

Compound NMR Spectra

A Catch and Anchor Approach to Combat both Toxicity and Longevity of Botulinum Toxin A

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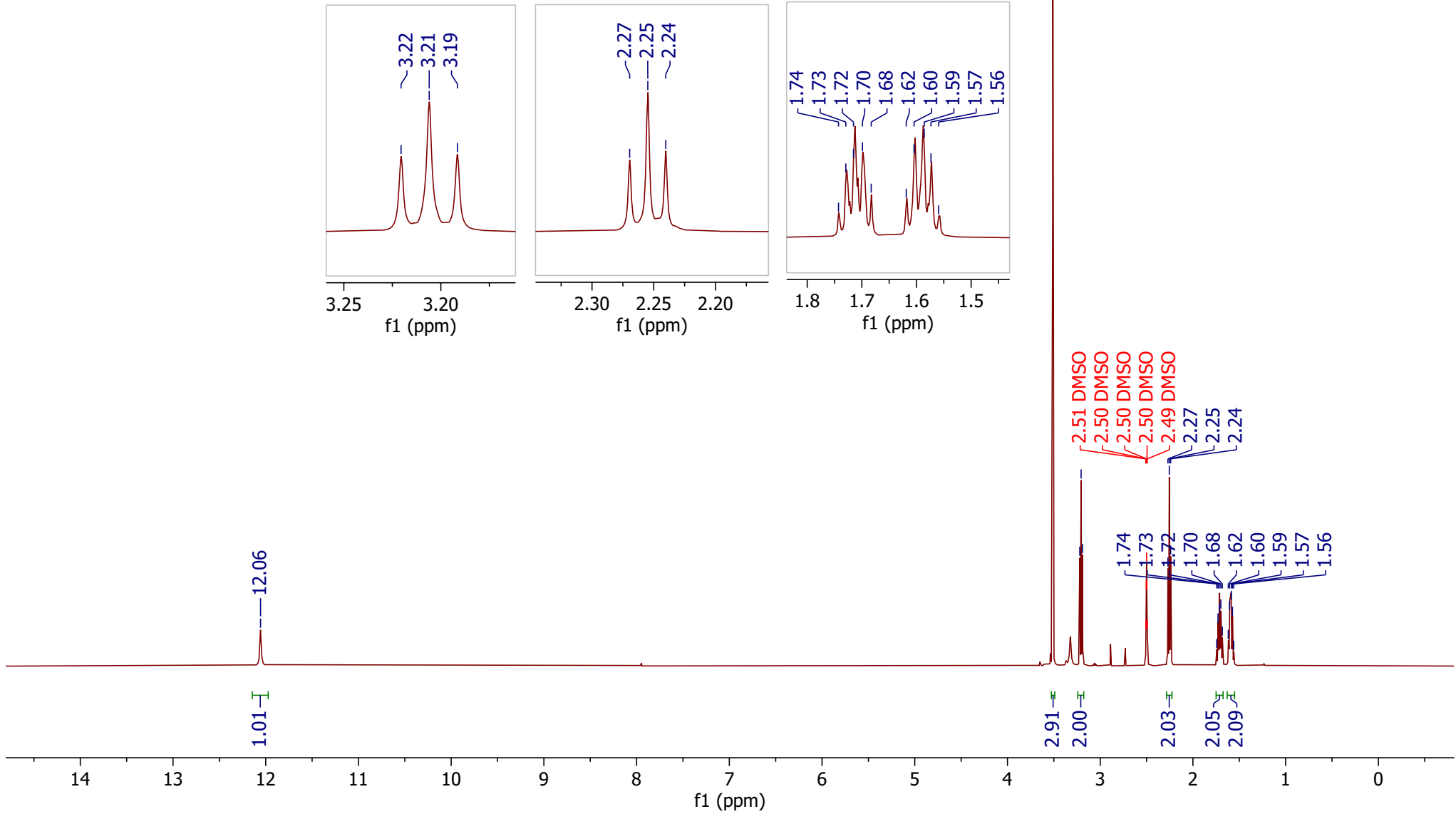
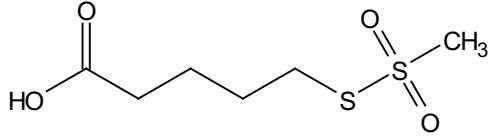
[¶] Department of Chemistry and Biochemistry, University of California San Diego, 9500 Gilman Drive, La Jolla, California 92093, United States.

[⊥]Department of Bacteriology, University of Wisconsin, 1550 Linden Drive, Madison, Wisconsin 53706, United States

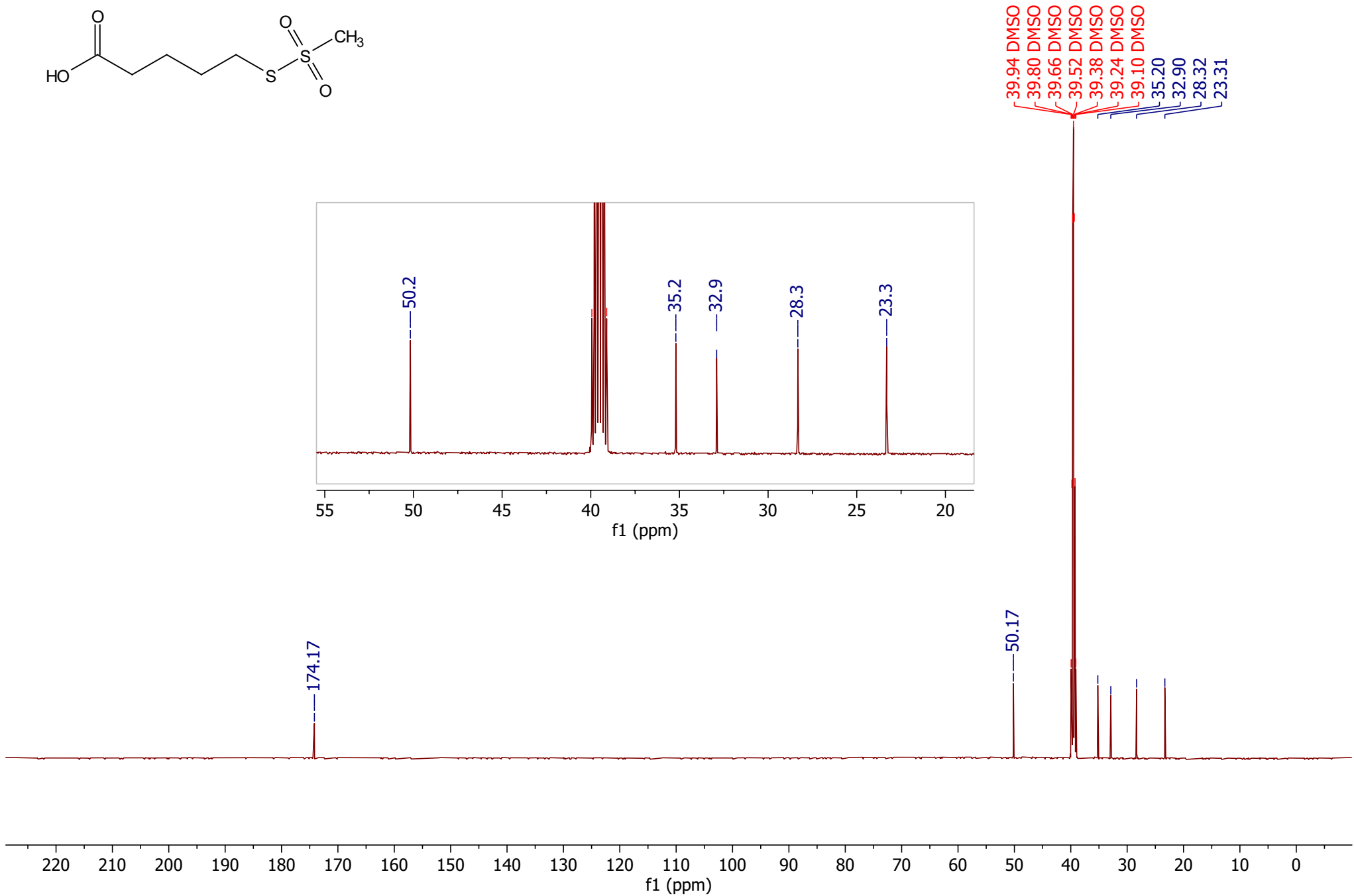
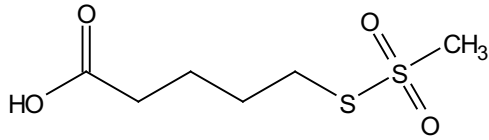
[‡]These authors contributed equally

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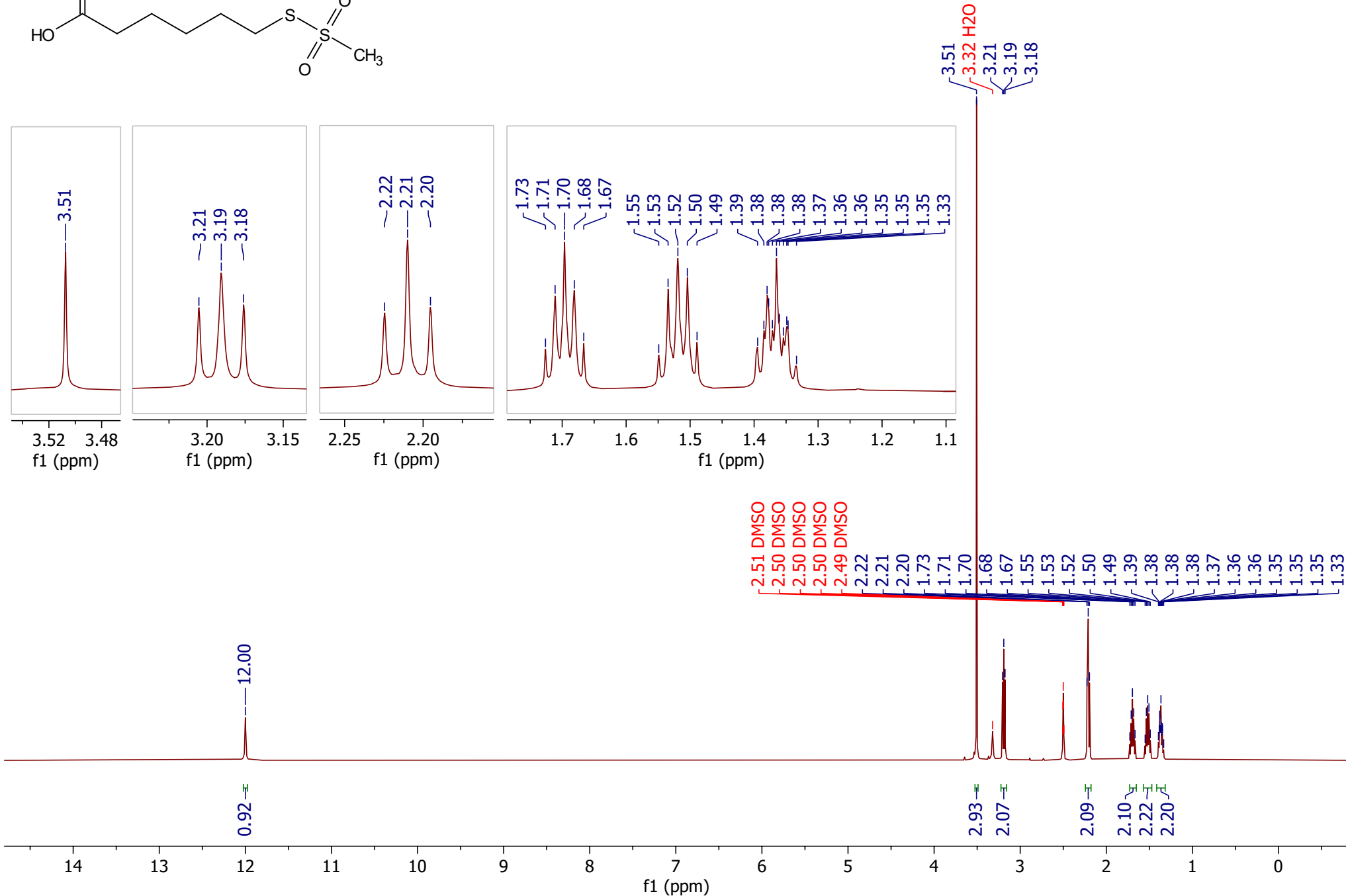
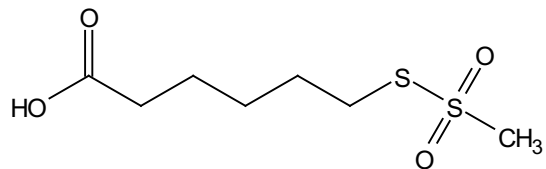
Compound 12
1H NMR (500 MHz, DMSO-d6)



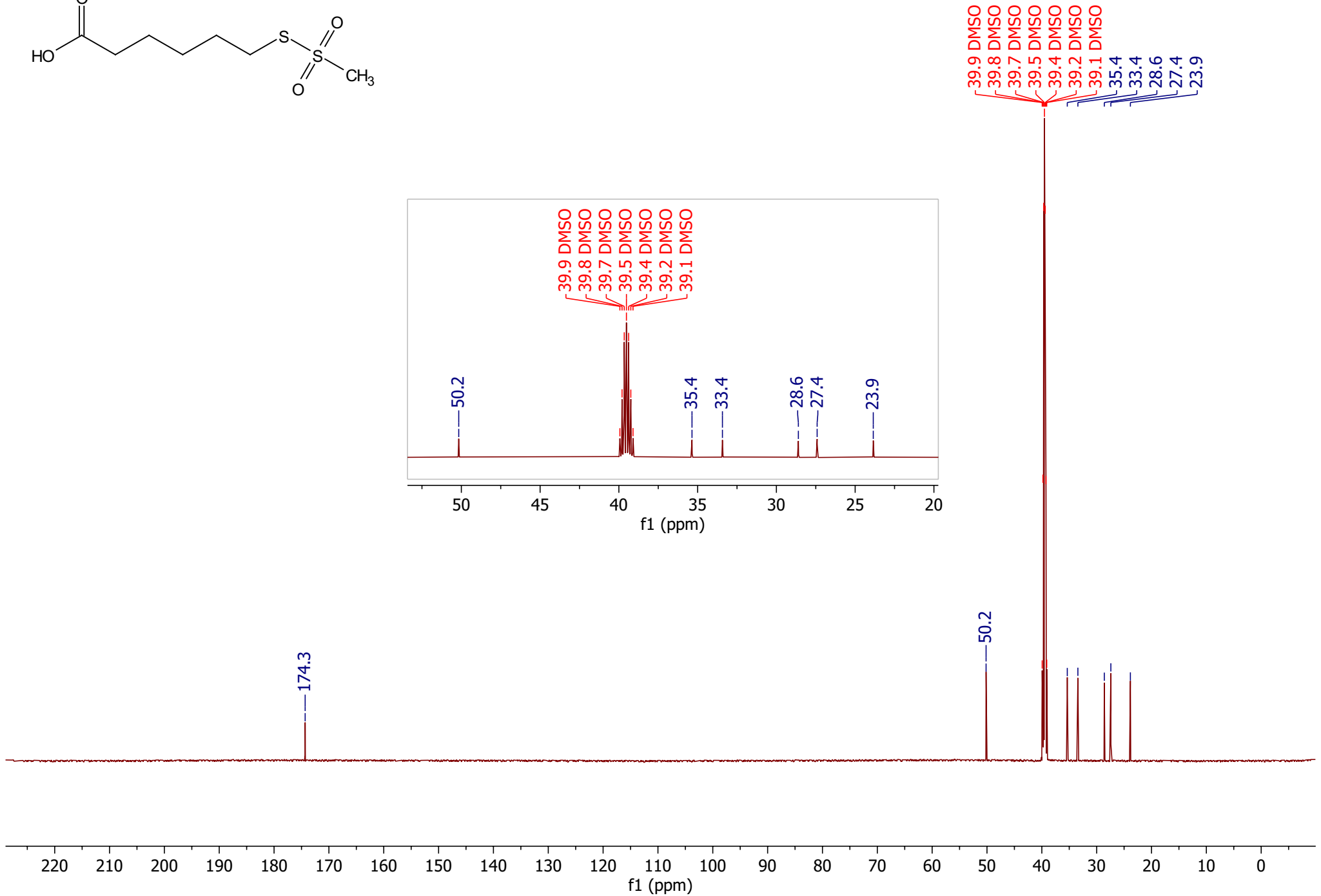
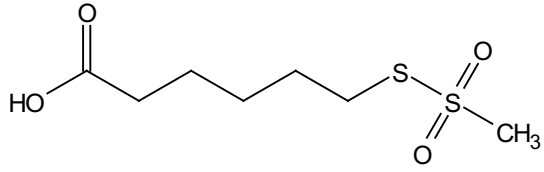
Compound 12
¹H NMR (151 MHz, DMSO-d6)



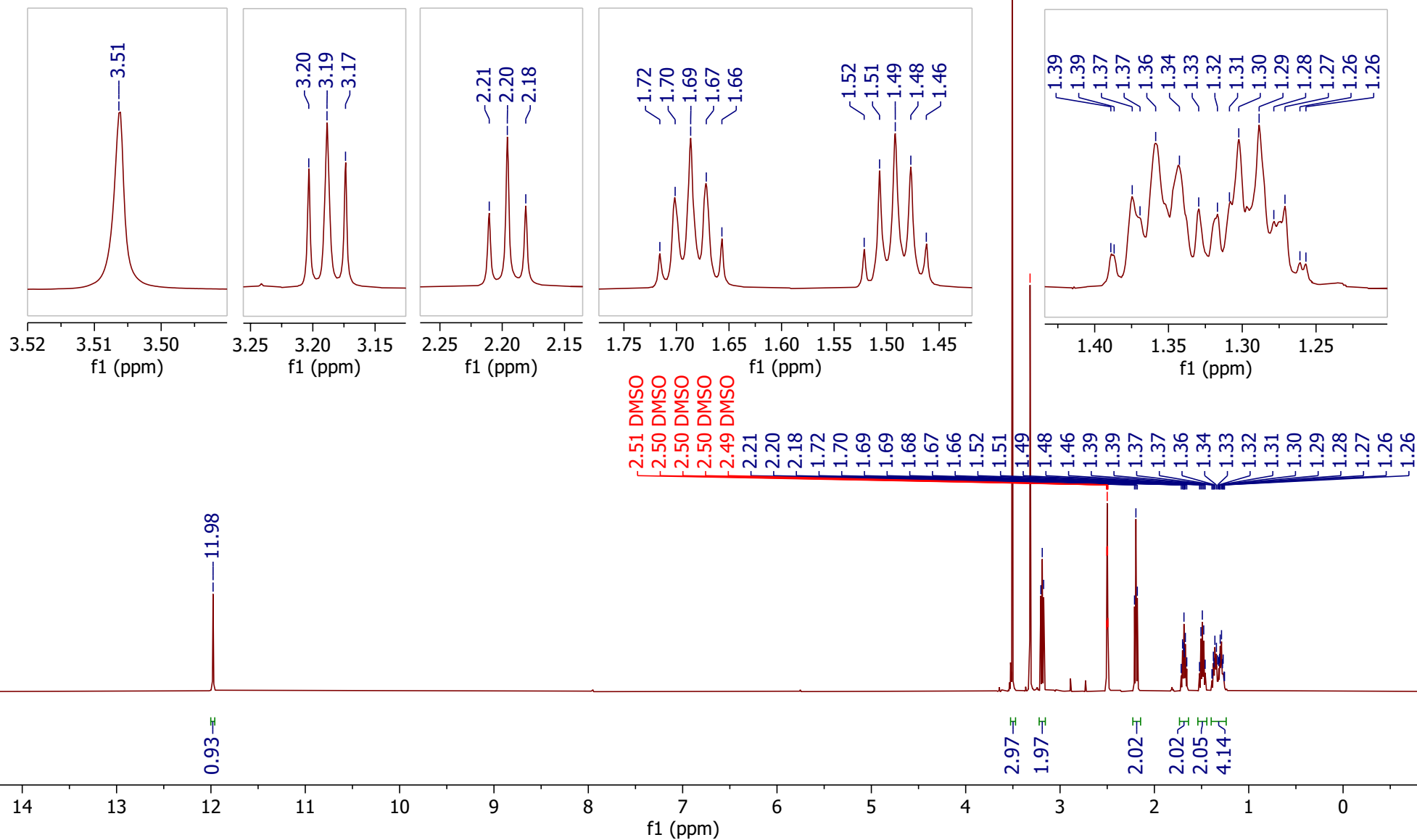
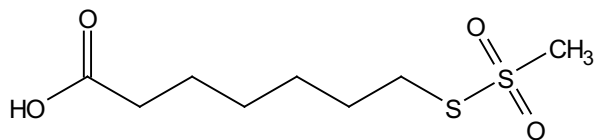
Compound 13
¹H NMR (500 MHz, DMSO-d6)



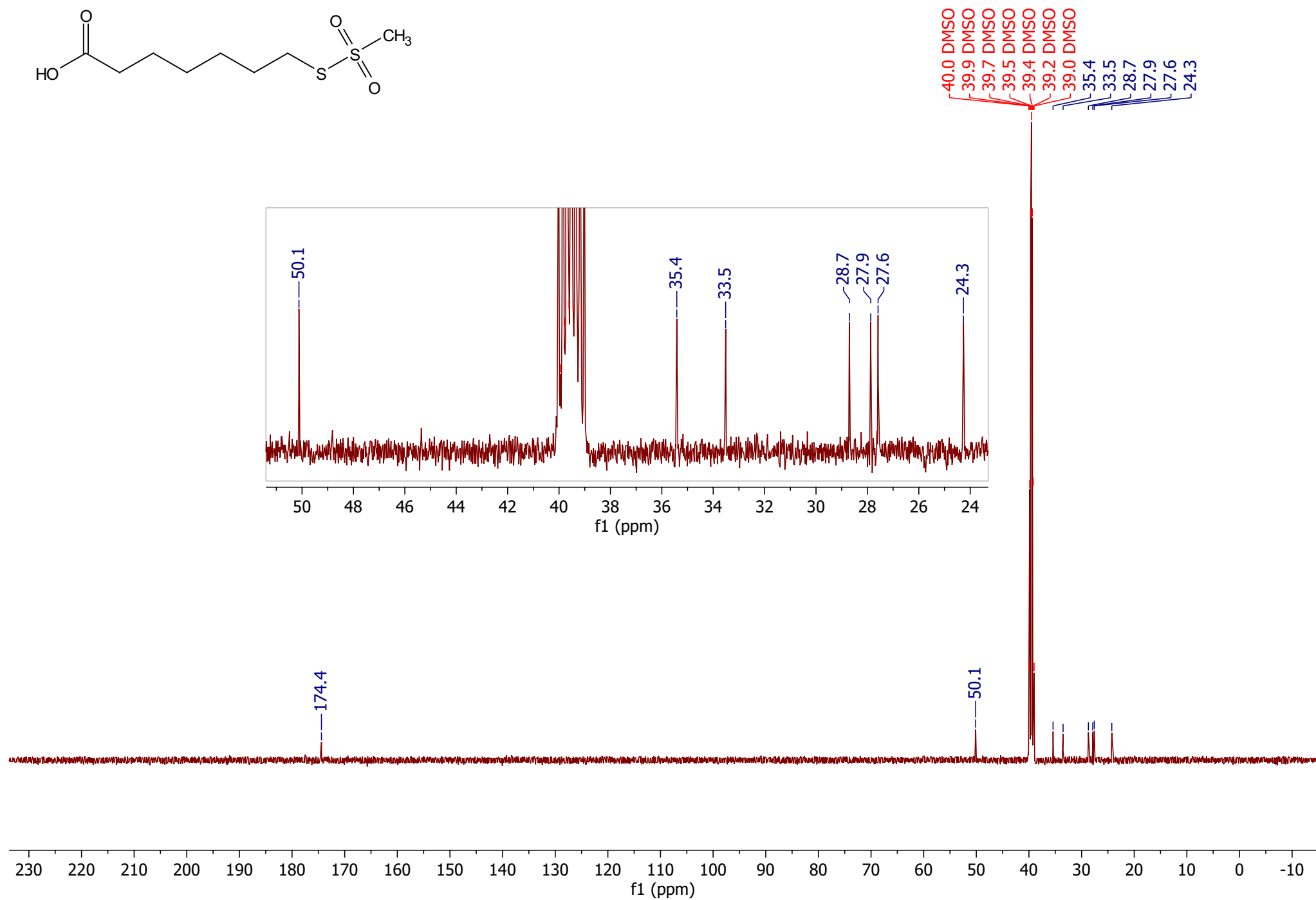
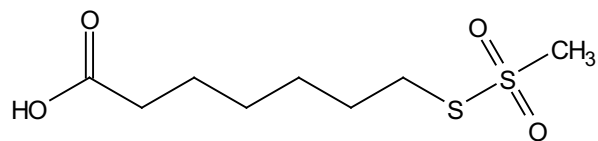
Compound 13
¹H NMR (151 MHz, DMSO-d6)



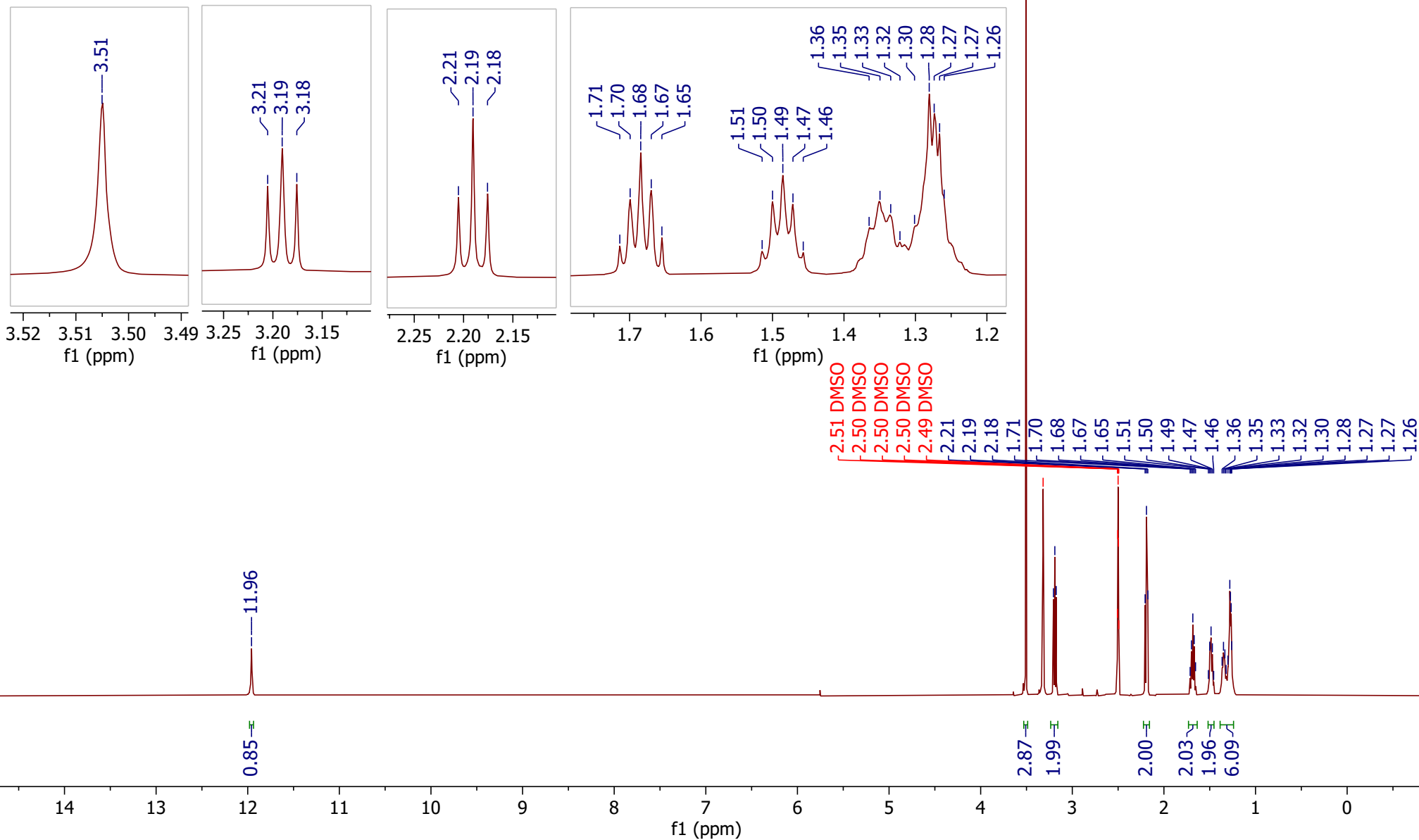
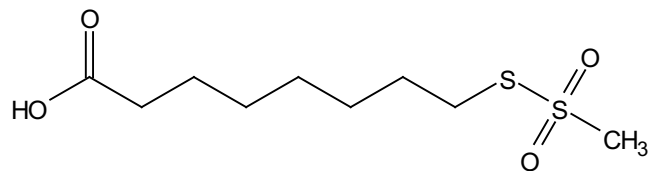
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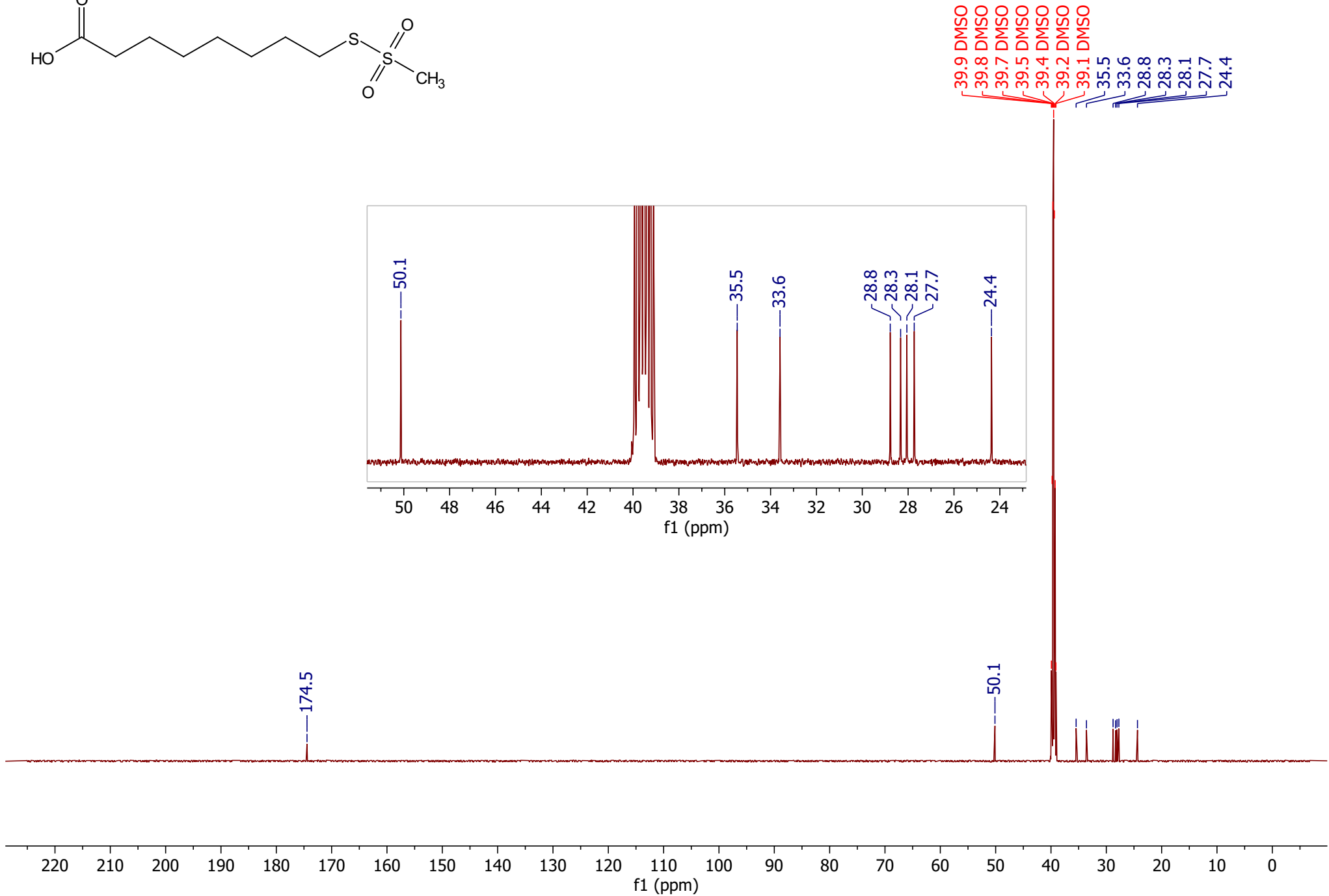
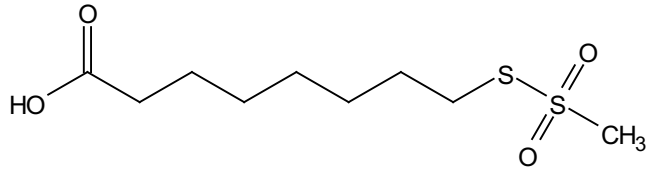
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¹H NMR (126 MHz, DMSO-d6)



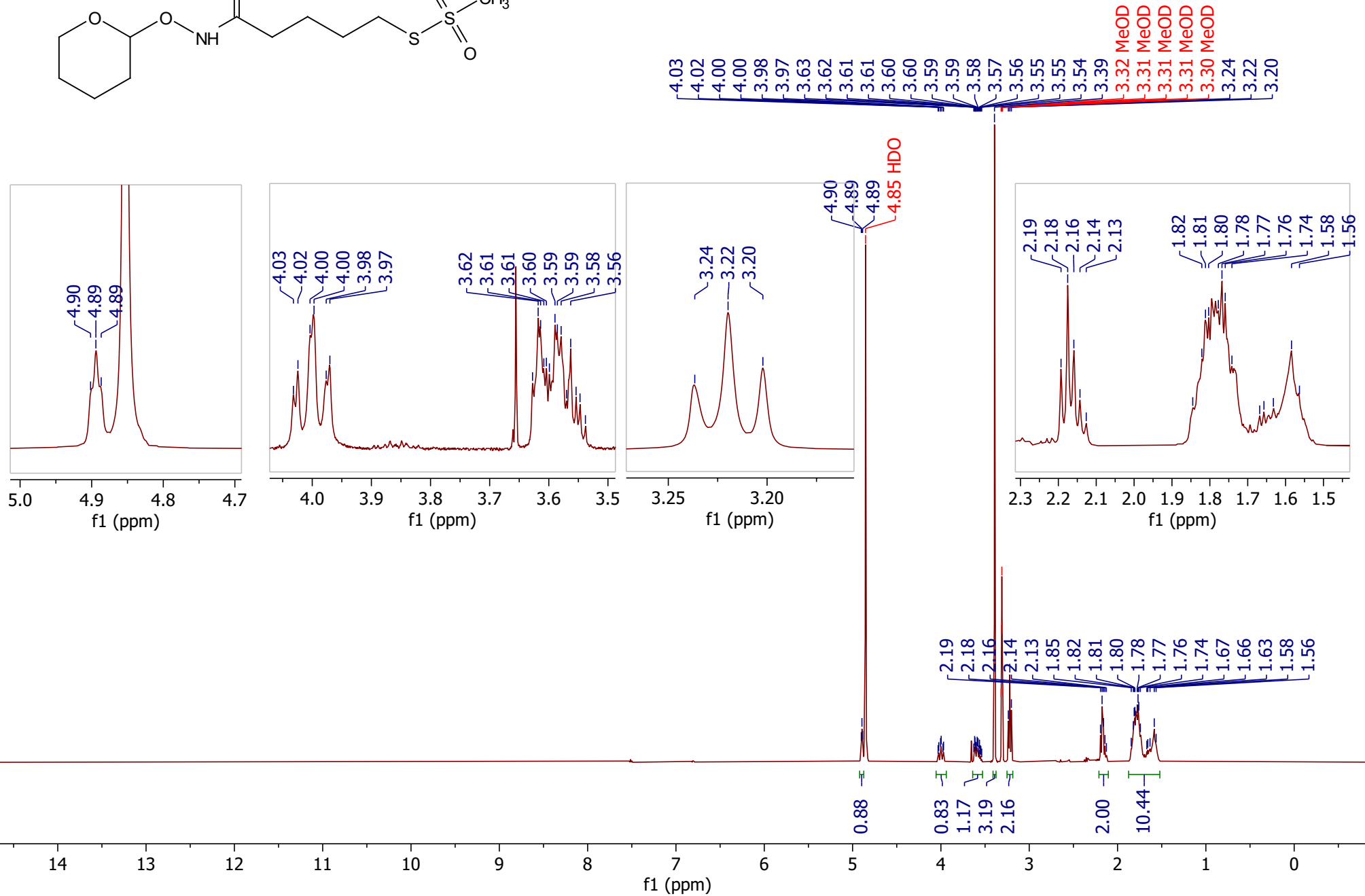
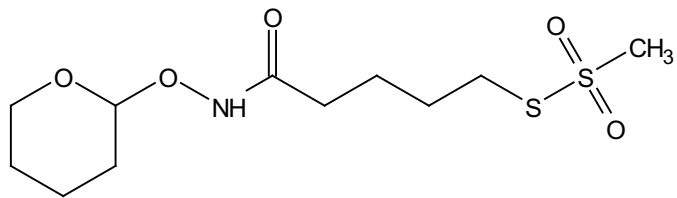
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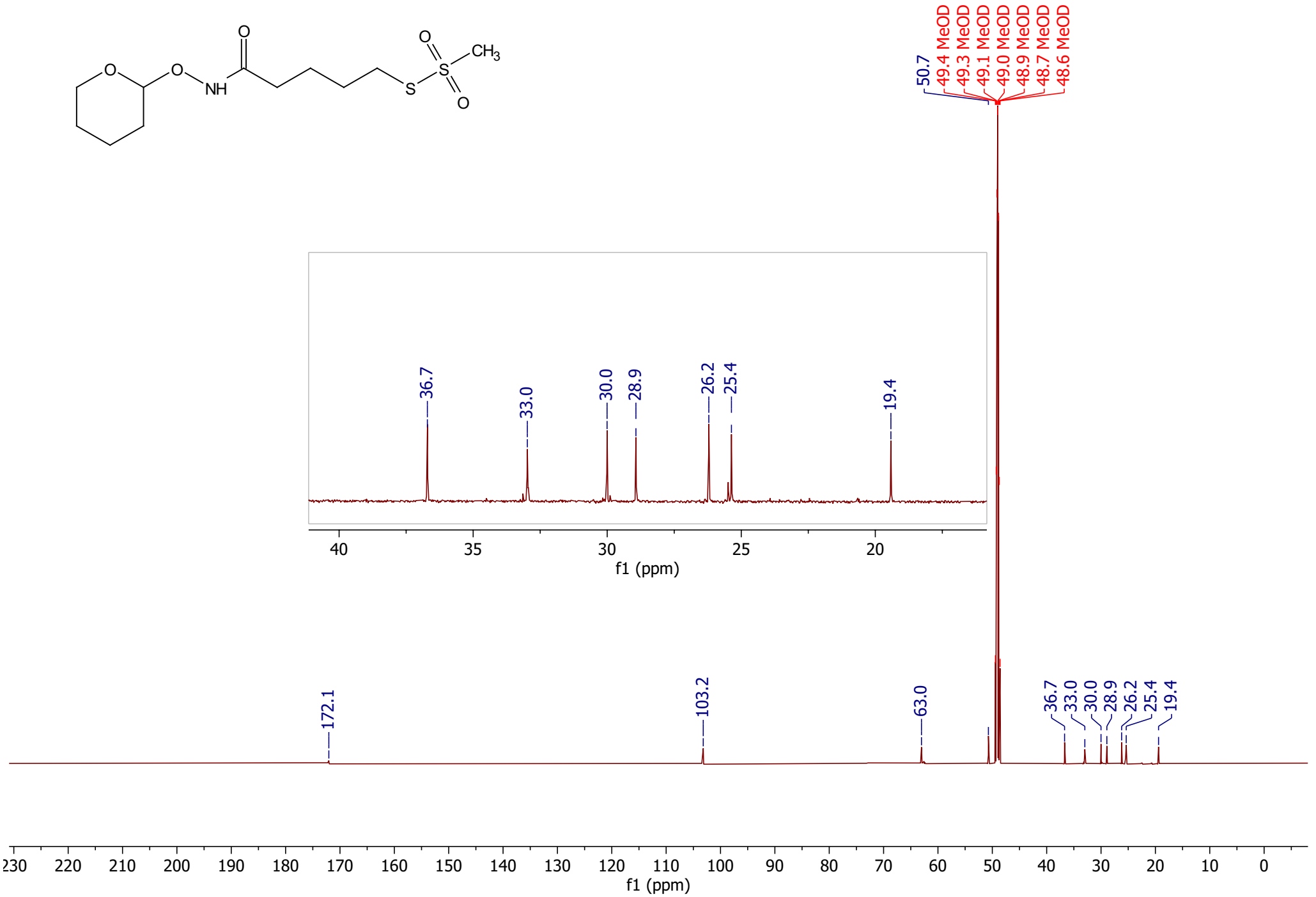
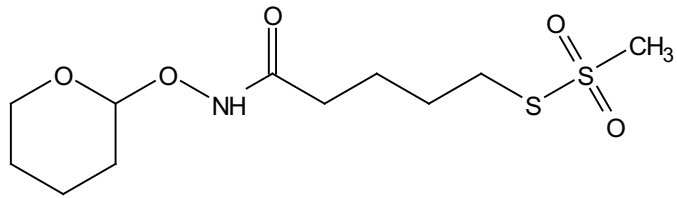
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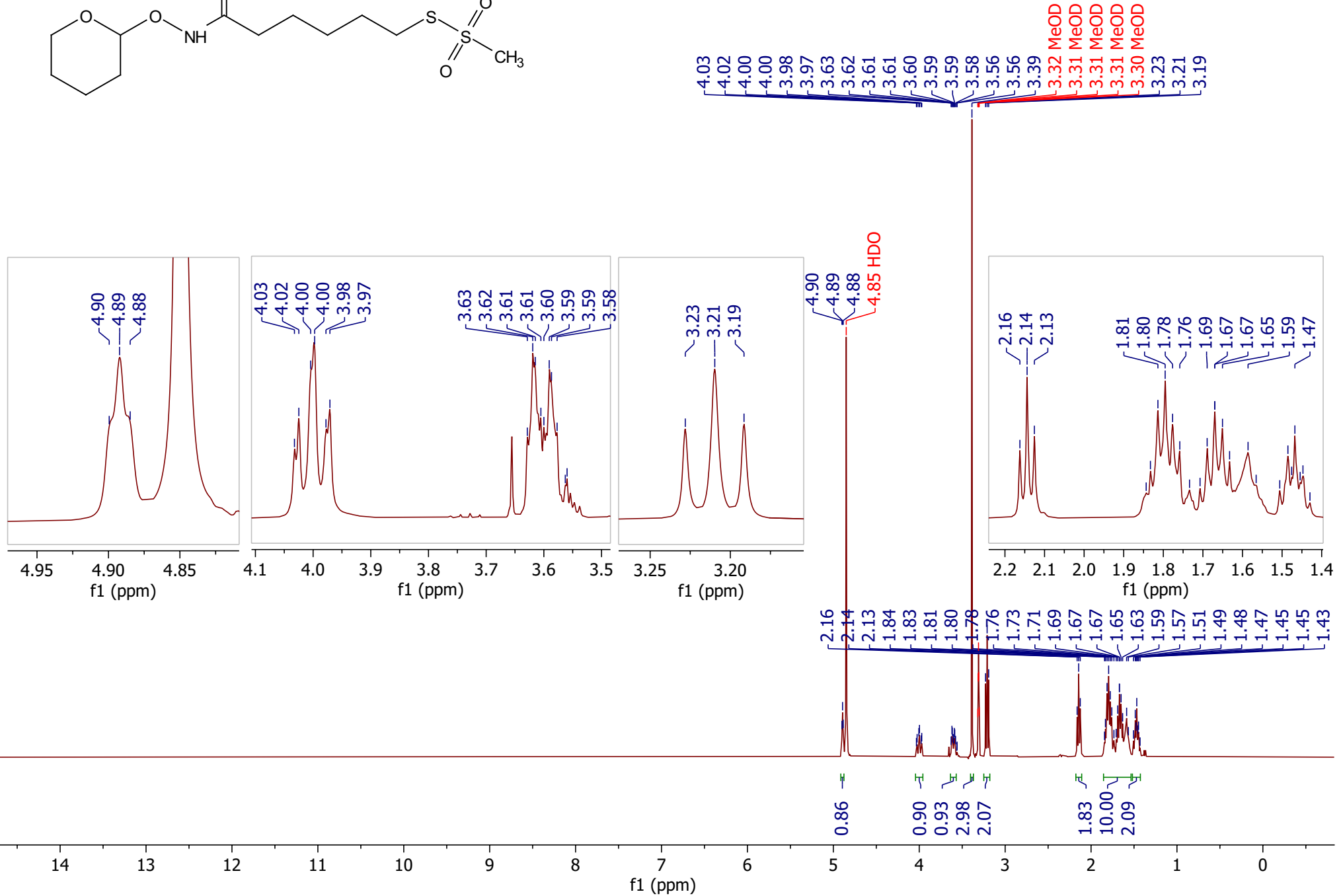
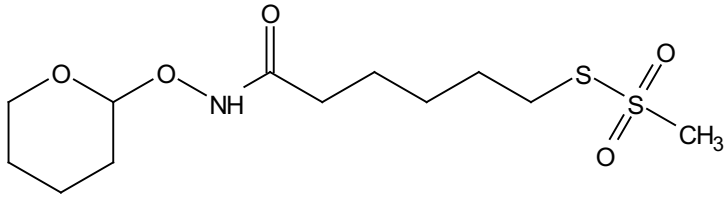
Compound 16
¹H NMR (400 MHz, MeOD-d4)



