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# 多环芳香硫化合物的定量结构-气相色谱保留指数关系

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# Quantitative structure-gas chromatographic retention relationship of polycyclic aromatic sulfur heterocycles using molecular electronegativity-distance vector

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摘要 应用分子电性距离矢量(MEDV)对114个多环芳香硫化合物(PASHs)进行结构表征,通过多元线性回归建立了PASHs的气相色谱保留指数与MEDV参数之间的定量结构-保留值关系模型;同时采用逐步回归分析进行变量筛选,继而以留一法交互检验对所得优化模型进行预测能力评价,所建立的模型的相关系数为0.9947,交互检验相关系数为0.9940,表明该优化模型具有良好的稳定性和预测能力。此外,通过将样本集按2:1分成校准集和测试集预测,统计分析结果显示所建的模型具有良好的相关性和稳定性。本文所建的定量结构-保留值关系(QSRR)模型为预测PASHs的气相色谱保留指数提供了一个便捷有效的新方法。

关键词： 气相色谱保留指数 定量结构-保留指数关系 分子电性距离矢量 多环芳香硫化合物

Abstract： The chemical structures of 114 polycyclic aromatic sulfur heterocycles (PASHs) have been studied by molecular electronegativity-distance vector (MEDV). The linear relationships between gas chromatographic retention index and the MEDV have been established by a multiple linear regression (MLR) model. The results of variable selection by stepwise multiple regression (SMR) and the powerful predictive abilities of the optimization model appraised by leave-one-out cross-validation showed that the optimization model with the correlation coefficient (R) of 0.9947 and the cross-validated correlation coefficient (RCV) of 0.9940 possessed the best statistical quality. Furthermore, when the 114 PASHs compounds were divided into calibration and test sets in the ratio of 2:1, the statistical analysis showed our models possesses almost equal statistical quality, the very similar regression coefficients and the good robustness. The quantitative structure-retention relationship (QSRR) model established may provide a convenient and powerful method for predicting the gas chromatographic retention of PASHs.

Keywords： gas chromatographic retention index quantitative structure-retention relationship (QSRR) molecular electronegativity-distance vector polycyclic aromatic sulfur heterocycles

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