Working With Multiple Datasets

Inputing more than one dataset:

PolySNAP 2 can analyse multiple different datasets of the same samples at the same time. This is done by switching from *Single Dataset* to *Multiple Datasets* in the option at the top of the main input window.

The main input window will then expand to provide extra sections for entering up to four different data sources. Once the details of each dataset has been entered individually analysis can begin. Be sure to specify the data type correctly (Powder, Raman, other...) as some processing options are method specific.

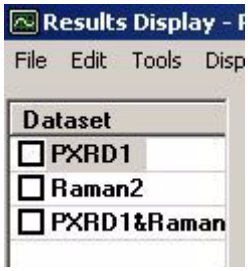
Combined results:

A seperate analysis will be performed on each individual dataset as normal, but additional analysis will also be performed on every combination of datasets in turn. Combined results can be more informative than looking at them individually, and in addition is also a useful tool for checking the agreement between different datasets. Consistency between different types of data creates confidence in the results. In certain circumstances there may be unusual samples that might go unnoticed in a single dataset, but will become apparent when different datasets are combined and there is found to be poor agreement on that sample. See the *PolySNAP* tutorial on multiple datasets for examples of these.

The datasets must be of the same sample set for the results to be meaningful; and for the program to run properly the number of files and filenames must be consistent across the datasets being used, otherwise the wrong samples will be compared, and the results would be meaningless.

Uses:

Multiple results are useful when looking at datasets which all contain data on the same set of samples. These datasets can be of the same type (*e.g.* three different PXRD datasets taken over a range of temperatures or over a period of time) or different types of data (*e.g.* a powder X-Ray dataset, a raman dataset and a DSC dataset). Therefore as well as highlighting samples that appear inconsistent across different types of data, looking at the results could also quickly indicate which samples change over a certain experimental variable.



The datasets are listed in a menu on the left-hand side of the display screen and can be switched between by clicking on the **names** of the different dataset (*e.g.* Raman2). The primary original datasets are listed first (*e.g.* PXRD, Raman), followed by the combined analyses (*e.g.* Raman&PXRD)

Comparing Datasets

Datasets can be selected by clicking on the **checkboxes** in the dataset list. Once selected up to four datasets can be visually compared next to each other by selecting ***Compare Results*** from the *Tools* menu. This opens a new window where the 3D plots (see Figure 1.a) and dendrograms (see Figure 1.b) from the selected datasets are plotted on the same screen for easy comparison. Switch between the different types of display using the drop-down menu in the upper left.

Figure 1.a - 3D plots in the comparison window

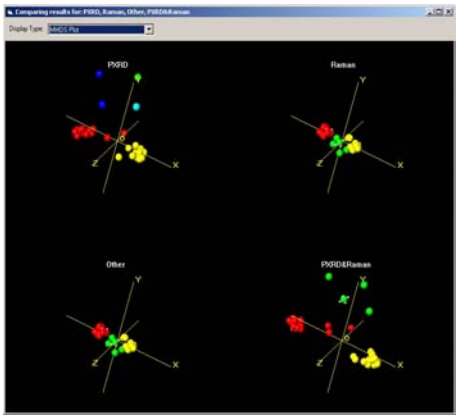
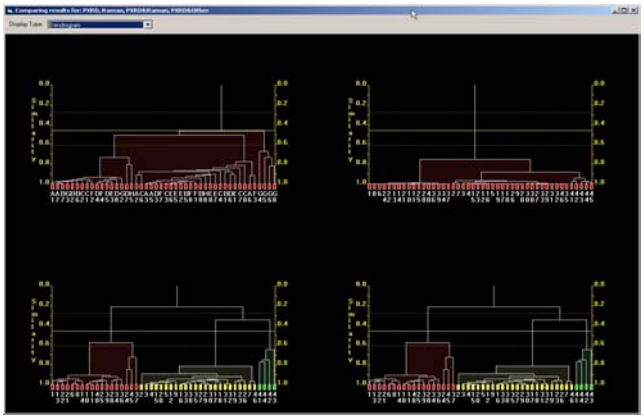


Figure 1.b - Dendrograms in the comparison window



Comparing results in this way only gives you a snapshot of the current clustering in each of the datasets; you cannot for example alter the cut level in this window, though you can zoom and rotate the displays. For full interaction with different sets of results simultaneously, you can ***Create New Results Viewer Window*** from the *Display* m enu. This is of most use when multiple monitors are available, and each results viewer window can be on a separate screen. Up to four windows can be opened at once.

Viewing Samples

Selecting patterns in any of the display panes shows the selected samples in the lower region of the results window. You can easily switch between viewing any of the different dataset profiles of the overlaid patterns by using the tabs at the far-left to move between viewing the PXRD, Raman, or Other profiles for these samples.