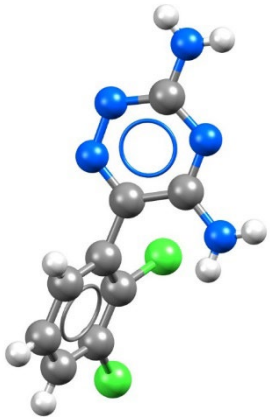
Measuring and Calculating Objects in Mercury

MER-005

2022.3 CSD Release



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Introduction

Mercury is the visualisation and analysis software of the Cambridge Structural Database (CSD). Mercury is used in investigating and analysing crystal structures with features that allows a user to generate packing diagrams, display and asses the strength of intermolecular interaction networks, calculate and display voids, create BFDH theoretical crystal morphologies and more (features availability subject to appropriate licence). With Mercury you can visualise 3D structures from the CSD as well as your own. You can also produce high-quality publication-ready images, frames for videos, and 3D print files.

Before beginning this workshop, ensure that you have installed Mercury. Please contact your site administrator or workshop host for further information.

Learning Outcomes

In this workshop we will learn about analysis tools in Mercury, specifically we will learn how to:

- Measure distances, angles and torsions.
- Calculate and display centroids and planes.

This workshop will take approximately **25 minutes** to be completed.

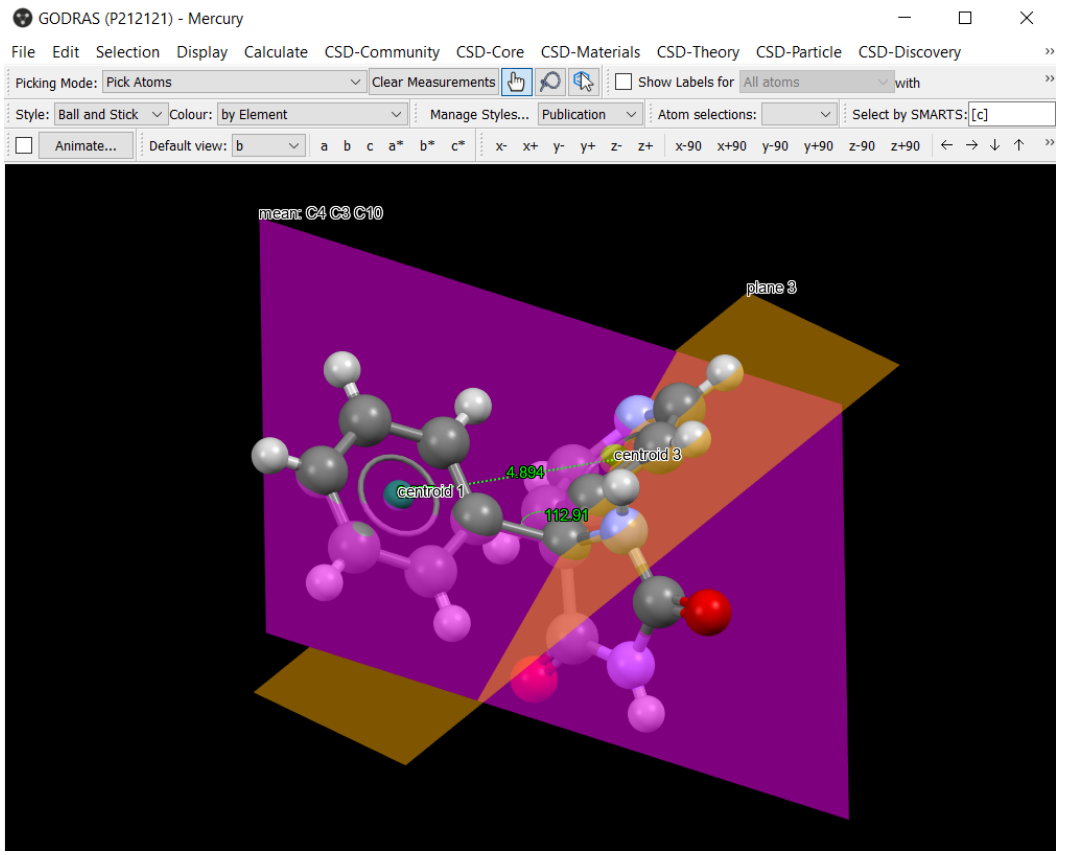
Note: The Glossary at the end of this handout contains useful terminology for the exercises.

Pre-required Skills

To complete this workshop, you would need to be comfortable with basics of Mercury visualization, including navigating the Mercury interface, editing styles and colours, and displaying packing diagrams. If you are not, we recommend the Structure Visualization Workshop (MER-001), available on this page.

Materials

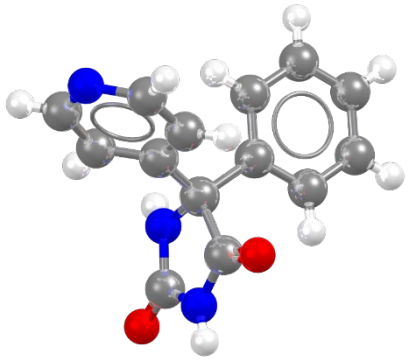
There are no additional materials required for this workshop.



Example 1. Measuring Distances, Angles and Torsions

Mercury's analysis features include the tools to measure distances, angles, and torsions among atoms and other user-defined objects, such as centroids and planes.

In the following exercises, we will learn how to measure distances, angles, and torsions between bonded and non-bonded atoms, how to calculate and display centroids and planes, and how to use them for measurements.



*High-resolution image of 5-(4-pyridyl)-5-phenylhydantoin (refcode: **GODRAS**).*

This example will show you how to measure distances, angles, and torsions for a molecule in Mercury.

1. Open Mercury by clicking the desktop icon, or launching from the Start menu, Launchpad (macOS) or command line (Linux).

