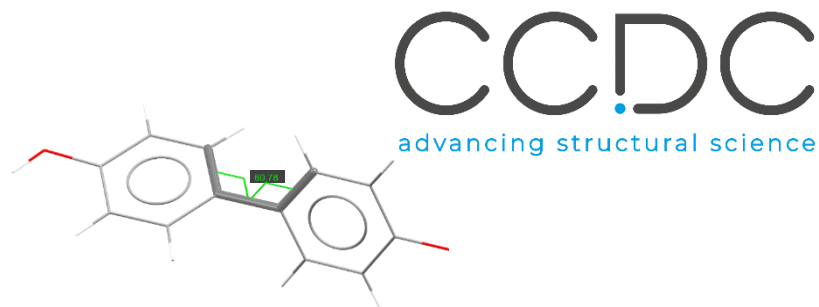


In-depth analysis of molecular geometries with industrial use-cases in Mogul

2021.2 CSD Release



CCDC Virtual Workshops

1

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Introduction

Structural chemists can use the Mogul Geometry Check tool to validate the three-dimensional [conformation](#) of a particular molecule. The data from structures in the CSD can be used to show the most likely values a particular bond, angle, [torsion](#) or ring should adopt. The information obtained from a Mogul check can help identify inconsistencies within a crystal structure and can suggest values to be used for restraints during refinement. In addition, Mogul can also be run on 3D coordinates generated [in silico](#) as a validation of calculated structures.

The examples from this handout demonstrate approaches to gain more insights from your data and to interpret critically the results obtained from Mogul.

Objectives

In this workshop you will learn:

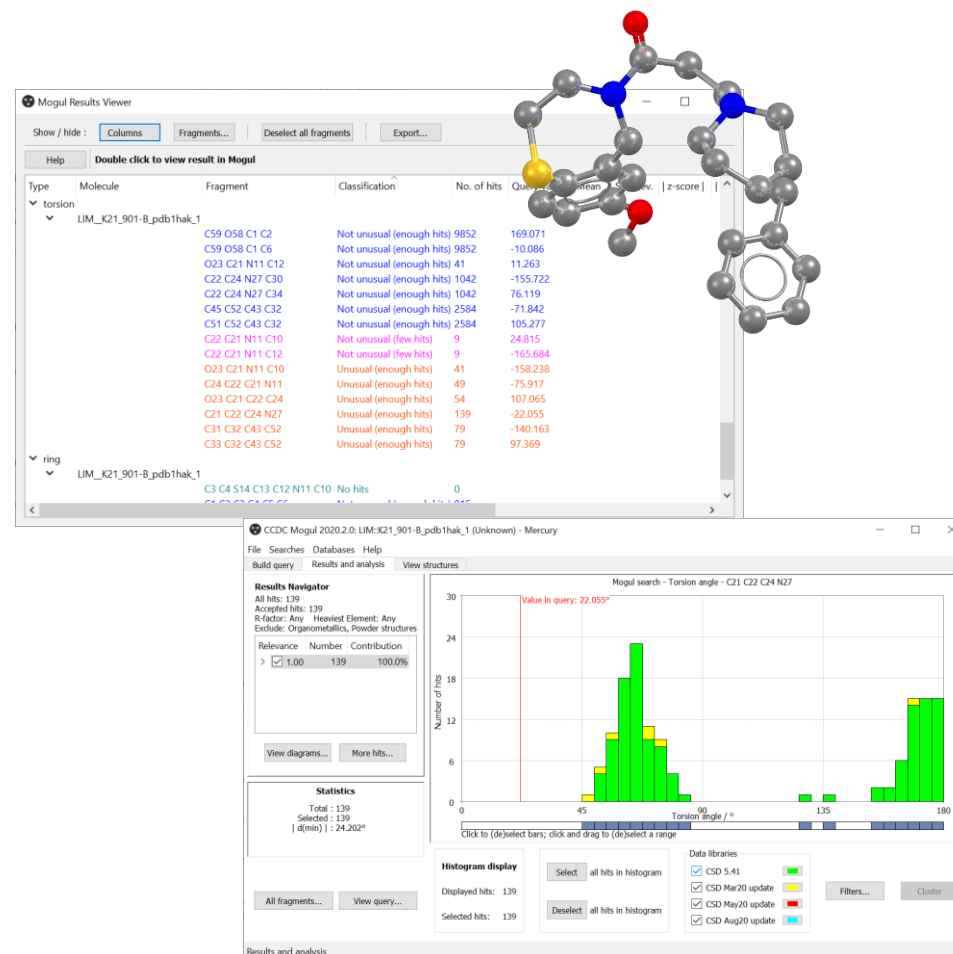
- How to apply filters for the Mogul Geometry Check search.
- How to restrict the visualisation of the results to specific parts of the histogram and why you would do that.
- What to look for when analysing not unusual or unusual torsion angles.
- How to complement Mogul Geometry Check with ConQuest 3D search and Mercury analysis.

The exercises in this handout will take approximately **25 minutes** to be completed.

Note: This handout was realised using the 2021.2 release of the CSD (data Sep21). Your results (e.g., number of hits and histogram colours) might differ based on the CSD version you are using.

Pre-required skills

The following exercises assume you have a working knowledge of the program Mercury, namely, how to display and manipulate structures from a 3D coordinates file, and basic knowledge of Mogul, namely how to run a search and how to access and read the results table.



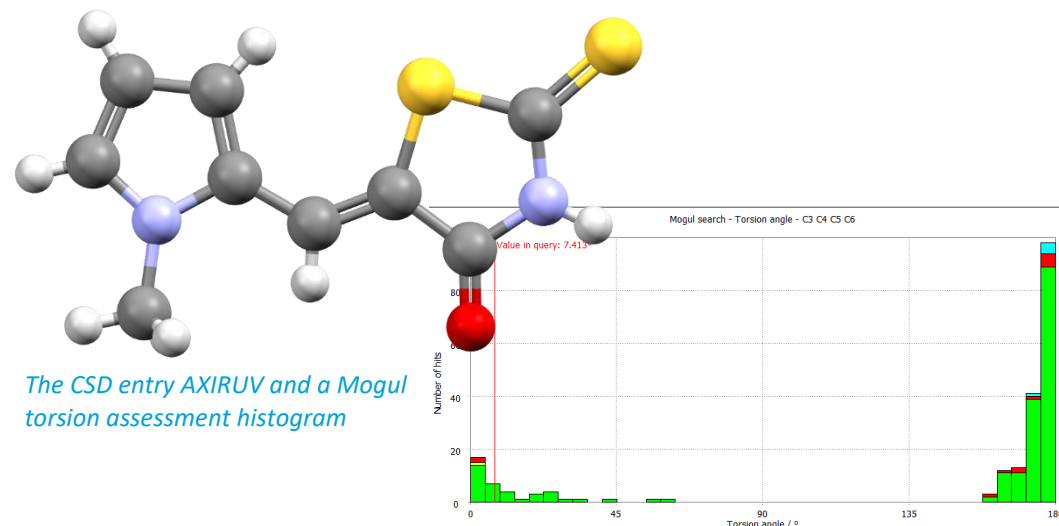
Example of the Mogul geometry assessment interface.

Note: The words in *Blue Italic* in the text are reported in the [Glossary](#) at the end of this handout.

Example 1. Using Mogul to assess intramolecular geometry: torsion angles.

By using the statistical distributions of similar [fragments](#), Mogul can confirm your 3D geometry is appropriate, or flag values that are too far outside the norm.

In this example, you will use Mogul to assess the torsion angles of a given molecule and investigate patterns in the distribution. You will find results for four different torsion angles, all resulting as “Not unusual” and will be guided to further analyse one of them as its value falls into a minor population of the resulting histogram.



1. Launch Mercury and type AXIRUV in the Structure Navigator toolbar.
2. To start a geometry analysis, click the CSD-Core menu and then click *Mogul Geometry Check* from the dropdown menu.
3. This brings up the *Mogul Search Settings* dialogue box. You can typically use the defaults in this window, but we are interested in the torsion angle between the rings. To streamline our search, we will select Torsion Angle in the Fragment Types option and tick the boxes for *Apply Filters*, *Exclude Organometallics*, and *Exclude Powder structures*. We will leave the remaining default options as is.
4. Click **Search** to start.
5. A dialogue box will pop up to warn you that you are going to check the entire molecule. Click **OK** to continue.
6. The search will begin to run. You can follow its progress in the *Search Progress* dialogue box.

7. When the search is complete, your results will be displayed in the **Mogul Results Viewer**.
8. The results are colour-coded. Unusual values are typically flagged in **orange**, however there are no unusual values here. Please, be aware that the number of hits might differ based on the version of the data update. The data in this workshop are obtained with the CSD Sep21 update.
9. Clicking on each entry in the **Mogul Results Viewer** will highlight the corresponding value in the Mercury display window. Although the entries are not unusual, it is useful to review the angle distribution. Double-click on the last entry C3 C4 C5 C6 to bring up the data from the Mogul library.
10. The red line marks the value of the angle from your molecule (the query).
11. The histogram shows the data from the CSD, colour coded by update. (Note: you can click the colour swatches under Data libraries to change the colour.)
12. To see which structures contribute to a certain bar on the histogram, first click **Deselect** (all the bars will turn grey), and then click the bar directly under the red query line. This will highlight that specific bar of the histogram in colour.

