

Modeling toxicity by using supervised Kohonen neural networks.

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Counterpropagation neural network is shown to be a powerful and suitable tool for the investigation of toxicity. This study mined a data set of 568 chemicals. Two hundred eighty-two objects were used as the training set and 286 as the test set. The final model developed presents high performances on the data set $R^2 = 0.83$ ($R^2 = 0.97$ on the training set, $R^2 = 0.59$ on the test set). This technique distinguishes itself also for the ability to give to the expert two-dimensional maps suitable for the study of the distribution/clustering of the data and the identification of outliers.

Adres publiczny

<http://dx.doi.org/10.1021/ci0256182>

Strona internetowa wydawcy

<https://www.acs.org/content/acs/en.html>