

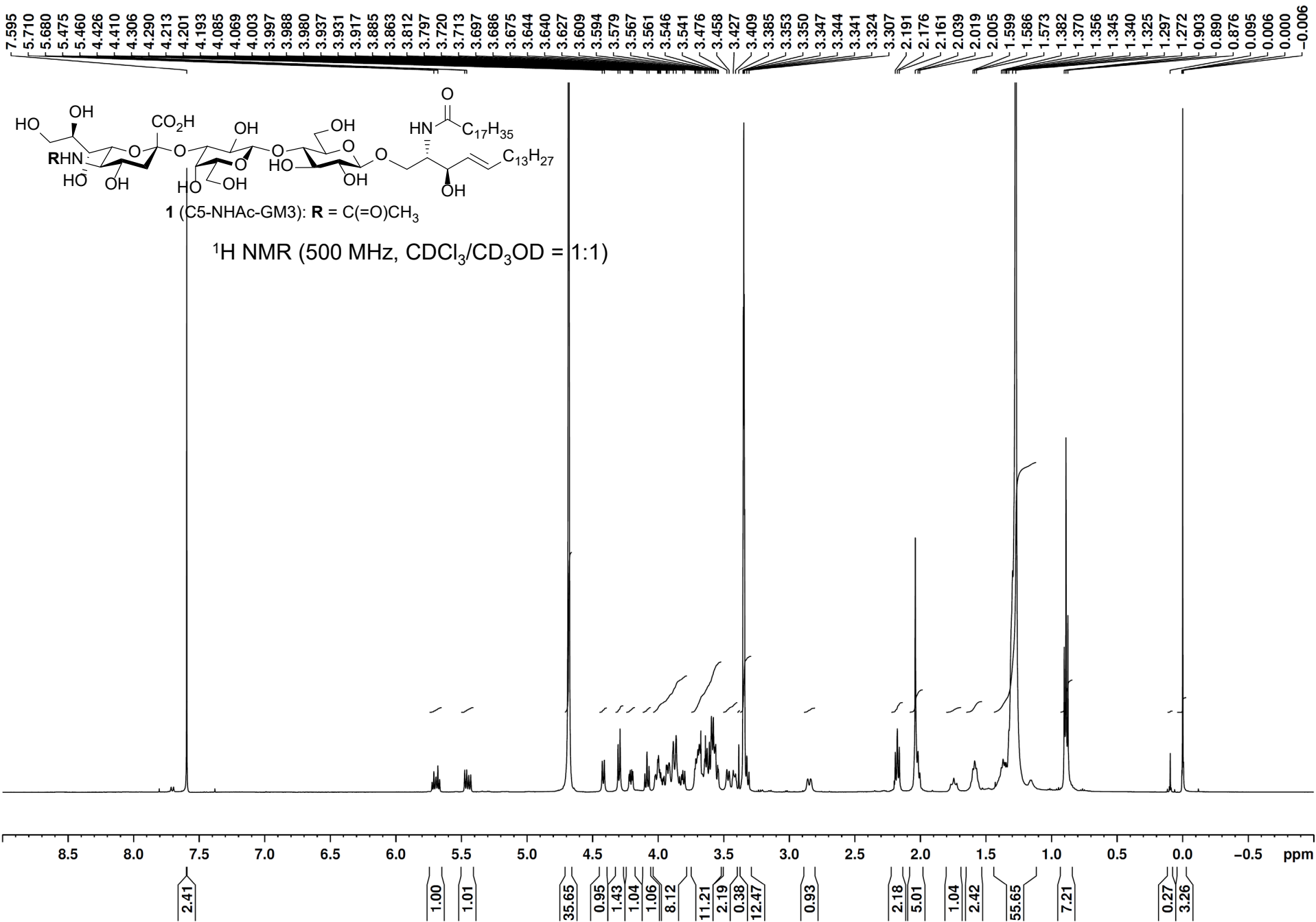
Supplementary information for

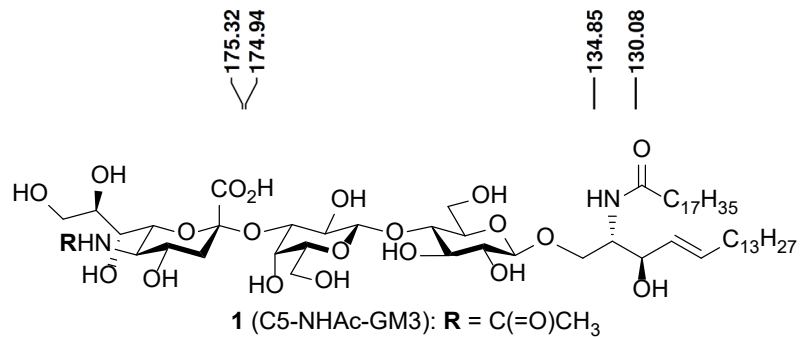
Efficient diversification of GM3 ganglioside via late-stage sialylation
and dynamic glycan structural studies with ^{19}F solid-state NMR

Maina Takahashi, Junya Shirasaki, Naoko Komura*, Katsuaki Sasaki,
Hide-Nori Tanaka, Akihiro Imamura, Hideharu Ishida, Shinya Hanashima*,
Michio Murata and Hiromune Ando*

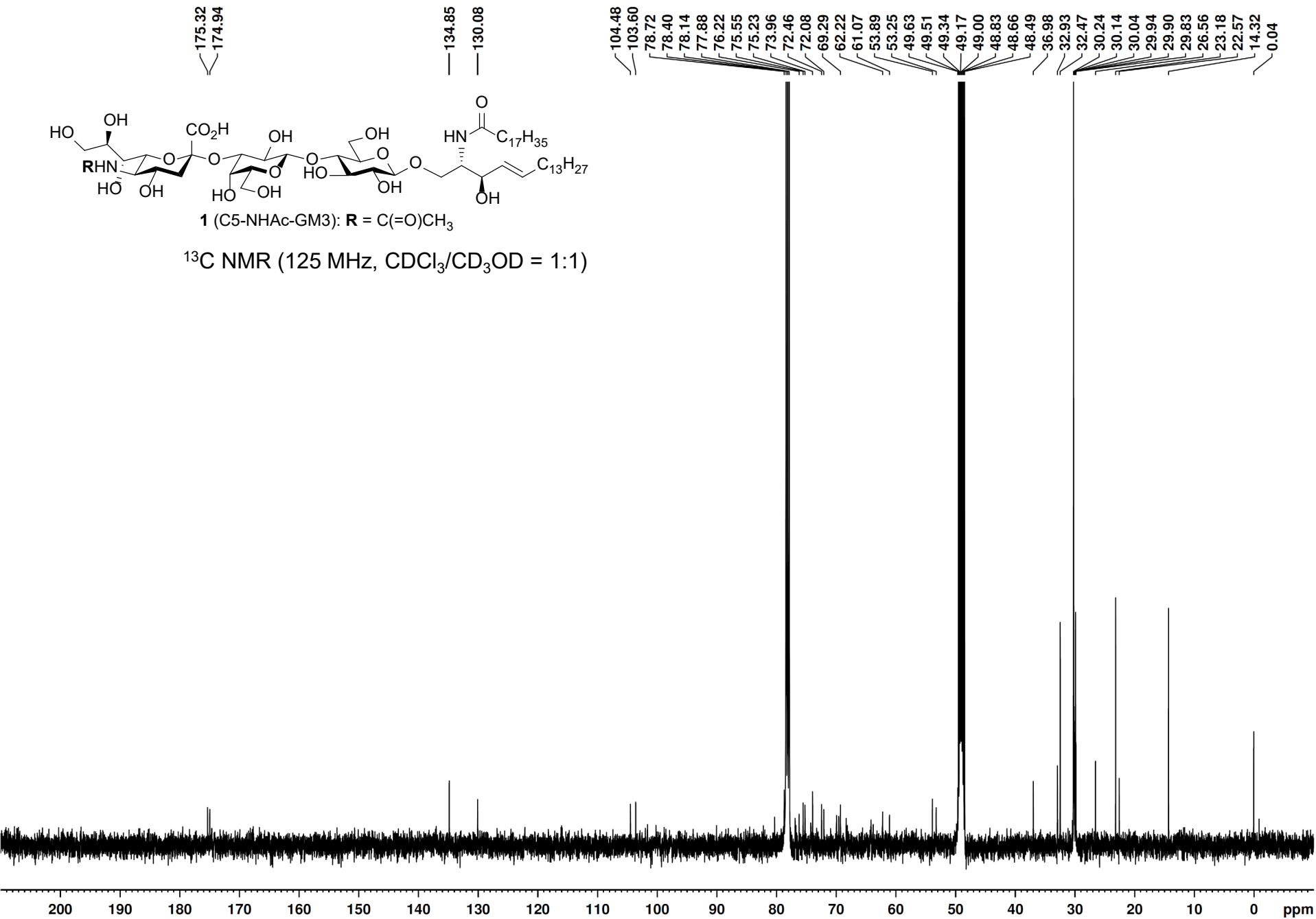
This PDF file includes:

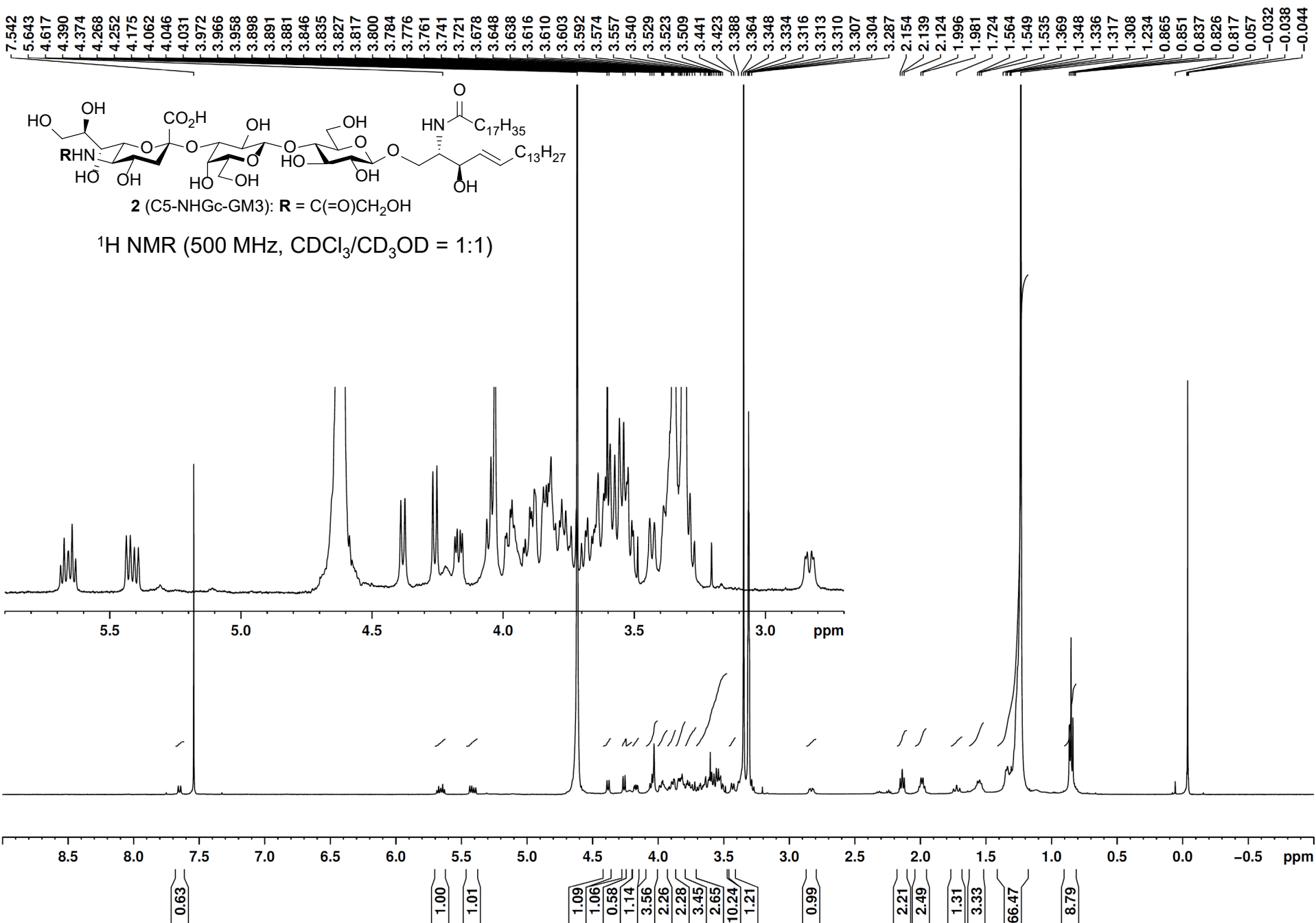
Copies of ^1H and ^{13}C NMR spectra of new compounds

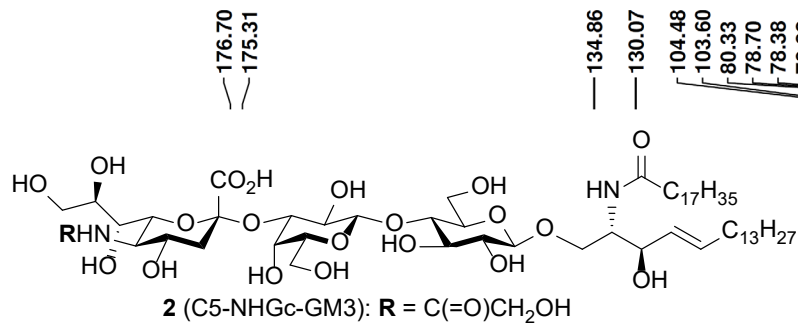




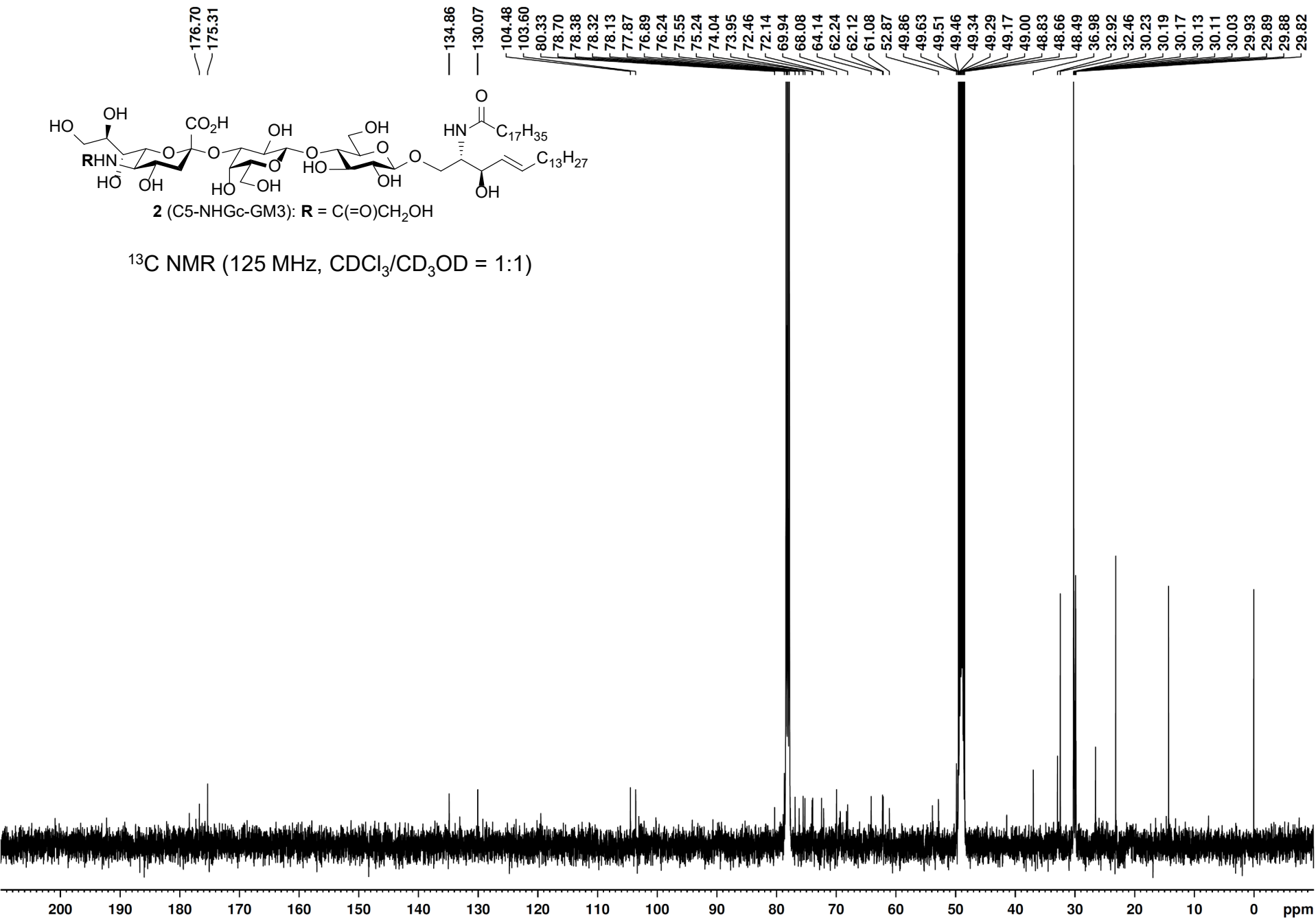
^{13}C NMR (125 MHz, $CDCl_3/CD_3OD = 1:1$)

