

Supporting Information: Synthesis of Cross-linked DNA Containing Oxidized Abasic Site Analogues

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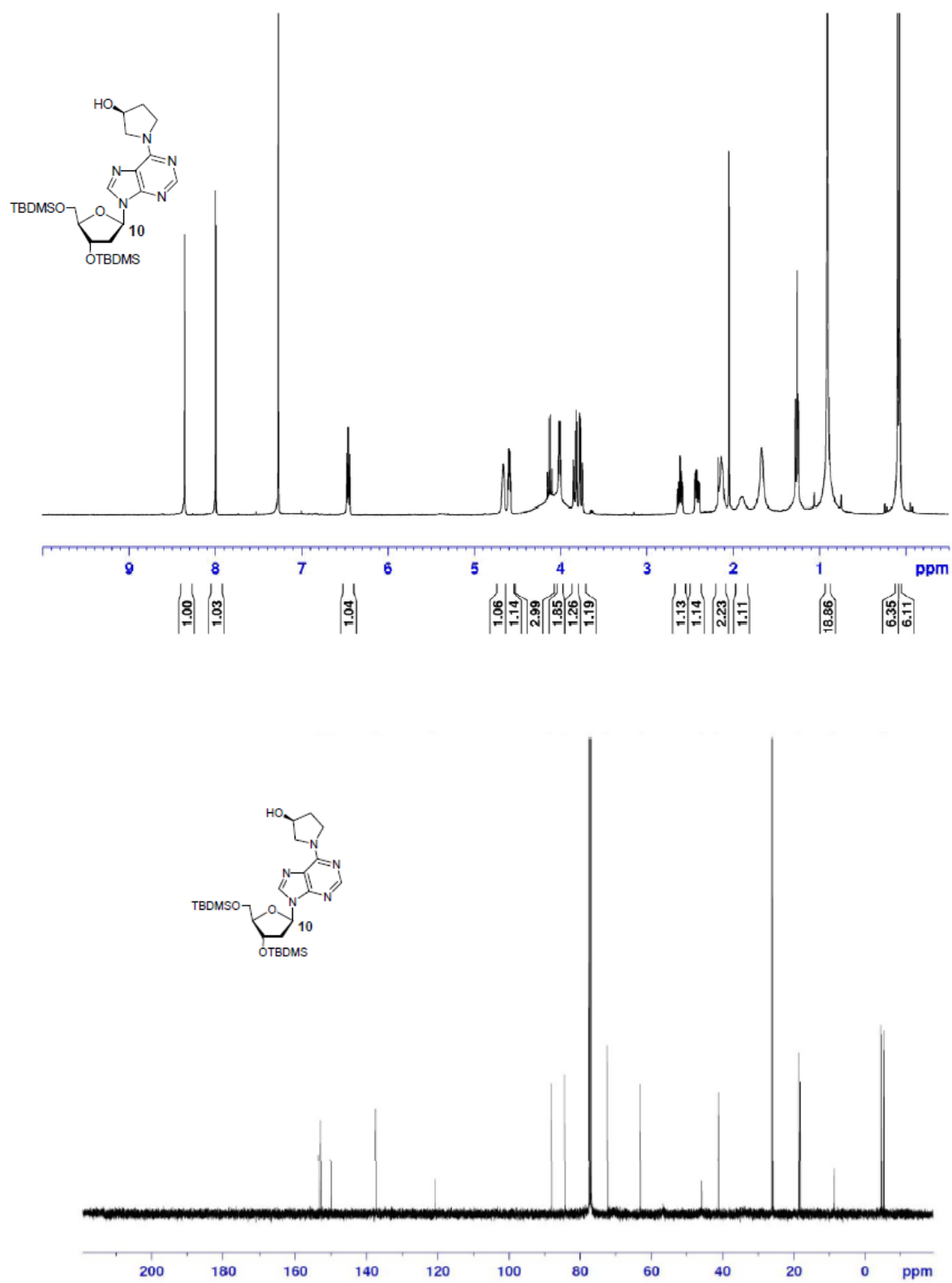


Figure S1. ^1H and ^{13}C NMR spectra of 10.

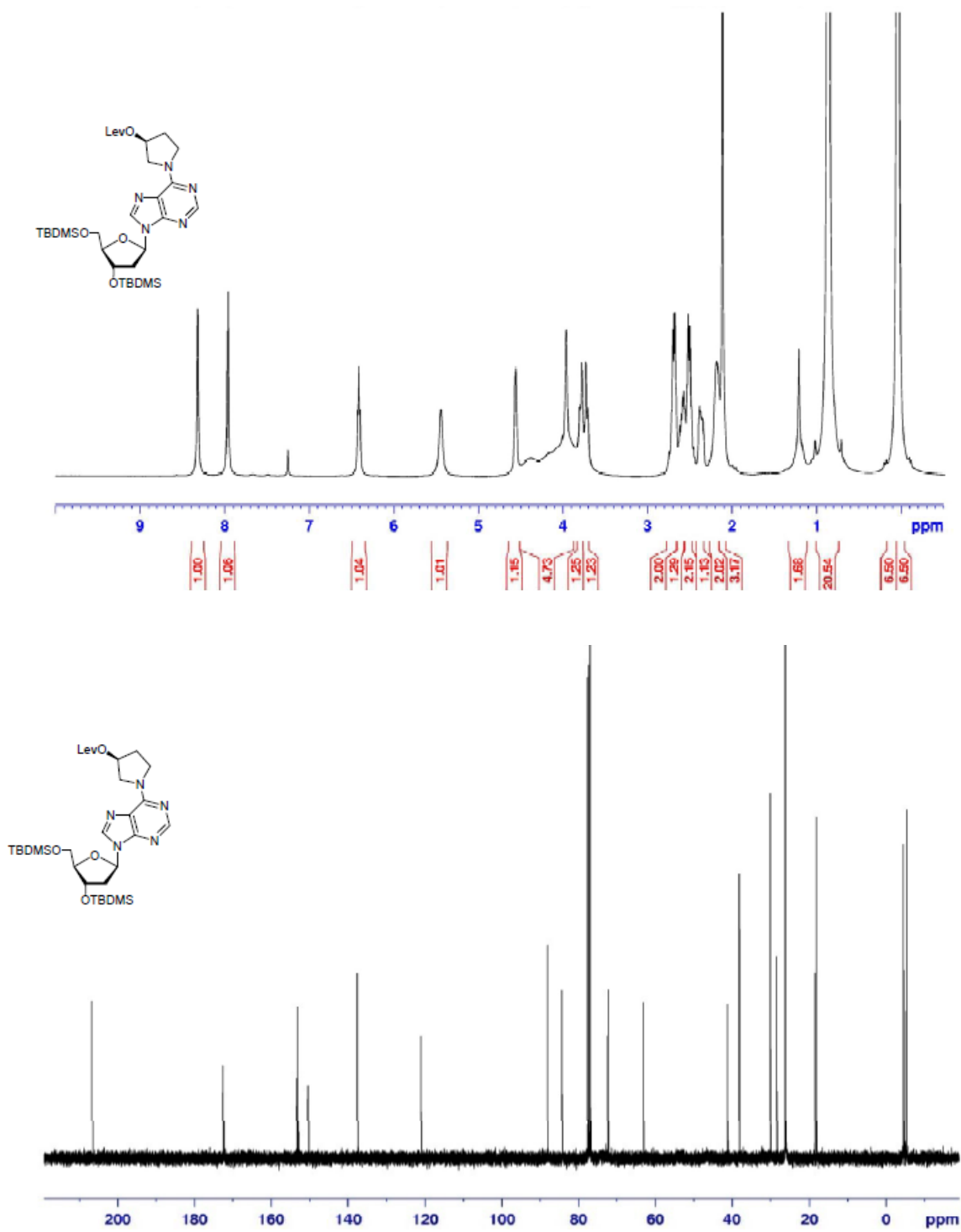


Figure S2. ^1H and ^{13}C NMR spectra of levulinyl protected 10.

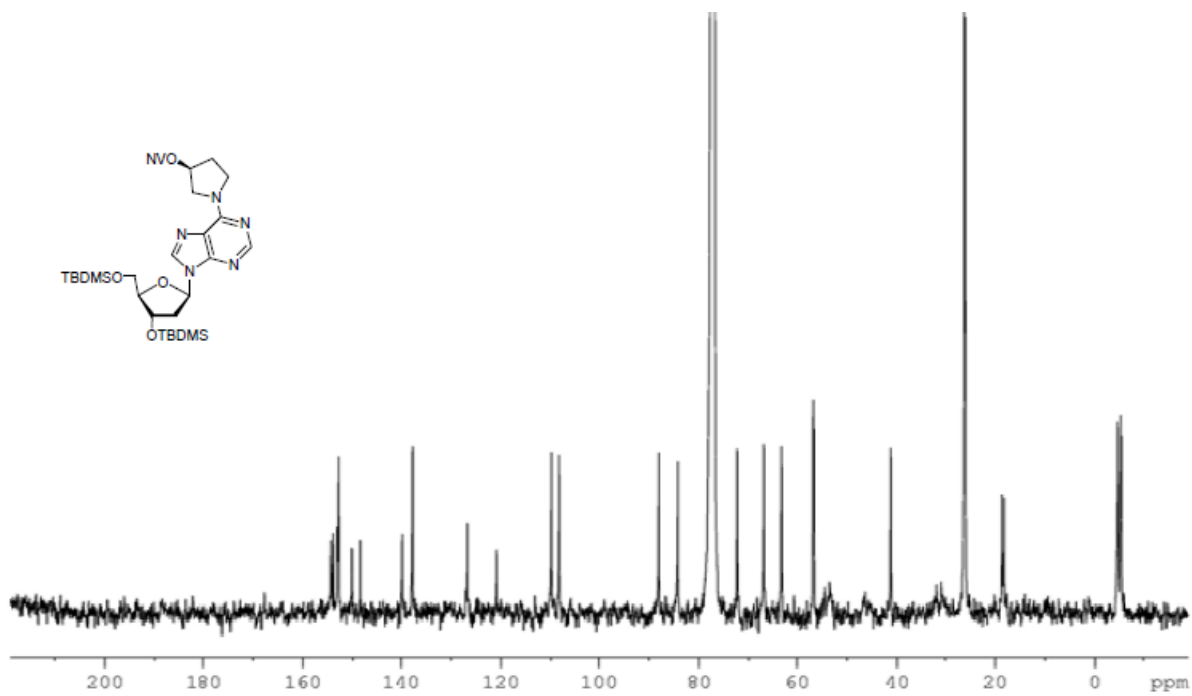
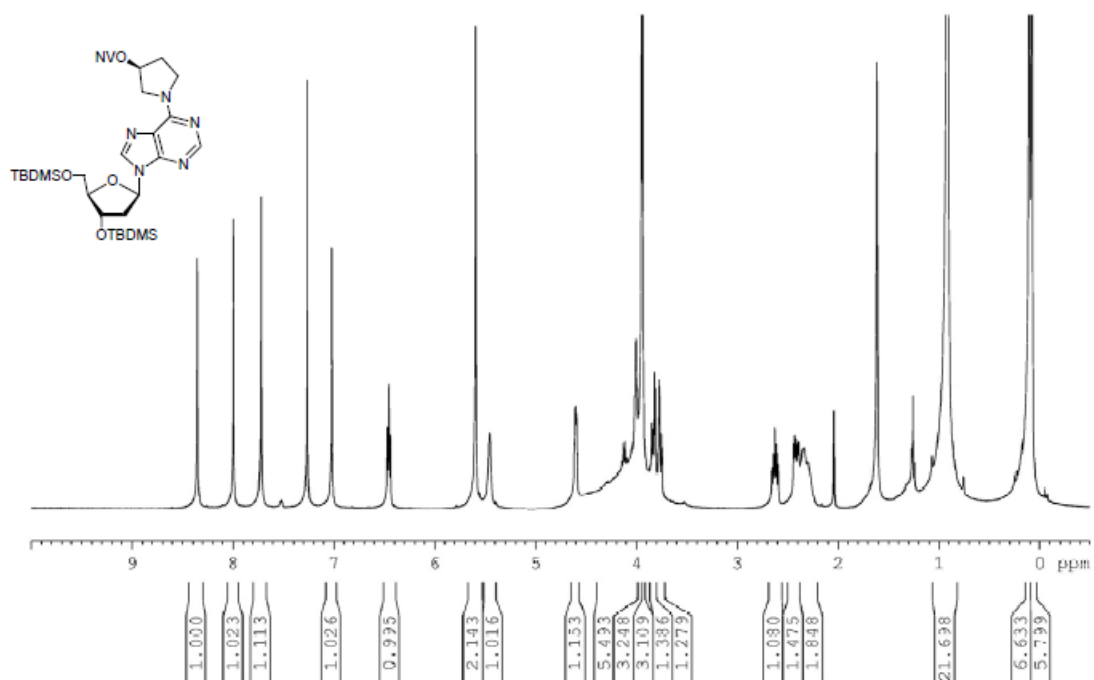


Figure S3. ¹H and ¹³C NMR spectra of nitroveratryloxycarbonyl protected **10**.

