The γ-Hydroxy-1,N^2-Propano-2'-Deoxyguanosine DNA Adduct Conjugates the N-Terminal Amine of the KWKK Peptide via a Minor Groove Carbinolamine Linkage

Supporting Information

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Running Title: Acrolein-Induced DNA-Peptide Conjugate

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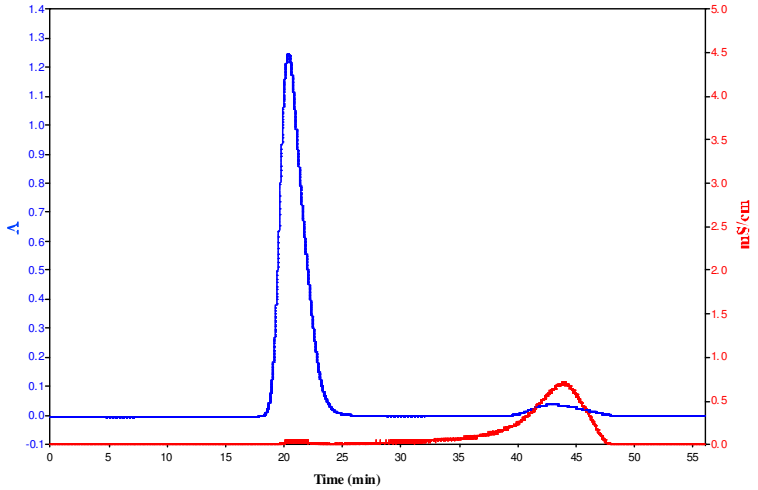

Figure S1. Gel filtration of the reaction mixture by Sephadex G-25. The first peak was DNA-peptide conjugates. The blue line represents the UV/vis absorption at 254 nm and the red line represents the conductivity of the solution.

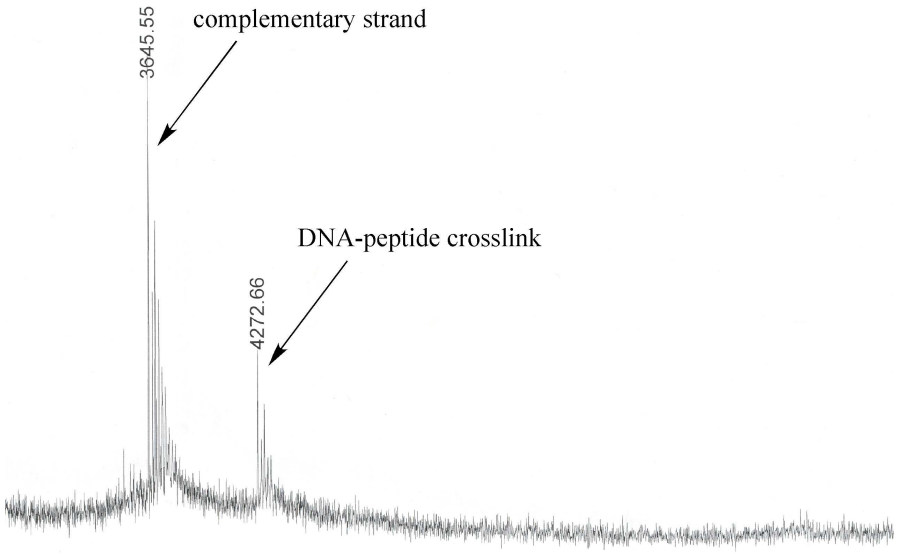

Figure S2. MALDF-TOF MS of the DNA-KWKK conjugates. The plot shows the molecular weights of DNA-peptide conjugates and complementary strand (calc. 4272.5[M-H_2O-1] and 3645.2[M-1], respectively).

