SUPPORTING INFORMATION

for

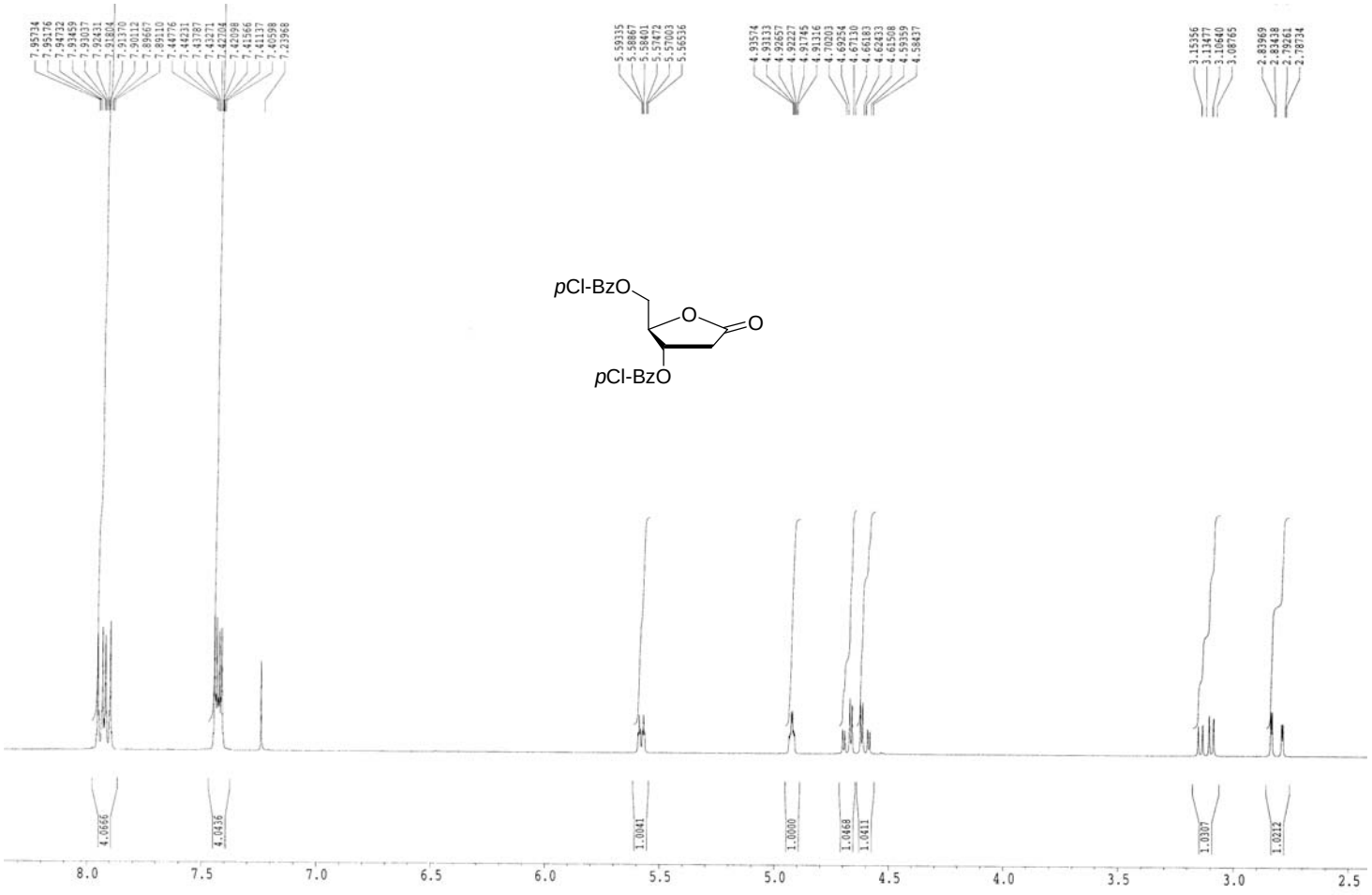
Diastereocontrolled Electrophilic Fluorination of 2-Deoxyribonolactone: Syntheses of All Corresponding 2-Deoxy-2-fluoro-lactones and 2'-Deoxy-2'-fluoro-NAD$^+$s

By Yana Cen, Anthony A. Sauve*

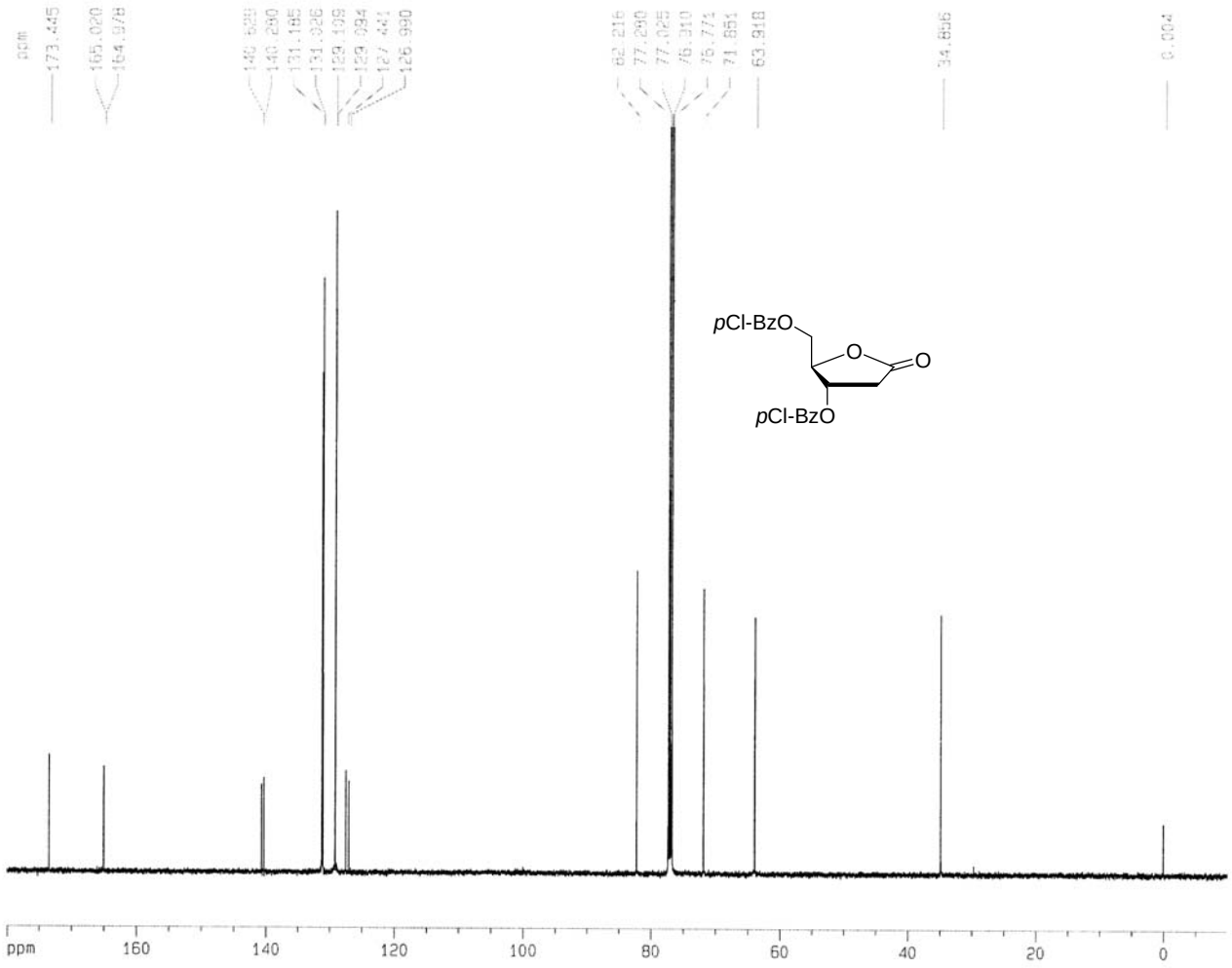
General S2
^{1}H and ^{13}C NMR spectra S3-

General

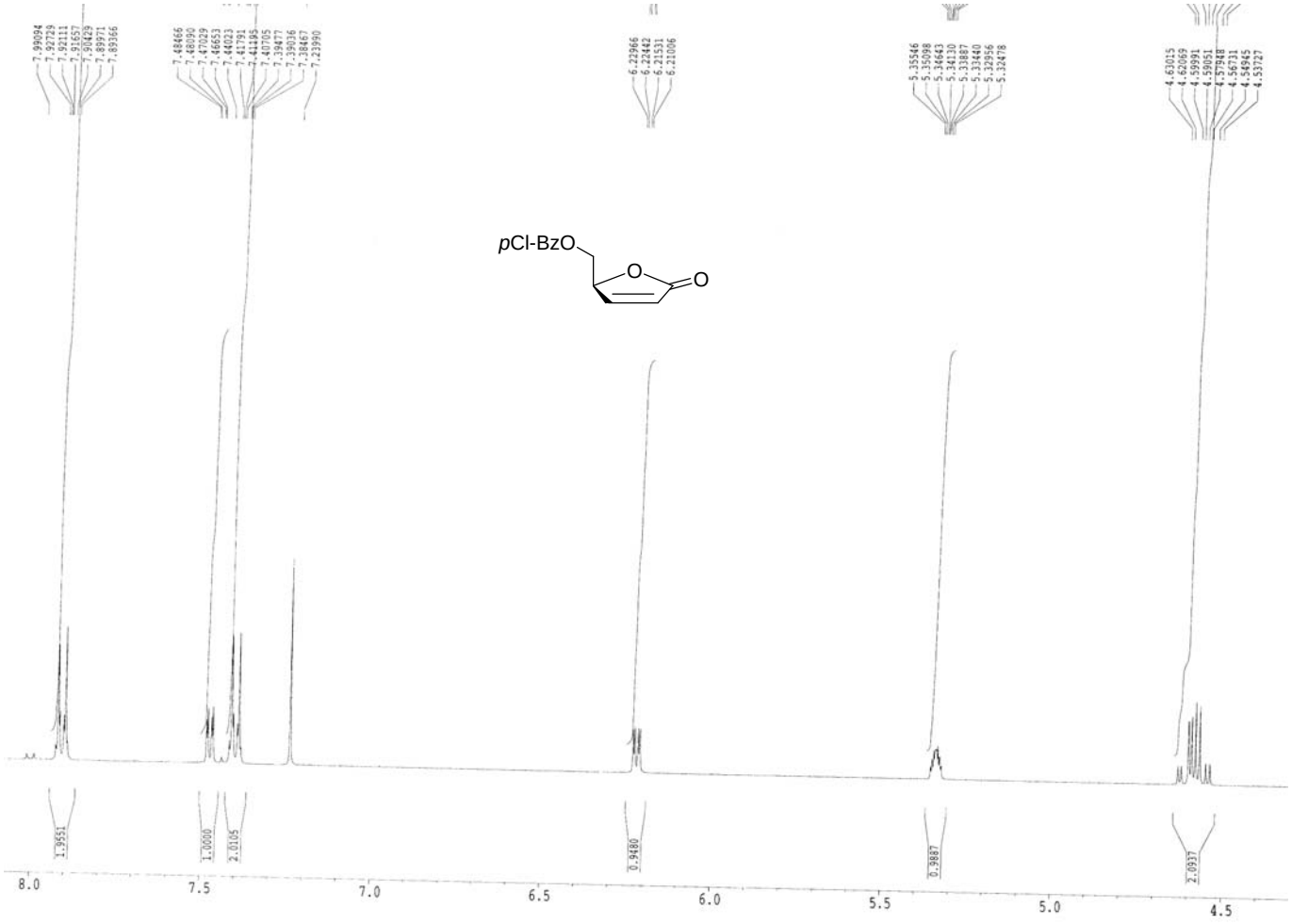
^{1}H and ^{13}C NMR spectra were obtained using either a 400 MHz, 500 MHz or a 600 MHz spectrometer. Melting points were uncorrected. 2-deoxy-1-methyl-3,5-di-*O*-(*p*-chlorobenzoyl)-D-ribofuranose was prepared by the method of Fox.[47] Pyrophosphatase was purchased from New England Biolabs (M0296S).Yeast nicotinamide mononucleotide adenyltransferase was cloned from yeast genomic DNA and integrated into a pet28 bacterial expression vector and expressed in CodonPlus (Stratagene) cells. After induction with 1mM IPTG for three hours, cells were pelleted and resuspended in 10 pellet volumes of 10 mM Tris buffer 500 mM NaCl pH 7.5 containing 10000 units of egg white lysozyme (Sigma, L6876) and broken by 3 freeze-thaw cycles. 50 units of DNase (Sigma, D4263) and $MgCl_2$ (final concentration 25 mM) were then added to destroy DNA and the lysate mixed until non-viscous. The lysate was pelleted again and the supernatant was incubated on nickel chelating resin (Gbiosciences 786-281) and purified by Ni-affinity chromatography using imidazole as an eluant. The purified protein was flash frozen in 20% glycerol and 2.5 mM DTT for later use.



