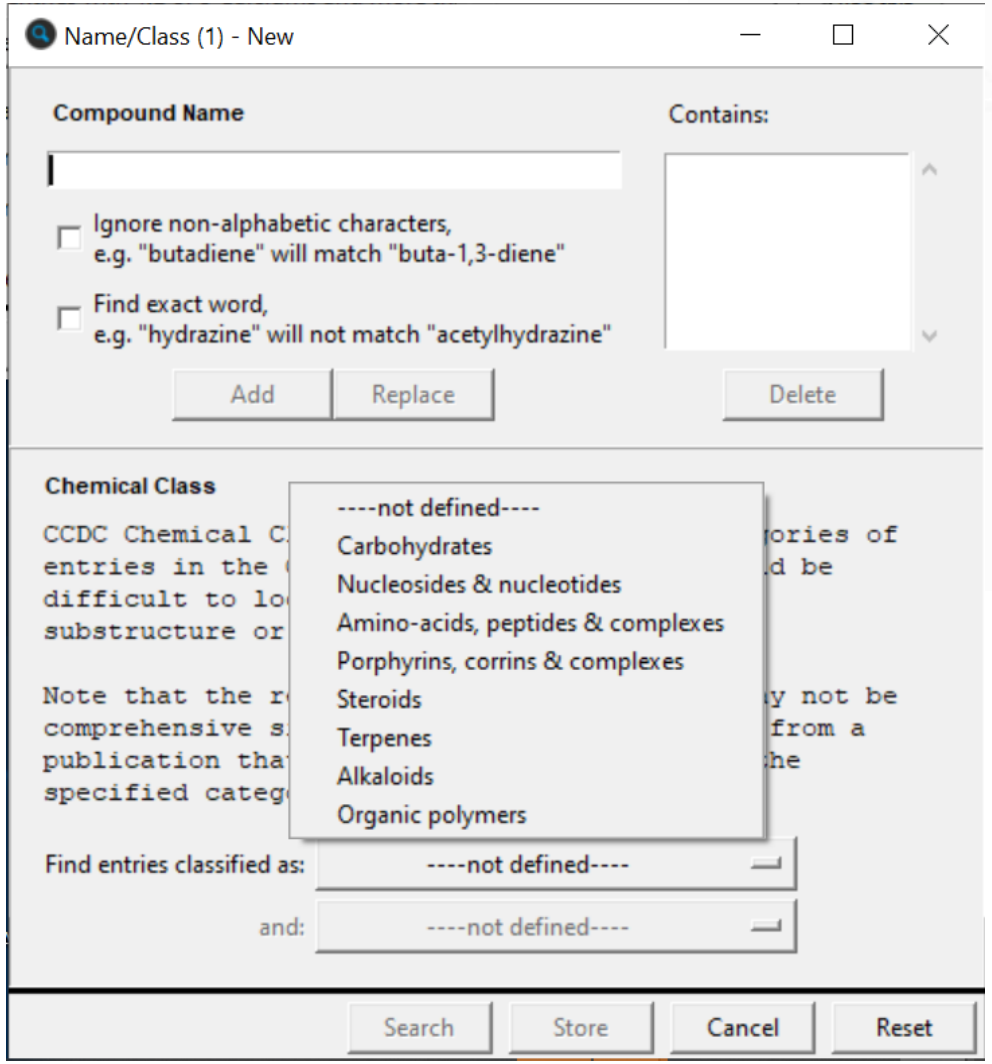
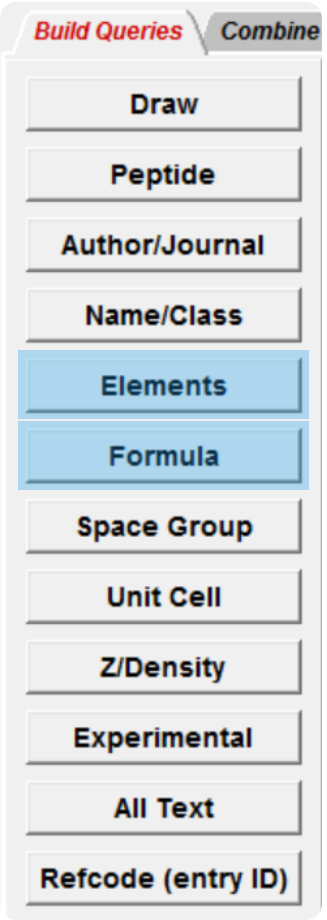
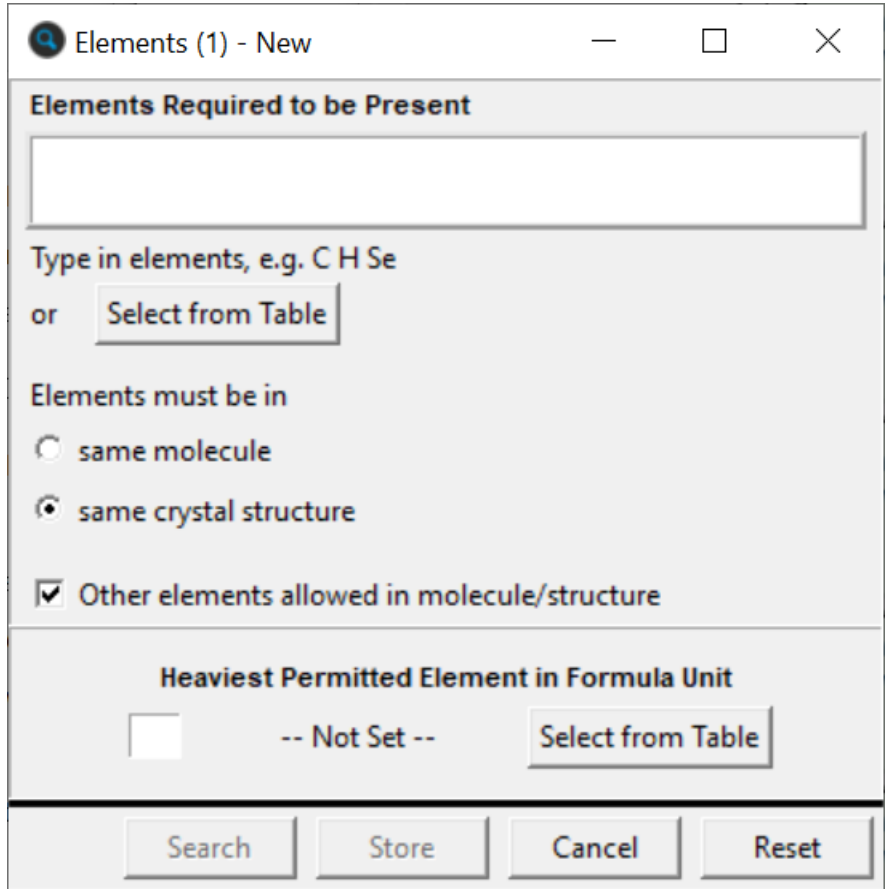
ConQuest – Compound name search

