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研究论文

微量热法研究丹皮酚及其两种同分异构体与γ-环糊精在水溶液中的相互作用

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摘要 在298.15 K下利用纳瓦级等温滴定微量热法研究了γ-环糊精与丹皮酚(Pae)及其两种同分异构体(2'-羟基-5'-甲氧基苯乙酮, Hma; 4'-羟基-3'-甲氧基苯乙酮, Ace)在水溶液中的相互作用, 并结合核磁共振对其相互作用的微观结构进行了表征. 试验表明, γ-环糊精与三种药物分子都是1∶1结合, 其中Pae, Hma与γ-环糊精相互作用过程是焓驱动, 而Ace与γ-环糊精相互作用却是焓-熵共驱动; ^{1}H NMR 谱表明 Pae, Ace 与γ-环糊精形成典型的包结物, 其中 Pae 分子从 *g*-环糊精空穴的小口端进入, Ace分子从 *g*-环糊精空穴的大口端进入, 而 Hma 与γ-环糊精之间只是以弱相互作用结合而非包结作用. 结果显示γ-环糊精对三种同分异构体具有明显的分子识别功能.

关键词 γ-环糊精 丹皮酚 分子识别 微量热 核磁共振

分类号

A Microcalorimetric Study on Interaction of γ-Cyclodextrin with Paeonol and Two of Its Isomers in Aqueous Solution

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Abstract The interaction between γ-cyclodextrin (γ-CD) and paeonol (Pae) as well as two of its isomers [4'-hydroxyl-3'-methoxyacetophone (Ace) and 2'-hydroxyl-5'-methoxyacetophone (Hma)] in aqueous solution has been studied with nano-Watt-scale isothermal titration calorimetry (ITC) at 298.15 K. The microcosmic structure of the host-guest combination has been characterized by ^{1}H NMR spectra at 298 K. The experiments indicate that γ-cyclodextrin binds with each drug molecule in the same 1∶1 stoichiometry. The binding processes of Pae and Hma with γ-cyclodextrin are enthalpy driven while that of Ace with γ-cyclodextrin is predominantly entropy-driven. The ^{1}H NMR spectra data have provided clear evidence of the inclusion interaction of γ-cyclodextrin with Pae and Ace, which shows that Pae molecule penetrates into the molecular cavity of the γ-CD from the secondary rim whereas Ace does from the primary rim. But Hma binds with γ-cyclodextrin by weak interaction rather than inclusion interaction. Therefore, both thermodynamic parameters and ^{1}H NMR spectra demonstrate that γ-CD molecule can evidently recognize the three kinds of isomer molecules.

Key words γ-cyclodextrin paeonol molecular recognition microcalorimetry ^{1}H NMR

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