

# Supporting Information: DNA Damage and Interstrand Cross-link Formation Upon Irradiation of Aryl Iodide C-Nucleotide Analogues

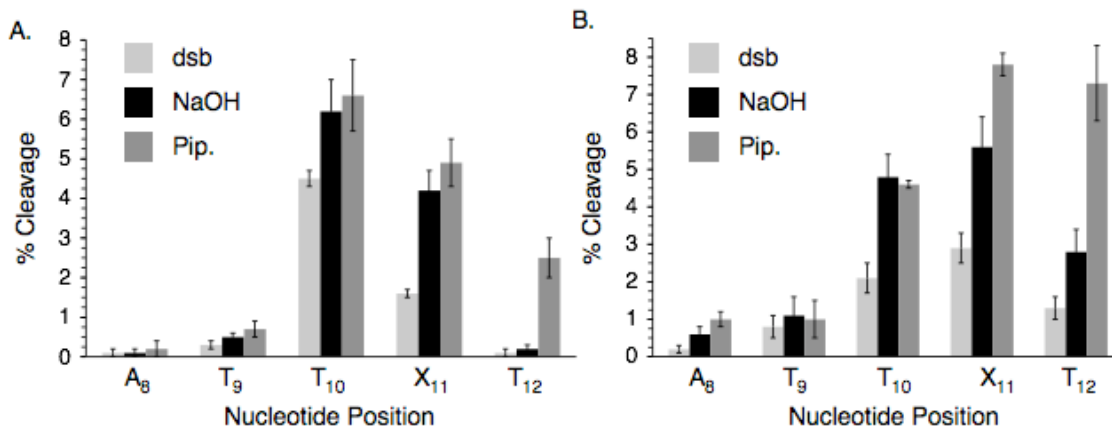
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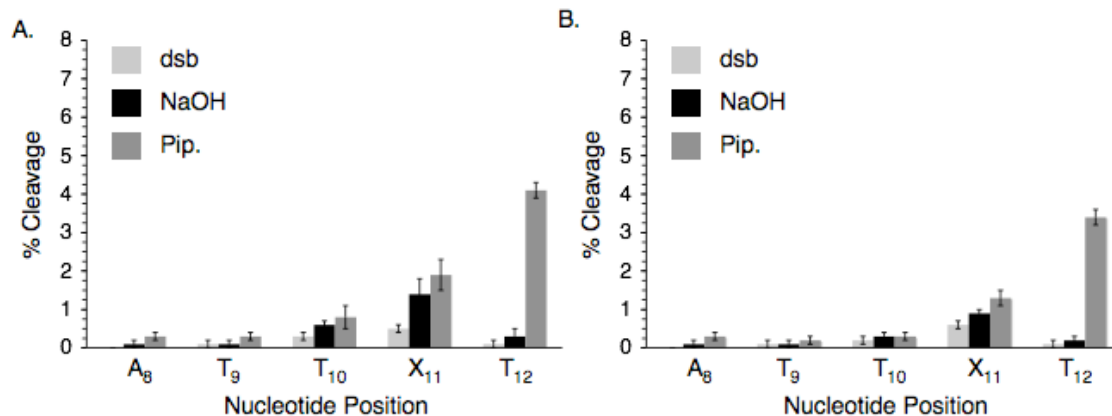
mgreenberg@jhu.edu

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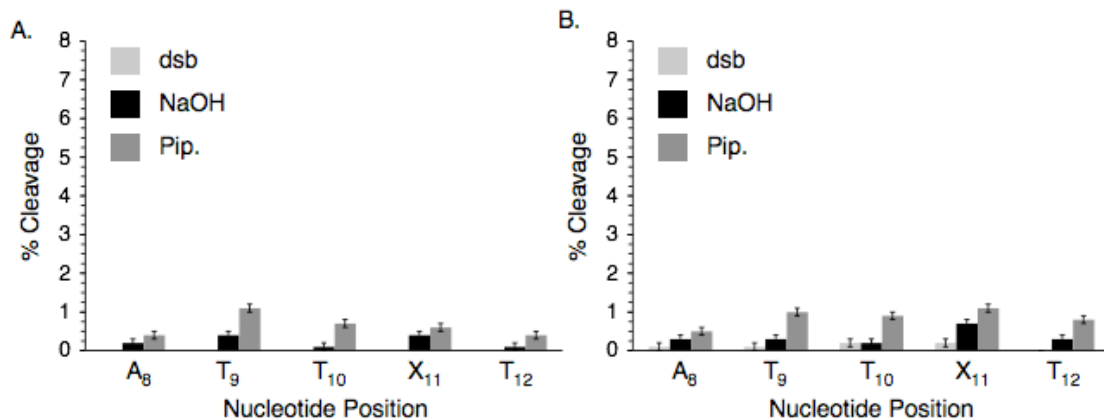
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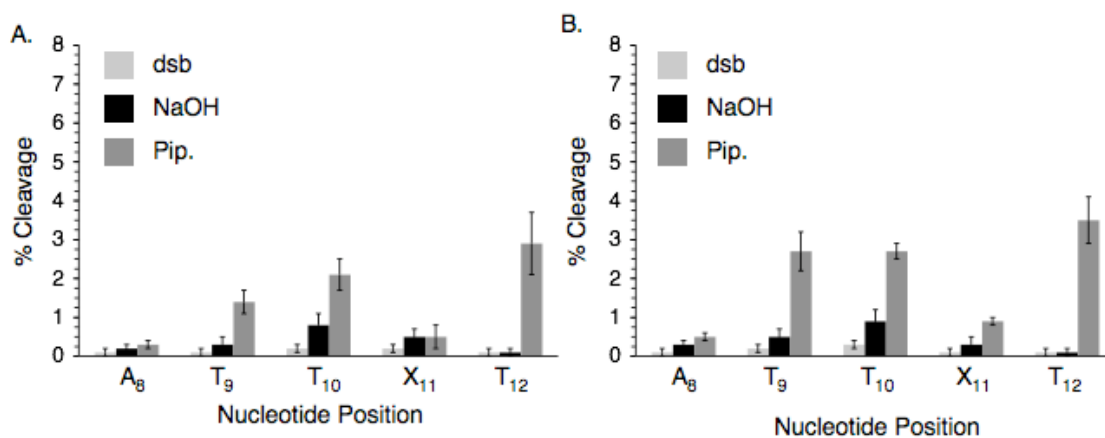
**Supporting Information Figure 1.** Direct strand scission and alkali-labile lesion formation when duplex DNA (**11**) containing **IT** is photolyzed. A. Anaerobic photolysis of 3'-<sup>32</sup>P-**11**. B. Aerobic photolysis of 3'-<sup>32</sup>P-**11**. dsb, direct strand breaks; NaOH, photolysate treated with 0.1 M NaOH at 37°C; Pip., photolysate treated with 1.0 M piperidine at 90°C.



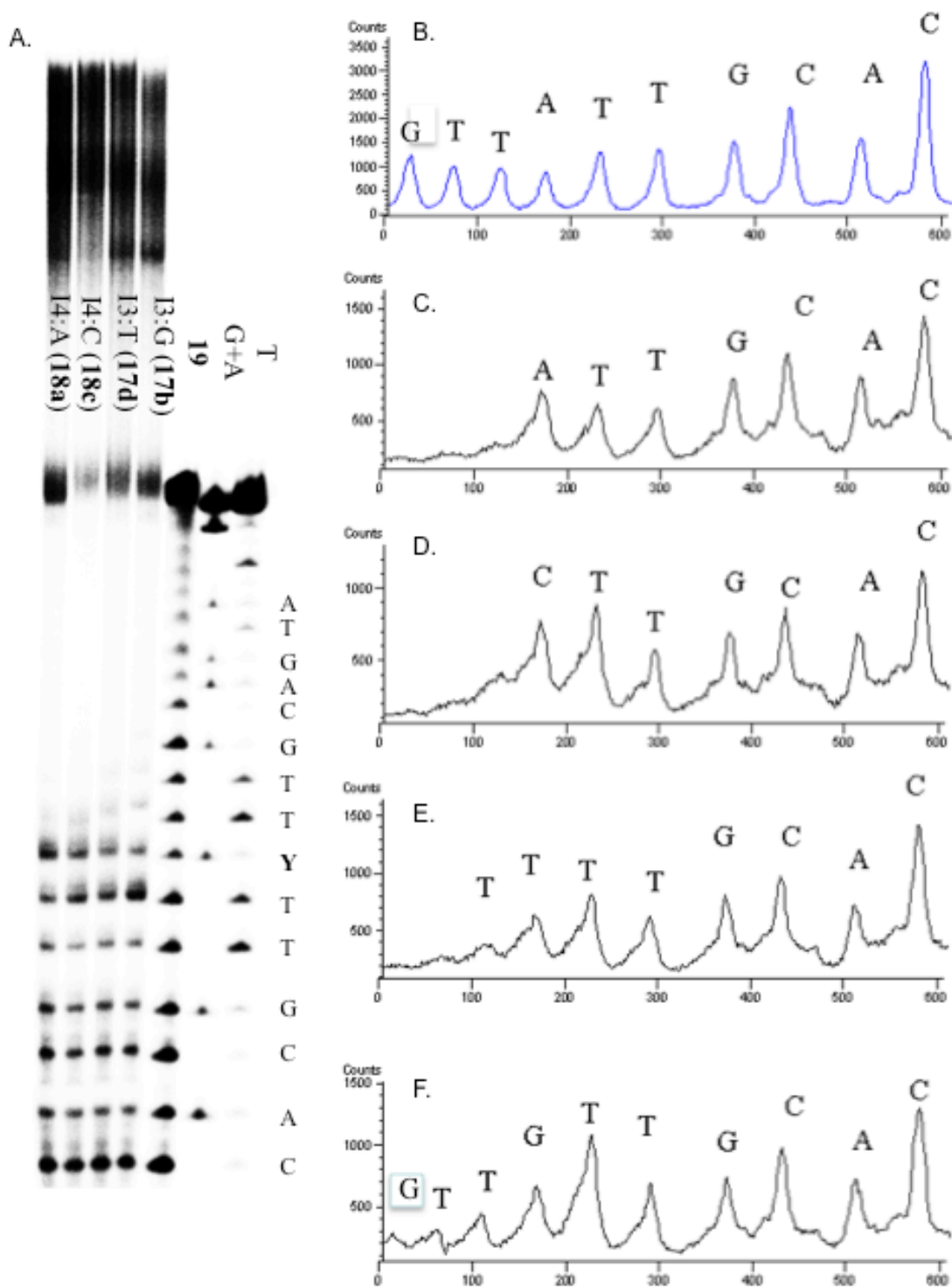
**Supporting Information Figure 2.** Direct strand scission and alkali-labile lesion formation when duplex DNA (**12**) containing **I2** is photolyzed. A. Anaerobic photolysis of 3'-<sup>32</sup>P-**12**. B. Aerobic photolysis of 3'-<sup>32</sup>P-**12**. dsb, direct strand breaks; NaOH, photolysate treated with 0.1 M NaOH at 37°C; Pip., photolysate treated with 1.0 M piperidine at 90°C.