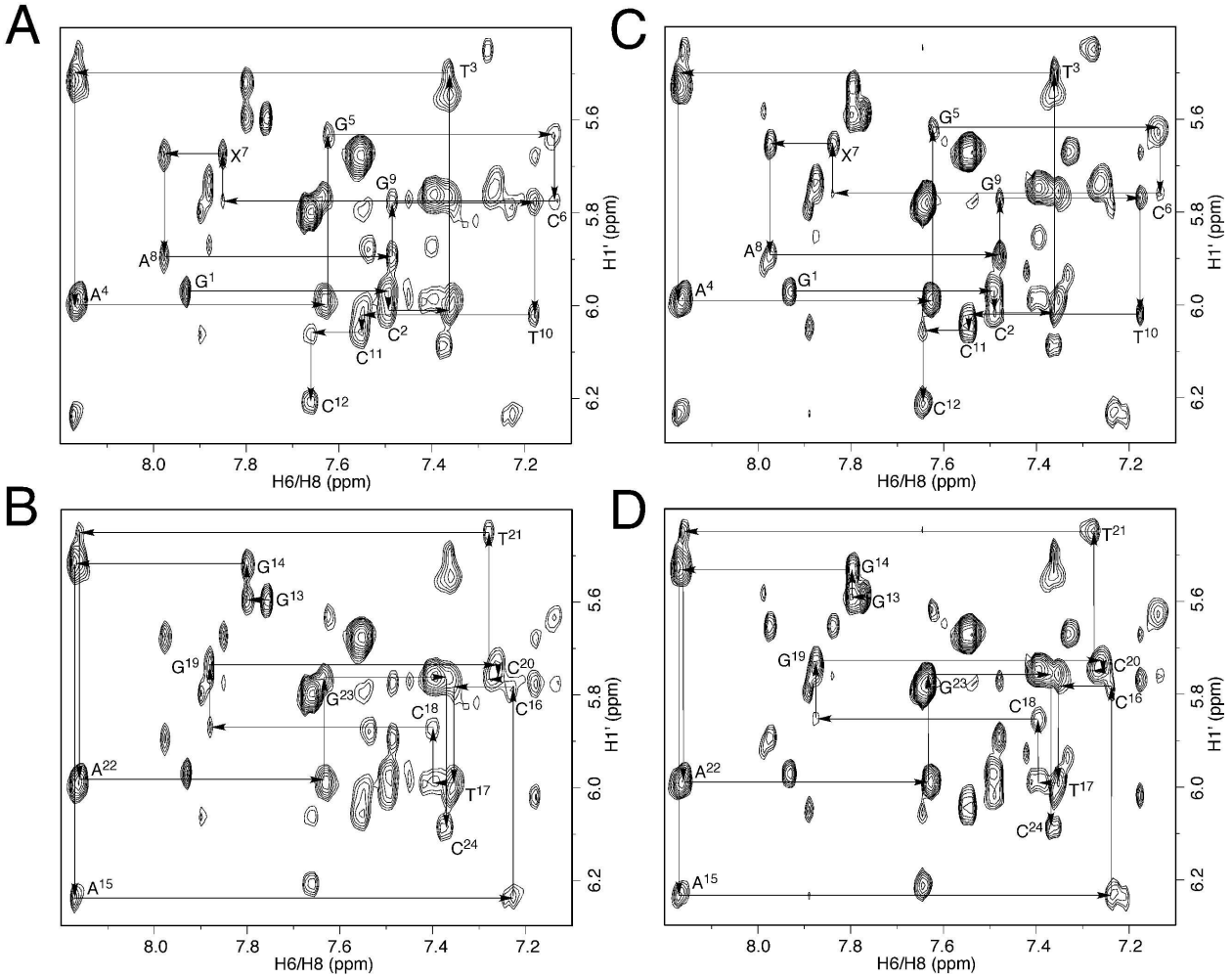

Figure S3. NOE connectivity of base aromatic H6/H8 protons with deoxyribose H1' protons. Expansions of NOESY showing complete NOE connectivities of base H6/H8 protons with 2′-deoxyribose H1′ protons of the major DNA-peptide conjugate: (A) conjugated strand at pH 5.3, (B) complementary strand at pH 5.3, (C) conjugated strand at pH 8.9, and (D) complementary strand at pH 8.9.

