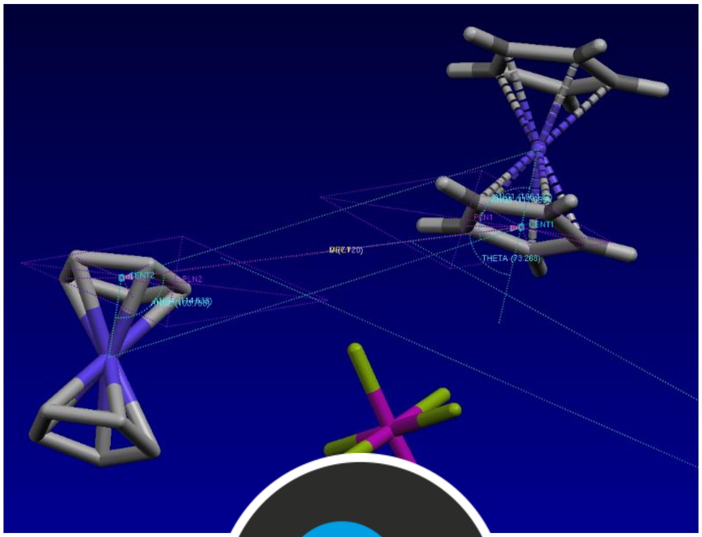
Advanced Geometry Searching in ConQuest

(CQ-008)

Developed using 2025.3 CSD Software release and CSD 6.01



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Contents

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 references to name a few. The chemical *substructure* search in ConQuest also includes the ability to define chemical constraints such as charge, hybridization state and cyclicity and to define 3D geometric parameters that can be used to generate measurement data during the search. Geometric objects such as planes, centroids and vectors can also be created and used to generate measurement data for advanced analysis; this is the focus of this workshop. ConQuest can export data in formats suitable for the Mercury Data Analysis program, for combined data analysis and structure visualisation.

Learning Outcomes

By the end of this workshop, you will be able to:

- Create a substructure search in ConQuest.
- Define centroids, planes and vectors, and distances and angles derived from them.
- Export measurements from ConQuest.
- View structures and analyse data in Mercury.

This workshop will take approximately ***25 minutes*** to be completed if you use the data supplied in the Materials section for the Analysing Data in Mercury part of this workshop. If you choose to run the ConQuest search, allow an additional 30 minutes for it to complete. The words in *Blue Italic* in the text are linked and reported in the Glossary at the end of this handout.

Pre-required Skills

If you have no previous experience with ConQuest, we recommend working through Example 1 in this self-guided workshop https://www.ccdc.cam.ac.uk/media/Introduction-to-ConQuest.pdf.

Materials

A ZIP file containing relevant files can be downloaded here. The folder contains a CSV file, which can be used in step 1 of the Analysing Data in Mercury part of this workshop if you do not have time to complete the ConQuest search. Alternatively, you can open the CQS file in ConQuest instead of running the search in step 44 of Searching in ConQuest. To do so, go to **File > Open > Search…** in ConQuest.

Example: Aromatic Interaction in Sandwich Complexes

Stacking interactions between *aromatic ligands* coordinated to transition metals have been studied by researchers, including Malenov *et al*.[1] who searched for non-covalent interactions between *sandwich* and *half-sandwich* type complexes with aromatic ligands of different ring sizes. It was reported that unsubstituted aromatic rings generally form two types of stacking interaction which are distinguished by the degree of horizontal displacement: small (offset < 3.0 Å) and large (offset > 4.5 Å). In this example, we will take a subset of the complexes studied, namely sandwich complexes with one unsubstituted cyclopentadienyl (Cp) ligand, to demonstrate the general approach to 3D structure searching.

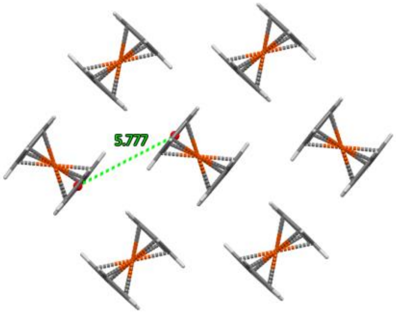

Figure 1. A section of the CSD entry FEROCE04 with a potential parallel displaced stacking interaction highlighted.

Interaction Geometry

The goal of the ConQuest search is to find instances of the parallel displaced stacking type of aromatic interaction, as shown in the Figure 2, below.

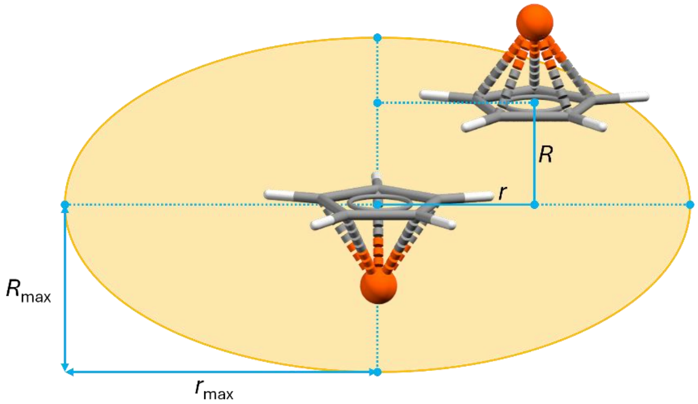

Figure 2. Stacking interactions between aromatic ligands in organometallic compounds can be defined according to the ellipse $\frac{r^2}{r_{\max}^2} + \frac{R^2}{R_{\max}^2} \leq 1$ as shown in the diagram. For Cp, r_{max} = 7.5 Å and R_{max} = 4.0 Å.

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[1] D. P. Malenov, D. Z. Vojislavljević-Vasilev and S. Zarić, *Crystallogr. Rev.*, 31, 2025, 60-95 DOI: 10.1080/0889311X.2025.2545799

In ConQuest, we cannot measure the horizontal (*r*) and vertical components (*R*) directly. Instead, we can define *centroids* (Ω_1 and Ω_2, Figure 3), and the vector joining them, **d**. We can then define mean planes for each of the C_5 rings and calculate the angle between the normal to the plane containing Ω_1 and **d**, θ. The angle between the mean planes, φ, should be less than 10° for stacking interactions, as shown in Figure 3.

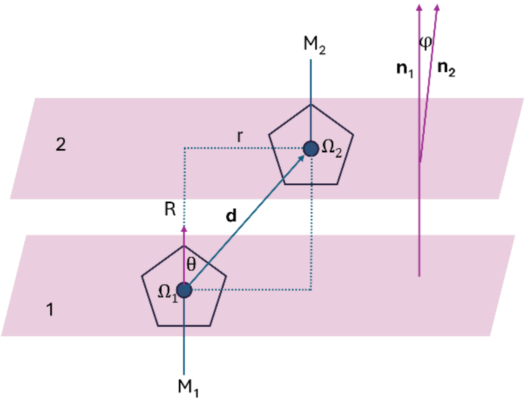


Figure 3. The geometry of aromatic interactions between metal cyclopentadienyl fragments. θ is angle between plane normal and vector from centroid Ω_1 to centroid Ω_2.

The components, $r = |\mathbf{d}|\ \sin(\theta)$ and $R = |\mathbf{d}|\ \cos(\theta)$ can be calculated in Mercury and filters applied to limit the data to the boundary of the ellipse in Figure 2.

A puzzle-type packing motif is often found in sandwich complex crystal structures (see Figure 3). This also leads to a parallel arrangement of aromatic ligands, but this arrangement is not an aromatic stacking interaction; rather, it is an intermolecular metal-ligand interaction.

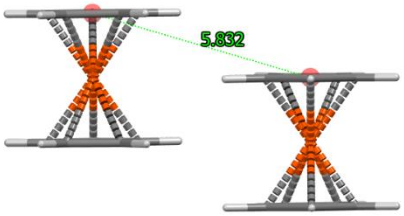


Figure 4. A pair of ferrocene molecules from CSD entry FEROCE24. Centroid-to-centroid distance shown.

To avoid measuring instances of this interaction, further constraints should be applied as shown in Figure 5. The next section guides you through setting up these geometrical constraints in combination with a sandwich complex substructure.

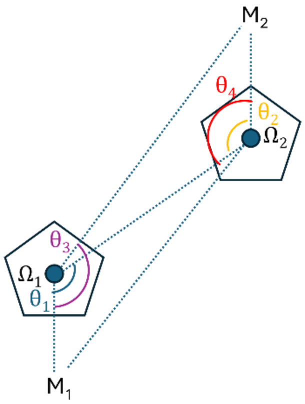
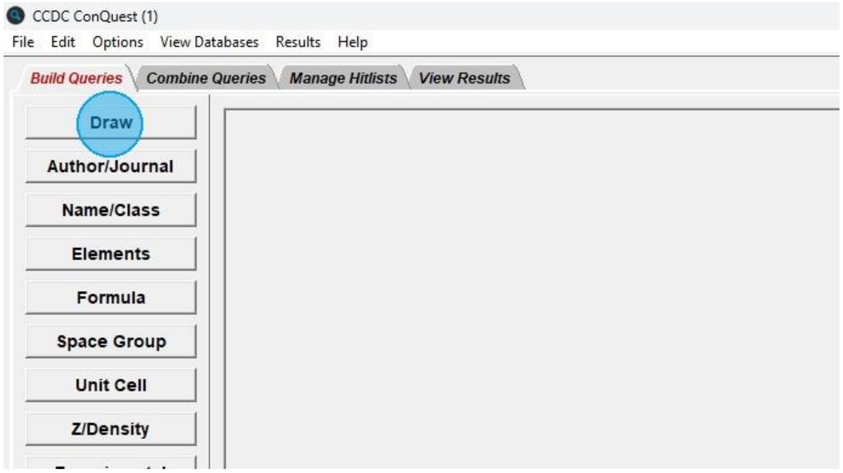


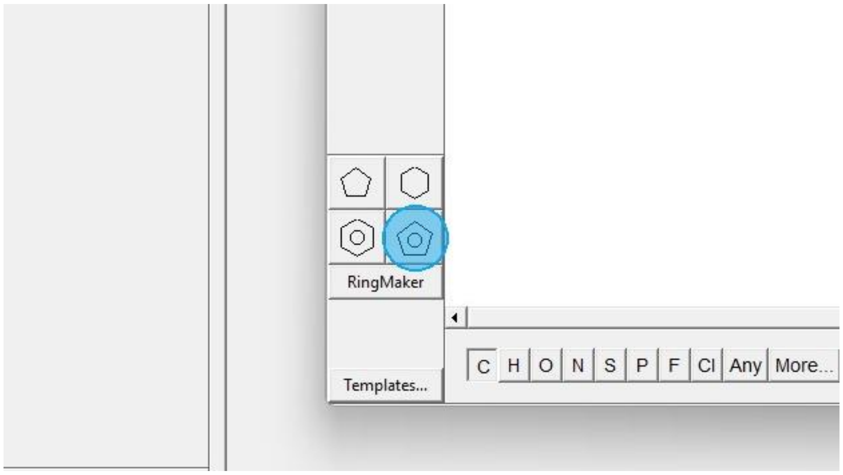
Figure 5. Additional geometrical constraints to avoid measuring puzzle-type packing features. Ω_1 and Ω_2 are the C_5 ring centroids, θ_1, θ_2, θ_3 and $\theta_1 > 90°$ for true aromatic interaction features.

Searching in ConQuest

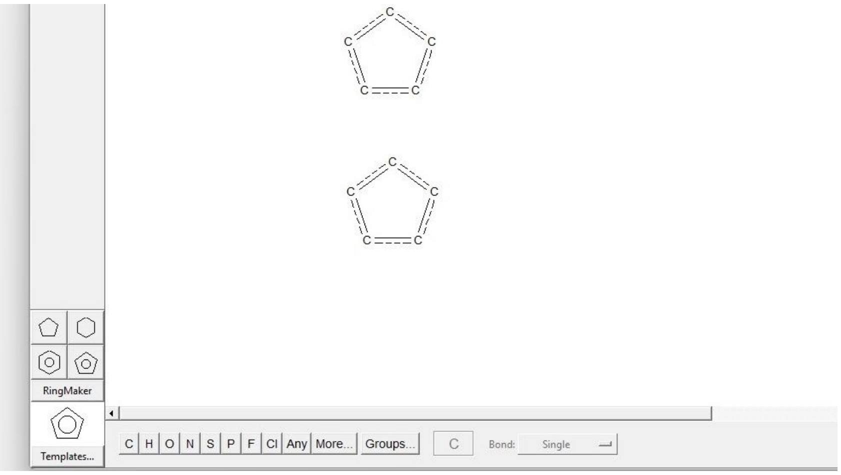
1. Open ConQuest from the Start menu or by clicking the desktop icon. Go to the **Build Queries** tab and click on **Draw**.



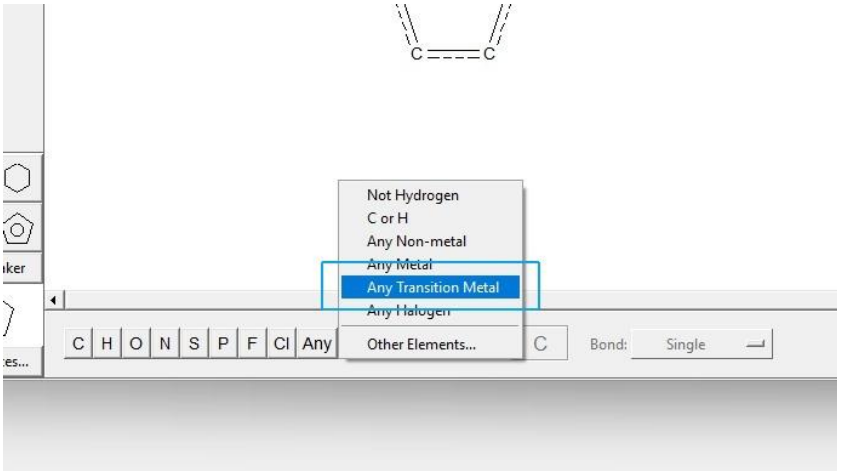
2. Click the Cp template icon.



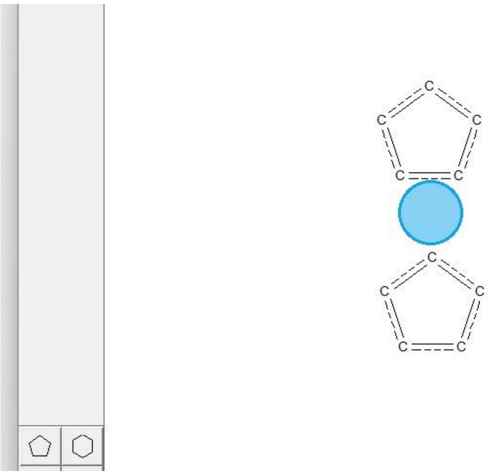
3. Click in the sketcher twice to add two Cp rings, on above the other, as shown.



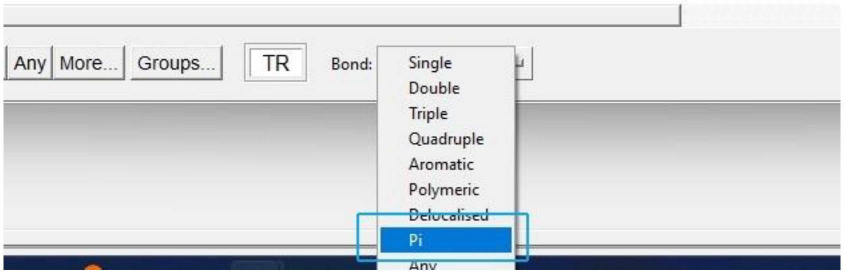
4. Click on the **More**... drop-down menu at the bottom and select **Any Transition Metal**. You should see TR in the box next to Groups.



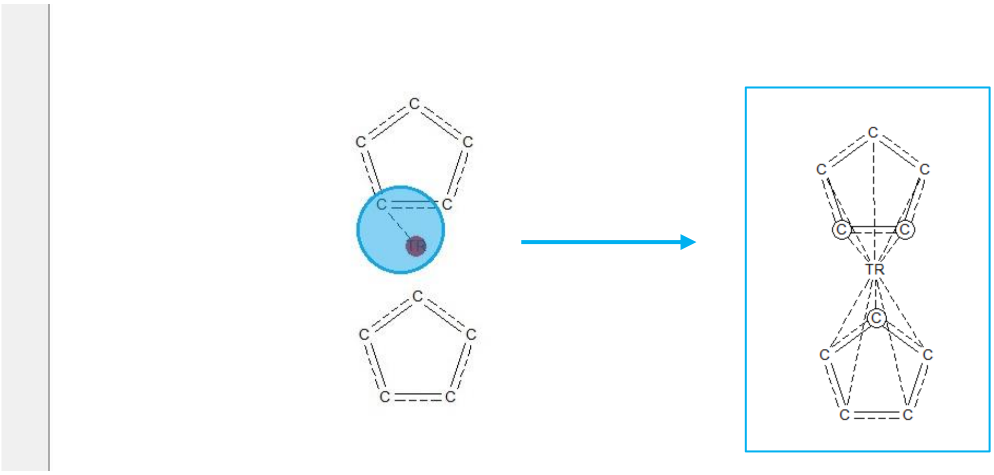
5. Click in the visualiser area in between the Cp rings to add a transition metal



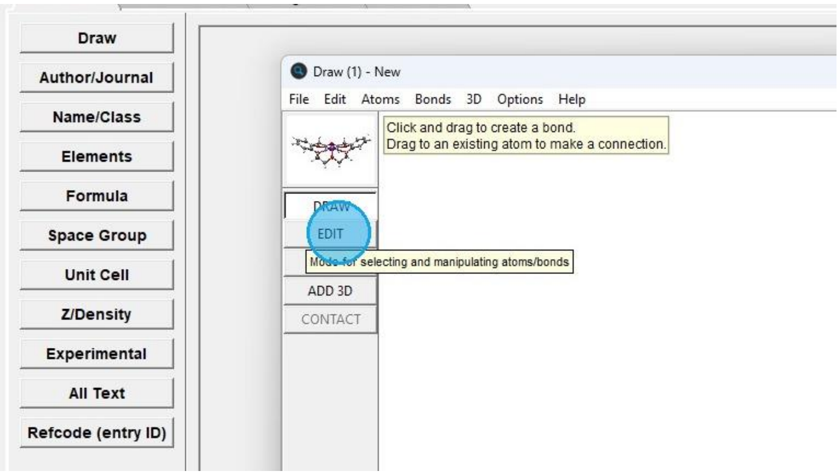
6. Click on the **Bond** drop-down menu and select **Pi** from the bond types.



7. Click on the transition metal 'TR', drag to a carbon atom of the Cp ring and release to add a bond. Repeat this process until all 10 metal-carbon bonds have been added.



