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研究论文

电拓扑状态预测有机磷酸酯类化合物的气相色谱保留指数

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摘要 以原子类型电拓扑状态指数(ETSI)有效表征35个有机磷酸酯类化合物(OP)的分子结构, 应用基于预测的变量选择与模型化(VSMP)方法建立OP化合物在3种不同固定相上的气相色谱保留指数(RI)与分子结构(ETSI)的定量相关模型. 结果表明, 影响不同固定相上OP色谱保留的主要结构因素都是由7个ETSI描述子对应的子结构碎片, 即: $=CH_2$,≡C—, aaC—, =O, —O—, Cl和Br. 其中子结构aaC—, =O和—O与OP化合物母体骨架密切相关, 而$=CH_2$,≡C—, —Cl和—Br反映支链或取代基的变化. 通过多元线性回归法建立OP化合物在三个固定相上的定量结构-保留相关模型(QSRR)发现, 各QSAR模型的估计相关系数均在0.99以上, LOO检验相关系数在0.98以上, 表明模型具有良好估计能力与稳定性. 应用28个OP训练集样本构建的QSRR模型预测外部7个检验集RI结果表明训练集模型具有良好预测能力.

关键词 电拓扑指数 有机磷酸酯 定量结构-保留相关 基于预测的变量选择与模型化方法(VSMP)

分类号

Prediction of Gas Chromatographic Retention Indices of Organophosphates by Electrotopological State Index

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Abstract Electrotopological state index (ETSI) for atom types was used to describe the structures of 35 organophosphates and a quantitative linear relationship between the ETSI descriptors and gas chromatographic retention indices (RI) was developed using the variable selection and modeling based on prediction (VSMP). It was found that some main structural factors influencing the RI of organophosphates are 7 substructures such as $=CH_2$, ≡C—, aaC— (where "a" refers to a chemical bond in the aromatic ring), =O, O, Cl and Br, which were related to the molecular skeleton of organophosphates, substituent groups on phenyl ring, and alkyls binding to the bond of P—O. Three best 7-variable models, with the calibrated correlation coefficient of $r>0.99$ and the validated correlation coefficient of $q>0.98$ for three stationary phases, were built by multiple linear regression, which shows a good estimation ability and stability of models. A prediction power for the external samples was validated by the model built from the training set with 28 organophosphates.

Key words electrotopological state index organophosphate quantitative structure-retention relationship variable selection and modeling based on prediction

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