

论文

桥联双 $\beta$ -环糊精对N-[4-(1-芘基)]丁酰-D/L-苯丙氨酸的手性识别及机理研究

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摘要:

利用紫外-可见吸收和荧光发射光谱, 结合非线性最小二乘法拟合曲线以及分子力学(MM2)模拟系统地研究了手性分子N-[4-(1-芘基)]丁酰-D/L-苯丙氨酸(PDP和PLP, 总称PPs)与 $\beta$ -环糊精( $\beta$ -CD)、2-位硒桥联双 $\beta$ -CD(2-SeCD)和2-位碲桥联双 $\beta$ -CD(2-TeCD)的包结能力大小及这3个环糊精对PPs手性识别能力的差异和识别机理. 研究表明, PPs不能与单疏水空腔的 $\beta$ -CD形成很好的包结复合物, 与具有较长桥联链的2-TeCD结合能力最强. 2-TeCD与PDP和PLP的结合常数分别为 $2.33 \times 10^4$ 和 $6.07 \times 10^3$  L/mol, 对PPs的手性识别比达到KD/KL=3.84, 高于2-SeCD(KD/KL=2.61). 用MM2模拟得出了PPs与这两个双环糊精形成复合物的三维结构: PPs的绝大部分位于双环糊精两个空腔之间, 但是在这两个复合物中, 苯环与芘环所成的二面角不同. 此外, PPs与这两个双环糊精作用时均存在明显的氢键相互作用, 且2-TeCD强于2-SeCD.

关键词: N-[4-(1-芘基)]丁酰-D/L-苯丙氨酸; 硒、碲桥联双 $\beta$ -环糊精; 非线性最小二乘法拟合; 分子模拟

Chiral Discrimination of N-[4(1-pyrene)butyroyl]-D/L-phenylalanine in Binding with Tellurium/Selenium Bridged-bis- $\beta$ -cyclodextrins

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Abstract:

The binding ability and chiral discrimination of  $\beta$ -cyclodextrin( $\beta$ -CD), 2,2'-diseleno-bridged  $\beta$ -cyclodextrins(2-SeCD)and 2,2'-ditelluro-bridged  $\beta$ -cyclodextrins(2-TeCD)with PPs were investigated in aqueous solution by using UV-Vis and fluorescence spectroscopy as well as MM2 calculation. The stability constants of complexes were obtained by using least-square curve fitting. From the results of UV-Vis and fluorescence spectroscopy, it was shown that  $\beta$ -CD could not form inclusion complexation with PPs while 2-SeCD and 2-TeCD could. The binding ability between 2-TeCD and PDP was higher ( $K_s=2.33 \times 10^4$  L/mol) than that of 2-SeCD/PDP( $K_s=3.03 \times 10^3$  L/mol). Meanwhile, the high chiral discrimination of PPs was also performed in binding with 2-TeCD(KD/KL=3.84)and 2-SeCD (KD/KL=2.61). Furthermore, the MM2 calculation illustrates that PPs were located between the two cavities of 2-SeCD or 2-TeCD, however, the dihedral angle between phenyl ring and pyrene ring was different from each other when they were included in two bis-cyclodextrins. Meanwhile, MM2 also demonstrates that the intermolecular hydrogen bonding interaction in 2-TeCD/PPs complex was relative stronger than that in 2-SeCD/PPs.

Keywords: N-[4(1-pyrene)butyroyl]-D/L-phenylalanine; 2,2'-Diseleno bridged bis- $\beta$ -cyclodextrin; 2,2'-

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收稿日期 1900-01-01 修回日期 1900-01-01 网络版发布日期

DOI:

基金项目:

通讯作者: 吴玉清

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#### 参考文献:

郝雅琼,王立旭,马立军,吴玉清,刘俊秋,罗贵民,杨光弟. 桥联双β-环糊精对N-[4-(1-萘基)]丁酰-D/L-苯丙氨酸的手性识别及机理研究.高等学校化学学报,2006,27(5): 920-924

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