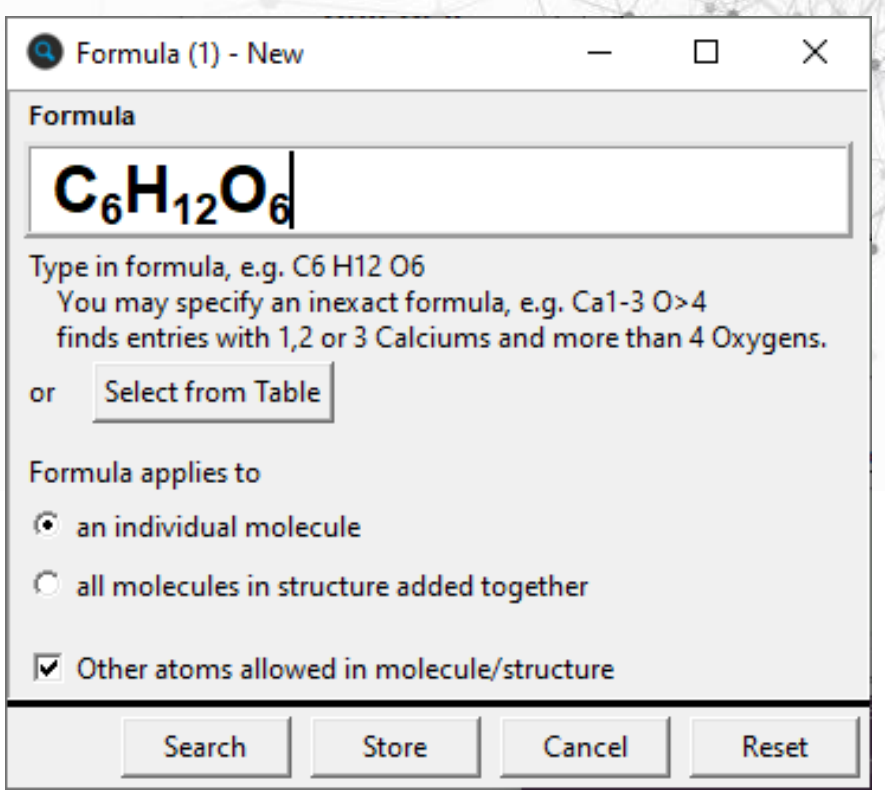




ConQuest – Elements and formula search

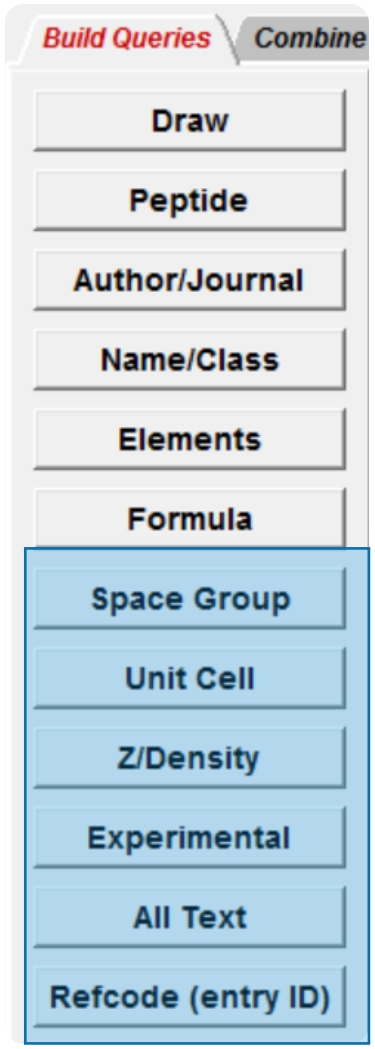


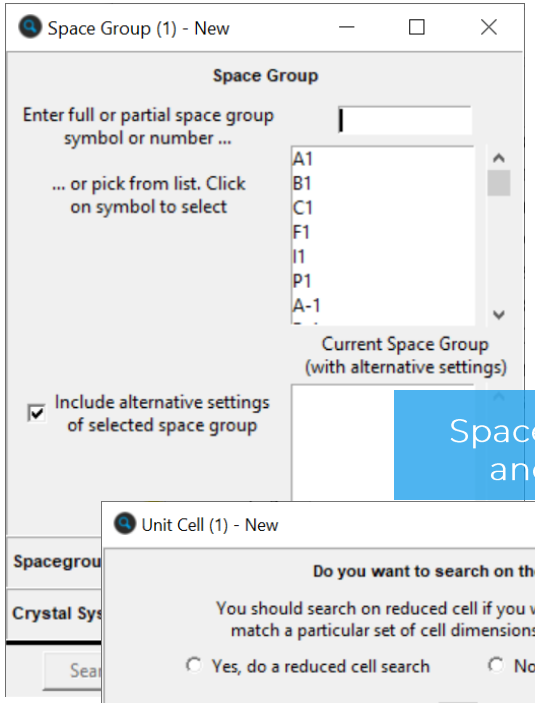