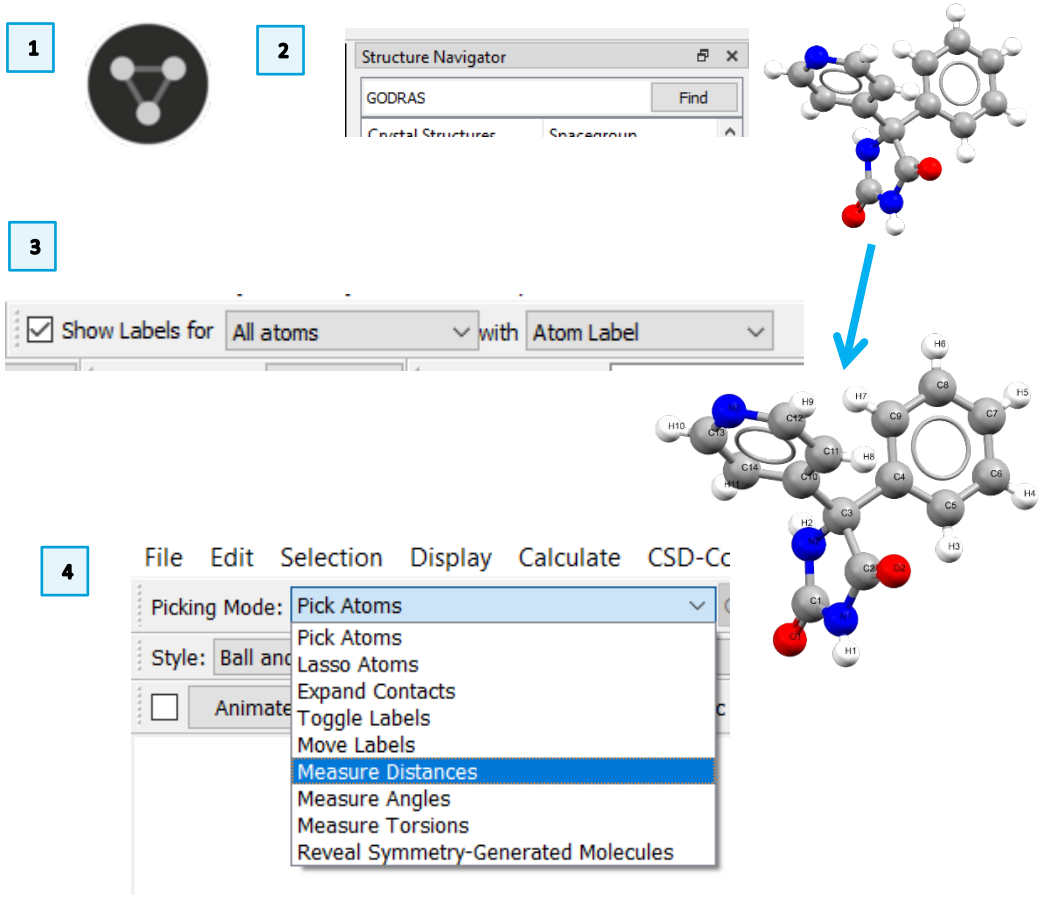
2. Type the refcode **GODRAS** in the **Structure Navigator** toolbar to load the structure of theophylline into the viewer.

3. To better identify atoms, you can add labels by ticking *Show Labels for* at the top right of the Mercury window. Adjust the options as needed.

4. To measure distances, we need to change Picking Mode (top left) to *Measure Distances*. You will notice that the cursor has now a "plus"-shape.

5. You can now measure the length of a bond by clicking on two bonded atoms. In this example we click on atom C3 and then atom C4. You can see the value of the length appearing on the bond. The unit is Angstrom. The distance between C3 and C4 in GODRAS is 1.533 Å.

6. You can measure more bonds lengths by repeating **Step 5** on other pairs of bonded atoms.



7. You can measure the distance between any two atoms by clicking on them as in **Step 5**. In this example, we measure the distance between C4 and C10. The measurement, in this case, appears above a dotted line. The distance between C4 and C10 is 2.551 Å.

8. To measure the distance between other pairs of non-bonded atoms, simply repeat **Step 5**.

9. To remove these measurements, right click on a measurement and select *Clear All Measurements*. You can clear individual measurements by selecting Delete Measurement instead.

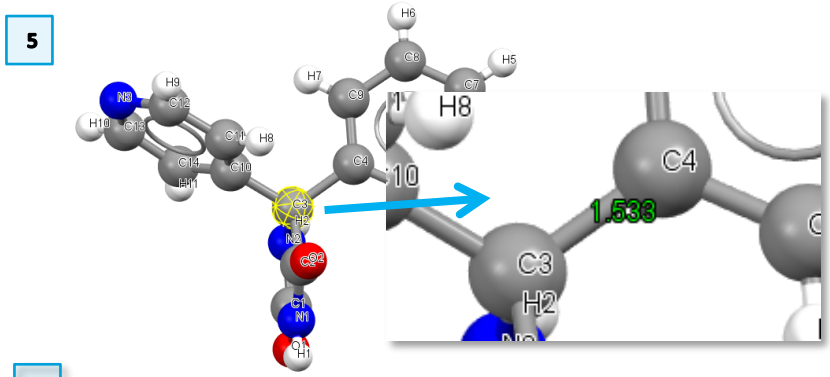
10. We will now move to measuring angles. To do so, from *Picking Mode* select *Measure Angles*.

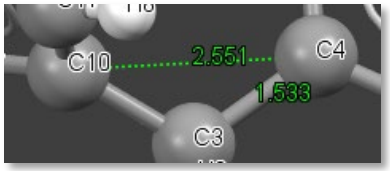
11. To measure an angle between bonded atoms, click on three consecutive atoms. In this example, we measure the C10-C3-C2 angle by clicking on them in this order. The angle's value appears in green over the central atom, and the angle is highlighted with a dotted arch. The value of the C10-C3-C2 is 108.07° in degrees.

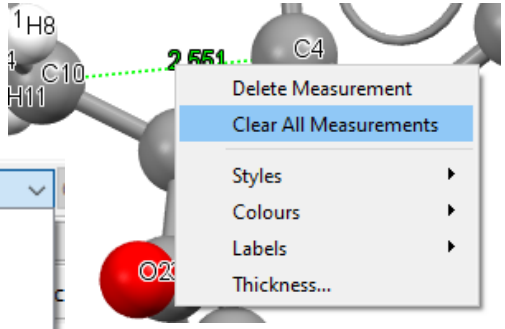
12. As with measuring distances, you can measure angles also among non-bonded atoms. To do so, simply select three atoms in the appropriate order. In this example, we measure the C2-N2-C10 angle by clicking on the atoms in this order. The value of the angle is 62.32°.

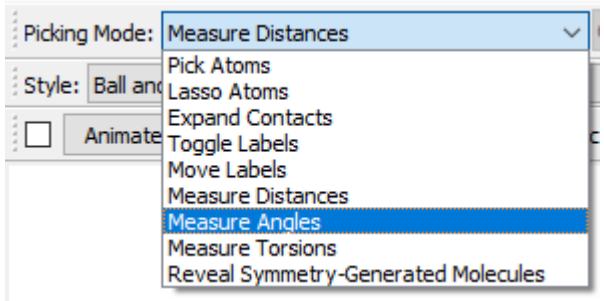
13. You can measure more angles by repeating **Step 11** on other groups of three bonded atoms.

