

cluster analysis

Cluster analysis is the clustering, or grouping, of large data sets (*e.g.*, chemical and/or pharmacological data sets) on the basis of similarity criteria for appropriately scaled variables that represent the data of interest. Similarity criteria (distance based, associative, correlative, probabilistic) among the several clusters facilitate the recognition of patterns and reveal otherwise hidden structures.

Source:

PAC, 1997, 69, 1137 (*Glossary of terms used in computational drug design (IUPAC Recommendations 1997)*) on page 1140