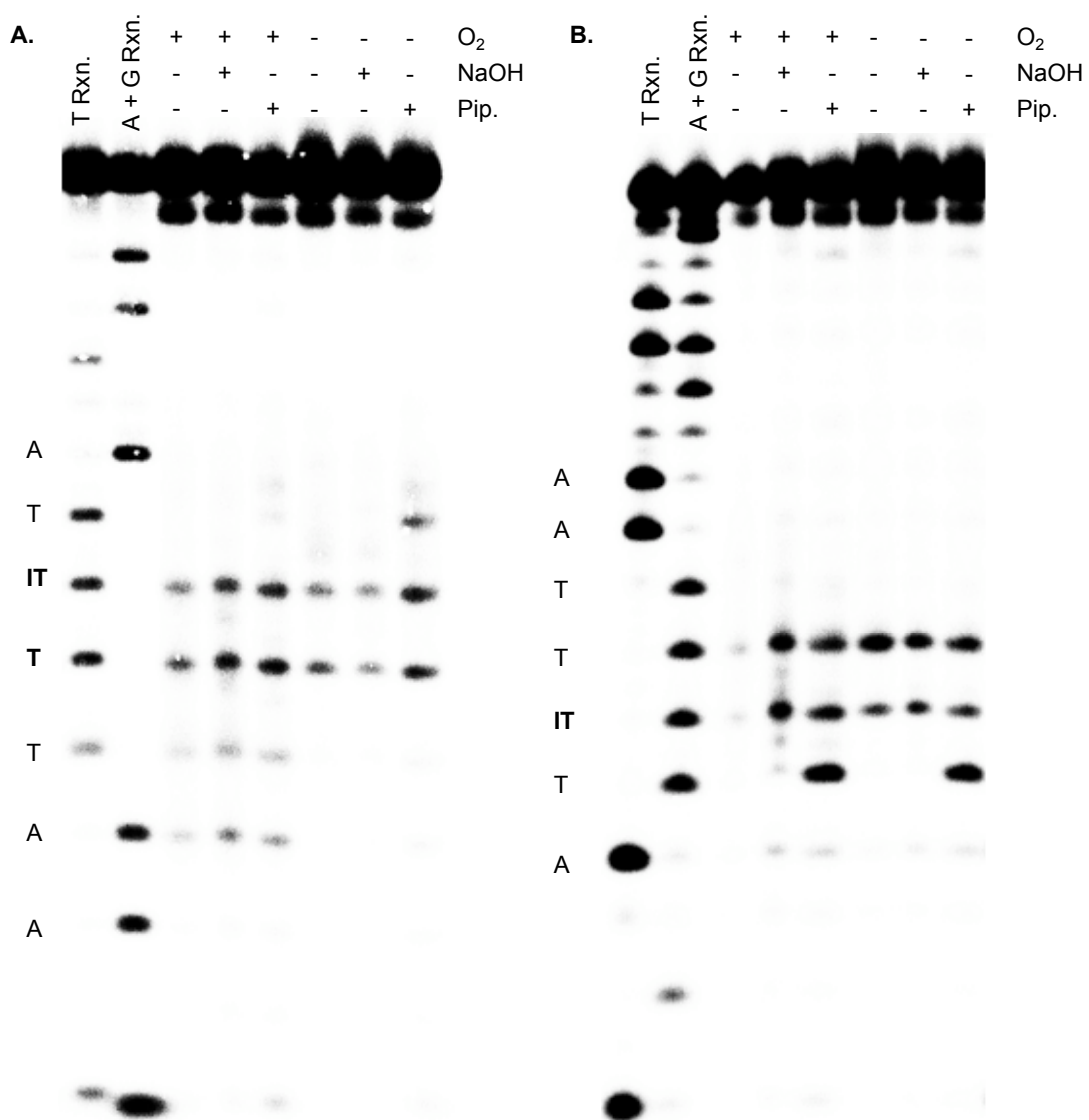
**Supporting Information Figure 3.** Direct strand scission and alkali-labile lesion formation when duplex DNA (**14**) containing **I4** is photolyzed. A. Anaerobic photolysis of 3'-<sup>32</sup>P-**14**. B. Aerobic photolysis of 3'-<sup>32</sup>P-**14**. dsb, direct strand breaks; NaOH, photolysate treated with 0.1 M NaOH at 37°C; Pip., photolysate treated with 1.0 M piperidine at 90°C.



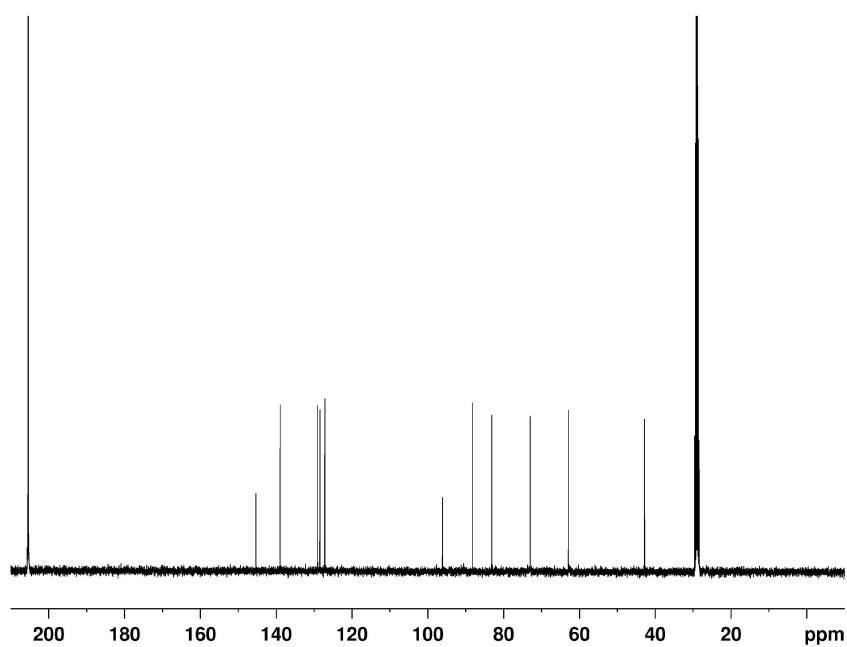
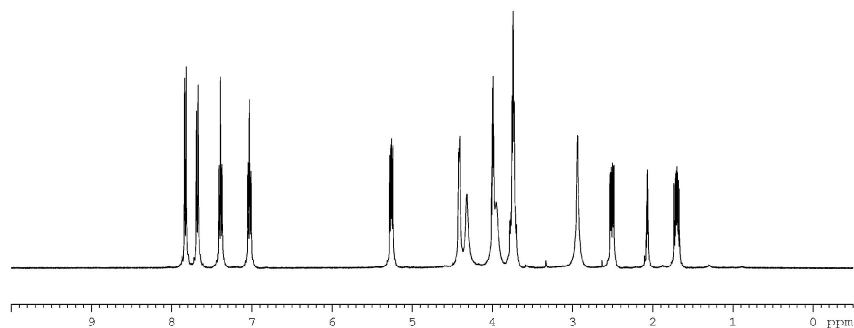
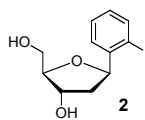
**Supporting Information Figure 4.** Direct strand scission and alkali-labile lesion formation when duplex DNA (**13**) containing **I3** is photolyzed. A. Anaerobic photolysis of 3'-<sup>32</sup>P-**13**. B. Aerobic photolysis of 3'-<sup>32</sup>P-**13**. dsb, direct strand breaks; NaOH, photolysate treated with 0.1 M NaOH at 37°C; Pip., photolysate treated with 1.0 M piperidine at 90°C.



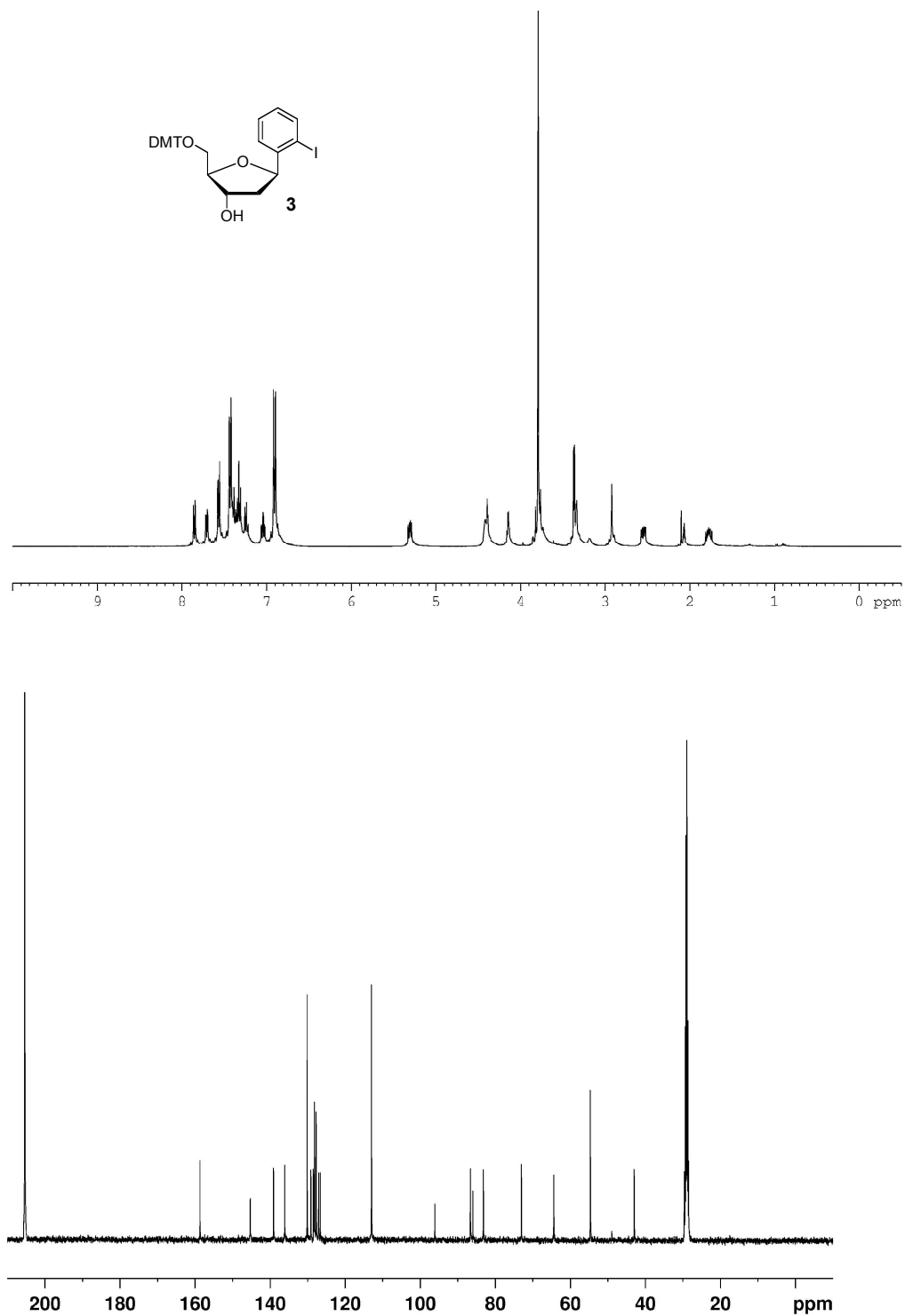
**Supporting Information Figure 5.** Hydroxyl radical digestion of cross-linked DNA produced upon UV-irradiation. A. Sample autoradiogram of 5'-<sup>32</sup>P-labeled cross-links in which the strand opposite the aryl iodide nucleotide analogue is radiolabeled. B. Control, noncross-linked DNA (19) C. 18a D. 18c E. 17d F. 17b.



