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Modeling of the antioxidant activity of a series of pulvinic acid and coumarine derivatives using CP-ANN and SVR

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The evolutionary emergence of antioxidants is explained by the need for protection of biological macromolecules from damage caused by highly reactive free radicals, which are the products of many reactions with single electron transfers. Reactions of free radicals with DNA and proteins can in turn cause mutations and/or lead to cell death. Because of the wish to minimize these harmful effects there is an increasing need for the discovery of new safe and potent antioxidants.

In vitro experiments were employed for the determination of the antioxidant potential of compounds, where the source of free radicals was the exposure of H_2O_2 to UV radiation. Activity was expressed as the percentage of thymidine that remained intact under these conditions after the addition of antioxidant. Then *in silico* modeling was used for the development of predictive models of the antioxidant activity, which could be later employed for the prediction of activity of new potential antioxidants.

The dataset consisted of 79 derivatives of pulvinic acid, 23 derivatives of coumarine and 9 unrelated compounds. Because we suspect the structure-activity relationship is non-linear, we applied counter propagation artificial neural networks (CP-ANN) for the modeling. The quality of the models was assessed using 10-fold cross-validation on the training set. The model chosen for further optimization has a squared correlation coefficient of 0.754 for the training set and 0.627 for the cross-validation. We will compare the results of the CP-ANN model with the support vector regression (SVR) prediction model for the same set of compounds.

Biography

Rok Martinčič has graduated as Master of Pharmacy in 2011 from the University of Ljubljana. Since then he is a Ph.D. student in the field of Biomedicine, working with QSAR modeling at the Laboratory of Chemometrics at the National Institute of Chemistry, Slovenia.

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