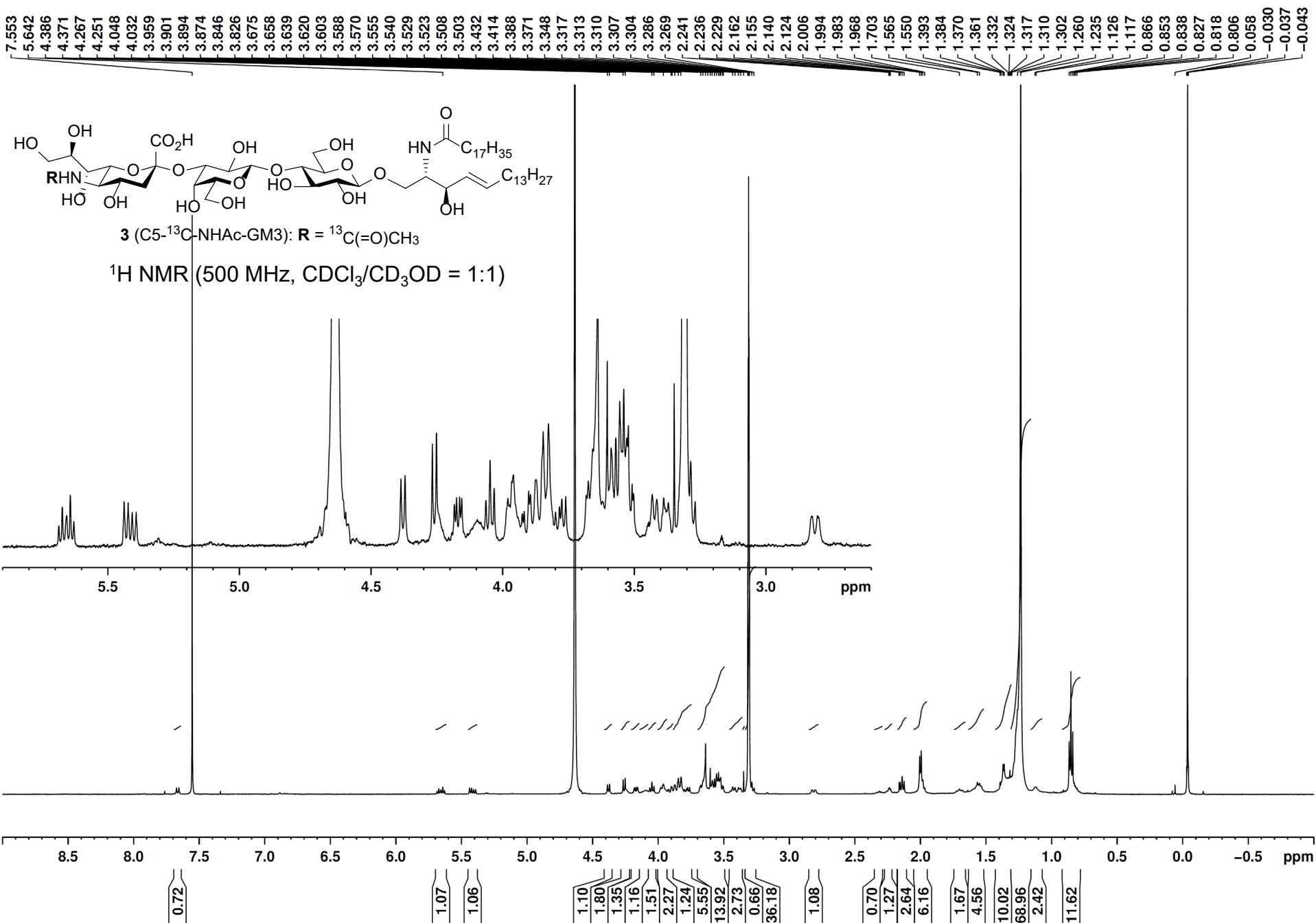






^{13}C NMR (125 MHz, $\text{CDCl}_3/\text{CD}_3\text{OD} = 1:1$)

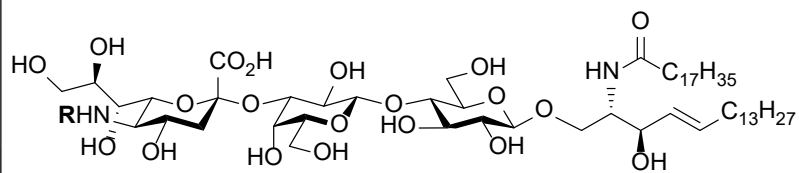




175.32
174.93

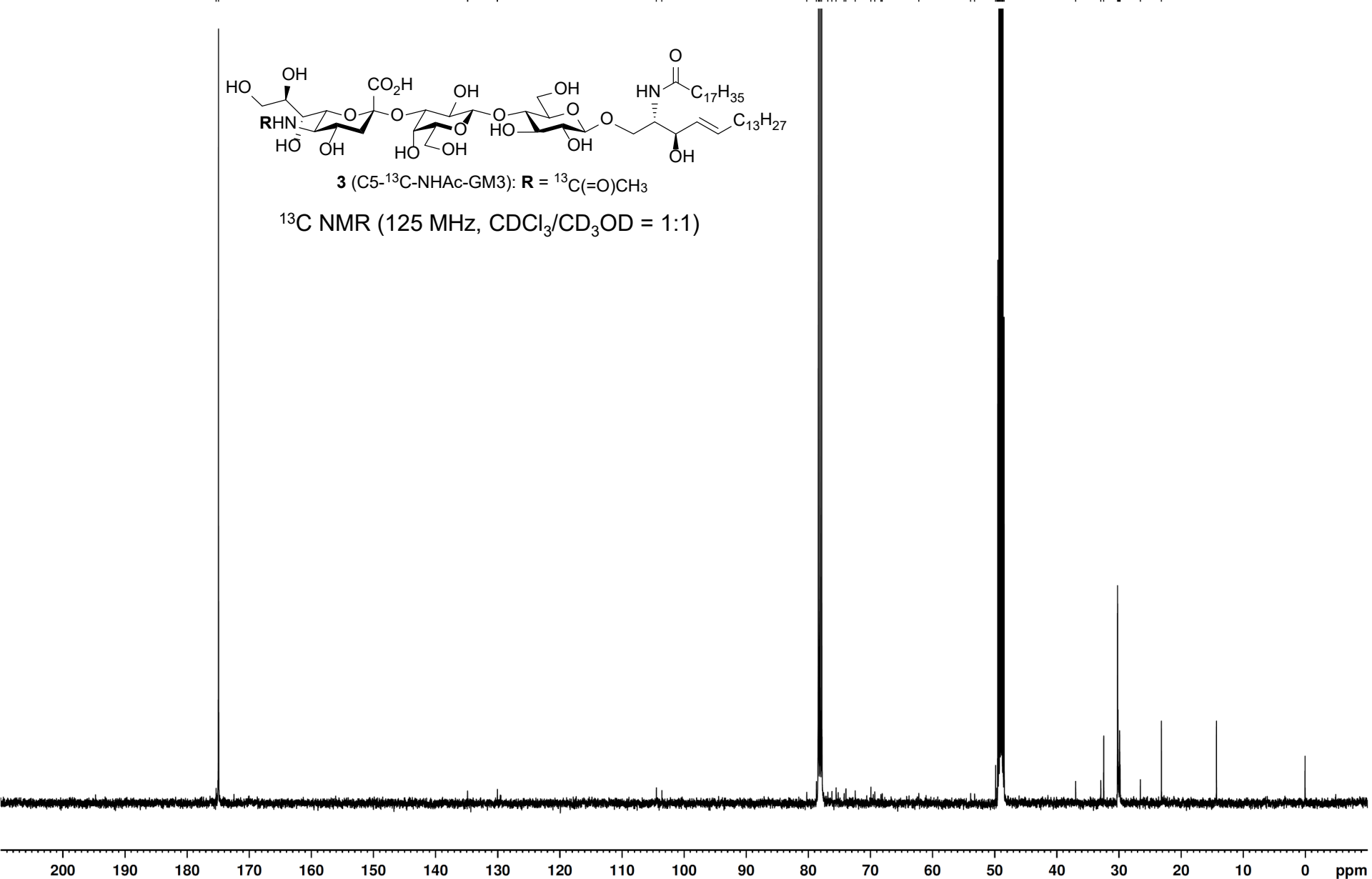
134.87
130.06

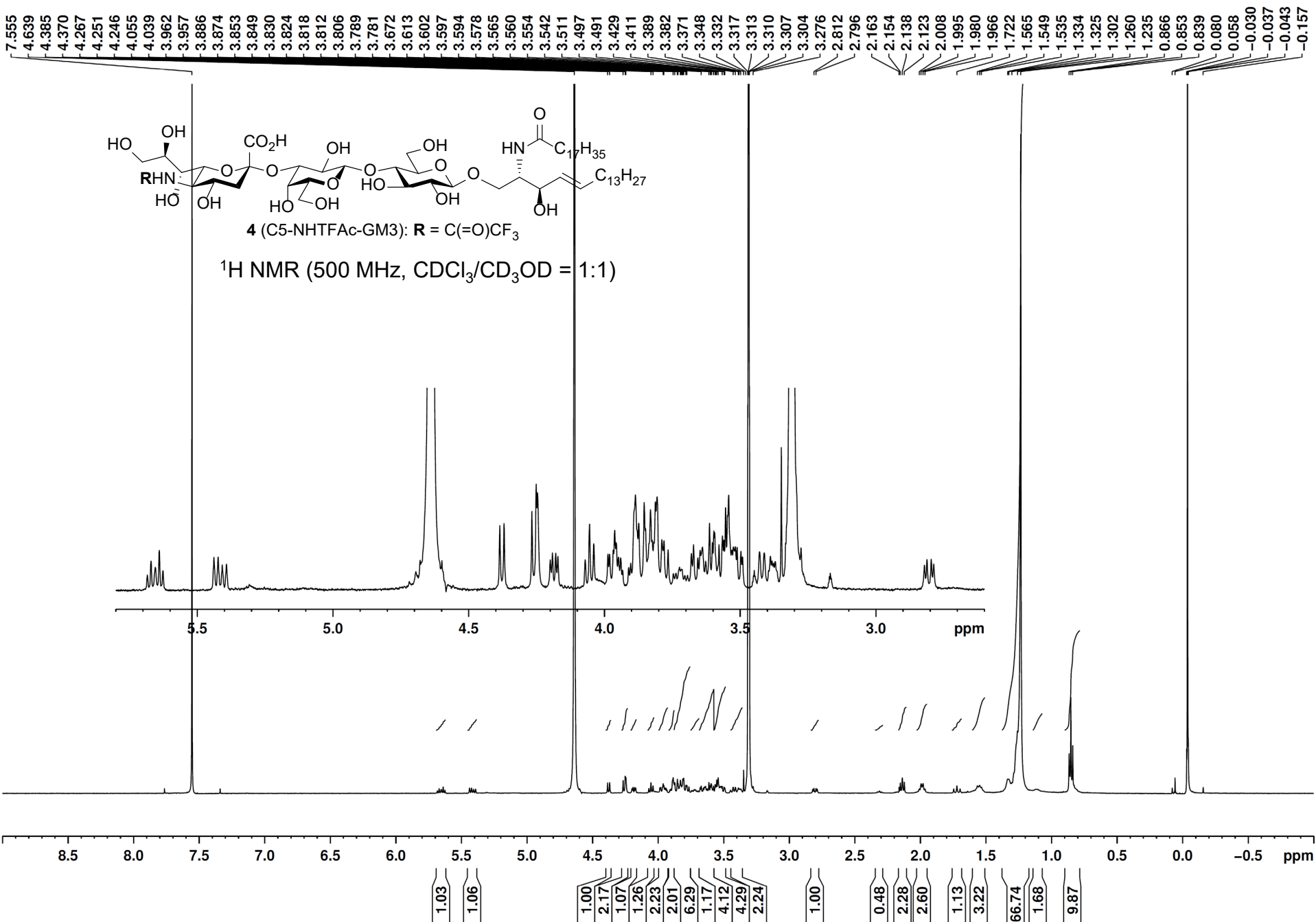
104.47
103.59
80.26
78.70
78.39
78.32
78.13
77.87
76.86
76.21
75.53
74.24
73.96
72.46
69.93
69.31
68.31
68.11
62.22
53.88
53.25
49.86
49.66
49.51
49.46
49.35
49.29
49.17
49.00
48.83
48.66
48.49
36.98
32.92
32.46
30.23
30.17
30.13
30.11
30.03
29.94
29.89
29.82
26.56
23.17

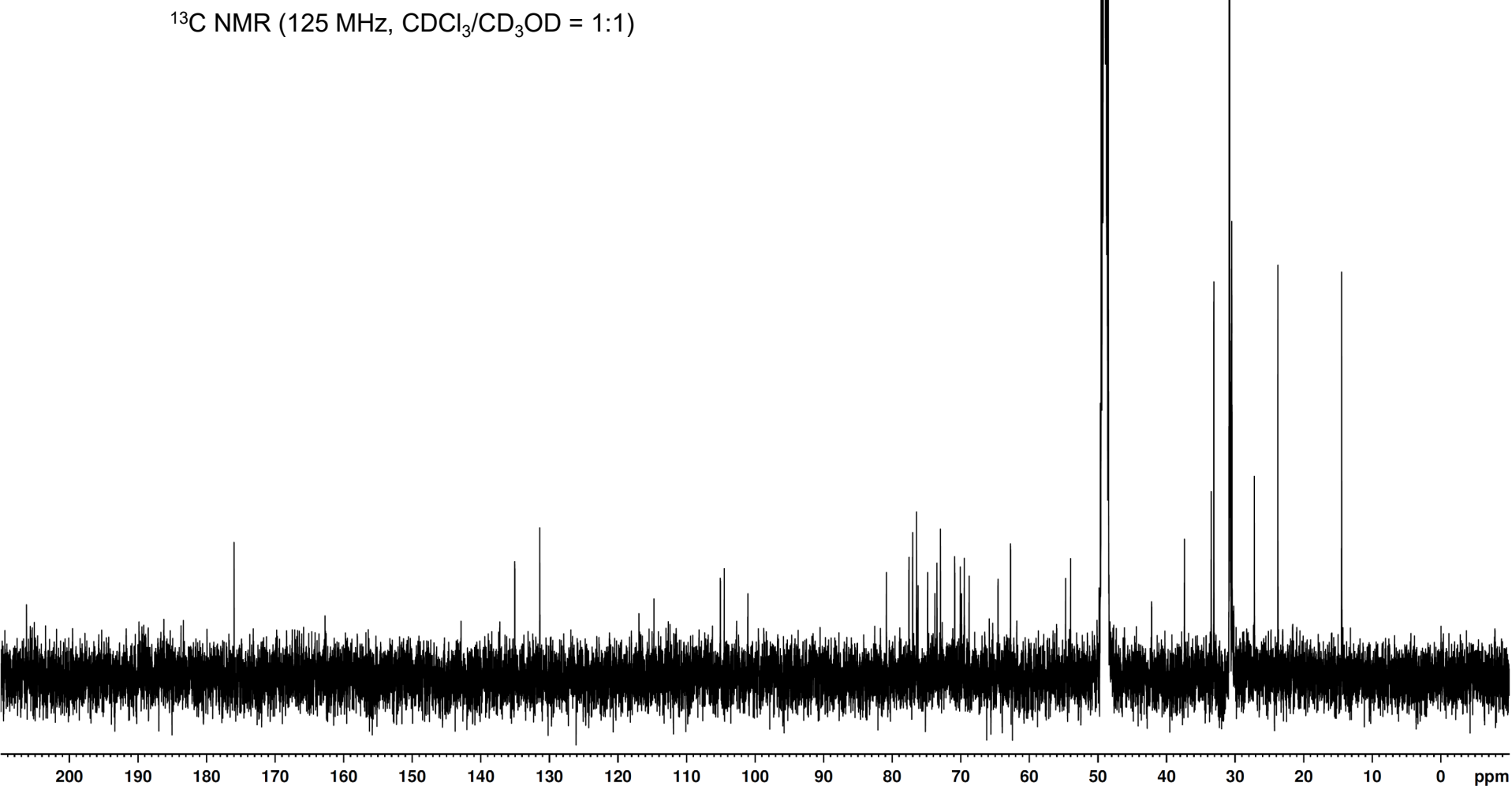
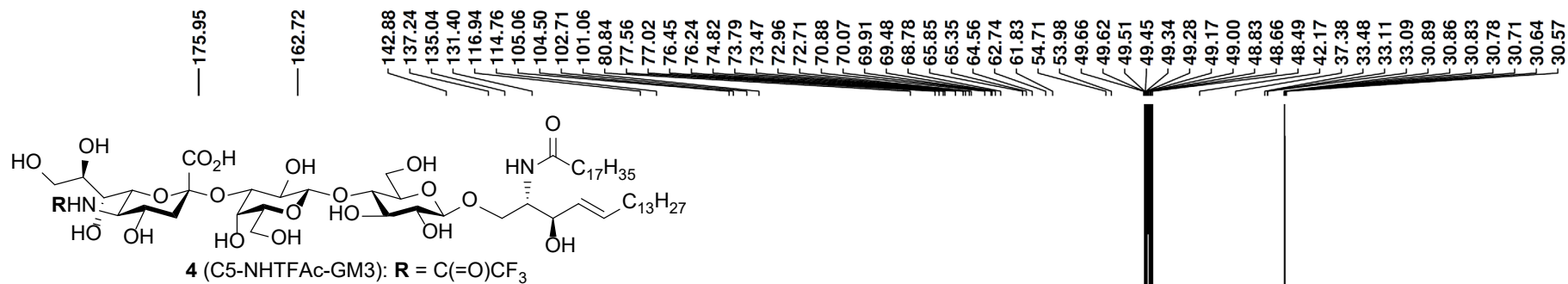