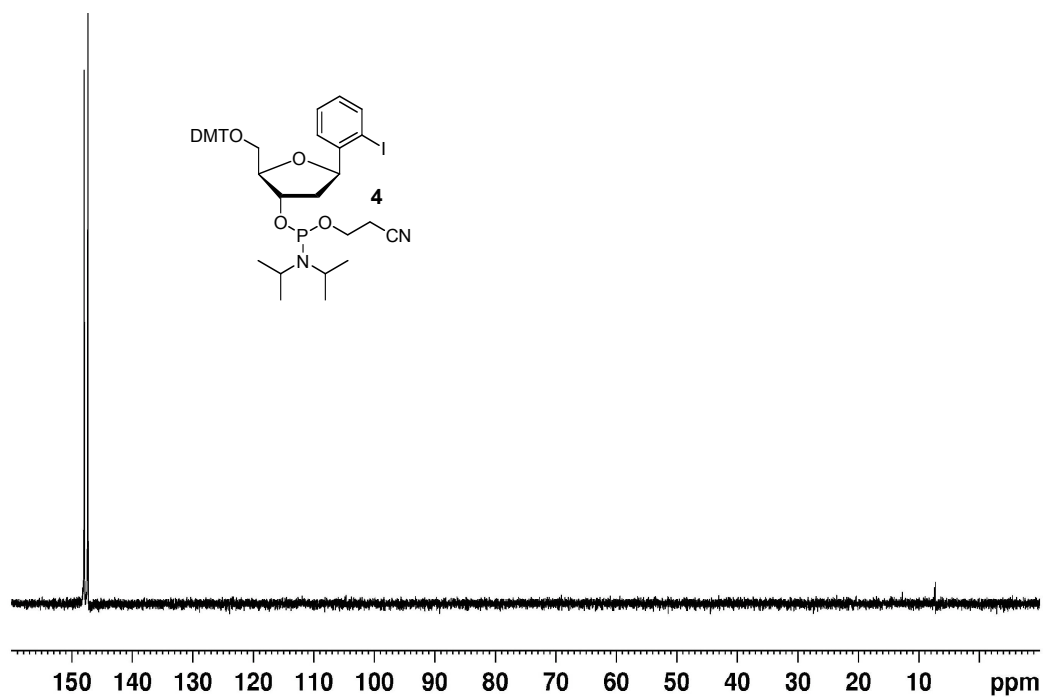
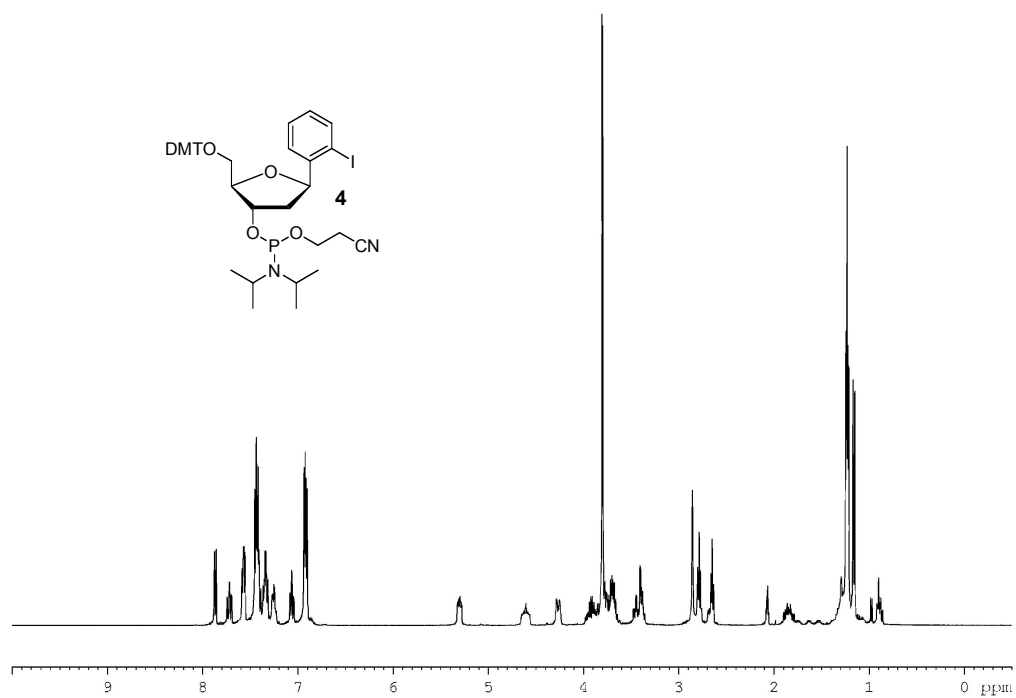
**Supporting Information Figure 6.** Sample autoradiograms from UV-irradiation of IT in 11. A. 5'-<sup>32</sup>P-11. B. 3'-<sup>32</sup>P-11.



Supporting Information Figure 7. NMR spectra of **2**. Top: <sup>1</sup>H NMR Bottom: <sup>13</sup>C NMR.

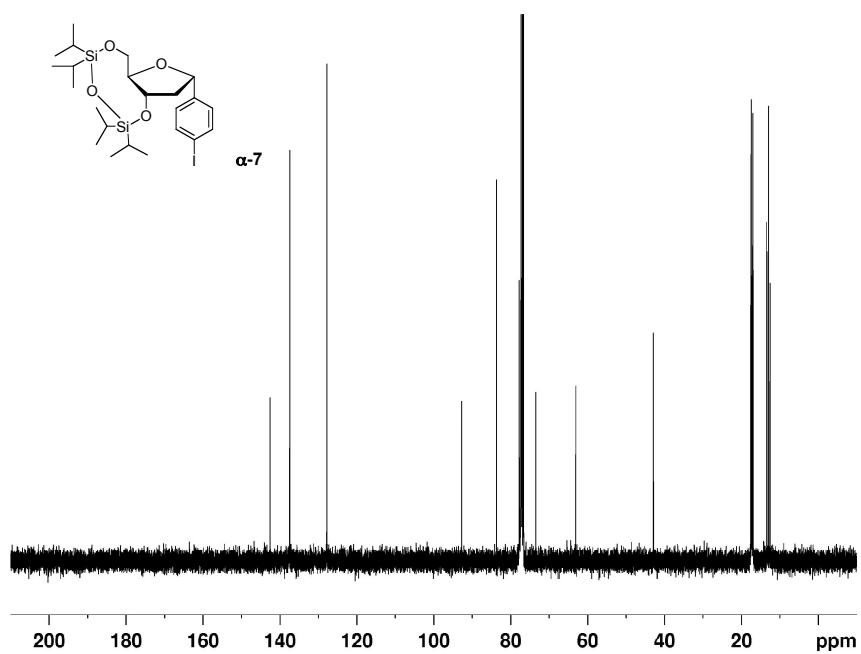
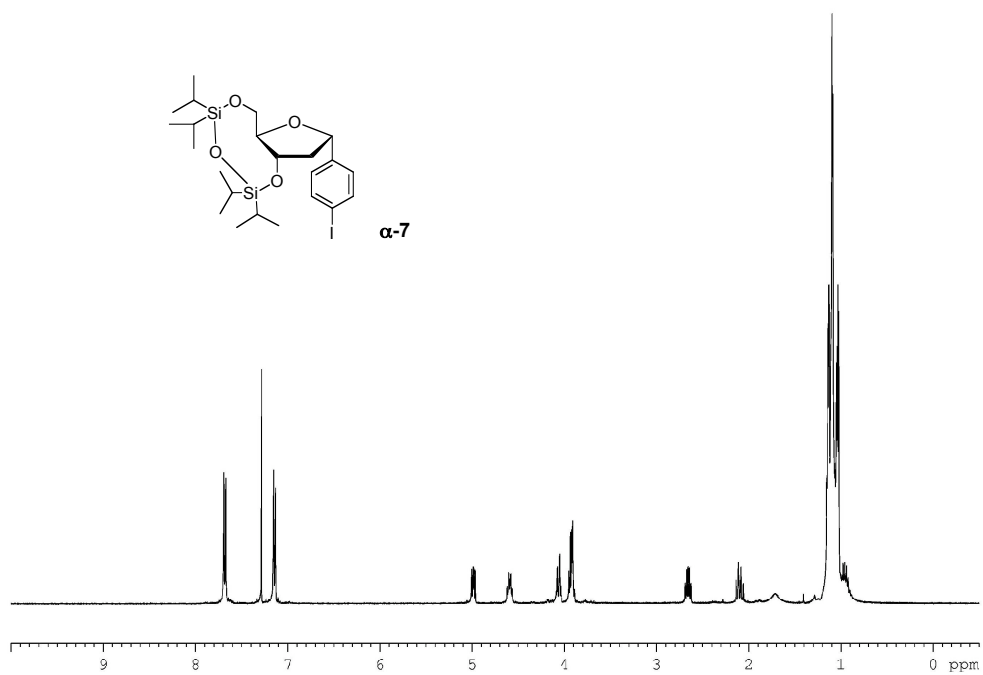