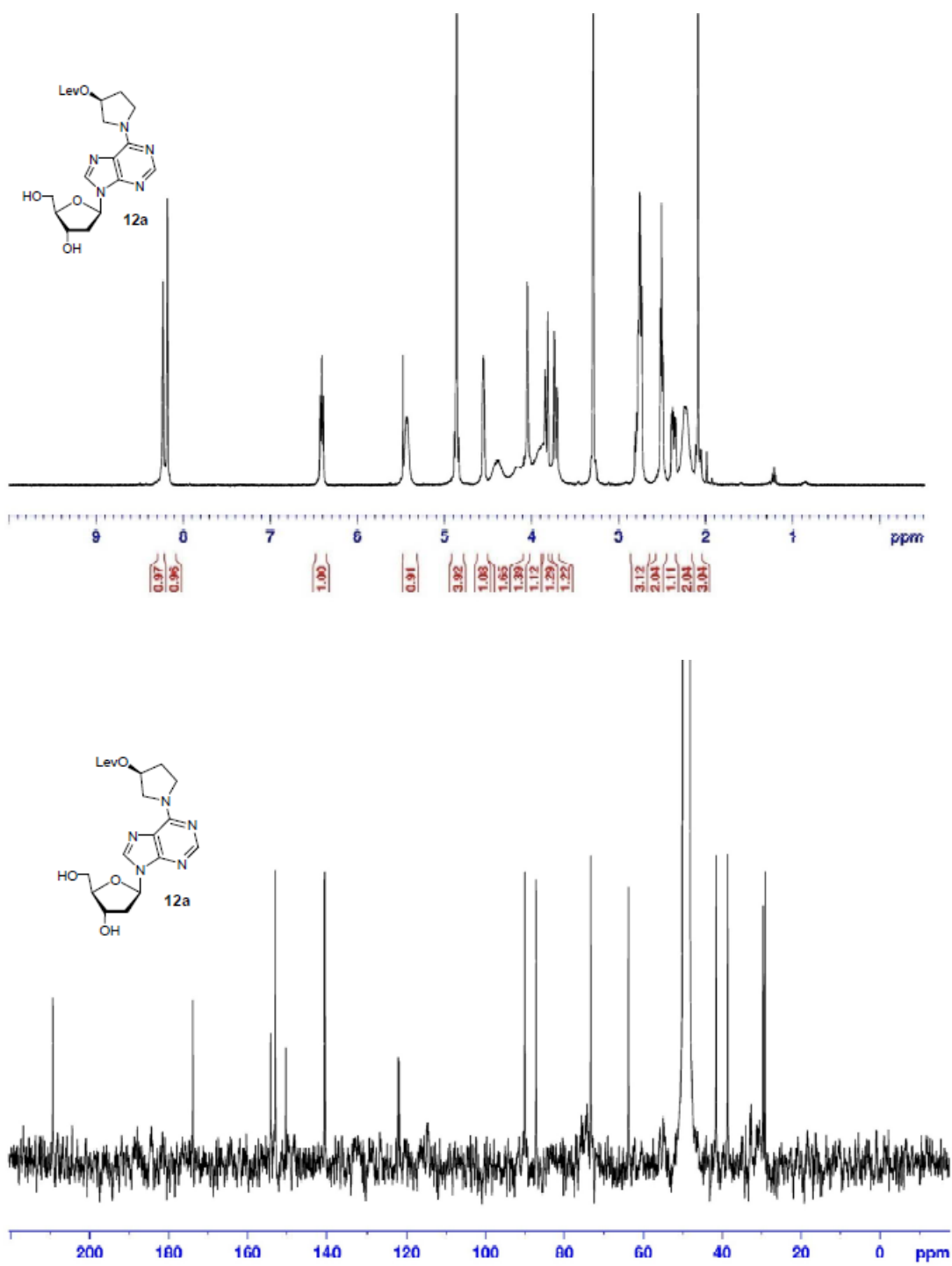


Figure S4. ^1H and ^{13}C NMR spectra of 12a.

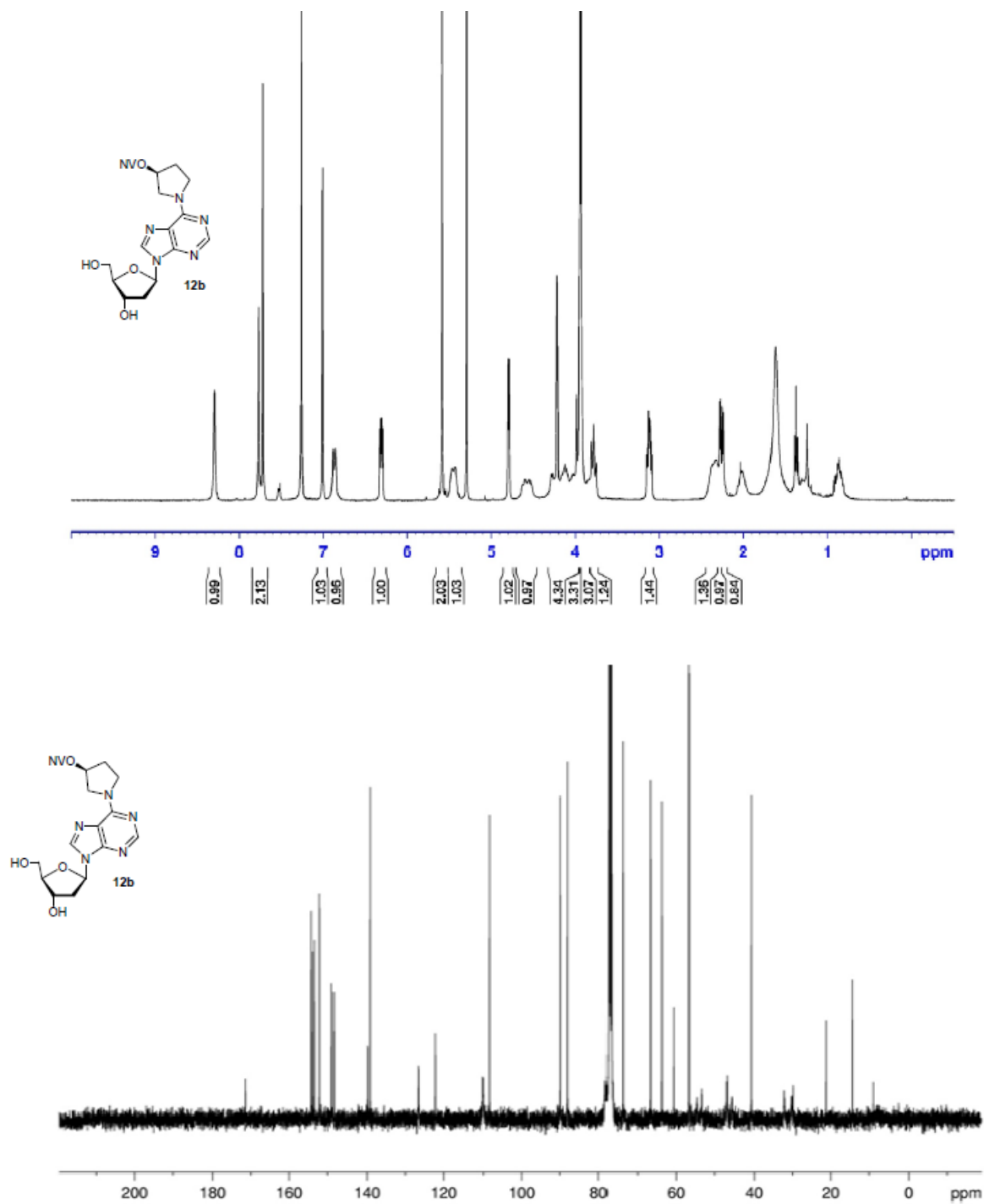


Figure S5. ^1H and ^{13}C NMR spectra of **12b**.

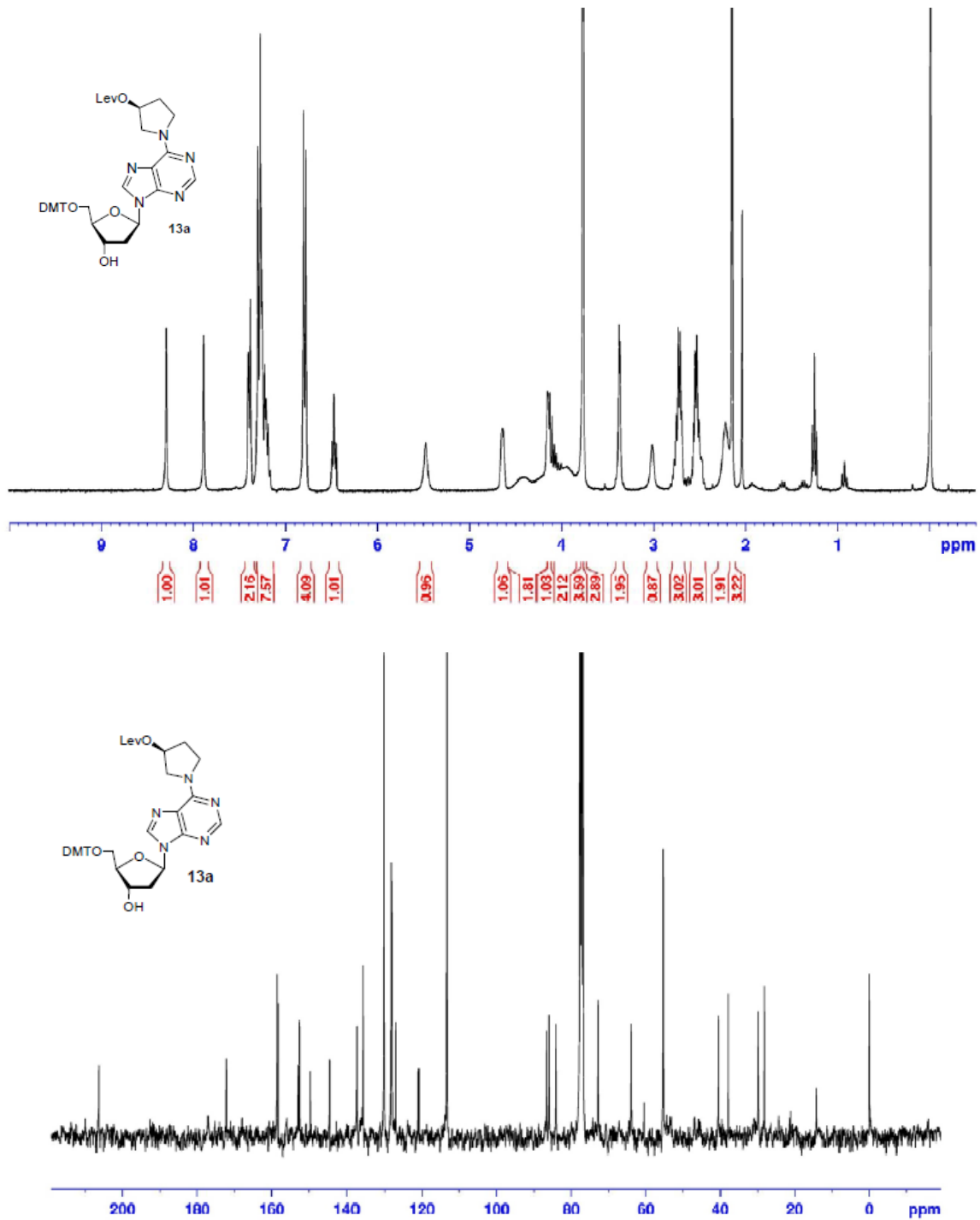


Figure S6. ¹H and ¹³C NMR spectra of 13a.

