## **Preparing and Importing Your Data**

## In the ConQuest Program:

Draw the search fragment of interest.

Click the *Add 3D* button in the *Draw* window and define at least **one** distance in the fragment. This can be any interatomic distance, it does not matter which one is defined. Perform the database search as normal.

## **Exporting results:**

This is performed in three steps:

(1) Save the search file by selecting Save Search As... from the File menu (e.g. save as search.cqs).

(2) Save coordinate file by selecting *Export Entries As...* from the *File* menu. Select the options as follows:

Export Entries: sear	ch1	
Select file type:		
COORD	-	
Select what to expo	rt:	
C Current entry of	only 💽 Al	I selected entries
Select options:		
Fractional	O Orthogon	al
O All Coordinates	Hit Fragmender	nent Only
Either: Edit Filename	and Save	Or: Save via
tings\andrla\Desktop\s	earch1.cor Save	File Popup
	0%	Cancel
🗖 Keep window open	when finished	

Click *File pop-up* to save into the same output folder and with the same basic filename used in (1).

(3)	Save parameters	file by	selecting	Export	Parameters a	ind Data	from the	File menu.
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🕌 Export Files			×
S S	elect the items you wish to in	clude from the choices below	
File type: Vista ( .tab ) 🛁	Field Separator: 🧾 💻	[	
Include Defined Pa	rameters		
Crystal data			
R-factor	🥅 Space Gp. Symbol	🥅 Space Gp. Number	□ □ No. of Coordinates
🗖 Z Value	🗖 Z Prime	🔲 Study Temp.	🗖 Calc. Density
Cell data			
n a	Г Ь	Г с	🗖 Alpha
🗖 Beta	🗖 Gamma	🔲 Cell Volume	🔲 Reduced Cell a
🔲 Reduced Cell b	🔲 Reduced Cell c	🔲 Reduced Cell Alpha	🔲 Reduced Cell Beta
🗖 Reduced Cell Gamma	Reduced Cell Volume		A.2000.035
	0%		Reset Cancel Save

Leave all default options (*i.e.* Include Defined Parameters should be selected, save as type should be Vista) and save using to the same folder and with the same basic filename as in (1) and (2).

The selected destination folder should now contain five files, all with the same basic filename. The ones used in *d*SNAP are **search.fgd**, **search.cor** and **search.cqs** (optional but recommended). The files search.fgn and search.tab are also produced, but are not used in the analysis.

## **Open** *d***SNAP**:

Select Run New Analysis... from the welcome window or Run On... from the File menu.

Click on the top *File* button to select one of the saved files (either the FGD or COR file may be selected).

Select a folder to save the dSNAP output files in. This cannot be the same location as the input folder. The user must have write privileges in this location. Click OK.

*d*SNAP will now perform analysis on the dataset returned by the original search and display the results. See chapters 2 and 3 of the main program manual for more detailed instructions.

**N.B.** There is a known issue with defining hydrogen atoms in the ConQuest search. If some hydrogen atoms are defined explicitly and others implicitly (as in Fig. 1, where the hydroxyl hydrogen has been defined explicitly and the alkyl hydrogen atoms implicitly), dSNAP will not run and an error message will be generated. However, dSNAP will run successfully in cases where all hydrogen atoms are defined explicitly (as in Fig. 2) or all are defined implicitly (as in Fig. 3).

