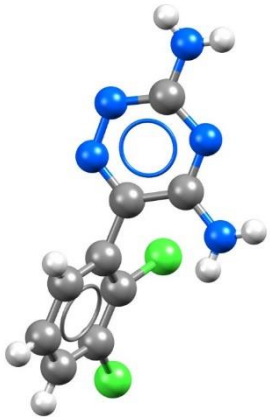
Searching and analysing molecular geometries using ConQuest and Mercury (CQ-006)

Developed using
2023.1 CSD Release
CSD version 5.44 (April 2023)



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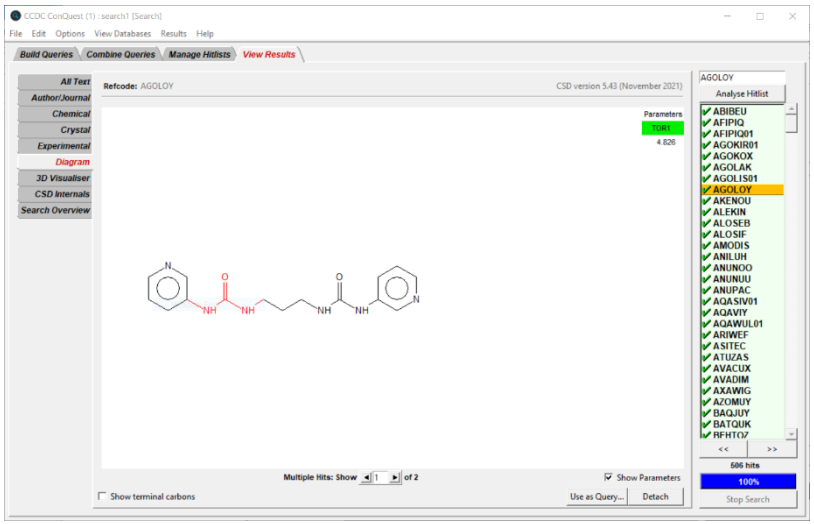
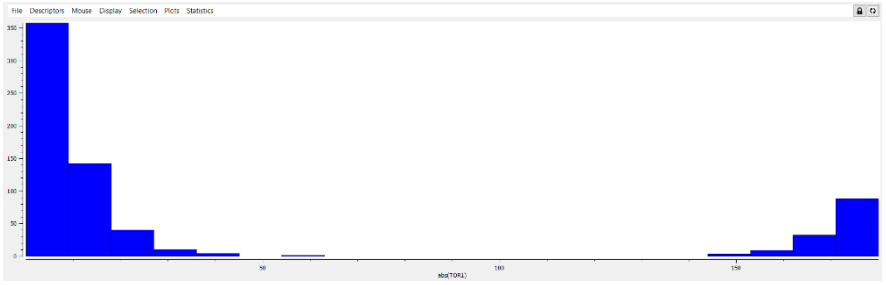
Introduction

ConQuest is the desktop search interface to the Cambridge Structural Database (CSD). All textual, numeric and structural data stored within the CSD can be searched using ConQuest. ConQuest provides an extensive range of flexible search options including searching based on compound name, formula, elemental composition, and literature search to name a few. The data from structures in the CSD can be used to show the most likely values a particular bond, angle, *torsion* or ring would adopt. This information can be included in the ConQuest search parameters with further analysis carried out in Mercury.

Before beginning this workshop, ensure that you have a registered copy of CSD-Core or CSD-Enterprise installed on your computer. Please contact your site administrator or workshop host for further information.





Learning Outcomes

After completing this workshop, you will be able to:

- Add 3D parameters in your ConQuest search.
- Use the data analysis function in Mercury.
- Explore conformation using ConQuest search results.

This workshop will take approximately **30** minutes to be completed. The words in *Blue Italic* in the text are reported in the Glossary at the end of this handout. A review of the ConQuest interface is also at the end of this handout.

