10.1071/CH21140_AC
Australian Journal of Chemistry

Supplementary Material for

The Synthesis, Structural Characterisation and Chemoselective Manipulation of Certain Functionalized Cyclic Sulfates Derived from Chiral, Non-Racemic and Polysubstituted Bicyclo[2.2.2]octane-2,3-diols

Martin G. Banwell,[a,]* Antony L. Crisp,[b] BoRa Lee,[b] Ping Lan,[a]

Hannah Bollard,[b] Jas S. Ward,[b] and Anthony C. Willis[b]

[a]Institute for Advanced and Applied Chemical Synthesis, Jinan University,

Guangzhou, 510632, China

and

[b]Research School of Chemistry, Institute of Advanced Studies,

The Australian National University, Canberra, ACT 2601, Australia

*Corresponding author. Email: mgb@rsc.anu.edu.au

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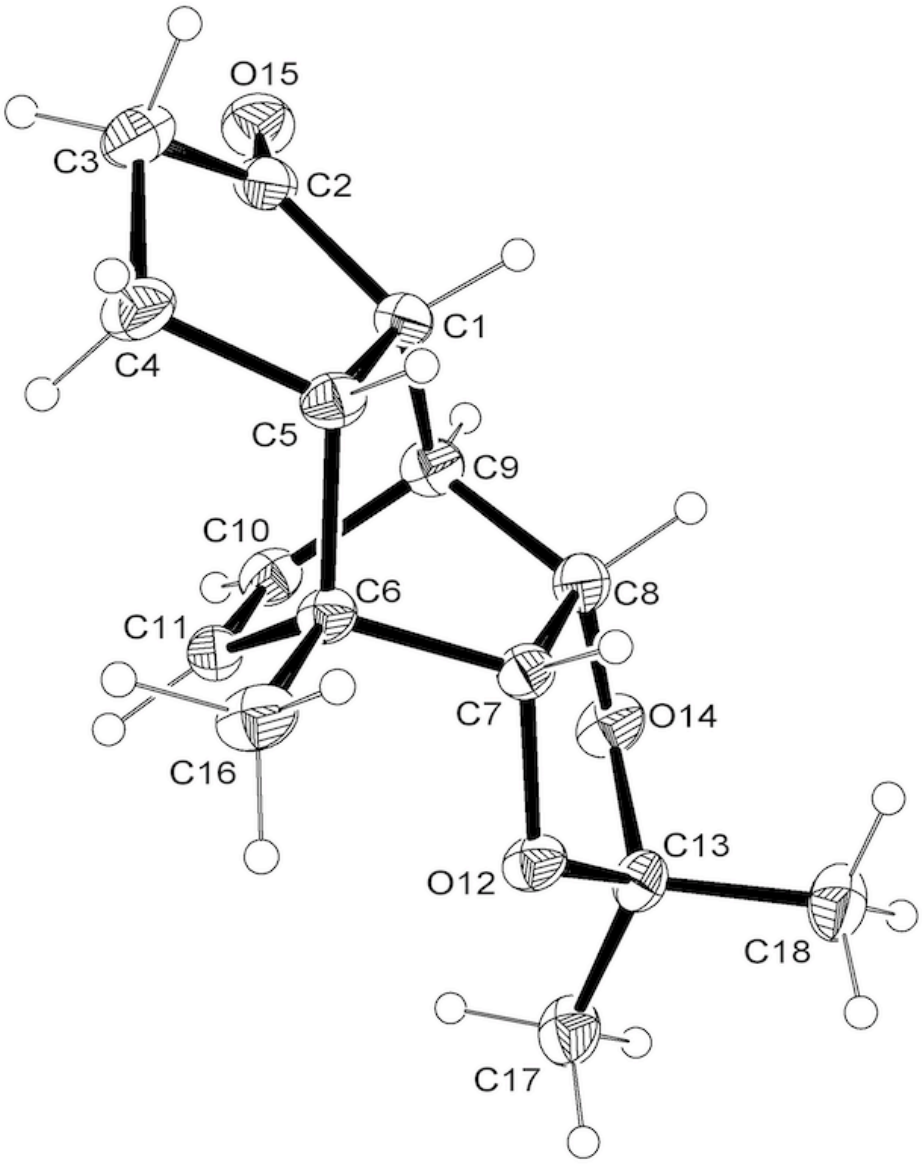


Figure S1: Plot arising from the single-crystal X-ray analysis of compound **13** – thermal ellipsoids at 50% probability (crystal grown by slow evaporation of a sample dissolved in dichloromethane/hexane) (CCDC 2082646).

