高等学校化学学报 2007 28 (1): 117-120 ISSN: 0251-0790 CN: 22-1131/O6

研究论文

苯砜基羧酸酯类急性毒性的QSAR研究

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收稿日期 2006-3-23 修回日期 网络版发布日期 2007-1-8 接受日期

摘要 采用密度泛函理论方法, 在B3LYP/6-31G(*d*)理论水平下, 计算了56种苯砜基羧酸酯类化合物的量子化学参数. 计算结果表明， 酯基连接的烷烃链亲水性越小, 毒性越大; 苯环连接的取代基亲水性越大, 毒性越大; 分子的体积越大, 毒性越小; 分子产生氢键的能力越大, 毒性越小; 分子最高占据轨道能量越高, 毒性越大.

关键词 苯砜基羧酸酯 急性毒性 密度泛函 QSAR

分类号 O641

DOI:

QSAR Study of Acute Toxicities of Phenylsulfonyl Carboxylate Compounds

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Received 2006-3-23 Revised Online 2007-1-8 Accepted

Abstract Based on the theoretical linear solvation energy relationship(LSER) parameters, a new QSAR model was established to correlate the acute toxicities of 56 phenylsulfonyl carboxylate compounds. All the descriptors were derived from quantum chemical computation at B3LYP/6-31G(*d*) level of theory. Compared with the model from TLSER, the new model has a better expression and prediction because more samples have been used. The model is shown below and its adequacy is $R=0.94$, $R^2_{adj}=0.88$, $F=61.62$, $q^2=0.83$.

$$-\lg EC_{50}=a\times E_{HOMO}+b\times P+c\times q_{10}+d\times q_1+e\times \mu+f\times q_H+costant$$

The computation results show that the smaller of the hydrophilicity of the substituent at the ester group, the bigger the acute toxicity; the bigger the hydrophilicity of the substitute attached to the benzene ring, the bigger the acute toxicity; the bigger the volume of the molecule, the smaller the toxicity; the bigger the ability of the molecule to form H-bonding, the smaller the toxicity; the higher the energy of HOMO, the bigger the toxicity. The present study may be helpful for probing the mechanism of action in acute toxicity of phenylsulfonyl carboxylate compounds and understanding the phenylsulfonyl carboxylate chemistry.

Key words Phenylsulfonyl acetate; Acute toxicity; Density function theory; QSAR

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