

Supporting Information

A New Chemical Probe for the Detection of Cancer-Linked Galectin-3

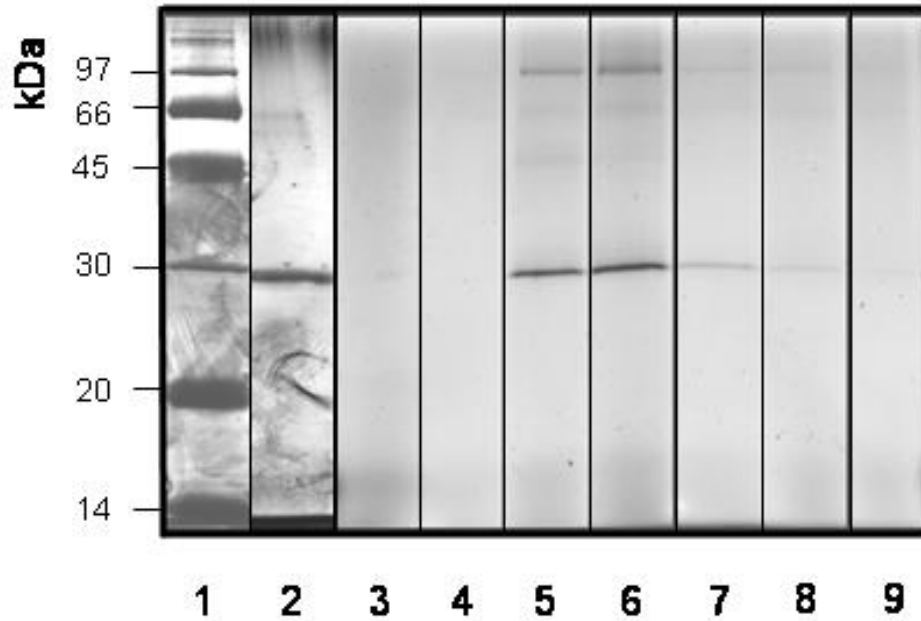
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Netherlands

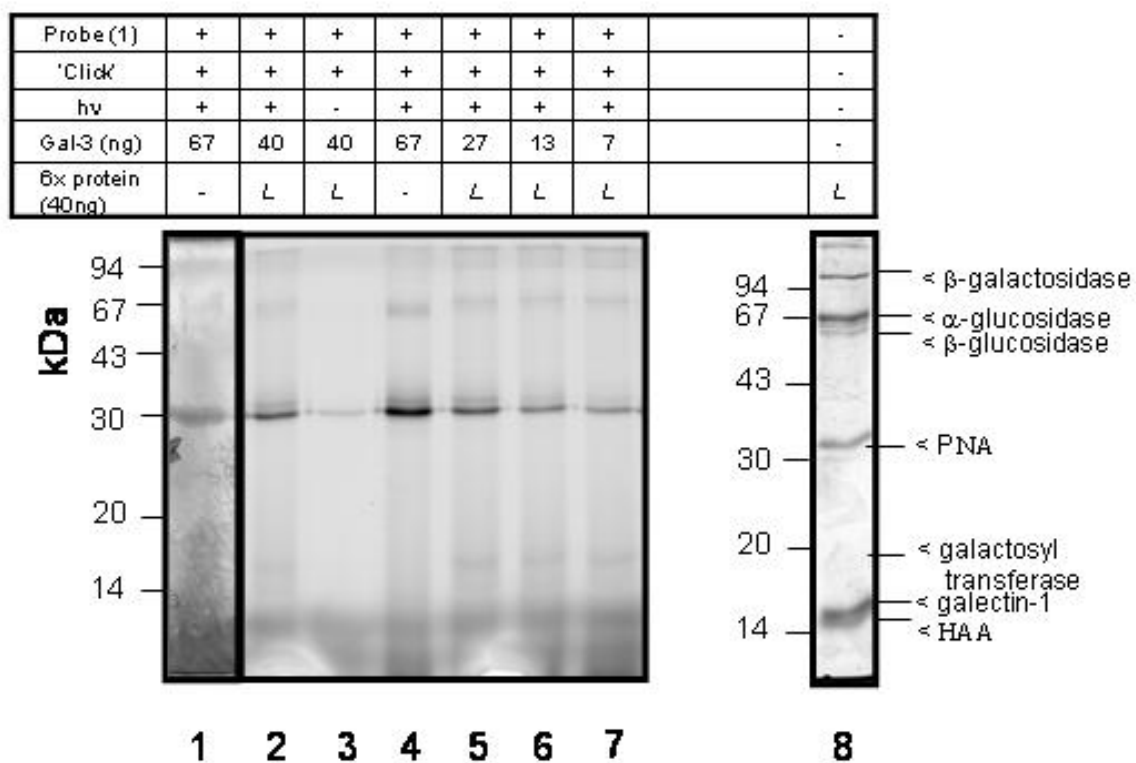
Galectin-3 labeling studies in presence of protein mixture I

Probe (1) [μ M]	-	-	-	10	10	5	2	1	0.5
'Click'	-	-	+	+	+	+	+	+	+
hv	-	-	+	-	+	+	+	+	+
Gal-3 (ng)	-	+	+	+	+	+	+	+	+
6x protein	+	-	+	+	+	+	+	+	+



Effect of probe concentration on labeling intensity in the presence of protein mix I. Lanes 1 and 2 are silver stained, lanes 3-9 fluorescent pictures.

Galectin-3 labeling studies in presence of protein mixture II



Selectivity of probe 1 for galectin-3 in presence of protein mixture II

Monovalent probe 3 concentration-dependent labeling studies.