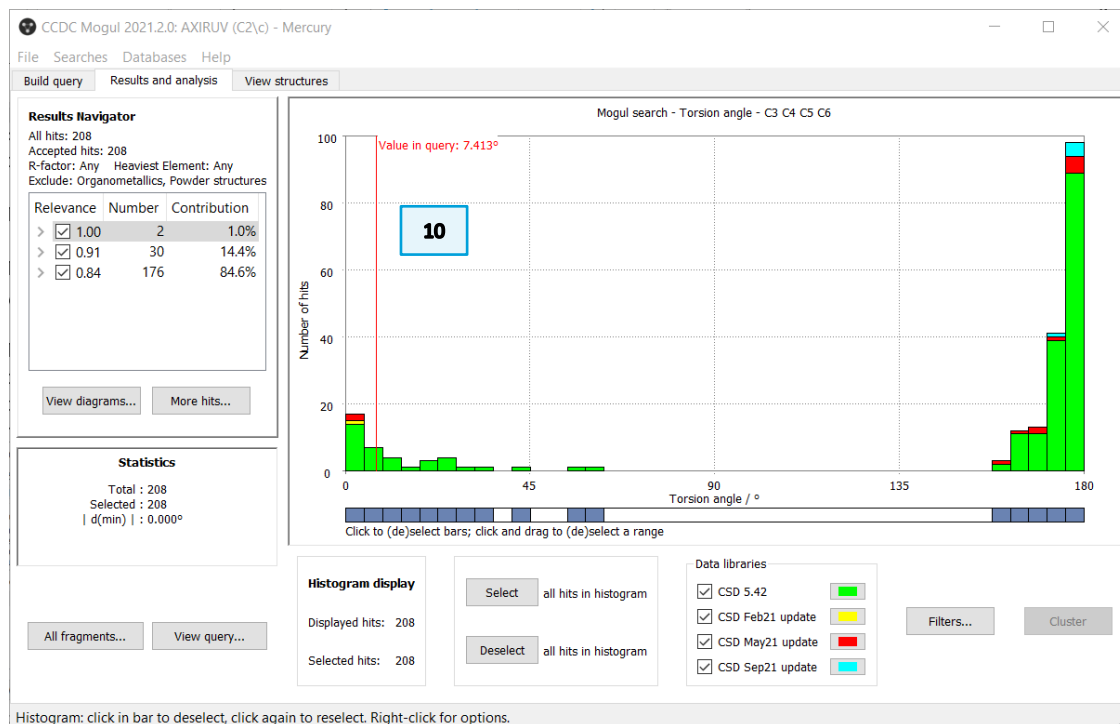
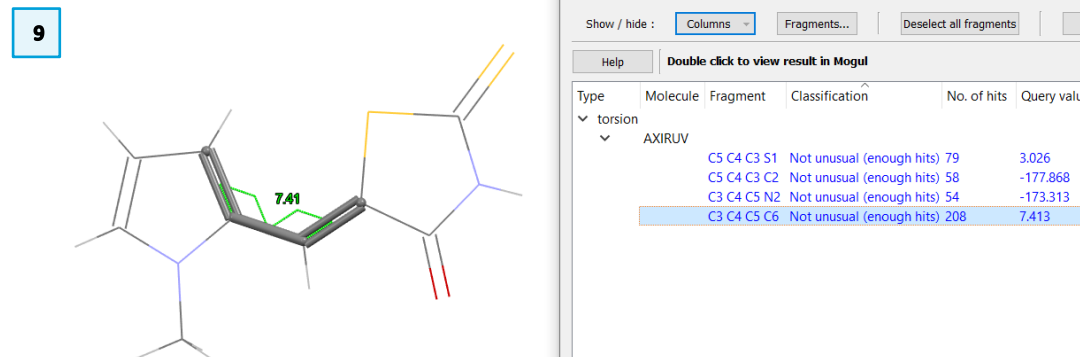
7

Mogul Results Viewer

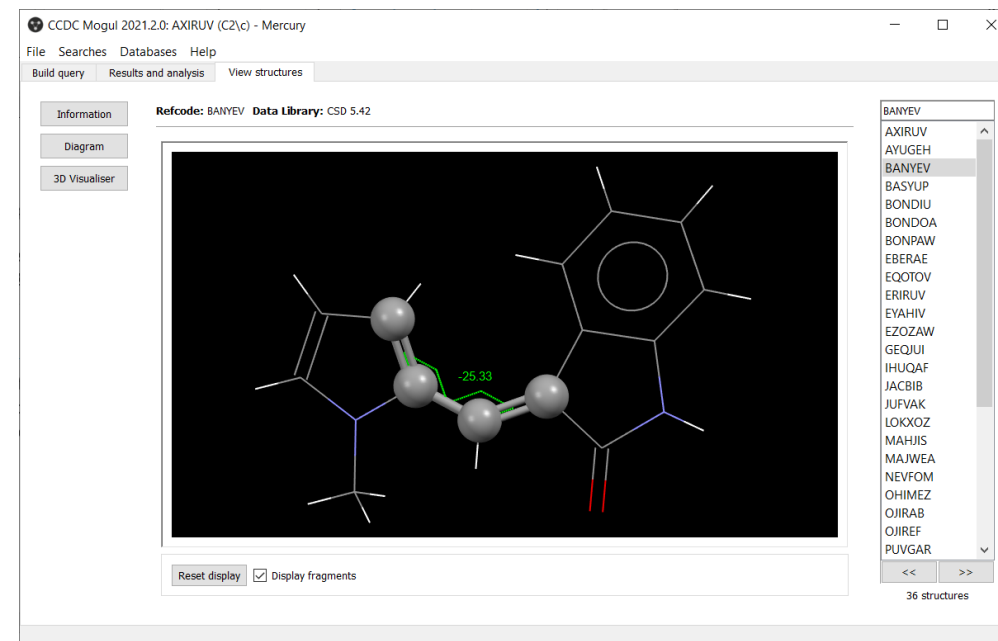
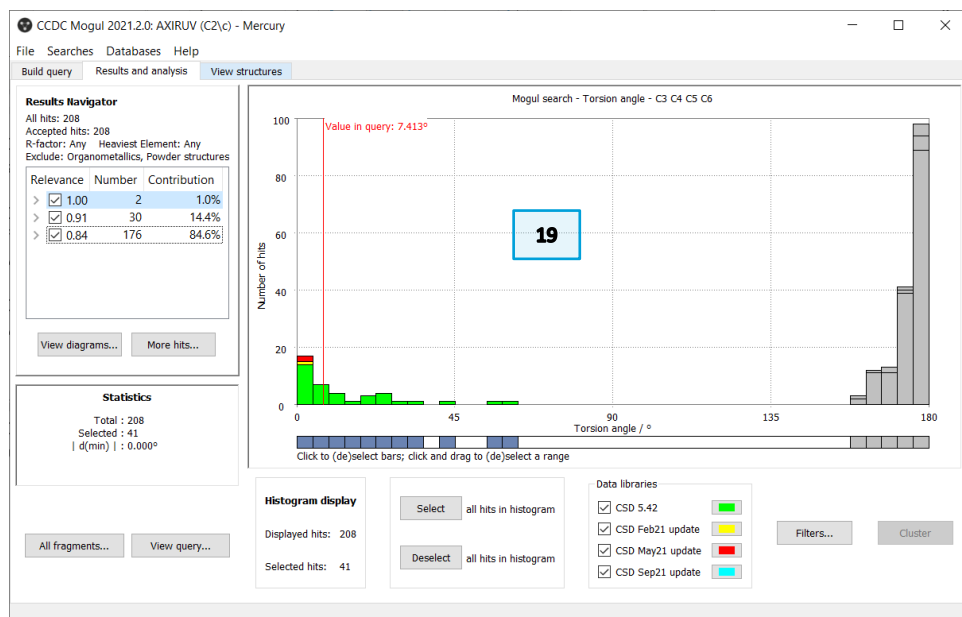
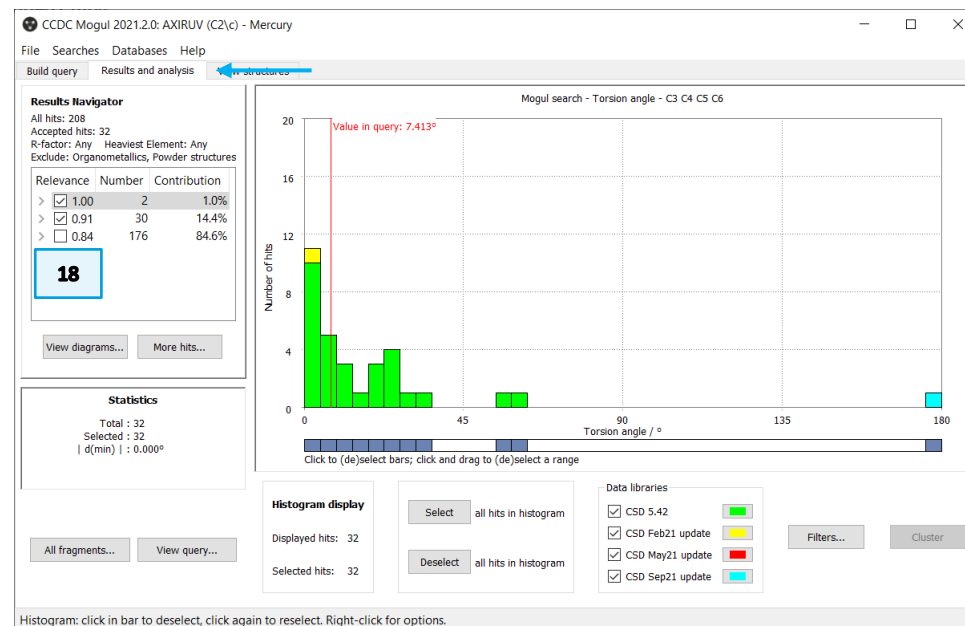
Show / hide: Columns Fragments... Deselect all fragments Export...

