عنوان مقاله:

An improved structure models to explain retention behavior of atmospheric nanoparticles

محل انتشار:

فصلنامه ارتباطات شیمی ایران, دوره 2, شماره 1 (سال: 1392)

تعداد صفحات اصل مقاله: 16

نویسندگان:

Sharmin Esmaeilpoor - *Department of Chemistry, Payame Noor University, P.O. BOX ۱۹۳۹۵-۴۶۹۷ , Tehran, Iran*

Zahra Shirzadi - *Department of chemistry, Islamic Azad University, Shahreza Branch, Isfahan, Iran*

Hadi Noorizadeh - *Department of Chemistry, Payame Noor University, P.O. BOX ۱۹۳۹۵-۴۶۹۷ , Tehran, Iran*

خلاصه مقاله:

The quantitative structure-retention relationship (QSRR) of nanoparticles in roadside atmosphere against the comprehensive two-dimensional gas chromatography which was coupled to high-resolution time-of-flight mass spectrometry was studied. The genetic algorithm (GA) was employed to select the variables that resulted in the best-fitted models. After the variables were selected, the linear multivariate regressions [e.g. the partial least squares (PLS)] as well as the nonlinear regressions [e.g. the kernel PLS (KPLS) and Levenberg- Marquardt artificial neural network (L-M ANN)] were utilized to construct the linear and nonlinear QSRR models. The correlation coefficient cross validation (Q^2) and relative error for test set L-M ANN model are 0.939 and 4.89, respectively. The resulting data .indicated that L-M ANN could be used as a powerful modeling tool for the QSPR studies

کلمات کلیدی:

Atmospheric nanoparticles, QSRR, GA-KPLS, Levenberg -Marquardt artificial neural network