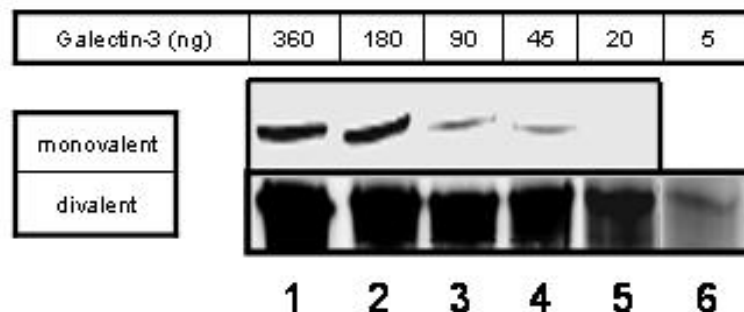
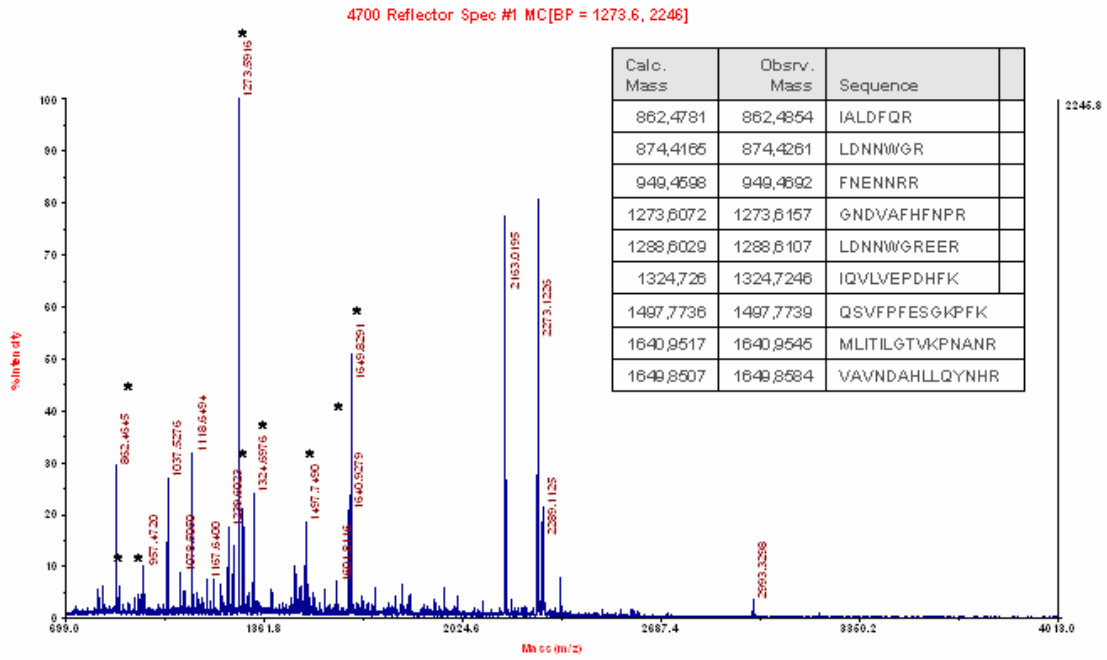


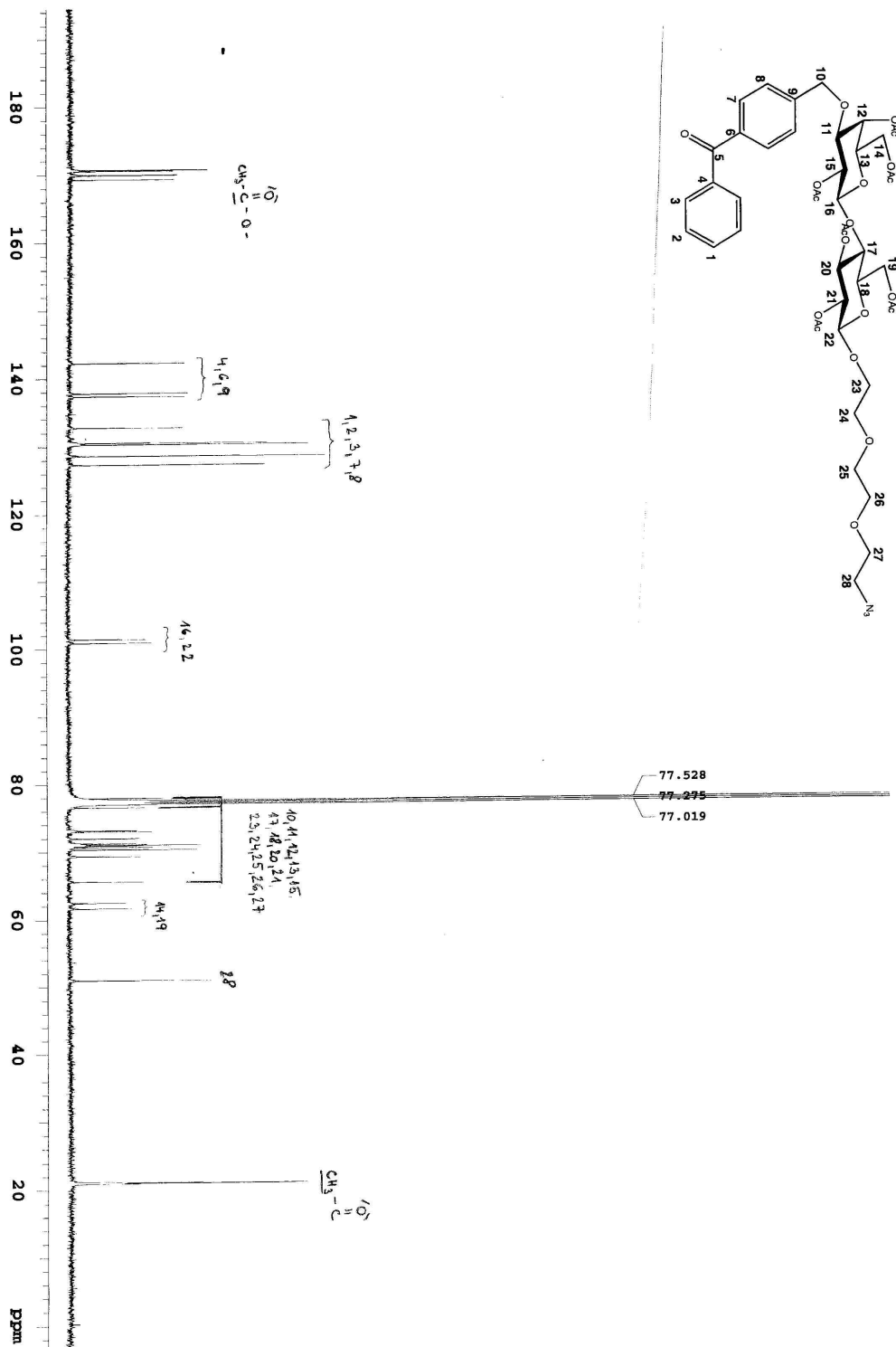
Figure 3 Galectin-3 labeling studies with variation of Galectin-3 quantity at 5 μ M monovalent probe 3 or divalent probe 1.