**Supporting Information Figure 8.** NMR spectra of **3**. Top:  $^1\text{H}$  NMR Bottom:  $^{13}\text{C}$  NMR.

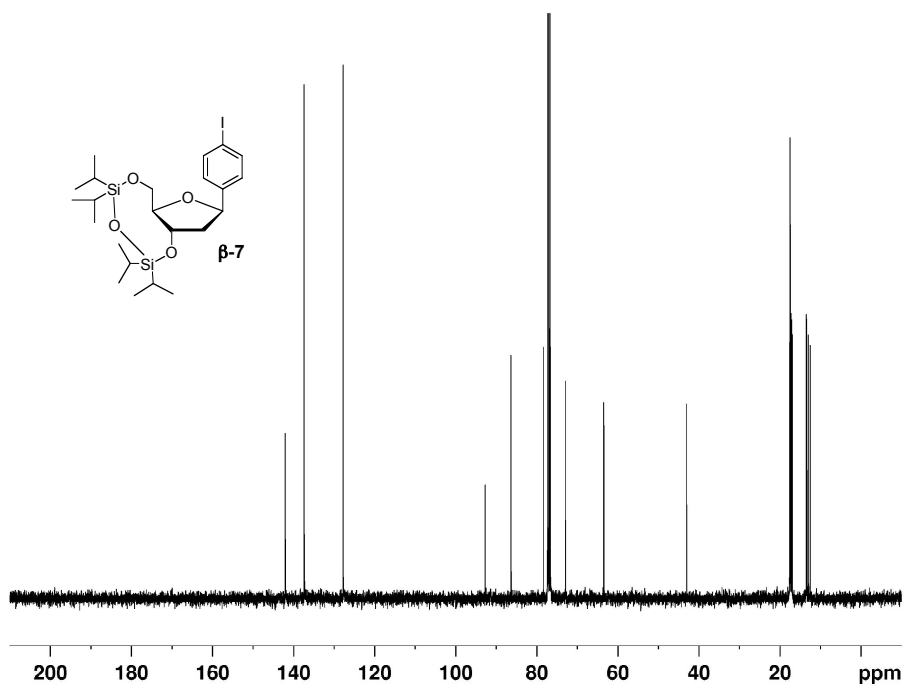
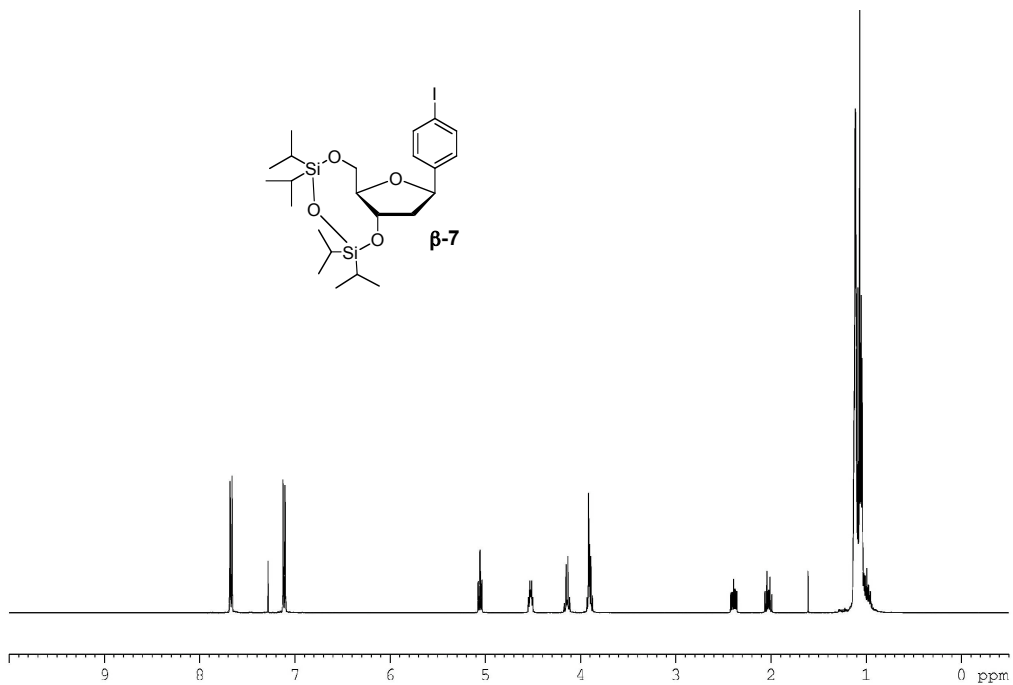


Supporting Information Figure 9. NMR spectra of **4**. Top:  $^1\text{H}$  NMR Bottom:  $^{31}\text{P}$  NMR.