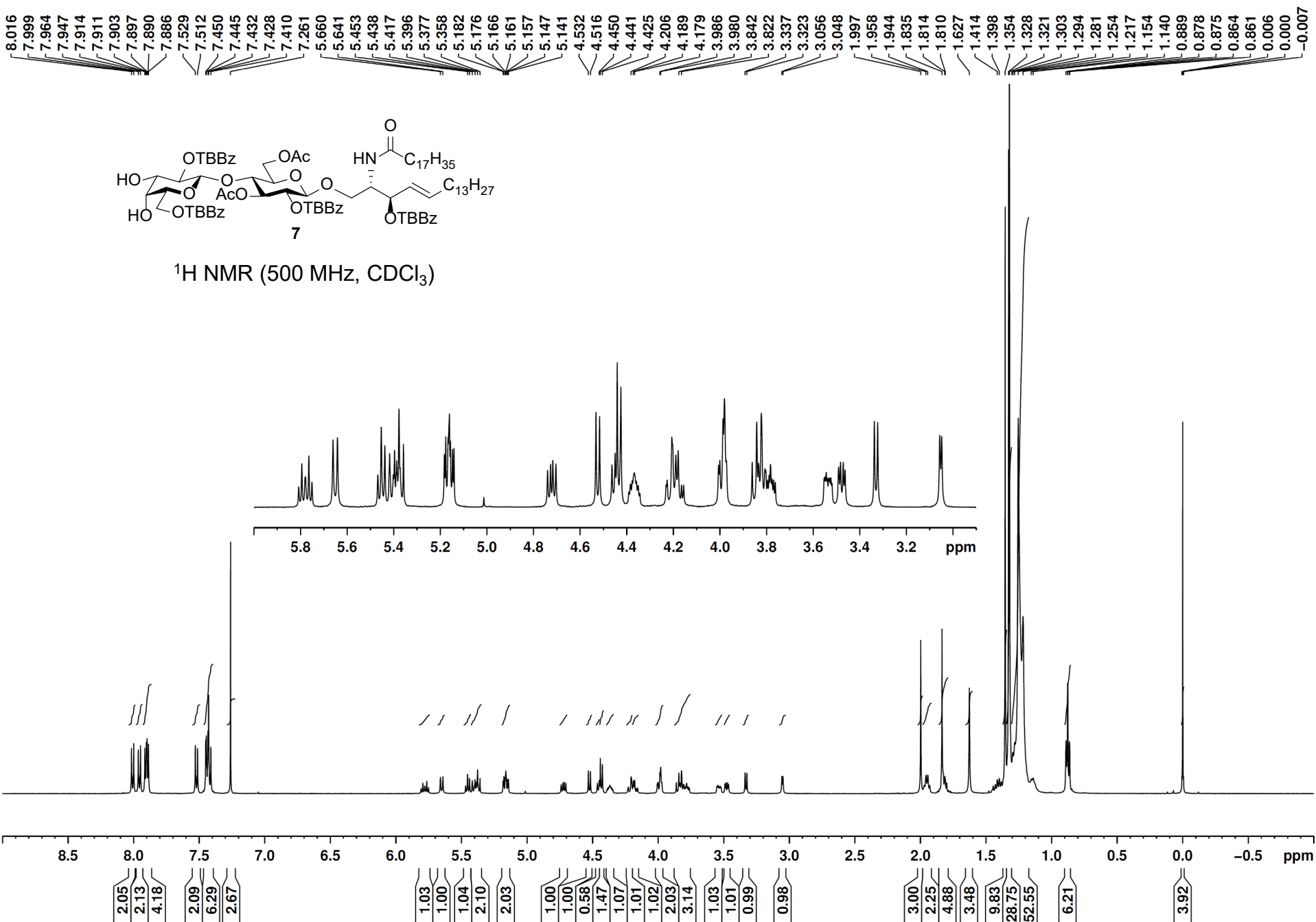
3 (C5- ^{13}C -NHAc-GM3): **R** = $^{13}\text{C}(=\text{O})\text{CH}_3$

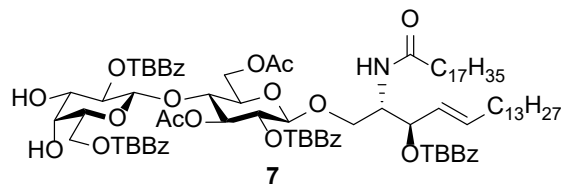
^{13}C NMR (125 MHz, $\text{CDCl}_3/\text{CD}_3\text{OD} = 1:1$)



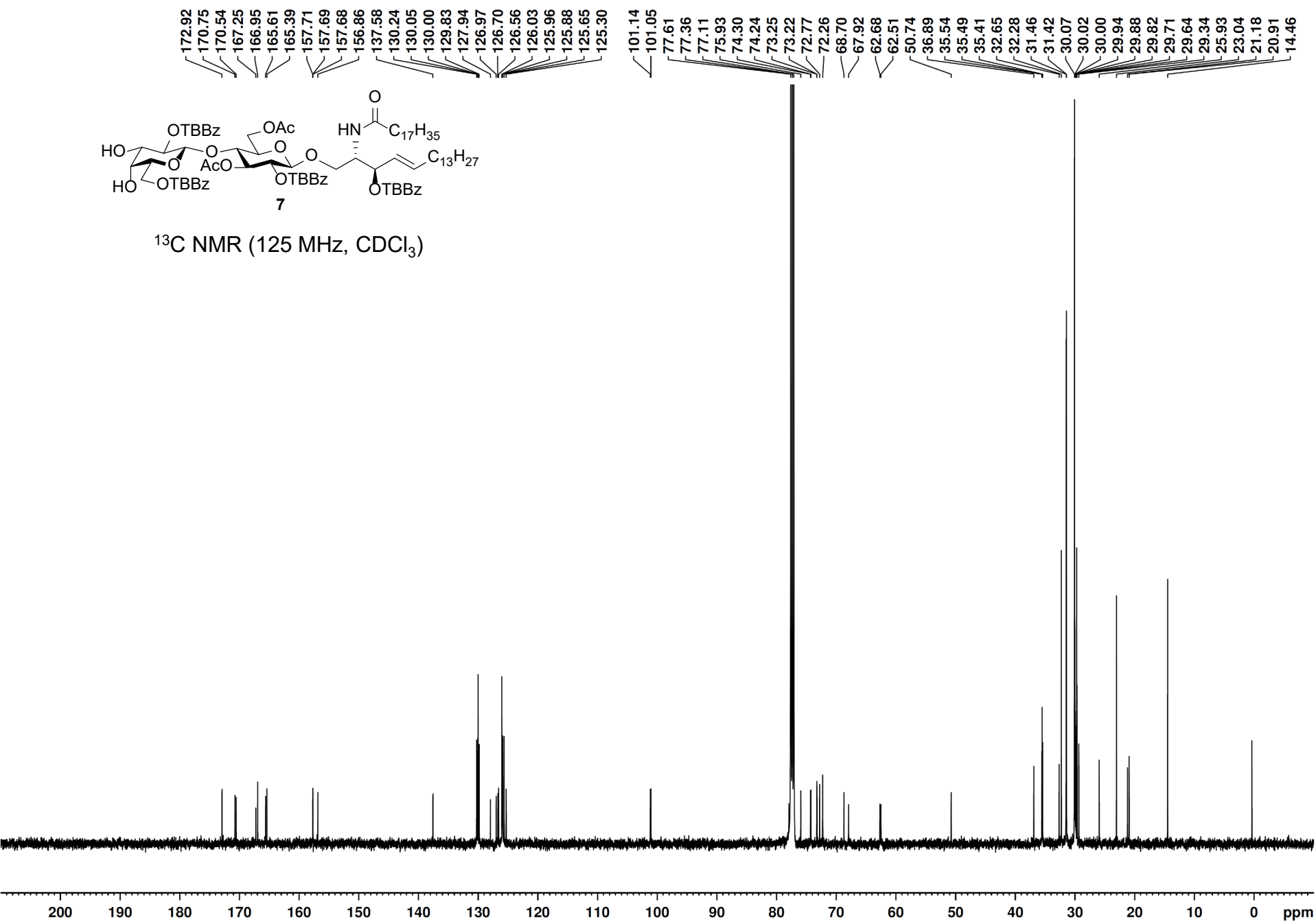


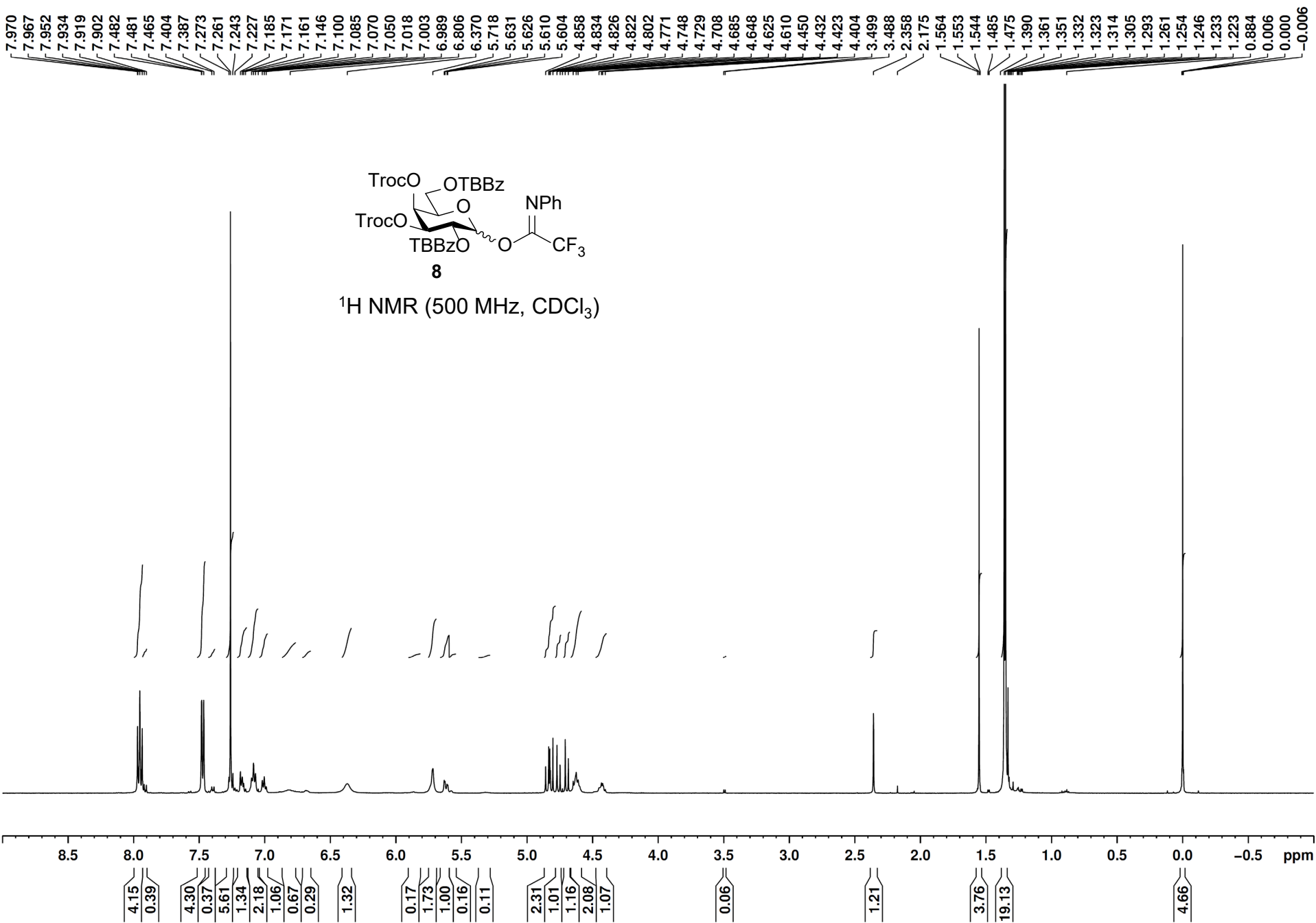


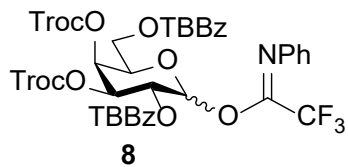




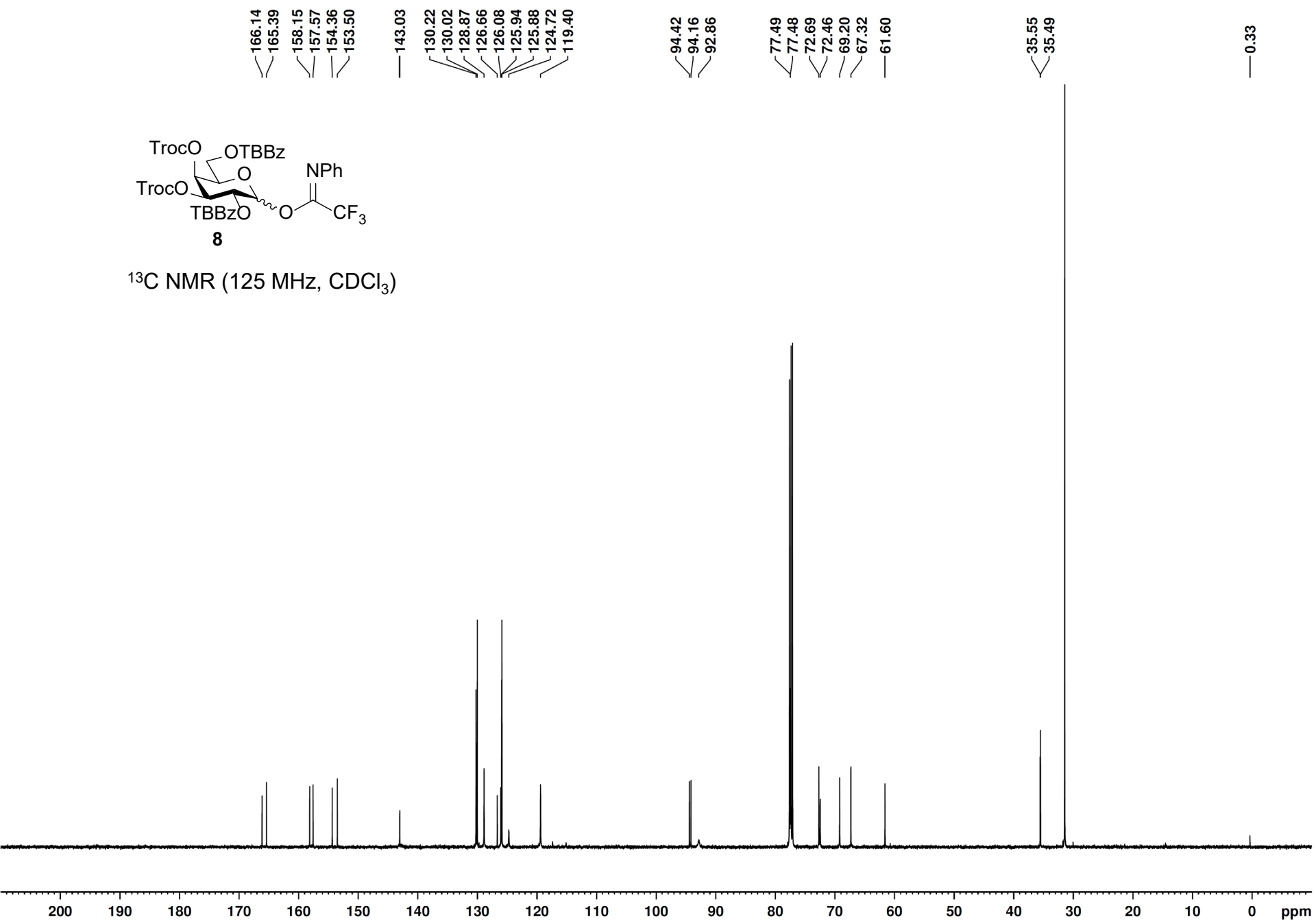
¹³C NMR (125 MHz, CDCl₃)