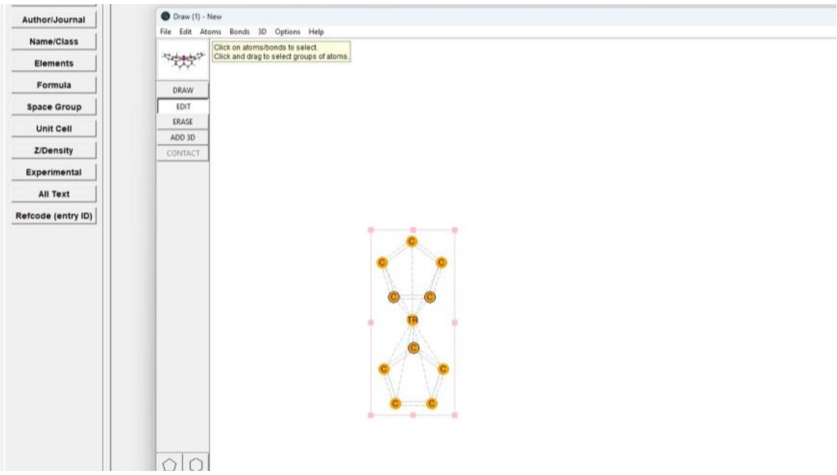
8. Click **Edit**.



Click and drag to create a bond.
Drag to an existing atom to make a connection.

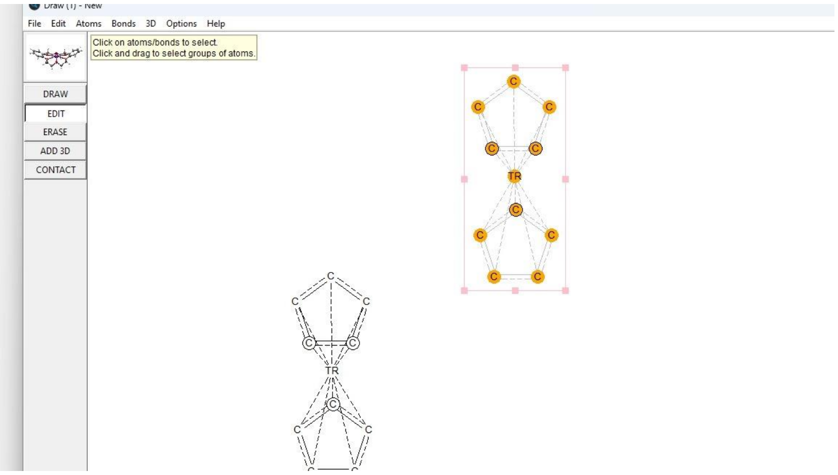
Mode for selecting and manipulating atoms/bonds

9. Left-click and drag a box around the metallocene substructure using the mouse, then press Ctrl + C



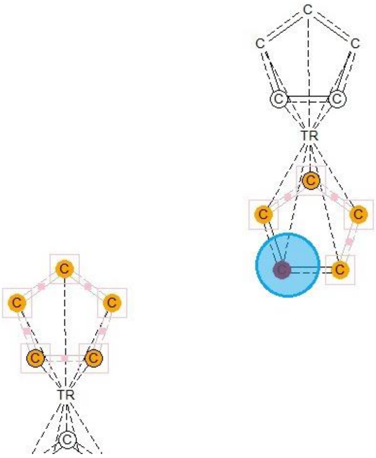
Click on atoms/bonds to select.
Click and drag to select groups of atoms.

10. Press Ctrl + V and reposition the second metallocene above and to the right of the first one. We shall refer to the lower left substructures as “1” and the upper right one as “2”. This will be important when we create geometric objects involving each substructure. Click in an empty area of the sketcher to deselect the molecule.

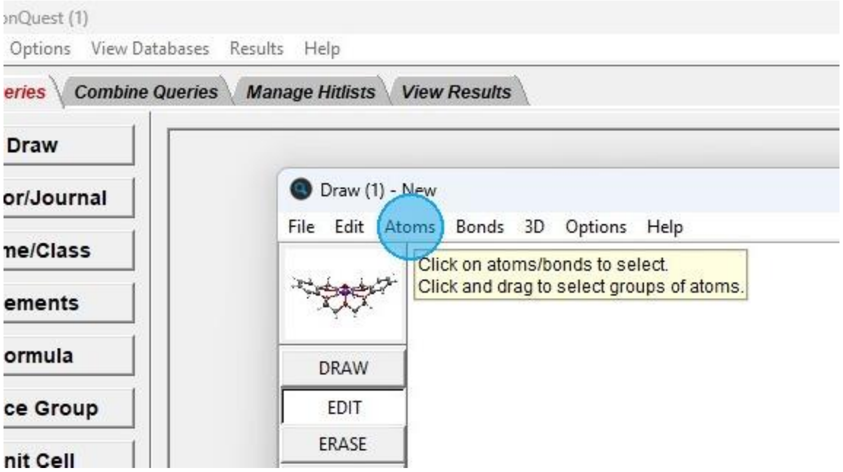


Click on atoms/bonds to select.
Click and drag to select groups of atoms.

11. We now need to add hydrogens to the substructure. These only need to be added to the pair of rings that we will specify as interacting (using geometric constraints, in the following steps). The other Cp ring can have substituents, so we should not add hydrogens to them. Hold down Shift and click on the carbon atoms in the upper ring of substructure 1 and the lower ring of substructure 2. They will be highlighted in orange.

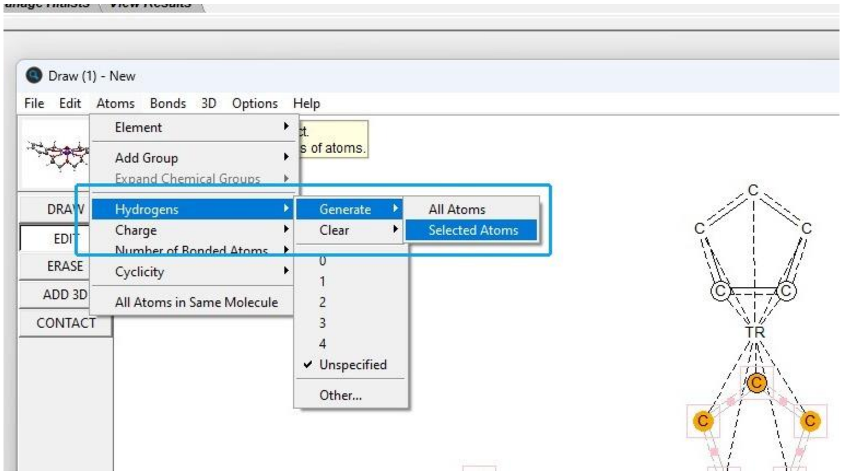


12. From the top menu, click **Atoms**.

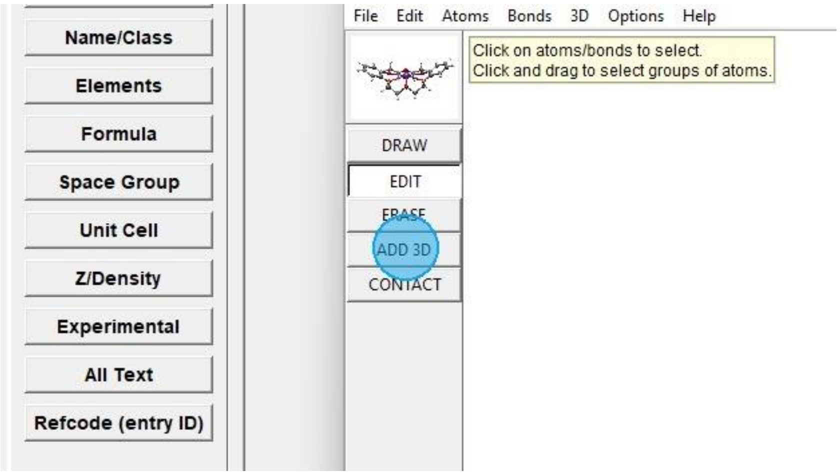


Click on atoms/bonds to select.
Click and drag to select groups of atoms.

13. Select **Hydrogens > Generate > Selected Atoms**.

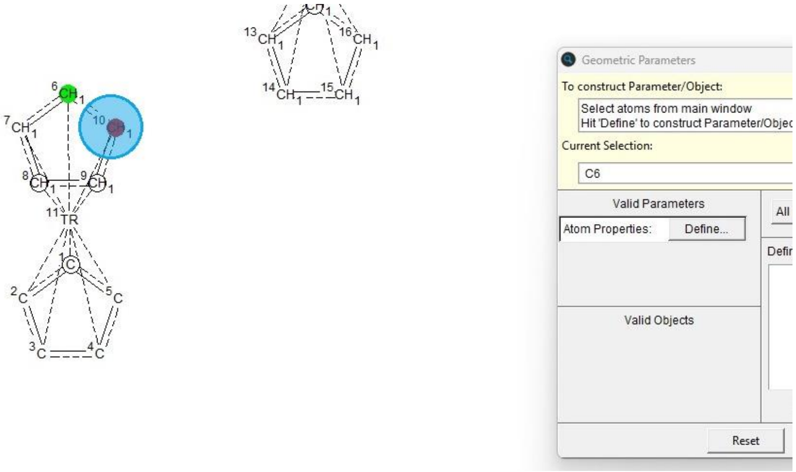


14. Click **ADD 3D**.



Click on atoms/bonds to select.
Click and drag to select groups of atoms.

15. The Geometric Parameters window will appear. This is where we can define the constraints needed to match the conditions discussed in the Interaction Geometry section and where we define the 3D parameters that we will be needed for the analysis section later. Click on each atom of the upper Cp ring of substructure 1. They will become highlighted green as they are selected.


Geometric Parameters

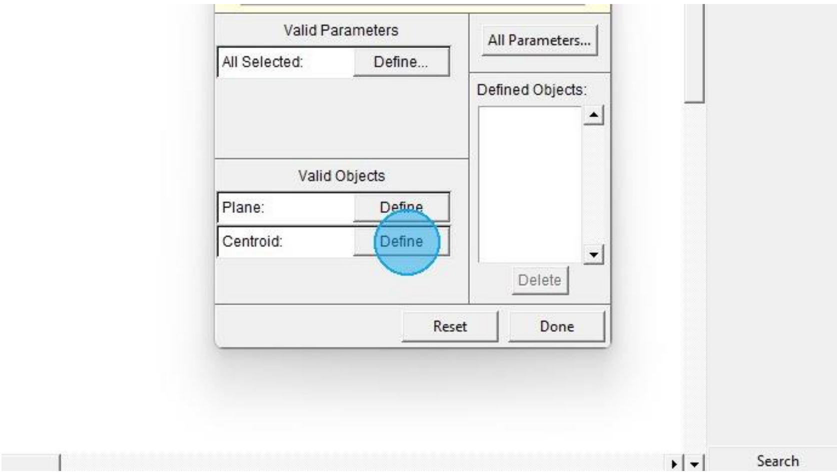
To construct Parameter/Object:

Select atoms from main window
Hit 'Define' to construct Parameter/Objec

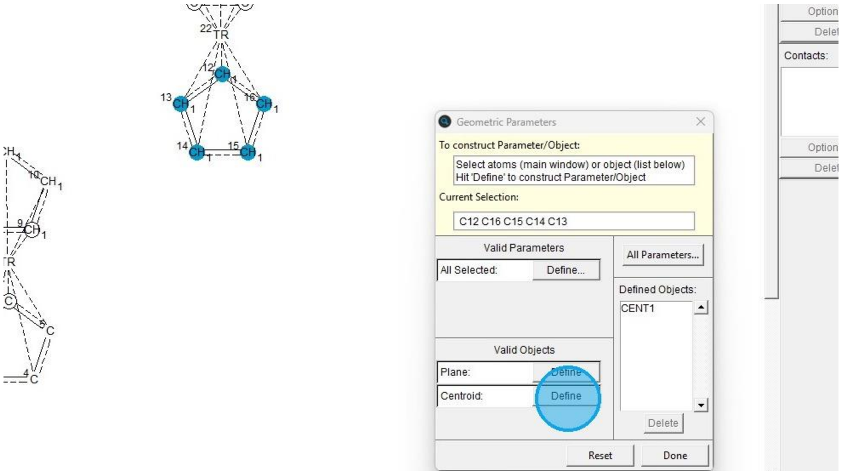
Current Selection:

C6

16. Click **Define**, next to Centroid.



17. Repeat this process to define the centroid for the lower ring of substructure 2.



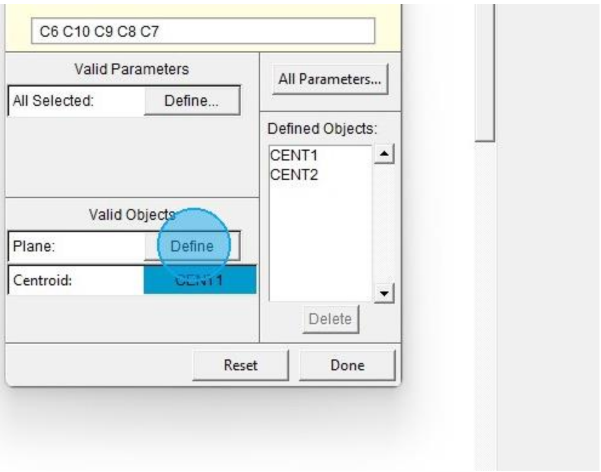
To construct Parameter/Object:

Select atoms (main window) or object (list below)
Hit 'Define' to construct Parameter/Object

Current Selection:

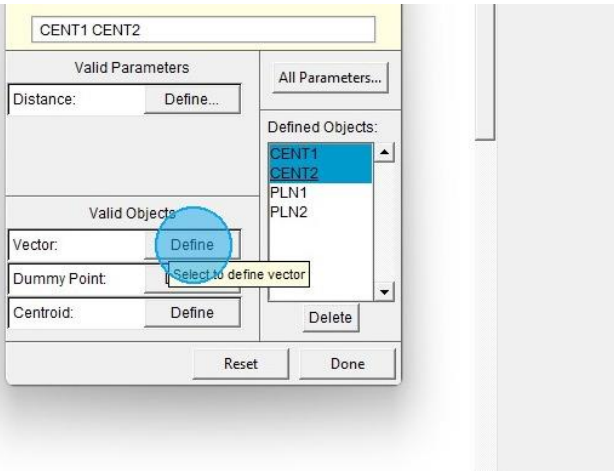
C12 C16 C15 C14 C13

18. Select the atoms in the upper ring of substructure 1 and click **Define** next to Plane. This will define mean planes involving the carbon atoms of the Cp ring. Do the same for the lower ring of substructure 2.



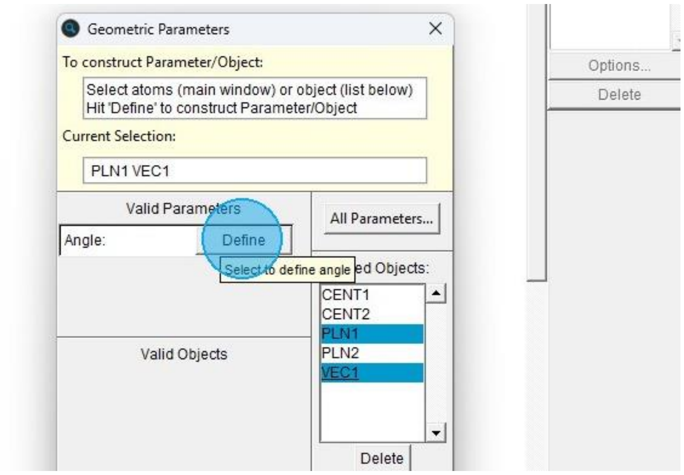
C6 C10 C9 C8 C7

19. When you have completed these steps you should see CENT1, CENT2, PLN1 and PLN2 in the Defined objects panel. Click on **CENT1**, then **CENT2**. Click **Define** next to Vector.



CENT1 CENT2

20. Next, click **PLN1** and **VEC1**. Then click **Define** next to Angle. This will calculate the angle between the plane normal and the inter-centroid vector, which we will use later to calculate the components of the centroid-centroid distance.