Labeling studies with variation of Galectin-3 quantity (probe 3). An aliquot of 5 μ L of monovalent probe 3 (50 μ M in water) or 1 (50 μ M in water : DMSO 20:1) was added to varying amounts of galectin-3 (20, 10, 5, 2.5, 1.1 μ L of 125 μ g/mL stock solution and 2.8 μ L of a 12.5 μ g/mL stock solution respectively), and the total volume was adjusted to 50 μ L in HEPES buffer. The samples were then photoincubated, “clicked” to the fluorescent dye 2, loaded onto the gel and visualized as described above. The experiments for probe 1 were performed similarly.

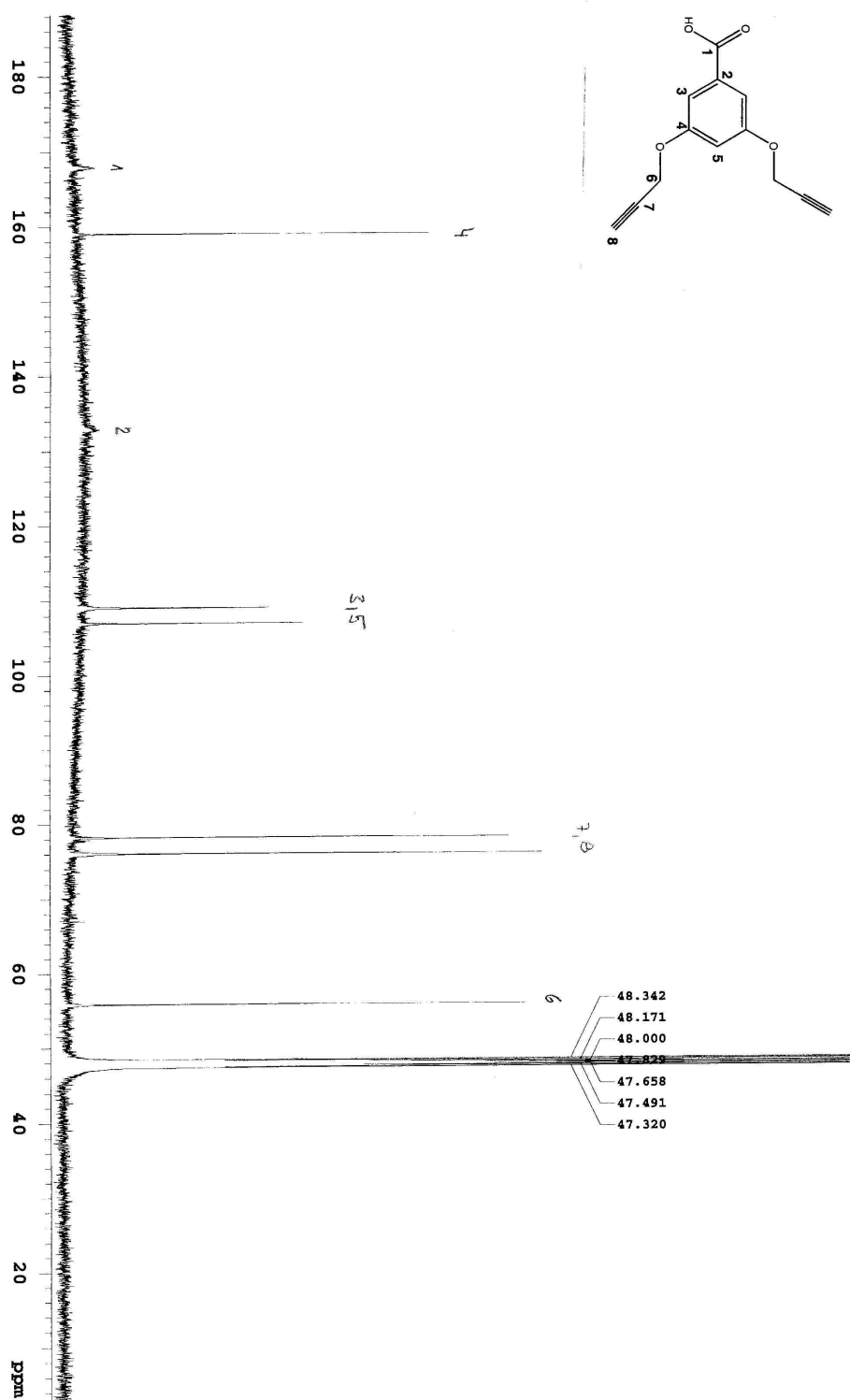


MALDI spectrum of the excised protein band indicated in figure 2, lane 6. Asterisks indicate 9 peptides from a tryptic digest of galectin-3

