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# Environmental toxicity prediction using computational tools: prediction of potential hazardous effects of chemicals in *Lactuca sativa* seed germination

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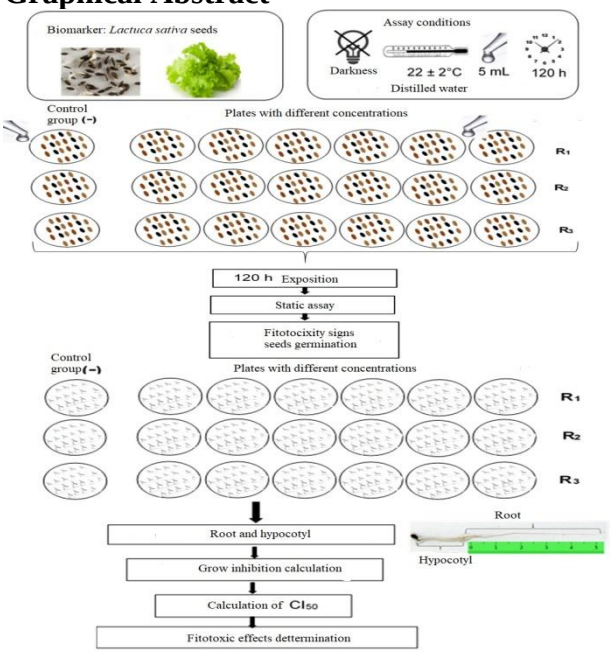
**Graphical Abstract**




**Abstract.**

*The main aim of the study was to develop quantitative structure-activity relationship (QSAR) models for the prediction of phytotoxicity effects of chemical compounds on the Lactuca sativa seeds germination. A database of 73 compounds, assayed against L. sativa and Dragon's molecular descriptors are used to obtain a QSAR model for the prediction of the phytotoxicity. The model is carried out with QSARINS software and validated according to OECD principles. The best model showed good value for the determination coefficient ($R^2$ = 0.917) and others parameters appropriate for fitting (s = 0.256 and $RMSE_{tr}$= 0.236). The validation results confirmed that the model has*

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| | *good robustness and stability ($Q^2_{LOO}$ = 0.874 and $Q^2_{LMO}$= 0.875), an excellent predictive power ($R^2_{ext}$ = 0.896) and was product of a non-random correlation ($R^2_{Y\text{-}scr}$ = 0.130 and $Q^2_{Y\text{-}scr}$ = -0.265). Finally, we can say that this model is a good predictor tool to predict the toxicity over L. sativa of chemical compounds.* |

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