

**Supporting Information: Interstrand Cross-Link and Bioconjugate Formation in RNA From a
Modified Nucleotide**

Jack L. Sloane and Marc M. Greenberg*

Department of Chemistry, Johns Hopkins University, 3400 N. Charles St., Baltimore MD 21218.

mgreenberg@jhu.edu

Contents:

1. **Figure S1.** ^1H NMR and ^{13}C NMR spectra of **8**. (S2)
2. **Figure S2.** ^1H NMR and ^{13}C NMR spectra of **9**. (S3)
3. **Figure S3.** ^1H NMR and ^{13}C NMR spectra of **10**. (S4)
4. **Figure S4.** ^1H NMR and ^{13}C NMR spectra of **11**. (S5)
5. **Figure S5.** ^1H NMR and ^{31}P NMR spectra of **12**. (S6)
6. **Figure S6.** ^1H NMR of **7**. (S7)
7. **Figure S7.** ^1H NMR of oxidation of **9** by H_2O_2 with H_2O solvent suppression. (S8)
8. **Figure S8.** MALDI-TOF MS of **13**. (S9)
9. **Figure S9.** MALDI-TOF MS of **14**. (S9)
10. **Figure S10.** MALDI-TOF MS of **15**. (S10)
11. **Figure S11.** LC-MS of ICL **23**. (S10)
12. **Figure S12.** MALDI-TOF MS of the glycine adduct (**24a**). (S11)
13. **Figure S13.** MALDI-TOF MS of the phenylalanine adduct (**24b**). (S11)
14. **Figure S14.** Histogram of hydroxyl radical cleavage of ICL from **19a** (**23**). (S12)
15. **Figure S15.** Histogram of hydroxyl radical cleavage of ICL from **21b** (**9** opposite cytidine). (S12)
16. **Figure S16.** Histogram of hydroxyl radical cleavage of ICL from **21a** (**9** opposite guanosine). (S13)
17. **Figure S17.** Histogram of hydroxyl radical cleavage of ICL from **21c** (**9** opposite guanosine). (S13)

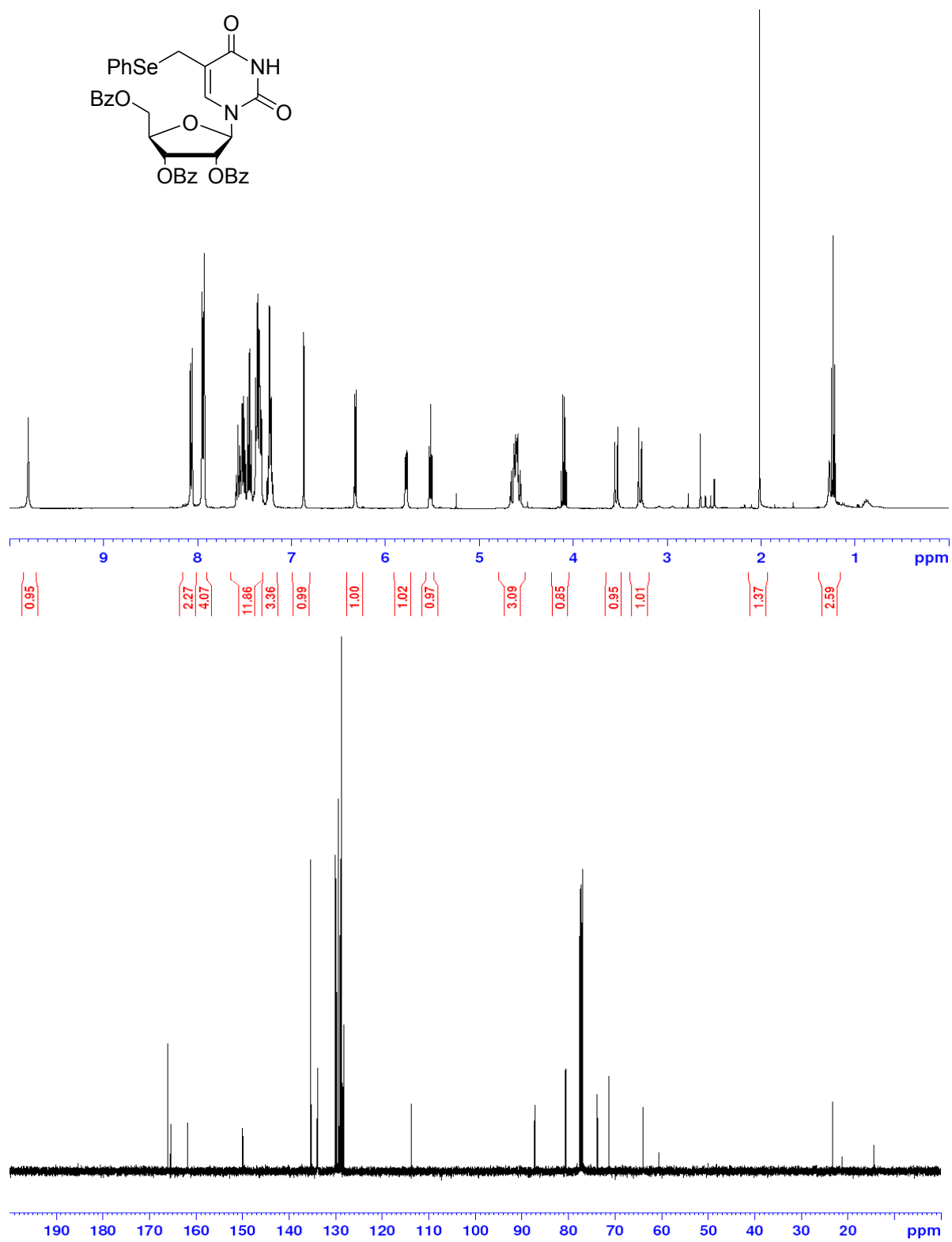


Figure S1. ^1H NMR and ^{13}C NMR spectra of **8**.

