Interactions of boronated and non-boronated intercalants in small nucleic acid models

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Intercalant molecules are aromatic molecules that bind between nucleic-acid bases in DNA. The presence of the intercalant disrupts the DNA structure, interfering with replication. It is possible that boronated intercalants may be used in the cancer treatment; boron neutron capture therapy. In this work, we examine the interaction energies between boronated and non- boronated intercalant molecules and segments of DNA. Differences in interaction energy, with respect to boronation or the particular base pairs binding the intercalant, provide information about the most likely locations for these intercalants to bind to DNA. The six complexes of four DNA bases (AT..TA,GC..CG, etc), each with the intercalant bound in between, were optimized using ONIOM(DFT/3-21G:AM1) with the DNA bases and intercalant in the upper-level and the sugar-phosphate back-bone in the lower-level. All interaction energies in the systems were calculated with MP2 and DFT with the 6-31+G* basis set. Complexes were examined with and without charge on the phosphate groups. The results show trends for the intercalant's preferred binding location and the effect of charge on binding.

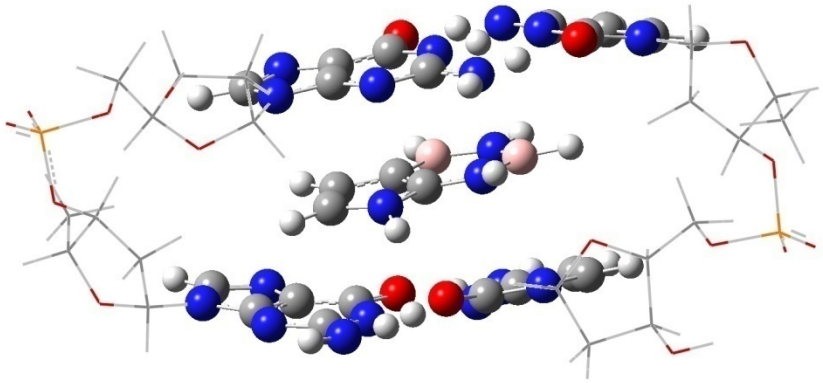

Figure 1: Boronated intercalant in complex with GGICC