

QSAR Modeling of Germination Activity of a Series of 5-(4-Substituent-Phenoxy)-3-Methylfuran-2(5H)-One Derivatives with Potential of Strigolactone Mimics toward *Striga hermonthica*

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Abstract : The present study is based on molecular modeling of a series of twelve 5-(4-substituent-phenoxy)-3-methylfuran-2(5H)-one derivatives which have potential of strigolactones mimics toward *Striga hermonthica*. The first step of the analysis included the calculation of molecular descriptors which numerically describe the structures of the analyzed compounds. The descriptors ALOGP (lipophilicity), AClogS (water solubility) and BBB (blood-brain barrier penetration), served as the input variables in multiple linear regression (MLR) modeling of germination activity toward *S. hermonthica*. Two MLR models were obtained. The first MLR model contains ALOGP and AClogS descriptors, while the second one is based on these two descriptors plus BBB descriptor. Despite the breaking Topliss-Costello rule in the second MLR model, it has much better statistical and cross-validation characteristics than the first one. The ALOGP and AClogS descriptors are often very suitable predictors of the biological activity of many compounds. They are very important descriptors of the biological behavior and availability of a compound in any biological system (i.e. the ability to pass through the cell membranes). BBB descriptor defines the ability of a molecule to pass through the blood-brain barrier. Besides the lipophilicity of a compound, this descriptor carries the information of the molecular bulkiness (its value strongly depends on molecular bulkiness). According to the obtained results of MLR modeling, these three descriptors are considered as very good predictors of germination activity of the analyzed compounds toward *S. hermonthica* seeds. This article is based upon work from COST Action (FA1206), supported by COST (European Cooperation in Science and Technology).

Keywords : chemometrics, germination activity, molecular modeling, QSAR analysis, strigolactones

Conference Title : ICACCE 2016 : International Conference on Applied Chemistry and Chemical Engineering

Conference Location : Copenhagen, Denmark

Conference Dates : August 15-16, 2016