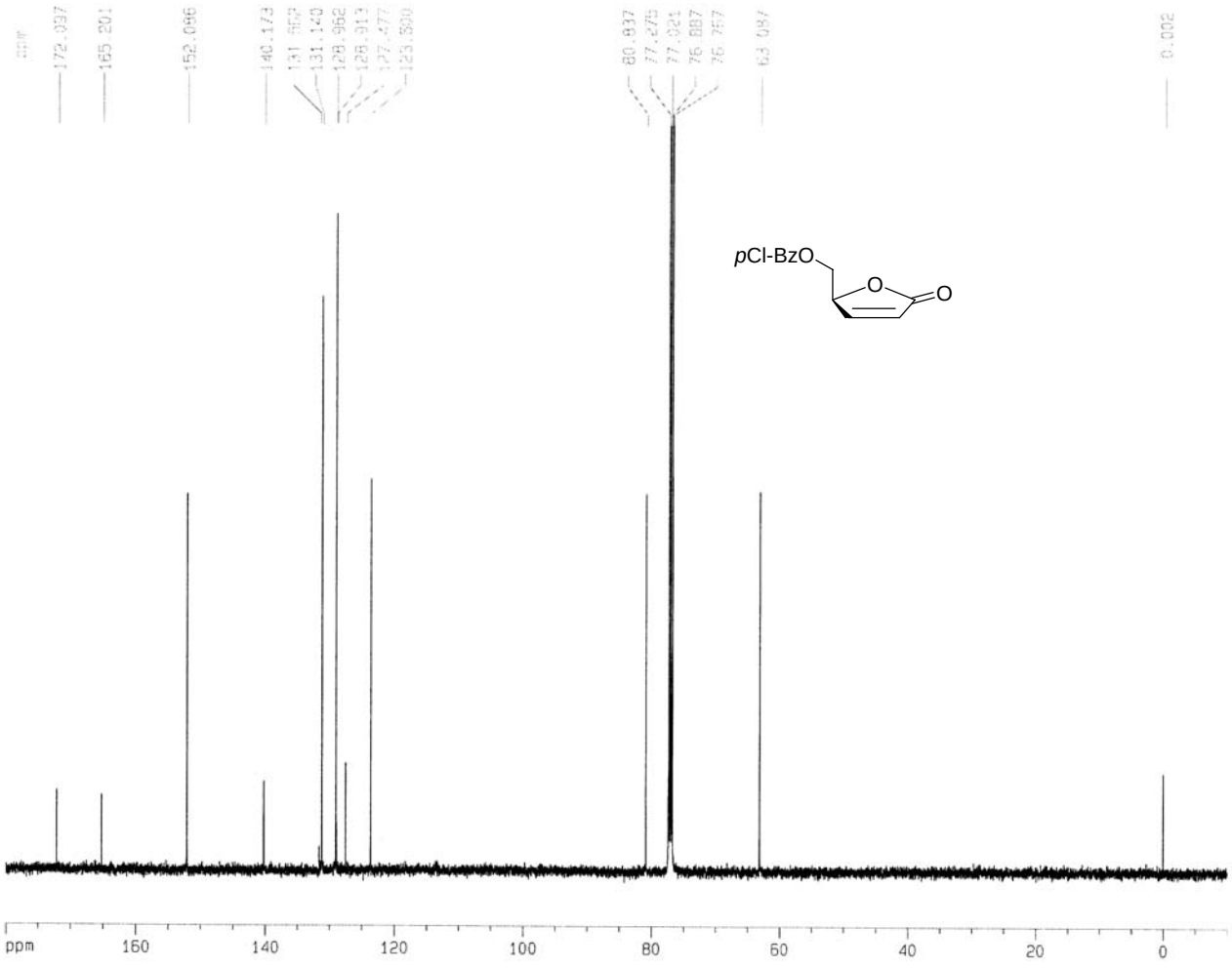
^{1}H NMR spectrum of **5**



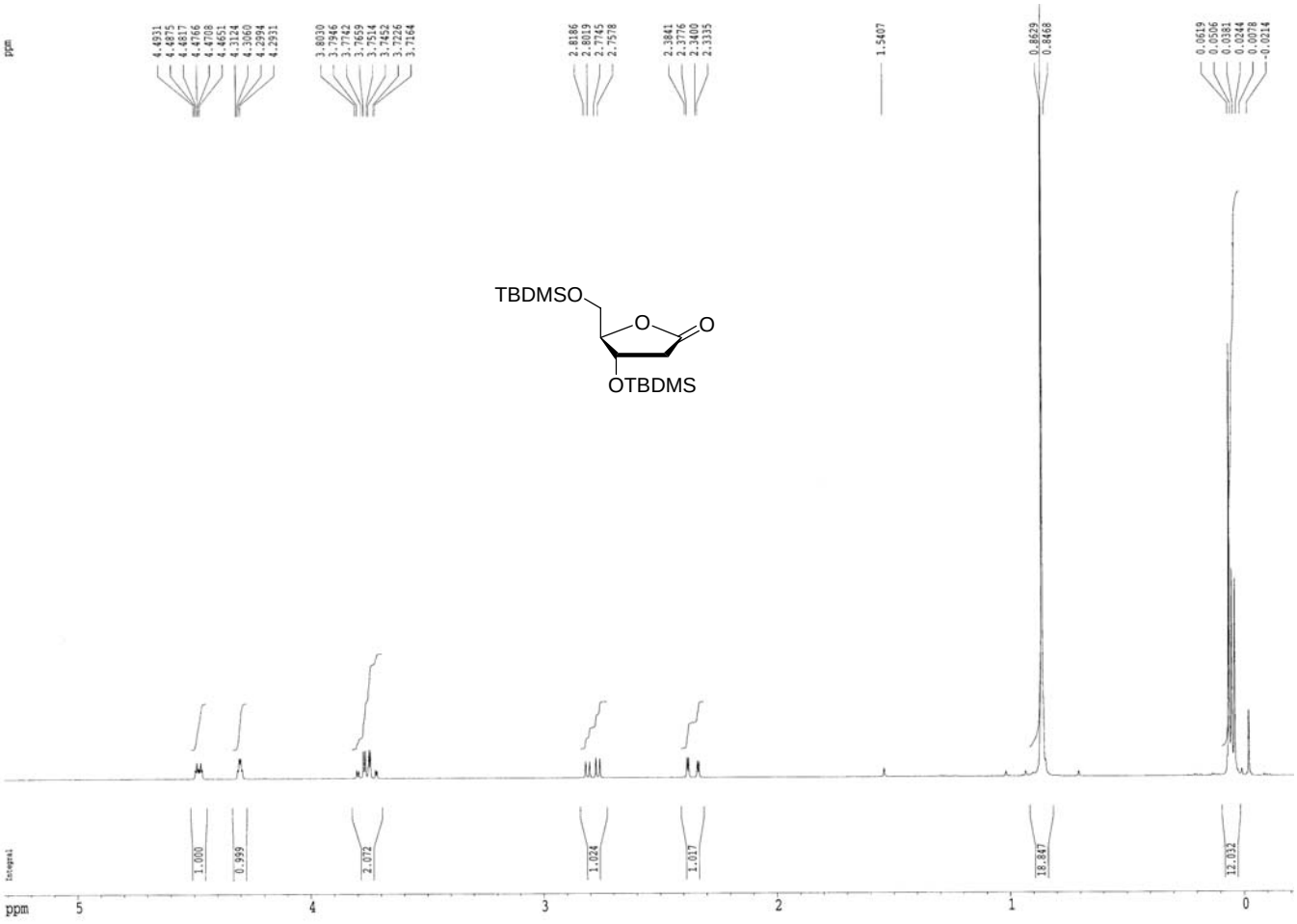
^{13}C NMR spectrum of **5**



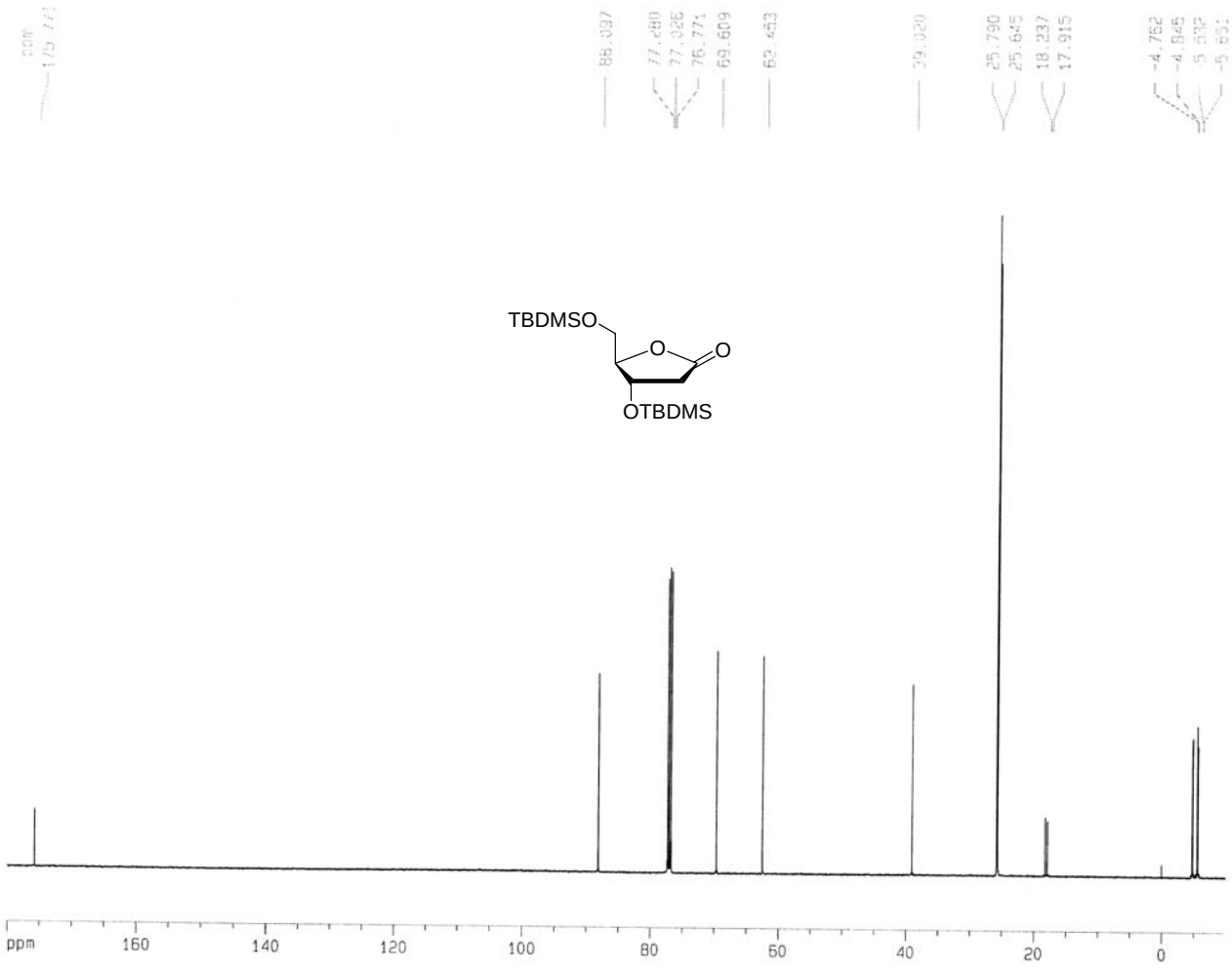
^{1}H NMR spectrum of **6**



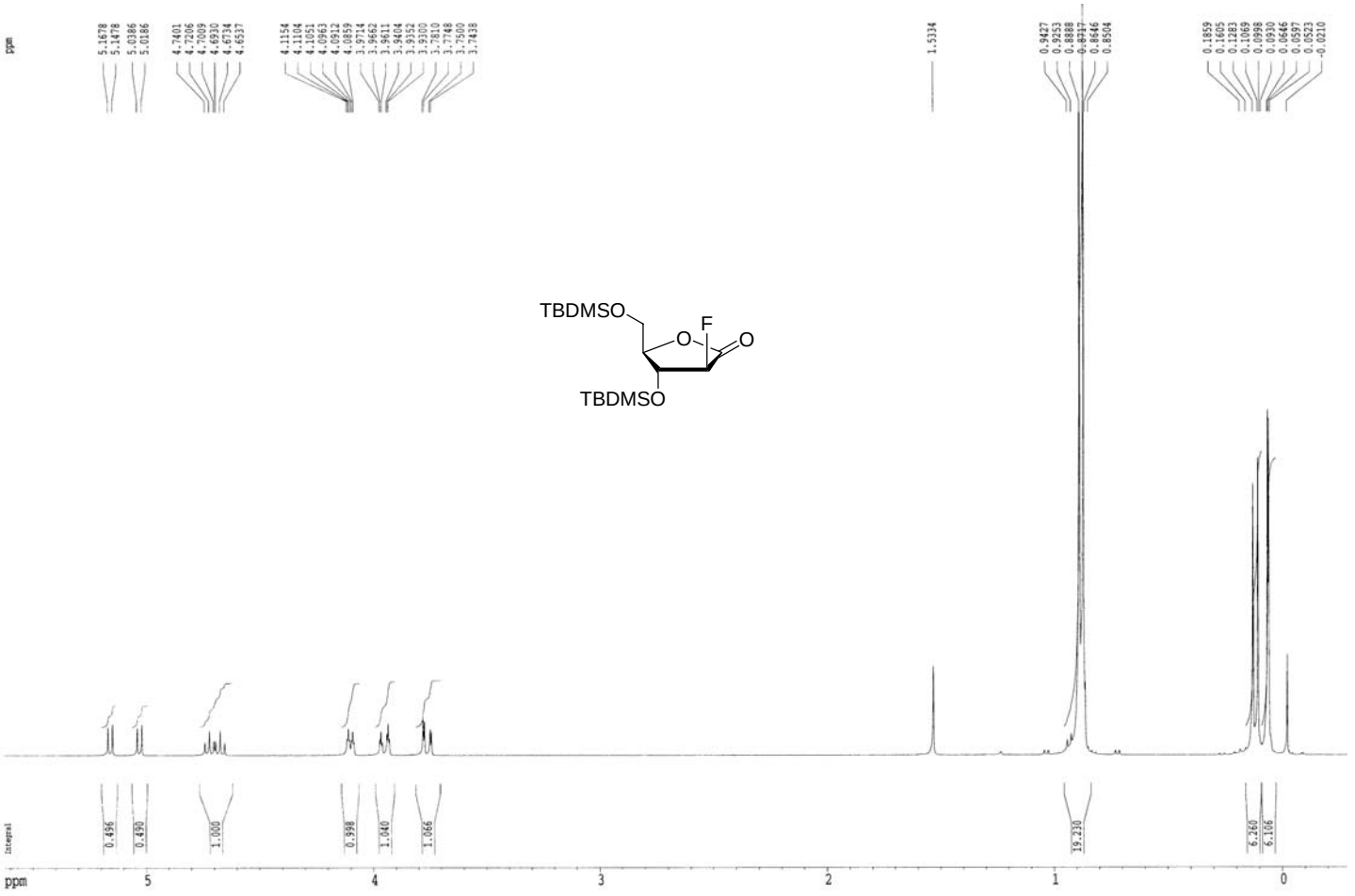
^{13}C NMR spectrum of **6**



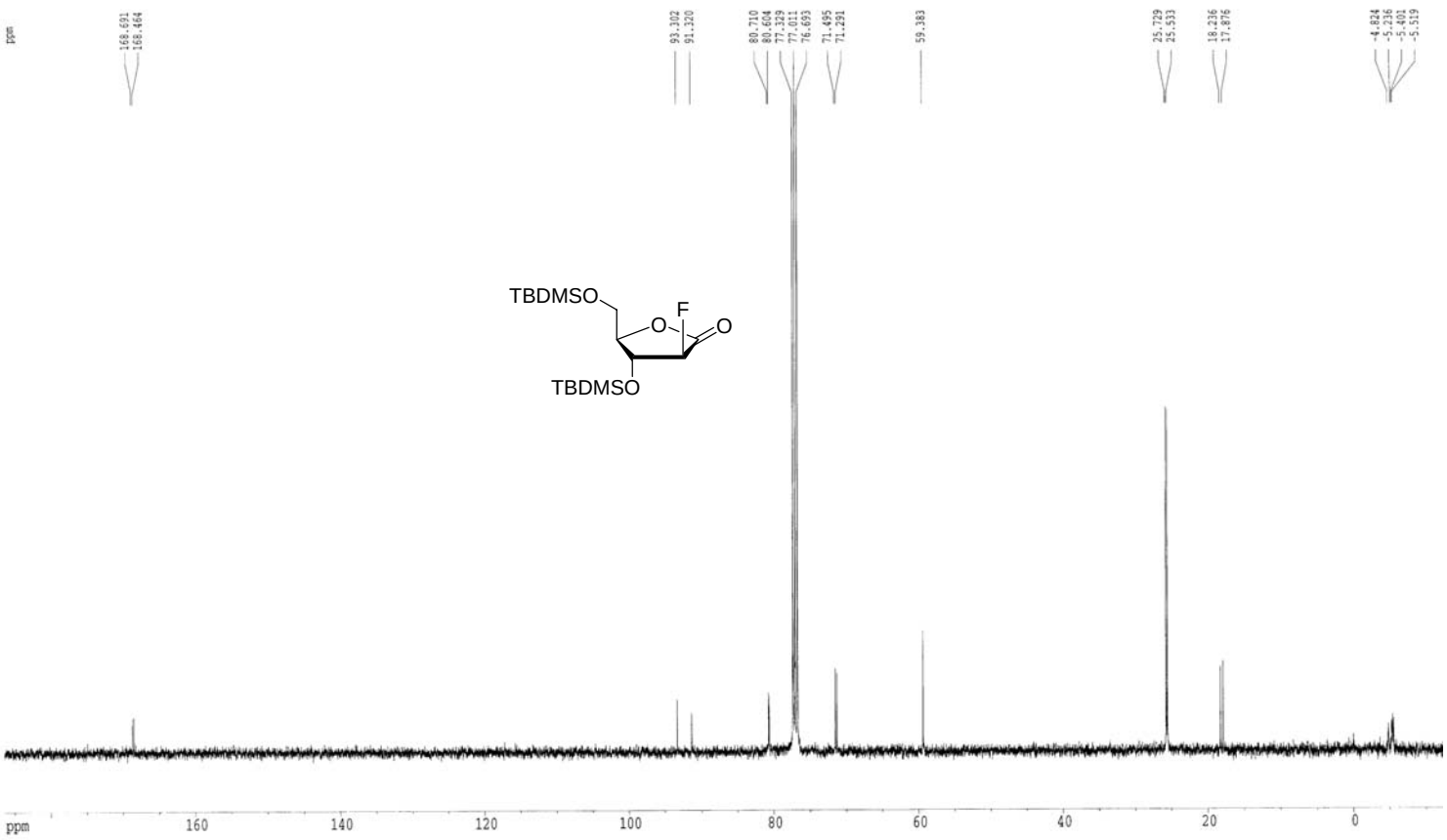
^{1}H NMR spectrum of **7**



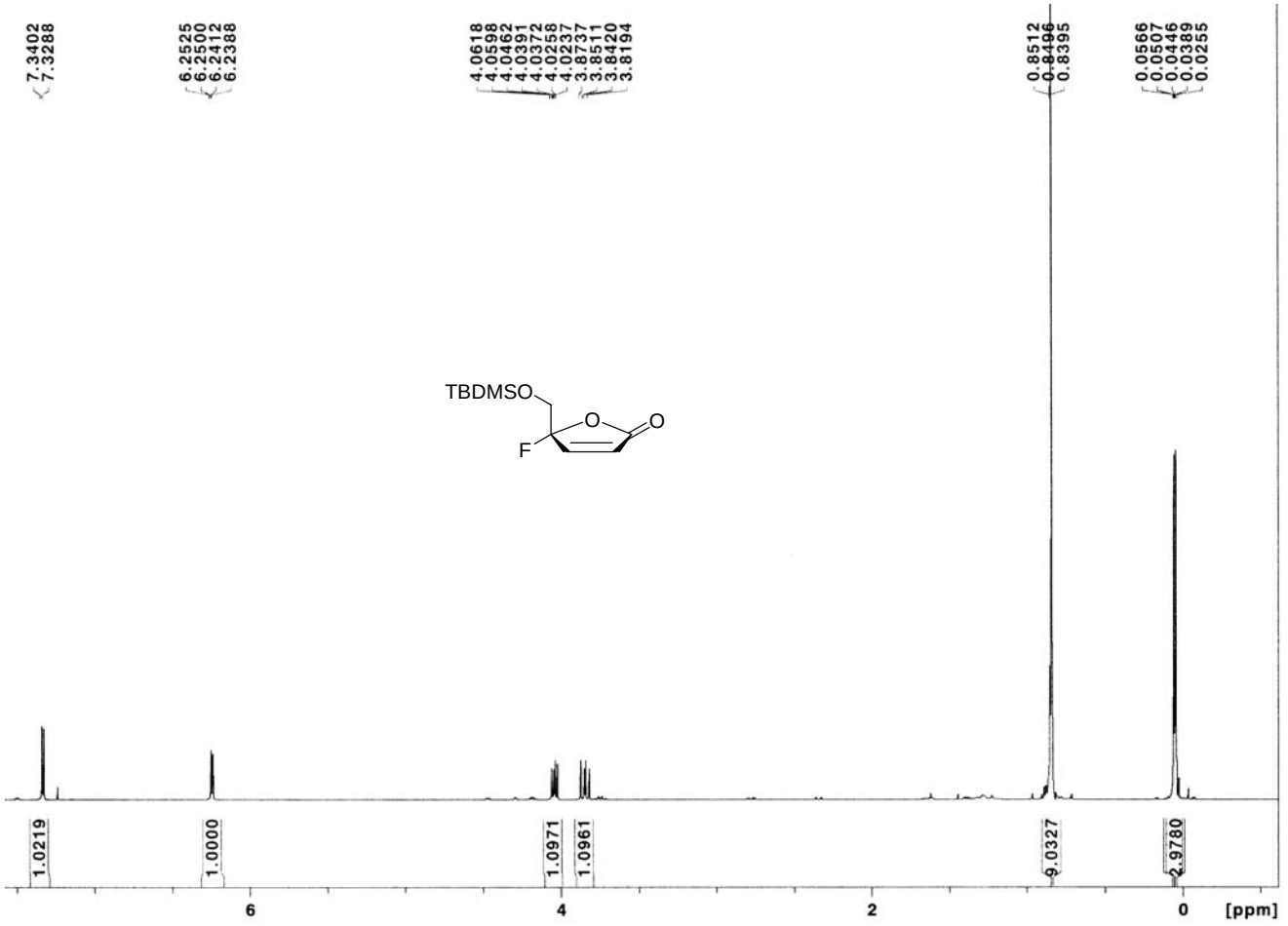
^{13}C NMR spectrum of **7**



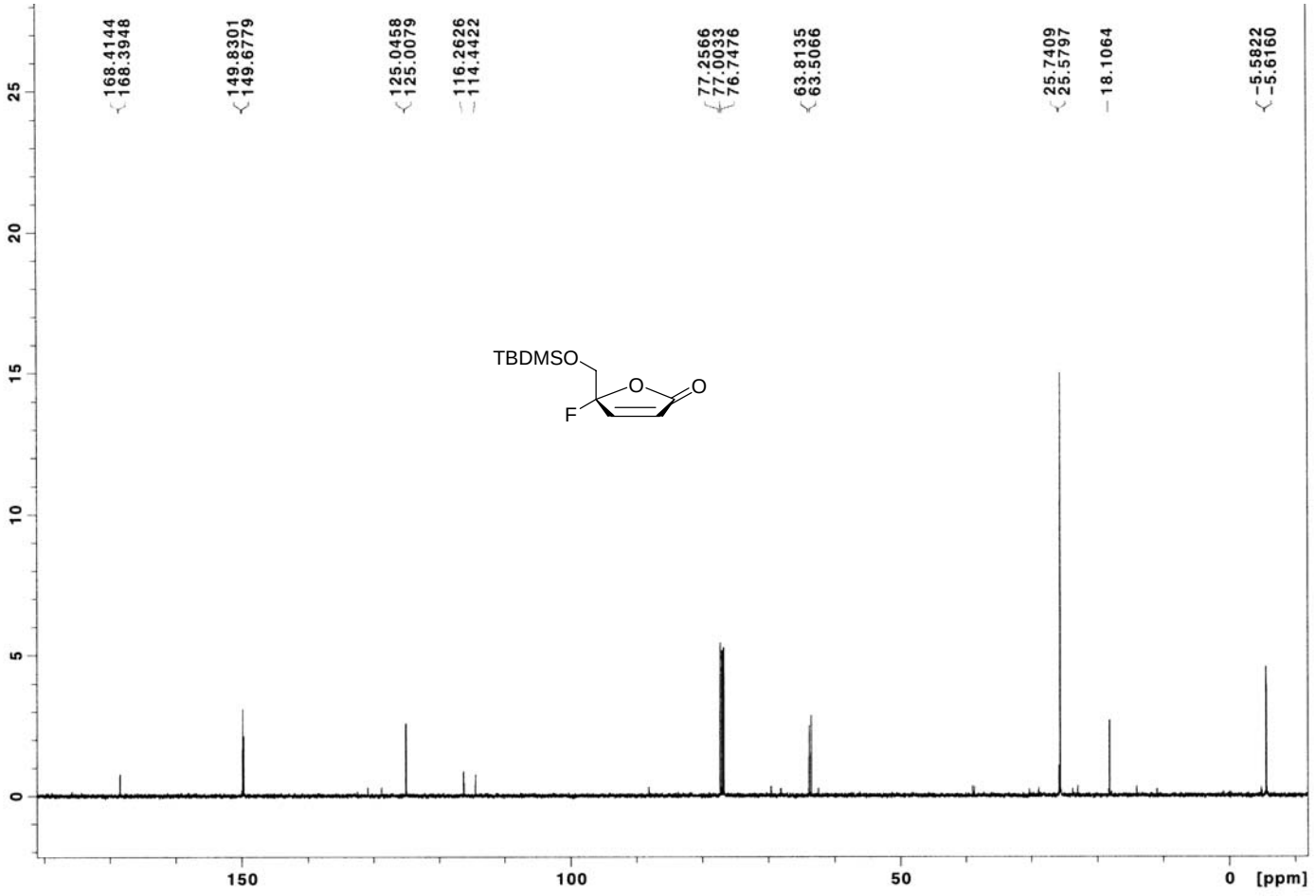
^{1}H NMR spectrum of **8**



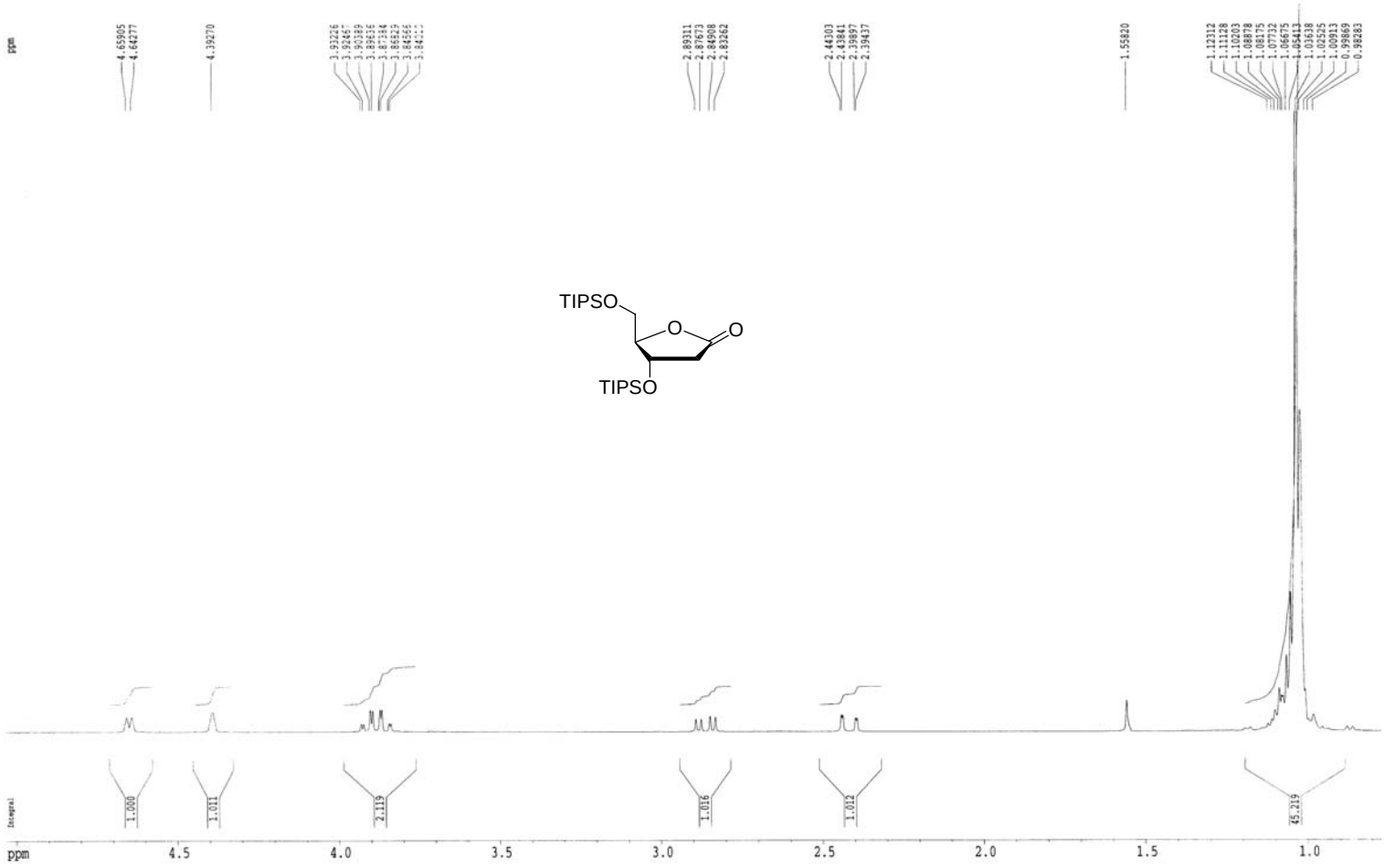
^{13}C NMR spectrum of **8**



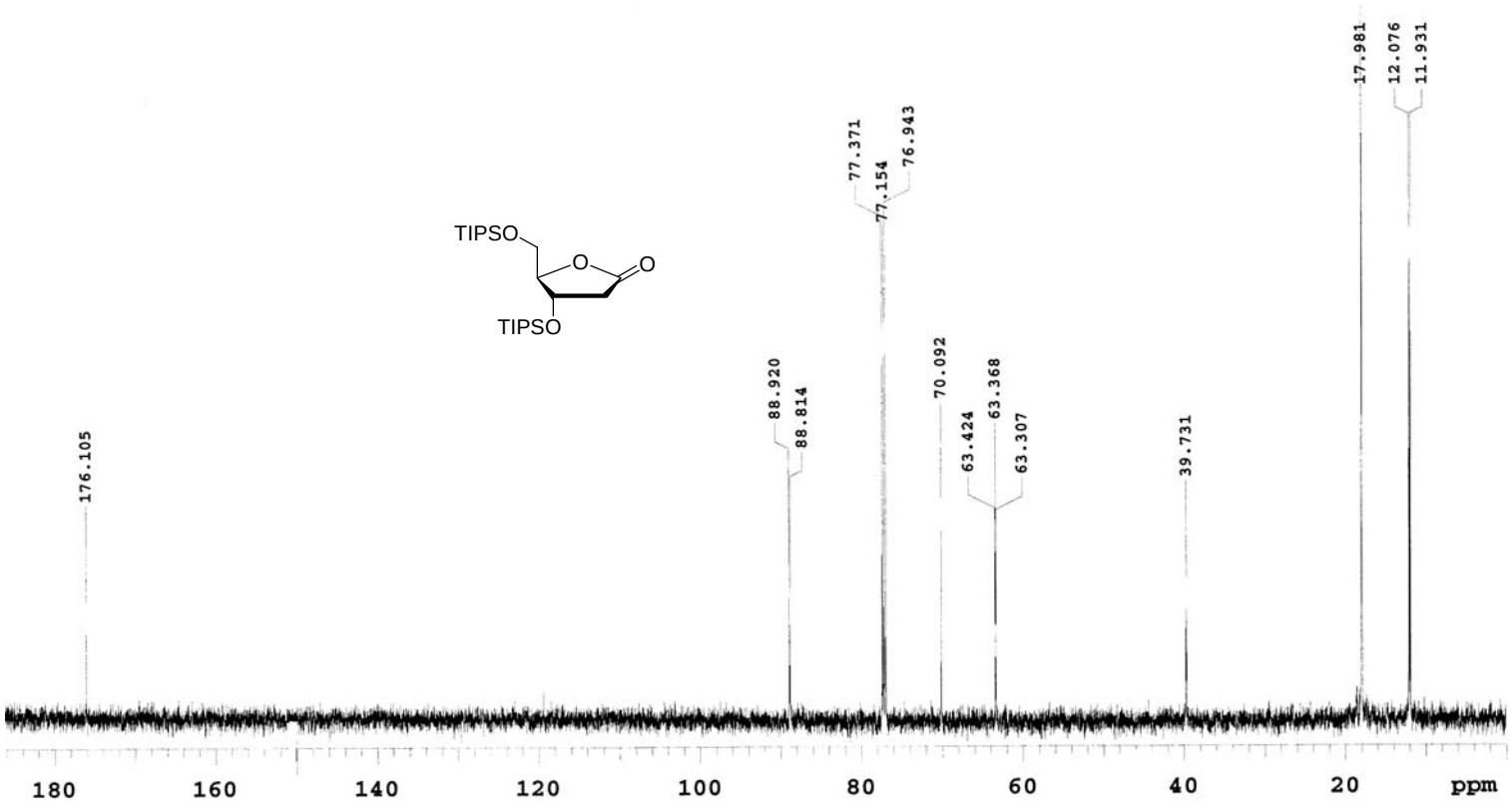
^{1}H NMR spectrum of **9**



