ELECTRONIC SUPPLEMENTARY INFORMATION

DNA Fragment Conformations in Adducts with Kiteplatin.

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Table S1. Temperature dependence of the H8 signals (ppm) of (*cis*-1,4-DACH)Pt(d(TGGT)) in D_2O.

(*cis*-1,4-DACH)Pt(d(TGGT))	**5 °C**	**25 °C**	**40 °C**
3′-G H8	9.15	9.06	9.00
5′-G H8	8.17	8.20	8.22

Table S2. ^{31}P NMR data (ppm) for (*cis*-1,4-DACH)Pt(d(TGGT)) at different temperatures.

T, °C	**GpG**	**GpT**	**TpG**
5	-3.03	-4.23	-4.39
25	-2.95	-4.09	-4.17
40	-2.87	-3.40	-3.40

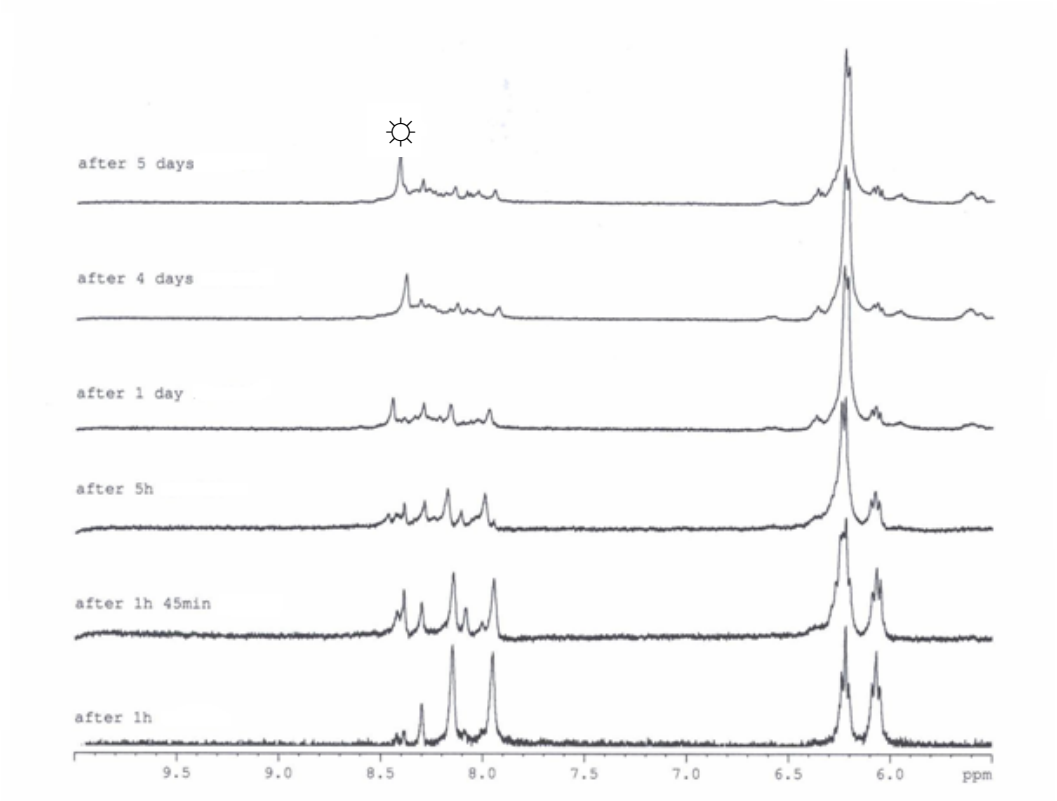

Figure S1. H8 and H1' regions of the ^{1}H NMR (400 MHz) spectra (collected at 25 °C) used to monitor the reaction between $[Pt(OD_2)_2(cis\text{-}1,4\text{-DACH})]^{2+}$ and d(GpG) in D_2O (pH ~3.1). The symbol ☼ designates an impurity (at 8.42 ppm in the final spectrum; likely formate from plastic pipette tips).

