

Supporting Information File 2

for

Total synthesis of the endogenous inflammation resolving lipid resolvin D2 using a common lynchpin

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Email: Mark A. Rizzacasa* - masr@unimelb.edu.au

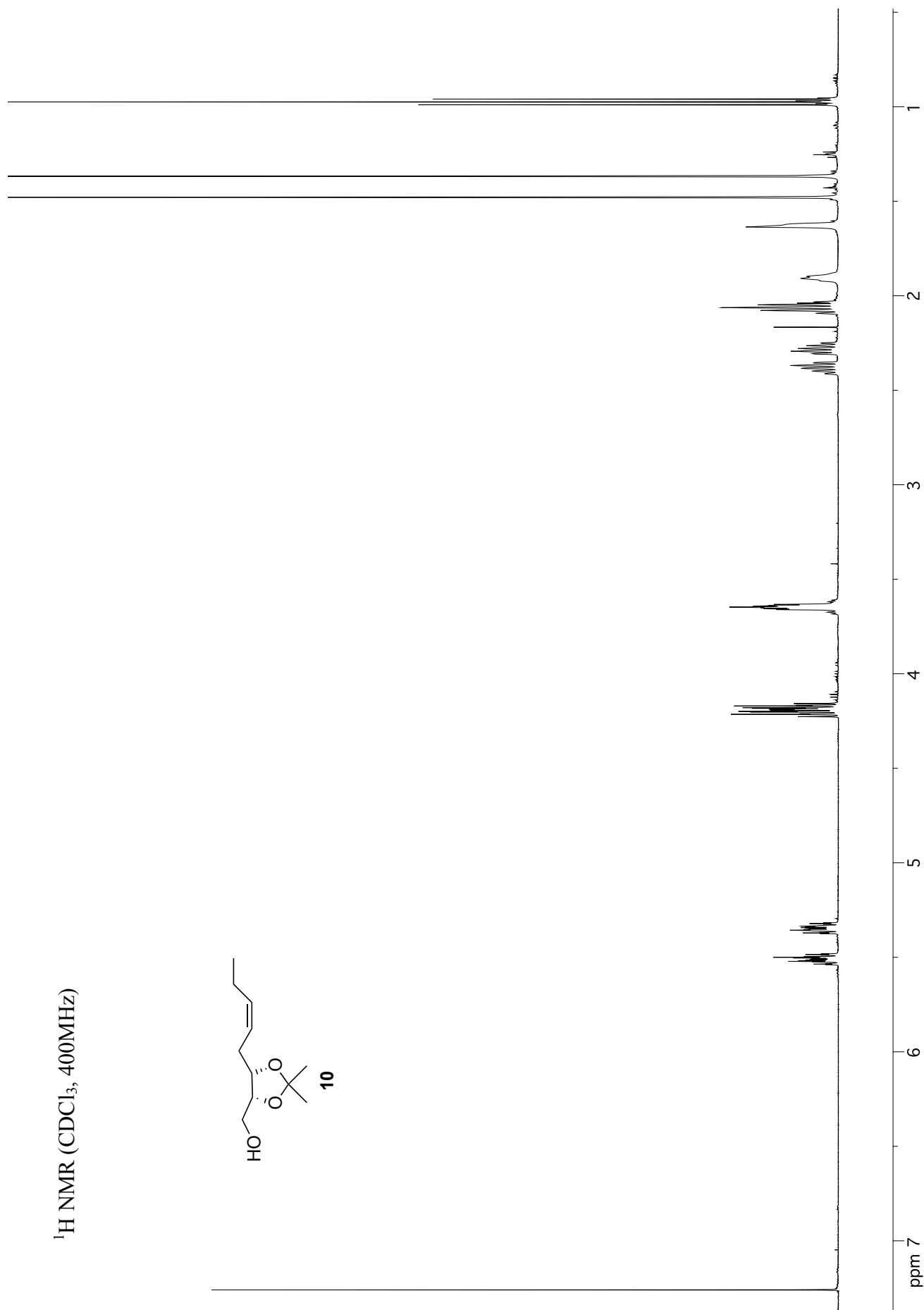
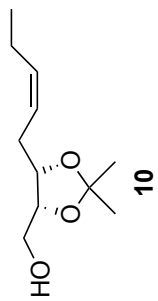
* Corresponding author

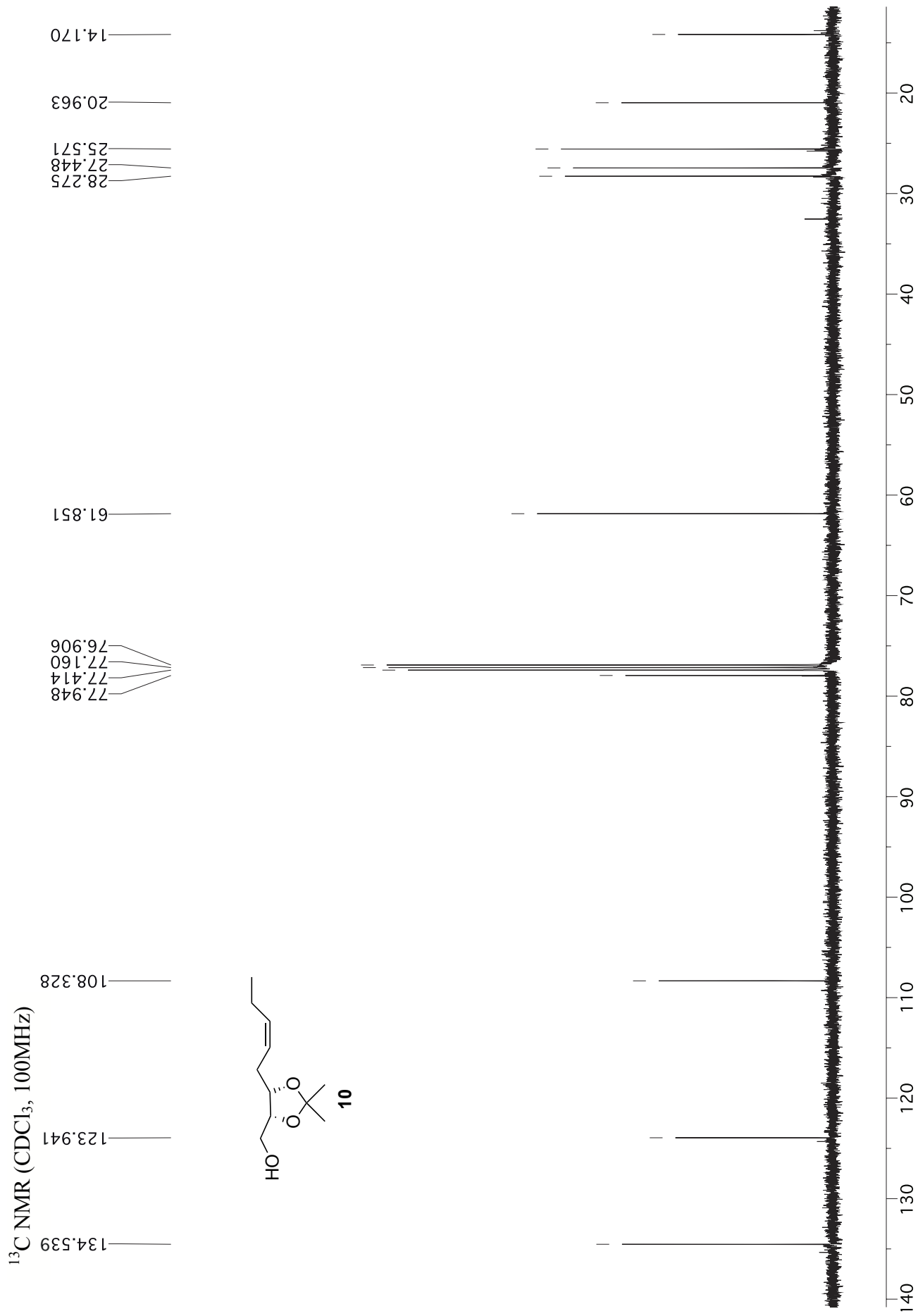
¹H and ¹³C NMR spectra of all intermediates and the mass spectrum of RvD2 (1)

¹ H NMR spectrum of alcohol 10	S3
¹³ C NMR spectrum of alcohol 10	S4
¹ H NMR spectrum of aldehyde 7	S5
¹³ C NMR spectrum of aldehyde 7	S6
¹ H NMR spectrum of enyne 11	S7
¹³ C NMR spectrum of enyne 11	S8
¹ H NMR spectrum of Z-isomer of 11	S9
¹³ C NMR spectrum of Z-isomer of 11	S10
¹ H NMR spectrum of enyne 12	S11
¹³ C NMR spectrum of enyne 12	S12
¹ H NMR spectrum of vinyl iodide 4	S13
¹³ C NMR spectrum of vinyl iodide 4	S14

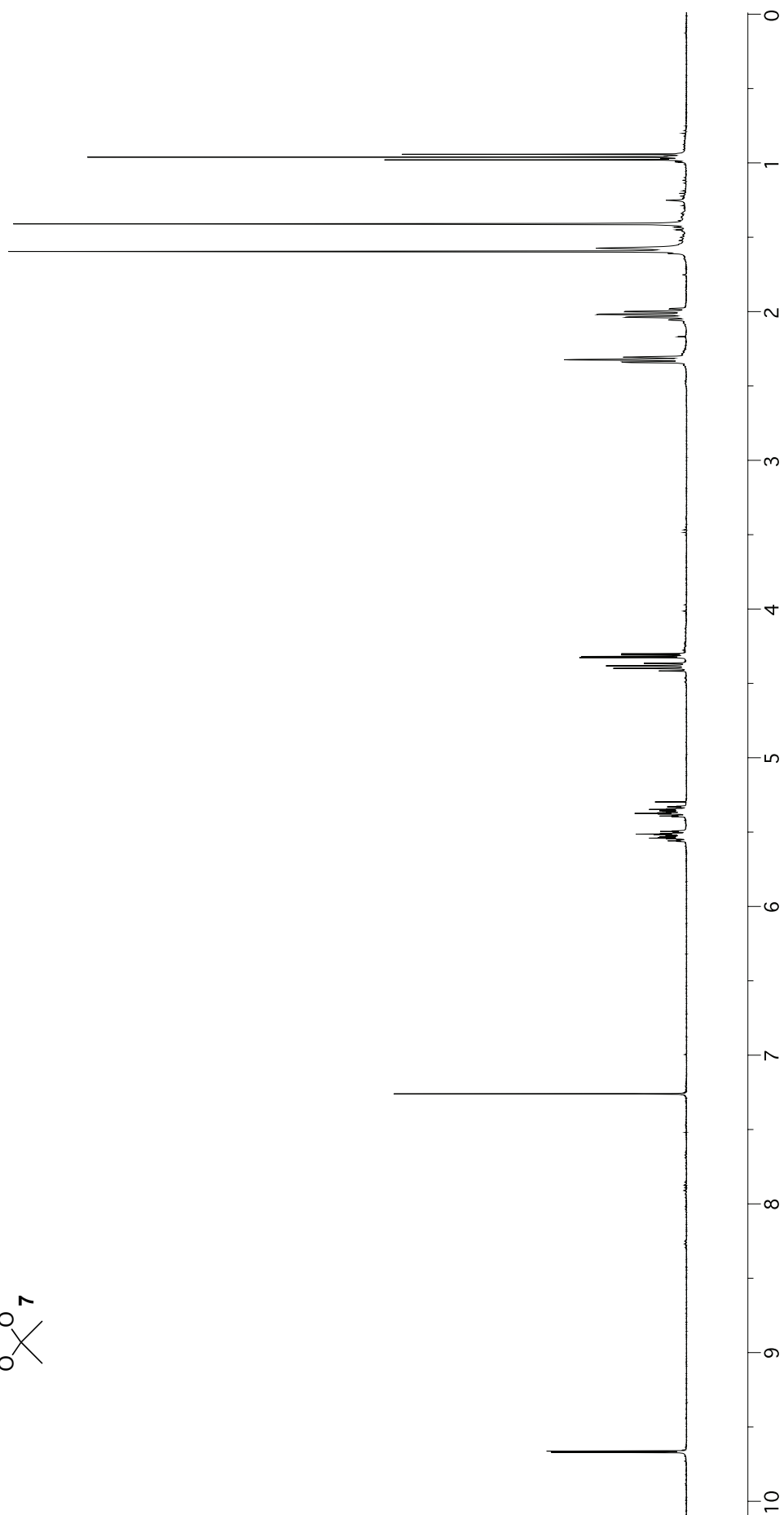
¹ H NMR spectrum of diol 14	S15
¹³ C NMR spectrum of diol 14	S16
¹ H NMR spectrum of bis-(S)-Mosher ester	S17
¹ H NMR spectrum of bis-TES ether 15	S18
¹³ C NMR spectrum of bis-TES ether 15	S19
¹ H NMR spectrum of alkene 16	S20
¹³ C NMR spectrum of alkene 16	S21
¹ H NMR spectrum of aldehyde 5	S22
¹³ C NMR spectrum of aldehyde 5	S23
¹ H NMR spectrum of enyne 17	S24
¹³ C NMR spectrum of enyne 17	S25
¹ H NMR spectrum of Z-isomer of enyne 17	S26
¹³ C NMR spectrum of Z-isomer of enyne 17	S27
¹ H NMR spectrum of enyne 3	S28
¹³ C NMR spectrum of enyne 3	S29
¹ H NMR spectrum of alkyne 18	S30
¹³ C NMR spectrum of alkyne 18	S31
¹ H NMR spectrum of triol 19	S32
¹³ C NMR spectrum of triol 19	S33
¹ H NMR spectrum of RvD2 methyl ester 20	S34
¹³ C NMR spectrum of RvD2 methyl ester 20	S35
¹ H NMR spectrum of RvD2 1	S36
¹³ C NMR spectrum of RvD2 1	S37
Low resolution mass spectrum of RvD2 1 (negative ion mode)	S38

¹H NMR (CDCl₃, 400MHz)