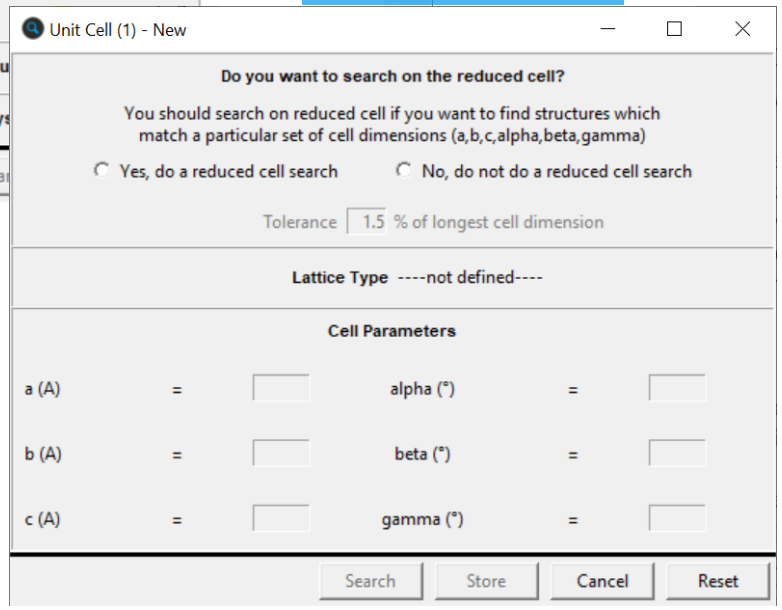


CCDC

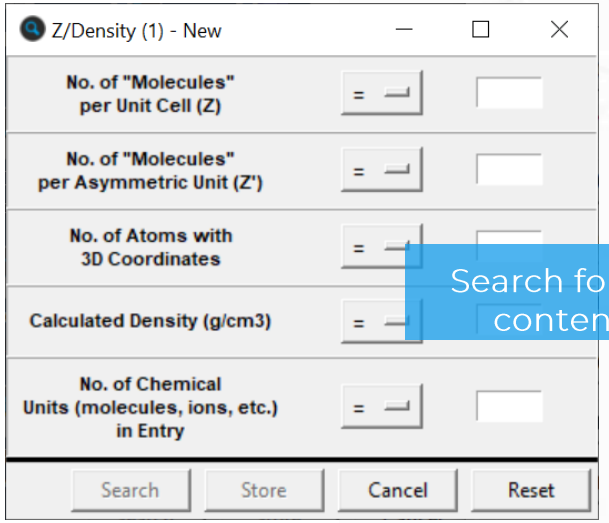
Other searches



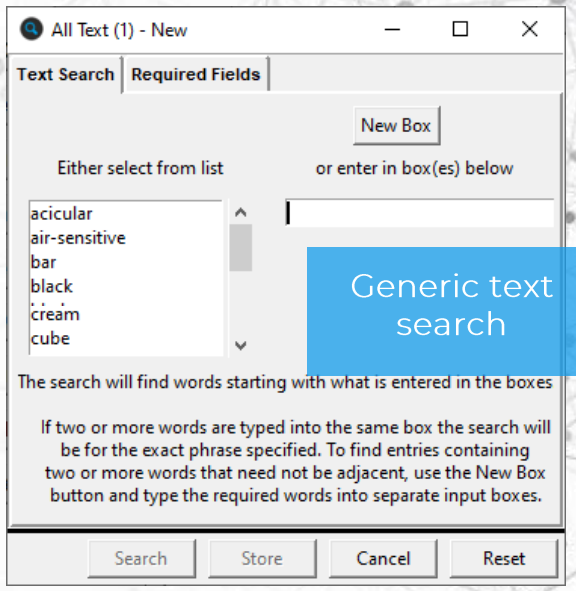




