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研究论文

白喉毒素活性中心的量子化学计算与**149**位突变体的酶学动力学

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摘要 通过量子化学计算确定白喉毒素分子催化区活性中心的关键氨基酸残基, 评价其取代后的酶活性的改变, 为导向性抗癌药物研究提供高效杀伤细胞工具.
结合目前关于白喉毒素结构与功能的研究状况和量子化学计算结果, 将白喉毒素催化区的第149位酪氨酸突变为苯丙氨酸, 对其酶活性和与底物的结合能力进行评价. Y149位酪氨酸位于正电中心, 起受电子作用, 与野生白喉毒素相比, 苯丙氨酸突变体的酶催化活性增加约一倍, 而与底物结合能力没有变化. Y149是酶活性中心的关键氨基酸残基, 对其取代能够影响蛋白质的生物活性.

关键词 白喉毒素 量子化学 酶促动力学

分类号

Quantum Chemistry Calculation and Enzymatic Kinetics of Site-149 Mutant in Diphtheria Toxin Active Center

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Abstract Essential amino acid residues in diphtheria toxin catalytic domain were determined by quantum chemistry calculation and the enzymatic activities of mutant in the active-site were tested in order to provide high effective cytotoxin for target anticancer drugs. According to the research on relationships between diphtheria toxin structure and function, associated with the results of quantum chemistry calculation, Tyr-149 in diphtheria toxin catalytic domain was replaced by Phe, and the activity of enzyme and capacity of binding substrate were tested. Tyr-149 is located in strong positive electricity centre and has the capacity to receive electrons, so it is an active amino acid residue. Compared with the wild diphtheria toxin, the enzymic activity of Phe-mutant was elevated, and its NAD binding capacity showed slight change. Y149 is an important amino acid residue lying in active centre of diphtheria toxin catalytic domain and substitution on it could influence the bioactivity of protein.

Key words diphtheria toxin quantum chemistry enzymic kinetics

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