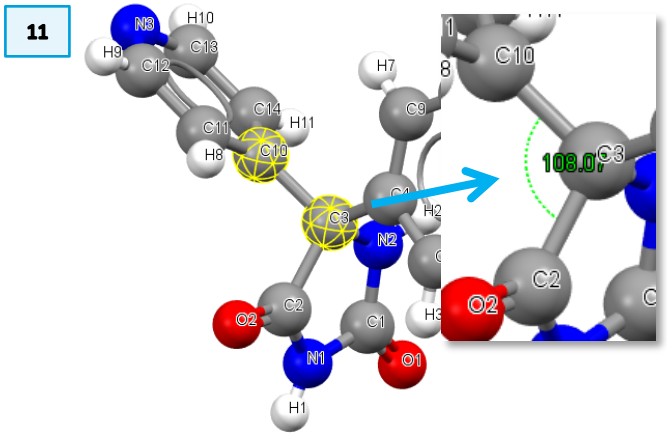
14. To delete all measurements, repeat **Step 9**.

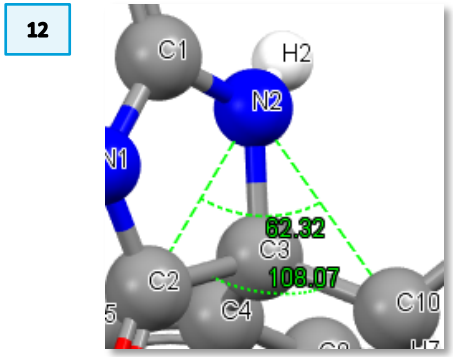












15. Next, we are going to measure torsional angles. To measure dihedrals, or torsion angles, we need to change *Picking Mode* to *Measure Torsions*.

16. In this case, we will need to select four atoms in the correct order. As with distances and angles, torsion angles can be measured for both bonded and not bonded atoms. We will see an example for each case. To measure the torsion between atoms N2, C3, C4, C5, select them in this order. The two planes employed for the calculations are represented by green squares and the measurement appears in green. Units are degrees. The N2-C3-C4-C5 torsion is -76.03°.

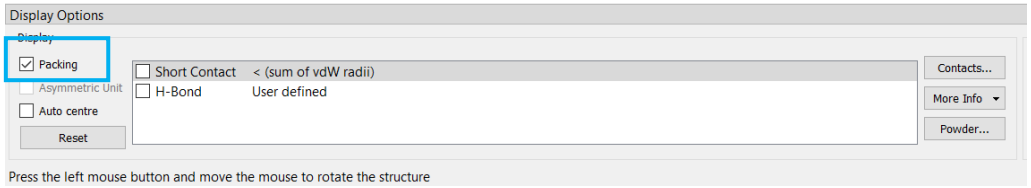
17. Repeat the procedure in **Step 16** for a group including non-bonded molecules, for example C1-N1-C3-C5. The C1-N1-C3-C5 torsion is -98.55°.

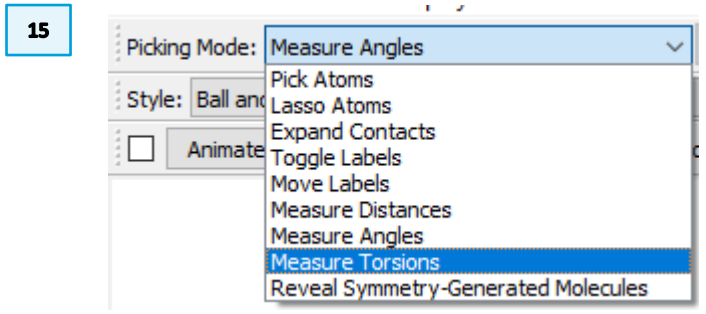
18. To view these measurements in a table, click on *More Info* > *Torsions List…* at the bottom of the Mercury window. In the pop-up window you can see the measured torsion angles, and save them as a document (.tsv, .csv, and .txt formats available).

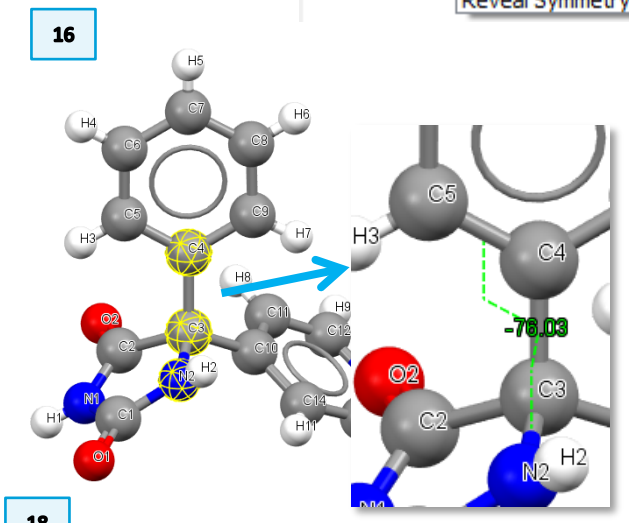
19. In this window you can click on *Distances* or *Angles* to visualize and save measurements of distances and angles. If you have cleared measurements along the way of this exercise, these tables will be empty.