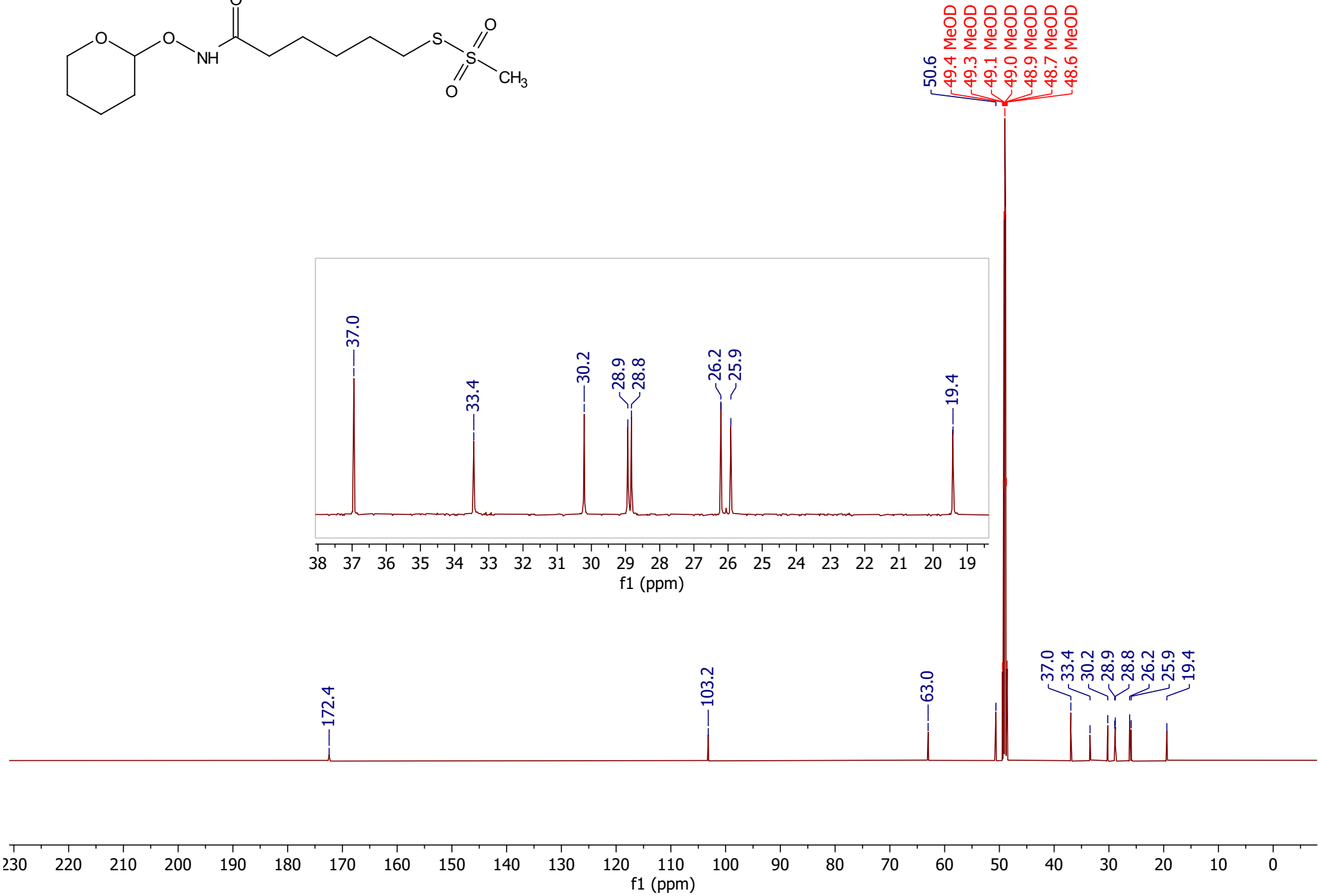
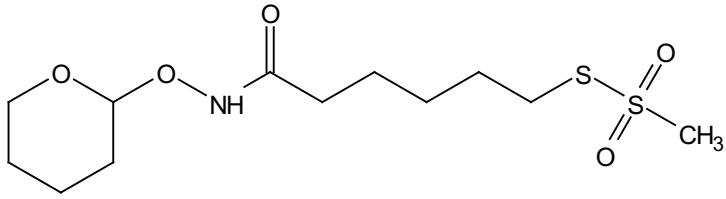
Compound 16
¹H NMR (151 MHz, MeOD-d4)



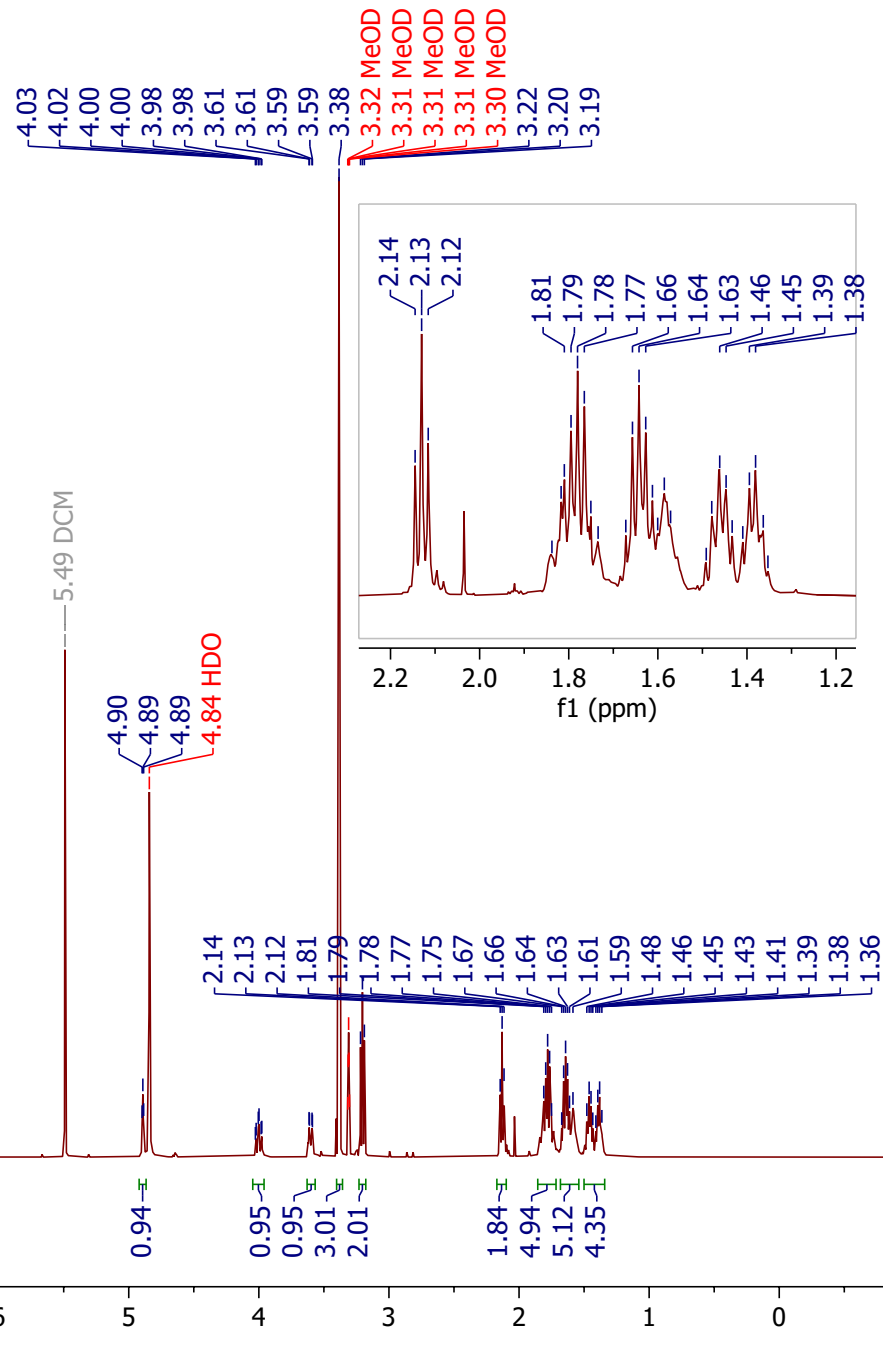
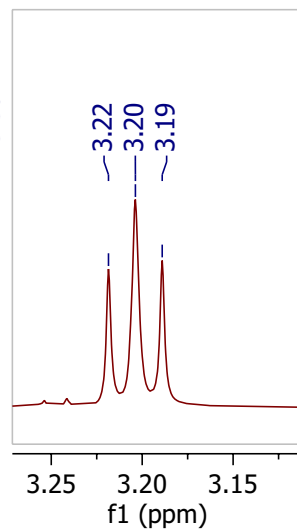
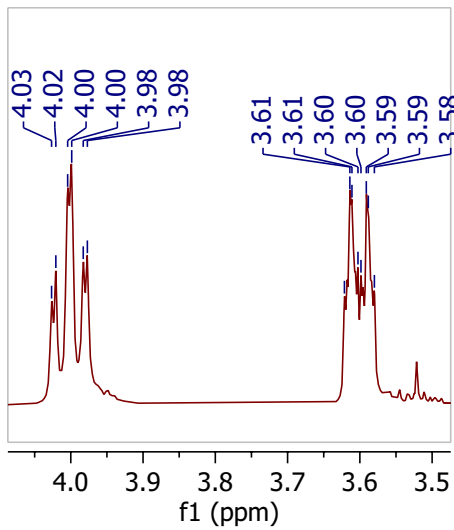
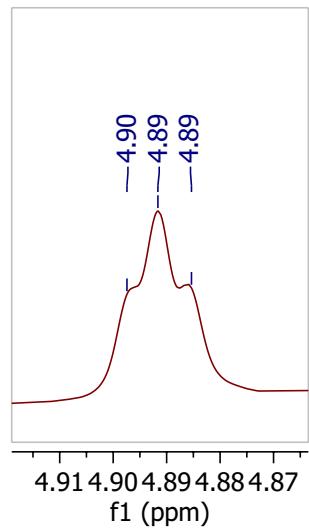
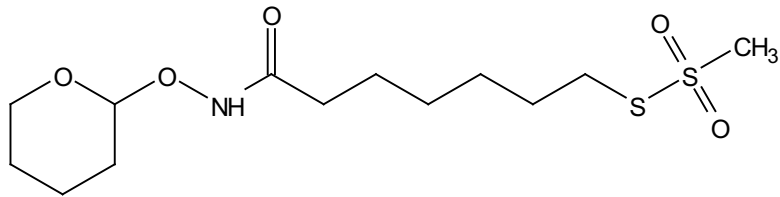
Compound 17
¹H NMR (400 MHz, MeOD-d4)



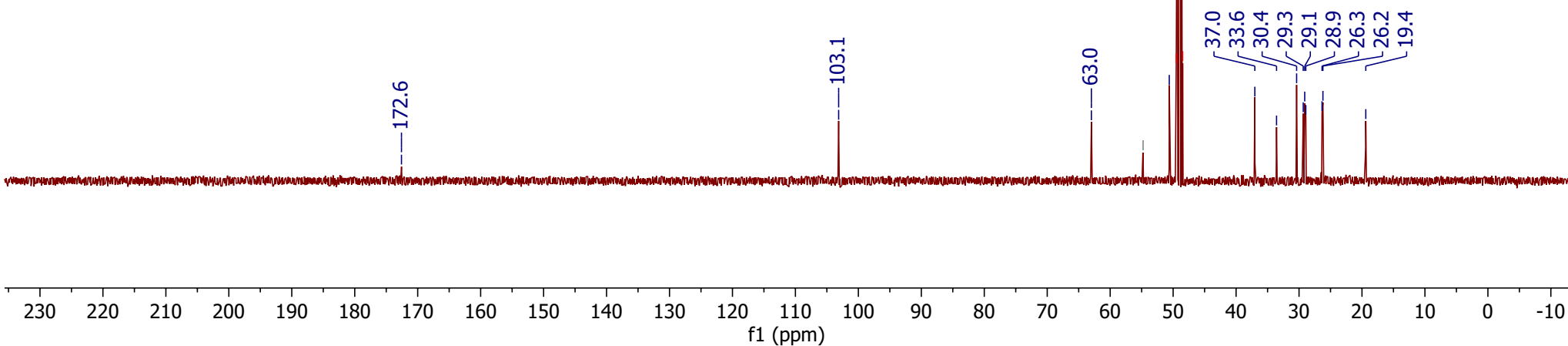
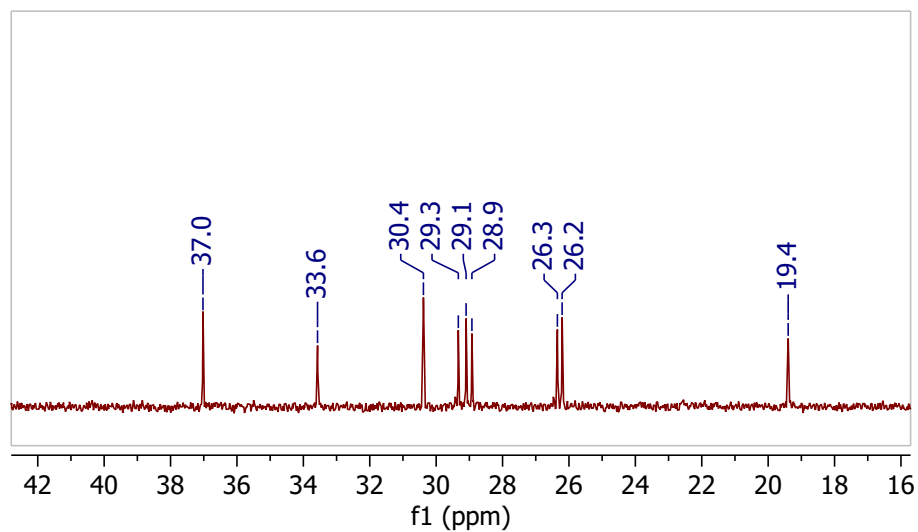
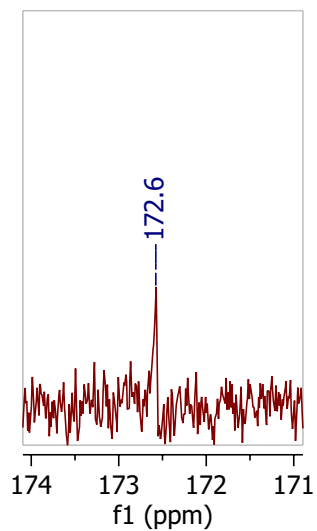
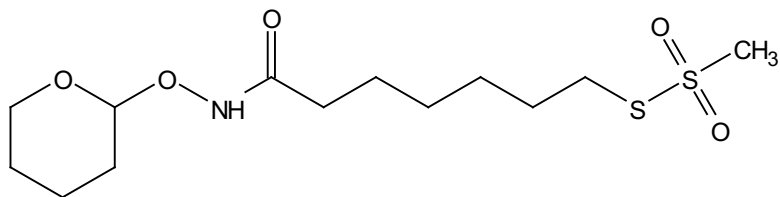
Compound 17
¹H NMR (151 MHz, MeOD-d4)



Compound 18
¹H NMR (500 MHz, MeOD-d4)

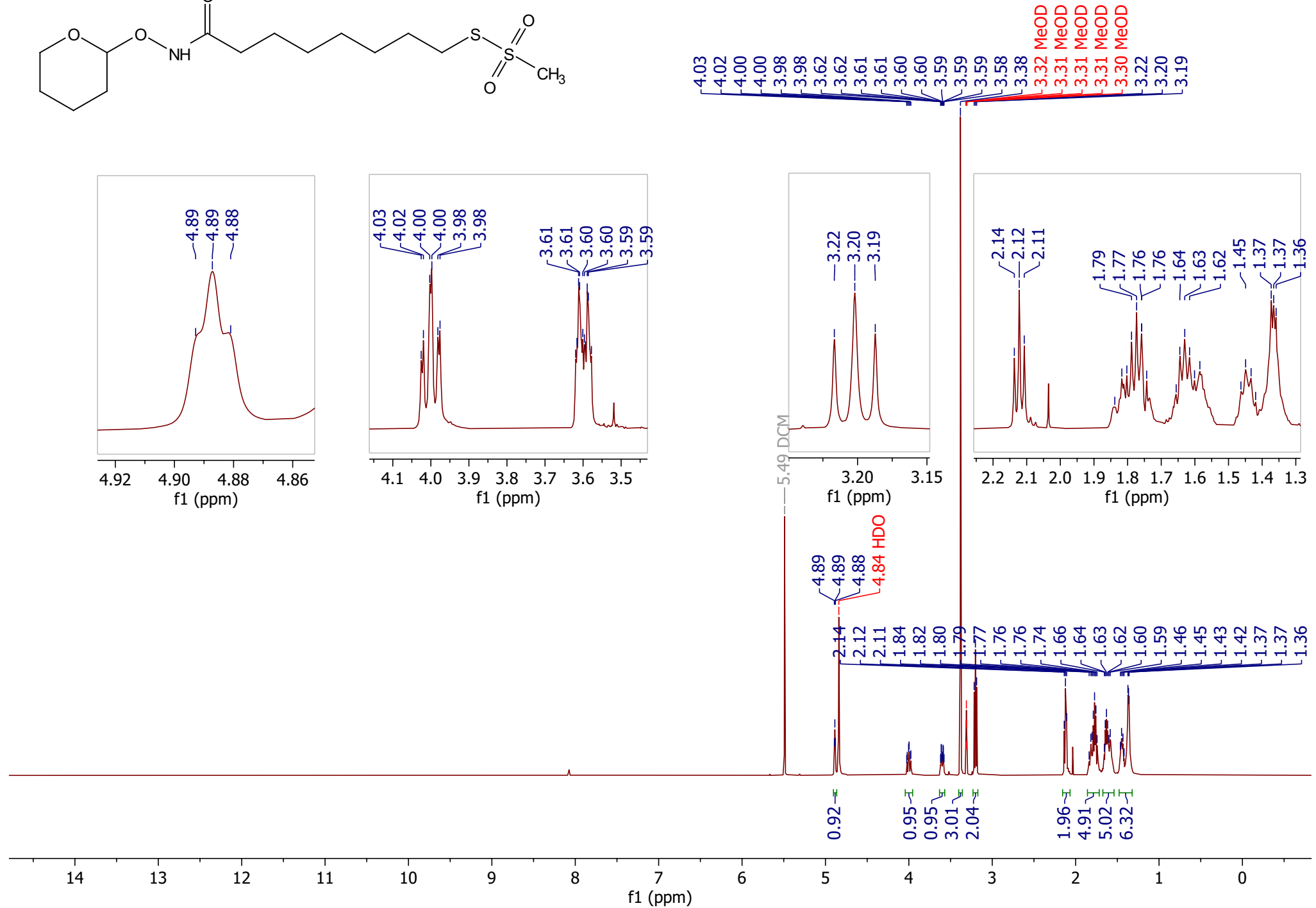
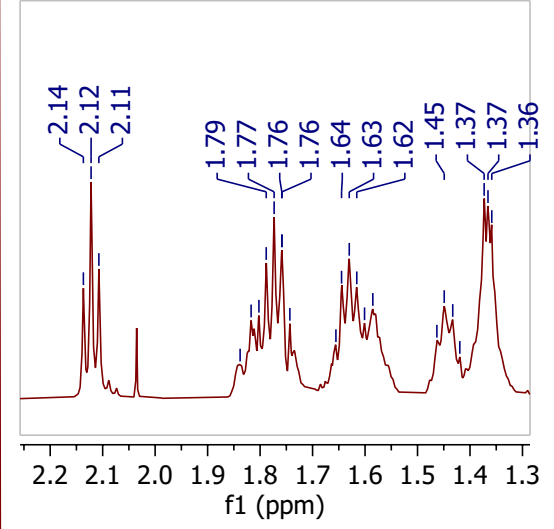
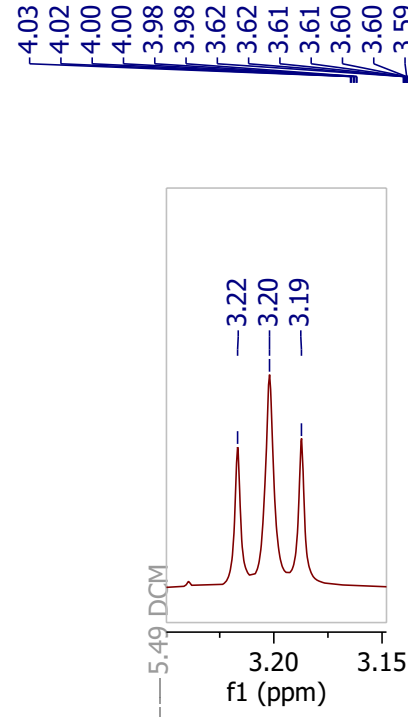
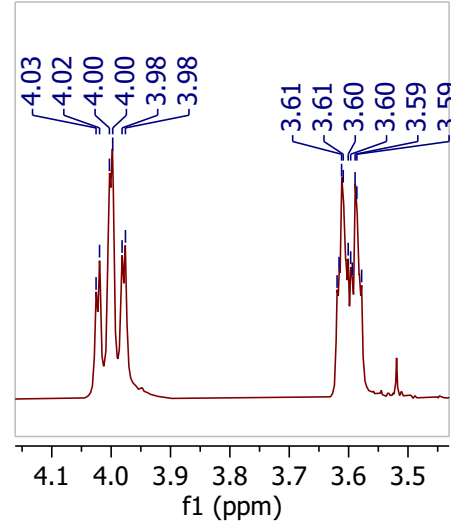
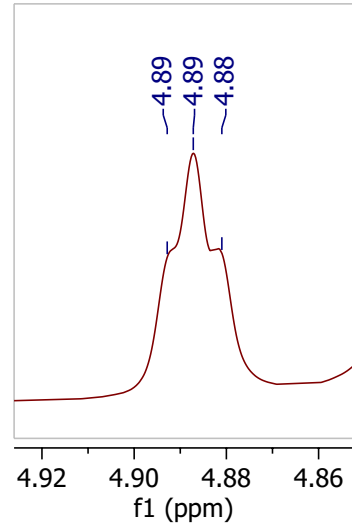
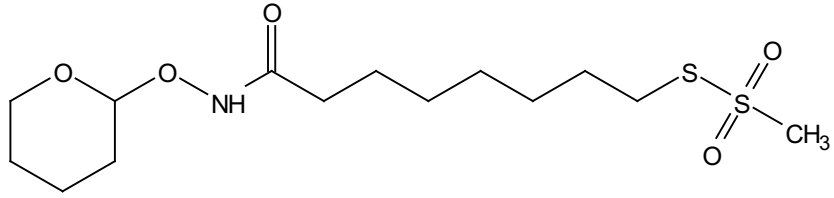


Compound 18
¹H NMR (126 MHz, MeOD-d4)

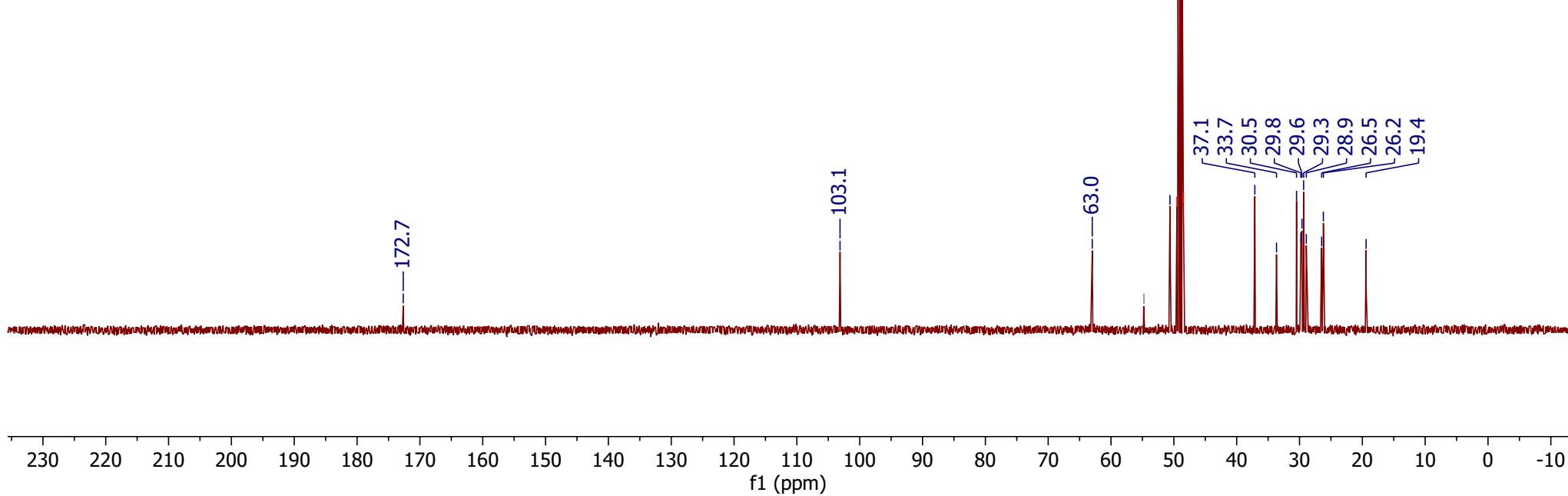
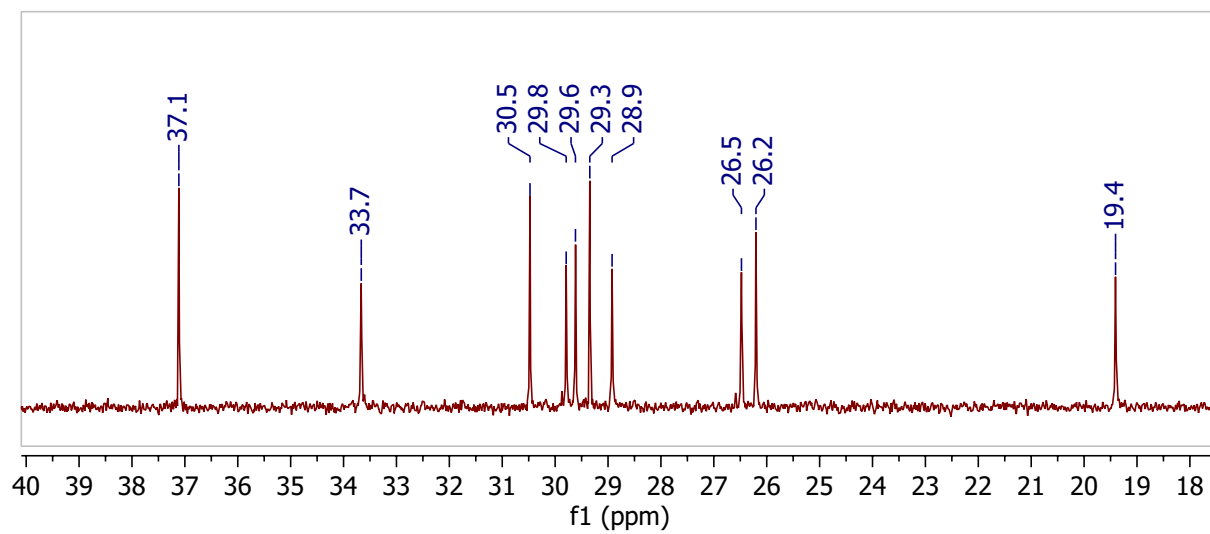
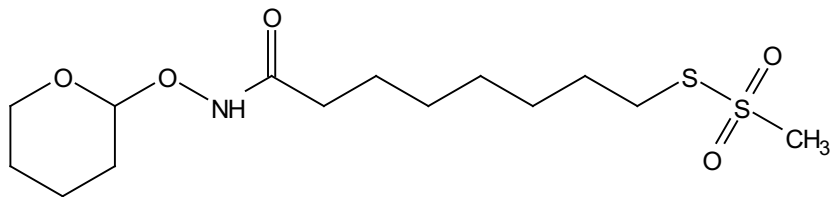


54.8 DCM
50.6
49.5 MeOD
49.3 MeOD
49.2 MeOD
49.0 MeOD
48.8 MeOD
48.7 MeOD
48.5 MeOD

Compound 19
¹H NMR (500 MHz, MeOD-d4)

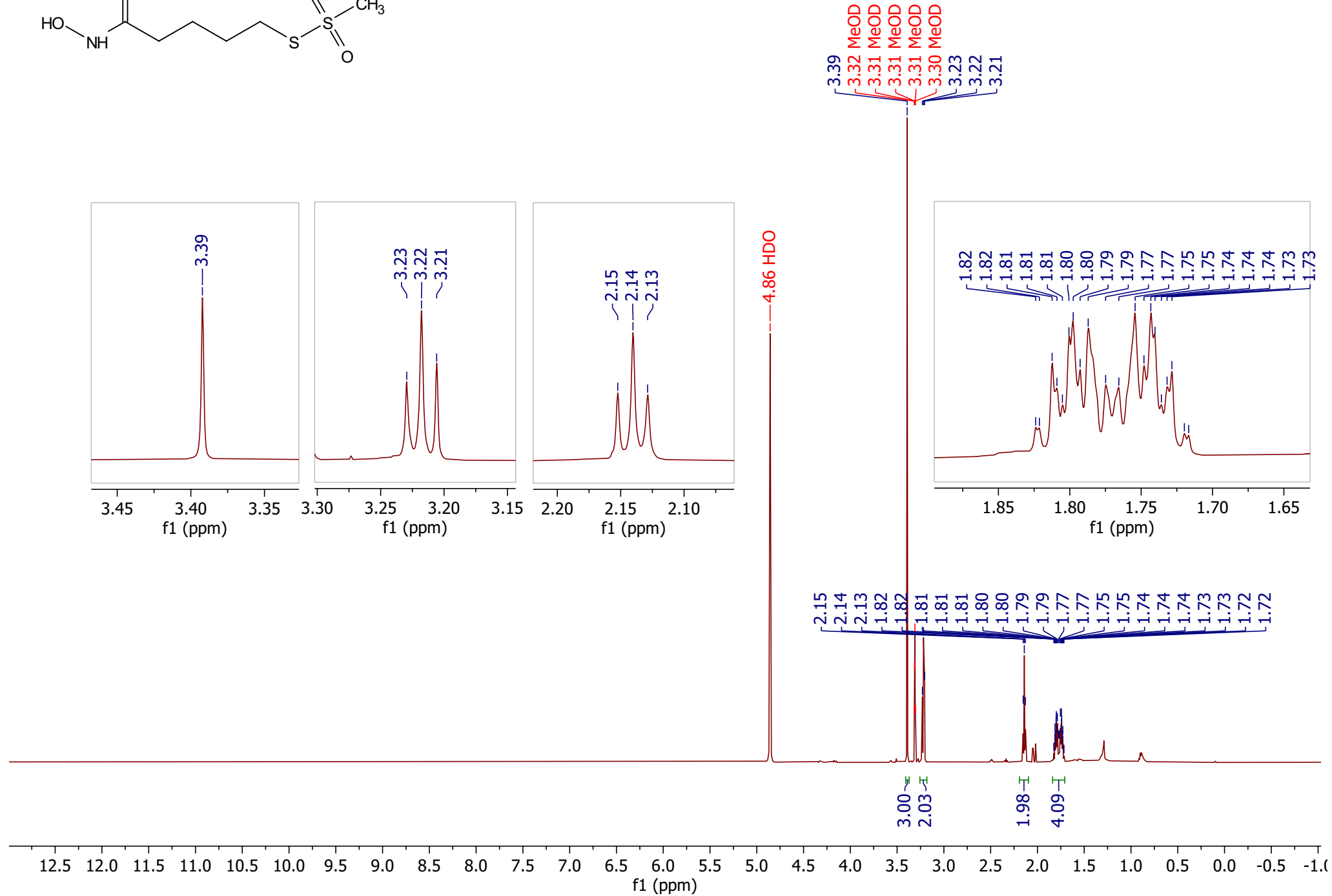
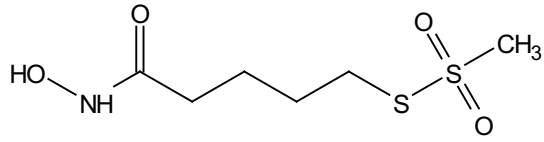


Compound 19
¹H NMR (126 MHz, MeOD-d4)

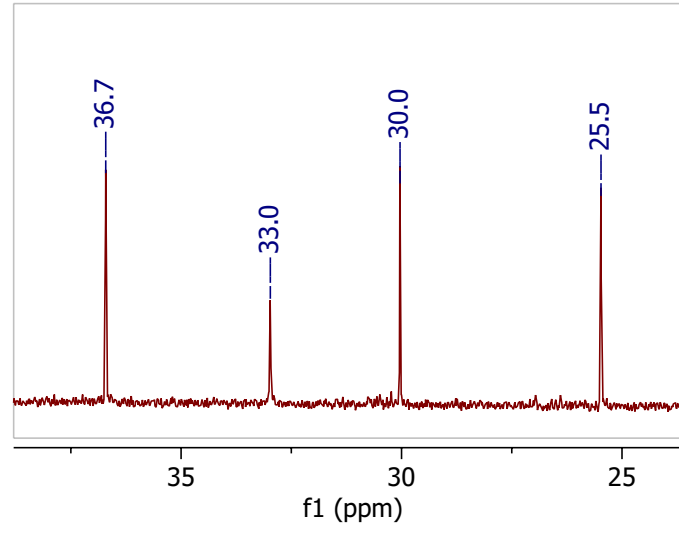
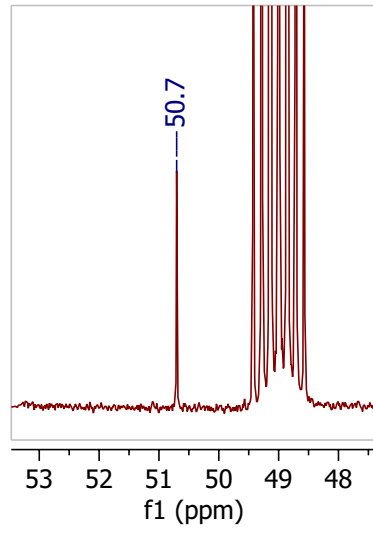
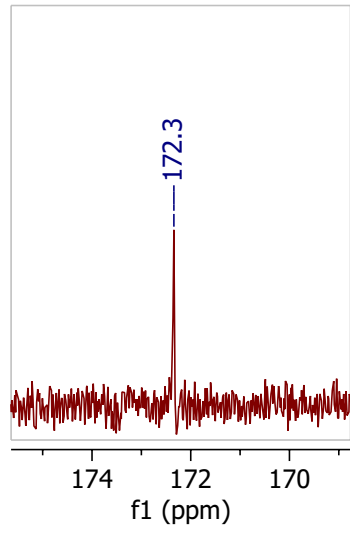
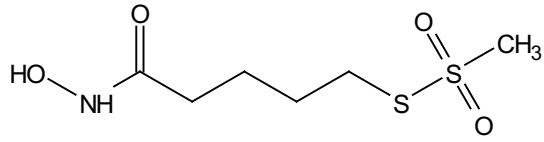


54.8 DCM
50.6
49.5 MeOD
49.3 MeOD
49.2 MeOD
49.0 MeOD
48.8 MeOD
48.7 MeOD
48.5 MeOD

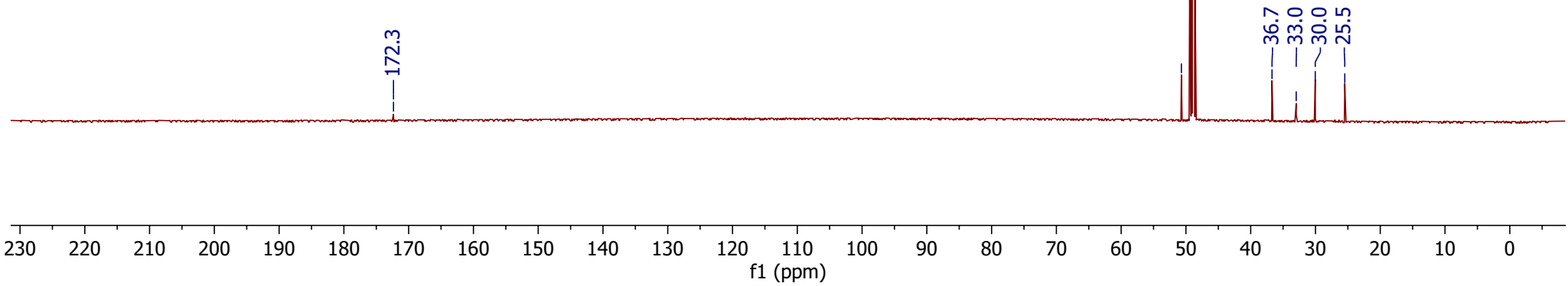
Compound 20
¹H NMR (600 MHz, MeOD-d4)



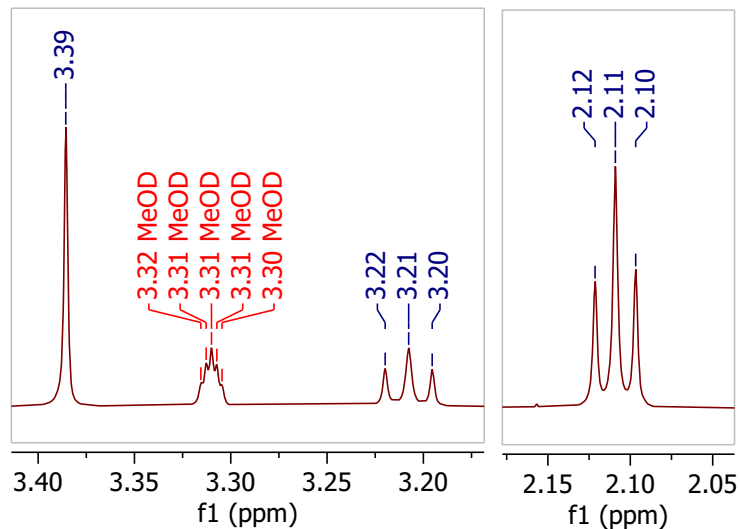
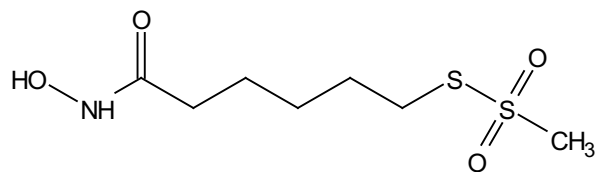
Compound 20
¹H NMR (151 MHz, MeOD-d4)



50.7
49.4 MeOD
49.3 MeOD
49.1 MeOD
49.0 MeOD
48.9 MeOD
48.7 MeOD
48.6 MeOD

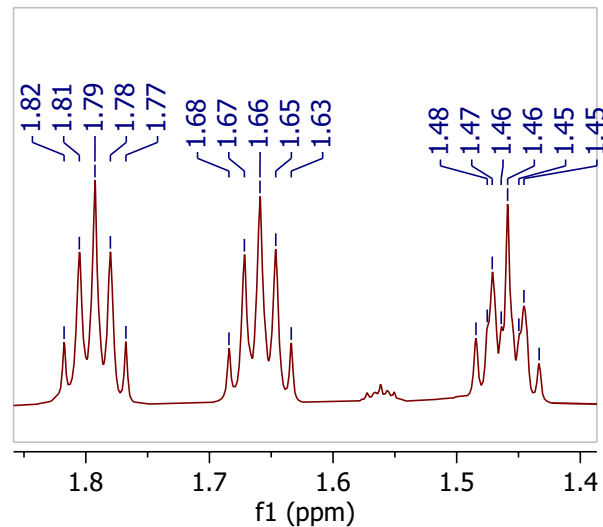


Compound 21
¹H NMR (600 MHz, MeOD-d4)



4.86 HDO

3.39
3.32 MeOD
3.31 MeOD
3.31 MeOD
3.31 MeOD
3.30 MeOD
3.22
3.21
3.20



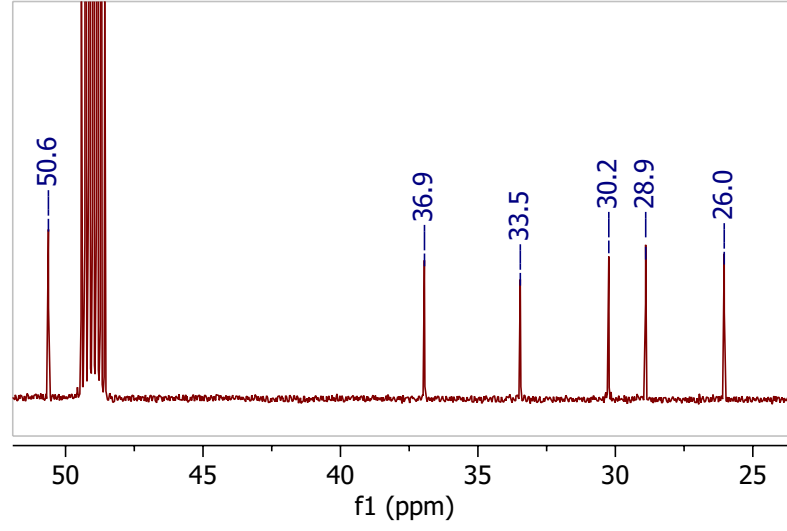
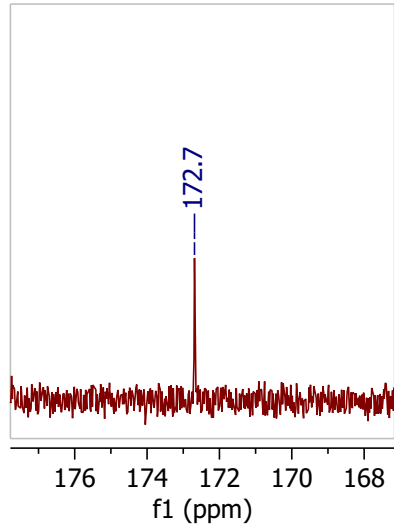
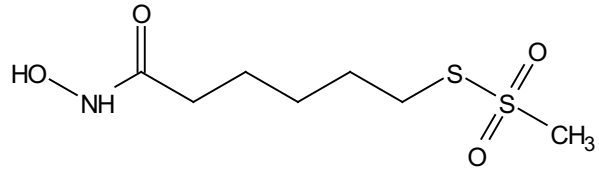
2.12
2.11
2.10
1.82
1.81
1.79
1.78
1.77
1.68
1.67
1.66
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1.48
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1.46
1.46
1.45
1.45
1.43

3.00
2.01

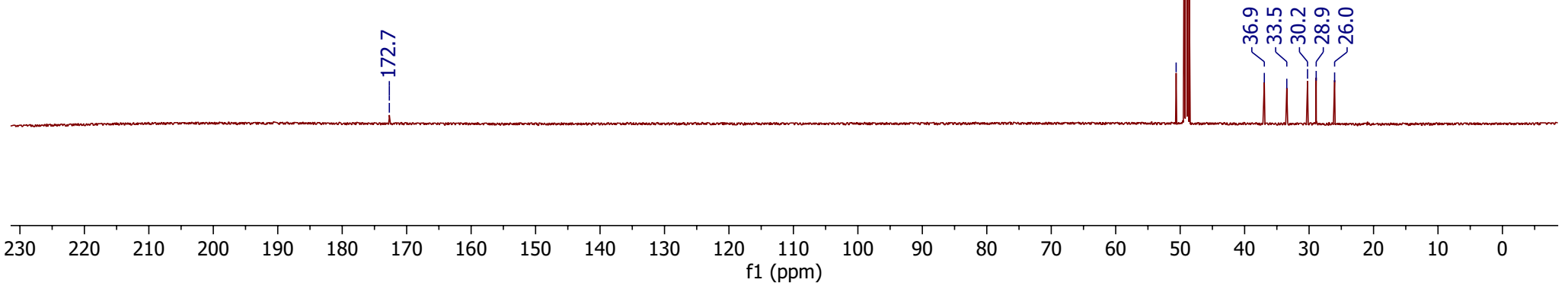
1.86
2.04
2.03
2.01

12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

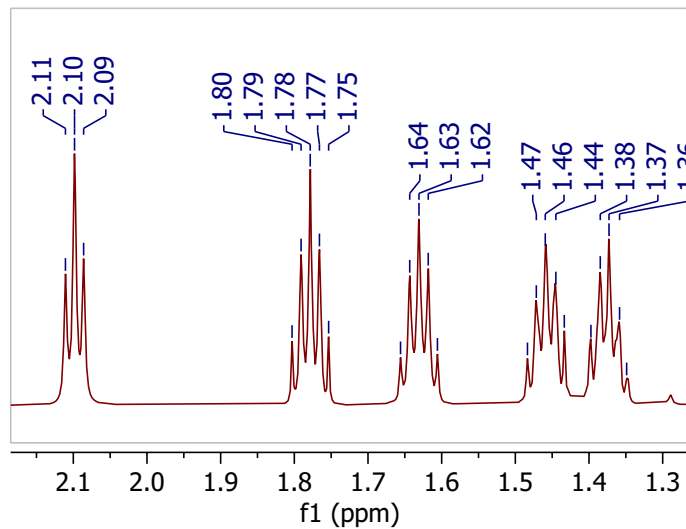
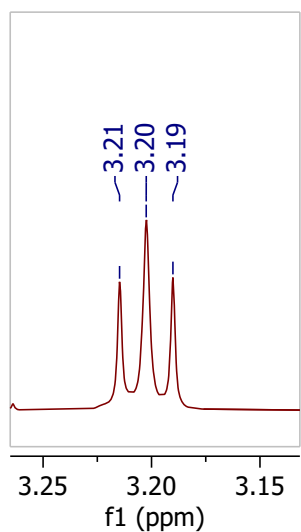
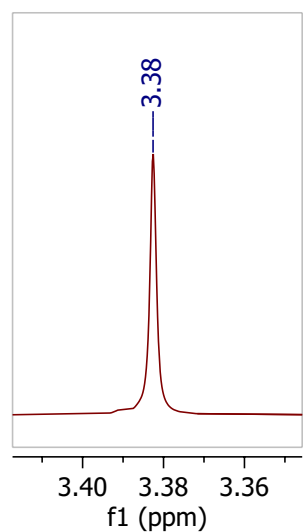
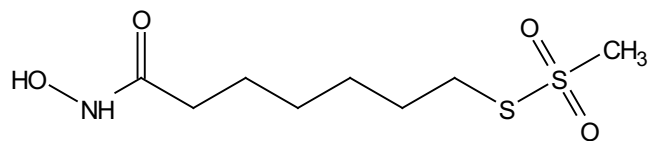
Compound 21
¹H NMR (151 MHz, MeOD-d4)