Pre-required Skills

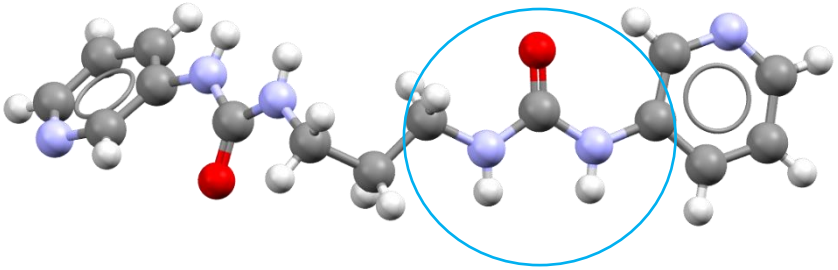
The following exercises assume you have a working knowledge of the programs ConQuest and Mercury, namely, how to conduct basic structural search in ConQuest and how to display and manipulate structures in Mercury. You can find the basics of visualization in Mercury as a CSDU module or as a self-guided workshop in the CSD-Core workshop area on our website. You can also find ConQuest workshops in the CSD-Core workshop area.

Materials

There are no additional materials required for this workshop.

Urea conformation in the CSD

There are over 1.2 million structures in the CSD providing a wealth of structural data. Structural chemists can use tools in the CSD portfolio to validate the three-dimensional conformation of a particular molecule or to verify the most observed conformer for a molecule. There are a couple of ways to explore conformation in the CSD, including Mogul Geometry Check. However, in this workshop, we will explore how to define parameters of interest in a ConQuest search and analyse the results using the data analysis tool in Mercury. We will investigate the preferred *conformation* of a urea in the CSD.



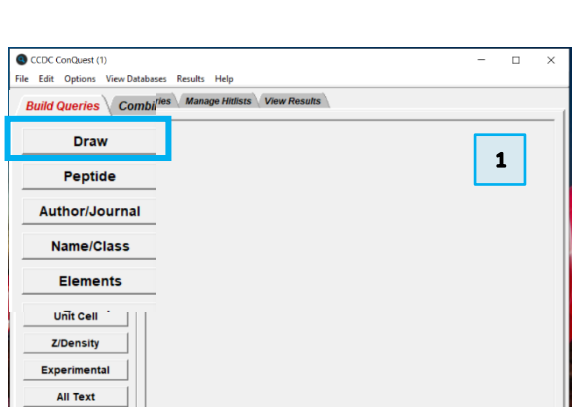
N,N”-propane-1,3-diylbis(3-(3-pyridinyl)urea) molecule, refcode AGOLOY with the urea substructure highlighted

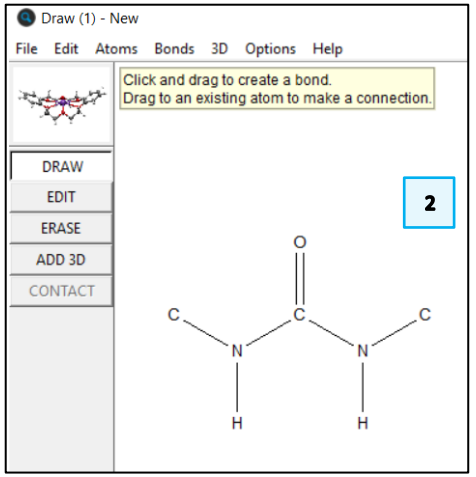
1. Launch ConQuest by clicking the ConQuest Icon on your desktop or launching it from the Start or Applications menu Open the sketcher by clicking the **Draw** button.

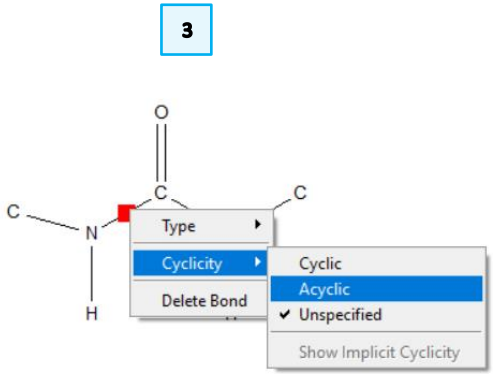
2. Sketch the urea molecule, if you need a refresher on how to sketch, a review of the ConQuest interface is at the end of this handout.