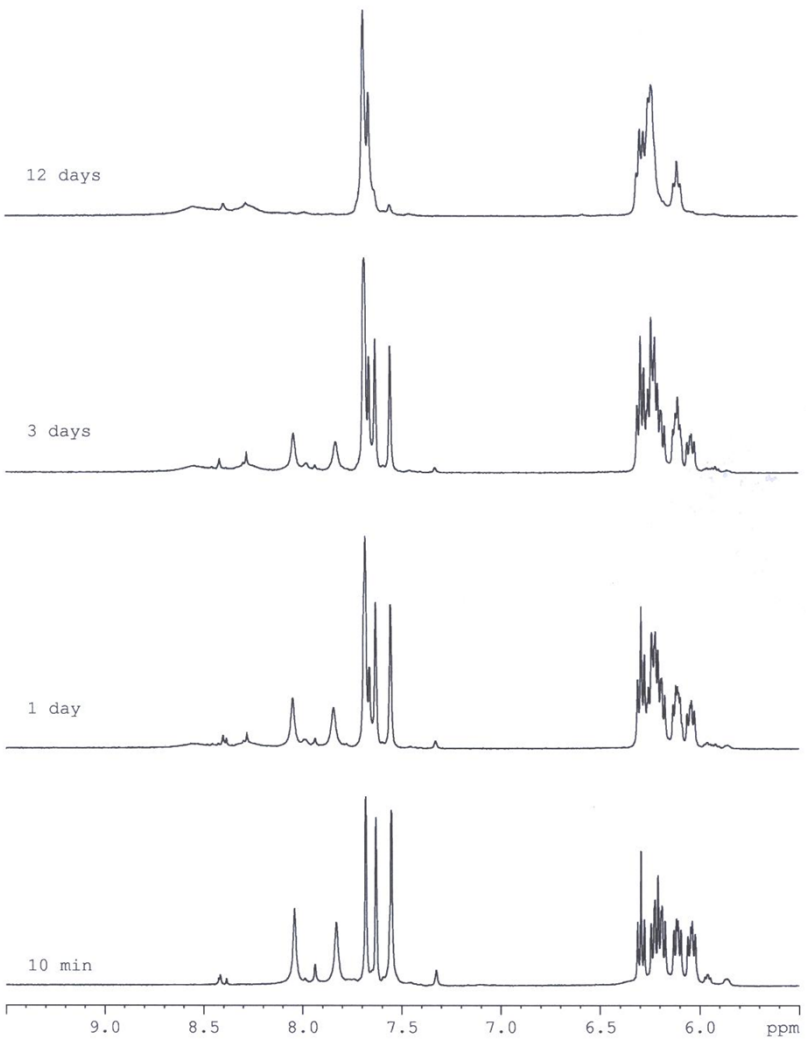

Figure S2. ^{1}H NMR (400 MHz) spectra (region of H8, H6 and H1' resonances) monitoring the reaction of $[Pt(OD_2)_2(cis\text{-}1,4\text{-DACH})]^{2+}$ with d(GGTTT) in D_2O (pH ~4).