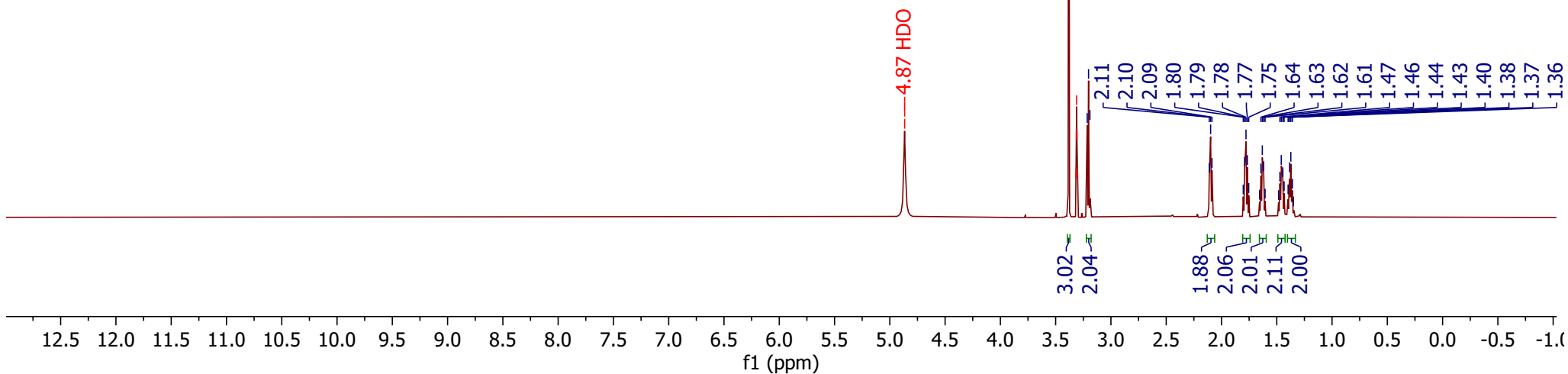
50.6
49.4 MeOD
49.3 MeOD
49.1 MeOD
48.9 MeOD
48.7 MeOD
48.6 MeOD



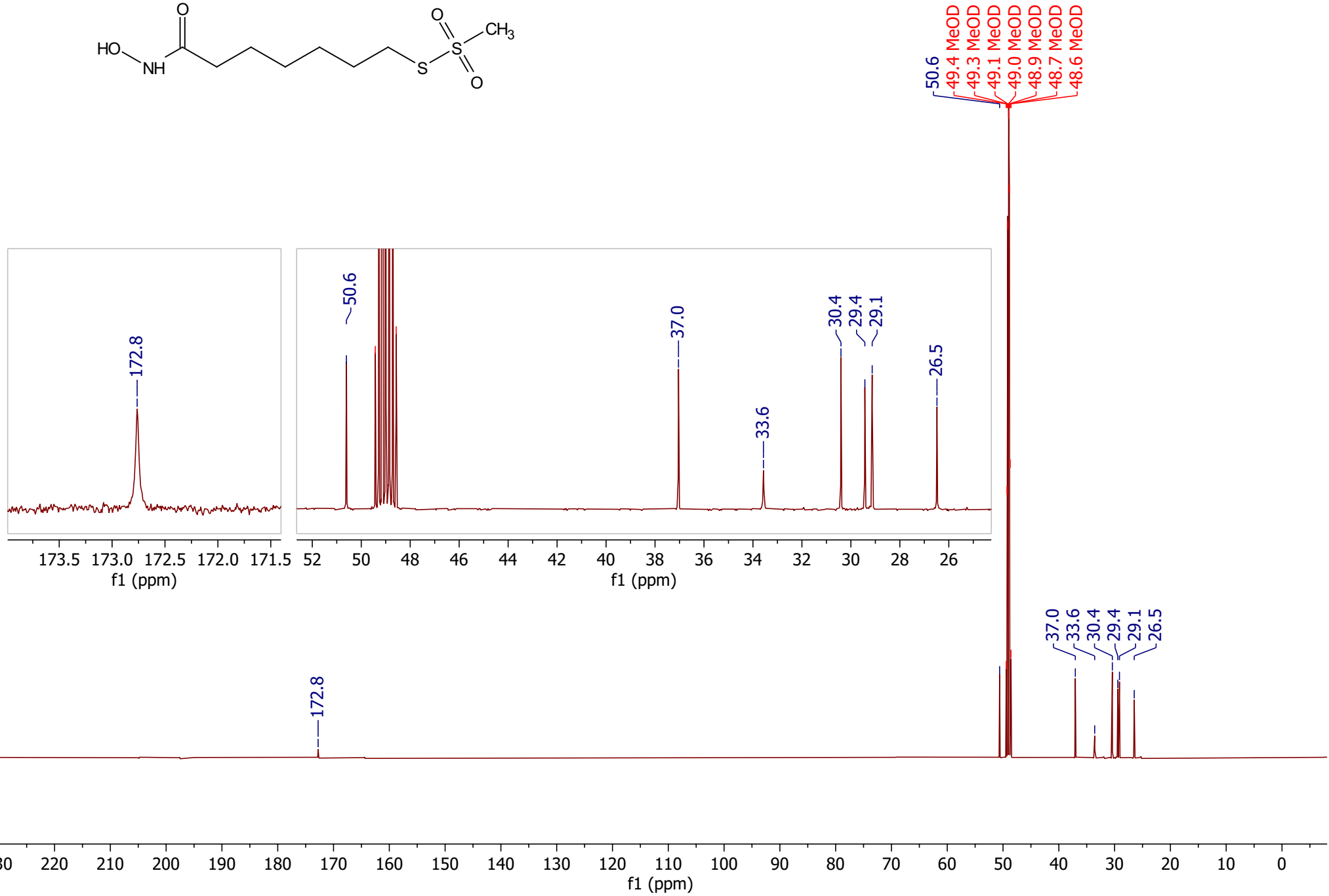
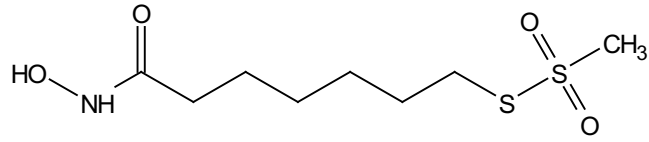
Compound 22
¹H NMR (600 MHz, MeOD-d4)



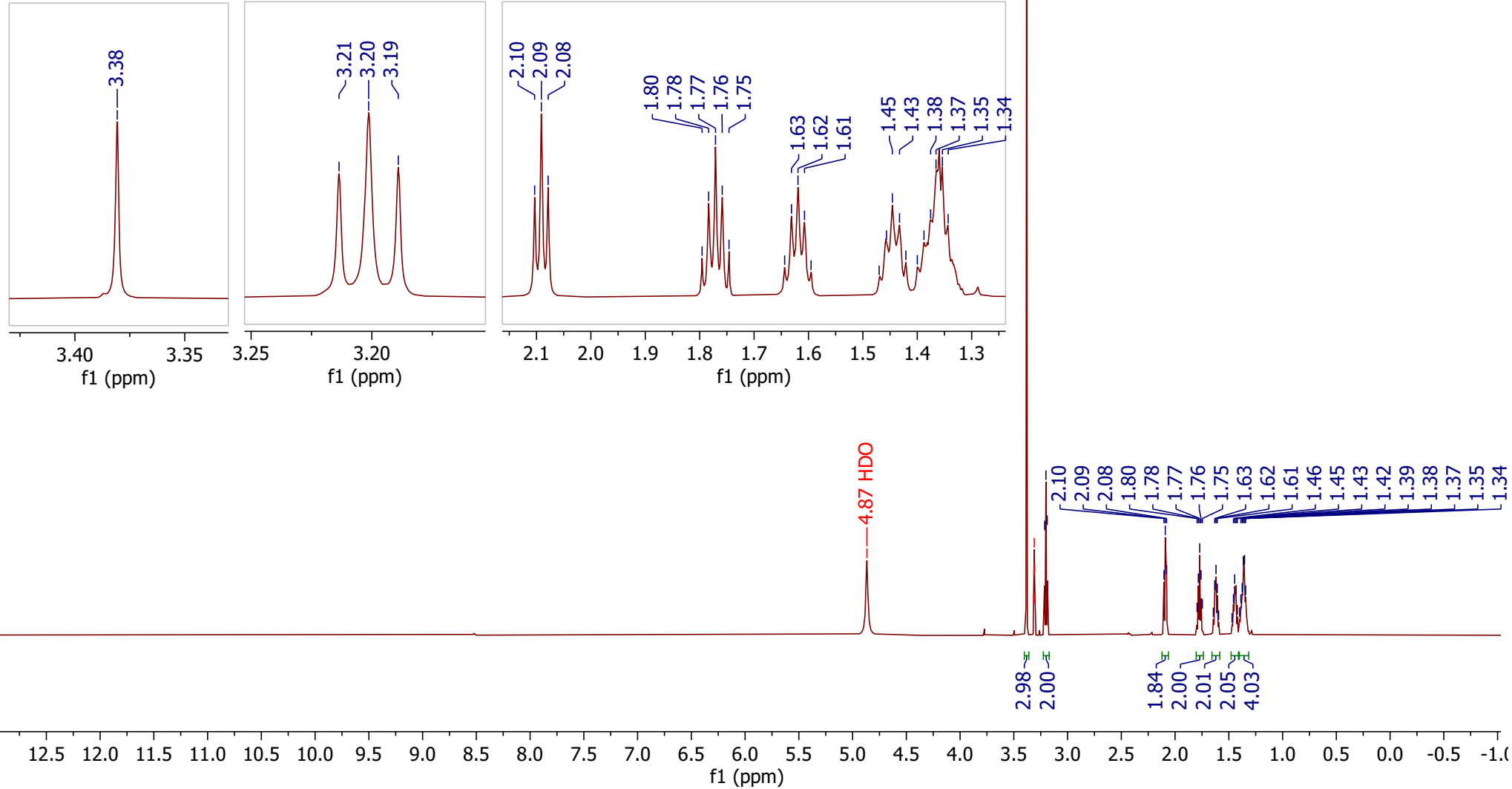
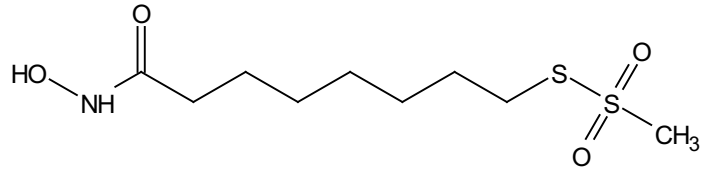
3.38
3.32 MeOD
3.31 MeOD
3.31 MeOD
3.31 MeOD
3.30 MeOD
3.21
3.20
3.19



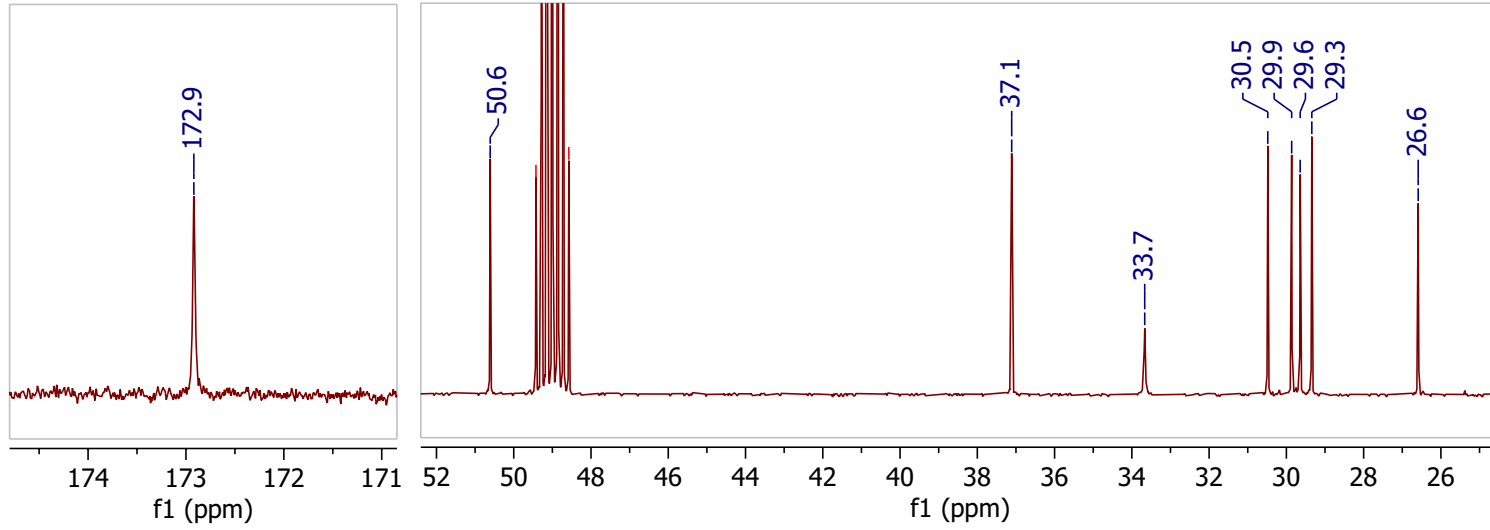
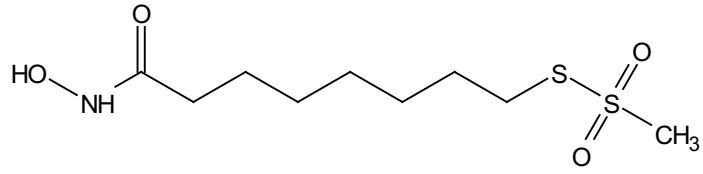
Compound 22
¹H NMR (151 MHz, MeOD-d4)



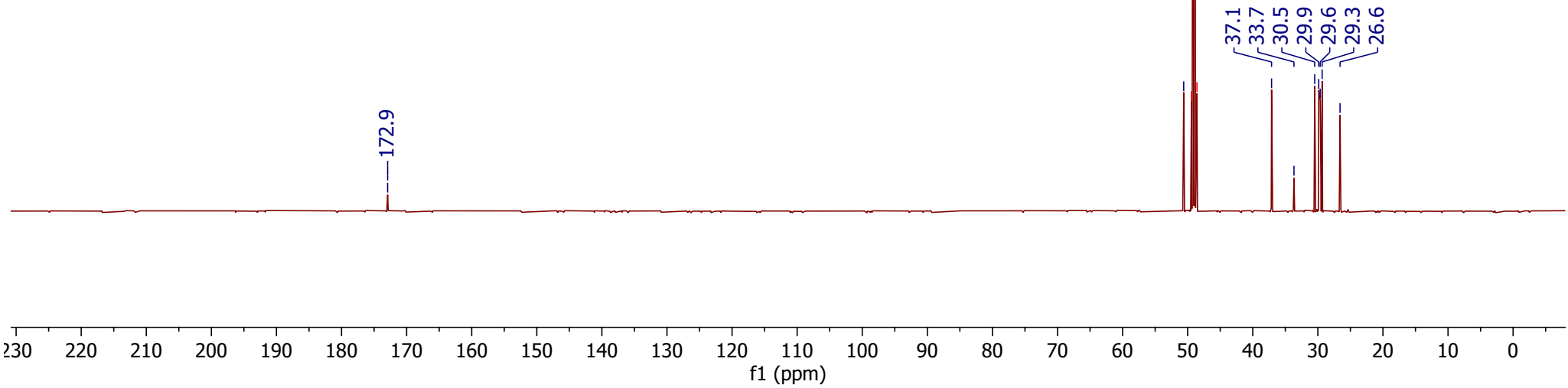
Compound 23
¹H NMR (600 MHz, MeOD-d4)



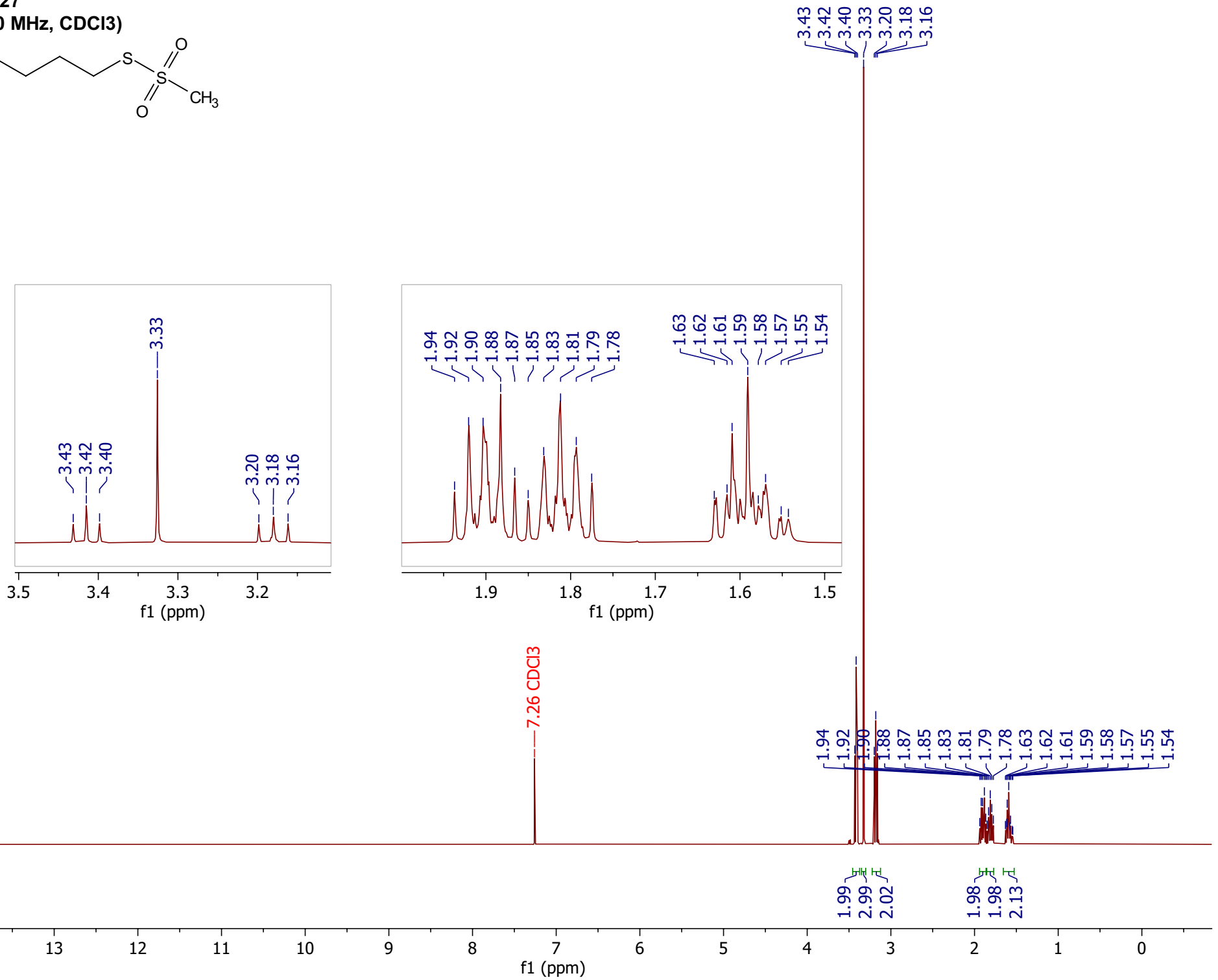
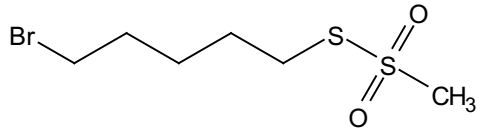
Compound 23
¹H NMR (151 MHz, MeOD-d4)



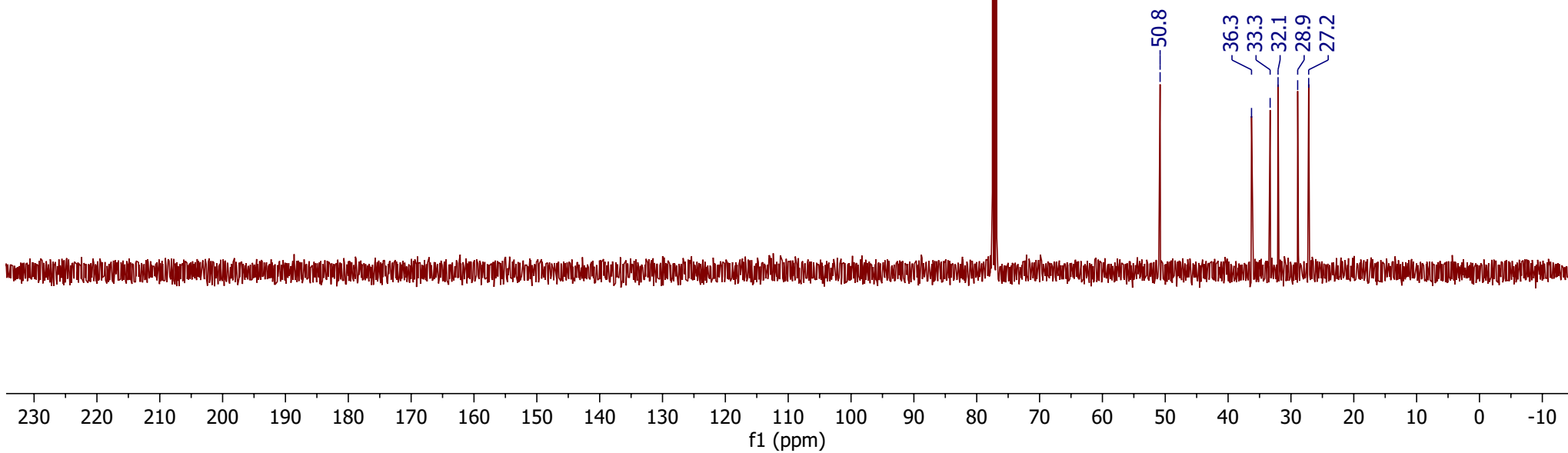
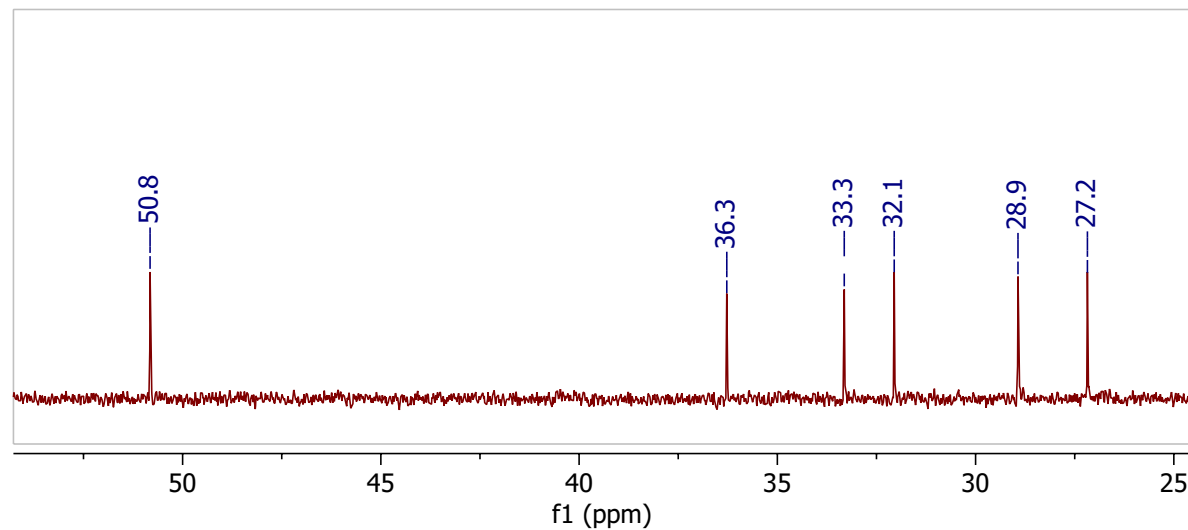
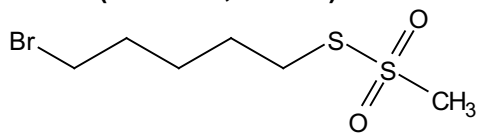
50.6
49.4 MeOD
49.3 MeOD
49.1 MeOD
49.0 MeOD
48.9 MeOD
48.7 MeOD
48.6 MeOD



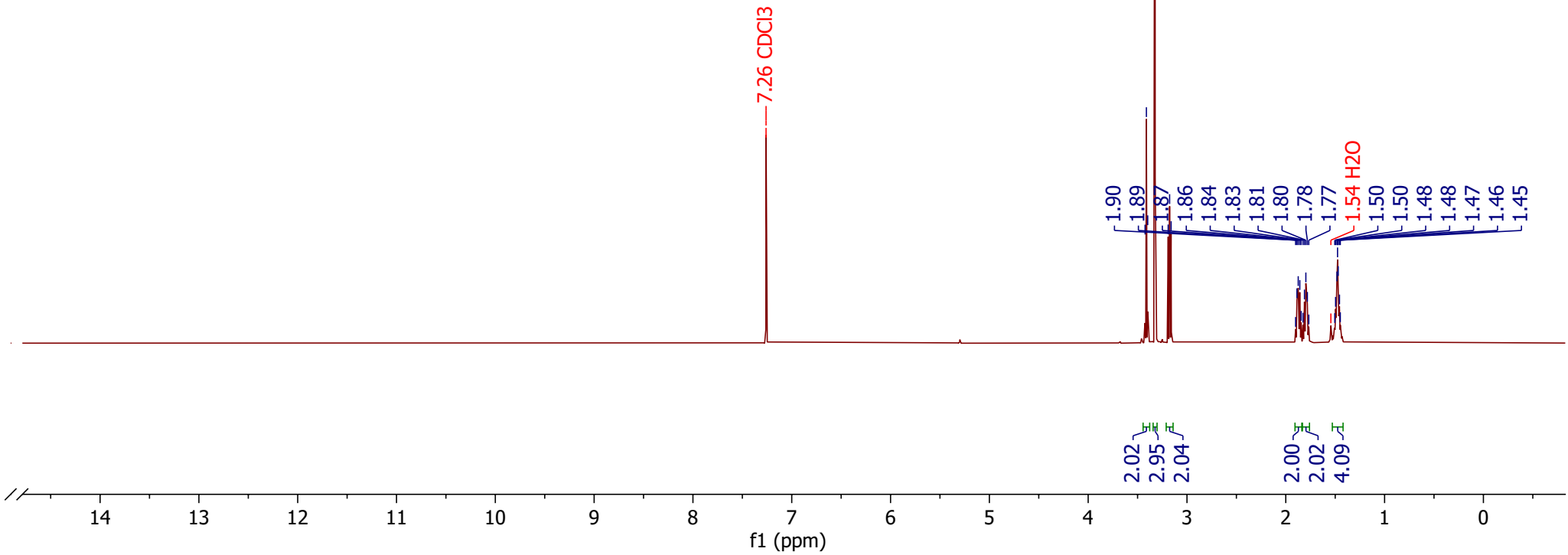
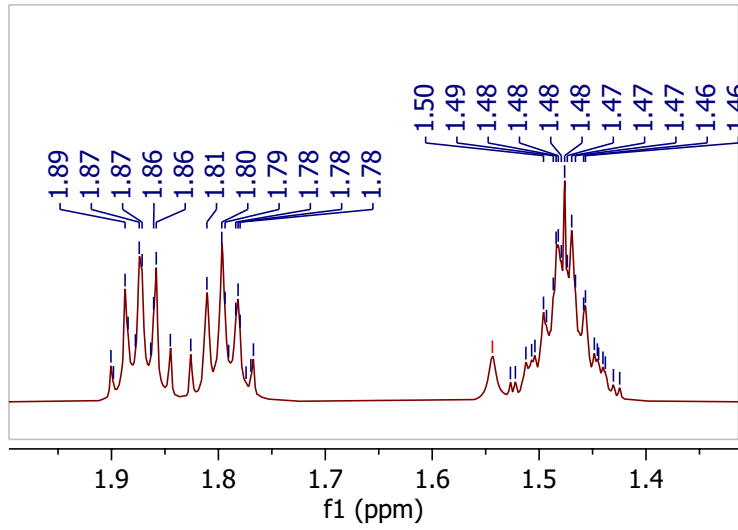
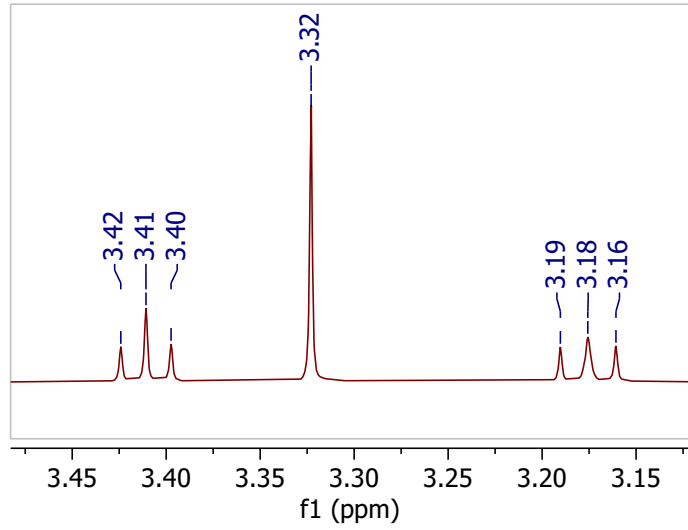
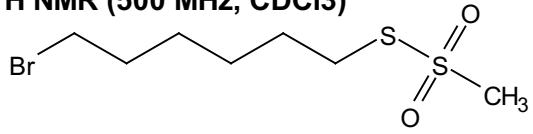
Compound 27
¹H NMR (400 MHz, CDCl₃)



Compound 27
¹³C NMR (101 MHz, CDCl₃)

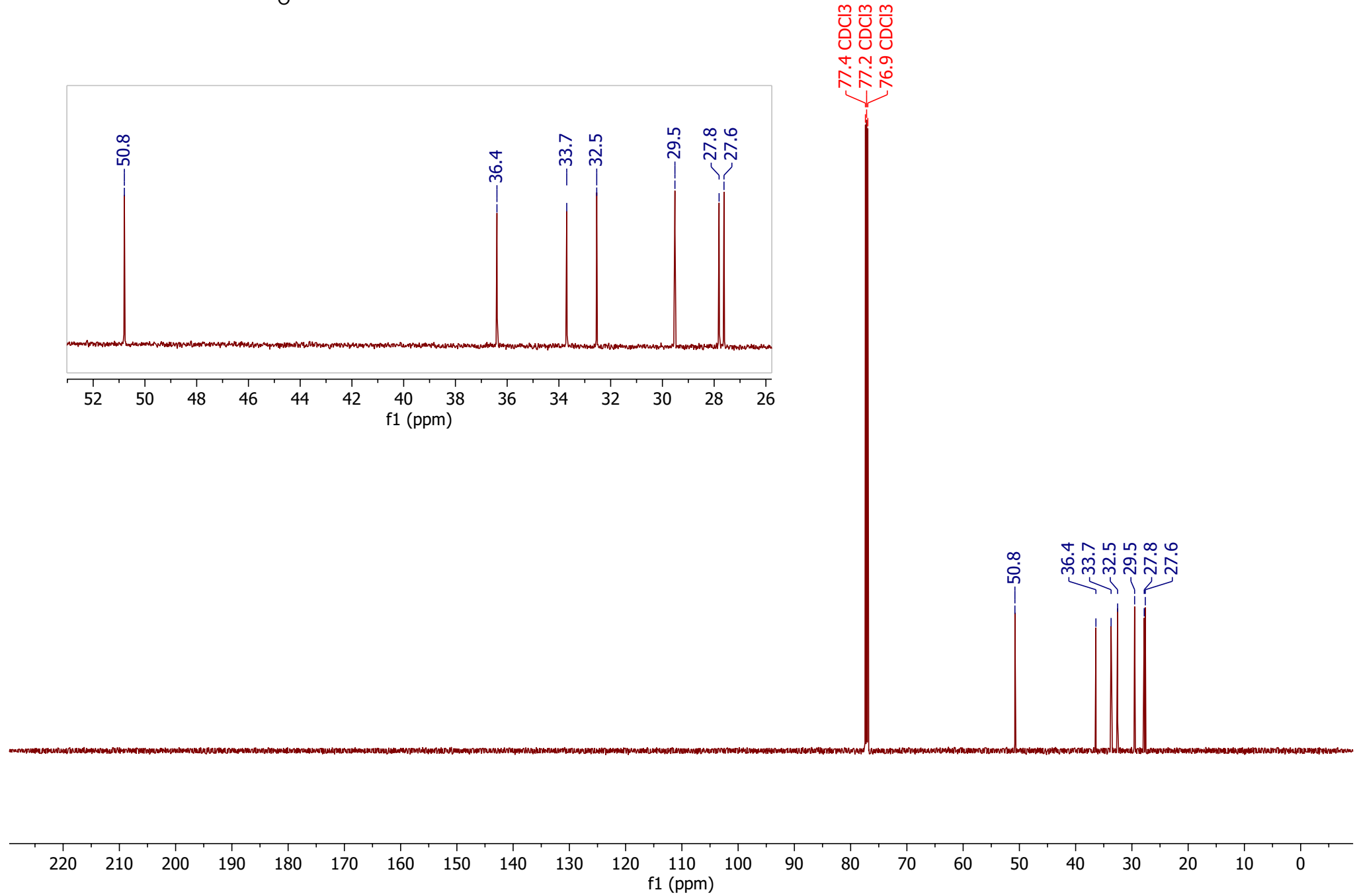
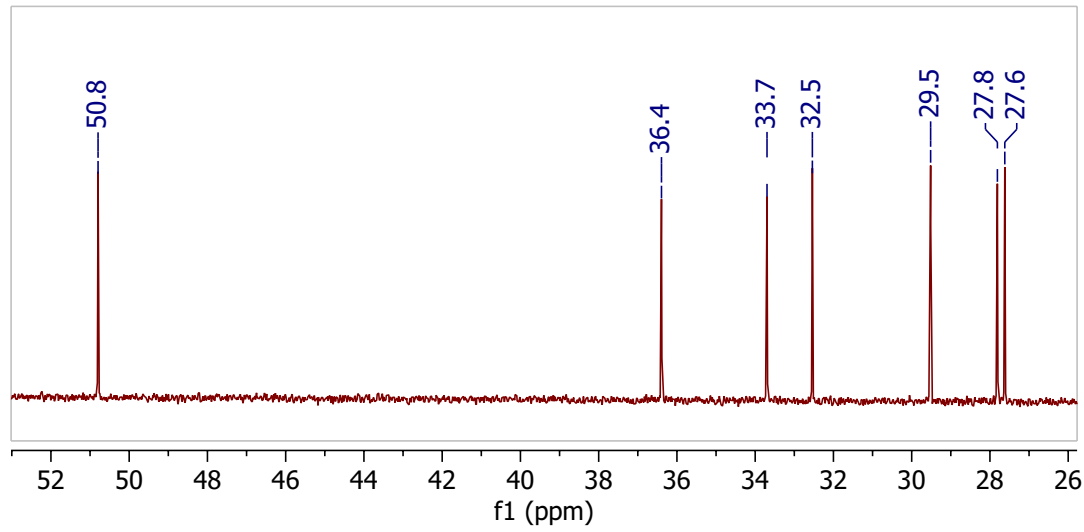
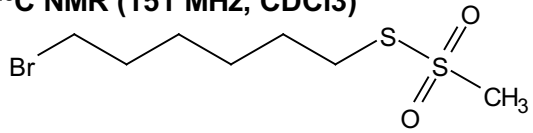


Compound 28
¹H NMR (500 MHz, CDCl₃)

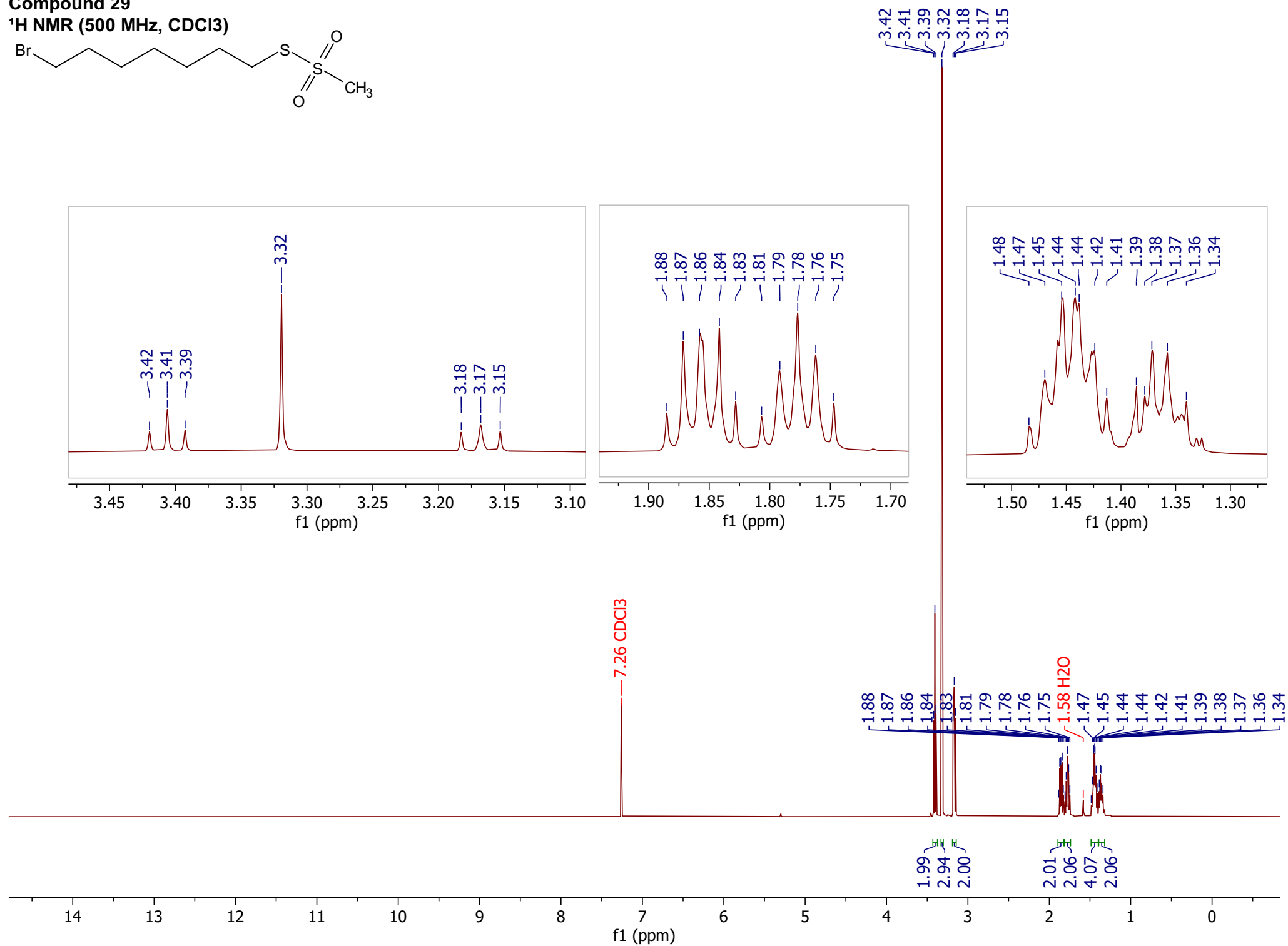
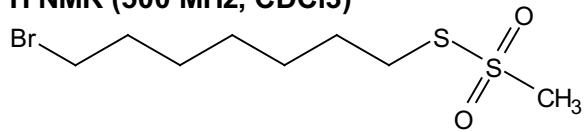


Compound 28

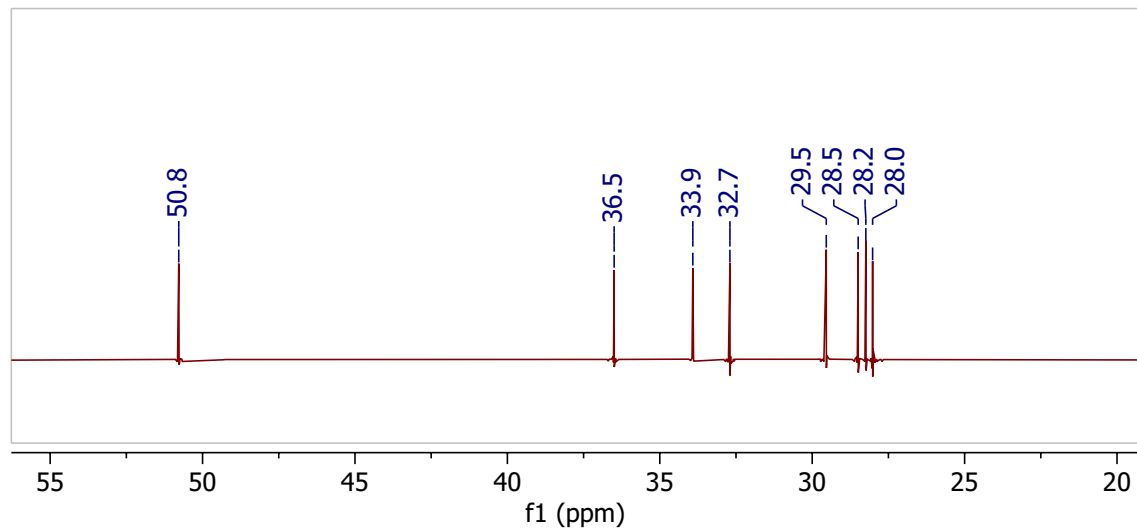
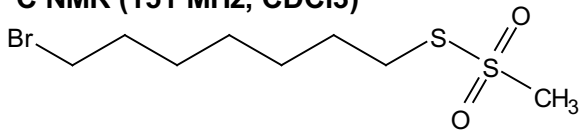
¹³C NMR (151 MHz, CDCl₃)



Compound 29
1H NMR (500 MHz, CDCl3)



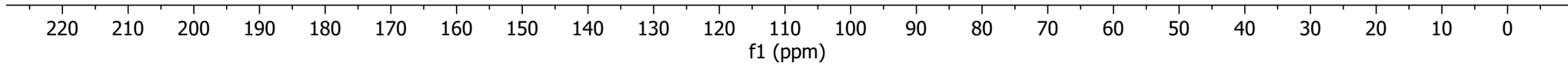
Compound 29
¹³C NMR (151 MHz, CDCl₃)



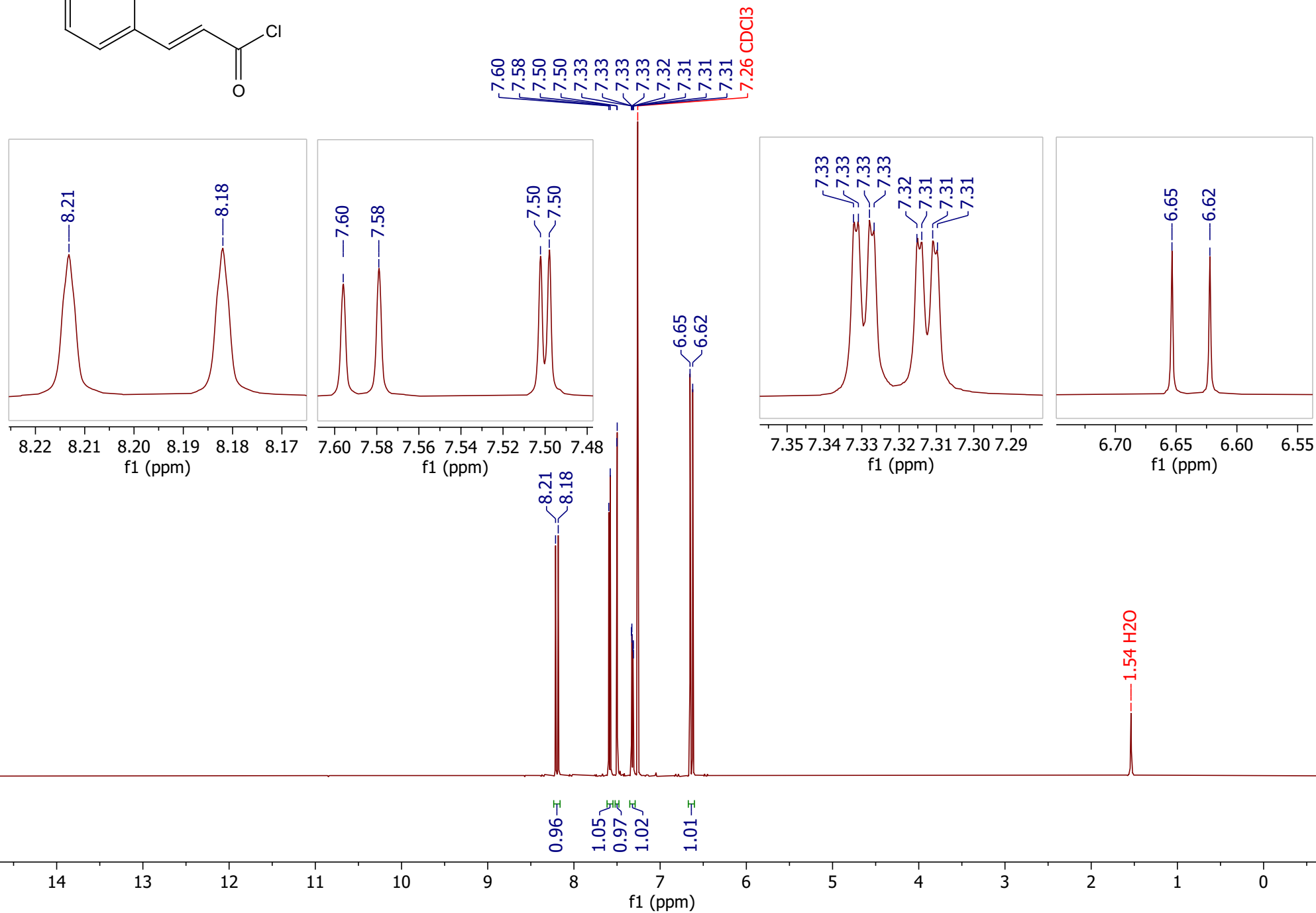
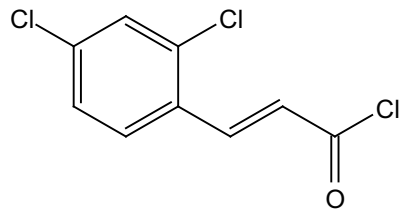
77.4 CDCl₃
77.2 CDCl₃
76.9 CDCl₃