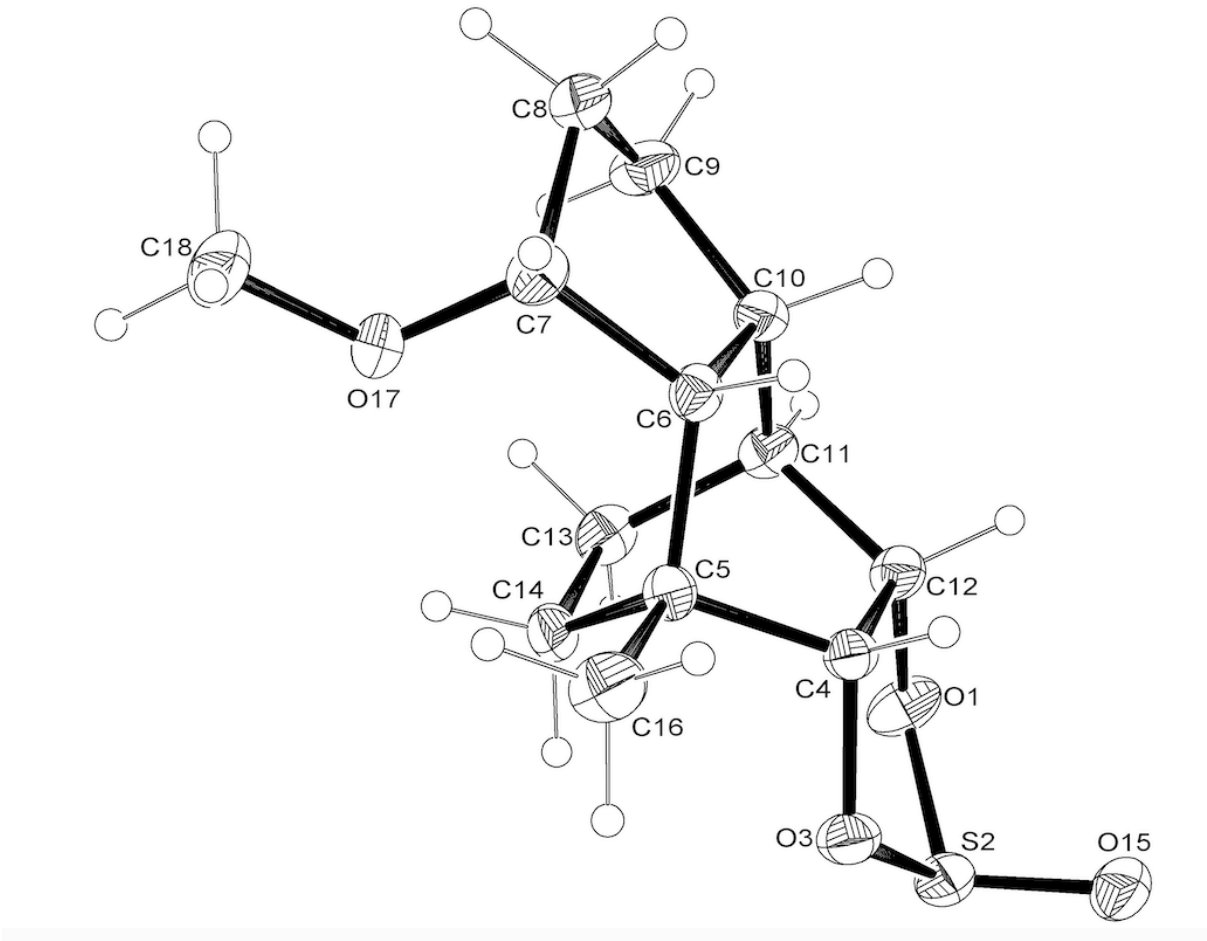


Figure S2: Plot arising from the single-crystal X-ray analysis of compound **16** – thermal ellipsoids at 50% probability (crystal grown by slow evaporation of a sample dissolved in dichloromethane/hexane) (CCDC 2082647).

