Supporting Information: DNA Interstrand Cross-Linking Upon Irradiation of Aryl Halide C-Nucleotides.

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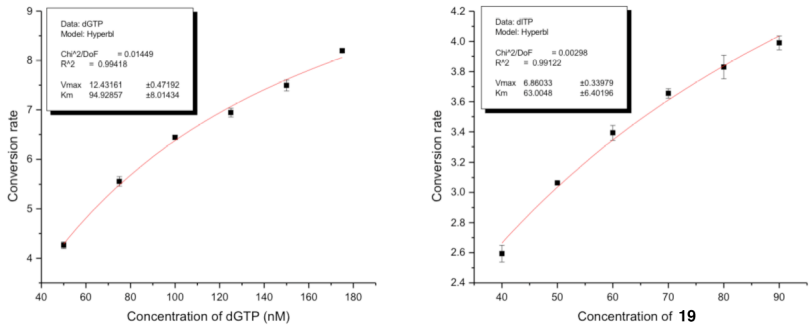
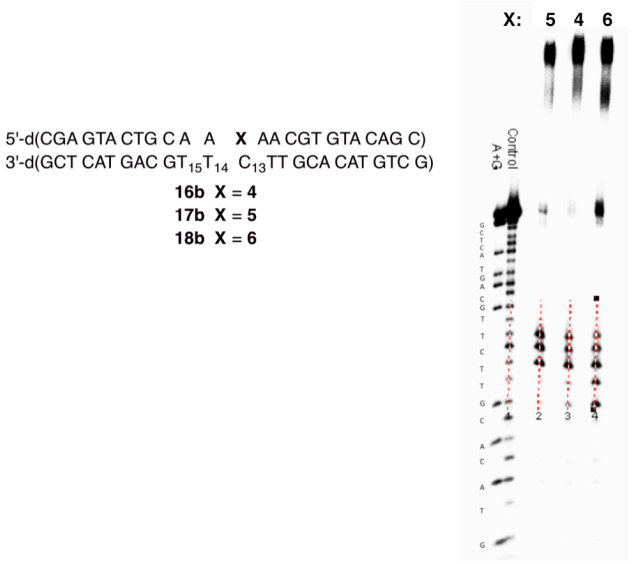
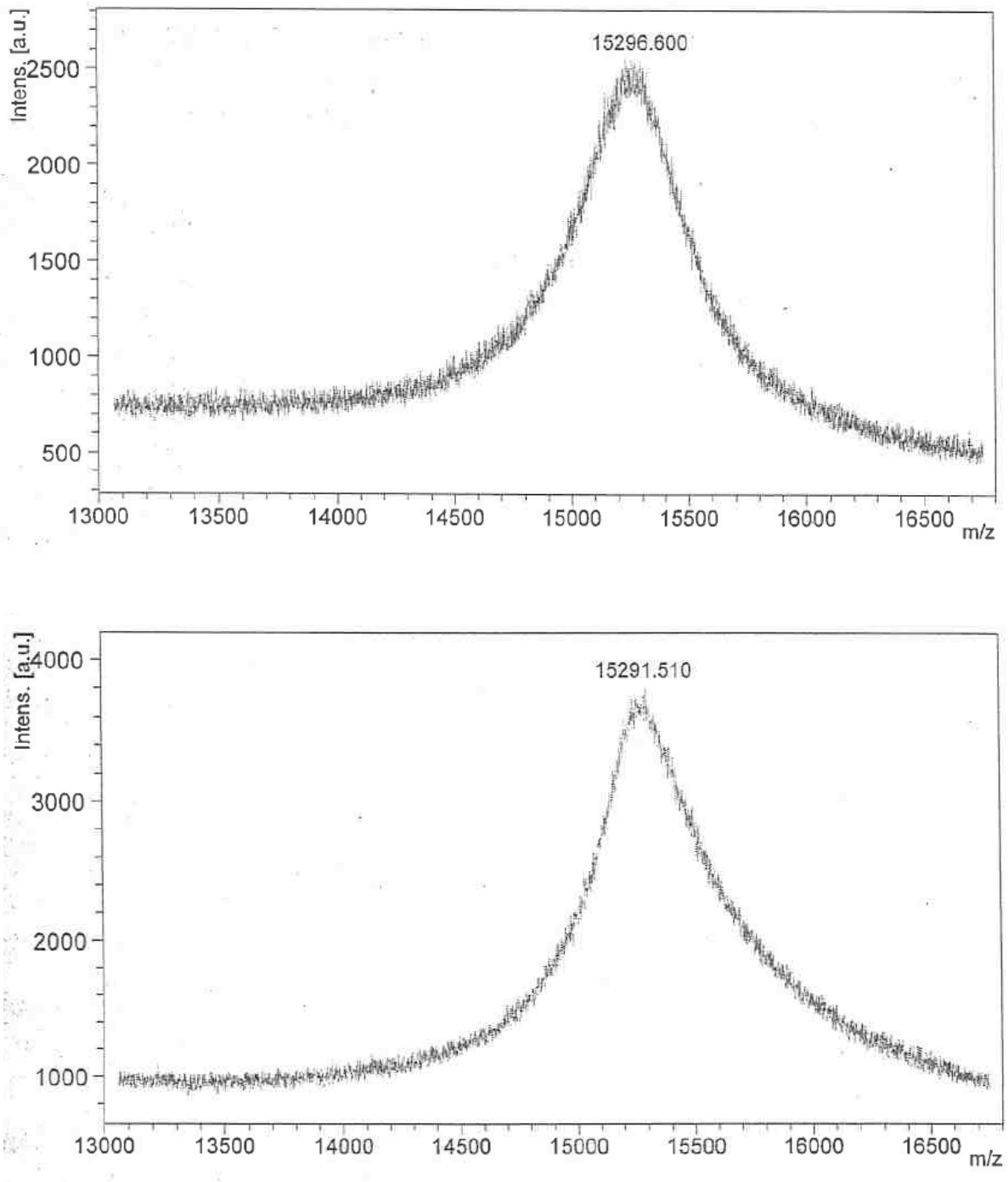
Contents:



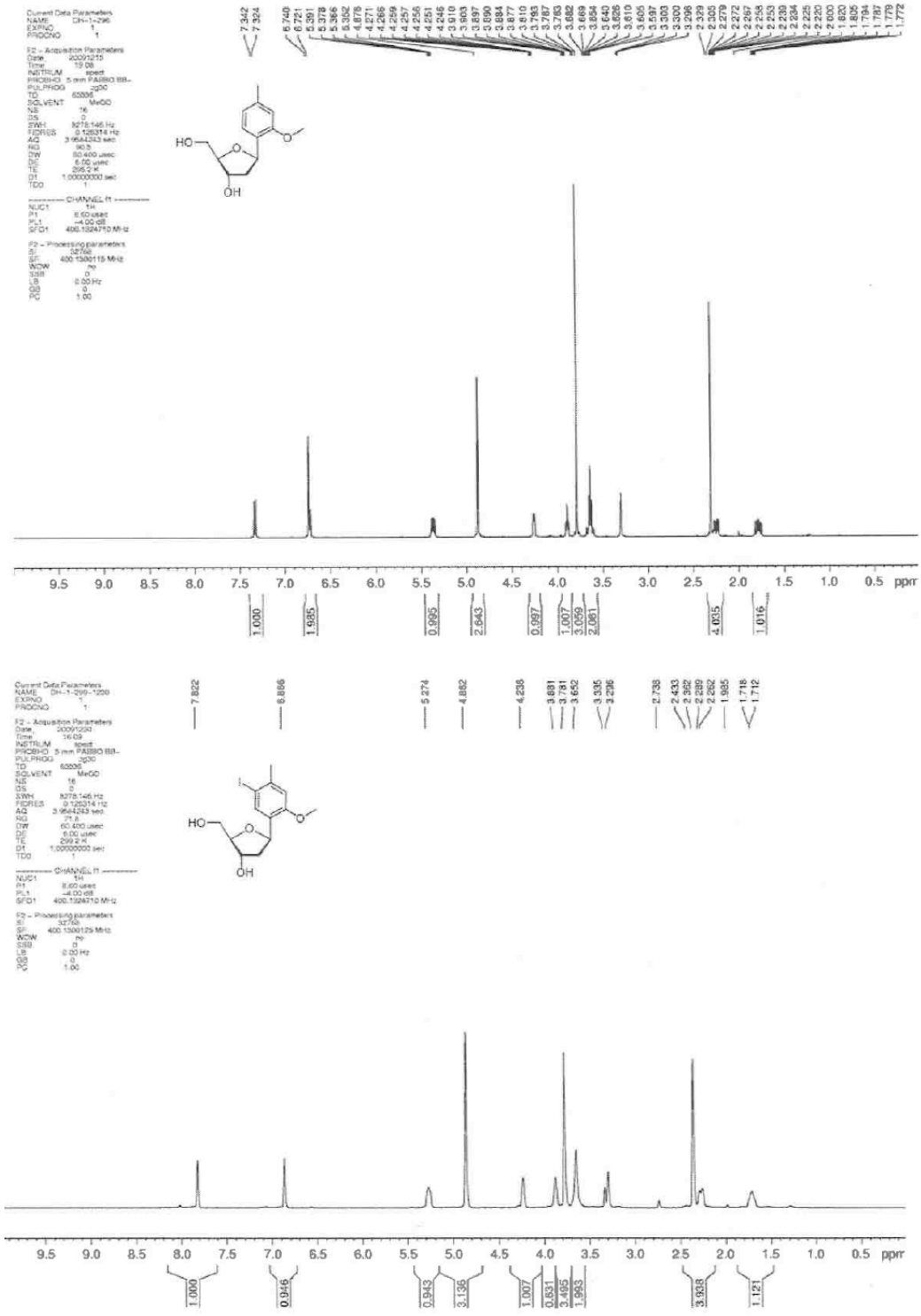
Supporting Information Figure 2. Steady-state nucleotide incorporation by Deep Vent (exo$^-$) opposite dC in 5'-^{32}P-**20**. (Left) dGTP as substrate; (Right) **19** as substrate.



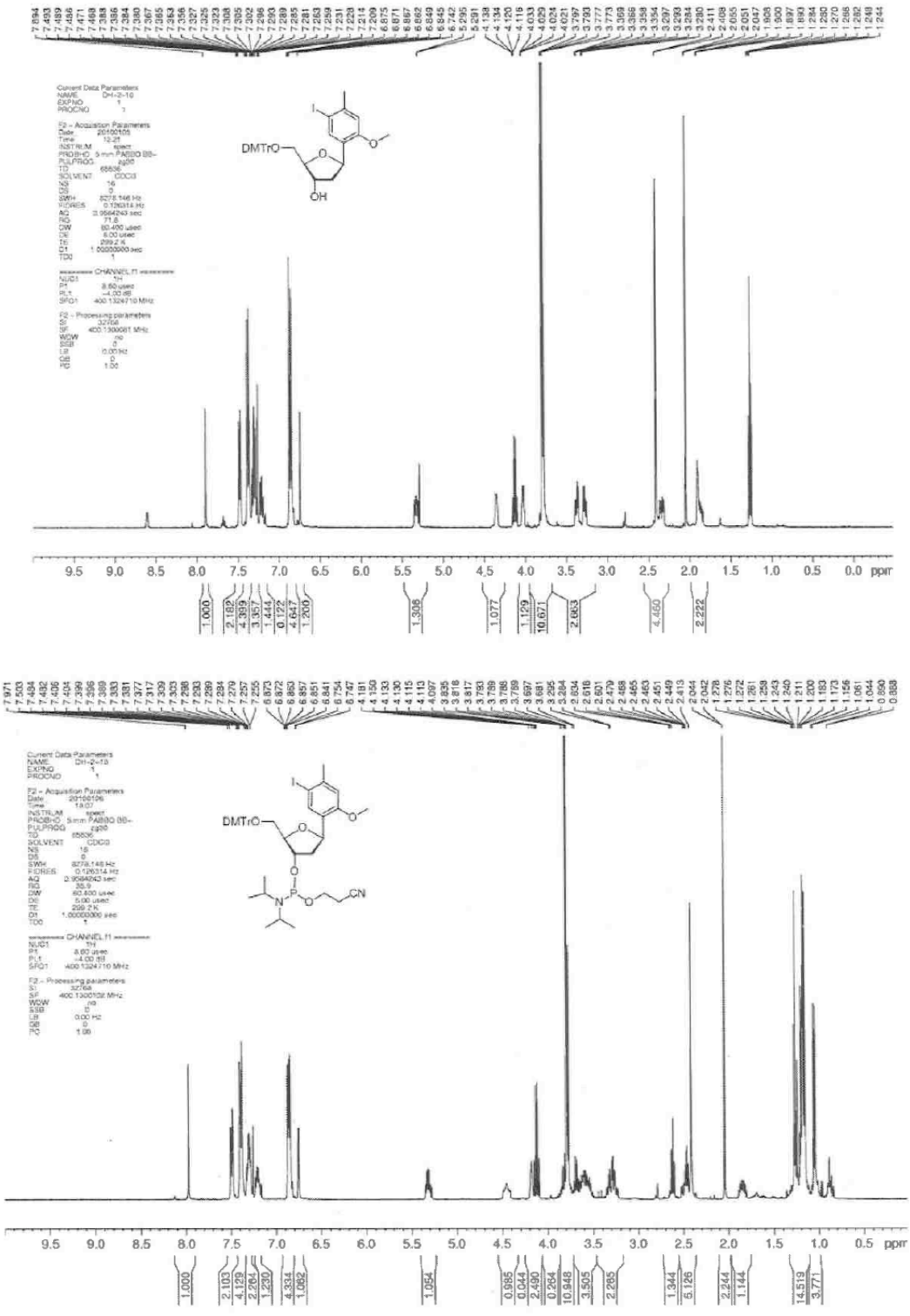
Supporting Information Figure 2. Sample autoradiogram of hydroxyl radical digestion of cross-linked DNA produced upon UV-irradiation of **16b**-**18b**. The strand opposite the C-nucleotide is 5'-^{32}P-labeled.