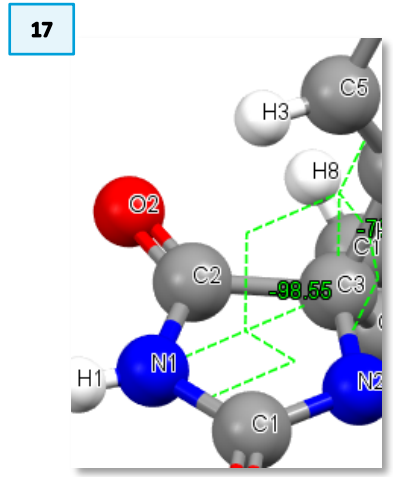
Tips and Tricks

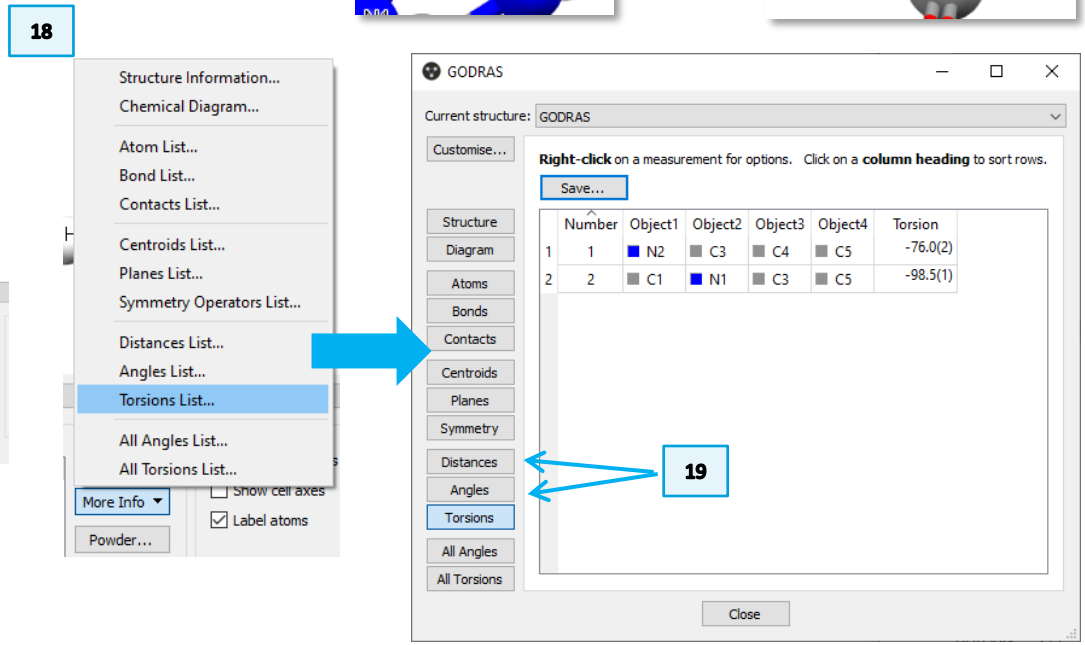
You can measure distances, angles, and torsions also for atoms not belonging to the same molecule. To try this, you will need to visualise more molecules. You can do so for example by ticking *Packing* in the *Display Options* toolbar. You can now repeat **Steps 4** & **5, 10** & **11,** and **15** & **16** for atoms belonging to different molecules.











Example 2. Calculating Centroids and Planes

In this example we will see how to calculate and display centroids and planes in Mercury and how it is possible to use them to measure distances, angles, and torsions.

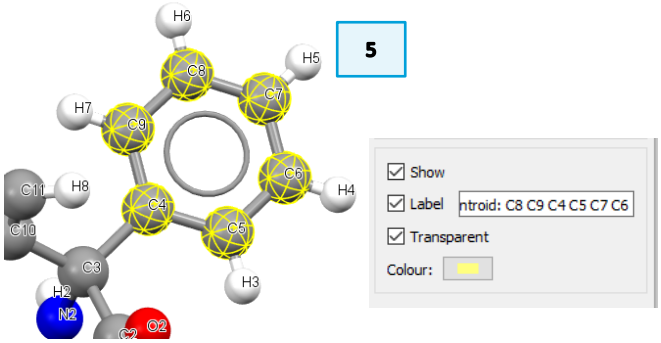
1. For Example 2, we will be using the same molecule as Example 1, i.e., **GODRAS**. Before proceeding with the rest of the exercise, make sure you clear all measurements following the directions in **Step 9** Example 1, and go back to the view as in **Step 3** above. In *Picking Mode* select *Pick Atoms*.

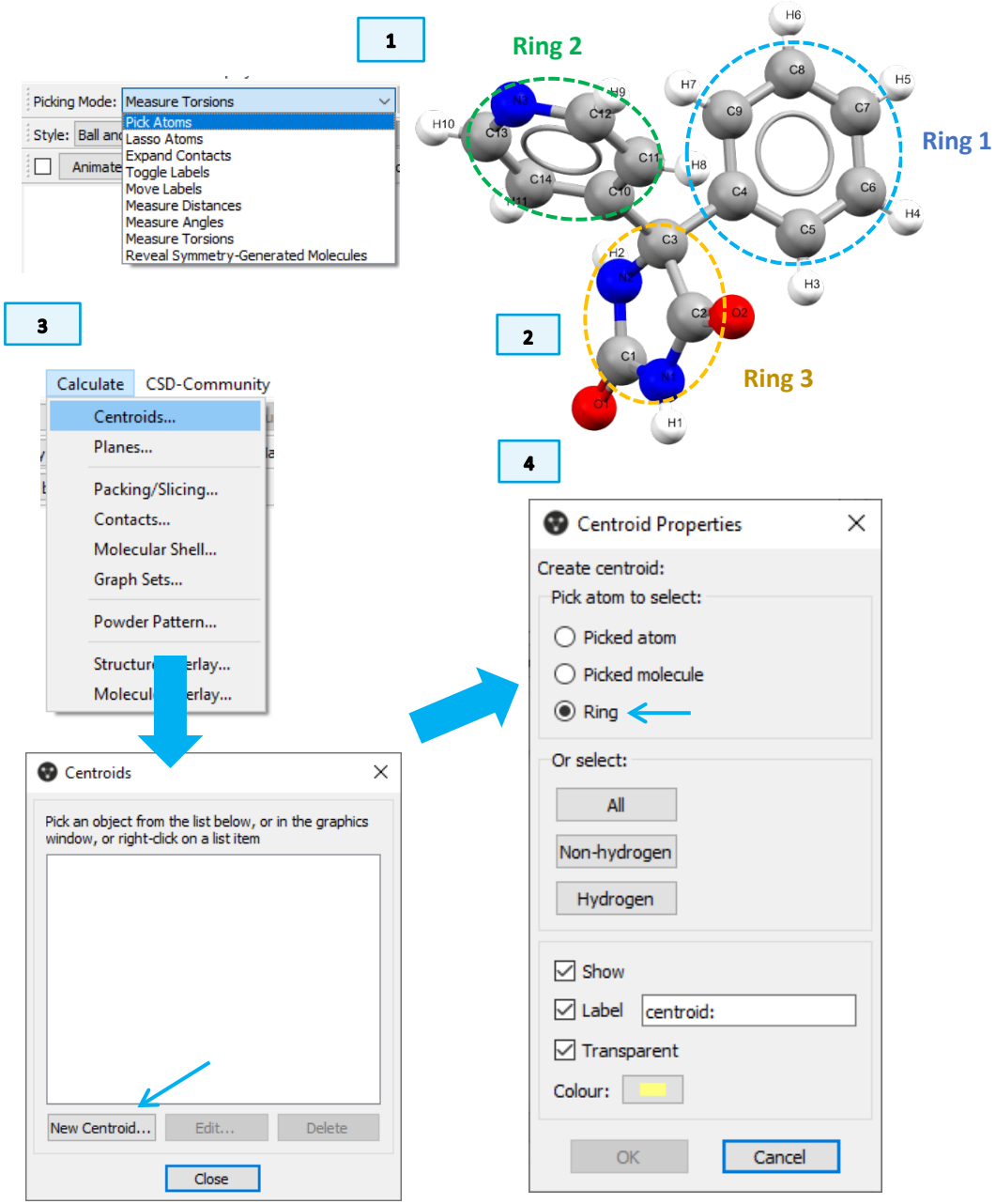
2. In this exercise, when referring to the three rings in this molecule, we will identify them as **Ring 1** = C4, C5, C6, C7, C8, C9; **Ring 2** = C10, C11, C12, N3, C13, C14; **Ring 3** = C1, N1, C2, C3, N2.