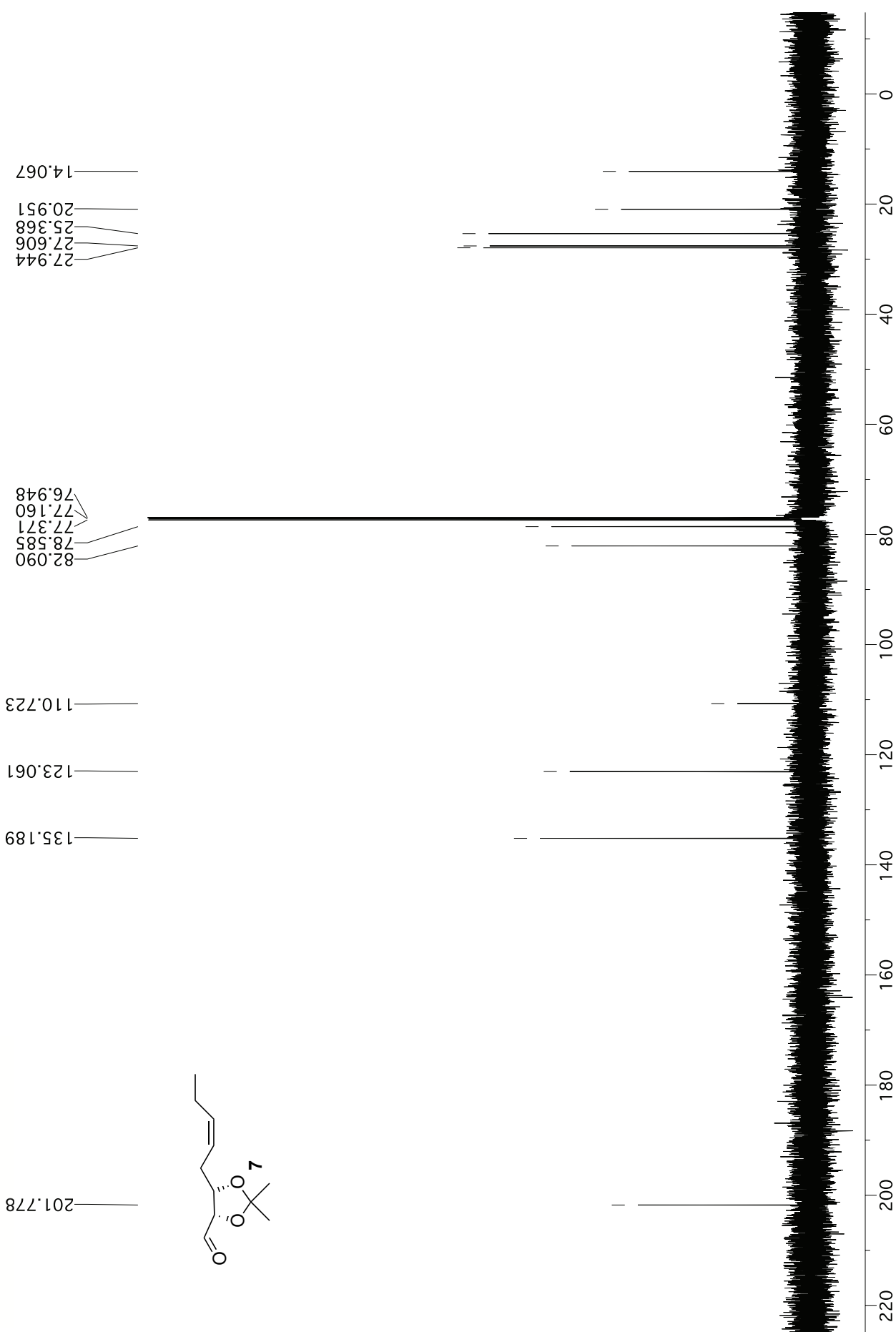




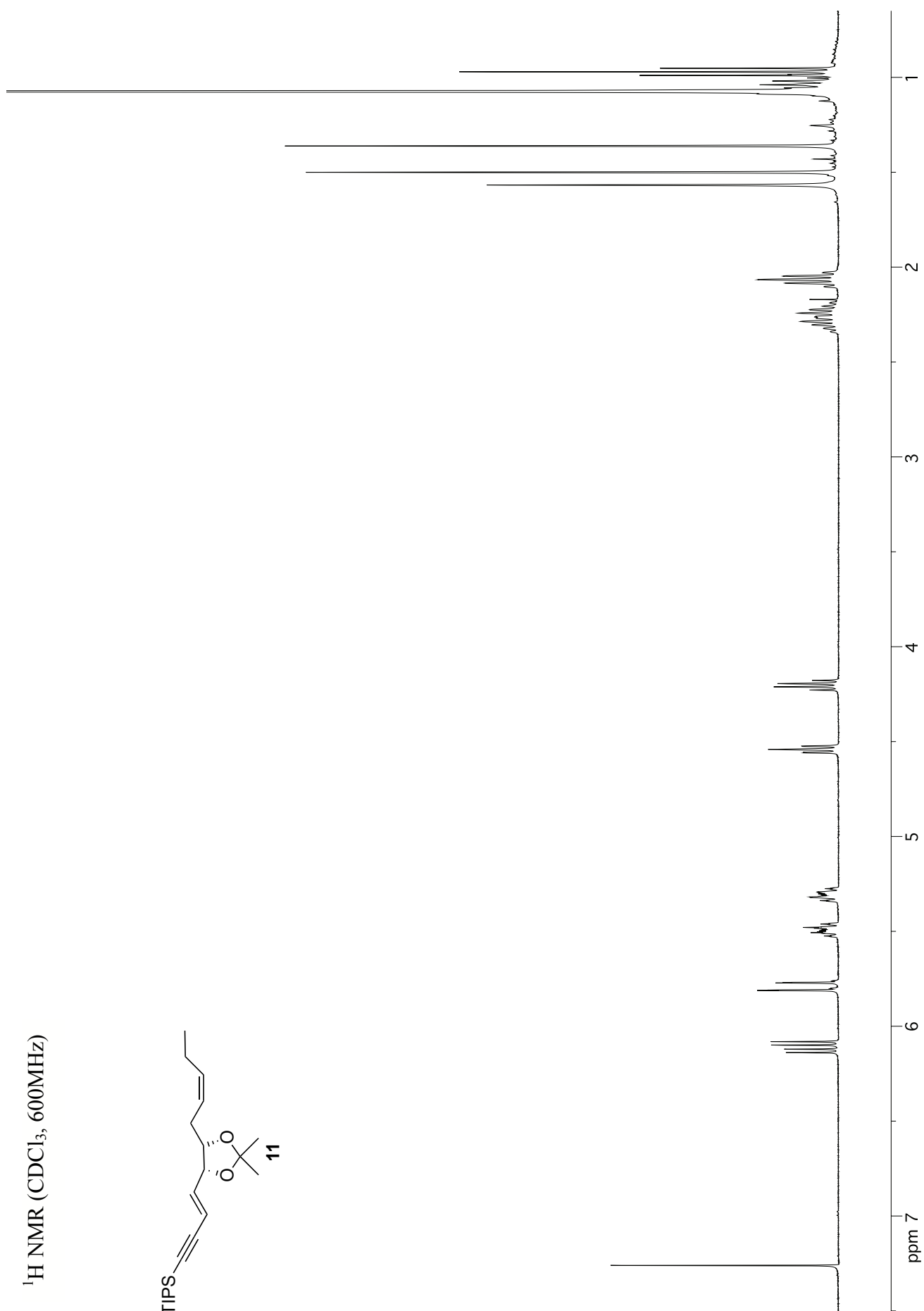
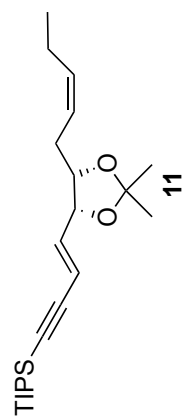
¹H NMR (CDCl₃, 400MHz)

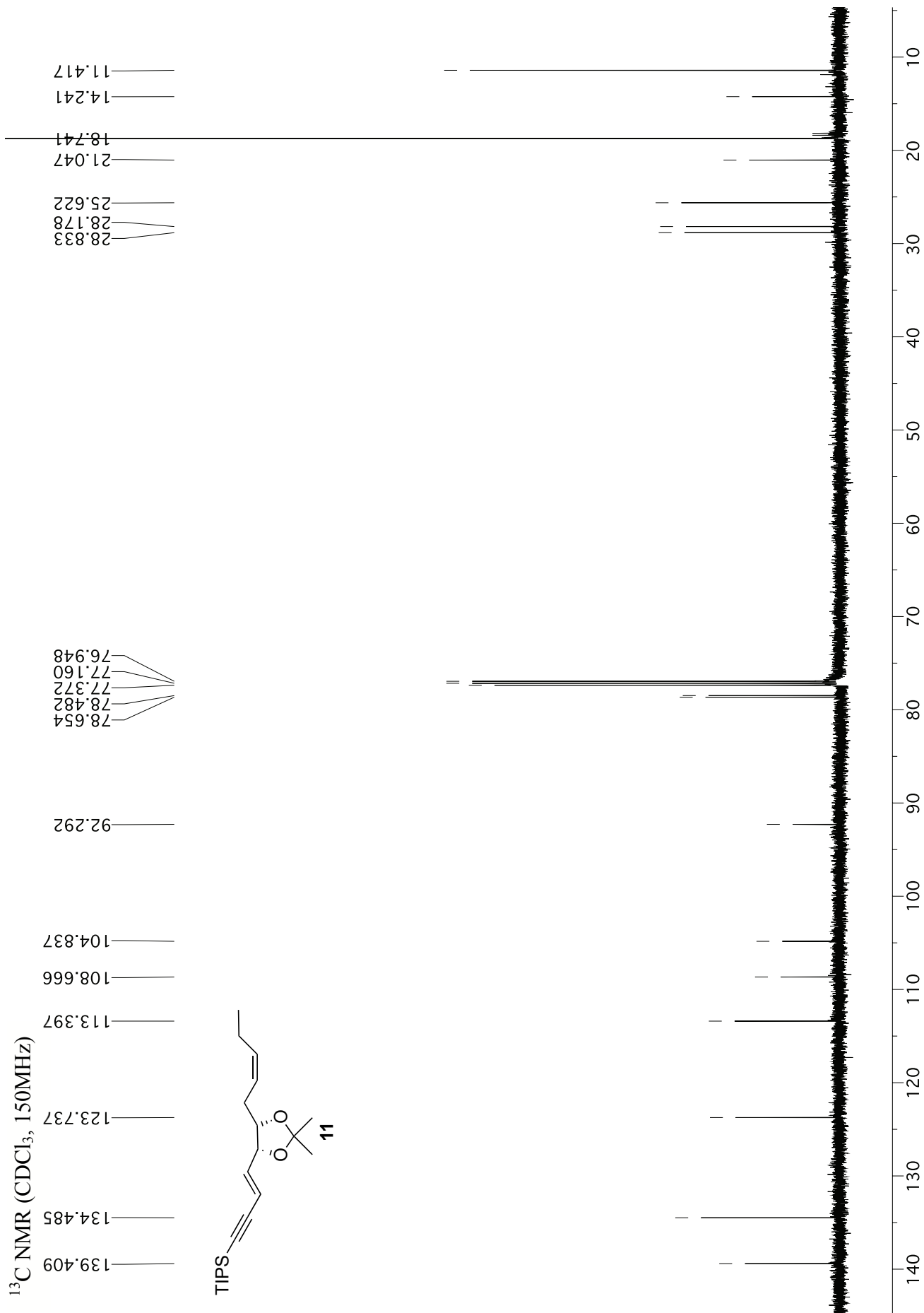


^{13}C NMR (CDCl_3 , 100MHz)

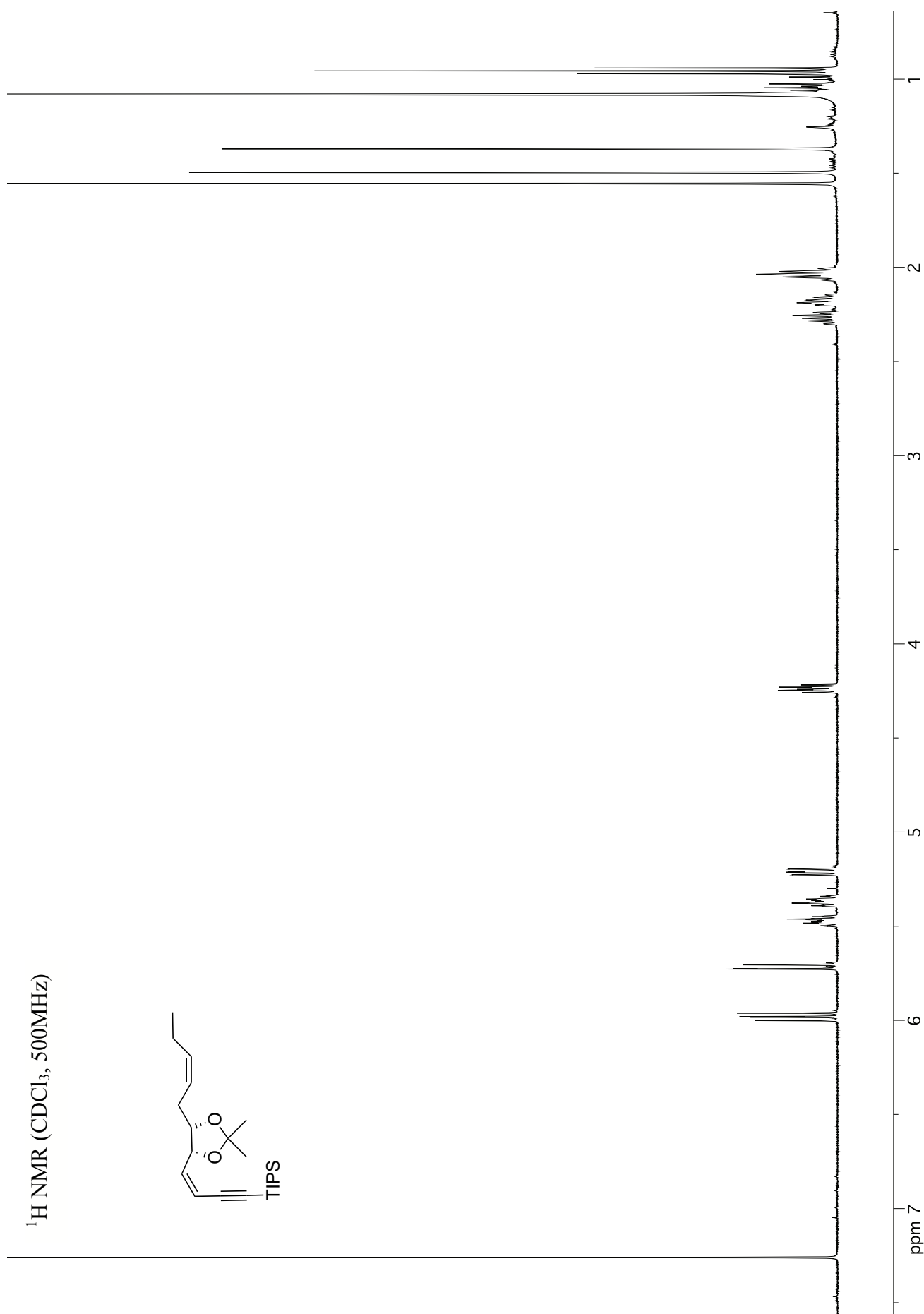
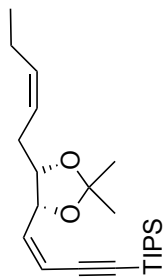


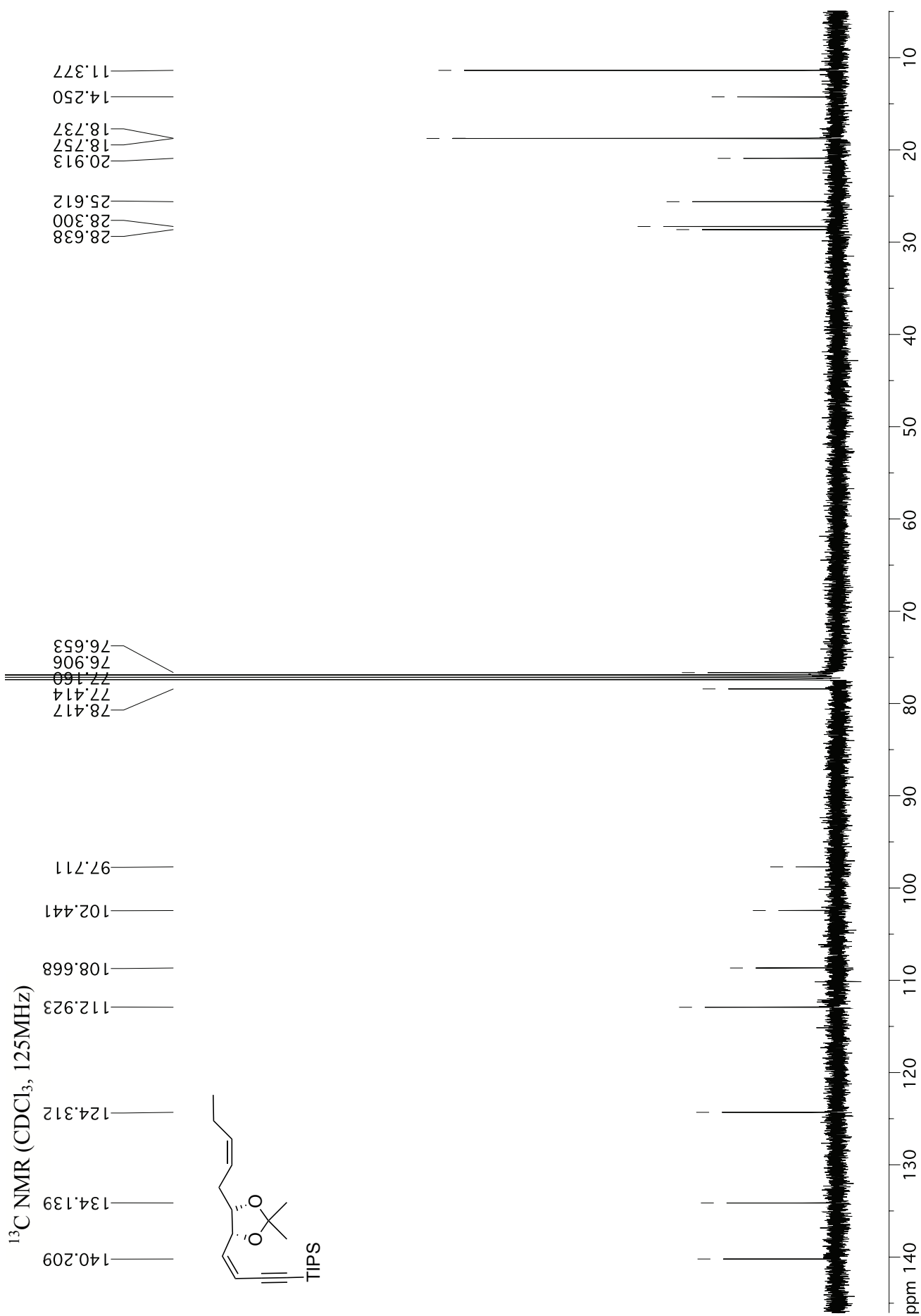
^1H NMR (CDCl_3 , 600MHz)