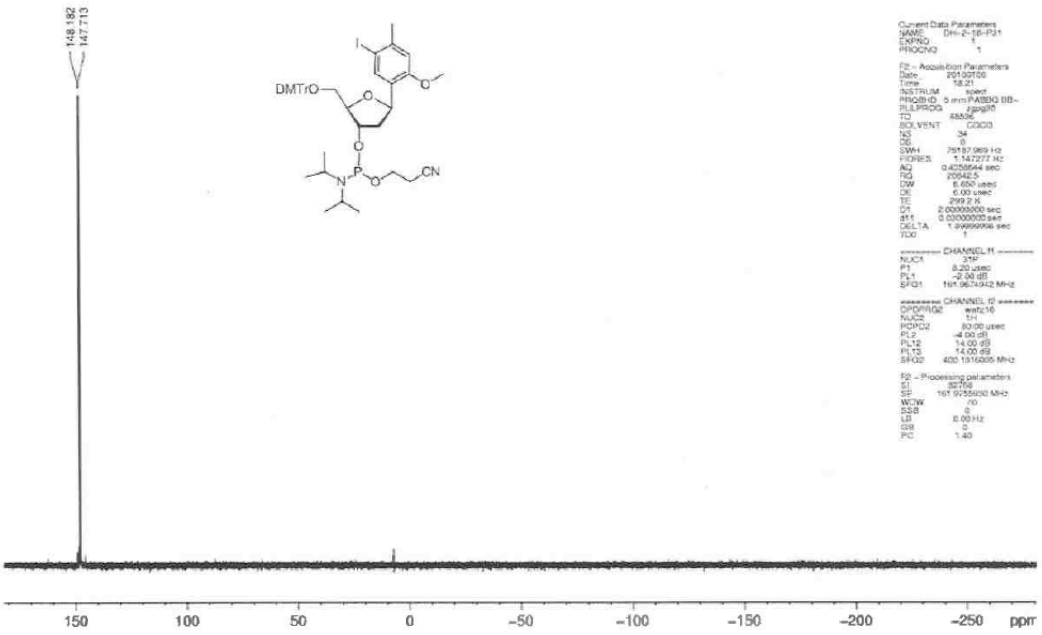
Supporting Information Figure 3. MALDI-TOF MS of interstrand cross-link products from irradiation of C-nucleotide containing duplexes. Top: from irradiation of **16b**. Calc'd mass: 15,293.0, Observed mass: 15,296.6. Bottom: from irradiation of **18b**. Calc'd mass: 15,279.0, Observed mass: 15,291.5.



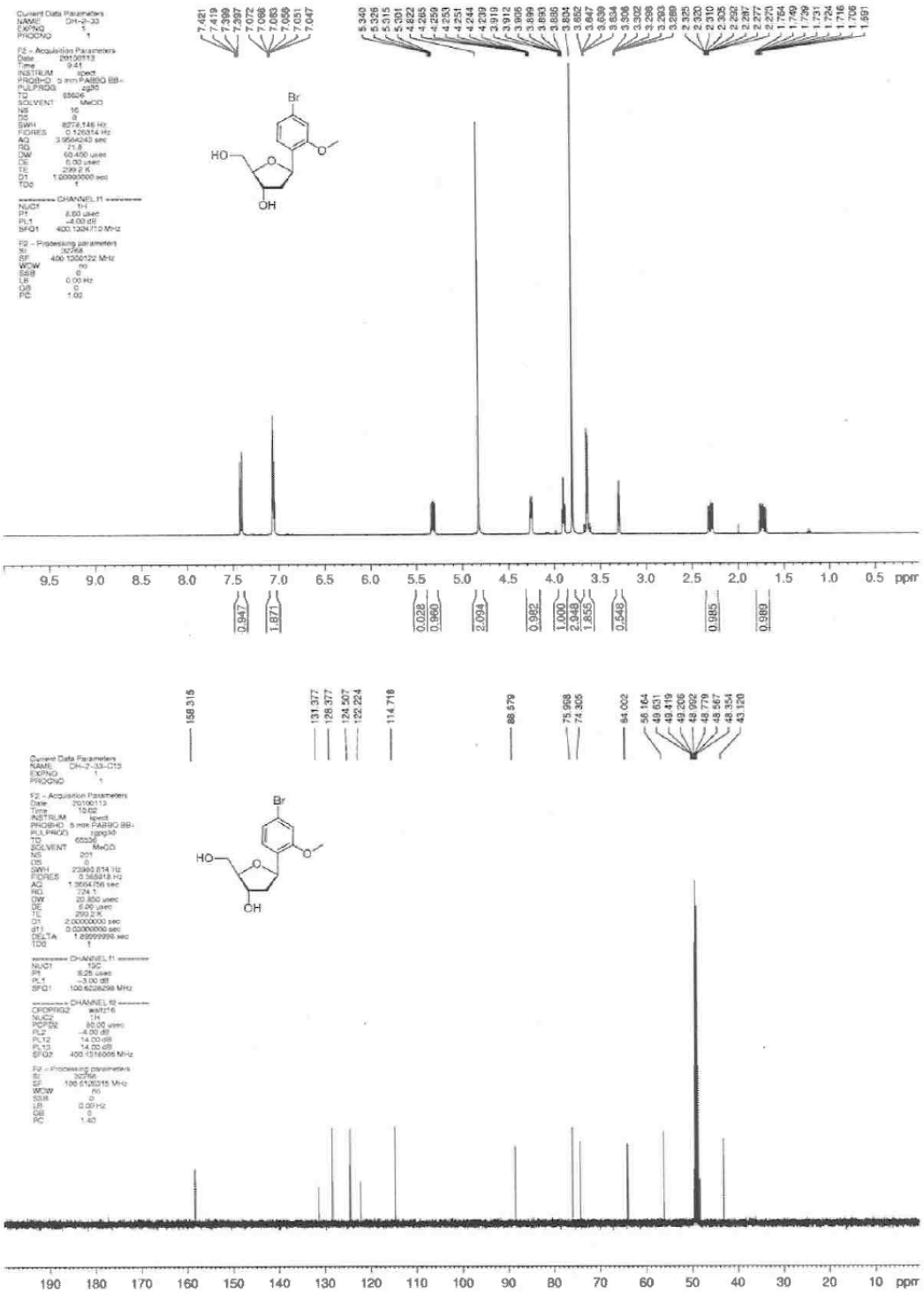
Supporting Information Figure 4. NMR spectra of known compounds used to prepare oligonucleotide **13**.