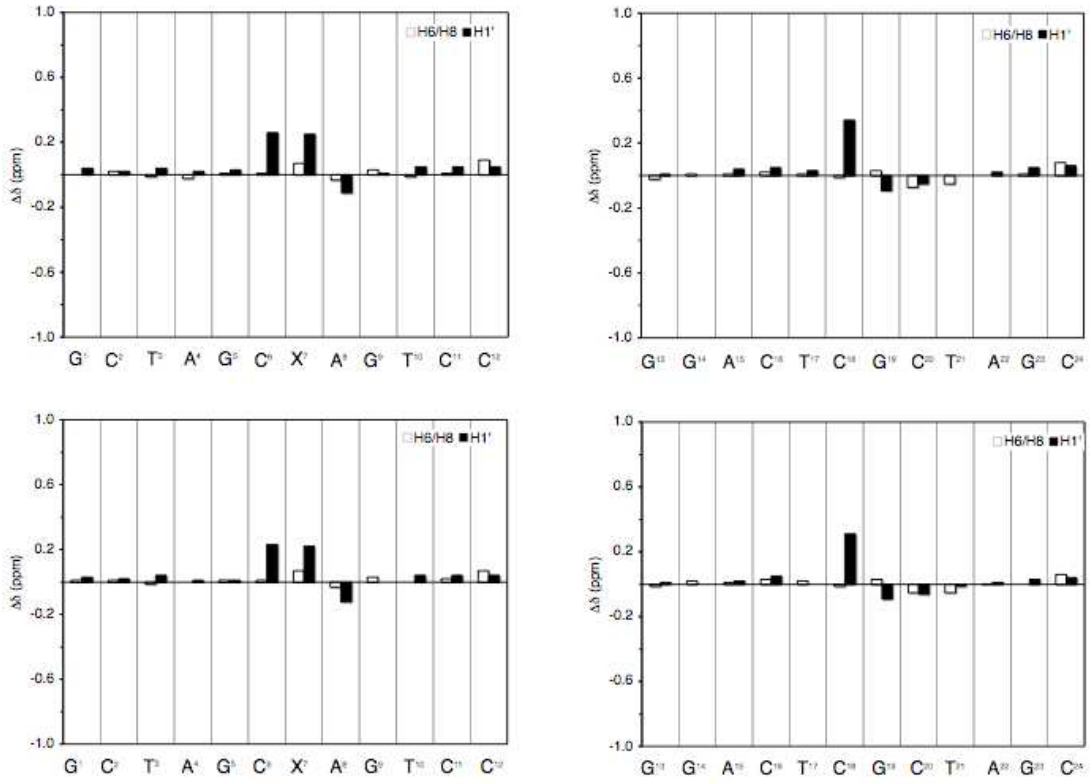

Figure S4. Chemical shift perturbations. The major DNA-peptide conjugate compared with unmodified DNA duplex: (A) conjugated strand at pH 5.3, (B) complementary strand at pH 5.3, (C) conjugated strand at pH 8.9, and (D) complementary strand at pH 8.9.

