技术及应用

单能电子诱发DNA损伤的理论计算

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摘要 利用径迹结构的方法模拟了单能电子从入射DNA水溶液到最终产生DNA损伤的早期物理和化学变化过程。着重研究了直接能量沉积导致碱基损伤的判断方法、DNA损伤穷举分类的定义及计算机实现方法,以及确定自由基产生位置的随机抽样方法。结果表明:物理、化学径迹与DNA的反应主要以NB(no break)的形式存在,而在链断裂中,主要也以易修复的单链断裂(SSB)为主;在为数不多的双链断裂(DSB)中,复杂DSB占到相当数量的份额。验证了DNA是辐射作用主要"靶"的假定。

关键词 <u>DNA损伤</u> <u>径迹结构</u> <u>直接损伤</u> <u>间接损伤</u> <u>自由基</u>

分类号

Theoretical Calculation of Monoenergetic Electron Induce d DNA Damage

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Abstract The track structure method was used to model the early physical and chemical event fr om the incidence of monoenergetic electrons to DNA solution to the production of final DNA da mage. The judgmental method of base damage induced by direct energy deposition, the exhaustiv e definition of classification of DNA damage and realization method on computer and the rando m sampling method for confirming the position of free radicals were introduced. The majority of in teractions in DNA are in the form of no break, and most of the strand breaks are the SSBs which are easy to repair. In a small number of DSBs, the complex DSBs account for a considerable number of shares. The basic assumption that DNA is the main target of radiation reaction is validated.

Key words DNA damage _ track structure _ direct damage _ indirect damage _ free radical

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