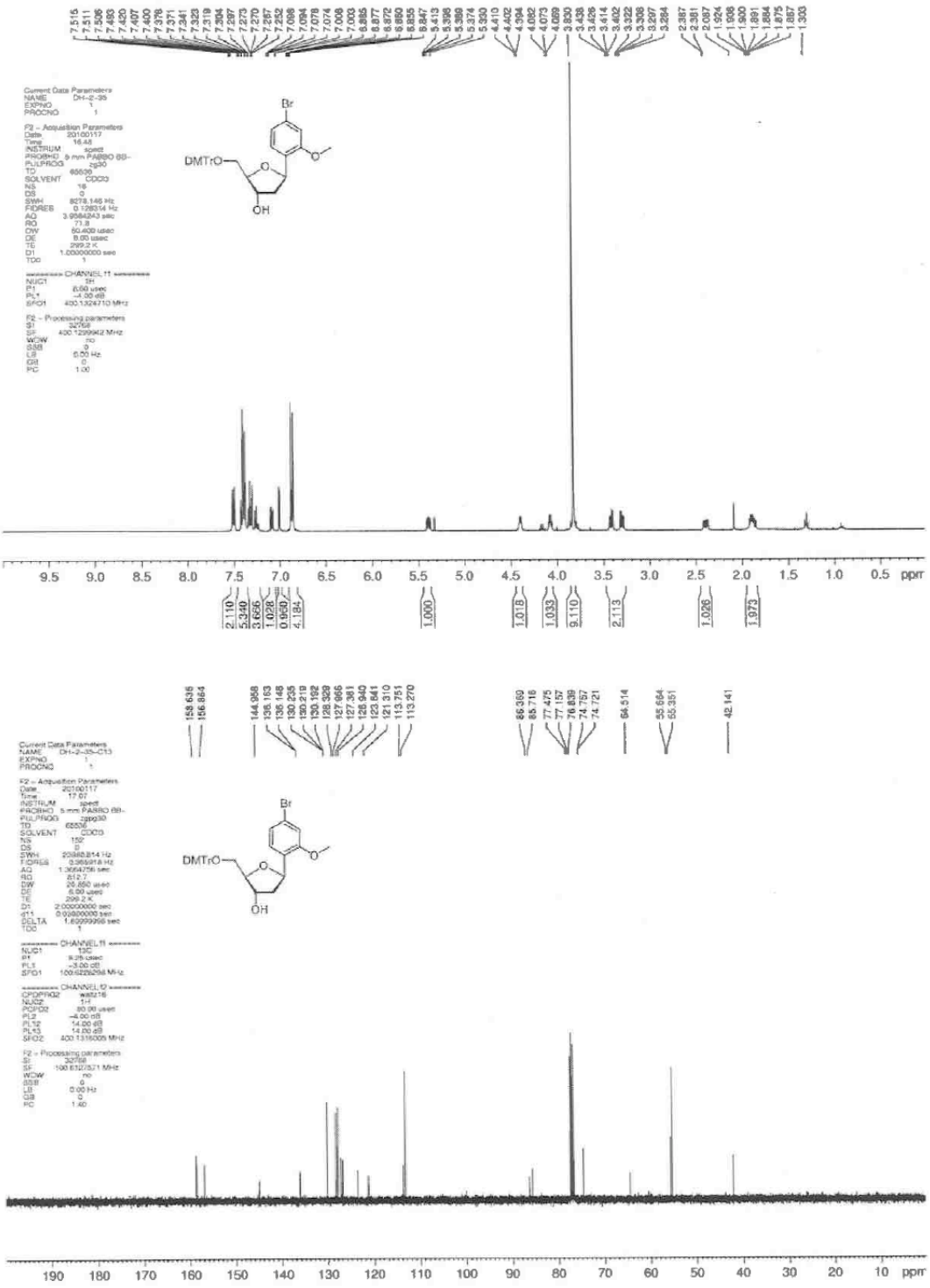
Supporting Information Figure 4 (continued). NMR spectra of known compounds used to prepare oligonucleotide **13**.