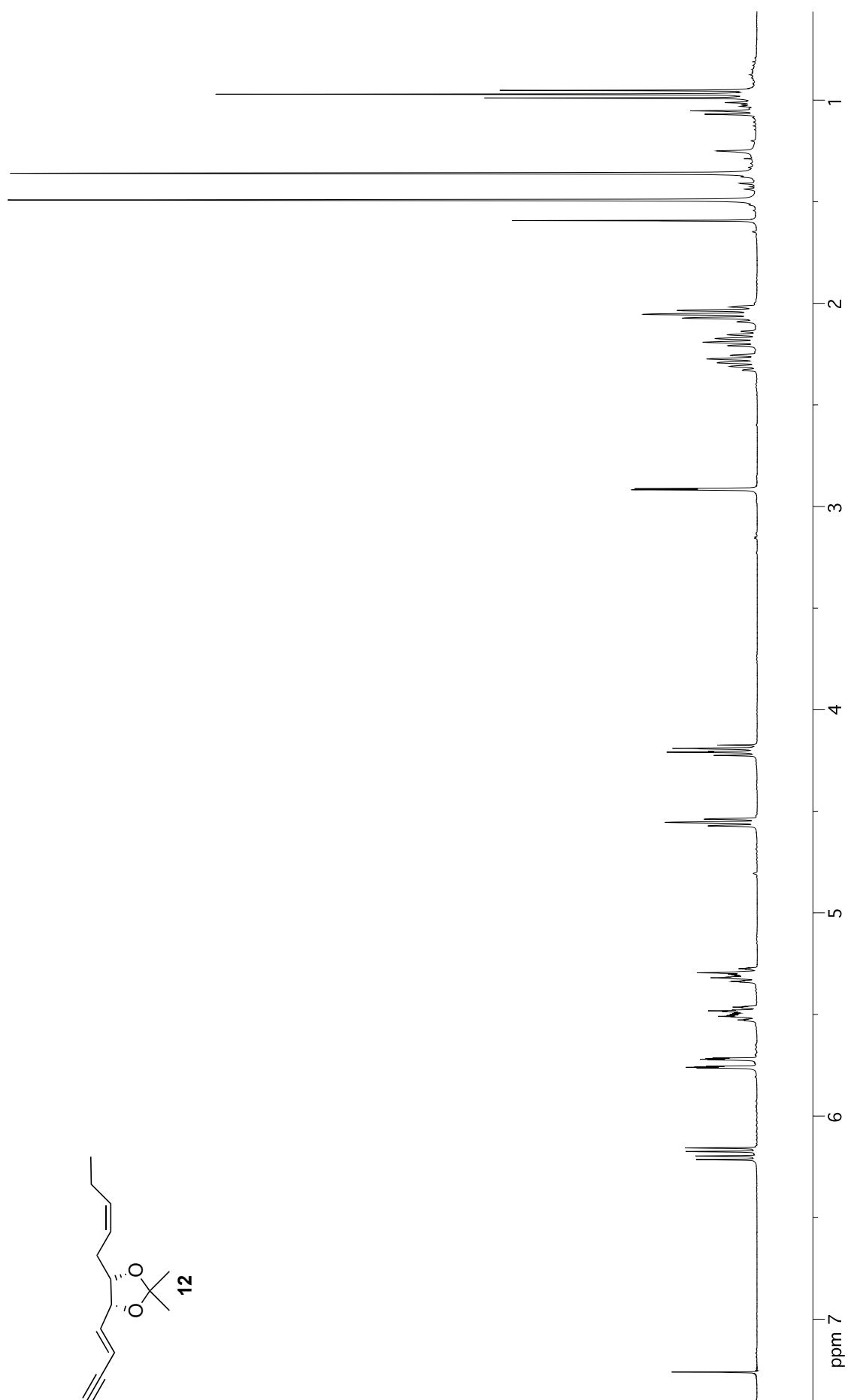
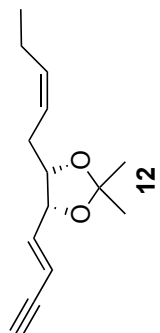


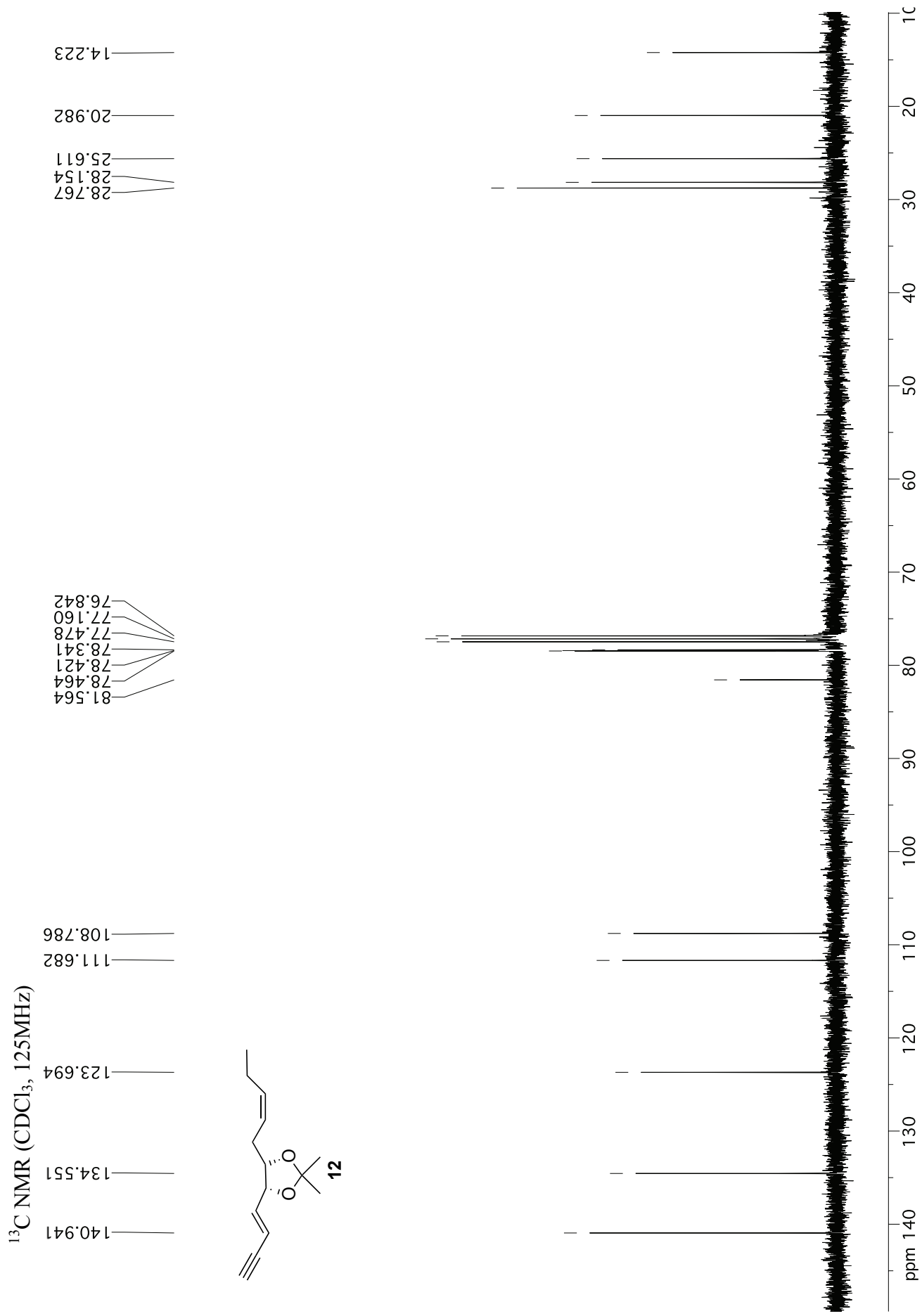
^1H NMR (CDCl_3 , 500MHz)



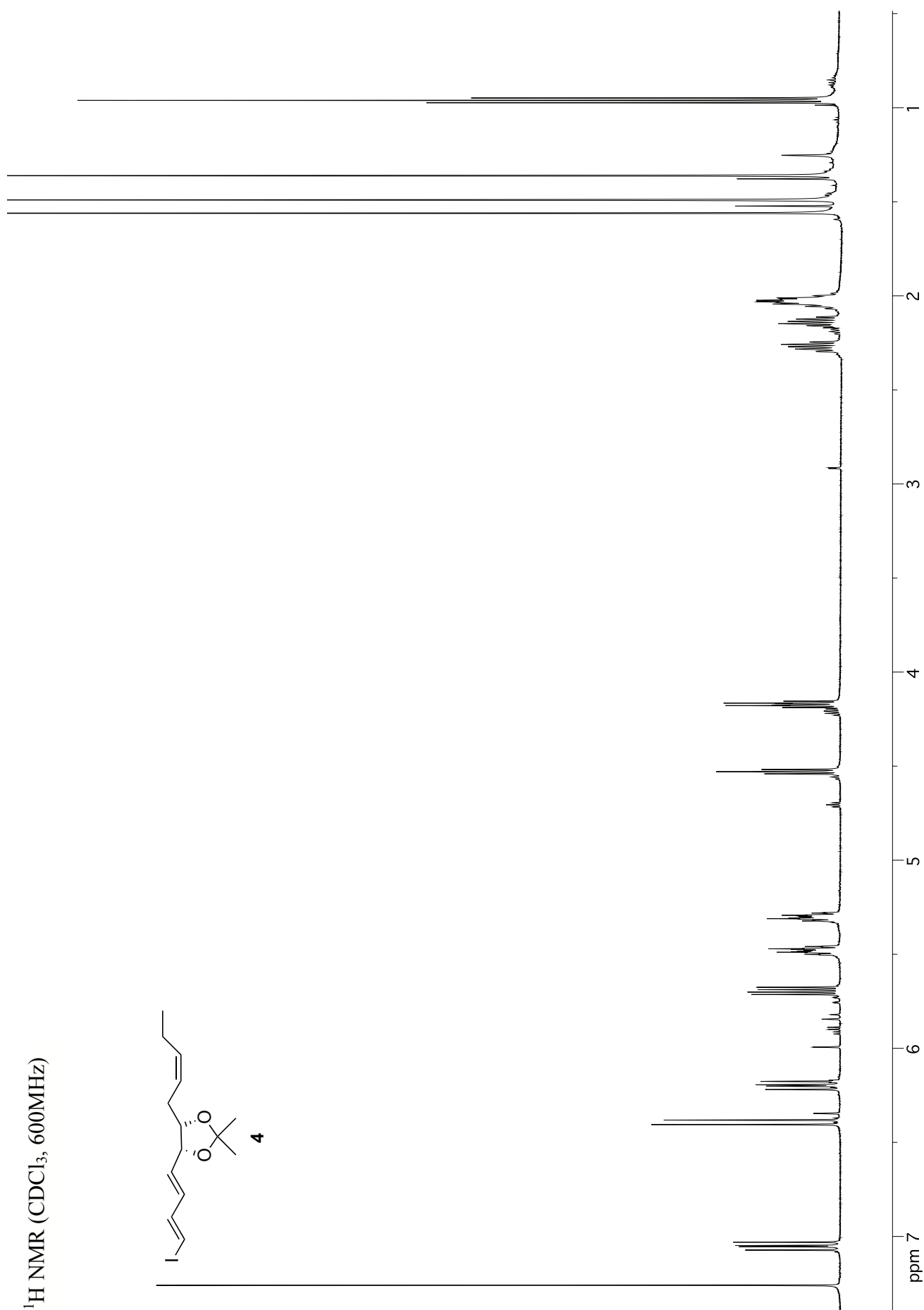
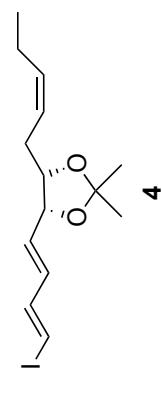


¹H NMR (CDCl₃, 500MHz)



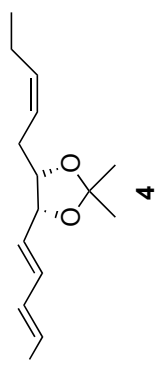


¹H NMR (CDCl₃, 600MHz)



¹³C NMR (CDCl₃, 150MHz)

144.440
134.349
132.838
130.109
123.967

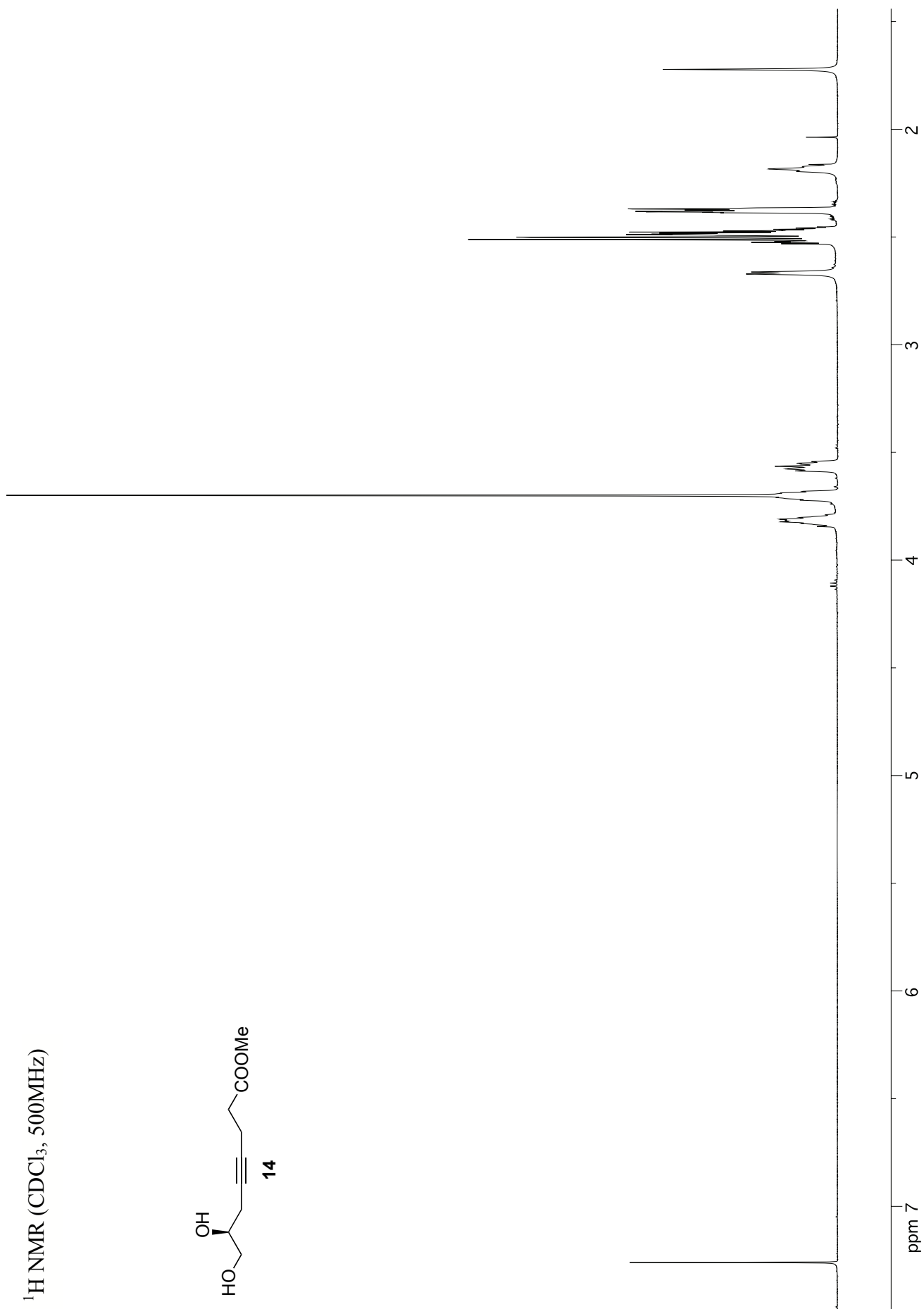
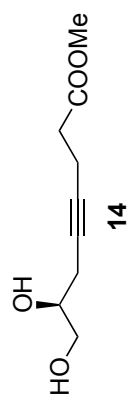