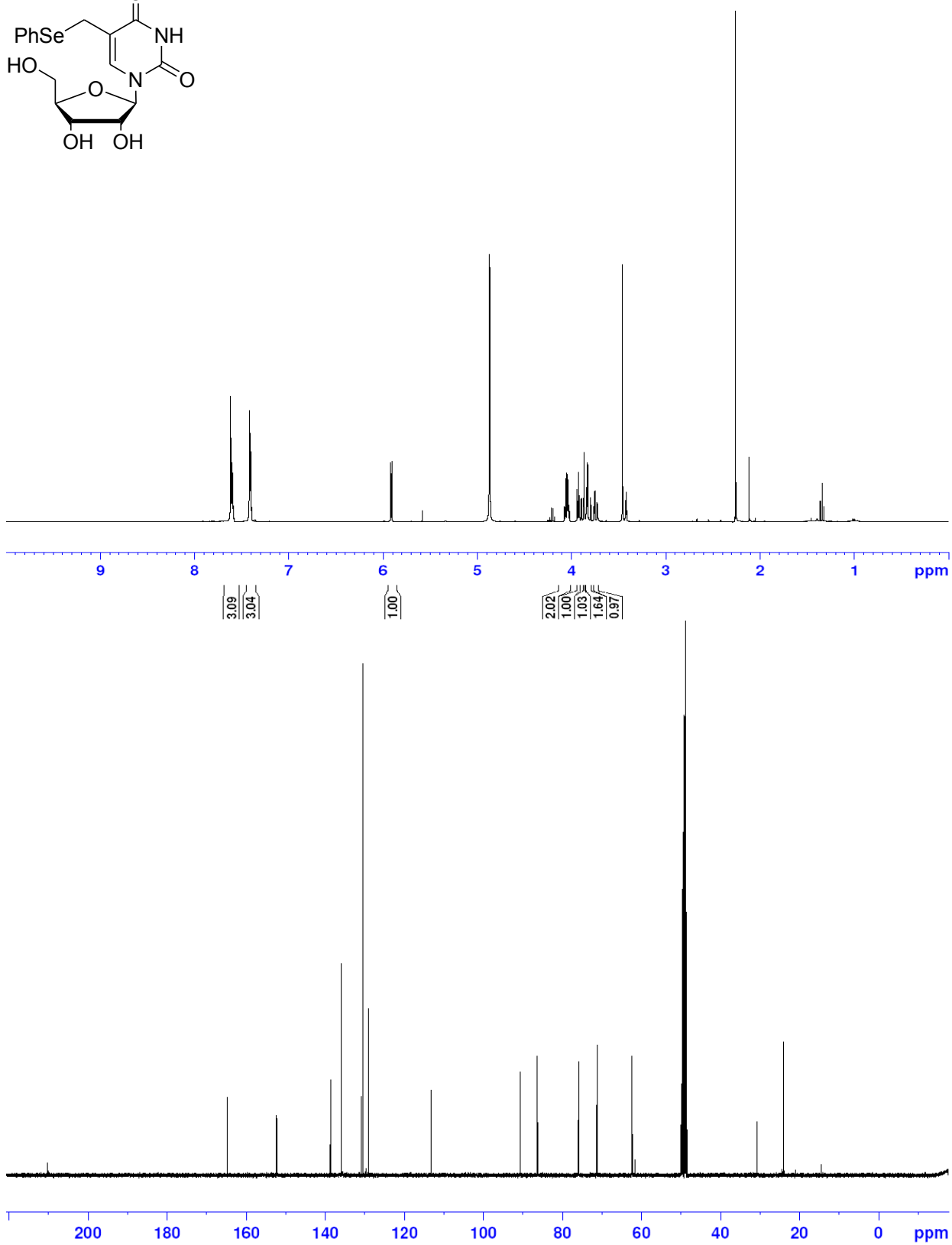
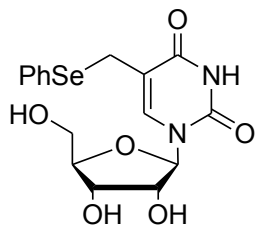


Figure S2. ^1H NMR and ^{13}C NMR spectra of 9.

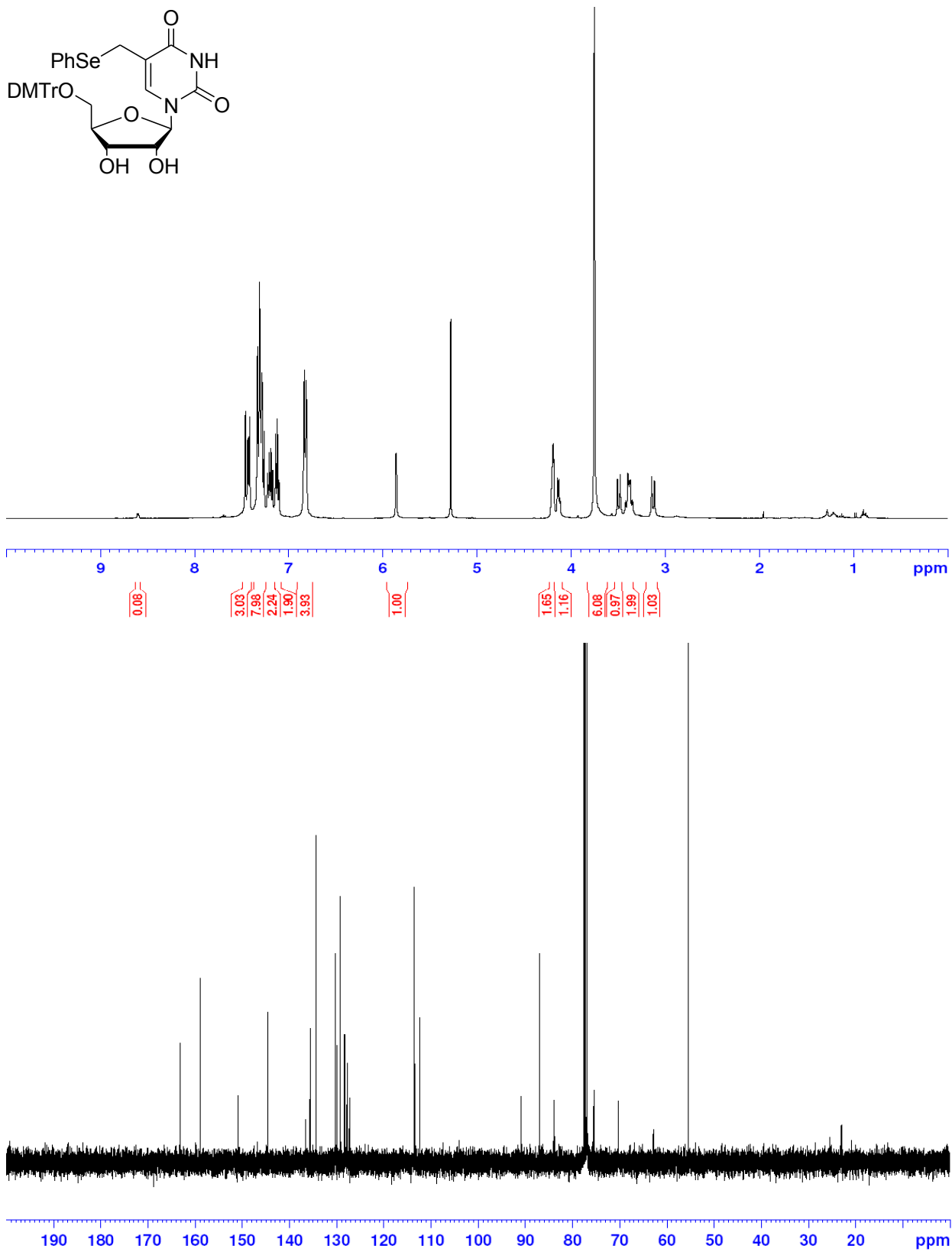


Figure S3. ^1H NMR and ^{13}C NMR spectra of **10**.