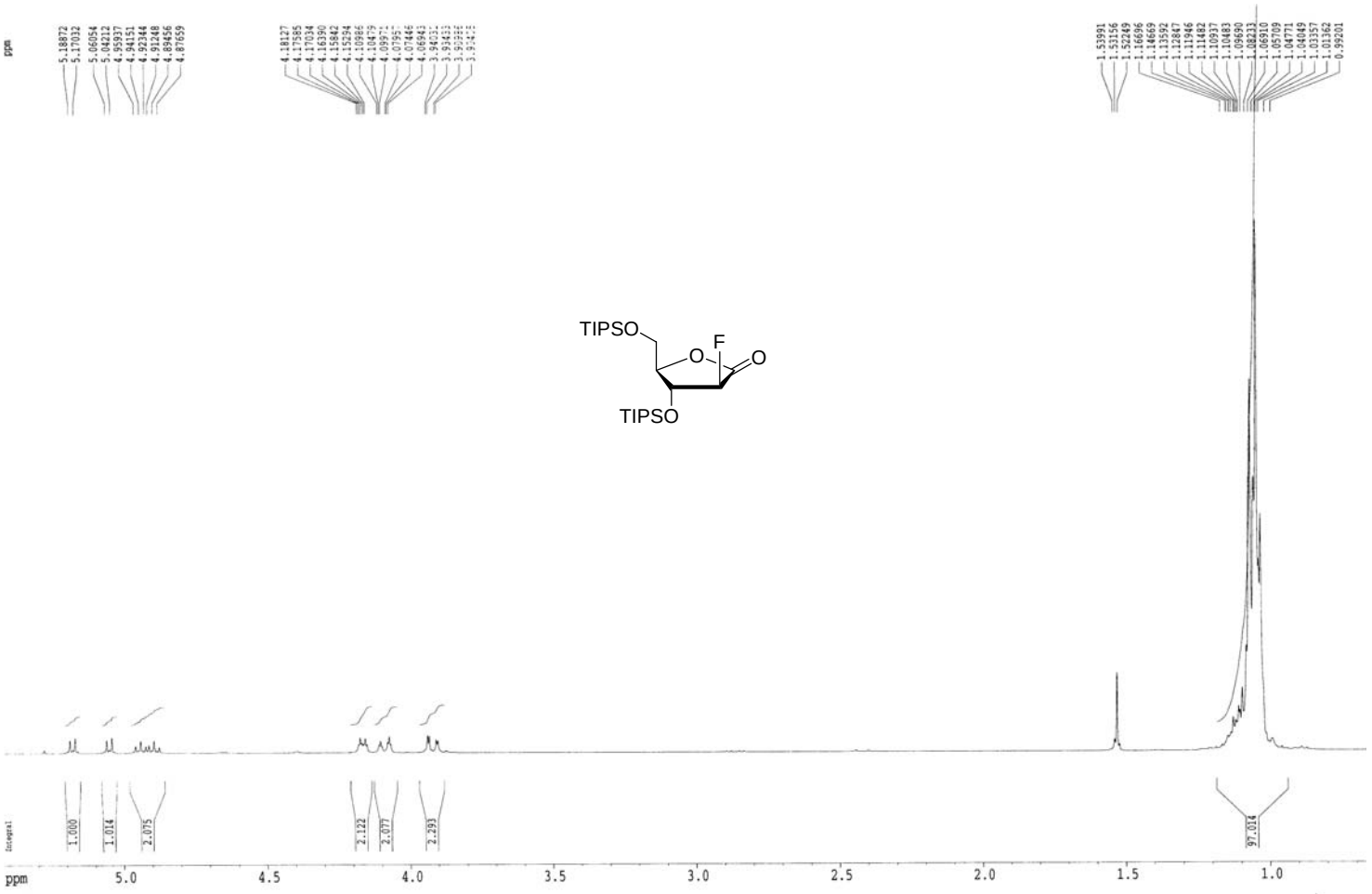
^{13}C NMR spectrum of **9**



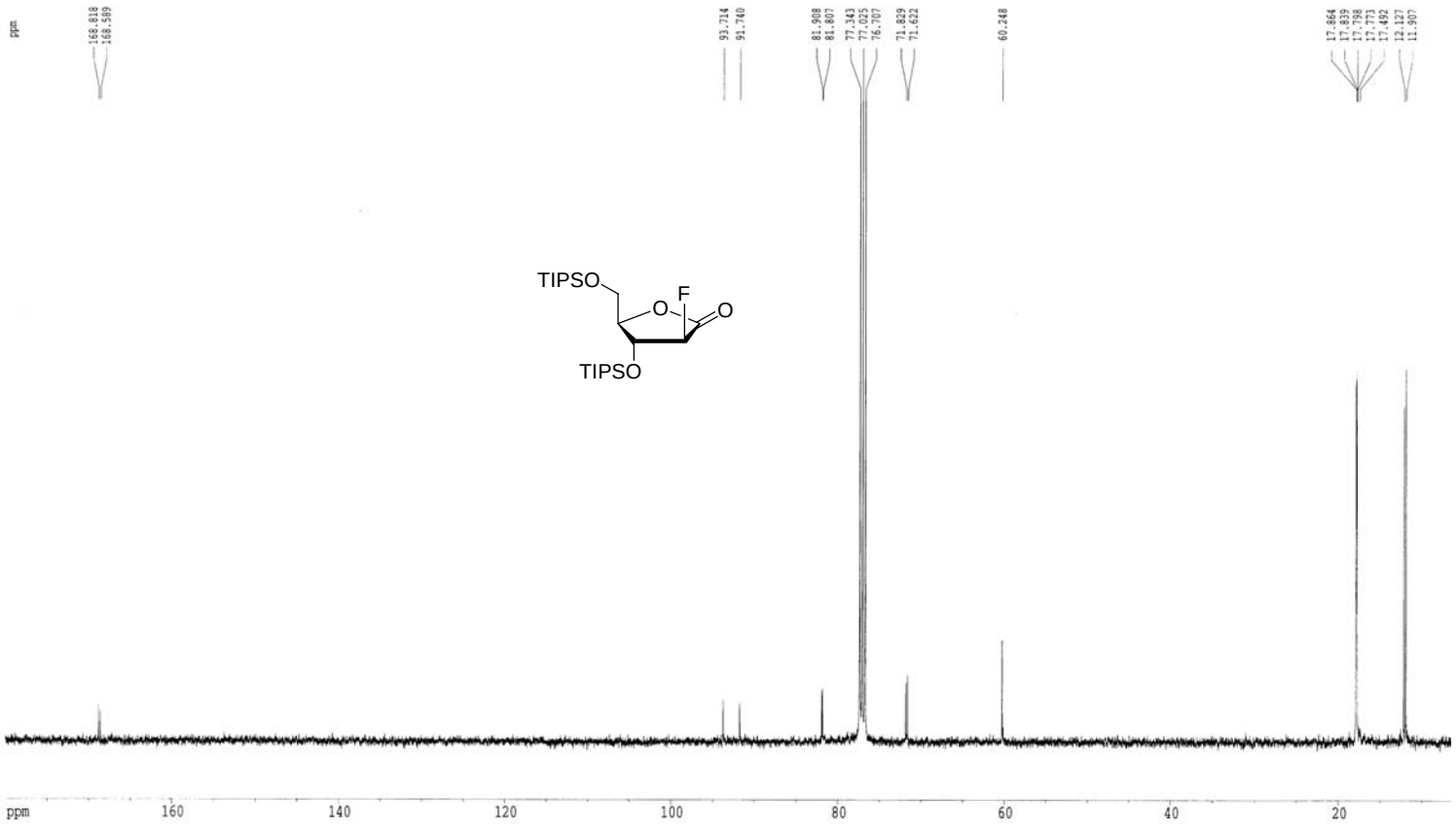
^{1}H NMR spectrum of **10**



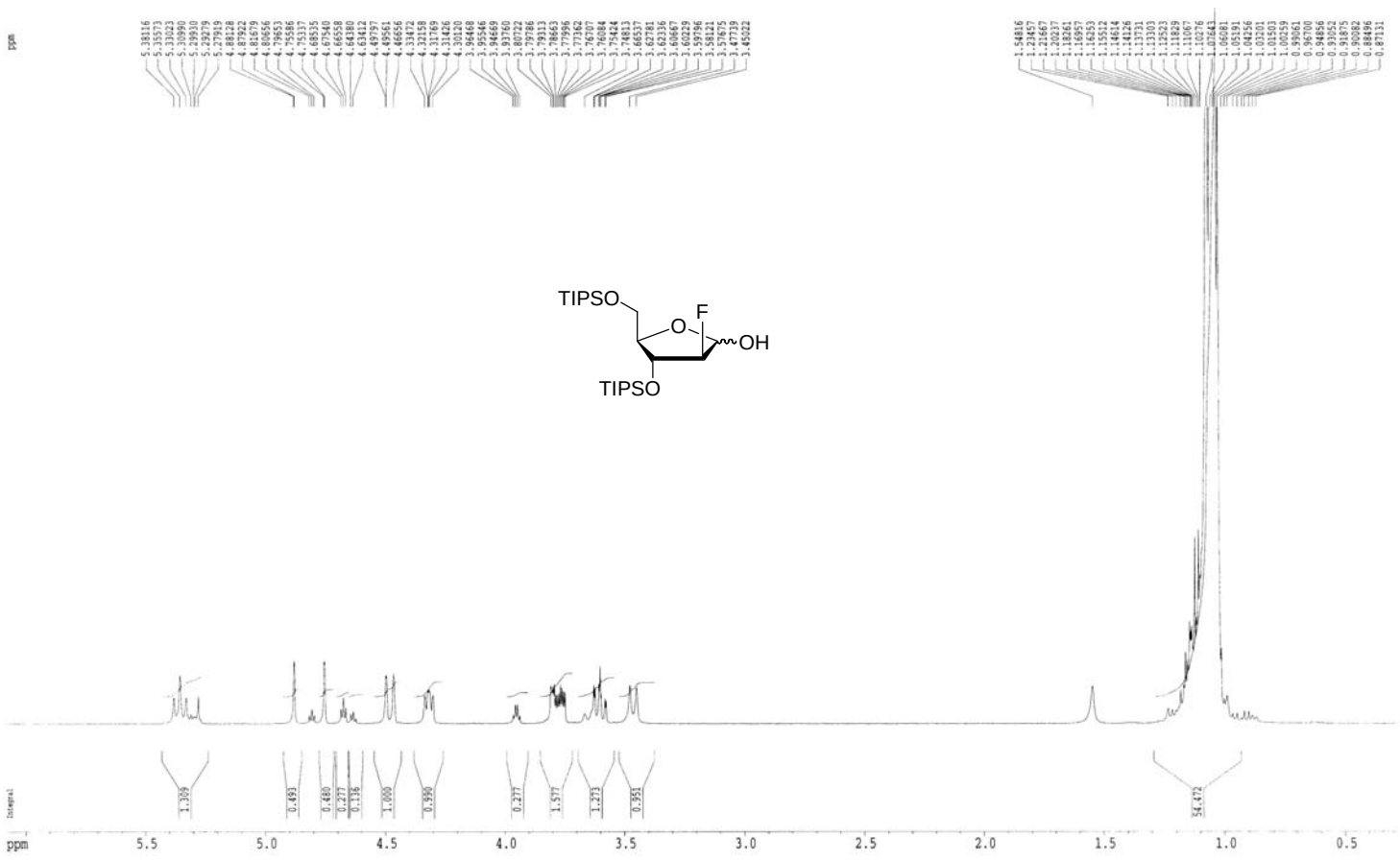
^{13}C NMR spectrum of **10**



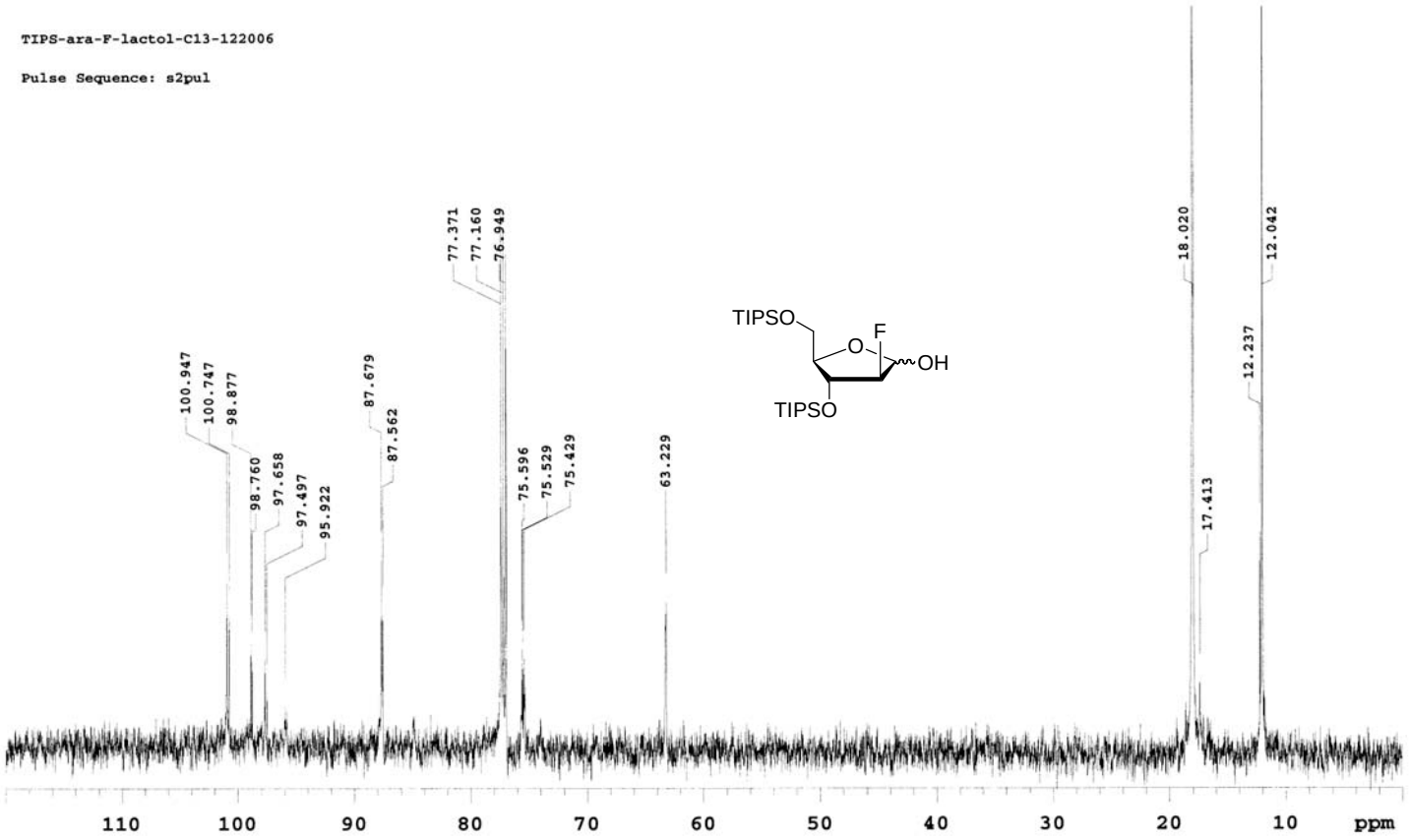
^{1}H NMR spectrum of **11**



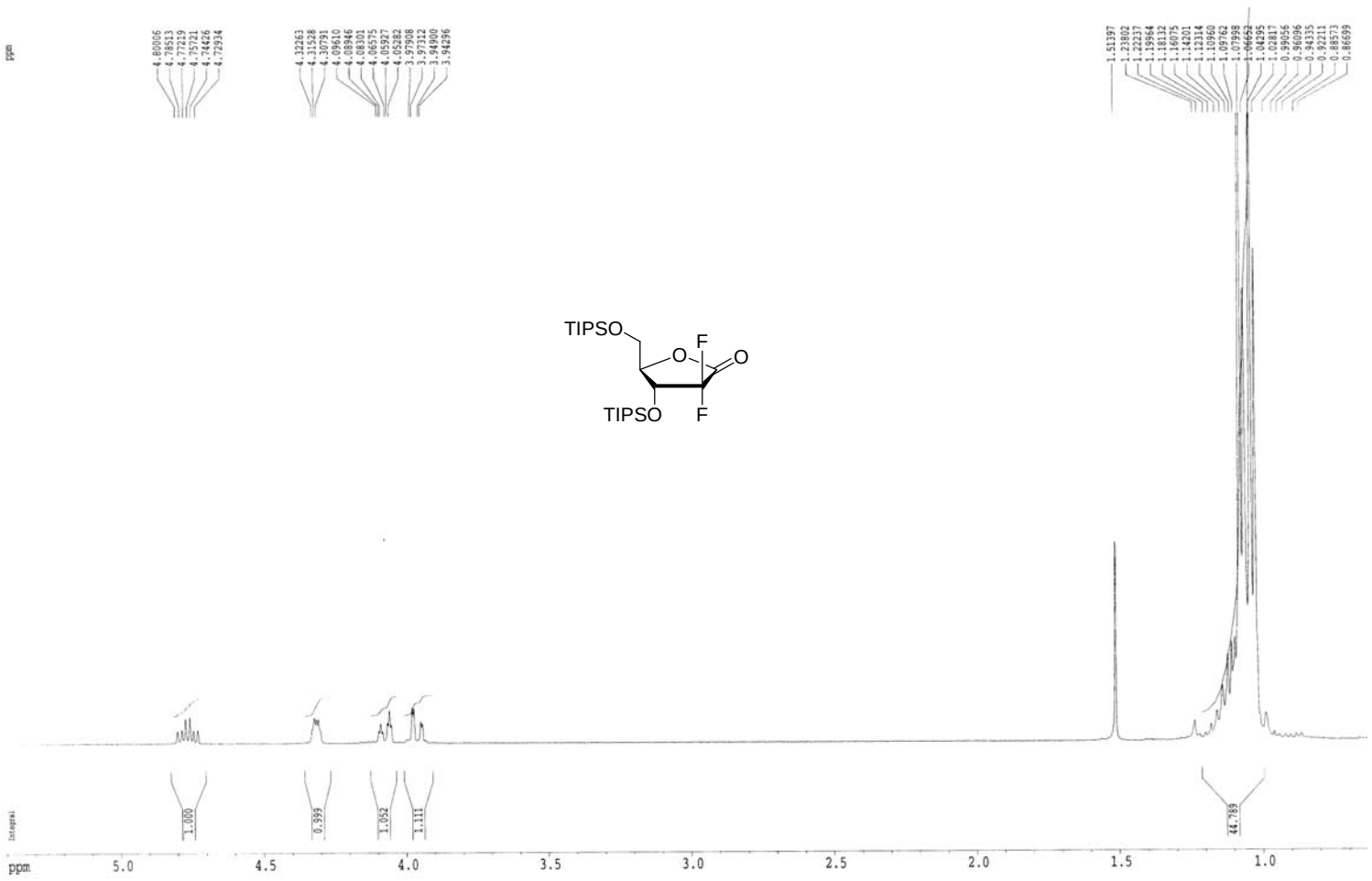
^{13}C NMR spectrum of **11**



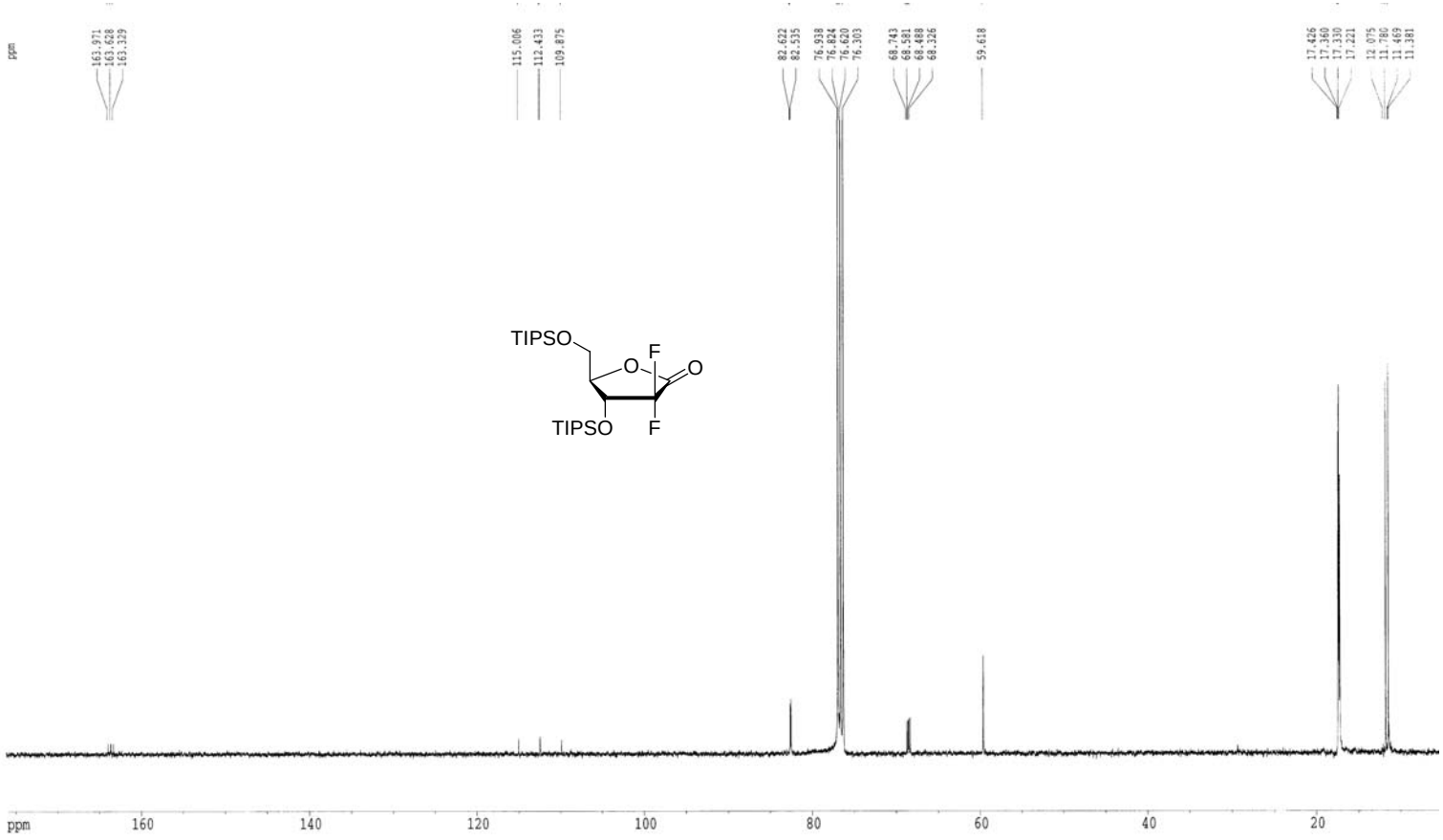
^{1}H NMR spectrum of **12**



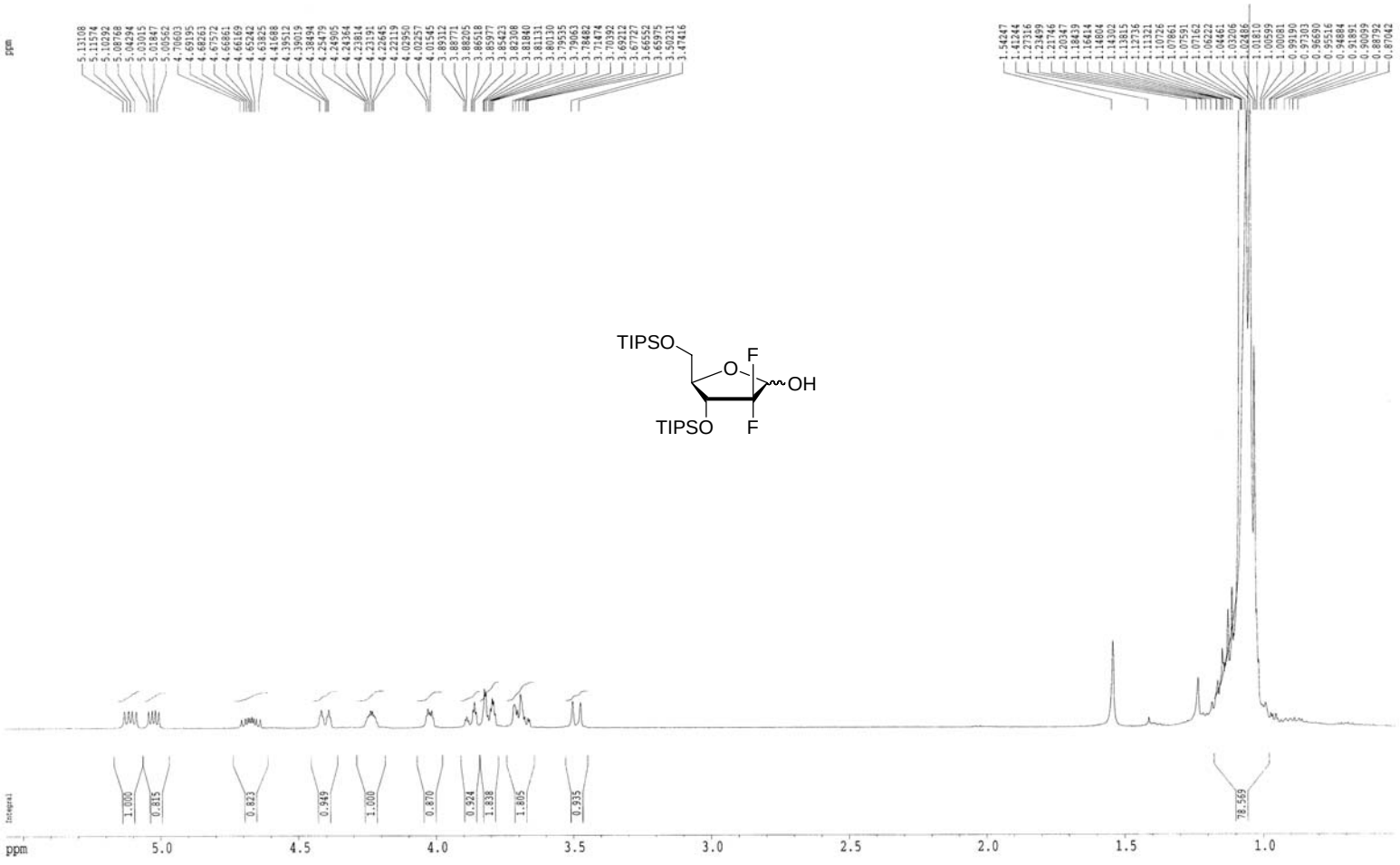
^{13}C NMR spectrum of **12**



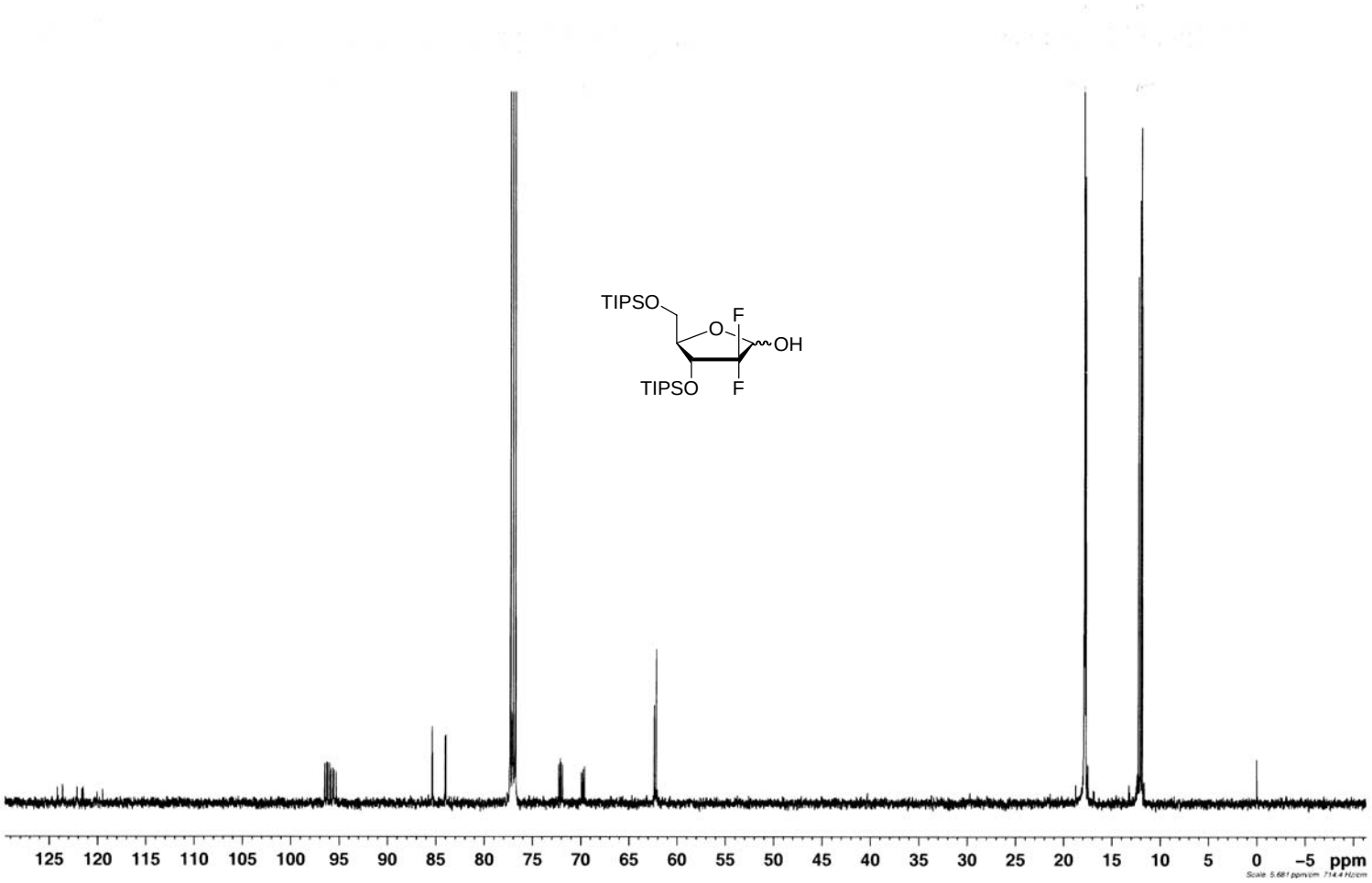
^{1}H NMR spectrum of **13**



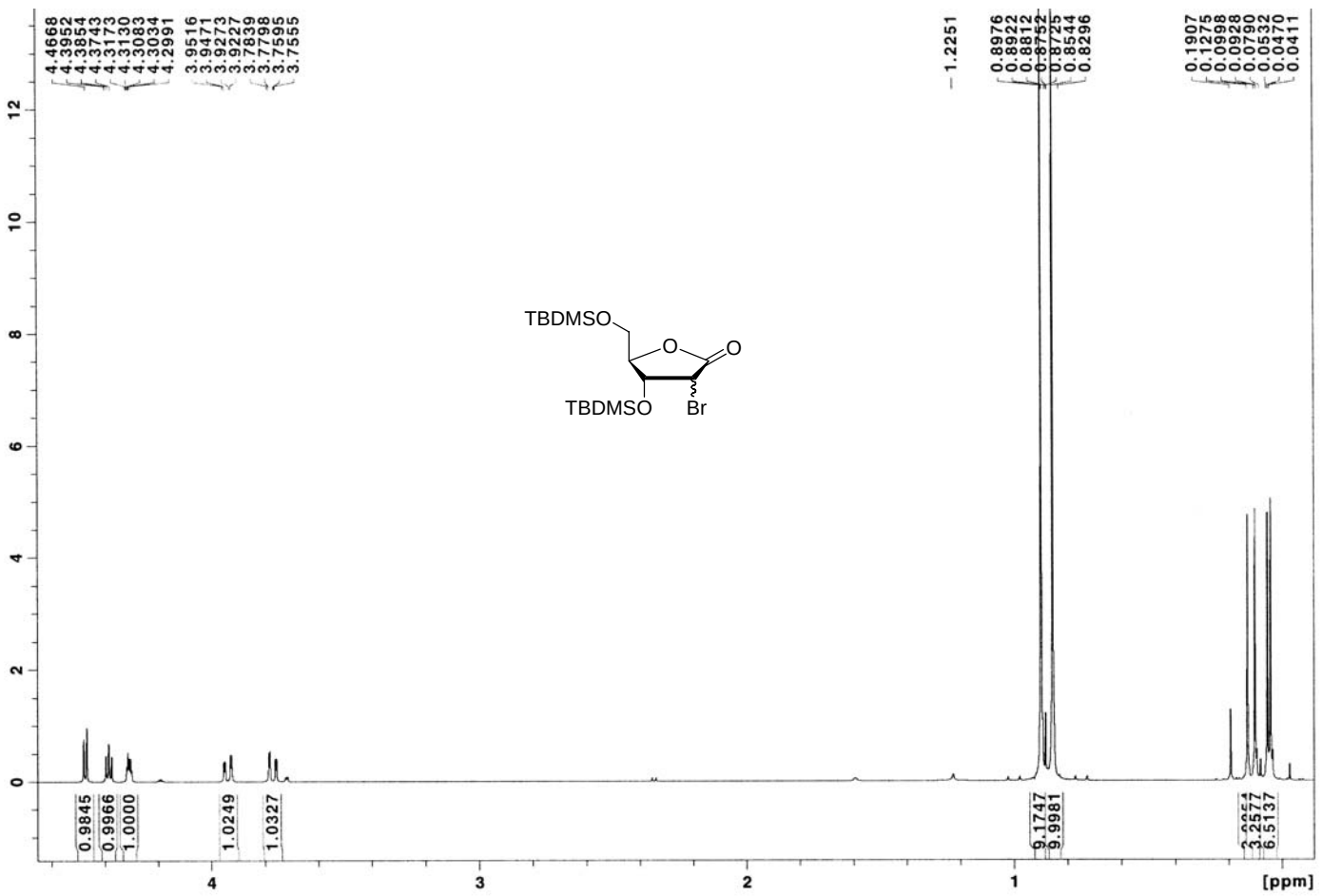