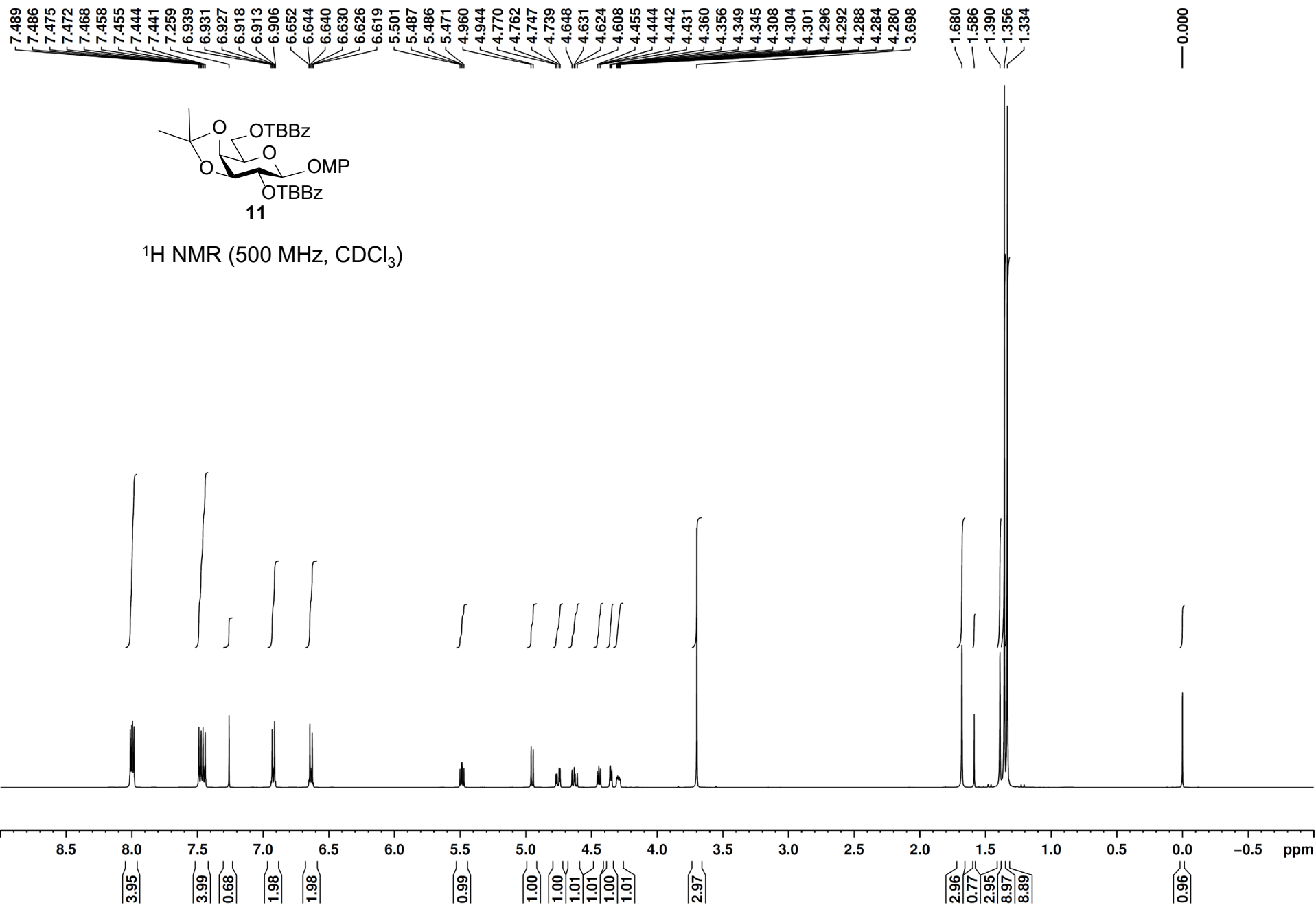
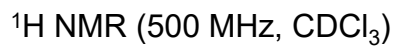


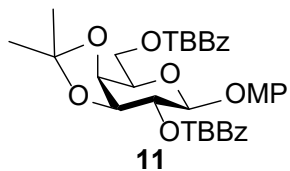




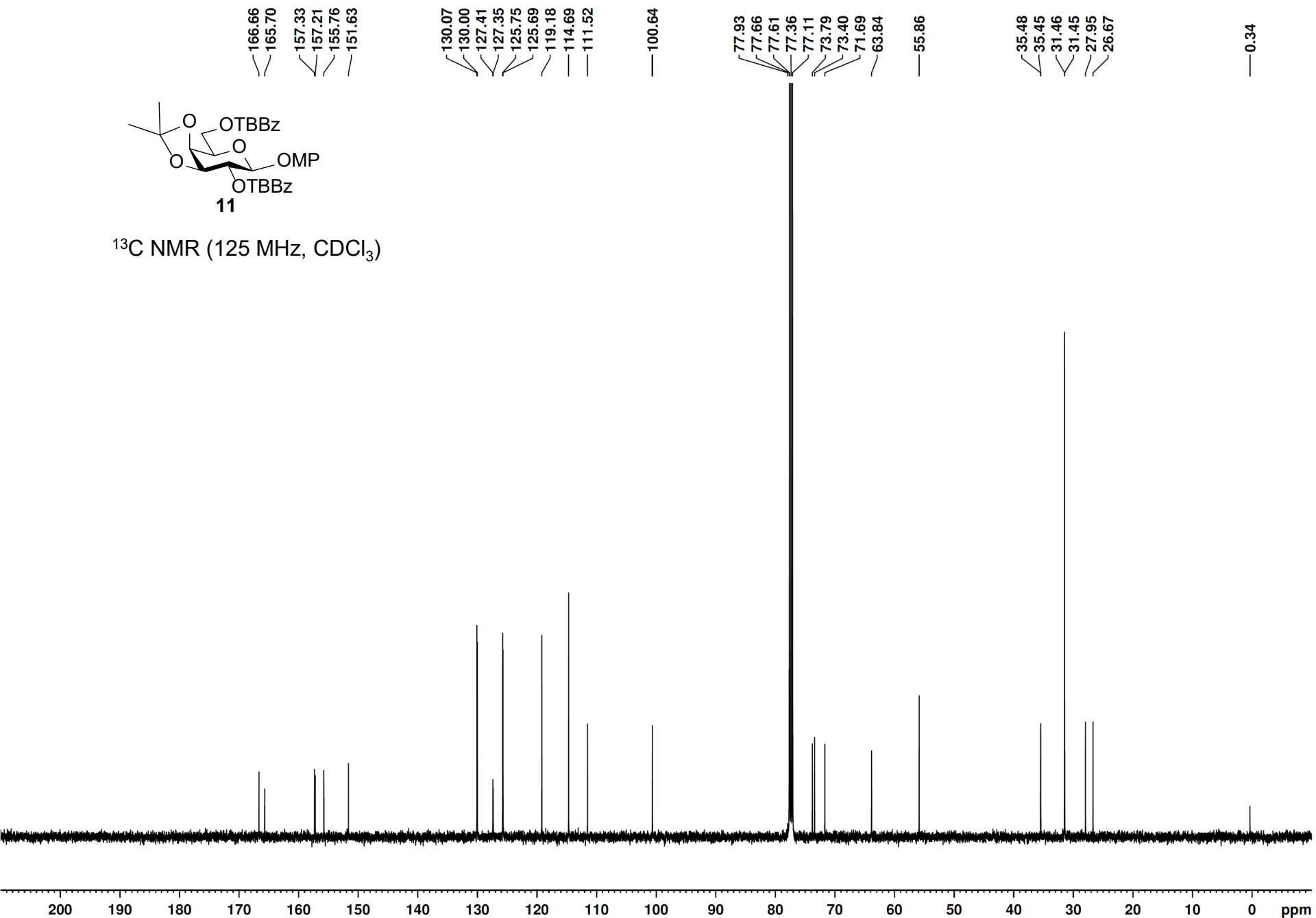
¹³C NMR (125 MHz, CDCl₃)







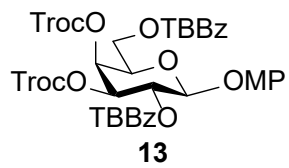
^{13}C NMR (125 MHz, CDCl_3)



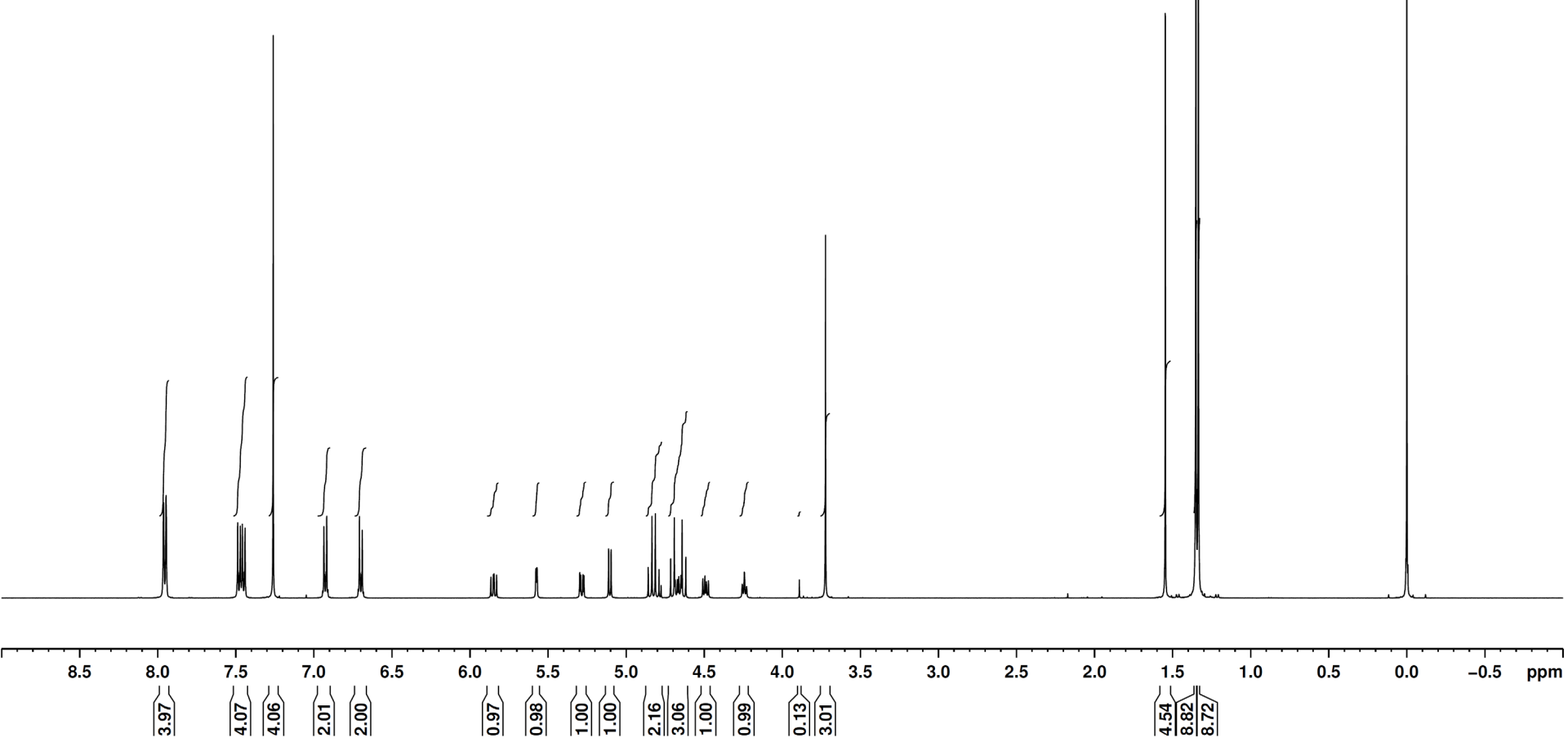
7.488
7.484
7.474
7.471
7.466
7.457
7.454
7.444
7.440
7.260
6.935
6.931
6.922
6.917
6.708
6.703
6.694
6.690
5.866
5.850
5.845
5.829
5.577
5.571
5.297
5.290
5.276
5.269
5.112
5.096
4.858
4.835
4.813
4.789
4.776
4.715
4.691
4.686
4.672
4.663
4.649
4.641
4.618
4.509
4.495
4.486
4.473
4.256
4.243
4.229
3.890
3.723

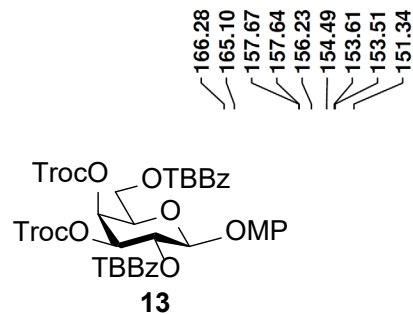
1.547
1.351
1.335

0.000

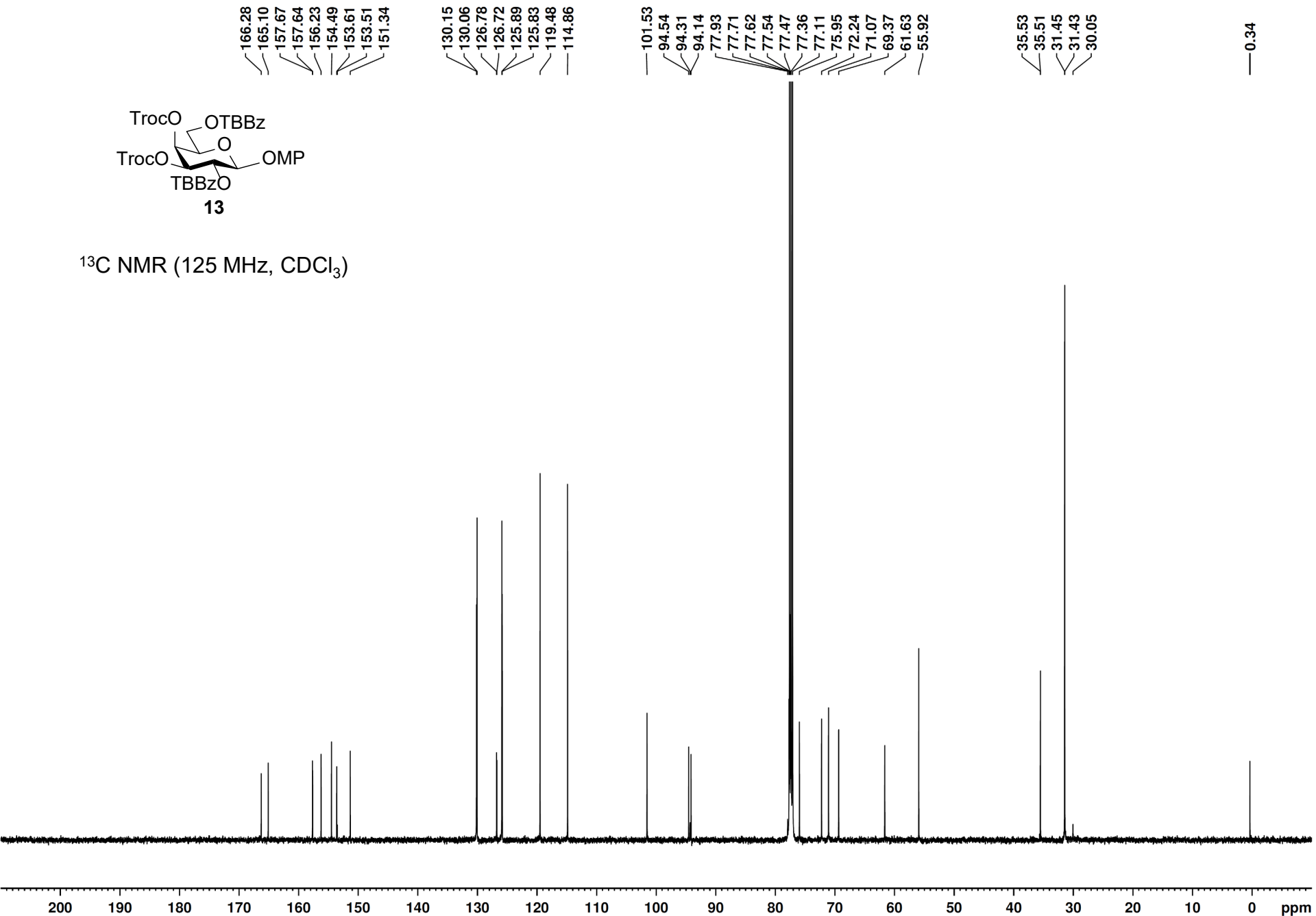


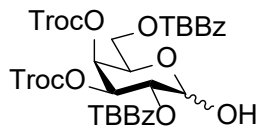
¹H NMR (500 MHz, CDCl₃)





