Exploring Structure Correlations Using Mercury and ConQuest

Developed using 2024.2 CSD Release

Table of Contents

Introduction	2
Learning Outcomes	2
Pre-required Skills	2
Materials	2
Example 1. The Dimerization of Group 11 L–M–X Halo complexes	3
Part 1. Building search queries in ConQuest	
Part 2. Data analysis in Mercury	11
Conclusion	17
Further exercises	17
Summary	
Next Steps	18
Glossary	
Basics of Mercury Visualization	
Review. ConQuest Interface	21
Review. Draw Window	22
ConQuest sketching conventions	22





Introduction

ConQuest is the desktop search interface to the Cambridge Structural Database (CSD). It provides an extensive range of flexible search options including substructure searching with the tandem capability of retrieving defined geometrical parameters, subject to structural and chemical constraints. ConQuest can export results directly to Mercury, which is the desktop crystal structure visualization software. Mercury additionally acts as the interface to many other CSD applications, including a comprehensive data analysis package which is dynamically linked to the structure visualizer. We will harness this functionality in this workshop to explore structure correlations in metal complexes.

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

Learning Outcomes

After completing this workshop, you will be able to:

- Draw a substructure query in ConQuest
- Add defined 2D and 3D parameters to the search query
- Run a combination search and export results to Mercury
- Perform calculations in the Data Analysis Module
- Select, plot and filter data according to specified criteria

We recommend attempting Part 1 or Part 2, each of which take approximately **25** *minutes* to be completed. The words in <u>Blue Italic</u> in the text are reported in the <u>Glossary</u> at the end of this handout.

Pre-required Skills

Basic familiarity with the ConQuest and Mercury interfaces is desirable, however, summary guides are provided at the end of this document.

Materials

You can download the files for this workshop here.



Example 1. The Dimerization of Group 11 L–M–X Halo complexes

Interpreting the correlation between two structural parameters within a family of related compounds as providing snapshots of chemical reaction pathways is one of the fields of study that has benefitted most from the wealth of data contained in the CSD. One such system, investigated by Echeverría and Alvarez¹, is the dimerization of Group 11 and Group 12 metal halides. The abundance of structures bearing a dimeric L–M–X motif provides hundreds of measurements of bond distances (as well as formally non-bonded contact distances) and valence angles which can be used as the starting point for structure correlation studies.

In this example, we will search the CSD for $(MX)_2$ fragments formed by the association of L–M–X units, where L is any ligand, M is one of Cu, Ag or Au, and X is Cl, Br or I. In so doing, we will collect the M–X···M distance and the L–M–X valence angles, and search for correlations between them.

Part 1. Building search queries in ConQuest

We will build two queries in such a way that we can deploy them simultaneously in a structure search. The use of consistent labels means the data retrieved can be combined in the second half of this tutorial.

Important: it is vital that you keep track of the labels you use for atoms and parameters in the following steps. We strongly recommend that you use the labelling scheme shown in Figure 1.

Tip: When defining parameters, it is advisable to use more memorable symbols in the labels; we suggest M, E and X for metal, halogen and ligand, respectively. The numbers 1 and 2 in Figures 1a and 1b refer to the fragment of the dimer.

¹ J. Echeverría and S. Alvarez, *Cryst. Growth Des.*, 2024, **24**, 4743–4747. https://doi.org/10.1021/acs.cgd.4c00335







Figure 1. Suggested atom labelling schemes for (a) bonded and (b) non-bonded dimers. The labels 1B, QA and X are used in ConQuest to refer to *atom type*. The superscript numbers visible in (c) when defining 3D parameters refer to the order in which the atom was added to the draw window. **If you edit the structure, these numbers will change.**

- 1. Open ConQuest from the Start Menu or by clicking on the desktop icon
- 2. Click on the **Draw** button from the **Build Queries** tab to bring up the Draw Window.
- 3. From the bottom toolbar, click on **More...**and then **Other Elements** to bring up the periodic table.
- 4. First, we will select the Group 11 metals. Click on **1B** at the top of the group and then click **Apply**.
- 5. Click in the **Draw** window to add "1B" atoms, corresponding to M1 and M2 in Figure 1a.
- Reopen the periodic table as in Step 3 (click Reset if 1B is still selected). Select Multi Pick from the *picking mode* section, then click on Cl, Br and I and click Apply.
- 7. Ensure that *Single* is selected from the *Bond*: drop down menu. Click, drag and release on the 1B atoms sequentially in the **Draw** window to add "QA" atoms, corresponding to E1 and E2 in Figure 1a.
- 8. From the bottom toolbar, click **Any** and click, drag and release to add "X" atoms, corresponding to X1 and X2 in Figure 1a.





CI Any More...



Х

Groups.

-1R

-QA

-1B-

CQ-007

9. Draw single bonds between the QA and 1B atoms

We will next define 3D parameters. All parameters except *Atom Labels* can be renamed, so we recommend that these are defined in the order suggested.

- 10. From the left-hand toolbar, click **Add 3D** to bring up the **Geometric Parameters** window.
- 11. In the **Draw** window, click on the atoms corresponding M1 and E2 in Figure 1a (in the image to the right, these are labelled as ¹1B and ⁴QA, respectively). Next to *Distance* in the define parameters window, click **Define**. Tip: the labels ⁿatom (like ¹1B) depend on the order they were drawn in; this is why we recommend relabelling according to Figure 1a.
- 12. In the Geometric Parameters window, click **Options...**and in the *RENAME:* field, type "M1E2" and click OK.

Select atoms from main window Hit 'Options' to set constraints or Current Selection:	change options	Modify options and hit 'Apply' when done.
Valid Parameters Distance: DIST1 Options	All Parameters Defined Objects:	LIMIT: From to (Å) © Range © Value +/- tolerance RENAME: M1E2
Valid Objects	Delete	Clos







 \times

Apply









- 13. Repeat **Steps 11–12** for the atoms corresponding to M2 and E1 in Figure 1a (these are labelled ²1B and ³QA in the image to the right). Note you may need to deselect the previous atoms first. Edit the name to "M2E1".
- 14. Click on the atoms corresponding to X1, M1 and E1 in Figure 1a, in that order. In the image to the right, these are labelled ⁵X, ¹1B and ³QA. Next to *Angle:* click **Define**.
- 15. Use the procedure in Step 12 to rename ANG1 to "X1M1E1".
- 16. Repeat **Steps 13–15** for the atoms corresponding to X2, M2 and E2 in Figure 1a (in the diagram to the right, these are labelled ⁶X, ²1B and ⁴QA, respectively). Rename this angle "X2M2E2".
- 17. Define the distance between the two metal atoms (M1 and M2 in Figure 1a, and ¹1B and ²1B in the figure to the right, respectively). Name this parameter "M1M2".
- 18. Select only the atom corresponding to M1 in Figure 1a (this is ¹1B in the image to the right, highlighted green). In the Geometric Parameters window, click **Define** next to *Atom Properties:*. In the All Parameters window that appears, tick **Atom label** and **OK**.
- 19. Repeat the procedure for the remaining atoms in this order (as in Figure 1a): E1, M2, E2 (these are labelled ³QA, ²1B and ⁴QA in the image on the right). Do not attempt to change the default labels, as this will cause an error. When you are finished, click Done in the Geometric Parameters window.
- 20. In the 3D parameters box at the top right-hand side of the Draw window, you should see a list of all the parameters you have defined. There should be nine defined parameters; you may need to scroll to see them all.