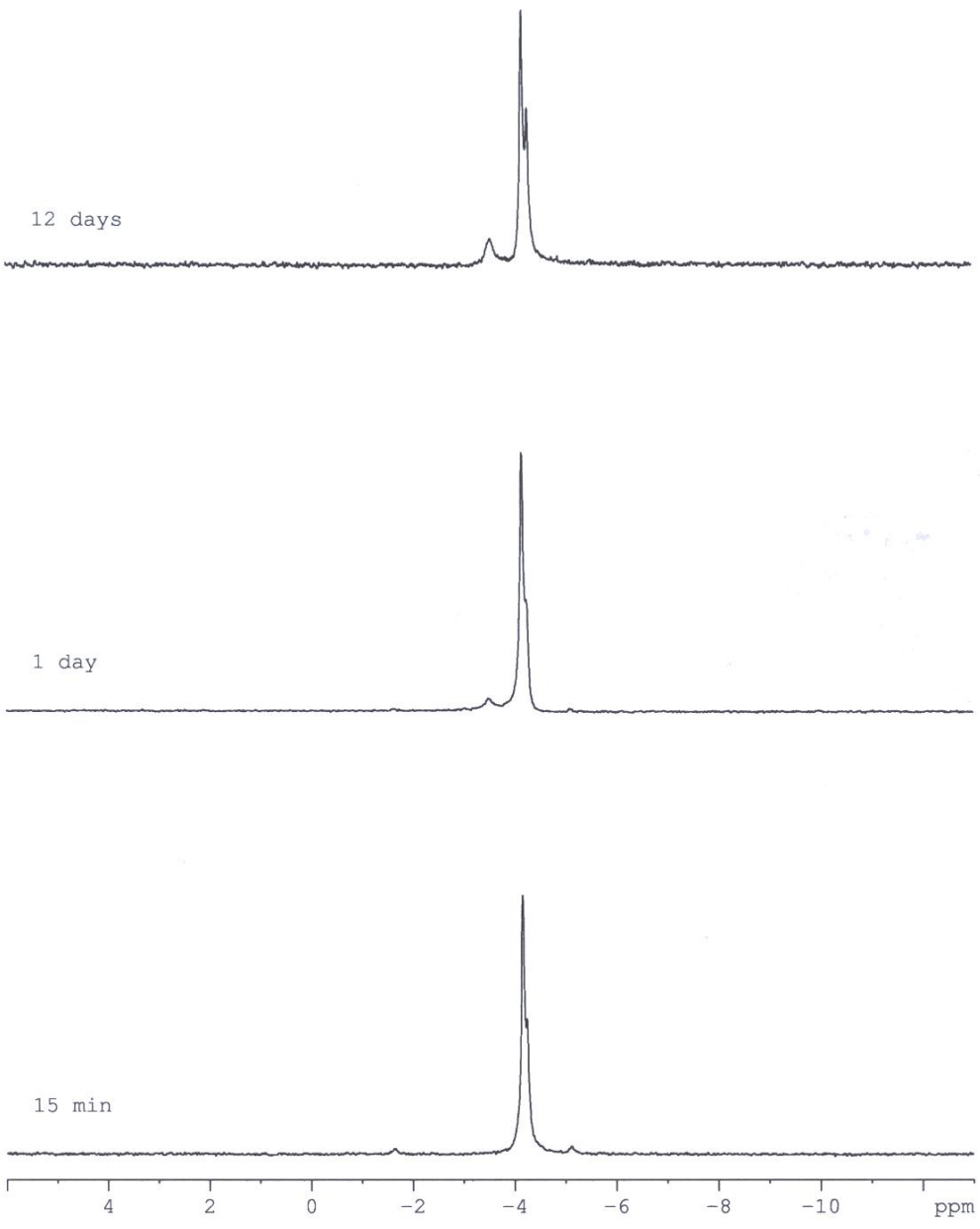

Figure S3. ^{31}P NMR (161.98 MHz) spectra monitoring the reaction of $[Pt(OD_2)_2(cis\text{-}1,4\text{-DACH})]^{2+}$ with d(GGTTT) in D_2O (pH ~4, 25 °C).