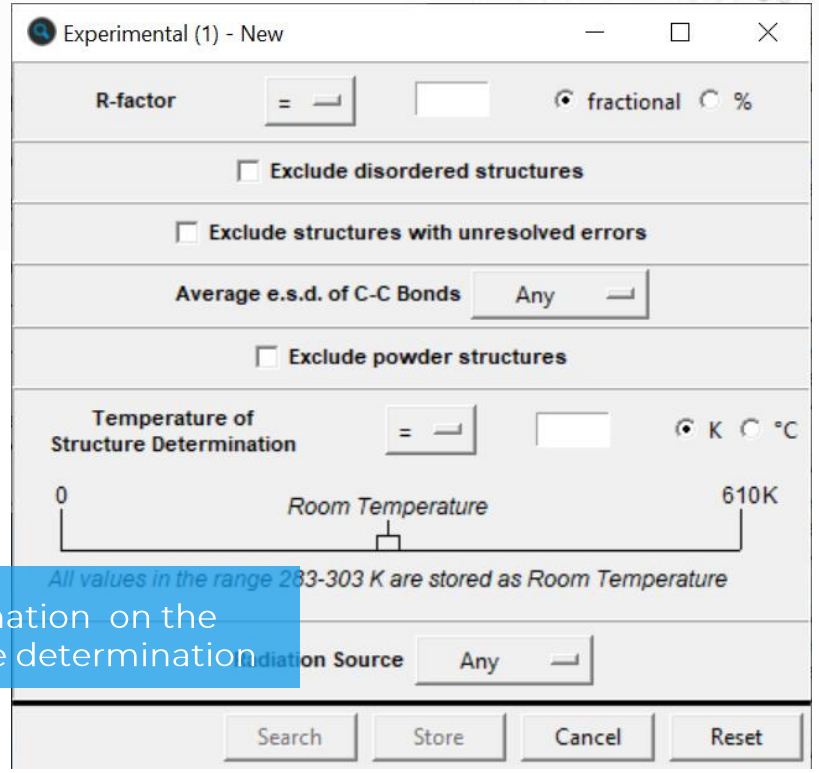
Space group and cell



Search for cell contents

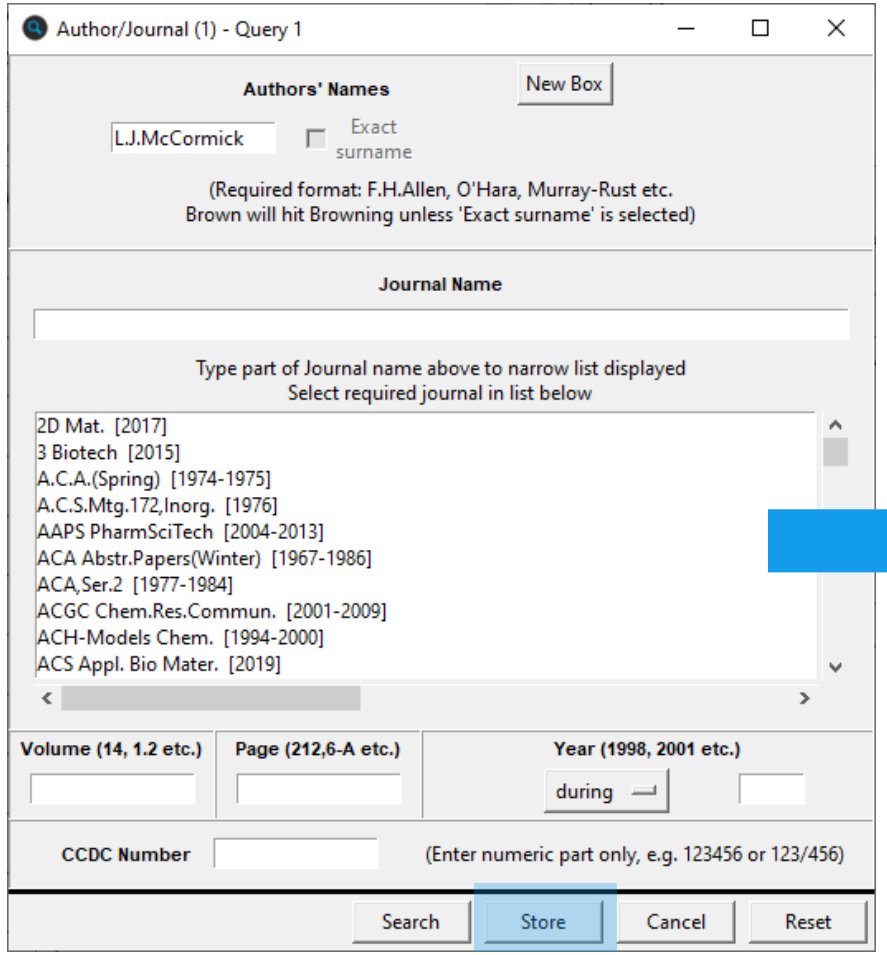