36.5
33.9
32.7
29.5
28.5
28.2
28.0

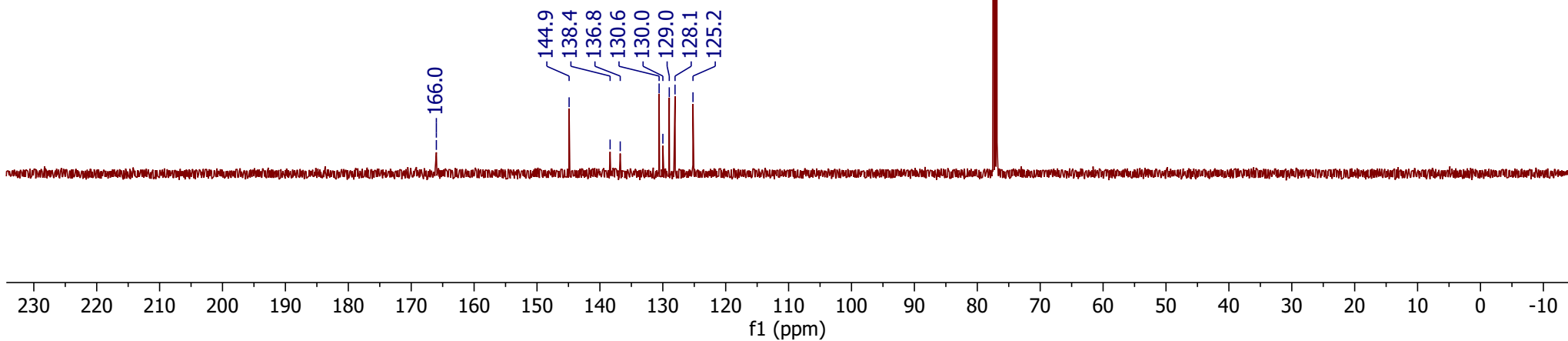
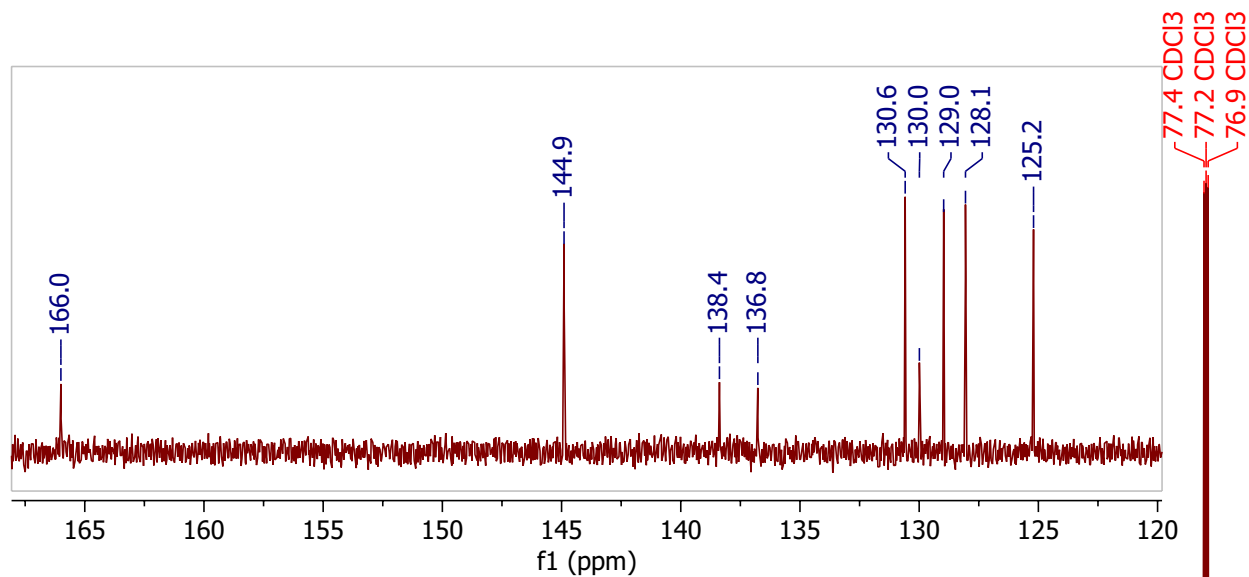
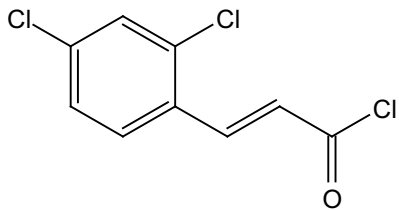
50.8



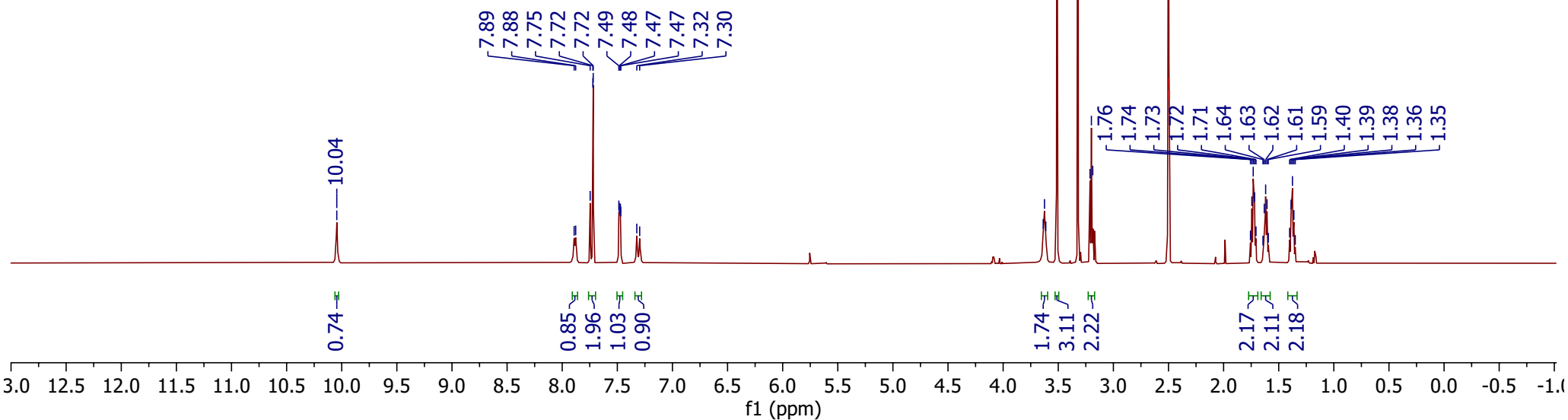
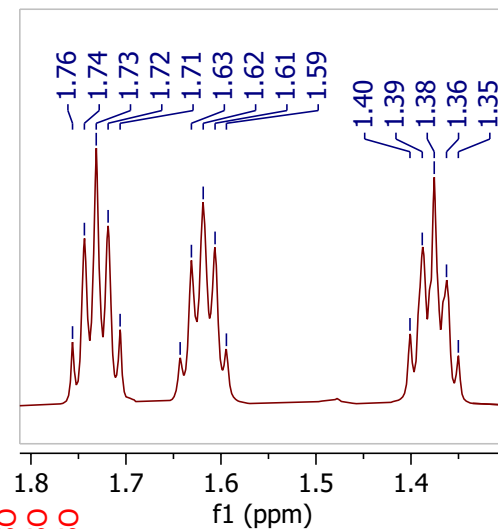
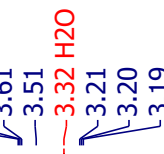
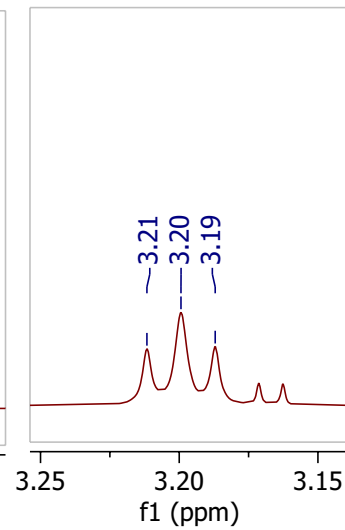
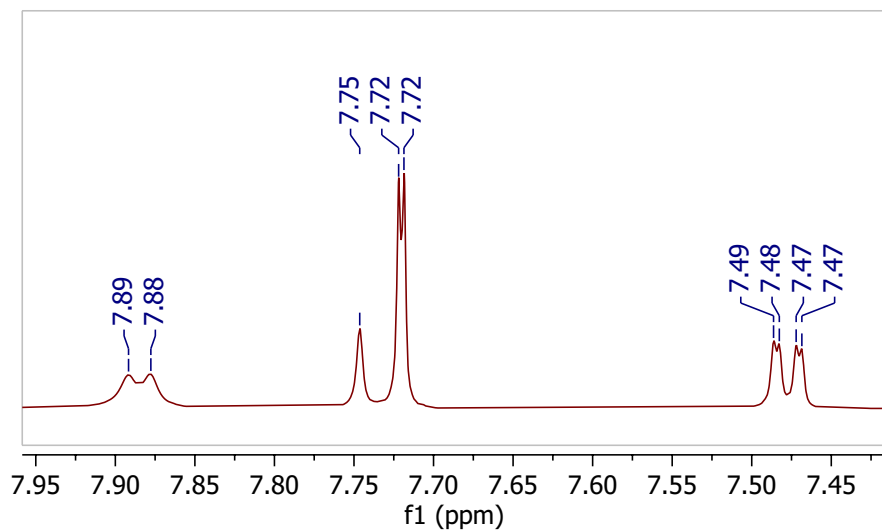
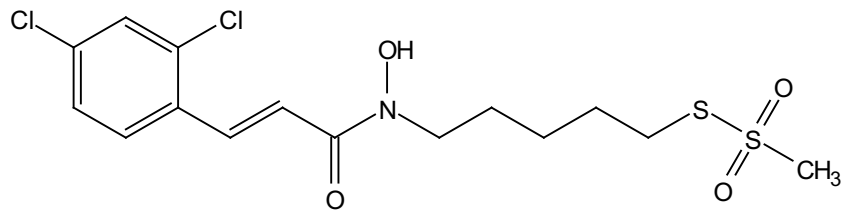
Compound 30
1H NMR (500 MHz, CDCl3)



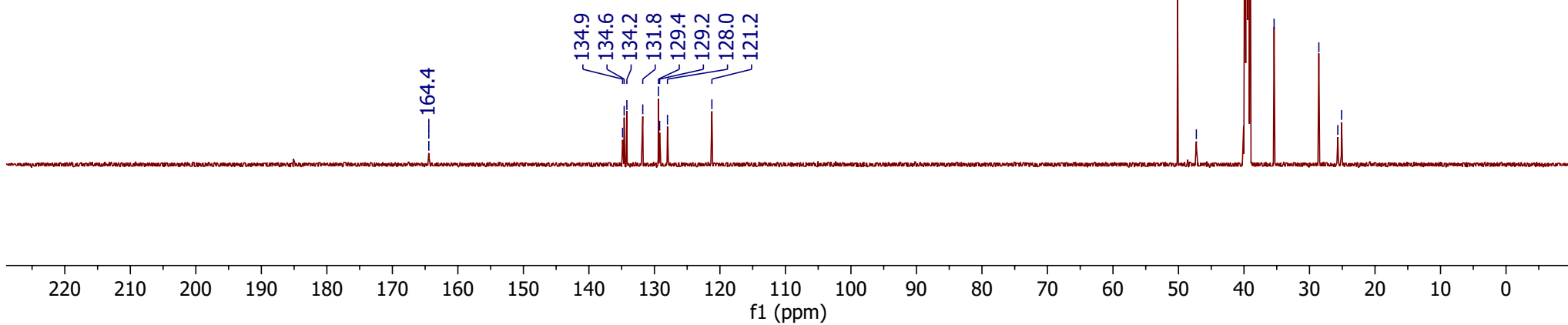
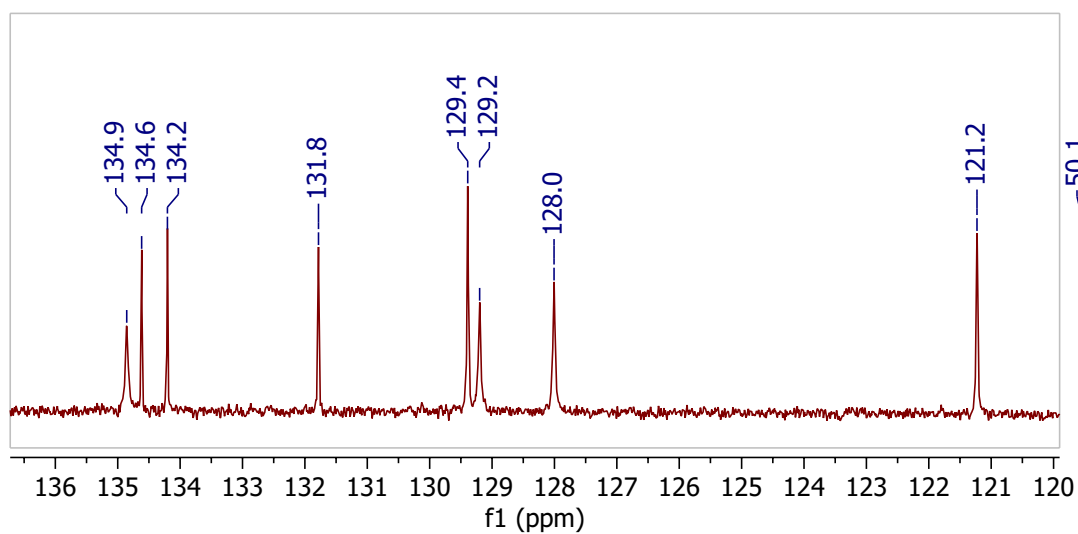
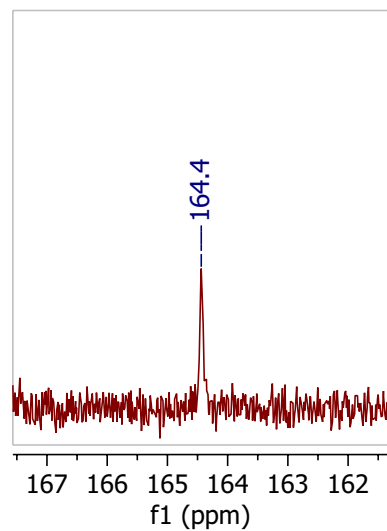
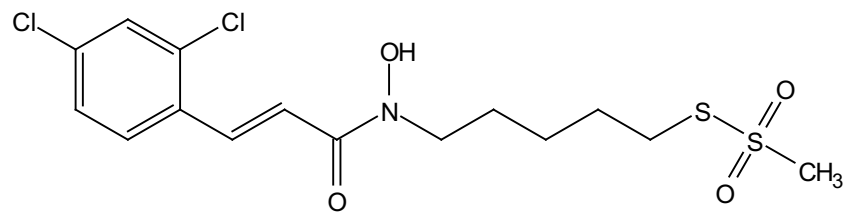
Compound 30
¹³C NMR (126 MHz, CDCl₃)



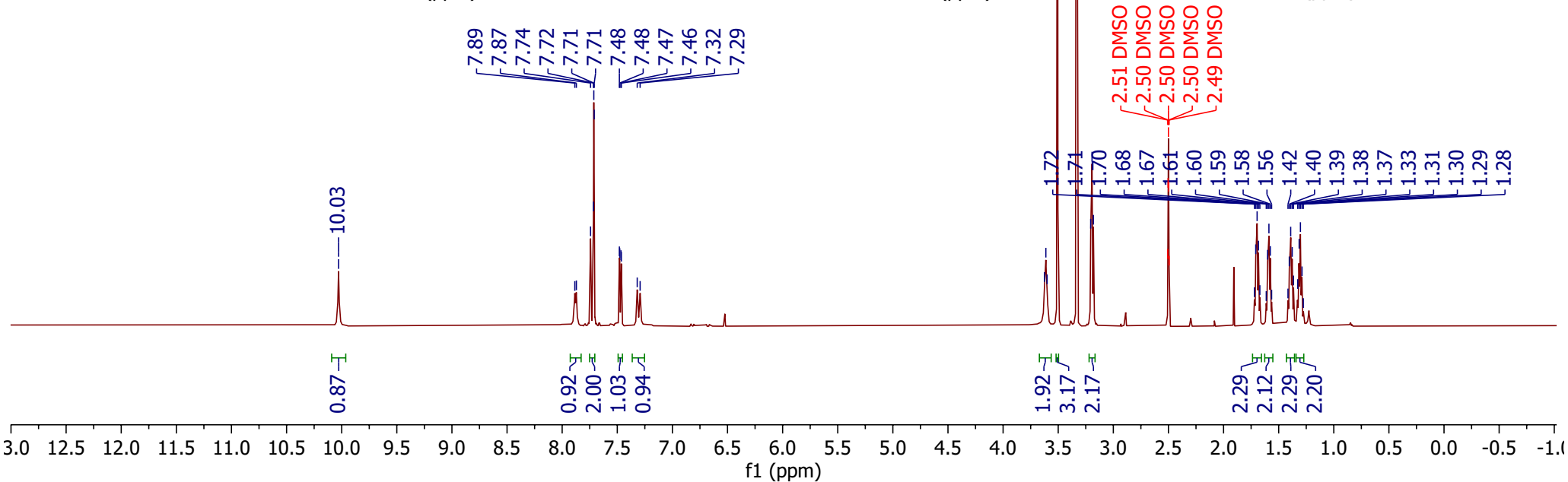
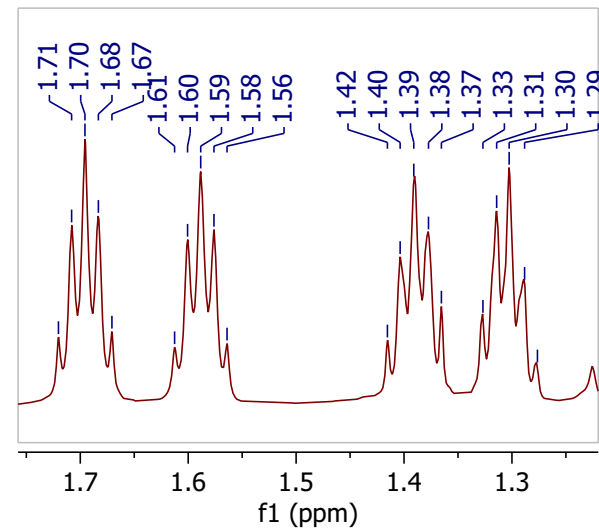
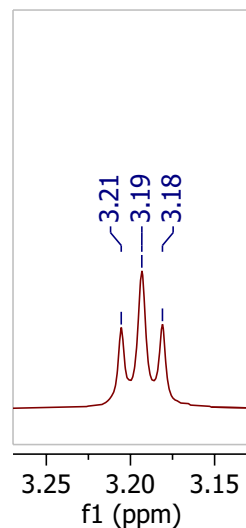
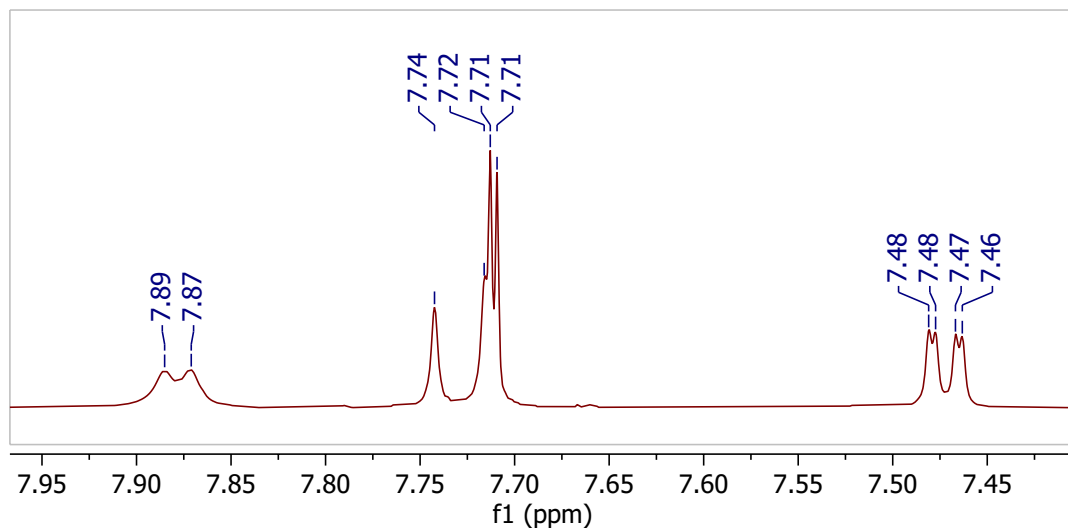
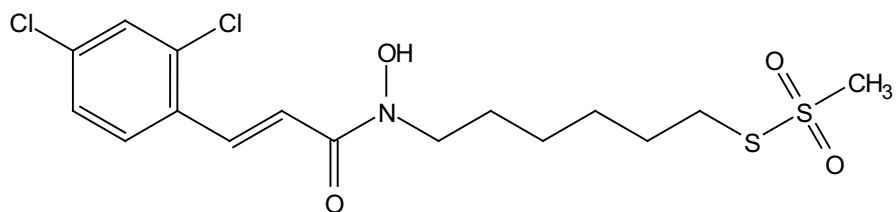
Compound 31
¹H NMR (600 MHz, DMSO-d6)



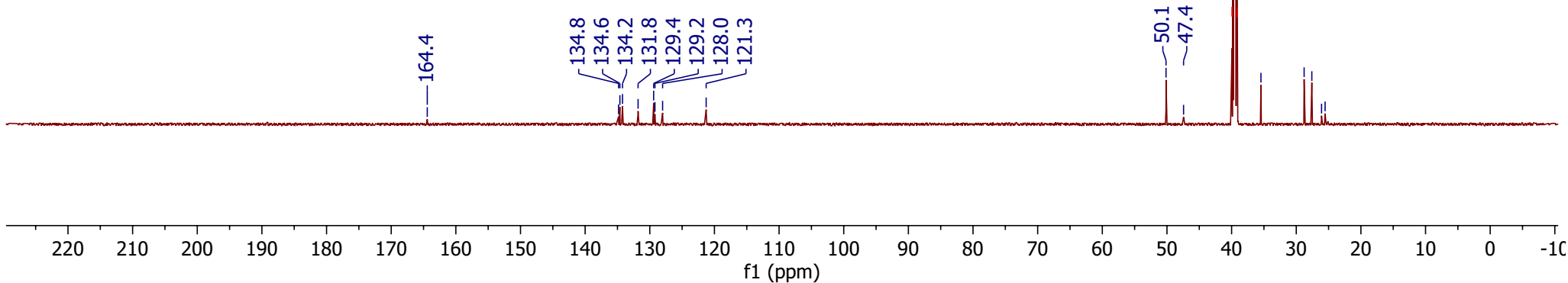
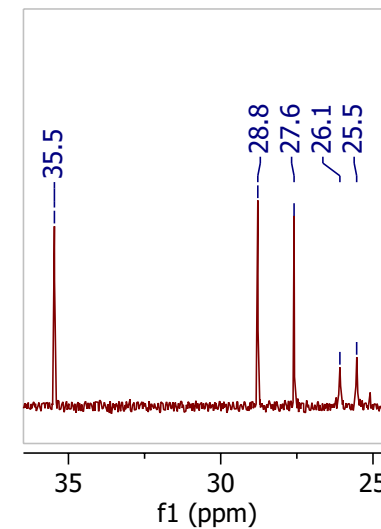
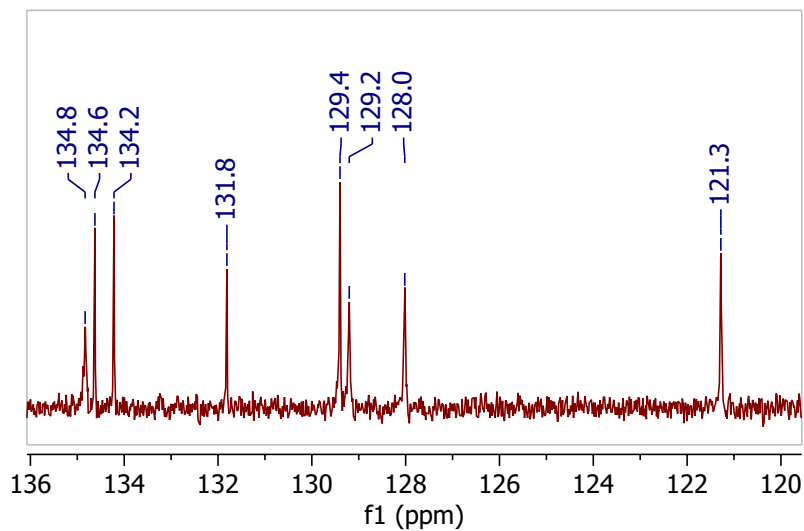
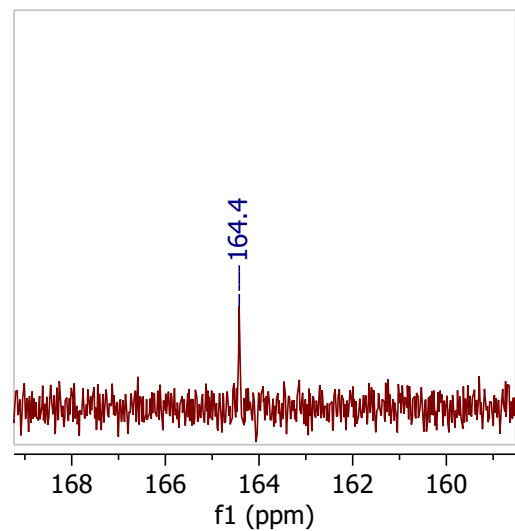
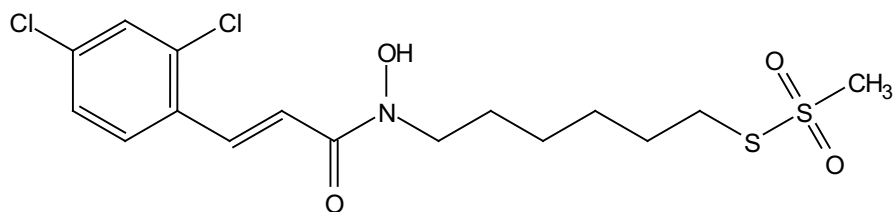
Compound 31
¹H NMR (151 MHz, DMSO-d6)



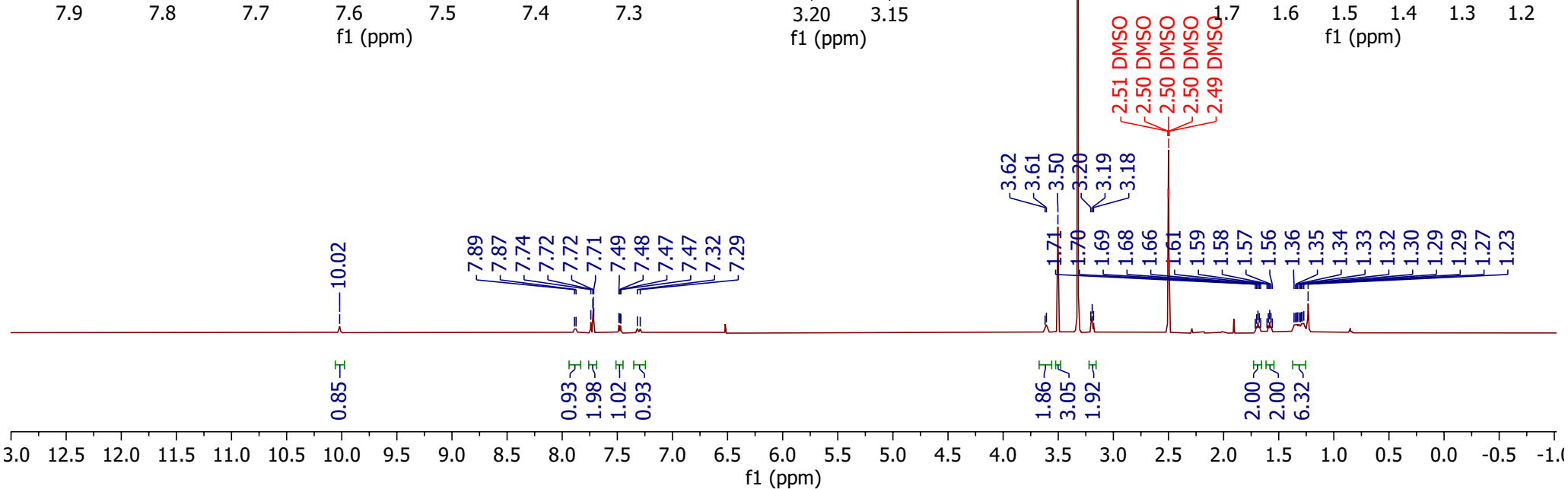
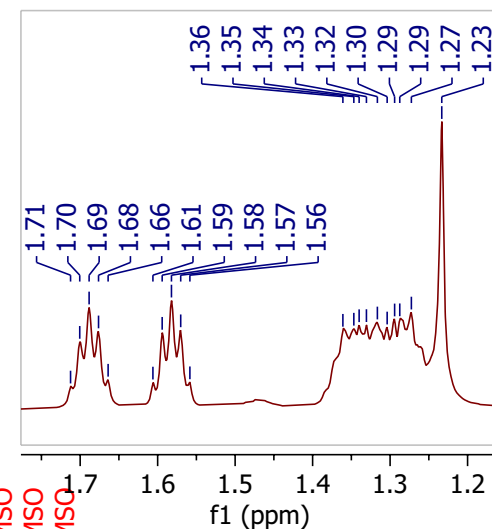
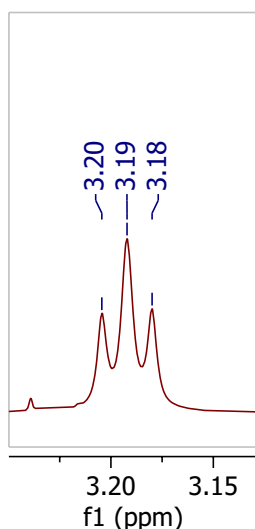
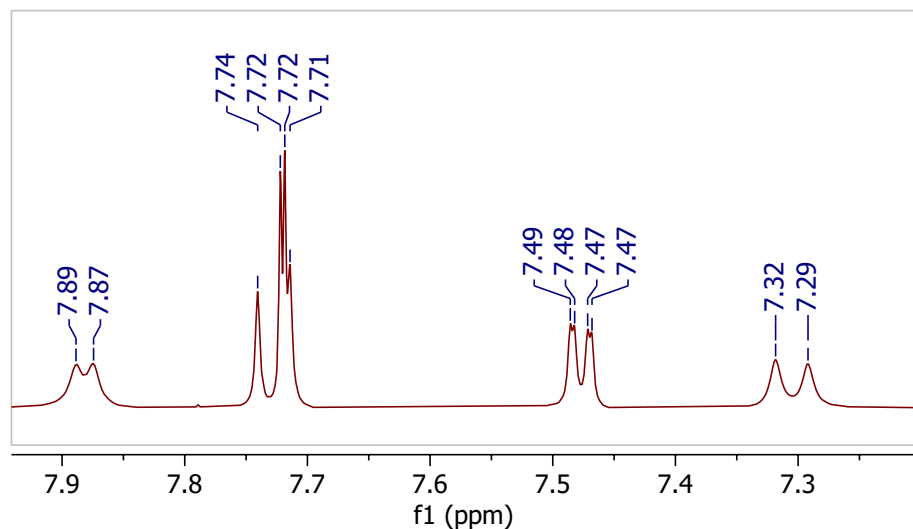
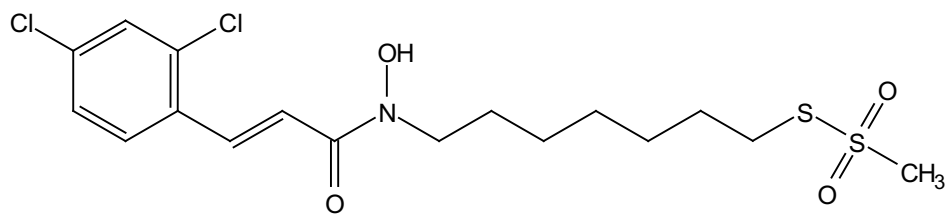
Compound 32
¹H NMR (600 MHz, DMSO-d₆)



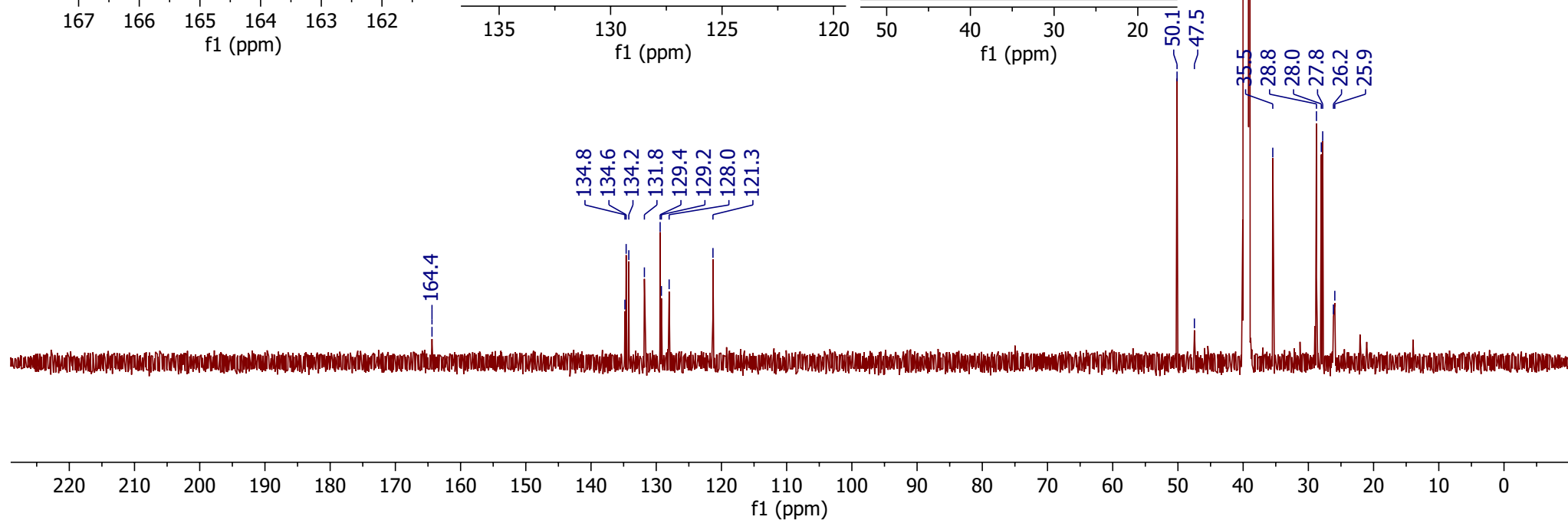
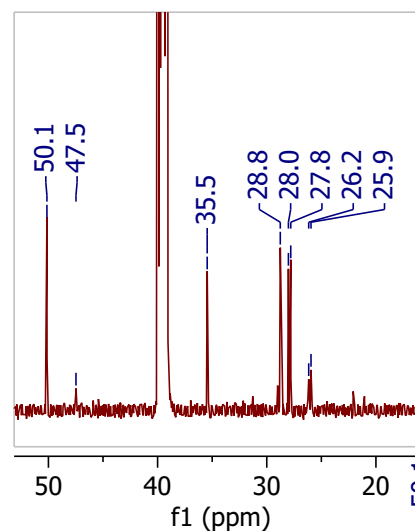
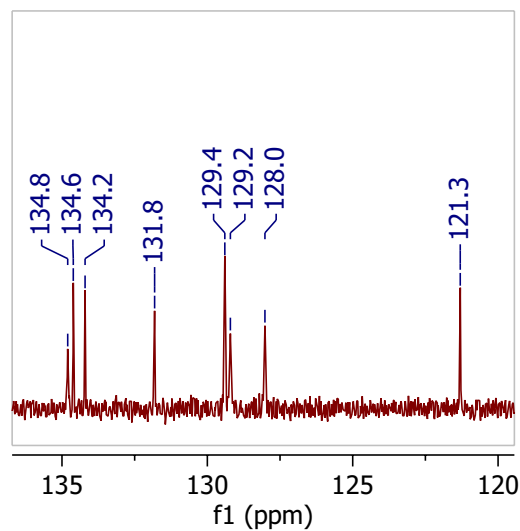
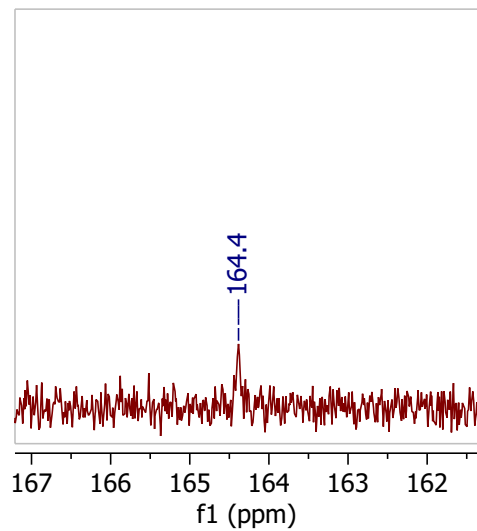
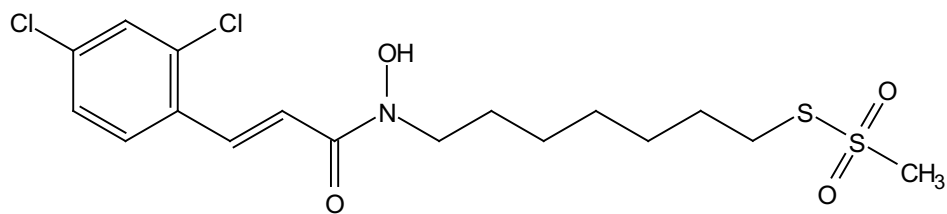
Compound 32
¹H NMR (151 MHz, DMSO-d6)



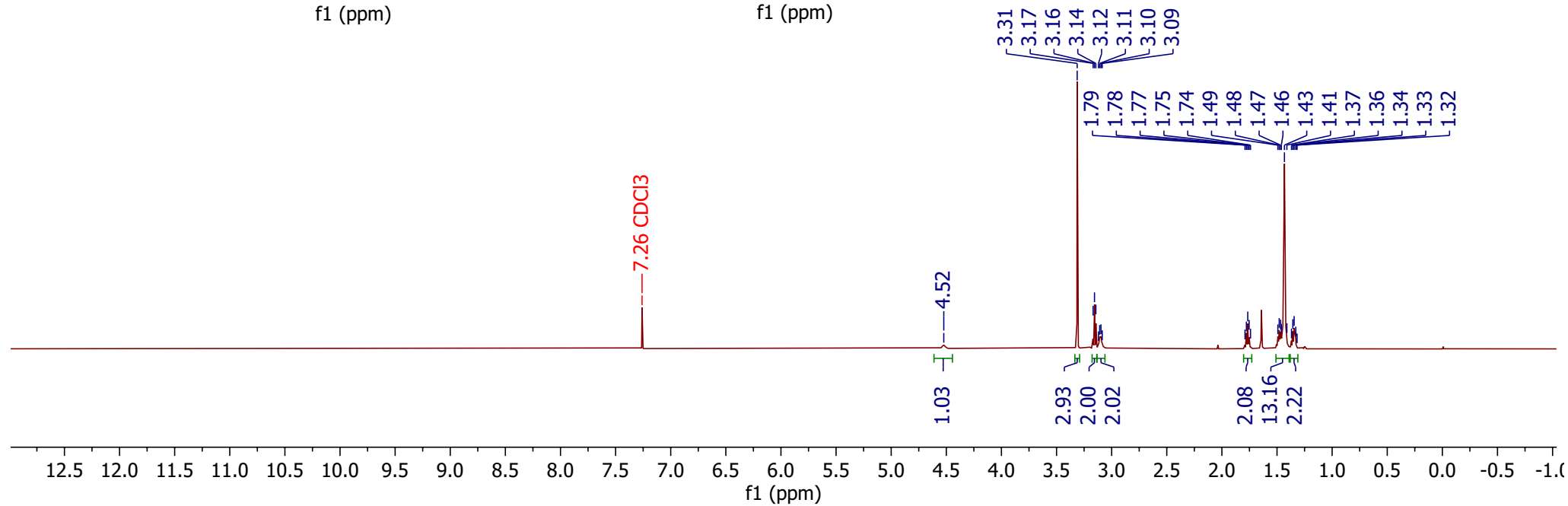
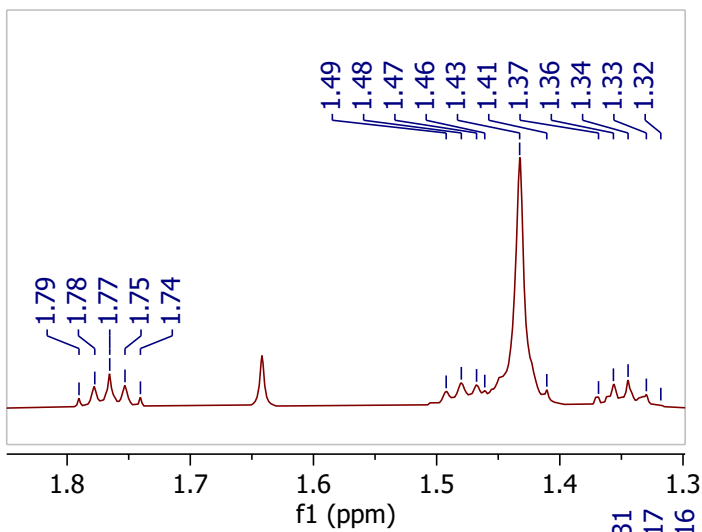
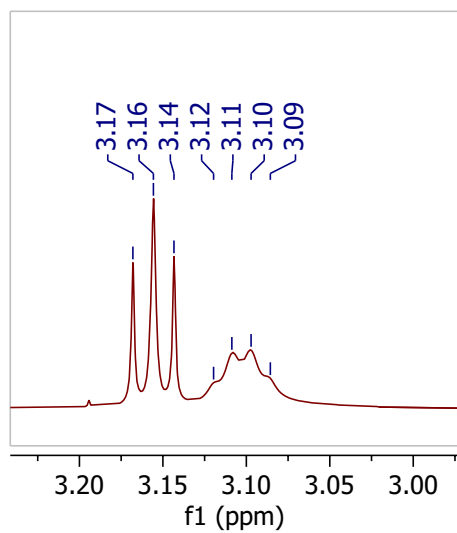
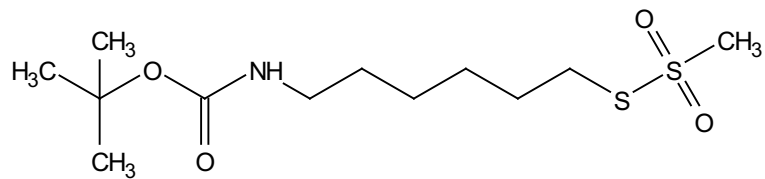
Compound 33
¹H NMR (600 MHz, DMSO-d6)



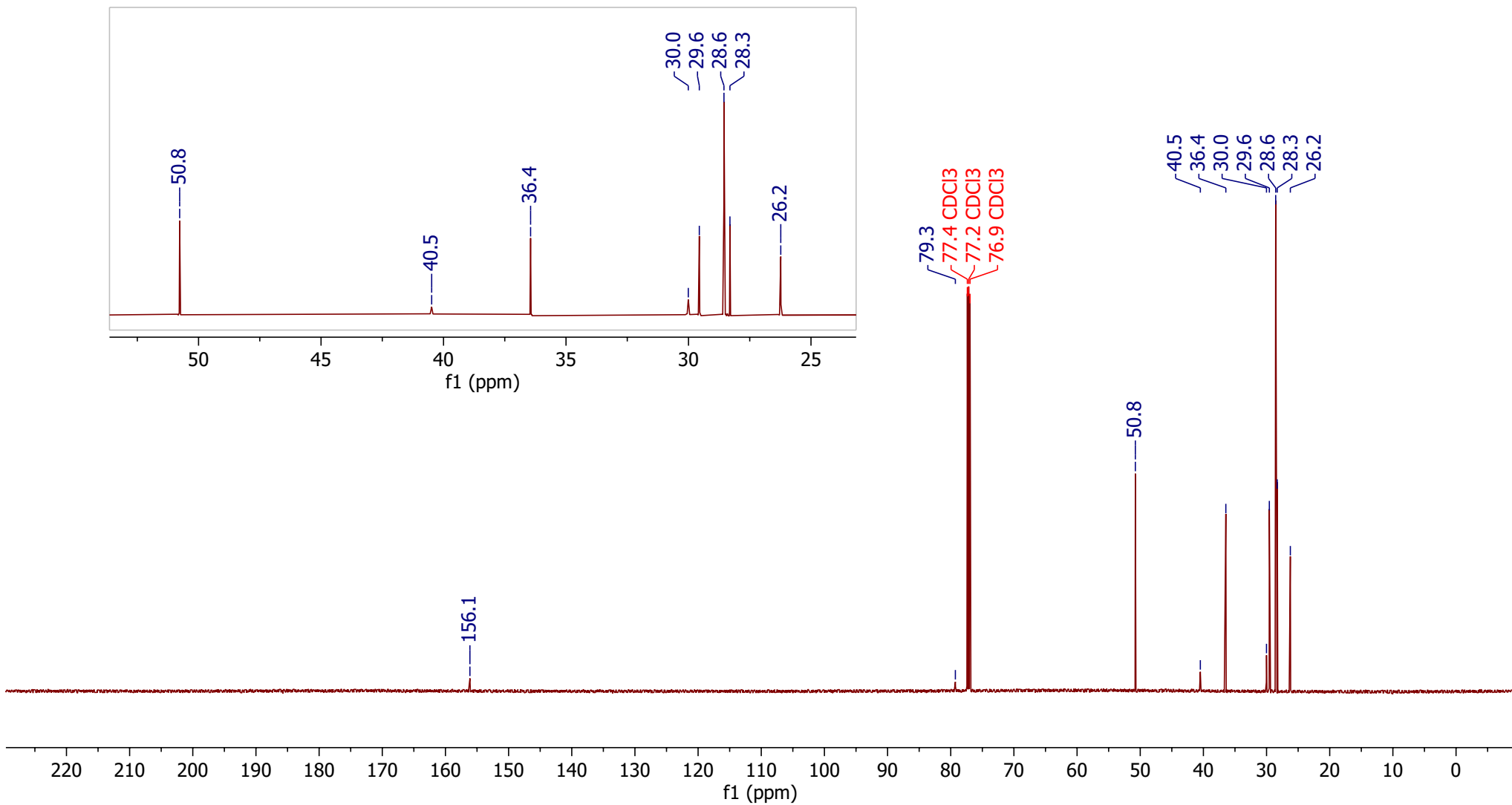
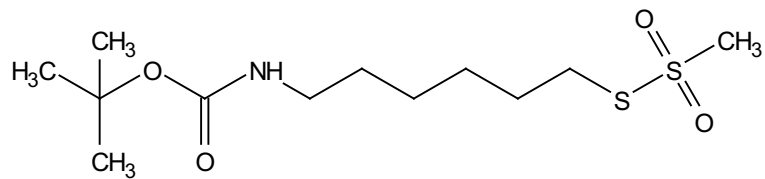
Compound 33
¹H NMR (151 MHz, DMSO-d6)