Help Double click to view result in Mogul

Type	Molecule	Fragment	Classification	No. of hits	Query value	Mean	Std. dev.	z-score	x - mean	Minimum	Maximum	Median	d(min)	Local density
torsion	AXIRUV													
	C5 C4 C3 S1		Not unusual (enough hits)	79	3.026					0.000	1.000			
	C5 C4 C3 C2		Not unusual (enough hits)	58	-177.868					0.000	1.000			
	C3 C4 C5 N2		Not unusual (enough hits)	54	-173.313					0.000	0.481			
	C3 C4 C5 C6		Not unusual (enough hits)	208	7.413					0.000	0.139			



17. Scroll through the refcodes to view the 3D structures that populate this region. You will notice that the angles are in most instances part of a macrocycle (large ring), which has an effect on the torsion angle. Our query is not part of a macrocycle and thus, it is reasonable that while there are more hits in this region, they have a low relevance value in our search.
18. Click the *Results and analysis* tab and untick the 0.84 Relevance row to view the change to the histogram. The histogram has now 32 hits (with the data update used to prepare this exercise) and our query falls in the populated area of the histogram.
19. Tick the 0.84 Relevance row to view the full histogram, then select the angles in the less populous region. Click the *View structures* tab and select **3D Visualiser**. Scroll through the refcodes and you will see that the structures that populate this region are not part of macrocycles and closer to our query structure.

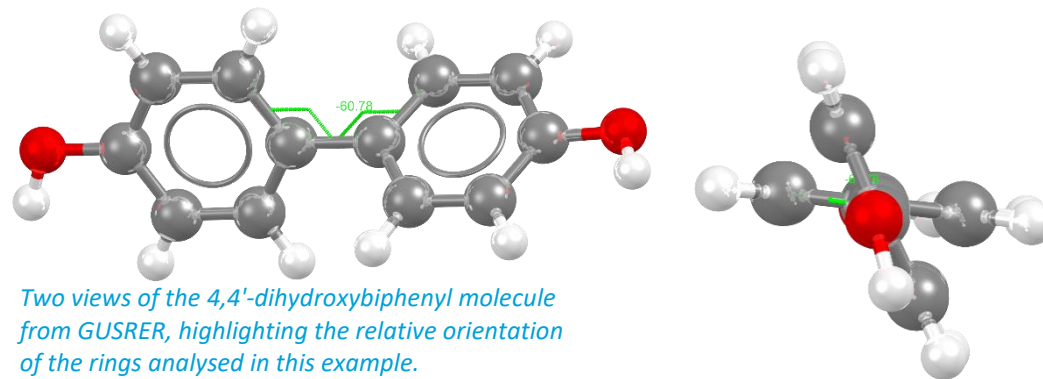


Conclusions for Example 1

In this exercise we have performed a Mogul Geometry Check on a molecule from the CSD. We have learnt how to analyse our results, reviewing relevant and less relevant structures and how those determinations are made.

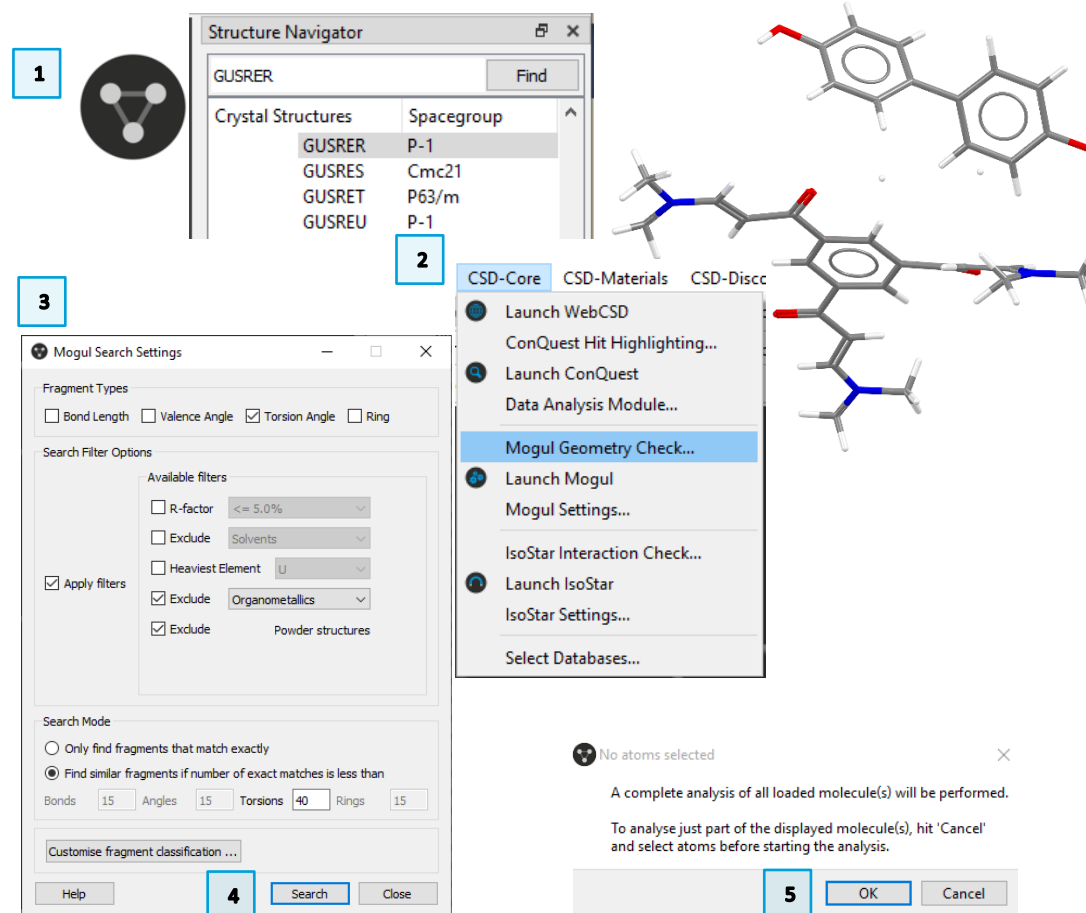
Example 2. Using Mogul to explain activity data

In this example you will see how to investigate unusual torsions in Mogul and how to complement the Mogul analysis with ConQuest and Mercury to gain more insights into your structure.



Two views of the 4,4'-dihydroxybiphenyl molecule from GUSRER, highlighting the relative orientation of the rings analysed in this example.

1. Launch Mercury and type GUSRER in the Structure Navigator toolbar. You will see that the structure has two components.
2. To start a geometry analysis, click the CSD-Core menu and then click *Mogul Geometry Check* from the dropdown menu.
3. This brings up the *Mogul Search Settings* dialogue box. For this example, we are interested in torsion angles. To streamline our search, we will select only Torsion Angle in the Fragment Types option and tick the boxes for *Apply Filters*, *Exclude Organometallics*, and *Exclude Powder structures*. We will leave the remaining options as the default.
4. Click **Search** to start.
5. A dialogue box will pop up to warn you that you are going to perform the check for all loaded molecules. Click **OK** to continue.
6. The search will begin to run. You can follow its progress in the *Search Progress* dialogue box.



The image illustrates the workflow for performing a Mogul analysis in Mercury. It includes screenshots of the Structure Navigator, the CSD-Core menu, the Mogul Search Settings dialog, and the confirmation dialog.

Step 1: Structure Navigator showing GUSRER.

Step 2: CSD-Core menu with Mogul Geometry Check... selected.

Step 3: Mogul Search Settings dialog. Fragment Types: ☐ Bond Length, ☐ Valence Angle, ☒ Torsion Angle, ☐ Ring. Search Filter Options: ☒ Apply filters, ☐ Exclude Solvents, ☐ Heaviest Element U, ☒ Exclude Organometallics, ☒ Exclude Powder structures. Search Mode: ☒ Find similar fragments if number of exact matches is less than. Bonds: 15, Angles: 15, Torsions: 40, Rings: 15. Search button highlighted.

Step 4: Confirmation dialog: No atoms selected. A complete analysis of all loaded molecule(s) will be performed. To analyse just part of the displayed molecule(s), hit 'Cancel' and select atoms before starting the analysis. OK button highlighted.

7. When the search is complete, your results will be displayed in the **Mogul Results Viewer**.
8. The results are colour-coded. Unusual values are typically flagged in **orange**. In this example we can see that the unusual values here are found only in one of the two molecules, the 4,4'-dihydroxybiphenyl (listed as GUSRER_2 in the **Mogul Results Viewer**). Please be aware that the number of hits might differ based on the version of the data update. The data in this workshop are obtained with the CSD Sep21 update.
9. The four torsion angles analysed for the 4,4'-dihydroxybiphenyl are all representative of the relative rotation between the two aromatic rings. We will investigate C26-C25-C31-C30. Click once on the entry in the **Mogul Results Viewer** to highlight the corresponding value in the Mercury display window. Then double-click to open the Mogul interface with the histogram.
10. From the histogram we can see that the orientation in our molecule (red line, value 60.784°) is very unusual, compared to data in the CSD that show a preferred orientation at around 35° and 145°.

7

Mogul Results Viewer

Show / hide : Columns Fragments... Deselect all fragments Export...