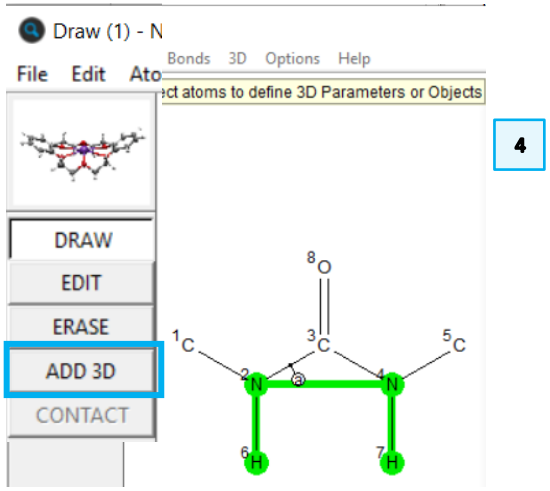
3. We want to omit rings in the dihedral angle of interest to limit our results to ureas. Right-click on the C-N bond and click on **Cyclicity** and select *Acyclic*.

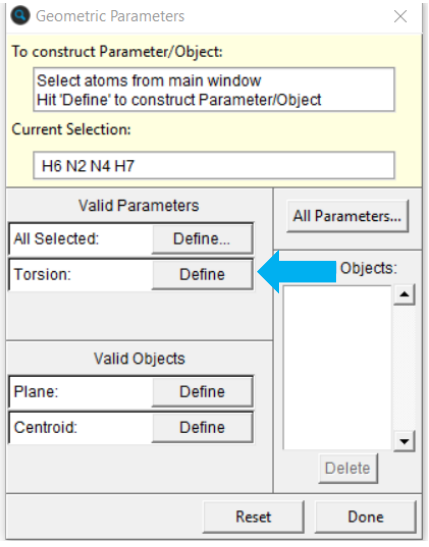
4. Now we define the dihedral angle of interest. Click on **ADD 3D** to launch the Geometric Parameters window. Select the H-N-N-H angle in order and click **Define** next to Torsion. Since signs of individual torsion angles can be ignored, we can use the Apply Function option to take the absolute value of the angles.