108.597

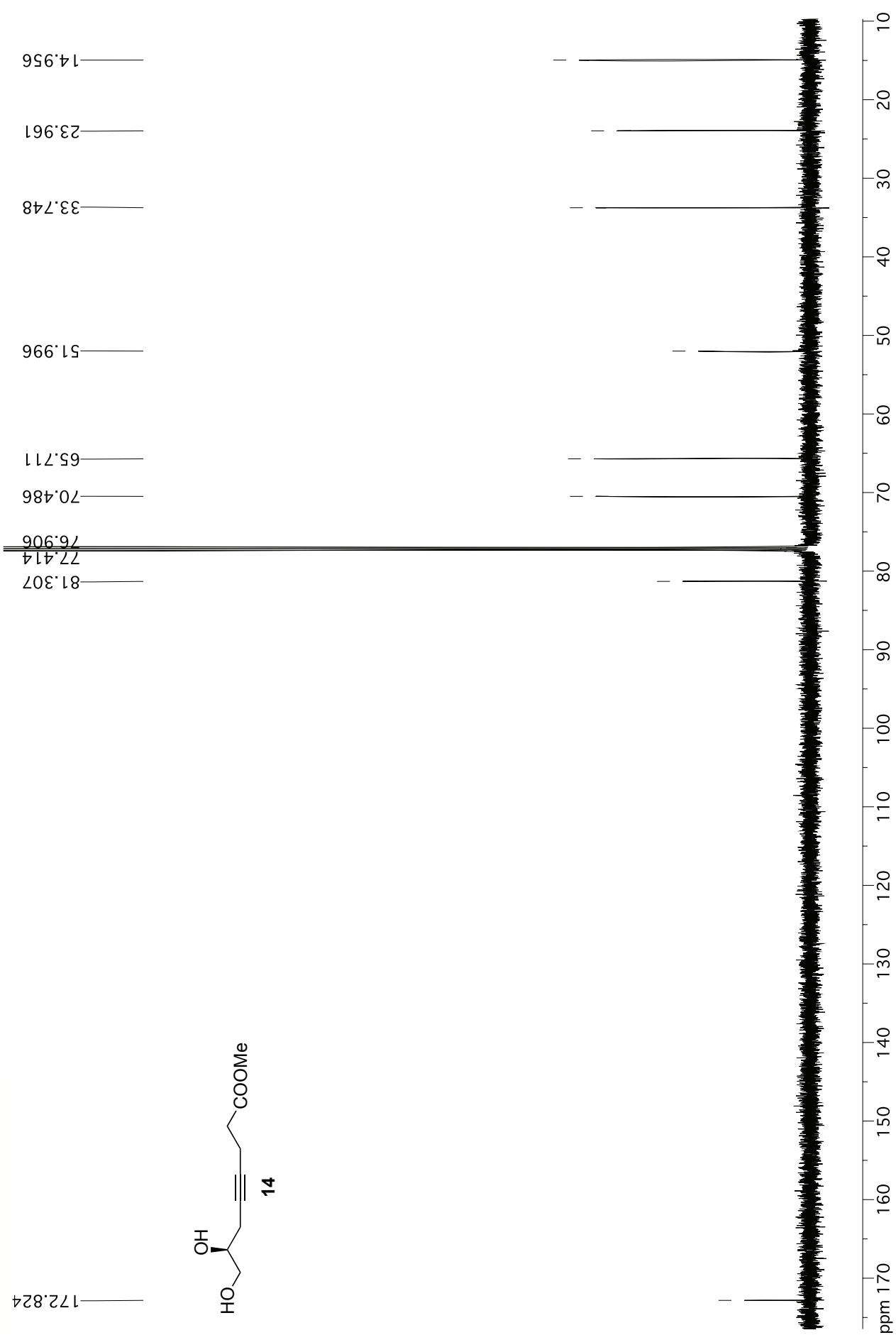
80.517
78.554
78.409
77.371
77.160
76.948

28.829
28.271
25.676
20.985
14.252

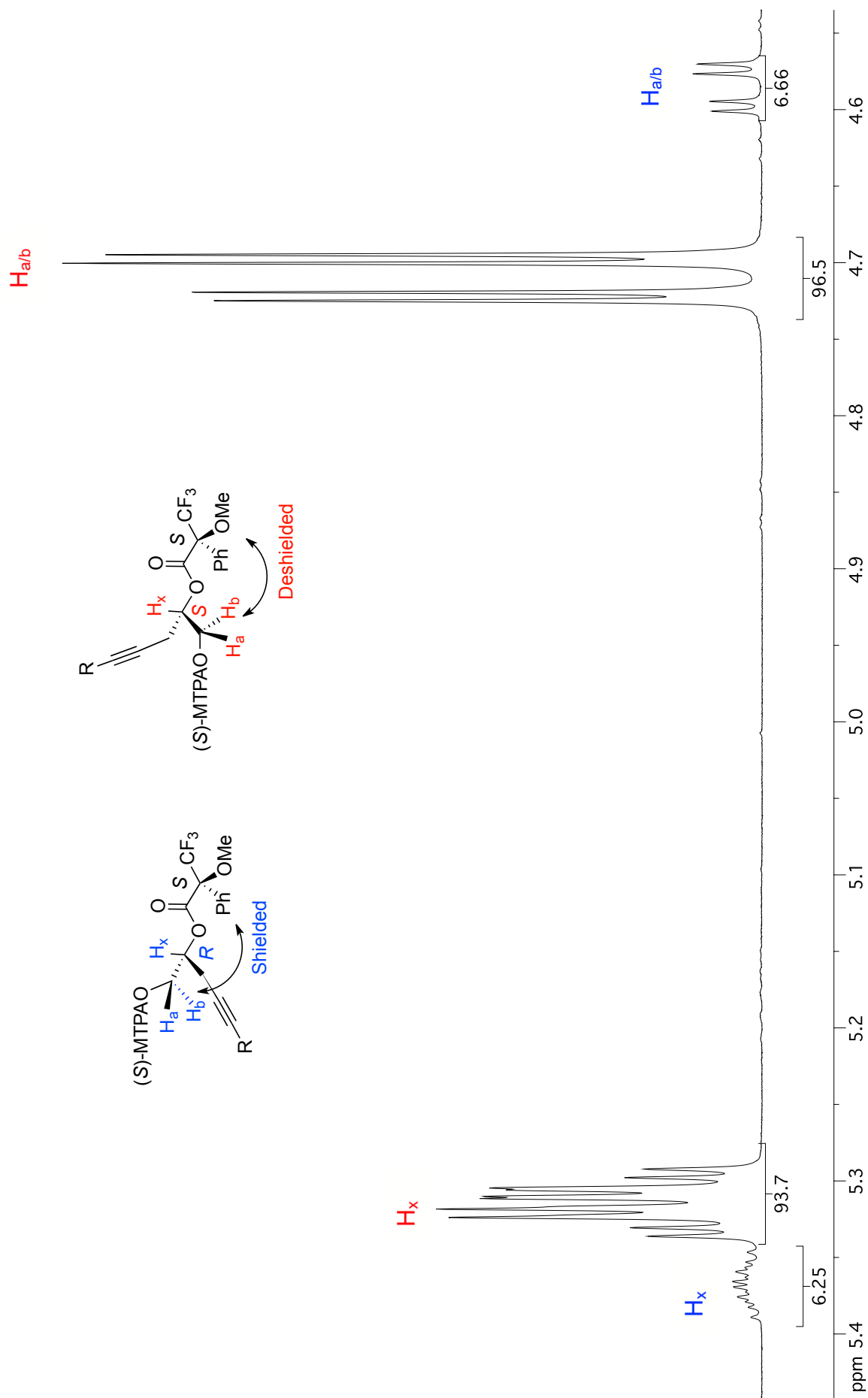
^1H NMR (CDCl_3 , 500MHz)



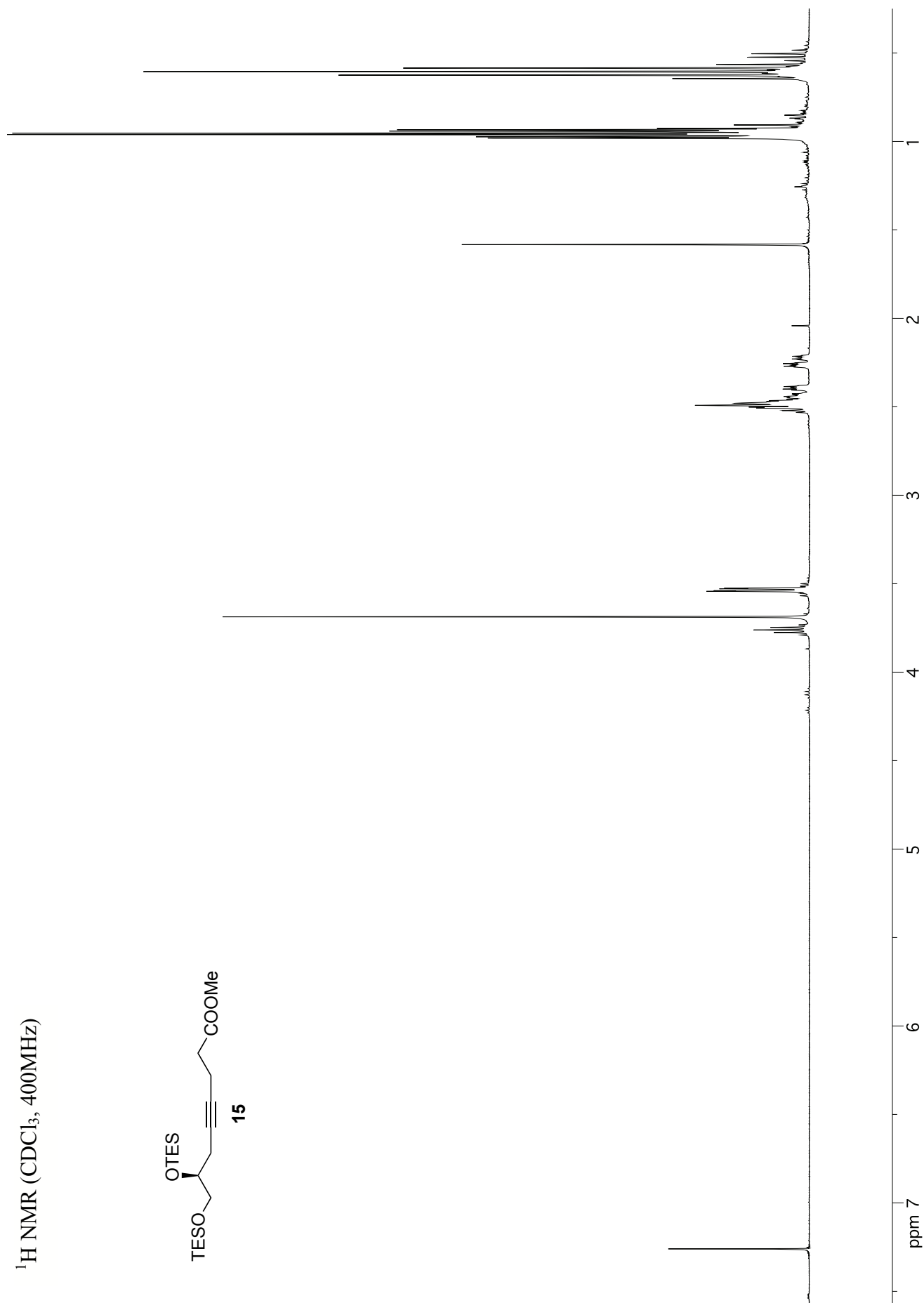
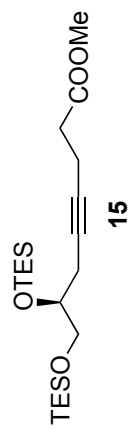
^{13}C NMR (CDCl_3 , 125MHz)



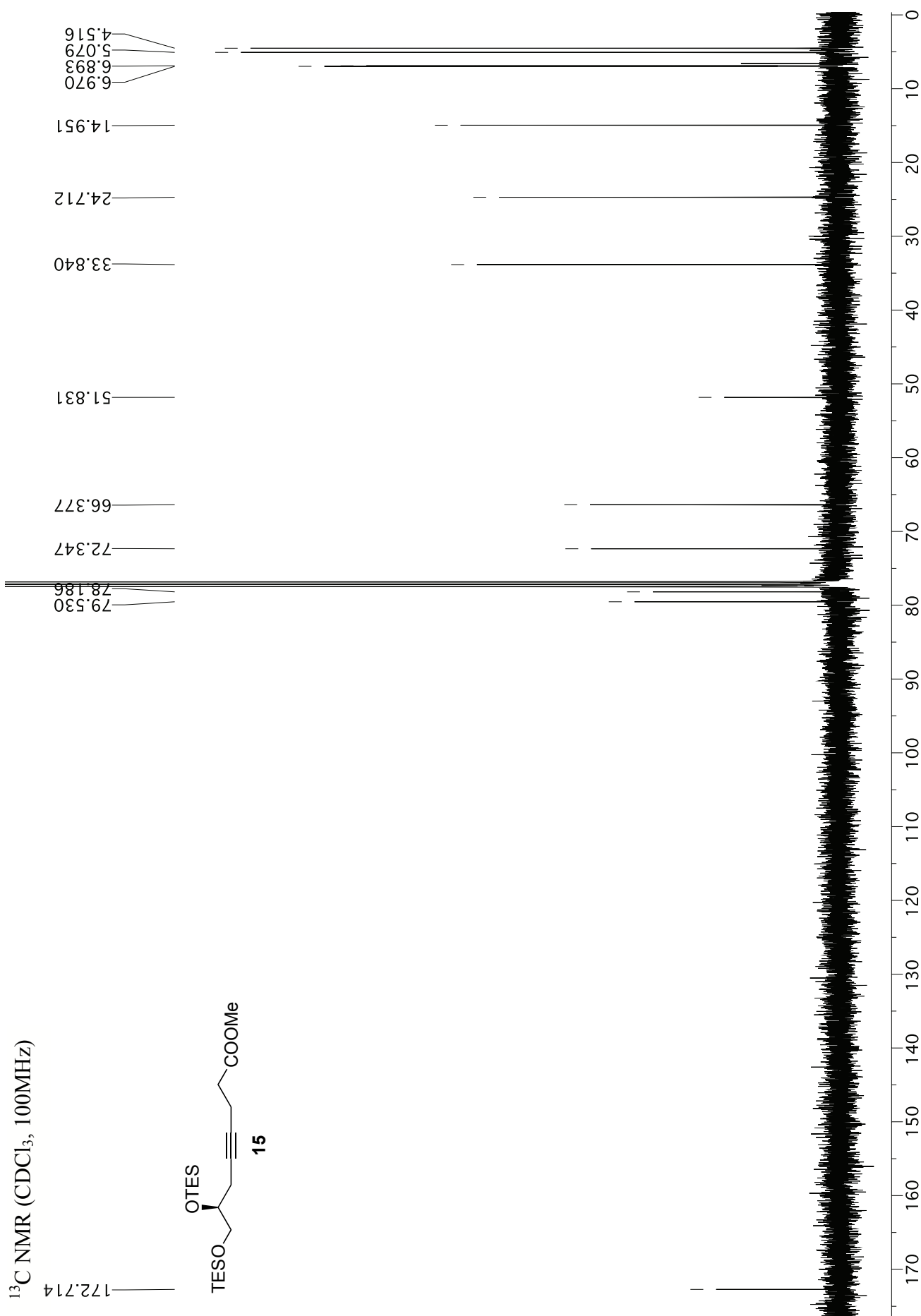
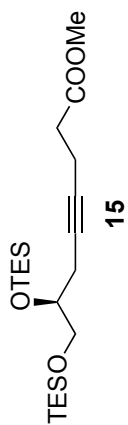
^1H NMR (CDCl_3 , 400MHz)