Help Double click to view result in Mogul

Type	Molecule	Fragment	Classification	No. of hits	Query value	Mean	Std. dev.	z-score	x - mean	Minimum	Maximum	Median	d(min)	Local density
▼	torsion													
		GUSRER_1												
		C8 C9 N1 C10	Not unusual (enough hits)	298	-177.041							0.000		0.490
		C8 C9 N1 C11	Not unusual (enough hits)	298	1.084							0.000		0.493
		C13 C14 N2 C15	Not unusual (enough hits)	298	-176.999							0.000		0.490
		C13 C14 N2 C16	Not unusual (enough hits)	298	-2.494							0.000		0.497
		C18 C19 N3 C20	Not unusual (enough hits)	298	179.441							0.000		0.473
		C18 C19 N3 C21	Not unusual (enough hits)	298	3.913							0.000		0.497
		O1 C7 C1 C2	Not unusual (enough hits)	3718	-1.915							0.000		0.254
		O1 C7 C1 C6	Not unusual (enough hits)	3718	175.403							0.000		0.277
		C2 C1 C7 C8	Not unusual (enough hits)	3630	-179.606							0.000		0.221
		C6 C1 C7 C8	Not unusual (enough hits)	3630	-2.289							0.000		0.231
		O1 C7 C8 C9	Not unusual (enough hits)	63	-1.719							0.000		0.968
		C9 C8 C7 C1	Not unusual (enough hits)	60	175.851							0.000		0.967
		C7 C8 C9 N1	Not unusual (enough hits)	83	-177.857							0.000		1.000
		O2 C12 C3 C2	Not unusual (enough hits)	3718	-173.322							0.000		0.310
		O2 C12 C3 C4	Not unusual (enough hits)	3718	9.098							0.000		0.364
		C2 C3 C12 C13	Not unusual (enough hits)	3630	8.972							0.000		0.335
		C4 C3 C12 C13	Not unusual (enough hits)	3630	-168.607							0.000		0.347
		O2 C12 C13 C14	Not unusual (enough hits)	63	-5.571							0.000		0.968
		C14 C13 C12 C3	Not unusual (enough hits)	60	171.980							0.000		1.000
		C12 C13 C14 N2	Not unusual (enough hits)	83	-177.790							0.000		1.000
		O3 C17 C5 C4	Not unusual (enough hits)	3718	-152.428							0.000		0.169
		O3 C17 C5 C6	Not unusual (enough hits)	3718	28.516							0.000		0.140
		C4 C5 C17 C18	Not unusual (enough hits)	3630	30.428							0.000		0.140
		C6 C5 C17 C18	Not unusual (enough hits)	3630	-148.628							0.000		0.113
		O3 C17 C18 C19	Not unusual (enough hits)	63	4.748							0.000		0.968
		C19 C18 C17 C5	Not unusual (enough hits)	60	-178.300							0.000		0.950
		C17 C18 C19 N3	Not unusual (enough hits)	83	-173.394							0.000		1.000
▼		GUSRER_2												
		C24 C25 C31 C30	Unusual (enough hits)	9241	-121.171							0.134		0.018
		C26 C25 C31 C30	Unusual (enough hits)	9241	60.784							0.025		0.010
		C24 C25 C31 C32	Unusual (enough hits)	9241	57.675							0.065		0.016
		C26 C25 C31 C32	Unusual (enough hits)	9241	-120.371							0.014		0.015

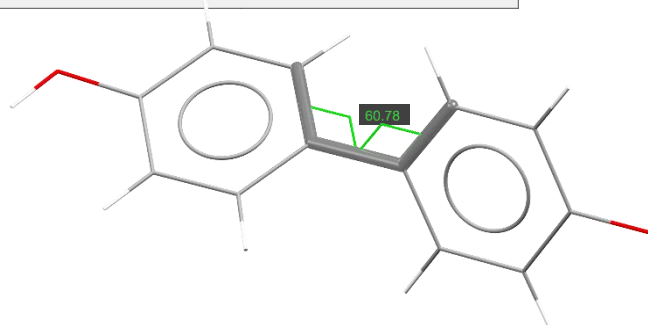
9

Mogul Results Viewer

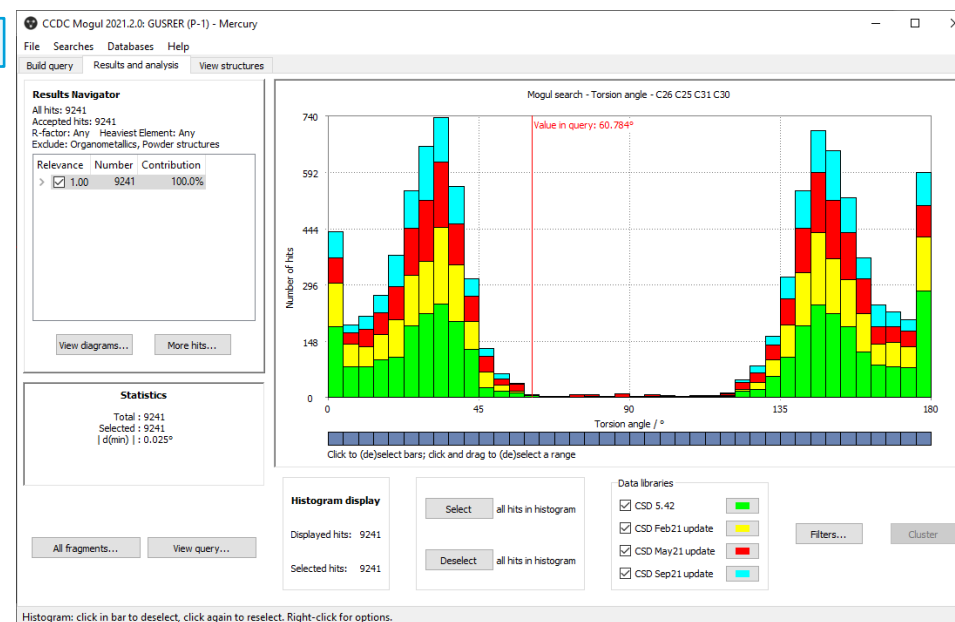
Show / hide : Columns Fragments... Deselect all fragments Export...

Help Double click to view result in Mogul

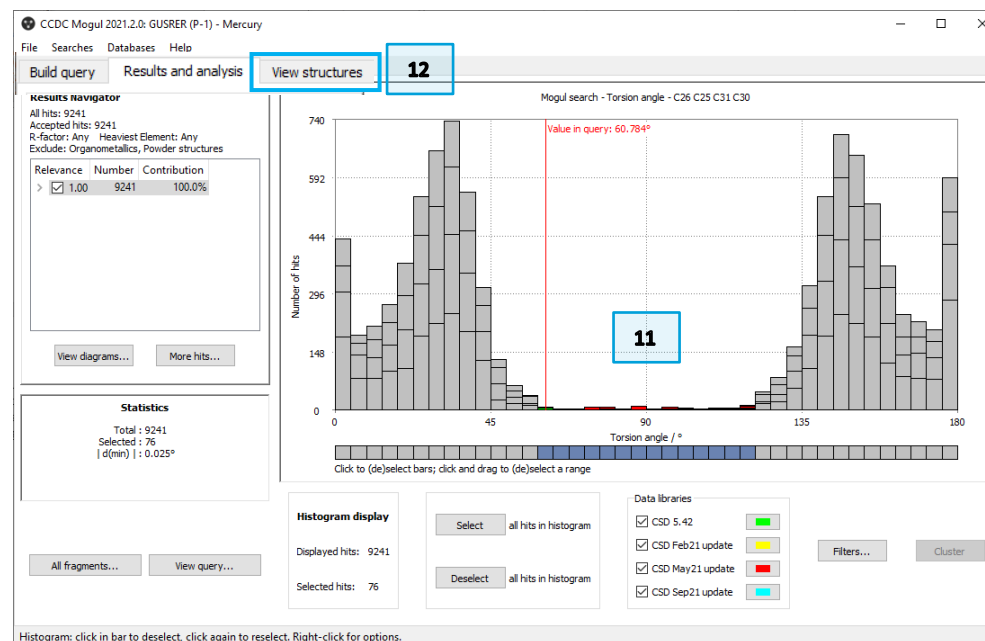
Type	Molecule	Fragment	Classification	No. of hits	Query value	Mean
▼	GUSRER_2	C17 C18 C19 N3	Not unusual (enough hits)	83	-173.394	
		C24 C25 C31 C30	Unusual (enough hits)	9241	-121.171	
		C26 C25 C31 C30	Unusual (enough hits)	9241	60.784	
		C24 C25 C31 C32	Unusual (enough hits)	9241	57.675	
		C26 C25 C31 C32	Unusual (enough hits)	9241	-120.371	



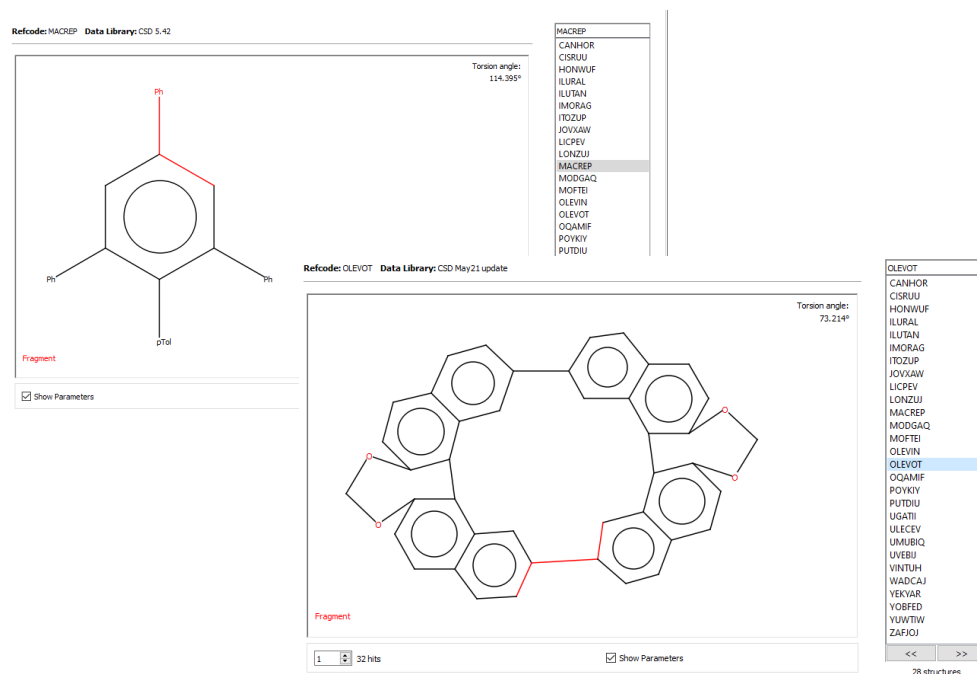
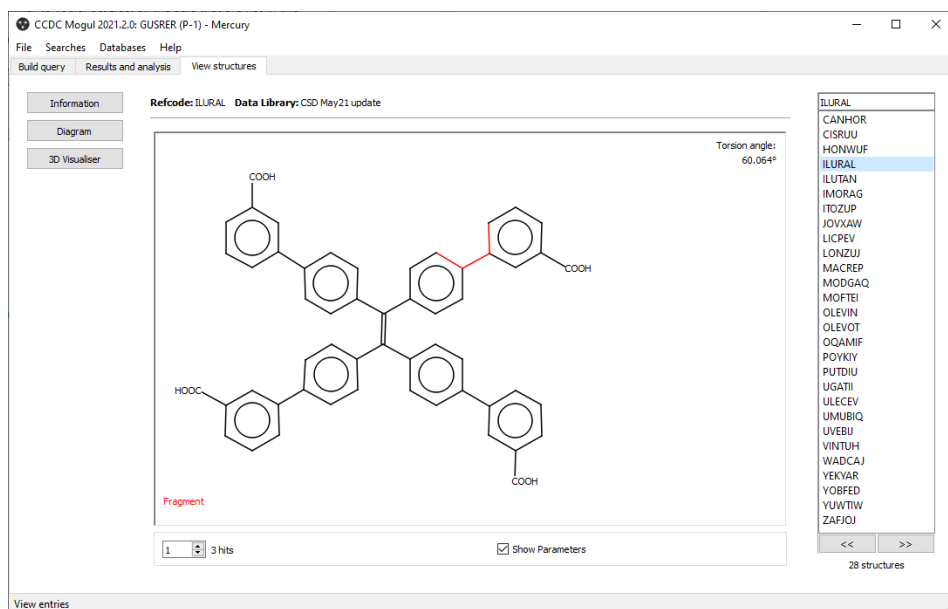
10



