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QSAR Modeling of Sulfonylurea Herbicides

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Sulfonylureas inhibit the biosynthesis of branched-chain amino acids in plants by inhibiting the enzyme ALS, and are widely used worldwide for selective weed control in various field-crops such as wheat, cotton, oil seed rape and corn, orchards (such olive groves) and vegetables (including tomato and potato) in pre-planting and post-planting applications. Some of these herbicides are highly persistent in the soil, with a long-term residual activity that results in damage to sensitive plants even several years after application to the soil.

The pKa constant is a measure of the acidity of a molecule or compound and itsis an important parameter in many chemical and biological processes, and its value can have significant effects on the behavior of molecules and compounds. The behavior of pesticides and their metabolites in the environment are largely dependent on their physicochemical properties. In case of ionisable pesticides, their pKa, values determine the degree of ionisation in water at the pH of the soil or biological system, and this in turn determines their effective lipophilicity. Accurate pKa values are therefore necessary to model pesticide behavior.

Herbicides SMILES codes was collected online from for PubChem database. pKa values were taken from Pesticide Properties Database (PPDB) website, a comprehensive source of data on pesticide chemical, physical and biological properties.

The experimental database in this study (modeling set), was divided into: 75% training set and 25% test set herbicides. QSAR (quantitative structure–activity relationships) models where created by training set, while model's efficacy after creation were estimate by test set. To build and test the MLR models, several variable selection methods such as Stepwise (SW), Forward (FW) and Best model selection with 2, 3 and 4 descriptors (BM2, BM3 and BM4), were used.

Initial QSAR models were assess according to R^2 values: 0.464 for SW and FW; 0.532 for BM2; 0.672 for BM3 and 0.719 for BM4, which is the statistically promising model.

Keywords: Sulfonylurea herbicides, pKa values, QSAR modeling, MLR