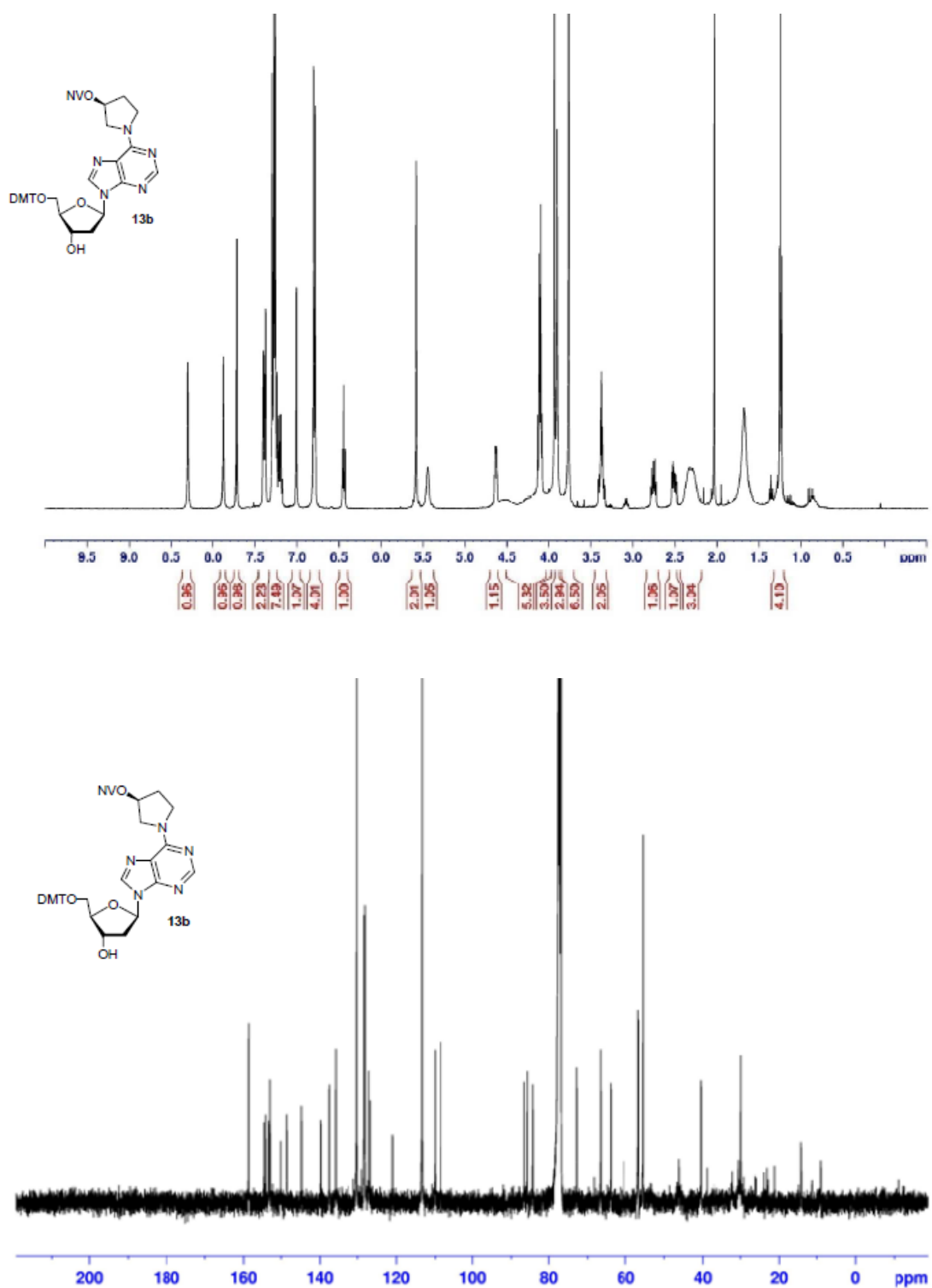


Figure S7. ^1H and ^{13}C NMR spectra of 13b.

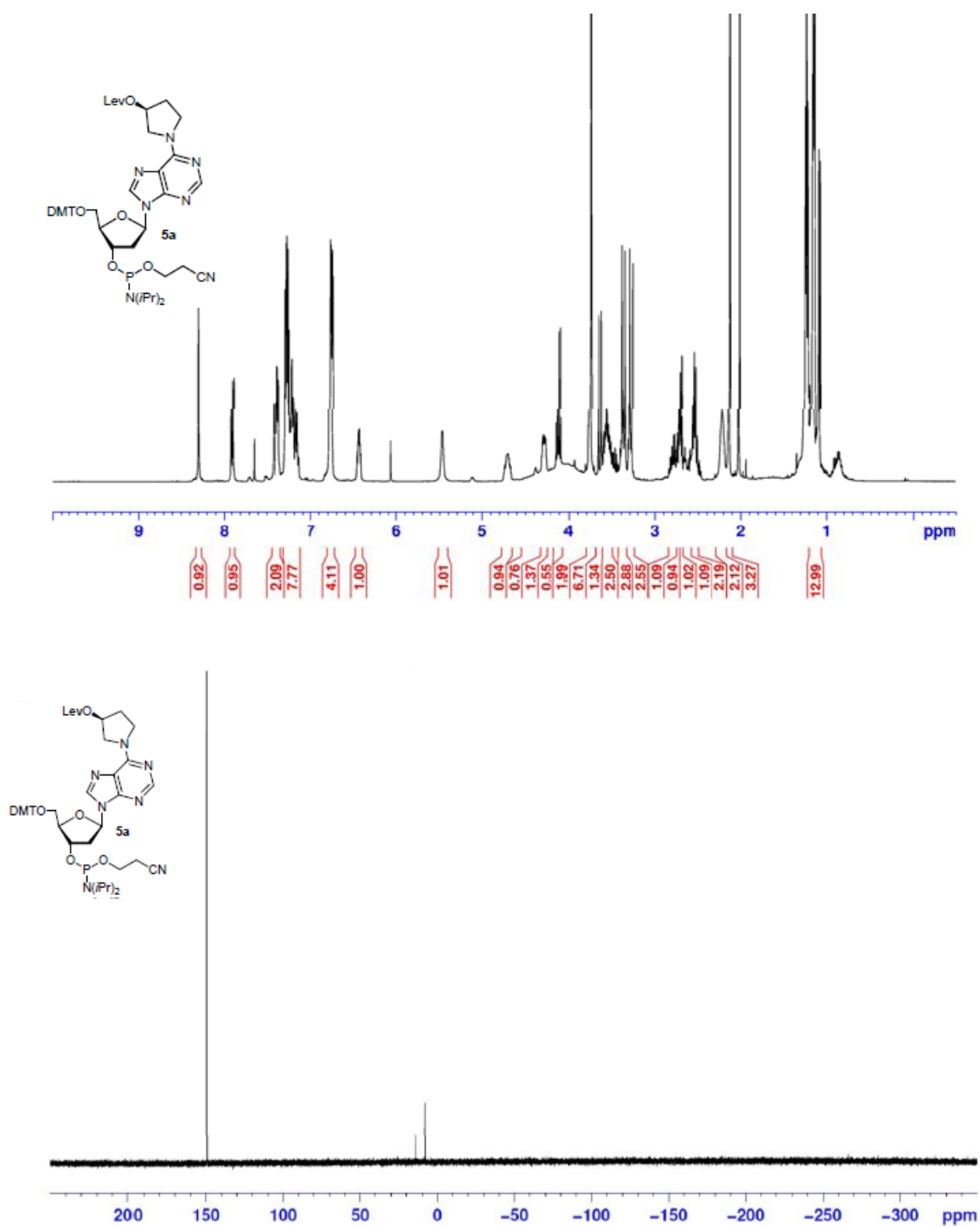


Figure S8. ^1H and ^{31}P NMR spectra of 5a.

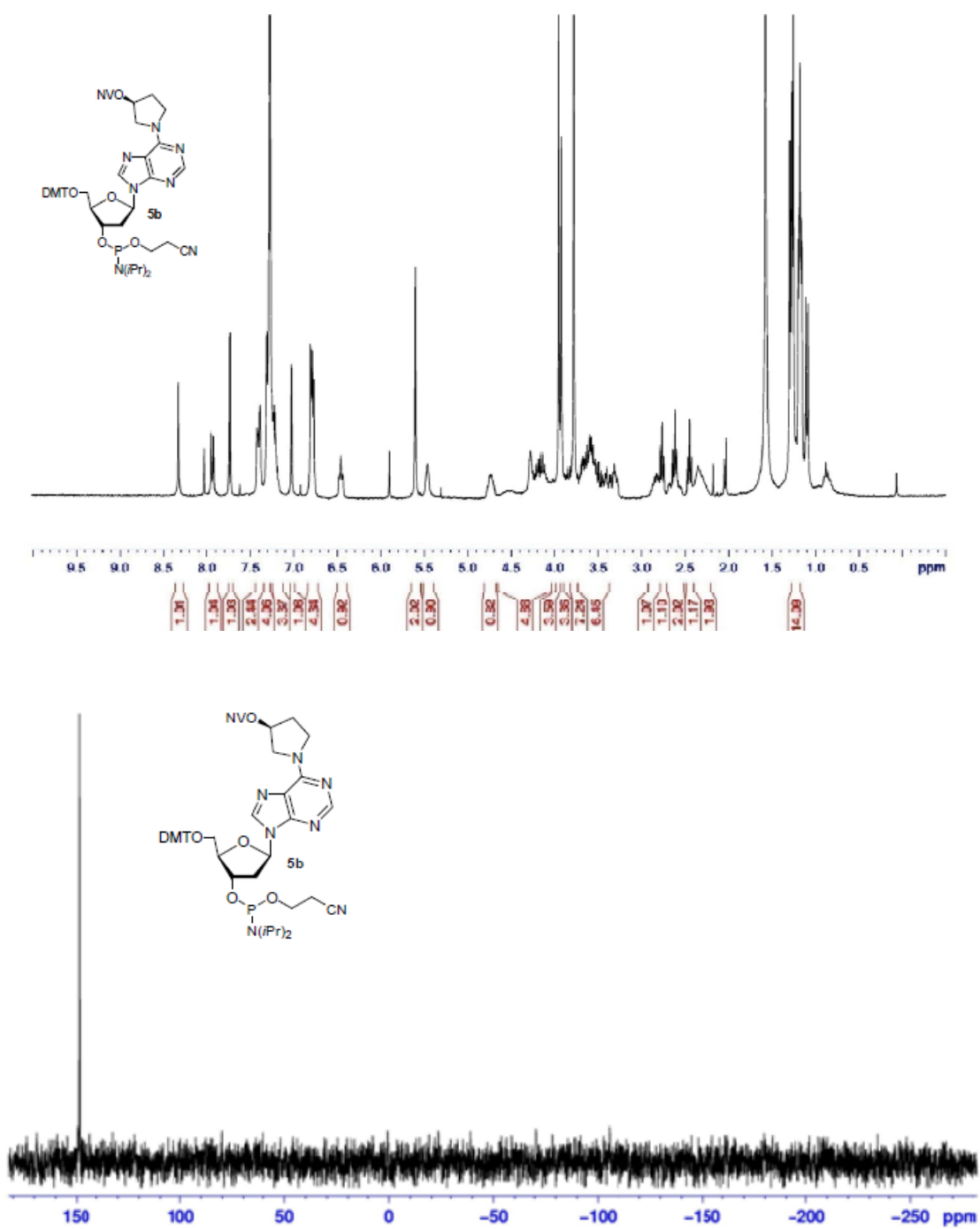


Figure S9. ¹H and ³¹P NMR spectra of **5b**.

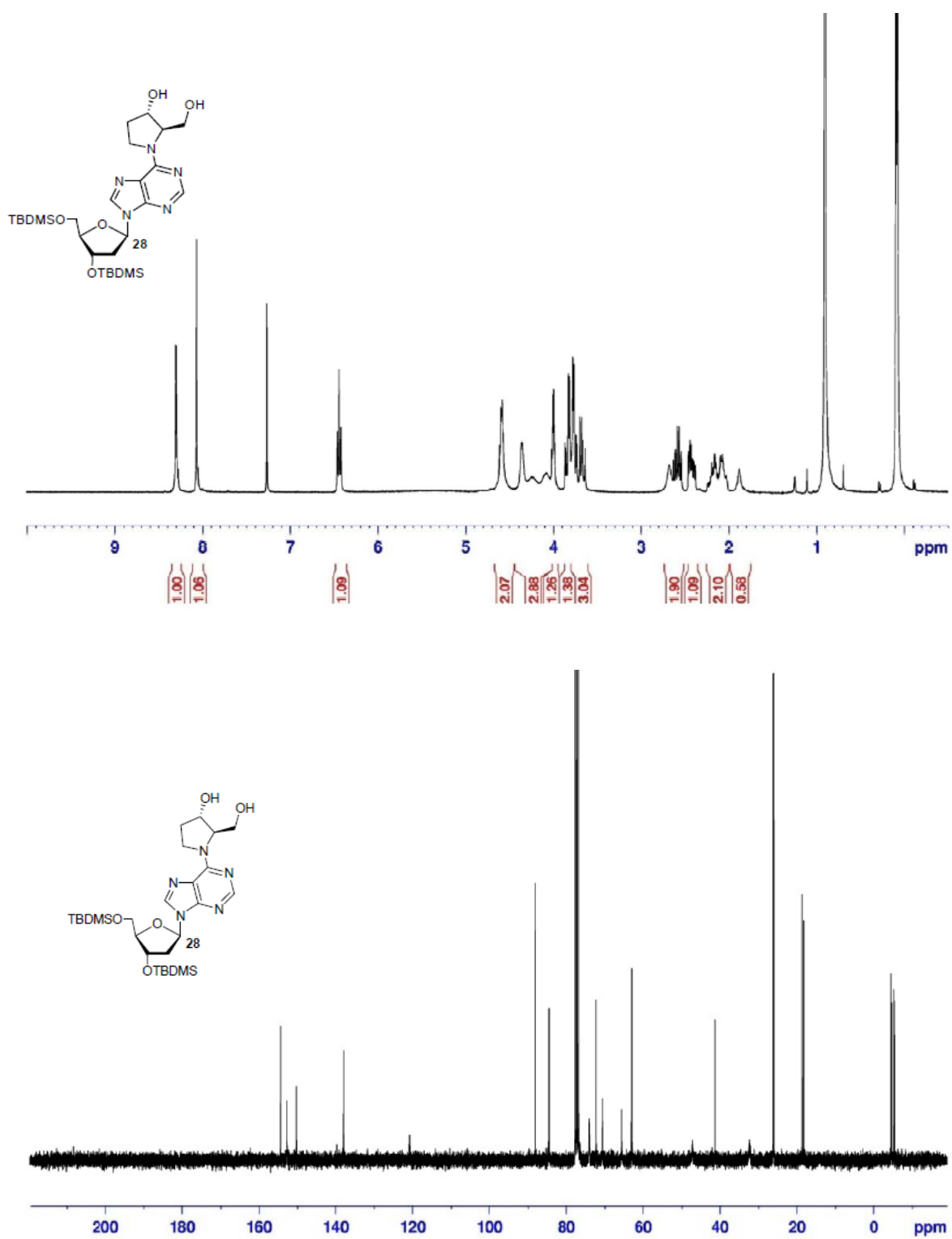


Figure S10. ^1H and ^{13}C NMR spectra of **28**.