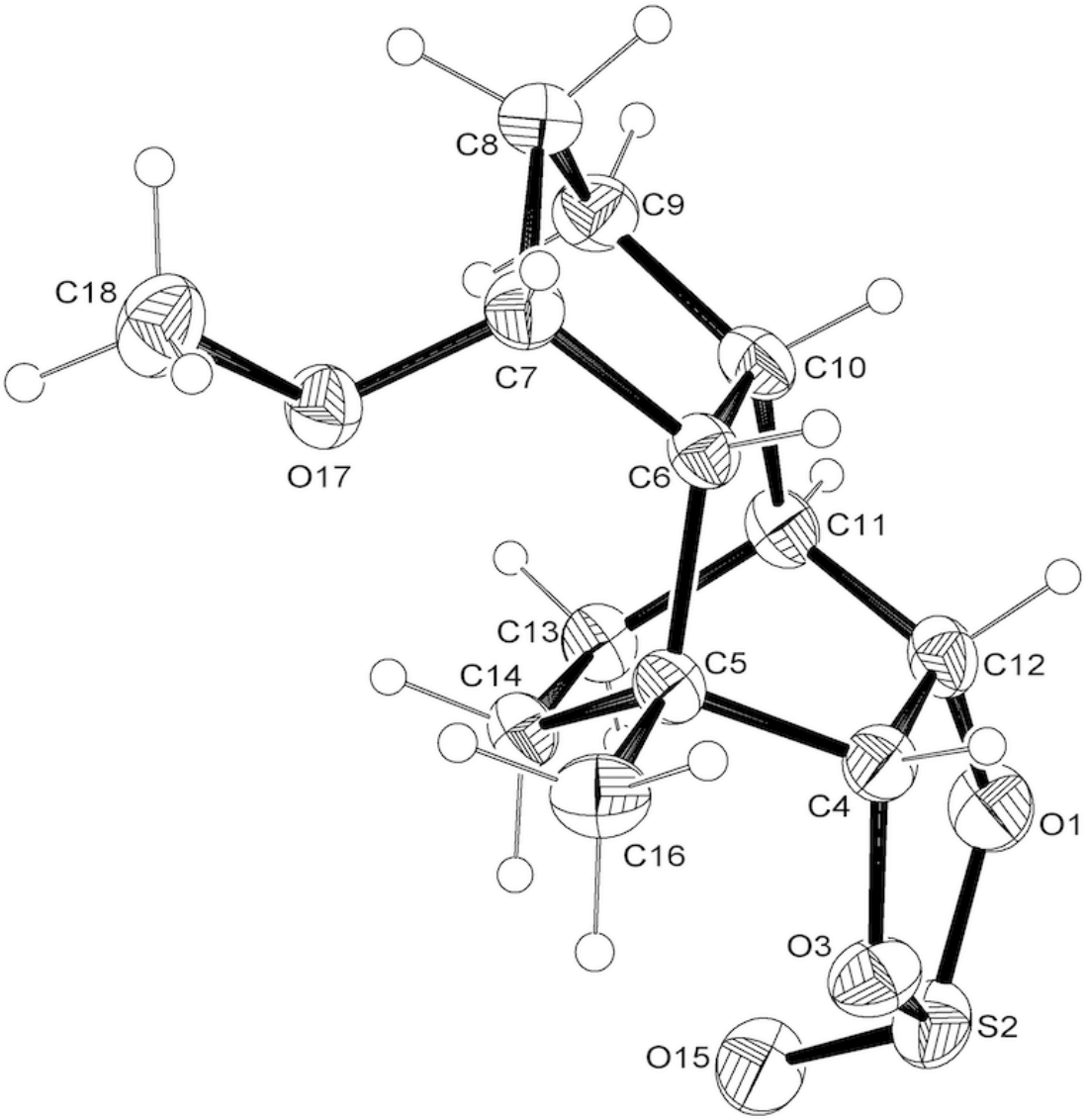


Figure S3: Plot arising from the single-crystal X-ray analysis of compound **17** – thermal ellipsoids at 50% probability (crystal grown by slow evaporation of a sample dissolved in dichloromethane/hexane) (CCDC 2082648).