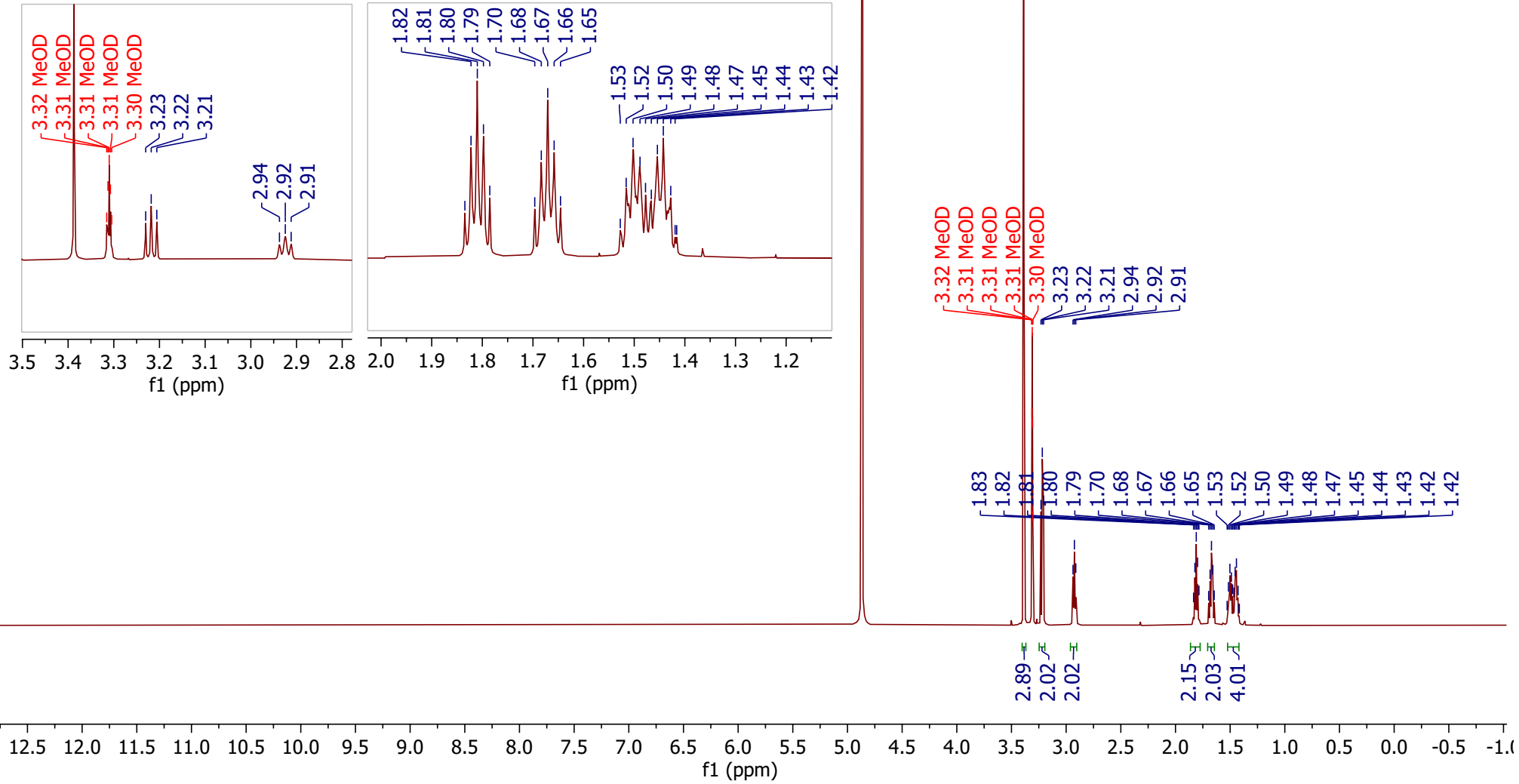
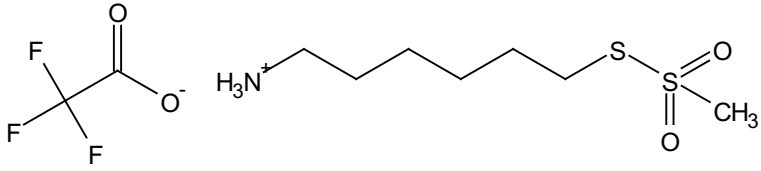
Compound 35
1H NMR (600 MHz, CDCl3)



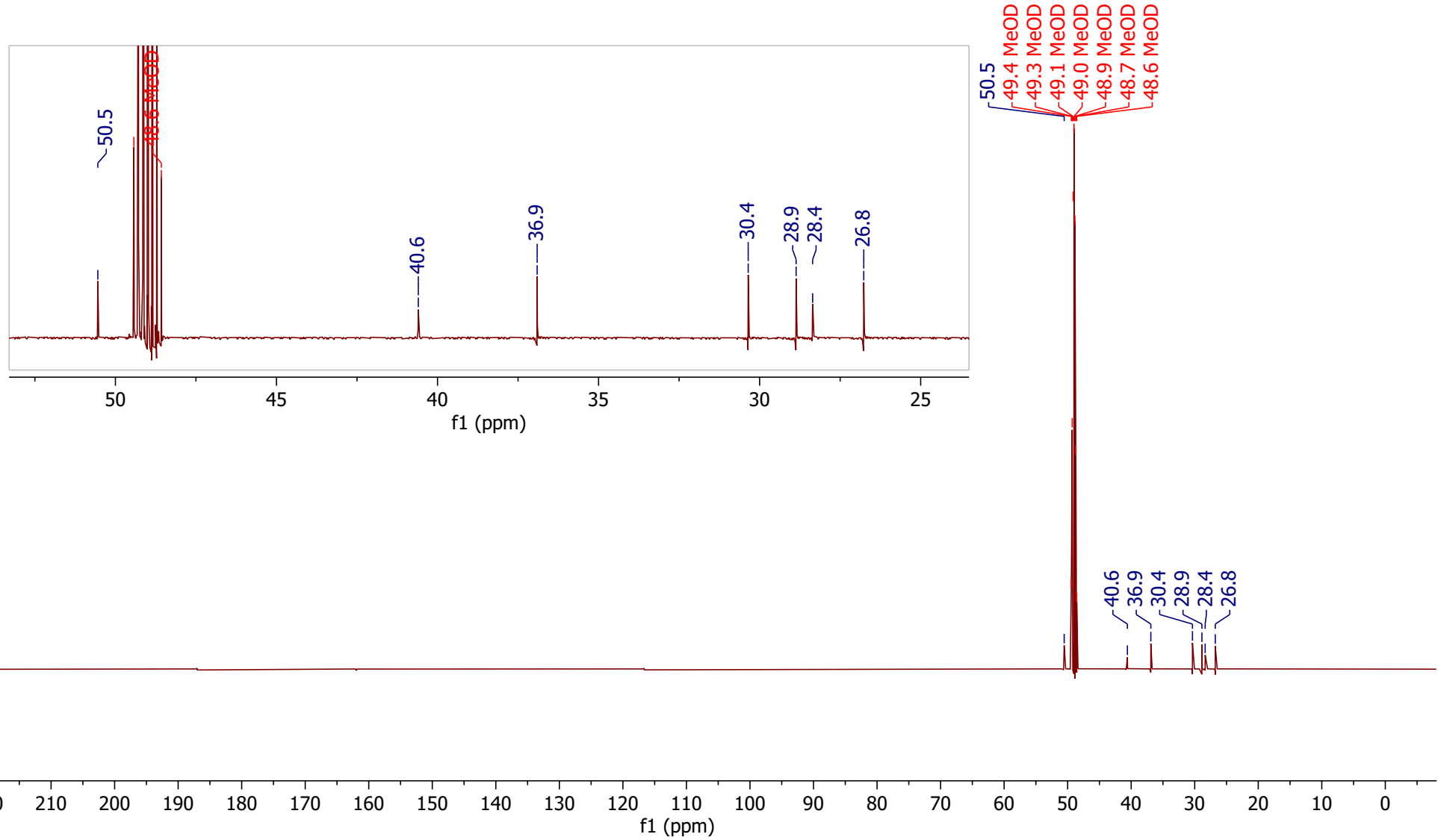
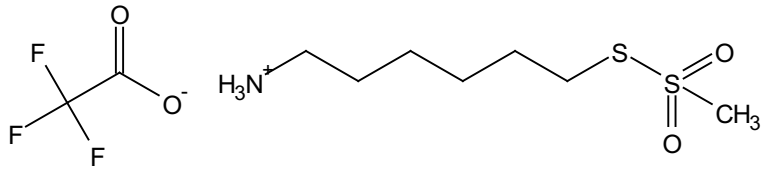
Compound 35
¹³C NMR (151 MHz, CDCl₃)



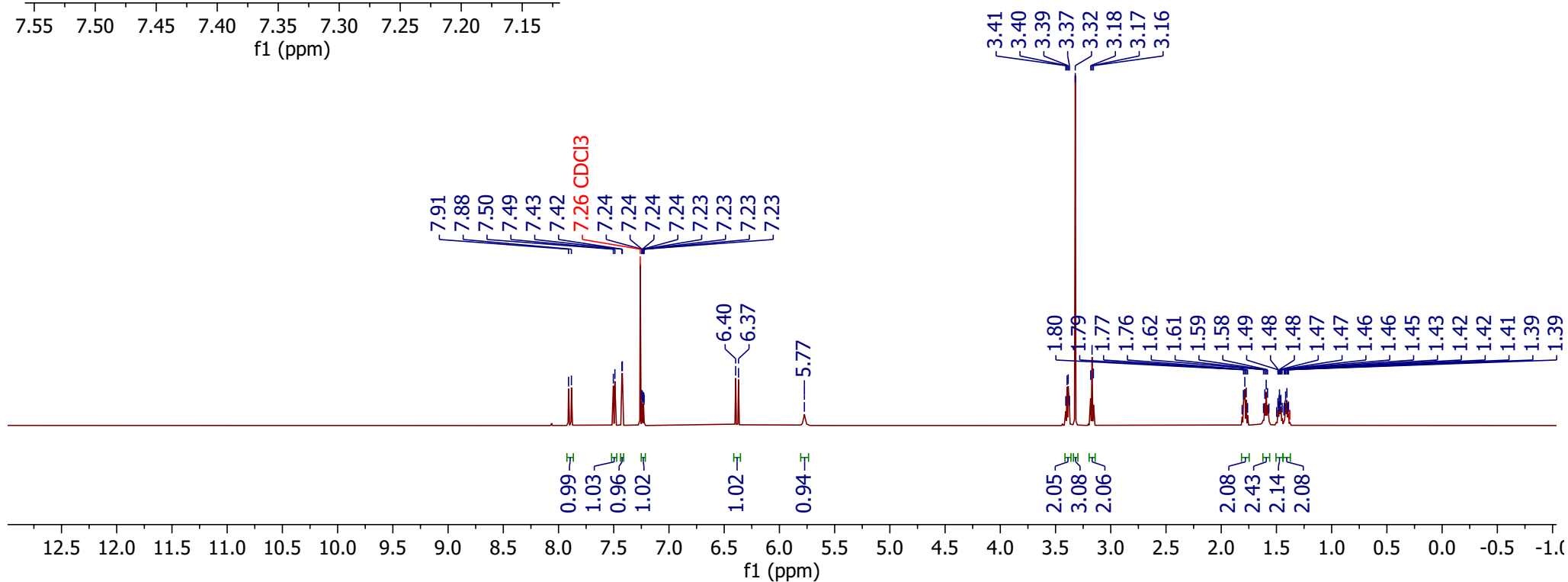
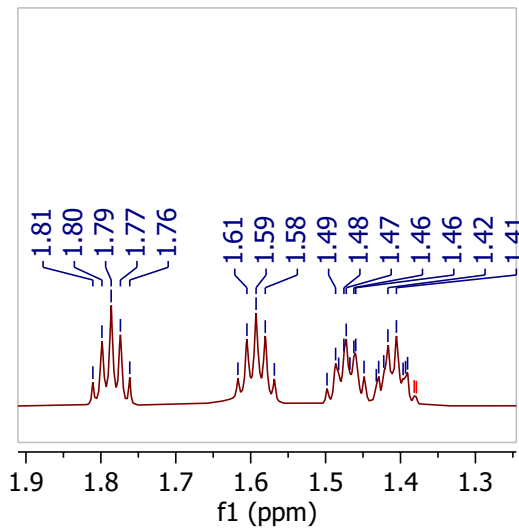
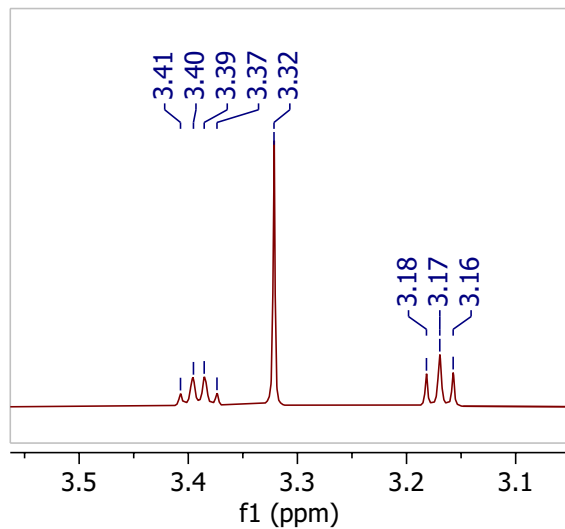
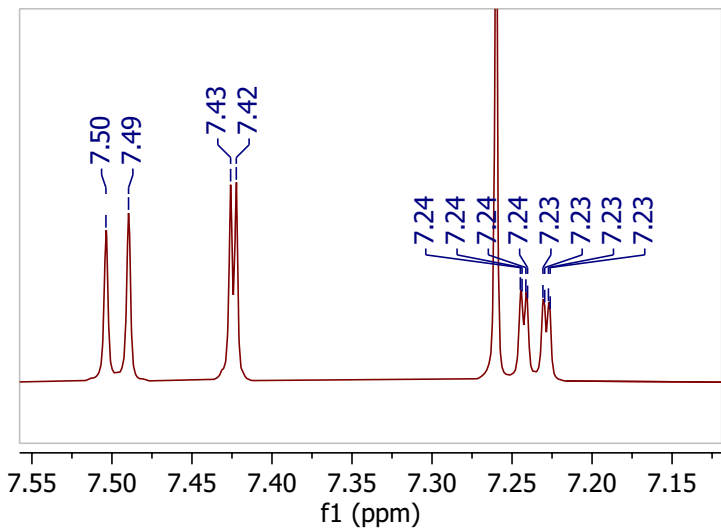
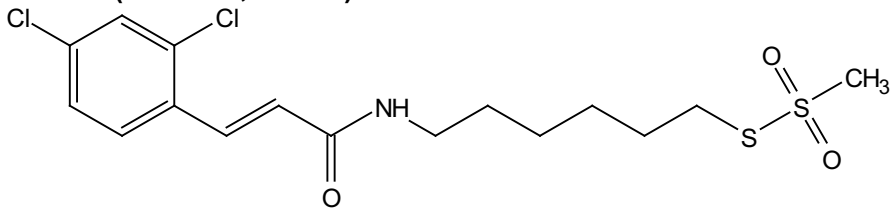
Compound 36
¹H NMR (600 MHz, MeOD-d4)



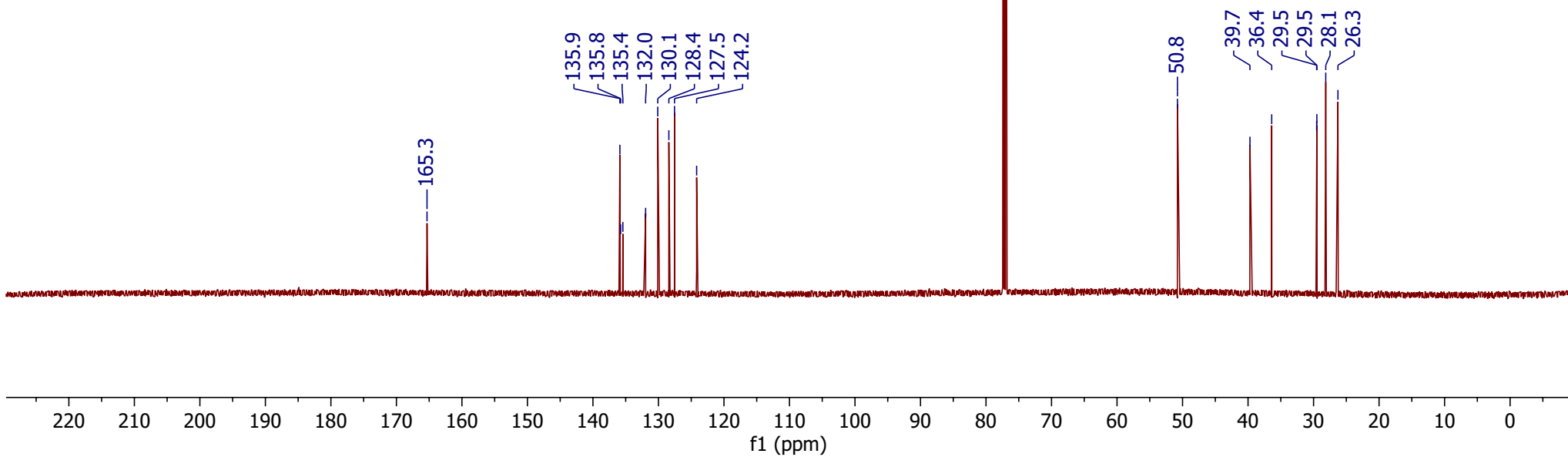
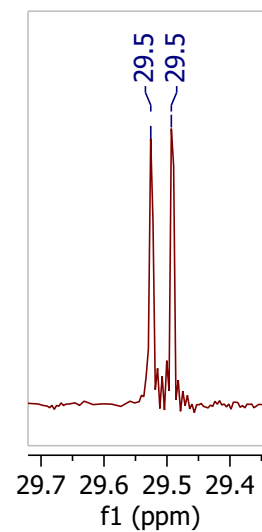
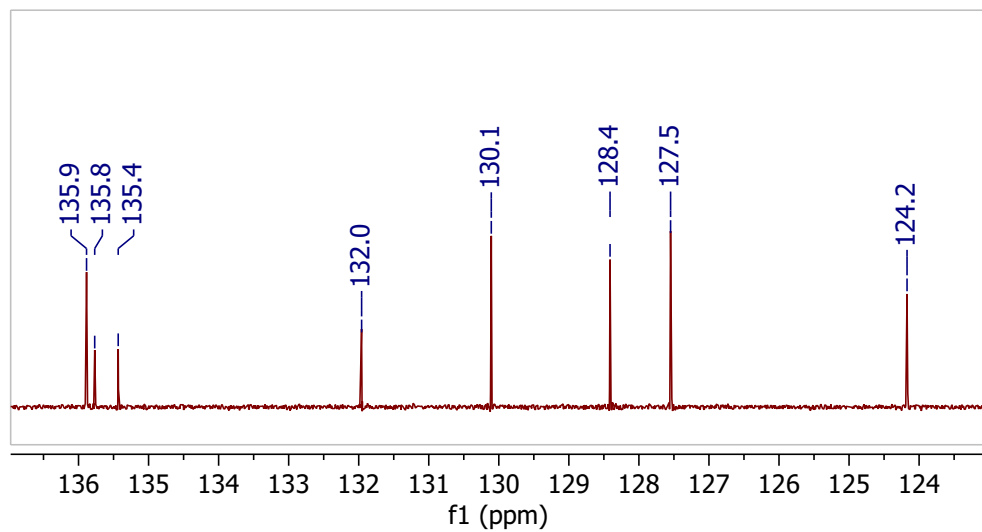
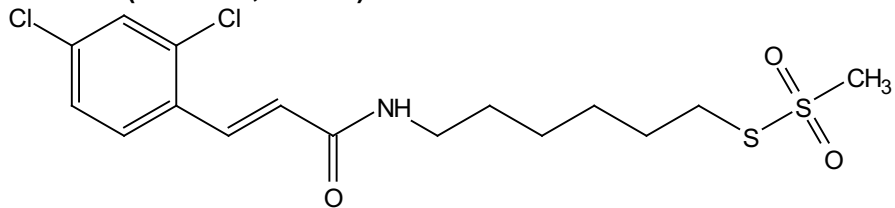
Compound 36
¹H NMR (151 MHz, MeOD-d4)



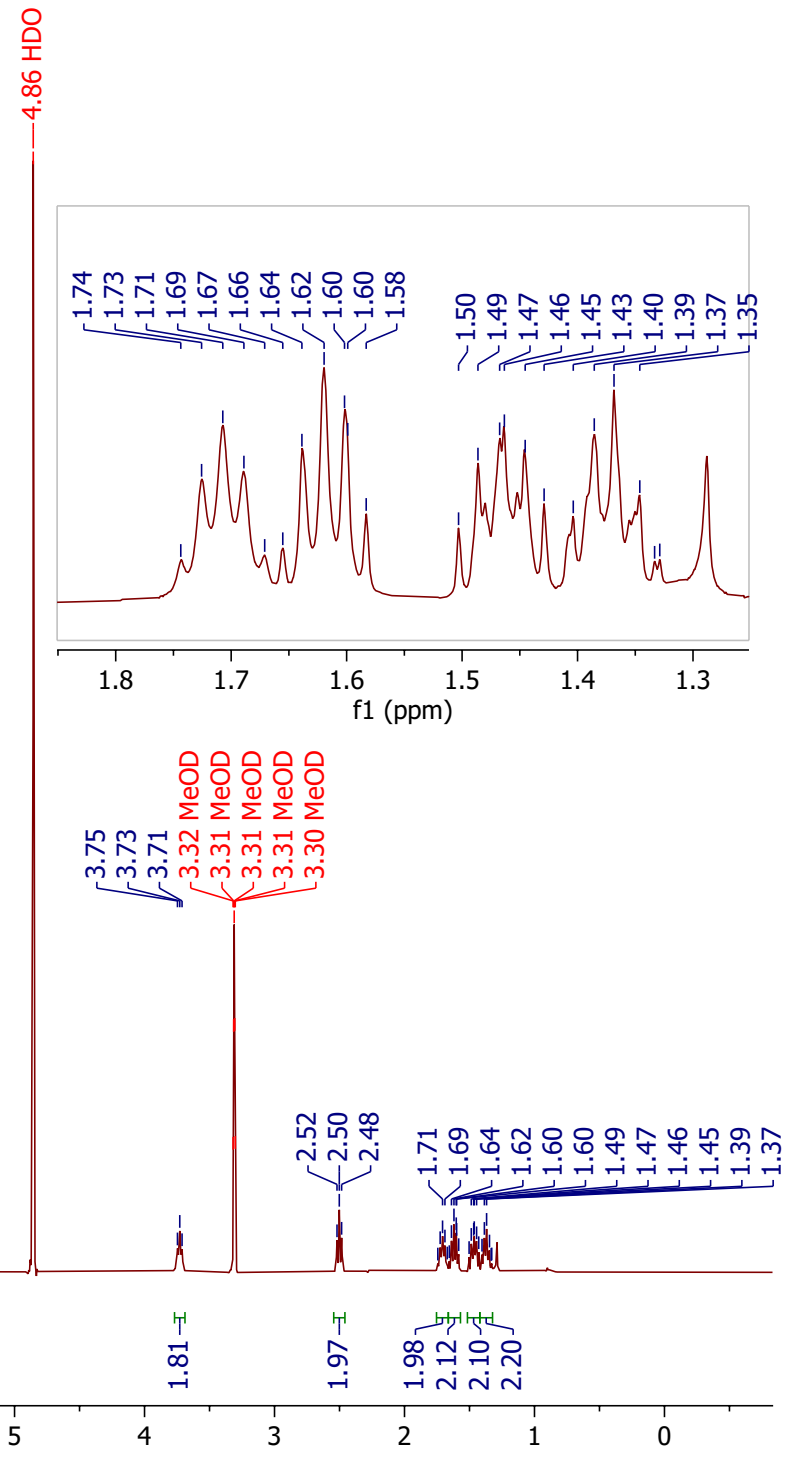
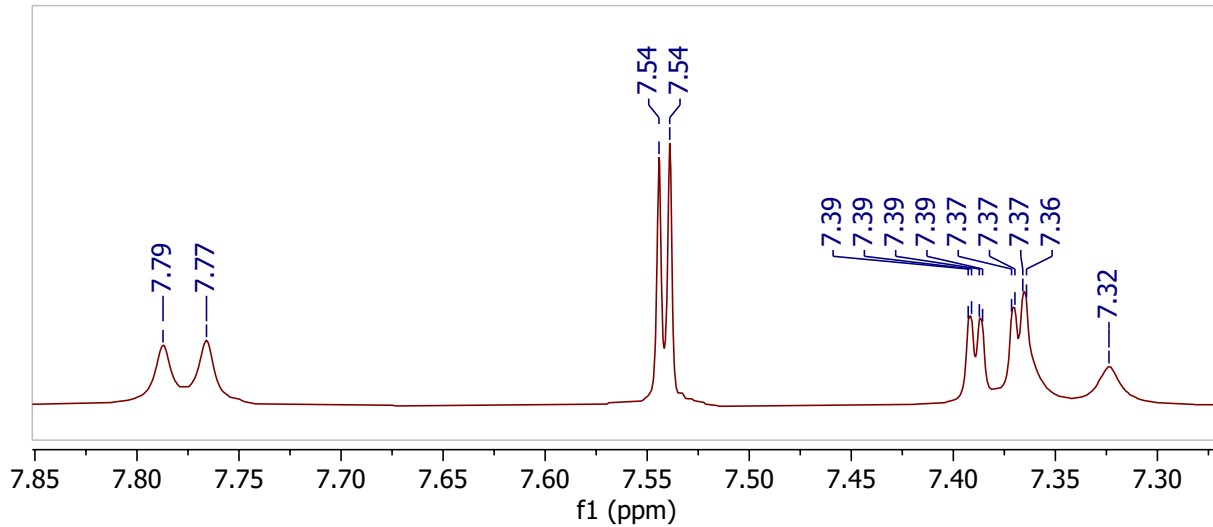
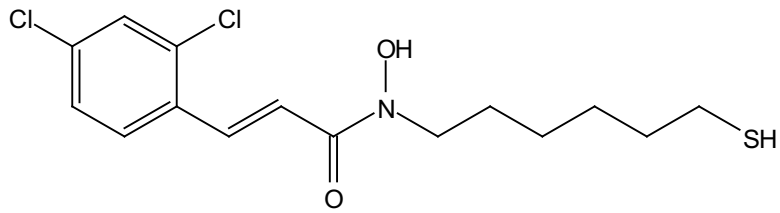
Compound 37
¹H NMR (600 MHz, CDCl₃)



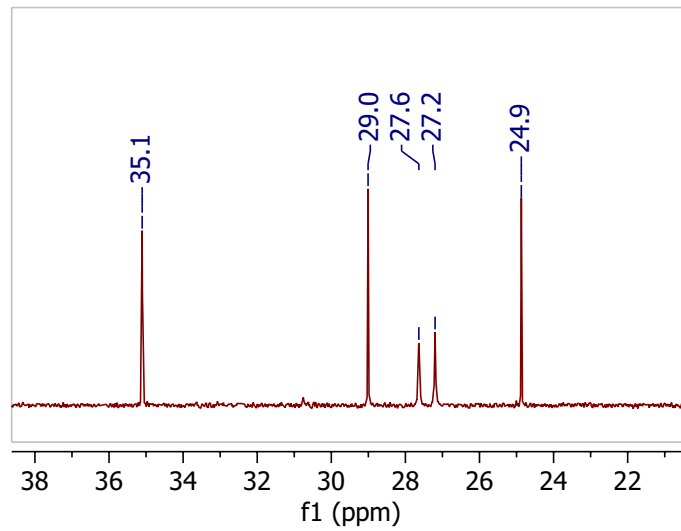
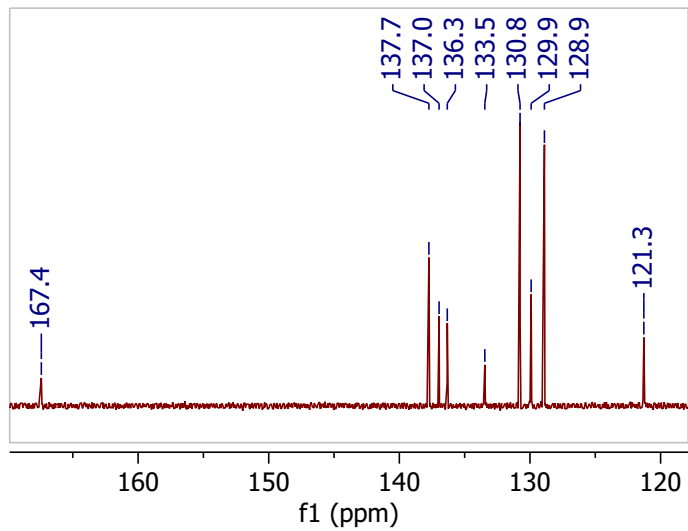
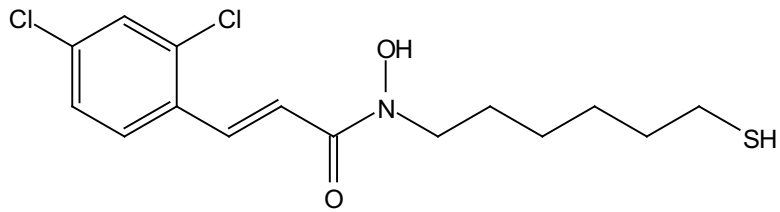
Compound 37
¹³C NMR (151 MHz, CDCl₃)



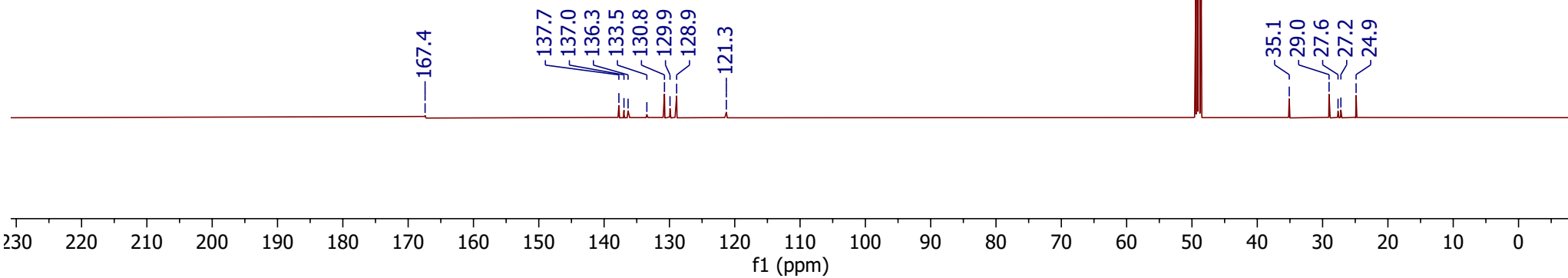
Compound 38
¹H NMR (400 MHz, MeOD)



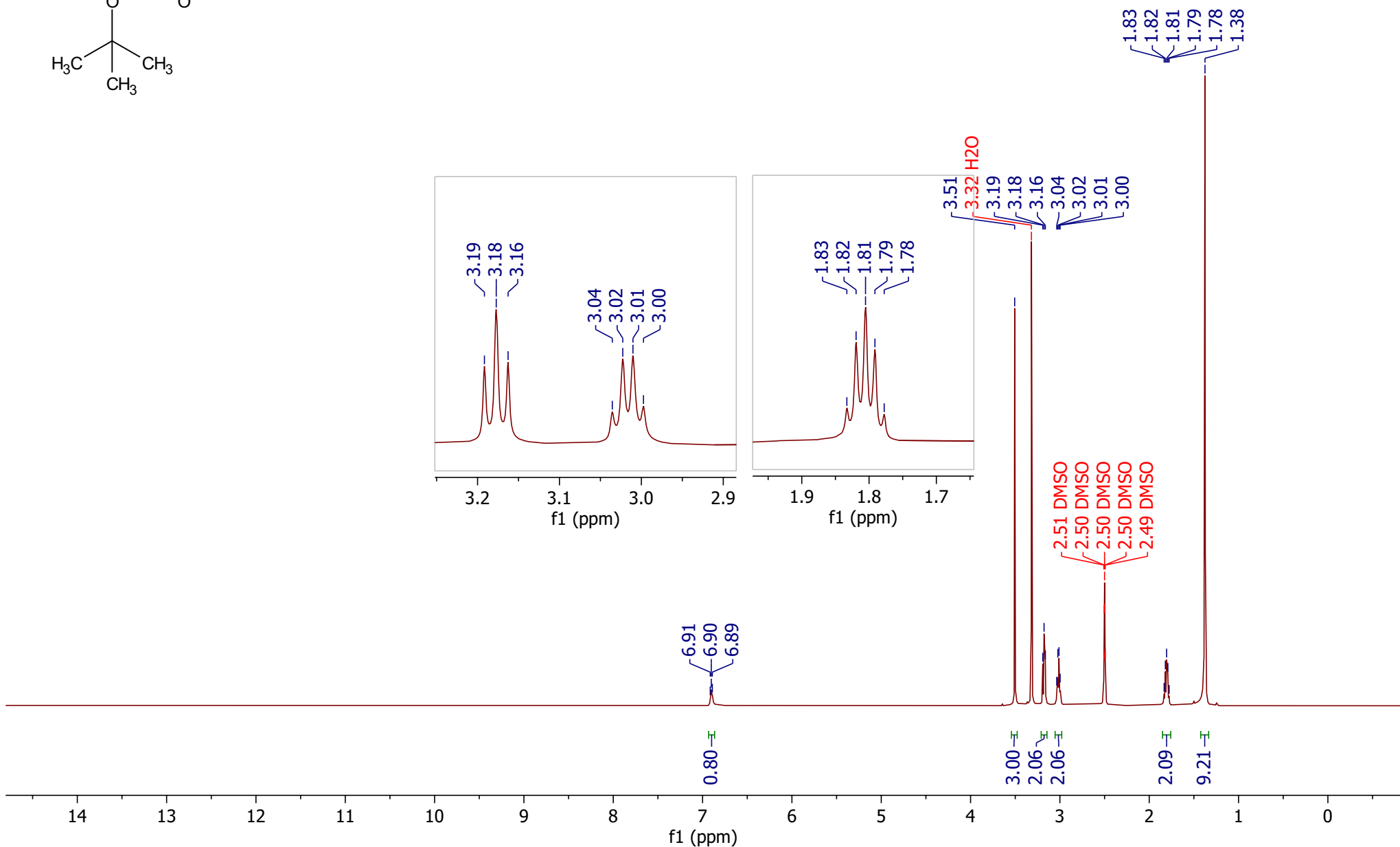
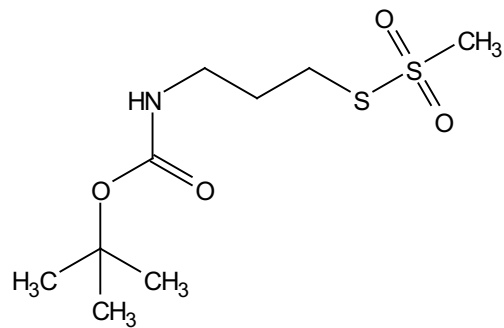
Compound 38
¹³C NMR (151 MHz, MeOD)



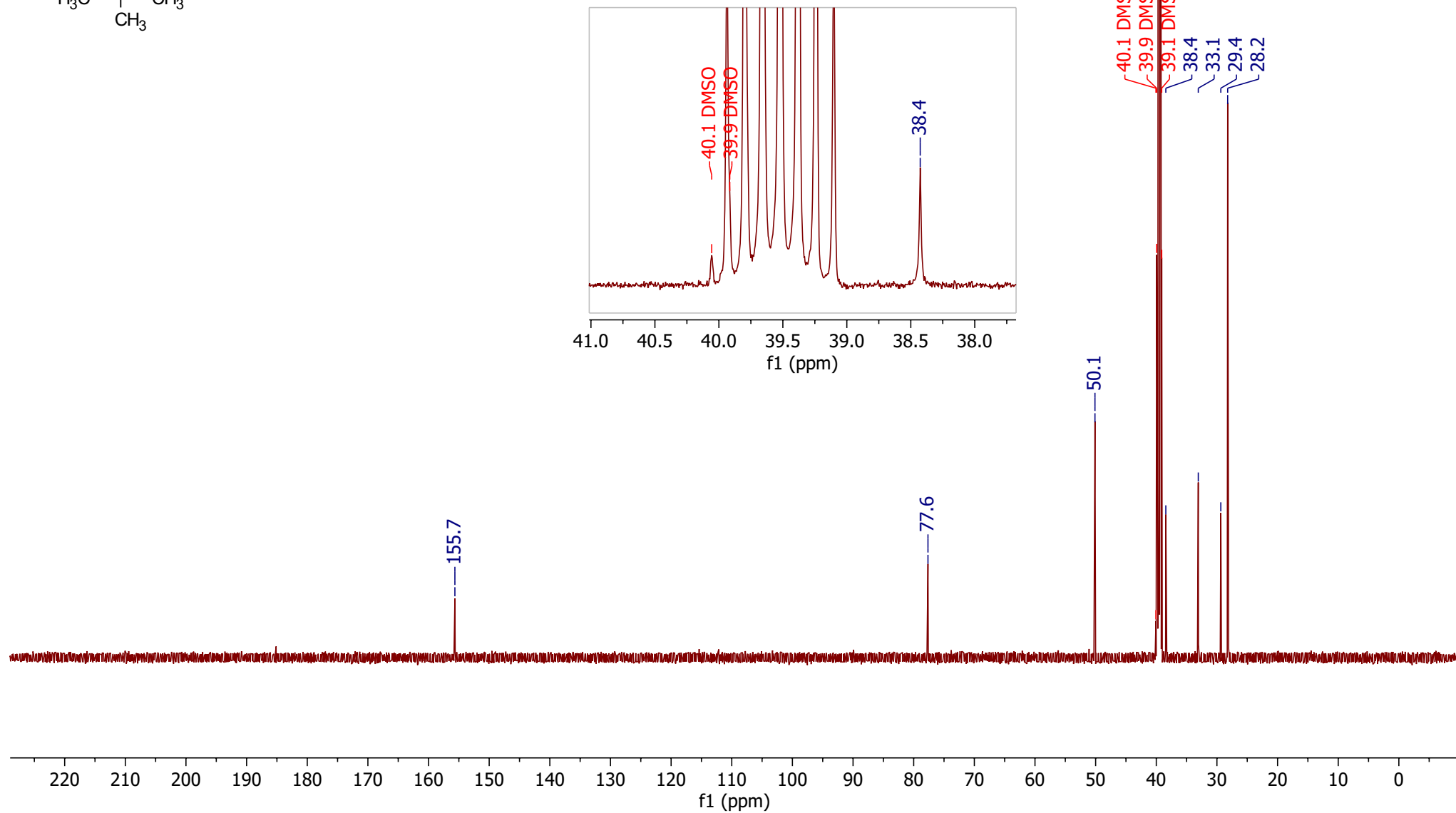
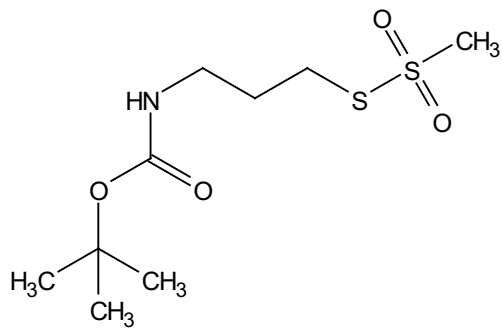
49.4 MeOD
49.3 MeOD
49.1 MeOD
49.0 MeOD
48.9 MeOD
48.7 MeOD
48.6 MeOD



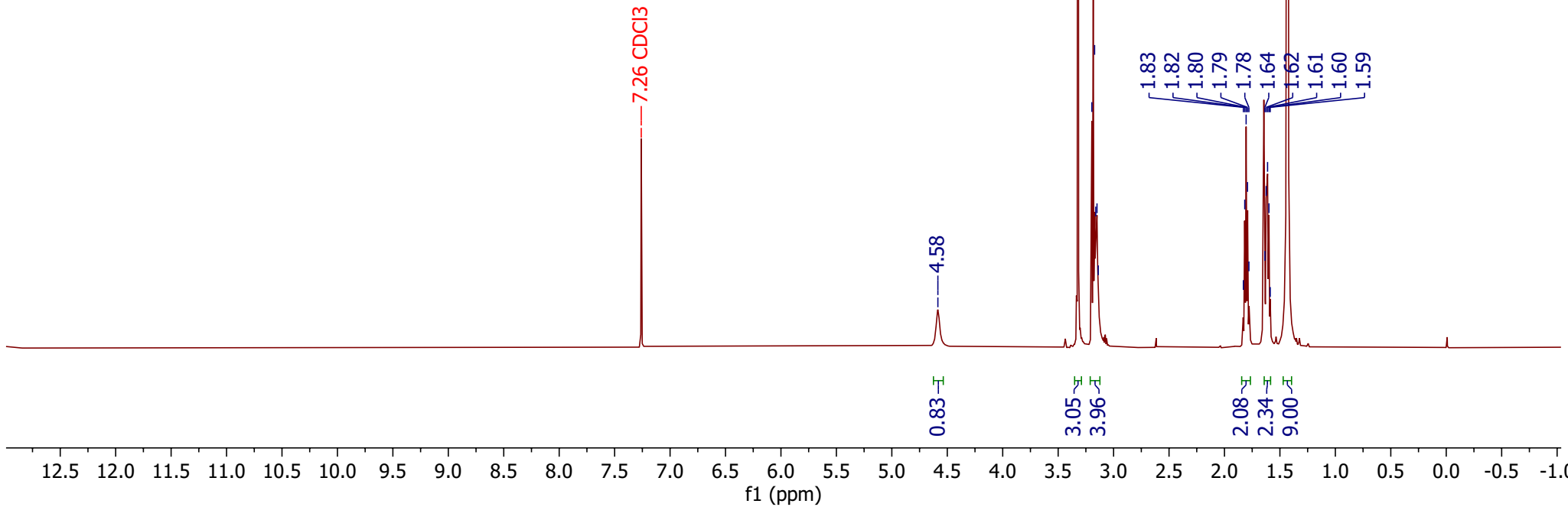
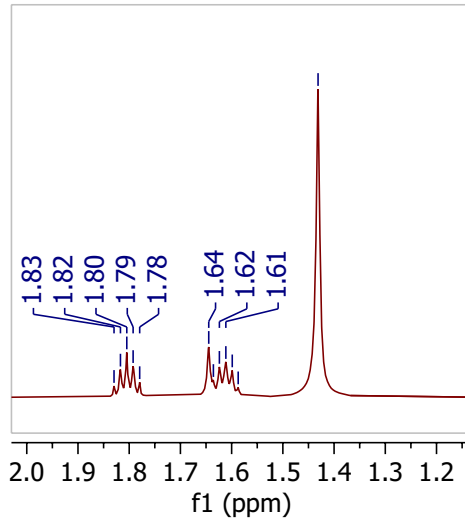
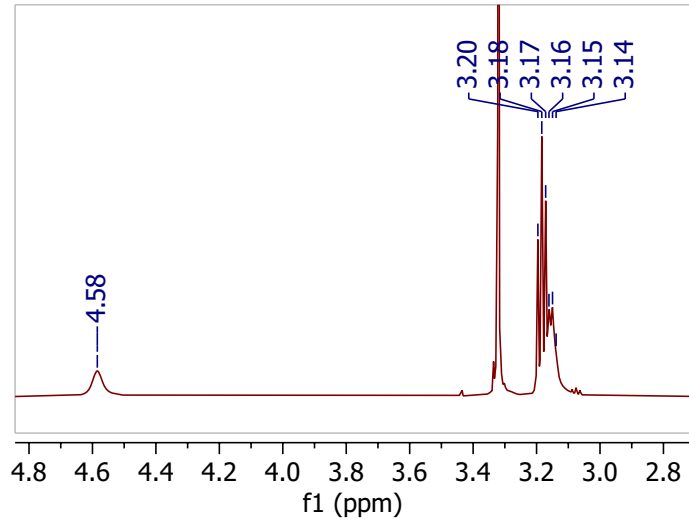
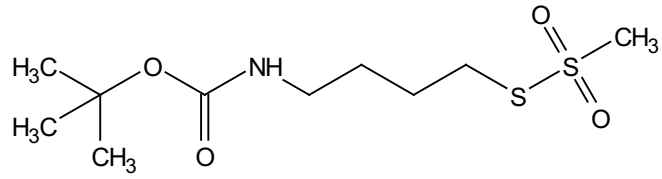
Compound 43
¹H NMR (500 MHz, DMSO-d6)