¹³C NMR spectrum of 4

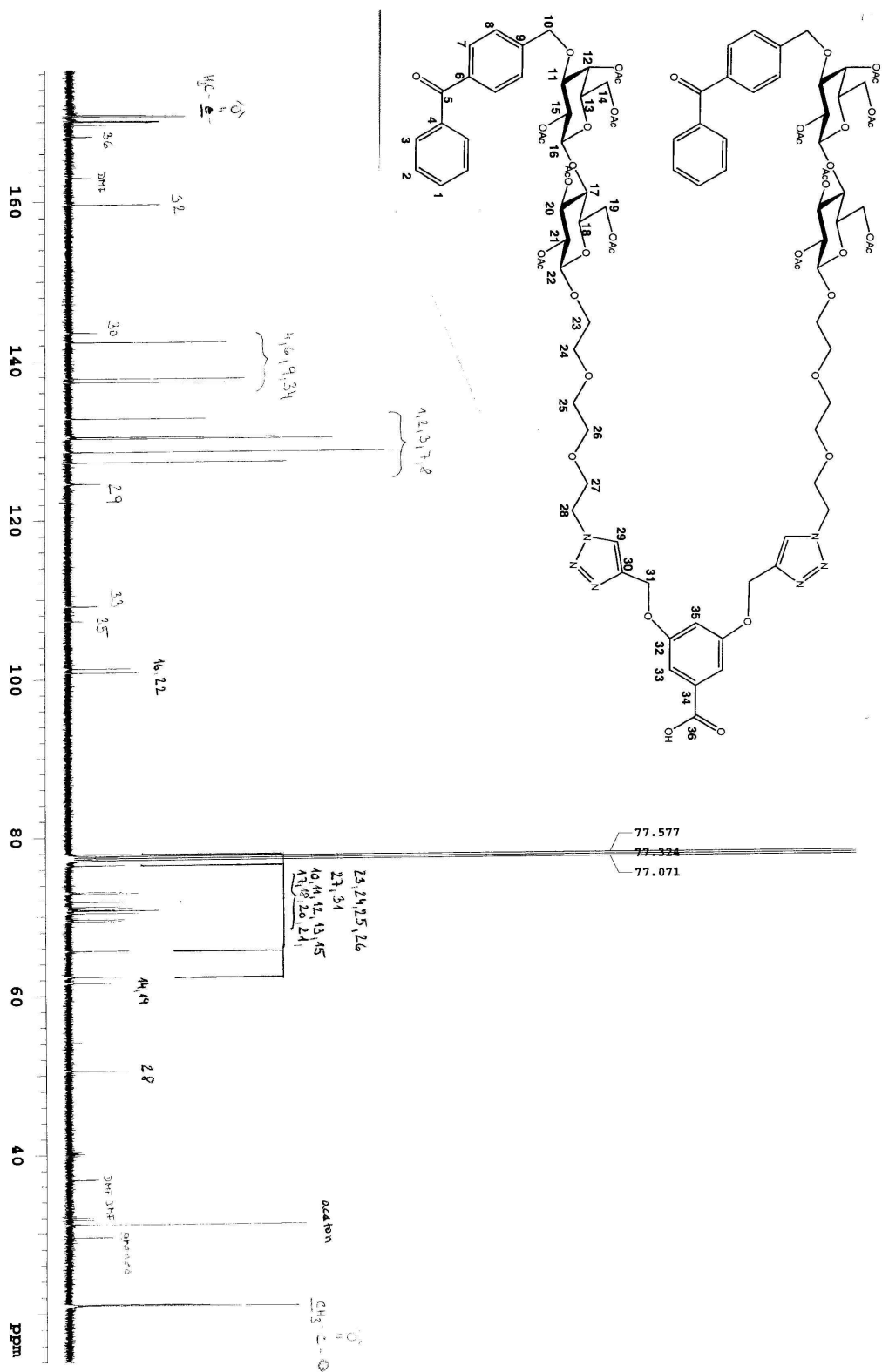


^{13}C NMR spectrum of 5

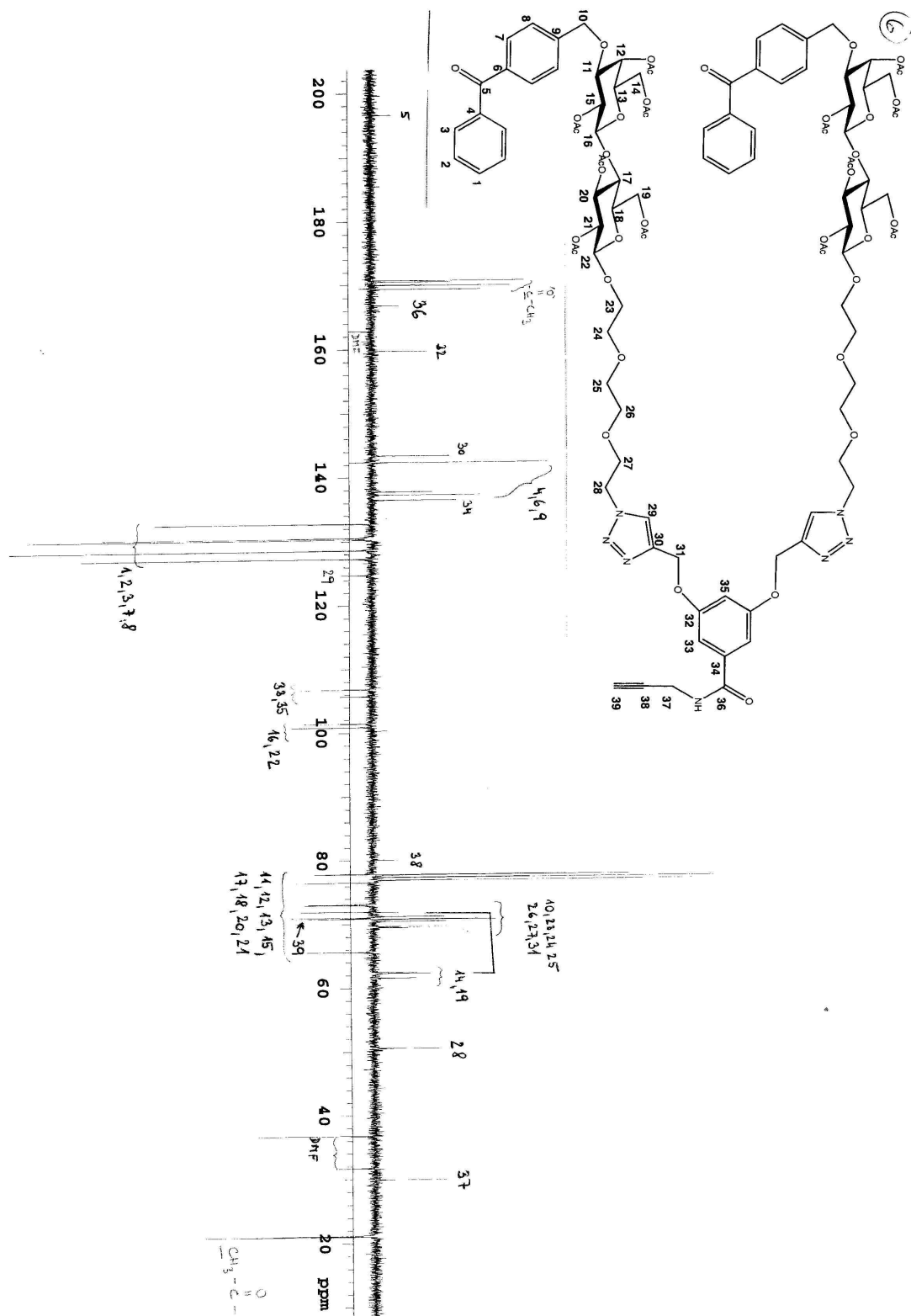


(1)