^{13}C NMR spectrum of **13**



^{1}H NMR spectrum of **14**



^{13}C NMR spectrum of **14**



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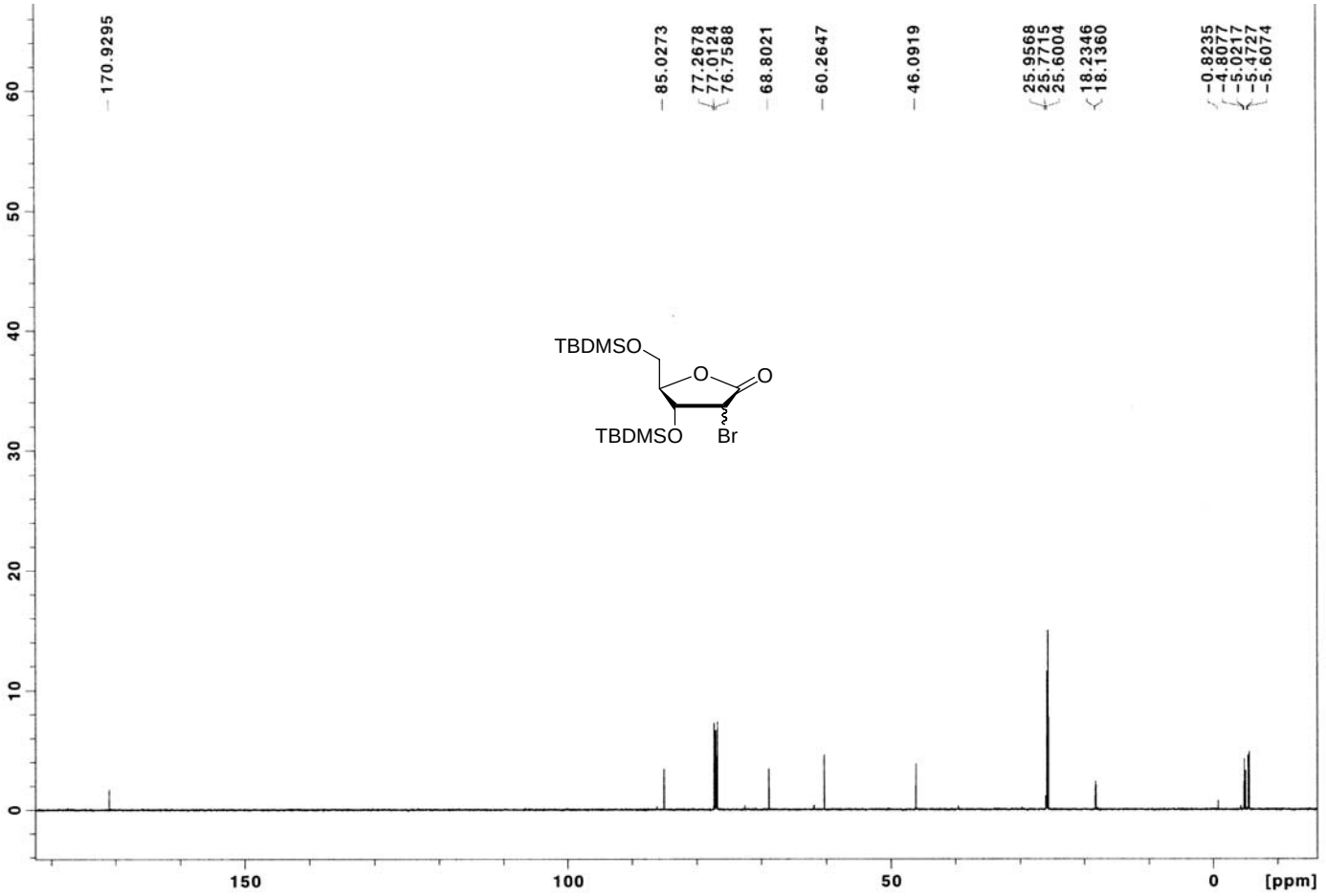

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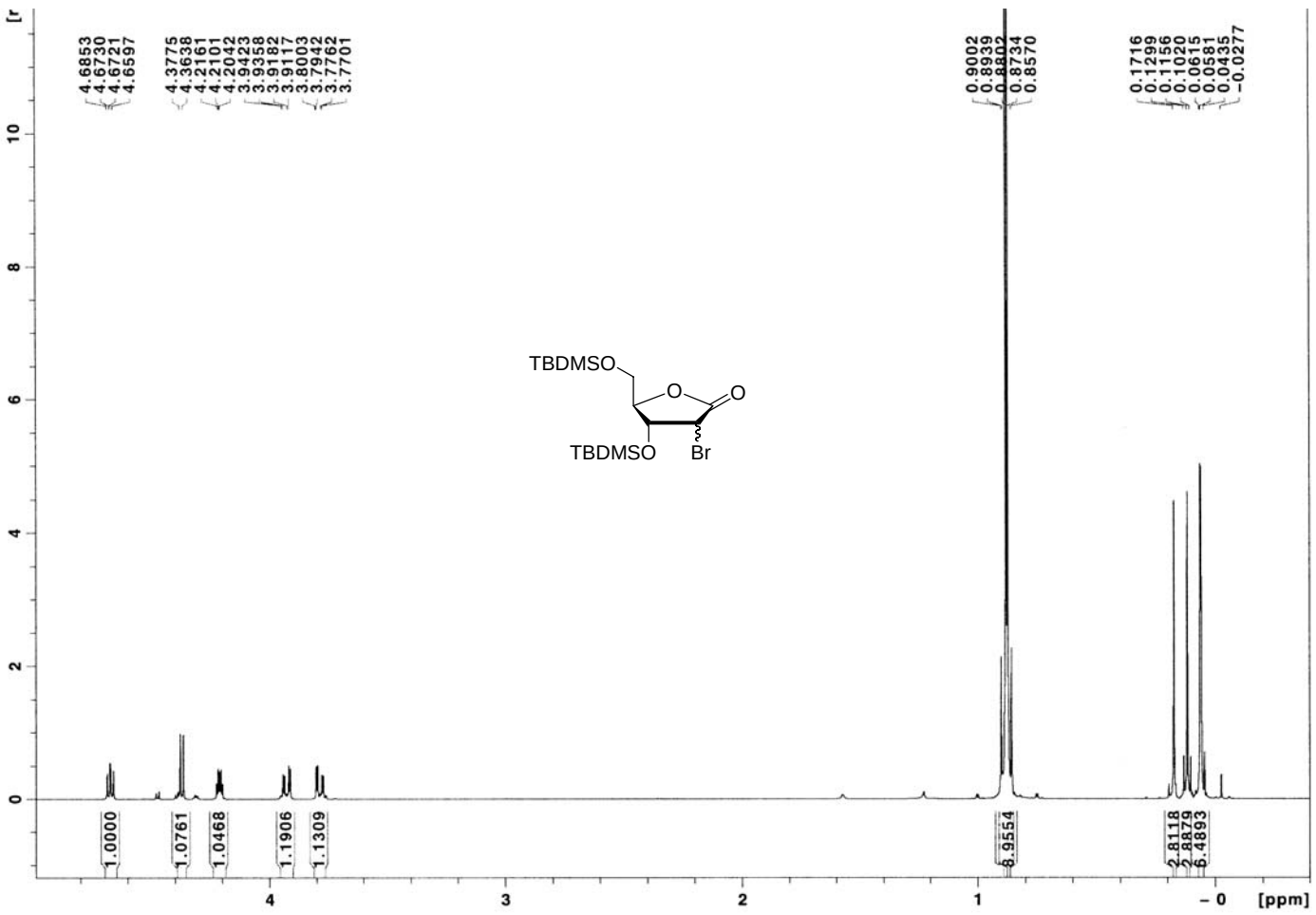

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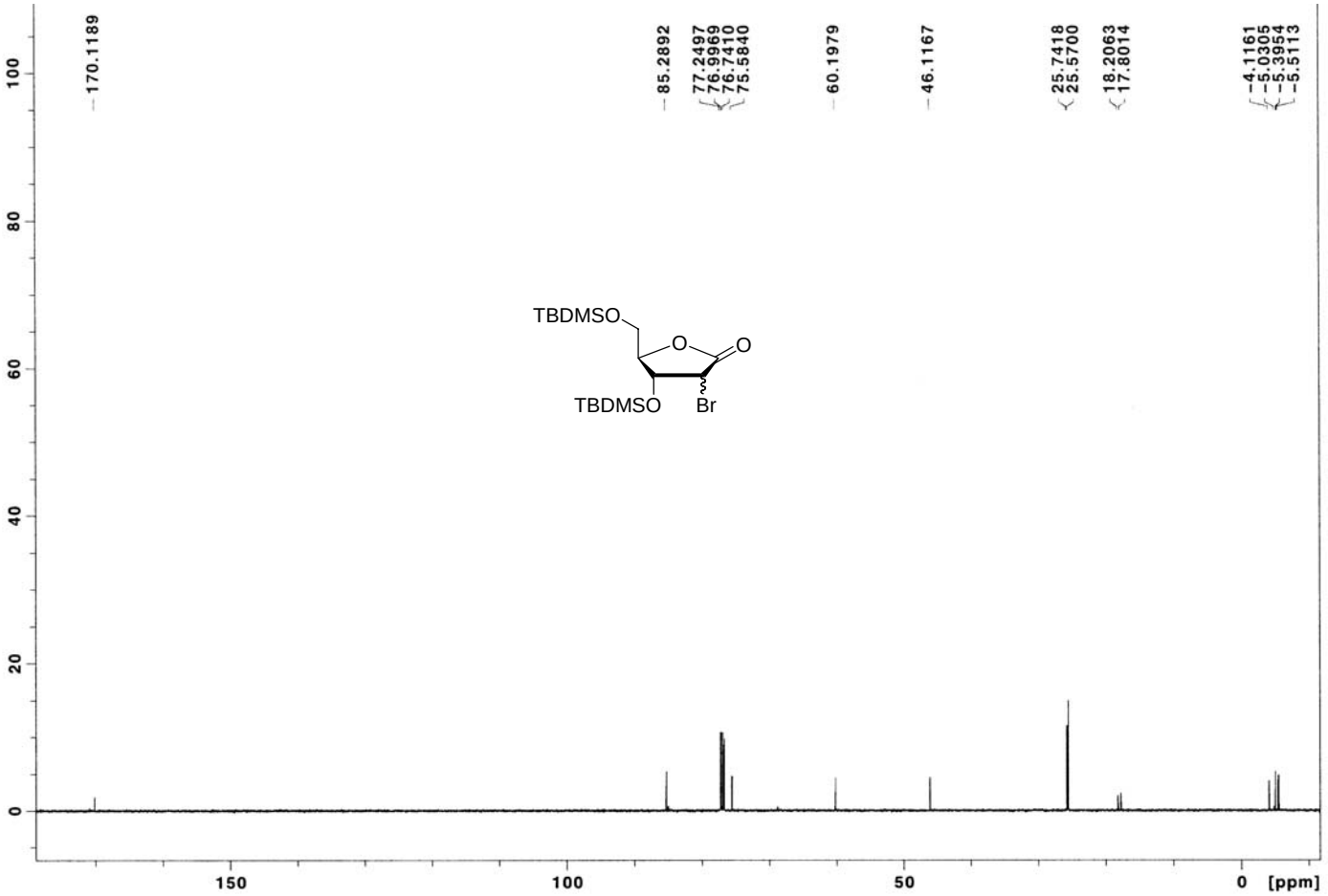

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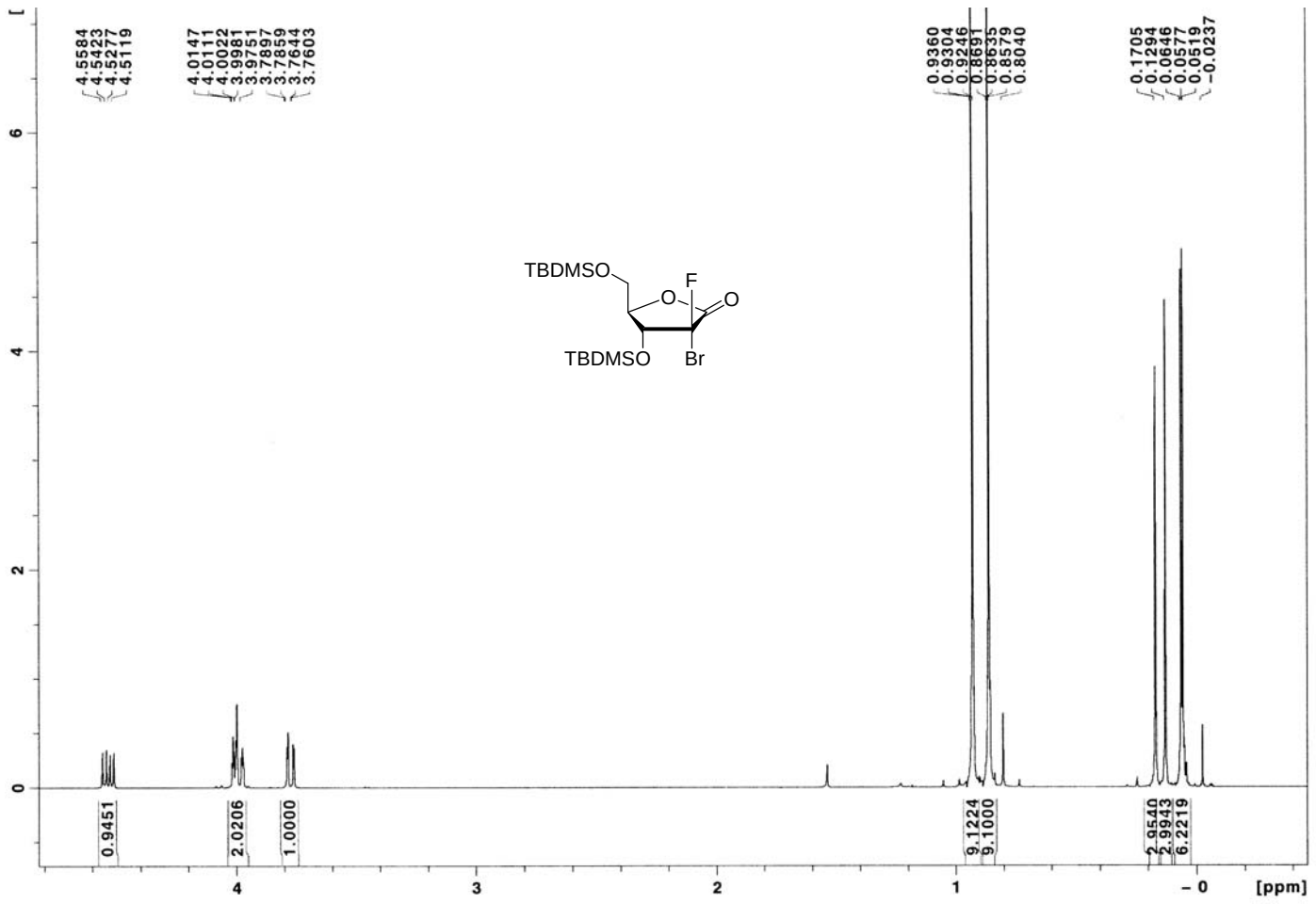
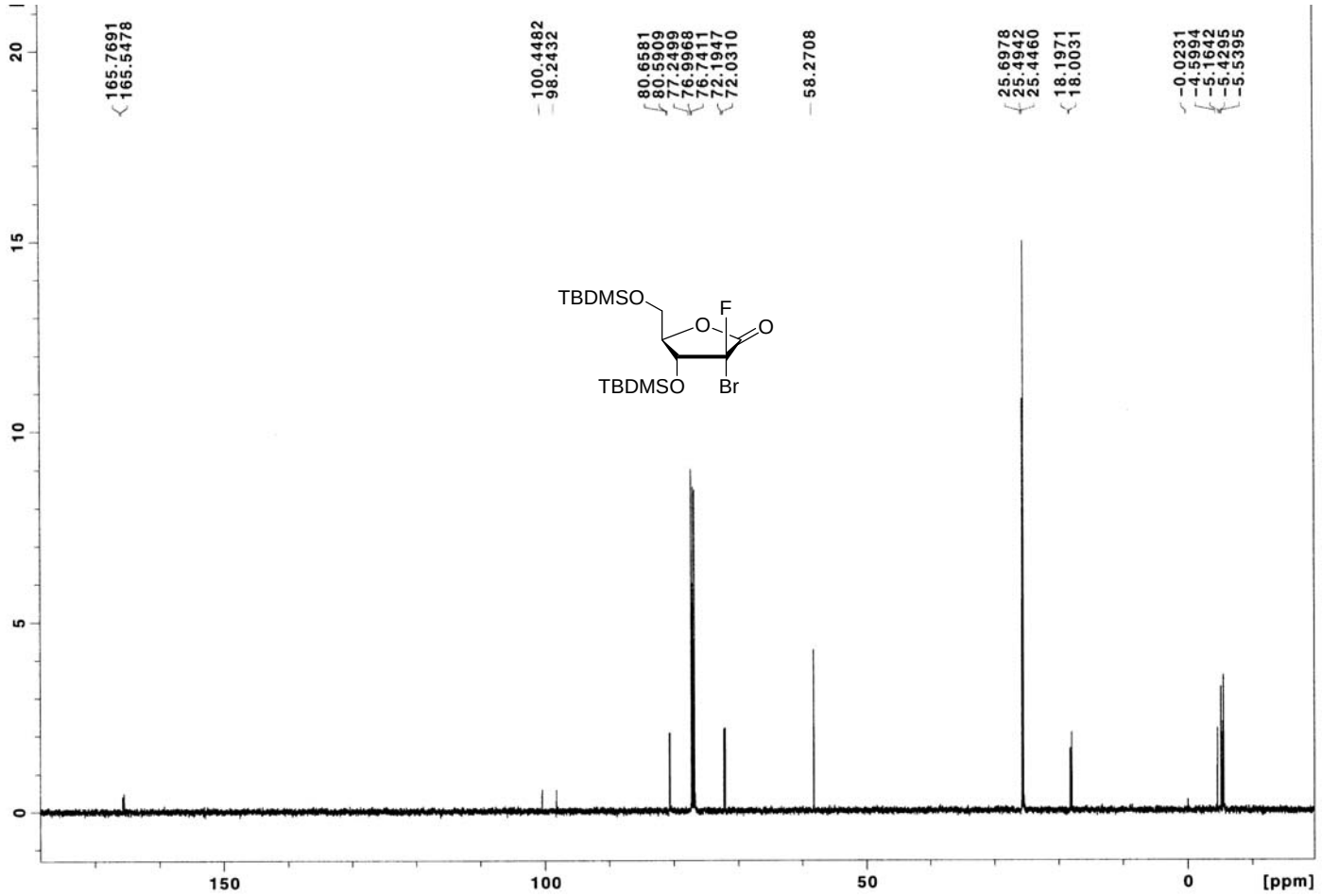


^{1}H NMR spectrum of **16**



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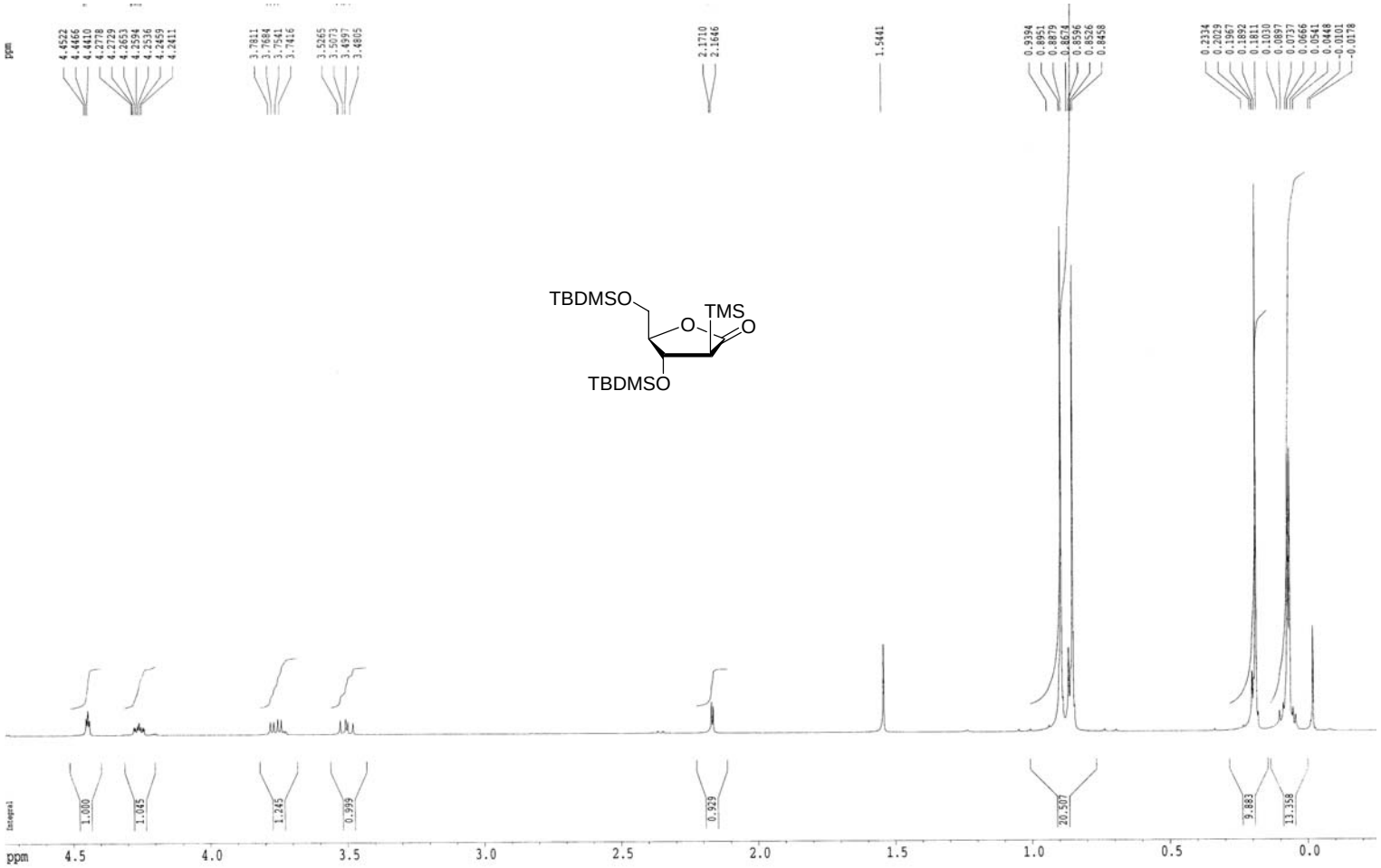