3. To calculate centroids, go to *Calculate > Centroids…* . In the *Centroids* window that appears click *New Centroid* to calculate our first centroid. This brings up another window with the *Centroids Properties*.

4. Our first centroid will be for **Ring 1**. In *Centroid Properties*, under *Create Centroid: Pick atom to select:* tick *Ring*. In this way by selecting one atom belonging to the ring we will be able to select the entire ring.

5. Now, on the Mercury interface, select one atom (any atom) belonging to Ring 1. You will see that the entire ring has indeed been selected. The *Label* in *Centroid Properties* now includes the labels of the atoms in Ring 1.





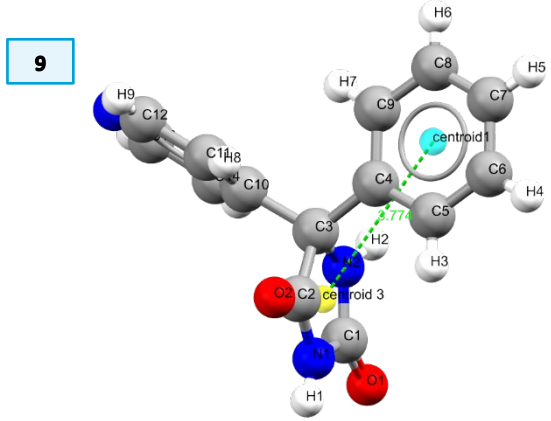
6. For clarity, change the *Label* in *Centroid Properties* to "*centroid 1*", and the *Colour* to blue (clicking on it, selecting the new colour, and then *OK*). When you are done, click *OK* to create the new centroid.

7. Centroid 1 has now been calculated and represented on the molecule. You can also find it listed in the window.

8. To calculate and display the centroid of **Ring 3**, repeat **Steps 3 to 6** selecting this time an atom from Ring 3. Edit the *Label* to *"centroid 3"* and the *Colour* to yellow.

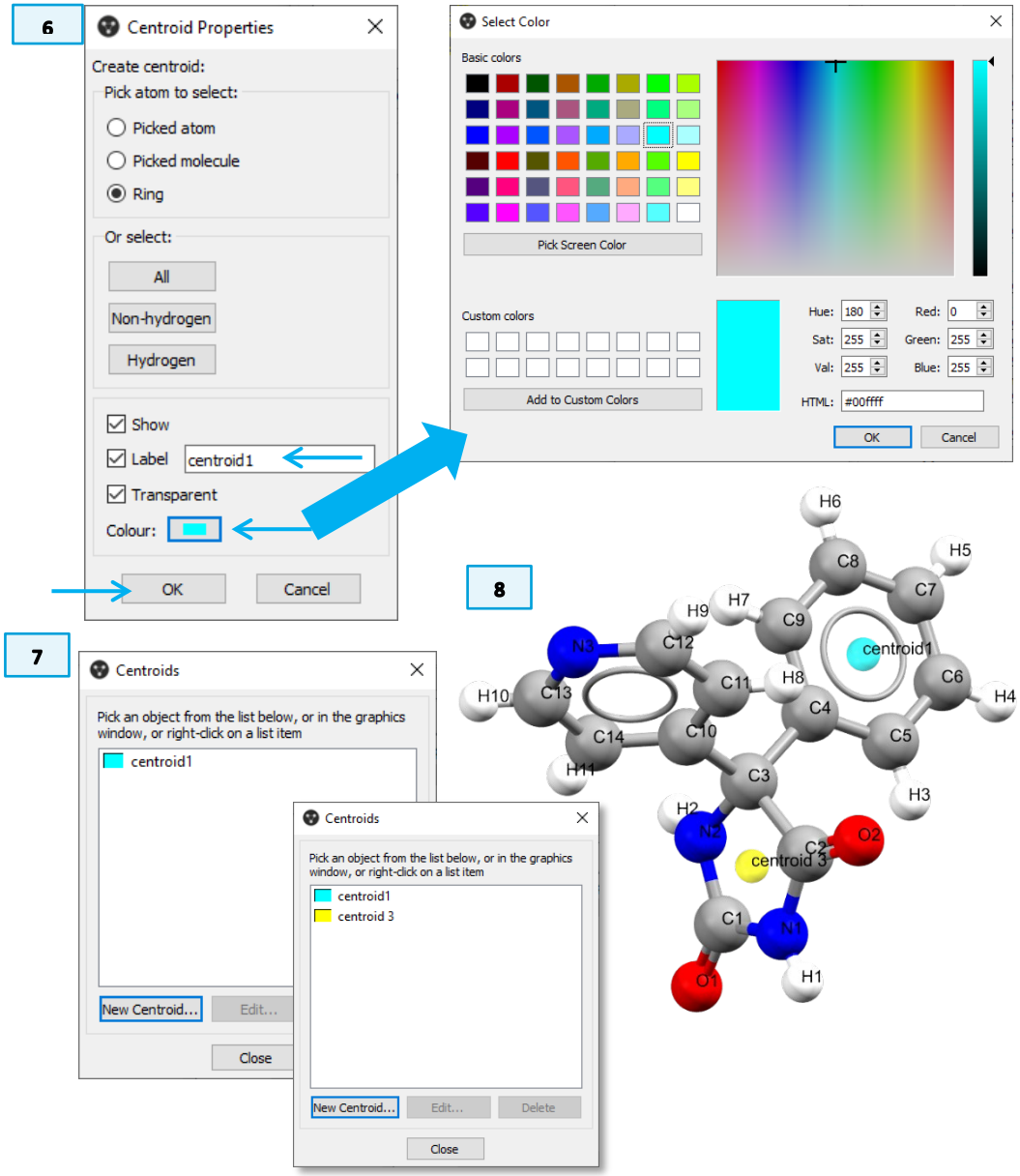
9. Centroids can be used for calculations of distances, angles, and torsions with other atoms. First, we measure the distance between *centroid 1* and *centroid 3*. To do so, repeat **Steps 4** & **5** from Example 1, selecting this time the two centroids we have just calculated. The distance between centroids 1 and 3 is 3.774Å.

10. For clarity, clear all measurements (**Step 9** of Example 1) and change the *Picking Mode* back to *Pick Atoms* (**Step 1** of Example 2). If you try the Exercise below, clear measurements after that as well.



Exercise

- What is the distance between centroid 1 and N3?
- Try and measure angles and torsions using these centroids and other atoms of your choice. To do so, follow **Steps 10** & **11,** and **15** & **16** from Example 1.



11. We will now move to calculating planes. You will notice that the procedure is very similar to what we have just done to calculate centroids. Go to *Calculate* > *Planes…* . In the *Planes* window that appears click *New Plane* to calculate our first plane. This brings up another window with the *Plane Properties*.