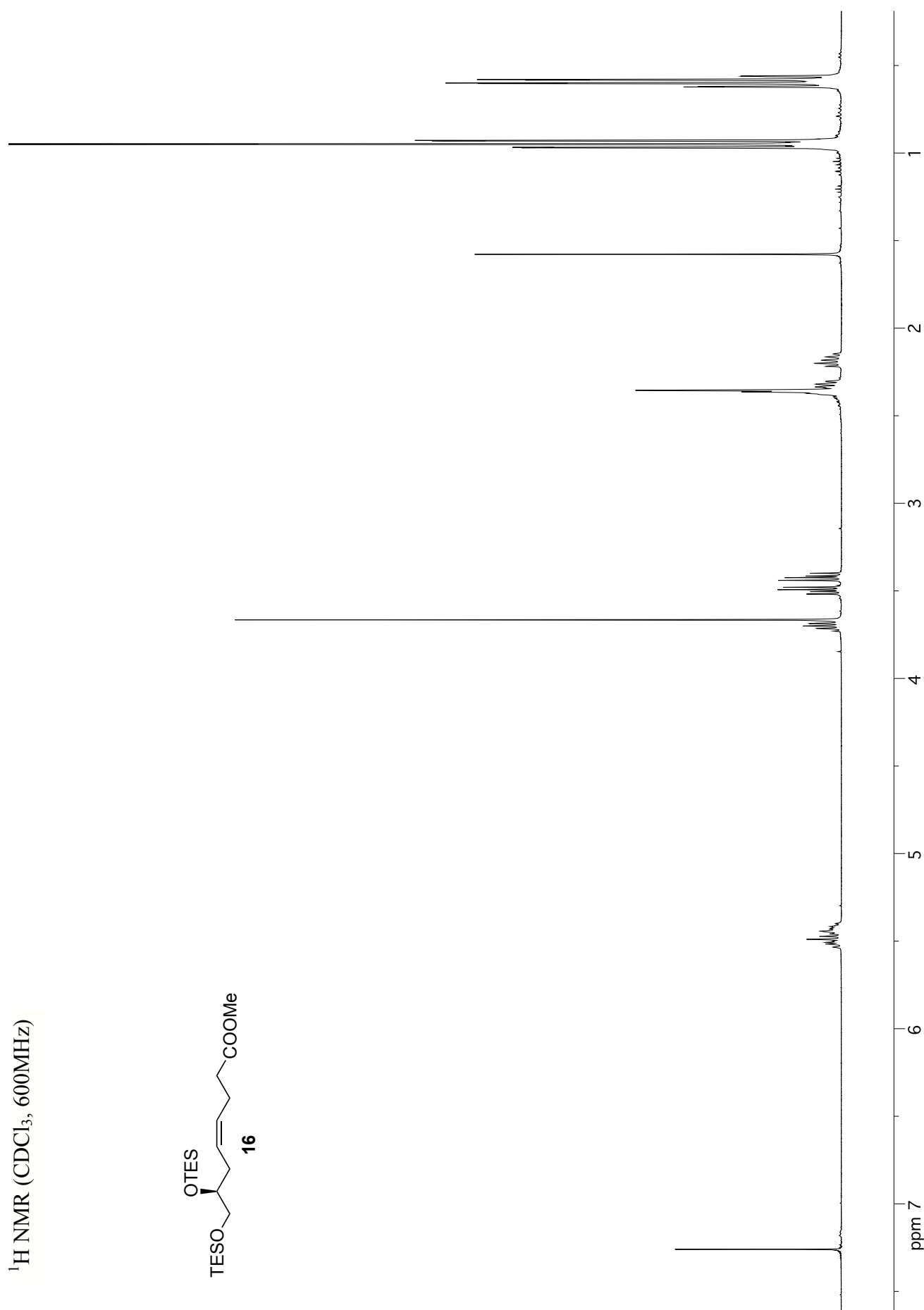
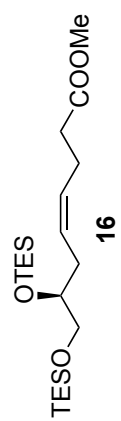
¹H NMR (CDCl₃, 400MHz)



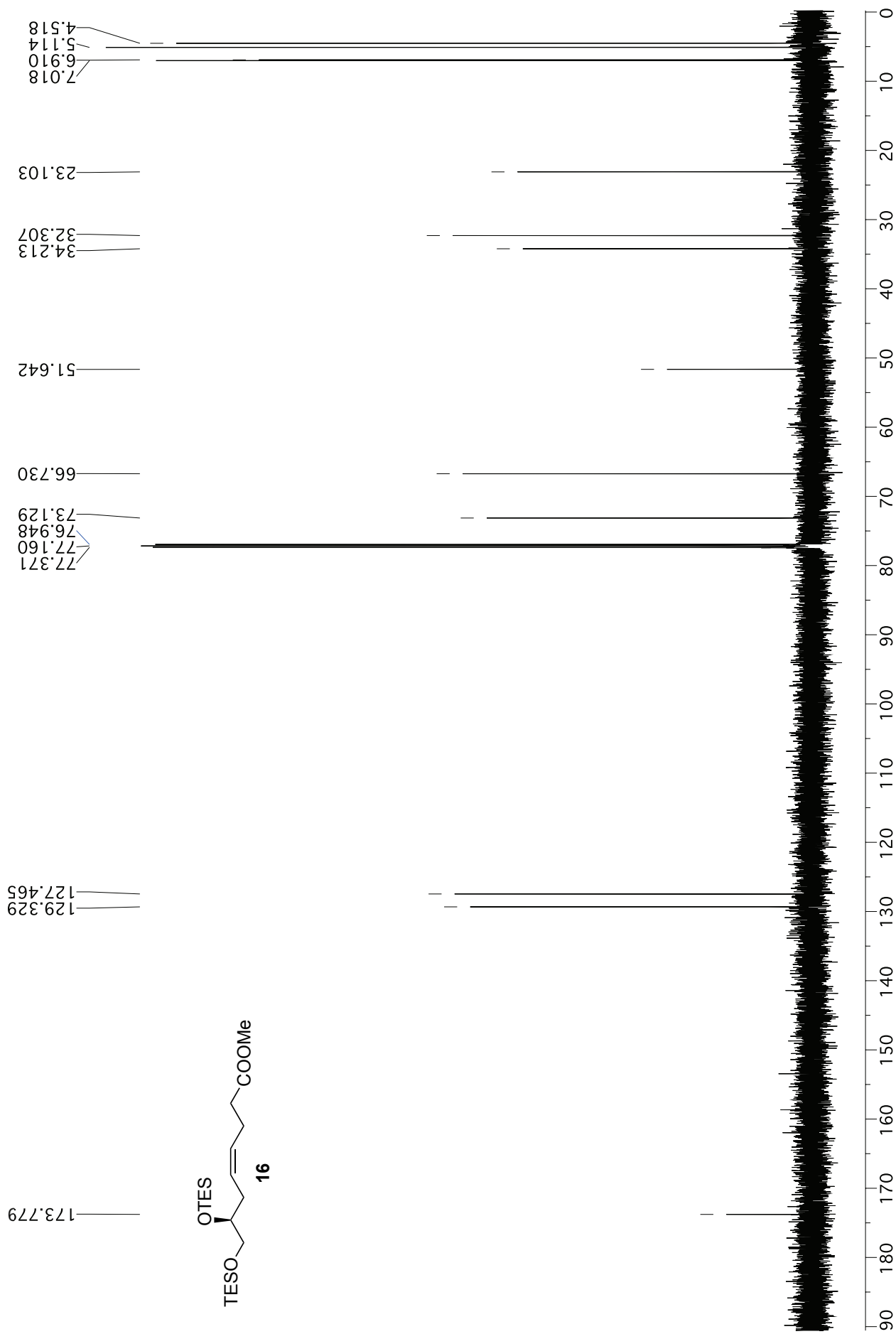
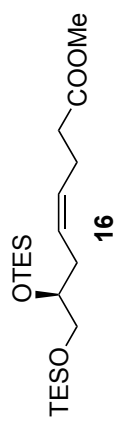
^{13}C NMR (CDCl_3 , 100MHz)



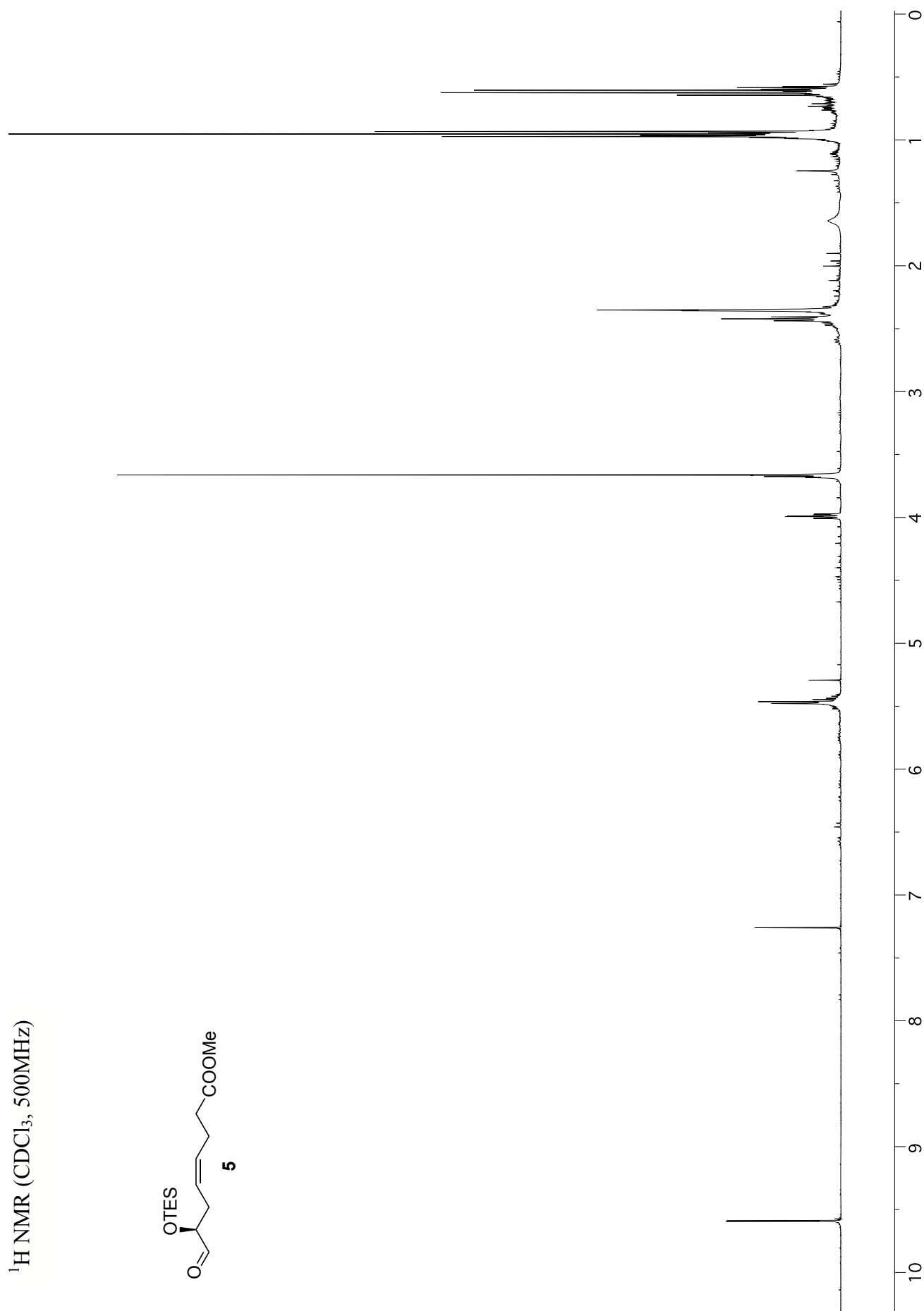
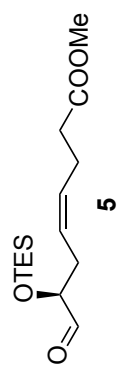
¹H NMR (CDCl₃, 600MHz)



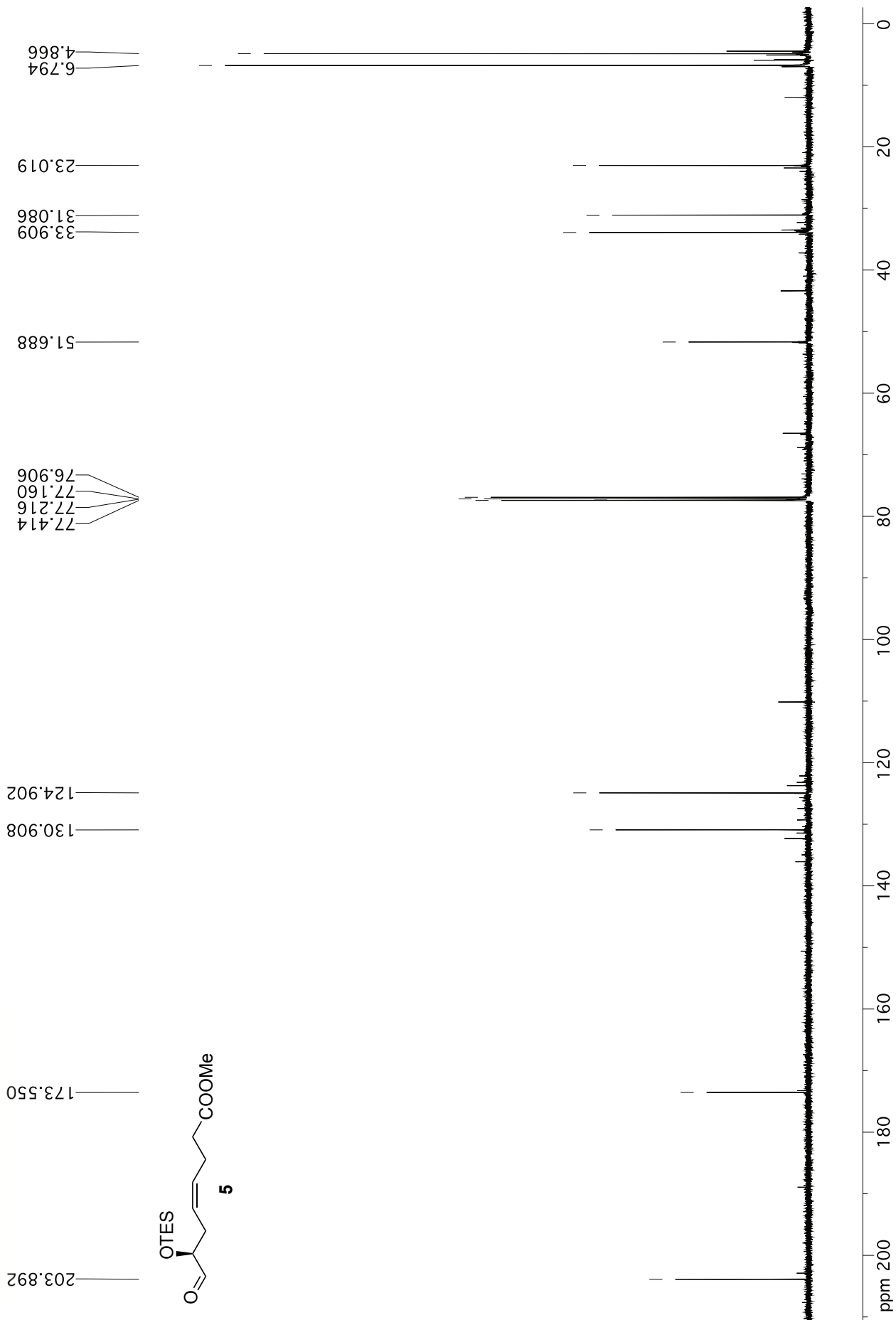
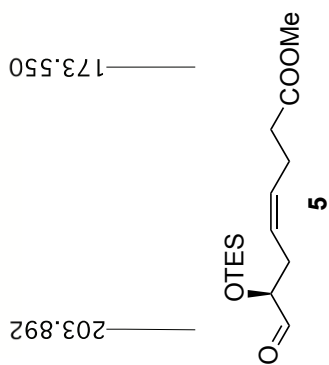
^{13}C NMR (CDCl_3 , 150MHz)