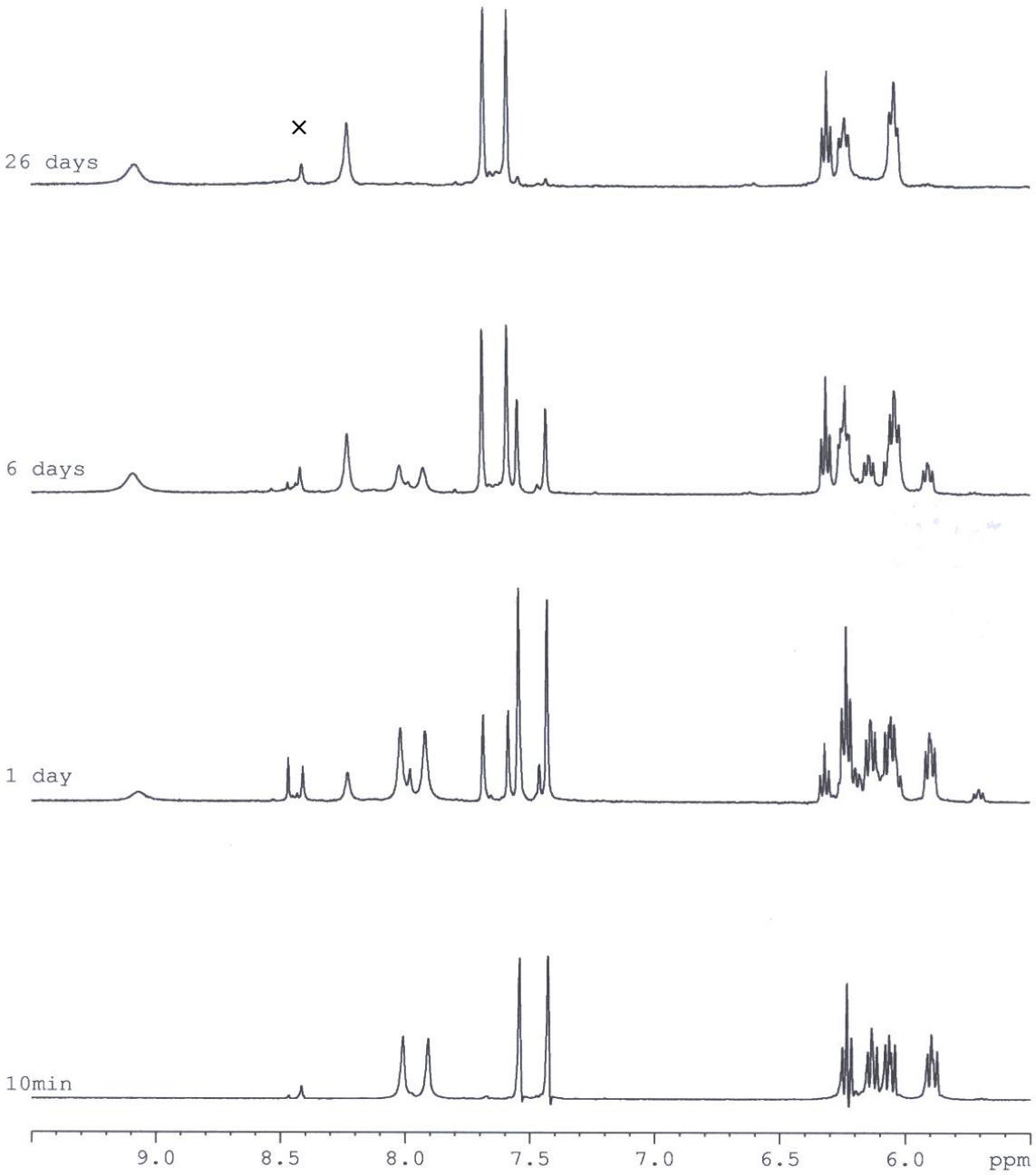

Figure S4. ^{1}H NMR (400 MHz) spectra in the region of H8, H6 and H1' resonances, monitoring the reaction of $[Pt(OD_2)_2(\textit{cis}\text{-}1,4\text{-DACH})]^{2+}$ with d(TGGT) in D_2O (pH ~4). × indicates an impurity present in the solvent (likely formate from plastic pipette tips).