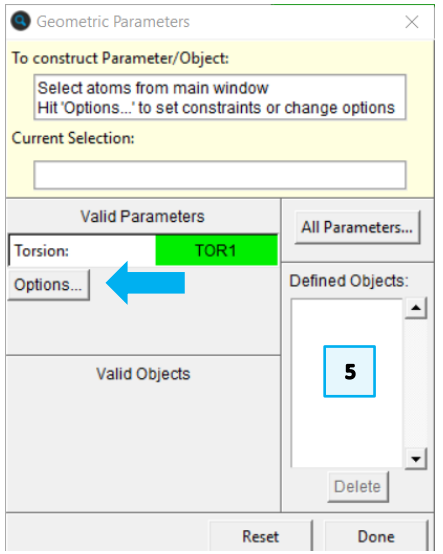




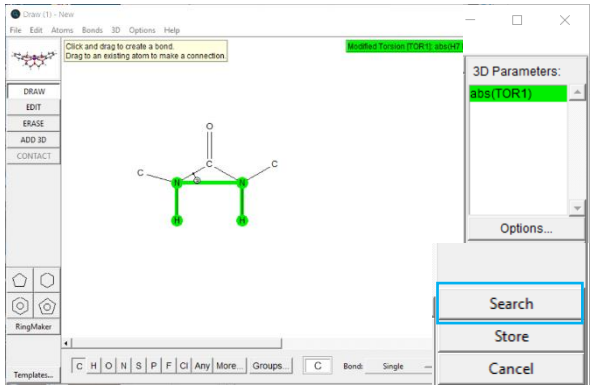






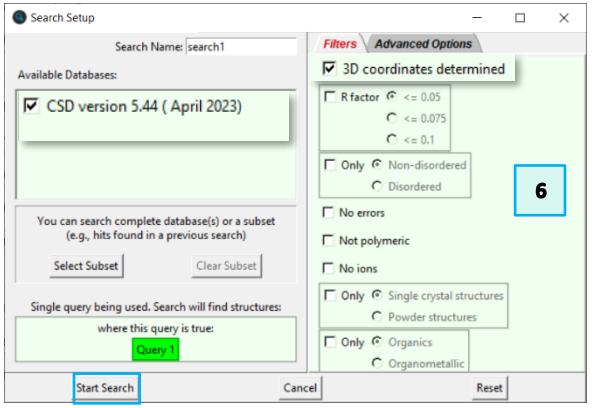


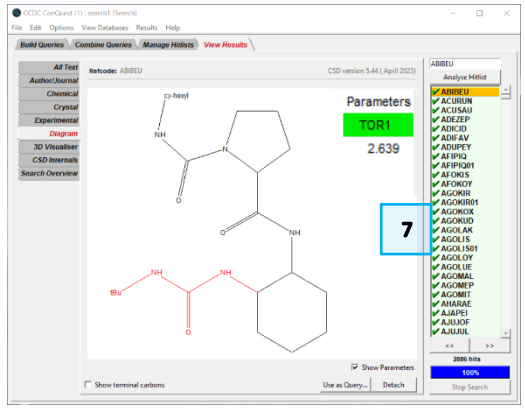
5. In the Geometric Parameters window, click on **Options** under TOR1 to launch the 3D Limits and Options window. In the *APPLY FUNCTION* drop down menu, select **Absolute** and click **OK** and click **Done** in the Geometric Parameters windows. You should be returned to the Draw window with the abs(TOR1) parameter defined. We are now ready to conduct our search. Click Search to launch the Search Setup window.



6. We want to search the entire database for structures that match our sketched substructure. In the *Search Setup* window, make sure to tick the box for "3D coordinates determined". Click **Start Search** to begin the search.

7. There should be at least 2886[1] structures returned. Note that the value for the torsion angle parameter you defined is shown in the upper right corner of the *View Results* tab. You can use the arrow keys to scroll through the refcodes to investigate the hits returned by this query.

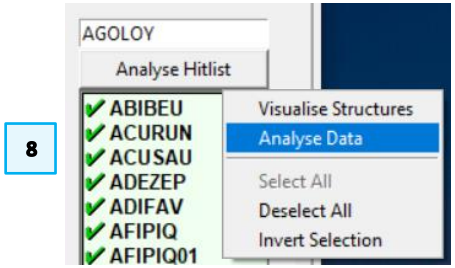


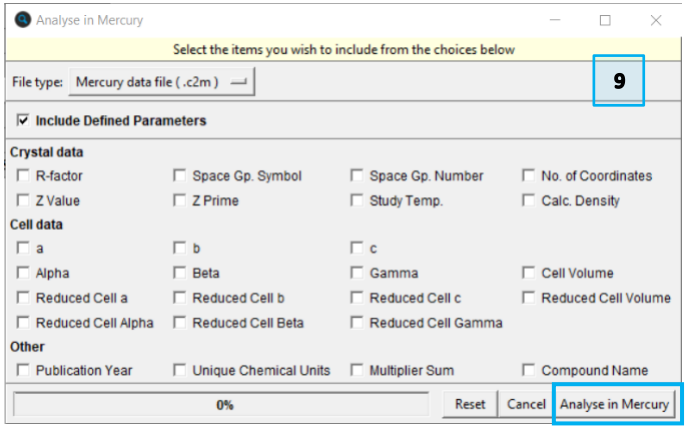


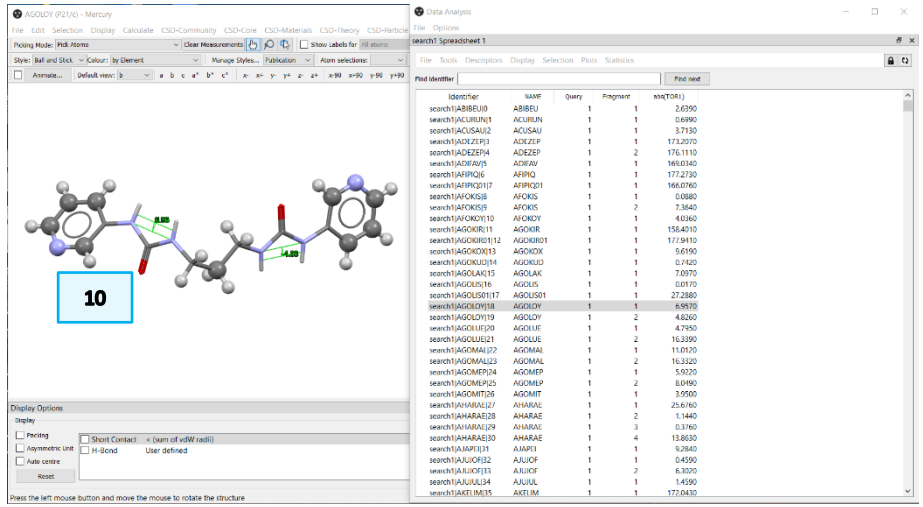
8. We can use Mercury's **Data Analysis** module to further analyse the data. To launch this, click the **Analyse Hitlist** button and choose *Analyse Data* from the drop-down menu.

