

How is the 'property space' plot created?

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Tuesday, 29 September 2009 19:55 - Last Updated Tuesday, 16 February 2016 13:45

Property chemical space plots can use either 'Visual Clustering' (tSNE - t-Distributed Stochastic Neighbour Embedding) or Principal Component Analysis (PCA) to enable visualization of the distribution of compounds with respect to their properties. Groups of compounds with a similar profile of properties will cluster together in these types of space. Additionally, if specific descriptors are expected to correlate with an important property, these may be imported into StarDrop and used to define a chemical space. Thus, the diversity of selections with respect to these descriptors may be visualized to aid in library design.