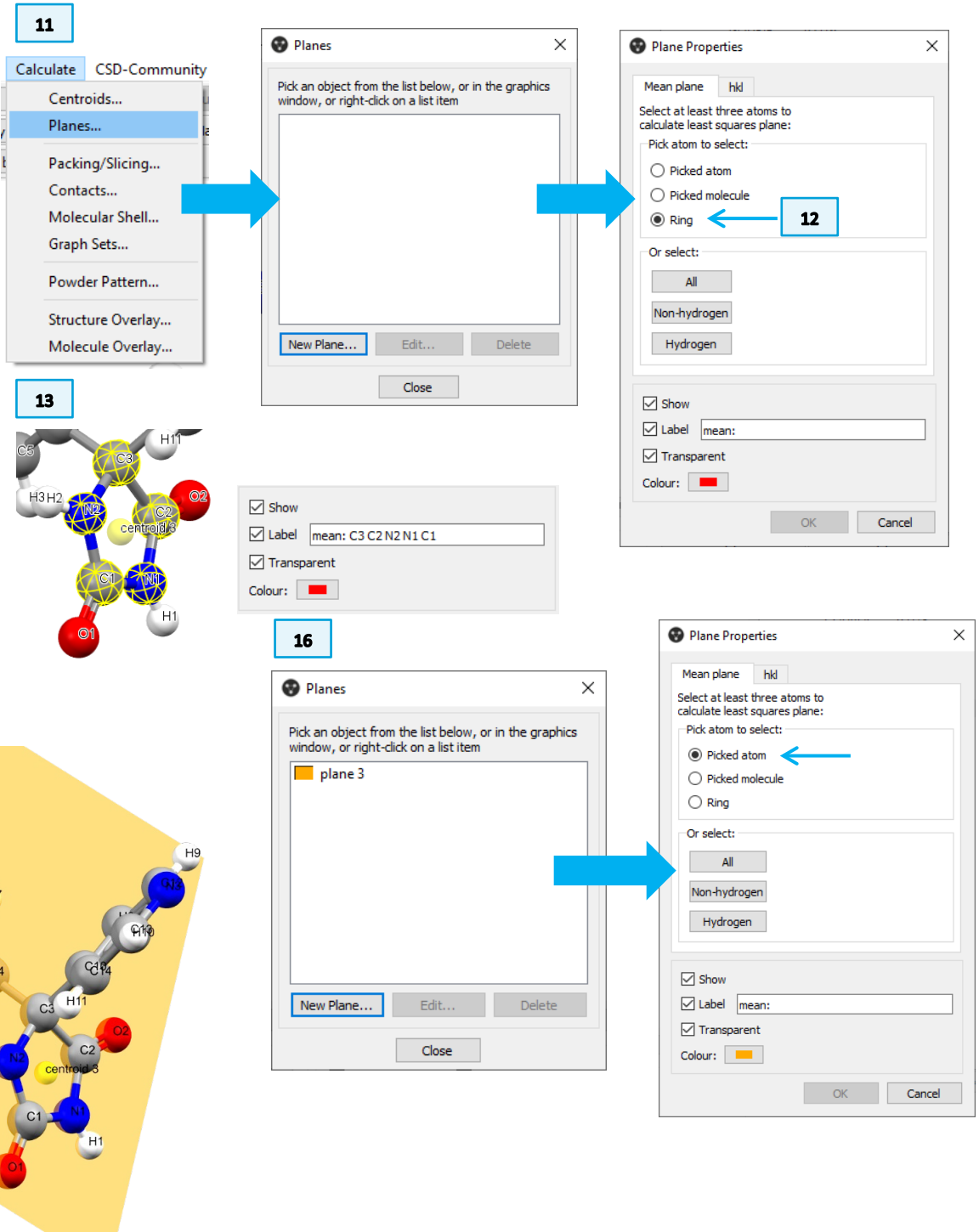
12. Our first plane will be for **Ring 3**. In *Plane Properties*, in the *Mean Plane* tab, under *Pick atom to select:* tick *Ring*.

13. On the Mercury interface, select one atom (any atom) belonging to Ring 3. As for centroids, you will see that the entire ring selected. The *Label* in *Plane Properties* now includes the labels of the atoms in **Ring 3**.

14. Change the *Label* in *Plane Properties* to "*plane* 3", and the *Colour* to orange (see **Step 6**). When you are done, click *OK* to create the new plane.

15. Plane 3 has now been calculated and represented on the molecule. You can also find it listed in the window.

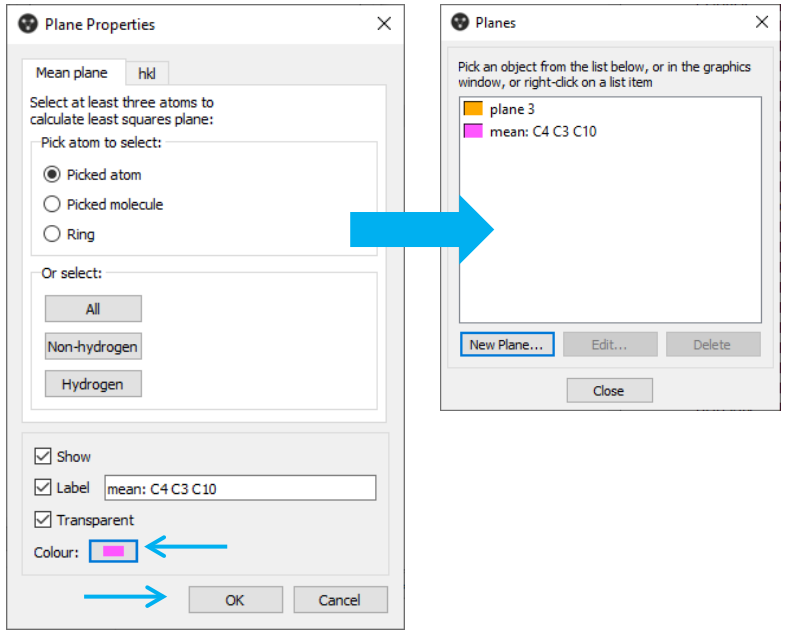
16. Next, we define the plane on which atoms C3, C4, and C10 lie. Please note that you could calculate a mean plane for more than three atoms, but for this example we will use these three. To calculate a new plane, in the *Planes* window click again *New Plane*. This time in *Plane Properties*, in the *Mean Plane* tab, under *Pick atom to select:* tick *Picked atom*.



17. On the Mercury interface, select the three atoms of interest: C3, C4, and C10. The *Label* in *Plane Properties* is now *"mean: C4 C3 C10"*.

18. In *Plane Properties* change only the *Colour* to pink (see **Step 6**). When you are done, click *OK* to create the new plane.