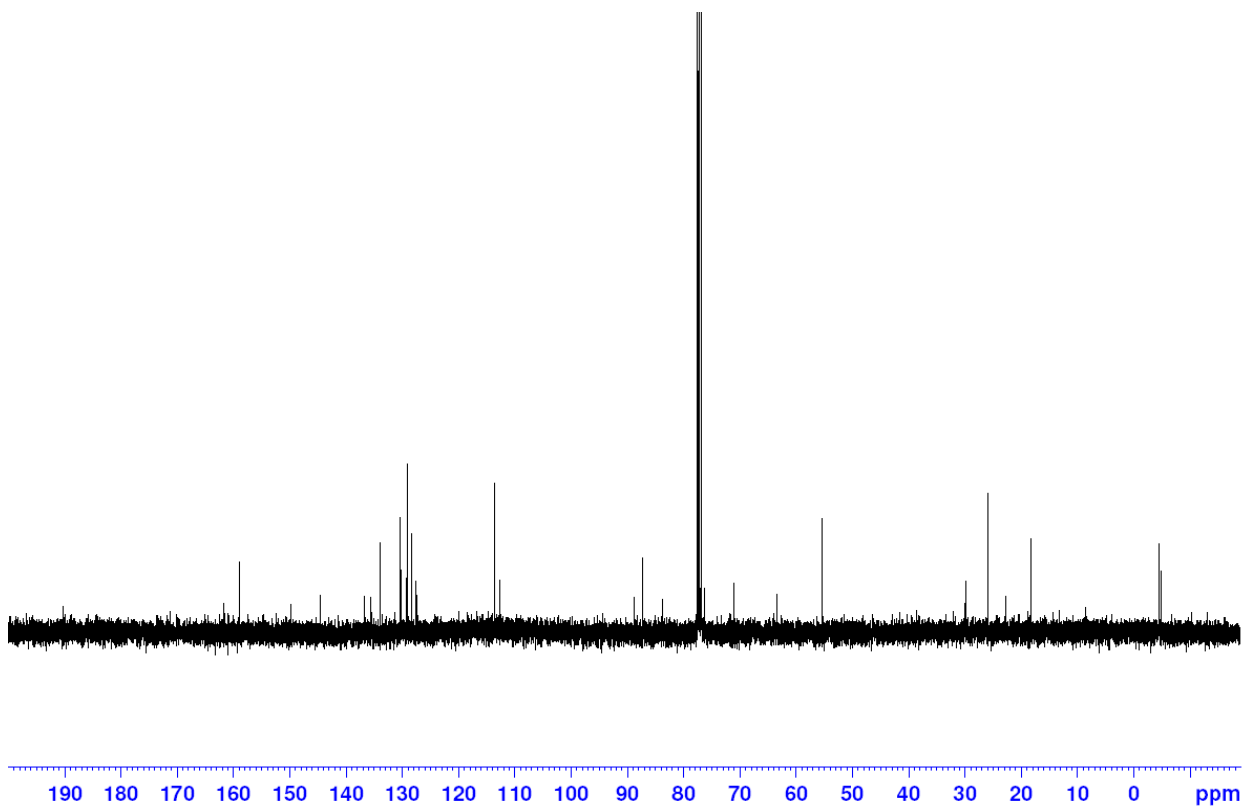
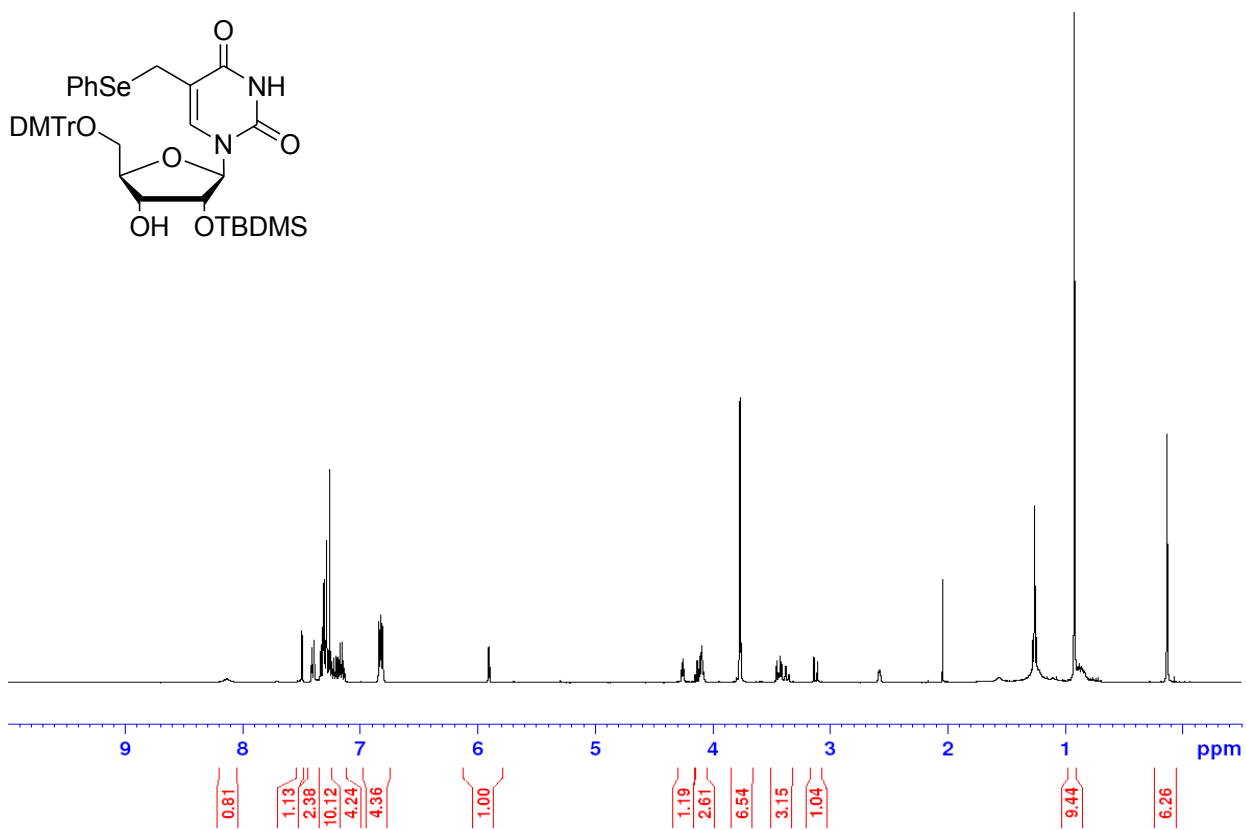
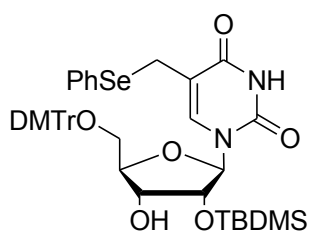


Figure S4. ^1H NMR and ^{13}C NMR spectra of **11**.

