

三种金属硫蛋白聚合物静电效应的研究

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摘要 考察了三种金属硫蛋白(大鼠金属硫蛋白亚型II,兔肝金属硫蛋白亚型I和兔肝金属硫蛋白亚型II)的单体、二聚体和三聚体在pH为5.6-8.5和10.6

两种缓冲条件下的静电势分布。其中大鼠金属硫蛋白亚型II的结构直接来自于晶体数据,兔肝金属硫蛋白亚型I和II的结构则通过同源蛋白模型搭建。三种金属硫蛋白的静电势通过有限差分方法求解Poisson-Boltzmann方程得到。对于三种金属硫蛋白的二聚体,pH为5.6-8.5时,单体和单体之间的静电势分布具有明显的互补性;但pH≥10.6时,这种互补性会大大削弱。对于三种金属硫蛋白的三聚体,单体和二聚体之间主要表现为静电排斥,而且pH在10.6下的静电排斥力明显强于pH为5.6-8.5时的静电排斥。

关键词 [金属硫蛋白](#) [高聚物](#) [静电势](#)

分类号 [Q5](#)

Electrostatic interactions in three types of metallothioneins aggregates

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Abstract The electrostatic potential calculations were carried out on three types of metallothioneins. The structure of MT-II in rat liver was obtained directly from protein data bank, while other two structures of MT-I and MT-II in rabbit were constructed by homology modeling. The electrostatic potential was calculated by solving the Poisson-Boltzmann equation using the finite difference method. In each dimer, two monomers exhibited apparent electrostatic complementarity in buffers of pH 5.6-8.5. But when pH was increased to 10.6, the electrostatic complementarity would be reduced significantly. For all trimers, the electrostatic interactions between the monomer and dimer were unfavorable. Moreover, the electrostatic repulsion would be significantly enhanced when the pH value was changed to 10.6.

Key words [METALLOTHIONEIN](#) [HIGH POLYMER](#) [ELECTROSTATIC POTENTIAL](#)

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