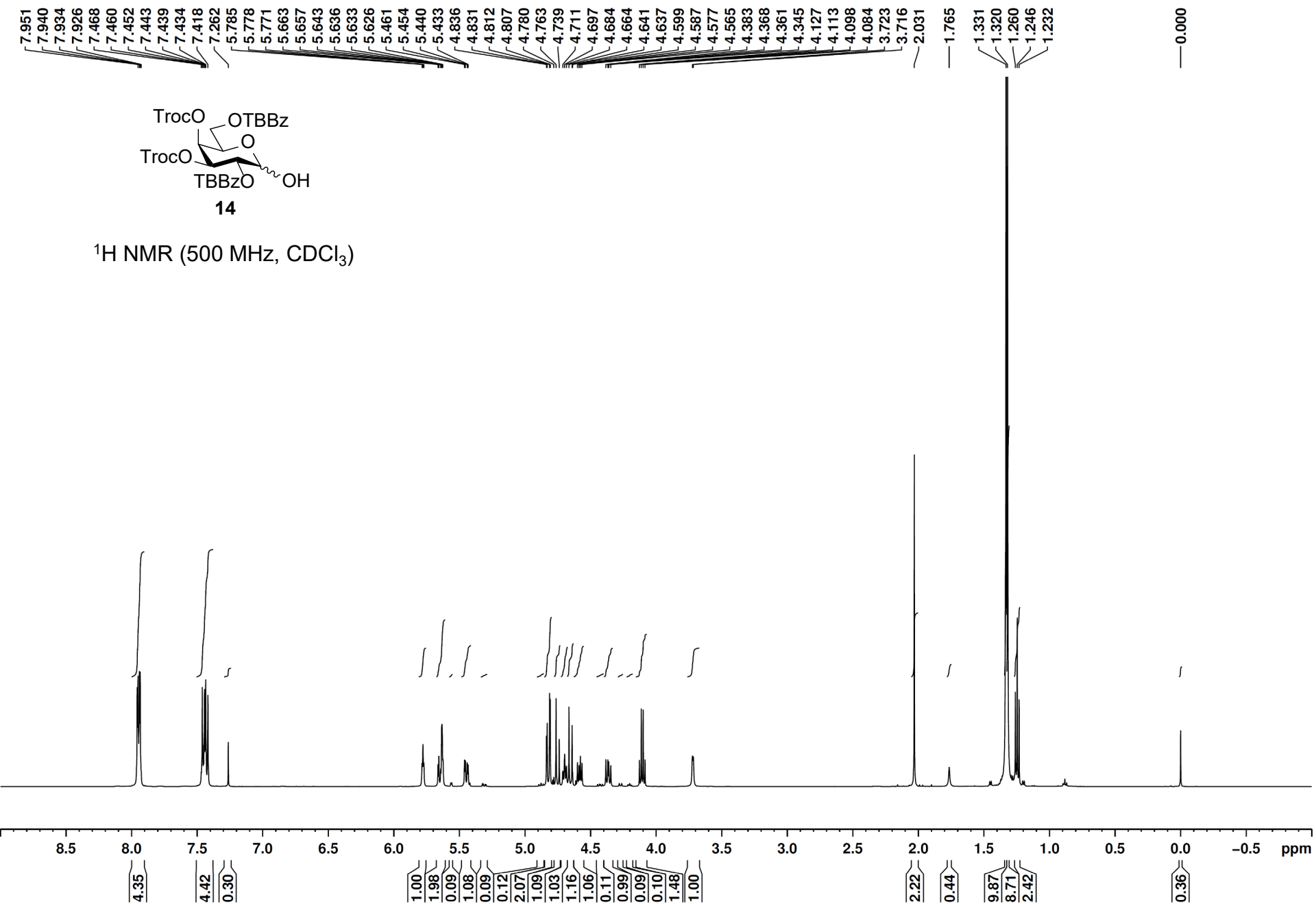
^{13}C NMR (125 MHz, CDCl_3)

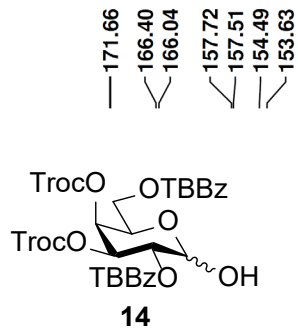




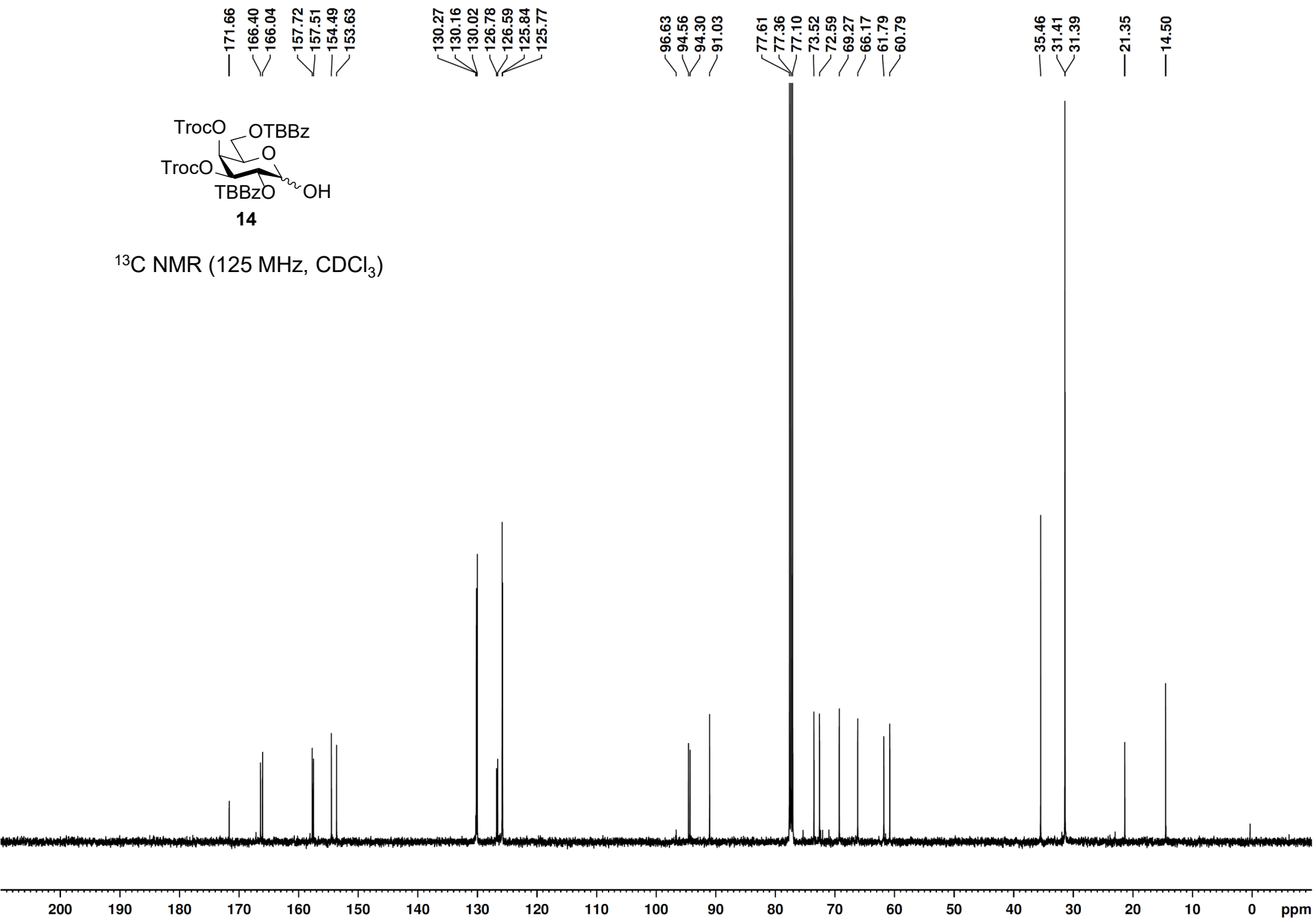
14

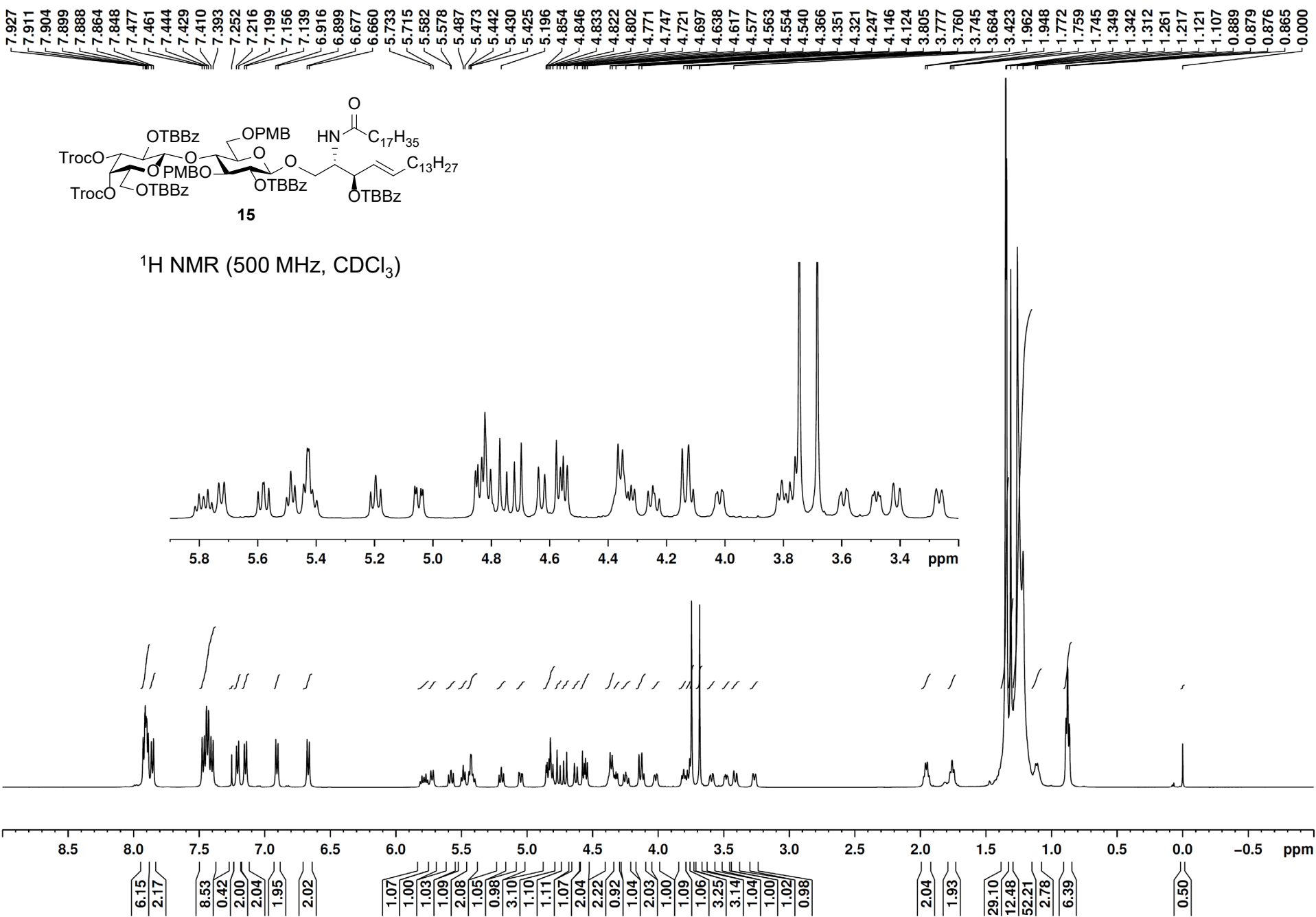
^1H NMR (500 MHz, CDCl_3)