¹H NMR (CDCl₃, 500MHz)



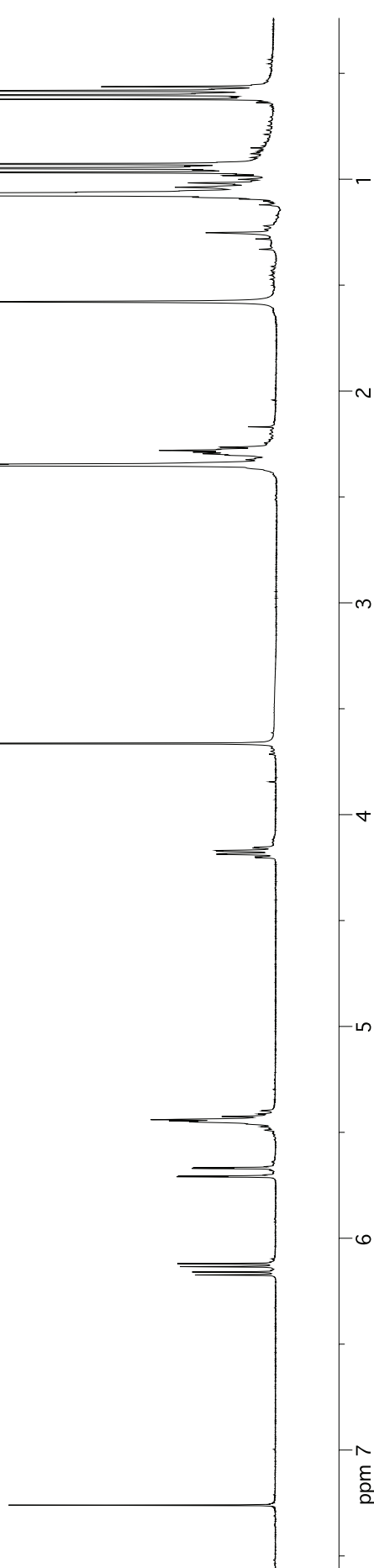
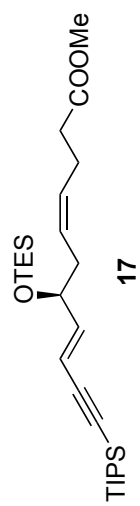
^{13}C NMR (CDCl₃, 125MHz)

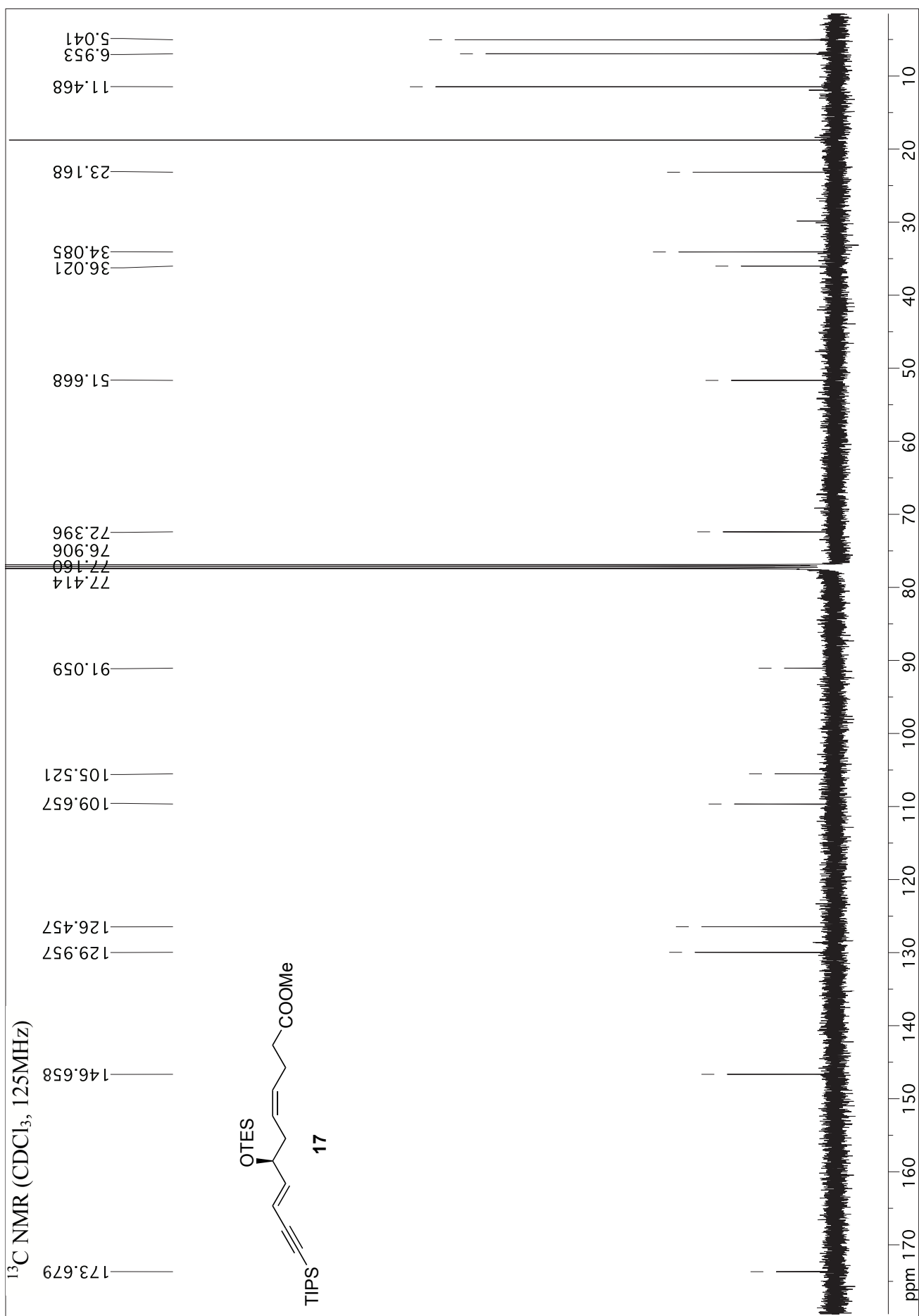


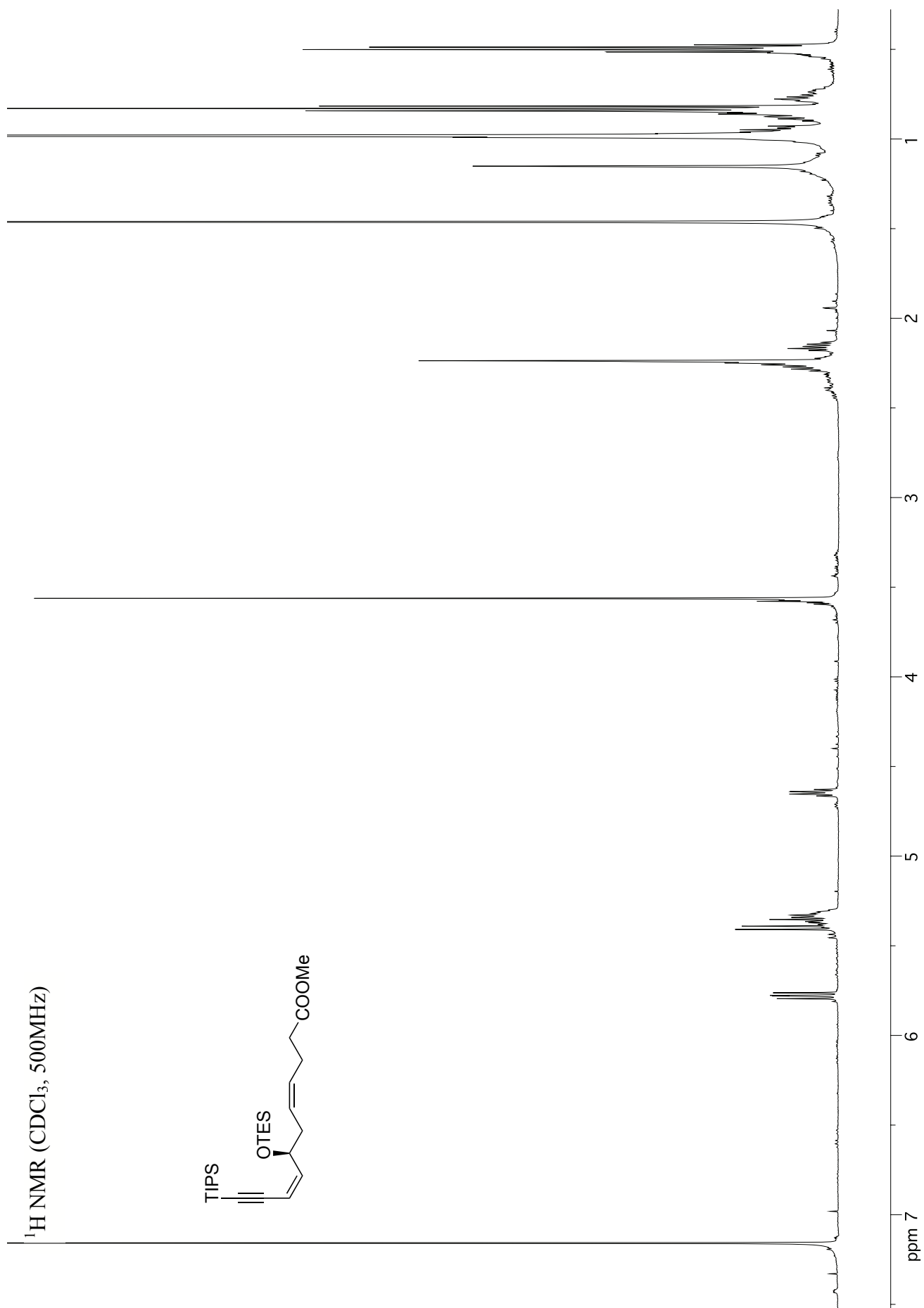
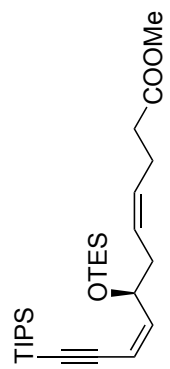
¹H NMR (CDCl₃, 500MHz)

CCOC(=O)C/C=C/[C@H](C#CC)C(=O)O[Si](C)(C)C **17**

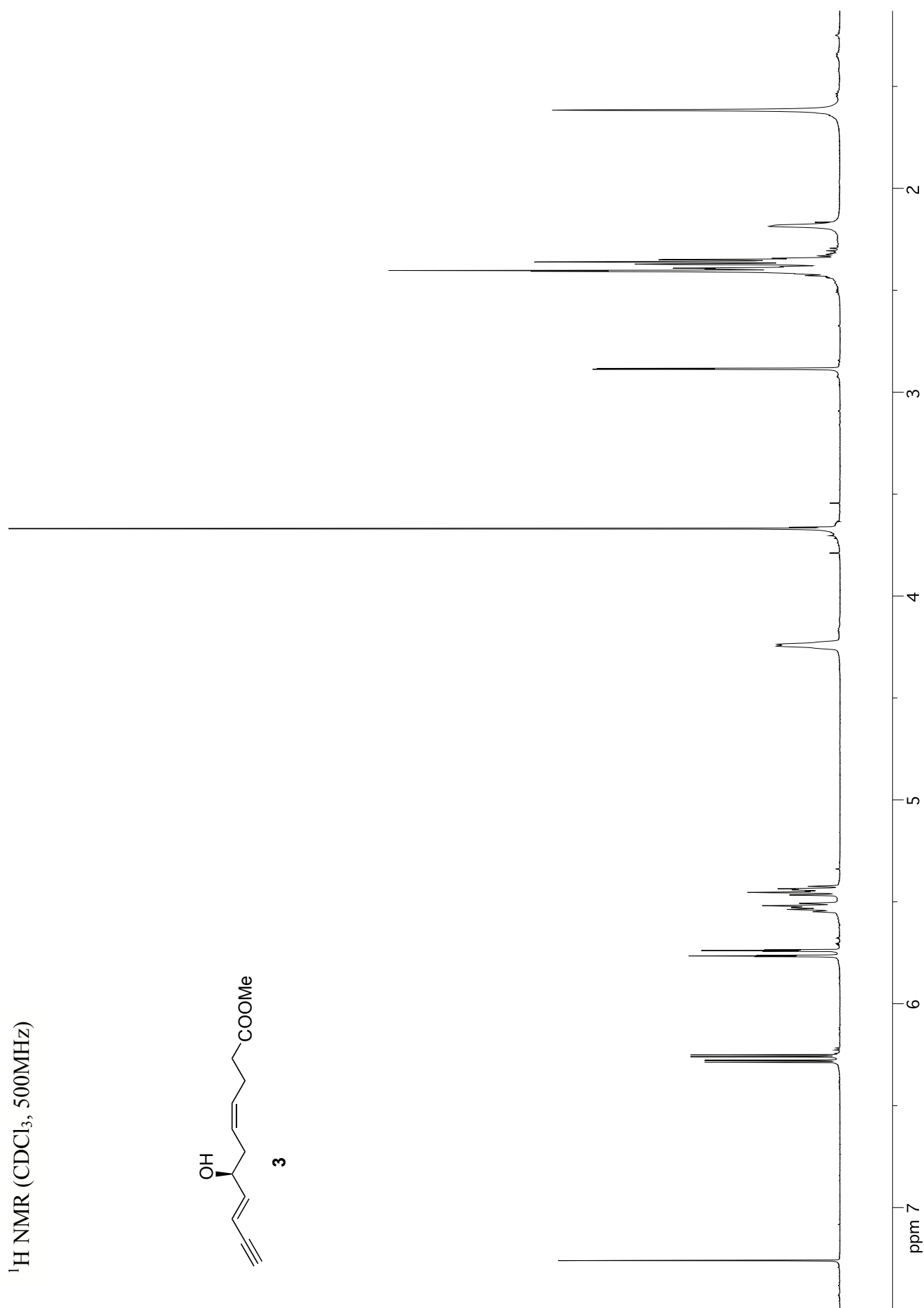
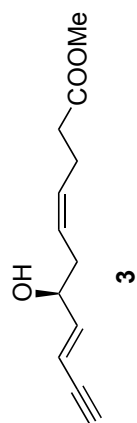
ppm