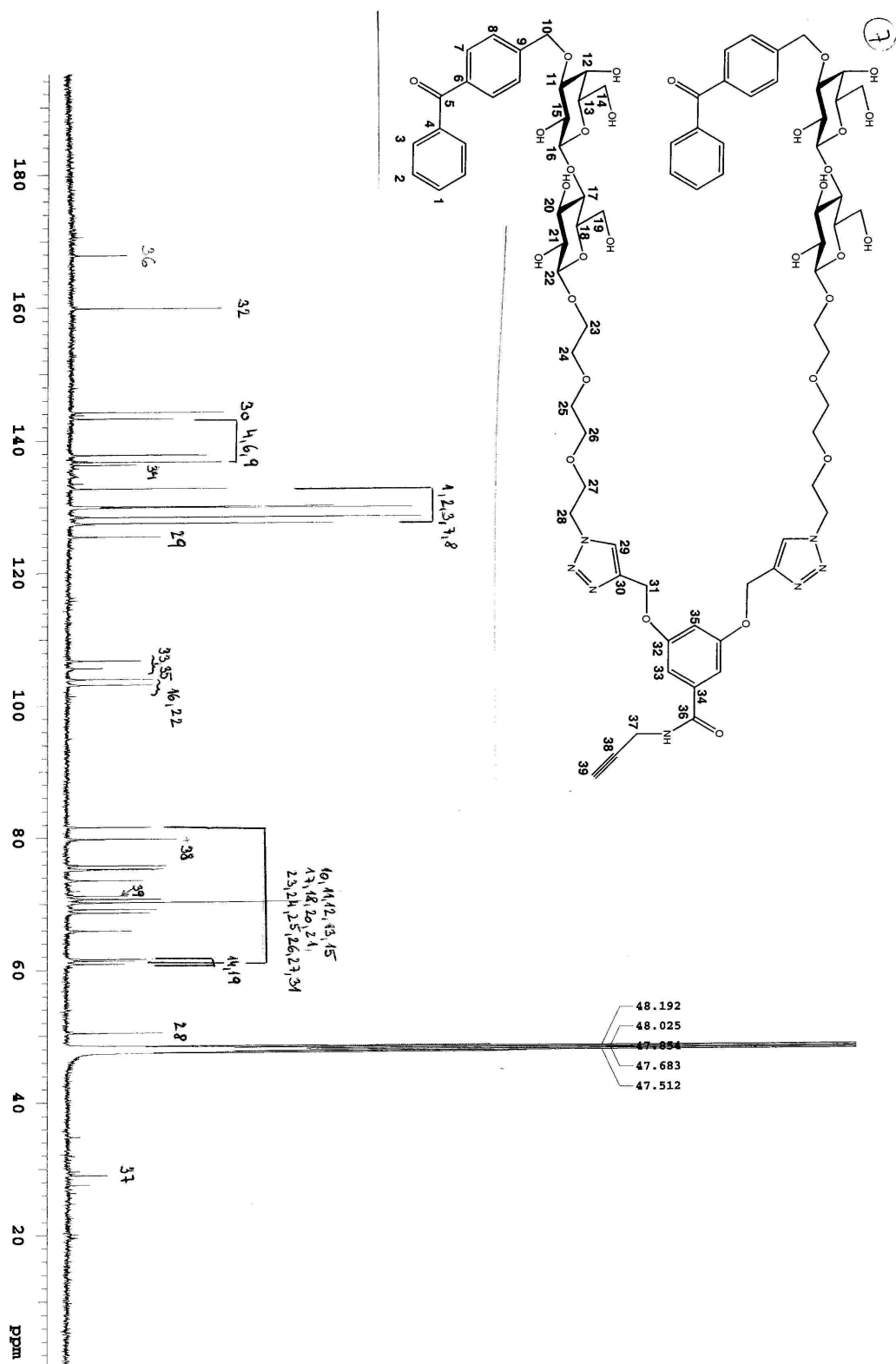
¹³C NMR spectrum of 6



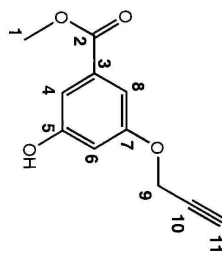
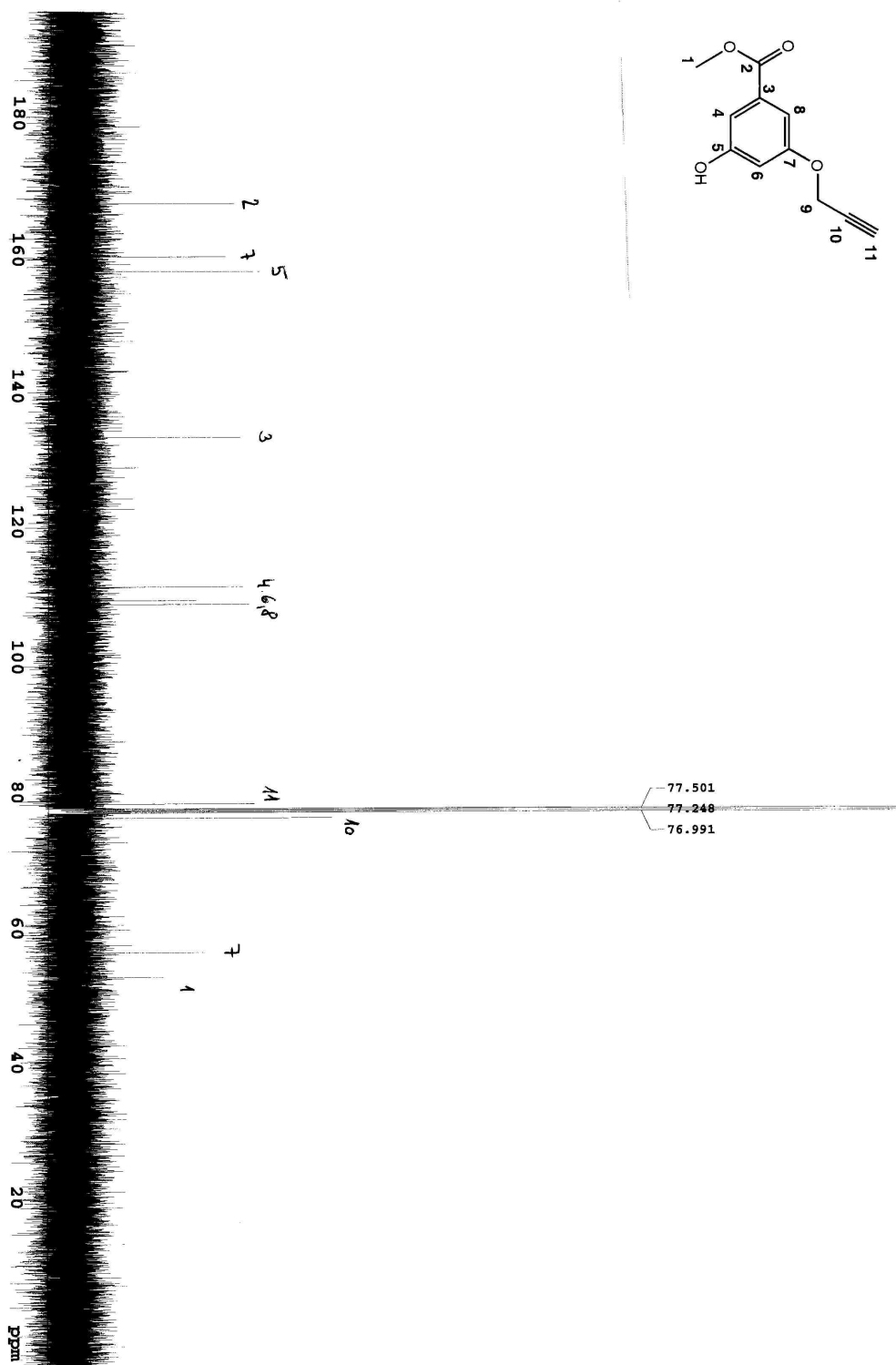
¹³C NMR spectrum of protected **1**