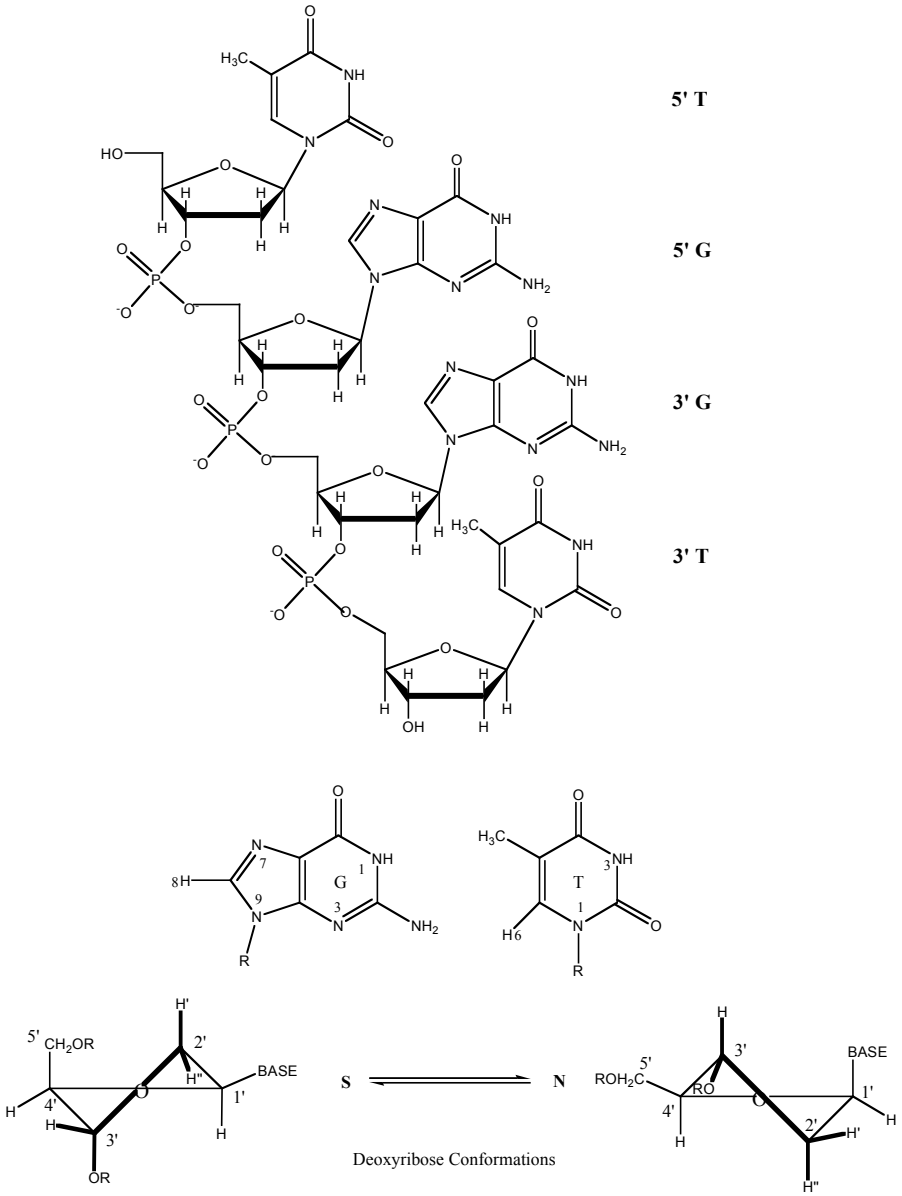

Figure S5. Schematic representation of d(TGGT) with the base and deoxyribose proton-numbering scheme. The S and N conformations of the deoxyribose moieties are also depicted.