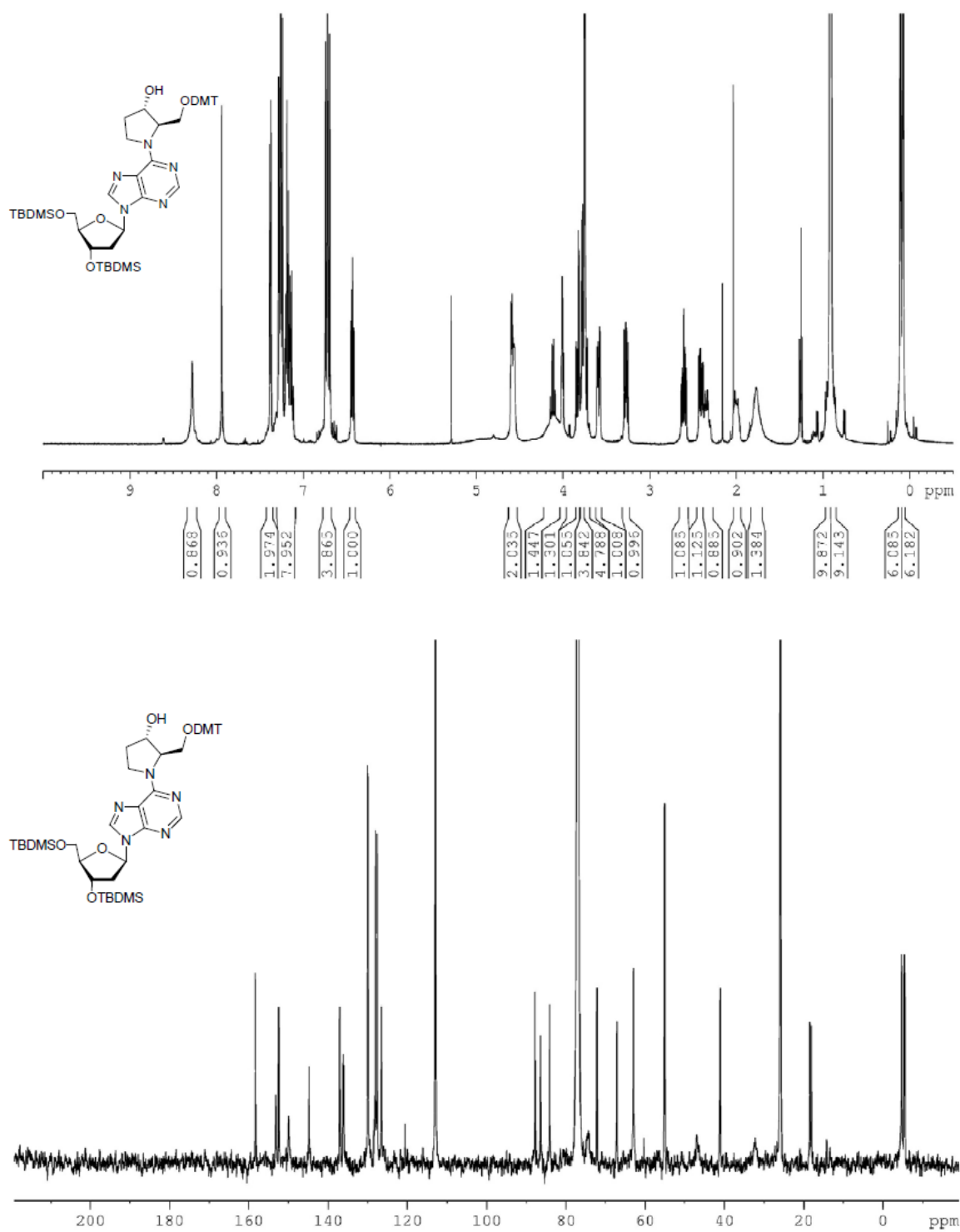


Figure S11. ^1H and ^{13}C NMR spectra of DMT protected **28**.

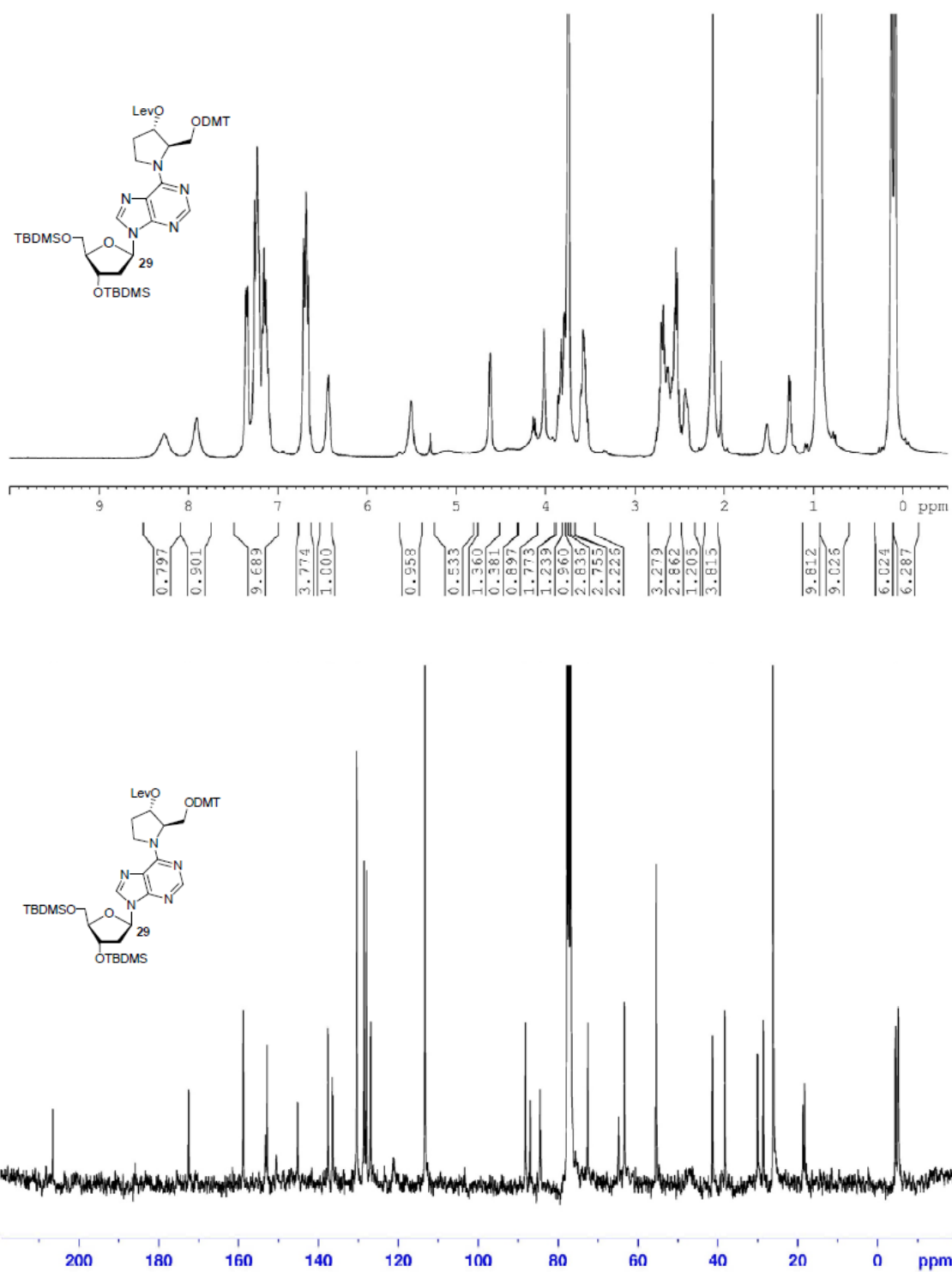


Figure S12. ^1H and ^{13}C NMR spectra of **29**.

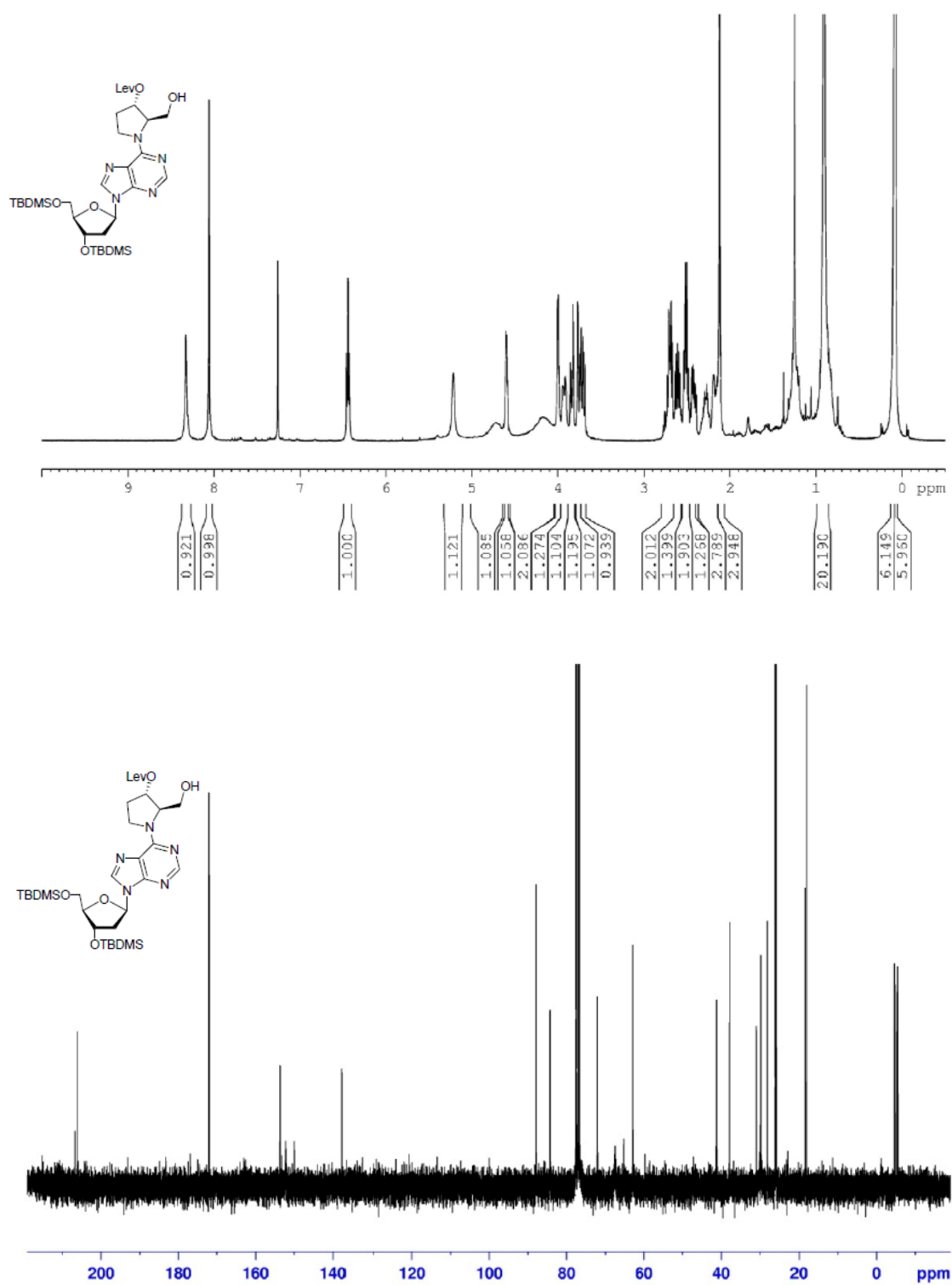


Figure S13. ¹H and ¹³C NMR spectra of DMT deprotected 29.