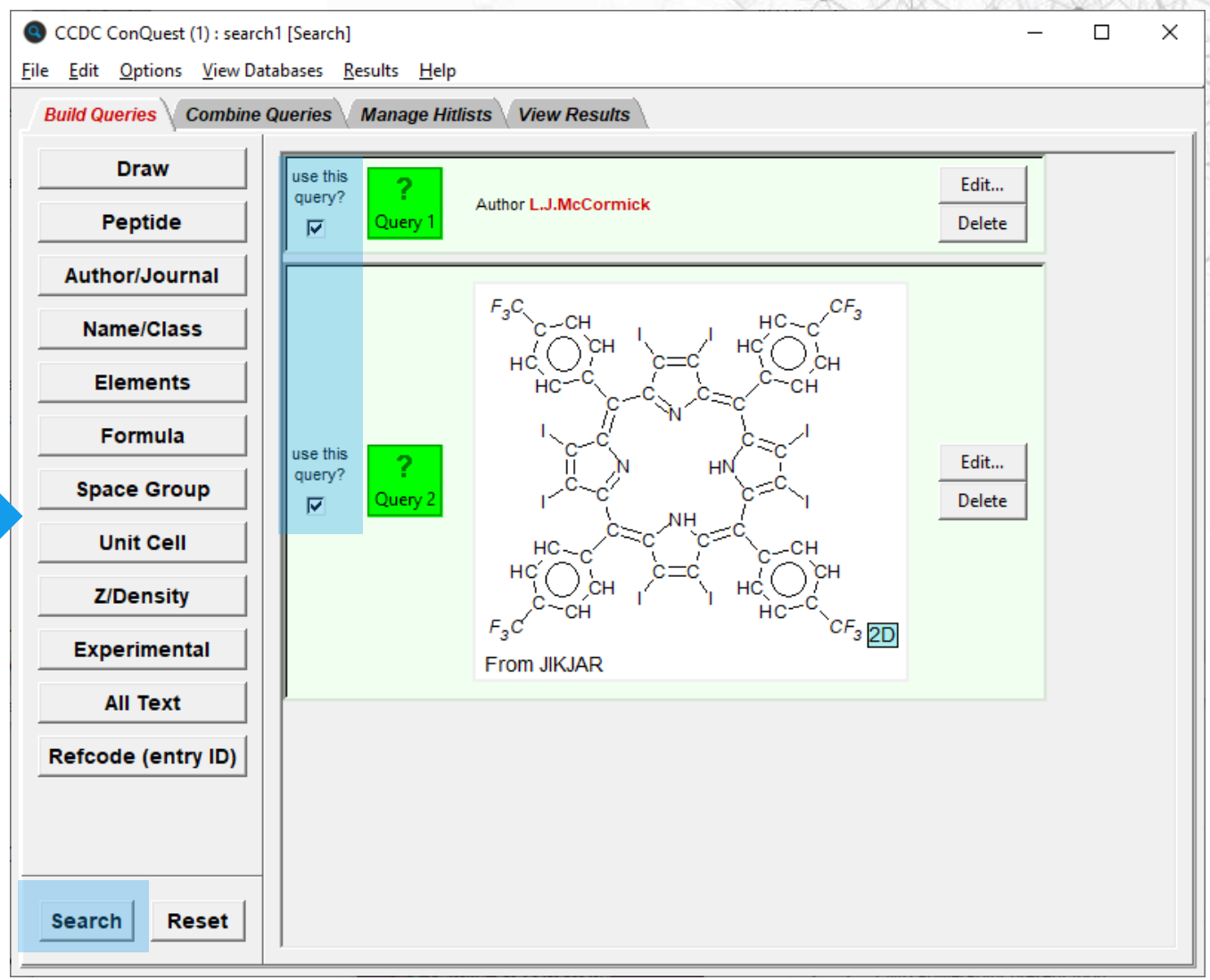
Generic text search



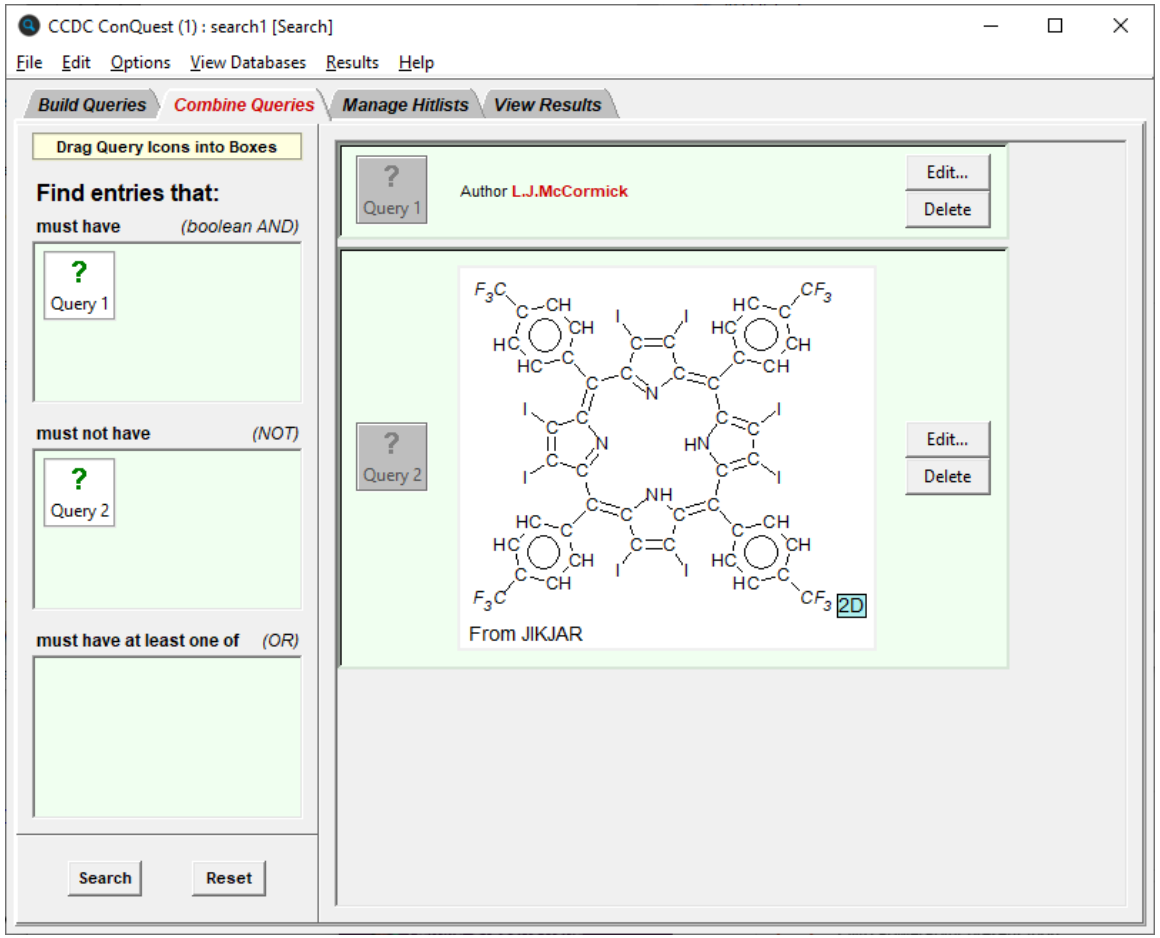
information on the structure determination