LAB1 LAB2 LAB3

Options.

- 21. Right click on the 1B atoms (which correspond to M1 and M2 in Figure 1a) and from the drop-down menu, select *Number of Bonded Atoms > 3*. The superscript "T3" will appear next to these atoms.
- 22. Click **Store** at the bottom right-hand side of the **Draw** window.

We will now create a second query, as shown in Figure 1b, which involves the same fragments but with <u>non-bonded contacts</u> between them.

- 23. In the **Build Queries** area, next to *Query 1*, click **Edit...**. This brings up another instance of the query that we constructed earlier.
- 24. Click on **Erase** in the left-hand toolbar, then click on the bonds between the 1B and QA atoms.
- 25. Click on Draw, then right click on the 1B atoms and select *Number of Bonded Atoms > 2*.
- 26. From the 3D Parameters section on the top right-hand side of the **Draw** window, click on M1E2 and click **Options**.
- 27. Next to CONTACT: click Create





- 8
- 28. Click **Define** to bring up the Non-bonded Contact definition.
- 29. Click **Edit** this will bring up another window with more options to customise the contact settings.
- 30. Ensure that the **Shorter than sum of VdW radii** is selected and leave the additional value as "+0.0". Click **Set Radii...**
- 31. We will update the default *van der Waals radii* to the following values: Cu, 2.38; Ag, 2.53; Au, 2.32; Cl, 1.82; Br, 1.86; I, 2.04. Type the element symbol and the new van der Waals radius, being sure to click **Store Value** after each change made. Click **OK** after all changes have been made.
- 32. Click OK in the Non-bonded Contacts Definition window(s).



33. Click Apply and Close the 3D Limits and Options window.

PARAMETER: M1E2 -	(Distance)
Modify options and	d hit 'Apply' when done.
Contact Distance:	CON1 Edit
This distance parameter is associated with a non-bonded contact. You can change its name or	Defined Contact: 1B1 QA4 * Inter-molecular Distance within sum of VdW + 0.0 Å
'Edit' the contact definition.	Distance within sum of vow + 0.0 A

28 Non-bonded Contact Defini × CONTACT: <new> Hit 'Define' to create contact or deselect atoms.</new>	29 Non-bonded Contact Definition CONTACT: CON1
ATOM: 1B1 ATOM: QA4 C Centroid C Centroid Closest Atom C Closest Atom Define Cancel OK	Hit 'Edit to change settings or 'Cancel' to close window. ATOM: 1B1 ATOM: QA4 C Centroid C Centroid C Iosest Atom C Iosest Atom Define Define Distance within sum of VdW + 0.0 Å
	Cancel OK



31	🕲 VdW Radii Setup		—		×
	Enter element symbol and VdW Radius Element: Cu VdW Radius: 2.38 Store Value	Curren Co Cr Cs Cu D Dy Er	nt Settin 2.0 2.0 2.0 1.4 2.0 2.0 2.0 2.0	igs (An	gstroms)
		Defa	ults C	ancel	ОК

- 34. Click on M2E1 in the *3D Parameters* box and repeat and repeat Steps 27–30 and 32–33 for the parameter M2E1 (you should not need to change vdW radii again).
- 35. Click **Store** from the bottom right-hand side toolbar. When prompted if you wish to overwrite the query, press **No**. This will ensure that a separate query is created.
- *36.* At this point, it is recommended that you save these queries, by selecting *File* > *Save Queries* > *All Queries...* and save it in a convenient location. These can be re-opened in another ConQuest session if needed.
- 37. Click on the **Combine Queries** tab and drag both Query 1 and Query 2 to the box *must have at least one of (OR)*
- 38. Click Search to launch the Search Setup window.

Build Queries Combine Queries	Manage Hitlists View Results	
Drag Query Icons into Boxes Find entries that: must have (Doolean AND)	Query 1 QA = CI Br I	Edit Delete
must not have (1/07)	$\begin{array}{c} X \stackrel{TZ}{=} 1B - QA \\ QA \stackrel{TZ}{=} 1B - X \\ QA = CI Br I \end{array}$	Edit Delete
must have at least one of (OR) ? ? Query 1 Query 2		
38		





Choose a suitable search name, such as "group 11 halides" and tick *R factor* <=0.075, Only Non-disordered and Only Single crystal structures. Leave all other settings as default.

40. Click Start Search.

- 41. The search should return a <u>hitlist</u> of 700 <u>refcodes</u> based on CSD 5.45 + 3 updates; your value may differ depending on your installation. You can scroll through the hits if you wish; you will notice that where a non-bonded dimer has been identified, the 3D parameter is highlighted pink, whereas it is highted green for the directly bonded dimers.
- 42. You can save the search results by going to File > Save Search As...



9 Search Setup	– 🗆 X
Search Name: group 11 halides	Filters Advanced Options
Available Databases: 🔲 Show Updates separate	ely 🗖 3D coordinates determined
CSD version 5.45 (November 2023) + 2 updates	Image: R factor C ≤= 0.05 Image: C = 0.075 C ≤= 0.1 Image: R factor C = 0.1 Image: R factor C = 0.1
You can search complete database(s) or a subset (e.g., hits found in a previous search) Select Subset	No errors
Summary of queries to be used. Search will find structur where at least one of these queries is true: Query 1 Query 2	es: C Powder structures C Only © Organics C Organometallic
40 Start Search	Cancel Reset



3a

Press the left mouse button and move the mouse to rotate the structure

Part 2. Data analysis in Mercury

In this section we will analyse ConQuest search data in Mercury. If you are attempting this part independently, please start from Step 2(b) using the .c2m file supplied in the workshop materials, otherwise begin at Step 1.

