Spectroscopic Characterization of Interstrand Carbinolamine Crosslinks Formed in the 5'-CpG-3' Sequence by the Acrolein-Derived γ-OH-1,N^2-Propano-2'-deoxyguanosine DNA Adduct [†]

Supporting Information

Revised Manuscript

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Running Title: Acrolein Carbinolamine DNA Crosslink

Figure S1. The parameterization of the carbinolamine crosslink, for the AMBER 8.0 forcefield.

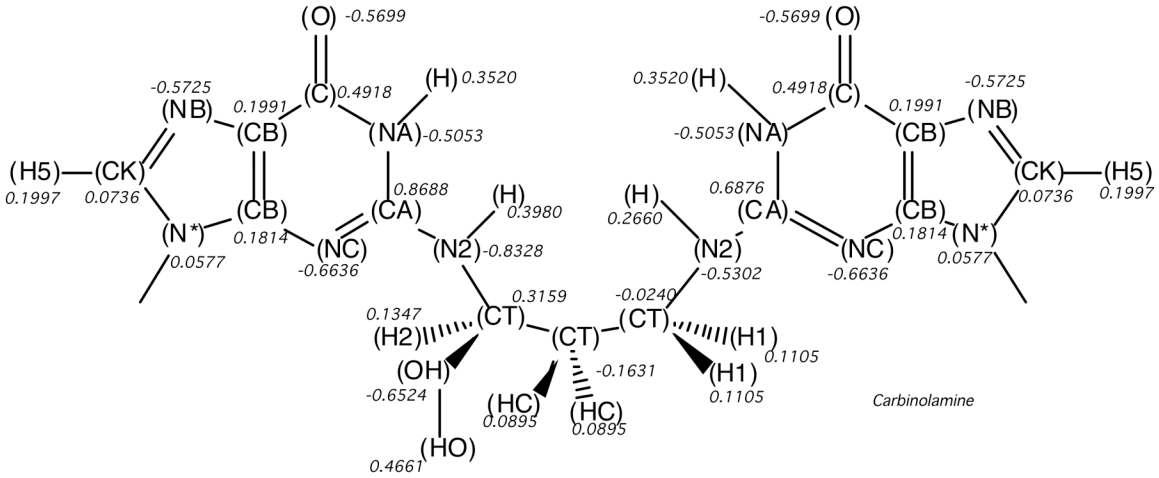
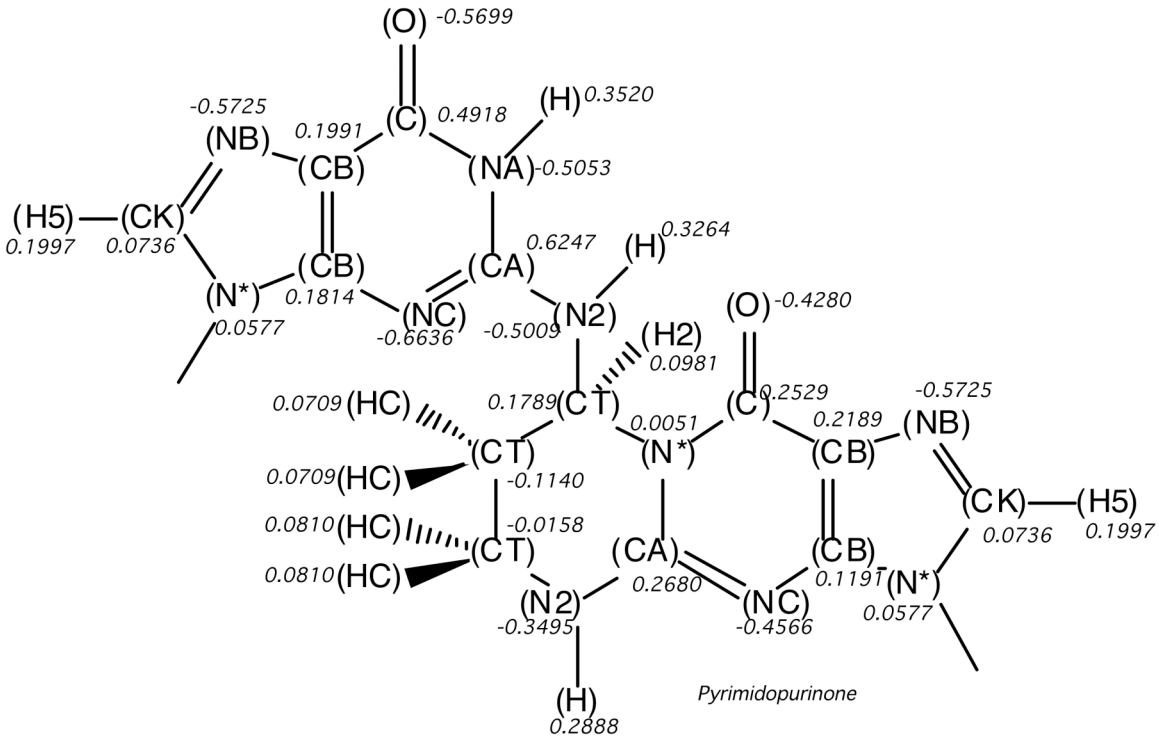


Figure S2. The parameterization of the pyrimidopurinone crosslink, for the AMBER 8.0 forcefield.



Complete References 37 and 39.

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