X Pert Highscore Plus.rar

X'PERT HIGHSCORE AND HIGHSCORE PLUS

Cluster analysis is a four step process that automatically produces:

- a correlation matrix
- a dendrogram
- a principal components analysis 3-D score plot
- and individual clusters

Cluster analysis automatically sorts all closely related scans of an experiment into clusters, and marks the most representative scan of each cluster as well as outlying patterns. It is useful for non-ambient experiments, mining samples and soil mapping, for synthesis experiments such as zeolites, and for finding polymorphs and solvates in drug development.
PANalytical's cluster analysis module uses several algorithms from common statistical packages, from the literature, and also some that are proprietary to PANalytical. X'Pert HighScore Plus supports the cluster analysis of an unlimited number of scans, while X'Pert HighScore can cluster up to a maximum of 50 scans per analysis.
XRD data can now be cross-linked with other data. Spearmans Rho, Pearsons R and overall rank correlation methods are used to compare and cluster non-XRD (eg. Raman) data. The overall speed of cluster analysis is 8 - 10 times higher than in previous versions.

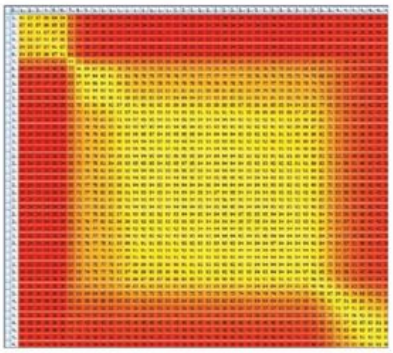
Cluster analysis greatly simplifies the analysis of large amounts of data

1. Cross-comparison of all scans in an experimental group, resulting in a color-coded **matrix of similarities**.

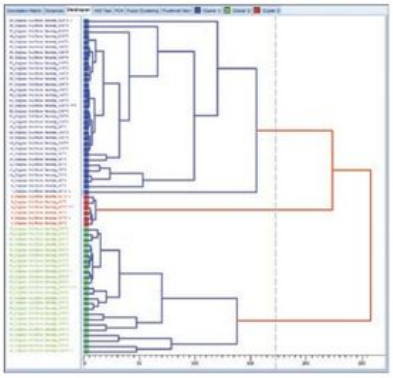
2. Agglomerative hierarchical cluster analysis puts the scans in different classes defined by their similarity, producing a **dendrogram**. The number of clusters is determined by statistical methods or manually, and the most representative scan within each cluster is determined. The representative scans can then be further processed for phase identification, quantification and so on.

3. Principal components analysis (PCA) can be carried out as a separate and independent method to visualize and judge the quality of the clustering.

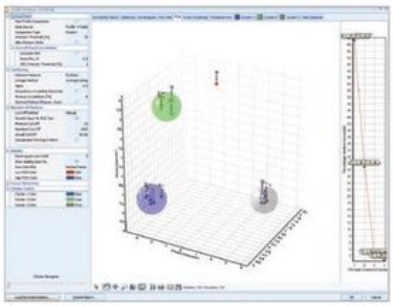
4. Individual clusters of scans are displayed on separate tabs, as well as any unclustered or outlying scans.



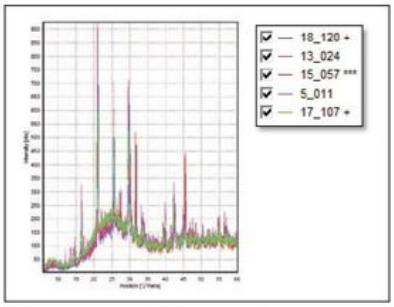
1. Correlation matrix



2. Dendrogram and cut-off value



3. 3D score plot from principal components analysis allows visual confirmation of the observed clusters with confidence spheres



4. Similar scans sorted into one cluster

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