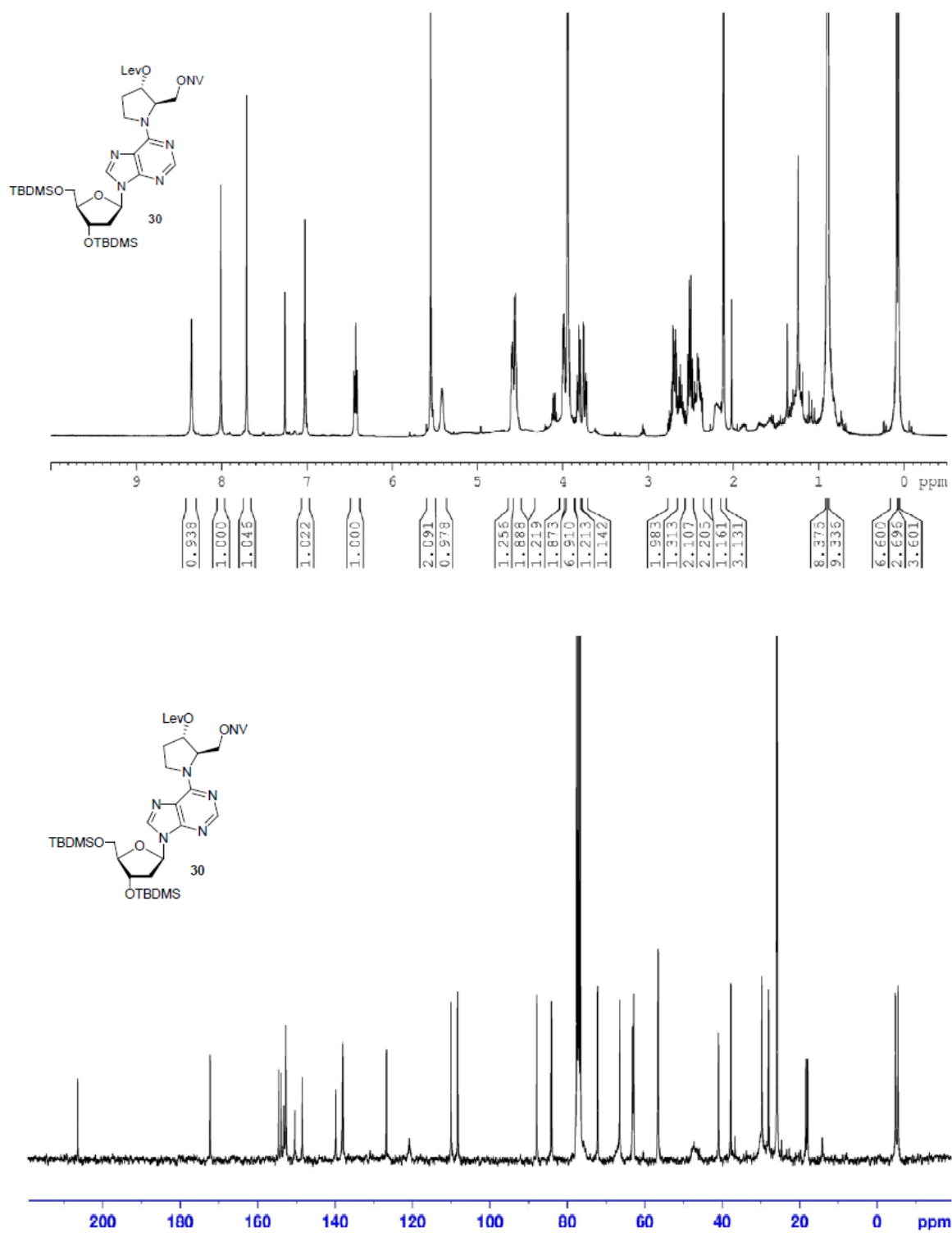


Figure S14. ^1H and ^{13}C NMR spectra of 30.

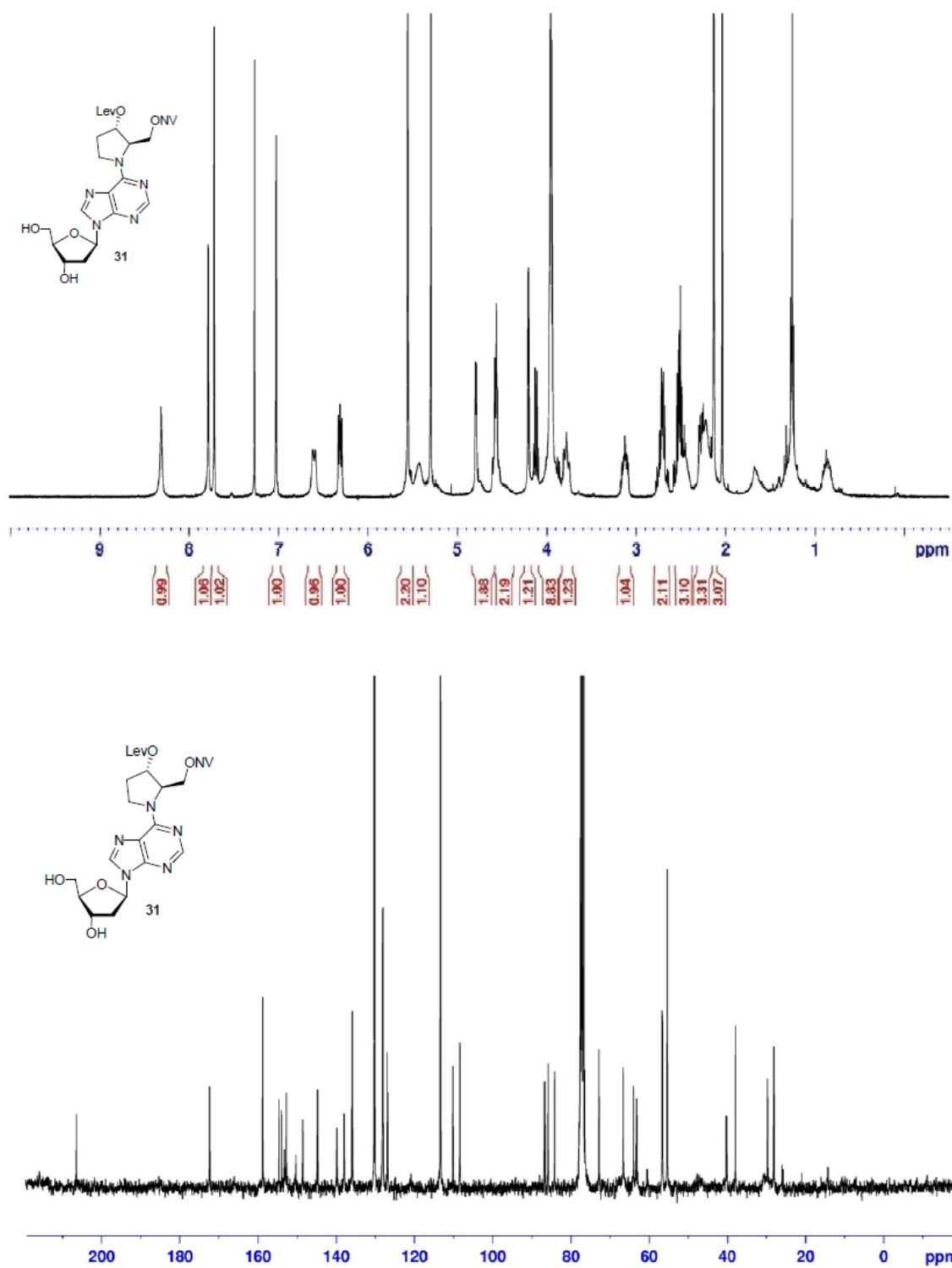


Figure S15. ^1H and ^{13}C NMR spectra of 31.

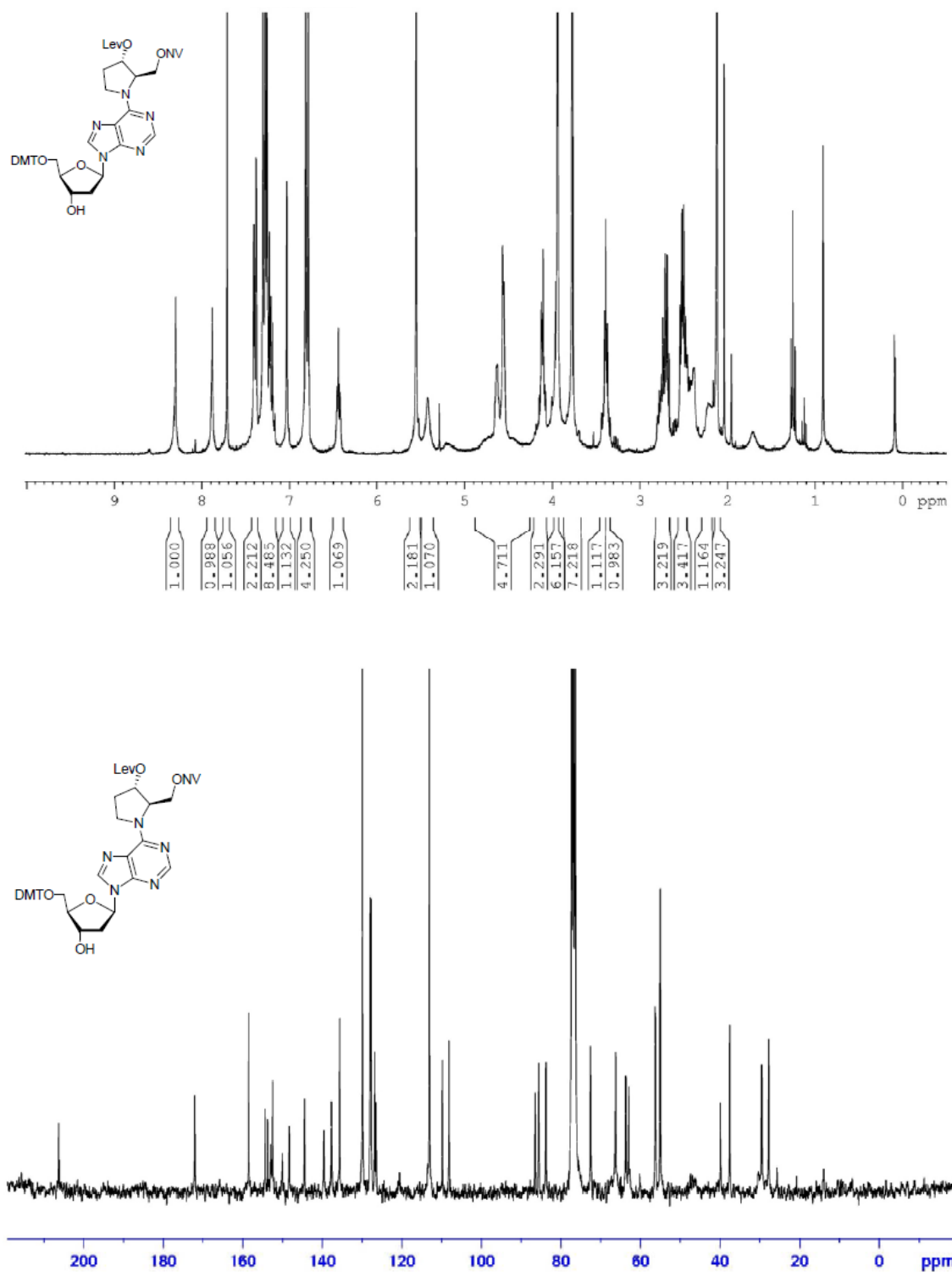


Figure S16. ^1H and ^{13}C NMR spectra of DMT protected 31.