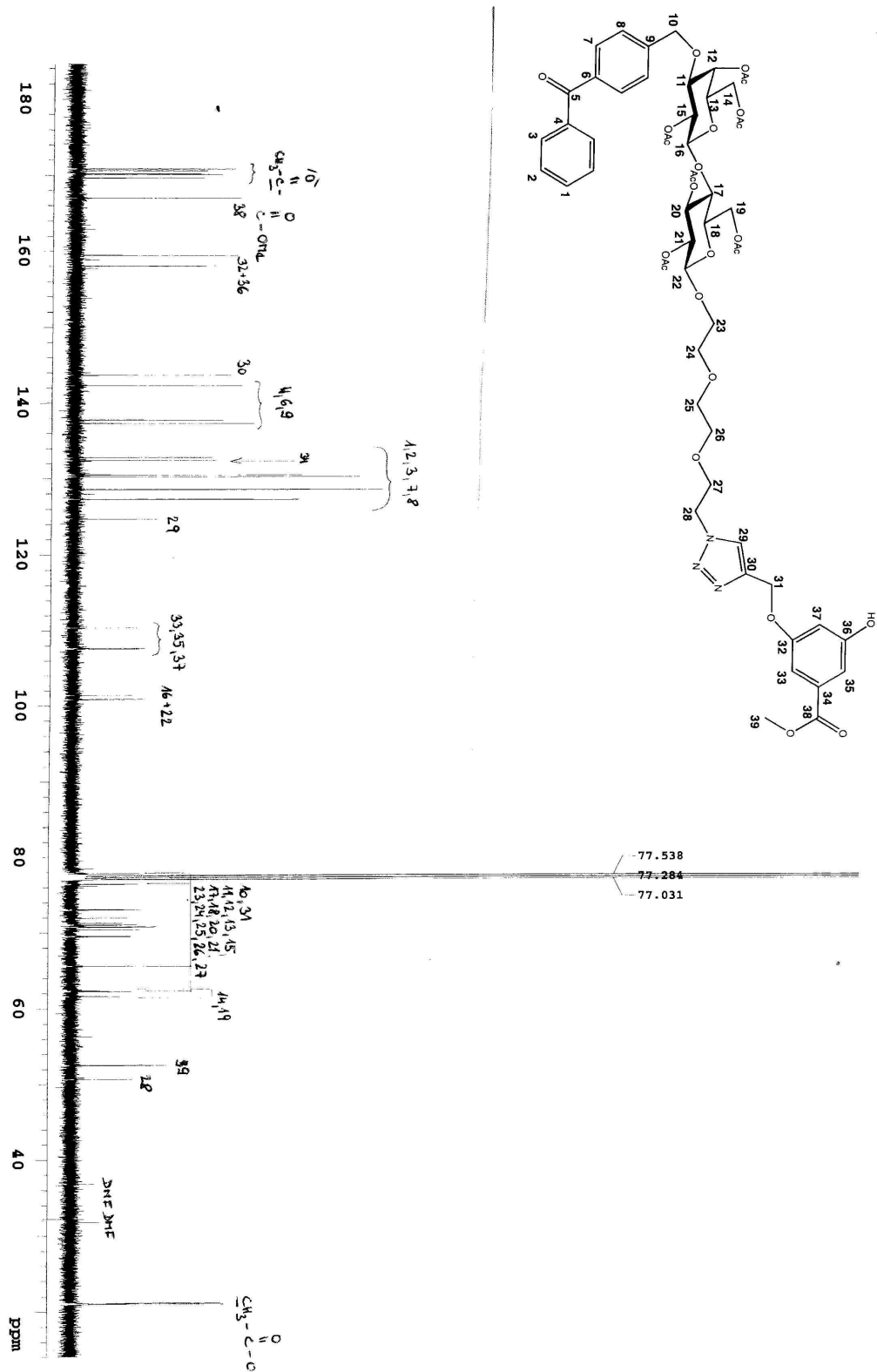
¹³C NMR spectrum of 1



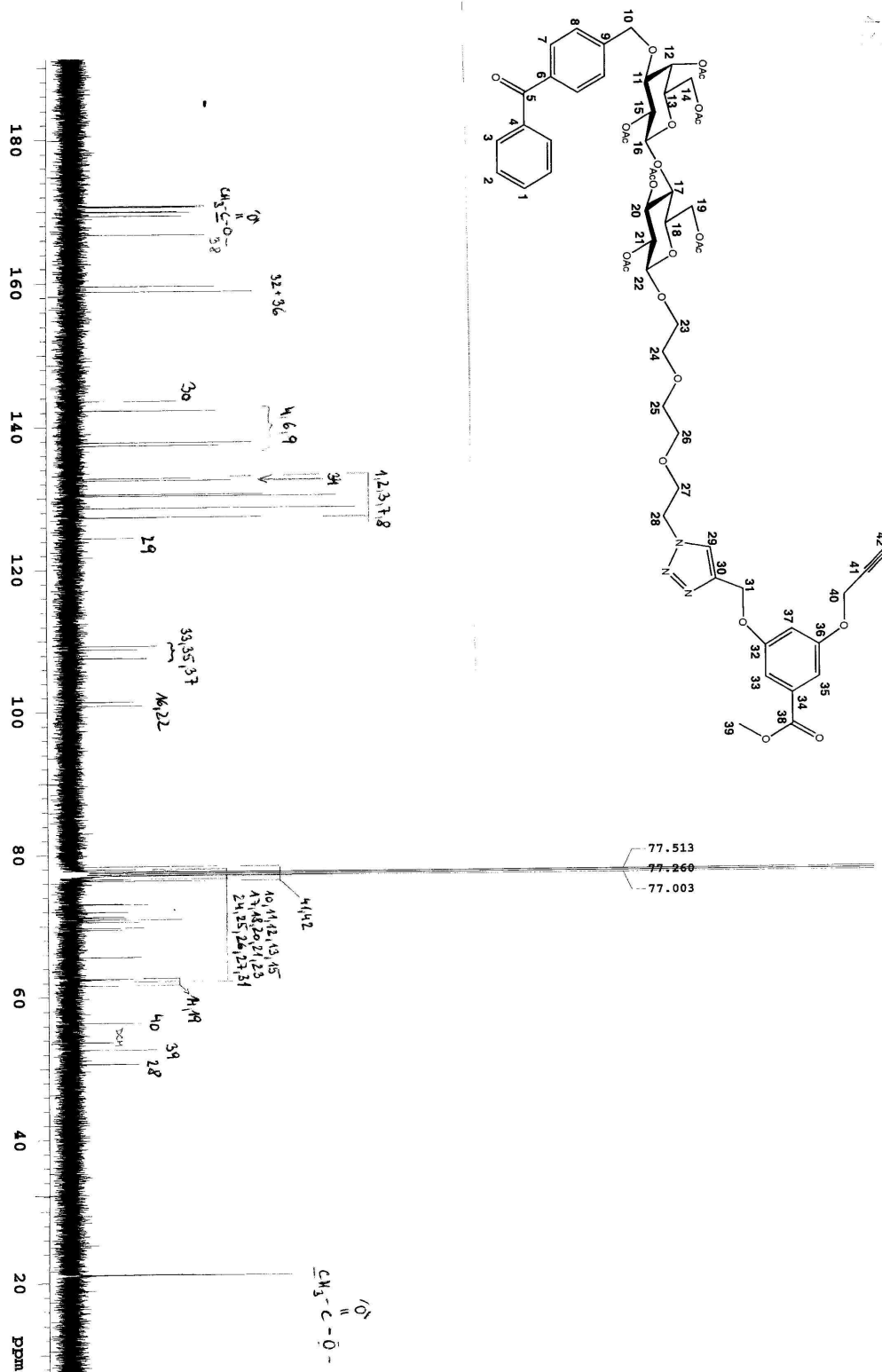
^{13}C NMR spectrum of monofunctionalized 7