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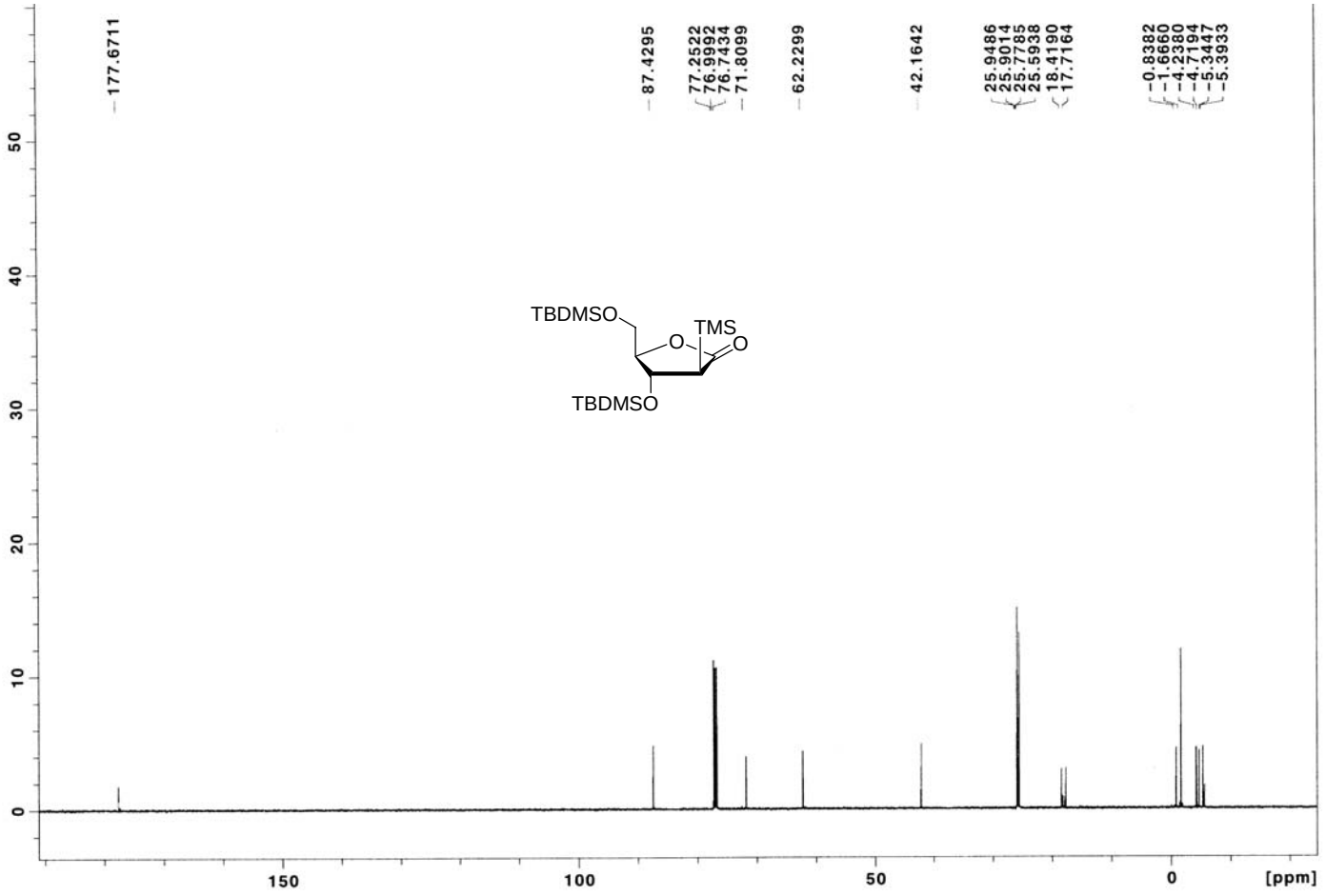
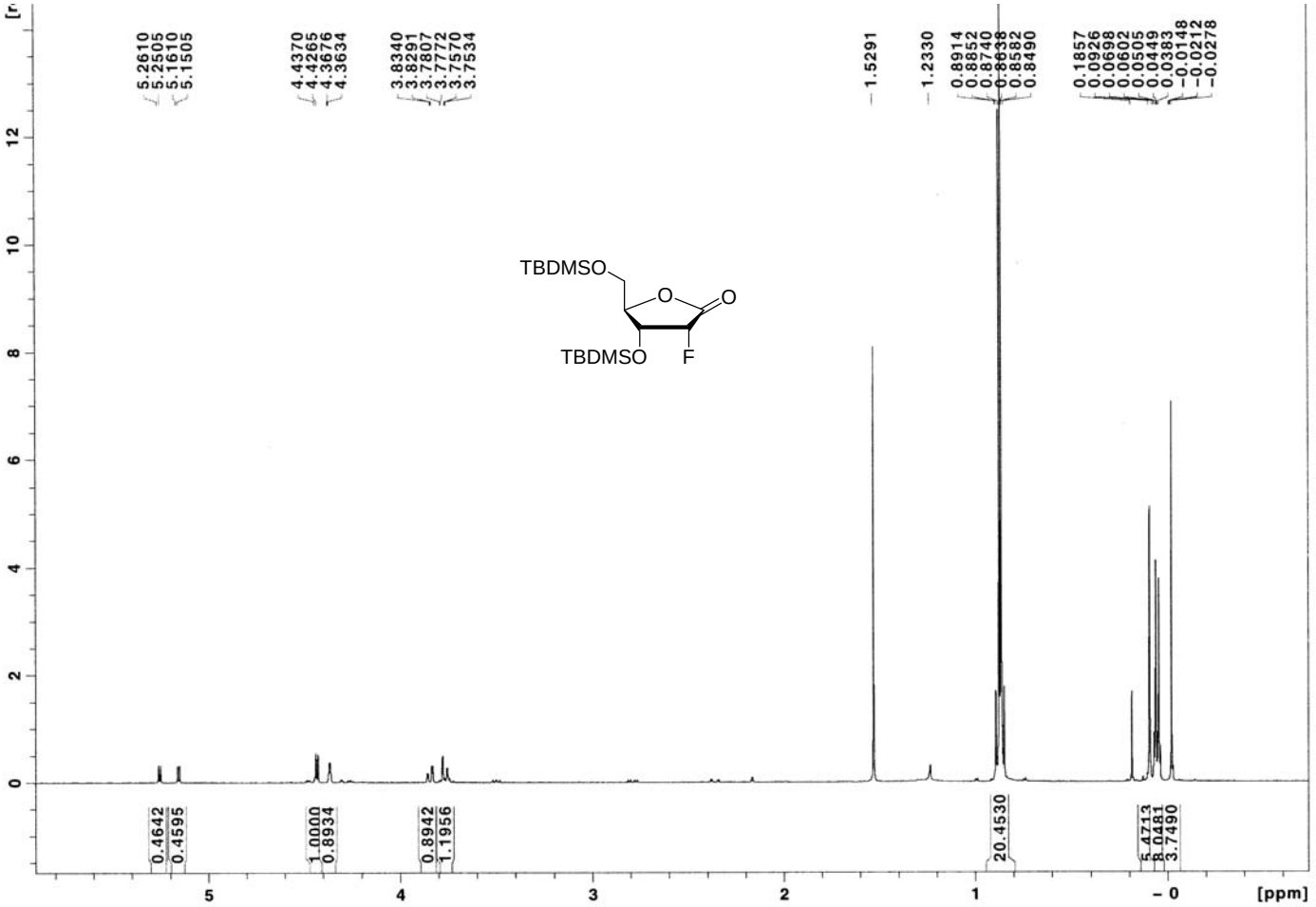


^{13}C NMR spectrum of **17**



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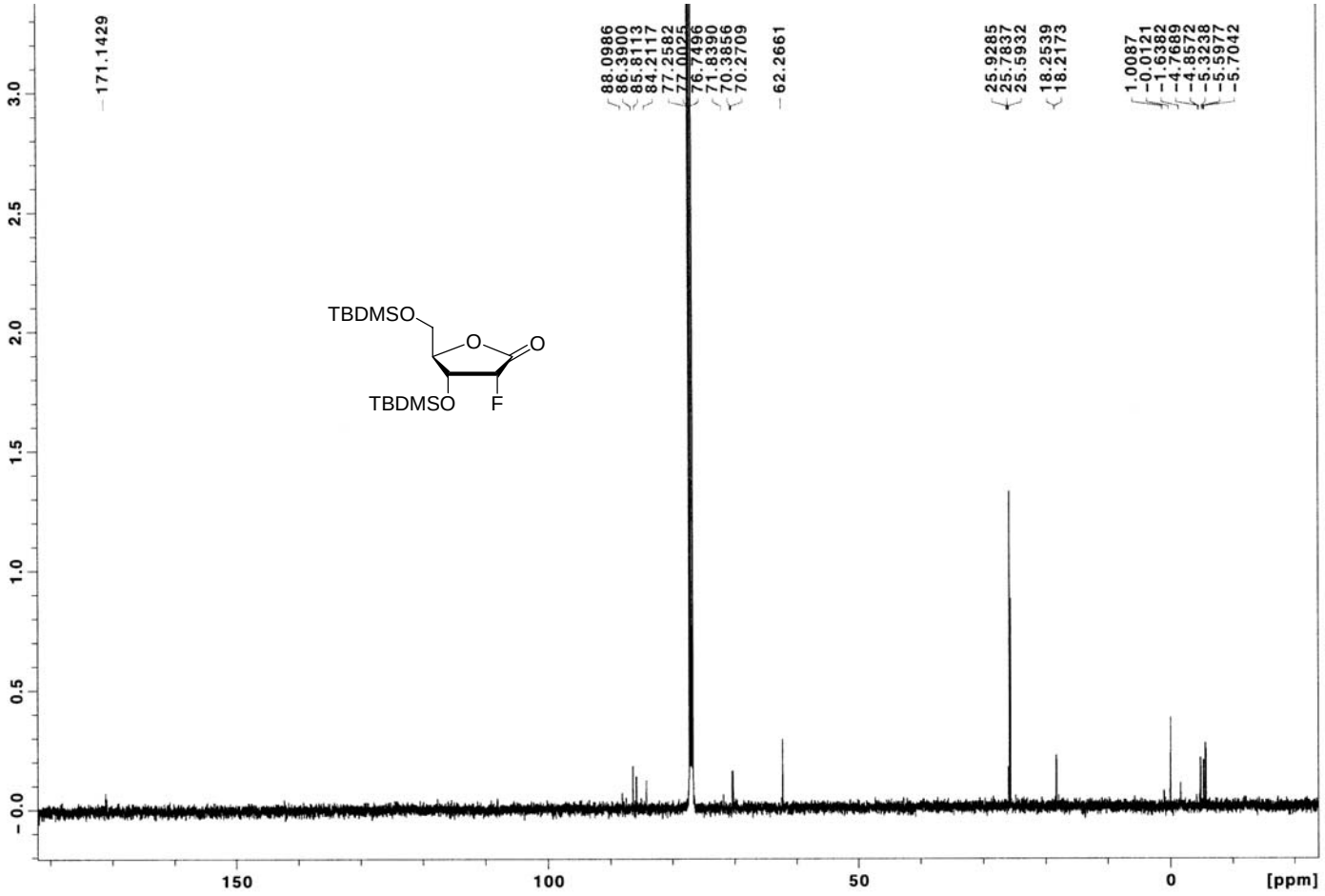
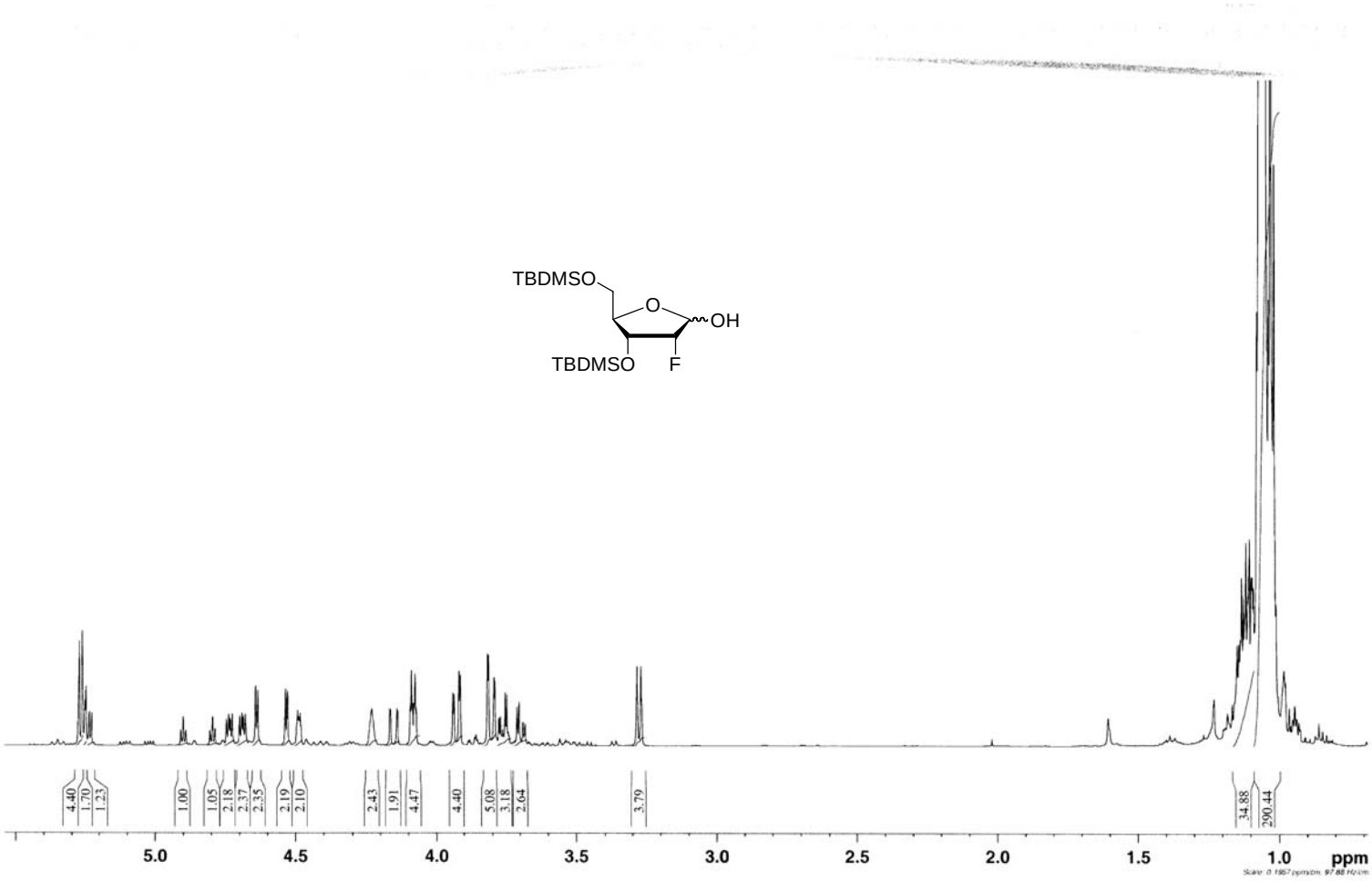
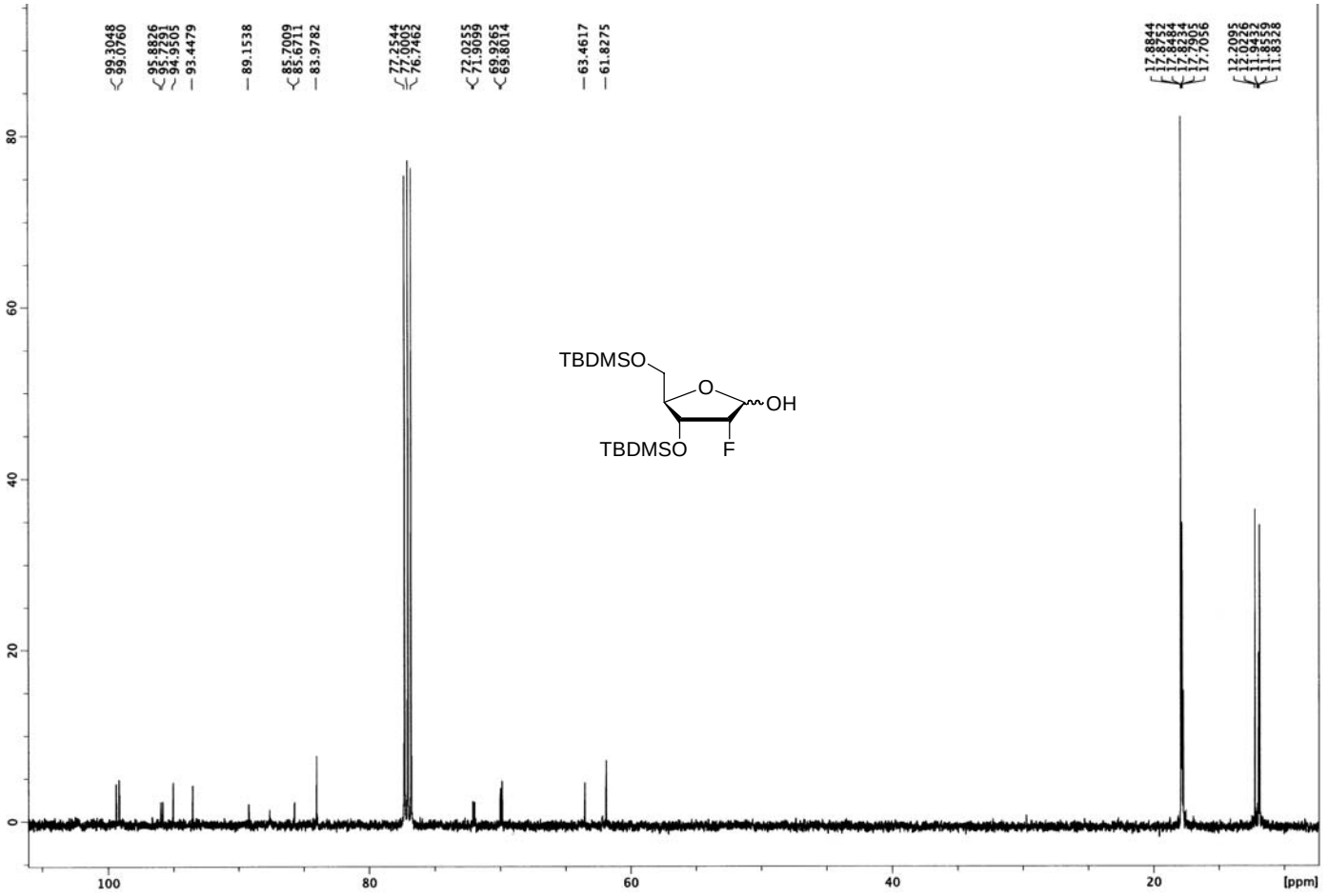