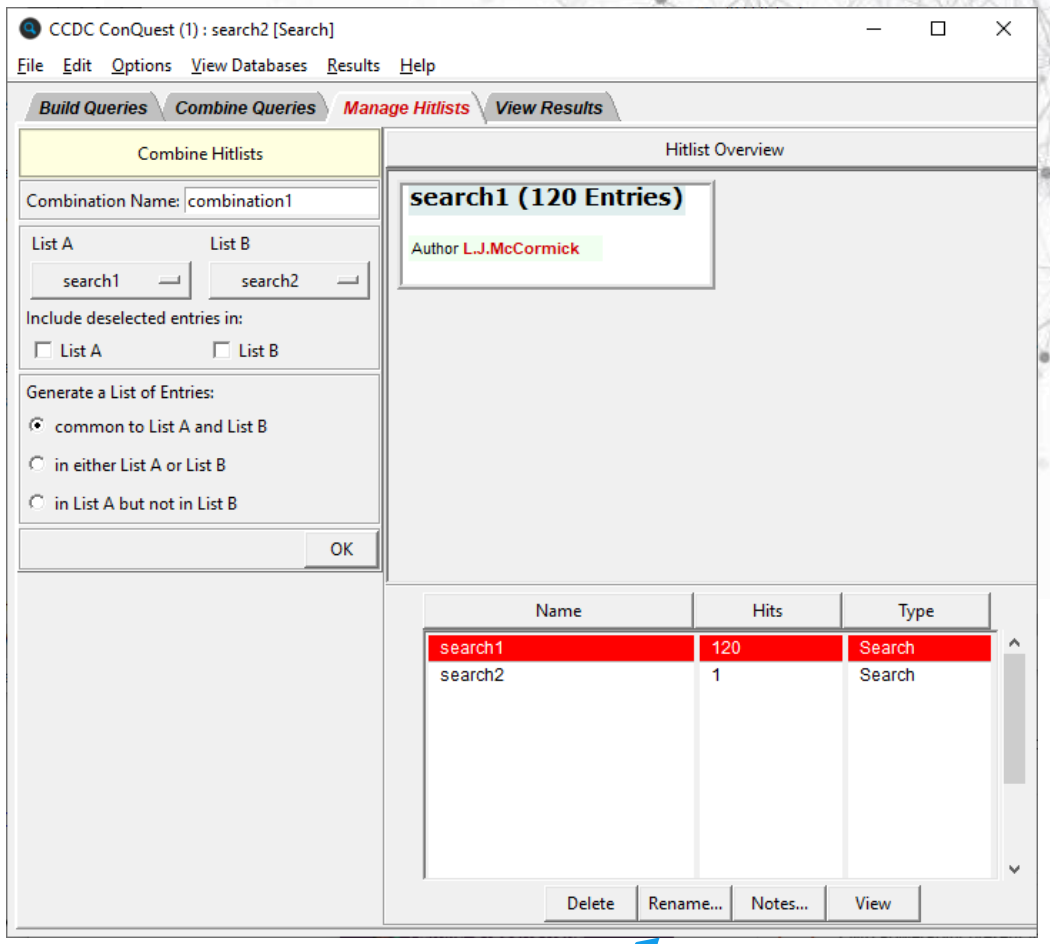
Storing and searching





Combining queries and managing hitlists





Tip - You can rename a search