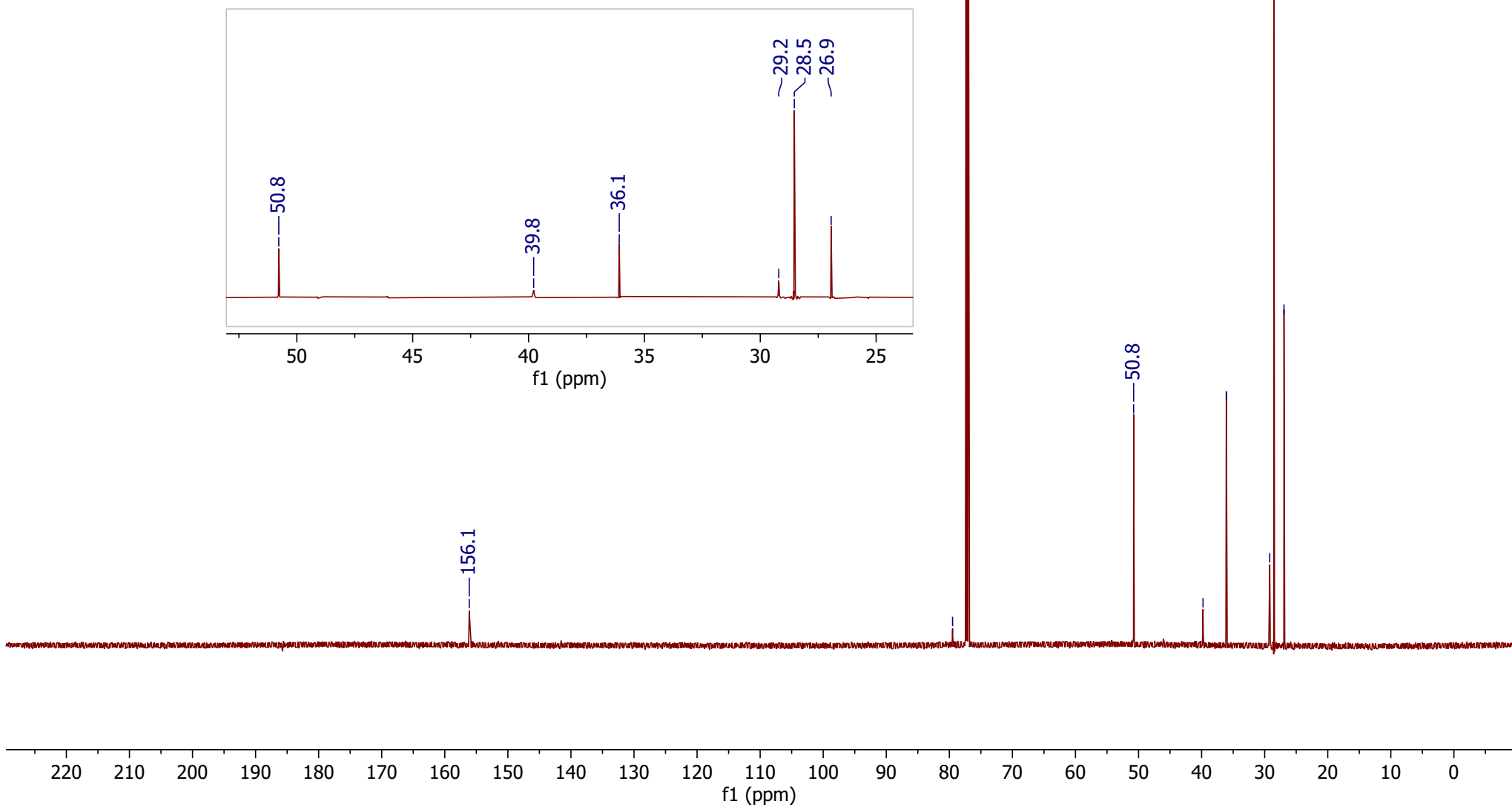
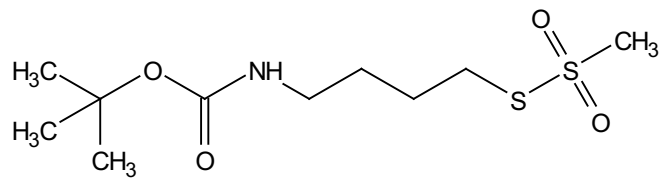
Compound 43
¹H NMR (151 MHz, DMSO-d6)



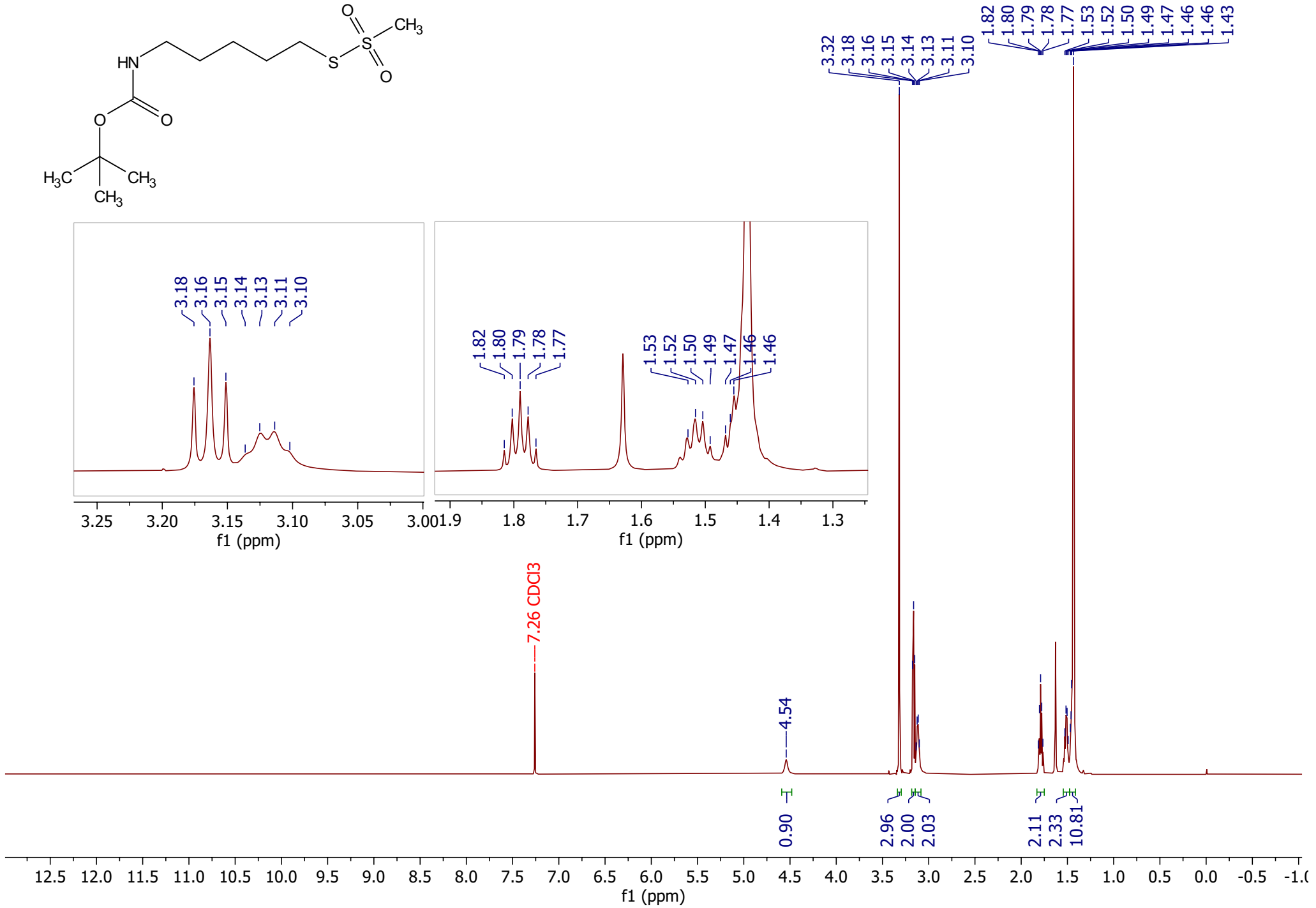
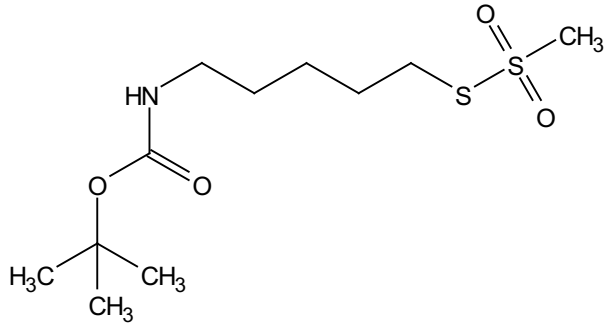
Compound 44
¹H NMR (600 MHz, CDCl₃)



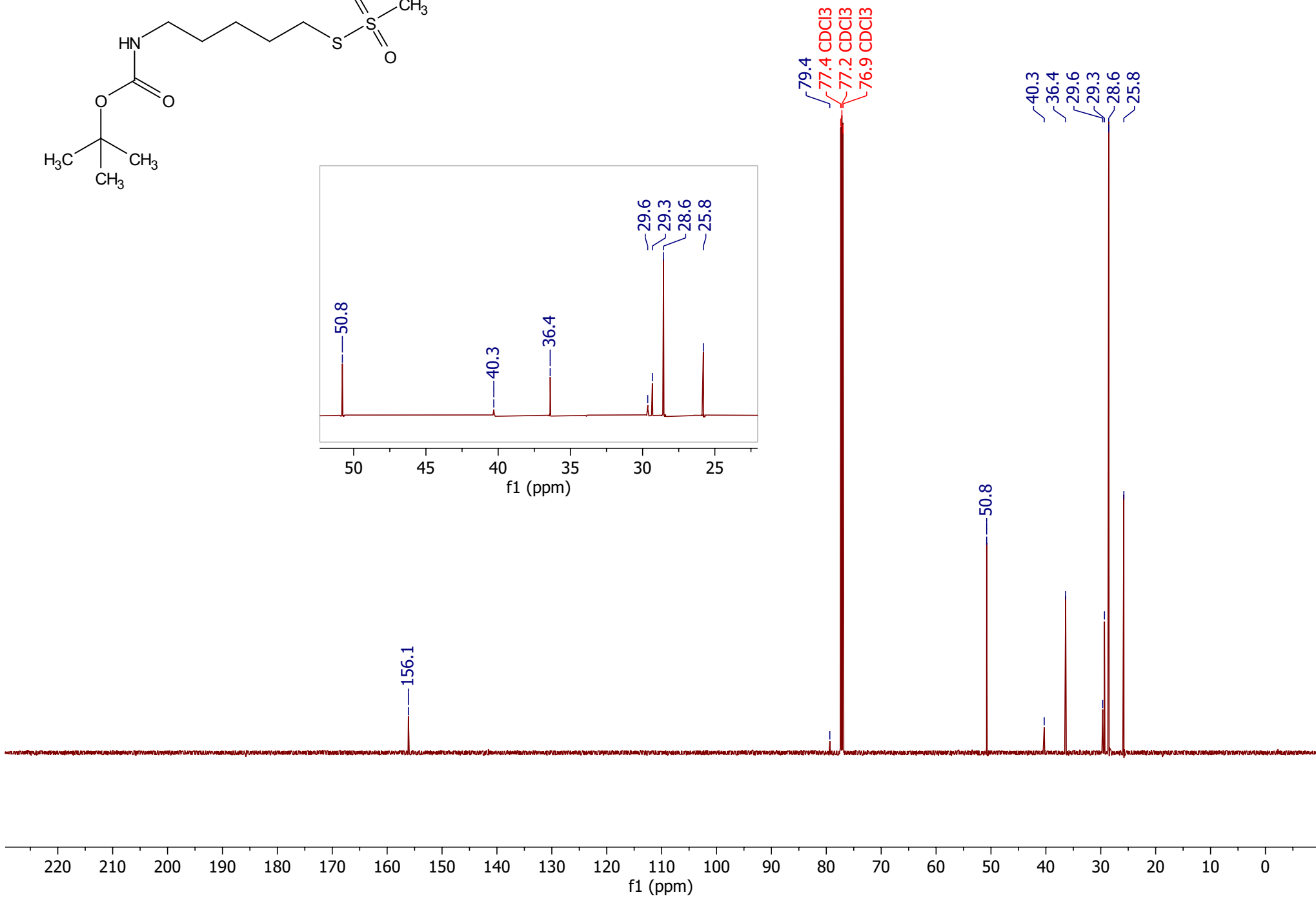
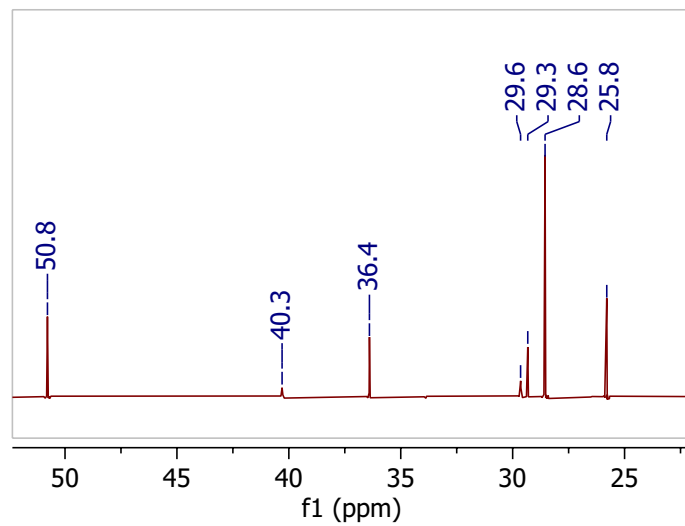
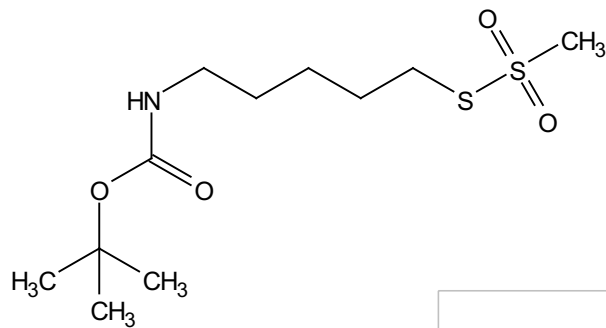
Compound 44
¹³C NMR (151 MHz, CDCl₃)



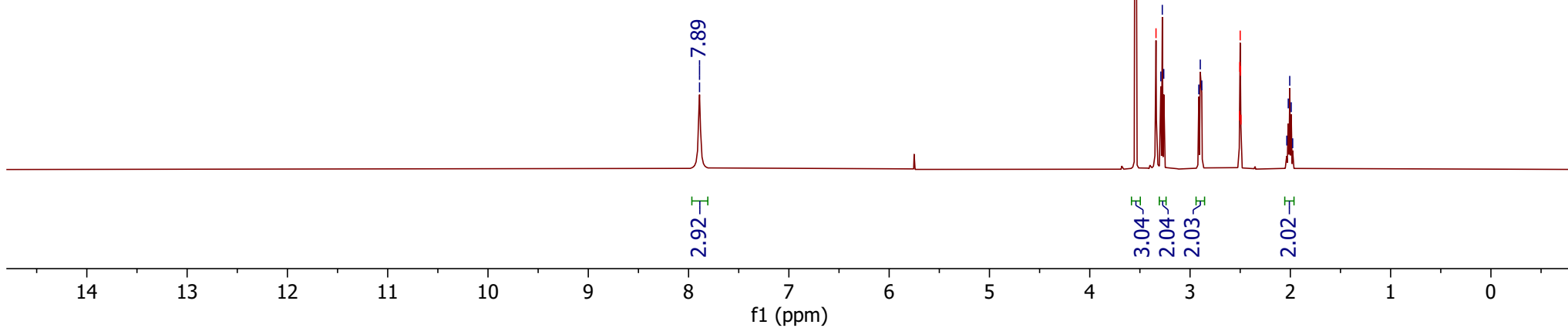
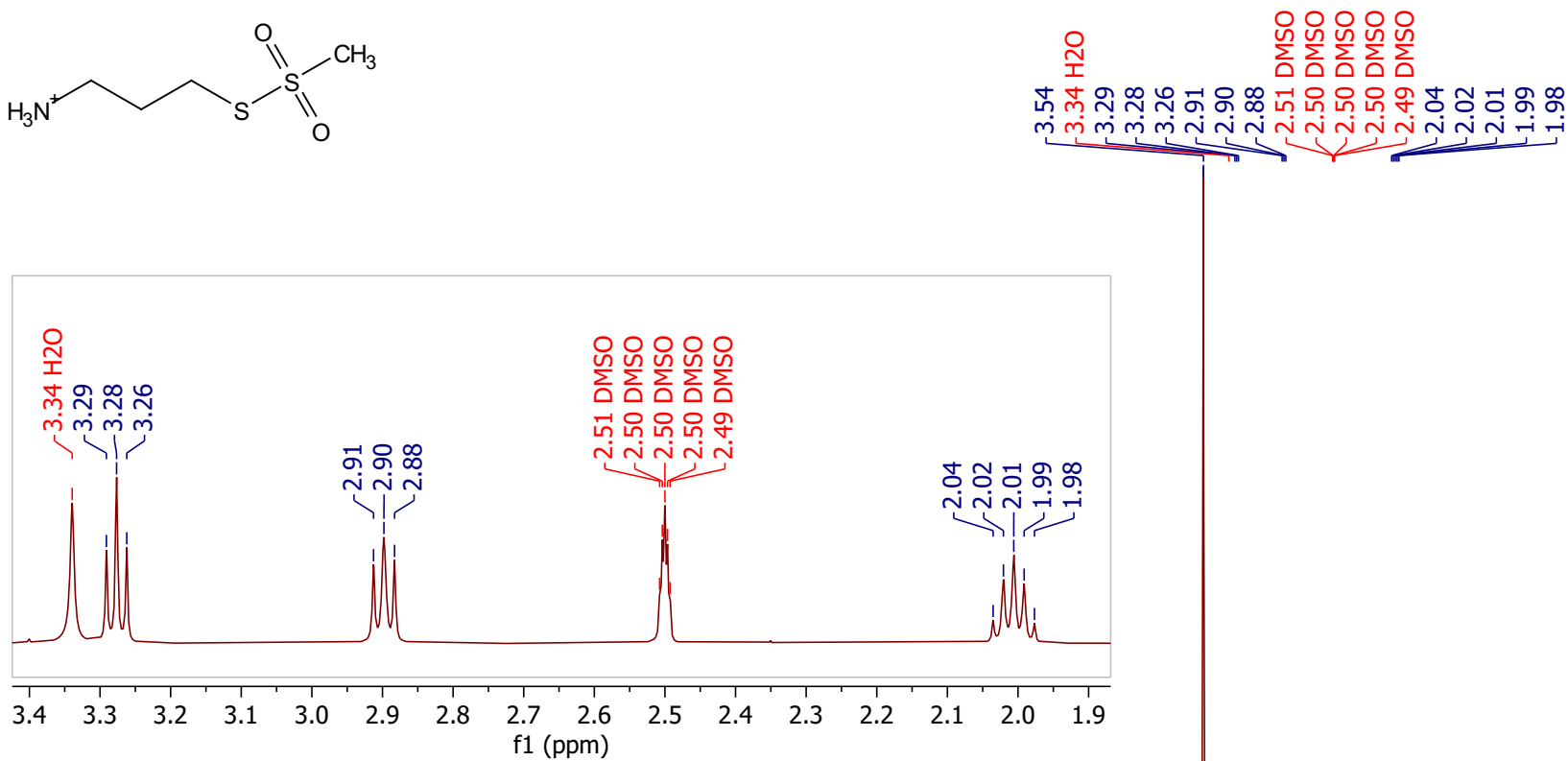
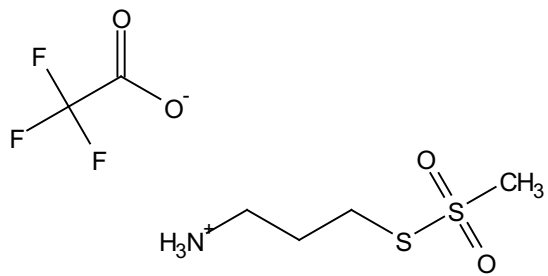
Compound 45
¹H NMR (600 MHz, CDCl₃)



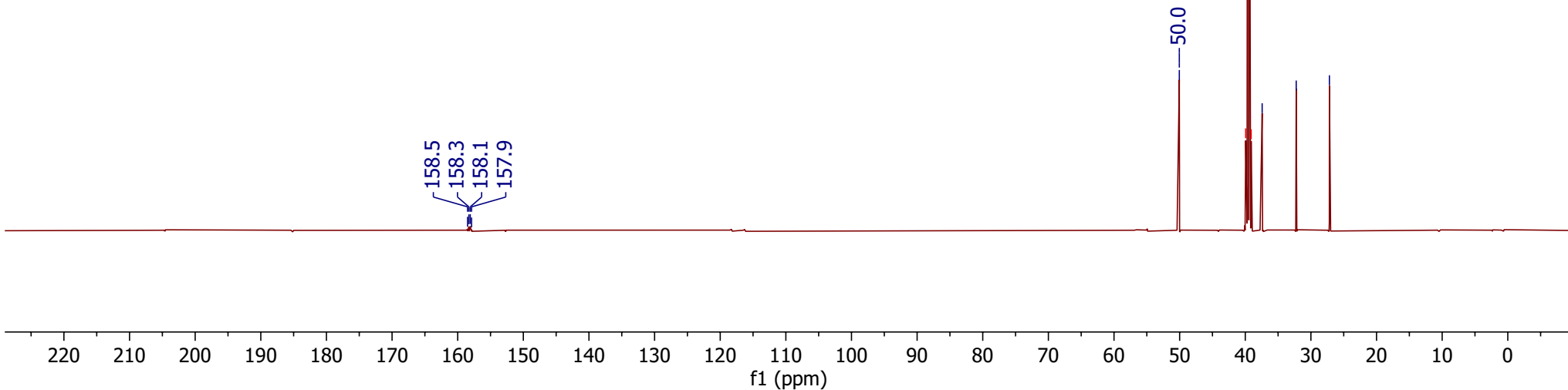
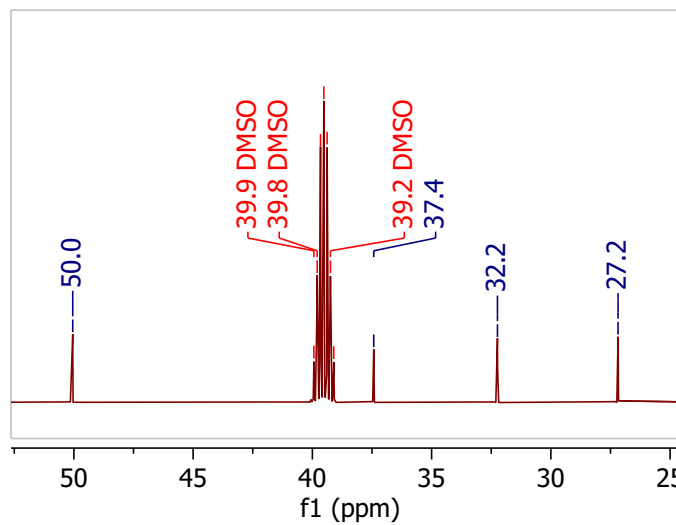
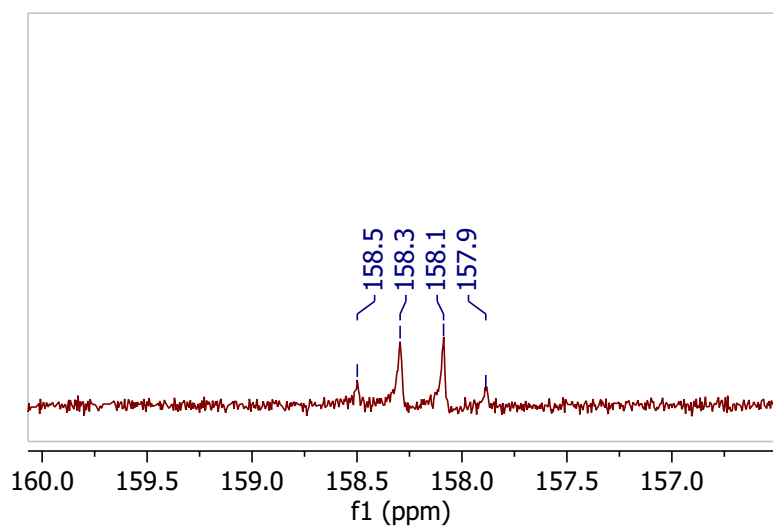
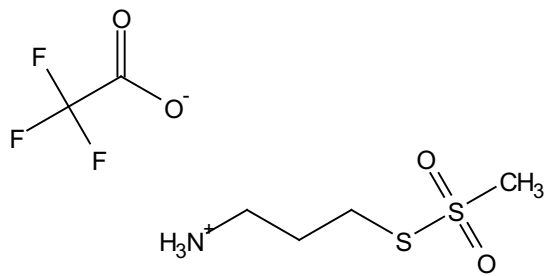
Compound 45
¹³C NMR (151 MHz, CDCl₃)



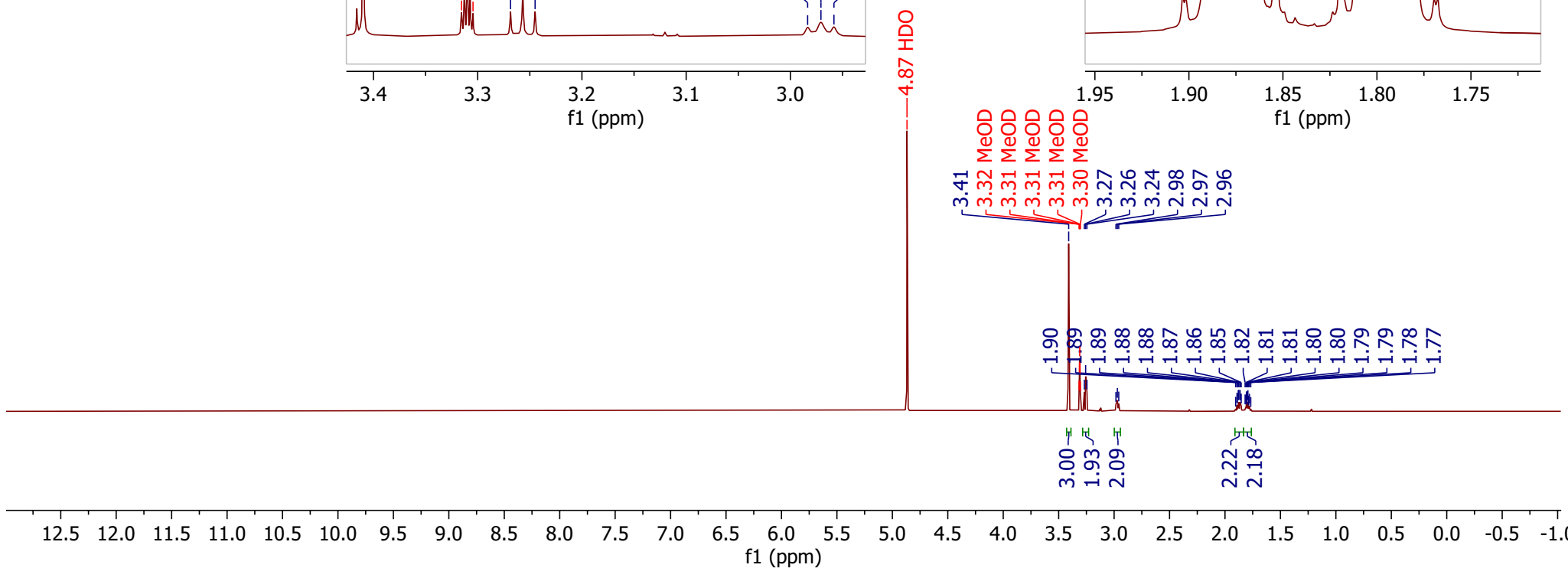
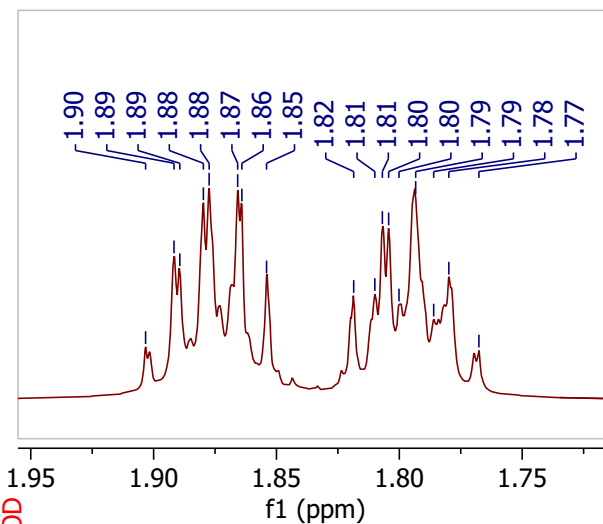
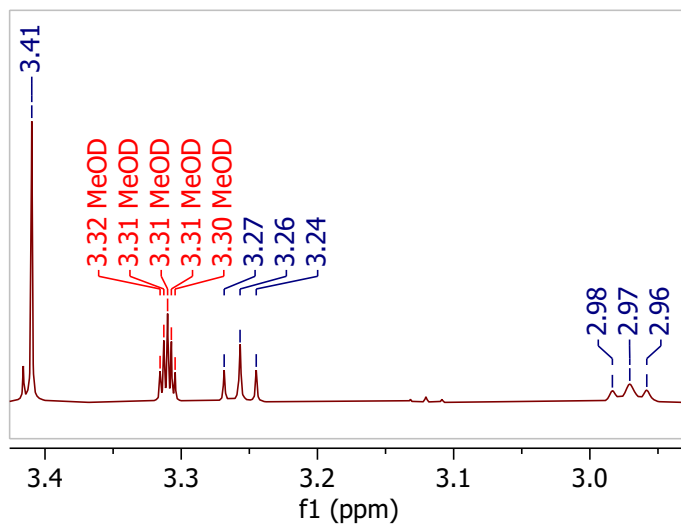
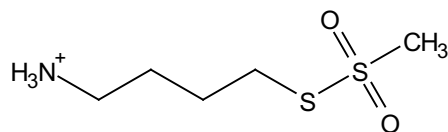
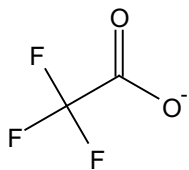
Compound 4
1H NMR (500 MHz, DMSO-d6)



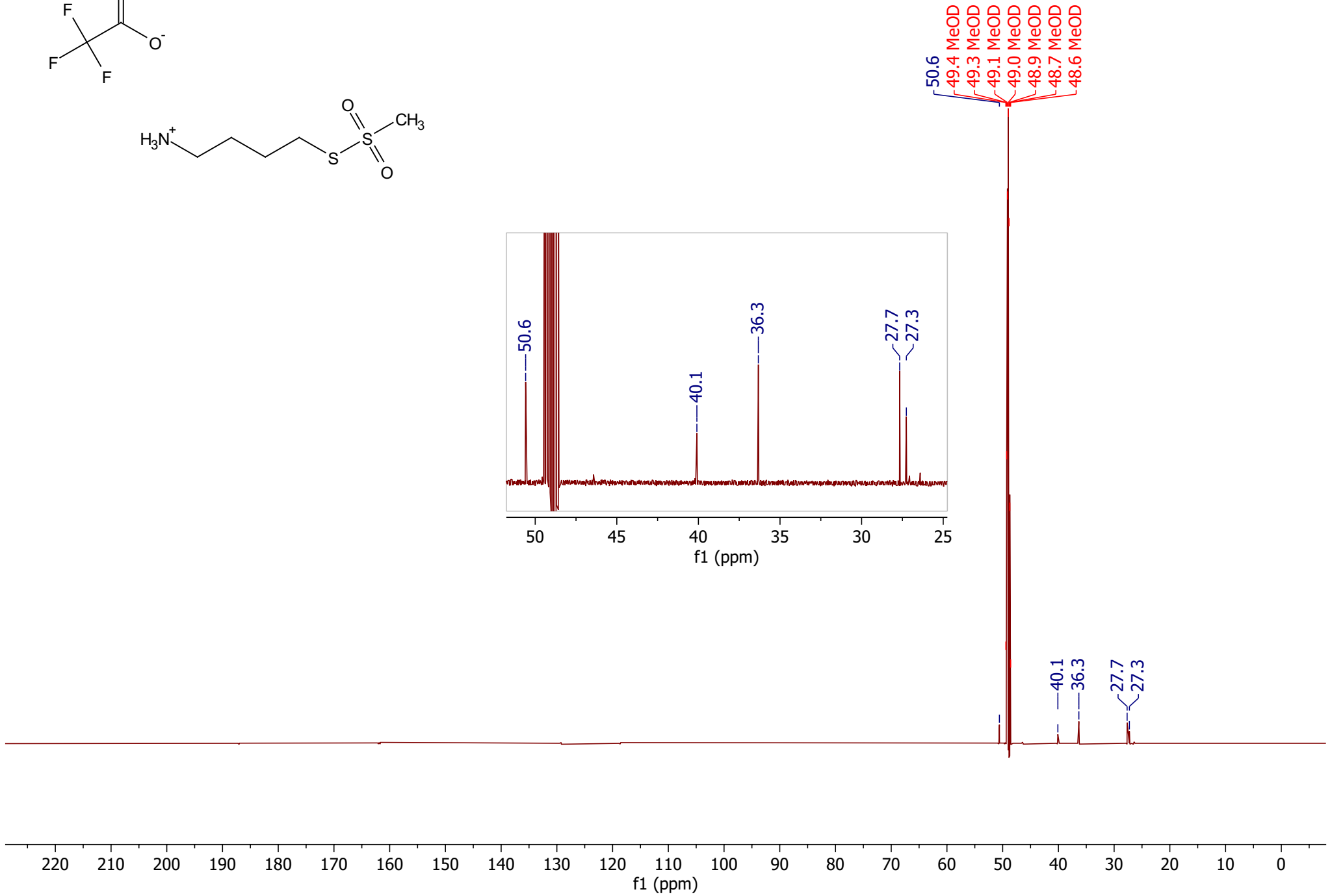
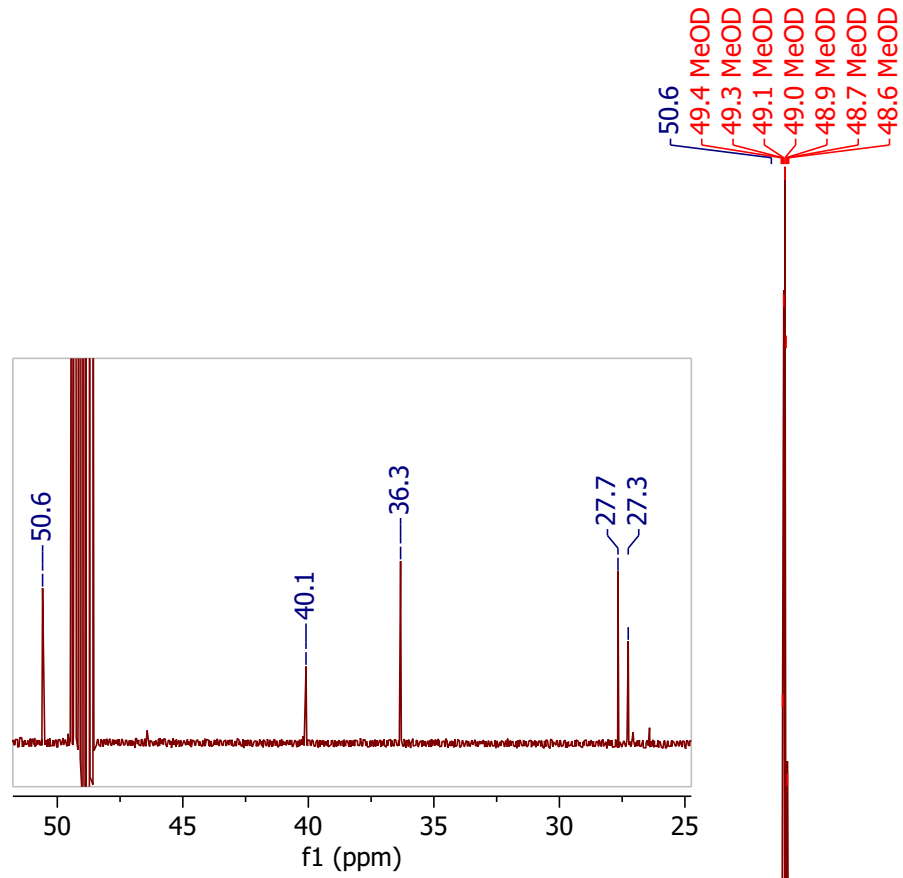
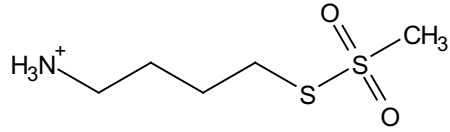
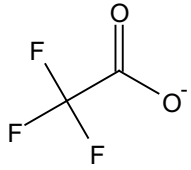
Compound 4
¹H NMR (151 MHz, DMSO-d6)



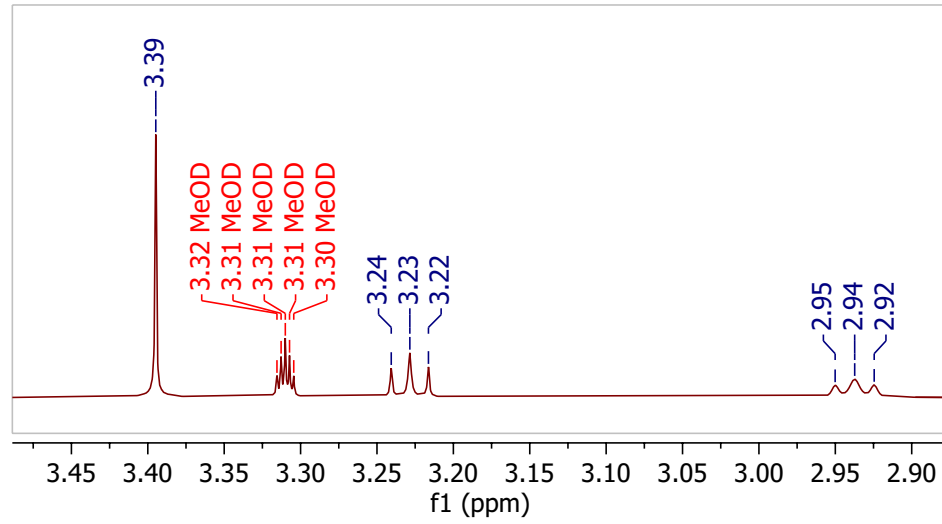
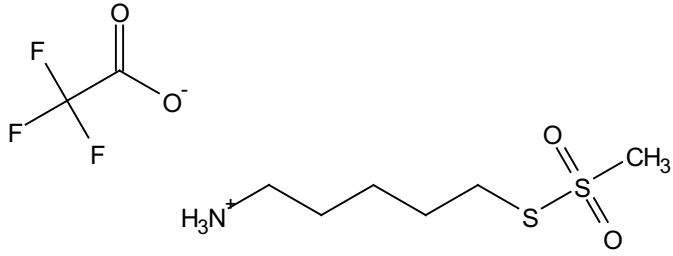
Compound 46
¹H NMR (600 MHz, MeOD-d4)



Compound 46
¹H NMR (151 MHz, MeOD-d4)

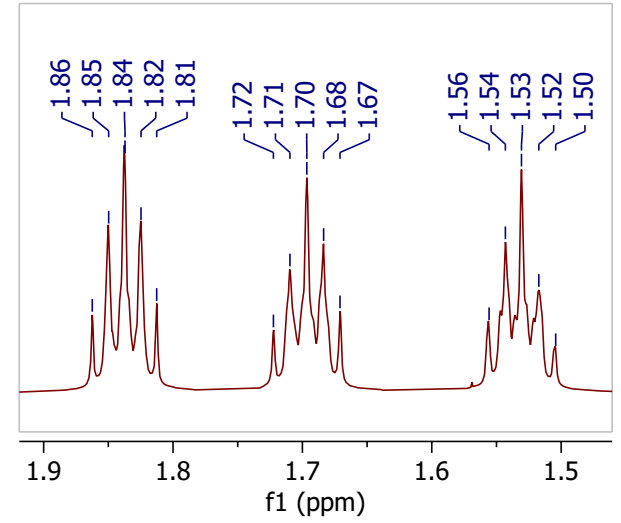


Compound 47
¹H NMR (600 MHz, MeOD-d4)



4.87 HDO

3.39
3.32 MeOD
3.31 MeOD
3.31 MeOD
3.31 MeOD
3.30 MeOD
3.24
3.23
3.22
2.95
2.94
2.92

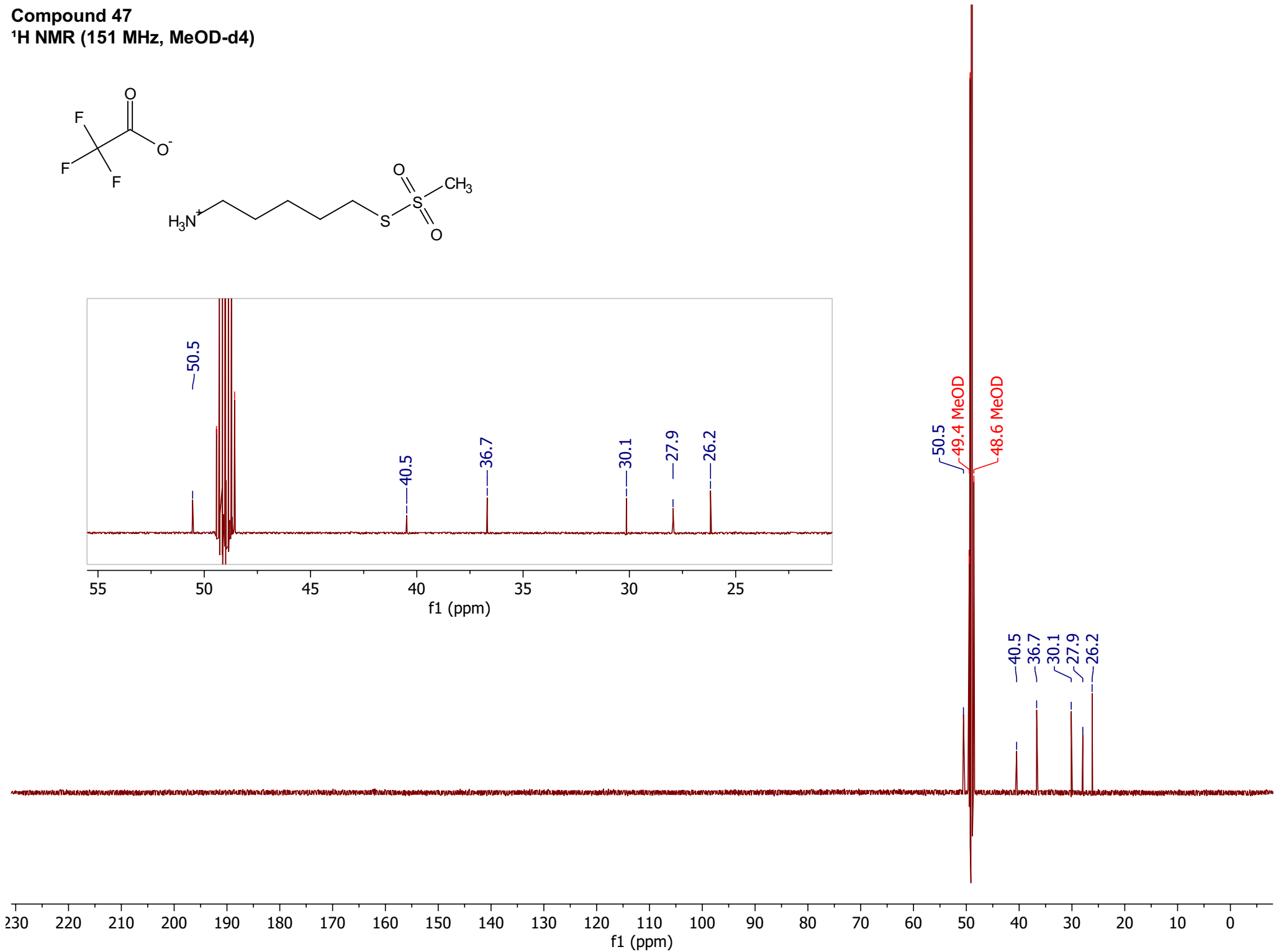
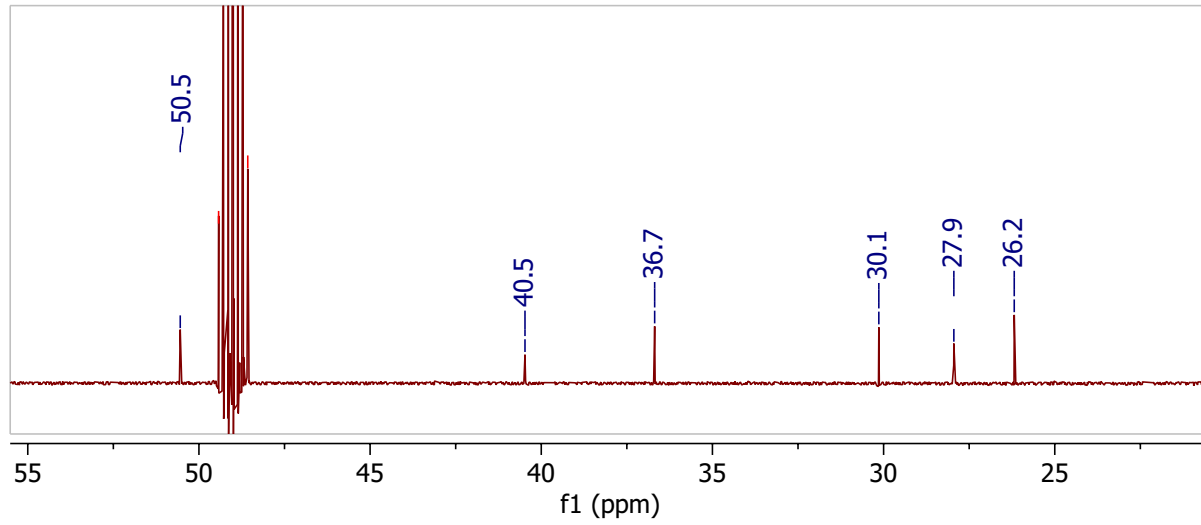
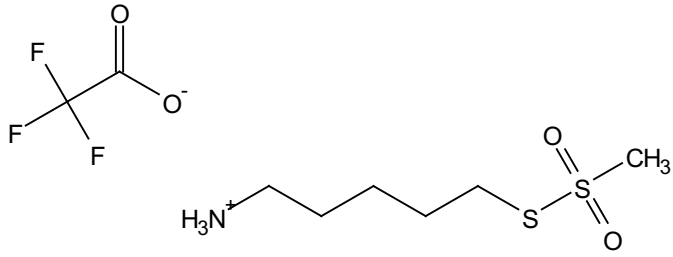