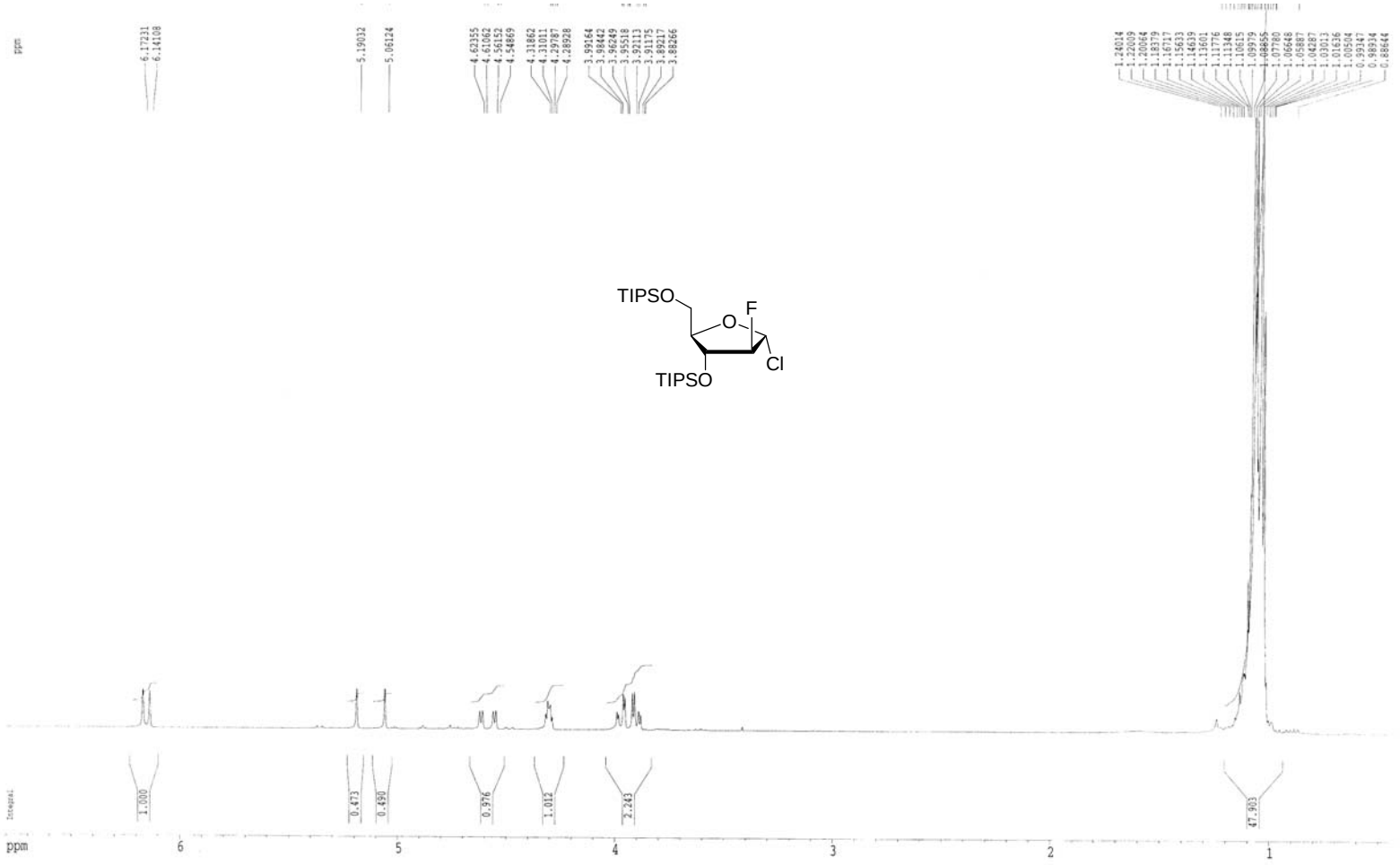
^{13}C NMR spectrum of **18**



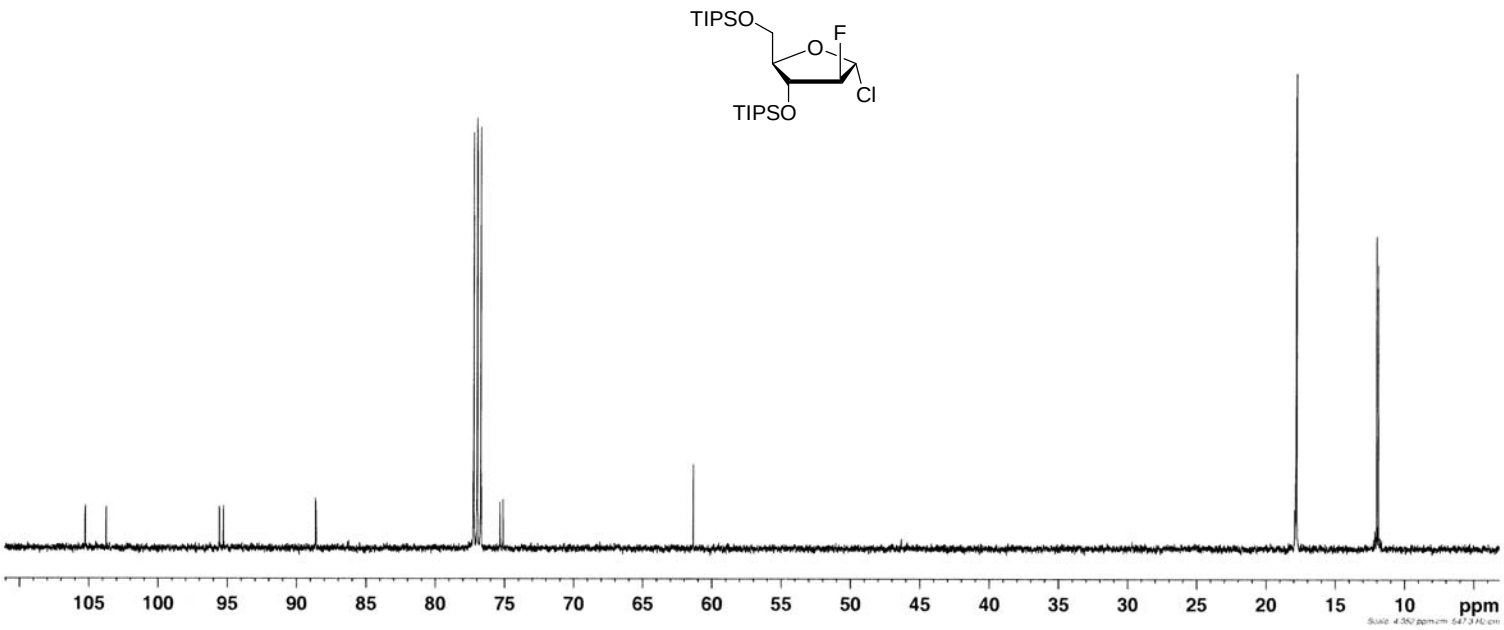
^{1}H NMR spectrum of **19**



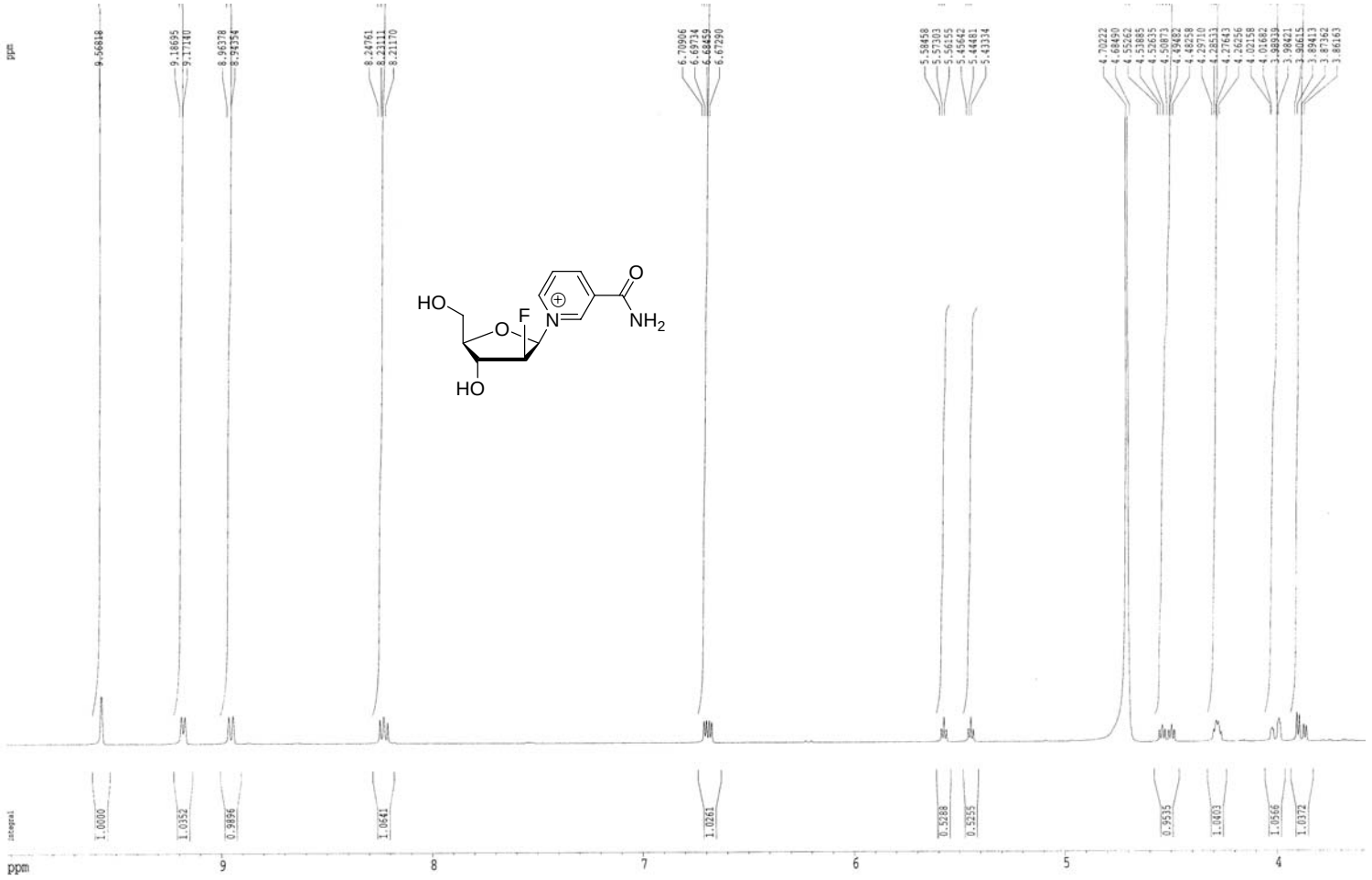
^{13}C NMR spectrum of **19**



^{1}H NMR spectrum of **20**



^{13}C NMR spectrum of **20**



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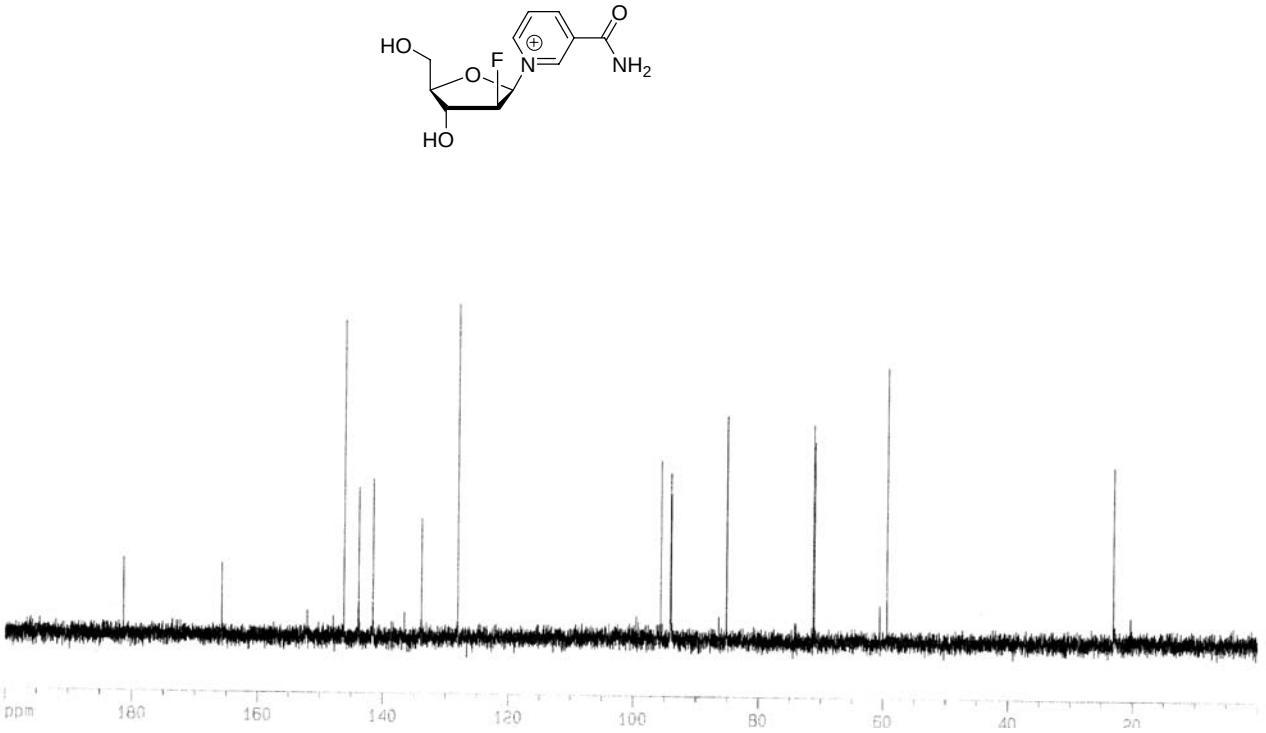

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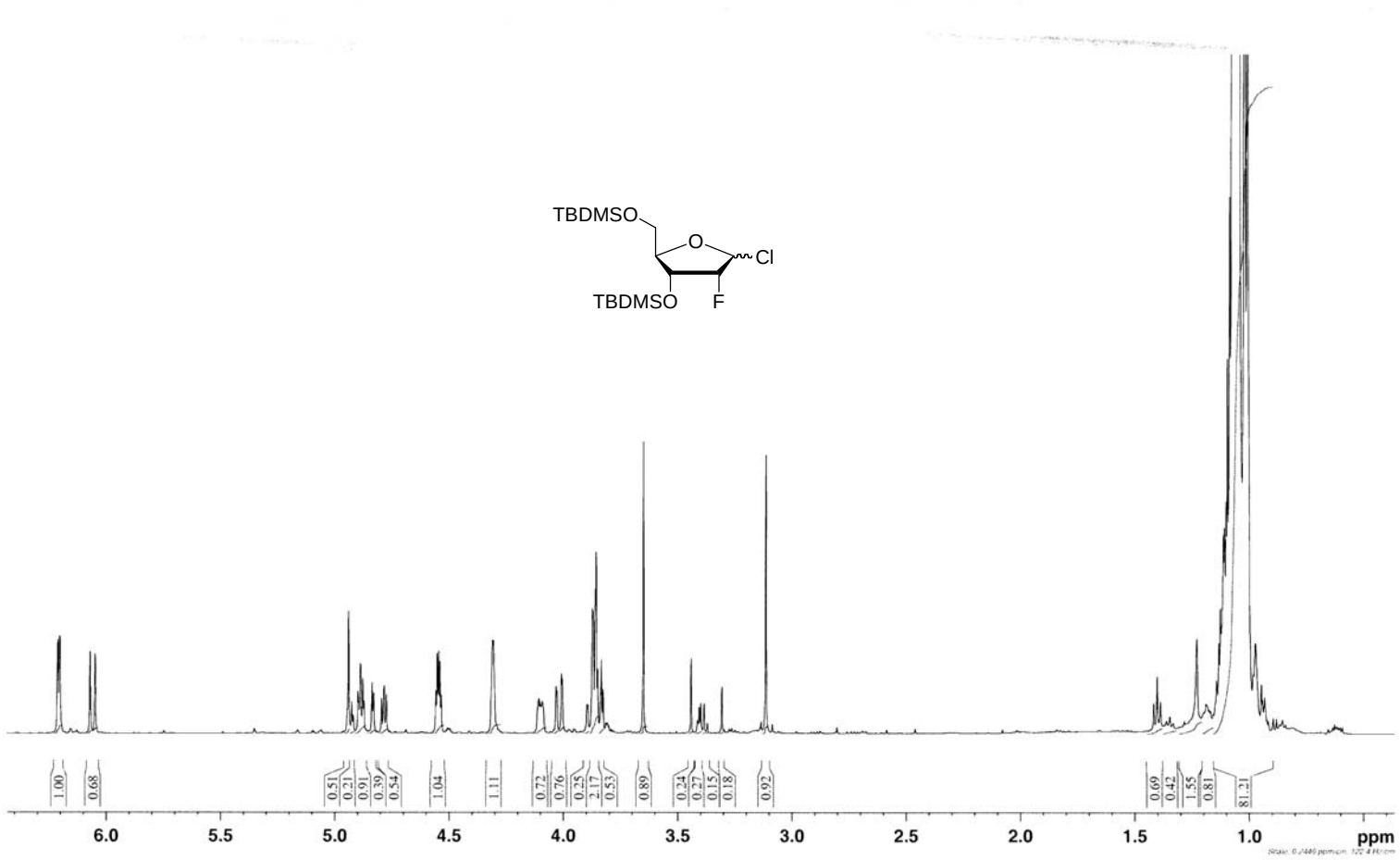
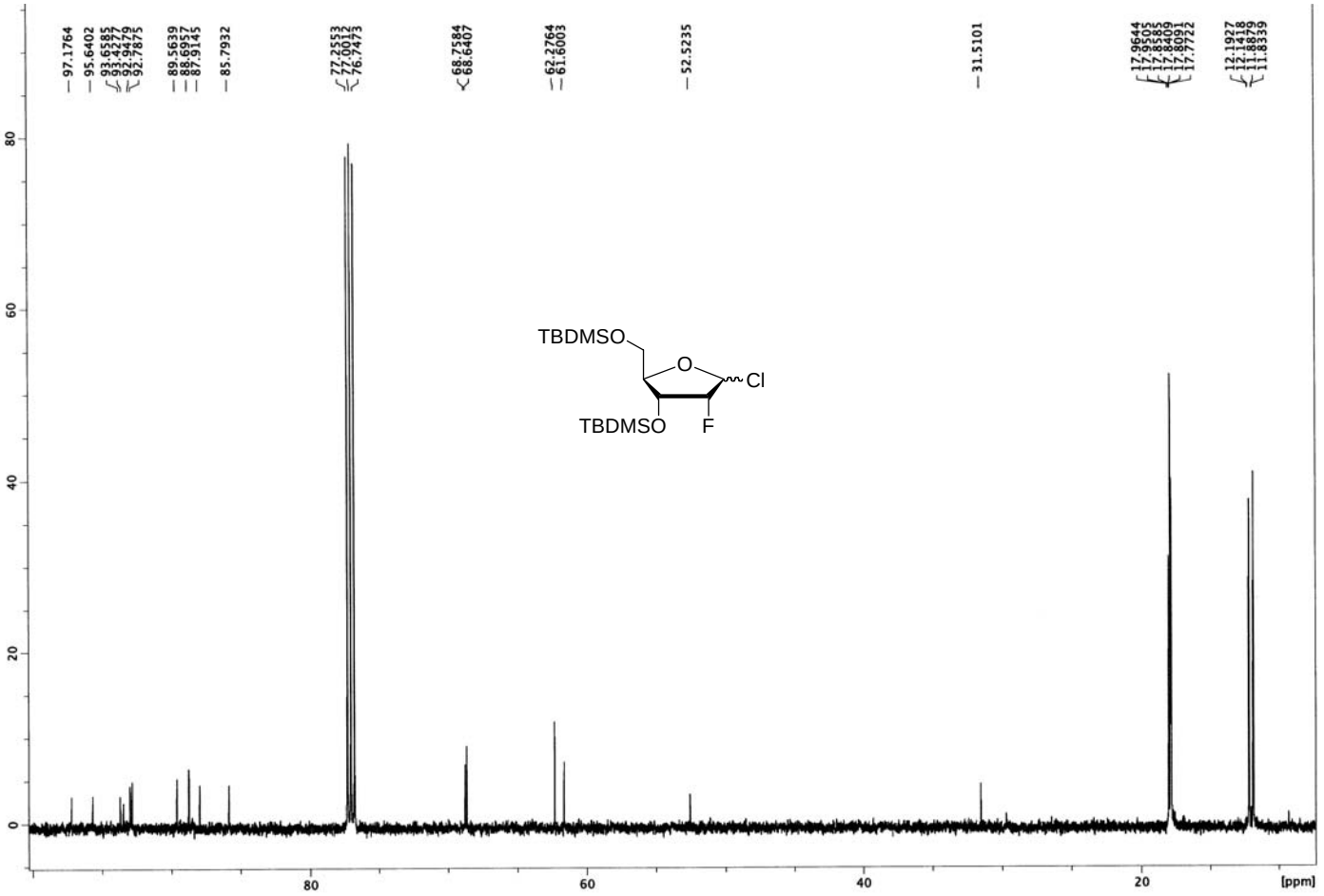
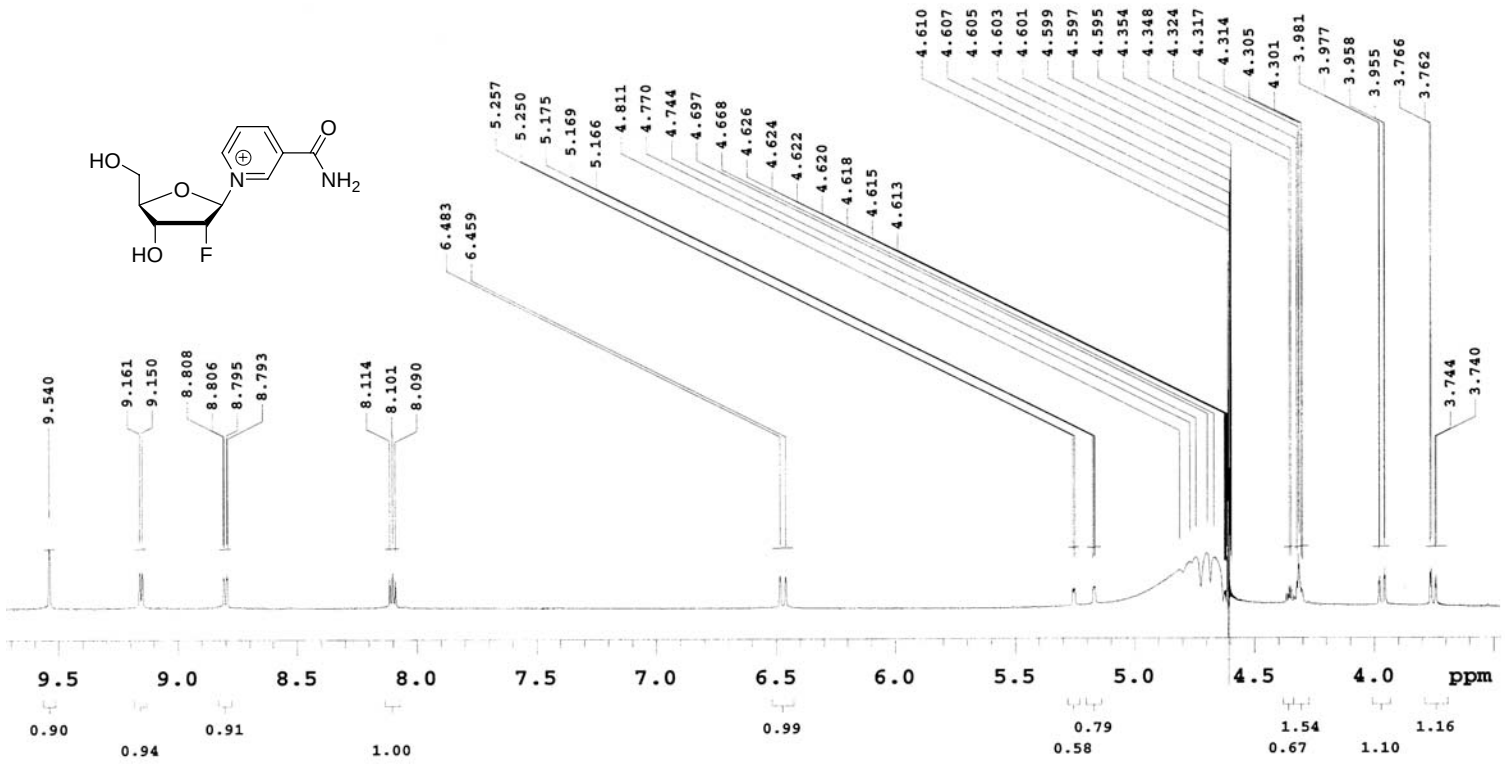


