

研究论文

苏氨酸在昆虫抗冻蛋白抗冻活性中的作用

周艳霞¹, 张勇¹, 谭宏伟¹, 贾宗超², 陈光巨¹

1. 北京师范大学化学学院, 北京 100875;
2. Department of Biochemistry, Queen's University, Ontario K7L3N6, Canada

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摘要 设计系列昆虫抗冻蛋白CfAFP突变体, 通过分子动力学模拟确定各突变体与冰晶的最佳作用模式, 并用半经验分子轨道方法AM1和PM3研究了其与冰晶的相互作用. 结果表明, TXT面上的苏氨酸在蛋白与冰晶相互识别和结合过程中十分关键, 对CfAFP与冰晶间相互作用的贡献大, 用其它疏水或亲水氨基酸残基替换都将削弱抗冻蛋白与冰晶的相互作用强度, 从而降低蛋白的抗冻活性. 但是, 在维系蛋白和冰晶结构匹配的基础上, 疏水基团的增加加强了抗冻蛋白与冰晶的结合, 从而增加蛋白的抗冻活性.

关键词 [昆虫抗冻蛋白](#) [基因突变](#) [亲水作用](#) [疏水作用](#) [分子动力学模拟](#)

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Role of Threonine on Antifreeze Activity of Insect Antifreeze Protein

ZHOU Yan-Xia¹, ZHANG Yong¹, TAN Hong-Wei¹, JIA Zong-Chao², CHEN Guang-Ju¹

1. Institute of Chemistry, Beijing Normal University, Beijing 100875, China;
2. Department of Biochemistry, Queen's University, Ontario K7L3N6, Canada

Abstract A series of mutants of the insect antifreeze protein(CfAFP) were designed, their best ice-binding modes were generated by using molecular dynamic simulations, and the interaction energy with ice was computed by semi-empirical molecular orbital methods AM1 and PM3. The results show that the contribution to the CfAFP-ice interaction of the threonine residues depends on the position and number in CfAFP, and Thr residues in TXT-motif play key roles on the recognition and binding of CfAFP and ice. Replacement of thr by other kinds of hydrophilic or hydrophobic amino residues reduced the interaction with ice, resulting in a moderate loss of antifreeze activity. Additionally, based on the structure complement of CfAFP and ice, increasing the size of hydrophobic residues could gain more stable interaction with ice and enhance the antifreeze activity.

Key words [Insect antifreeze protein](#) [Mutagenesis](#) [Hydrophilicity](#) [Hydrophobicity](#) [Molecular dynamics](#)

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通讯作者 陈光巨 gjchen@bnu.edu.cn

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