Geometric Parameters

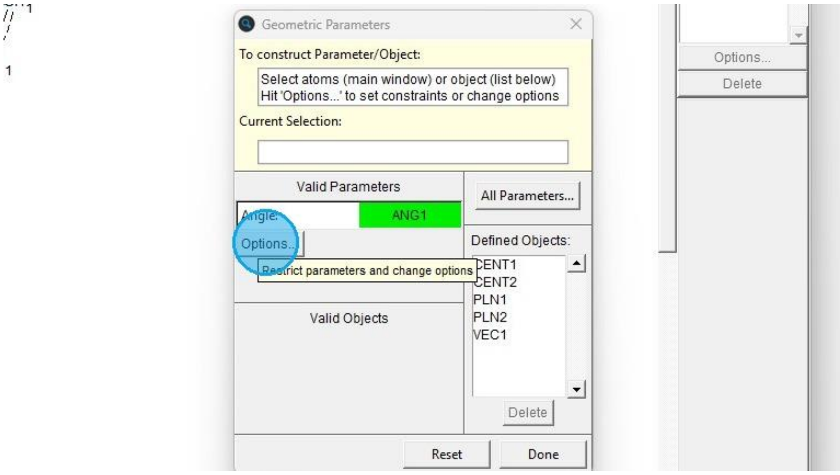
To construct Parameter/Object:

Select atoms (main window) or object (list below)
Hit 'Define' to construct Parameter/Object

Current Selection:

PLN1 VEC1

21. Click **Options**.



Geometric Parameters

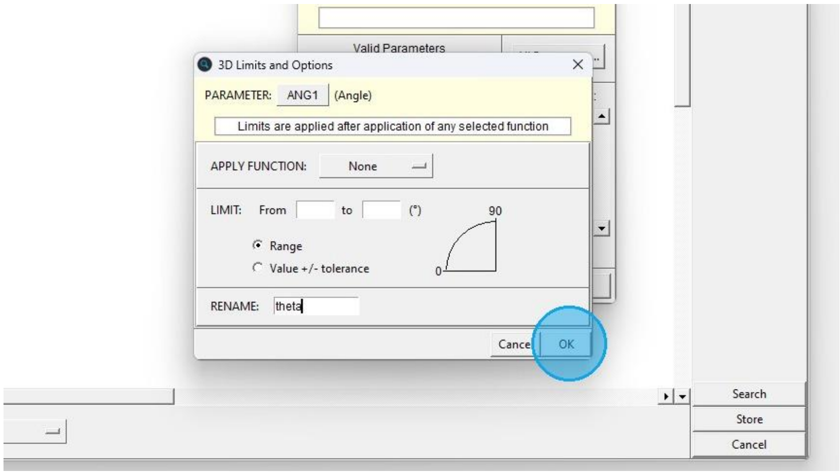
To construct Parameter/Object:

Select atoms (main window) or object (list below)
Hit 'Options...' to set constraints or change options

Current Selection:

Restrict parameters and change options

22. In the RENAME: box, type "theta", then click **OK**.



3D Limits and Options

PARAMETER: ANG1 (Angle)

Limits are applied after application of any selected function

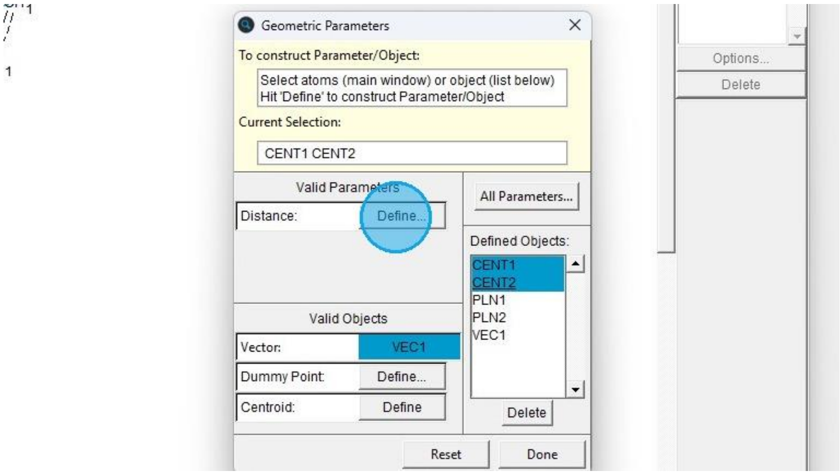
APPLY FUNCTION: None

LIMIT: From to (°)

● Range
○ Value +/- tolerance

RENAME: theta

23. In the Geometric Parameters window, click on **CENT1** and **CENT2**, then click **Define** next to Distance.



Geometric Parameters

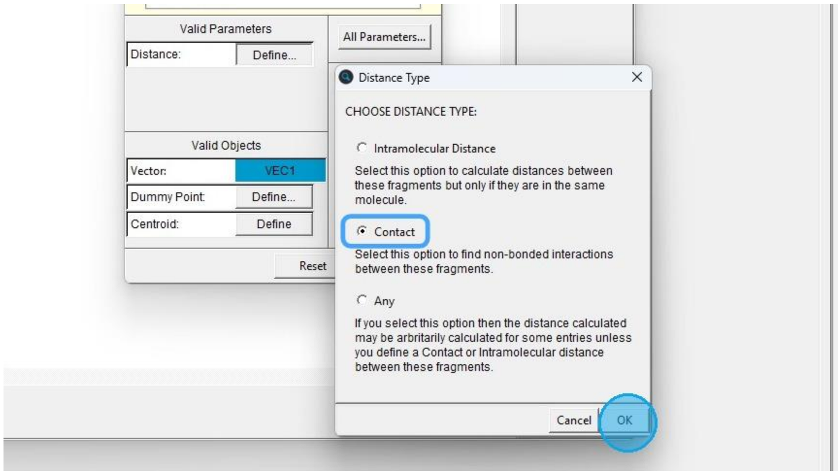
To construct Parameter/Object:

Select atoms (main window) or object (list below)
Hit 'Define' to construct Parameter/Object

Current Selection:

CENT1 CENT2

24. We need to tell ConQuest what type of distance to measure. In this example, we are looking for intermolecular interactions, therefore, choose the **Contact** option in the Distance Type window. Then click **OK**.



CHOOSE DISTANCE TYPE:

○ Intramolecular Distance

Select this option to calculate distances between these fragments but only if they are in the same molecule.

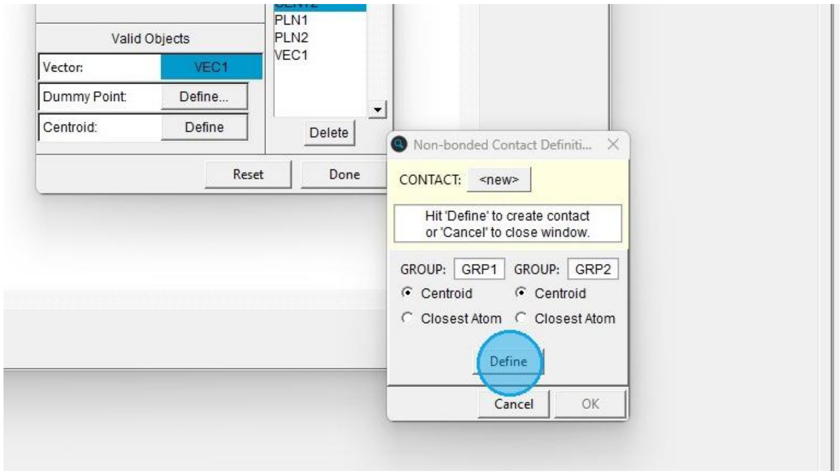
● Contact

Select this option to find non-bonded interactions between these fragments.

○ Any

If you select this option then the distance calculated may be arbritarily calculated for some entries unless you define a Contact or Intramolecular distance between these fragments.

25. In the Non-bonded Contact Definition window, click **Define.**



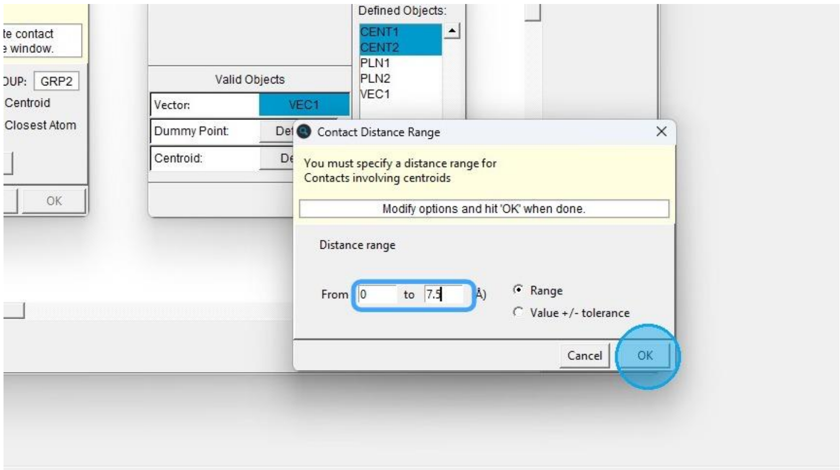
CONTACT: <new>

Hit 'Define' to create contact or 'Cancel' to close window.

GROUP: GRP1
● Centroid
○ Closest Atom

GROUP: GRP2
● Centroid
○ Closest Atom

26. We need to define a distance range for an intermolecular contact to get reasonable results. From the introduction we know the maximum possible distance is 7.5 Å. Therefore, type from 0 to 7.5 in the text boxes (ensuring **Range** is ticked). We will apply the ellipse boundary conditions later on. Click **OK**.



Contact Distance Range

You must specify a distance range for Contacts involving centroids

Modify options and hit 'OK' when done.

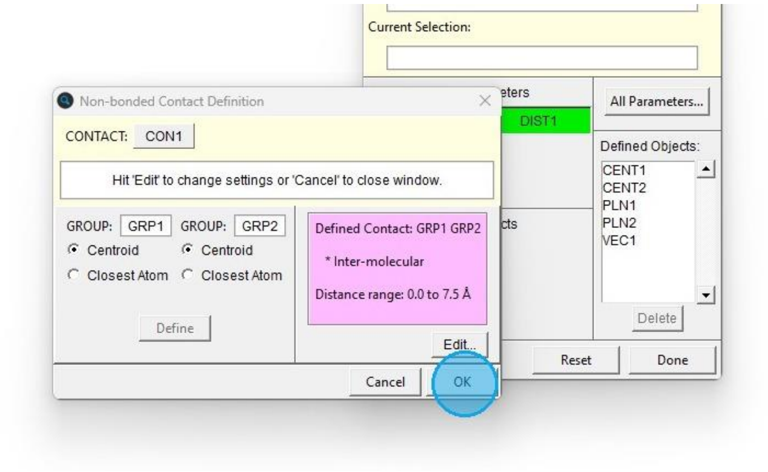
Distance range

From 0 to 7.5 Å)

● Range

○ Value +/- tolerance

27. Click **OK** in the Non-Bonded Contact Definition window.



Non-bonded Contact Definition

CONTACT: CON1

Hit 'Edit' to change settings or 'Cancel' to close window.

GROUP: GRP1 ● Centroid ○ Closest Atom

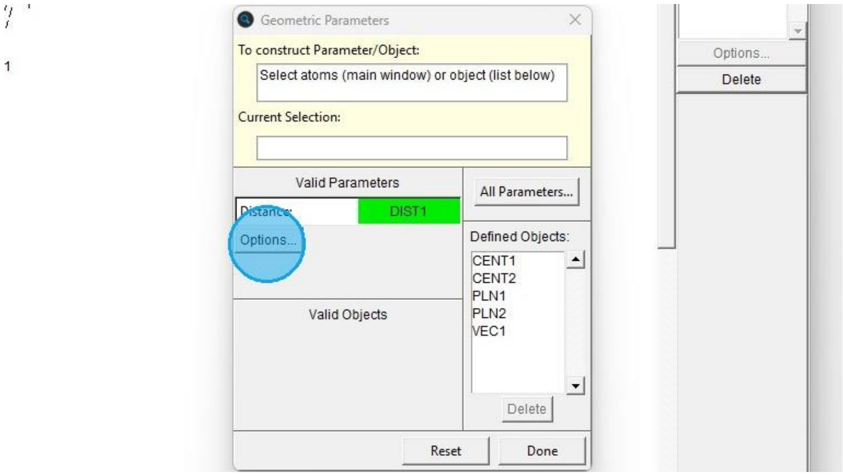
GROUP: GRP2 ● Centroid ○ Closest Atom

Defined Contact: GRP1 GRP2

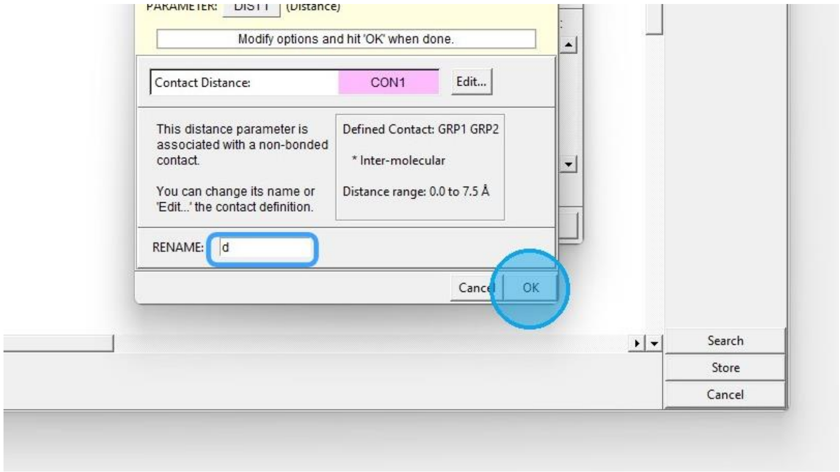
* Inter-molecular

Distance range: 0.0 to 7.5 Å

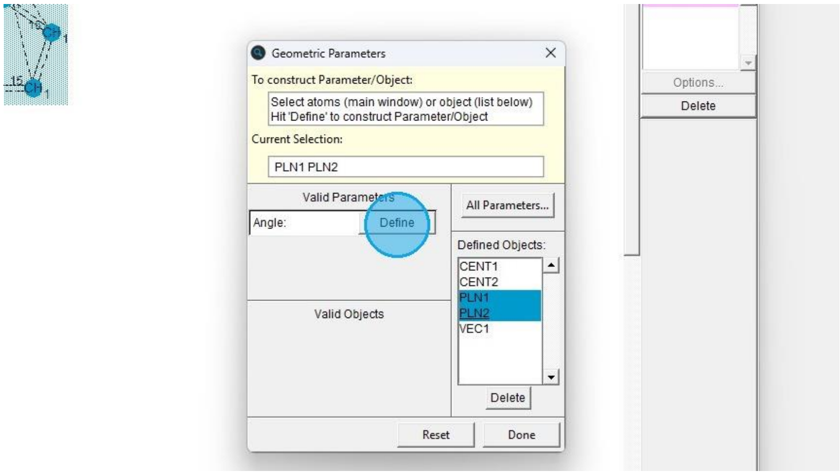
28. Click **Options**.



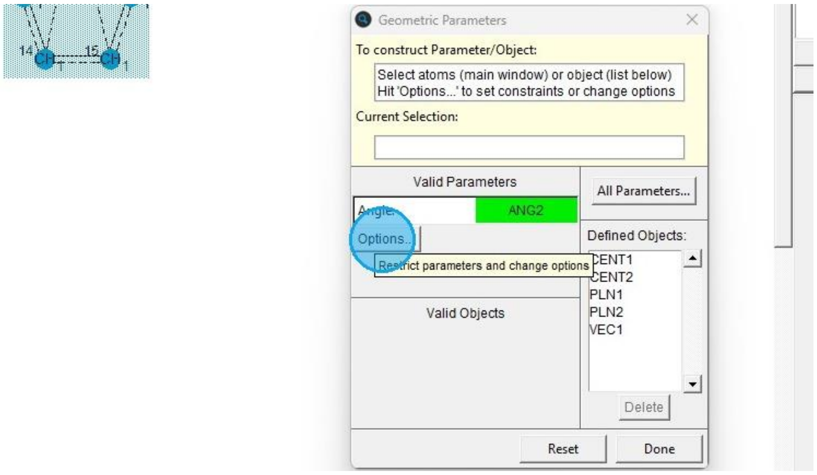
29. Rename the parameter "d", then click **OK**.



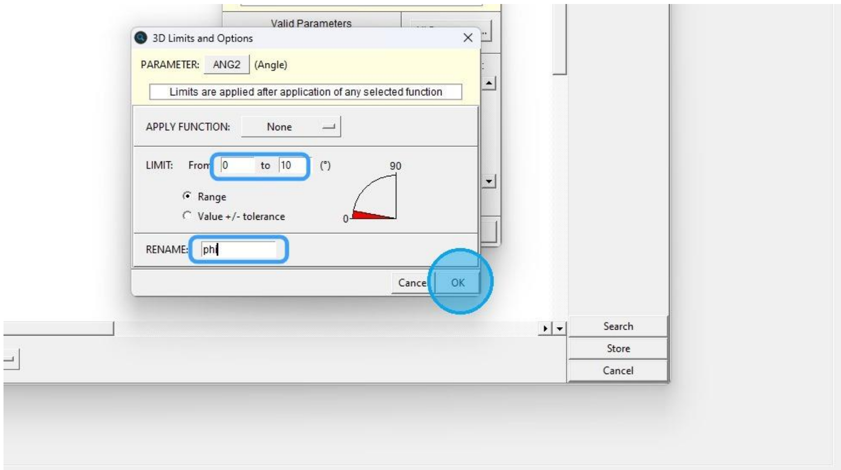
30. We next need to restrain the rings to be parallel within a certain tolerance. We can do this by defining the angle between their mean planes. Click **PLN1** and **PLN2**, then click **Define** next to Angle.



31. Click **Options**.



32. In the LIMIT range, type 0 for the lower limit and 10 for the upper limit. Also rename the parameter "phi". Click **OK**.



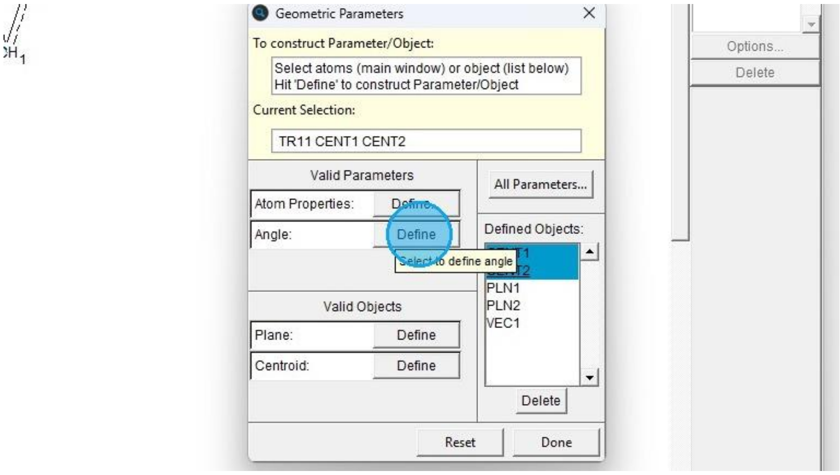
PARAMETER: ANG2 (Angle)

LIMIT: From 0 to 10

● Range

RENAME: phi

33. We next need to apply some constraints to the angles between the substructures to avoid irrelevant interactions (see Figure 5). Recall that (1) and (2) refer to the lower and upper substructures, respectively; click, in order, **TR**(1) **CENT1 CENT2**. You can see this highlighted green in the next step. click **Define** next to Angle.



