

[PDF文档](#)

# 四种结构类型的蛋白质设计方法

刘赞<sup>1</sup>、王屹华<sup>1</sup>、王宝翰<sup>2</sup>、王存新<sup>\*1</sup>、陈慰祖<sup>1</sup>

1 北京工业大学生命科学与生物工程研究院

2 中国科学院生物物理研究所

给出了以疏水-亲水模型为基础的蛋白质设计方法，该方法以物理学原理为基础，以相对熵作为优化的目标函数。对四种不同结构类型的天然结构的真实蛋白质进行了检测，分析了影响检测成功率的主要因素，结果表明，该方法是普适的，可用于对不同结构类型的蛋白质设计序列。

## AN APPROACH TO DESIGN PROTEINS OF FOUR STRUCTURAL CLASSES

A design method for identifying the correct hydrophobic or polar class of residues was presented in previous work. This approach is based entirely on the physical principle and the relative entropy is used as a minimization object function. The algorithm is used to perform the design on target conformations corresponding to the native states of four structural classes of real proteins. The failure to increase the design success score are also analyzed and discussed. The method is general and can be extended to design proteins of different structural classes.

关键词