

Stereospecific Formation of Interstrand Carbinolamine DNA Crosslinks by Crotonaldehyde- and Acetaldehyde-Derived α -CH₃- γ -OH-1,N²-Propano-2'-deoxyguanosine Adducts in the 5'-CpG-3' Sequence

Supporting Information

Revised Manuscript

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Running Title: Crotonaldehyde Carbinolamine DNA Crosslinks

Figure S1. The parameterization of the carbinolamine and the pyrimidopurinone crosslinks for the AMBER 8.0 forcefield.

