# **6-dimensional Plot**

As well as the 3-dimensional plots that aid in visualising the make up of the clusters, *PolySNAP* also contains a 6-dimensional plot that allows various experimental variables to be plotted onto the display. In this way it can be established if there are any trends where an experimental factor may have had an influence on the results.



The plot is fully interactive and in this way the effects of different parameters on the results can be easily and quickly investigated.

## Toolbar

When the 6-dimensional plot is open a toolbar is displayed running along the top of the display which contains the options needed to customise the plot to display the relevant information.

| 🔠 Cell Display 🚮 Dendrograms 🛛 🕊 3D Plot (MMDS) ** | 🗶 3D Plot (PCA) 🧏 6D Plot 📐 Advanced 🔠 | Numerical Results 🛛 🗛 View Logfile 📄 Report Writer      |
|--|--|---|
| Plot:  MMDS C PCA with  Ball Size as  Mass         | 💌 🔽 Ball Colour as Total Volume 💌      | ✓ Ball Shape as         Solvent         ✓         Apply |

## **Type of plot:**

The 6-dimensional plot can be set up either to display the results according to the MMDS (Metric Multi-Dimensional Scaling) plot or the PCA (Principal Component Analysis) plot.

## **Different options:**

There are then three options that allow different variables to included on the plot. To activate these options click on the relevant tick-box and select the appropriate variable from the drop-down menu. These include:

#### **Shape Dimension**

A series of various shapes can be used to represent the samples in the dataset on the plot. These can be used to identify groups of samples which have been grouped together on the basis of:

Solvent, Antisolvent, Counterion or Sample Presentation.

#### **Size Dimension**

The relative size of the sample representations (ball, cone, square, etc) on the 6D plot can be used to represent the differences (or similarities) between samples in:

Mass, Total Volume, Stirrer Rate, Initial Temperature, Cooling Rate, Isolation Temperature, Reaction Time, Antisolvent Volume,

#### **Colour Dimension**

In a similar manner to the shape dimension the colour given to the different sample representations can be used to identify groups of samples which have been grouped together on the basis of:

Mass, Total Volume, Stirrer Rate, Initial Temperature, Cooling Rate, Isolation Temperature, Reaction Time, Antisolvent Volume or Heating Rate. Dendrogram colours can also be used.

By controlling these three additional dimensions extra information can be gathered on the factors that may be affecting the results. After the conditions have been set clicking *Apply* in the toolbar will refresh the plot with the new settings applied.

Sample preparation information can be read in from either the data file headers, or a separate CSV file specified at the time of analysis. It is also possible to edit the expected variables and the order in which they come in. Full details of how this is done are given in the manual.

| 🔽 Ball Shape as | Solvent 💌                         |
|-----------------|-----------------------------------|
|                 | Solvent<br>Antisolvent            |
|                 | Counterion<br>Sample Presentation |