9. If you are interested in analysing other parameters, you can tick them off in the dialogue box that appears. We will skip this step for now. Simply click **Analyse in Mercury.**

10. This will launch the Mercury app with the refcode list loaded and the **Data Analysis** window. The **Data Analysis** window is often hidden behind the main Mercury app, so you may have to minimise Mercury to see it.







[1] As of version 2023.1 of the CSD.

Data Analysis in Mercury.

Now that you have performed the search and obtained the torsion angle parameter, we can use the data analysis module in Mercury to visualize the values.

1. Look at the **Data Analysis** window. This shows all the data from your defined geometric parameter, sorted by refcode.

2. To view the distribution of torsion angles in this hitlist, click the ***abs(TOR1)*** header in the column to highlight the column, then click *Plots* from the top menu and then select *Histogram.*

3. Most of the urea containing structures in the CSD adopt a cis conformer. Click on the bar of the histogram around 0 degrees to highlight the corresponding entries in the spreadsheet.

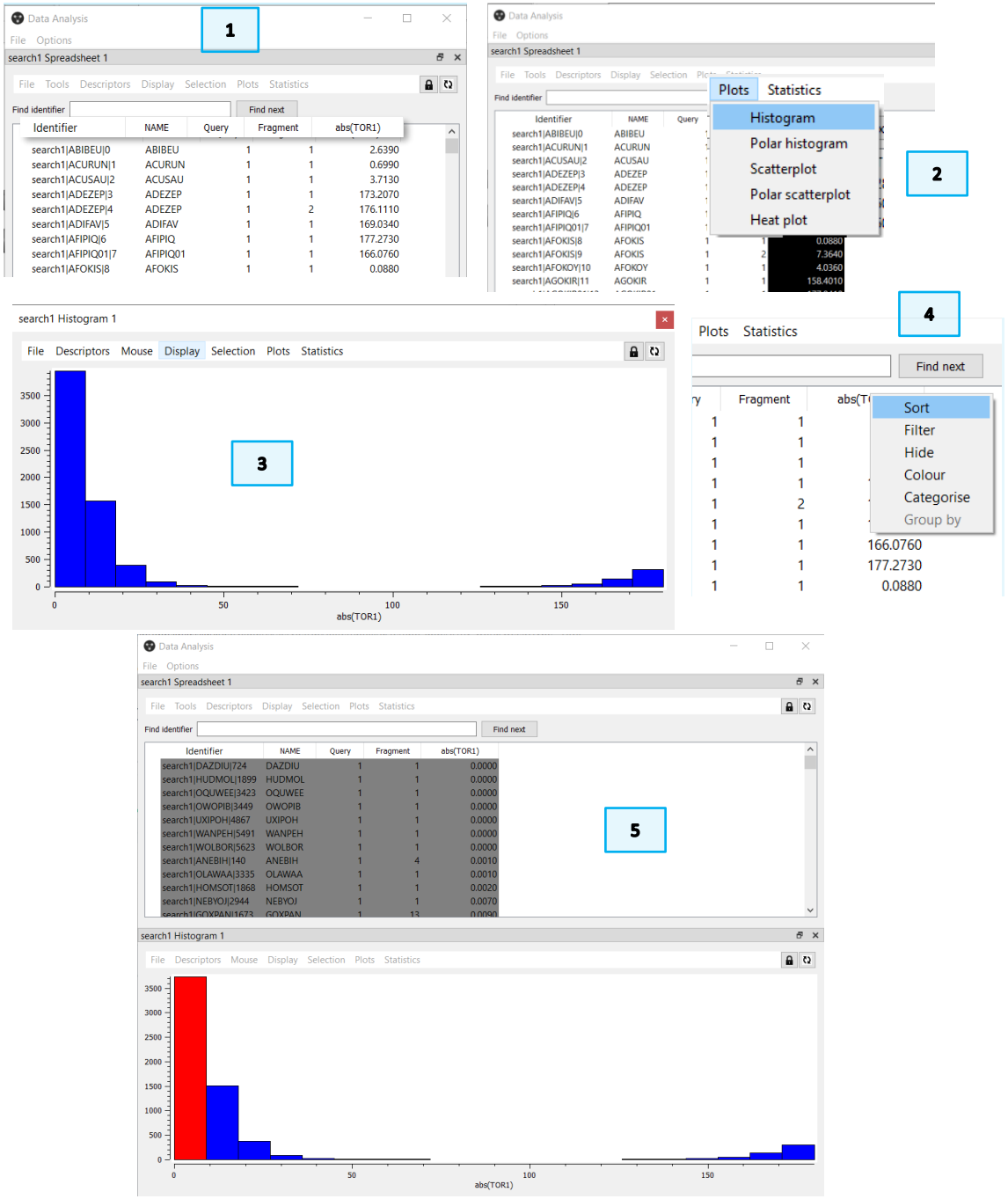
4. It will be easier to scroll through the refcodes in that region by sorting the spreadsheet by abs(TOR1). Right-click on the **abs(TOR1)** heading and click *Sort*.

