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Supplementary Material

NMR Evidence for Specific Intercalation of Δ-Rh(phen)$_2$phi^{3+} in [d(GTCGAC)]$_2$

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Figure 1S: Temperature dependence of the 1-D NMR spectrum of Δ-Rh(phen)$_2$phi^{3+} - [d(GTCGAC)]$_2$ (1:1, 3 mM) at 500 MHz. The sample was buffered with 50 mM phosphate containing 0.2 M NaCl (D_2O), uncorrected pD = 7.0. The region from 9.5 to 5 ppm is shown for clarity. These spectra illustrate that the complex is in the intermediate to fast exchange regime over this temperature range. Note the broad resonances between 6.0 and 7.0 ppm for two of the phi protons which shift dramatically with temperature in contrast to three phenanthroline resonances near 9 ppm which are considerably sharper and exhibit a smaller temperature dependence in their chemical shifts.

Figure 2S: Expanded NOESY contour plot (mixing time, 300 ms) of Δ-Rh(phen)$_2$phi^{3+} - [d(GTCGAC)]$_2$ (0.75:1, 3 mM) at 320 K. The sample was buffered with 50 mM phosphate containing 0.6 M NaCl (D_2O), uncorrected pD = 7.0. The contour plot correlates the base protons (7.0 - 8.5 ppm) to the H1' protons (6.5 - 5.0 ppm). The labeled cross peaks correspond to NOEs between the base protons and the H1' protons of the sugar residue of the 5'-nucleotide. The numbering scheme for the bases is given from the 5'-end of the oligonucleotide. Dotted lines illustrate the NOE walk along the oligonucleotide. Due to the absence of a clear assignment for the T_2H1' proton, the internucleotide NOE at this step cannot be unambiguously located, and therefore it has not been labeled in the plot. Noteworthy is the absence of an internucleotide NOE at the 5'-CG-3' step.

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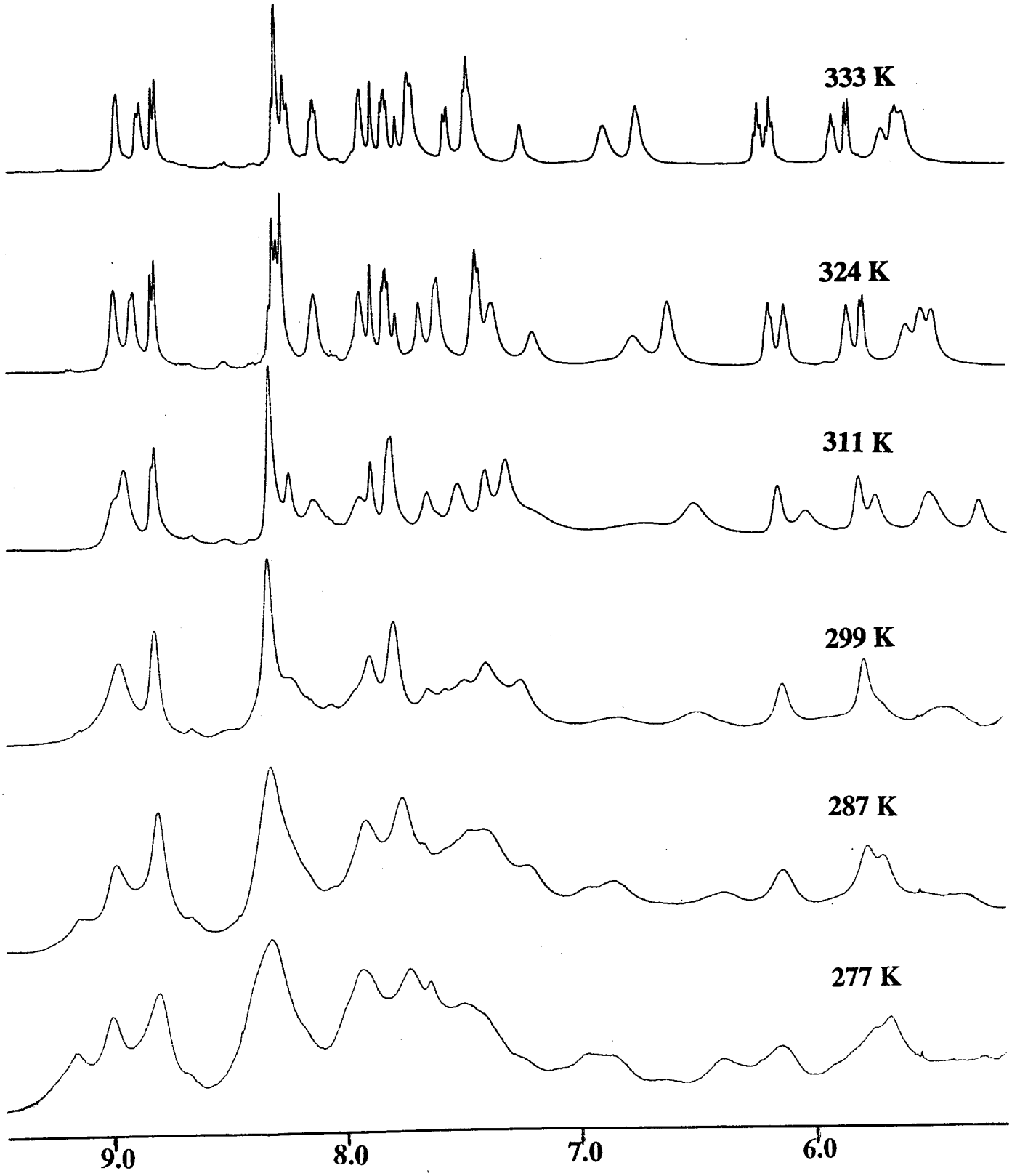