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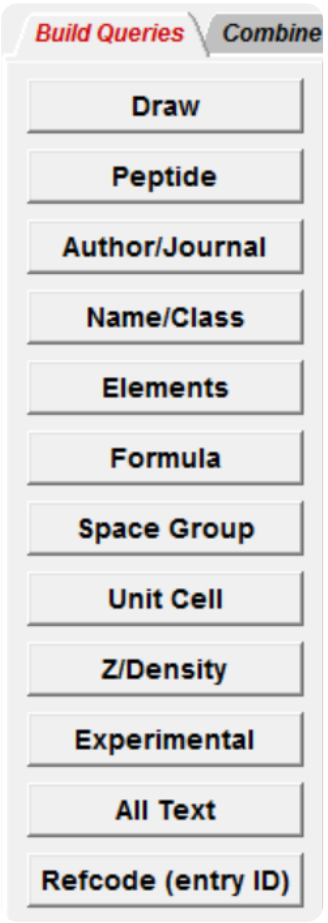
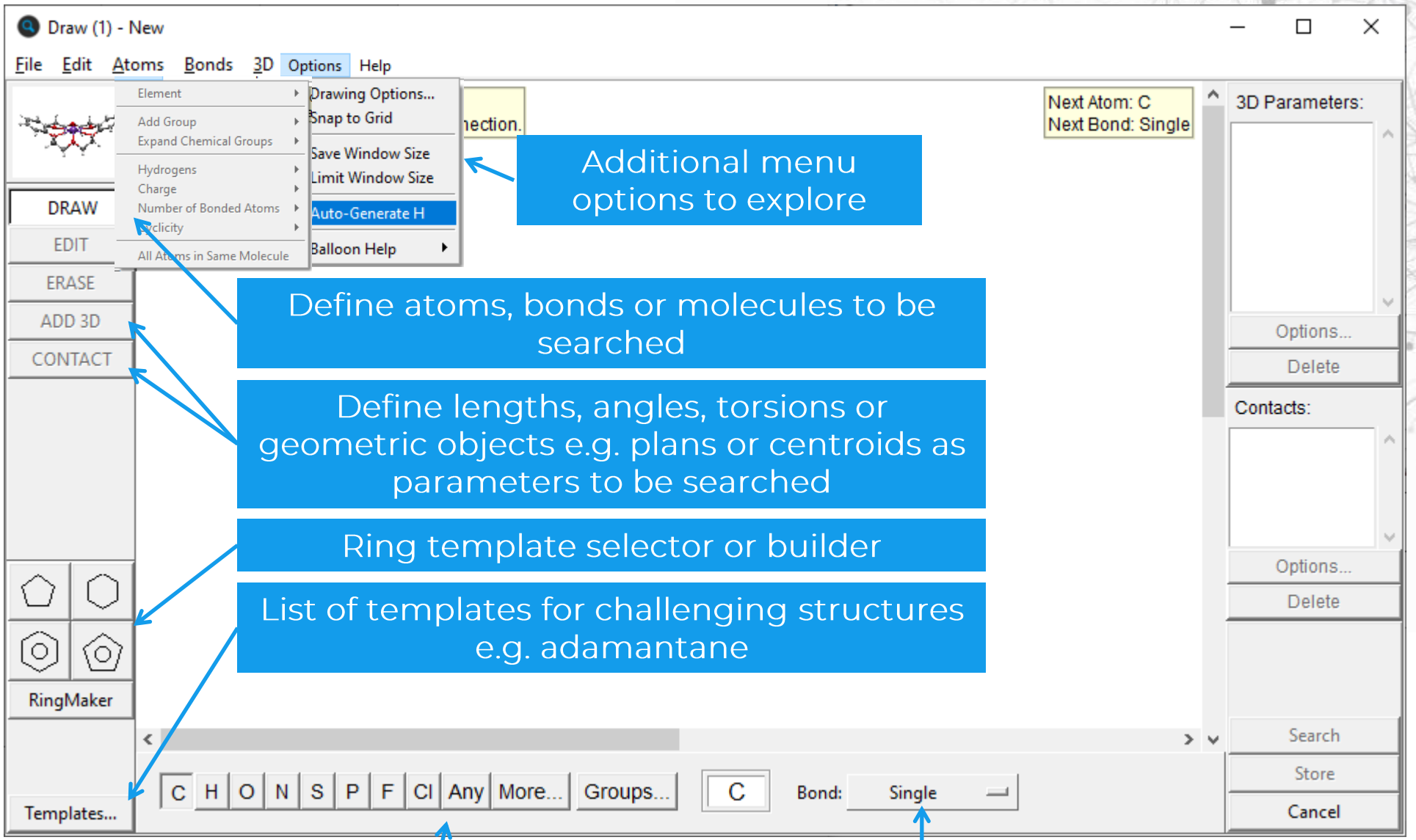
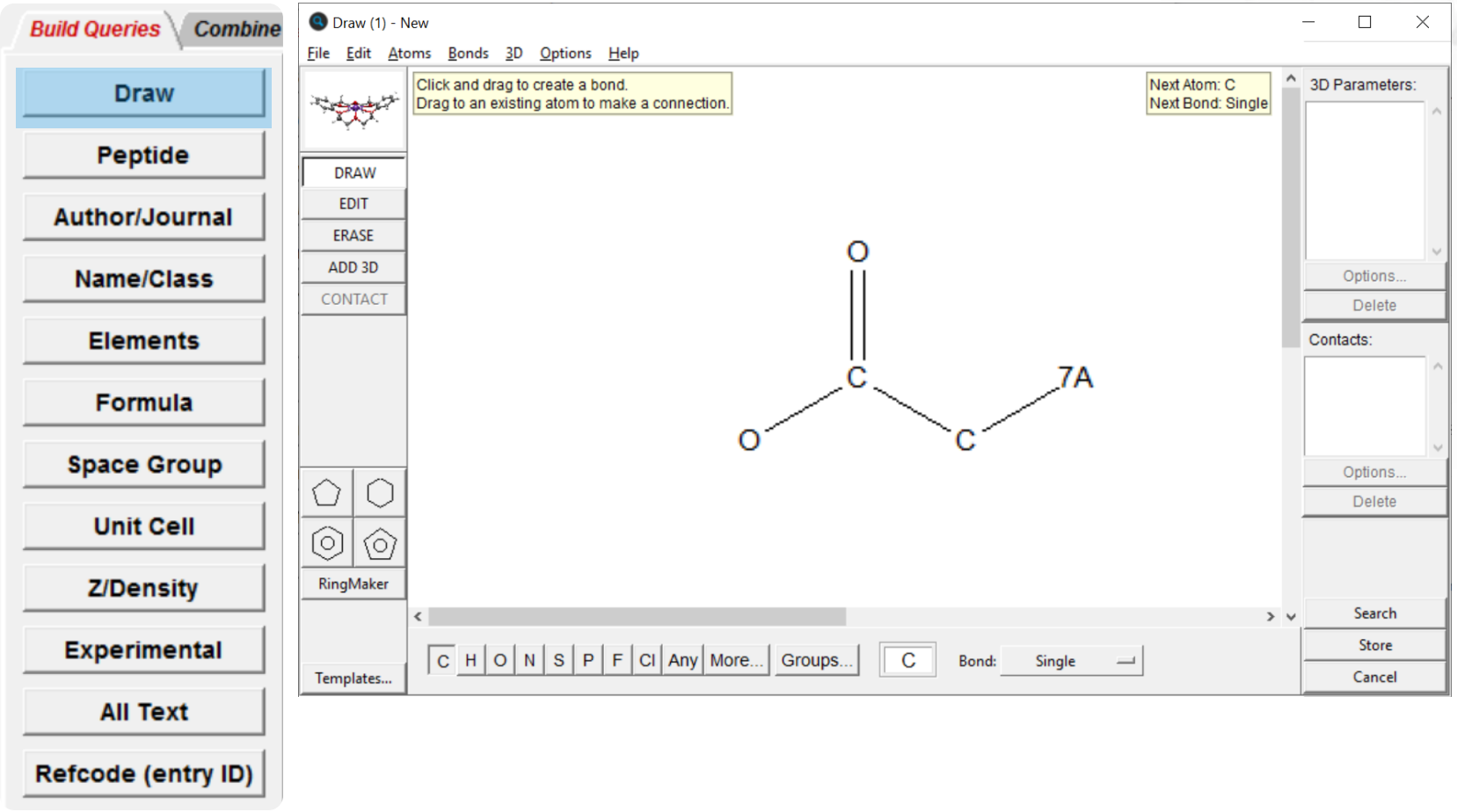
Draw