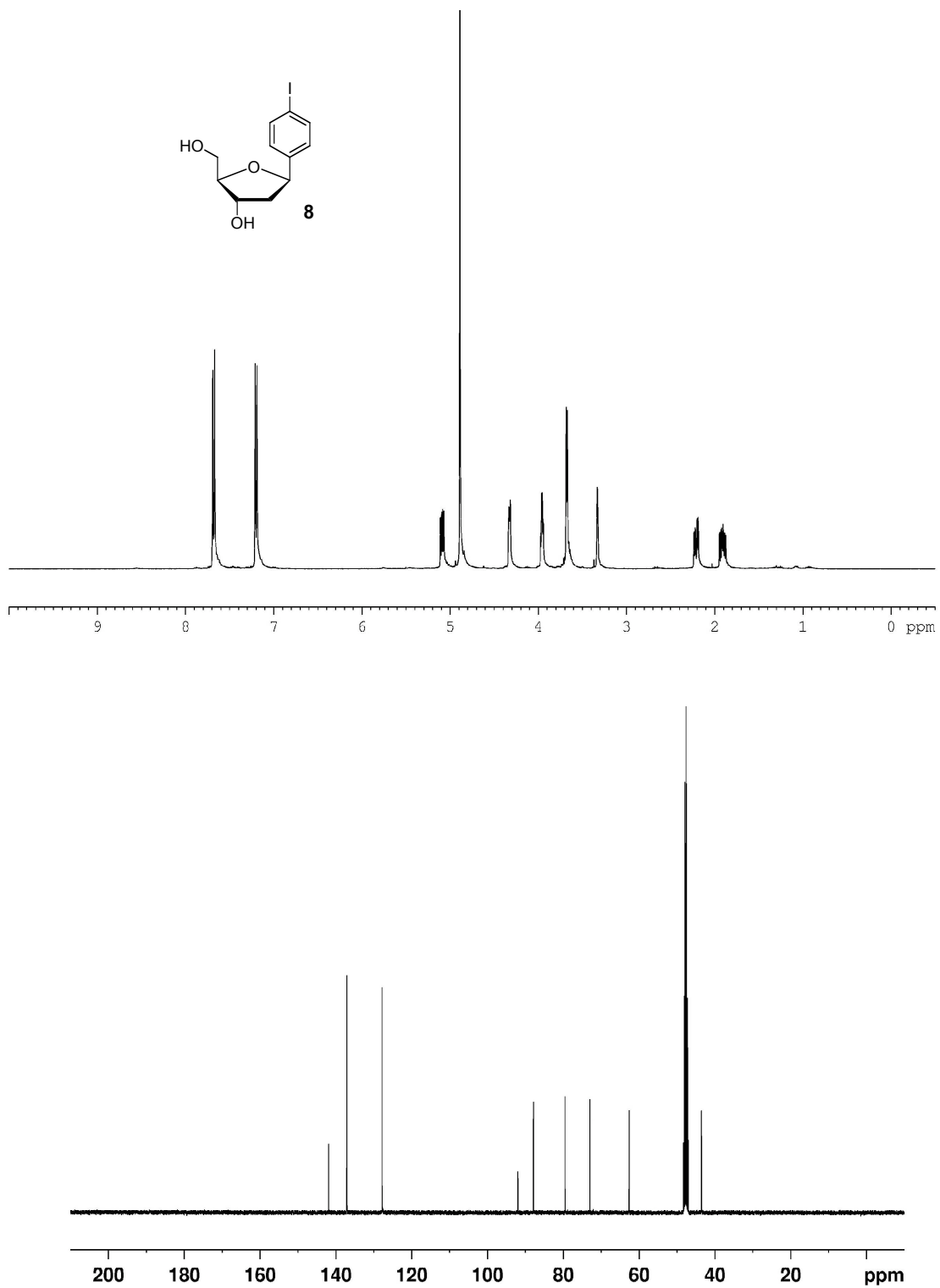




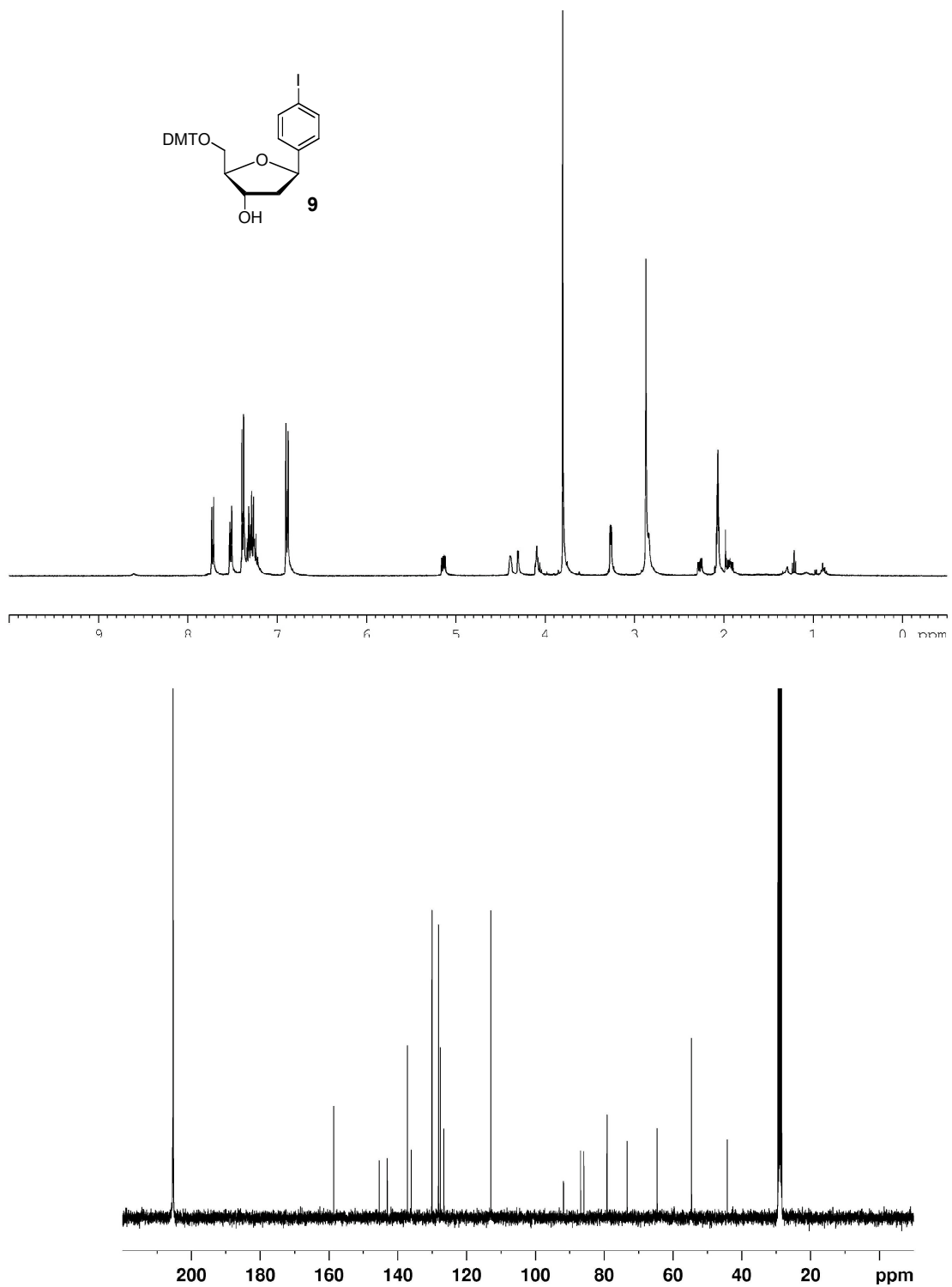
Supporting Information Figure 10. NMR spectra of  $\alpha$ -7. Top:  $^1\text{H}$  NMR Bottom:  $^{13}\text{C}$  NMR.



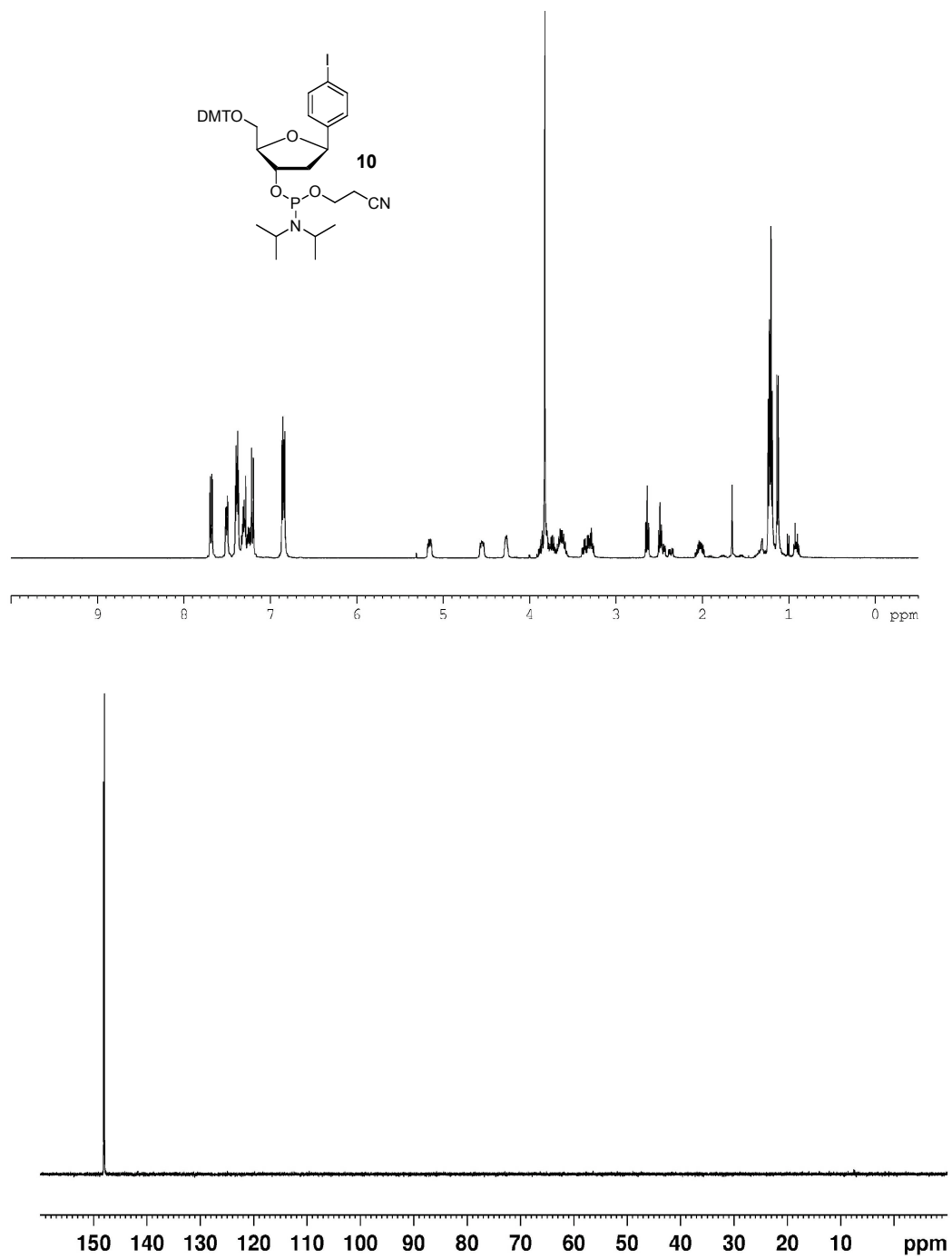
**Supporting Information Figure 11.** NMR spectra of  $\beta$ -7. Top:  $^1\text{H NMR}$  Bottom:  $^{13}\text{C NMR}$ .



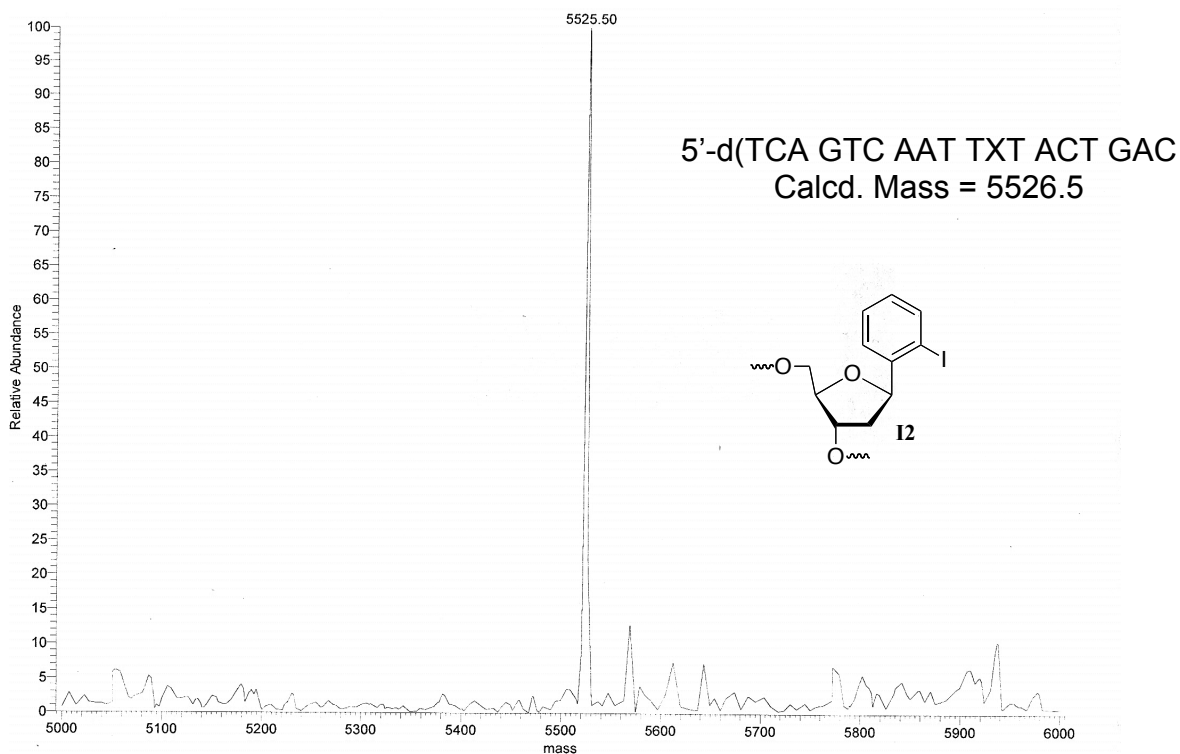
Supporting Information Figure 12. NMR spectra of **8**. Top:  $^1\text{H}$  NMR Bottom:  $^{13}\text{C}$  NMR.



