

Energetic analysis of base-pair stability and DNA decamers containing 7,8-dihydro-8-oxoguanine

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DNA base-pair mutations have been implicated in aging and cancer. 8-Oxo-2'-deoxyguanosine (OdG) is an abundant DNA lesion for which analogues have been developed and experimentally tested. In this work we have utilized the OPLSAA/GBSA (water) molecular mechanics method to analyze and compare the energetics of normal (dG:dC and dA:dT) and damaged (XdG(anti):dC and XdG(syn):dA where X=O, C, Cl, Br and I) base-pairs. A comparison of structural and geometrical differences and similarities will be presented. In addition, the structural and energetic effects of various base pairs will be examined using a model 10 unit DNA strand.