11. To see structures that contribute to the central part of the histogram (~60° to ~120° (please keep in mind that by symmetry these are equivalent) and assess whether these are similar to the query molecule, deselect all the bars that are not in this area by clicking and dragging the mouse arrow on the squares under the range of histogram bars to deselect. The deselected bars will turn grey.
12. Click *View Structures* to access the visualisation tab and inspect the structures that contribute to this part of the histogram.
13. Scroll through the structures and **reflect on the following questions**: Are these molecules similar to the one we are studying, e.g., do they have oxygen substituents on the two aromatic rings? Can you identify a pattern or any similarity among these structures that might explain why they are adopting this unusual orientation of the rings? You can switch between the Diagram and 3D visualisation if needed.
14. We observe different types of structures (macrocycles, different substituents attached to the aromatic rings), but there is not an obvious pattern that might explain the unusual torsion angle.

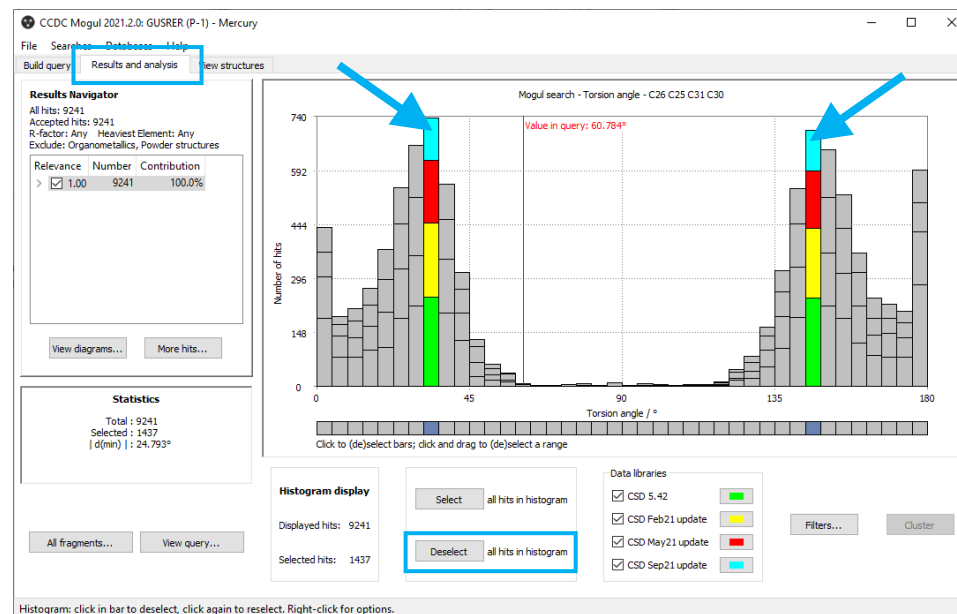
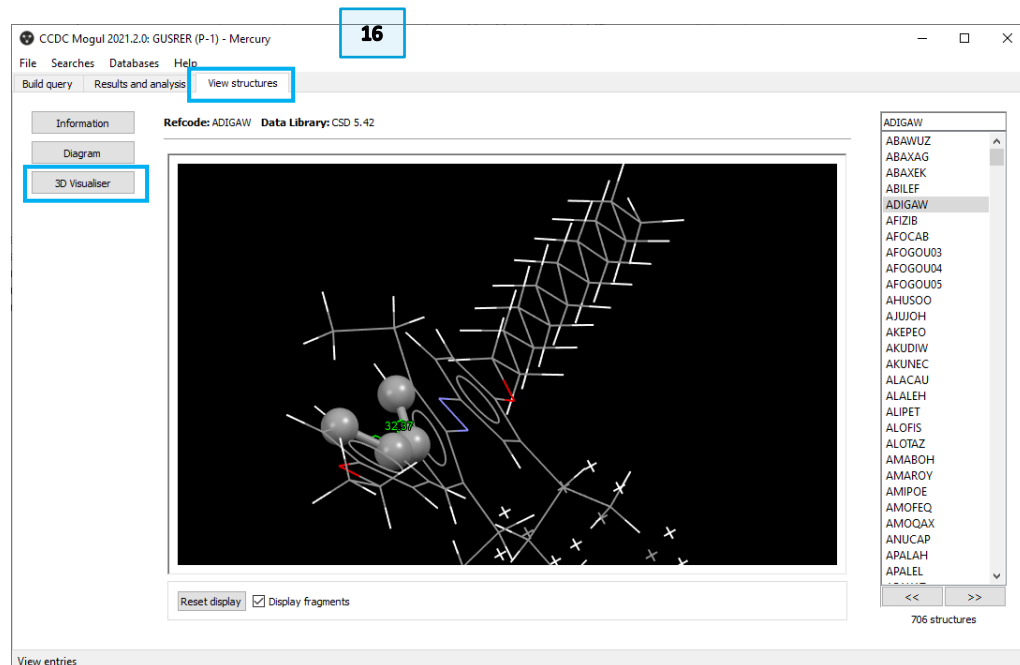


13



15. To see what the most common orientation looks like, go back to the *Results and analysis* tab, deselect all the bars using the **Deselect** button, and then click the two highest populated columns (~35° and ~145°) to select them.

16. Go to the *View structures* tab, and investigate these structures in the **3D Visualiser** to assess what the most common torsion angle looks like.



17

17

Bonus Example: Learn more about this unusual torsion using ConQuest

To investigate further how unusual this torsion is, we will perform a search in ConQuest of 4,4'-dihydroxybiphenyl and analyse the value of the torsion in our reference structure compared with other structures.

17. Launch ConQuest and in the **Build Queries** tab click **Refcode (entry ID)**. In the textbox enter the refcode of the structure we are investigating, GUSRER, then click **Find**.

18. This will bring you to the **View Results** tab, where the first result is the structure of interest.

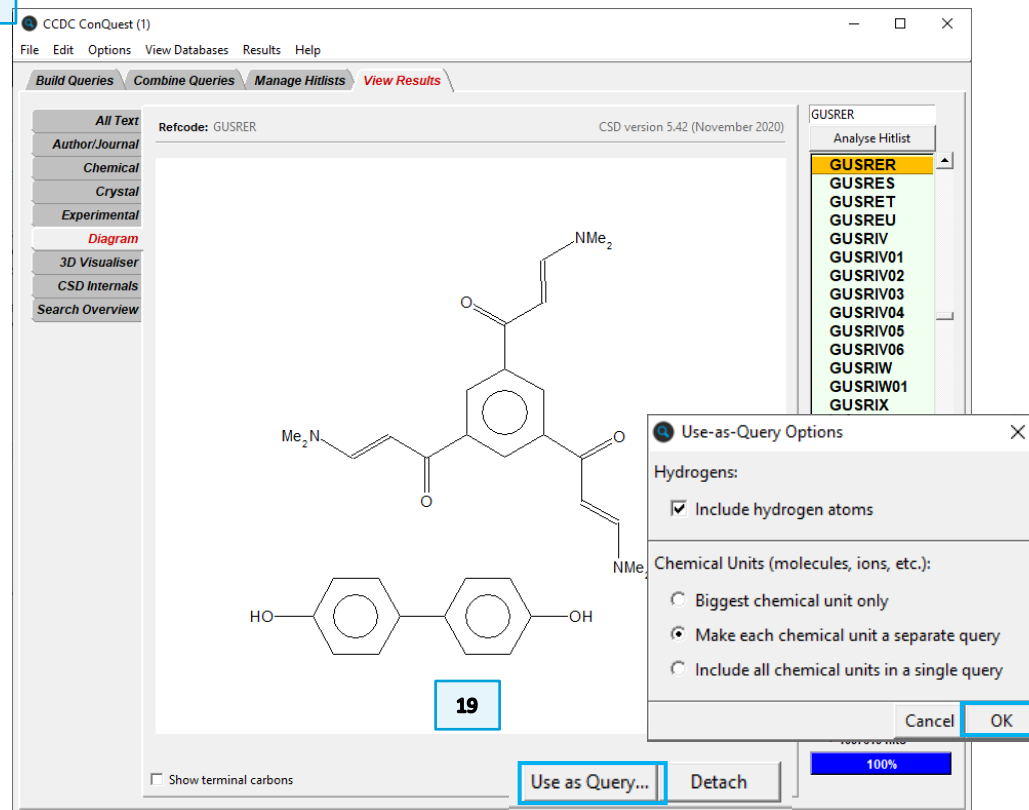
19. We want to use the 4,4'-dihydroxybiphenyl molecule as the starting point for our next search. We click on **Use As Query** and select the options *Include hydrogen atoms* and *Make each chemical unit a separate Query*, then click **OK**.