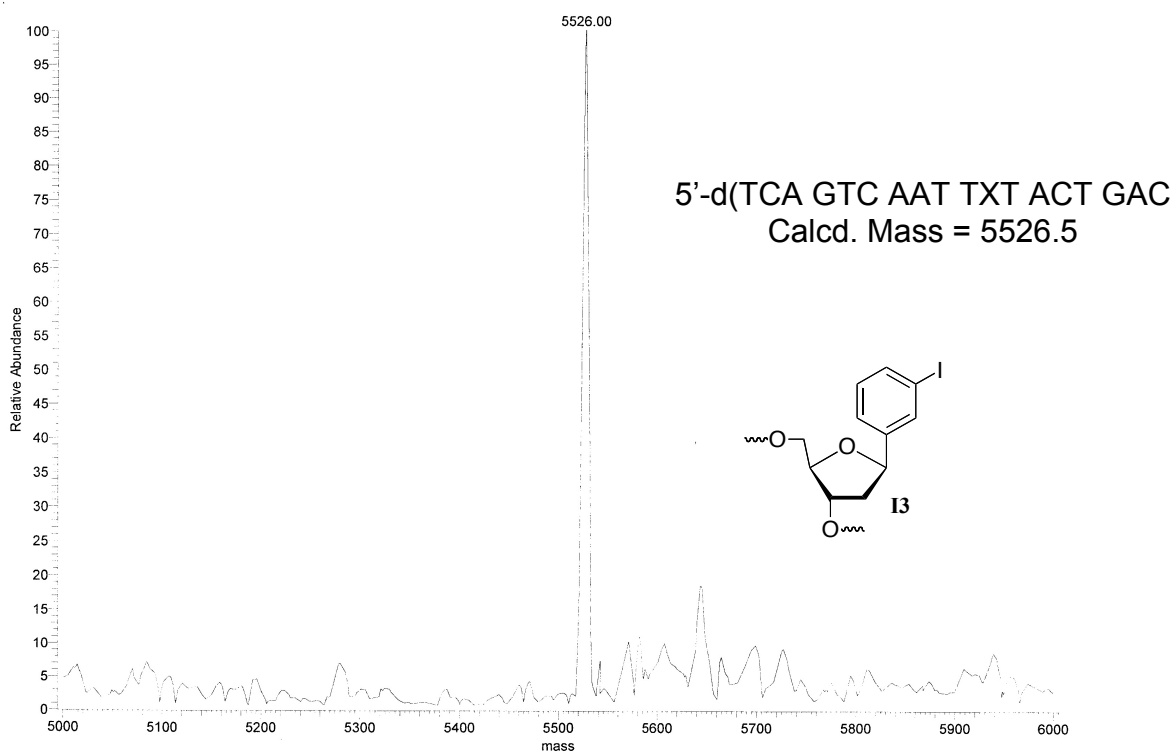
Supporting Information Figure 13. NMR spectra of **9**. Top:  $^1\text{H}$  NMR Bottom:  $^{13}\text{C}$  NMR.



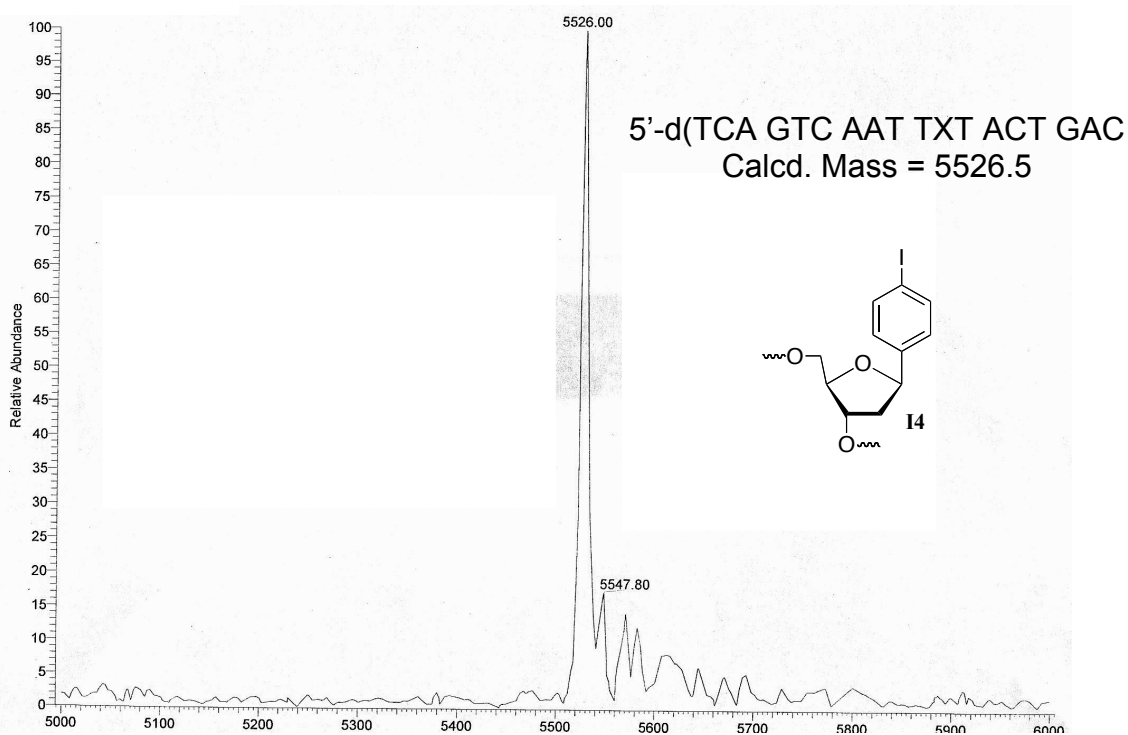
**Supporting Information Figure 14.** NMR spectra of **10**. Top: <sup>1</sup>H NMR Bottom: <sup>31</sup>P NMR.



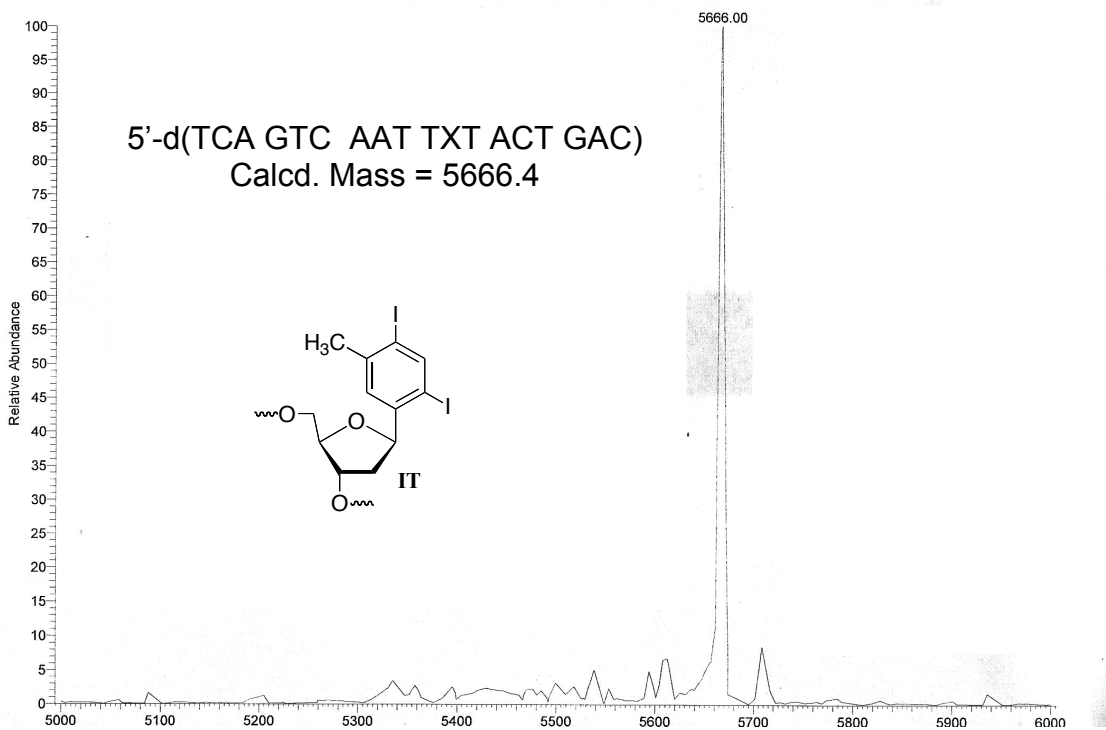
Supporting Information Figure 15. ESI-MS of 18mer containing **I2**.



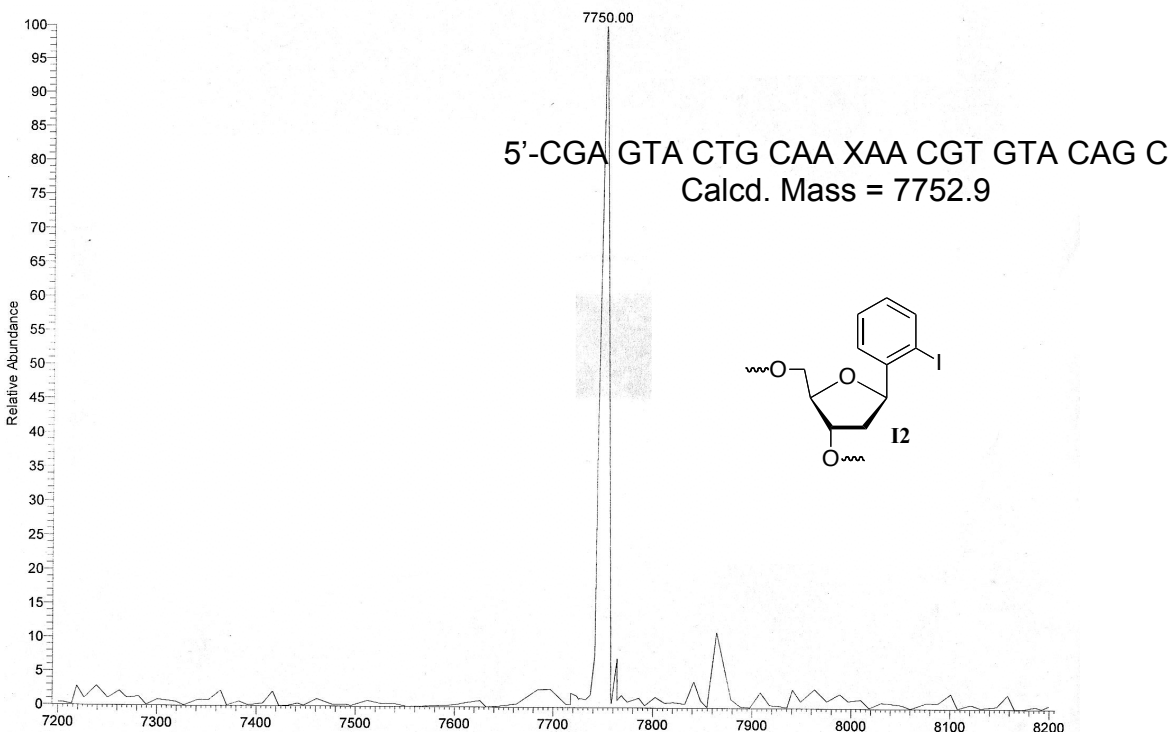
Supporting Information Figure 16. ESI-MS of 18mer containing **I3**.