Geometric Parameters

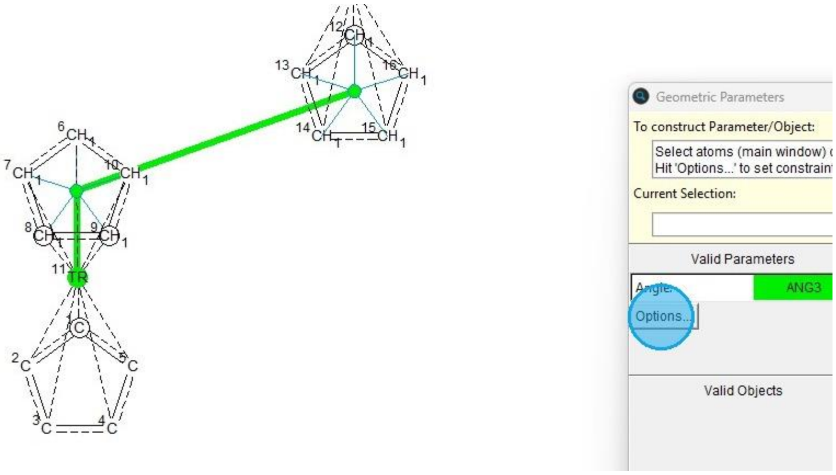
To construct Parameter/Object:

Select atoms (main window) or object (list below)
Hit 'Define' to construct Parameter/Object

Current Selection:

TR11 CENT1 CENT2

34. Click **Options**.



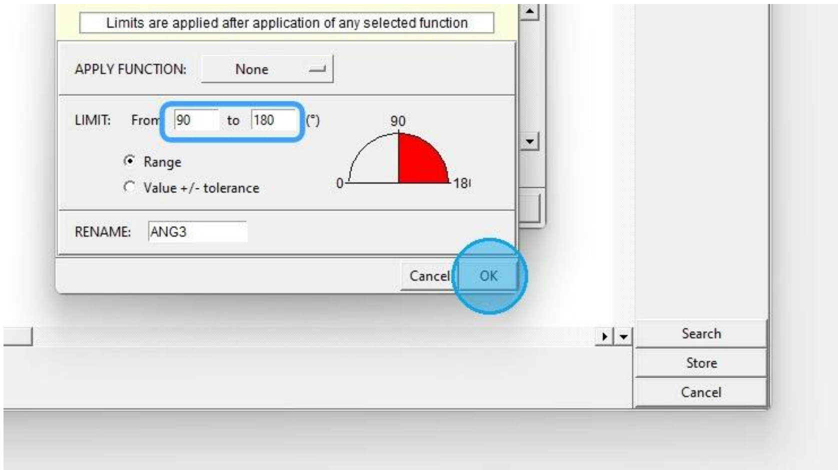
Geometric Parameters

To construct Parameter/Object:

Select atoms (main window)
Hit 'Options...' to set constrain

Current Selection:

35. Limit the angle range from 90 to 180° and click **OK**.



Limits are applied after application of any selected function

APPLY FUNCTION: None

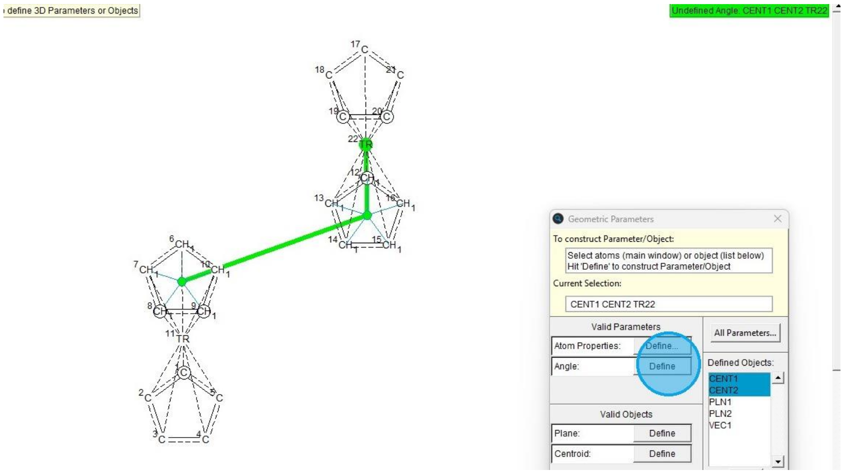
LIMIT: From 90 to 180 (°)

● Range

○ Value +/- tolerance

RENAME: ANG3

36. Following previous two steps, define the angle given by **CENT1 CENT2 TR**(2) as shown in the image below and constrain the angles from 90 to 180°.



define 3D Parameters or Objects

Undefined Angle: CENT1 CENT2 TR22

Geometric Parameters

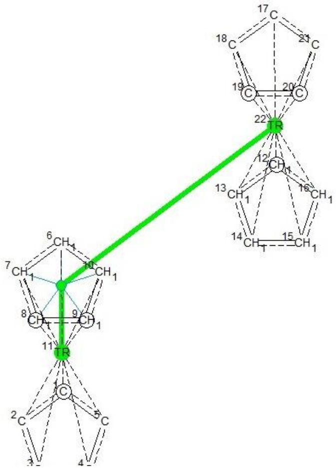
To construct Parameter/Object:

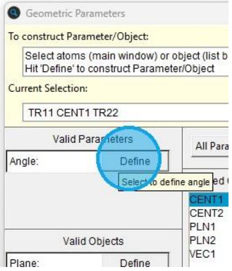
Select atoms (main window) or object (list below)
Hit 'Define' to construct Parameter/Object

Current Selection:

CENT1 CENT2 TR22

37. Define the angle given by **TR**(1) **CENT1 TR**(2) as shown in the image below and constrain the angles from 90 to 180°.





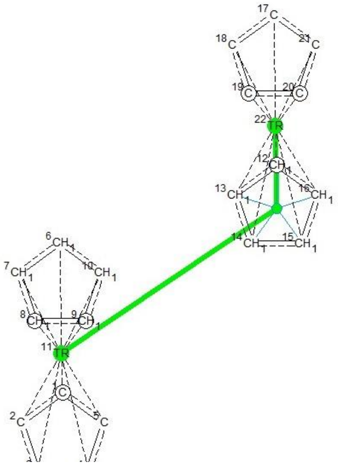
To construct Parameter/Object:

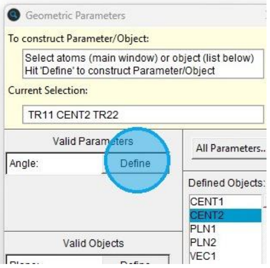
Select atoms (main window) or object (list b
Hit 'Define' to construct Parameter/Object

Current Selection:

TR11 CENT1 TR22

38. Define the angle given by **TR**(1) **CENT2 TR**(2) as shown and constrain the angle to be between 90 and 180°.





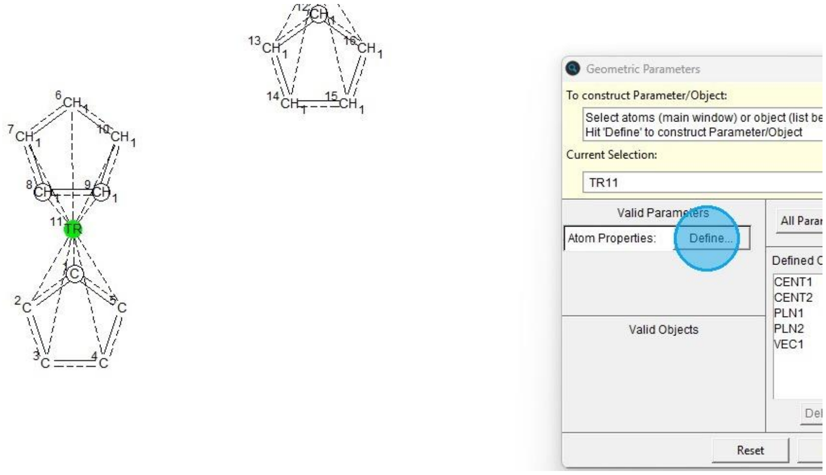
To construct Parameter/Object:

Select atoms (main window) or object (list below)
Hit 'Define' to construct Parameter/Object

Current Selection:

TR11 CENT2 TR22

39. Next, we will define the number of connected atoms to each transition metal. One to nine connected atoms can be added as constraints in the search, however since we will have a minimum of 10, we will need to gather the number of connected atoms in the search and apply a filter post search. Click on **TR**(1) and click **Define** next to Atom Properties.

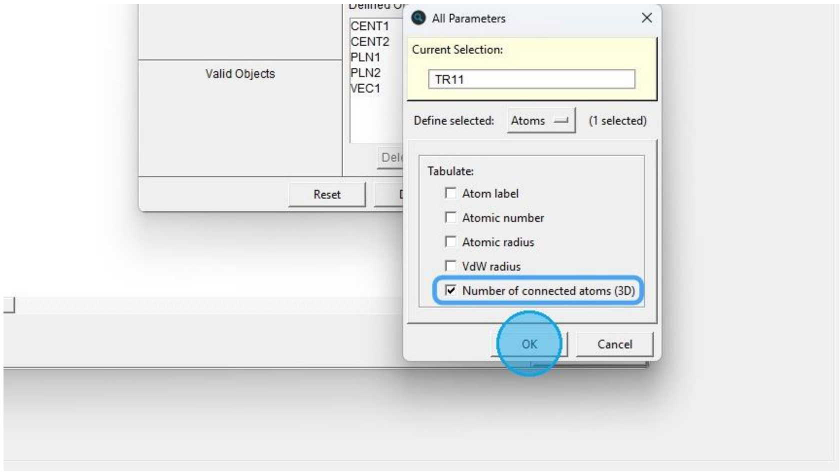


To construct Parameter/Object:

Select atoms (main window) or object (list be
Hit 'Define' to construct Parameter/Object

Current Selection: TR11

40. Tick the box for **Number of connected atoms**, then click **OK**.

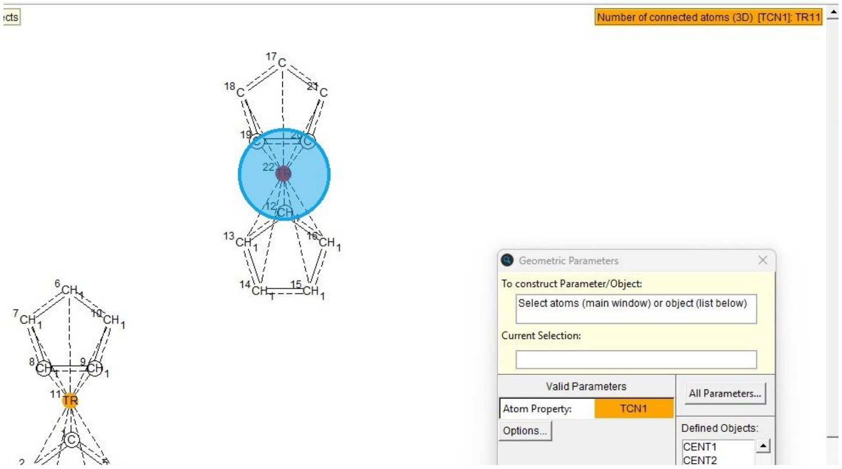


Current Selection: TR11

Define selected: Atoms (1 selected)

☐ Atom label
☐ Atomic number
☐ Atomic radius
☐ VdW radius
☑ Number of connected atoms (3D)

41. Repeat the preceding two steps to define the number of connected atoms for **TR**(2).


Number of connected atoms (3D) [TCN1]: TR11

Geometric Parameters

To construct Parameter/Object:

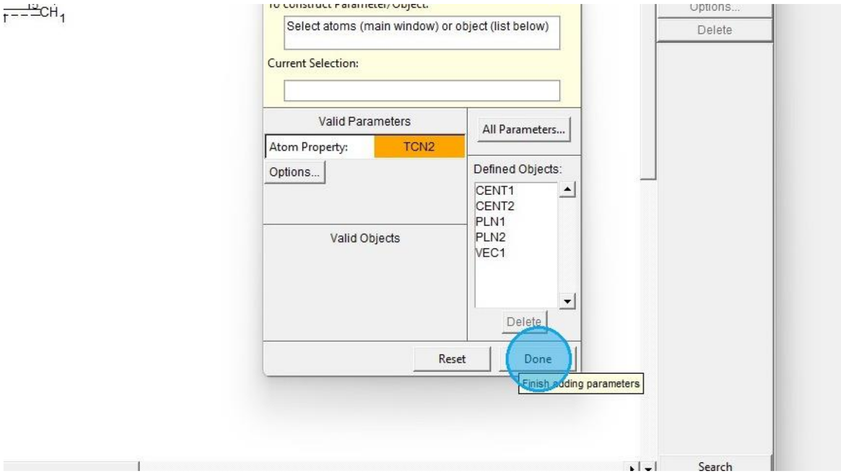
Select atoms (main window) or object (list below)

Current Selection:

Atom Property: TCN1

Defined Objects:
CENT1
CENT2

42. Click **Done** in the Geometric Parameters window.


Select atoms (main window) or object (list below)

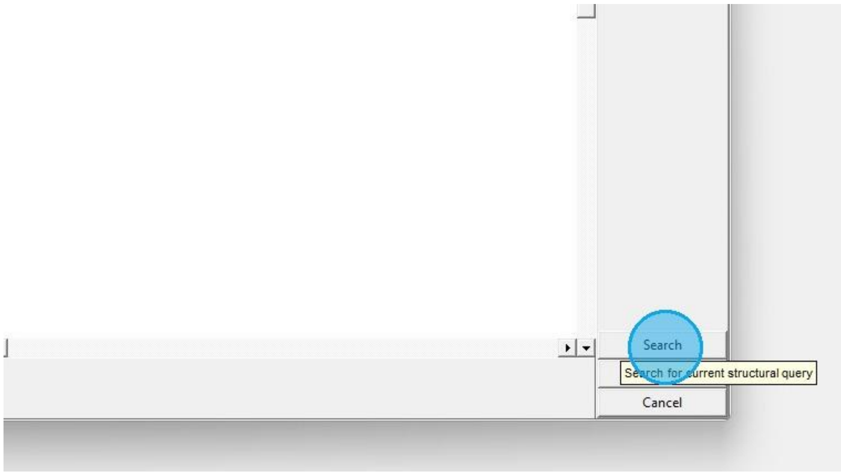
Current Selection:

Atom Property: TCN2

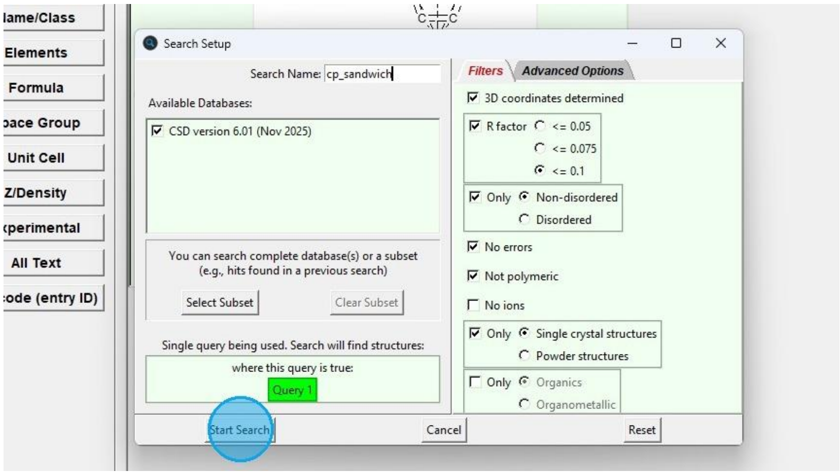
Defined Objects:
CENT1
CENT2
PLN1
PLN2
VEC1

Finish adding parameters

43. Click **Search**.


Search for current structural query

44. Give the search a suitable name, such as cp_sandwich, then in the Filters tab, check **3D coordinates determined**, **R factor <=0.1**, **Only Non-disordered**, **No errors**, **Not polymeric** and **Only Single crystal structures**. When you are ready, click **Start Search**. The search will take about **30 mins** to run so we recommend proceeding to the Analysing Data in Mercury section on page 29 at this point and using the search data supplied here. You can complete this section later.



Search Setup

Search Name: cp_sandwich

Available Databases:

☑ CSD version 6.01 (Nov 2025)

You can search complete database(s) or a subset (e.g., hits found in a previous search)

Single query being used. Search will find structures:

where this query is true:

Query 1

Filters

☑ 3D coordinates determined

☑ R factor ○ <= 0.05 ○ <= 0.075 ● <= 0.1

☑ Only ● Non-disordered ○ Disordered

☑ No errors

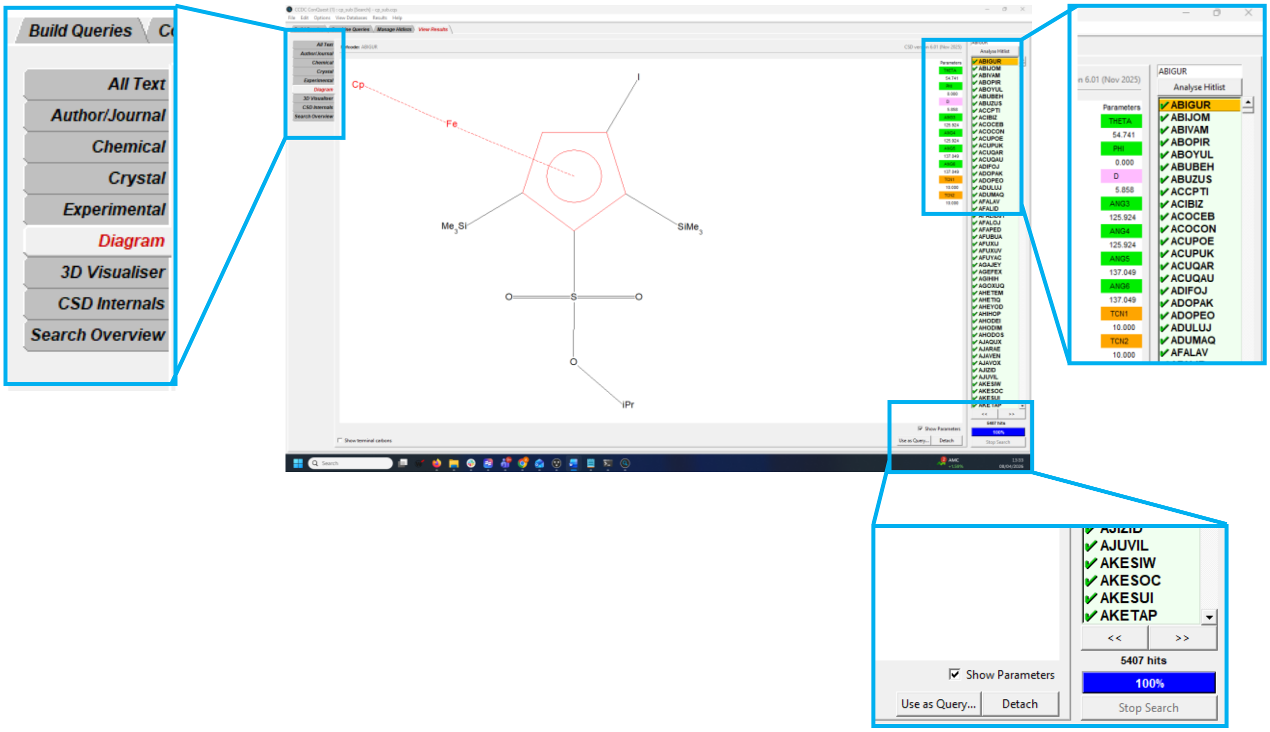
☑ Not polymeric

☐ No ions

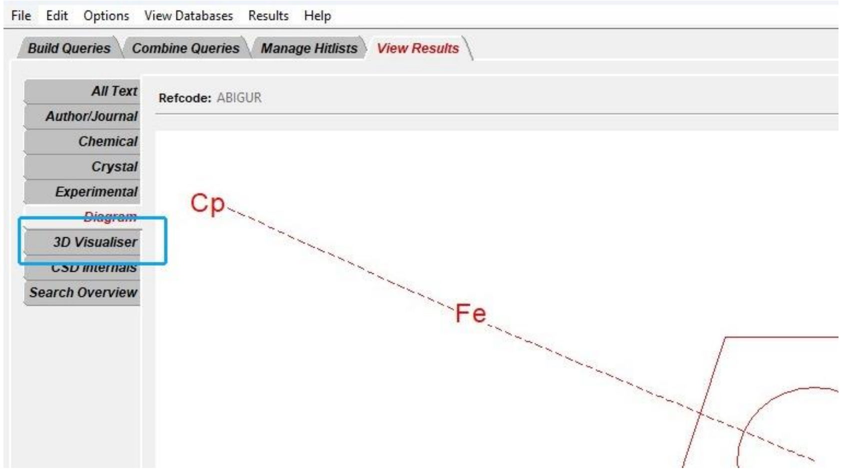
☑ Only ● Single crystal structures ○ Powder structures

☐ Only ● Organics ○ Organometallic

45. As the search runs, the refcodes of hits will appear in the right-hand side of the window. By default, the 2D diagram tab is selected and the first set of measurements are displayed at the top right of the diagram. Other tabs can be used to access other information and the 3D structure.