20. This will bring us back to the Build Queries tab, where we can see the two molecules as Query 1 and Query 2. 4,4'-dihydroxybiphenyl is Query 2. Untick *use this query?* for Query 1.

21. We now need to set up a search to analyse the torsional angle for molecules in structures in the CSD like the one we are studying. Click **Edit** for Query 2 to access the **Draw** window. **Steps 17 to 21** enabled us to have the diagram of the molecule we need in a fast and efficient way. Otherwise, you could have drawn it directly from the Draw tab at **Step 17**.

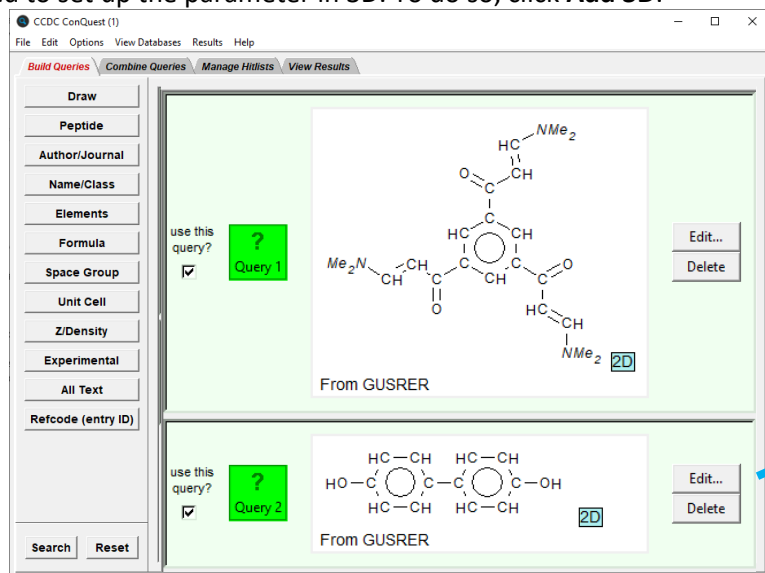
22. To access the measurements of the torsional angle during our search, we need to set up the parameter in 3D. To do so, click **Add 3D**.

18

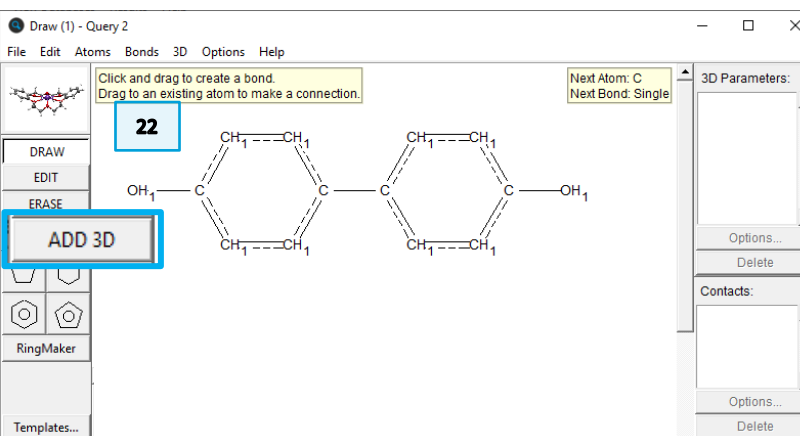


19

20

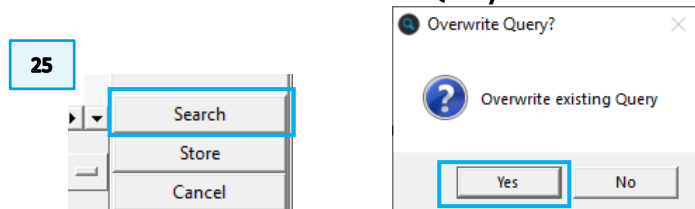


21



22

23. Now click on the four carbon atoms involved in the torsion, in order: C5, C2, C1, C4. In the **Geometric Parameters** pop-up, click **Define** next to *Torsion*, then click **Done**.
24. You could include all four the torsional angles relevant to the relative rotation of the two rings. If you wish to do so, repeat **Step 23** for the C5-C2-C1-C3 torsion, the C6-C2-C1-C3 torsion and the C6-C2-C1-C4 torsion. For this example we will not add any more torsions.
25. Now, click **Search**. When asked “**Overwrite Query?**” click **Yes**.

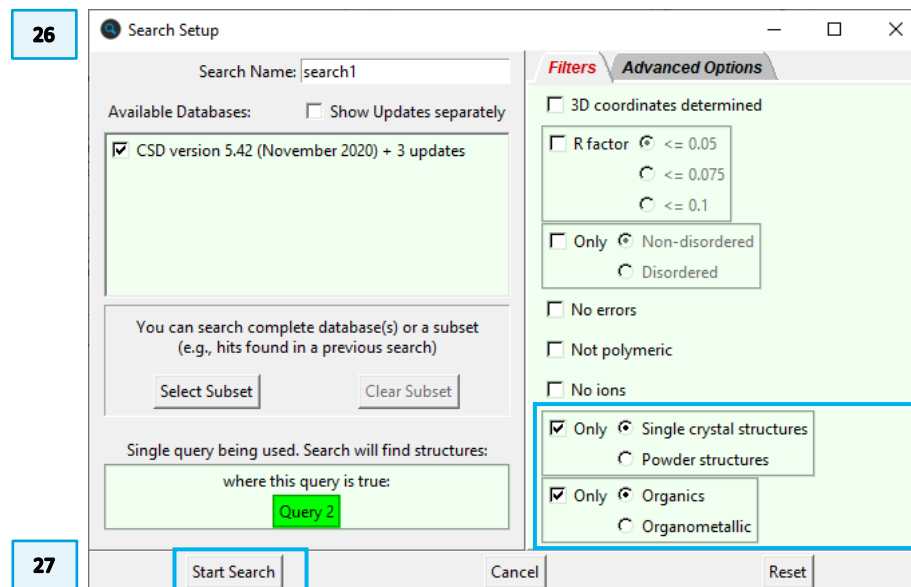
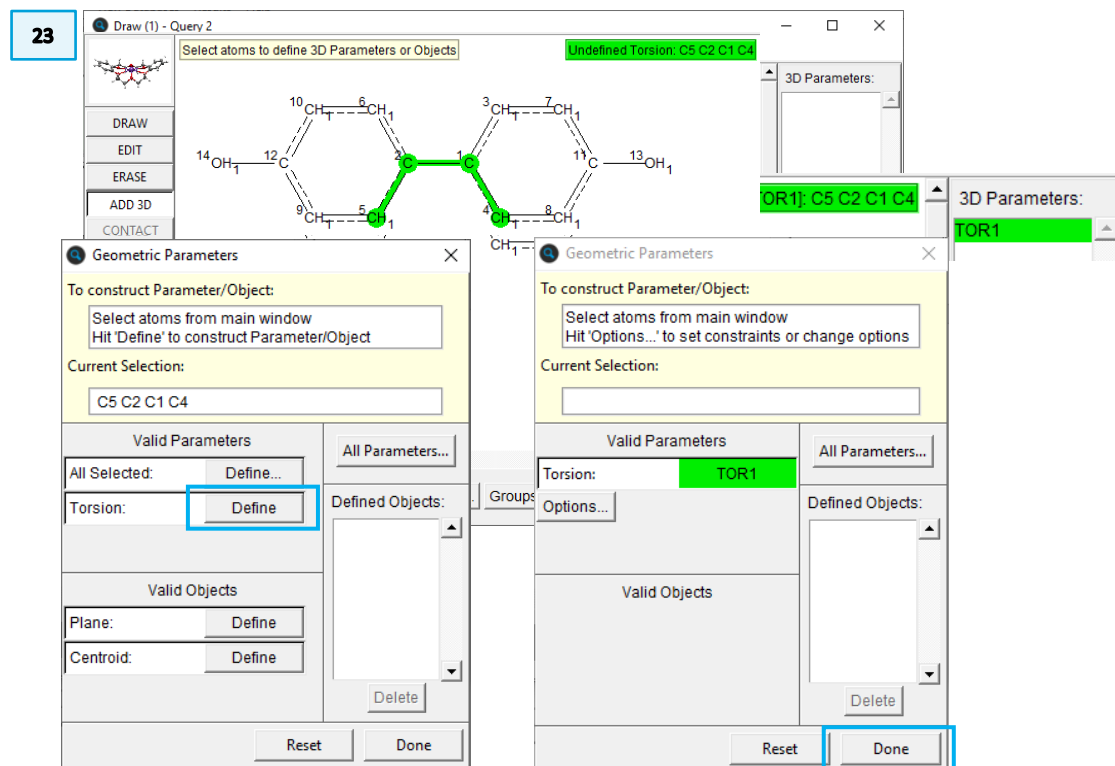


26. In the **Search Setup** window, tick as **Filters Only – Single crystal structures** and **Only – Organics**. This will make the search consistent with the Mogul analysis performed before.