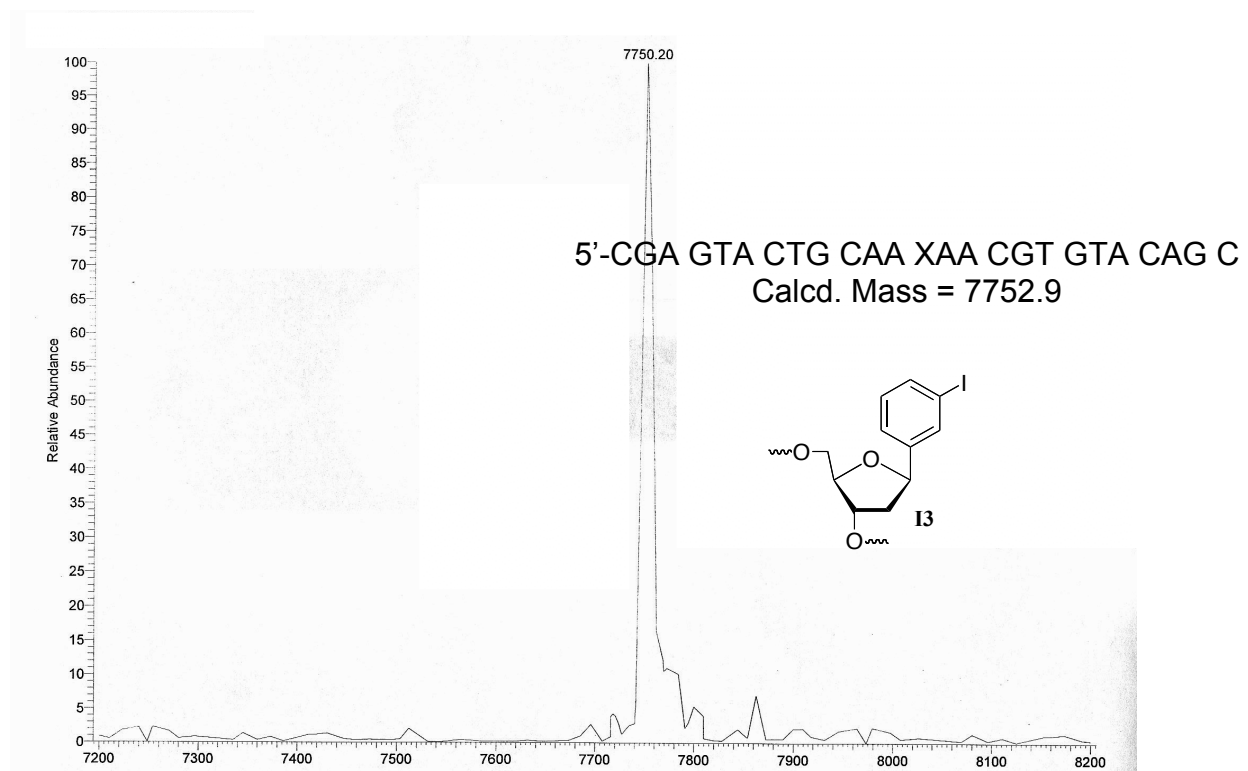
Supporting Information Figure 17. ESI-MS of 18mer containing **I4**.



Supporting Information Figure 18. ESI-MS of 18mer containing **IT**.

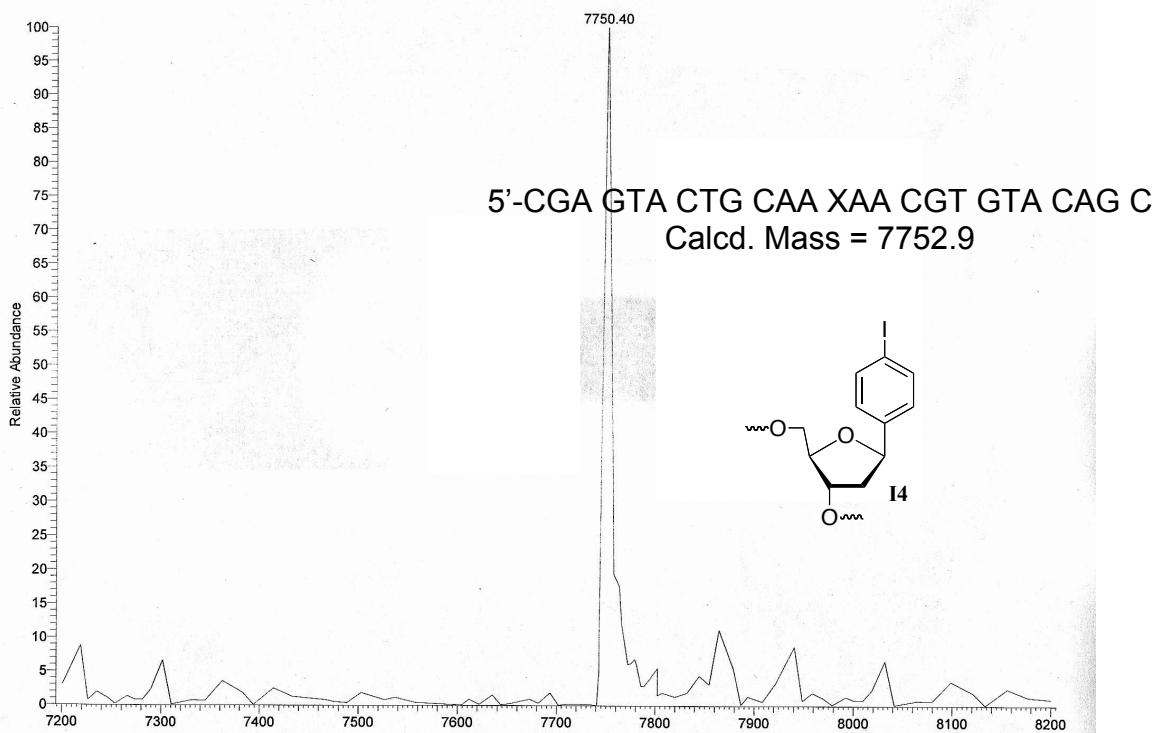


Supporting Information Figure 19. ESI-MS of 25mer containing **12**.

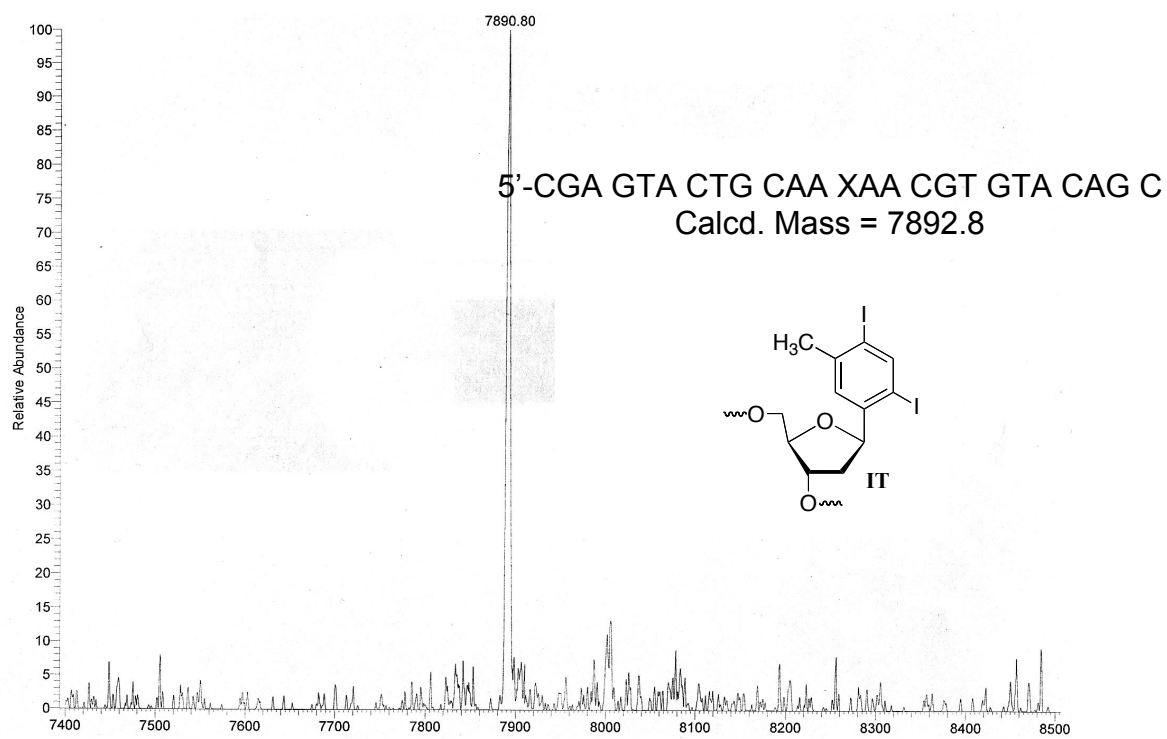


Supporting Information Figure 20. ESI-MS of 25mer containing **13**.

