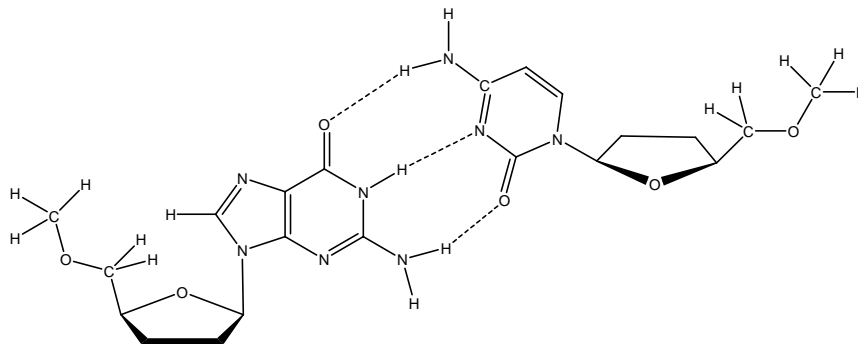


# “Energetic Analysis of base-pair stability and DNA containing 7,8-dihydro-8-oxogaunine”

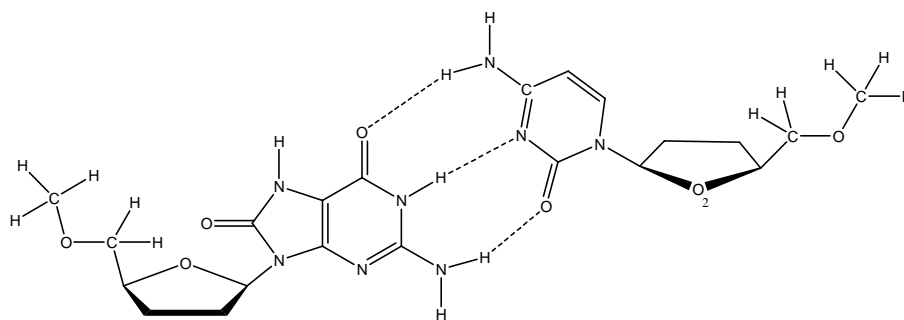
Tyler Steele, Anna Parker, Carol Parish and Michelle Hamm

Department of Chemistry, University of Richmond

DNA base-pair mutations have been implicated in aging and cancer. 8-Oxo-2'-deoxygaunosine (OdG) is an abundant lesion for which analogues have been developed and experimentally tested. In this work we have utilized quantum mechanics to analyze and compare the structures and energetics of normal (dGanti:dC) and damaged (XdGanti:dC and XdGsyn:dA, where X=O,S,C) base-pairs. As well, the energetic information for the syn versus anti conformations was analyzed. All geometry optimizations were done using the B3LYP functional with the 6-31G\* basis set in the presence of the polarizable continuum model (PCM) for water (all methods as employed by Gaussian 03.)



dGanti:dC



OdGanti:dC