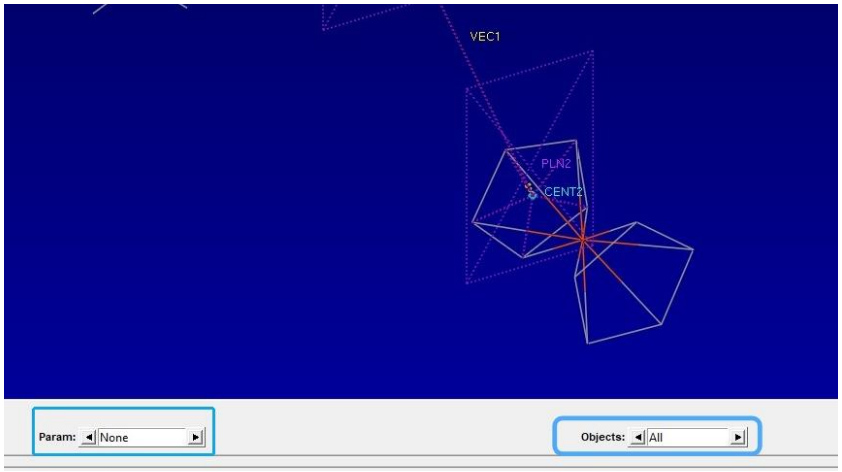


46. Click **3D visualiser**.



Refcode: ABIGUR

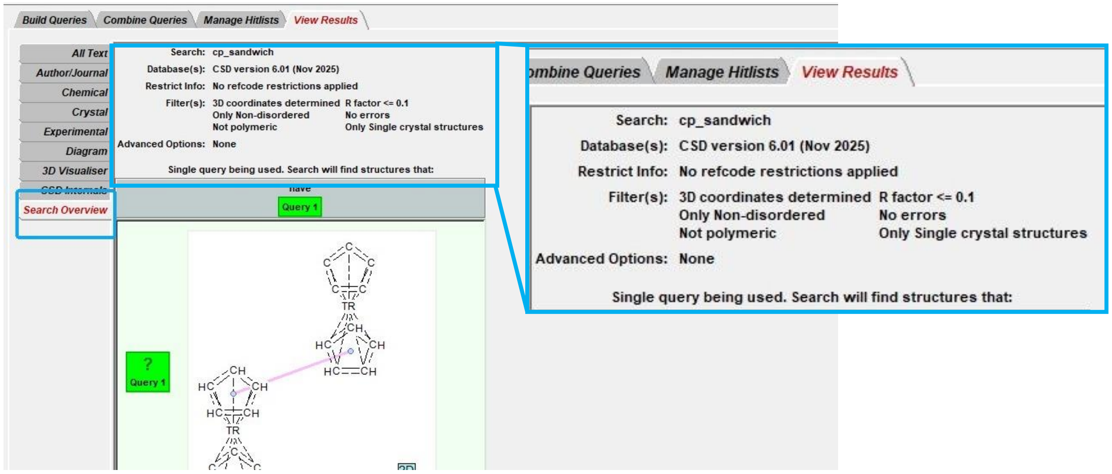
47. The 3D visualiser will appear. The measurements of the defined parameters are shown on the structure but to make it easier to visualise, you can scroll through them using the buttons next to Param. Objects (centroids, vectors) can be controlled in the same way.



Param: None

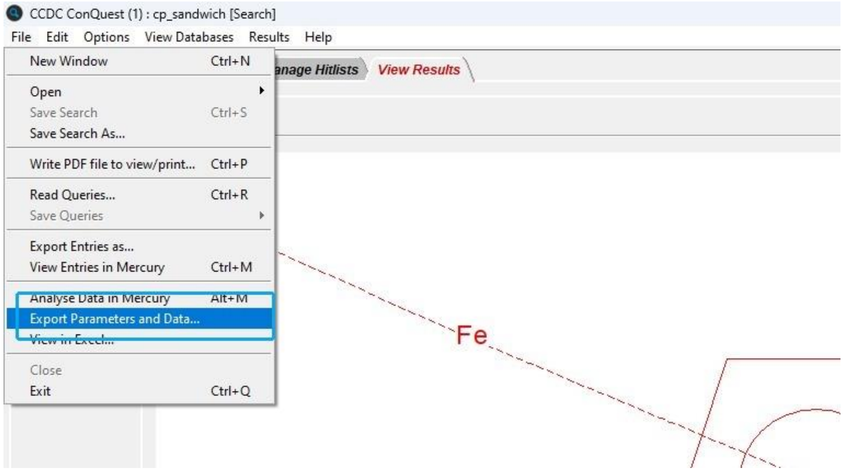
Objects: All

48. Click on the **Search Overview** tab to see a summary of the substructure query and the search settings used. Tip: This can be useful if you want to write up results for publications.

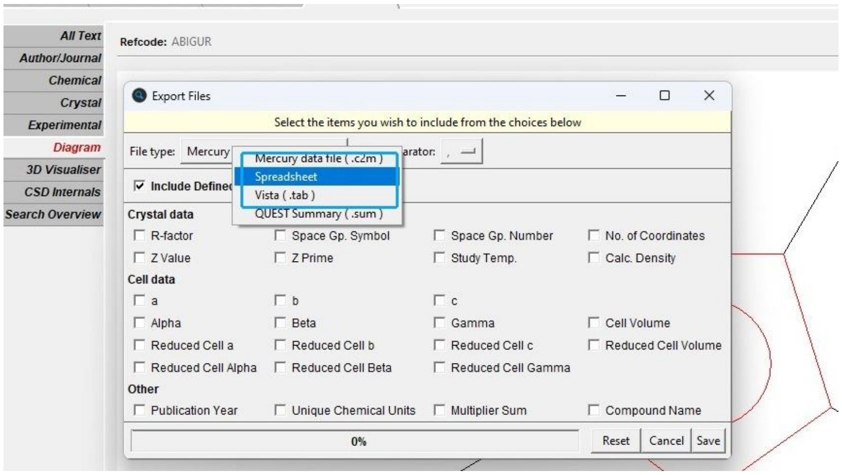


Search: cp_sandwich
Database(s): CSD version 6.01 (Nov 2025)
Restrict Info: No refcode restrictions applied
Filter(s): 3D coordinates determined R factor <= 0.1
Only Non-disordered No errors
Not polymeric Only Single crystal structures
Advanced Options: None
Single query being used. Search will find structures that:

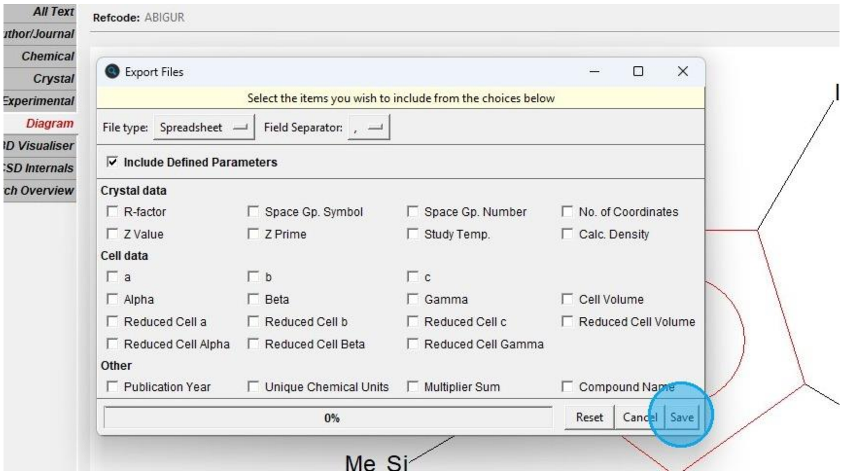
49. From the top menus, click **File > Export Parameters and Data**.



50. In the drop-down menu next to file type, select **Spreadsheet**.

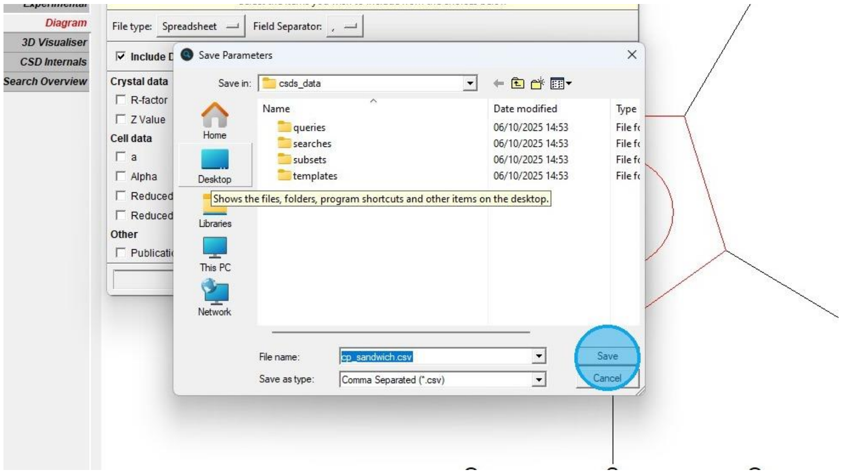


51. Click **Save**.



File type: Spreadsheet
Field Separator: ,
☑ Include Defined Parameters

52. Using the File Explorer, navigate to where you want to save the file, choose a suitable name and click **Save**.

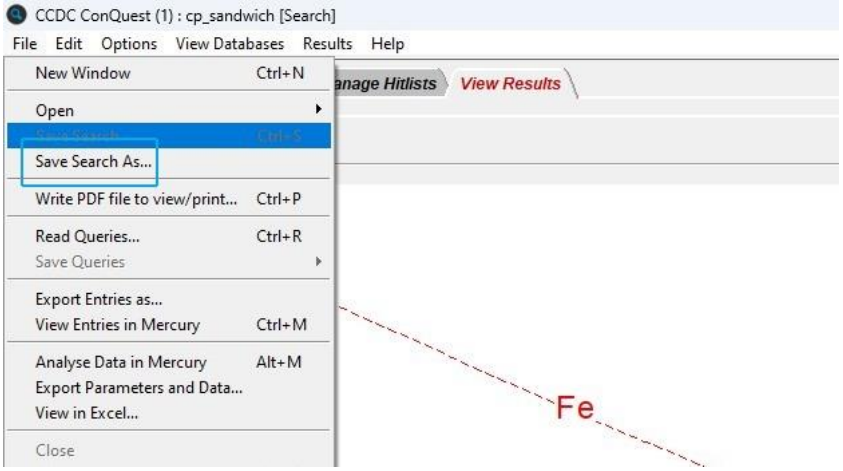


Save in: csds_data

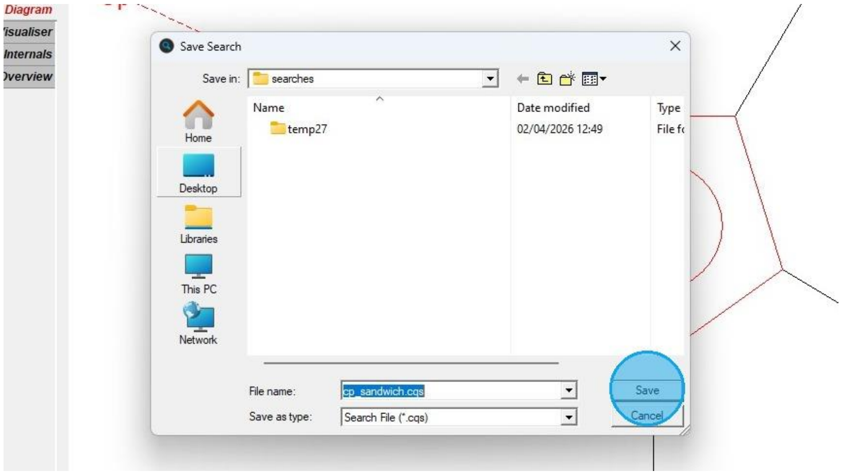
Name	Date modified	Type
queries	06/10/2025 14:53	File fo
searches	06/10/2025 14:53	File fo
subsets	06/10/2025 14:53	File fo
templates	06/10/2025 14:53	File fo

File name: cp_sandwich.csv
Save as type: Comma Separated (*.csv)

53. Click **File > Save Search As**. This will allow you to reopen the session later should you wish to.



54. Navigate to a suitable location, choose a file name and click **Save**.



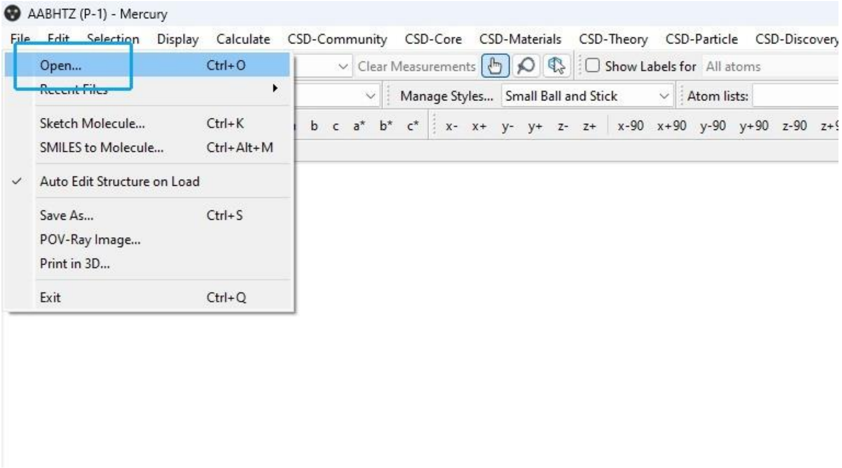
Save in: searches

File name: cp_sandwich.cqs

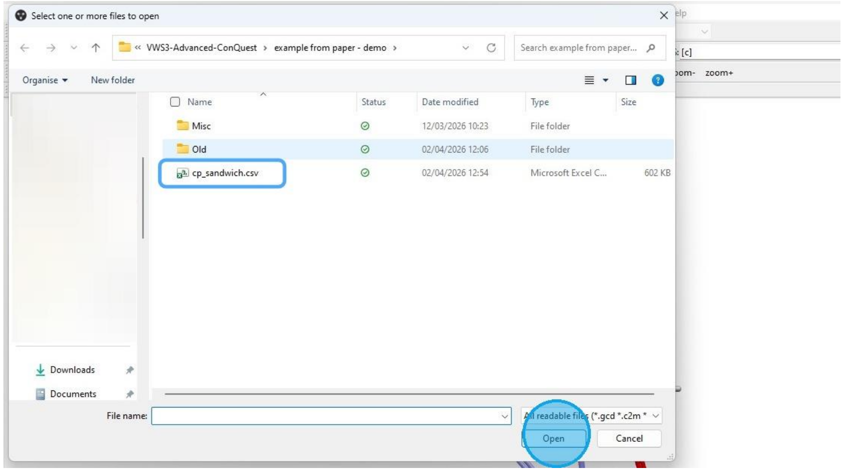
Save as type: Search File (*.cqs)

Analysing Data in Mercury

1. Open Mercury from the Start menu or click on the desktop icon. From the top menus, choose **File > Open**.

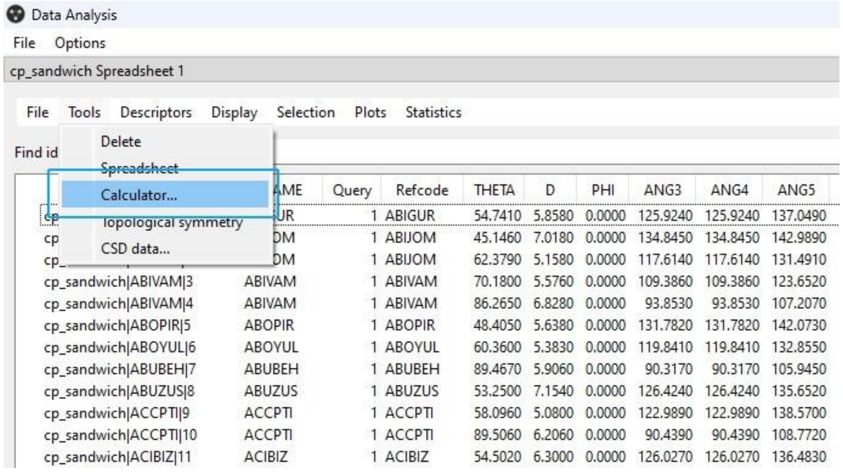


2. Navigate to the CSV file that was exported from ConQuest in the first part of this example (or use this one here). Select the file and click **Open**. The data will be loaded as a spreadsheet in the Data Analysis Module.



Name	Status	Date modified	Type	Size
Misc	✓	12/03/2026 10:23	File folder	
Old	✓	02/04/2026 12:06	File folder	
cp_sandwich.csv	✓	02/04/2026 12:54	Microsoft Excel C...	602 KB

3. You will see headers corresponding to the parameters defined in ConQuest, in addition to Identifier, Name and Query and Refcode. Identifier and Name are automatically generated from the CSV file by the Data Analysis module. Click **Tools > Calculator**.