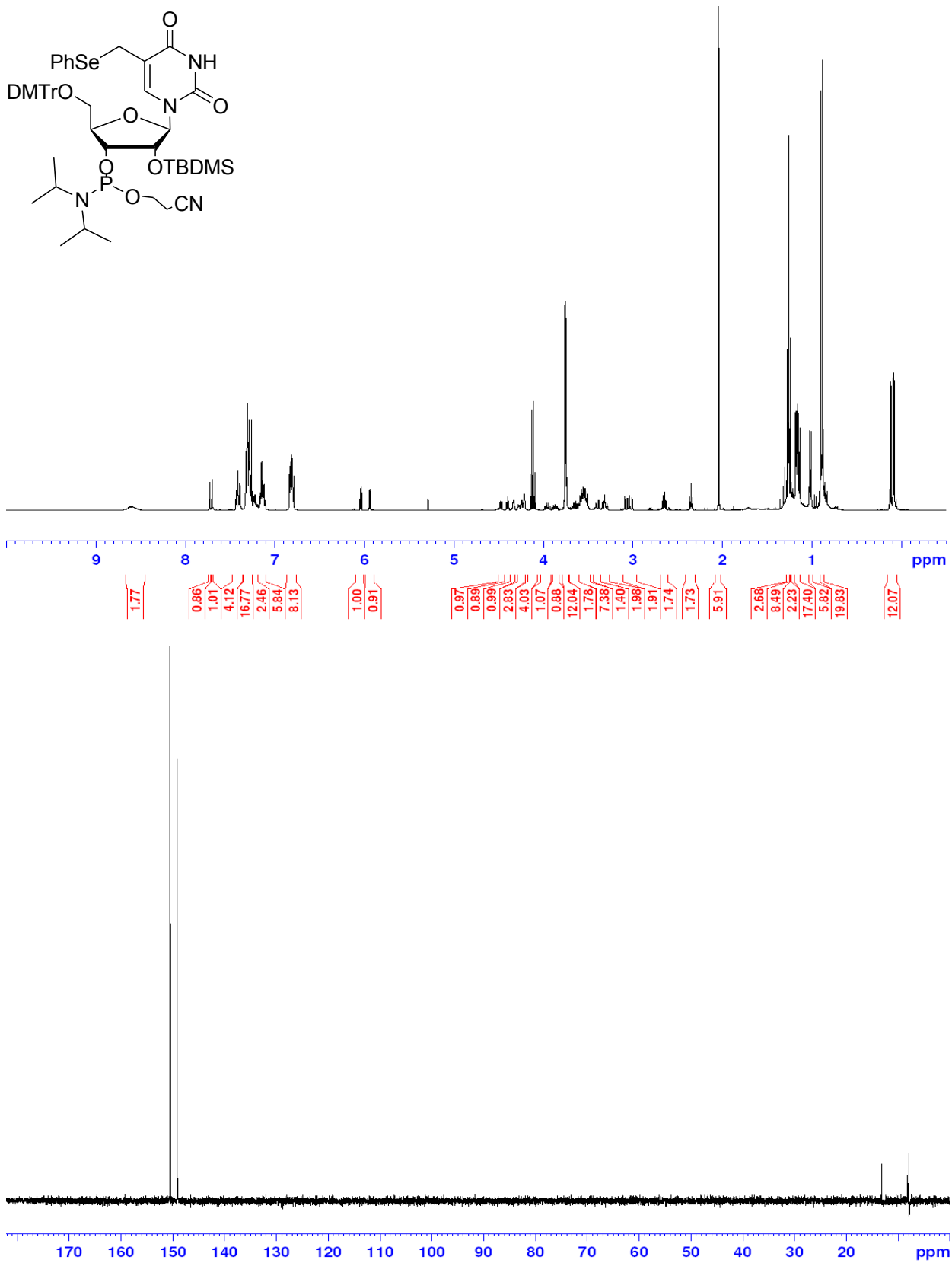


Figure S5. ¹H NMR and ³¹P NMR spectra of **12**.

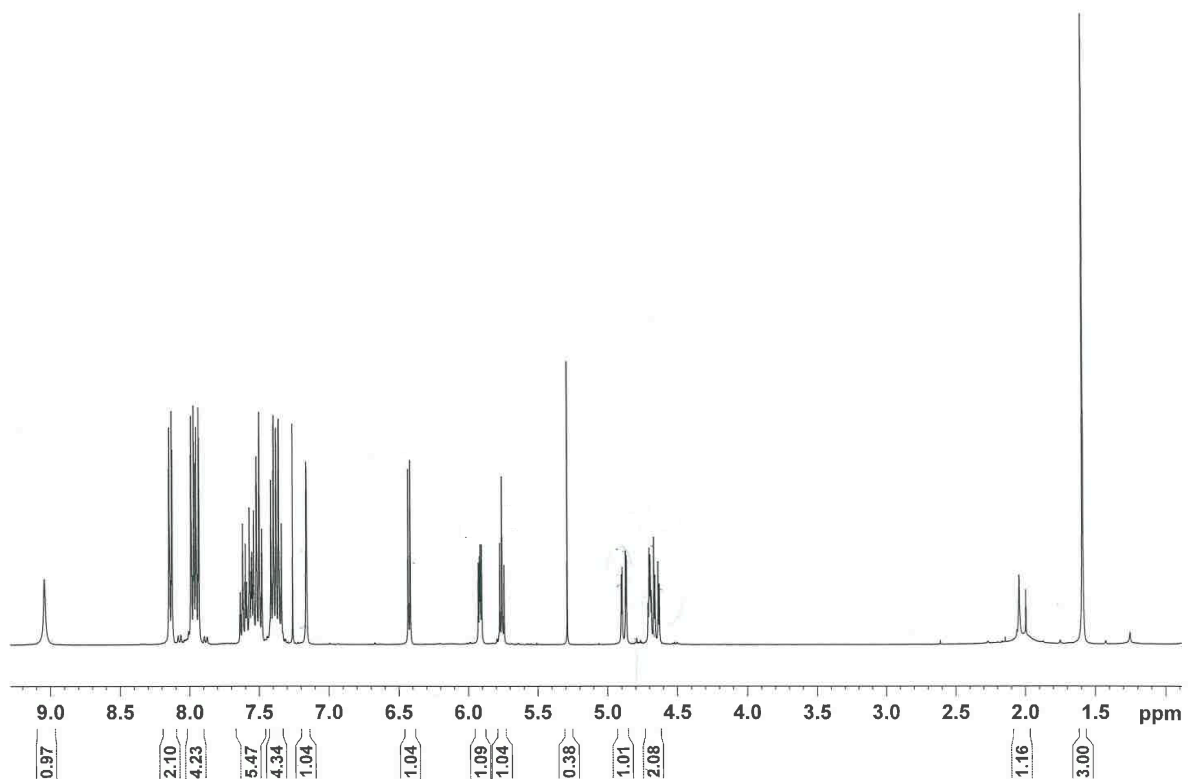


Figure S6. ^1H NMR of 7.

