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2D-QSAR Studies on flavonoids as α -glucosidase inhibitors

Aicha Laoud¹, Khaireddine Kraim^{1,2}, Youcef Saihi¹ and Fouad Ferkous¹

¹Université Badji Mokhtar, Algérie

²Ecole Normale Supérieure de l'Enseignement Technologique (ENSET), Algérie

Due to their huge use in traditional medicine, the flavonoids have been paying attention of researchers for several decades in order to improve their therapeutic effects. In addition to the proved biological activities such as antioxidant, antitumoral anticancer, recently, several researches have been focused on flavonoids and their use as antidiabetic drugs and specifically as α -glucosidase inhibitors. In order to improve the inhibition of α -glucosidase by flavonoid derivatives, it was used QSAR as efficient approach to model the inhibition of α -glucosidase using a data set composed of 56 molecules, derived from flavonoid, divided into training and test sets. Genetic algorithms and multiple linear regressions as features election and training algorithms have been used respectively. As a results, the model presented good statistical parameters ($R^2=0.86$, $Q^2_{loo}=0.80$, $Q^2_{ext}=0.53$) and has more predictive power as requested from Tropsha.

aicha.laoud@gmail.com