27. Then click **Start Search**.

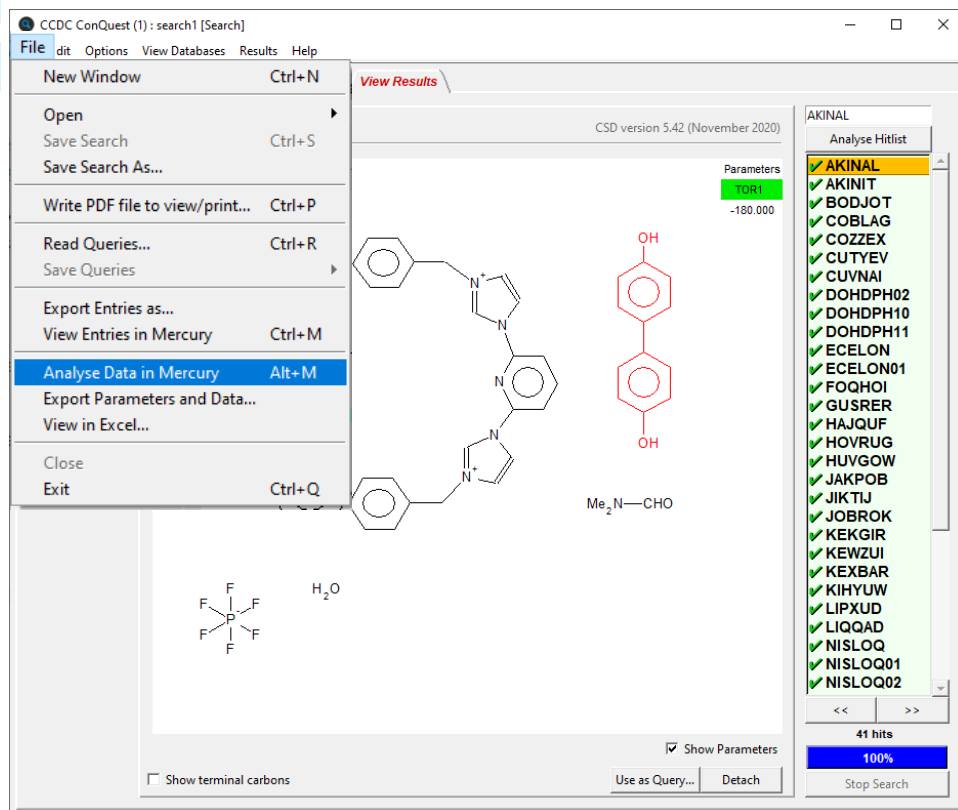
28. With version CSD version 5.42 and 3 data updates (Feb, May, Sep 2021), we obtain 41 hits that we can see in the *View Results* tab. You can scroll through the hitlist and see which entries are in the list and in the 2D Diagram. You will see the fragment we looked for in red and the value of the torsion at the top right of the visualisation window.

29. We want to analyse more systematically the value of the torsion. To do so, we will need to export the data to Mercury. Go to **File > Analyse Data in Mercury**.



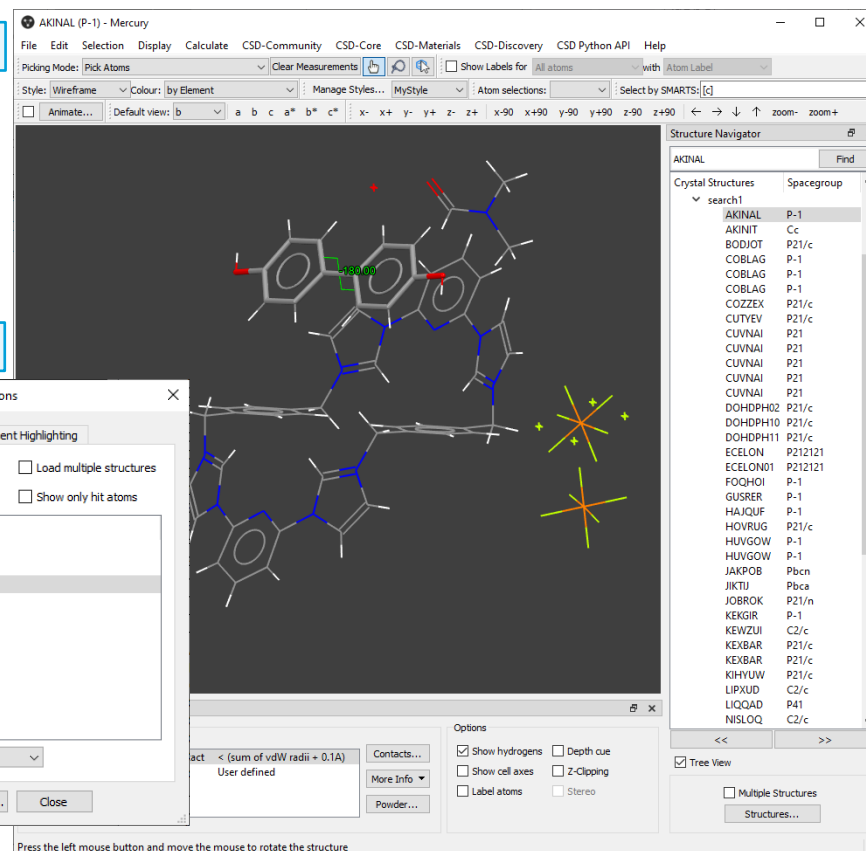
28

29



30

31a



31b

30. In the **Analyse in Mercury** pop-up ensure the option *Include Defined Parameters* is ticked. You may select other parameters if you want to include them in your analysis. Click the **Analyse in Mercury** button at the bottom right to proceed. This will automatically bring you to a new Mercury window.

31. In Mercury you have three new windows open:

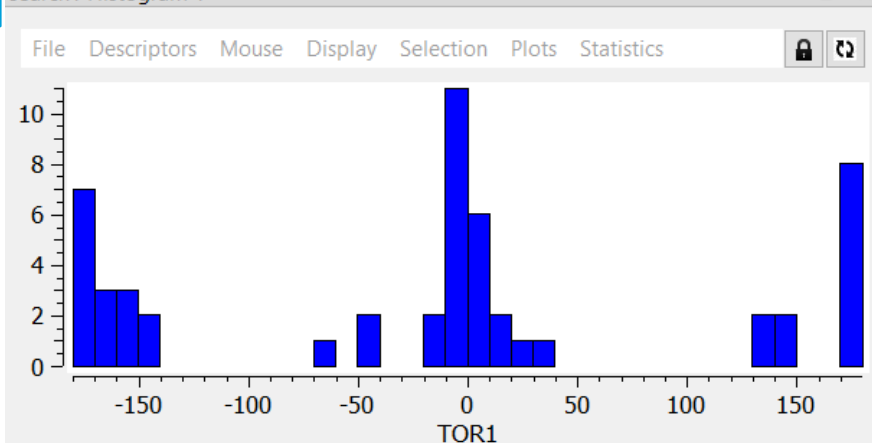
- The Mercury interface with the list of refcodes from the search in the **Structure Navigator**. The torsion angle value is highlighted on the structure in the 3D view.
- The **Hit Fragment Display Options**. This is not of interest for this example, so we can close it.
- The **Data Analysis** window, which we will use to analyse the data.

32. In the **Data Analysis** table, select the column for the torsion angle under investigation, clicking on **TOR1**. To generate a histogram with the measurements go to **Plots > Histogram**.

33. The histogram will appear at the bottom of the **Data Analysis** window. **Observe the data:** what do you notice? Where are the clusterings for this distribution? How does it compare to the one obtained from Mogul?

33

search1 Histogram 1



34. From this distribution, we can see clustering towards 180° and 0°, so it seems that this molecule prefers to have the two aromatic rings near in plane with one another, rather than twisted.

35. To compare the torsion in the molecule from the structure under investigation with this distribution, we can click on the row corresponding to the refcode GUSRER in the **Data Analysis** table and this will highlight the value on the histogram and show the structure in the Mercury interface. To see all structures in a bar of the histogram, click on the bar and you will see the corresponding rows highlighted in the table.

36. We can see that the 4,4'-dihydroxybiphenyl molecule in the structure with refcode GUSRER is the only result with an angle of ~60°. Searching for the relative orientation of two aromatic rings with *para* OH substituents shows

31c

Data Analysis

search1 Spreadsheet 1

Identifier	NAME	Query	Fragment	TOR1
search1 AKINAL 0	AKINAL	2	1	-180.0000
search1 AKINIT 1	AKINIT	2	1	179.2200
search1 BODJOT 2	BODJOT	2	1	-1.6030
search1 COBLAG 3	COBLAG	2	1	0.3670
search1 COBLAG 4	COBLAG	2	2	0.3960
search1 COBLAG 5	COBLAG	2	3	24.5390
search1 COZZEX 6	COZZEX	2	1	-180.0000
search1 CUTVEV 7	CUTVEV	2	1	-1.1460
search1 CUVNAI 8	CUVNAI	2	1	-10.3710
search1 CUVNAI 9	CUVNAI	2	2	-13.3170
search1 CUVNAI 10	CUVNAI	2	3	15.7090
search1 CUVNAI 11	CUVNAI	2	4	6.4690
search1 CUVNAI 12	CUVNAI	2	5	8.7870
search1 DOHDPH02 13	DOHDPH02	2	1	-0.3010
search1 DOHDPH10 14	DOHDPH10	2	1	-2.5790
search1 DOHDPH11 15	DOHDPH11	2	1	-180.0000
search1 ECELON 16	ECELON	2	1	172.1010
search1 ECELON01 17	ECELON01	2	1	145.1610
search1 FOQHOI 18	FOQHOI	2	1	0.0910
search1 GUSRER 19	GUSRER	2	1	-60.7840
search1 HAJQUF 20	HAJQUF	2	1	-179.8350
search1 HOVRUG 21	HOVRUG	2	1	-154.7800
search1 HUVGOW 22	HUVGOW	2	1	180.0000
search1 HUVGOW 23	HUVGOW	2	2	180.0000
search1 JAKPOB 24	JAKPOB	2	1	-0.0970
search1 JIKTUJ 25	JIKTUJ	2	1	178.3640
search1 JOBROK 26	JOBROK	2	1	-0.3420
search1 KEGIR 27	KEGIR	2	1	-178.2630
search1 KEVZUI 28	KEVZUI	2	1	-149.7260