- 1. At the top of the results list in the **View Results** tab, click *Analyse Hitlist > Analyse Data*.
- (a) The Analyse in Mercury window will appear. There are many details that you can export, but all we require is **Include Defined Parameters**. Ensure this is selected and that the *File type* is set to *Mercury data file (.c2m)*, and press analyse in Mercury. **OR** (b) Open Mercury S from the desktop or *Start* menu, go to *File > Open*, select "group 11 halides.c2m" and click **Open**.
- 3. Three windows will appear: (a) the **Mercury visualizer** window, with the search results displayed in the **Structure Navigator** (b) the **Hit Fragment Display Options** and (c) **Data Analysis**. You can experiment with the Hit Fragment Display options if you wish, but we do not require it, so it may be closed. The remainder of the workshop will focus on the **Data Analysis** window.



lab(LAB4)

I1B

CI1

CI2

Br2B

I2B CI1

CI2

Br2

I1D

I1D

CI1

Br4

Br2

Br6

11

Br1

CI2

Br2B

Br2D

CI1A

11

lab(LAB2)

11

CI1

CI1

Br2

12

CI1

CI2

Br2

11

l1 Cl1

Br3

Br1

Br6

I2A

Br1

Cl2

Br2

Br2

11

CI1

lab(LAB3)

Cu1B

Cu1

Cu2

Cu1B

Cu1B

Au1

Au2

Au2

Cu1D

Cu1D

Aq1

Cu4

Cu2

Au2

Au1

Ag1

Au2

Cu1B

Cu1D

Au1

Ag1A

BOJYOS (P21/c) - Mercury		- 🗆 × .	😌 Hit Fragment Display Options	X Data Analysis
File Edit Selection Display Calculate CS	D-Community CSD-Core CSD-Materials CSD-Theory CSD-Particle CSD-Di	scovery CSD Python API Help		File Options
Picking Mode: Pick Atoms	Clear Measurements D O Show Labels for All atoms	✓ with Atom Label	Fragment Selection Fragment Highlighting	group 11 halides Spreadsheet 1
Style: Wireframe V Colour: by Element	V Manage Styles Small Ball and Stick V Atom selections:	 Select by SMARTS: [c] 	Tree view 🗌 Load multiple	tiple structures
Animate Default view: b	a b c a* b* c* x- x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-9	$10 \ z+90 \leftrightarrow \rightarrow \downarrow \uparrow zoom- \rightarrow Disorder; \rightarrow$	Select all Show only hil	y hit atoms File loots Descriptors Display Selection Plots Statistics
		Structure Navigator 🗗 🗙	Charles Wiles	Find identifier Find next
\searrow		BOJYOS Find	Structure Value	Identifier NAME Overy Fragment M1E2 M1M2 M2E1 X1M1E1 X2M2E2 lab(LAB
$\langle \bigcirc \rangle$		Countral Structures Spaceagroup	✓ BOJYOS	group 11 halidesi8 BOJYOS 1 1 2.2840 2.9380 2.3060 131.7340 130.7220 Cu1
$\langle O \rangle$		BOIVOE B31/6	* Query I	group 11 halides C CORZIS01 1 1 2.5780 2.6370 2.5780 122.1500 122.1500 Cu1
\sum		COR7/S01 P21/c	* Frag	group 11 halides[EF EFIBOO 2 1 3.2240 3.5770 3.2240 170.6490 170.6490 Cu1
	TAY T	FFIBOO P21/c	2.284	group 11 halides GL GIWMEI 1 1 2.3130 3.0070 2.3060 135.1840 128.6840 Cu1
\rightarrow (7)		GIWMEI P21/n	2.306	group 11 halides QI QIVTIC 1 1 2.4270 2.8630 2.4270 124.9780 124.9780 Cu1
YOI DE		QIVTIC P21/c	131.734	group 11 halides V VOFDED 1 1 2.5600 2.8560 2.5600 125.3510 125.3510 Cu1
$ 0\rangle$		VOFDED P21/n	130.722	group 11 halides YI YIVJUM 2 1 3.9670 5.1610 3.9670 173.6890 Au1
	133/73 2.306	YIVJUM P21/c	2.938	group 11 halides YI YIVJUM 2 2 4.0400 4.8530 4.0400 178.2210 178.2210 Au2
	280	YIVJUM P21/c	I Cu1	group 11 halides/Z ZODCII 2 1 4.1330 3.5770 4.1330 170.6290 170.6290 Au2
	2.284 130.72	ZODCII P-1	I Cl1	group 11 halides A ACURAV 1 1 2.5760 2.6520 2.5760 121.3840 121.3840 Cu1
L	$\lambda \vee \rightarrow \langle () \rangle$	ACURAV Pbca	I Cu2	group 11 halides A ACURAV01 1 1 2.5780 2.5970 2.5780 120.4260 L20.4260 Cu1
		ACORAA DO1/0	I Cl2	group 11 halides A AGOBAA 2 1 2.9850 3.9420 2.9850 165.0200 165.0200 Ag1
]()	$ \rangle \langle \rangle \langle \rangle \rangle = \langle \rangle \langle \rangle \rangle \langle \rangle \langle \rangle \rangle \langle \rangle \langle$	ABOBAA P21/II AHACAO P-1		group 11 halides A AHACAQ 1 1 2.4230 2.9140 2.4490 127.7900 135.4330 Cu3
		AHACAO P-1		group 11 halides A AHACAQ 1 2 2.4550 2.7850 2.4410 134.2600 126.8200 Cu1
14	\sim	AHOFIO P-1	Show parameters: All	group 11 halides A AHOFIO 2 1 4.1620 4.1990 4.1620 176.4190 176.4190 Au2
	/()/	ALEBIE C2/c		group 11 halides/AL ALEBIE 2 1 3.8560 2.9950 4.2100 176.1020 170.9300 Au2
		AMETOC P-1	Data Analysis Close	group 11 halides/A AMETOC 2 1 3.9650 3.4420 3.9650 174.1780 174.1780 Ag1
	7	ANIRAS P21/c		group 11 halides[A ANIRAS 2 1 4.0340 5.0940 4.0340 175.9290 175.9290 Au2
		AVUSIU P21/n		group 11 halides[AV AVUSIU 1 1 2.4180 2.8870 2.4180 125.5960 125.5960 Cu1
Disels: Ostions		AYARUQ Pbca		group 11 halidesjAY AYARUQ 1 1 2.4420 2.6770 2.4420 124.7710 124.7710 Cu1
Display Options	Online:	AYUSIZ C2/c		group in natioesjay AYUSIZ 2 1 3,6940 3,0290 3,6940 171,4720 171,4720 Au1
	Options Date in	<< >>		group 11 naildesja AZOXOE 1 1 2.8100 3.6580 2.8100 147.2790 147.2790 Ag1
Packing Short Contact < (si	um of vdW radii) Contacts Show hydrogens Depth cue	Tree View		R * -
Auto contro	r defined More Info More Info			
Auto dentre	Label atoms Stereo	Multiple Structures		
Reset	POWDEL	Structures		

3b

4. The headers of the columns in the spreadsheet correspond to the parameters that we defined in our search queries. You may need to expand the columns to read the headings properly (click and drag on the column dividers).