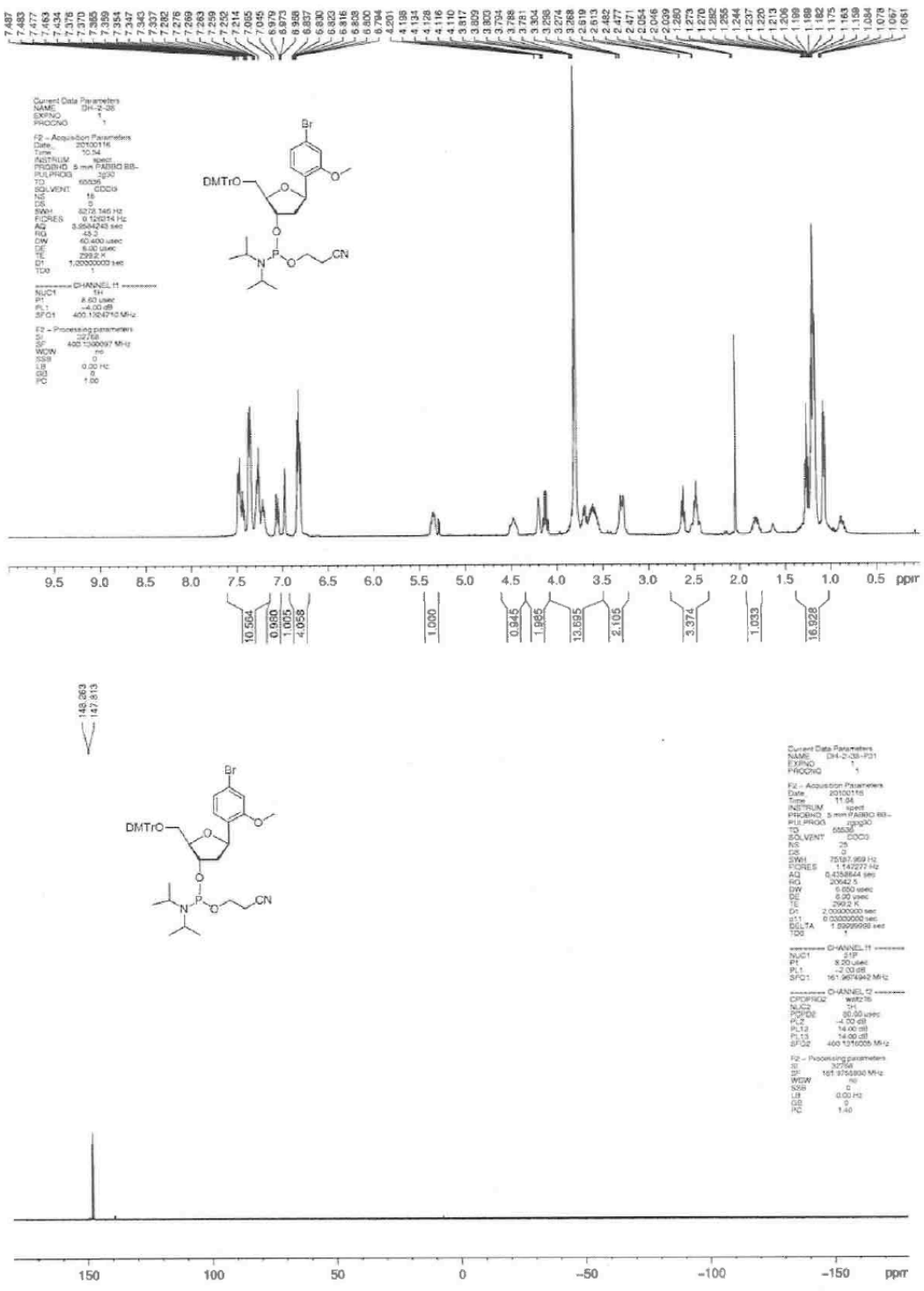
Supporting Information Figure 4 (continued). NMR spectra of known compounds used to prepare oligonucleotide **13**.



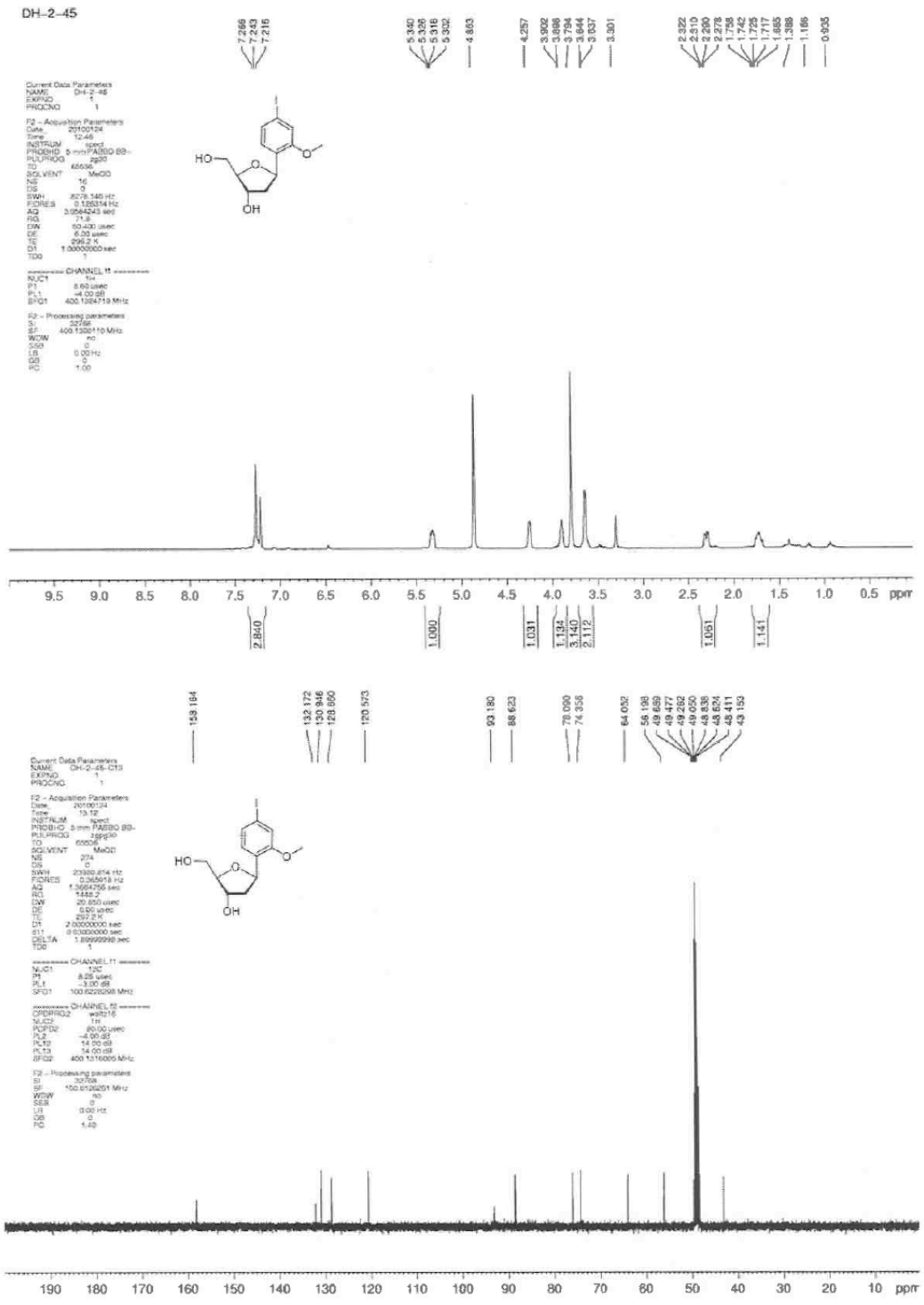
Supporting Information Figure 5. NMR spectra of **5**. Top: ^{1}H NMR Bottom: ^{13}C NMR.



