NONEXPERIMENTAL SCREENING OF THE WATER SOLUBILITY, LIPOPHILICITY, BIOAVAILABILITY, MUTAGENICITY AND TOXICITY OF VARIOUS PESTICIDES WITH QSAR MODELS AID

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Abstract: In our study the dataset containing 489 pesticides and their active substances of different classes of organic compounds was used for analysis. For compounds of analyzed dataset the values of lipophilicity, water solubility, toxicity, bioavailability and mutagenicity were predicted by developed QSAR models. The most environmentally hazardous substances were identified using prediction of QSAR models for pesticides. The satisfactory coincidence between the experimental values of investigated properties and their predicted values by QSAR models was obtained (coefficient of determination in the range 83-94 %).

Keywords: pesticides, toxicological analysis, QSAR, lipophilicity, RF method.