Dimers of the type we have searched for are known to form M…M interactions in some circumstances. The presence of such bonding may invalidate the bonding model we are using in describing M…Hal dimers. To filter these out, we can disregard examples where the M1M2 distance is less than 0.1 Å greater than the M1E2 and M2E1 distances.

- 5. Click *Tools > Calculator* from the top menus of the spreadsheet.
- From the available heading in the Name section, click M1M2. It will appear in the lower box as 'group 11 halides'.'M1M2'. In the box, type "-" (or click the minus button from the right hand) and then click on M1E2. In the New descriptor box give a suitable name, such as "M1M2 M1E2" and click Calculate.
- 7. The name of this calculation will appear in the left-hand box of the calculator and also in the spreadsheet as a new column.
- 8. Click **Clear** and repeat the procedure to calculate M1M2-M2E1. **Close** the calculator.

(LAB4)	M1M2 - M1E2
Cl1	0.6570
11	0.0670
Cl1	U 523U

	\sim
Na	me
\sim	group 11 halides
	X2M2E2
	X1M1E1
	Query
	M2E1
	M1M2 - M1E2
	M1M2
	M1E2
	Fragment

4												
Identifier	NAME	Query	Fragment	M1E2	M1M2	M2E1	X1M1E1	X2M2E2	(LAB1)	(LAB2)	(LAB3)	(LAB4)
group 11 halides BOJYOS 0	BOJYOS	1	1	2.2810	2.9380	2.2970	127.0820	129.2040	Cu1	Cl2	Cu2	Cl1

😵 Da	ita Ana	lysis		
File C)ptions			
group	11 hali	des Spreadsh	eet 1	
File	Tools	Descriptors	Display	Selecti
Find ic	D	elete		
	S	preadsheet		
	С	alculator		
g	То	opological syr	nmetry	BOJ
g	С	SD data		CO
g				_ EFIE



- 9. Right-click on the M1M2-M1E2 column header and select Sort from the dropdown menu. This will sort the column by numerical value. You may need to click twice to get the value in descending order.
- 10. Scroll down the spreadsheet until you find the row at which M1M2-M1E2 is less than 0.1 Å. Left-click on the row and drag to select all remaining rows below 0.1 Å.
- 11. From the top menu, click *Selection > Hide selected*.
- 12. Repeat steps 9–11 for the column M1M2-M2E1 to remove the small number of additional entries for which this value is less than 0.1 Å.
- 13. Make sure that no columns are selected by clicking the header of any columns that are currently highlighted. Click Ctrl + A to highlight the selected entries. From the top menu, select *Plots > Scatter plot*. In the resulting **Choose descriptors** menu, from the drop-down menus, select *X2M2E2* for the *X axis* and *M1E2* for the *Y axis*. Leave the **Colour** and **Size** boxes unchecked and click OK.

😌 Data Analy	sis							-		
File Options										
group 11 halide	es Spreadsheet 1									ð
File Tools	Descriptors Direla	v Selection	Plote	Intistics					0	1
The Tools	Descriptors Displa	y Selection	FIUS .	Judustics						1
Find identifier				Find n	ext					
	Identifier	NAME	Query	Fragment	M1E2	M1M2	M2E1	X1M1E1	X2M2E2	1
group 11	halides YUXBOJ 731	YUXBOJ	1	1	2.5730	2.8590	2.5770	126.7670	127.3530	C
group 11	halides YUXVUJ 734	YUXVUJ	2	3	3.1830	4.0030	3.1830	169.9650	169.9650	I A
group 11	halides[YUXWAQ]735	YUXWAQ	2	1	3.2670	4.2550	3.4260	163.4130	163.4130	I A
group 11	halides[YUXXEV]736	YUXXEV	2	1	2.9850	3.9910	3.0300	173.8580	173.8580	I A
group 11	halides[YUXXUL]738	YUXXUL	2	2	2.9470	3.0550	3.0120	165.9470	166.2840	I A
group 11	halides ZACGUF 740	ZACGUF	2	1	2.6930	3.2090	2.6930	156.8110	156.8110	C
group 11	halides ZATKIS 741	ZATKIS	1	1	2.7790	2.9700	2.7640	125.6920	120.3830	I A
group 11	halides ZATZOL 742	ZATZOL	1	1	2.2300	3.2790	2.2300	118.0840	118.0840	0
group 11	halides ZEHQEK 743	ZEHQEK	2	1	3.8390	4.0240	3.8390	180.0000	180.0000	I A
group 11	halides ZENDIF 744	ZENDIF	1	1	2.8070	3.1110	2.8070	124.0440	124.0440	I A
group 11	halides ZEQBEG 745	ZEQBEG	1	1	2.7730	3.5740	2.8710	138.3000	156.5860	I A
group 11	halides ZEQBIK 746	ZEQBIK	2	1	3.2870	4.0900	3.3730	176.5900	174.1380	I A
group 11	halides ZISKUH 750	ZISKUH	2	1	3.7010	4.1770	3.7010	176.4490	176.4490	I A
group 11	halides ZOMCAH 758	ZOMCAH	1	1	2.4090	3.7890	2.4090	114.5130	114.5130	I A
group 11	halides ZOMCIP 759	ZOMCIP	2	1	3.0430	3.9610	3.0430	176.5070	176.5070	I A
group 11	halides ZOMCOV 760	ZOMCOV	1	1	2.6320	3.1200	2.6320	130.2540	130.2540	I A
group 11	halides ZOTMOK 761	ZOTMOK	2	1	4.0540	4.5170	4.0540	178.9050	178.9050	I A
group 11	halides ZOWZUI 762	ZOWZUI	2	1	3.1210	4.0570	3.1210	165.3800	165.3800	I A
group 11	halides ZUHMIB 763	ZUHMIB	2	1	3.7650	4.8490	3.7650	177.2580	177.2580	A
group 11	halides ZUSTEP 764	ZUSTEP	2	1	3.5700	3.9290	3.5700	175.4830	175.4830	A
group 11	halides QOMYIE 767	QOMYIE	1	1	2.4750	3.8650	2.4750	98.1880	98.1880	A

😗 Choose	descriptors	×					
Choose bet	ween two and four descri	iptors					
X axis	X2M2E2	\sim					
Y axis	M1E2	\sim					
	Query	\sim					
🗌 Size	Query	\sim					
	OK Cancel						