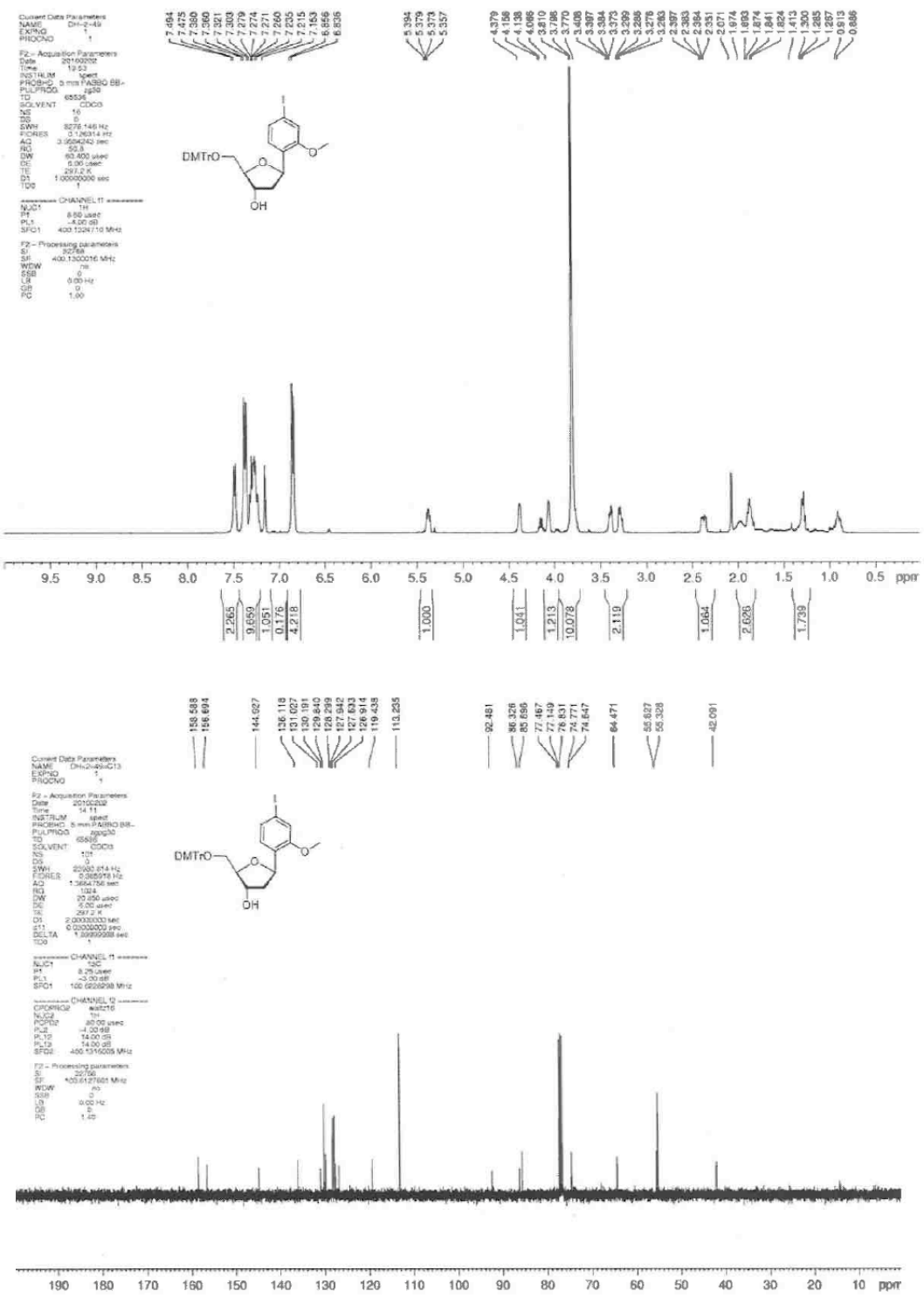
Supporting Information Figure 6. NMR spectra of dimethoxytritylated **5**. Top: ^{1}H NMR Bottom: ^{13}C NMR.



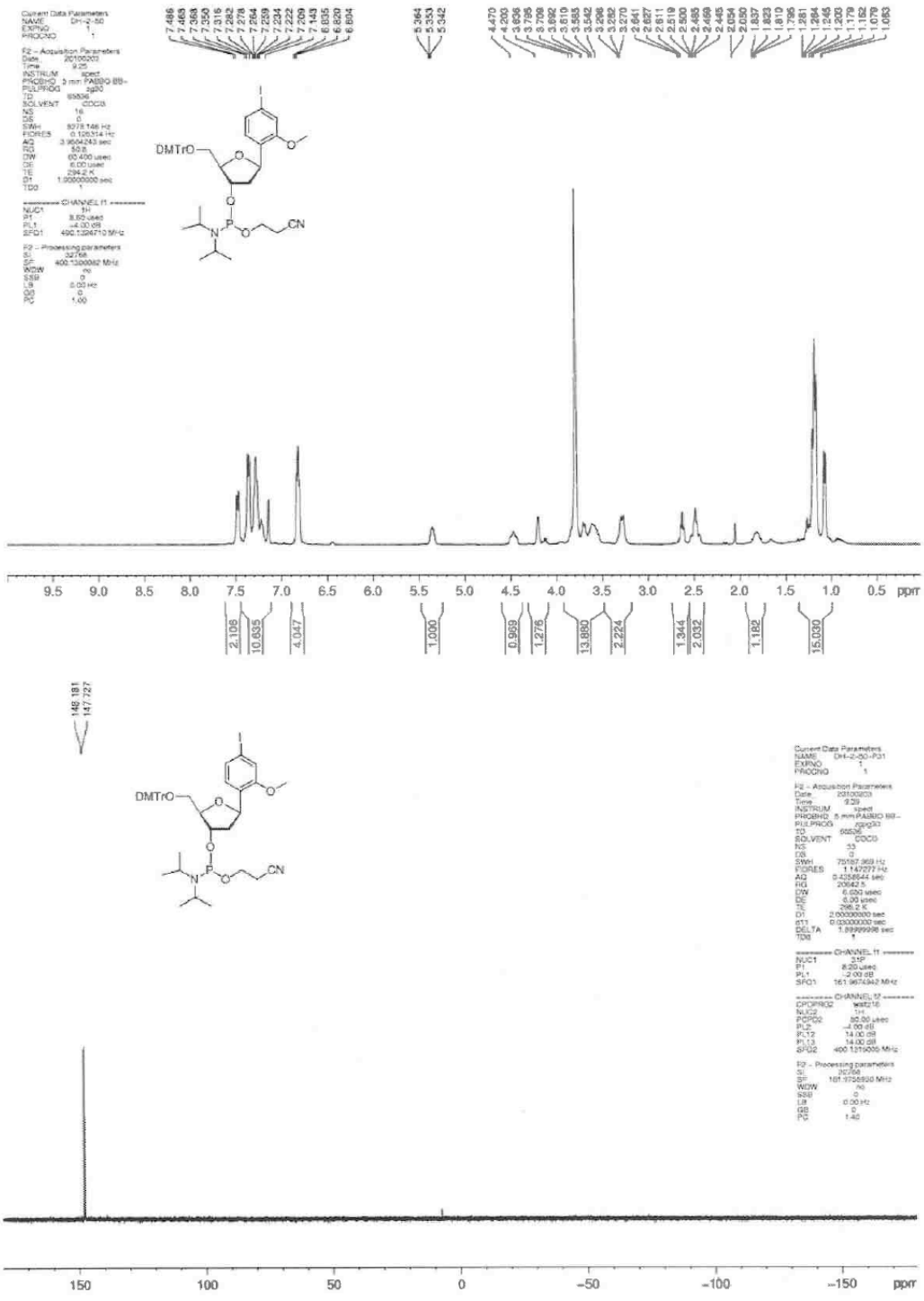
Supporting Information Figure 7. NMR spectra of **10a**. Top: ^{1}H NMR Bottom: ^{31}P NMR.