5. You should now see the highlighted refcodes in the spreadsheet that correspond to the angles clustered around 0 degrees. Clicking on each entry in the spreadsheet will place the corresponding structure in the Mercury display.

6. As you scroll through the highlighted refcodes, can you observe a trend in the structures clustered here? Review some of the structures in the 150 – 180-degree cluster (trans conformers).

Conclusion

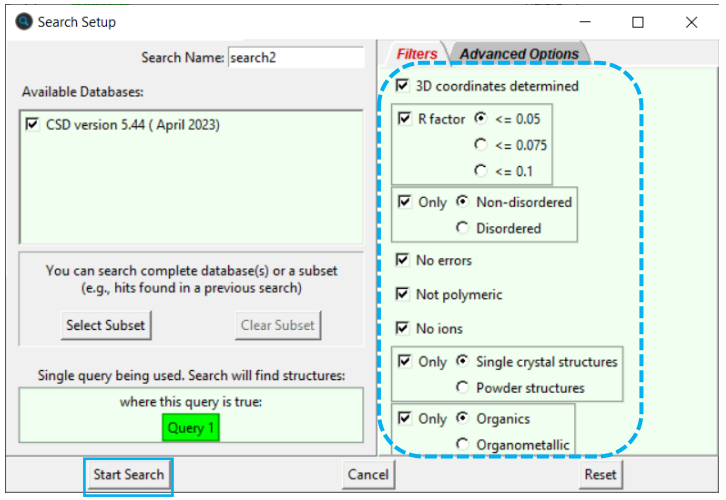
From the search of the CSD and plotting the results, we can see that the most observed conformer for urea in the CSD is the cis conformer.



Exercises

In the example above, we conducted a search of the entire database. How could the distribution of our histogram change if we defined a narrower search?

- Return to the ConQuest, using Query 1, include all the filters in the Search Setup window.
- Use the data analysis module in Mercury to create a histogram on your torsion angles. How does this distribution differ from our initial search?

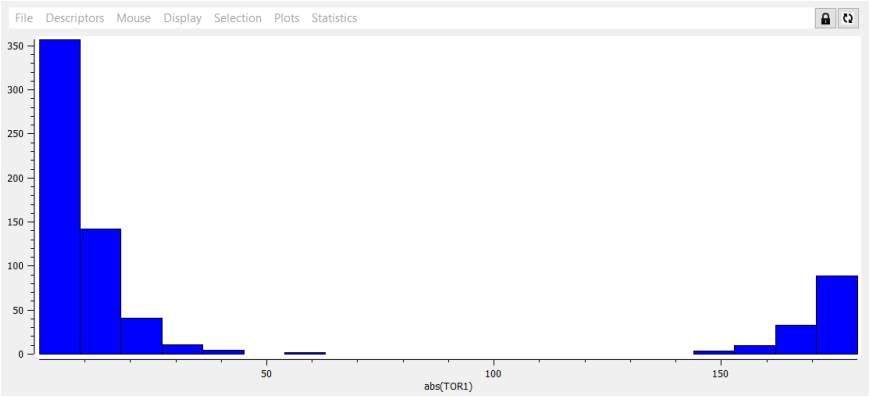


Summary

This workshop introduced how to use ConQuest searches and data analysis in Mercury to review conformation of a specific molecule.
In the example you have seen how to add 3D parameters to your query to mine the CSD for even more structural information. The data analysis window allows you to plot your data in a variety of ways, determine statistics on your datasets, and to perform calculations on the values of the parameters returned by the search.

