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Building QSAR model to predict antioxidant activity of flavonoids

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Summary: *A Quantitative Structure-Activity Relationship (QSAR) study was carried out on 32 flavonoids with their antioxidant activities. Multiple linear regression analysis was performedto generate correlation models. The most significant QSAR model (**I**) was obtained with* $R^2 = 0.986$; $R^2_{adj} = 0.981$; $Q^2_{LOO} = 0.975$; $R^2_{test} = 0.992$. *The accuracy of predictions given by the model were 99.32% and 99.28% for the training set and the test set, respectively. Model (**I**) wasused to predict antioxidant activities of 3 flavonoids and show reliable predictability based on experimental values. Results of the present study are expected to be useful in screening for potential antioxidant flavonoids.*