Tools Des														
IOOIS Des	criptors Display	Selection	Plots Statistic	:s										8
dentifier								Find next						
Picks	NAME	Query	Fragment	M1E2	M1M2	M2E1	X1M1E1	X2M2E2	(LAB1)	(LAB2)	(LAB3)	(LAB4)	M1M2 - M1E2	M1M2 - M2E1
	TETKUB	1	1	2.5690	2.6890	2.5690	118.9330	118.9330	Cu3	I2A	Cu3A	12	0.1200	0.12
	CUKDOD	2	1	3.4850	3.5960	3.5080	171.3340	173.8530	Au1	CI2	Au2	Cl4	0.1110	0.08
	YUXXUL	2	2	2.9470	3.0550	3.0120	165.9470	166.2840	Ag1	Cl1	Ag2	CI2	0.1080	0.04
	MASCIV	2	1	3.2440	3.3410	3.2610	172.3290	171.5570	Au1	Cl1	Au2	Cl2	0.0970	0.08
	KOFWOR	1	1	2.5810	2.6770	2.5810	119.2930	119.2930	Cu2	I2A	Cu2A	12	0.0960	0.09
	QICMOI	1	1	2.5720	2.6680	2.5720	120.4120	120.4120	Cu1	I1B	Cu1B	11	0.0960	0.09
	YITXAB	1	1	2.5780	2.6740	2.5780	124.8440	124.8440	Cu2	I1D	Cu2D	11	0.0960	0.09
	EDAPUV	1	1	2.5840	2.6760	2.5840	120.4150	120.4150	Cu1	I1D	Cu1D	11	0.0920	0.09
	XEXZEH	2	1	3.1460	3.2370	3.1460	168.1530	168.1530	Ag1	CI1	Ag1	Cl1	0.0910	0.09
	KALJOW	1	1	2.5700	2.6580	2.5700	120.1710	120.1710	Cu1	I1A	Cu1A	11	0.0880	0.08
	DOCSIY	1	1	2.5800	2.6630	2.8270	119.1910	146.6470	Cu1	12	Cu2	11	0.0830	-0.16
	ACURAV	1	1	2.5760	2.6520	2.5760	120.5760	120.5760	Cu1	I1D	Cu1D	11	0.0760	0.07
	FOGYAD	2	1	3.6690	3.7390	3.6690	175.2640	175.2640	Au1	Cl1	Au1	Cl1	0.0700	0.07
	NIBYON	1	3	2.6980	2.7660	2.5690	133.8590	121.0690	Cu4	15	Cu5	14	0.0680	0.19
	CORZIS01	1	1	2.5700	2.6370	2.5700	119.4720	119.4720	Cu1	I1B	Cu1B	11	0.0670	0.06
	FOGYEH	2	1	3.8210	3.8870	3.8210	177.9890	177.9890	Au1	Cl1	Au1	CI1	0.0660	0.06
	ETOKEE	1	1	2.5970	2.6620	2.5970	123.0910	123.0910	Cu2	I1B	Cu2B	11	0.0650	0.06
	NIBYON	1	2	2.6570	2.7190	2.6180	133.2450	121.4930	Cu2	13	Cu3	12	0.0620	0.10
	KAZJAZ	1	1	2.5370	2.5980	2.5370	103.8680	103.8680	Cu1	I1A	Cu1A	11	0.0610	0.06
	CIKDIJ	1	1	2.6100	2.6630	2.5840	124.6120	120.3130	Cu1	12	Cu2	11	0.0530	0.07
	IDALIK	1	1	2,5470	2.6000	2.5470	115.8630	115.8630	Cu1	11A	Cu1A	11	0.0530	0.05





- 14. A plot will now appear, probably below the spreadsheet. You can detach this by clicking the two windows symbol at the top of the plot window to position it somewhere more convenient.
- 15. The graph contains entries for different metal-halide pairs e.g. Cu–Cl and Au– I. We can filter based on the atom labels defined in the search to highlight particular combinations. Left-click on the LAB1 and LAB2 headings; they will become shaded black. Then from the Selection menu at the top of the spreadsheet, choose Filter.
- 16. In the filter window (you can detach it) you will see filters for LAB1 and LAB2. From the dropdown menu, select Starts with for both labels and type Cu for LAB1 and Cl for LAB2. This will filter the results, so we see the Cu-Cl dimers highlighted red in the plot window.