You should now be familiar with:

- Adding 3D parameters in your search.
- Conducting data analysis in Mercury.



Next Steps

After this workshop, you can explore more exercises in the self-guided workshops available in the CSD-Core (ConQuest) and CSD-Materials (Mercury) workshops area on our website.
https://www.ccdc.cam.ac.uk/community/training-and-learning/workshop-materials/ . Please see the ConQuest documentation for more details.

Feedback

We hope this workshop improved your understanding of ConQuest and you found it useful for your work. As we aim to continuously improve our training materials, we would love to get your feedback. Click on this link to a survey, it will take less than **5** minutes to complete. The feedback is anonymous. You will be asked to insert the workshop code, which for this self-guided workshop is CQ-006. Thank you!

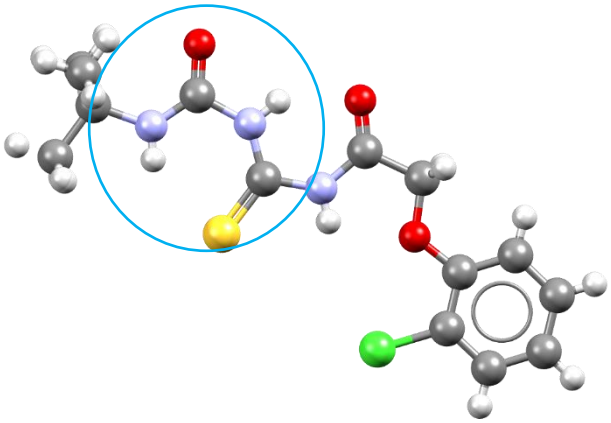
Glossary

Conformation

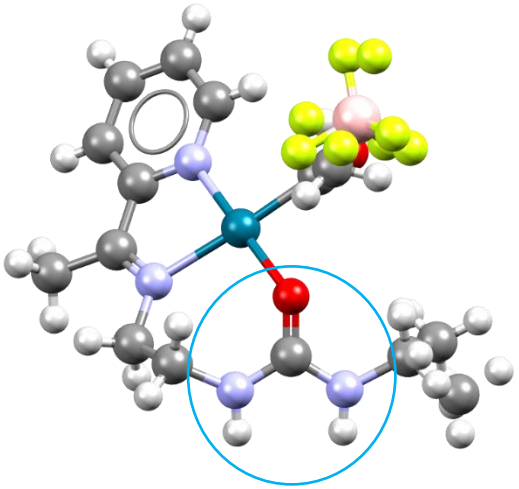
The shape, or more precisely, the spatial arrangement of a molecule is called conformation. The same molecule can present different conformations (different shapes).

Torsion Angles

Torsion angles are used to describe conformations around rotatable bonds. The torsion angle between 4 atoms A-B-C-D is the angle by which the vector A-B must be rotated in order to eclipse the vector C-D when views along the vector B-C.