18



19. So far, we have calculated two centroids (centroid 1 and centroid 3) and two planes (plane 3 and mean: C4 C3 C10). We will now use them for measuring distances, angles, and torsions.

20. To measure the distance between centroid 1 and plane 3, first under *Picking Mode* select *Measure Distances* (see **Step 4** in Example 1). Then click on centroid 1 and on one (any) point on plane 3. Please note: the point on plane 3 does not need to be the closest to centroid 1. The value of the distance appears, as before, in correspondence of a dotted line. The distance between centroid 1 and plane 3 is 2.438 Å.

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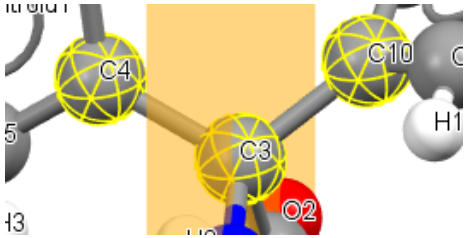

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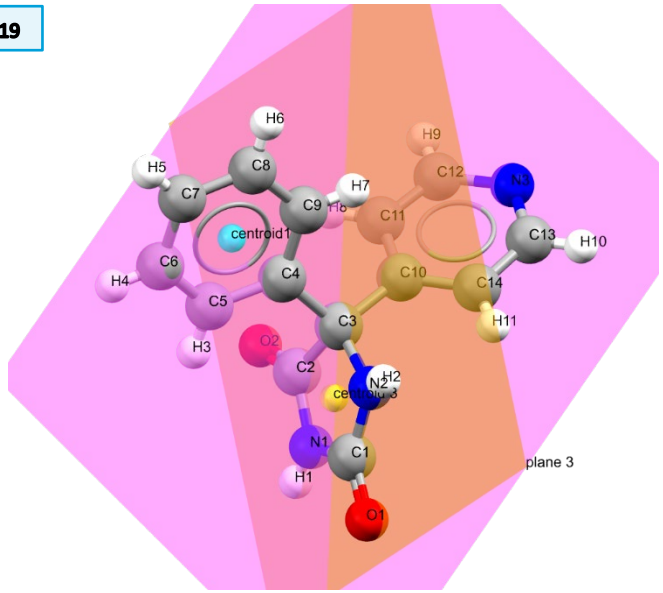

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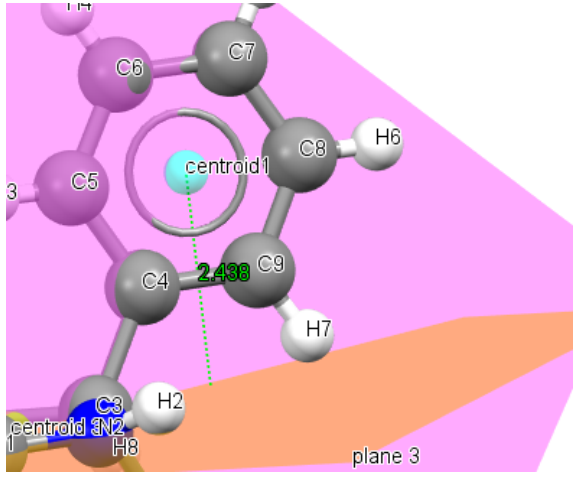
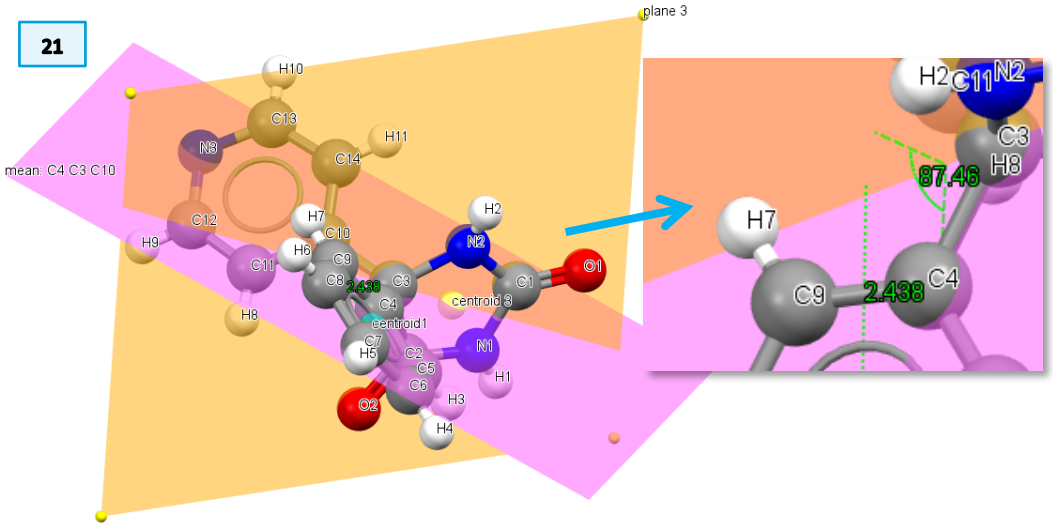


21. To measure the angle between the two planes that we calculated, under *Picking Mode* select *Measure Angles* (see **Step 10** in Example 1). Then click on plane 3 and on mean: C4 C3 C10. The angle is represented with a dotted arch as before and its value is 87.46°.

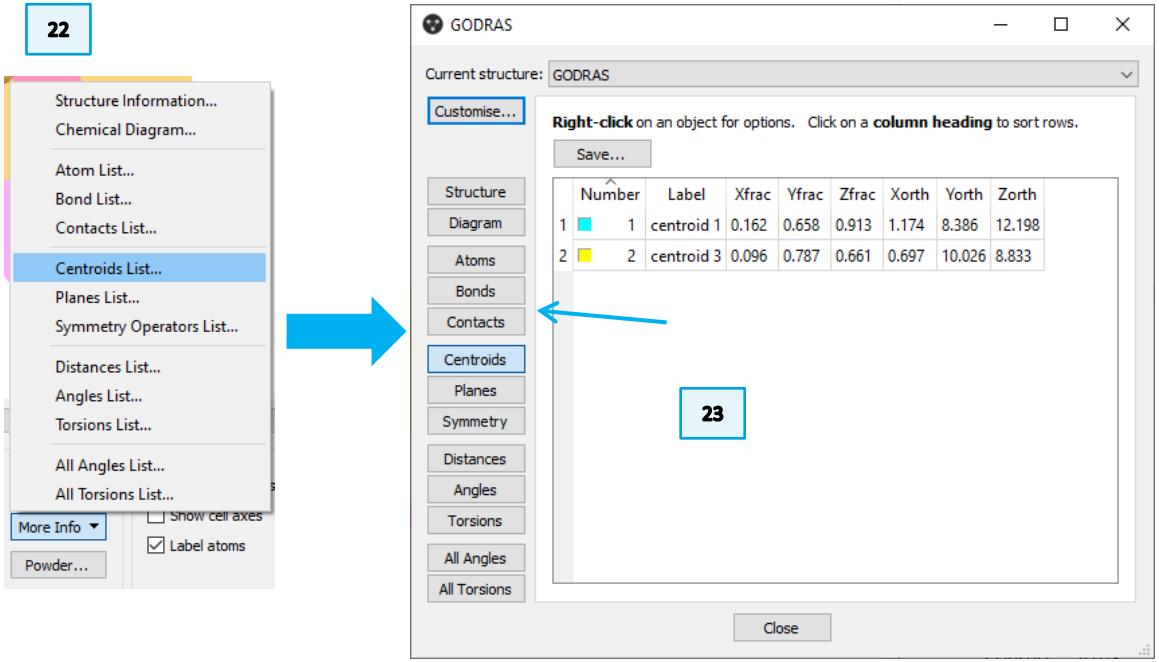
22. You can view the centroids and planes details listed in a table. Click on *More Info > Centroids List…* at the bottom of the Mercury window. In the pop-up window you can see the calculated centroids, and save them as a document (.tsv, .csv, and .txt formats available).