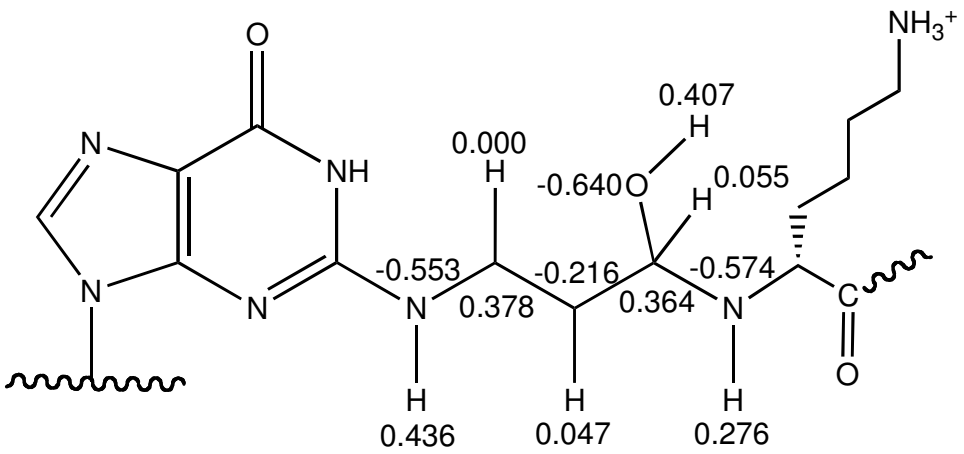

Figure S5. Force constants used for the carbinolamine linkage obtained from Gaussian calculation

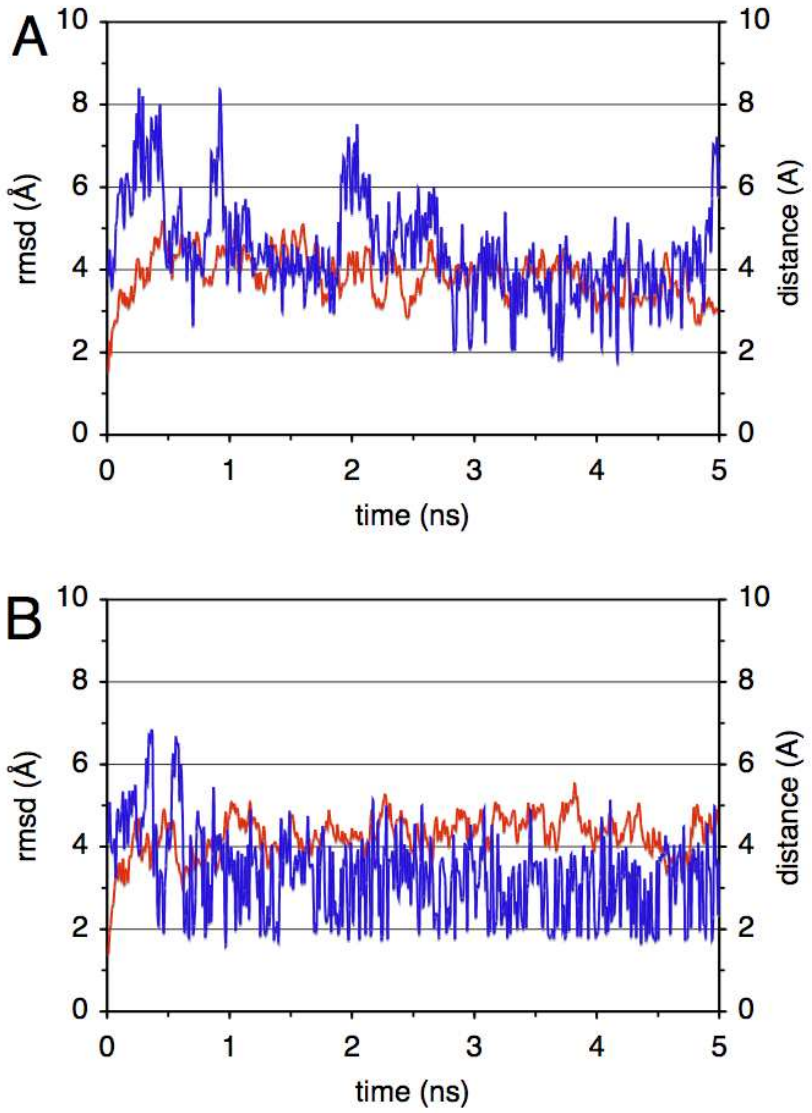

Figure S6. Molecular dynamics simulations of the *R*- and *S*-carbinolamine DNA-KWKK. (A) *R*-configuration, red lines represent the rmsd values of the trajectories compared to the starting structure, blue lines represent the distances between carbinol and A^{8} O4' in the trajectories; (B) *S*-configuration, red lines represent the rmsd values of the trajectories compared to the starting structure, blue lines represent the distances between carbinol and G^{19} O4' in the trajectories.