14

le Options oup 11 halides Spreadsheet 1 File Tools Descriptors Display Selection Plots Statistics Image: Statis												_	
oup 11 halides Spreadsheet 1 File Tools Descriptors Display Selection Plots Statistics Image: Control of	le Options												
File Tools Descriptors Display Selection Plots Statistics Image: Statistics Imag	oup 11 halid	es Spreadsheet 1											é
Identifier NAME Query Fragment MIE2 M1ML W2E1 X1M1E1 X2M2E2 lab(LAB1) lab(LAB2) l	File Tools	Descriptors Display	Selection	Plots	Statistics								A
Identifier NAME Query Fragment M1E2 M1M2 M2E1 X1M1E1 X2M2E2 lab(LAB1) lab(LAB2) lab(LAB2) group 11 halides/YUXNB0/731 YUXBO/ 1 1 2.5730 2.8590 2.5770 127.3530 Cu1 4 Cu2 group 11 halides/YUXNB0/731 YUXBO/ 1 1 2.5730 2.8590 2.5770 127.3530 Cu1 H Cu2 group 11 halides/YUXNURQ/735 YUXNAQ 2 1 3.2670 4.2550 3.4260 163.4130 163.4130 Ag1 Br1 Ag1 group 11 halides/YUXNURQ/735 YUXNAQ 2 1 2.9650 3.9910 3.0300 173.8580 Ag1 Cl1 Ag1 group 11 halides/YUXNURS/143 YUXNUL 2 2.9470 3.0500 173.8580 Ag1 Cl1 Ag1 group 11 halides/YUXNURS/141 ZATKIS 1 2.7790 2.7640 125.6591 105.8310 105.8310 Qu2 Cu2 Cu2 Cu2													
Identifier NAME Query Fragment M1E2 M1M2 M2E1 X1M1E1 X2M2E2 Iab(LAB1) Iab(LAB2) I	nd identifier						Find next						
group 11 halides/VLXBOJ/731 YUXBOJ 1 1 2.5730 2.6590 2.5770 126.7670 127.3530 Cu1 I4 Cu2 group 11 halides/VLXBOJ/731 YUXBOJ 2 3 31830 4.0030 31830 169.050 Ag1 Cl1 Ag1 group 11 halides/VLXBOJ/735 YUXMAQ 2 1 3.2670 126.7670 127.3530 Cu1 I4 Cu2 group 11 halides/VLXBAQ/755 YUXMAQ 2 1 3.2670 3.0200 173.4580 Ag1 Cl1 Ag1 group 11 halides/VLXBAQ/1736 YUX0UL 2 2.9470 3.0550 3.0120 165.9470 166.2840 Ag1 Cl1 Ag2 group 11 halides/VLXBAQ/1740 ZACGUF 2 1 2.6503 3.2900 2.69200 120.3830 Ag1 I2 Ag2 group 11 halides/ZACGUF/1740 ZATKIS 1 1 2.7900 2.7640 125.6920 120.3830 Ag1 I2 Ag2 group 11 halides/ZACGUF/1740 ZATKIS 1 1 2.2300 3.2790 2.2300 118.08		Identifier	NAME	Query	Fragment	M1E2	M1M2	M2E1	X1M1E1	X2M2E2	lab(LAB1)	lab(LAB2)	lab(L
group 11 halides/UXVU/J734 VUXVU/J 2 3 3.1830 4.0300 3.1830 169.050 Ag1 Cl1 Ag1 group 11 halides/VUXVVJ/734 VUXWAQ 2 1 3.2670 4.2550 3.4260 163.4130 69.050 Ag1 Br1 Ag1 group 11 halides/VUXVVJ/735 VUXWAQ 2 1 3.2670 4.2550 3.4260 163.4130 69.050 Ag1 Br1 Ag1 group 11 halides/VUXVUJ/738 VUXVU 2 2 2.9470 3.0550 3.0120 165.9470 166.2840 Ag1 Cl1 Ag2 group 11 halides/ZAKIS/TH ZAKGUF 2 1 2.9500 3.2790 2.6901 156.8170 Cu2 Cl2 Cu2 group 11 halides/ZAKIS/TH ZAKIS 1 1 2.7900 2.7400 156.840 118.0840 Cu1 Cu1 Ag2 group 11 halides/ZAKIS/TH ZAKIS 1 1 2.7900 2.2300 118.0840 118.0840 Cu1 Cu1 Cu1 Cu1 oup 11 halides/ZAKIS/TH ZAKIS 1 2.2	group 11	halides YUXBOJ 731	YUXBOJ	1	1	2.5730	2.8590	2.5770	126.7670	127.3530	Cu1	14	Cu2
group 11 halides/UXWAQ[725 102WAQ 2 1 3 2670 4.2550 3.4260 163.4130 63.4130 Ag1 Br1 Ag1 group 11 halides/UXWAQ[735 102WAQ 2 1 2.9650 3.9910 3.0300 173.8580 Ag1 Cl1 Ag1 group 11 halides/UXXEV[736 102WEV 2 1 2.9650 3.9910 3.0300 173.8580 Ag1 Cl1 Ag1 group 11 halides/UXXEV[736 102WEV 2 2.9470 3.0550 3.0500 165.4970 166.2480 Ag1 1 Ag1 group 11 halides/UXXEV[740 ZACGUF 2 1 2.6930 2.6930 156.810 10.2030 Ag1 12 Ag2 group 11 halides/ZATKIS/741 ZATKIS 1 1 2.7900 2.7640 125.6301 18.0840 Cu1 Cl1 Cu1	group 11	halides YUXVUJ 734	YUXVUJ	2	3	3.1830	4.0030	3.1830	169.9650	169.9650	Ag1	Cl1	Ag1
group 11 haildes/1VXXVI/736 YUXXV 2 1 2.9850 3.9910 3.0300 173.8580 Ag1 Cl1 Ag1 group 11 haildes/1VXXVI/738 YUXXVI 2 2 2.9470 3.0550 3.0120 165.9470 166.2840 Ag1 Cl1 Ag2 group 11 haildes/2XCGU/F740 ZACGUF 2 1 2.6930 3.0120 156.3110 156.8110 Cu2	group 11	halides YUXWAQ 735	YUXWAQ	2	1	3.2670	4.2550	3.4260	163.4130	163.4130	Ag1	Br1	Ag1
group 11 halides/UXXUL[738 YUXXUL 2 2 2,9470 3,0550 3,0120 165,8470 166,2840 Ag1 Cl1 Ag2 group 11 halides/ZATKIS/HZ ZATKS 1 2,6930 3,2090 2,6930 156,8110 Cu2 Cl2 Cu2 group 11 halides/ZATKIS/HZ ZATKS 1 1 2,2900 2,8700 2,7640 125,6920 120,830 Ag1 Cl1 Ag2 group 11 halides/ZATKIS/HZ ZATKS 1 1 2,2900 2,8700 126,800 126,800 Cu1 Cl1 Cu2 Cu2 group 11 halides/ZATKIS/HZ ZATKOL 1 1 2,2300 118,0840 118,0840 Cu1 Cl1 Cu1 Cu1<	group 11	halides YUXXEV 736	YUXXEV	2	1	2.9850	3.9910	3.0300	173.8580	173.8580	Ag1	Cl1	Ag1
group 11 halides/ZATCOUF740 ZACGUF 2 1 2.6930 2.6930 156.8110 Cu2 Cl2 Cu2 group 11 halides/ZATKIS/41 ZATKIS 1 1 2.7790 2.9700 2.7640 126.8920 120.8830 Ag1 I2 Ag2 group 11 halides/ZATKIS/ZATKIS/ZATKIS/ZATKIS/ZATKIS 1 1 2.2700 3.2790 2.2300 118.0840 Cu1 Cl1D Cu1 poup 11 halides/ZATKOLTAZ ZATZOL 1 1 2.2300 3.2790 2.2300 118.0840 Cu1 Cl1D Cu1 poup 11 halides/ZATZOLTAZ ZATZOL 1 1 2.2300 3.2790 2.2300 118.0840 Cu1 Cl1D Cu1 poup 11 halides/ZATZOLTAZ ZATZOL 1 1 2.2300 3.2790 2.2300 118.0840 Cu1 Cl1D Cu1 poup 11 halides/ZATZOLTAZ ZATZOL 1 1 2.2300 118.0840 Cu1 Cl1D Cu1 poup 11 halides/ZATZOLTAZ Selection	group 11	halides YUXXUL 738	YUXXUL	2	2	2.9470	3.0550	3.0120	165.9470	166.2840	Ag1	Cl1	Ag2
group 11 halides/ZATXOL/742 ZATKIS 1 1 2.7790 2.760 125.6920 120.3830 Ag1 I2 Ag2 group 11 halides/ZATXOL/742 ZATZOL 1 1 2.2300 3.2790 2.2300 118.0840 100.000 Cu1 CHD Cu1 poup 11 halides/ZATXOL/742 ZATZOL 1 1 2.2300 3.2790 2.2300 118.0840 118.0840 Cu1 CHD Cu1 poup 11 halides/ZATXOL/742 ZATZOL File Aws Mouse Display Selection Plots Statistics File Ag2 Cu1	group 11	halides ZACGUF 740	ZACGUF	2	1	2.6930	3.2090	2.6930	156.8110	156.8110	Cu2	CI2	Cu2
group 11 halides/ZATZOL/742 ZATZOL 1 1 2.2300 118.0840 Cu1 Cu1 Cu1 Cu1 oup 11 halides Scatterplot 1 File Axes Mouse Display Selection Plots Statistics Image: Cut = Cut	group 11	halides ZATKIS 741	ZATKIS	1	1	2.7790	2.9700	2.7640	125.6920	120.3830	Ag1	12	Ag2
oup 11 halides Scatterplot 1 File Axes Mouse Display Selection Plots Statistics 4 1/4	group 11	halides ZATZOL 742	ZATZOL	1	1	2.2300	3.2790	2.2300	118.0840	118.0840	Cu1	CI1D	Cu1D
oup 11 halides Scatterplot 1 File Axes Mouse Display Selection 4 1				-		-	-	-					-
File Axes Mouse Display Selection Plots Statistics	oup 11 balid	es Scatternlot 1										1	2
File Axes Mouse Display Selection Plots Statistics 4 1	sap in naliu	o soutterplot i										_	
4 =	File Aves	Mouse Display Se	election Plo	ts Statis	tics								
4	Aves											•	0
· 4	Aves												
	4												
	4												-
3	4									•	و بوش	- <u>.</u>	-
	4 3.500 3				Latiniza	. 14	s* .e		•		41	• \$7*7	*
3	3.500 3.500 2.500	an a	nida		1		.	•. •	•.		447	•	+
	3.500 3.500	esti o ti	nién			vic.	•:•	•	*	•	44/	••••	•



