

Classification of Different Classes of Pesticides Based on ADMET Properties

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Abstract : In the present study, *in silico* ADMET properties of different classes of pesticides were calculated to characterize these compounds in the domain of their absorption, distribution, metabolism, and excretion-toxicity. The pesticides cover different groups of insecticides, herbicides, fungicides, rodenticides and acaricides. *In silico* ADMET descriptors were calculated and used for classification through principal component analysis. The obtained model was described by five principal components with an eigenvalue higher than 1: 5.01, 3.88, 2.49, 1.23 and 1.04, covering 85.36% of the variance in total. From the scores plot and along with the first principal component following descriptors contributed the most regarding the compound positioning: FeSSIF (simulated intestinal fluid in fed state, -0.9432) and FaSSIF (simulated intestinal fluid in fasted state, -0.9432). The loadings plot indicated that almost all compounds were positioned in one group positioned on the positive end of the axis. On the negative end of the axis following herbicides were positioned: 2,4-DB, MCPB and dinoseb. The use of ADMET molecular descriptors coupled with principal component analysis provided useful information about studied compounds characteristics and grouping.

Keywords : pesticides, chemometrics, AMET, classification

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