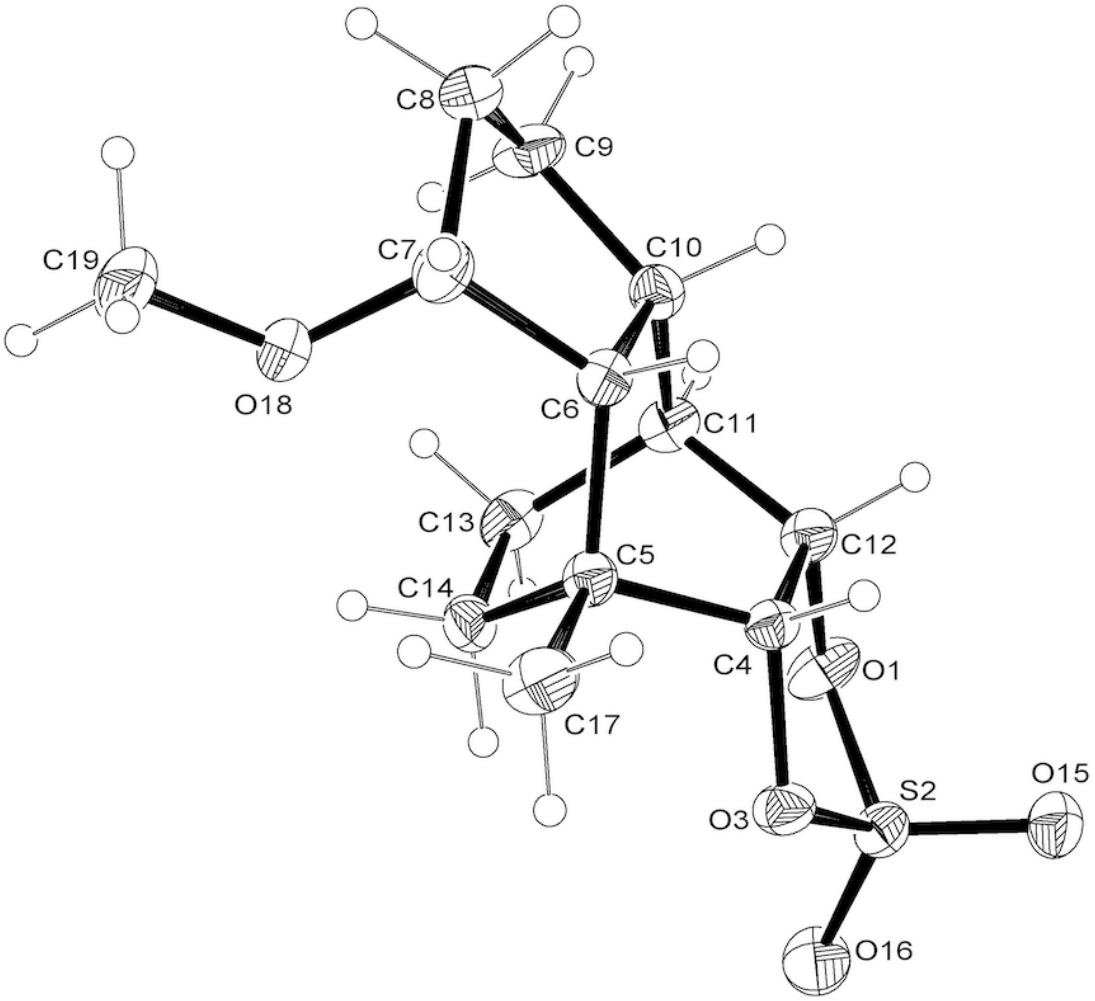


Figure S4: Plot arising from the single-crystal X-ray analysis of compound **18** – thermal ellipsoids at 50% probability (crystal grown by slow evaporation of a sample dissolved in dichloromethane/hexane) (CCDC 2082649).