Figure 1S

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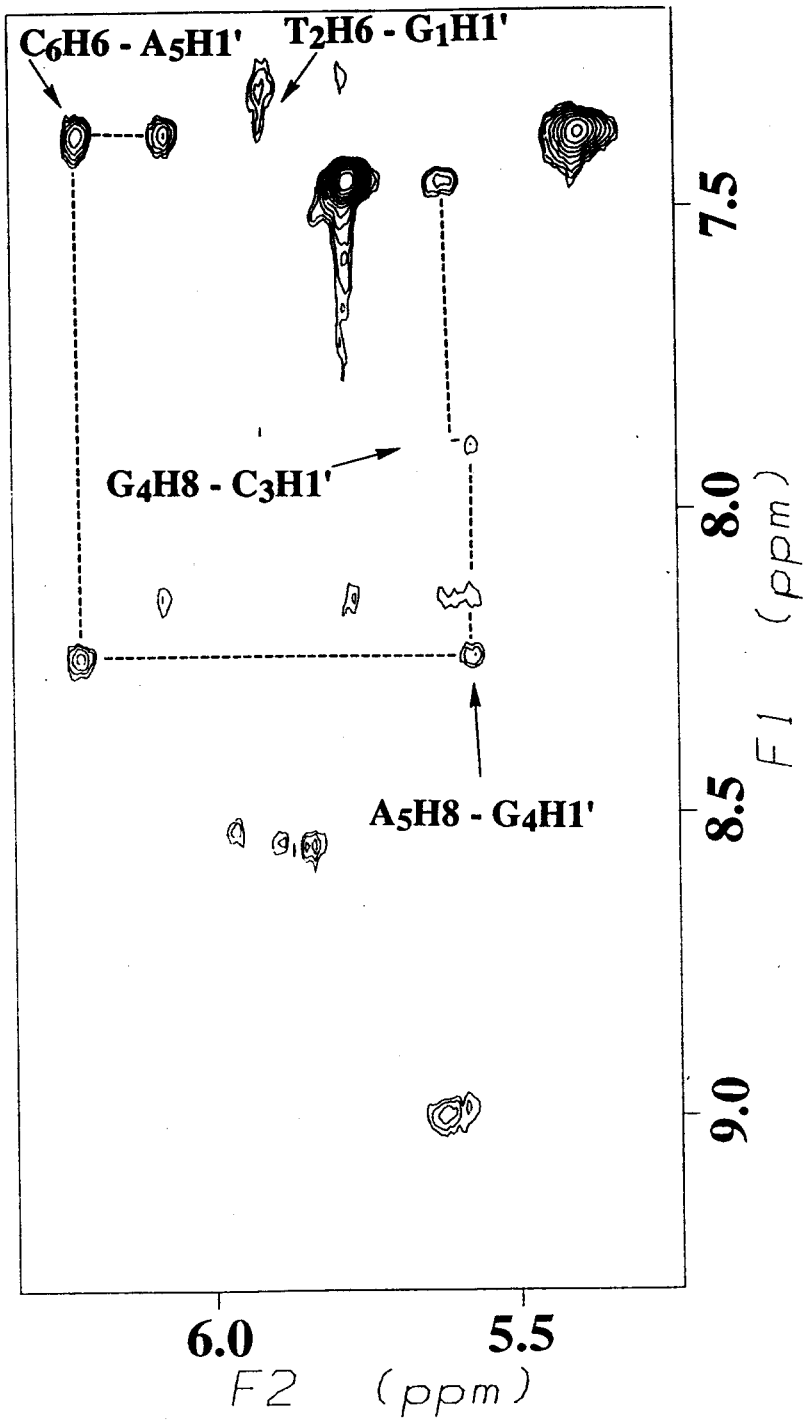

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Figure 2S