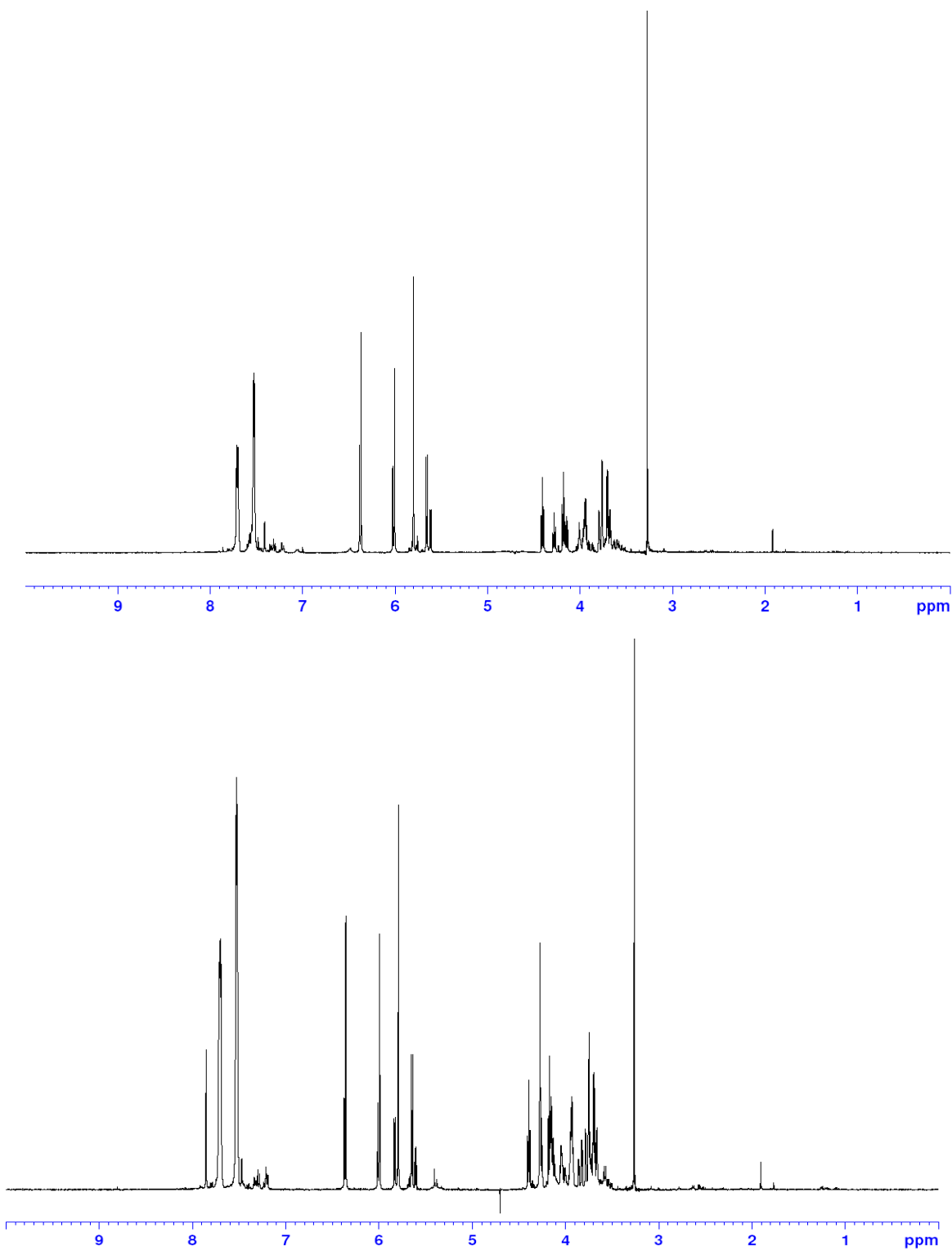


Figure S7. ¹H NMR of oxidation of **9** by H₂O₂ with H₂O solvent suppression. Top: After 15 min; Bottom: after 18 h.

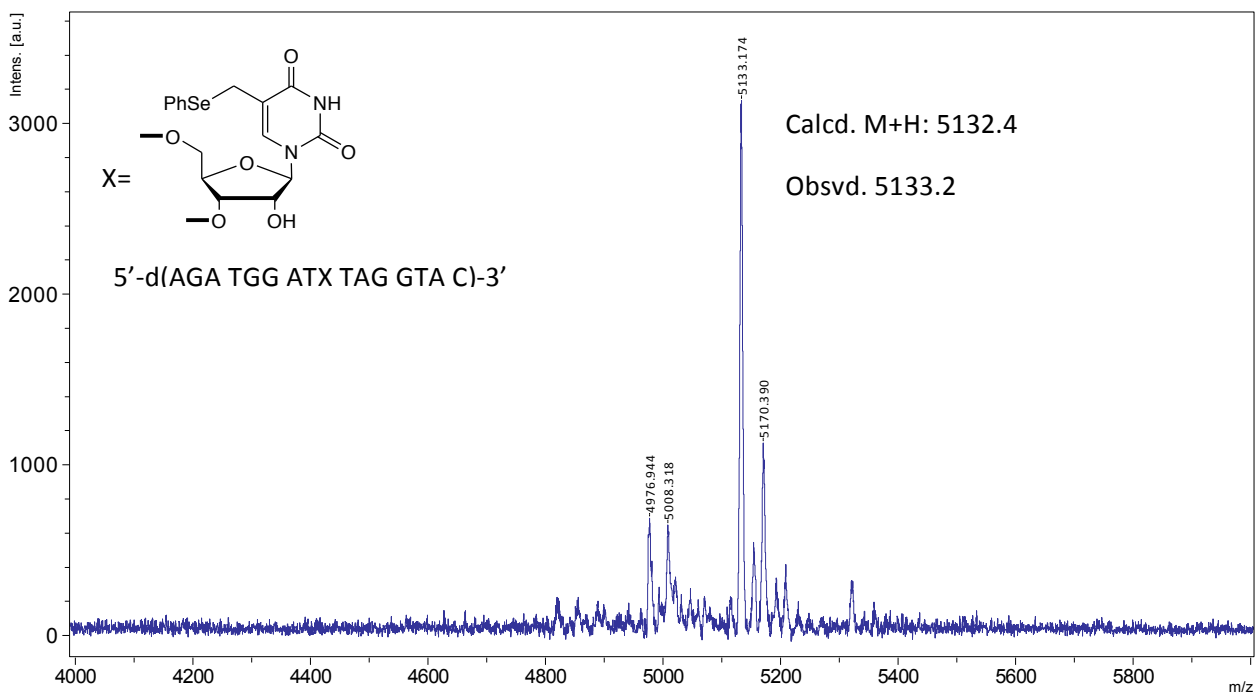


Figure S8. MALDI-TOF MS of **13**; m/z 4976 corresponds to photolyzed thymidine, m/z 5008 corresponds to the peroxy adduct, m/z 5170 corresponds to the potassium salt

