

pattern recognition

Pattern recognition is the identification of patterns in large data sets, using appropriate mathematical methodology. Examples are principal component analysis (*PCA*), *SIMCA*, partial least squares (*PLS*) and artificial neural networks (*ANN*).

Source:

PAC, 1997, 69, 1137 (*Glossary of terms used in computational drug design (IUPAC Recommendations 1997)*) on page 1148