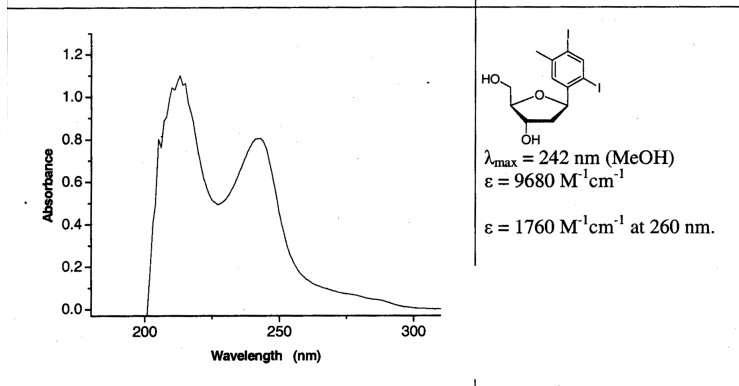
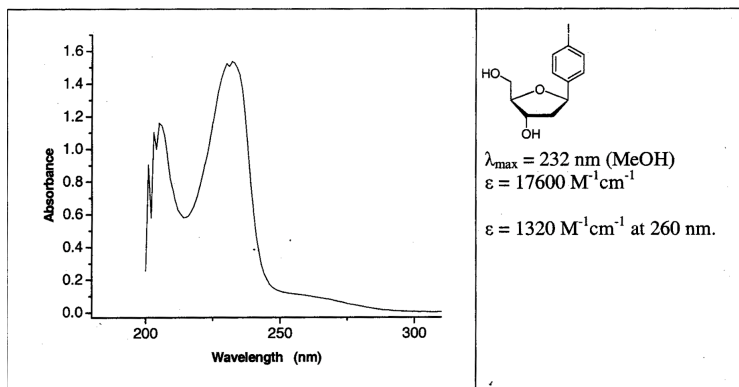
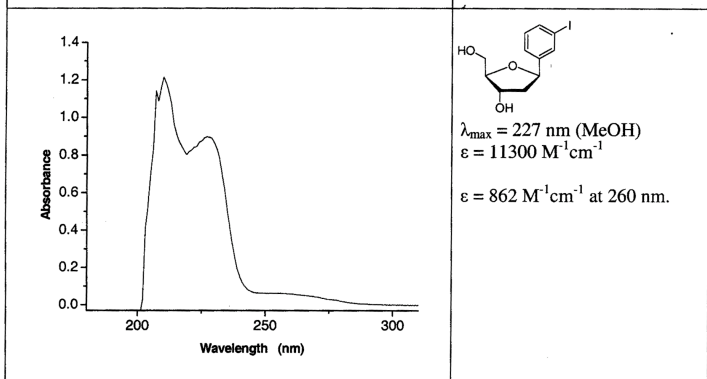
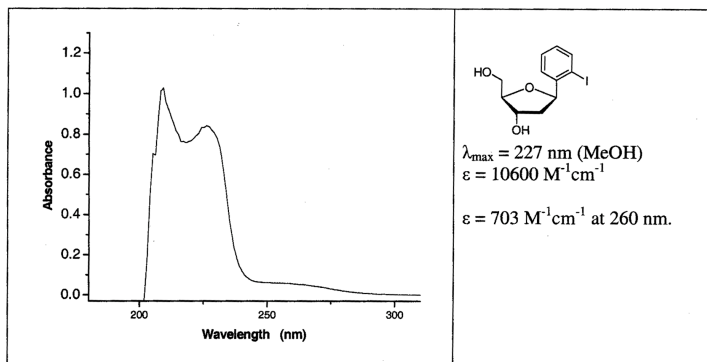




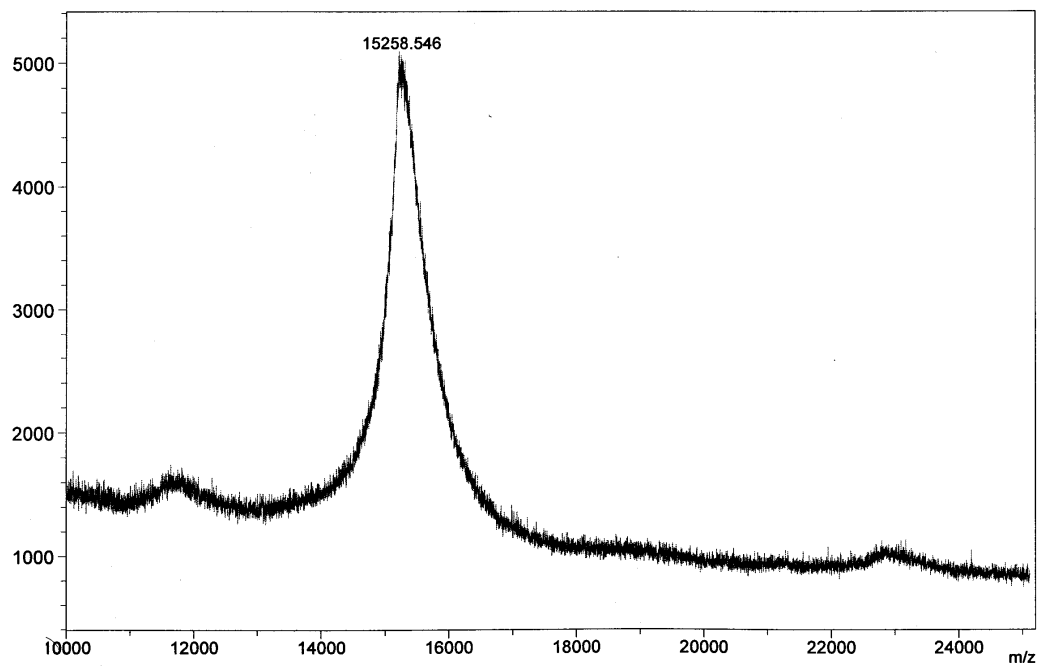
Supporting Information Figure 21. ESI-MS of 25mer containing I4.



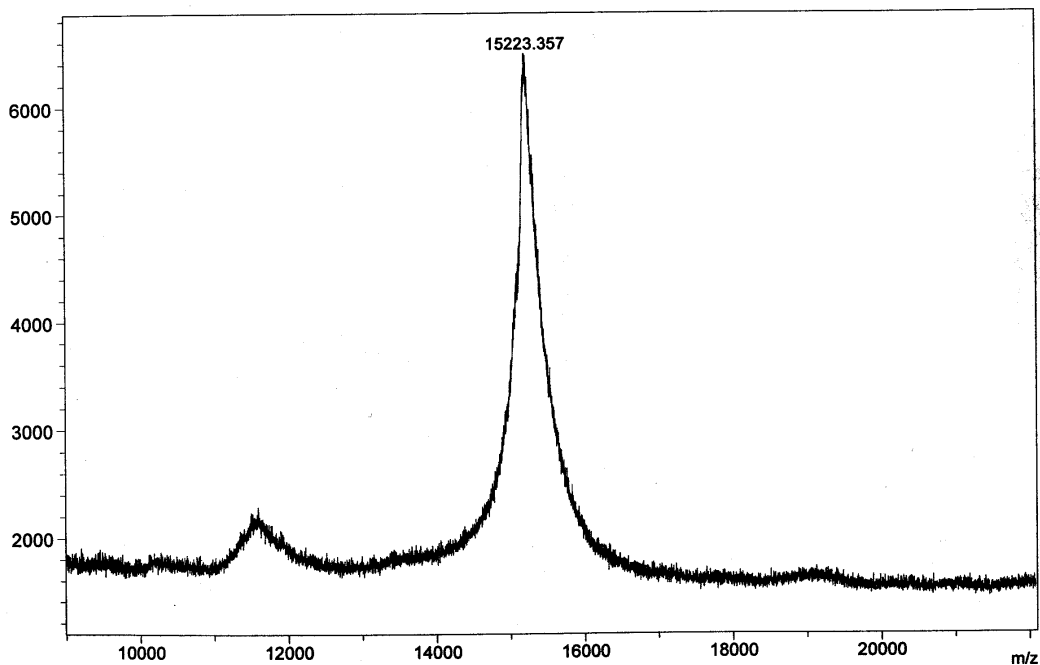
Supporting Information Figure 22. ESI-MS of 25mer containing IT.



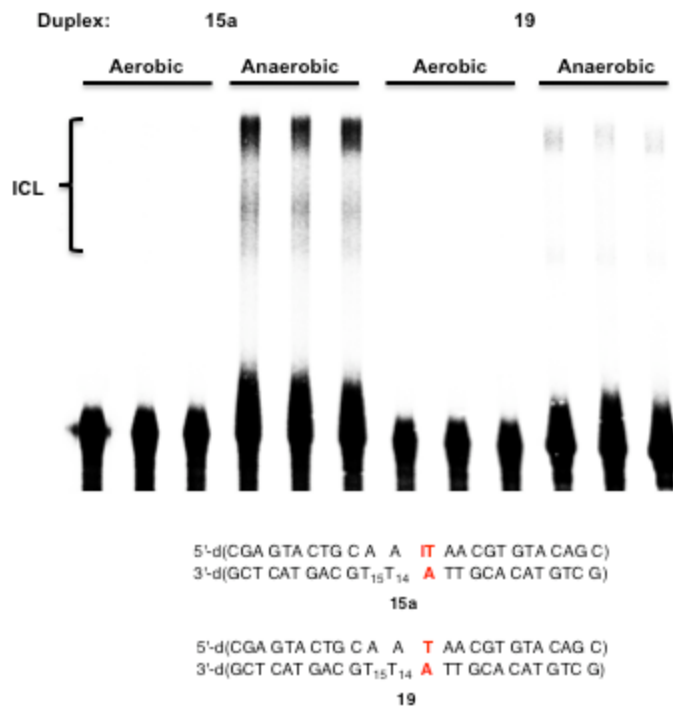
Supporting Information Figure 23. UV spectra of aryl iodide nucleosides.



**Supporting Information Figure 24.** MALDI-TOF MS of interstrand cross-link from I3 opposite dT (**17d**). Calc'd mass: 15,264. Calibrated using a synthetic oligonucleotide with mass: 5549.



**Supporting Information Figure 25.** MALDI-TOF MS of interstrand cross-link from I4 opposite dC (**18c**). Calc'd mass: 15,249. Calibrated using a synthetic oligonucleotide with mass: 5549.



**Supporting Information Figure 26.** Denaturing gel electrophoresis detection of cross-linked DNA. <sup>137</sup>Cs exposure: 700 Gy. (S20)

**Supporting Information Table 1.** Interstrand cross-link yields following <sup>137</sup>Cs irradiation (700 Gy) in the presence of t-BuOH.

	ICL Yield (%)			
<b>X</b>	<b>Y = A</b>	<b>Y = G</b>	<b>Y = C</b>	<b>Y = T</b>
<b>IT</b>	4.3 ± 0.8	3.8 ± 0.7	7.0 ± 1.2	4.5 ± 0.6
<b>2I</b>	1.4 ± 0.2	2.0 ± 0.2	1.8 ± 0.3	1.0 ± 0.3
<b>3I</b>	5.9 ± 0.1	7.4 ± 0.2	8.6 ± 0.6	8.7 ± 0.8
<b>4I</b>	17.5 ± 1.4	10.0 ± 0.6	18.8 ± 1.0	13.5 ± 1.8

<sup>a</sup>Yields are the average ± std. dev. of 3 samples.