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水溶液中的氨基酸桥联环糊精二聚体的分子识别

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摘要 采用荧光偏光方法研究了用2-氨基-L-1, 5-戊二酸衍生物和(1R,3R)-1-氨基-1, 3-二羧基环戊烷衍生物桥联的环糊精二聚体1和2(主体), 在298K、pH=7.4时, 与四个低分子量的多肽(客体, H-Trp-Trp-Arg-Arg-NH23; Adm-Trp-Arg-Arg-NH24; Adm-D-Trp-Arg-Arg-NH25; H-Trp-Trp-Trp-Trp-Arg-Arg-NH26)之间的相互作用。研究结果表明, 二聚体环糊精对于多肽的分子识别作用, 就主体而言, 即便是主体作用位点以外部分基团结构的改变, 对主-客体之间的分子识别也有重要影响, 并且两个空腔在组装客体过程中相互之间产生协同作用, 就客体而言, 多肽分子的链长、疏水性及其嵌入基团的极性、大小、形状等对包合物的形成与稳定均起重要作用。主-客体组装过程中产生负的焓变和正的熵变, 表明范德华-伦敦色散力、氢键和疏水相互作用是本文研究体系的主要包合驱动力。

关键词 [荧光偏光分析](#) [氨基酸](#) [环糊精](#) [二聚体](#) [分子识别](#) [多肽](#) [包合物](#)

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Molecular recognition of double cyclodextrin bridged with amino acid derivatives in aqueous solution

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Abstract The interaction between four peptides with low molecular weight (guest, H-Trp-Trp-Arg-Arg-NH2 3; Adm-Trp-Arg-Arg-NH24; Adm-D-Trp-Arg- Arg-NH25; H-Trp-Trp-Trp-Trp-Arg-Arg-NH26) and cyclodextrin dimers (host, 1,2) bridged with derivatives of glutamic acid or (1R, 3R)-1- aminocyclopentane-cis-1,3-dicarboxylic acid was investigated by using fluorescencepolarization method in aqueous buffer solution (pH 7.4) at 298 K. It was shown that the molecular recognition of a double cyclodextrin to a peptide is not only affected by the structure and properties of the bridging group between two cyclodextrins but also related to the chain length, hydrophobicity of a peptide and polarity, size and shape of the penetrating group. The changes in enthalpy (ΔH°) and entropy ($T\Delta S^{\circ}$) accompanying the complexation were determined in usual way. It was found that complexation is accompanied by negative changes in enthalpy and positive changes in entropy, indicating that van der Waals-Lodon dispersion, hydrogen bonding and hydrophobic interaction between a double cyclodextrin and a peptide are mainly responsiblefor the inclusion compound formation.

Key words [AMINO ACID](#) [CYCLODEXTRIN](#) [DIMER](#) [OLECULAR RECOGNITION](#) [POLYPEPTIDE CLATHRATES](#)

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