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## 研究论文

### DNA拓扑异构酶II的多态转换模型

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#### 摘要:

DNA拓扑异构酶II是一种分子马达, 它利用ATP水解产生的化学能, 切断一条双链DNA片段(G segment), 并让另一条双链DNA片段(T segment)从缺口处通过。对DNA拓扑异构酶II的工作循环研究将有助于阐明其工作机理。本文根据已有实验资料, 利用主方程方法构建了DNA拓扑异构酶II状态转变的随机跃迁模型, 求得系统各态的稳态解。进而推导出稳态下无机磷(Pi)浓度随时间的变化, 得到DNA拓扑异构酶II的最小工作周期约为0.78秒, 该结果同实验获得的DNA拓扑异构酶II工作周期为0.5~1秒一致。该模型定量地分析了DNA拓扑异构酶II的动力学行为。

关键词: DNA拓扑异构酶II 主方程 稳态 无机磷

### A Multi-States Model for DNA Topoisomerase II Cycle

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#### Abstract:

DNA topoisomerase II is a molecular motor that couples ATP hydrolysis to the transport of one DNA segment (T segment) through a transient break in another segment (G segment). The study of DNA topoisomerase II cycle is useful in elucidating the mechanism of DNA topoisomerase II work. Based on experiments, a master equation approach is used to model multi-states change of DNA topoisomerase II cycle. The non-equilibrium steady state solution describes the probability distribution of each state as a function of concentration of ATP. Moreover, the concentration of inorganic phosphate Pi as a function of time t and ATP concentration under steady state is obtained. By calculating the released velocity of Pi, we deduce that the minimized cycle of DNA topoisomerase II is 0.78 second. This result is consistent with the cycle of DNA topoisomerase II derived from experiments, which are in the range of 0.5~1 second. The conclusions demonstrate that the proposed model can qualitatively explain experiment results rather being satisfactory.

Keywords: DNA topoisomerase II Master equation Steady state Inorganic phosphate

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