32

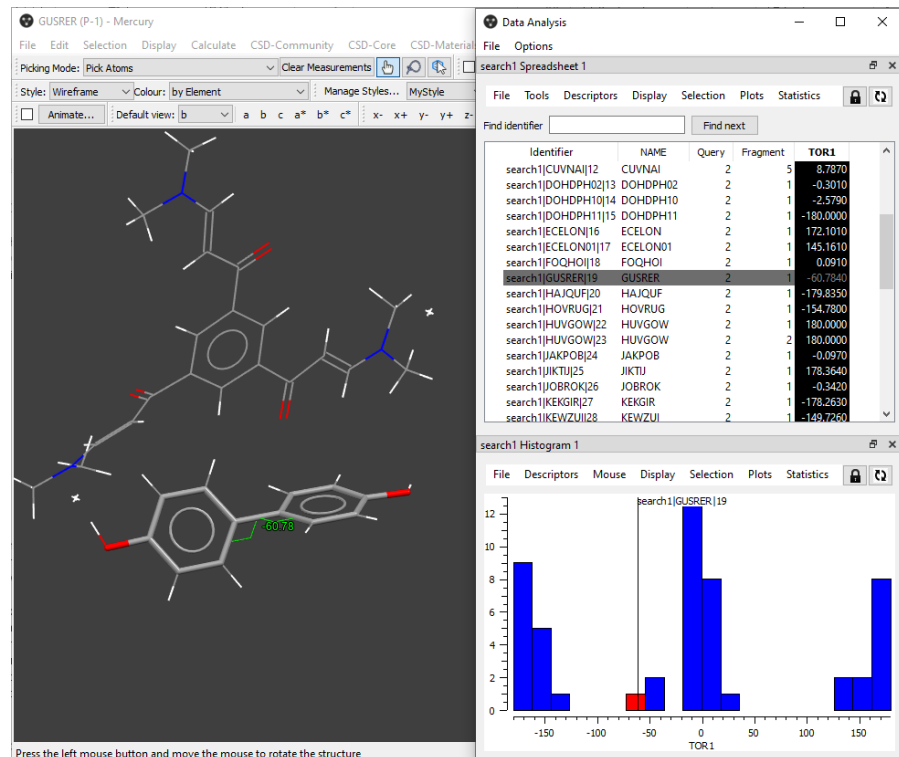
Data Analysis

search1 Spreadsheet 1

Identifier	NAME	Query	Fragment	TOR1
search1 AKINAL 0	AKINAL	2	1	-180.0000
search1 AKINIT 1	AKINIT	2	1	179.2200
search1 BODJOT 2	BODJOT	2	1	-1.6030
search1 COBLAG 3	COBLAG	2	1	0.3670
search1 COBLAG 4	COBLAG	2	2	0.3960
search1 COBLAG 5	COBLAG	2	3	24.5390
search1 COZZEX 6	COZZEX	2	1	-180.0000
search1 CUTVEV 7	CUTVEV	2	1	-1.1460
search1 CUVNAI 8	CUVNAI	2	1	-10.3710
search1 CUVNAI 9	CUVNAI	2	2	-13.3170
search1 CUVNAI 10	CUVNAI	2	3	15.7090
search1 CUVNAI 11	CUVNAI	2	4	6.4690
search1 CUVNAI 12	CUVNAI	2	5	8.7870

Plots > Histogram

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that the conformation adopted in GUSRER is highly unusual in this scenario, and even more unusual than indicated in the original Mogul analysis.

Conclusions for Example 2

This example shows how to combine advanced searches technique in the CSD-Core suite to analyse and validate structures.

The analysis performed with Mogul and ConQuest raises two questions that you might want to consider if a similar situation arises in your research while analysing your structure:

1. Is the refinement correct or is there anything that needs double-checking?
2. What is the reason driving such unusual geometry? E.g., a strong hydrogen bond network.

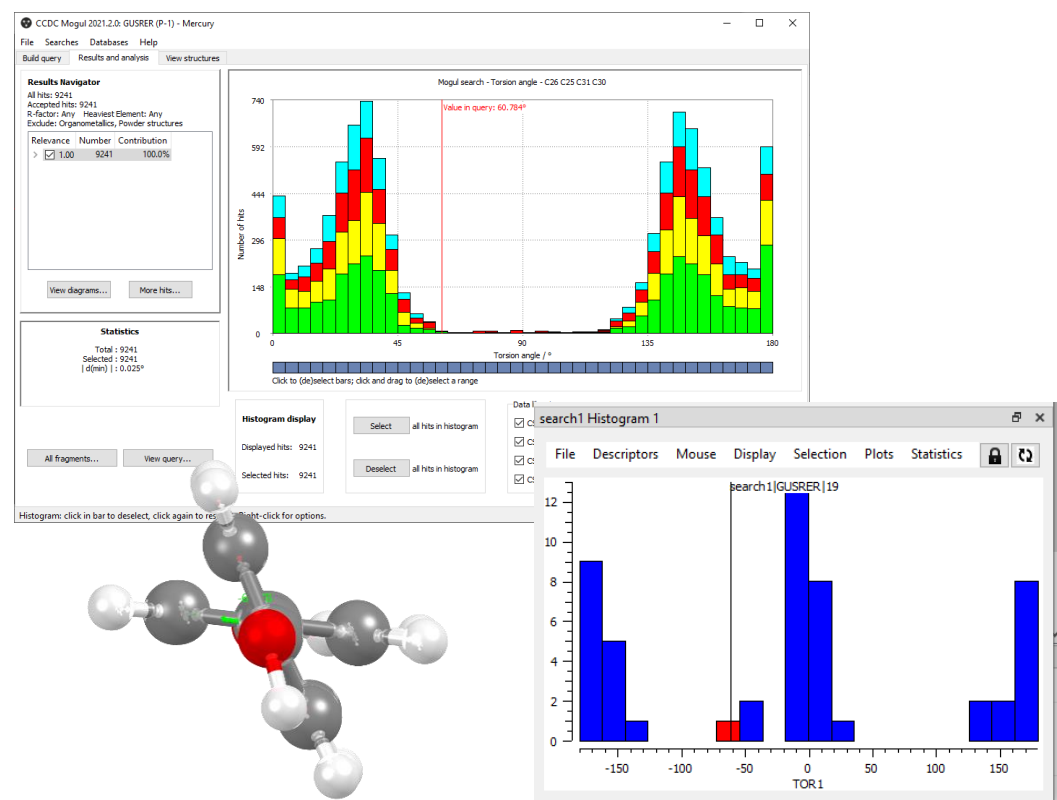
Extra tip!

When you export ConQuest result for analysis in Mercury, you can include more parameters. You can see the options available at Step 30. Including such information could complement the Mogul and ConQuest analysis performed and provide more insights.

Conclusions

After this workshop you will be able to perform an in-depth analysis of the geometry of a molecule in a structure of interest using Mogul in Mercury, with particular focus on torsion angles. In particular, you will:

- Know how to apply filters for the Mogul Geometry Check search.
- Know how to select and deselect specific bars of the histogram to restrict the visualisation of the results to specific parts of the histogram.
- Be familiar with looking for patterns and similarities in structures contributing to the same area of Mogul results.
- Know how to include or exclude structures contributing to the Mogul results based on their relevance.
- Be familiar with how to complement Mogul Geometry Check with ConQuest 3D search and Mercury analysis.



Next steps

After this workshop, you can explore more exercises in the self-guided workshops available in the [CSD-Materials workshops area](https://www.ccdc.cam.ac.uk/Community/educationalresources/workshop-materials/csd-materials-workshops/) on our website. We suggest trying the Full Interactions Maps workshop, which complement the Mogul geometry Check in the assessing of stability.

<https://www.ccdc.cam.ac.uk/Community/educationalresources/workshop-materials/csd-materials-workshops/>

You can also ask the workshop tutors for more challenging exercises or try with your own structures.

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).

Fragment

Fragment is the generic word used in Mogul for a bond, valence angle or torsion.

Hydrogen Bonds

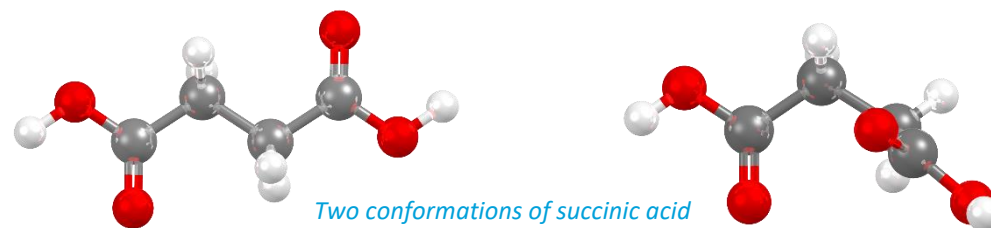
Hydrogen Bonding occurs between donor-acceptor interactions precisely involving hydrogen atoms. The H-bonds interactions are classified as: strong (mostly covalent), moderate (mostly electrostatic) and weak (electrostatic). Their strength is observed to be between 12 and 30 kJ/mol.

In silico

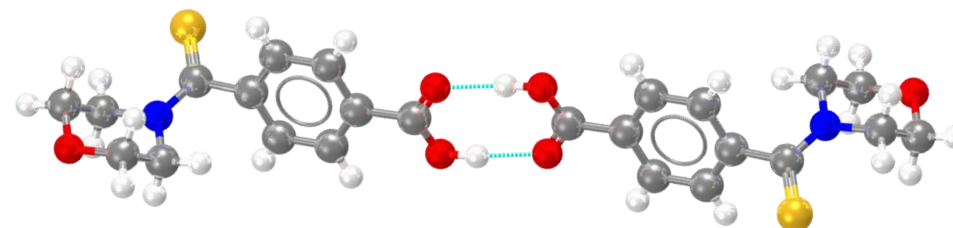
The expression *in silico* is used to refer to values that are generated via computer calculations or simulations.

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 viewed along the vector B-C.



Two conformations of succinic acid molecules, shown on refcodes SUCACB02 (left) and SUCACB19 (right)



In light blue, example of hydrogen bonds for refcode MULWIC.