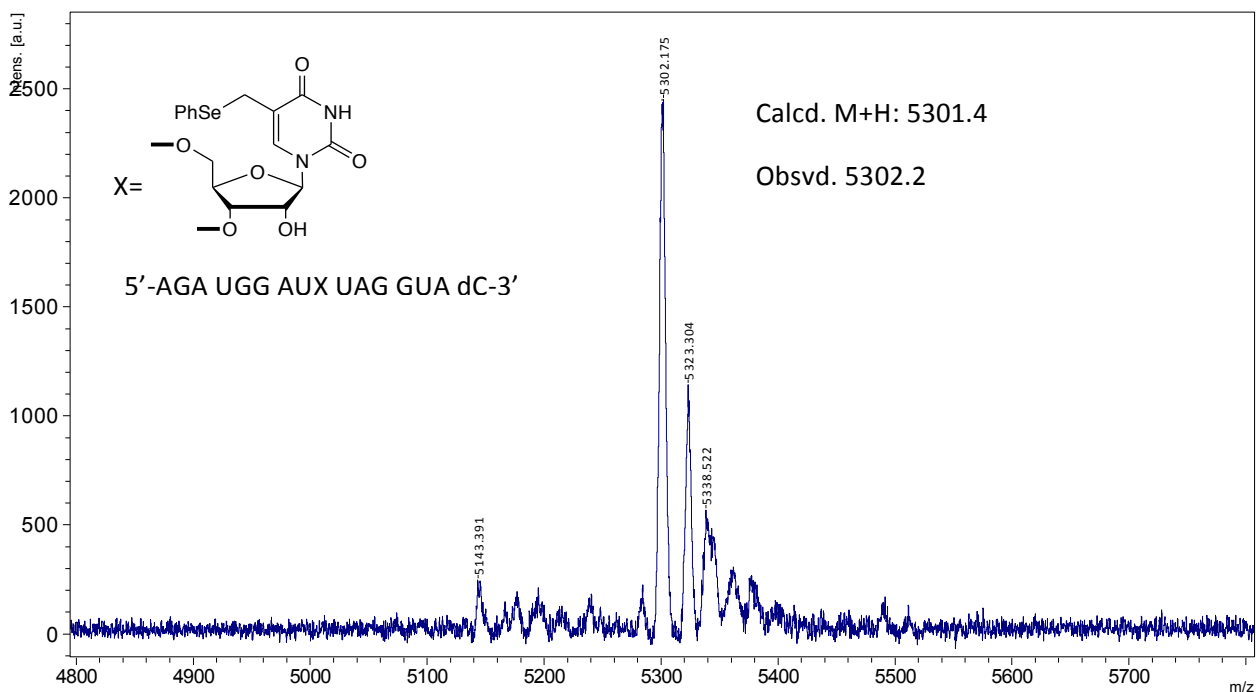


Figure S9. MALDI-TOF MS of **14**; m/z 5323 and 5338 correspond to the sodium and potassium salt, respectively; m/z 5143 corresponds to photolyzed thymidine

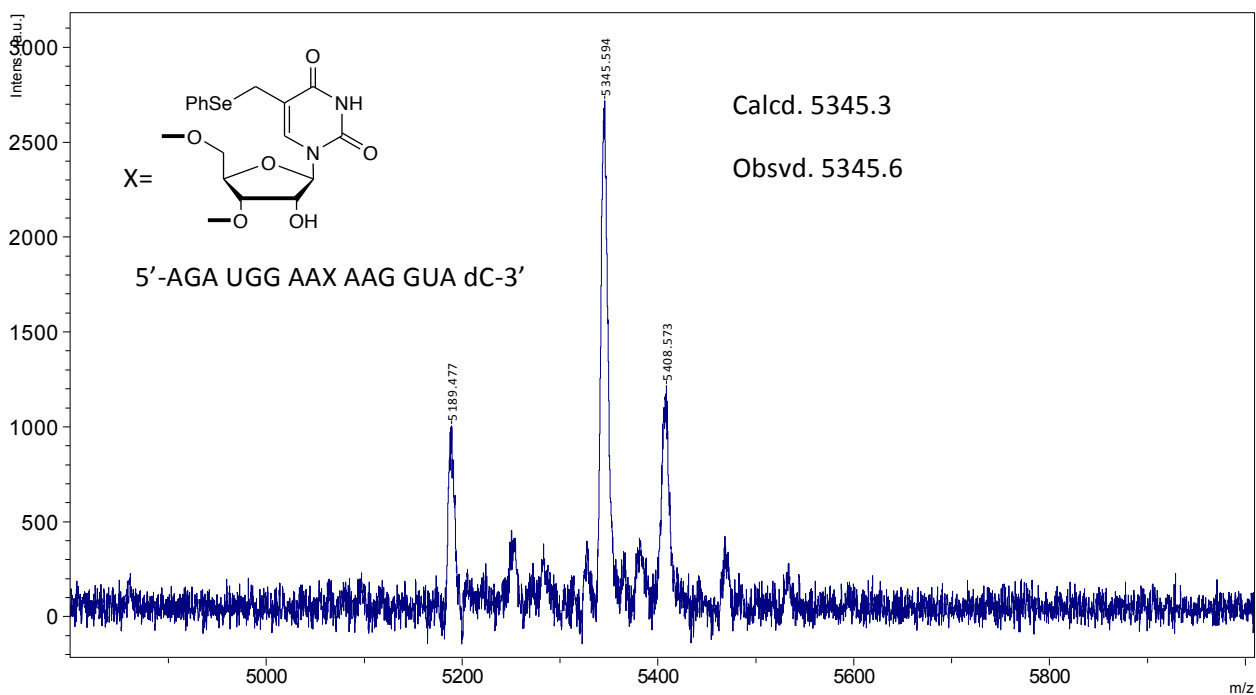


Figure S10. MALDI-TOF MS of **15**; m/z 5189 is photolyzed thymidine, m/z 5408 is the potassium salt

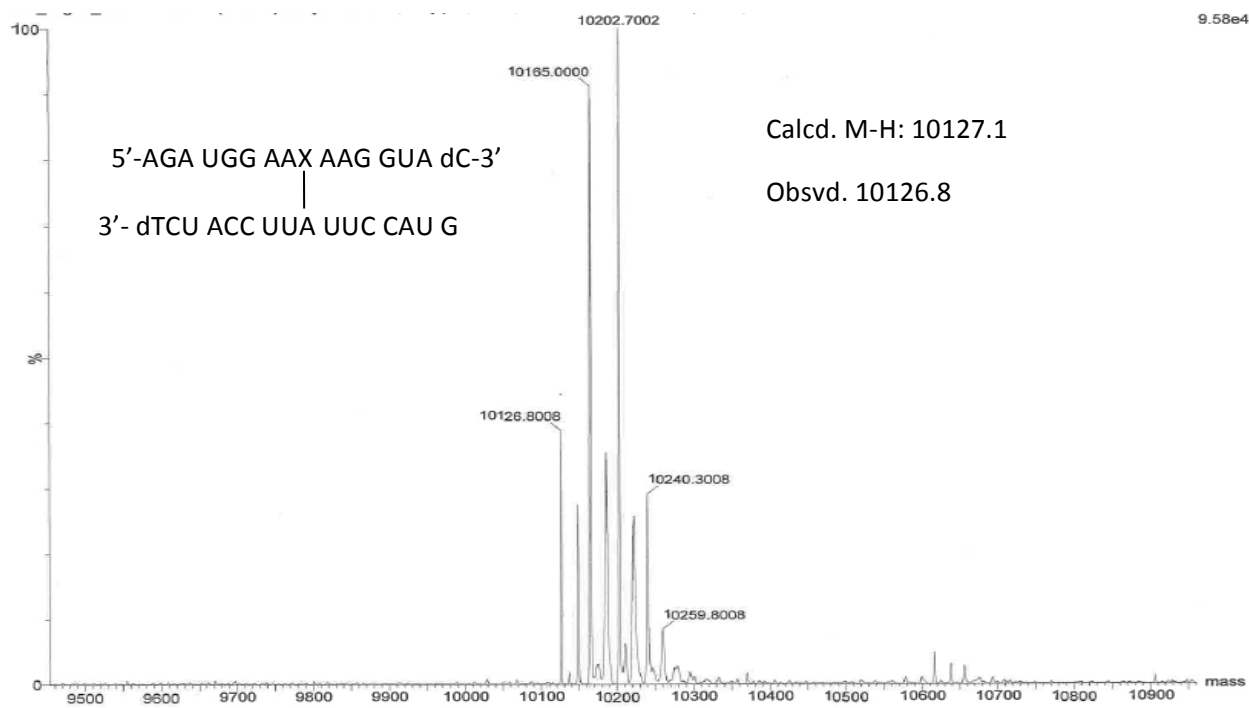


Figure S11. LC-MS of ICL **23**; m/z between 10165 and 10259 correspond to a mixture of sodium and potassium salts of the ICL