23. In this window you can click *Planes* to view and save the planes calculated.



Hints

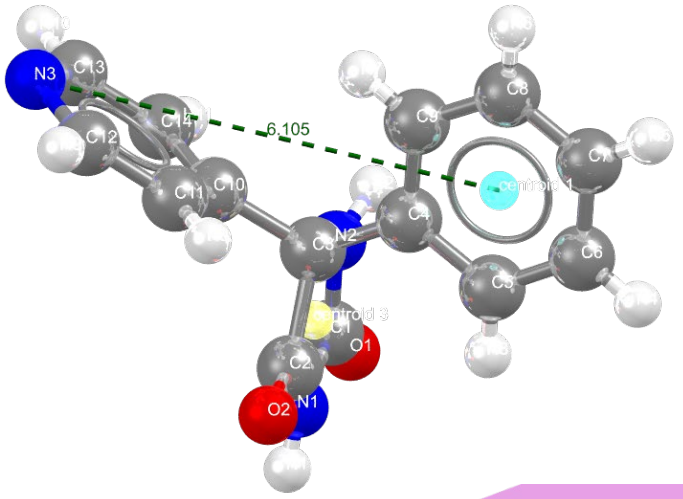
- What happens if you measure the distance between these planes?
- You can calculate centroids and planes for any selected group of atoms. You can try and investigate what happens if you define a plane using 4 or more atoms.
- With the packing visualisation on, define the centroid for each entire molecule and use them to explore distances, angles, and torsions.



Summary

In this workshop we used Mercury tools helpful in analysing crystal structures. You should now be familiar with:

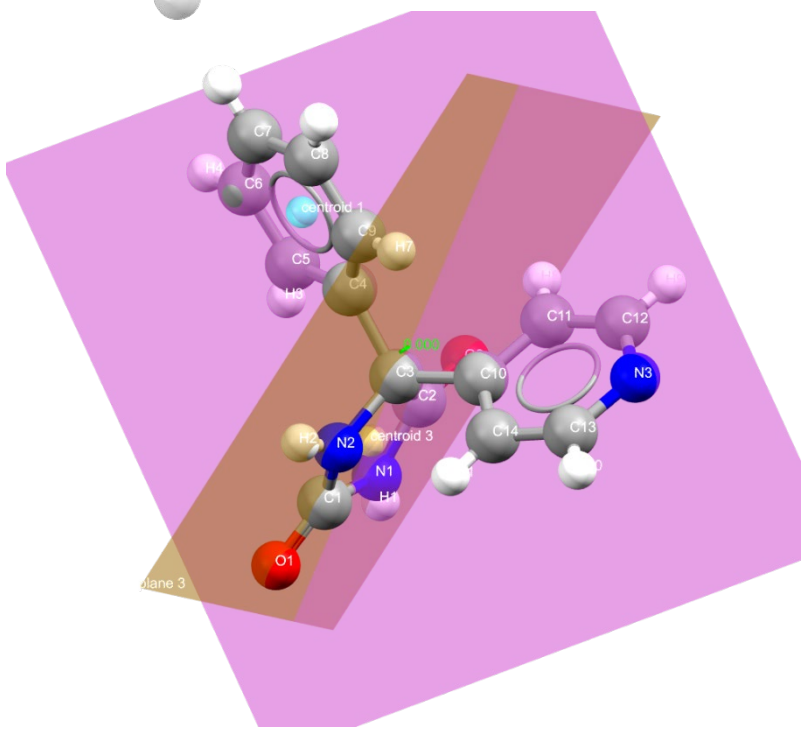
- Measuring distances, angles, and torsions.
- Displaying labels.
- Calculating centroids and planes.
- Viewing measurements and calculated objects from the More Info window.



Next Steps

If you want to continue exploring the conformation of a molecule and assess it with data from the CSD, you can use Mogul Geometry Check. The self-guided workshop on Mogul (MOG-001) is available on this page: https://www.ccdc.cam.ac.uk/community/training-and-learning/workshop-materials/csd-core-workshops/.

Other advanced analysis tools are available in Mercury with CSD-Materials and CSD-Discovery. Explore more features, such as the Aromatic Analyser, with more workshops on this page: https://www.ccdc.cam.ac.uk/community/training-and-learning/workshop-materials/csd-materials-workshops/.

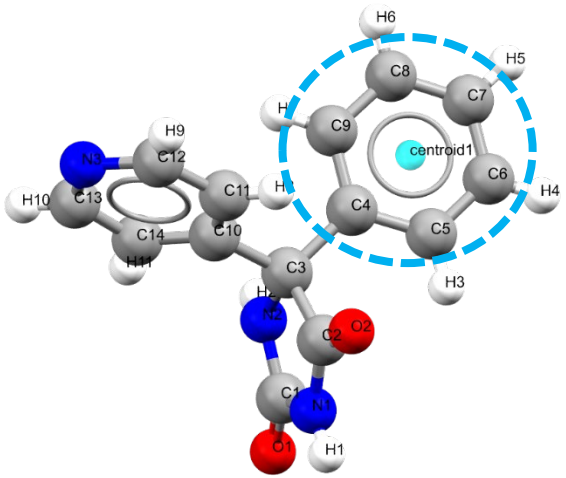


Feedback

We hope this workshop improved your understanding of Mercury 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 (https://www.surveymonkey.co.uk/r/CCDC-Online-Workshop, link also available from workshops webpage), 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 MER-005. Thank you!

Glossary

Centroid
In Mercury, the centroid is the geometric centre of a group of selected atoms.



Centroid for atoms C4, C5, C6, C7, C8, C9 of structure GODRAS