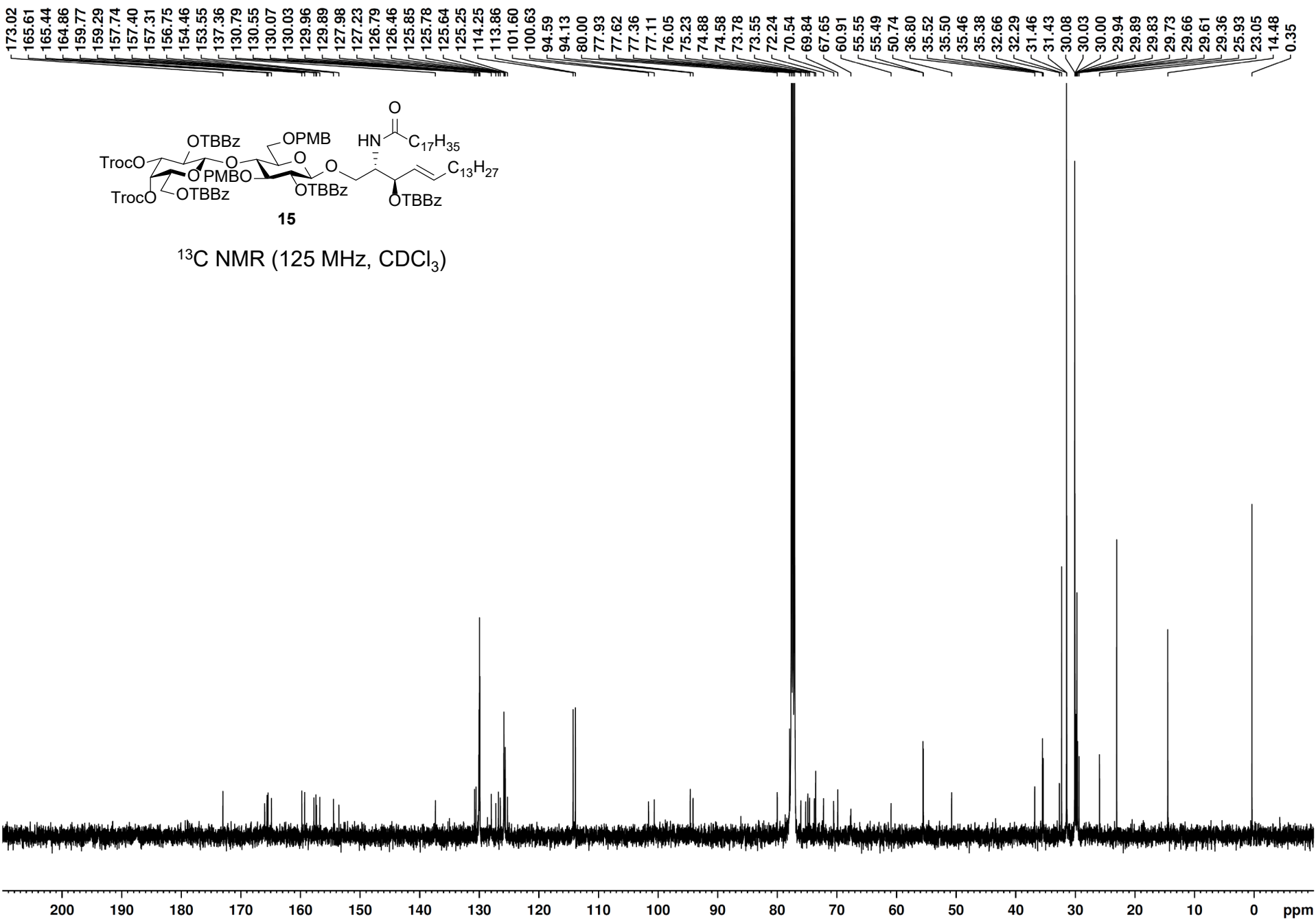


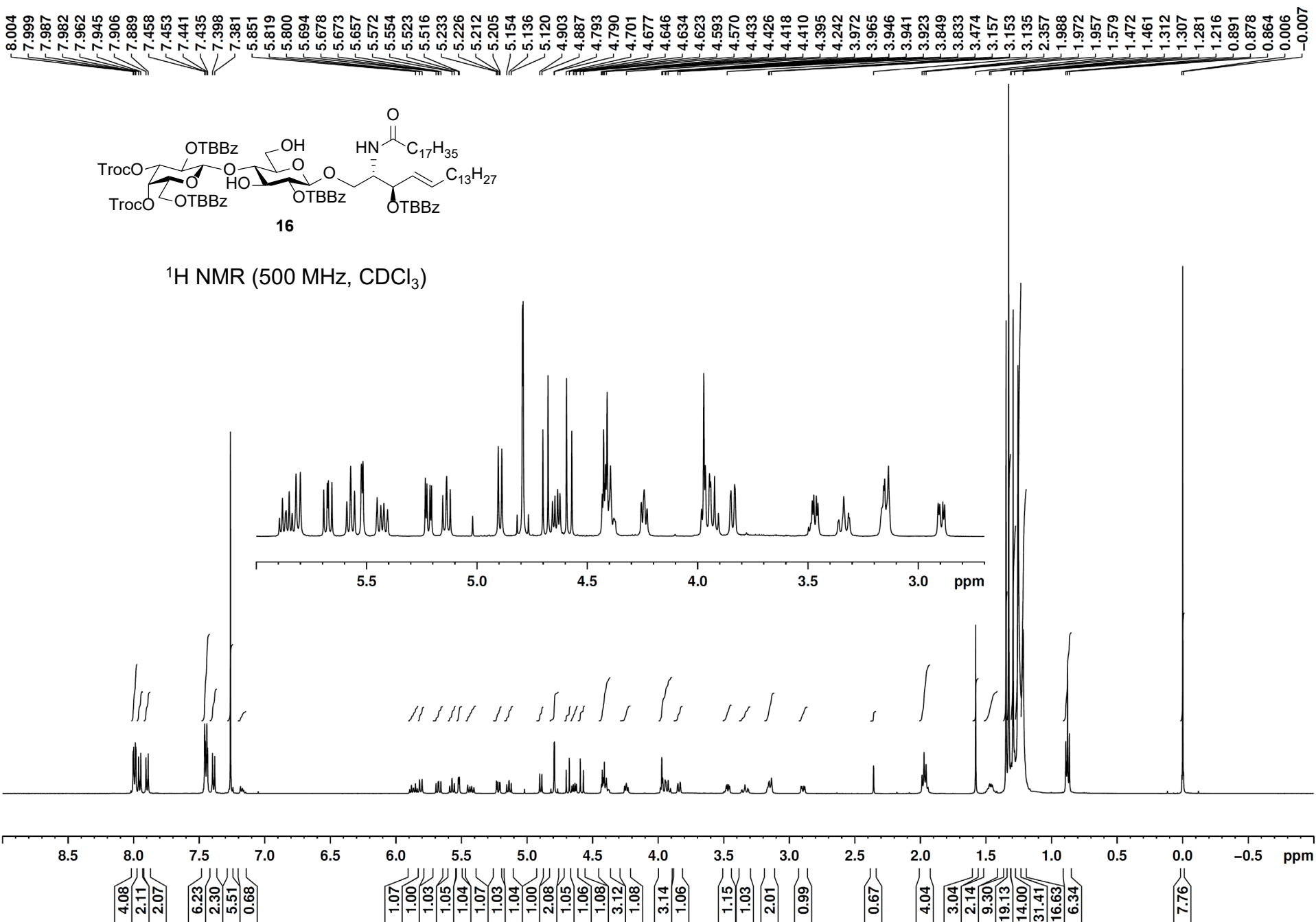


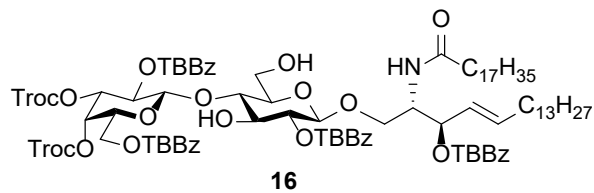
^{13}C NMR (125 MHz, CDCl_3)





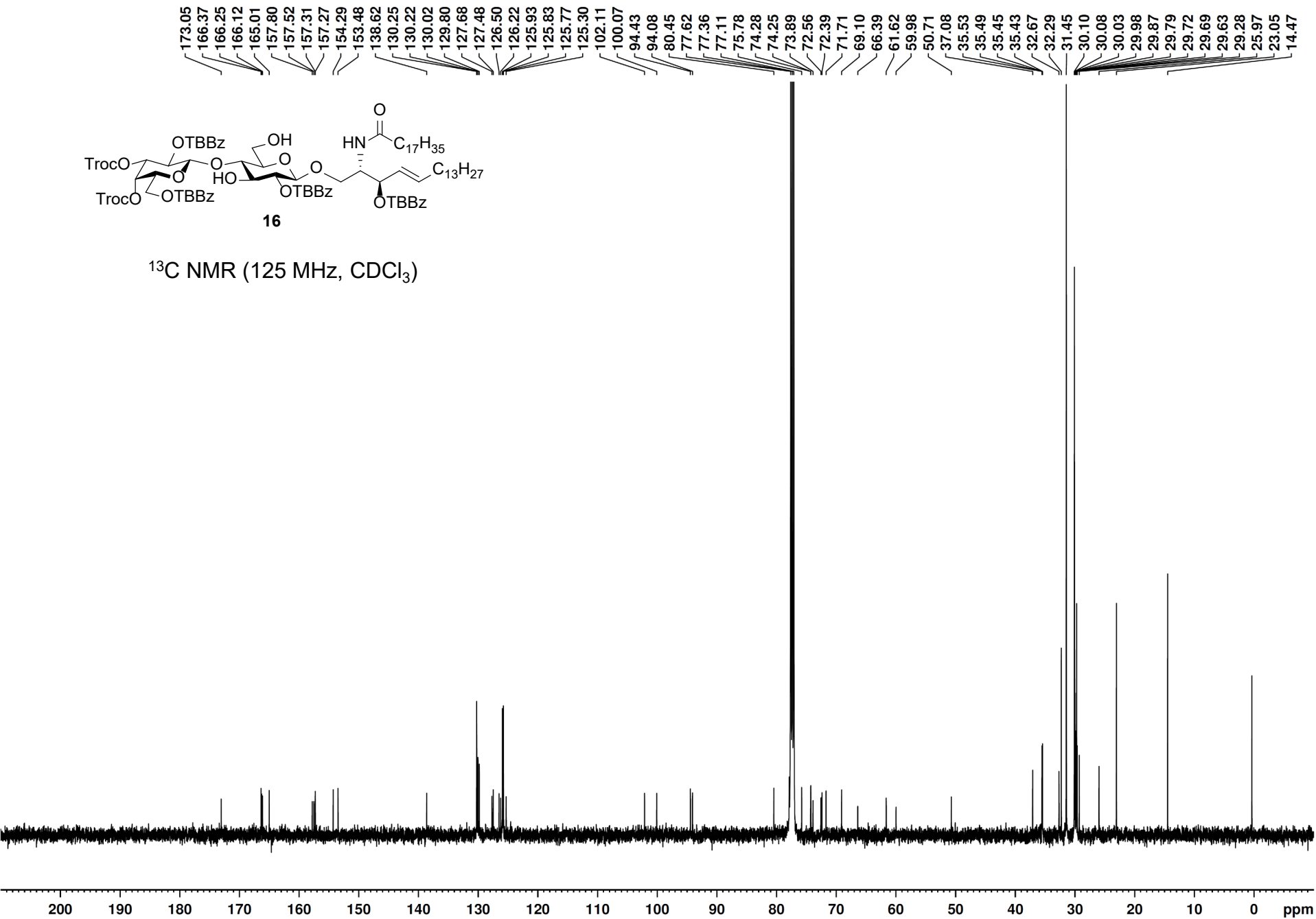


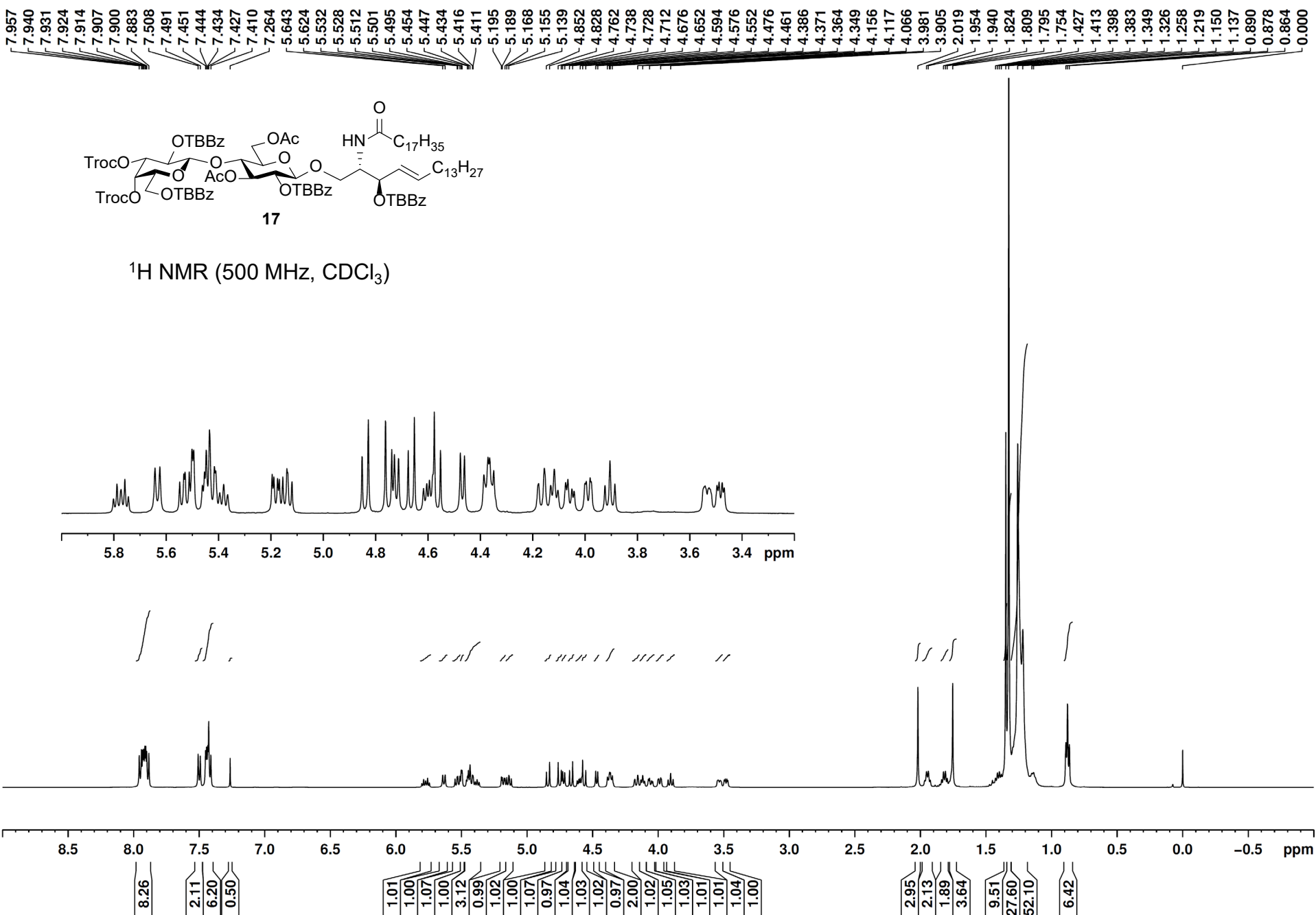




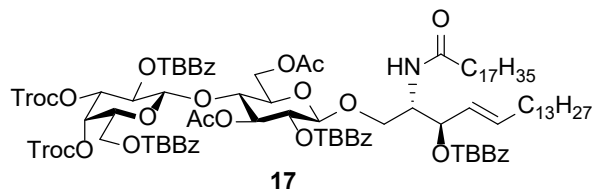
16

¹³C NMR (125 MHz, CDCl₃)



