[P2] Prediction of retention indices polycyclic aromatic hydrocarbons in gas chromatography

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Polycyclic aromatic hydrocarbons (PAHs) are of concern in environmental chemistry and toxicology [1]. Analysis and study of PAHs by gas chromatography (GC) on capillary columns, using the temperature programming, can provide a great amount of quantitatively precise, reproducible and comparable retention data for large sets of structurally diversified compounds. On the other hand, chemometrics is recognized as a valuable tool for accomplishing a variety of tasks in a chromatography laboratory. Chemometrics facilitates the interpretation of large sets of complex chromatographic and structural data [2].

In the present work, a QSRR study was performed on previously reported PAHs using quantum mechanics and other descriptors sources estimated by different approaches. The objective of the study is prediction of the retention indices for 209 PAHs taken from the literature [3]. Multiple linear regression was used to build QSRR model.

The proposed model presented high-quality fit, internal and external predictive powers. It is expected that the model can effectively predict retention indices of 209 PAHs (Figure 1) and if needed, others without experimental values. The leave-one-out, bootstrapping and Y-randomization test showed the model robustness and stability. The external validation with a test set selected from the original data by Kennard and Stone procedure showed that the model presents high external predictive power.

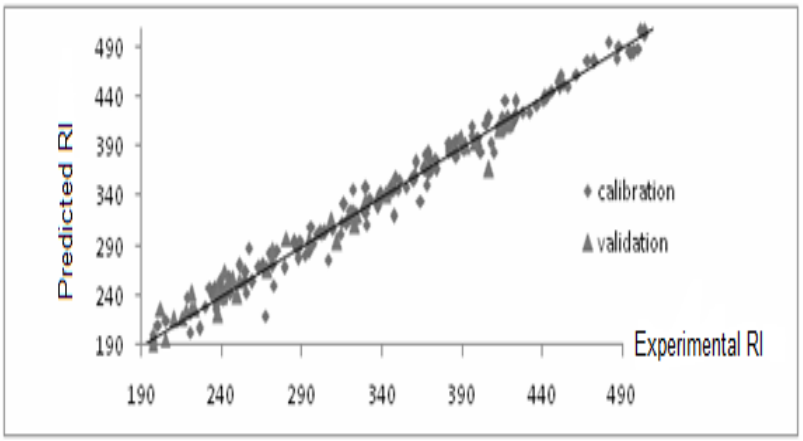

Figure 1: predicted *VS* experimental retention indices of the 209 PAHs stayed

A check of the applicability domain of the proposed model with the leverage approach is provided to ensure the reliability of new PAH' retention indices prediction.

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[3] M. L; D.L. V; C.M. W; M. N. Anal. Chem. 51 (1979) 768-773.