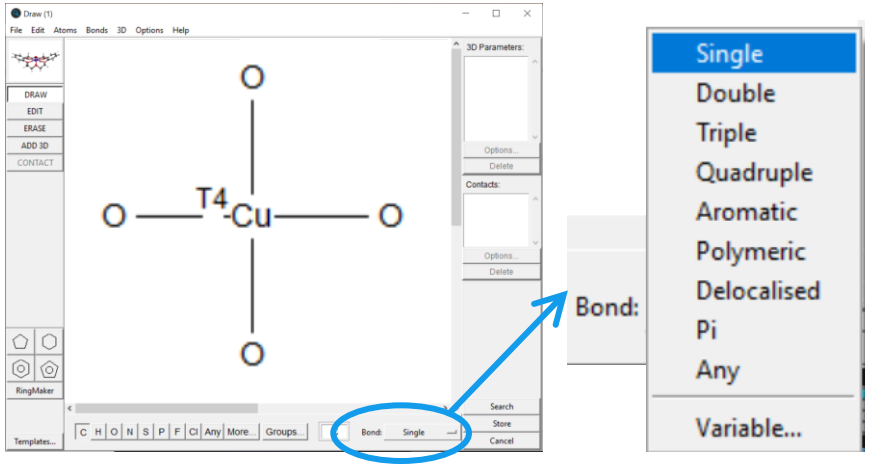

Build Queries
Combine
Draw
Peptide
Author/Journal
Name/Class
Elements
Formula
Space Group
Unit Cell
Z/Density
Experimental
All Text
Refcode (entry ID)

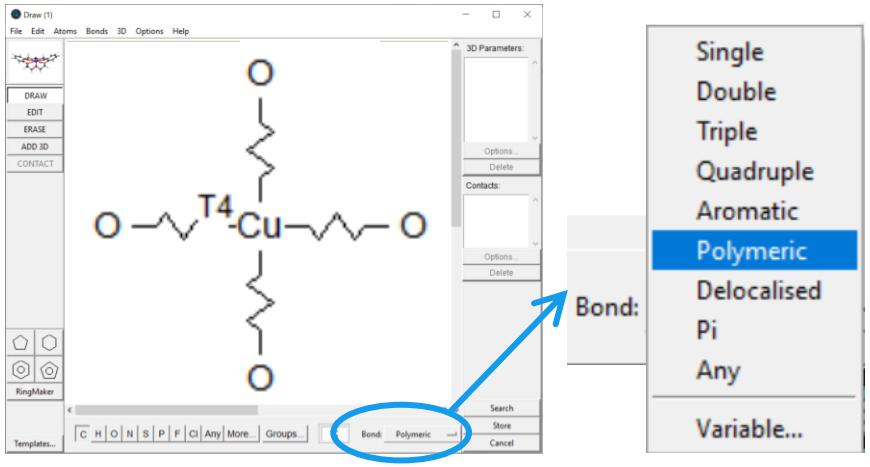

Draw (1) - New
File
Edit
Atoms
Bonds
3D
Options
Help
Element
Add Group
Expand Chemical Groups
Hydrogens
Charge
Number of Bonded Atoms
All Atoms in Same Molecule
Drawing Options...
Snap to Grid
Save Window Size
Limit Window Size
Auto-Generate H
Balloon Help
DRAW
EDIT
ERASE
ADD 3D
CONTACT
RingMaker
Templates...
Next Atom: C
Next Bond: Single
3D Parameters:
Options...
Delete
Contacts:
Options...
Delete
Search
Store
Cancel
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. plans 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

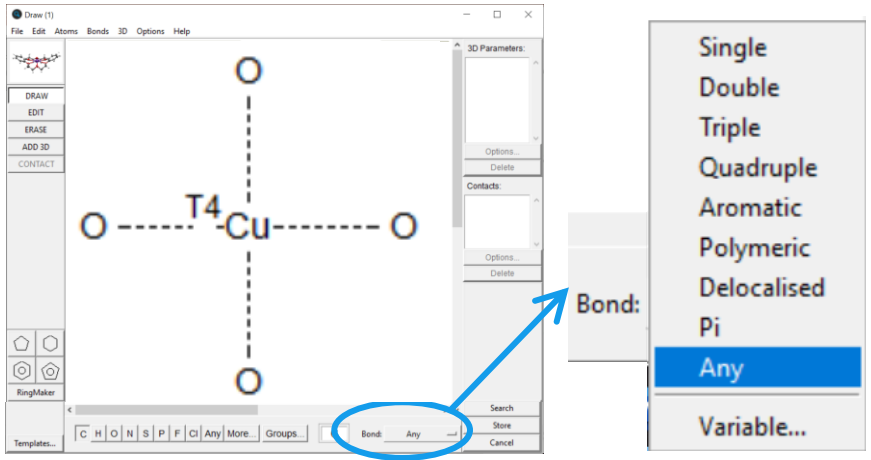
ConQuest – Draw/Structure search



Example of a search, where 7A represents any halogen







Using “Any” bond can help find more complicated structures such as polymers, delocalised and pi-bonded systems

Substructure found