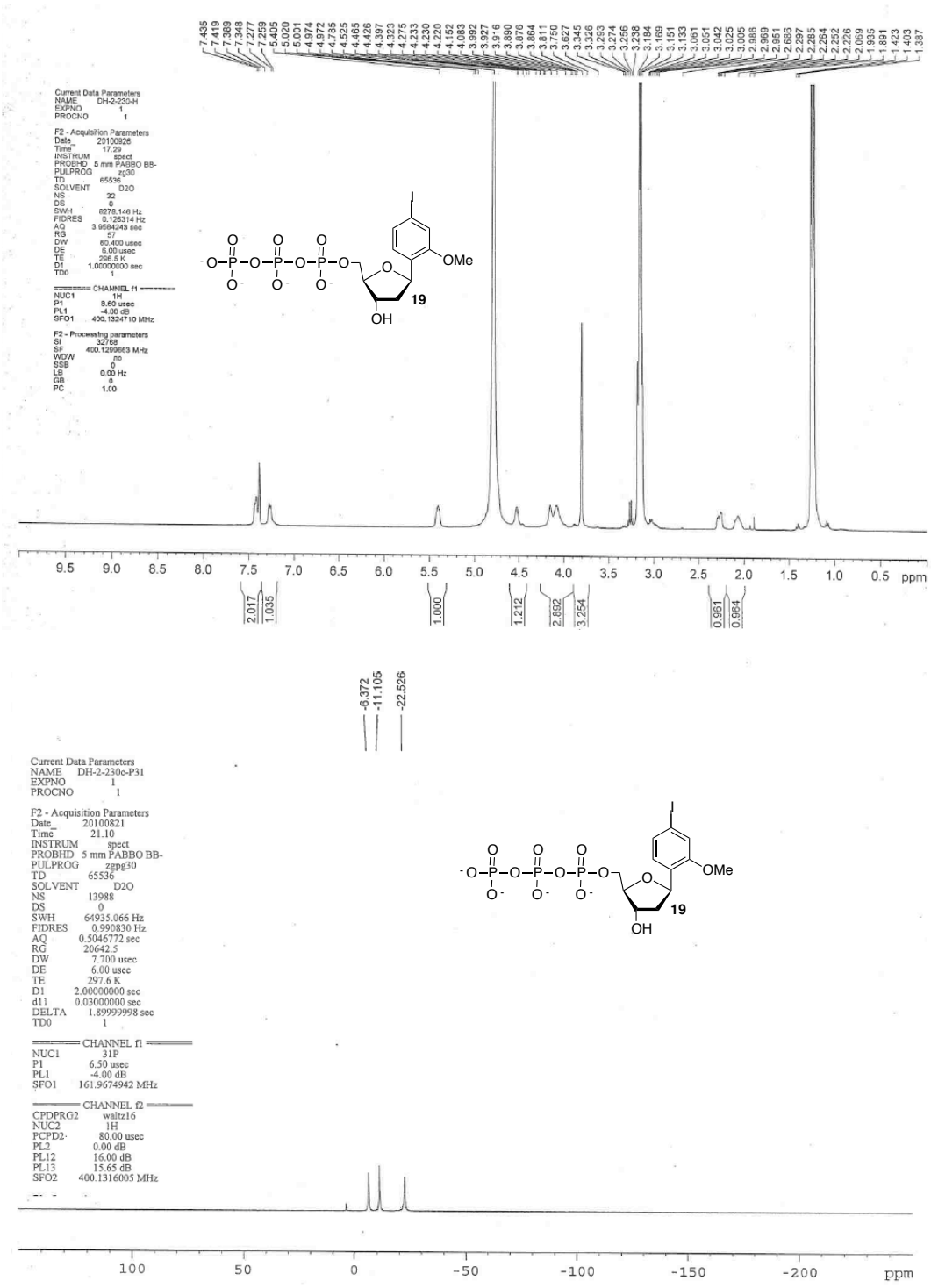
Supporting Information Figure 8. NMR spectra of **6**. Top: ^{1}H NMR Bottom: ^{13}C NMR.