				Sele	ction	Plots	Statistics
Ì	(LAB1)	(LAB2)			Hide Show	selecte / only s	d elected
)	Cu1	Cl2	(Show	ı all	
)	Cu1	Cl1	C		Selec	t all	
)	Cu1	Cl2	C		Dese	lect all	
)	Cu1	Br2B	C		Inver	t selecti	ion
)	Cu1	I2B	(Selec	tion	•
)	Au1	Cl1	1		Name	e select	ion
)	Au2	Cl2	1		Filter.		
)	Ag1	Cl1	1		Mana	ige	
)	Cu3	Br4	C				
	a (





- 17. Explore other possible metal-halide combinations. You can save the plots at any point from the plot window by going to *File > Export* and selecting as appropriate.
- 18. Untick the filters and close the filter window. You can reverse the filter process and select entries from the graph by clicking individually or dragging a box. The highlighted entries will turn red in the scatter plot and will be shaded grey in the spreadsheet.
- 19. Clicking on a single row will update the structure in the visualizer.





aroup 11 halid	los Epresdehest 1						-
group i i naliu	les spreausneer i						
File Tools	Descriptors Display	Selection	Plots Statistic	s			8
Find identifier			Find nex	t			
Pick	s NAME	Query	Fragment	M1E2	M1M2	M2E1	X1M1E
0	AYARUQ	1	1	2.4190	2.6770	2.4190	122.04
0	AZOXOE	1	1	2.4400	3.6580	2.4400	120.6
0	AZOYEV	1	1	2.5830	3.1230	2.5830	126.4
0	AZUGOU	2	1	3.7390	4.8110	3.7390	178.7
0	BESYAC	1	1	2.5060	3.6580	2.5060	113.5
0	BIBZOE	1	1	2.3870	3.7460	2.3870	106.5
0	BICVUH	1	1	2.5270	3.6770	2.5270	135.7
0	BIHHIN	1	1	2.4000	3.7660	2.4000	113.6
0	BIQWEF	2	1	3.1250	3.9300	3.1250	174.2
0	BIWNUR	2	2	4.0150	5.0210	4.0150	172.3
0	BIYMIF	1	1	2.5650	2.7240	2.5650	117.9
0	BIYMIF01	1	1	2.5840	2.7240	2.5840	125.73
0	BIYMIF02	1	1	2.5870	2.7290	2.5870	125.6

isplay Opt Display Packing

Asymmetric Unit

Auto centre

Reset

H-Bond

User defined



- 20. In the main spreadsheet, press Ctrl + A to select the entries then click *File* > *Export*. This will allow you to save out the data to a CSV file for further processing by other programs.
- 21. In the Export Spreadsheet window, you can select the columns you want to export by selecting from the *Available Items* area and clicking **Add** >> to move it to the *Selected Items*. We will select all with Ctrl+A and transfer them to the *Selected Items* using **Add** >>.
- 22. Select a suitable location using the Browse button and click Save.
- 23. To save the results in a format that can re-opened by Mercury, from the Data Analysis top menu (*not* the spreadsheet top menu). Click *File > Save database...*. Choose a suitable location and save the database. This can be reopened from *File > Load database* in the future.

22	•	Data Analysis		Save Database	×
23	File	Options		← → ∨ ↑ a octo → ConQuest-Me ∨ C Search ConQuest-Mercury Oroanise ▼ New folder	م وہ -
		Load database Save database	shee	Comments - F Name Status D Documents - F Name 2 Introductional Mat metal halides bonded and non bonded.sqlite 2	ate modifi 3/08/2024
		Main windows	rs [Ceneral Payslip Pictures Mecordings	
	_	Exit	NA	File name: stopp 11 metal holides Save as type: Databases ("sqlite *.db)	
				► Hide Folders Save Ca	ncel



Available Items (Right-click for options) Picks NAME Query Fragment M1E2 M1M2 M2E1 X1M1E1 ¥2M2E2	>> Nove Up Down
--	-----------------



Conclusion

In this example, we have seen how 3D geometric data from a large number of crystal structures can be used to elucidate structure correlations. We have verified that amongst group 11 metal halides, there is a correlation between the inter-dimer metal-halide bond length and the bond angle in the monomers. Furthermore, we have used the capabilities to the Mercury Data Analysis module to compare trends amongst different metal-halogen pairs and have established that there are indeed substantial differences.

Further exercises

If you have enjoyed this exercise, you can explore the results further:

- Plot M2E1 vs X1M1E1 using the Data Analysis module to check the same correlations are found.
- In the exported spreadsheet, combine the distance and angle data for all the fragments and plot graphs of the complete dataset.

Echeverría and Alvarez have proposed analysis of these data in terms of the *penetration index* which takes into account both van der Waals and covalent radii to give a more meaningful comparison of distances. The penetration index of two atoms, A and B, is defined as:

$$p_{AB} = 100 \times \frac{v_A + v_B - d_{AB}}{v_A + v_B - r_A - r_B}$$

where v_A and v_B are the van der Waals radii of A and B, r_A and r_B are the covalent radii of A and B, and d_{AB} is the interatomic distance.

• Calculate the penetration indices for the data, using the values in Table 1, and plot these against the L-M-X angles (see Figure 2).



Figure 2. Plot of X-M-L angle vs M...X percentage penetration.

Atom	van der Waals radius	Covalent radius
Cu	2.38	1.32
Ag	2.53	1.45
Au	2.32	1.36
Cl	1.82	1.02
Br	1.86	1.20
1	2.04	1.39

Table 1. Selected van der Waals and covalent radii.