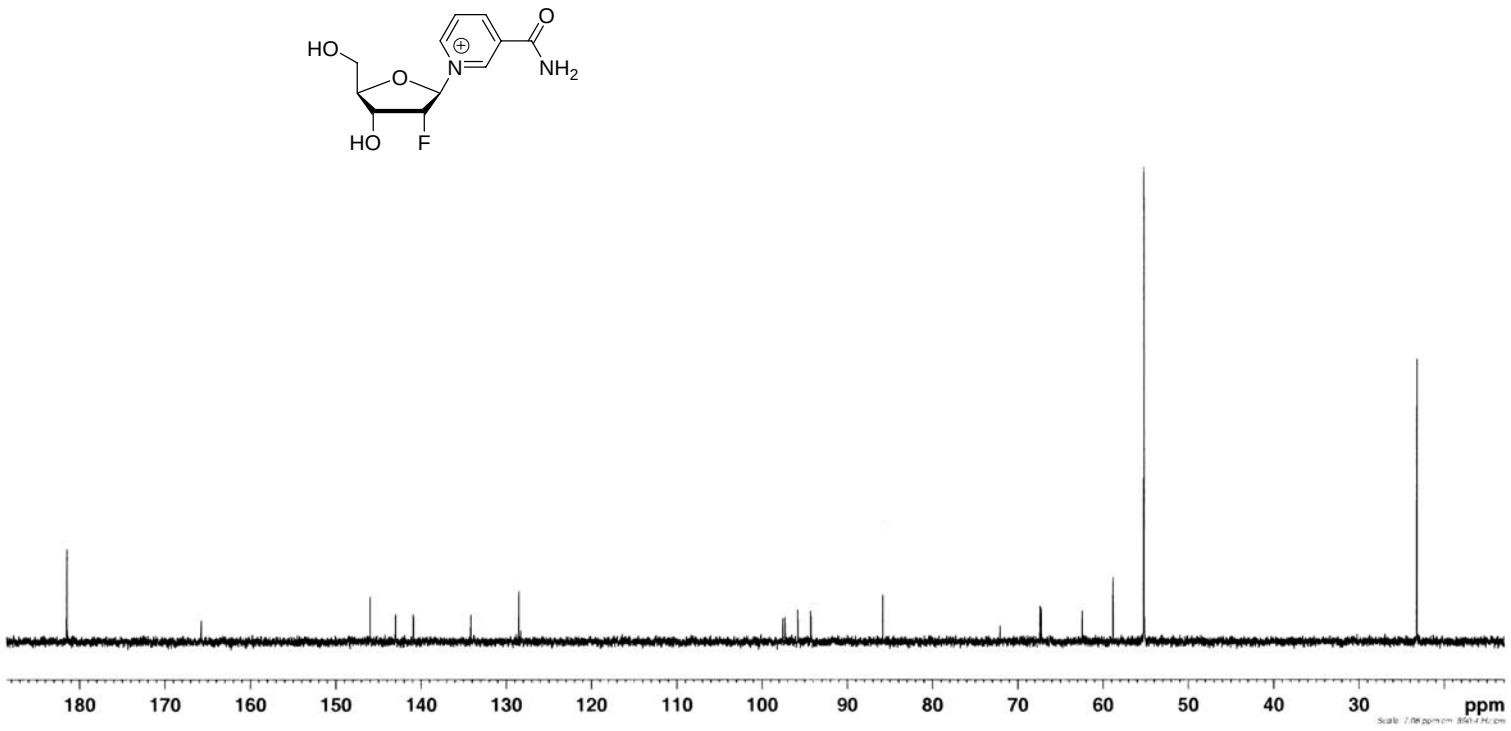
^{1}H NMR spectrum of **23**



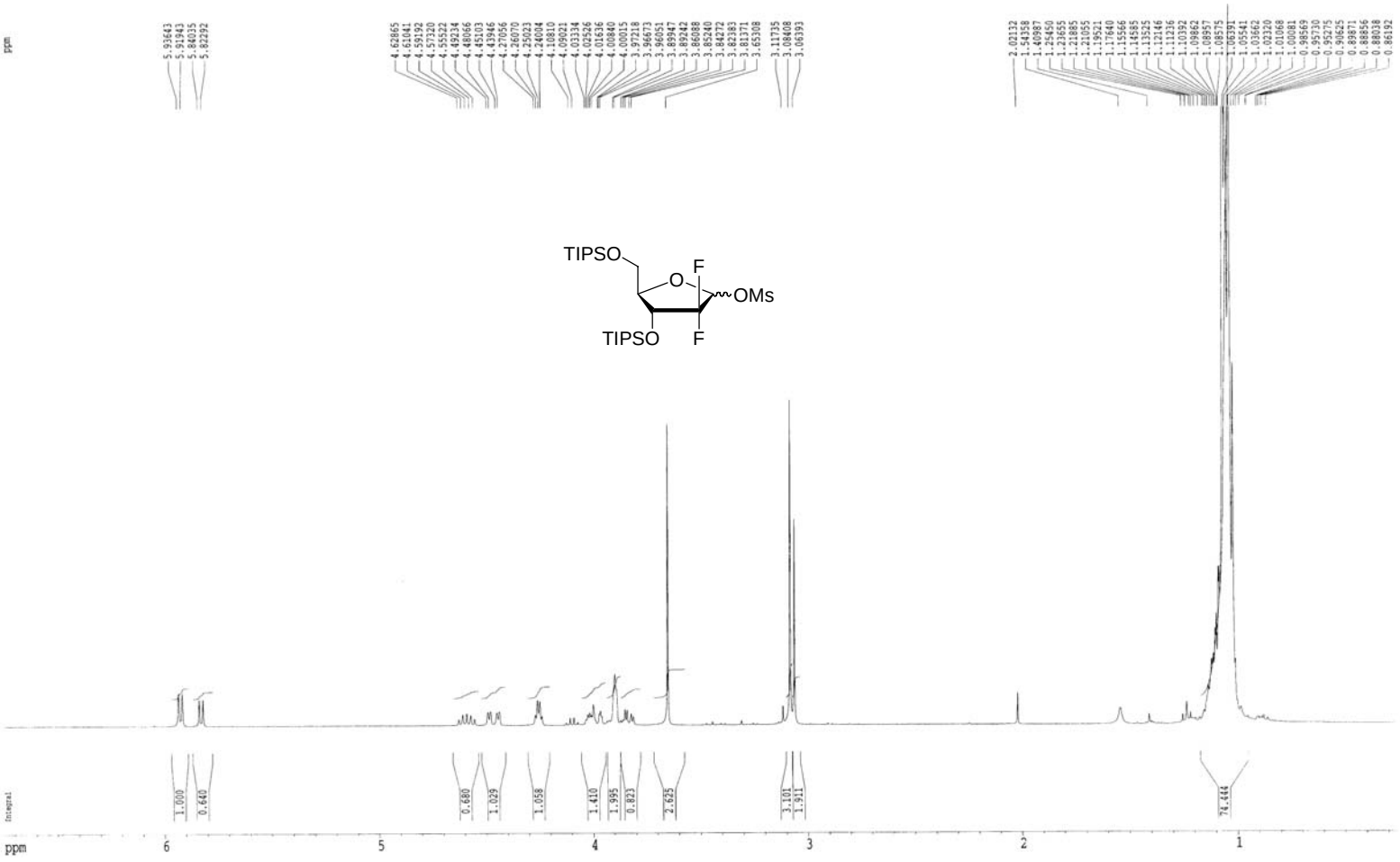
^{13}C NMR spectrum of **23**



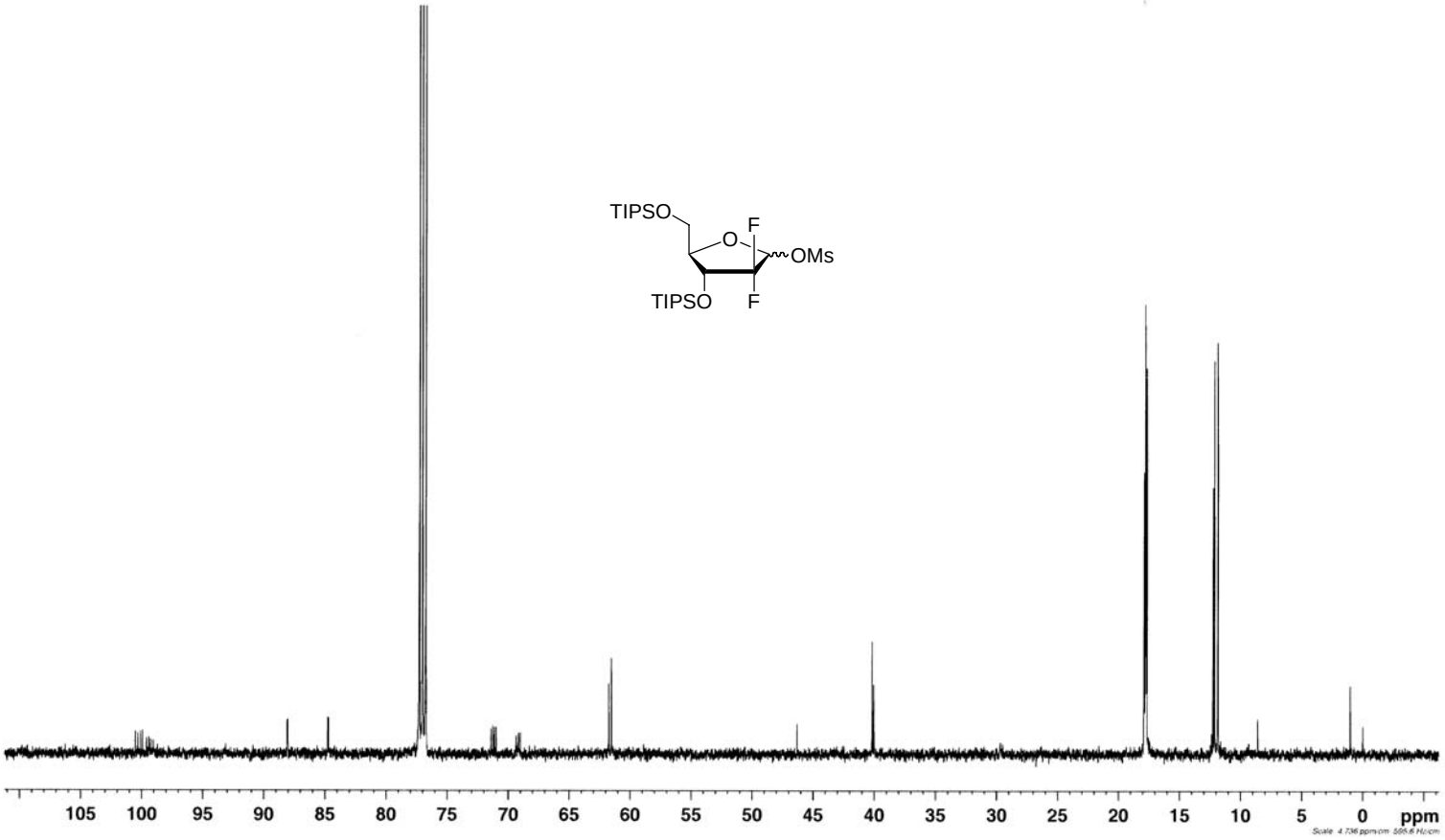
^{1}H NMR spectrum of **25**



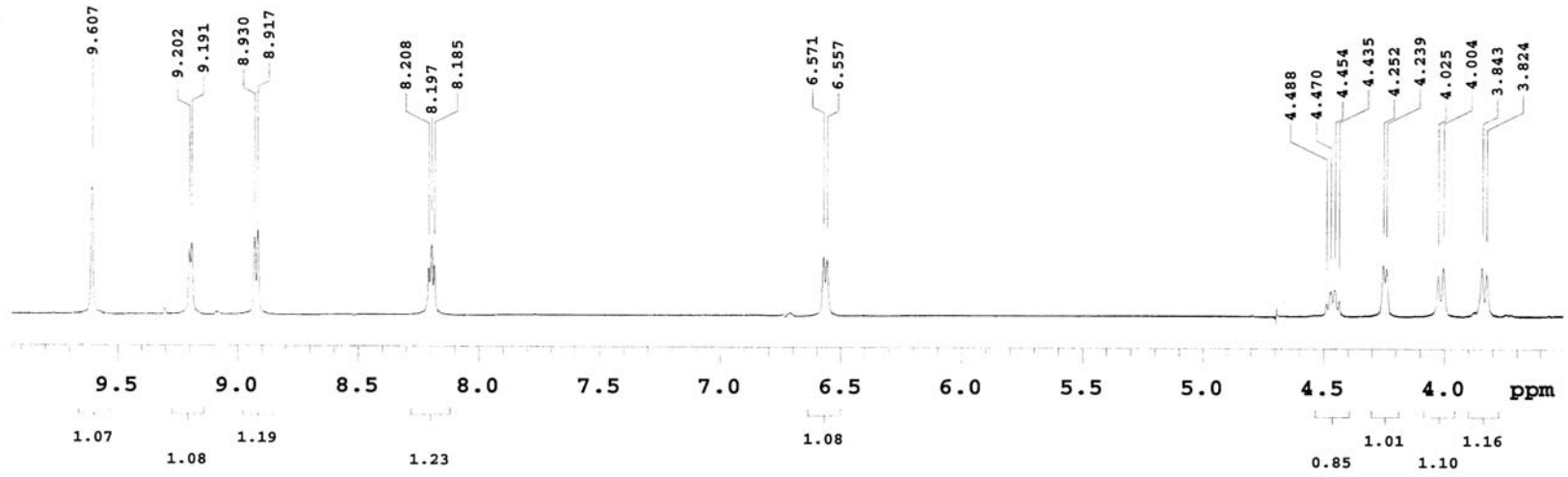
^{13}C NMR spectrum of **25**



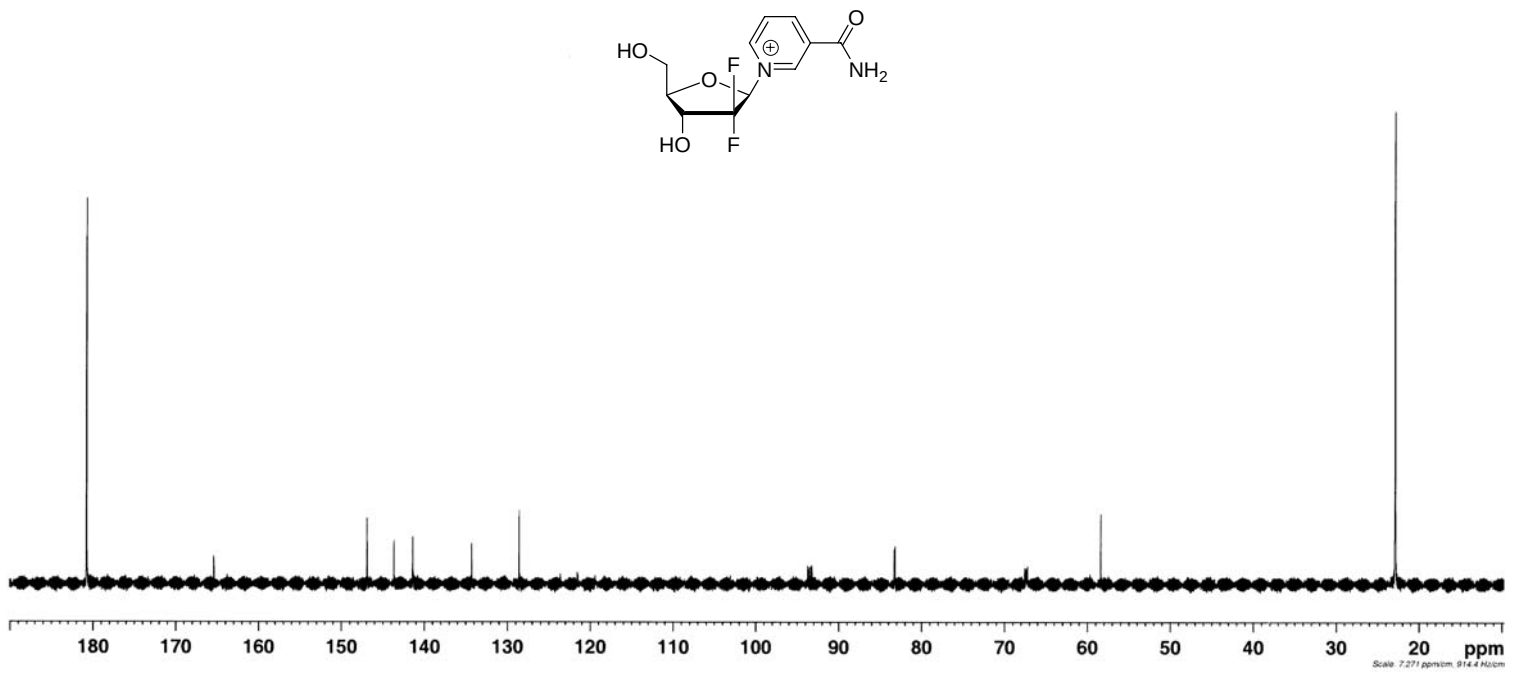
^{1}H NMR spectrum of **26**



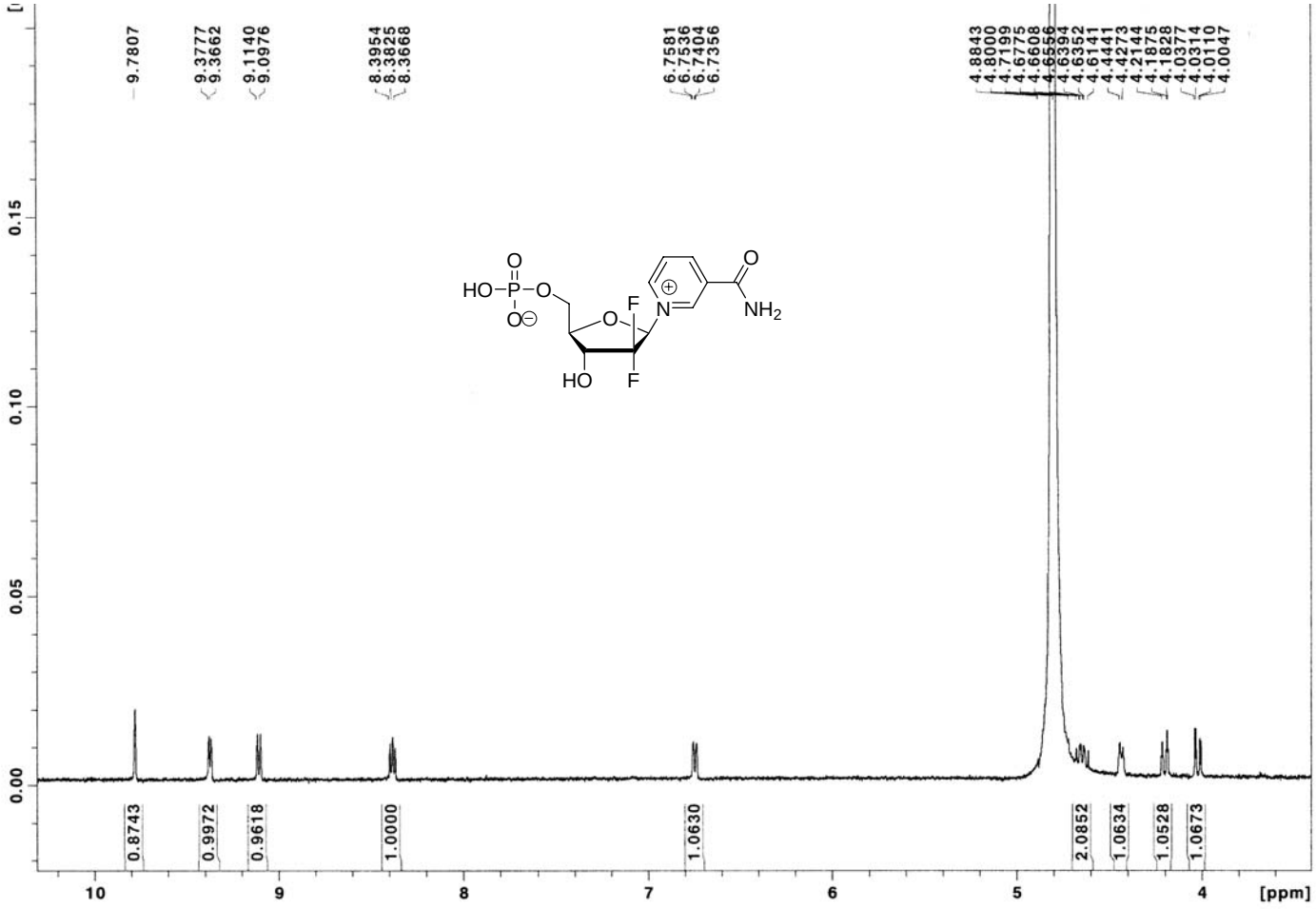
^{13}C NMR spectrum of **26**



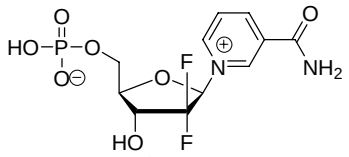
^{1}H NMR spectrum of **28**

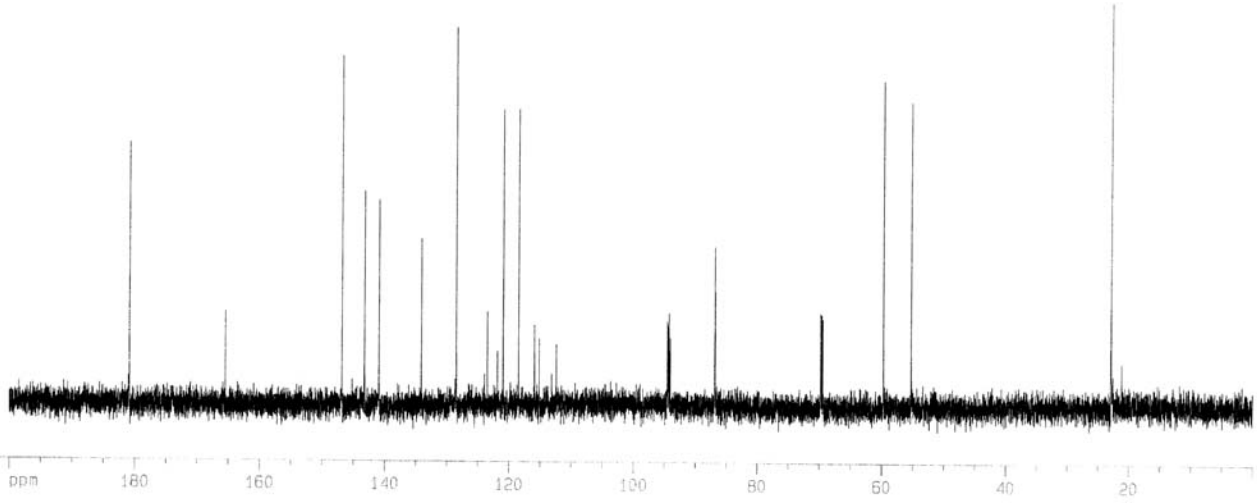


^{13}C NMR spectrum of **28**

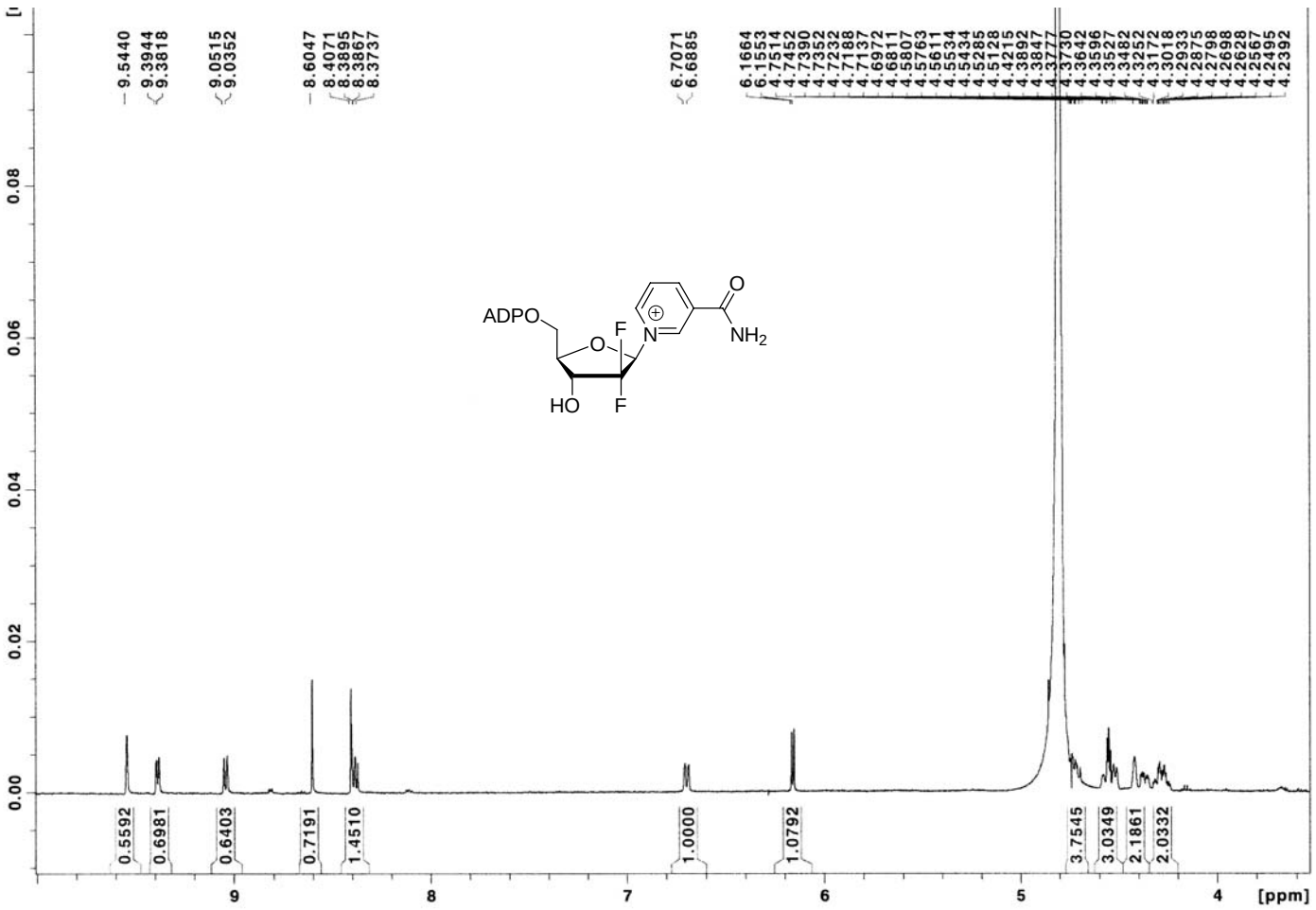


^{1}H NMR spectrum of **29**

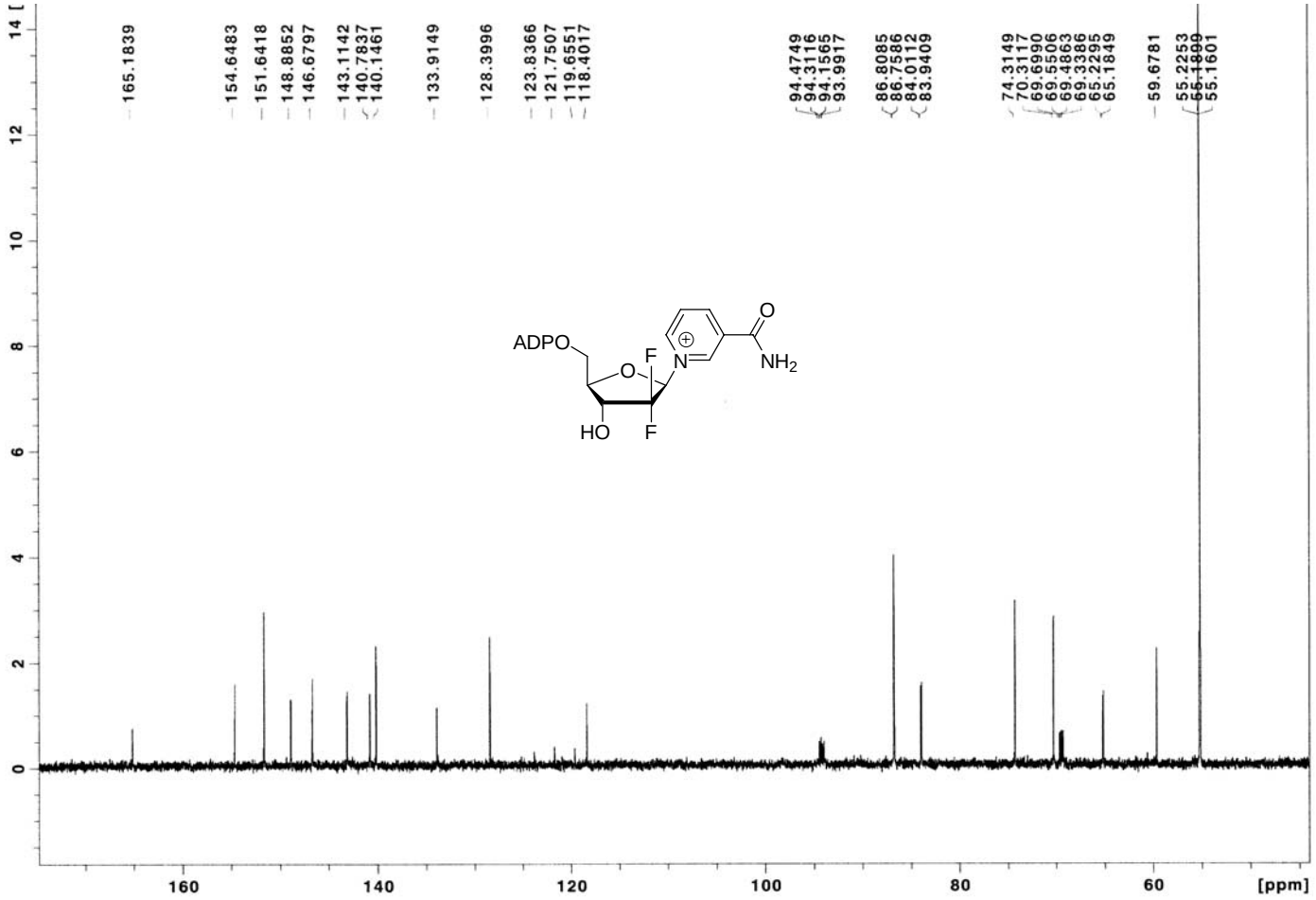




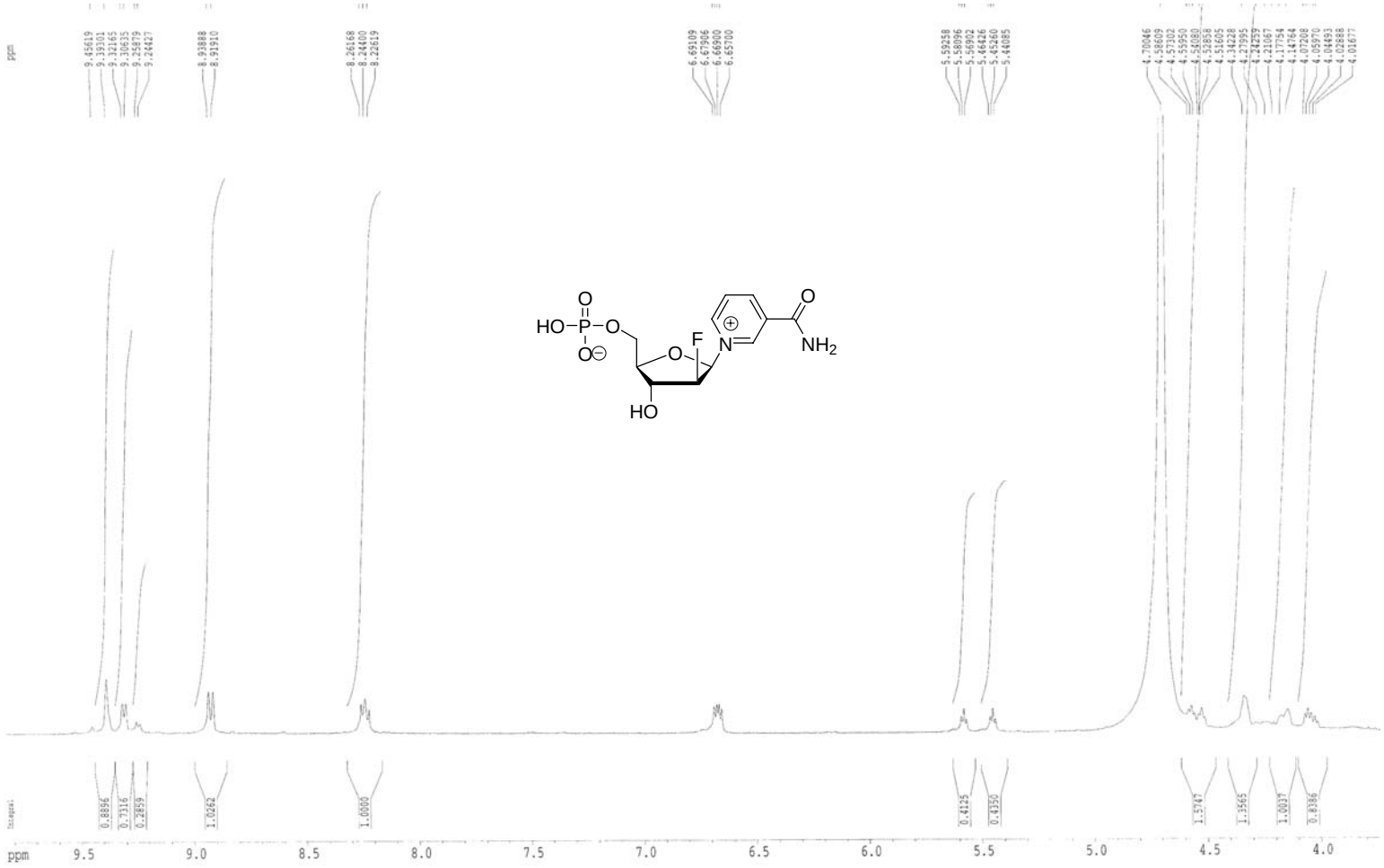