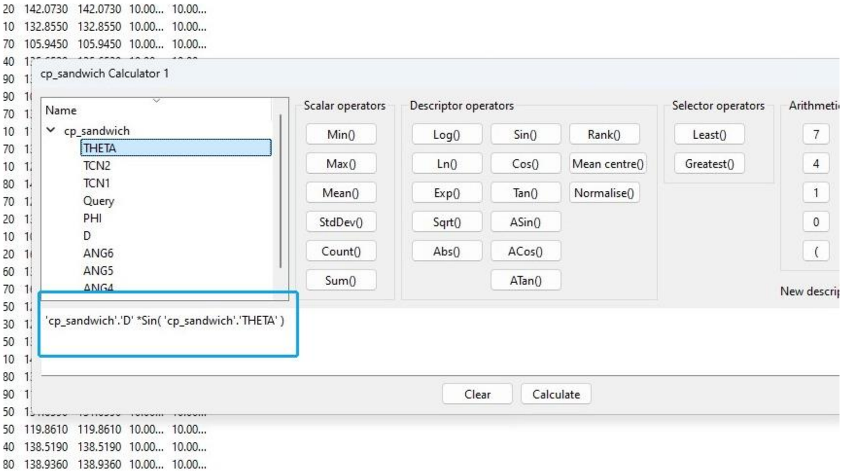


	AME	Query	Refcode	THETA	D	PHI	ANG3	ANG4	ANG5
cp	UR	1	ABIGUR	54.7410	5.8580	0.0000	125.9240	125.9240	137.0490
cp	OM	1	ABIJOM	45.1460	7.0180	0.0000	134.8450	134.8450	142.9890
cp_	OM	1	ABIJOM	62.3790	5.1580	0.0000	117.6140	117.6140	131.4910
cp_sandwich|ABIVAM|3	ABIVAM	1	ABIVAM	70.1800	5.5760	0.0000	109.3860	109.3860	123.6520
cp_sandwich|ABIVAM|4	ABIVAM	1	ABIVAM	86.2650	6.8280	0.0000	93.8530	93.8530	107.2070
cp_sandwich|ABOPIR|5	ABOPIR	1	ABOPIR	48.4050	5.6380	0.0000	131.7820	131.7820	142.0730
cp_sandwich|ABOYUL|6	ABOYUL	1	ABOYUL	60.3600	5.3830	0.0000	119.8410	119.8410	132.8550
cp_sandwich|ABUBEH|7	ABUBEH	1	ABUBEH	89.4670	5.9060	0.0000	90.3170	90.3170	105.9450
cp_sandwich|ABUZUS|8	ABUZUS	1	ABUZUS	53.2500	7.1540	0.0000	126.4240	126.4240	135.6520
cp_sandwich|ACCPTI|9	ACCPTI	1	ACCPTI	58.0960	5.0800	0.0000	122.9890	122.9890	138.5700
cp_sandwich|ACCPTI|10	ACCPTI	1	ACCPTI	89.5060	6.2060	0.0000	90.4390	90.4390	108.7720
cp_sandwich|ACIBIZ|11	ACIBIZ	1	ACIBIZ	54.5020	6.3000	0.0000	126.0270	126.0270	136.4830

4. We will first calculate the horizontal displacement (corresponding to *r* in the Interaction Geometry section). This can be calculated by multiplying the distance between the centroids (D) by the sine of the angle THETA. In the Name panel on the left-hand side of the calculator, click on D, then either type the asterisk sign (*) or click on it from the Arithmetic panel on the right-hand side. Next, either type Sin() or click on it in the Descriptor operators panel. Place the mouse cursor inside the brackets and click on THETA in the Name panel.

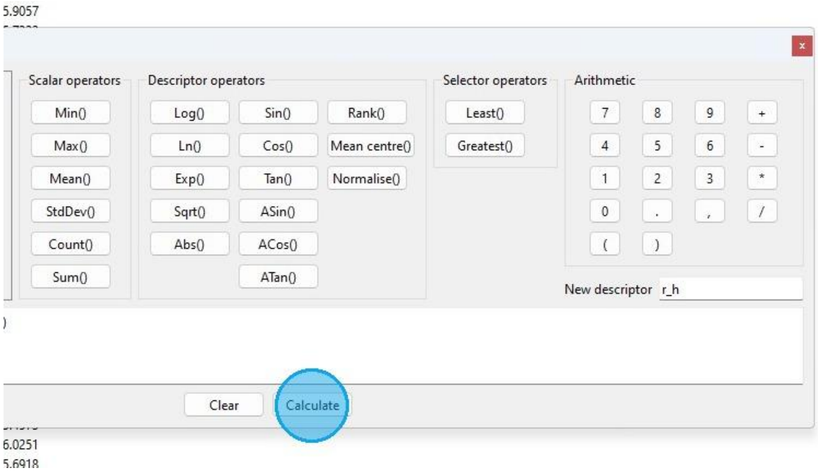
   If you used the parameter and search names we recommended, your formula should be:

   'cp_sandwich'.'D' * Sin('cp_sandwich'.'THETA')



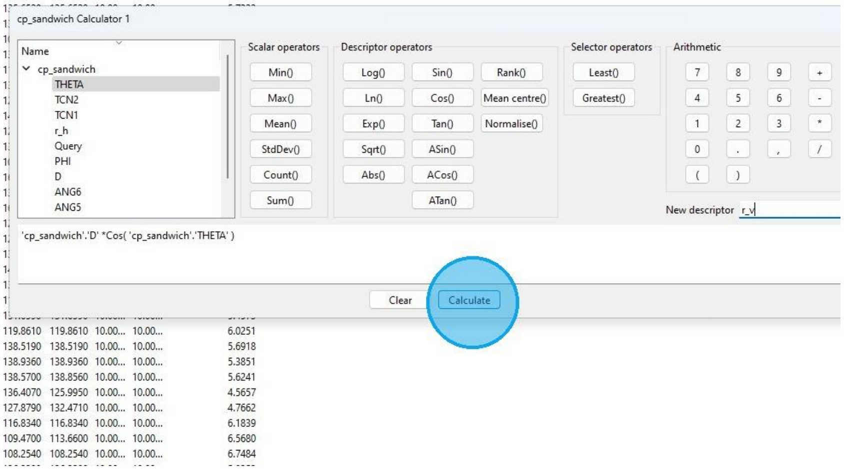
'cp_sandwich'.'D' *Sin('cp_sandwich'.'THETA')

5. Add a suitable name in the New descriptor field (we choose “r_h”, with h indicating the horizontal component), then click **Calculate**. The new parameter r_h will appear as a spreadsheet column and will also be available in the Name area of the Calculator.



New descriptor r_h

6. To calculate the vertical component, *R*, edit the formula by changing Sin to **Cos**, type a New descriptor (we suggest “r_v” where v indicates the vertical component) and click **Calculate**.



New descriptor r_v

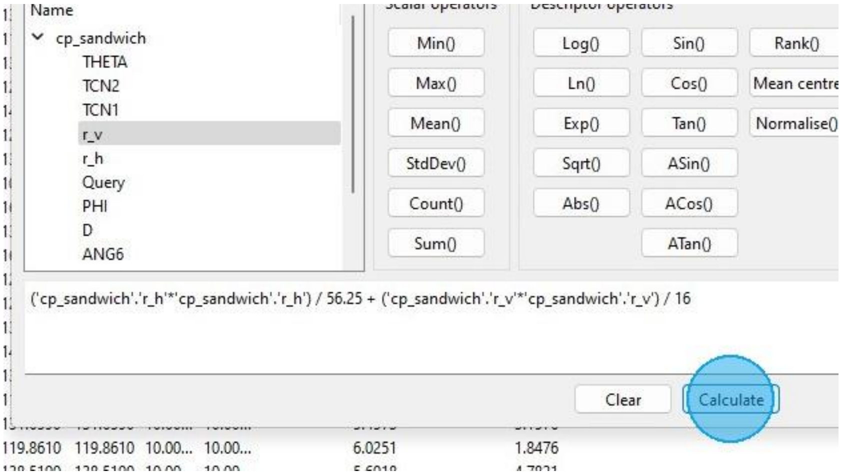
'cp_sandwich'.'D' *Cos('cp_sandwich'.'THETA')

```
119.8610  119.8610  10.00...  10.00...  6.0251
138.5190  138.5190  10.00...  10.00...  5.6918
138.9360  138.9360  10.00...  10.00...  5.3851
138.5700  138.8560  10.00...  10.00...  5.6241
136.4070  125.9950  10.00...  10.00...  4.5657
127.8790  132.4710  10.00...  10.00...  4.7662
116.8340  116.8340  10.00...  10.00...  6.1839
109.4700  113.6600  10.00...  10.00...  6.5680
108.2540  108.2540  10.00...  10.00...  6.7484
```

7. We next need to calculate a variable that can be used to apply the boundary conditions of the ellipse described in the Interaction Geometry section. If you used the parameter and search names we recommended, the formula should be:

('cp_sandwich'.'r_h' * 'cp_sandwich'.'r_h') / 56.25 + ('cp_sandwich'.'r_v' * 'cp_sandwich'.'r_v') / 16

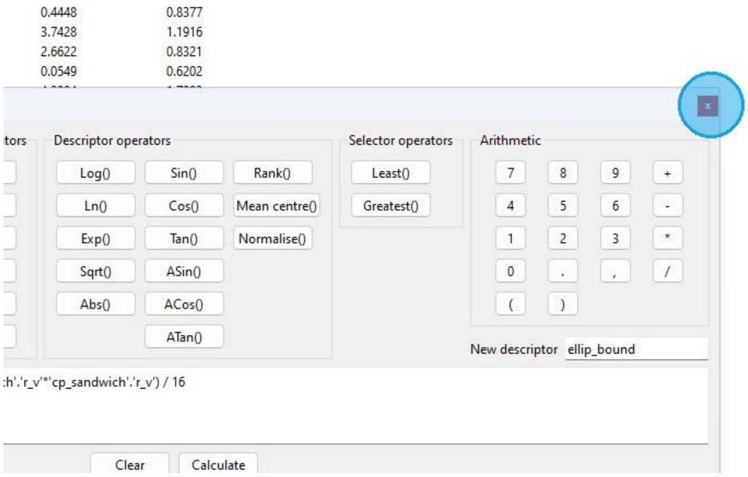
Give the new variable a suitable name such as “ellip_bound” and click **Calculate**.



('cp_sandwich'.'r_h'*'cp_sandwich'.'r_h') / 56.25 + ('cp_sandwich'.'r_v'*'cp_sandwich'.'r_v') / 16

```
119.8610  119.8610  10.00...  10.00...  6.0251  1.8476
```

8. When you are finished, close the Calculator.

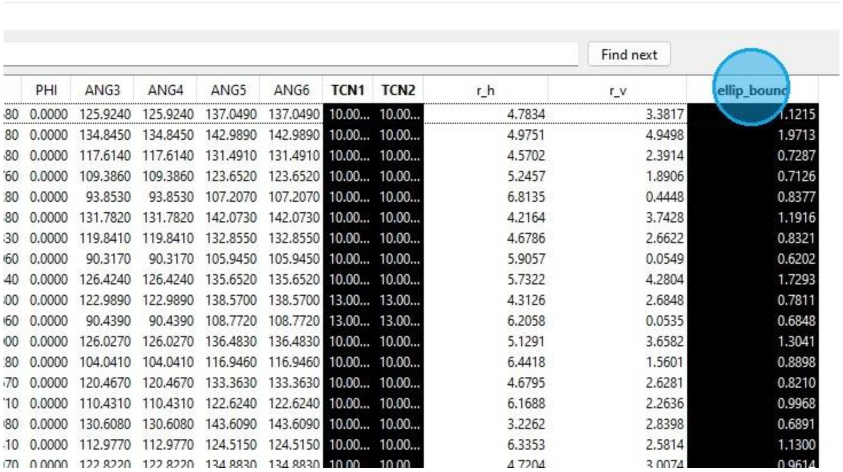


0.4448	0.8377
3.7428	1.1916
2.6622	0.8321
0.0549	0.6202

New descriptor ellip_bound

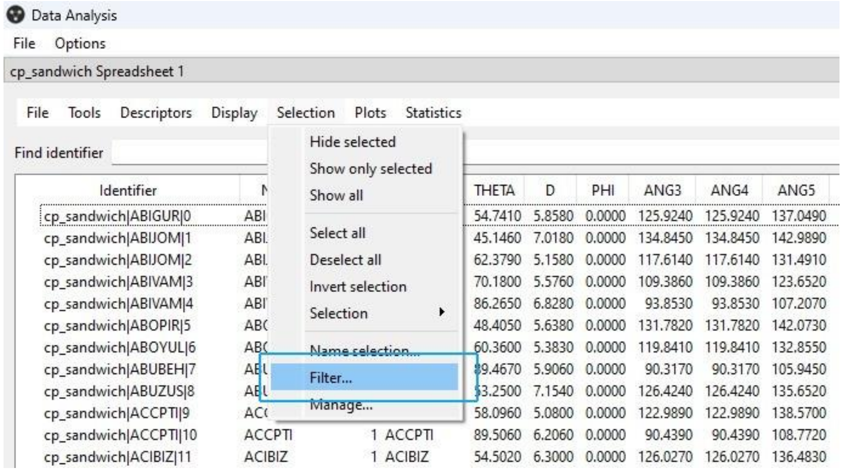
:h'.'r_v'*'cp_sandwich'.'r_v') / 16

9. Click on the column headers **TCN1**, **TCN2** and **ellip_bound**. They will become shaded in black, which indicates they are selected for further use.



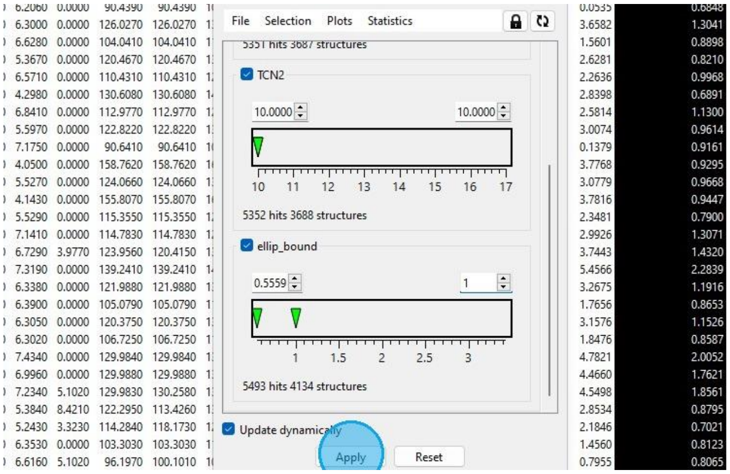
	PHI	ANG3	ANG4	ANG5	ANG6	TCN1	TCN2	r_h	r_v	ellip_bound
80	0.0000	125.9240	125.9240	137.0490	137.0490	10.00...	10.00...	4.7834	3.3817	1.1215
80	0.0000	134.8450	134.8450	142.9890	142.9890	10.00...	10.00...	4.9751	4.9498	1.9713
80	0.0000	117.6140	117.6140	131.4910	131.4910	10.00...	10.00...	4.5702	2.3914	0.7287
60	0.0000	109.3860	109.3860	123.6520	123.6520	10.00...	10.00...	5.2457	1.8906	0.7126
80	0.0000	93.8530	93.8530	107.2070	107.2070	10.00...	10.00...	6.8135	0.4448	0.8377
80	0.0000	131.7820	131.7820	142.0730	142.0730	10.00...	10.00...	4.2164	3.7428	1.1916
30	0.0000	119.8410	119.8410	132.8550	132.8550	10.00...	10.00...	4.6786	2.6622	0.8321
60	0.0000	90.3170	90.3170	105.9450	105.9450	10.00...	10.00...	5.9057	0.0549	0.6202
40	0.0000	126.4240	126.4240	135.6520	135.6520	10.00...	10.00...	5.7322	4.2804	1.7293
00	0.0000	122.9890	122.9890	138.5700	138.5700	13.00...	13.00...	4.3126	2.6848	0.7811
60	0.0000	90.4390	90.4390	108.7720	108.7720	13.00...	13.00...	6.2058	0.0535	0.6848
00	0.0000	126.0270	126.0270	136.4830	136.4830	10.00...	10.00...	5.1291	3.6582	1.3041
80	0.0000	104.0410	104.0410	116.9460	116.9460	10.00...	10.00...	6.4418	1.5601	0.8898
70	0.0000	120.4670	120.4670	133.3630	133.3630	10.00...	10.00...	4.6795	2.6281	0.8210
10	0.0000	110.4310	110.4310	122.6240	122.6240	10.00...	10.00...	6.1688	2.2636	0.9968
80	0.0000	130.6080	130.6080	143.6090	143.6090	10.00...	10.00...	3.2262	2.8398	0.6891
10	0.0000	112.9770	112.9770	124.5150	124.5150	10.00...	10.00...	6.3353	2.5814	1.1300
70	0.0000	122.8220	122.8220	134.8830	134.8830	10.00	10.00	4.7204	3.0074	0.9614

10. From the top menus, select **Selection > Filter**. The selected columns will be used to filter out irrelevant results.



Identifier	N			THETA	D	PHI	ANG3	ANG4	ANG5
cp_sandwich|ABIGUR|0	ABI			54.7410	5.8580	0.0000	125.9240	125.9240	137.0490
cp_sandwich|ABIJOM|1	ABI			45.1460	7.0180	0.0000	134.8450	134.8450	142.9890
cp_sandwich|ABIJOM|2	ABI			62.3790	5.1580	0.0000	117.6140	117.6140	131.4910
cp_sandwich|ABIVAM|3	ABI			70.1800	5.5760	0.0000	109.3860	109.3860	123.6520
cp_sandwich|ABIVAM|4	ABI			86.2650	6.8280	0.0000	93.8530	93.8530	107.2070
cp_sandwich|ABOPIR|5	ABC			48.4050	5.6380	0.0000	131.7820	131.7820	142.0730
cp_sandwich|ABOYUL|6	ABC			60.3600	5.3830	0.0000	119.8410	119.8410	132.8550
cp_sandwich|ABUBEH|7	ABU			89.4670	5.9060	0.0000	90.3170	90.3170	105.9450
cp_sandwich|ABUZUS|8	ABU			53.2500	7.1540	0.0000	126.4240	126.4240	135.6520
cp_sandwich|ACCPTI|9	ACC			58.0960	5.0800	0.0000	122.9890	122.9890	138.5700
cp_sandwich|ACCPTI|10	ACCPTI	1	ACCPTI	89.5060	6.2060	0.0000	90.4390	90.4390	108.7720
cp_sandwich|ACIBIZ|11	ACIBIZ	1	ACIBIZ	54.5020	6.3000	0.0000	126.0270	126.0270	136.4830

11. In the resulting Filter window, type an upper limit of 10 for TCN1 and TCN2, and a maximum value of 1 for the ellip_bound. You may need to scroll to see all of them. Applying these conditions ensures that we have conventional metallocene-like structures and that the ellipsoid equation in Figure 2 is satisfied. Click **Apply**. **Do not close the Filter window**.