1.86
1.85
1.84
1.82
1.81
1.72
1.71
1.70
1.68
1.67
1.56
1.54
1.53
1.52
1.50

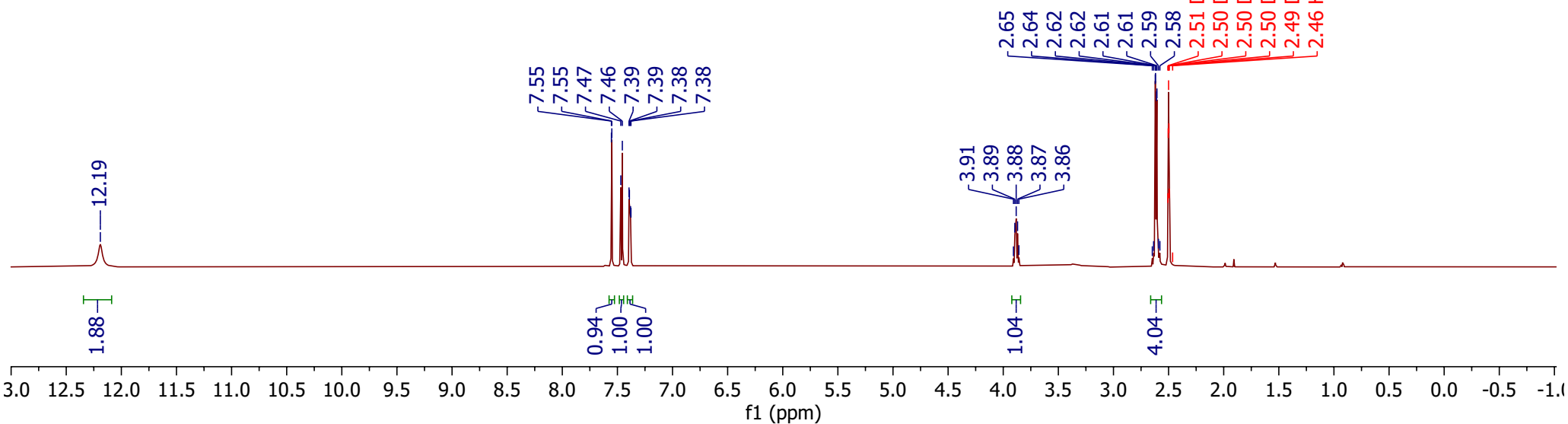
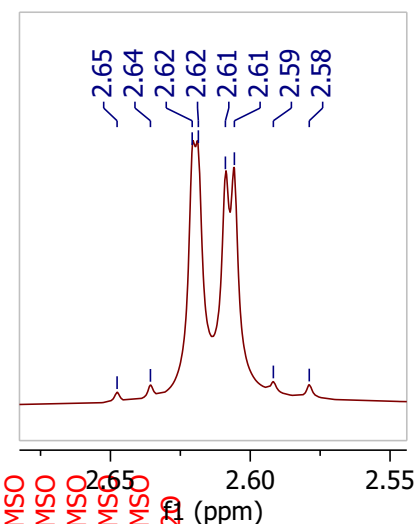
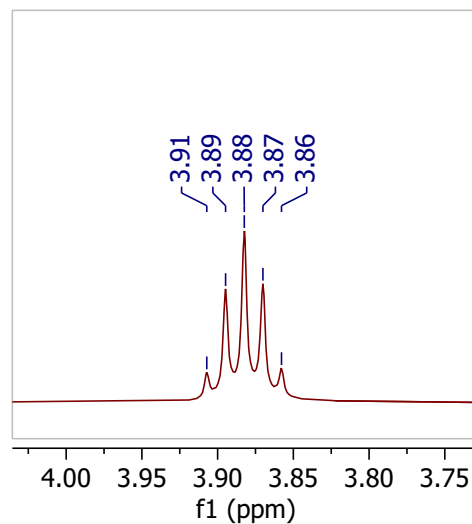
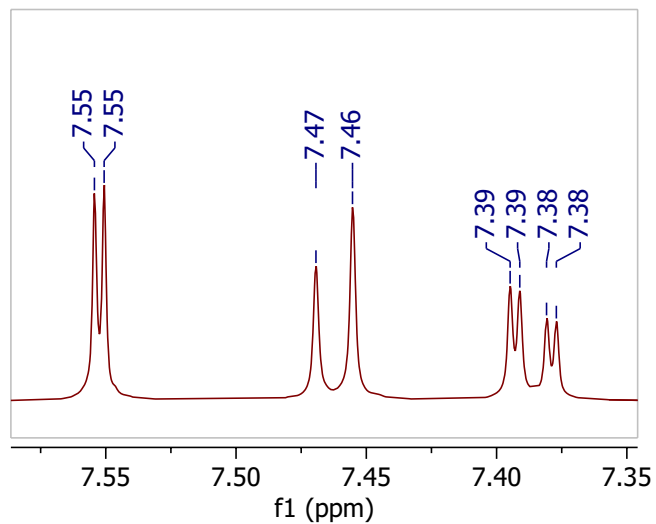
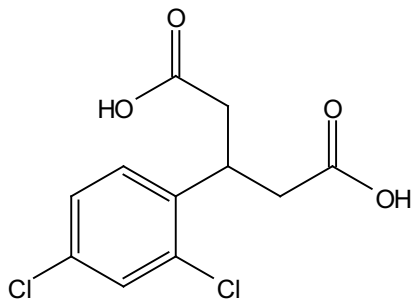
2.91
2.00
2.01
2.06
2.06
2.04

12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

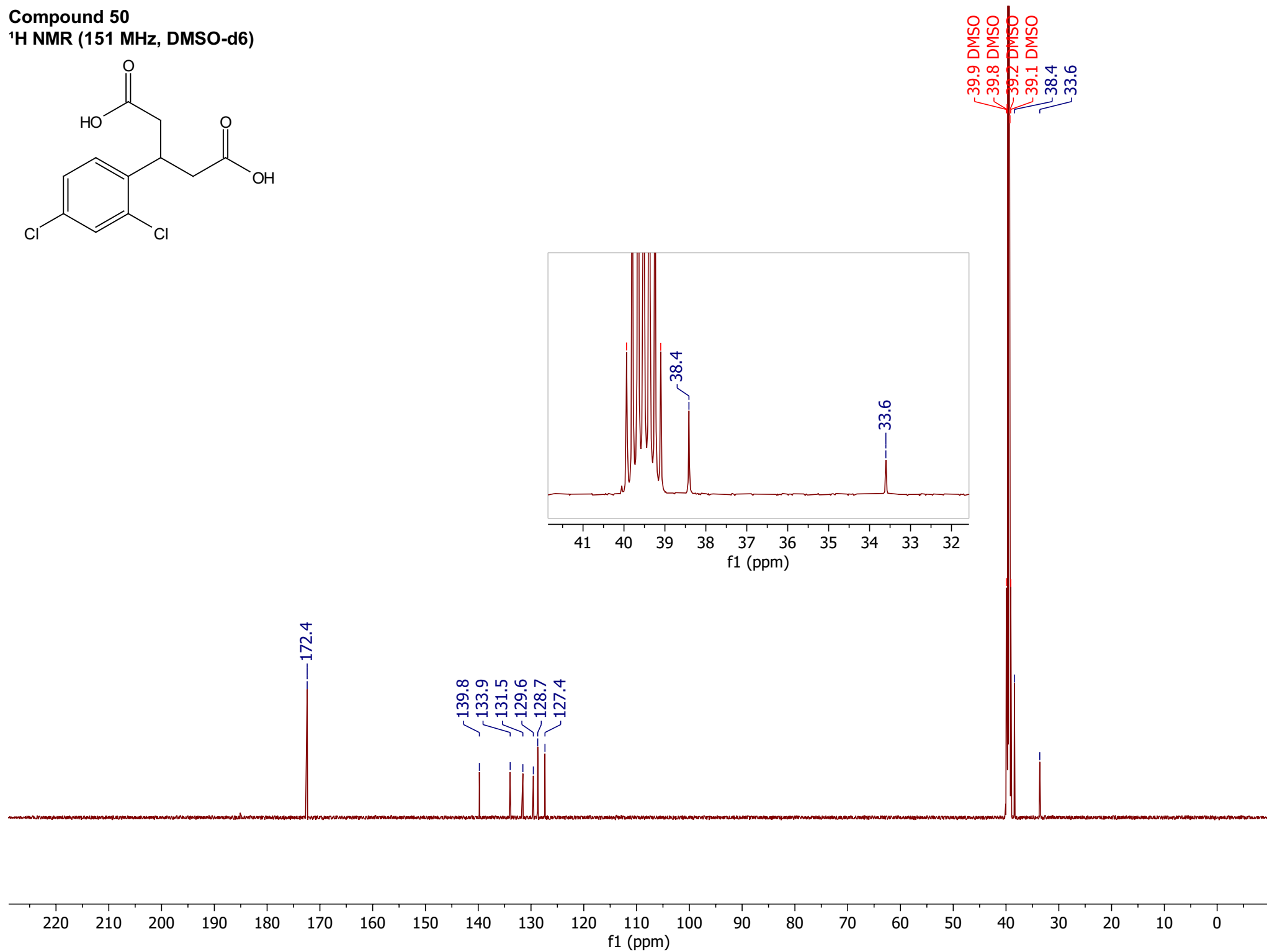
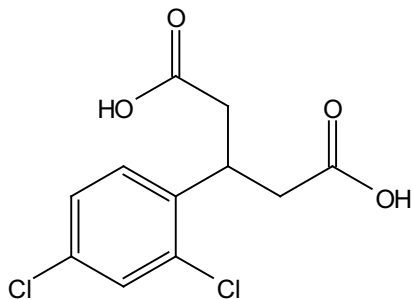
Compound 47
¹H NMR (151 MHz, MeOD-d4)



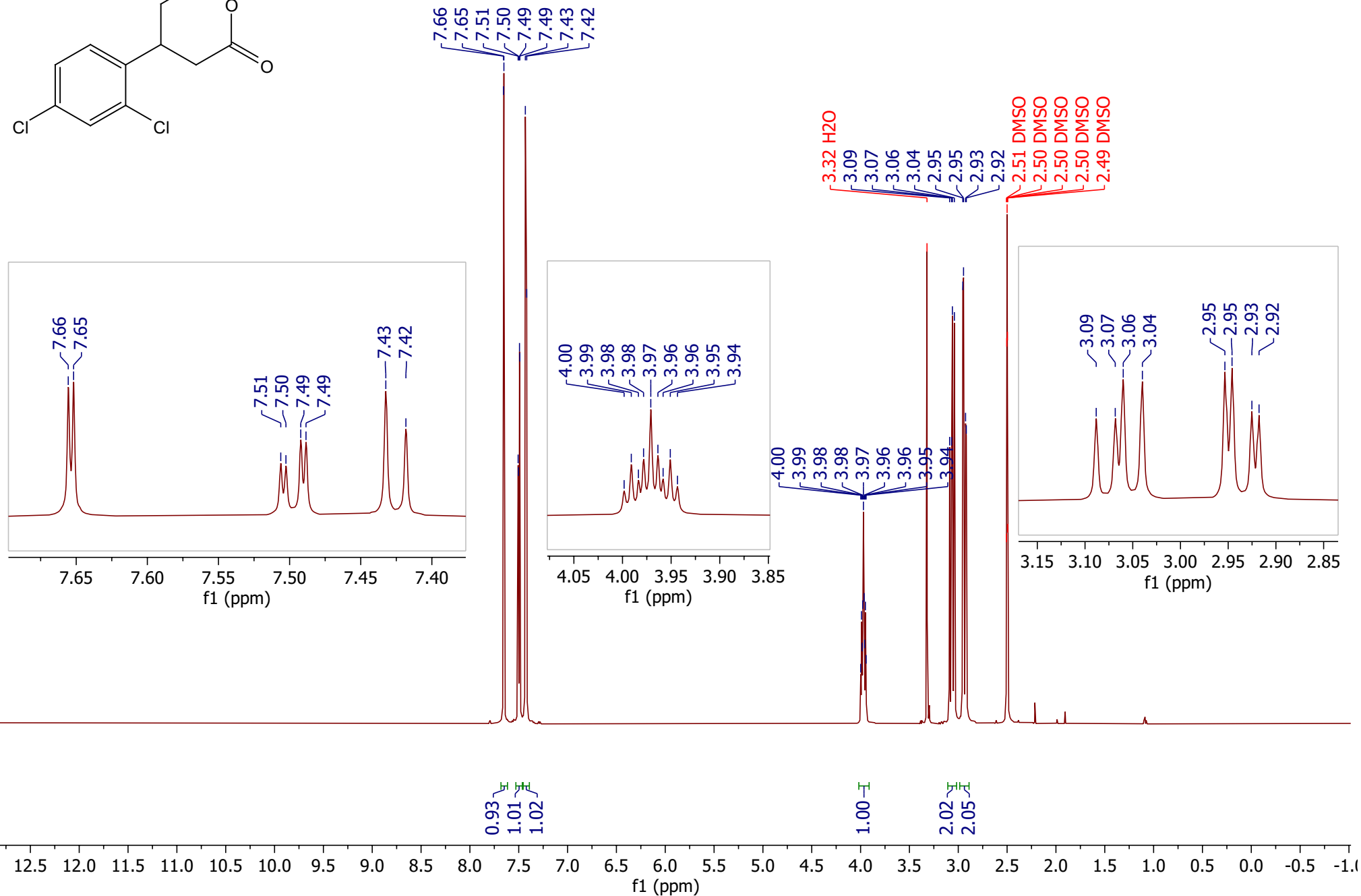
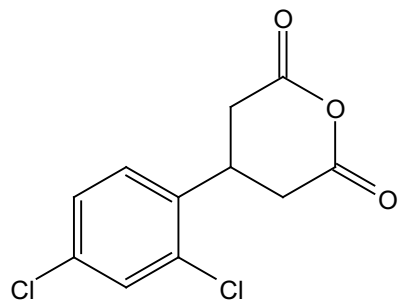
Compound 50
¹H NMR (600 MHz, DMSO-d6)



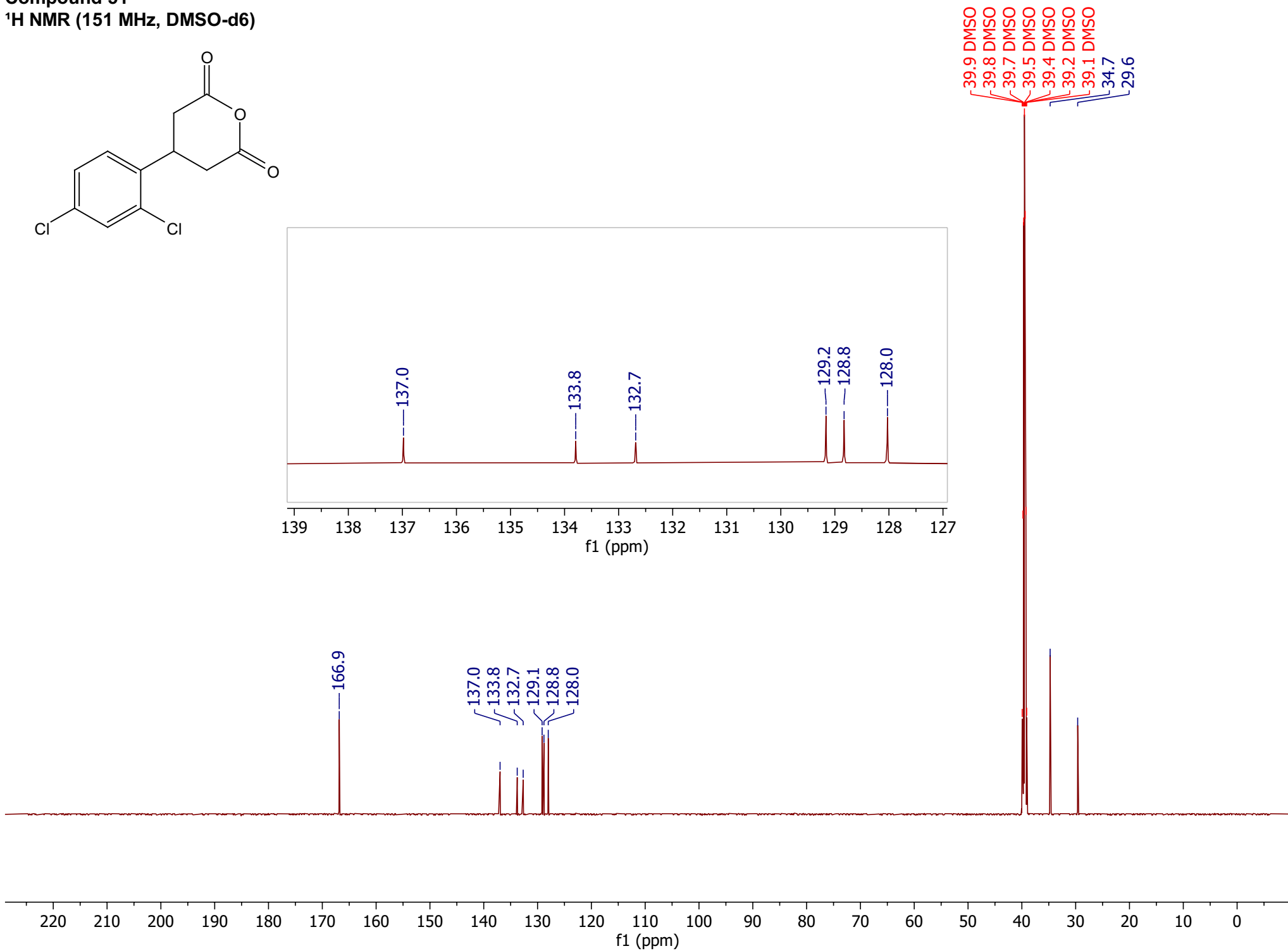
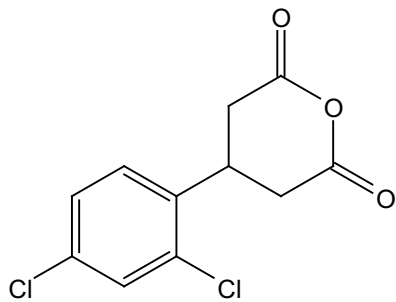
Compound 50
¹H NMR (151 MHz, DMSO-d6)



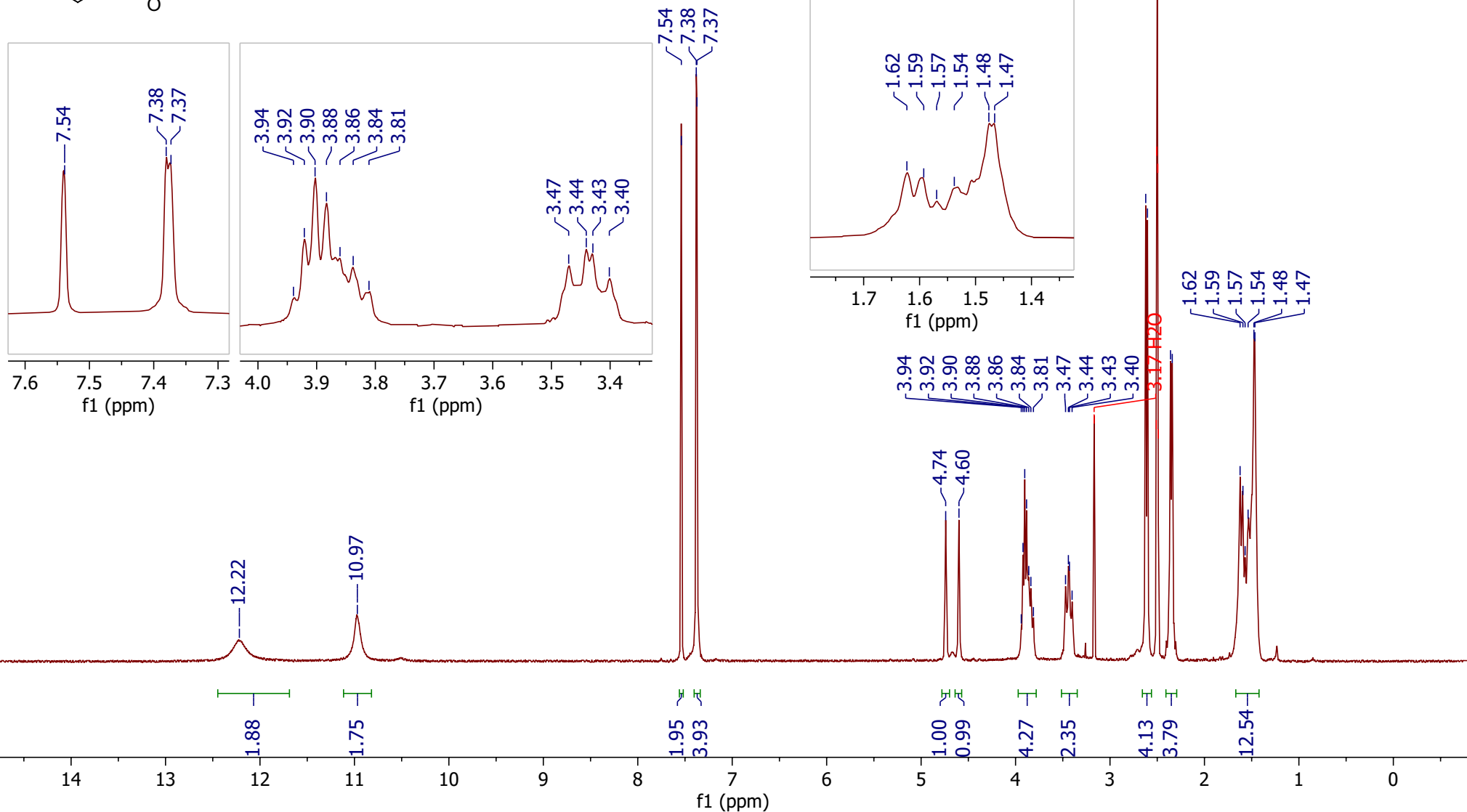
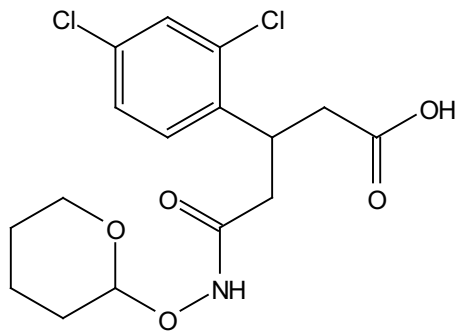
Compound 51
¹H NMR (600 MHz, DMSO-d6)



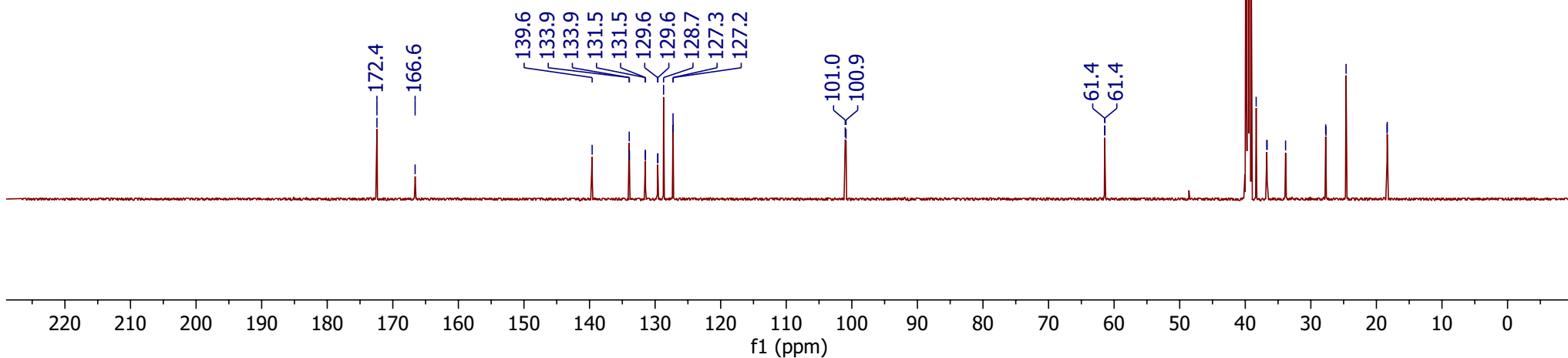
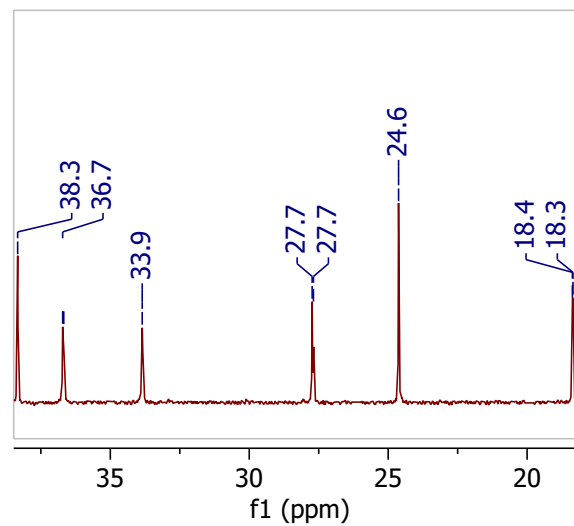
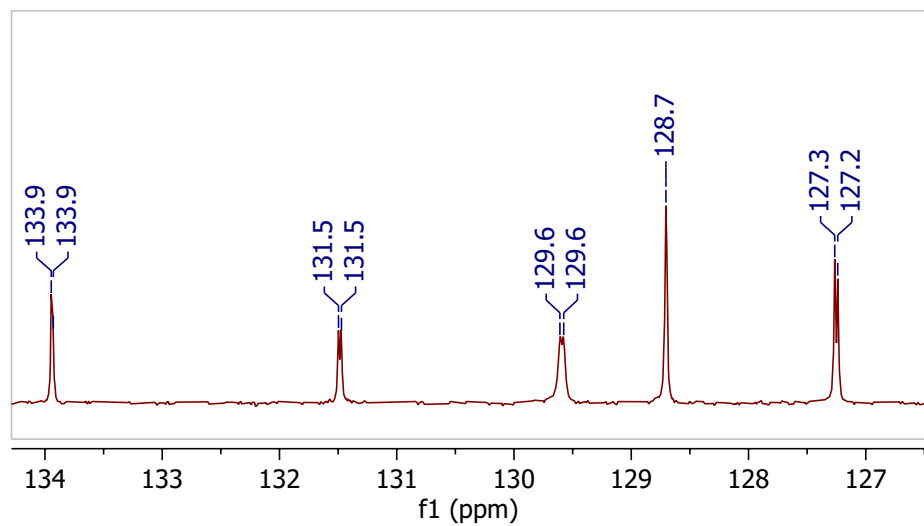
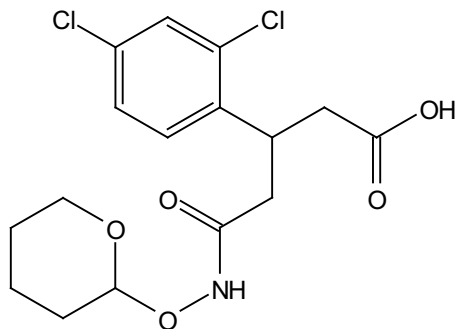
Compound 51
1H NMR (151 MHz, DMSO-d6)



Compound 52
¹H NMR (400 MHz, DMSO-d6)

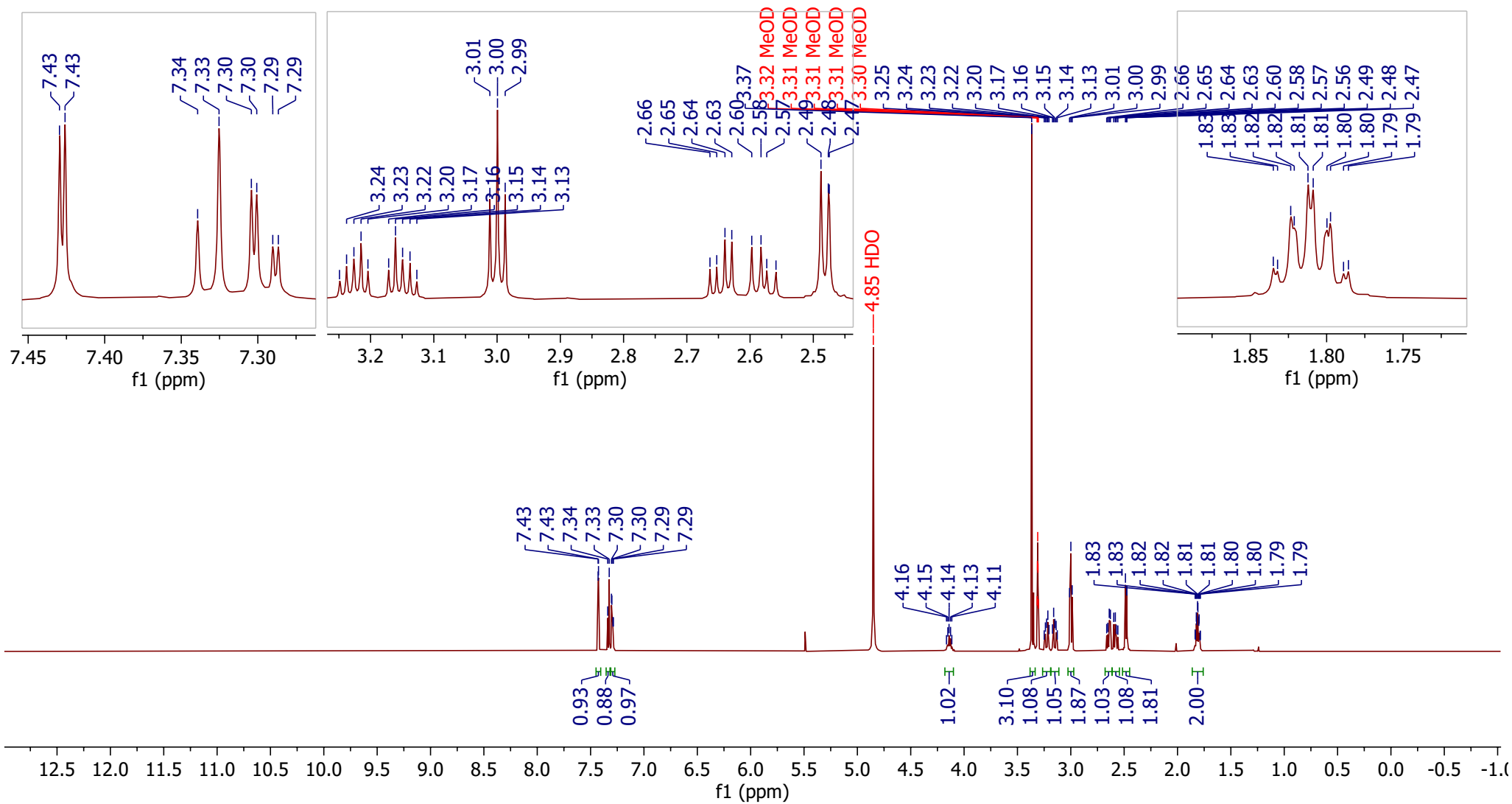
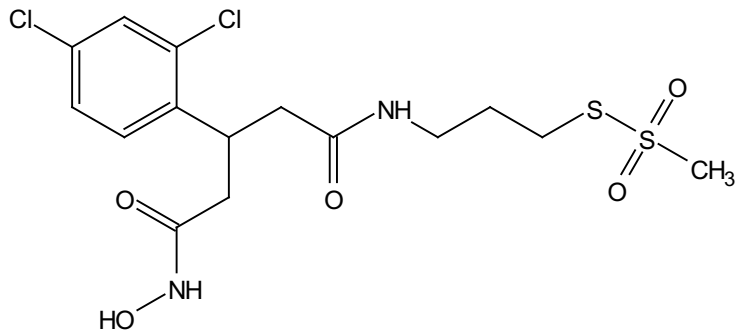


Compound 52
¹H NMR (151 MHz, DMSO-d6)

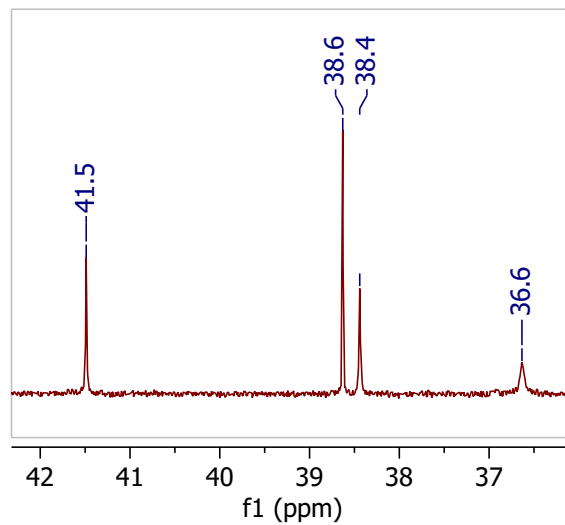
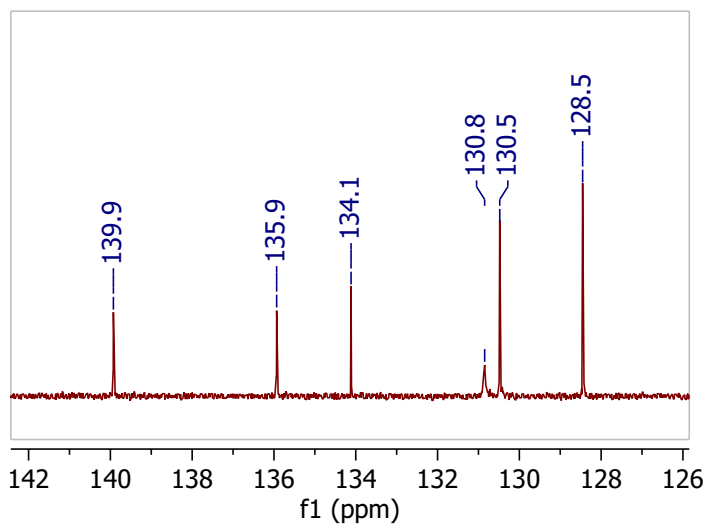
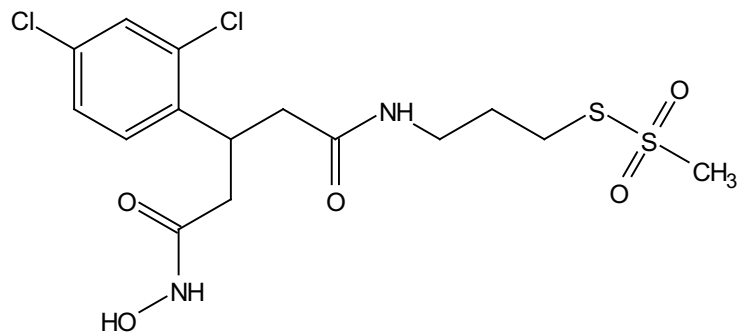


39.9 DMSO
39.8 DMSO
39.2 DMSO
39.1 DMSO
38.3
36.7
36.7
33.9
27.7
27.7
24.6
18.4
18.3

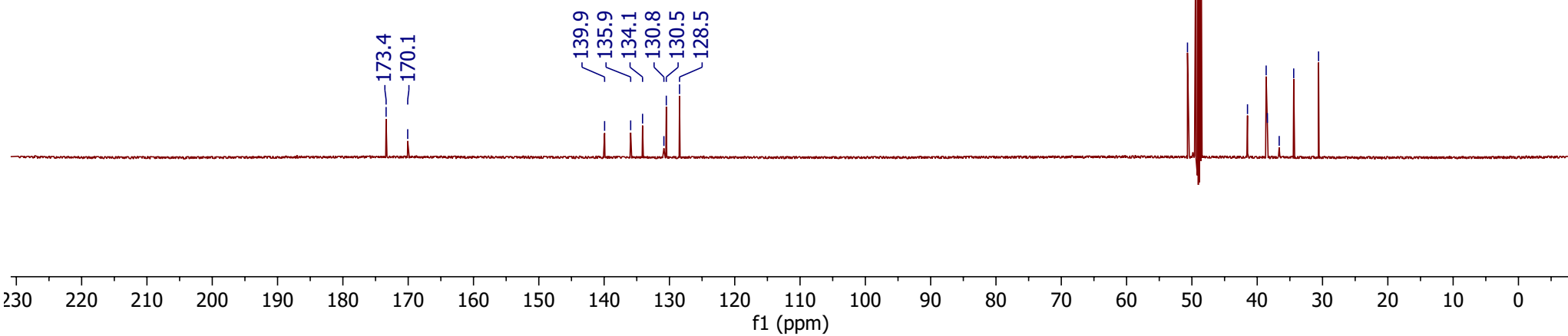
Compound 53
¹H NMR (600 MHz, MeOD-d4)



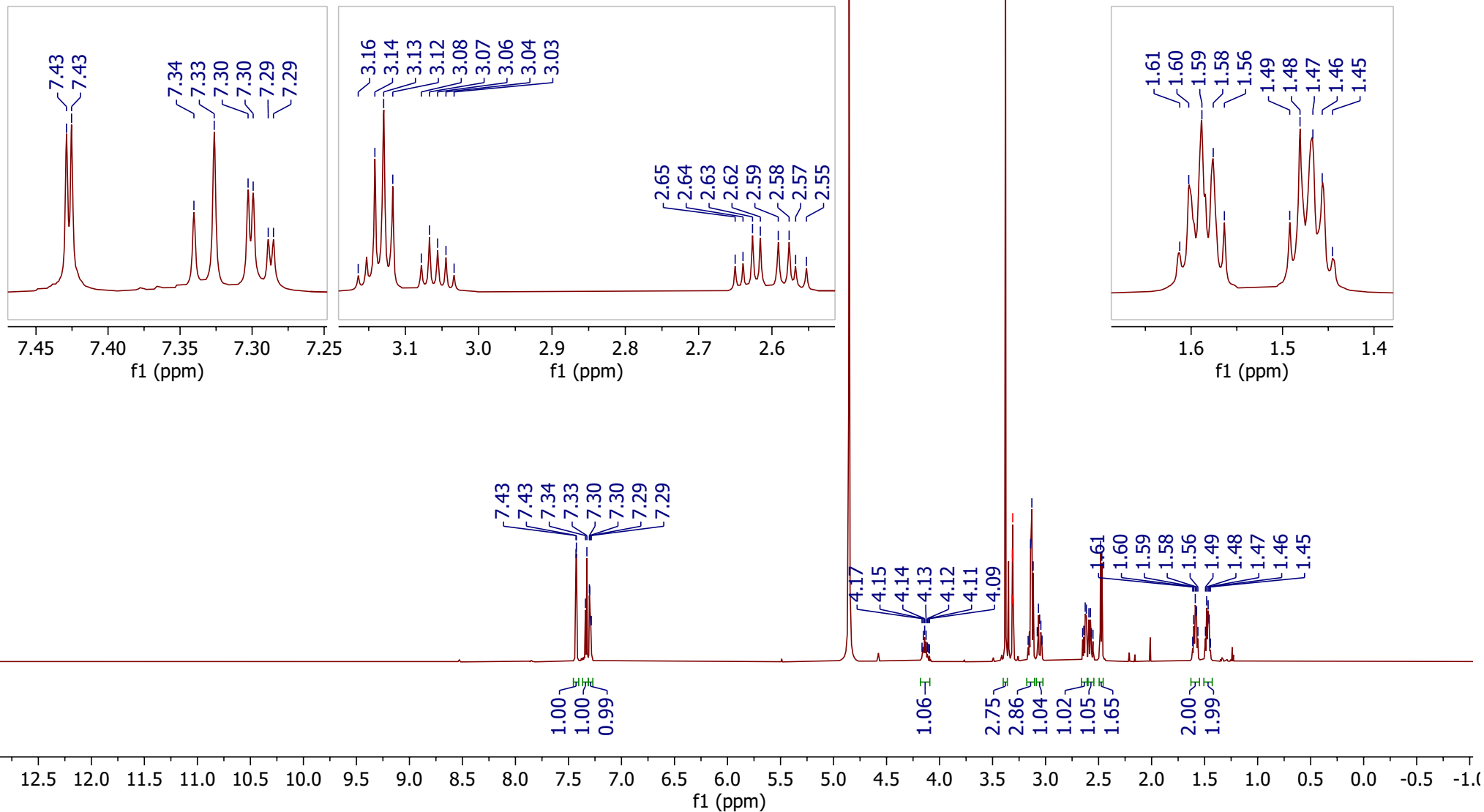
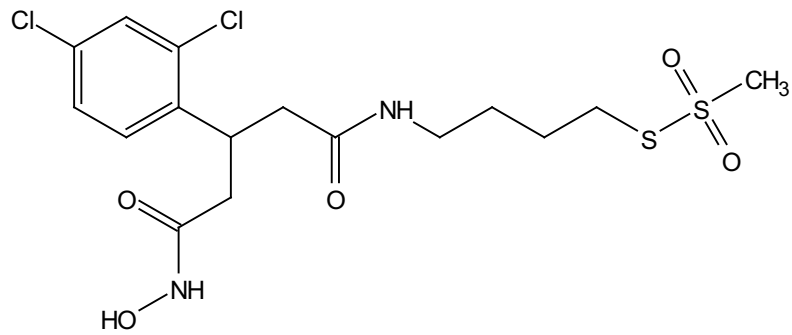
Compound 53
¹H NMR (151 MHz, MeOD-d4)



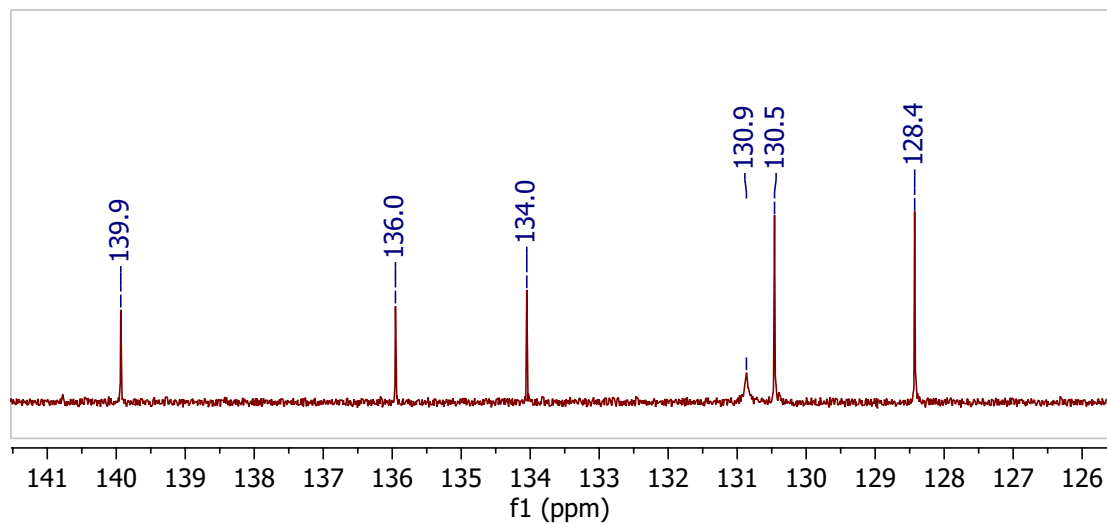
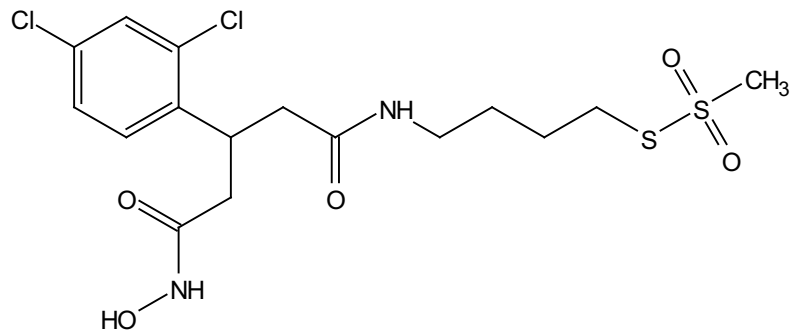
50.7
49.4 MeOD
49.3 MeOD
48.7 MeOD
48.6 MeOD
41.5
38.6
38.4
36.6
34.4
30.6



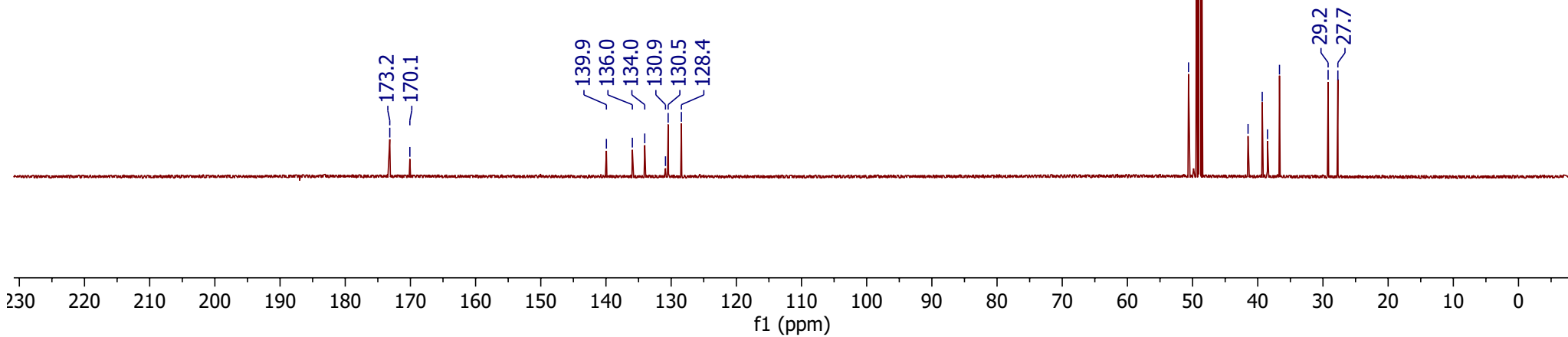
Compound 54
1H NMR (600 MHz, MeOD-d4)