¹³C NMR spectrum of 8



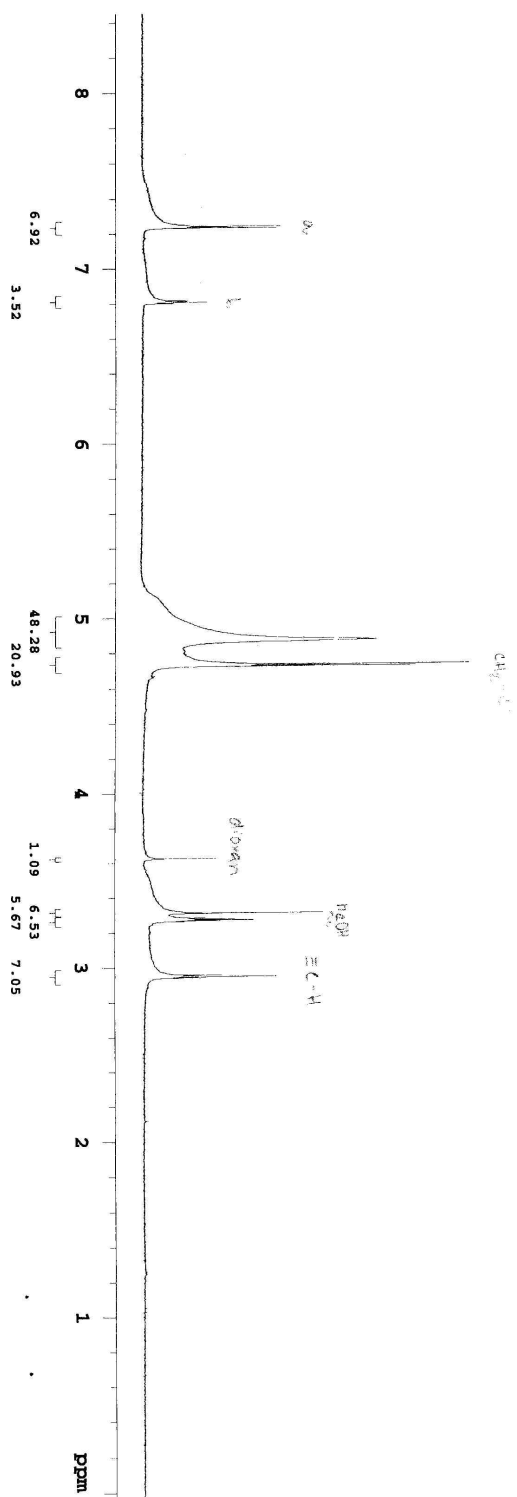
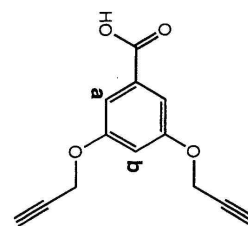
¹³C NMR spectrum of 9