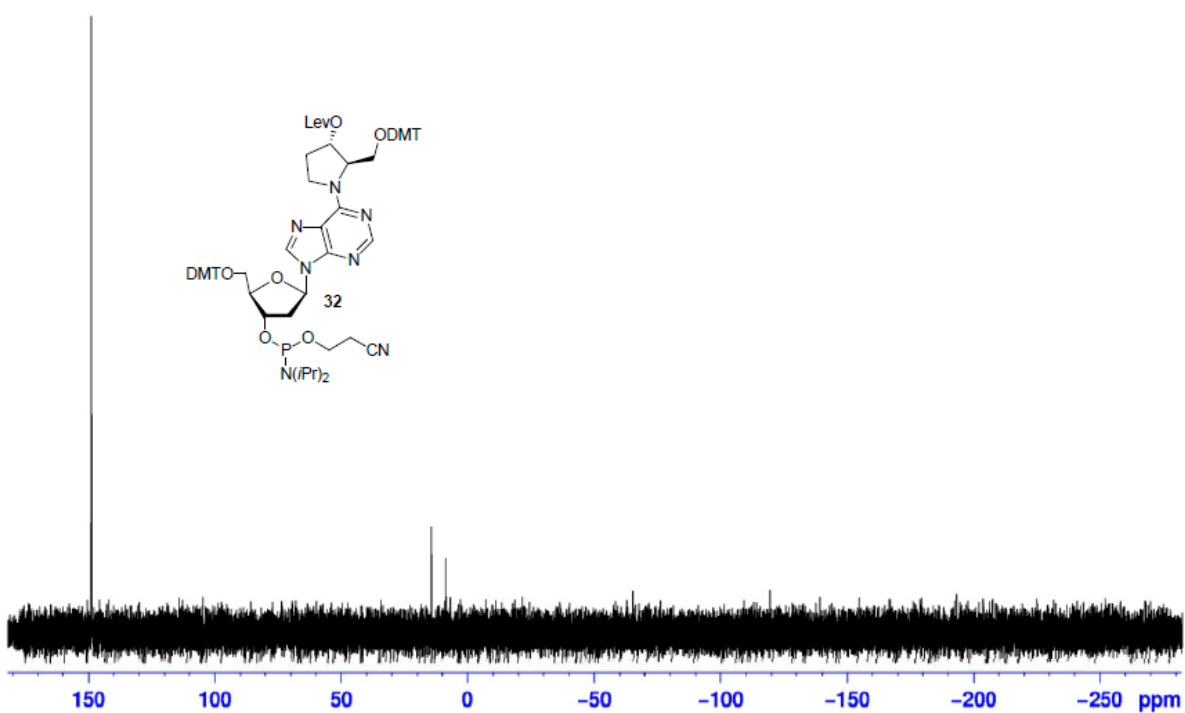
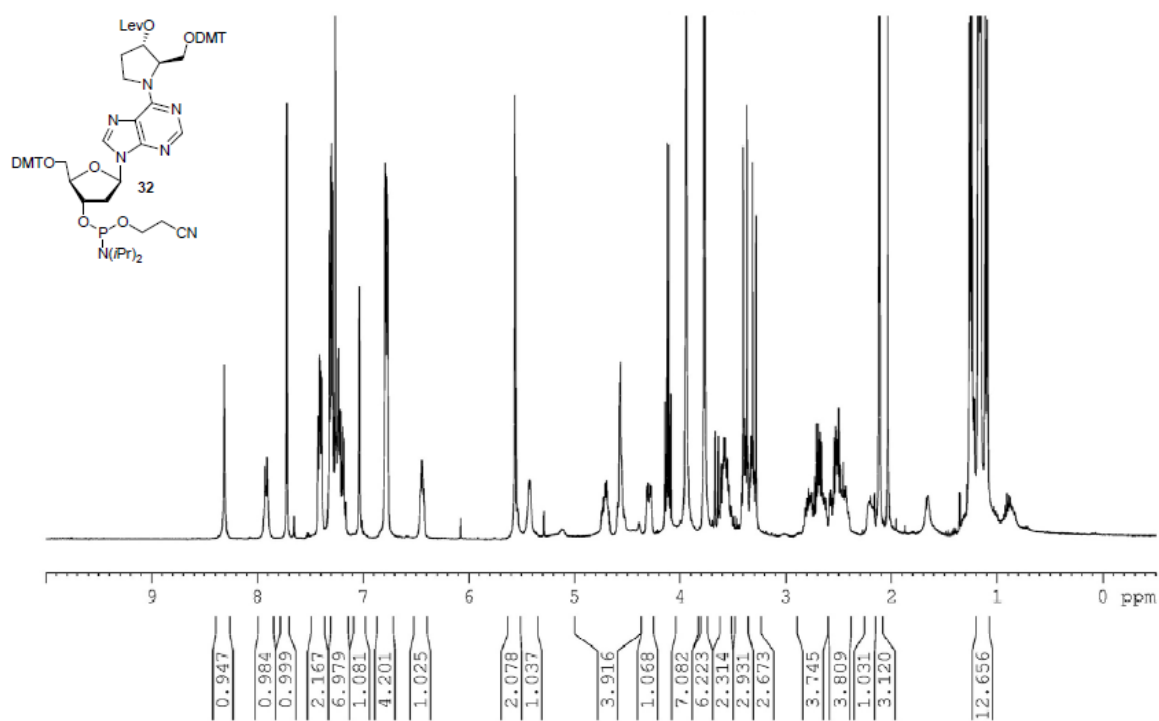


Figure S17. ¹H and ³¹P NMR spectra of 32.

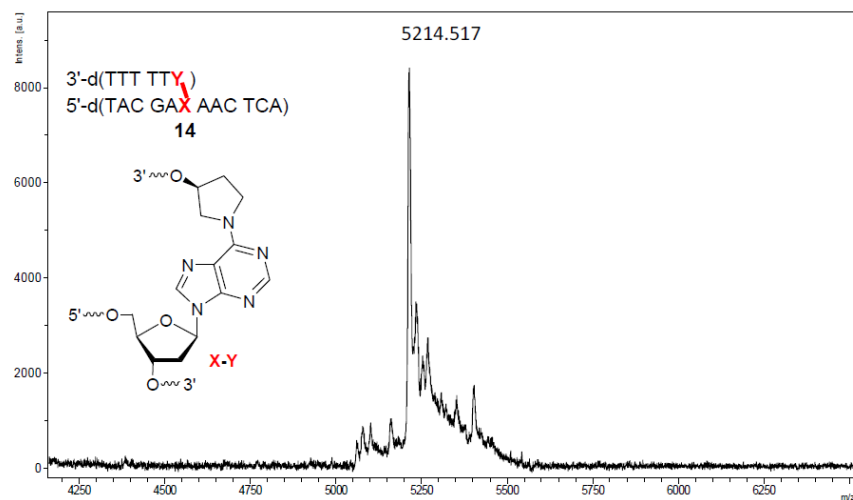


Figure S18. MALDI-TOF-MS of **14**. Calc'd mass 5213.422, observed mass 5214.517.

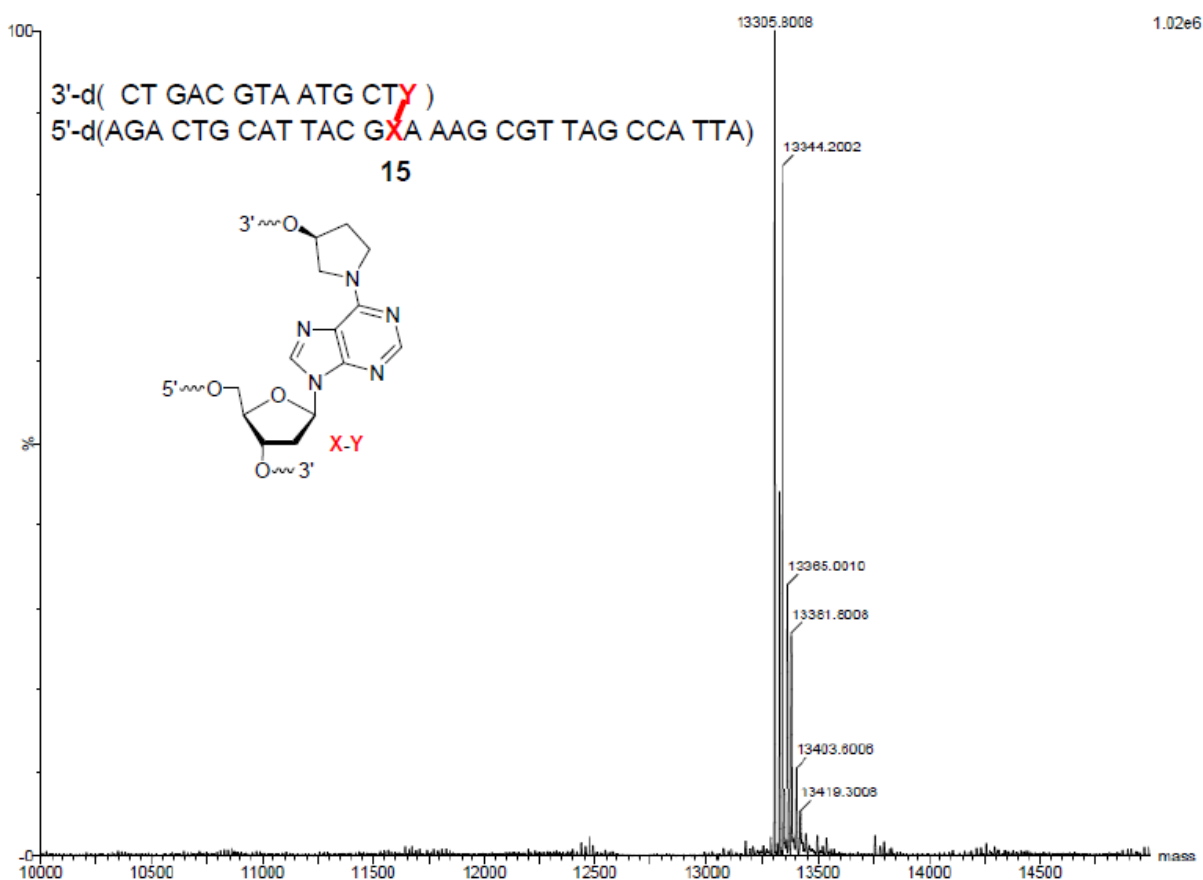


Figure S19. ESI-MS of **15**. Calc'd mass 13304.603, observed mass 13305.800, 13344.200 [M + K]⁺, 13365.001 [M + K + Na]⁺, 13381.800 [M + 2K]⁺, 13403.600 [M + 2K + Na]⁺, 13419.300 [M + 3K]⁺.

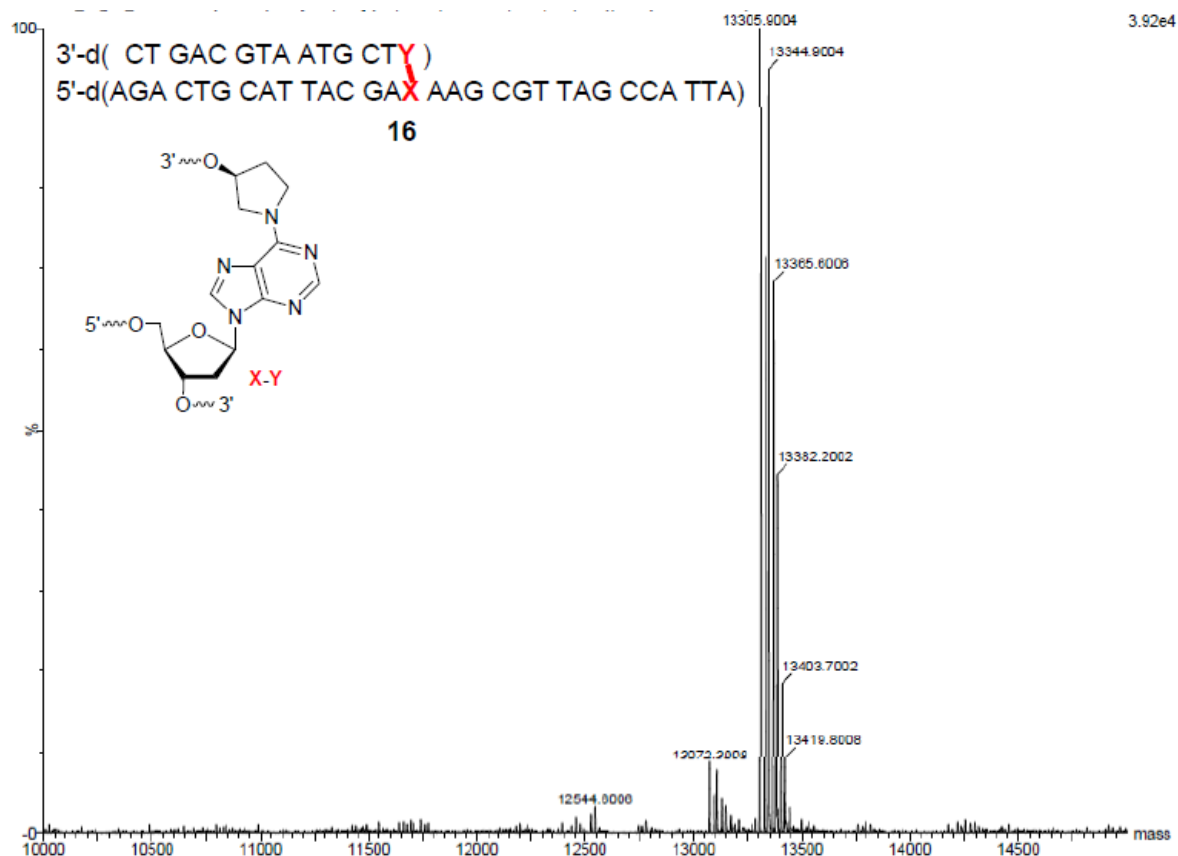


Figure S20. ESI-MS of **16**. Calc'd mass 13304.603, observed mass 13305.900, 13344.900 [M + K]⁺, 13365.601 [M + K + Na]⁺, 13382.200 [M + 2K]⁺, 13403.700 [M + 2K + Na]⁺, 13419.800 [M + 3K]⁺.