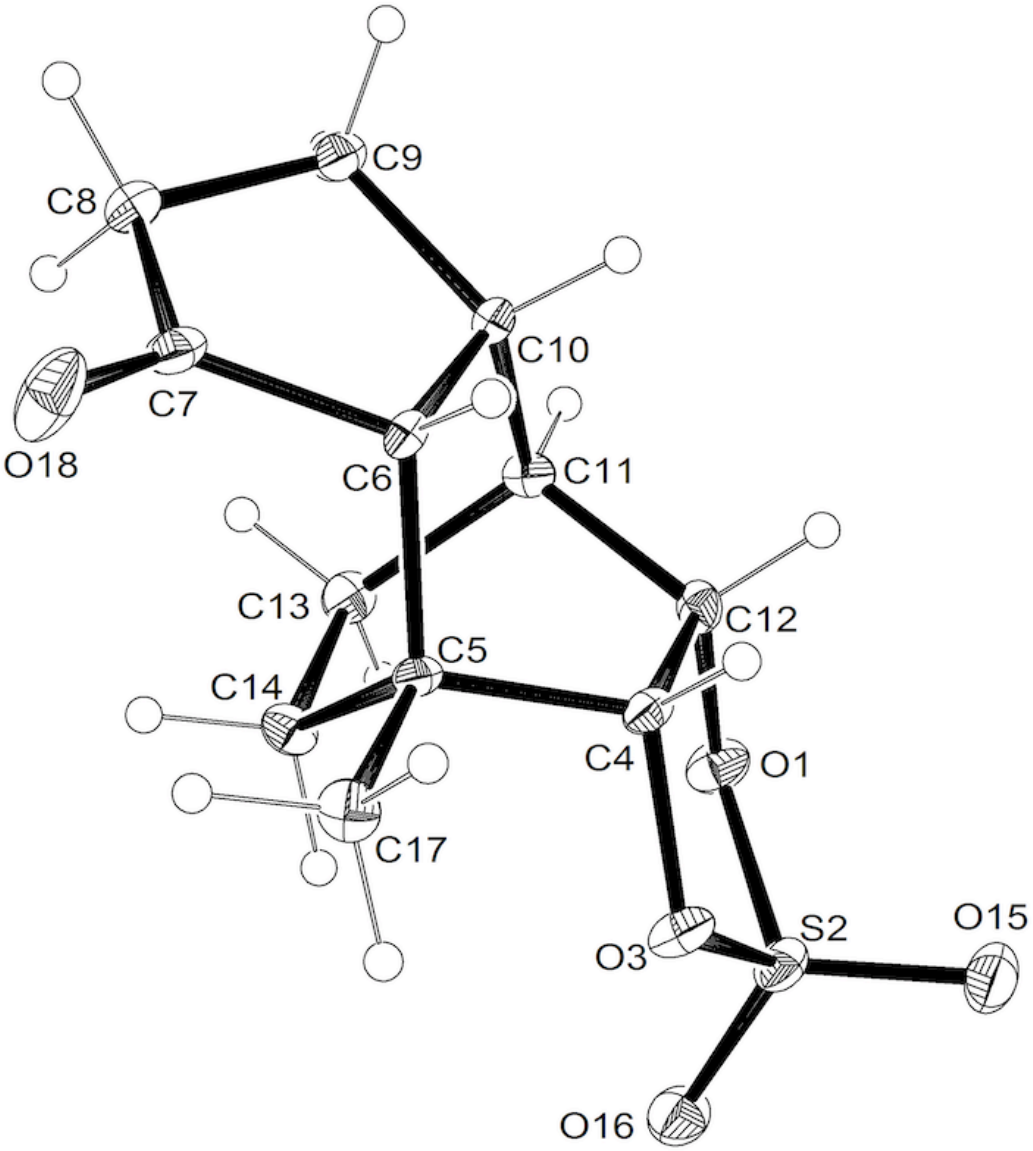


Figure S5: Plot arising from the single-crystal X-ray analysis of compound **23** – thermal ellipsoids at 50% probability (crystal grown by slow evaporation of a sample dissolved in dichloromethane/ethyl acetate) (CCDC 2082650).

