Preparing and Importing Your Data

In the ConQuest Program:

Draw the search fragment of interest.

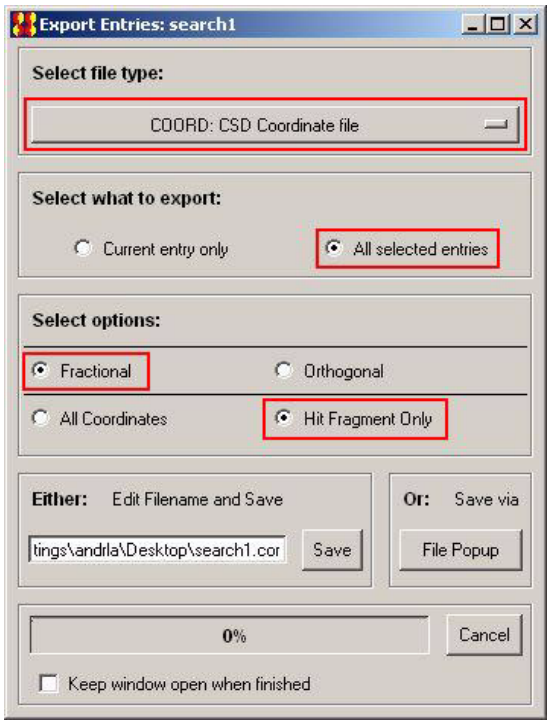
Click the *Add 3D* button in the *Draw* window and define at least **one** distance in the fragment. This can be any interatomic distance, it does not matter which one is defined. Perform the database search as normal.

Exporting results:

This is performed in three steps:

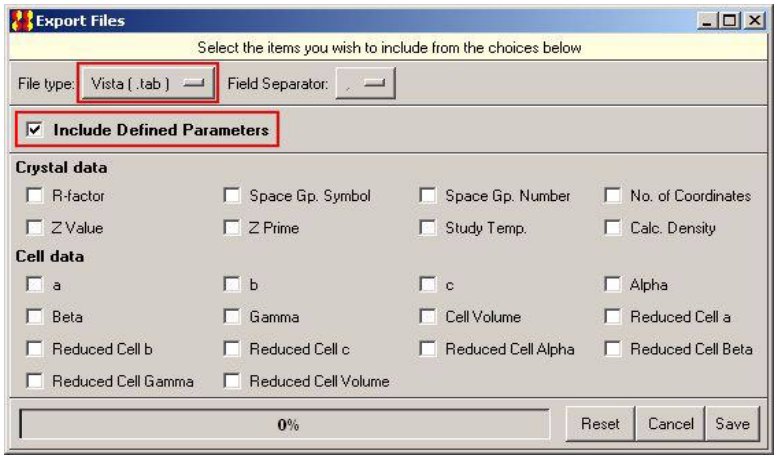
(1) Save the search file by selecting *Save Search As...* from the *File* menu (*e.g.* save as *search.cqs*).

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



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 and Data...* from the *File* menu.



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 *d*SNAP 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), *d*SNAP will not run and an error message will be generated. However, *d*SNAP 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).

Fig. 1

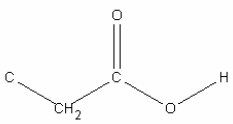


Fig. 2

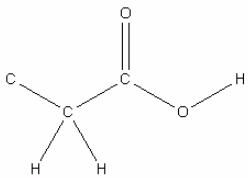


Fig. 3