研究论文

基于估计均方差的统计量**Sp**的修正变量选择法用于持久性有机污染物毒性研究

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摘要　　提出并详细说明基于估计均方差的统计量Sp的修正变量选择(MVSSp)方法. 采用分子电性距离矢量(MEDV)及其二次项表征多氯二苯并呋喃(PCDFs), 多氯二苯并二噁英(PCDDs)和多氯联苯(PCBs)三种持久性有机污染物异构体分子结构, 结合MVSSp方法选择适当的描述子, 建立了三种持久性有机污染物分别对芳烃受体(AhR)亲合性, 芳香羟化酶(AHH), 7-乙氧基异吩唑酮-脱乙基酶(EROD)诱导作用的定量结构活性相关(QSAR)模型, 模型的质量优于文献或相当, 讨论了这些实验毒性与分子结构关系. 这对研究和预测这些持久性污染物的毒性具有一定的指导意义.

关键词　　估计均方差的统计量Sp　变量选择　分子电性距离矢量　多氯二苯并二噁英　多氯二苯并呋喃　多氯联苯　毒性

分类号

Modified Variable Selection Based on Estimated Root Mean Square Statistic Sp for Studying Toxicity of Persistent Organic Pollutants

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Abstract　A modified variable selection based on the estimated root mean square statistic Sp (MVSSp), has been developed. The molecular electronegativity distance vector (MEDV) based on 13 atom type (MEDV) and their quadratic terms were used to describe the molecular structures of polychlorinated dibenzofurans (PCDFs), polychlorinated dibenzo-*p*-dioxins (PCDDs) and polychlorinated biphenyls (PCBs) isomers. With the choices of some appropriate descriptors by MVSSp, several QSAR models, between the MEDV and the abilities of three types of persistent organic pollutants (POPs) bound to the cytosolic aryl hydrocarbon receptor (AhR), the stimulating induction to aryl hydrocarbon hydroxylase (AHH) and 7-ethoxyresorufin O-deethylase (EROD), were built. The qualities of those models are not worse than those of literature. And then the relations between the experiment toxicities and the molecular structures were discussed. This study will help to provide a useful guideline for modeling and predicting the toxicity of POPs.

Key words　estimated root mean square statistic Sp　variable selection　MEDV　PCDDs　PCDFs　PCBs　toxicity

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