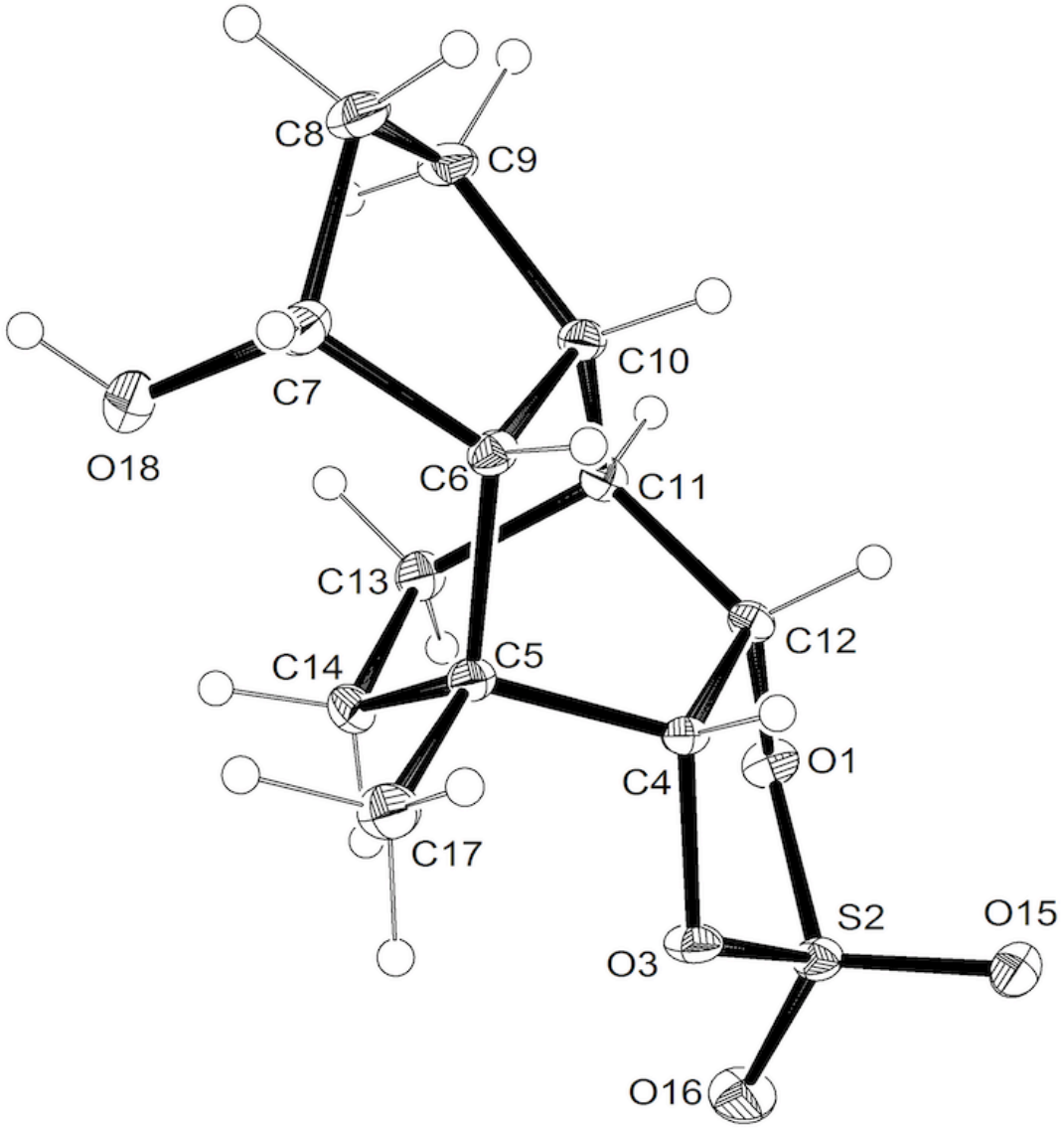


Figure S6: Plot arising from the single-crystal X-ray analysis of compound **25** – thermal ellipsoids at 50% probability (crystal grown by slow evaporation of a sample dissolved in dichloromethane/hexane/ethyl acetate/chloroform) (CCDC 2082651).