^{13}C NMR spectrum of **29**



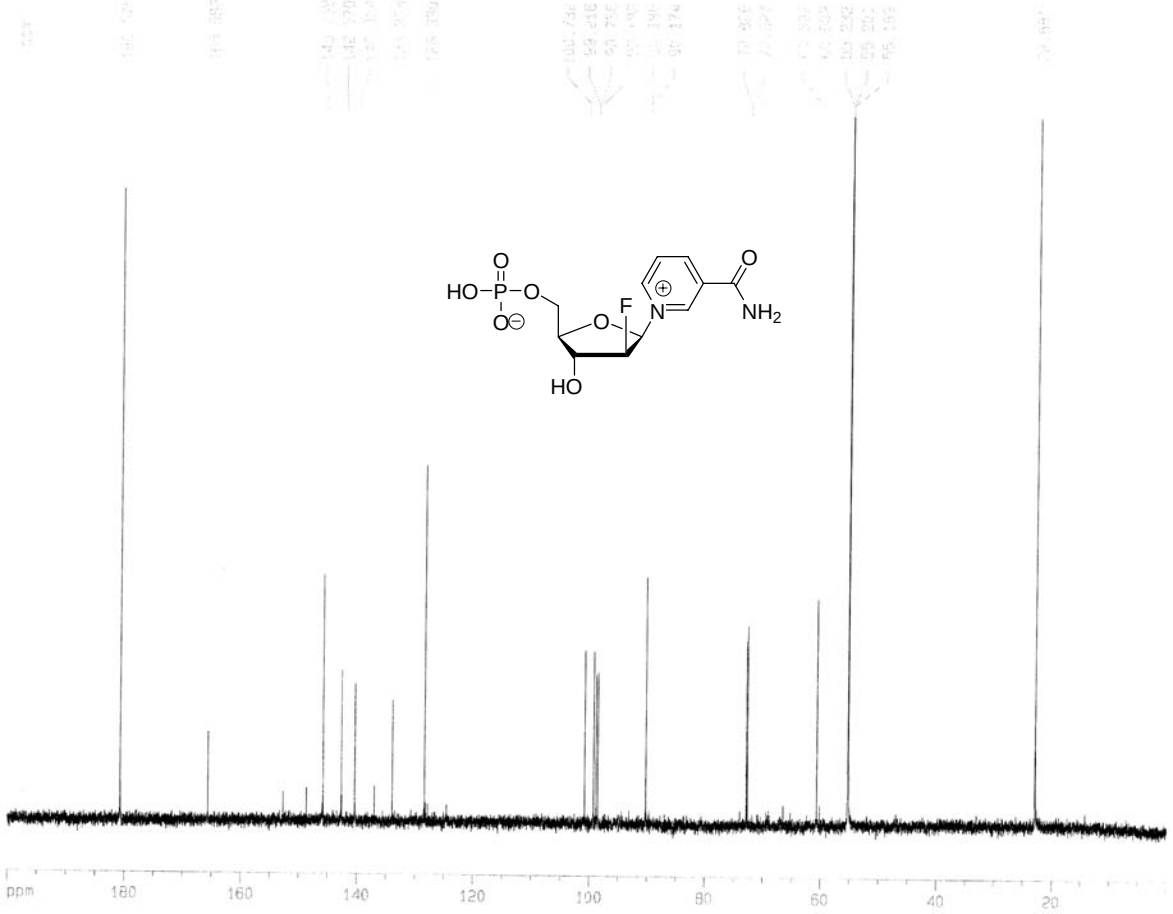
^{1}H NMR spectrum of **30**



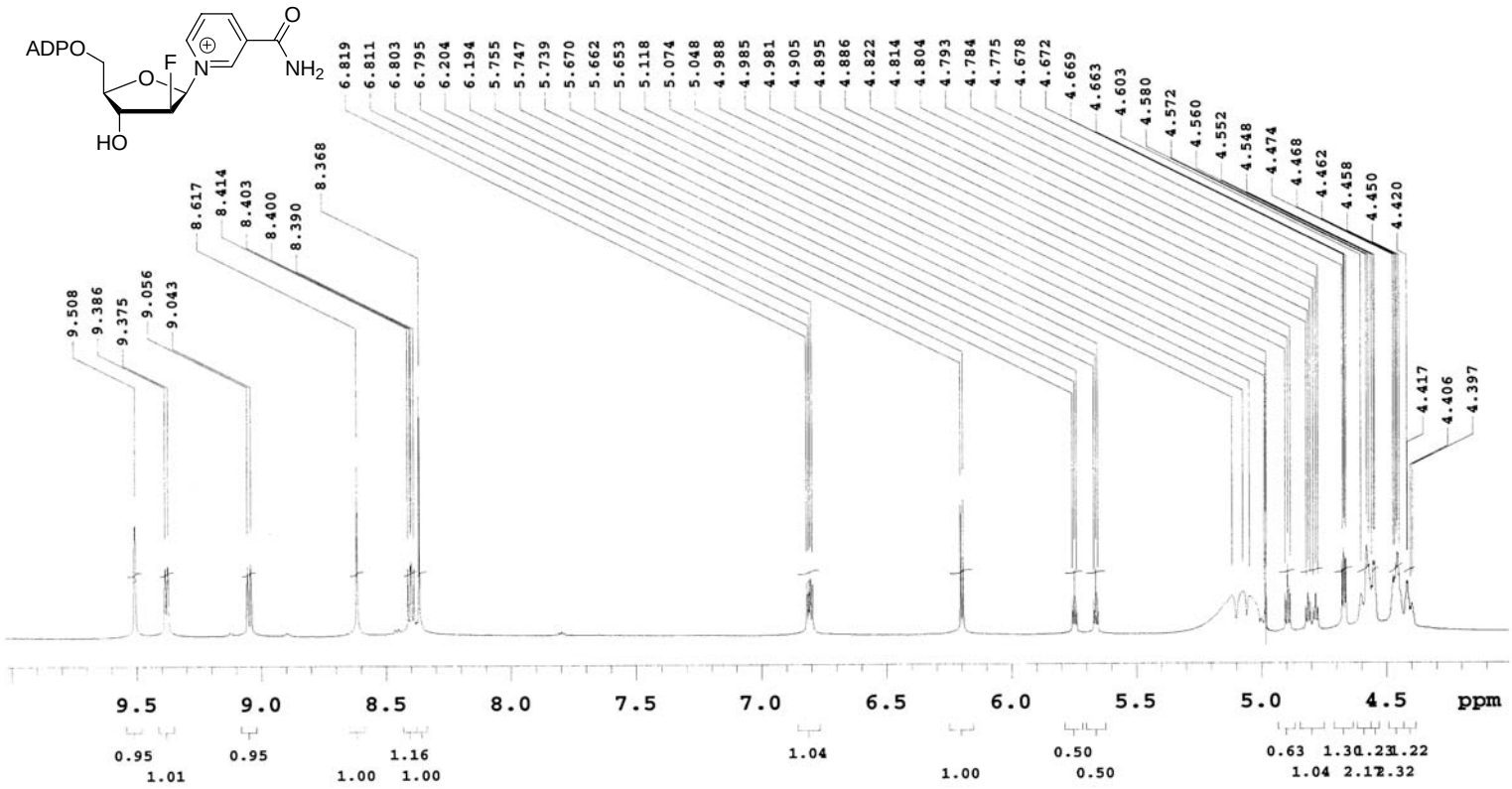
^{13}C NMR spectrum of **30**



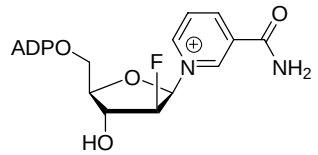
^{1}H NMR spectrum of **31**

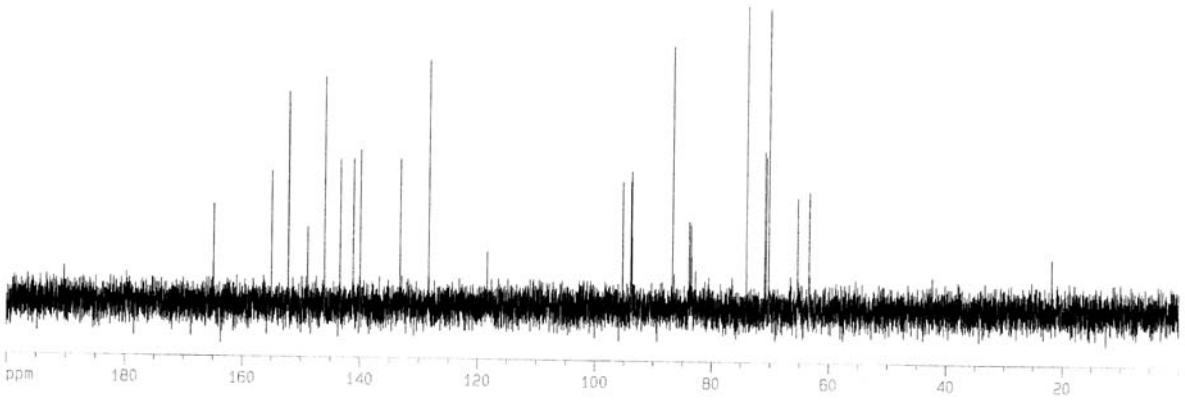


^{13}C NMR spectrum of **31**

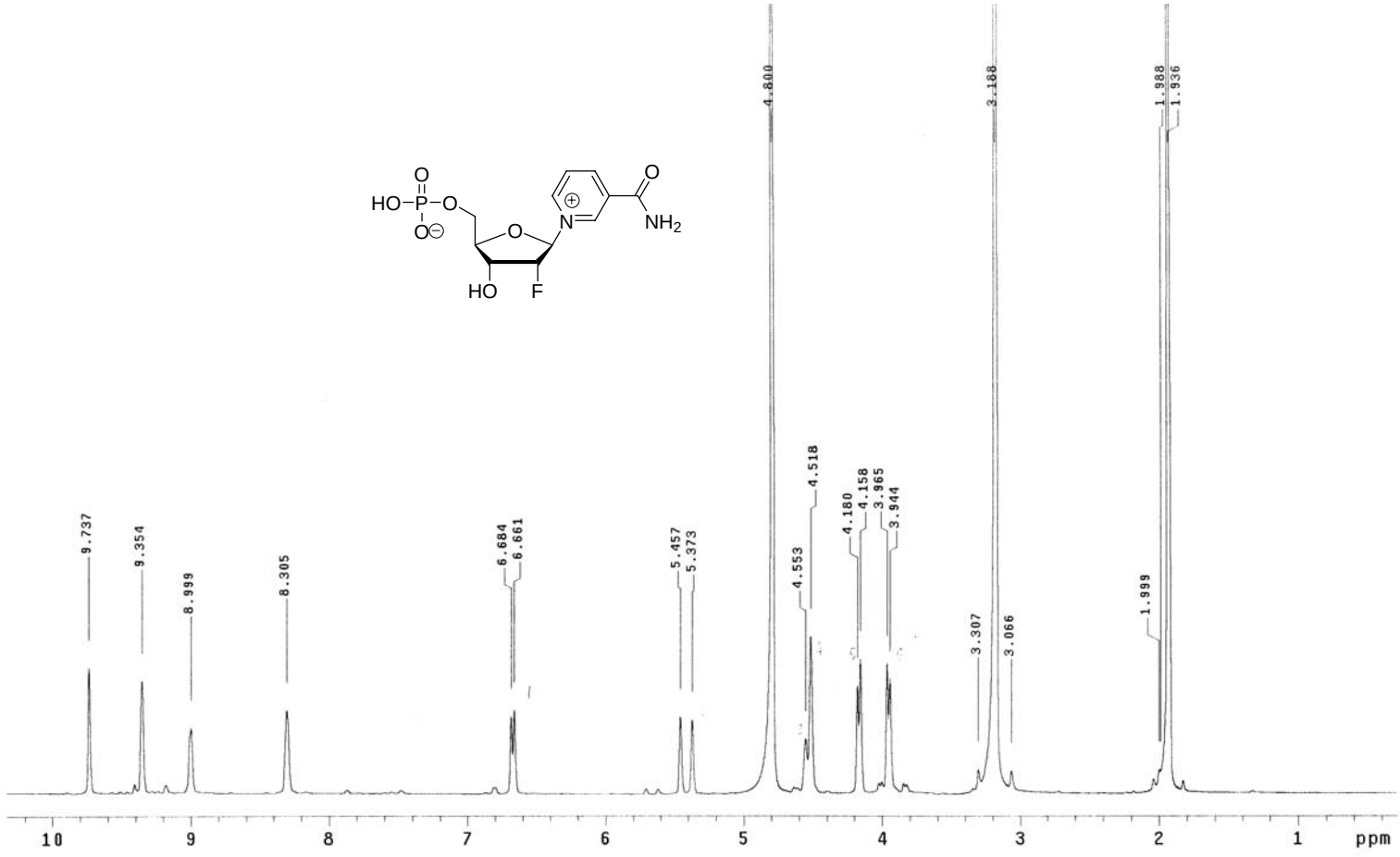


^{1}H NMR spectrum of **32**

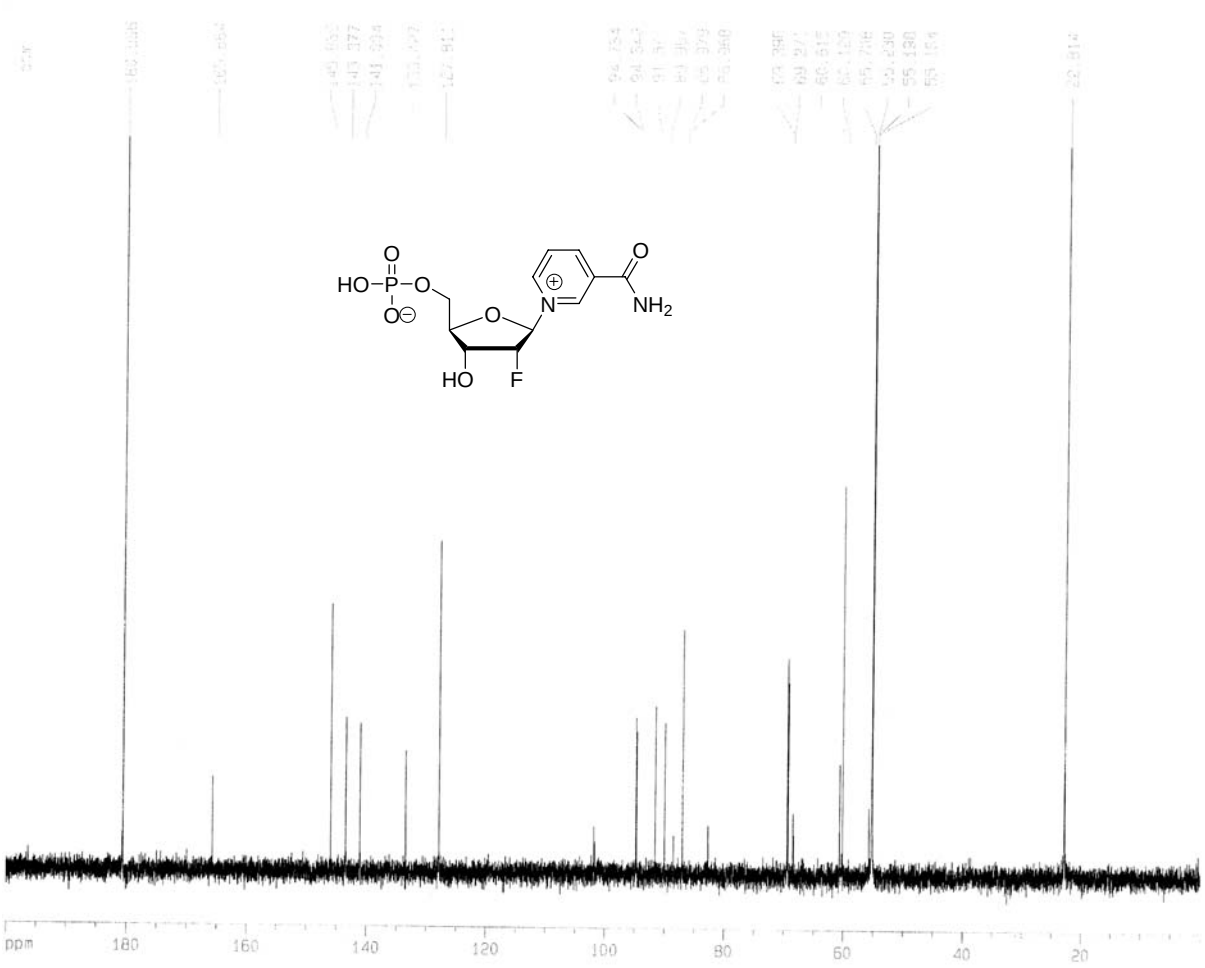




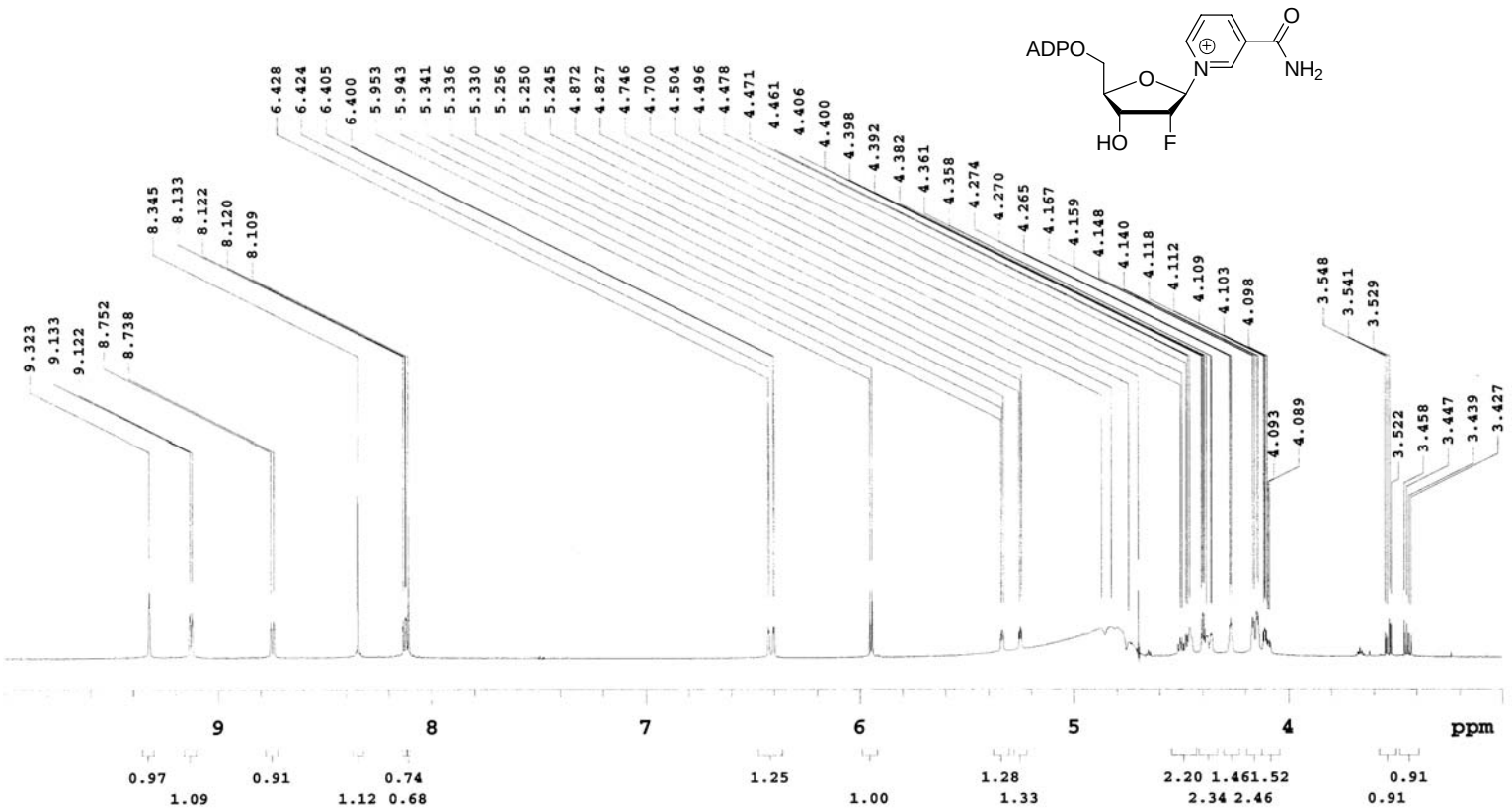
^{13}C NMR spectrum of **32**



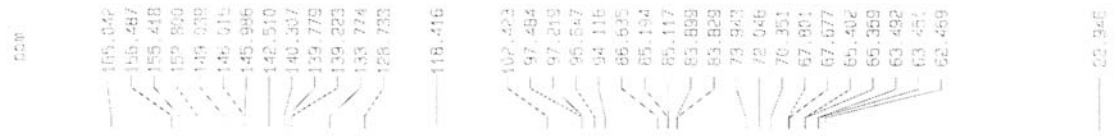
^{1}H NMR spectrum of **33**

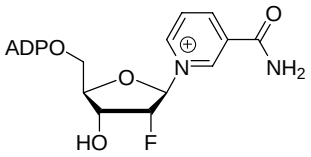


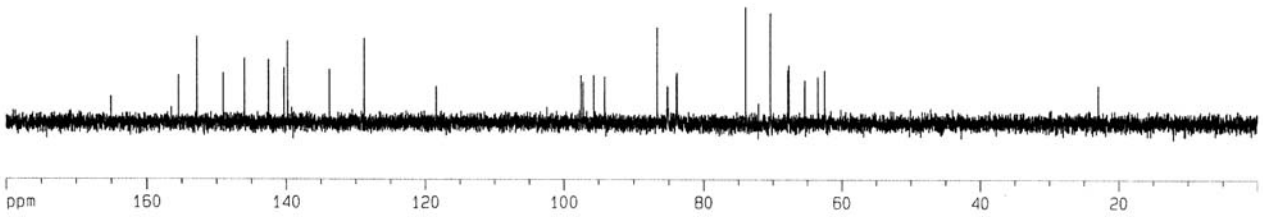
^{13}C NMR spectrum of **33**



^{1}H NMR spectrum of **34**







^{13}C NMR spectrum of **34**