5351 hits 3687 structures

☑ TCN2

10.0000 10.0000

5352 hits 3688 structures

☑ ellip_bound

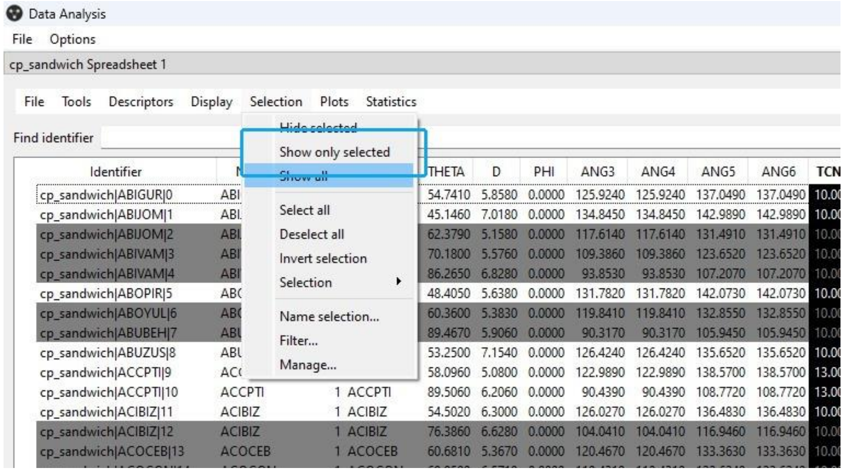
0.5559 1

5493 hits 4134 structures

☑ Update dynamically

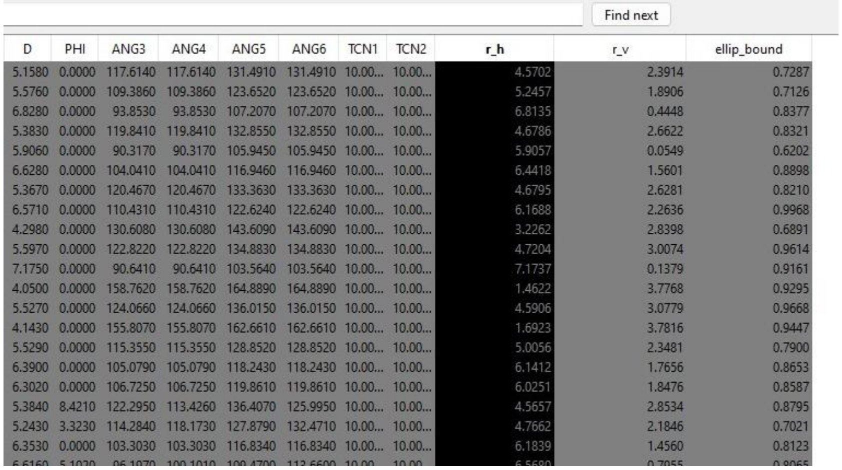
6.2060	0.0000	90.4390	90.4390	0.0535	0.6848
6.3000	0.0000	126.0270	126.0270	3.6582	1.3041
6.6280	0.0000	104.0410	104.0410	1.5601	0.8898
5.3670	0.0000	120.4670	120.4670	2.6281	0.8210
6.5710	0.0000	110.4310	110.4310	2.2636	0.9968
4.2980	0.0000	130.6080	130.6080	2.8398	0.6891
6.8410	0.0000	112.9770	112.9770	2.5814	1.1300
5.5970	0.0000	122.8220	122.8220	3.0074	0.9614
7.1750	0.0000	90.6410	90.6410	0.1379	0.9161
4.0500	0.0000	158.7620	158.7620	3.7768	0.9295
5.5270	0.0000	124.0660	124.0660	3.0779	0.9668
4.1430	0.0000	155.8070	155.8070	3.7816	0.9447
5.5290	0.0000	115.3550	115.3550	2.3481	0.7900
7.1410	0.0000	114.7830	114.7830	2.9926	1.3071
6.7290	3.9770	123.9560	120.4150	3.7443	1.4320
7.3190	0.0000	139.2410	139.2410	5.4566	2.2839
6.3380	0.0000	121.9880	121.9880	3.2675	1.1916
6.3900	0.0000	105.0790	105.0790	1.7656	0.8653
6.3050	0.0000	120.3750	120.3750	3.1576	1.1526
6.3020	0.0000	106.7250	106.7250	1.8476	0.8587
7.4340	0.0000	129.9840	129.9840	4.7821	2.0052
6.9960	0.0000	129.9880	129.9880	4.4660	1.7621
7.2340	5.1020	129.9830	130.2580	4.5498	1.8561
5.3840	8.4210	122.2950	113.4260	2.8534	0.8795
5.2430	3.3230	114.2840	118.1730	2.1846	0.7021
6.3530	0.0000	103.3030	103.3030	1.4560	0.8123
6.6160	5.1020	96.1970	100.1010	0.7955	0.8065

12. From the top menus, click **Selection > Show only selected**. This ensures that we will plot only the filtered data in the next steps.



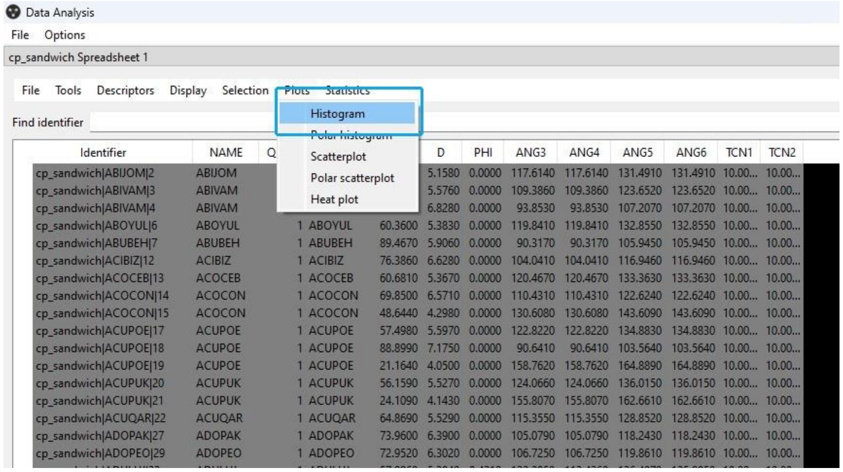
Identifier	N			THETA	D	PHI	ANG3	ANG4	ANG5	ANG6	TCN
cp_sandwich|ABIGUR|0	ABI			54.7410	5.8580	0.0000	125.9240	125.9240	137.0490	137.0490	10.0
cp_sandwich|ABIJOM|1	ABI.			45.1460	7.0180	0.0000	134.8450	134.8450	142.9890	142.9890	10.0
cp_sandwich|ABIJOM|2	ABI.			62.3790	5.1580	0.0000	117.6140	117.6140	131.4910	131.4910	10.0
cp_sandwich|ABIVAM|3	ABI			70.1800	5.5760	0.0000	109.3860	109.3860	123.6520	123.6520	10.0
cp_sandwich|ABIVAM|4	ABI			86.2650	6.8280	0.0000	93.8530	93.8530	107.2070	107.2070	10.0
cp_sandwich|ABOPIR|5	ABC			48.4050	5.6380	0.0000	131.7820	131.7820	142.0730	142.0730	10.0
cp_sandwich|ABOYUL|6	ABC			60.3600	5.3830	0.0000	119.8410	119.8410	132.8550	132.8550	10.0
cp_sandwich|ABUBEH|7	ABU			89.4670	5.9060	0.0000	90.3170	90.3170	105.9450	105.9450	10.0
cp_sandwich|ABUZUS|8	ABU			53.2500	7.1540	0.0000	126.4240	126.4240	135.6520	135.6520	10.0
cp_sandwich|ACCPTI|9	ACC			58.0960	5.0800	0.0000	122.9890	122.9890	138.5700	138.5700	13.0
cp_sandwich|ACCPTI|10	ACCPTI	1	ACCPTI	89.5060	6.2060	0.0000	90.4390	90.4390	108.7720	108.7720	13.0
cp_sandwich|ACIBIZ|11	ACIBIZ	1	ACIBIZ	54.5020	6.3000	0.0000	126.0270	126.0270	136.4830	136.4830	10.0
cp_sandwich|ACIBIZ|12	ACIBIZ	1	ACIBIZ	76.3860	6.6280	0.0000	104.0410	104.0410	116.9460	116.9460	10.0
cp_sandwich|ACOCEB|13	ACOCEB	1	ACOCEB	60.6810	5.3670	0.0000	120.4670	120.4670	133.3630	133.3630	10.0

13. Deselect the TCN1, TCN2 and ellip_bound columns, and select **r_h** by clicking on the column header.



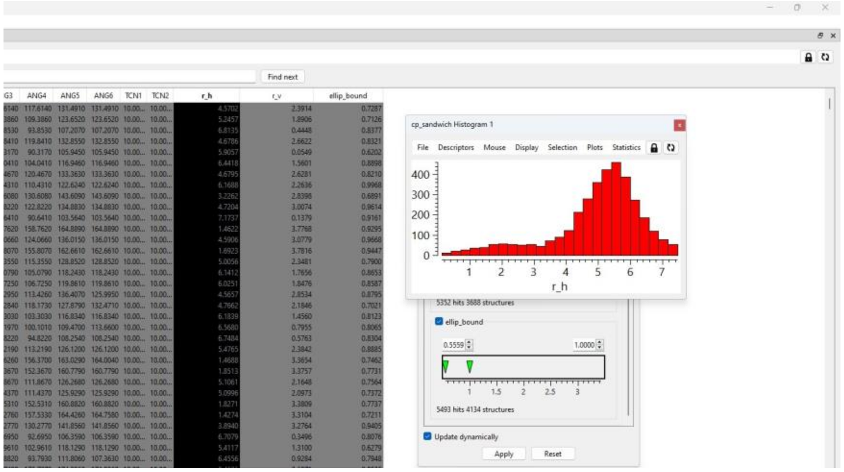
D	PHI	ANG3	ANG4	ANG5	ANG6	TCN1	TCN2	r_h	r_v	ellip_bound
5.1580	0.0000	117.6140	117.6140	131.4910	131.4910	10.00...	10.00...	4.5702	2.3914	0.7287
5.5760	0.0000	109.3860	109.3860	123.6520	123.6520	10.00...	10.00...	5.2457	1.8906	0.7126
6.8280	0.0000	93.8530	93.8530	107.2070	107.2070	10.00...	10.00...	6.8135	0.4448	0.8377
5.3830	0.0000	119.8410	119.8410	132.8550	132.8550	10.00...	10.00...	4.6786	2.6622	0.8321
5.9060	0.0000	90.3170	90.3170	105.9450	105.9450	10.00...	10.00...	5.9057	0.0549	0.6202
6.6280	0.0000	104.0410	104.0410	116.9460	116.9460	10.00...	10.00...	6.4418	1.5601	0.8898
5.3670	0.0000	120.4670	120.4670	133.3630	133.3630	10.00...	10.00...	4.6795	2.6281	0.8210
6.5710	0.0000	110.4310	110.4310	122.6240	122.6240	10.00...	10.00...	6.1688	2.2636	0.9968
4.2980	0.0000	130.6080	130.6080	143.6090	143.6090	10.00...	10.00...	3.2262	2.8398	0.6891
5.5970	0.0000	122.8220	122.8220	134.8830	134.8830	10.00...	10.00...	4.7204	3.0074	0.9614
7.1750	0.0000	90.6410	90.6410	103.5640	103.5640	10.00...	10.00...	7.1737	0.1379	0.9161
4.0500	0.0000	158.7620	158.7620	164.8890	164.8890	10.00...	10.00...	1.4622	3.7768	0.9295
5.5270	0.0000	124.0660	124.0660	136.0150	136.0150	10.00...	10.00...	4.5906	3.0779	0.9668
4.1430	0.0000	155.8070	155.8070	162.6610	162.6610	10.00...	10.00...	1.6923	3.7816	0.9447
5.5290	0.0000	115.3550	115.3550	128.8520	128.8520	10.00...	10.00...	5.0056	2.3481	0.7900
6.3900	0.0000	105.0790	105.0790	118.2430	118.2430	10.00...	10.00...	6.1412	1.7656	0.8653
6.3020	0.0000	106.7250	106.7250	119.8610	119.8610	10.00...	10.00...	6.0251	1.8476	0.8587
5.3840	8.4210	122.2950	113.4260	136.4070	125.9950	10.00...	10.00...	4.5657	2.8534	0.8795
5.2430	3.3230	114.2840	118.1730	127.8790	132.4710	10.00...	10.00...	4.7662	2.1846	0.7021
6.3530	0.0000	103.3030	103.3030	116.8340	116.8340	10.00...	10.00...	6.1839	1.4560	0.8123

14. From the top menus, click **Plots > Histogram**.

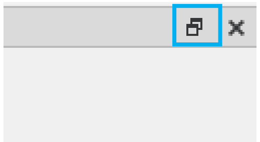


Identifier	NAME	Q			D	PHI	ANG3	ANG4	ANG5	ANG6	TCN1	TCN2
cp_sandwich|ABIJOM|2	ABIJOM				5.1580	0.0000	117.6140	117.6140	131.4910	131.4910	10.00...	10.00...
cp_sandwich|ABIVAM|3	ABIVAM				5.5760	0.0000	109.3860	109.3860	123.6520	123.6520	10.00...	10.00...
cp_sandwich|ABIVAM|4	ABIVAM				6.8280	0.0000	93.8530	93.8530	107.2070	107.2070	10.00...	10.00...
cp_sandwich|ABOYUL|6	ABOYUL	1	ABOYUL	60.3600	5.3830	0.0000	119.8410	119.8410	132.8550	132.8550	10.00...	10.00...
cp_sandwich|ABUBEH|7	ABUBEH	1	ABUBEH	89.4670	5.9060	0.0000	90.3170	90.3170	105.9450	105.9450	10.00...	10.00...
cp_sandwich|ACIBIZ|12	ACIBIZ	1	ACIBIZ	76.3860	6.6280	0.0000	104.0410	104.0410	116.9460	116.9460	10.00...	10.00...
cp_sandwich|ACOCEB|13	ACOCEB	1	ACOCEB	60.6810	5.3670	0.0000	120.4670	120.4670	133.3630	133.3630	10.00...	10.00...
cp_sandwich|ACOCON|14	ACOCON	1	ACOCON	69.8500	6.5710	0.0000	110.4310	110.4310	122.6240	122.6240	10.00...	10.00...
cp_sandwich|ACOCON|15	ACOCON	1	ACOCON	48.6440	4.2980	0.0000	130.6080	130.6080	143.6090	143.6090	10.00...	10.00...
cp_sandwich|ACUPOE|17	ACUPOE	1	ACUPOE	57.4980	5.5970	0.0000	122.8220	122.8220	134.8830	134.8830	10.00...	10.00...
cp_sandwich|ACUPOE|18	ACUPOE	1	ACUPOE	88.8990	7.1750	0.0000	90.6410	90.6410	103.5640	103.5640	10.00...	10.00...
cp_sandwich|ACUPOE|19	ACUPOE	1	ACUPOE	21.1640	4.0500	0.0000	158.7620	158.7620	164.8890	164.8890	10.00...	10.00...
cp_sandwich|ACUPUK|20	ACUPUK	1	ACUPUK	56.1590	5.5270	0.0000	124.0660	124.0660	136.0150	136.0150	10.00...	10.00...
cp_sandwich|ACUPUK|21	ACUPUK	1	ACUPUK	24.1090	4.1430	0.0000	155.8070	155.8070	162.6610	162.6610	10.00...	10.00...
cp_sandwich|ACUQAR|22	ACUQAR	1	ACUQAR	64.8690	5.5290	0.0000	115.3550	115.3550	128.8520	128.8520	10.00...	10.00...
cp_sandwich|ADOPAK|27	ADOPAK	1	ADOPAK	73.9600	6.3900	0.0000	105.0790	105.0790	118.2430	118.2430	10.00...	10.00...
cp_sandwich|ADOPEO|29	ADOPEO	1	ADOPEO	72.9520	6.3020	0.0000	106.7250	106.7250	119.8610	119.8610	10.00...	10.00...

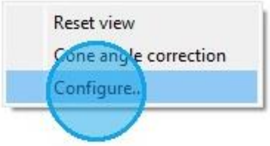
15. A histogram will appear. You can move this around and snap it to different panels, or have it as a separate tab. We will do the latter.



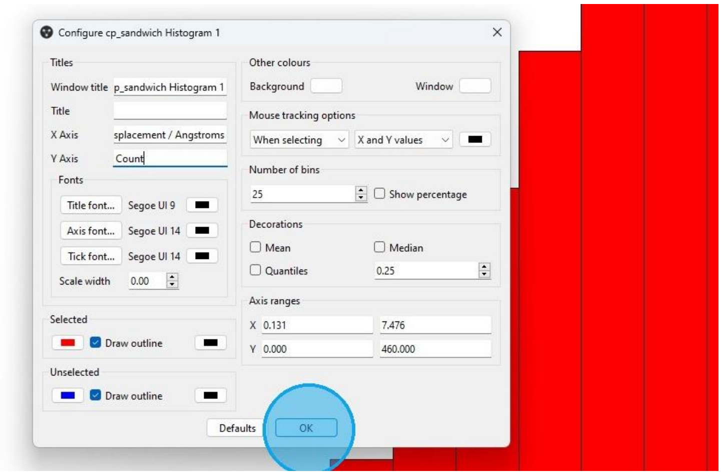
Tip: windows in the Data Analysis module can be detached using the windows symbol and snapped back into place by dragging and dropping.



16. Right-click in the histogram window and select configure from the pop-up menu.

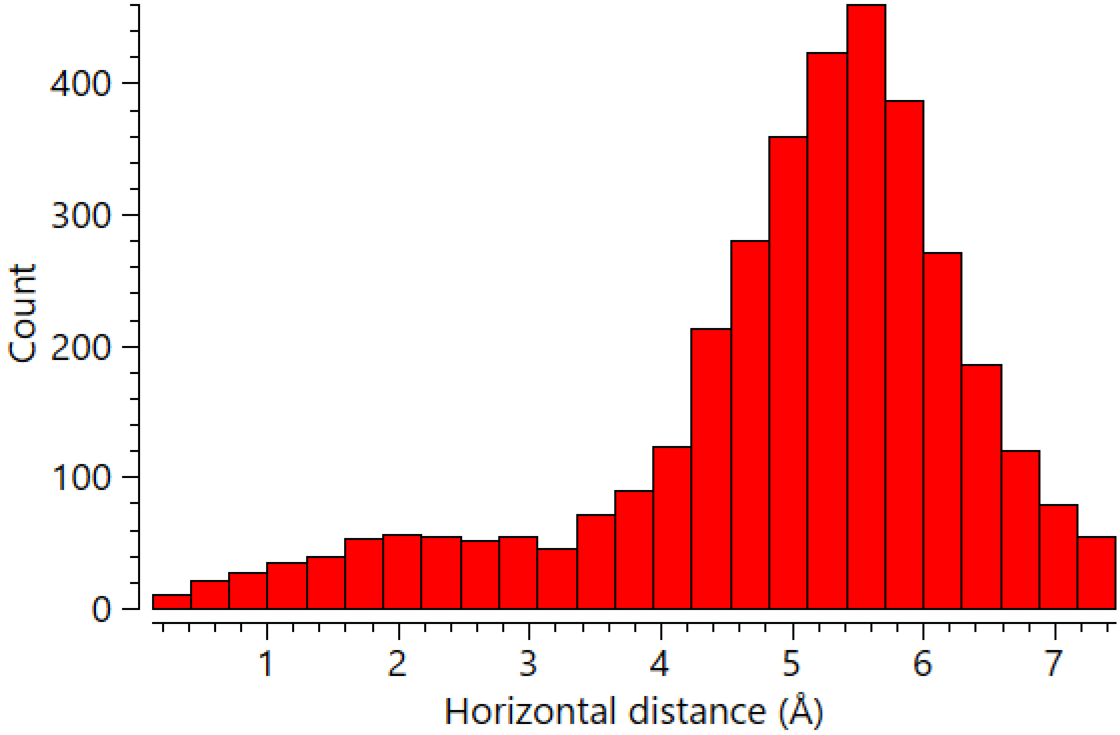


17. You can customise the histogram display, for example by editing/adding axis titles. When you are happy with your customisations click **OK**.