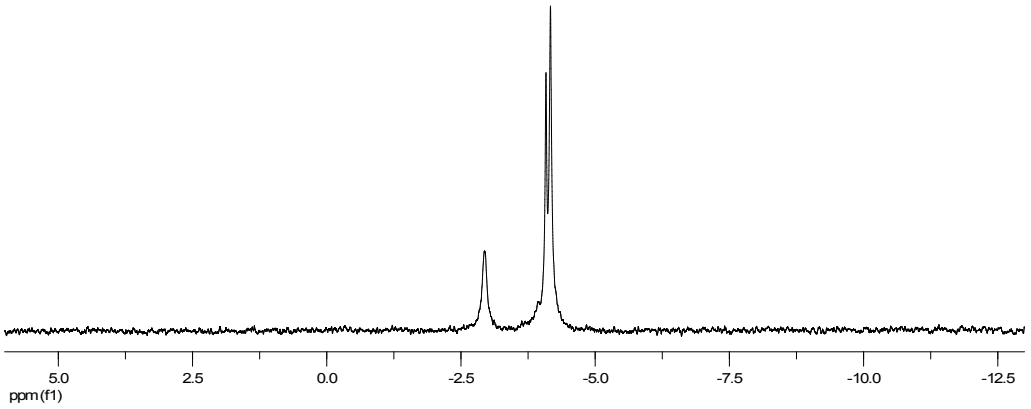

Figure S6. ^{31}P NMR (161.98 MHz) spectrum of the end product of the reaction between [Pt(OD_2)(*cis*-1,4-DACH)]$^{2+}$ and d(TGGT) in D_2O (pH ~4, 25 °C, 25 days after mixing).