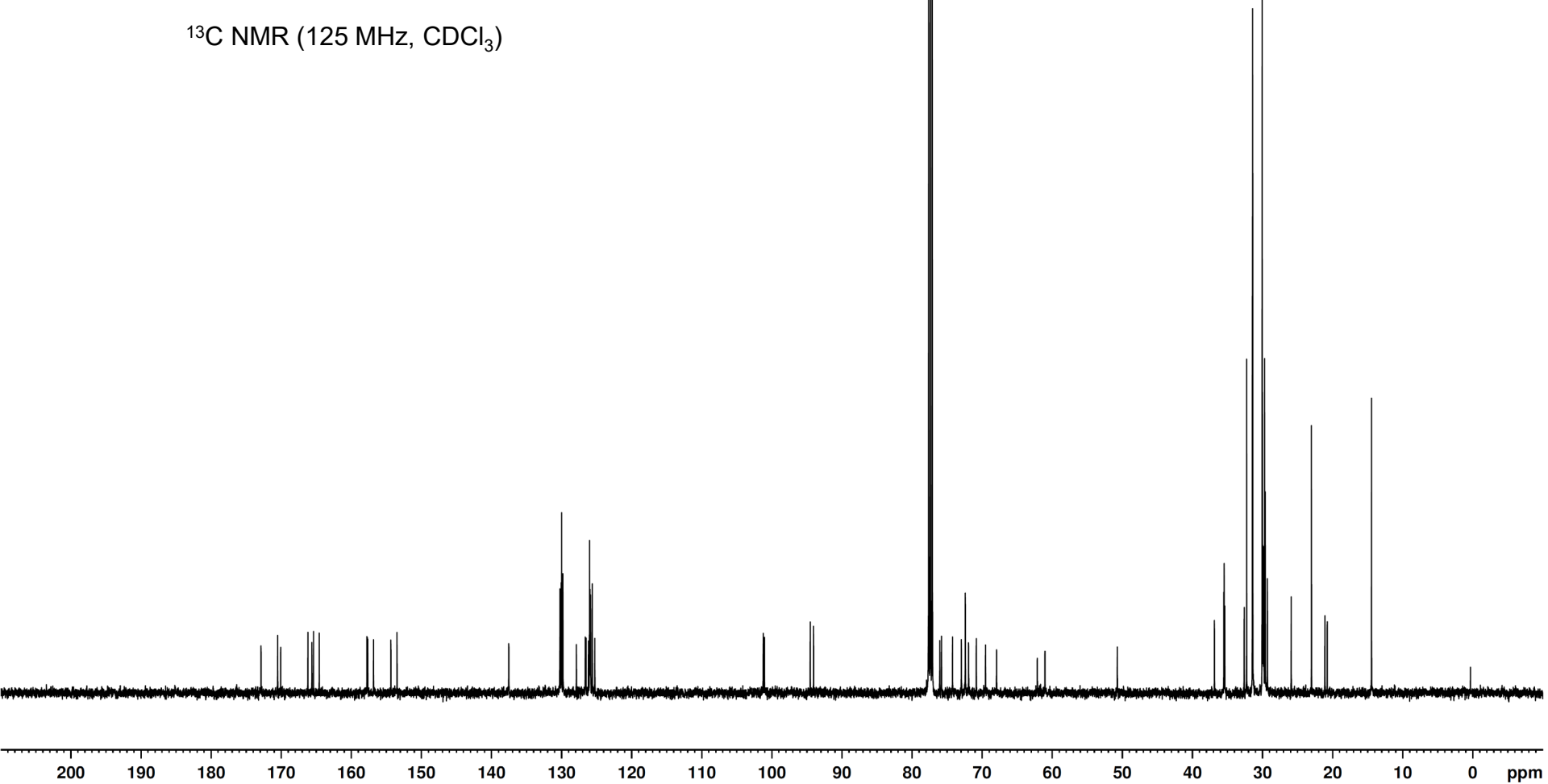


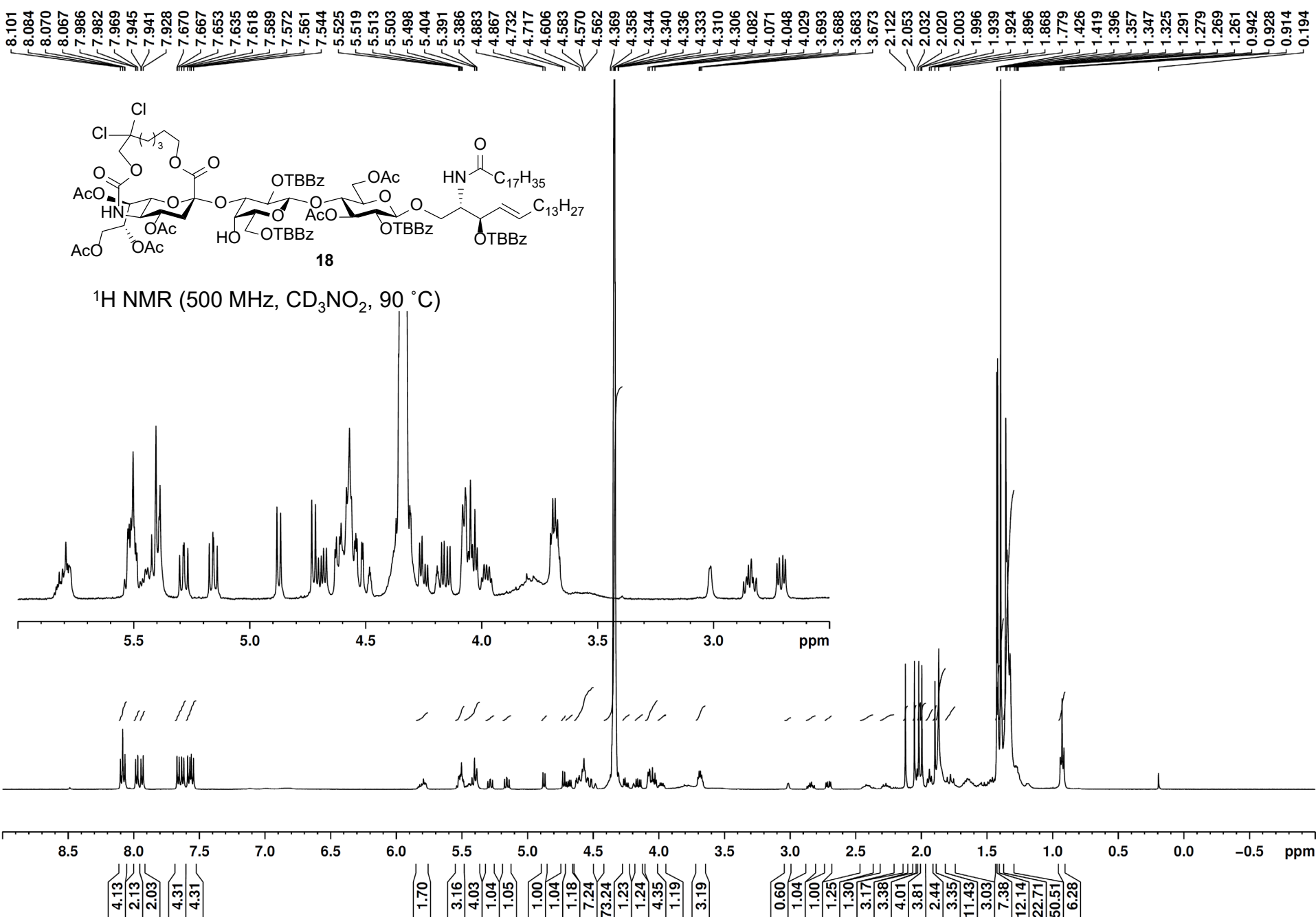
172.87 170.50 170.07 166.19 165.62 165.38 164.57 157.77 157.70 157.65 156.82 154.35 153.48 137.53 130.23 130.05 129.98 129.80 127.88 126.62 126.51 126.16 126.01 125.93 125.85 125.62 125.25 101.22 101.05 94.52 94.04 77.93 77.62 77.42 77.36 77.11 76.03 75.79 74.22 72.95 72.39 71.93 70.82 69.50 67.93 62.12 61.03 50.71 36.85 35.51 35.47 35.46 35.37 32.60 32.25 31.43 31.39 30.04 29.99 29.95 29.89 29.84 29.78 29.68 29.59 29.29 25.90 23.01

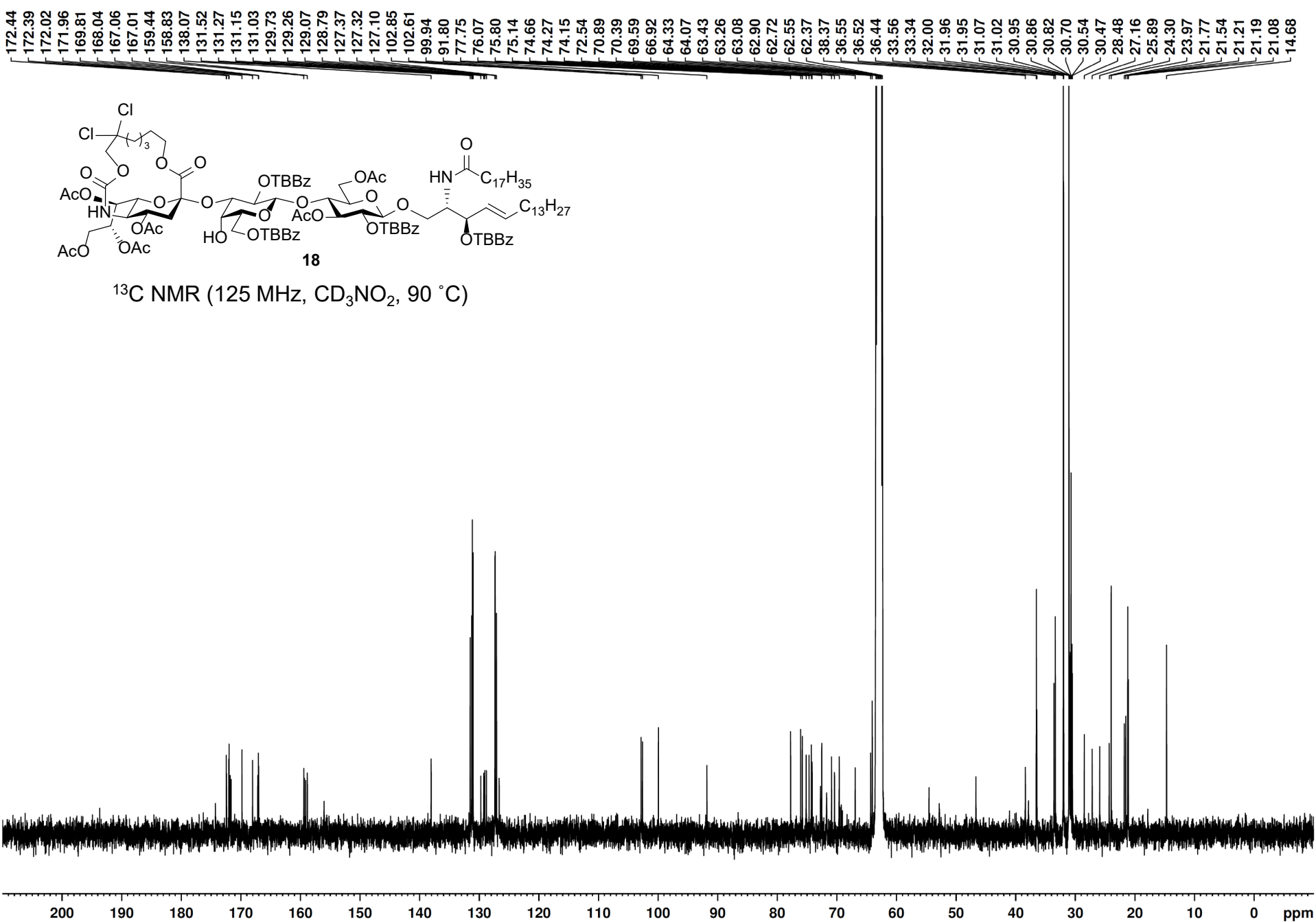


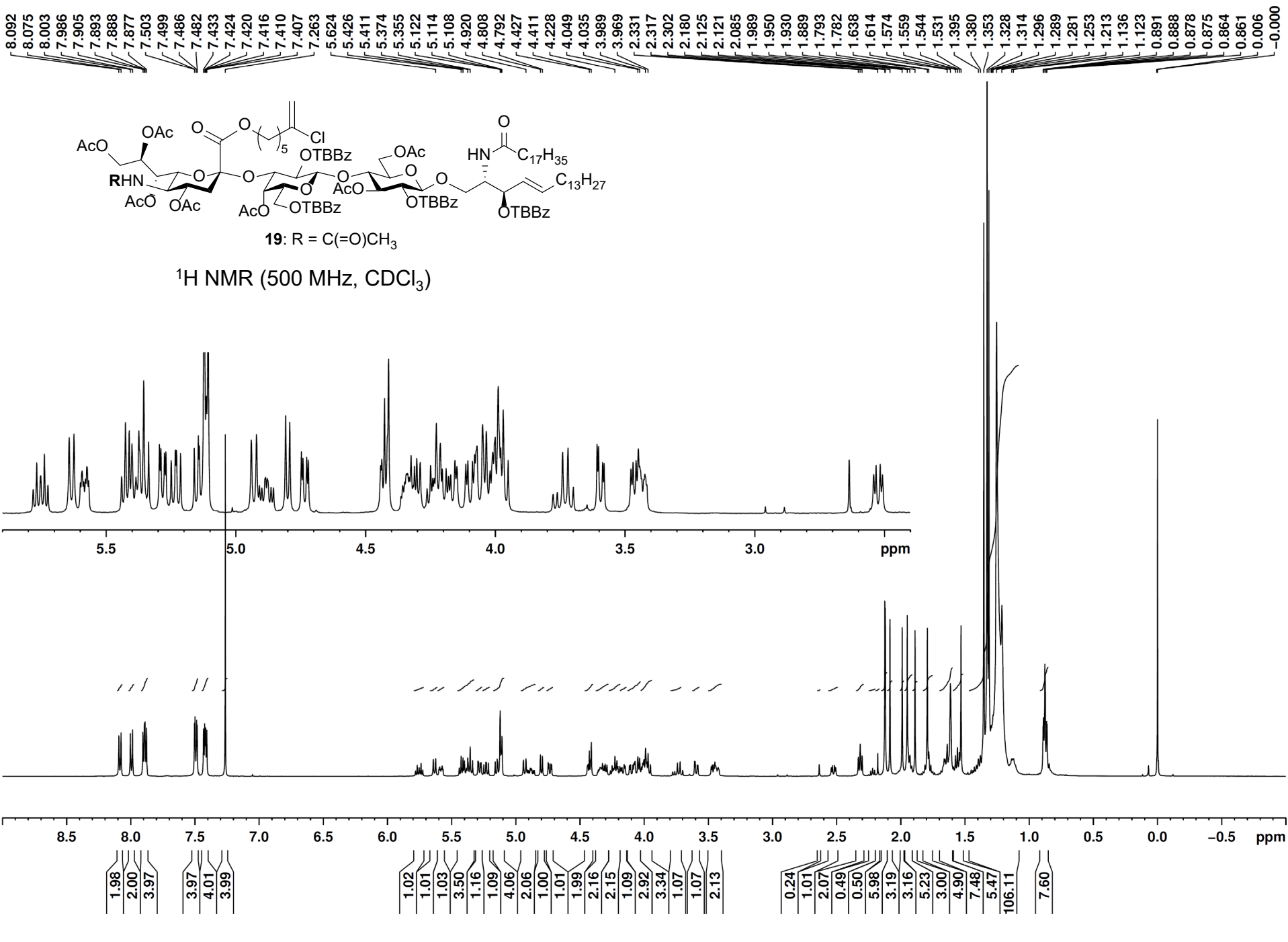
17

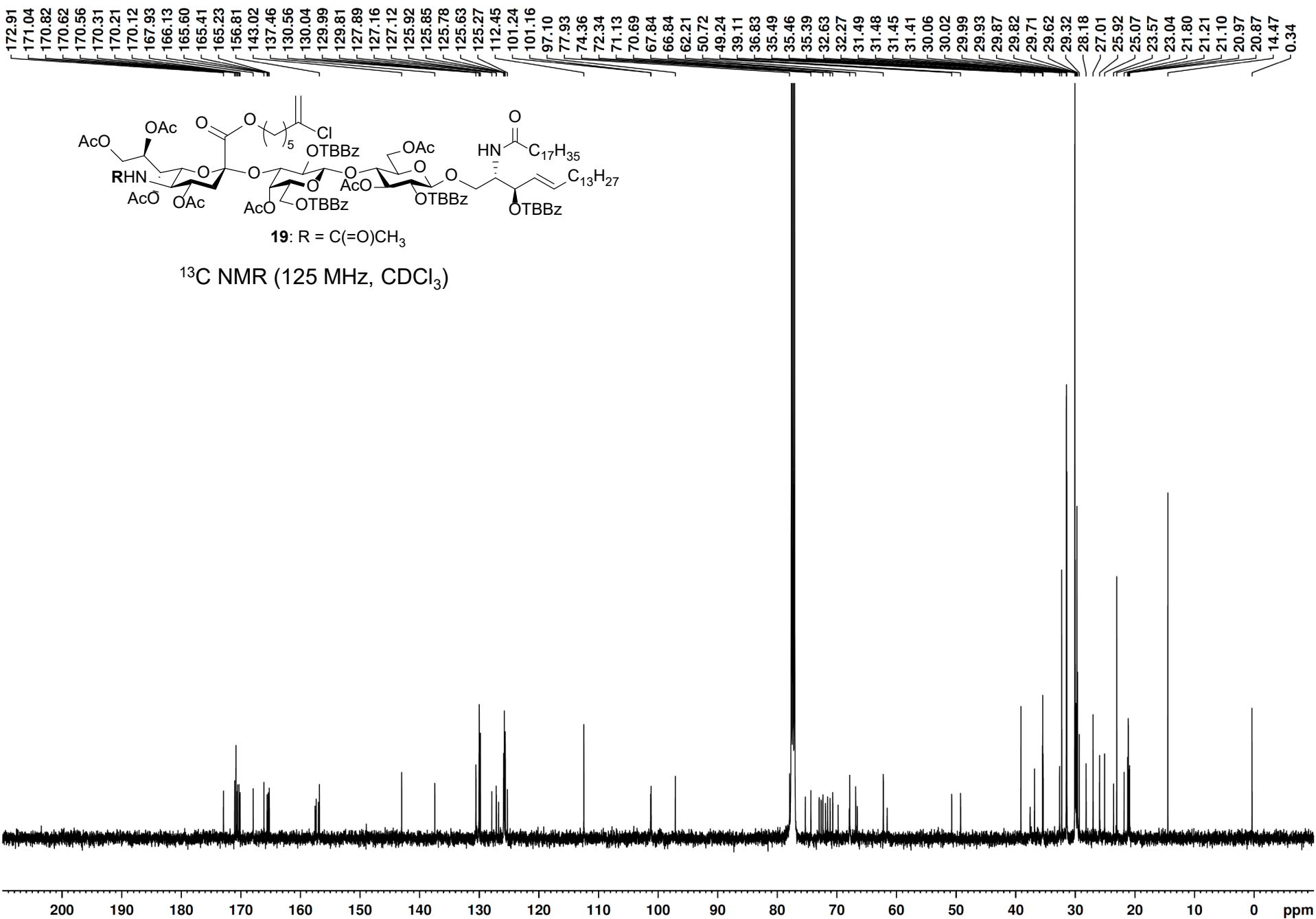
¹³C NMR (125 MHz, CDCl₃)

