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胆甾类分子钳对氨基酸衍生物的对映选择性识别

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摘要 用差紫外光谱滴定法考察了以脱氧胆酸作spacer的手性分子钳1～3对一系列α-氨基酸甲酯的对映选择性识别性能。结果表明，分子钳1和2与客体氨基酸甲酯形成1:1型超分子配合物，并显示较好的手性识别能力。分钳3对所考察的氨基酸甲酯均没有明显的识别作用。讨论了主-客体间尺寸/形状匹配、几何互补等因素对形成超分子配合物的影响，并利用计算机模拟作辅助手段对实验结果和现象进行了解释。

关键词 分子识别 氨基酸 对映体 甾族化合物 计算机模拟 超分子

分类号 Q51

enantioselective recognition of amino acid derivatives by chiral molecular tweezers derived from steroid cholic acid

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Abstract Molecular recognition properties of new chiral molecular tweezers based on deoxycholic acid 1～3 have been investigated using amino acid methyl esters. The association constants (K~a) and gibbs free energy changes (-△G°) have been measured by UV-visible spectroscopic titration for inclusion complexation of molecular tweezers 1～3 with some D/L-amino acid methyl esters in CHCl~3 at 25℃. The results indicate that the molecular tweezers 1 and 2 are favorable for complexation with D-amino acid methyl esters and molecular tweezer 3 fails to recognize all amino acid methyl esters examined. the supramolecular complexes formed from host 1 or 2 with various guest D/L-amino acid methyl esters consist of 1 : 1 host and guest molecules. The molecular recognition ability and enantioselectivity of receptors for amino acid methyl esters are discussed from in terms of size/shape-fit, complementary geometrical relationship and the weak intermolecular forces. A computer-aided study has been employed to elucidate the binding behavior of these molecular tweezers. Molecular modeling suggests that in these molecular tweezers the recognition ability come mainly from hydrogen bonding and van der Waals interaction. The size/shape-fit and geometrical complementary relationship between receptor and substrate play a pivotal role in the inclusion complexation of amino acid methyl esters with rceptor 1～3.

Key words OLECULAR RECOGNITION AMINO ACID ENANTIOMORPH STEROIDS COMPUTERIZED SIMULATION

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