Summary

In this workshop we have seen how to search for substructures in the CSD and retrieve 3D data from the hits. We subsequently saw how to analyse these results in Mercury. You should now be able to:

- Set up substructure searches in ConQuest
- Define 3D search parameters, including distances, angles and nonbonded contacts
- Run a combination search in ConQuest, with suitable filters
- Export search results to Mercury
- Use the calculator tool in the Data Analysis Module
- Plot selected data and apply filters
- Export data in spreadsheet format and save data as a database

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

Next Steps

If you have enjoyed this workshop, you might like to explore some of our other self-guided workshops which use ConQuest and Mercury. In particular, we would suggest "Using 3D information in Searches in ConQuest", "Intermolecular Interaction Searching in ConQuest" and "Searching and Analysing Metal-Organic Structures using ConQuest and Mercury".

Glossary

Hitlist

A hitlist is a subset of CSD entries which can include search results, refcode lists, or the results of combining these.

Nonbonded contact

This type of search can be used for finding intermolecular interactions such as hydrogen bonds, halogen-halogen interactions, intramolecular non-covalent interactions and generating tables of geometries for nonbonded interactions. Nonbonded contacts between atoms are defined in terms of distance limits.

Refcode

A refcode is a CSD entry identifier comprising six letters e.g. ABACOF. Two digits identifying additional structure determinations e.g. ABACOF03.

Van der Waals radius

The van der Waals radius of an element is one half of the distance between the closest approach of two non-bonded atoms of a given element.



Non-bonded contacts between Ag and Cl in CSD entry UPAFAU.

Basics of Mercury Visualization

Mercury is the CCDC's visualization software to view 3D structures of small molecules, generate images, and animations of molecules.

In the following we will see some of the basics of navigation and visualization in Mercury that you will find helpful to support your analysis.

In the Mercury interface we find:

- At the top: list of menus from which we can access visualization and analysis options, and other CSD components such as CSD-Materials.
- On the right-hand side: the Structure Navigator, with the database loaded (depending on your licence). The Structure Navigator allows you to select a refcode to visualize in the main Mercury window.
- Beneath the main display window: Display options toolbar. You can quickly view a packing diagram, display Hydrogen bonding and detailed information about the molecule using the More Info option.

Using the mouse to enhance visualization:



- Left mouse button and move rotate molecules.
- Middle Mouse wheel move molecules up and down.
- Right mouse button and move up and down zoom in and out of molecules.
- Shift + Left mouse button and move rotate in the plane molecules.
- Ctrl + Left mouse button and move translate molecules.

Right click:

- a) Near a molecule and
- b) Away from a molecule

AABHTZ (P-1) - Mercury

File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Theory CSD-Particle CSD-Discovery CSD Python API Help

AABHTZ (P-1) - Mercury				Structure Navigator		ð ×
File Edit Selection Display Calculate Picking Mode: Pick Atoms	CSD-Community CSD-Core CSD-Materia	Is CSD-Theory CSD-Particle CSD-Discovery CSD P Show Labels for All atoms with Atom Label	vthon API Help	AABHTZ		Find
Style: Ball and Stick v Colour: by Element	 Manage Styles Work 	Atom selections: V Select by SMARTS: [c]		Countral Structures	Spacegroup	^
Animate Default view: b 🗸	a b c a* b* c* x x+ y- y+ z-	$z + \begin{array}{ c c c c c c c c c c c c c c c c c c c$	' zoom- zoom+	Crystal Structures	spacegroup	
				AABHTZ	P-1	
				AACANI10	P21/c	
				AACANI11	P21/c	
				AACFAZ	Pbcn	
		-		AACFAZ10	Pbcn	
				AACMAL	P21/c	
				AACMHX10	Pbca	
		- • • •	•	AACRHA	Pncm	
		• • • • • • • • • • • • • • • • • • •	<u>.</u>	AACRHC	P-1	
				AACRUB	Cc	
				AACRUB01	C2/c	
				AADAMC	P21/c	
				AADMPY	P-1	
				AADMPY10	P-1	
				AADRIB	P21	
				AAGAGG10	P212121	
				AAGGAG10	P21	~
Display Options				<<	>>	
Display			Options		<	>
isplay Options						83
Display				Options		
Packing	Short Contact	< (sum of vdW radii)	Contacts	Show hydrogens	Depth cue	
Asymmetric Unit		Default definition		Show cell axes	Z-Clipping	
		Default definition	More Info 🔻			
Auto centre				Label atoms	Stereo	
			Powder			
Reset						



Review. ConQuest Interface

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

CCDC ConQuest (1) File Edit Options View Databases Resul	lts Heln			_		×
Build Queries Combine Queries Ma	anage Hitlists View	Results 3				
Draw						-1
Peptide						
Author/Journal						
Name/Class						
Elements						
Formula						
Space Group				_		
Unit Cell	Author/Journal (1) - N	Authors' Names	- C ×	-		
Z/Density	(Re	Exact sumame	Ab			
Experimental	Brown	will hit Browning unless 'Exact	surname' is selected)	-		
All Text	Туре	part of Journal name above to	narrow list displayed			
Refcode (entry ID)	2D Mat. [2017] 3 Biotech [2015] A.C.A.(Spring) [1974-19 A.C.S.Mtg.172,Inorg. [1 AAPS PharmSciTech [2 ACA abstr Paners(Wint	Select required journal in 975] 976] 004-2013] ev [1967-1986]	list below			
Search Reset	ACA,Ser.2 [1977-1984] ACGC Chem.Res.Comm ACH-Models Chem. [1 ACS Appl. Bio Mater. [2 <	nun. [2001-2009] 994-2000] 2019]	v >			
	Volume (14, 1.2 etc.)	Page (212,6-A etc.)	Year (1998, 2001 etc.) during —			
	CCDC Number	(Enter nu	meric part only, e.g. 123456 or 123/456)			
4c		Search	Store Cancel Reset			
Experimental (1) - New	- n x					4d
R-factor =	• fractional C %		All Text (1) - New Text Search Required Fields		-	
Exclude disordered structur	es			Ne	w Box	
Exclude structures with unresolve	ed errors		Either select from list	or en	ter in box(es)	below
Average e.s.d. of C-C Bonds Any			air-sensitive bar black			
Exclude powder structure	s		blade block blue			
Temperature of =	⊙кО°с		brown colorless column			
0 Room Temperature	610K		conductor cream cube v			
All values in the range 283-303 K are stored as Ro	om Temperature		The search will find words star	ting with what	is entered in ame box the	the boxes. search will
Radiation Source Any	_		be for the exact phrase s two or more words that ne button and type the requi	ecified. To fir ed not be adja red words into	id entries con icent, use the separate inp	New Box ut boxes.
Search Store	Cancel Reset		Search	Store	Cancel	Reset

Review. Draw Window

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

ConQuest sketching conventions

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