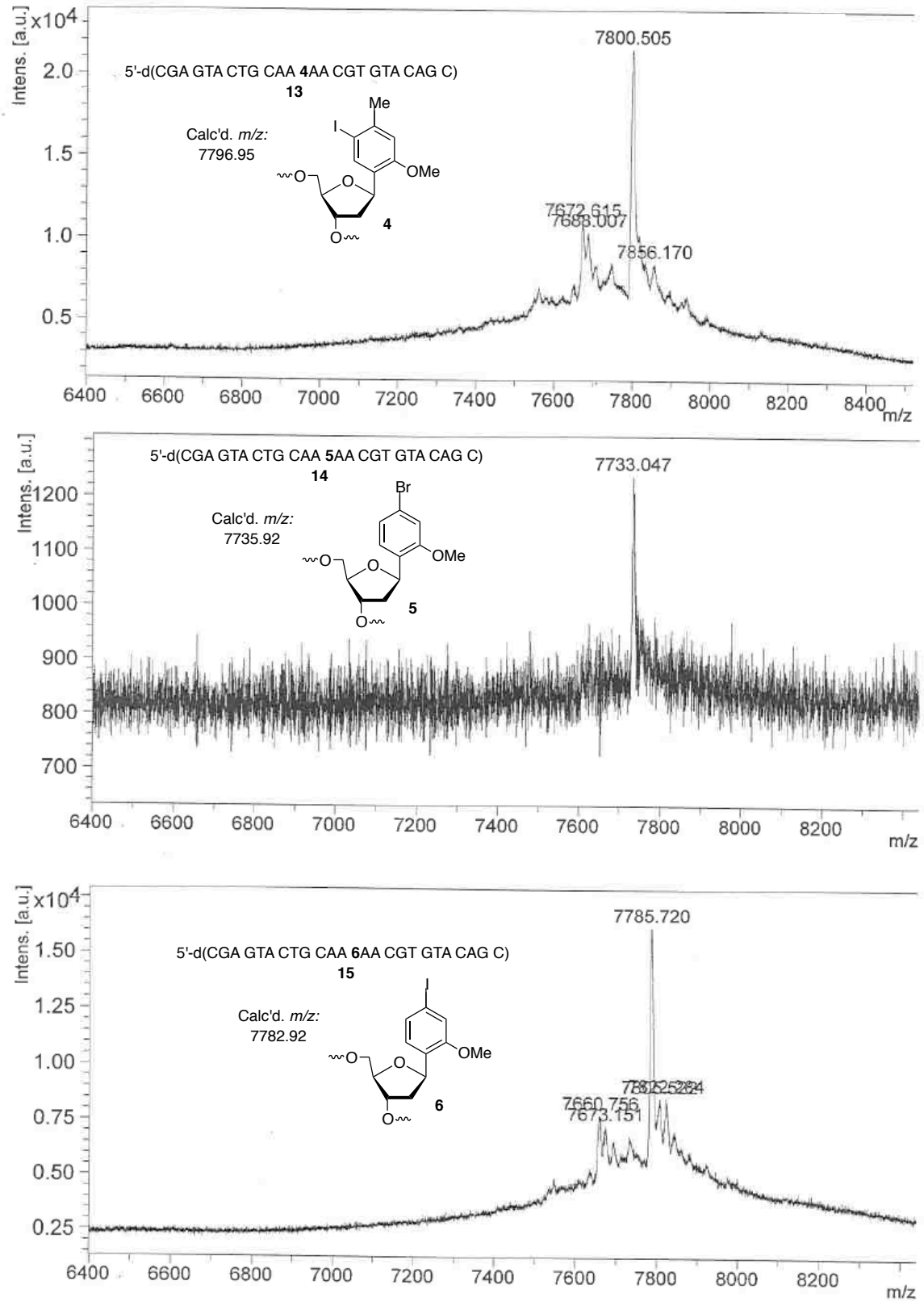
Supporting Information Figure 9. NMR spectra of dimethoxytritylated **6**. Top: ^{1}H NMR Bottom: ^{13}C NMR.



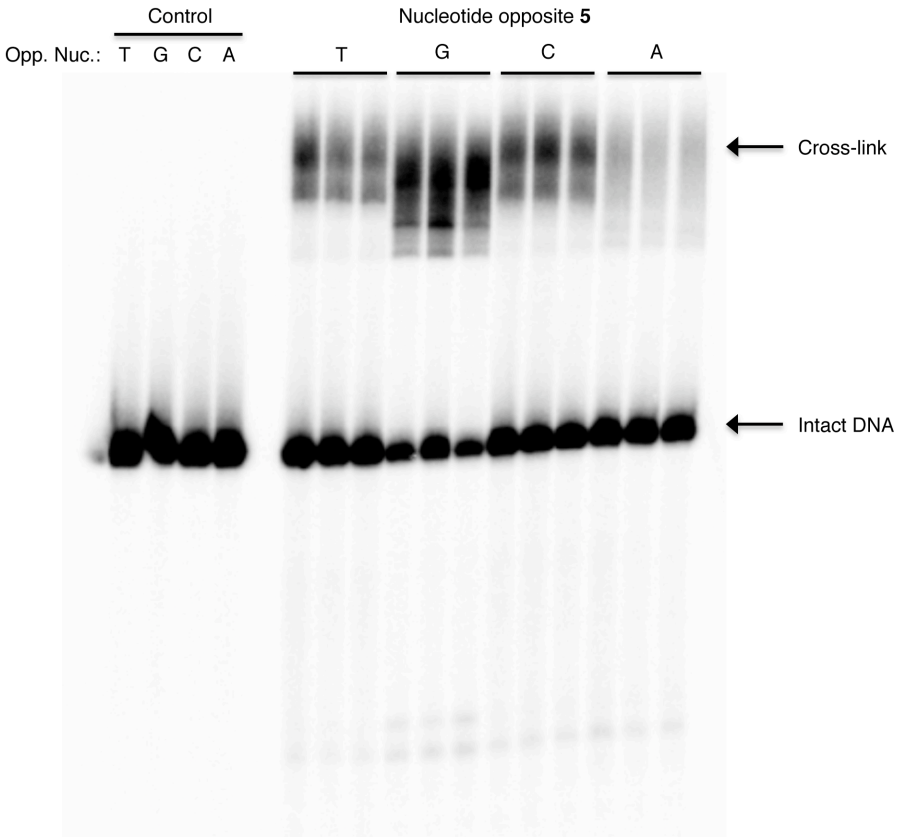
Supporting Information Figure 10. NMR spectra of **10b**. Top: ^{1}H NMR Bottom: ^{31}P NMR.



Supporting Information Figure 11. NMR spectra of **19**. Top: ^{1}H NMR Bottom: ^{31}P NMR.



Supporting Information Figure 12. MALDI-TOF MS of oligonucleotides containing C-nucleotides (**13**-**15**).



Supporting Information Figure 13. Sample ICL gel upon UV-irradiation of 5'-^{32}-P-**17a-d**. Controls correspond to otherwise identical duplex in which thymidine is substituted for **5**