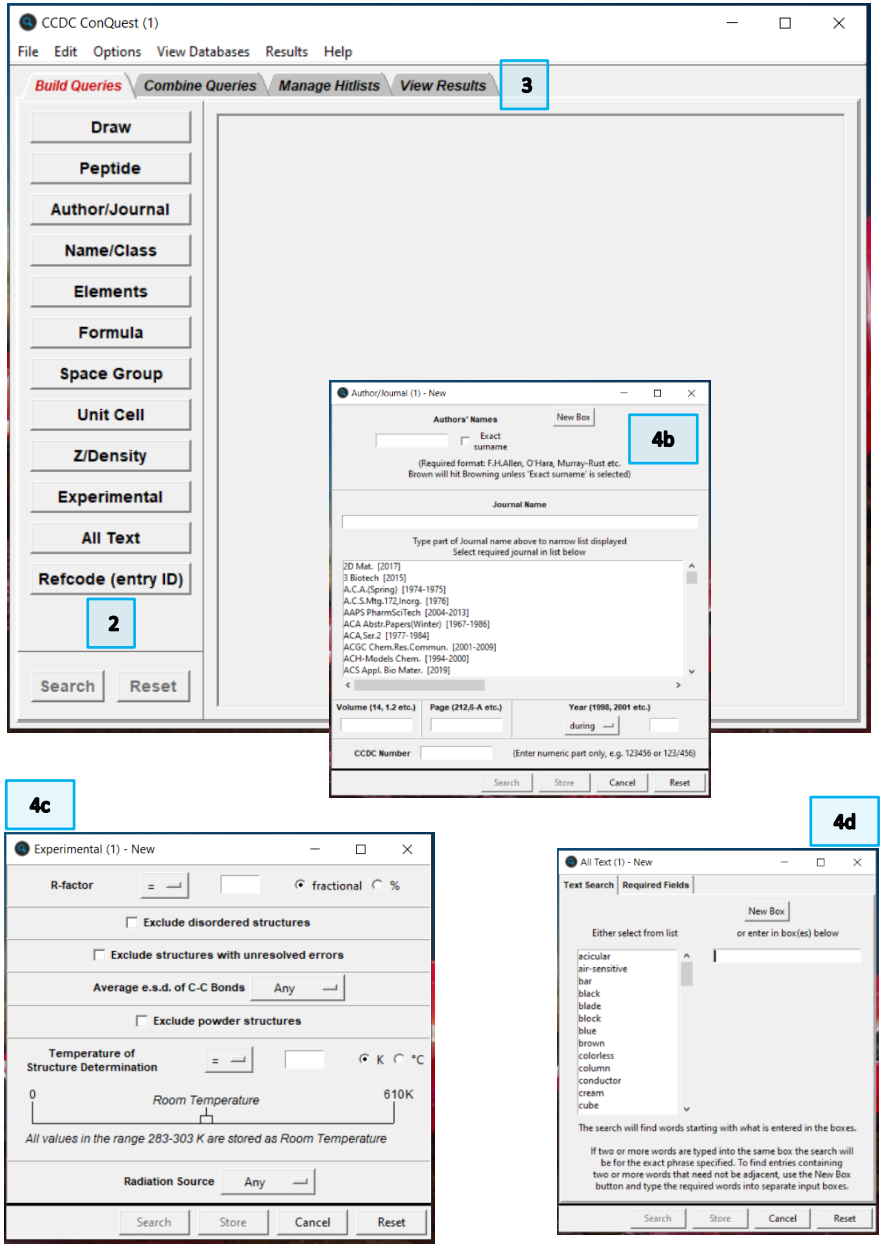
N-t-Butylaminocarbonyl-N-2-chlorophenoxyacetylthiourea structure (refcode LIDCEH) with the urea substructure in a trans conformation highlighted



(acetyl)-(1-(2-(1-(pyridin-2-yl)ethylideneamino)ethyl)-3-ethylurea)-palladium(ii) tetrafluoroborate structure (refcode, DEDDUM) with the urea substructure in a cis conformation highlighted

Review. ConQuest Interface

1. Launch ConQuest by clicking the ConQuest Icon on your desktop or launching it from the Start or Applications menu.
2. The ConQuest main window shows all the search routines you can perform on the left-hand side of the window.
3. The row of tabs across the top of the window will guide you through the steps of the search process.
4. Some example searches are
    a. Draw – substructure and 3D information searching
    b. Author/Journal – bibliographic searching
    c. Experimental – experimental set up searching
    d. All Text – generic text-based searching
5. The majority of the searching we will do in these tutorials will be substructure searching, so we will focus on the Draw tab here.



Review. Draw Window

All drawing takes place in the central white area of the *Draw* window. In addition to creating 2D chemical structure sketches, the *Draw* window allows for the inclusion of 3D parameters for searching or for filtering.

ConQuest sketching conventions

- Left click in the sketcher to insert the selected atom type
- Left click and drag to sketch two bonded atoms
- Use the **Edit** button to modify properties of or delete atoms, bonds or entire substructures
- Right-click on atoms or bonds to modify their properties
- Use the **Templates…** button to pick from a list of CSD editor devised and drawn substructures
- Use the **More…** button to find less frequently used element types, or generic atom type groups (e.g. halogens), or define custom element combinations (e.g. C or N or O).