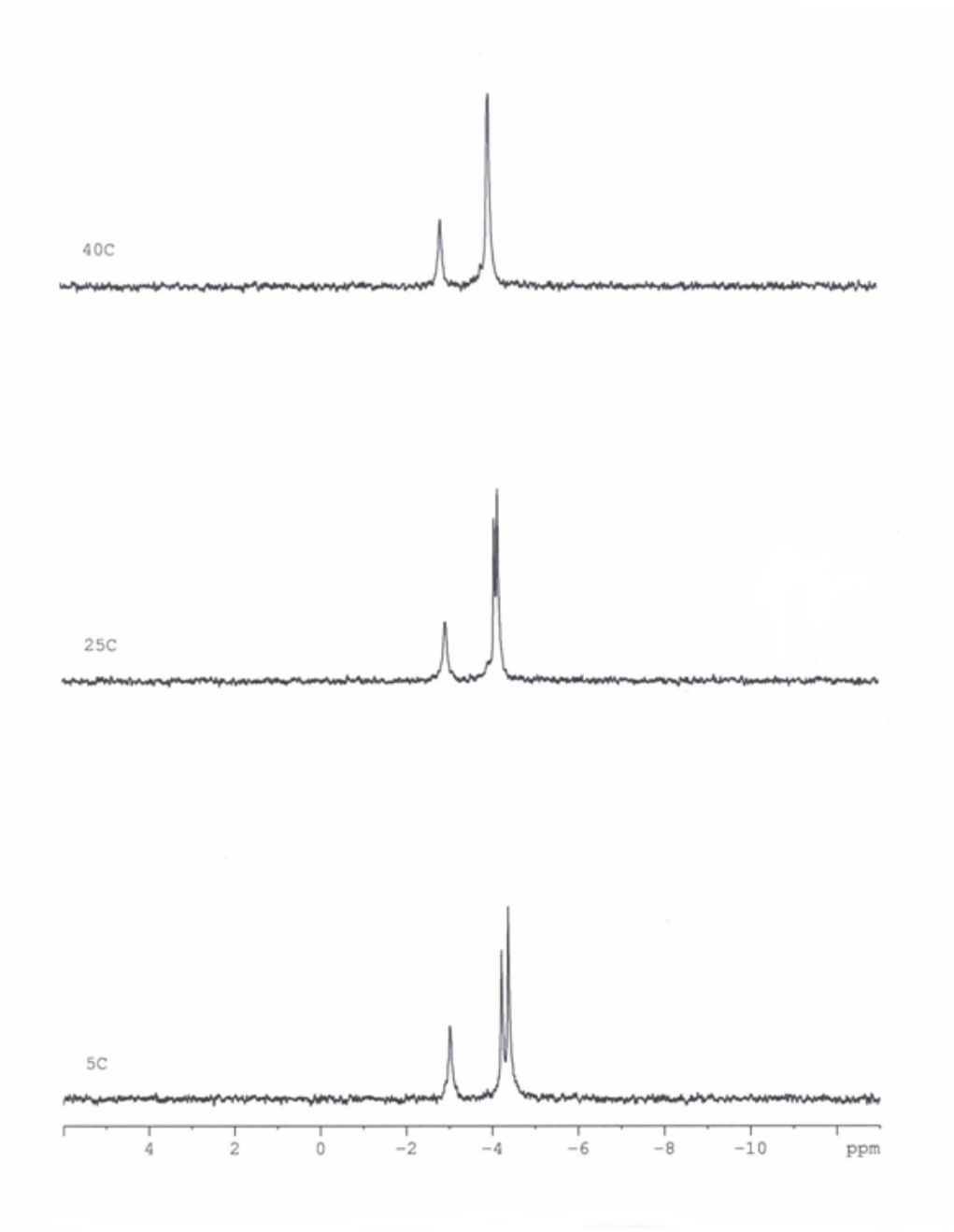

Figure S7. Temperature dependence (from 5 °C to 40 °C) of the ^{31}P NMR (161.98 MHz) spectrum of (*cis*-1,4-DACH)Pt(d(TGGT)) in D_2O solution (pH ~4).

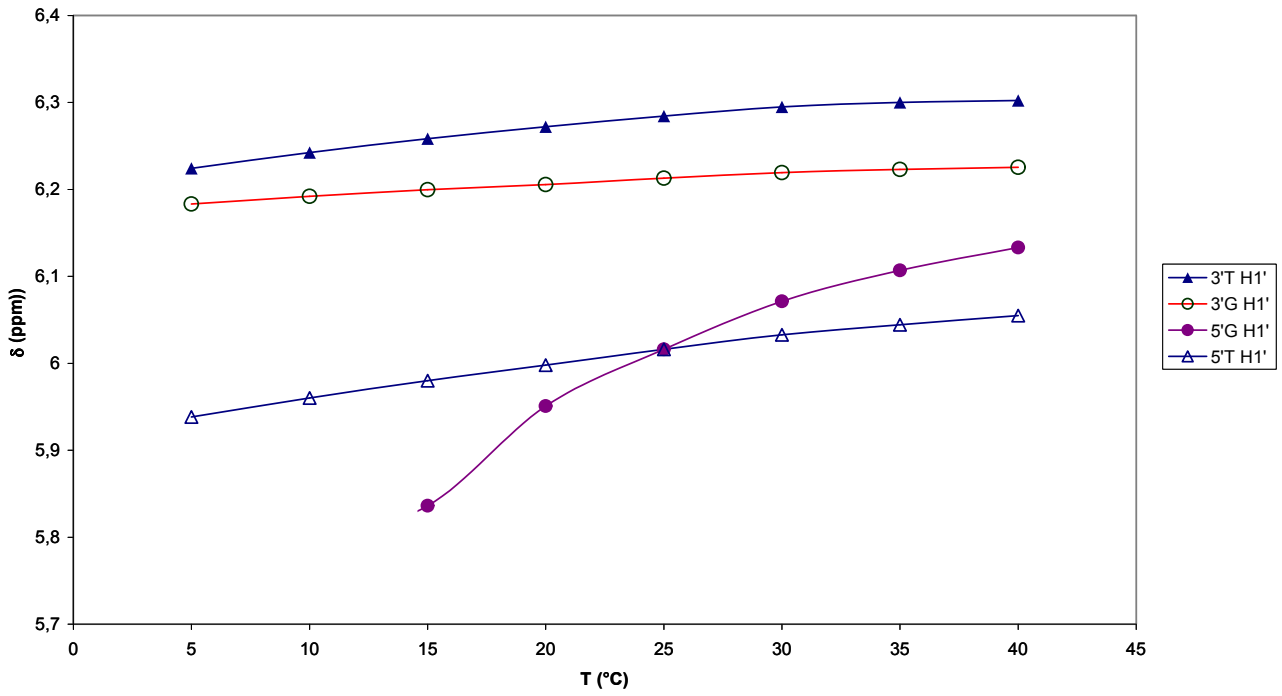

Figure S8. Temperature dependence of the H1' signals of (*cis*-1,4-DACH)Pt(d(TGGT)) in D_2O solution.