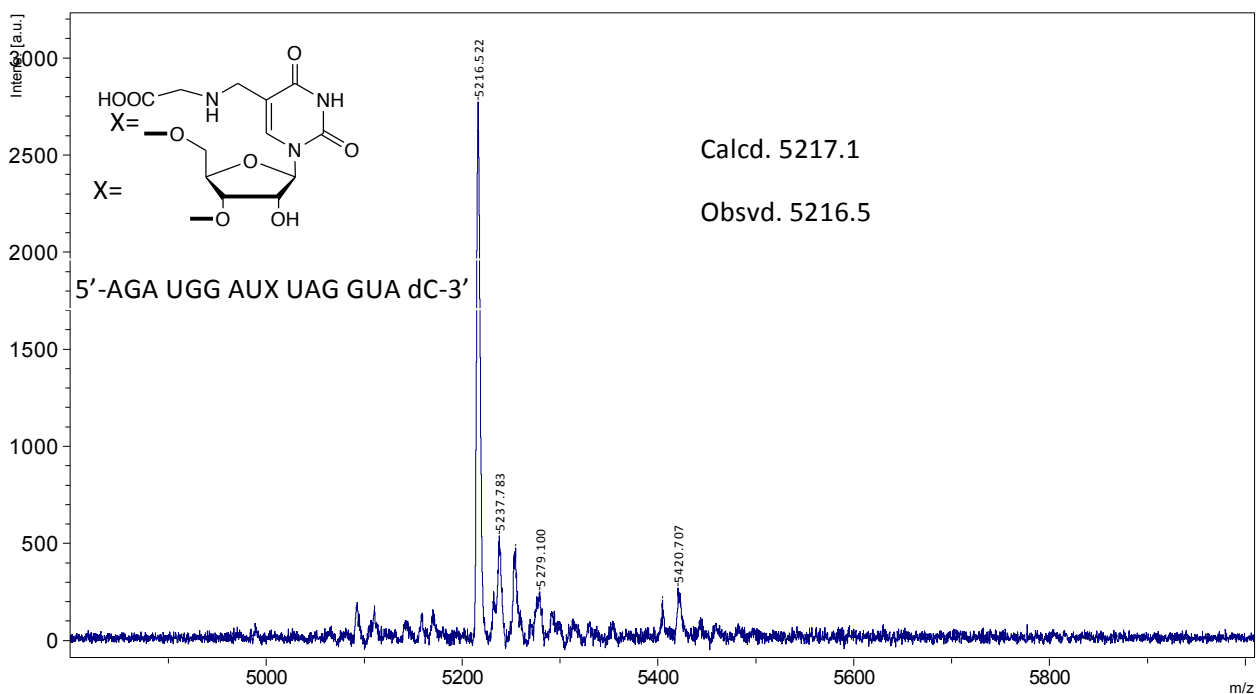


Figure S12. MALDI-TOF MS of the glycine adduct (**24a**); m/z greater than 5237 correspond to a mixture of sodium and potassium salts

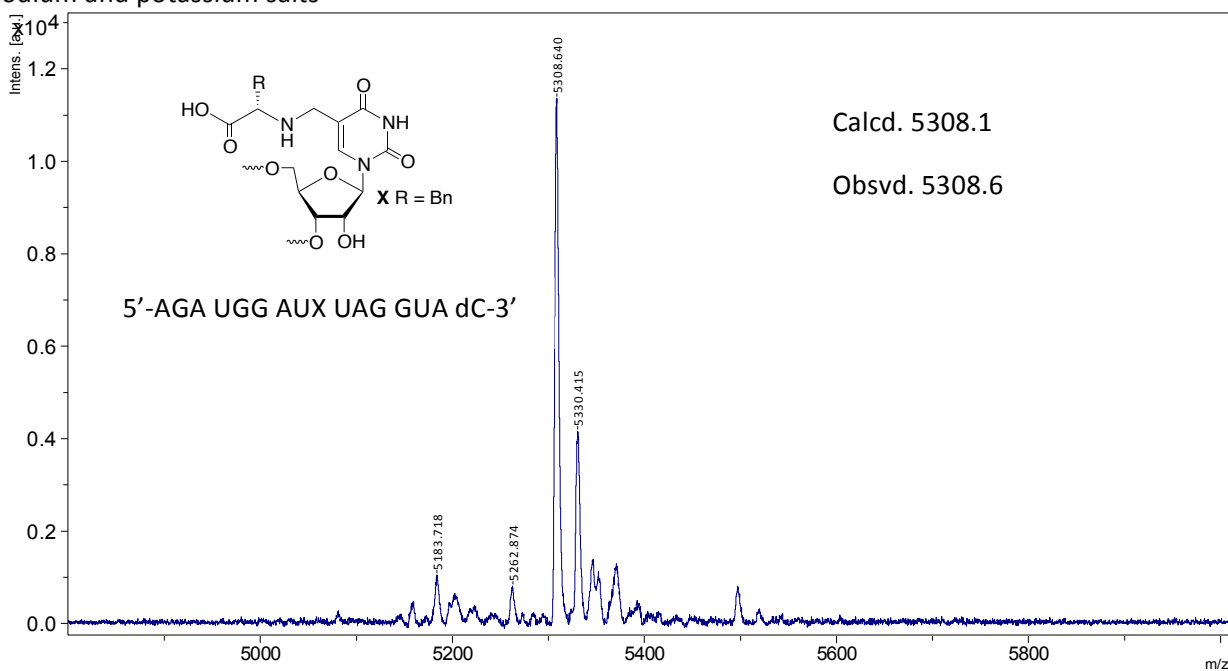


Figure S13. MALDI-TOF MS of the phenylalanine adduct (**24b**); m/z 5183 and 5262 corresponds to reaction side products, m/z greater than 5330 correspond to a mixture of sodium and potassium salts

