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论文

计算机模拟内毒素吸附剂吸附机理的研究

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摘要:

应用计算机模拟的方法研究了内毒素吸附剂的吸附机理. 模拟结果显示, 以二甲胺为配体的吸附剂, 当β位存在羟基时, 此羟基可与内毒素分子间形成氢键, 并形成一个八元环的稳定结构. 此时吸附剂与内毒素之间存在静电、 氢键、 疏水相互作用和八元环的协同作用. 同时模拟了羟基位于配体不同位置的吸附剂与内毒素的相互作用. 结果表明, 静电作用为主要的相互作用力, 羟基的位置对吸附剂的吸附能力影响显著.

关键词: 内毒素 计算机模拟 吸附机理

Studies on Adsorption Mechanisms of Adsorbents for Endotoxin

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Abstract:

It had been reported that a novel molecular recognition, in which there was a hydroxyl group at β site, had excellent adsorption capacity of endotoxin. In this work, the computer simulation method was used to investigate the interaction mechanism between the adsorbents and the endotoxin. The computer simulation showed that the hydroxyl group at β site of adsorbent with dimethylamine ligand could form H bond with endotoxin, as a result an eight membered ring was formed. The electrostatic interaction, hydrogen bond and cooperative effect of the eight membered ring were formed simultaneously. The interaction between a series of adsorbents model with hydroxyl group at different sites and endotoxin were investigated by computer simulation, too. The result indicated that electrostatic interaction was the main interaction force, and the site of hydroxyl group could affect the adsorption capacity of adsorbents obviously.

Keywords: Endotoxin Computer simulation Adsorption mechanism

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