Window title: p_sandwich Histogram 1
Title:
X Axis: splacement / Angstroms
Y Axis: Count
Title font...: Segoe UI 9
Axis font...: Segoe UI 14
Tick font...: Segoe UI 14
Scale width: 0.00
Selected: ☑ Draw outline
Unselected: ☑ Draw outline
Background
Window
Mouse tracking options: When selecting; X and Y values
Number of bins: 25 ☐ Show percentage
Decorations: ☐ Mean ☐ Median ☐ Quantiles 0.25
Axis ranges: X 0.131 7.476
Y 0.000 460.000

The final histogram should look like shown below. There may be differences depending on your CSD version and the number of bins in your histogram (we chose 25).



Conclusions

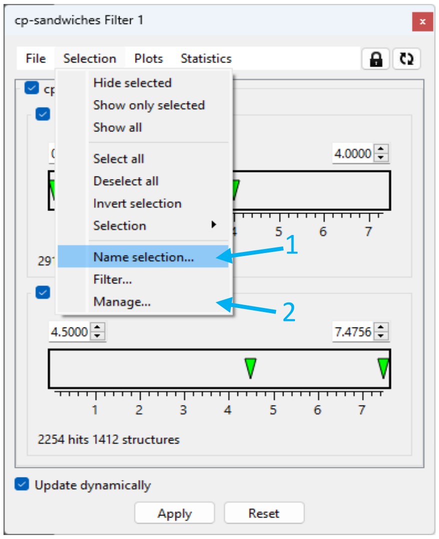
From the histogram it appears that there might be two possible distributions, one centred at smaller horizontal displacements, and one centred at larger horizontal displacement, which appear to overlap slightly somewhere around 3-4 Å. This is in keeping with the findings of Malenov *et al*. who note that small horizontal displacements are associated with stronger stacking interactions, but weaker stacking interactions at larger displacements are often preferred as they provide areas for additional interactions with neighbouring species in crystals, leading to more stable supramolecular structures.

Exercises

The data in the original study which included the searches relating to sandwich complexes was published in 2018[2], at which time the percentage of weaker interactions, at 4.5 ≤ r ≤ 7.5 Å, was 73.1% of all contacts measured. The number of structures in the CSD has increased substantially since that time.

Use the sliders in the filters in the Mercury Data Analysis module to evaluate the % of measurements in the range 4.5 ≤ r ≤ 7.5 Å in the data you have generated. How does it compare to the 2018 results?

Hint: name the selections for each particular combination of the sliders and see how many measurements are in each set with Manage Selections.



2254 hits 1412 structures

In this exercise, we have used trigonometry to calculate r and R. Can you think of another way of obtaining these parameters using distances only? How would you do it in ConQuest? Hint: think about how to obtain the normal distance of an object from a plane in ConQuest.

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[2] D. P. Malenov, I. S. Antonijević, M. B. Hall and S. Zarić, *CrystEngComm*, 20, 2018, 4506-4514, DOI: 10.1039/C8CE00597D

Summary

In this workshop we have seen how to create a substructure search in ConQuest to find aromatic interactions between metallocene molecules in crystal structures. Calculating centroids, planes and vectors automatically with 3D search options was an essential step in generating the data. By using the Mercury Data Analysis module, we have been able to confirm the predominance of larger horizontal offset aromatic interactions between metallocenes in crystal structures in the CSD.

For your reference, you can find the ConQuest user manual at this link.

Next Steps

If you have enjoyed this workshop, you might like to explore other examples of this type of analysis with ConQuest and Mercury. Self-guided workshops CQ-003 and QQ-007 give examples with organic and inorganic systems respectively and can be downloaded from the CSD-Core workshops webpage.

For further examples of filtering and working with selections in Mercury, you can watch this video.

How to Cite these Tools

ConQuest: I. J. Bruno, J. C. Cole, P. R. Edgington, M. Kessler, C. F. Macrae, P. McCabe, J. Pearson and R. Taylor, *Acta Cryst.*, **B58**, 389-397, 2002 DOI: 10.1107/S0108768102003324

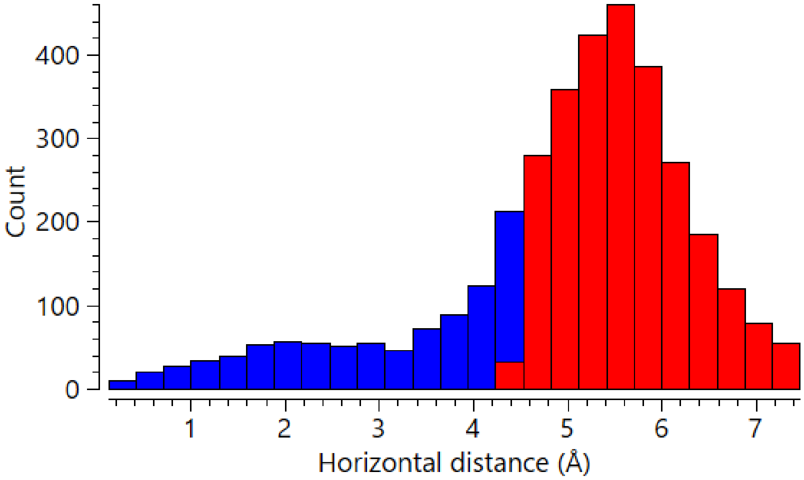
Mercury: C. F. Macrae, I. Sovago, S. J. Cottrell, P. T. A. Galek, P. McCabe, E. Pidcock, M. Platings, G. P. Shields, J. S. Stevens, M. Towler and P. A. Wood, *J. Appl. Cryst.*, **53**, 226-235, 2020 DOI: 10.1107/S1600576719014092

Feedback

We hope this workshop improved your understanding of 3D geometry searching in ConQuest and you found it useful for your work. As we aim to continuously improve our training materials, we would love to hear your feedback. Follow the link on the workshop homepage and insert the workshop code, which for this self-guided workshop is CQ-008. It will only take 5 minutes and your feedback is anonymous. Thank you!

Answers to Exercises

Using the data supplied in this workshop (derived from CSD version 6.01), the proportion of measurements for 4.5 ≤ *r* ≤ 7.5 Å (with 0 ≤ *R* ≤ 4.0 Å) is 2644 / 3548 = 74.5%, very similar to the proportion found in the 2018 study. Your findings may differ depending on your CSD version.



As an alternative to using trigonometry to obtain *r* and *R*, the normal distance of a centroid in one ring to the mean plane of the other ring – this is *R* – can be measured directly in ConQuest. The Pythagorean theorem can then be applied to calculate *r*. Note that it is not necessary to define vectors using this method, therefore it is simpler to implement and recommended.

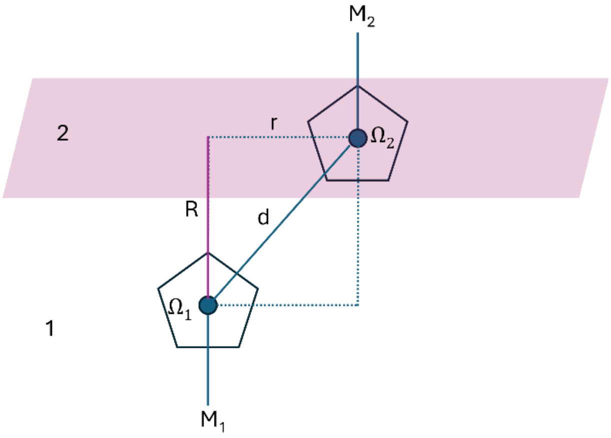
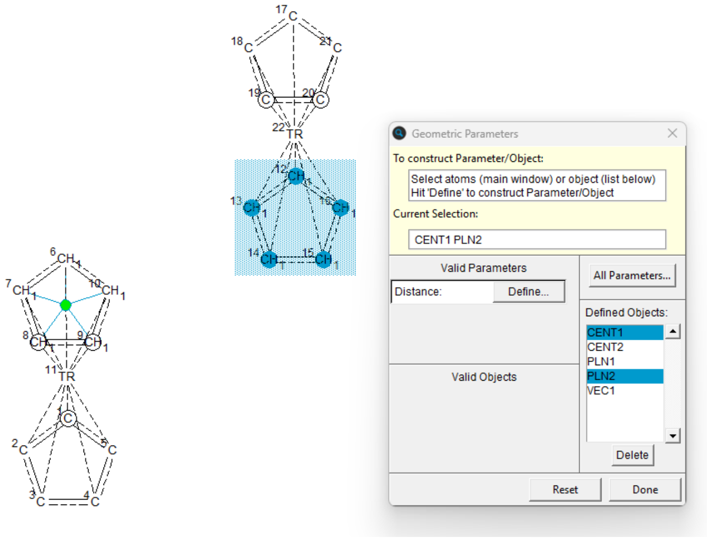


Figure 6. Alternative way of calculating *r* by measuring *R* directly. $r = \sqrt{d^2 - R^2}$.

In ConQuest, this would look like a Distance involving CENT1 and PLN2.



To construct Parameter/Object:

Select atoms (main window) or object (list below)
Hit 'Define' to construct Parameter/Object

Current Selection:

CENT1 PLN2

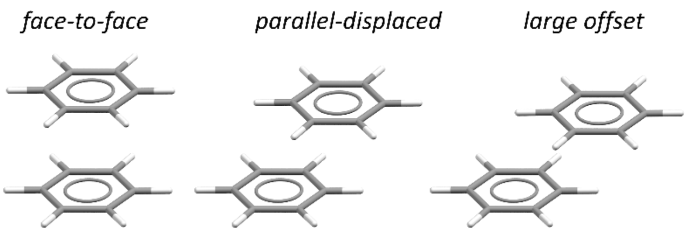
Glossary

Aromatic ligands

In organometallic chemistry, fully π-conjugated rings may be considered aromatic if they have 4*n* + 2 (n = integer) π electrons after accounting their formal charge in the complex. E.g. $C_4H_4^{2-}$, $C_5H_5^{-}$, C_6H_6, $C_7H_7^{+}$, $C_8H_8^{2-}$ and so on.

Aromatic stacking interaction

Aromatics stacking interactions are a subset of aromatic interactions, which are non-covalent forces involving aromatic systems such as benzene. Common geometries for aromatic interactions include face-to-face, edge-to-face and parallel-displaced. Face-to-face and parallel-displaced are subsets of the stacking geometry. Additionally, there is a large offset stacking geometry. These three stacking interactions are characterised by decreasing normal distances with increasing horizontal displacement.

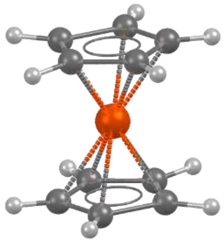

face-to-face *parallel-displaced* *large offset*

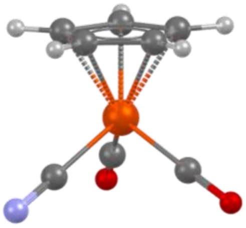
Centroid

A centroid is the geometric centre of a set of atoms; for aromatic ligands, it is the centre of the ring.

Sandwich and half-sandwich complexes

A sandwich complex is an organometallic compound in which a metal atom or ion is positioned between two parallel, typically aromatic ligands. Metallocenes, such as ferrocene (CSD refcode family FEROCE), are examples of sandwich complexes. In half-sandwich (or piano-stool) complexes, one aromatic ligand is replaced by other ligands, for example, in $CpFe(CO)_2CN$ (CSD refcode ACODUR)


FEROCE04

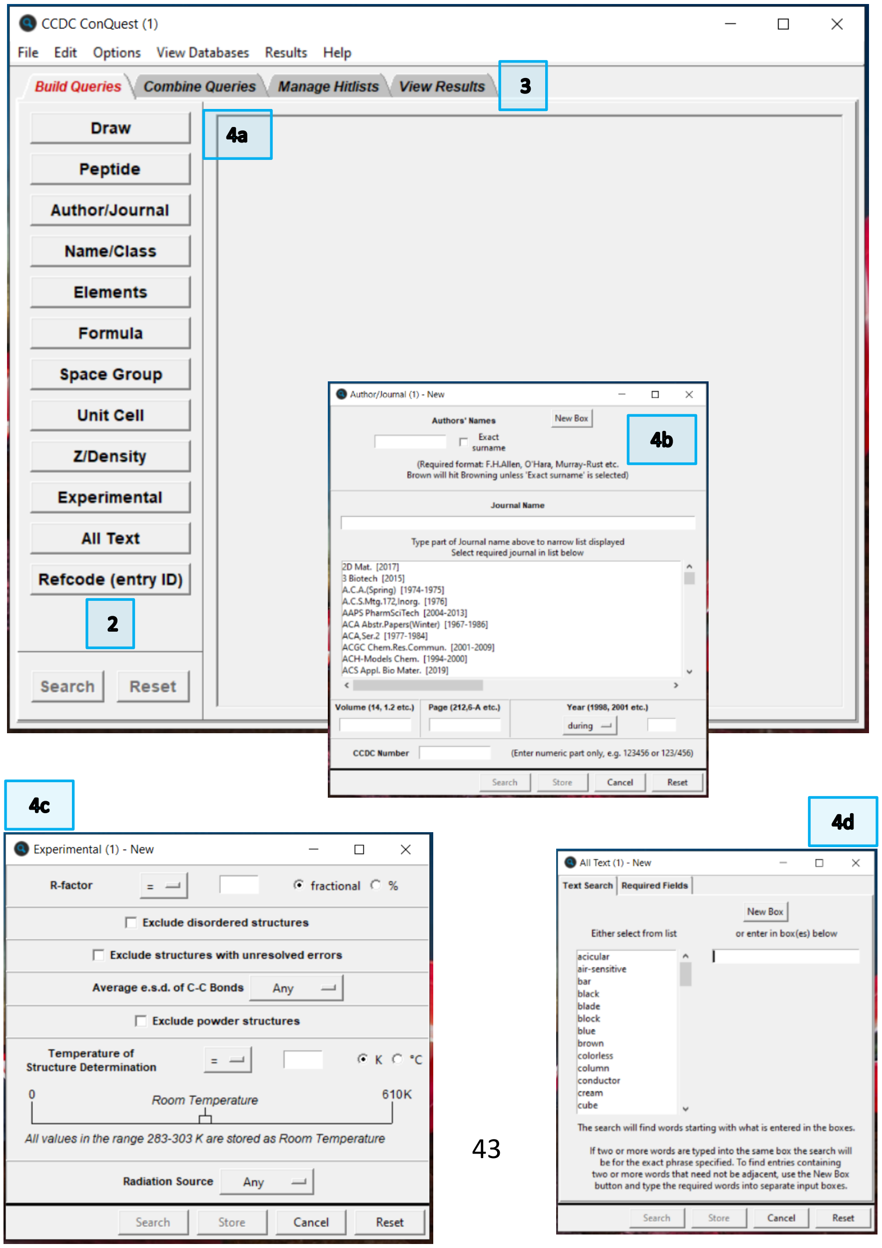

ACODUR

Substructure

A substructure of a structure is a specific smaller part of a structure. It does not need to be a complete molecule. For example, the C_6 ring of benzene is a substructure of both benzene and phenol but is not a complete molecule.

Review of the 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.



(Required format: F.H.Allen, O'Hara, Murray-Rust etc. Brown will hit Browning unless 'Exact surname' is selected)

Type part of Journal name above to narrow list displayed
Select required journal in list below

(Enter numeric part only, e.g. 123456 or 123/456)

All values in the range 283-303 K are stored as Room Temperature

The search will find words starting with what is entered in the boxes.

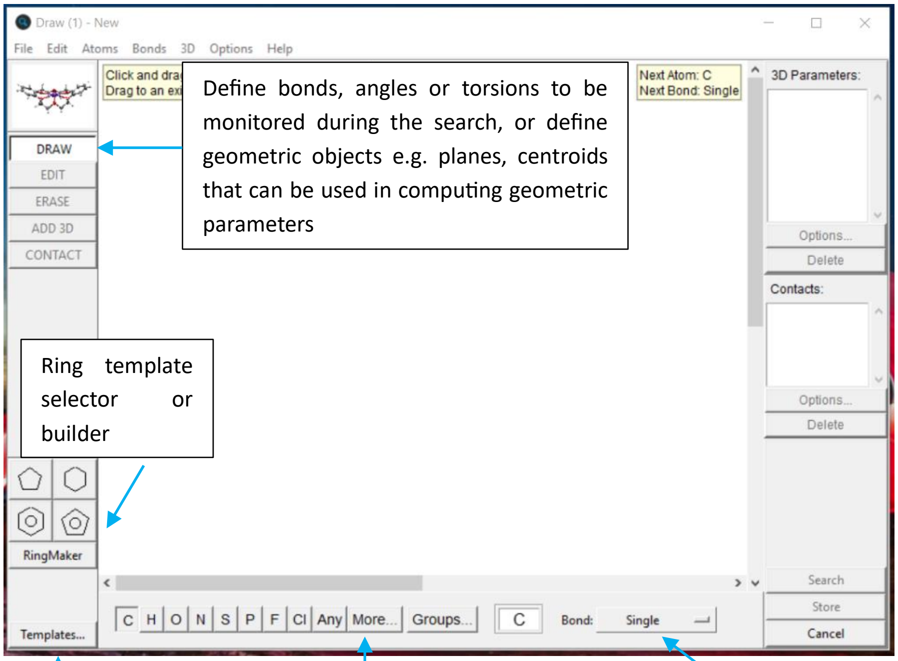
If two or more words are typed into the same box the search will be for the exact phrase specified. To find entries containing two or more words that need not be adjacent, use the New Box button and type the required words into separate input boxes.

Review of the 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).



Define bonds, angles or torsions to be monitored during the search, or define geometric objects e.g. planes, centroids that can be used in computing geometric parameters

Ring template selector or builder

List of templates for challenging substructures e.g. adamantane

Choice of specific or general atom types/functional groups

Choice of bond types