



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 in order 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 eigenvalue higher than 1: 5.01, 3.88, 2.49, 1.23 and 1.04, covering 85.36% of variance in total. From the scores plot and along the first principal component following descriptors contributed the most regarding the compounds 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 axis. On the negative end of axis following herbicides were positioned: 2,4-DB, MCPB and dinoseb as compounds with the highest values of FaSSIF (0.50-068) and FeSSIF (1.46-1.66).

The use of ADMET molecular descriptors coupled with principal component analysis provided useful information about studied compounds characteristics and grouping.

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