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Different Molecular Descriptors in Characterization and Classification of Pesticides

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Abstract : The present study is focused on in silico determination of different lipophilicity and physicochemical descriptors of a collection of different pesticides. The pesticides include herbicides, insecticides, fungicides, rodenticides and acaricides. A set of different molecular descriptors was calculated. The obtained molecular descriptors were used as input variables for pattern recognition chemometic approach – hierarchical clustering analysis. The clustering was done on the basis of Ward's method by calculating Euclidean distances. Clustering resulted in two well separated cluster. The first cluster consisted of two subclusters while in the second cluster atypical triazine herbicide hexazinone stood out. First cluster comprised of pesticides that had lower values of McGowan volume and Wiener index and higher values of diffusion coefficient while the second one contained compounds with higher values of McGowan volume and Wiener index and lower values of diffusion coefficient. The hexazinone was out of cluster based on its lowest diffusion coefficient value together with the highest values of diffusion coefficient In silico calculated lipophilicity and physicochemical descriptors together with hierarchical clustering analysis gave insight regarding the considered compounds grouping. Acknowledgement: The present research is supported by the project of Provincial Secretariat for Higher Education and Scientific Research of AP Vojvodina (Molecular engineering and chemometric tools: Towards safer and greener future, No. 002902513 2024 09418 003 000 000 001 04 002).

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