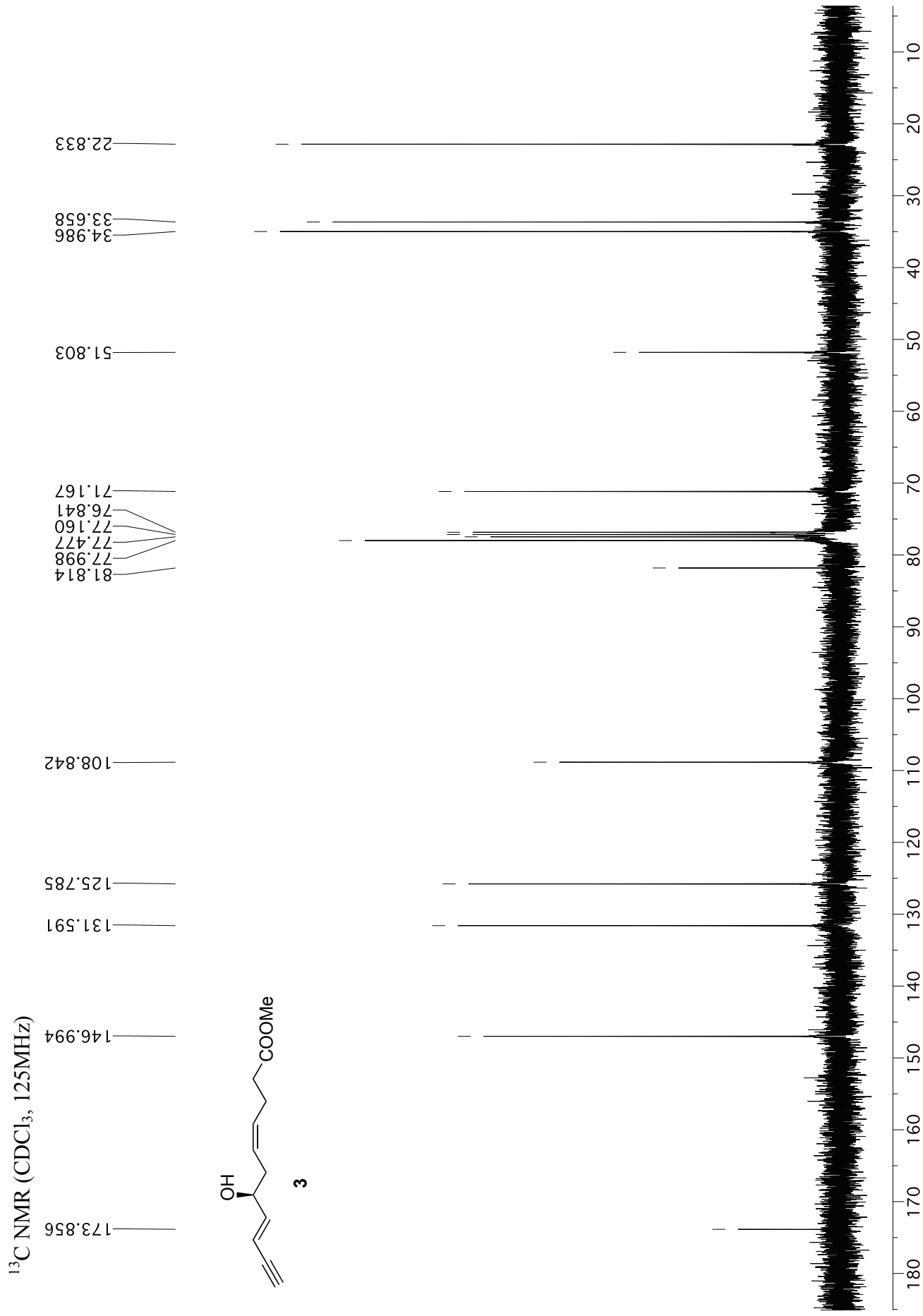




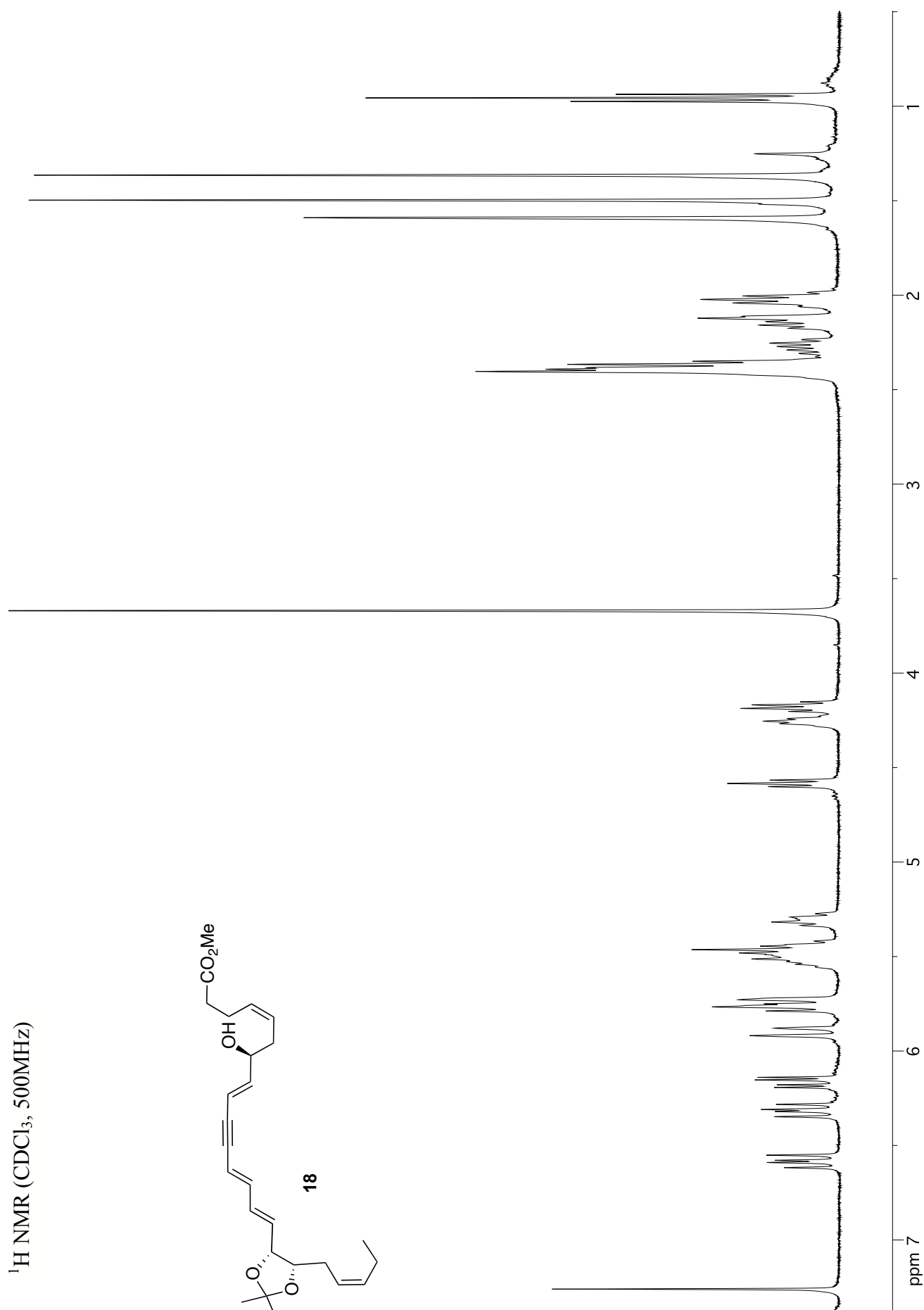
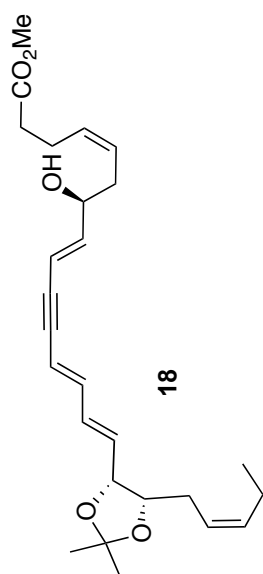
¹H NMR (CDCl₃, 500MHz)

¹H NMR (CDCl₃, 500MHz)

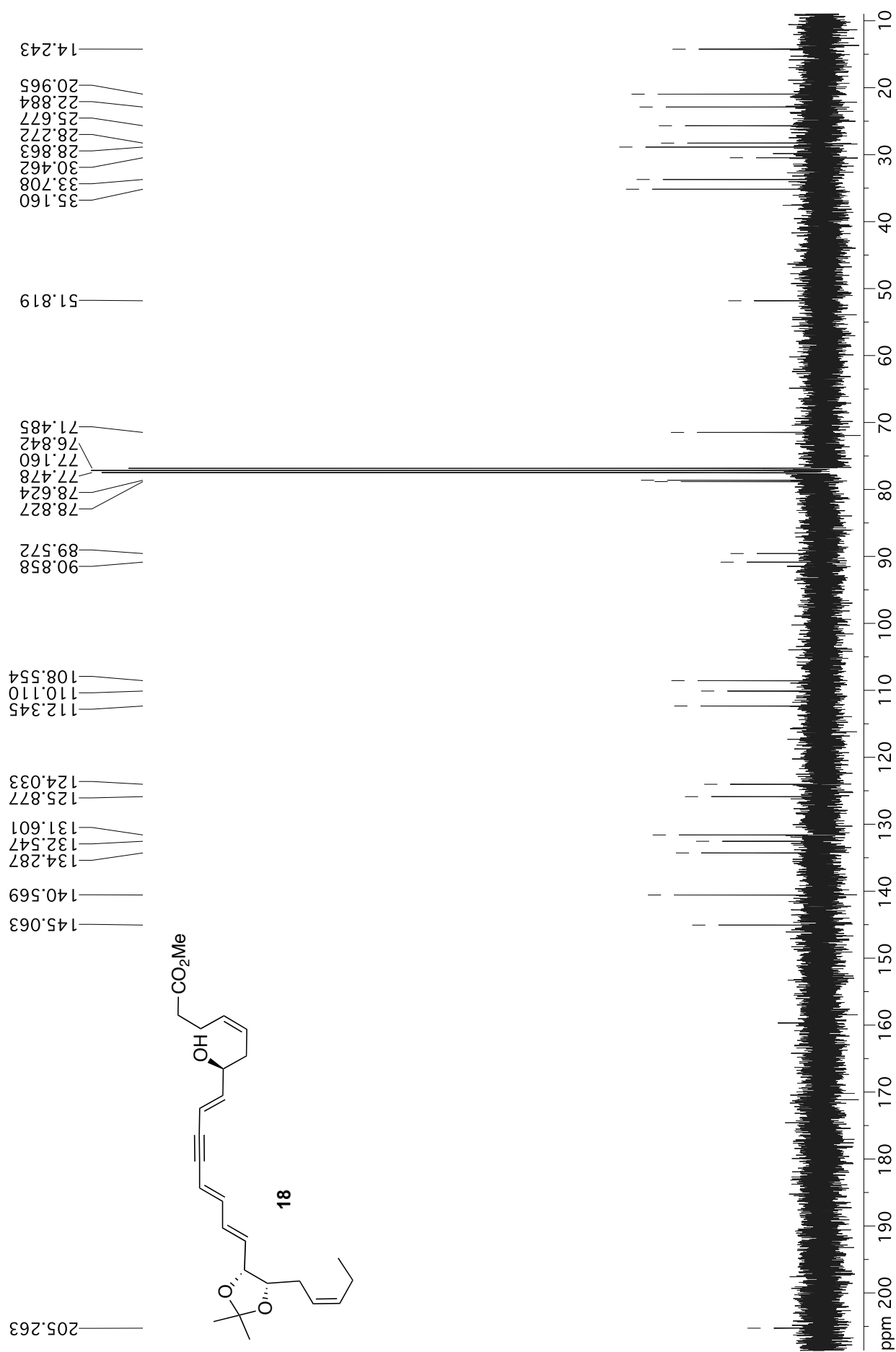




^1H NMR (CDCl_3 , 500MHz)



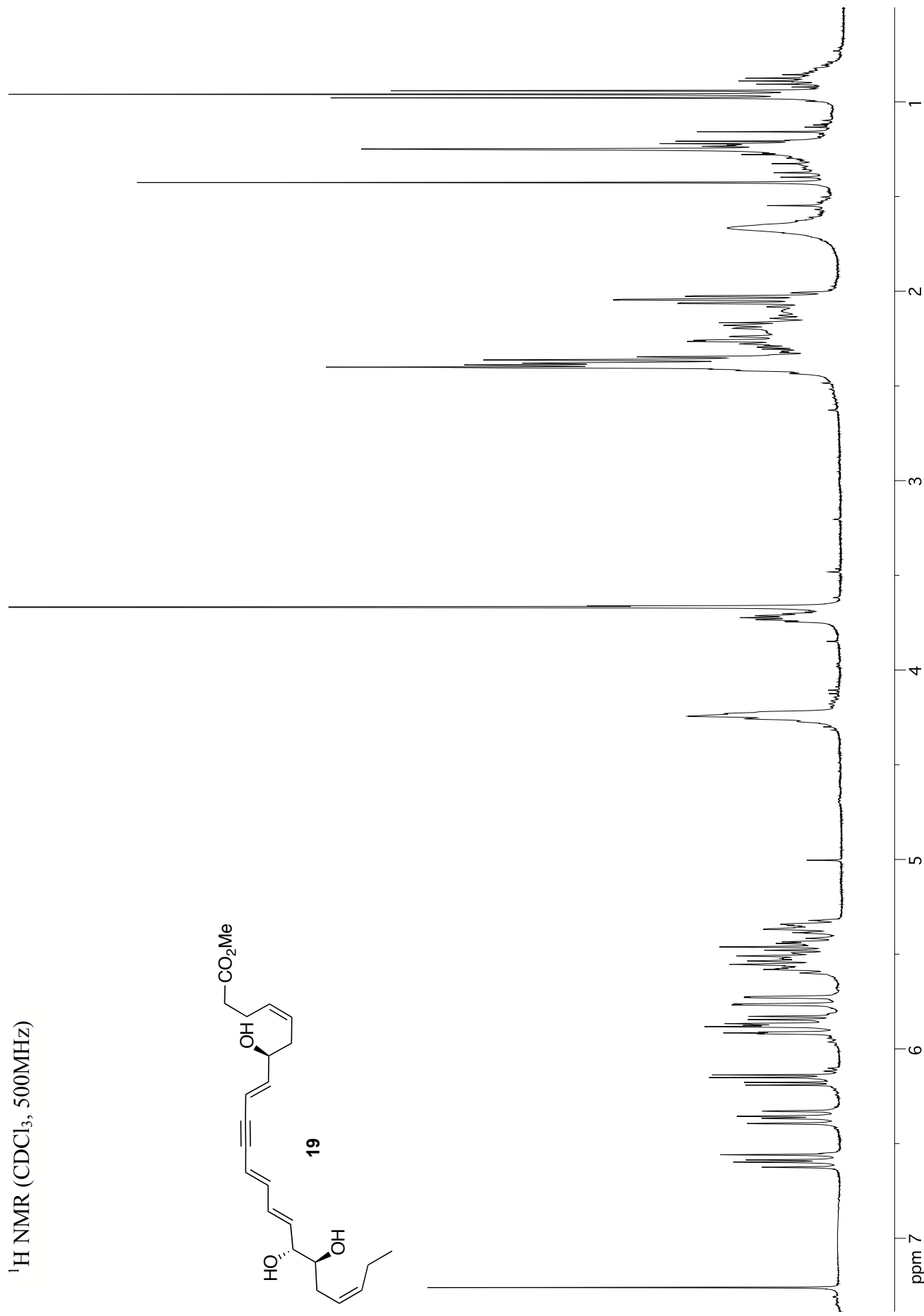
¹³C NMR (CDCl₃, 125MHz)



¹H NMR (CDCl₃, 500MHz)