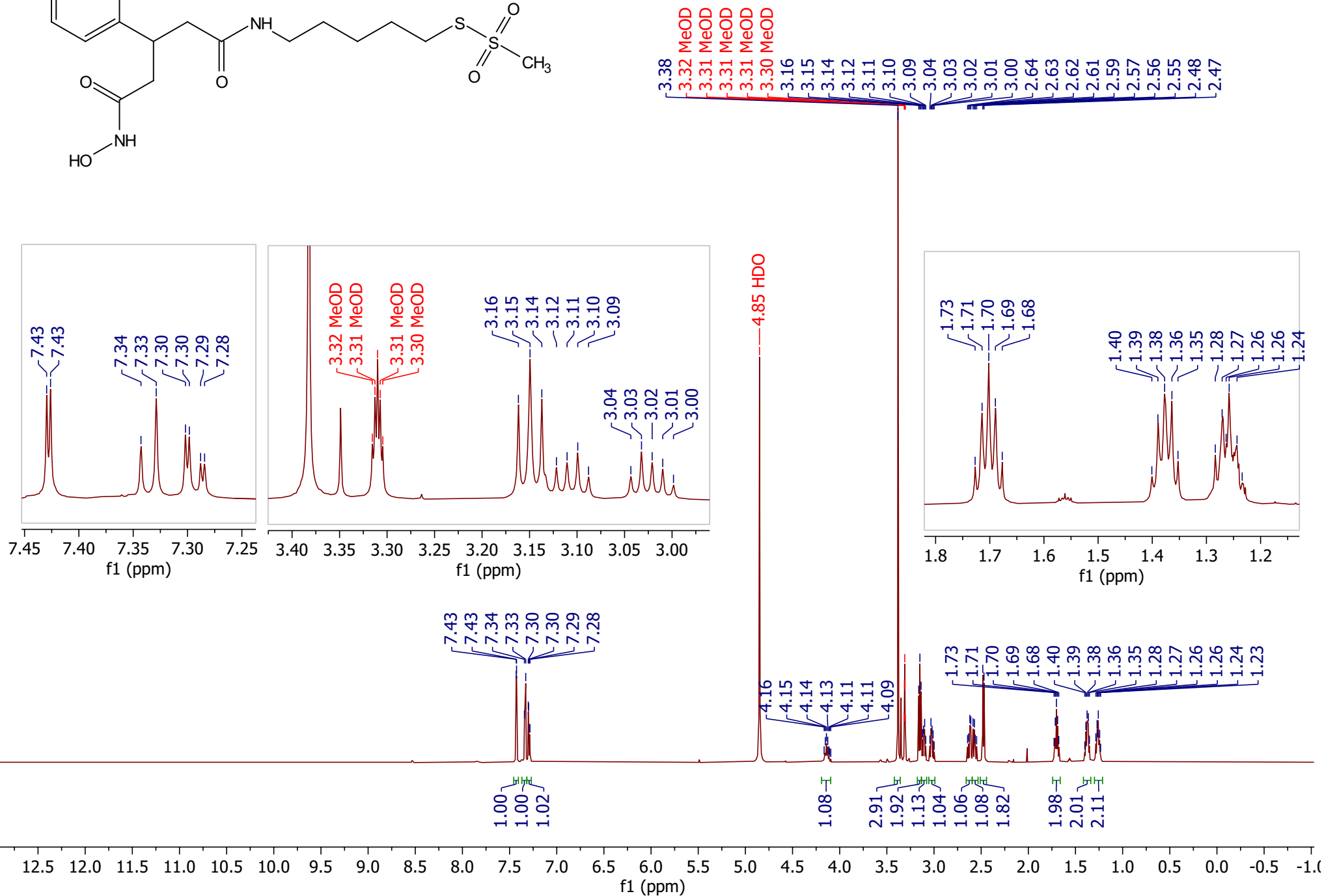
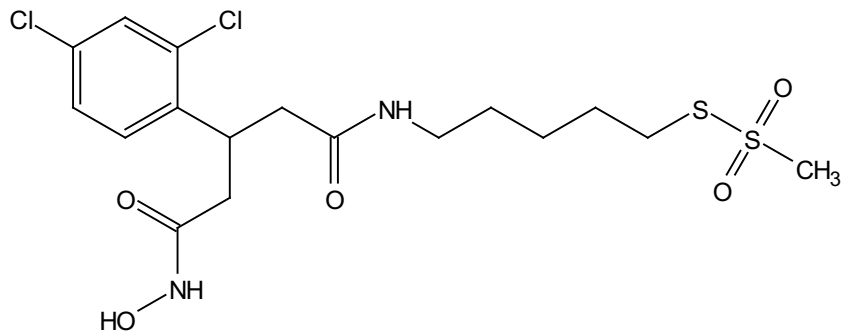
Compound 54
¹H NMR (151 MHz, MeOD-d4)



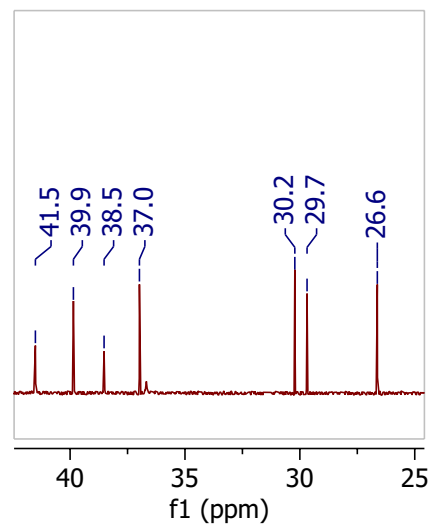
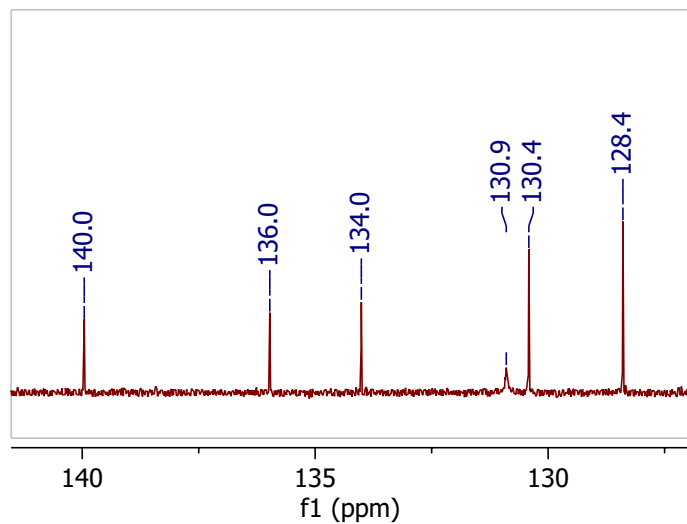
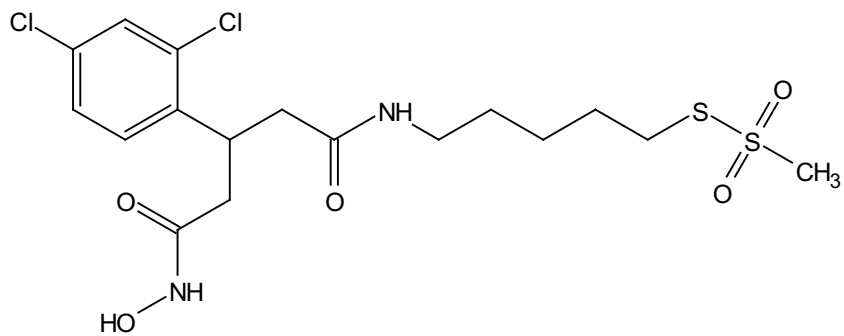
50.6
49.4 MeOD
49.3 MeOD
48.7 MeOD
48.6 MeOD
41.5
39.3
38.5
36.7



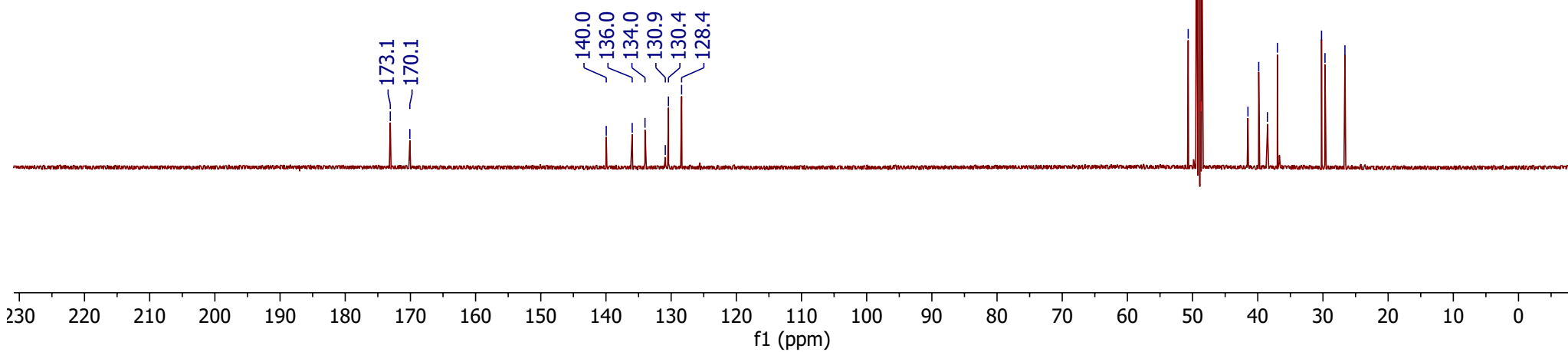
Compound 55
¹H NMR (600 MHz, MeOD-d4)



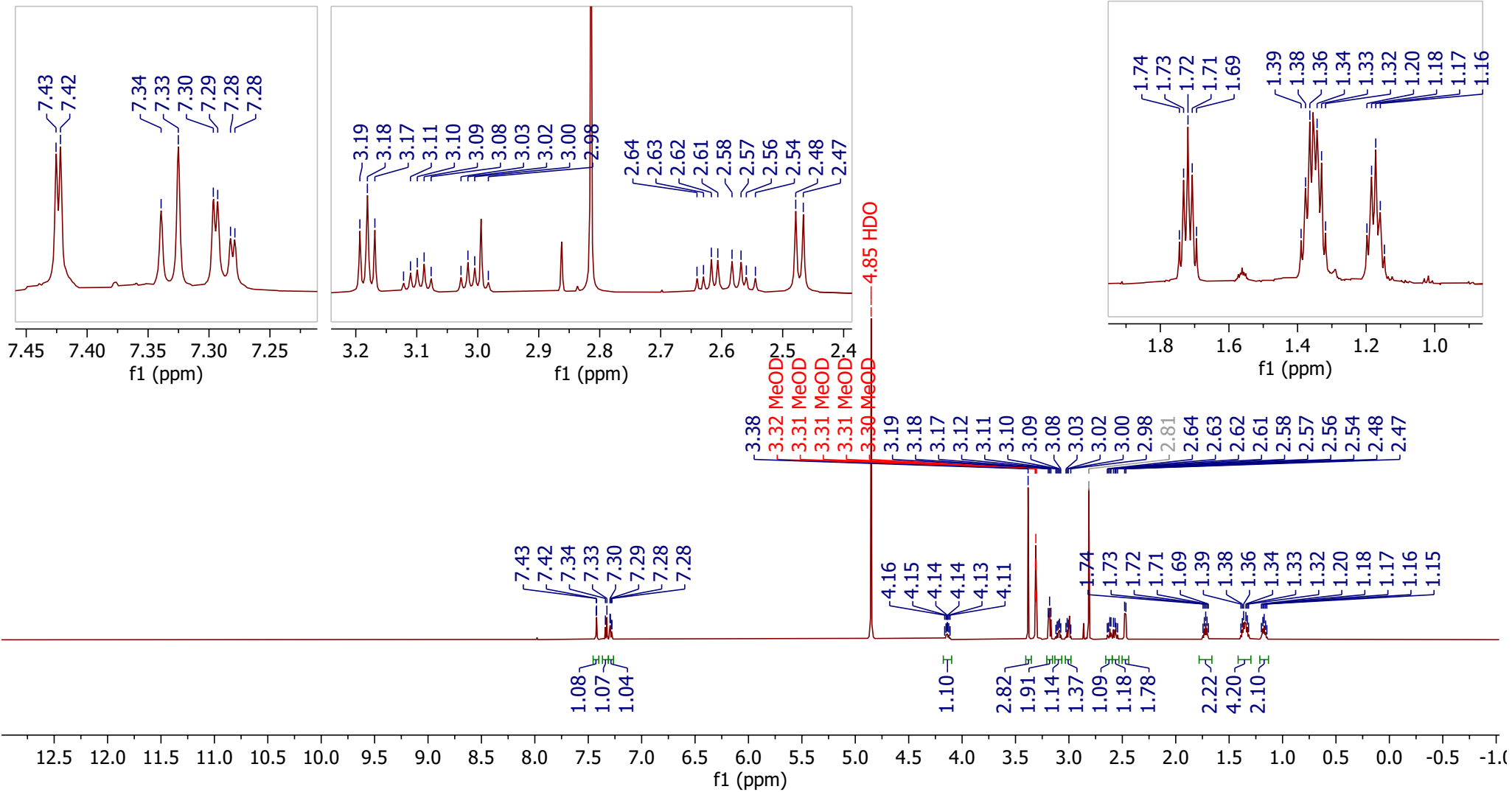
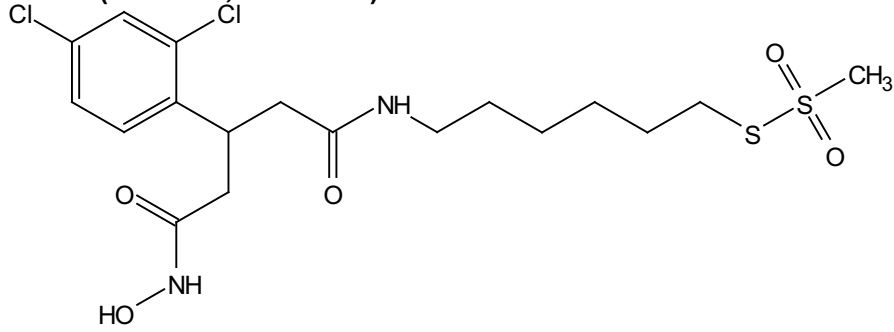
Compound 55
¹H NMR (151 MHz, MeOD-d4)



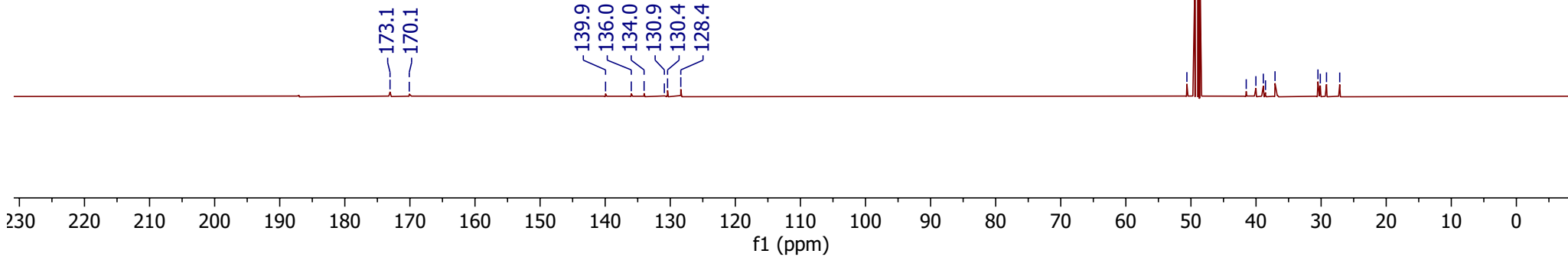
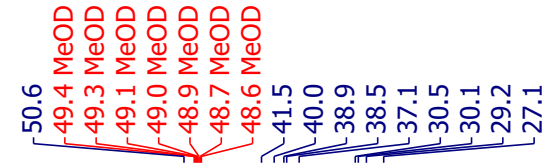
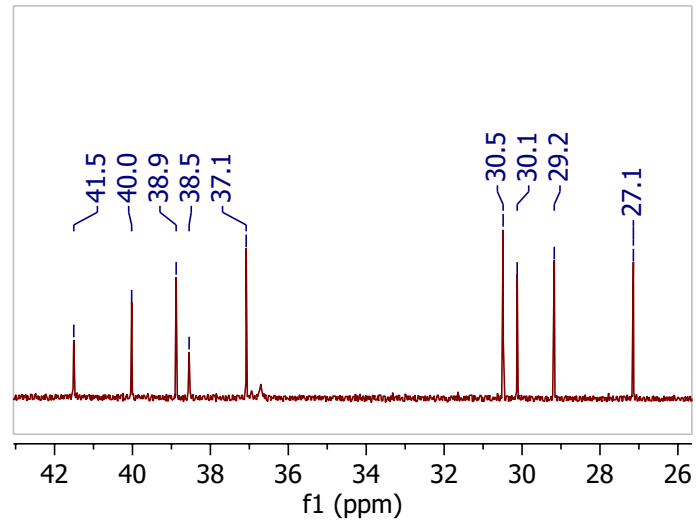
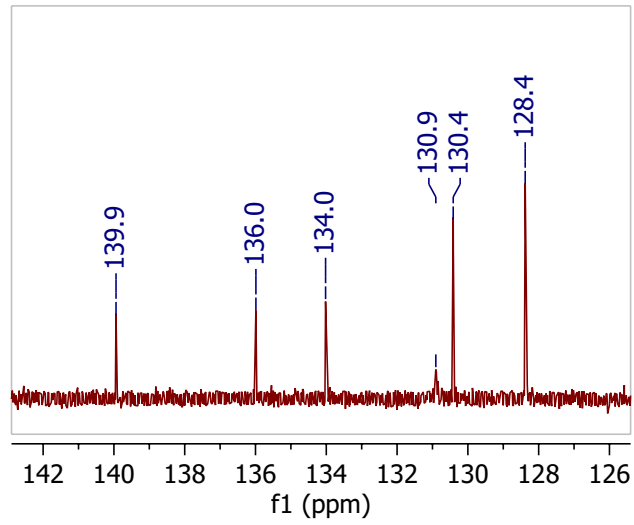
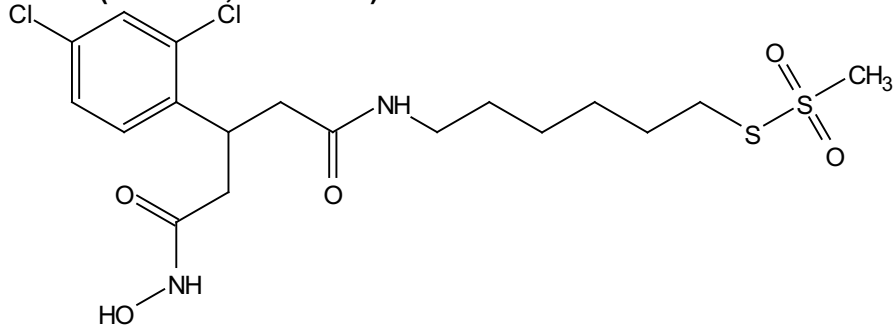
50.7 MeOD
49.4 MeOD
49.3 MeOD
48.7 MeOD
48.6 MeOD
41.5
39.9
38.5
37.0
30.2
29.7
26.6



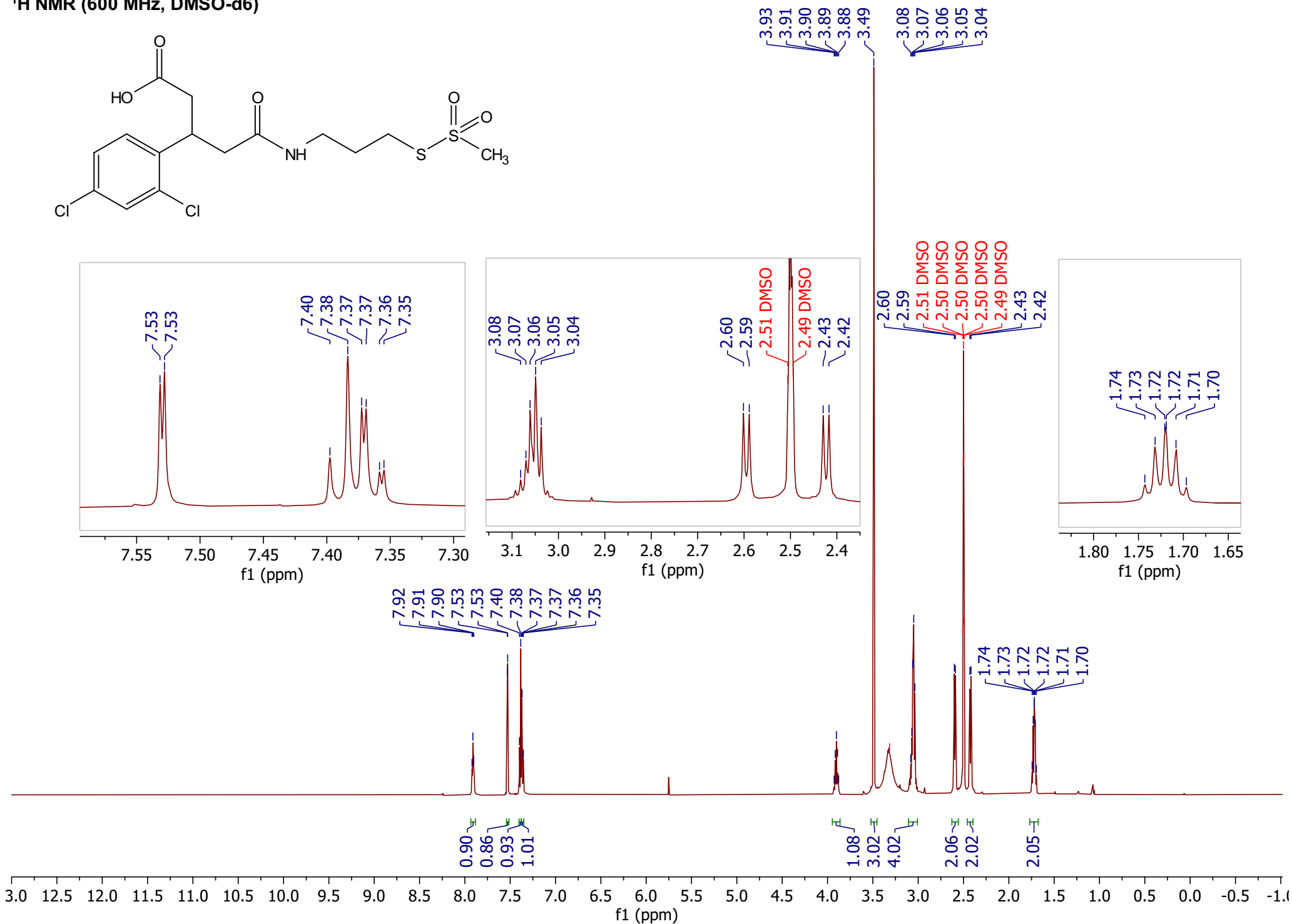
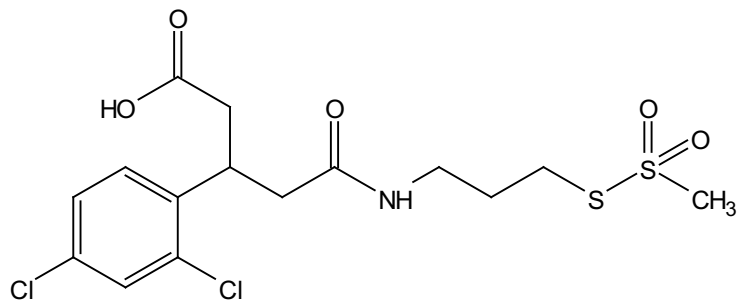
Compound 56
¹H NMR (600 MHz, MeOD-d4)



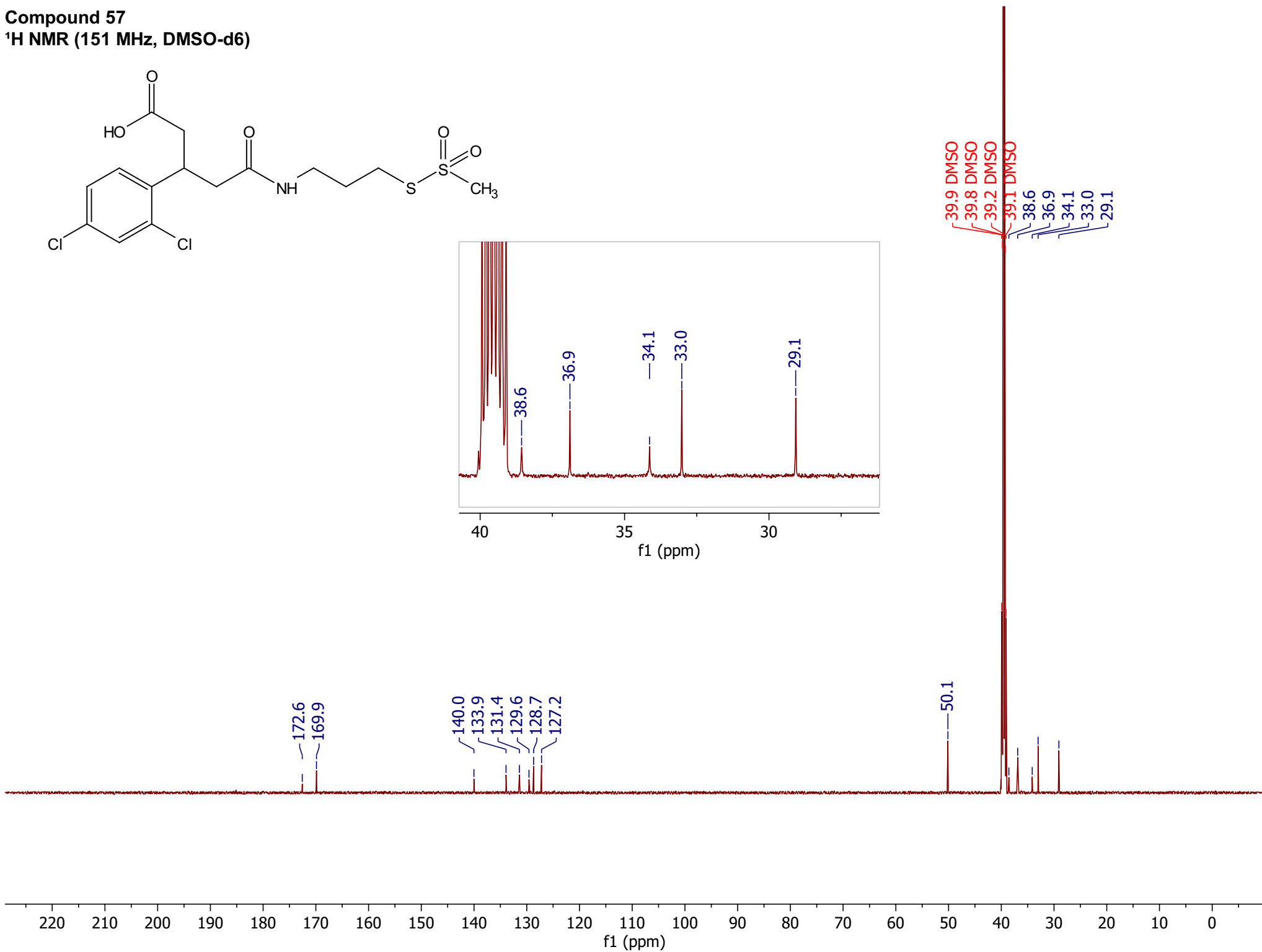
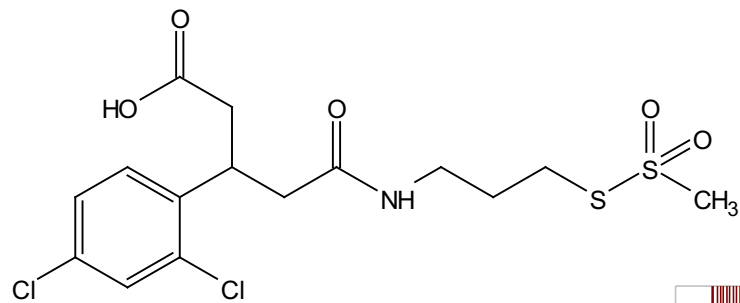
Compound 56
¹H NMR (151 MHz, MeOD-d4)



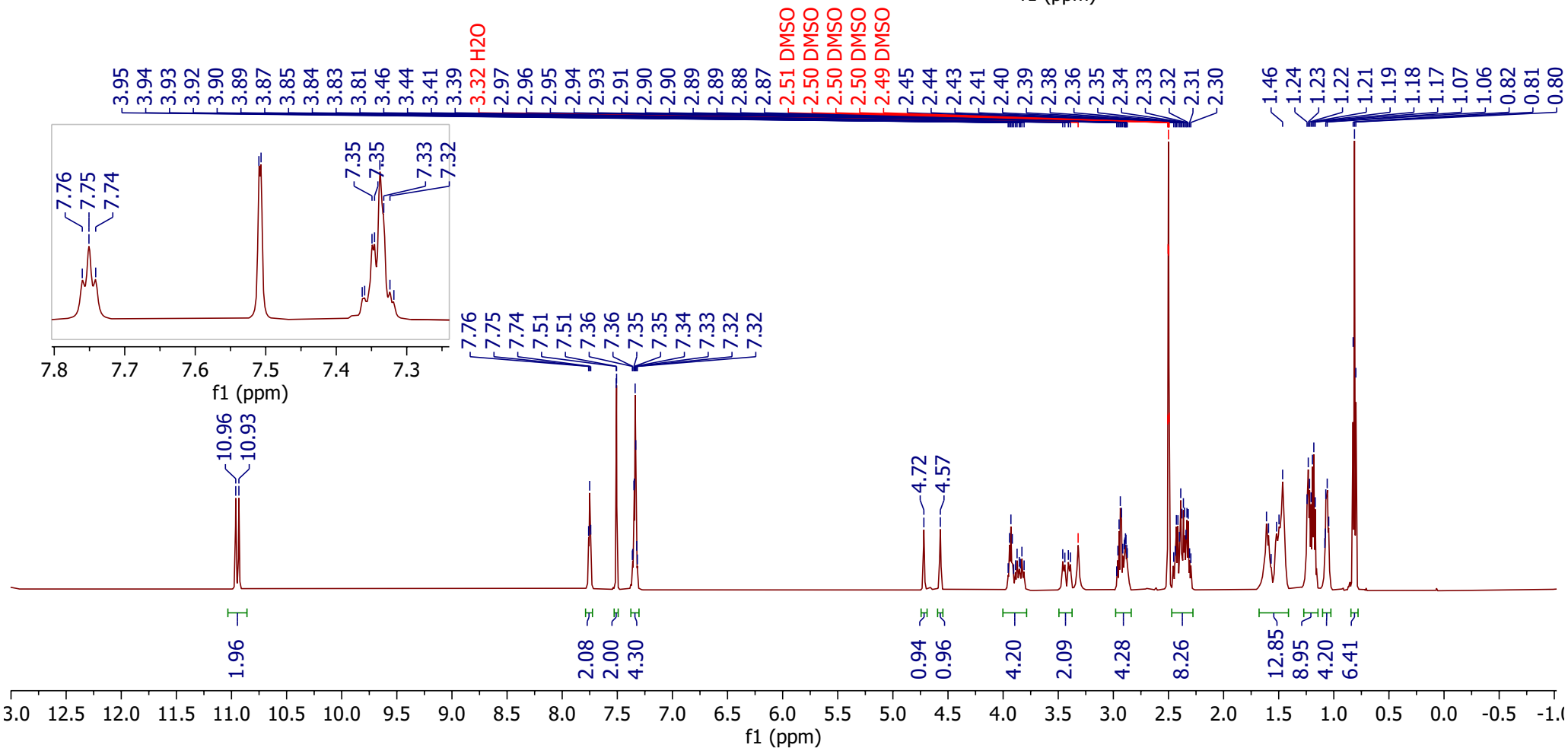
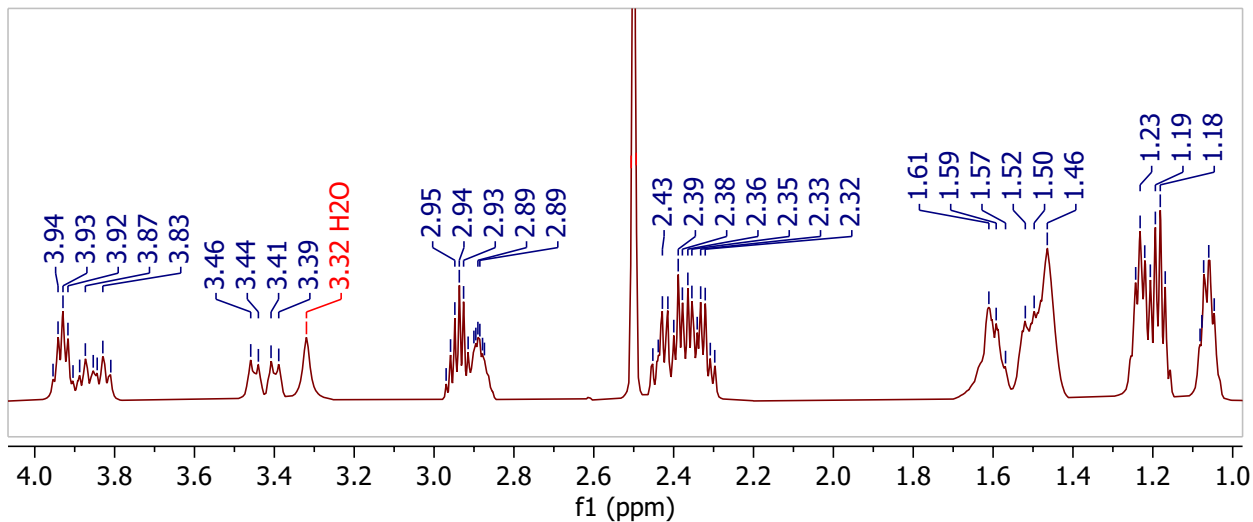
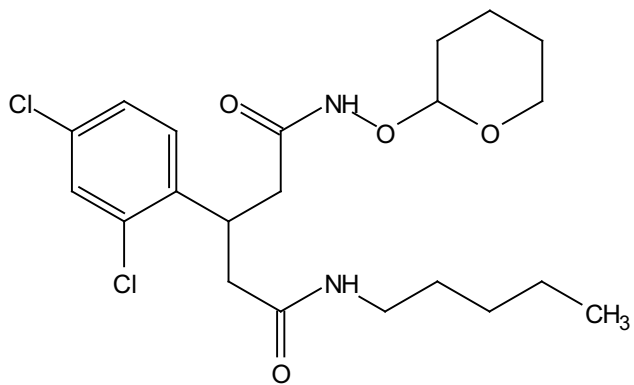
Compound 57
¹H NMR (600 MHz, DMSO-d6)



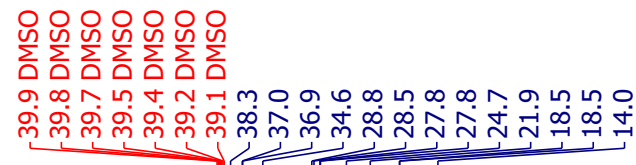
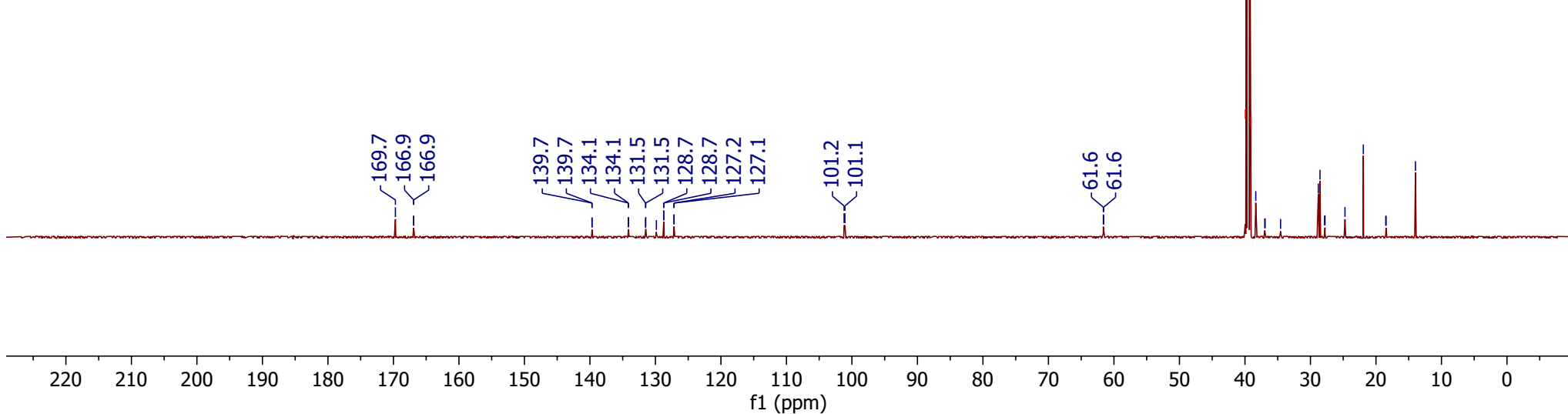
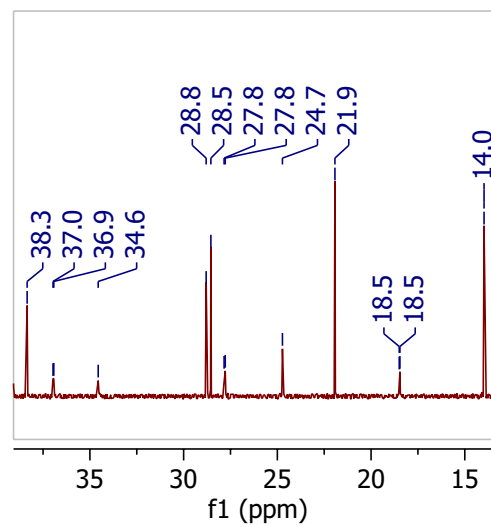
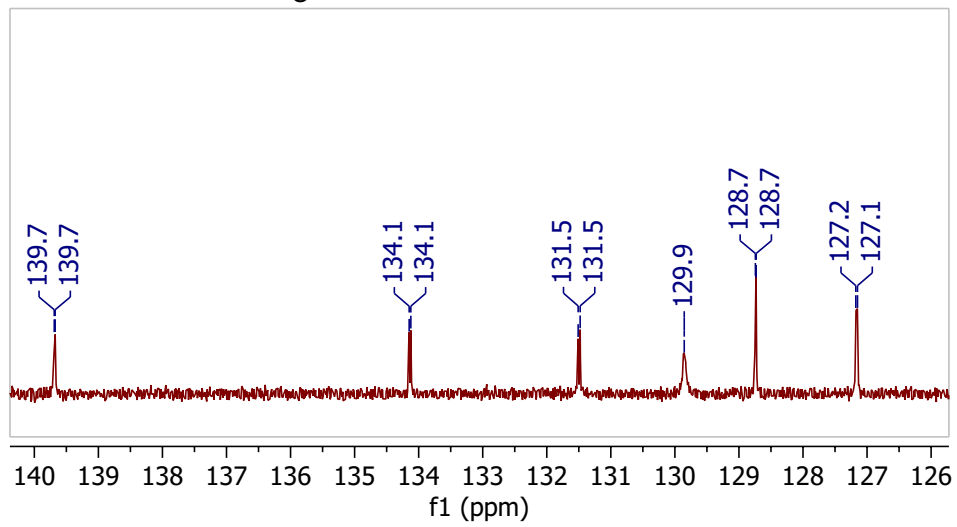
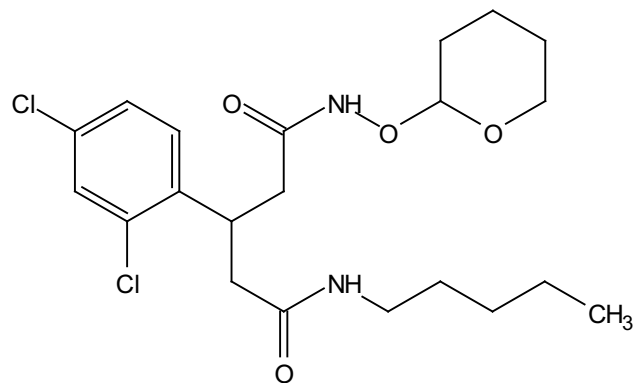
Compound 57
¹H NMR (151 MHz, DMSO-d6)



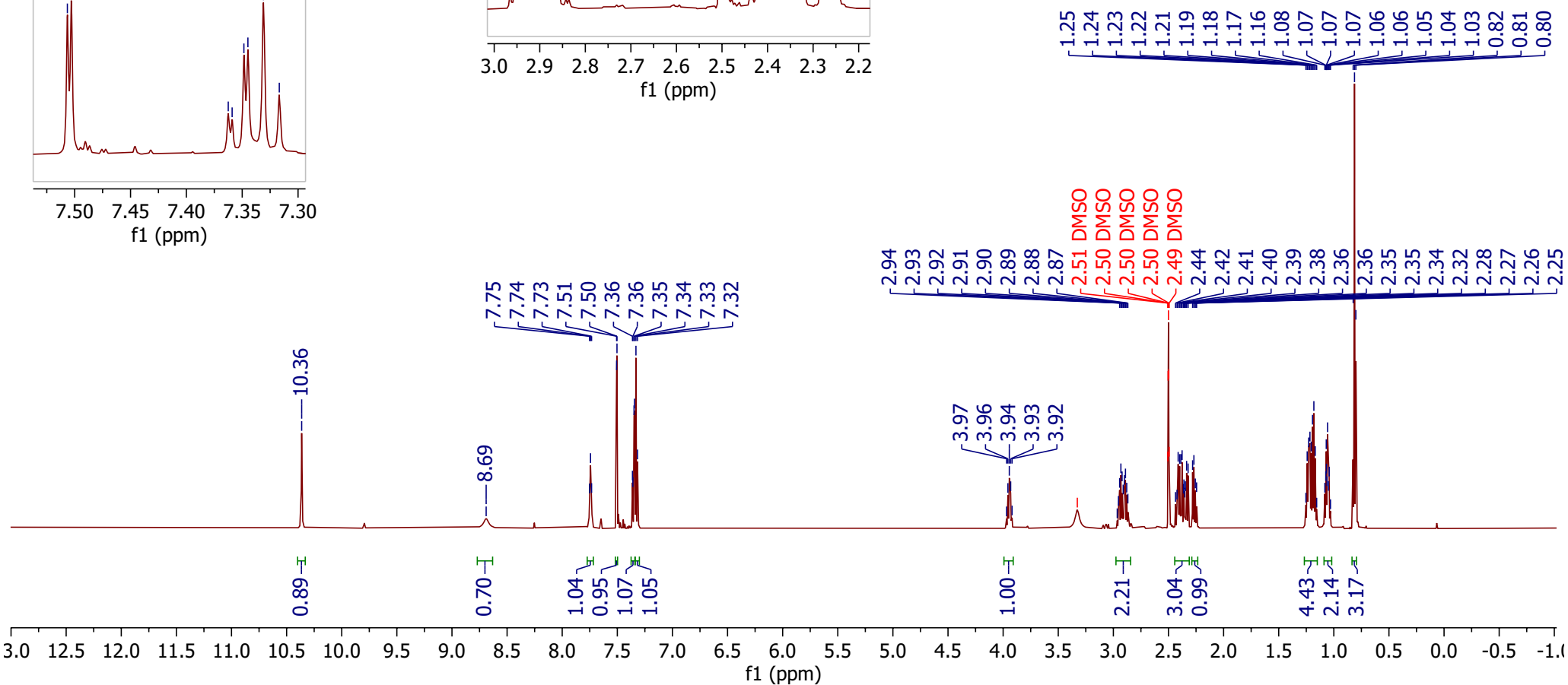
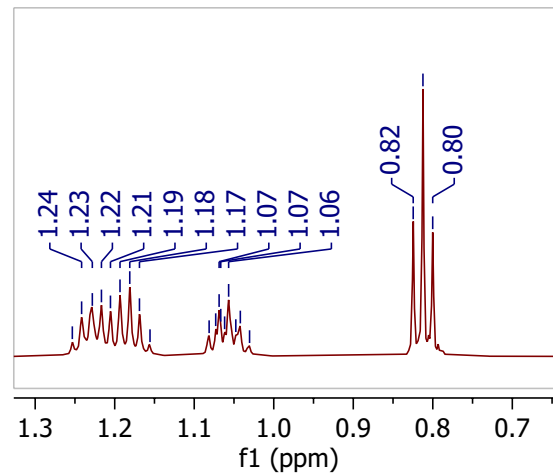
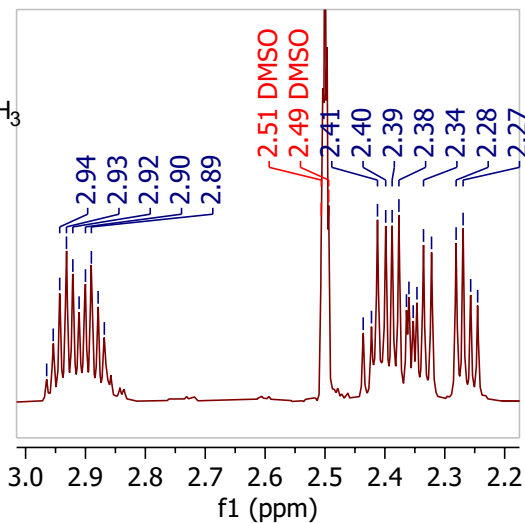
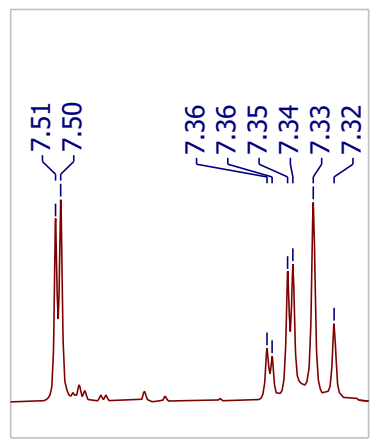
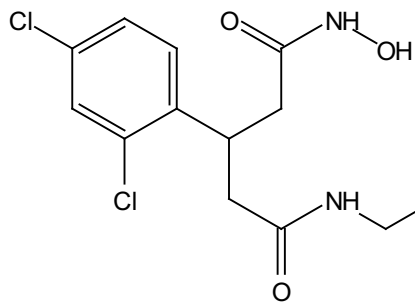
Compound 58
¹H NMR (600 MHz, DMSO-d₆)



Compound 58
¹H NMR (151 MHz, DMSO-d6)



Compound 59
¹H NMR (600 MHz, DMSO-d6)



Compound 59
¹H NMR (151 MHz, DMSO-d6)

