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FULL PAPERS

应用原子类型电拓扑状态指数与**VSMP**方法建立取代苯生物可降解性模型

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摘要 以电拓扑状态指数表征取代苯化合物的分子结构，通过本实验室发展的计算程序计算了51个取代苯中所含11种原子类型的电拓扑指数，应用基于预测的变量选择与建模方法进行变量优化选择，并建立优化电拓扑指数与生物可降解性之间的定量关系。结果表明，由多元线性回归方法构建的5-变量优化模型具有良好的稳定性和预测能力，
其中估计过程计算相对生物可降解性值与实验值之间的相关系数和均方根误差分别为0.9378和0.35，交互检验过程的相关系数与预测误差分别为0.9210和0.39。

关键词 变量选择,电拓扑状态指数,生物可降解性,取代苯,定量结构-活性相关

分类号

VSMP for Modeling the Biodegradability of Substituted Benzenes Based on ElectrotopologicaState Indices for Atom Typesl

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Abstract The electrotopological state (E-state) index was employed to characterize the structures of 51 substituted benzenes. Eleven E-state indices of the compounds were calculated by the computer program developed in our laboratory. The method for variable selection and modeling based on prediction (VSMP) was used to select an optimal combination of the variables from 11 E-state descriptors. Then the optimal descriptors were employed to model the relationship between the relative biodegradability of the substituted benzenes and their molecular structures. A novel 5-descriptor linear model was developed and the model has a high quality with the correlation coefficient and the root mean square error in estimation step being 0.9378 and 0.35, respectively, and these in leave-one-out cross-validation procedure being 0.9210 and 0.39, respectively.

Key words variable selection and modeling based on prediction electrotopological state index biodegradability substituted benzenes

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