19

ppm 7 6 5 4 3 2 1

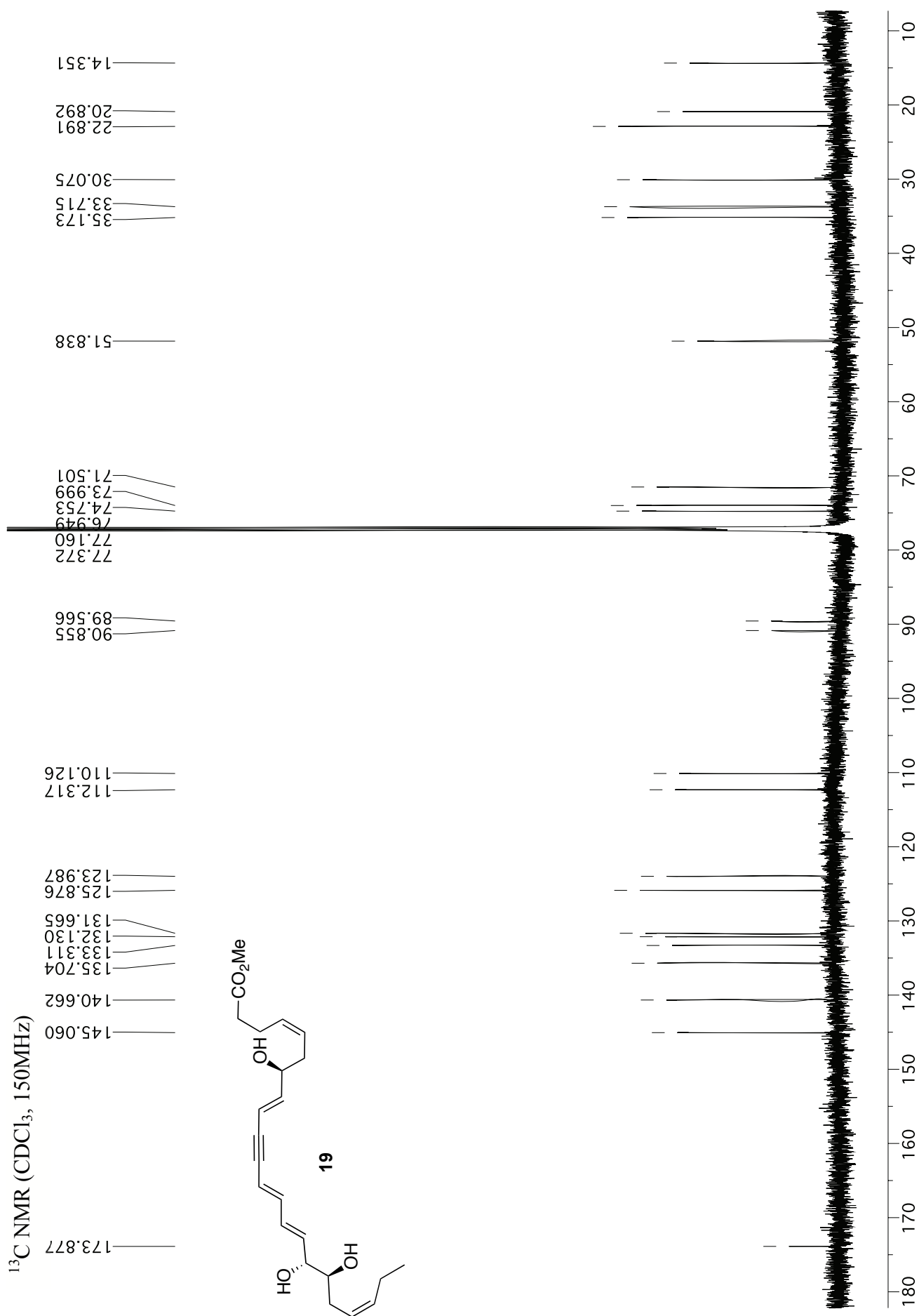


¹H NMR (CDCl₃, 500MHz)

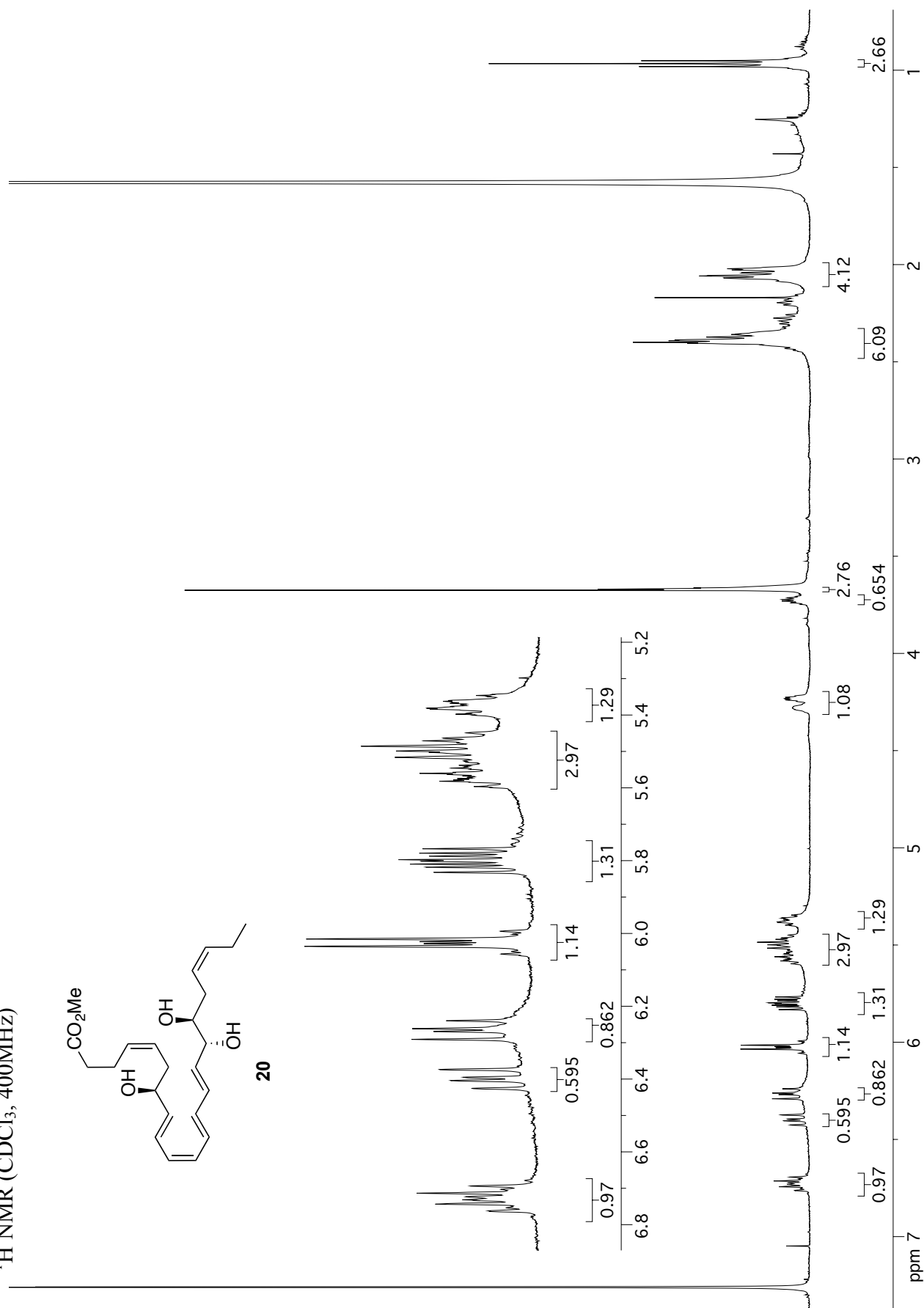
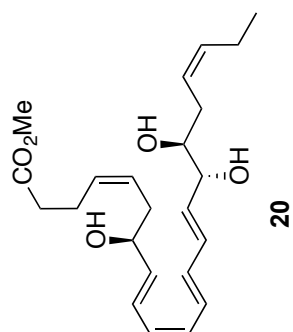
19

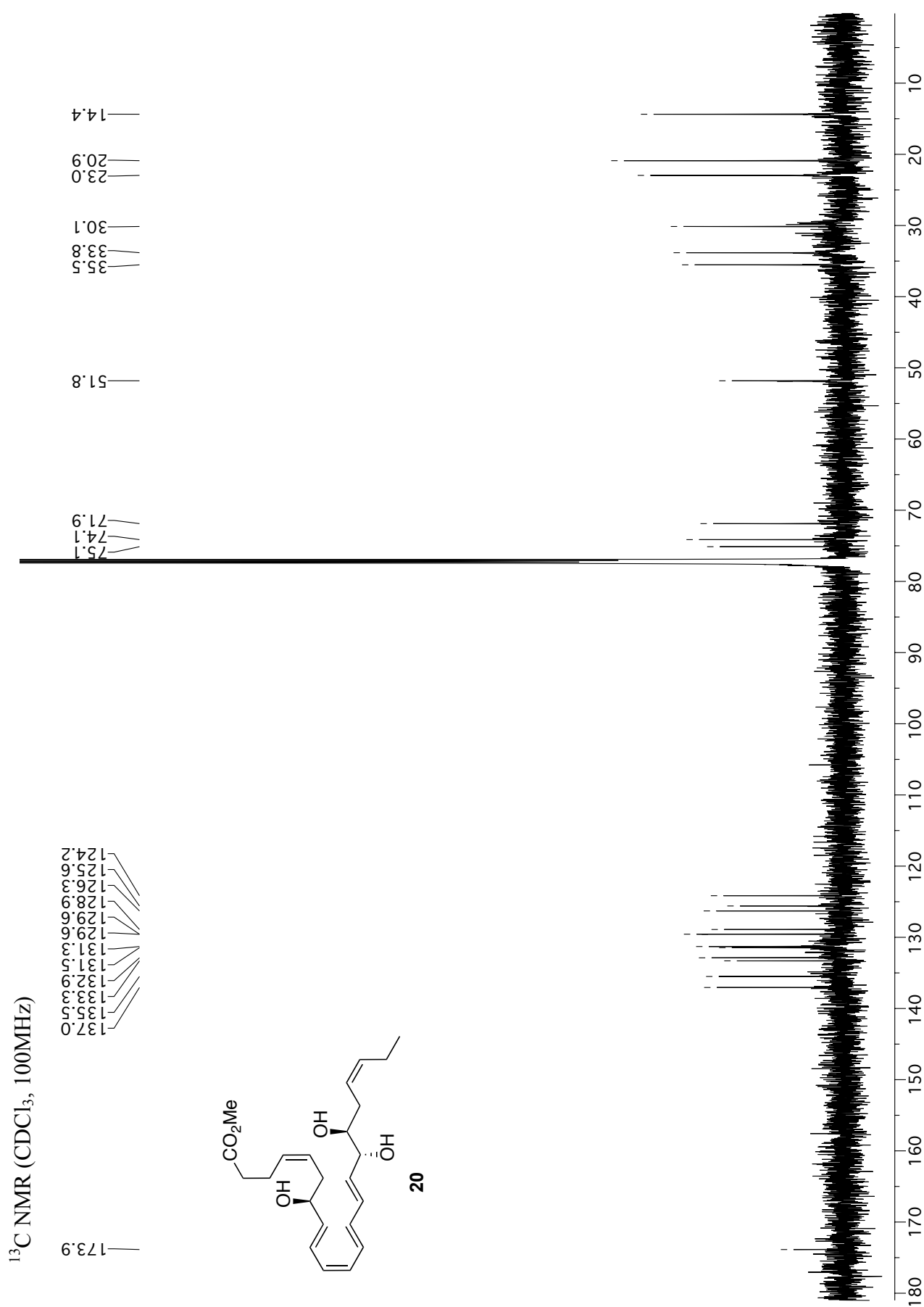
Chemical structure of compound **19** is shown above the spectrum. It is a complex molecule featuring a long chain with multiple functional groups, including a terminal hydroxyl group, a terminal ester group, and several internal hydroxyl groups. The structure is labeled **19**.

¹³C NMR (CDCl₃, 150MHz)

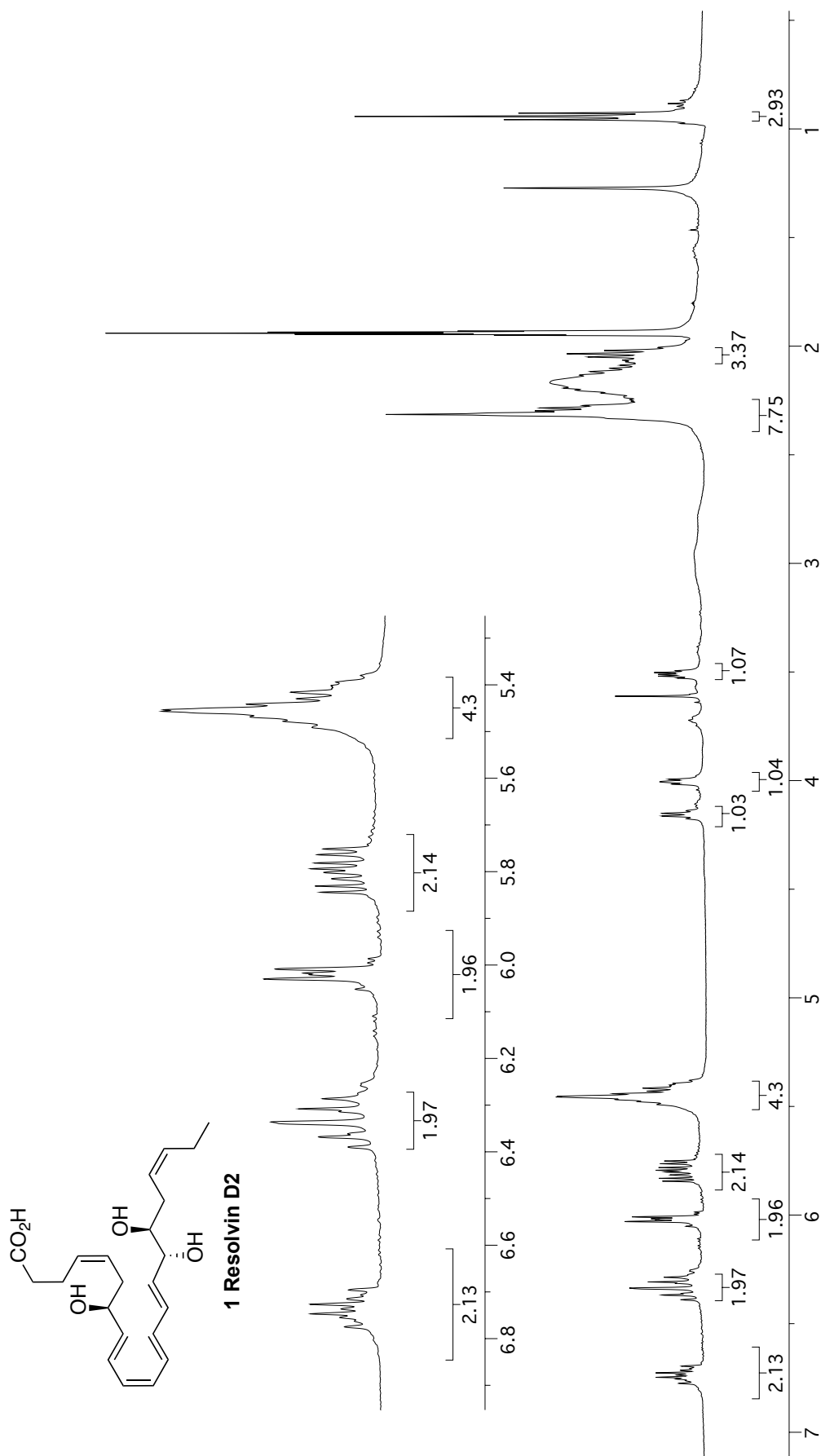


^1H NMR (CDCl_3 , 400MHz)





¹H NMR (CD₃CN, 500MHz)



^{13}C NMR (CD_3CN , 125MHz)

