

## عنوان مقاله:

Quantitative structure-retention relationships applied to chromatographic retention of ecotoxicity of anilines and phenols

## محل انتشار:

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## نویسندگان:

Mehrdad Shahpar - *Director of Ilam Petrochemical Company*

Sharmin Esmailpoor - *Department of Chemistry, Payame Noor University, Tehran, Iran*

## خلاصه مقاله:

Aniline, phenol, and their derivatives are widely used in industrial chemicals that consequently have a high potential for environmental pollution. Genetic algorithm and partial least square (GA-PLS), kernel partial least square (GA-KPLS) and Levenberg-Marquardt artificial neural network (L-M ANN) techniques were used to investigate the correlation between chromatographic retention ( $\log k$ ) and descriptors for modelling the toxicity to fathead minnows of anilines and phenols. Descriptors of GA-PLS model were selected as inputs in L-M ANN model. The described model does not require experimental parameters and potentially provides useful prediction for  $\log k$  of new compounds. Finally a model with a low prediction error and a good correlation coefficient was obtained by L-M ANN. The stability and prediction ability of L-M ANN model was validated using external test set techniques.

## کلمات کلیدی:

Ecotoxicity, Environmental hazard, Phenols, Anilines, Quantitative stature retention relationship

## لینک ثابت مقاله در پایگاه سیویلیکا:

<https://civilica.com/doc/723267>