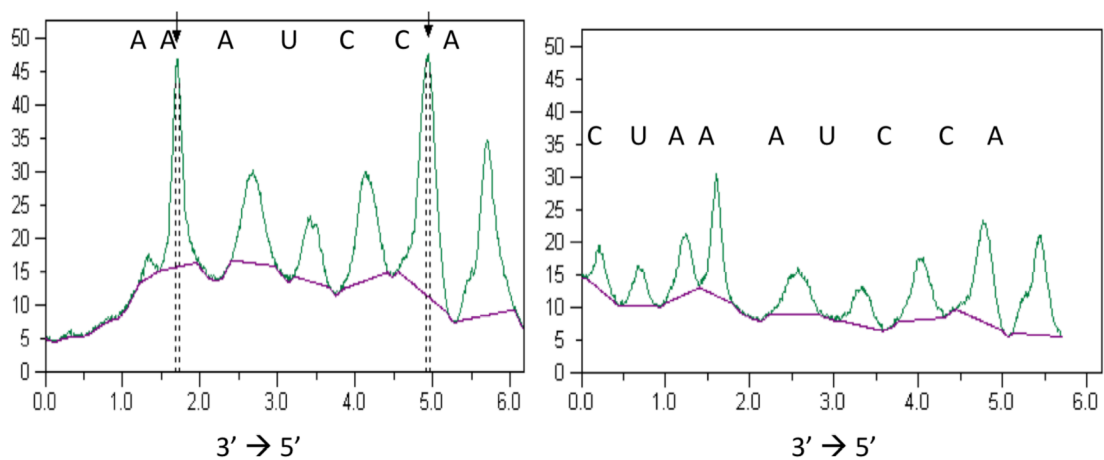


Figure S14. Histogram of hydroxyl radical cleavage of ICL from **19a** (**23**). Left: ICL; Right: Duplex precursor

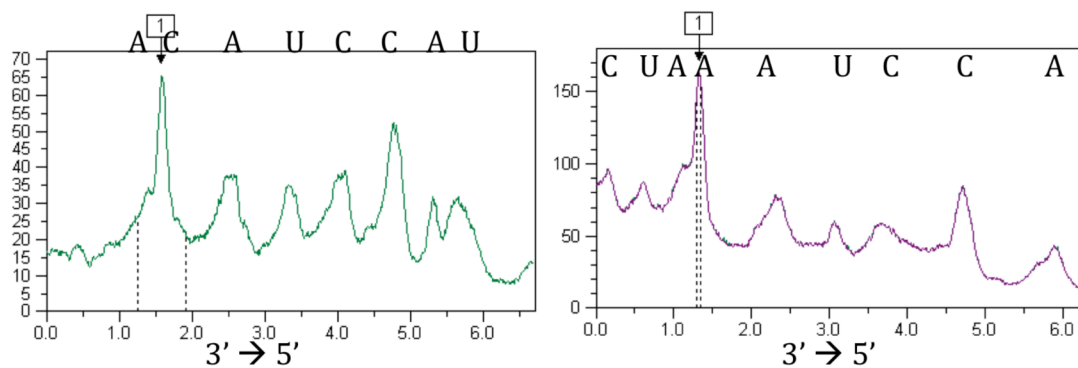


Figure S15. Histogram of hydroxyl radical cleavage of ICL from **21b** (**9** opposite cytidine). Left: ICL; Right: Duplex precursor

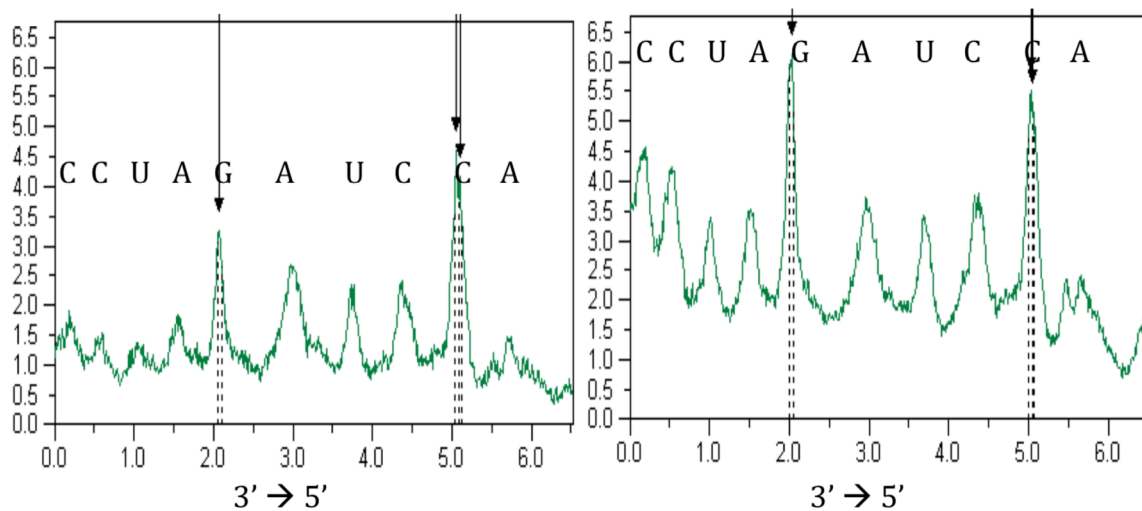


Figure S16. Histogram of hydroxyl radical cleavage of ICL from **21a** (9 opposite guanosine). Left: ICL; Right: Duplex precursor

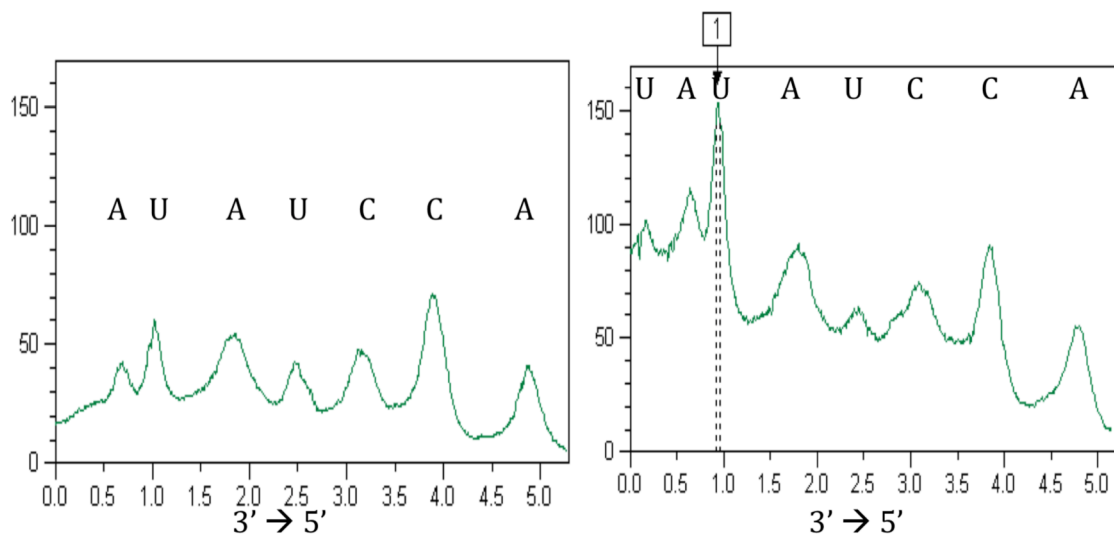


Figure S17. Histogram of hydroxyl radical cleavage of ICL from **21c** (9 opposite uridine). Left: ICL; Right: Duplex precursor