MODELING HERBICIDAL ACTIVITY OF A SUBSTITUTED TRIAZINES CLASS BY INTEGRATION OF COMPOUNDS COMPLEX STRUCTURAL INFORMATION

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Relationships between herbicidal activity and structure of a set of thirty 1,3,5-substituted-triazines was studied by applying an original methodology, through integration of compounds complex structural information by the use of Molecular Descriptors Family. The obtained models (mono-, bi-, tri-, and tetra-varied models) were assess and validate through the study of correlation coefficients, the cross validation leave-one-out scores, models stability defined as the differences between the squared correlation coefficient and the cross validation leave-one-out score, and in training versus test analysis. Comparison of the models with the previous reported model was performed by applying of the correlated correlation analysis. Analysis of the obtained models shows that the four-variated model, which has a squared correlation coefficient equal with 0.9885, obtains the best results. The prediction abilities of the four-varied model is justified by the cross validation leave-one-out score (0.9849), by the model stability, and by the results of training vs. test analysis ($p < 0.05$). Comparison of the correlation coefficient obtained by the four-varied model with previous reported model shows that the four varied model obtained significantly greater value ($p = 0.002$). It can be concluded that herbicidal activity of 1,3,5- substituted-triazines is of geometrical and topological nature, and is strongly dependent on the partial change and on the number of directly bonded hydrogen′s.