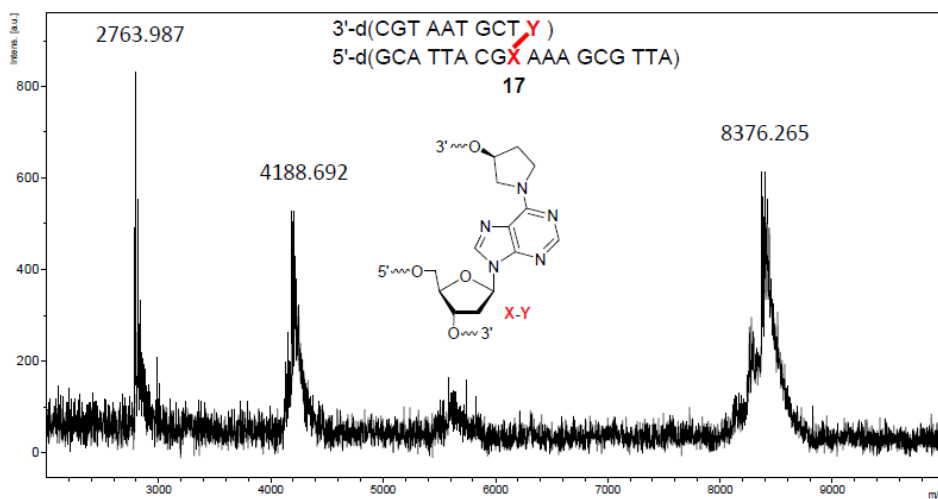


Figure S21. MALDI-TOF-MS of **17**. Calc'd mass 8377.514, observed mass 2763.987 ($z = -3$), 4188.692 ($z = -2$), 8376.265.

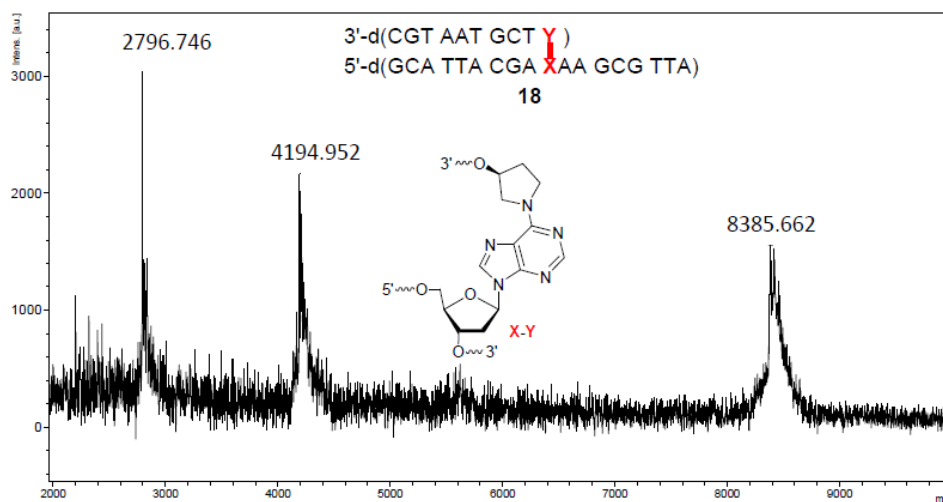


Figure S22. MALDI-TOF-MS of **18**. Calc'd mass 8377.514, observed mass 2796.987 ($z = -3$), 4194.692 ($z = -2$), 8385.662.

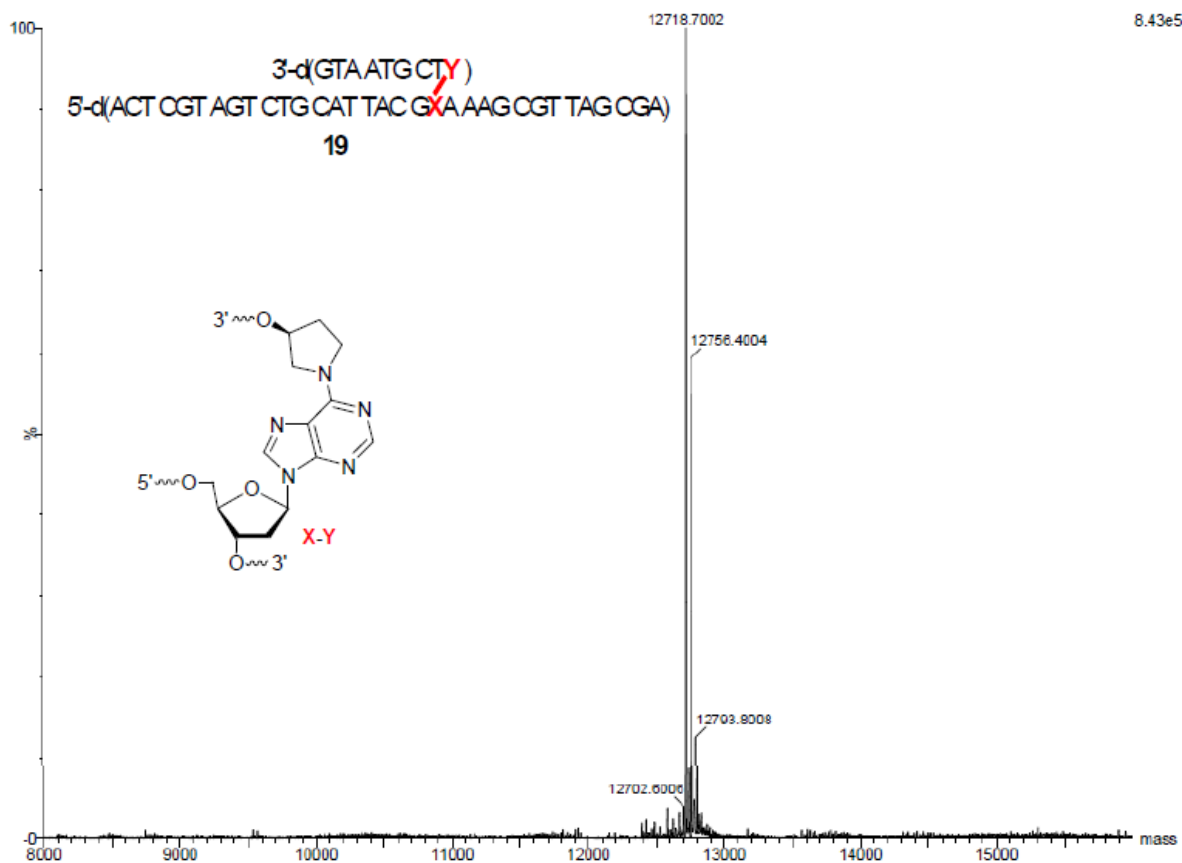


Figure S23. ESI-MS of **19**. Calc'd mass 12718.312, observed mass 12718.700, 12756.400 [$M + K$]⁺, 12793.800 [$M + 2K$]⁺.

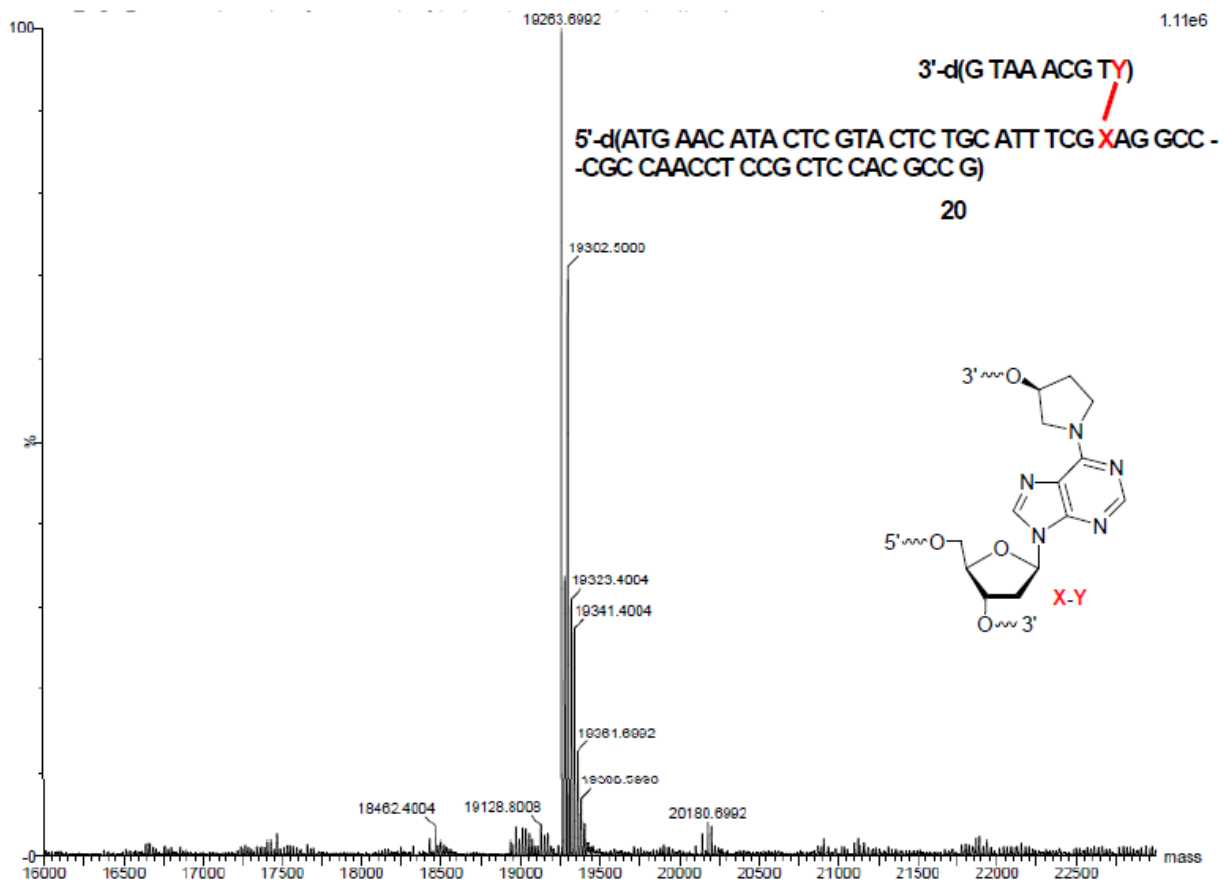


Figure S24. ESI-MS of **20**. Calc'd mass 19262.492, observed mass 19263.699, 19302.500 [M + K]⁺, 19223.400 [M + K + Na]⁺, 19341.400 [M + 2K]⁺, 19361.699 [M + 2K + Na]⁺, 19380.599 [M + 3K]⁺.

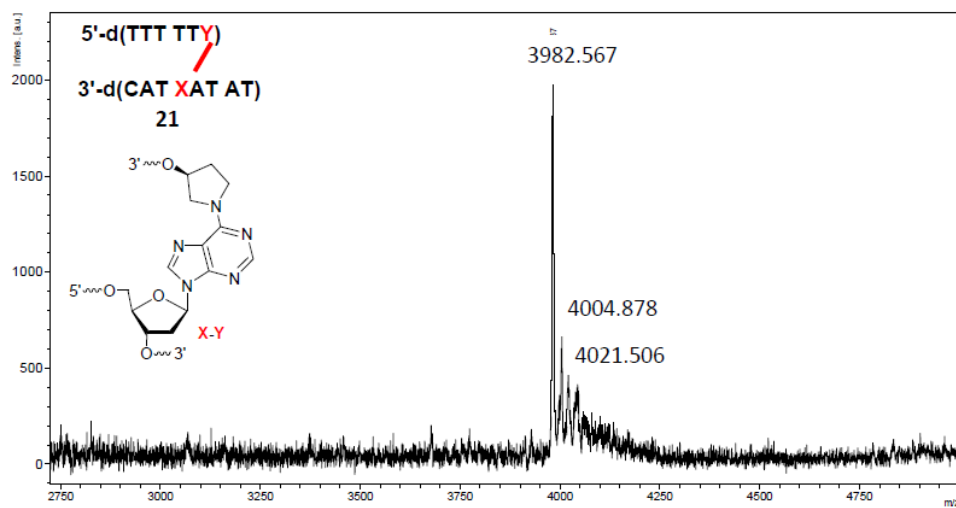


Figure S25. MALDI-TOF-MS of **21**. Calc'd mass 3983.611, observed mass 3982.567, 4004.878 [M + Na]⁺, 4021.506 [M + K]⁺.