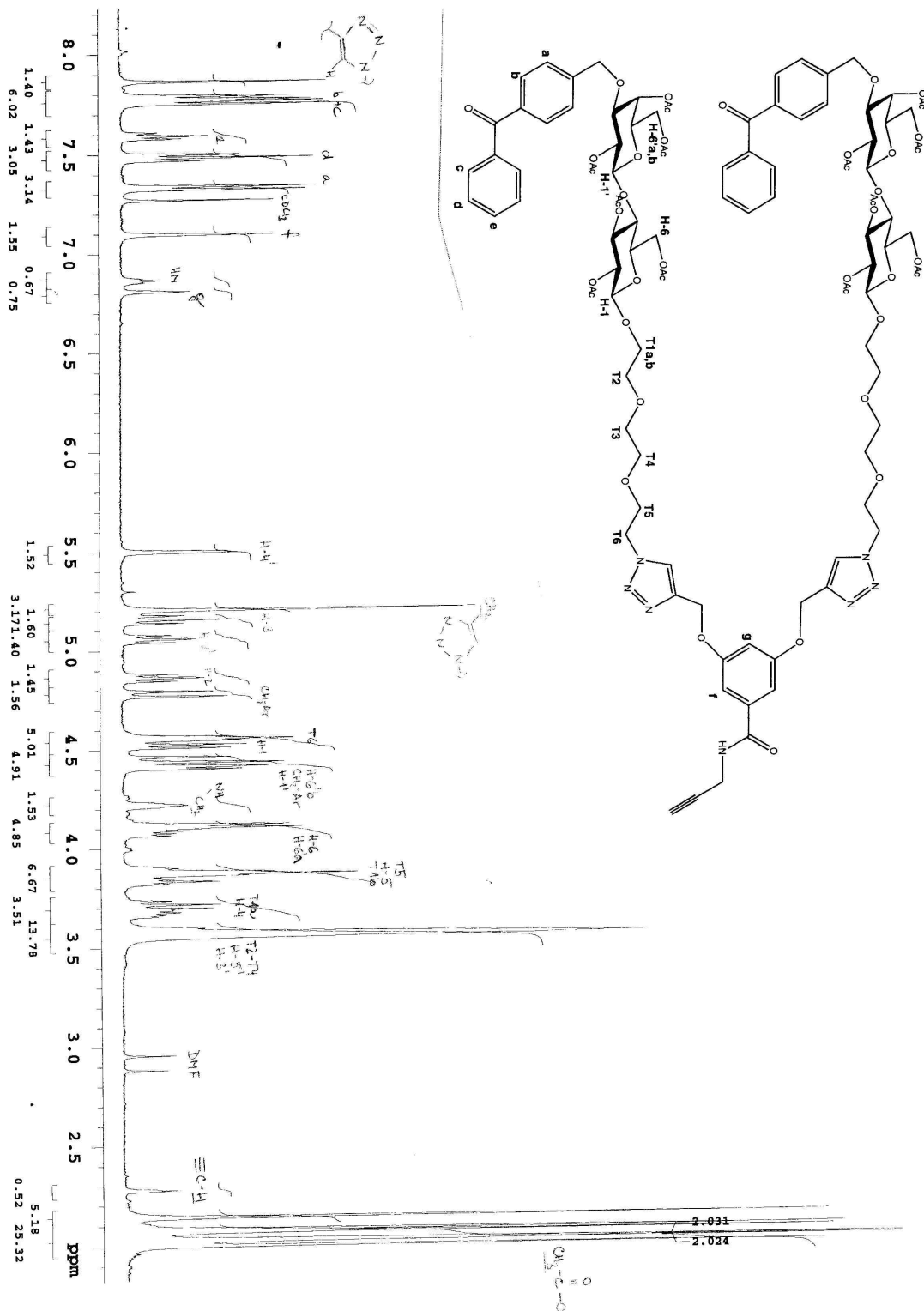
¹³C NMR spectrum of 3



¹H NMR spectrum of 5



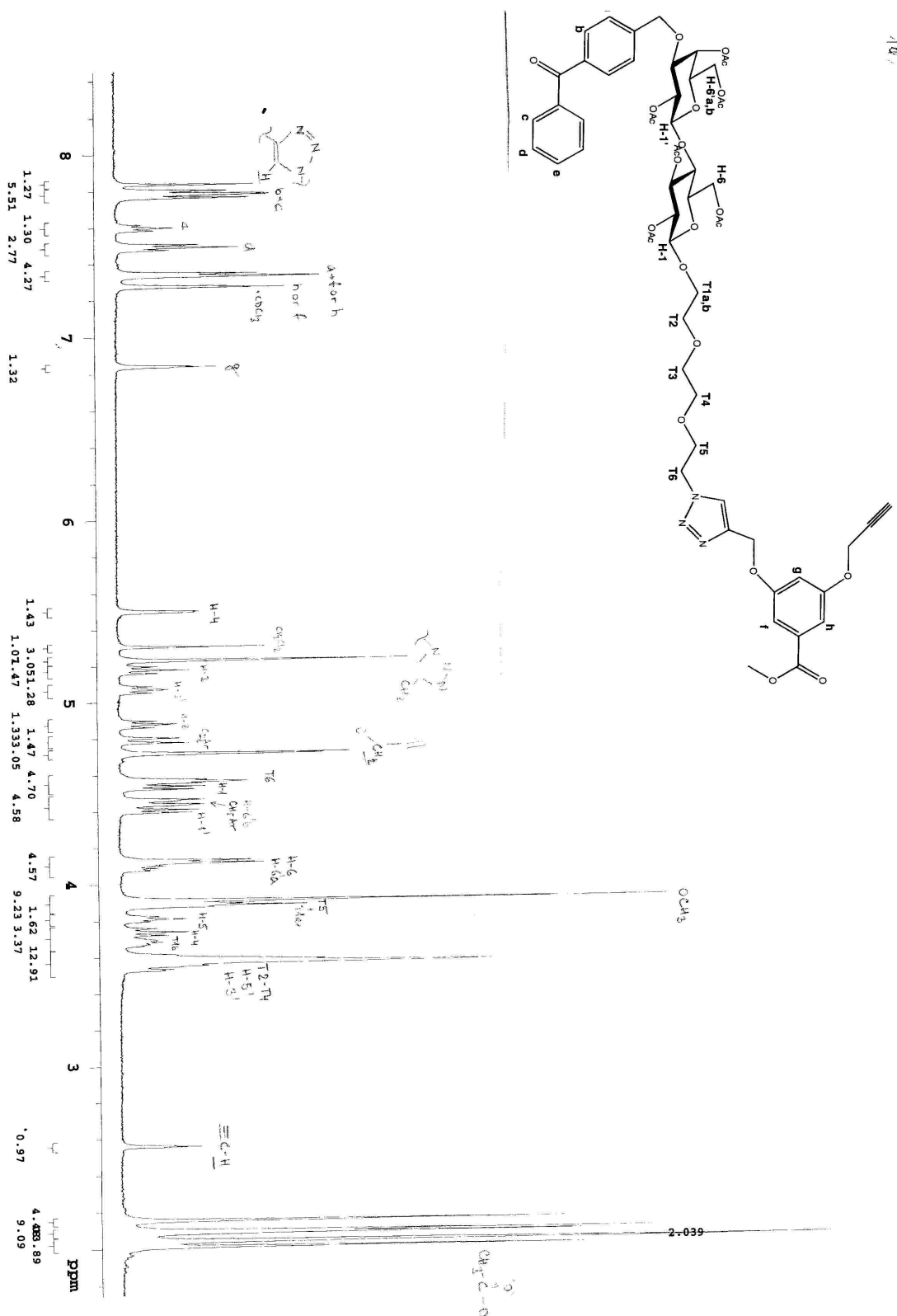
¹H NMR spectrum of protected 1



¹H NMR spectrum of monofunctionalized 7



¹H NMR spectrum of 9



¹H NMR spectrum of 3