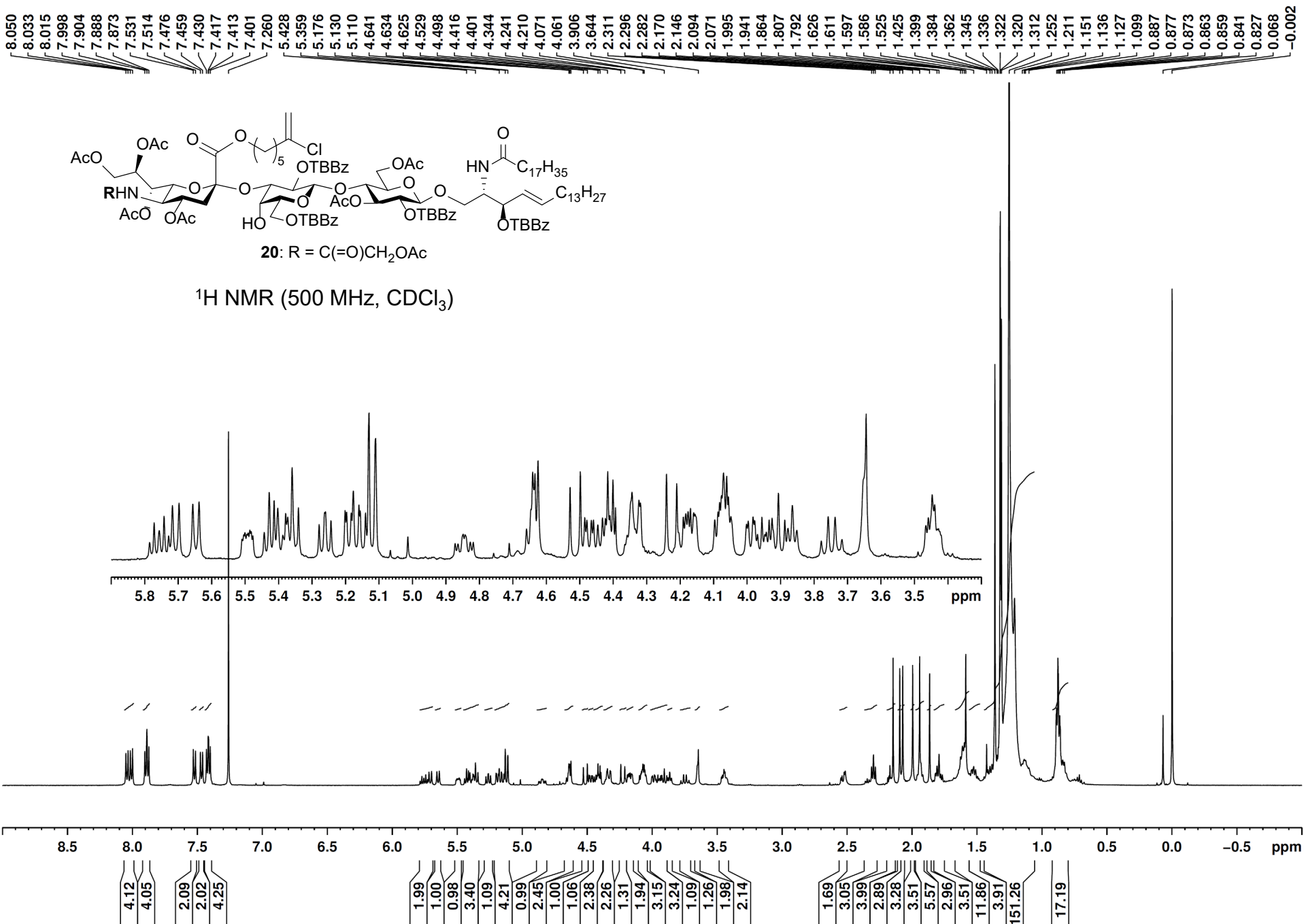


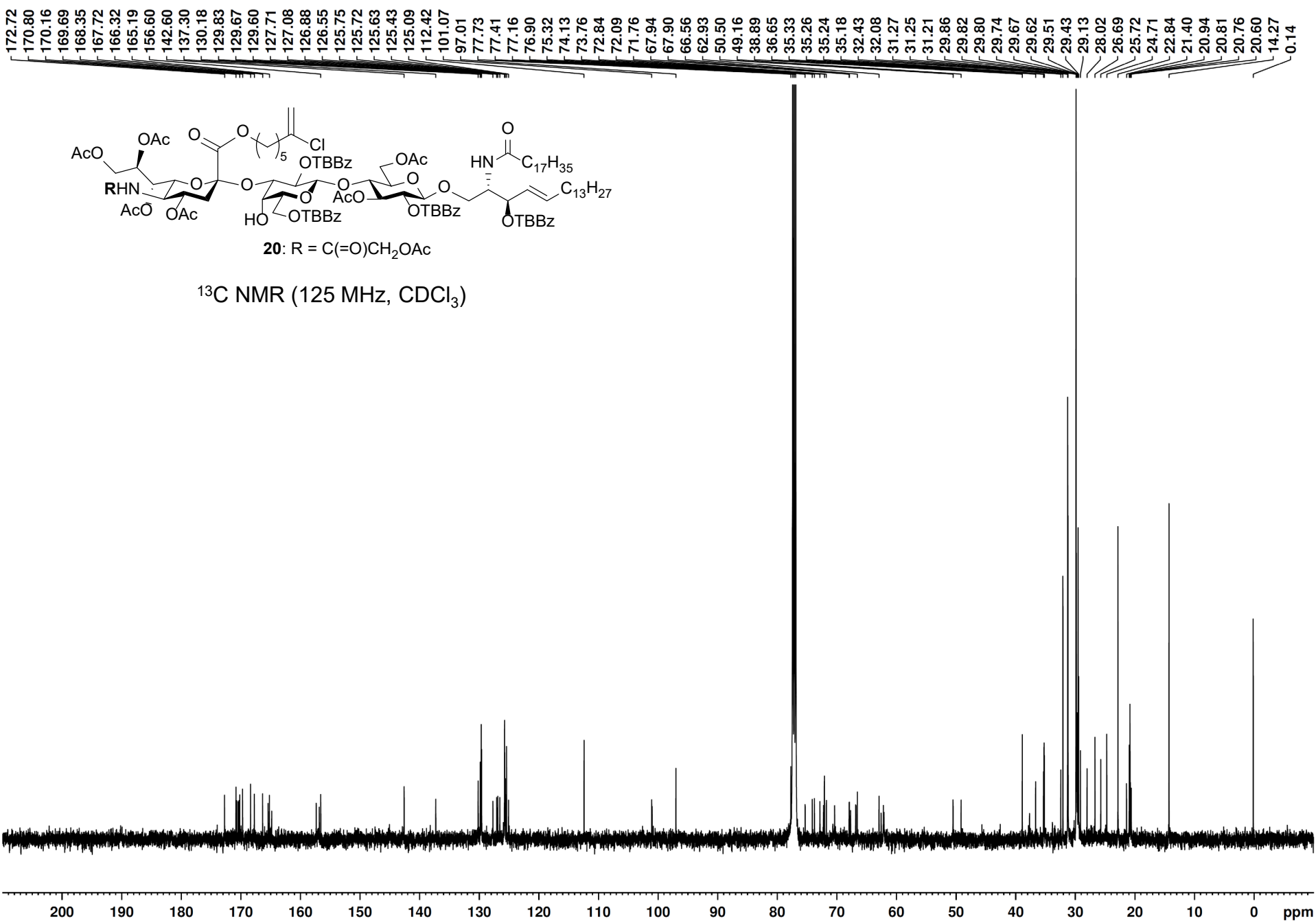


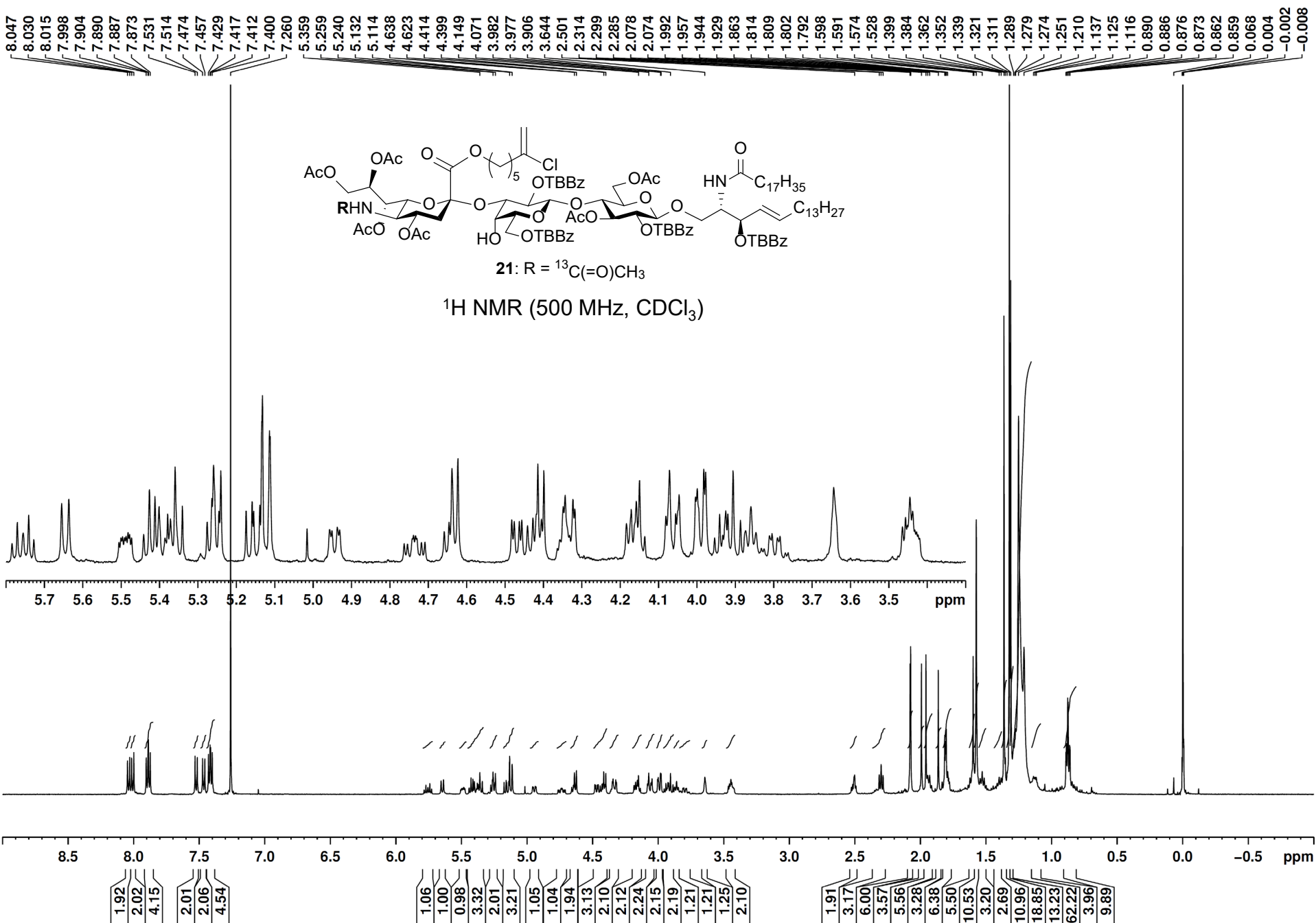


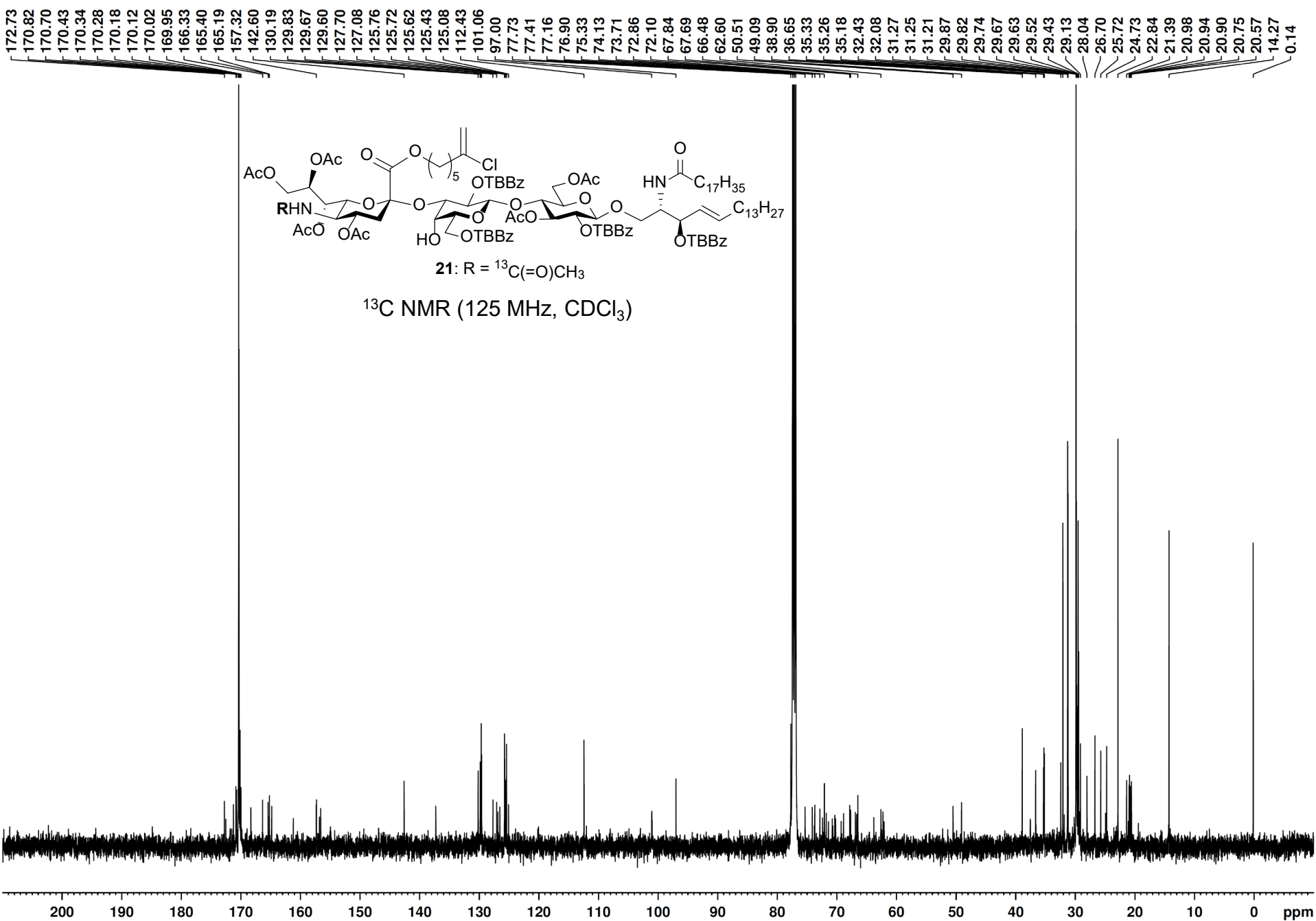


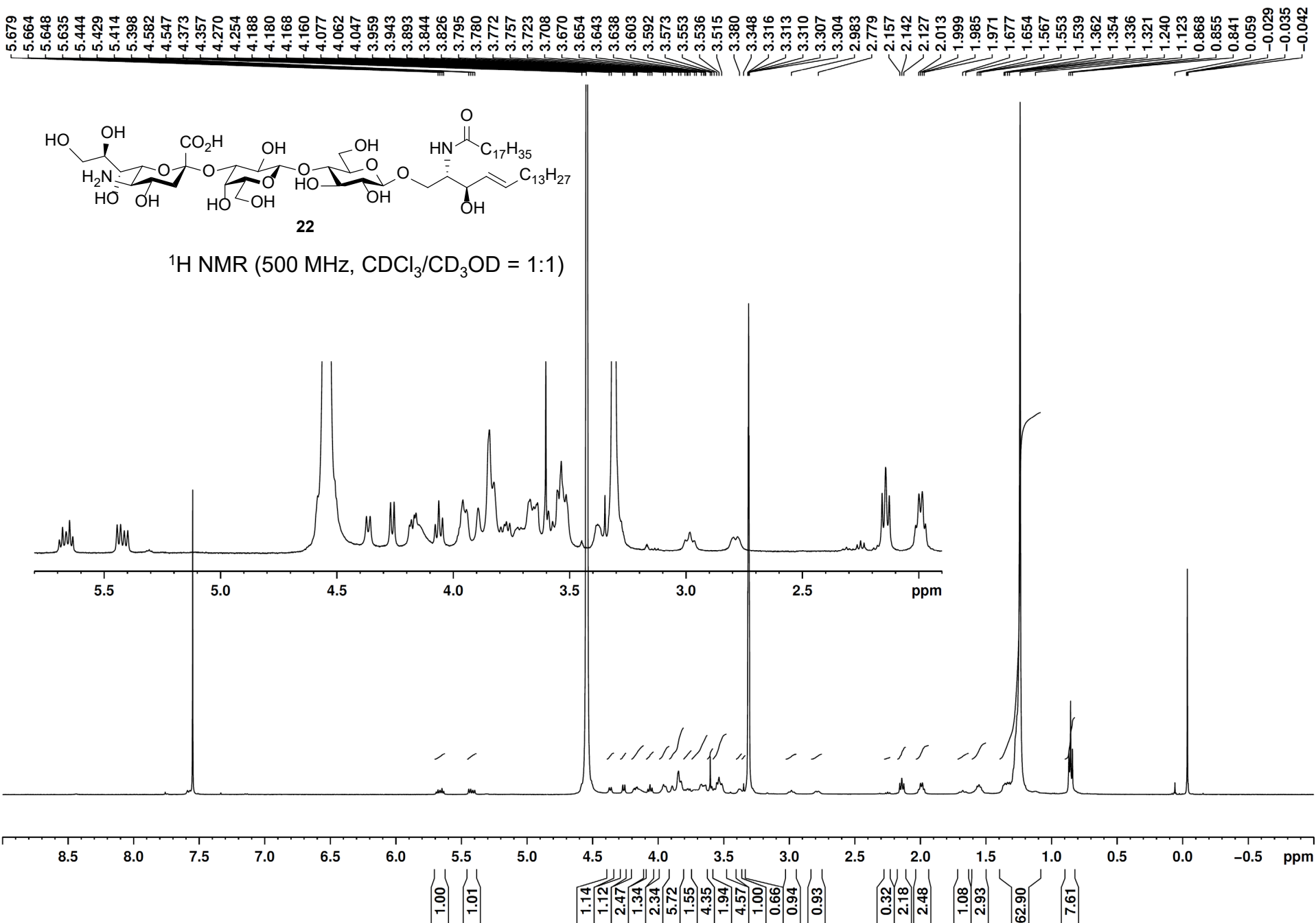


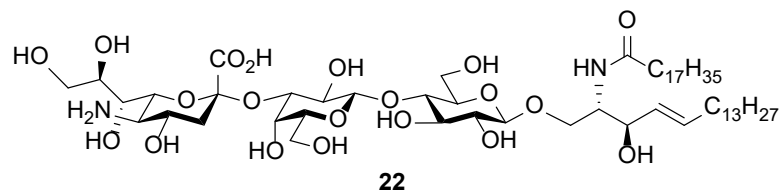












^{13}C NMR (200 MHz, $\text{CDCl}_3/\text{CD}_3\text{OD} = 1:1$)

