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## 论文

### 香豆素类中药有效成分与牛血清白蛋白结合的构效关系

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#### 摘要:

本文主要用荧光光谱(FS)、紫外光谱(UV)从药物分子结构角度研究五种香豆素类中药有效成分C I ~C V与牛血清白蛋白(Bovine Serum Albumin, BSA)结合时的构效关系.

关键词: 构效关系; 中药; 香豆素; 牛血清白蛋白; 荧光光谱

### Structure-performance Relationship of some Chinese Herb Components Containing Structural Unit of Coumarin During Binding to Bovine Serum Albumin

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#### Abstract:

The interaction between bovine serum albumin(BSA) and five active components of Chinese Herb C I ~C V containing structural unit of coumarin was investigated by ultraviolet(UV) and fluorescence spectroscopy(FS). The intrinsic fluorescence of BSA was quenched by pharmaceuticals via forming pharmaceutical-BSA complexes. The quenching mechanism is mainly a combination of static quenching with nonradiative energy transfer. The parameters of pharmaceutical-BSA binding process, such as statistic quenching constant KP, the apparent association constant KA, the value of binding site n, the efficiency of energy transfer E, the spatial distance r and  $\Delta G$  were obtained. The above parameters disclose the structural-performance relationship of pharmaceutical-BSA interaction as follows. The process of pharmaceutical-BSA binding is promoted strongly by both 4-methyl and 6-hydroxyl in coumarin molecule, but the latter must endure simultaneously some adverse effects caused by increment of molecular polarity and stereo hindrance. Decreasing the polarity of 7-substituent group and increasing the volume of substituting group destroys the pharmaceutical-BSA binding, and the effect is almost totally opposite to that of 6-hydroxyl.

Keywords: Structural-performance relationship; Chinese Herb; Coumarin; Bovine serum albumin; Fluorescence spectroscopy

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