



HCA and PCA in study of structure property relationships of newly synthesized hydantoins and its molecular descriptors

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Abstract

The biological activity of the molecule greatly depends on its structural properties. Numerical expressions of these properties are reflected in various molecular descriptors. In the paper molecular descriptors that are of interest for the activity of 29 newly synthesized hydantoins were analyzed using multivariate exploratory analysis. Hierarchical cluster analysis and principal component analysis had been used to visualize grouping patterns among molecular descriptors as well as investigated compounds. Recognition of the similarity between investigated compounds and grouping pattern gives a starting point for understanding deeper level of physiological processes which may also provide base for future development and further derivatization or modification to obtain more potent and selective drugs.

Keywords: HCA; PCA; hydantoins; molecular descriptors.