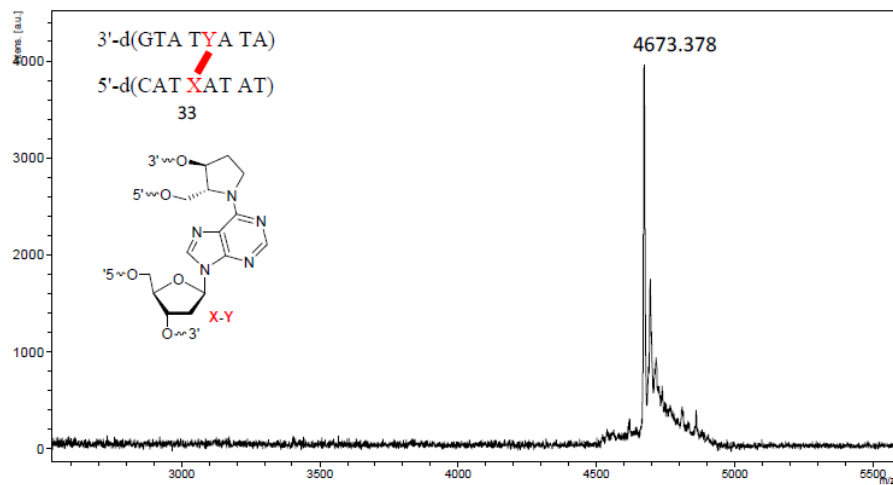


Figure S26. MALDI-TOF-MS of **33**. Calc'd mass 4674.102, observed mass 4673.378.

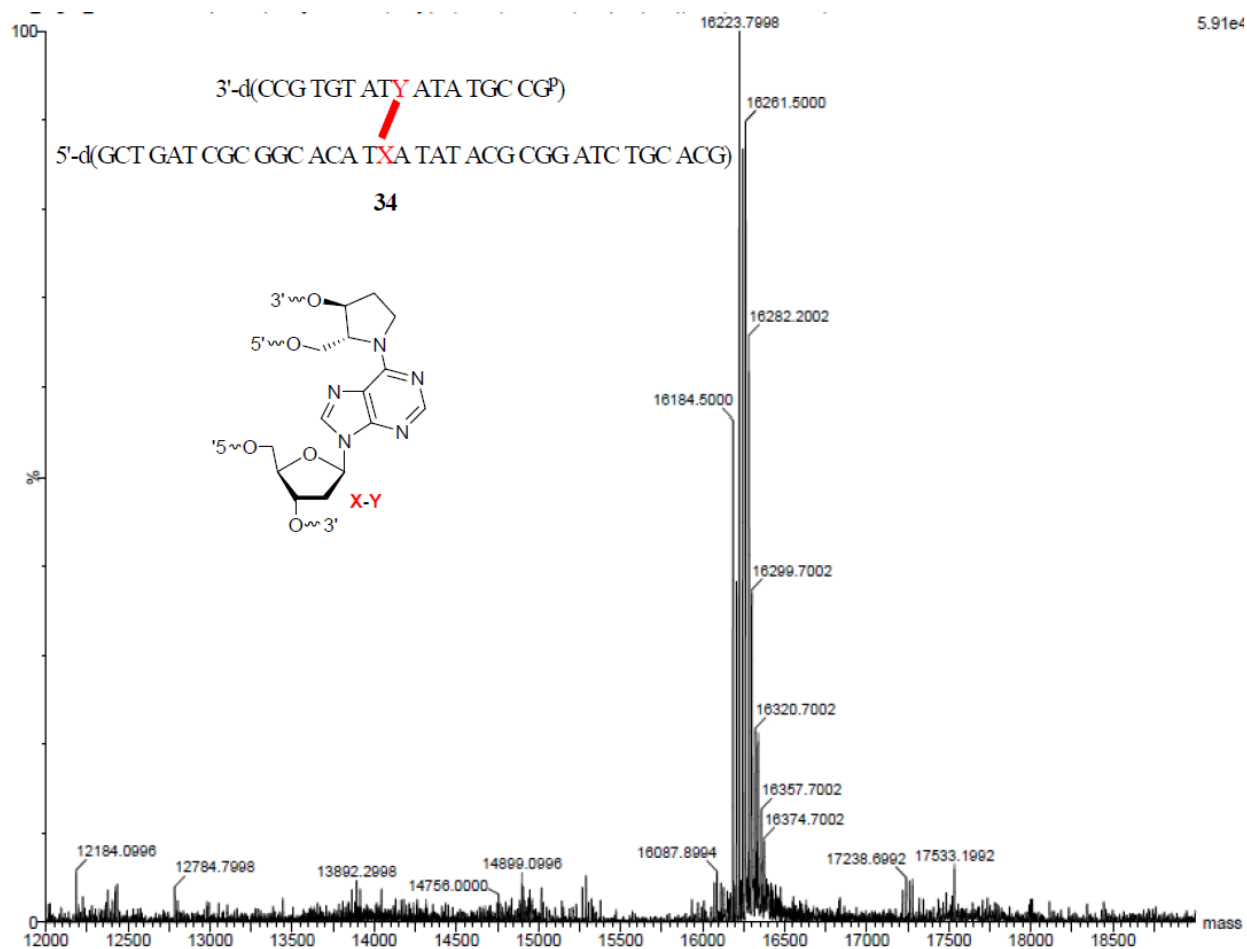


Figure S27. ESI-MS of **34**. Calc'd mass 16182.485, observed mass 16184.500, 16223.799 [M + K]⁺, 16261.500 [M + 2K]⁺, 16282.200 [M + 2K + Na]⁺, 16299.700 [M + 3K]⁺, 16320.700 [M + 3K + Na]⁺, 16357.700 [M + 4K + Na]⁺, 16374.700 [M + 5K]⁺.

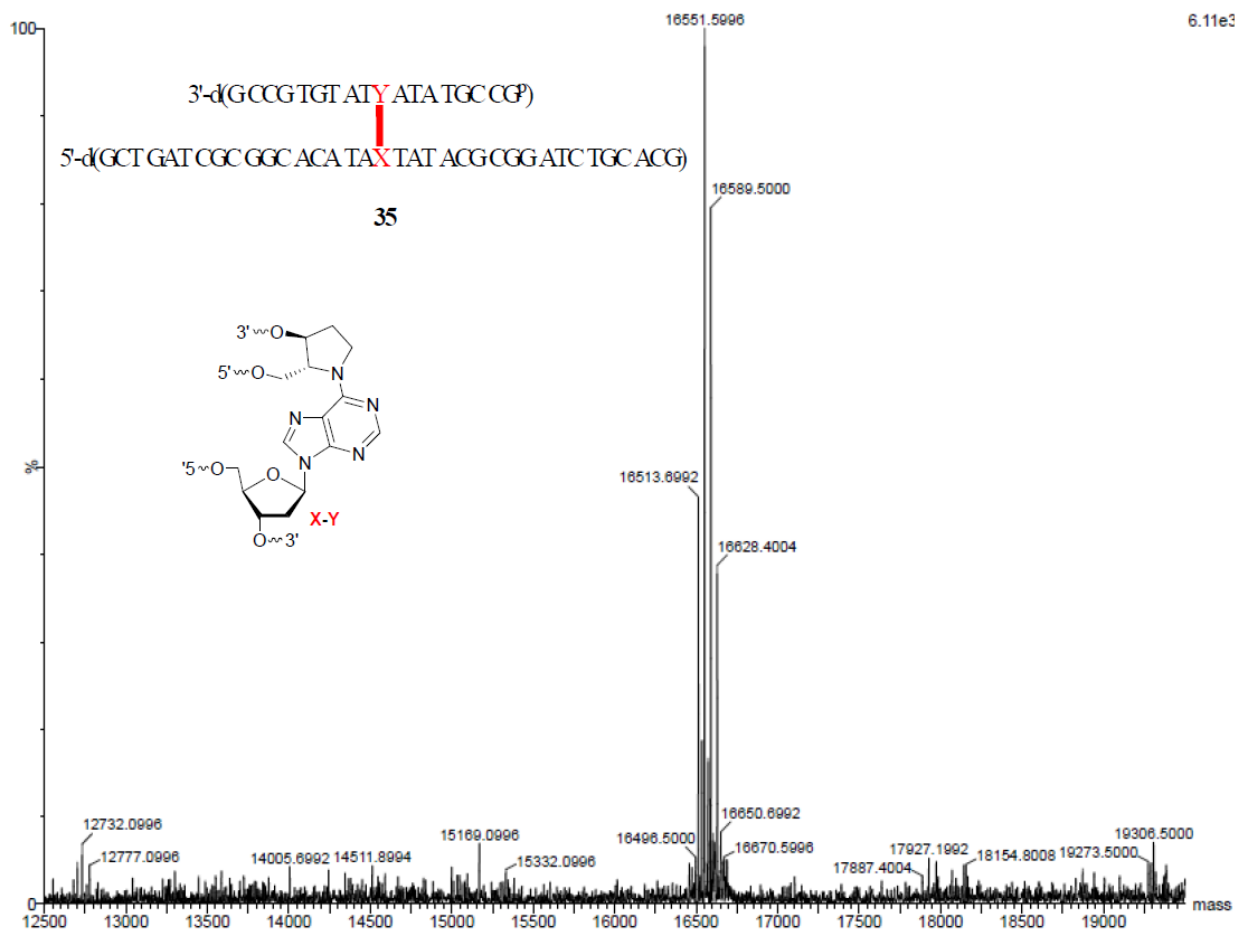


Figure S28. ESI-MS of **35**. Calc'd mass 16511.658, observed mass 16513.699, 16551.599 [M + K]⁺, 16589.500 [M + 2K]⁺, 16628.400 [M + 3K]⁺.

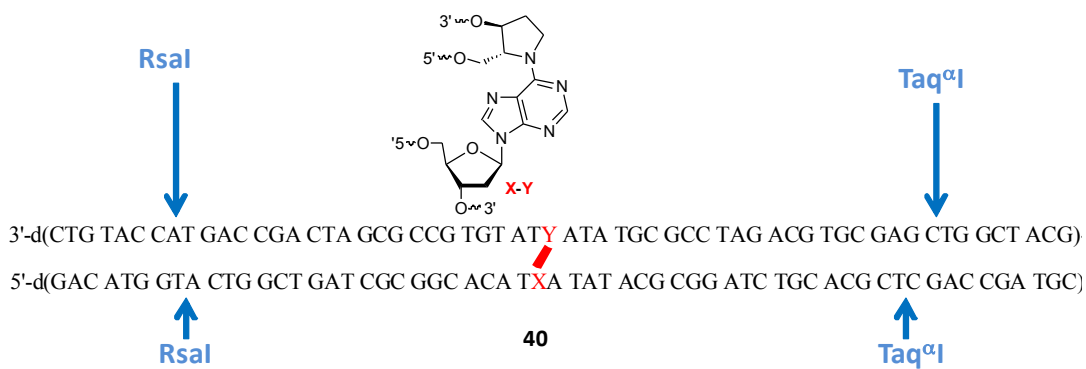


Figure S29. RsaI and Taq^I restriction enzyme sites on **40**.

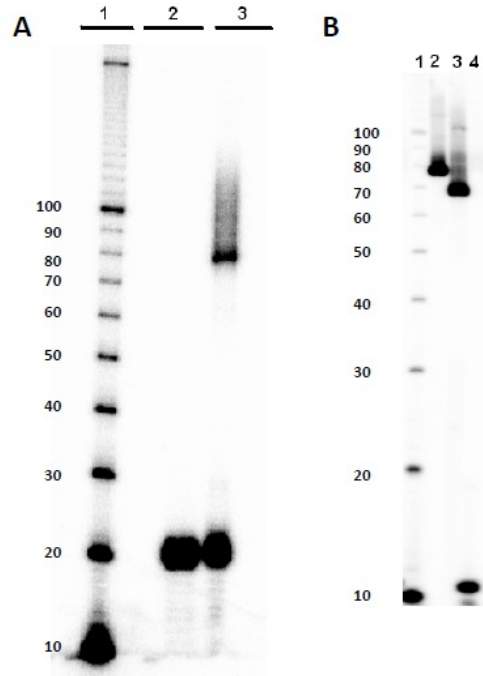


Figure S30. Ligation for constructing 5'-³²P-40 and restriction enzyme treatment of purified 5'-³²P-40. (Panel A) Representative 12% denaturing PAGE gel showing the ligation to construct 5'-³²P-40. Lane 1, 10 base pair DNA ladder. Lane 2, 5'-³²P-38. Lane 3, crude reaction to produce 5'-³²P-40. (Panel B) Representative 15% denaturing PAGE gel analysis of restriction enzyme treatment of purified 5'-³²P-40. Lane 1, 10 base pair DNA ladder. Lane 2, 5'-³²P-40 without any treatment. Lane 3, 5'-³²P-40 treated with RsaI. Lane 4, 5'-³²P-40 treated with TaqI.