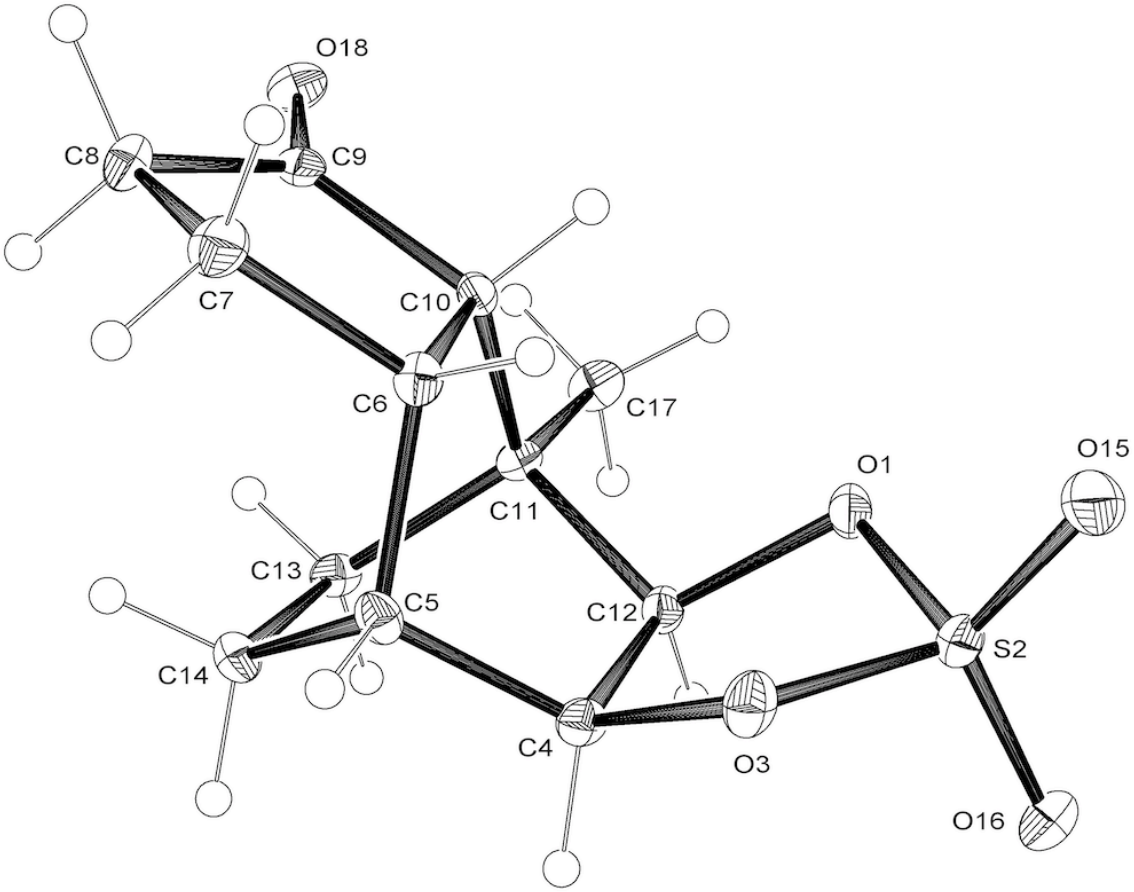


Figure S7: Plot arising from the single-crystal X-ray analysis of compound **33** – thermal ellipsoids at 50% probability (crystal grown by slow evaporation of a sample dissolved in dichloromethane/hexane/ethyl acetate) (CCDC 2082652).

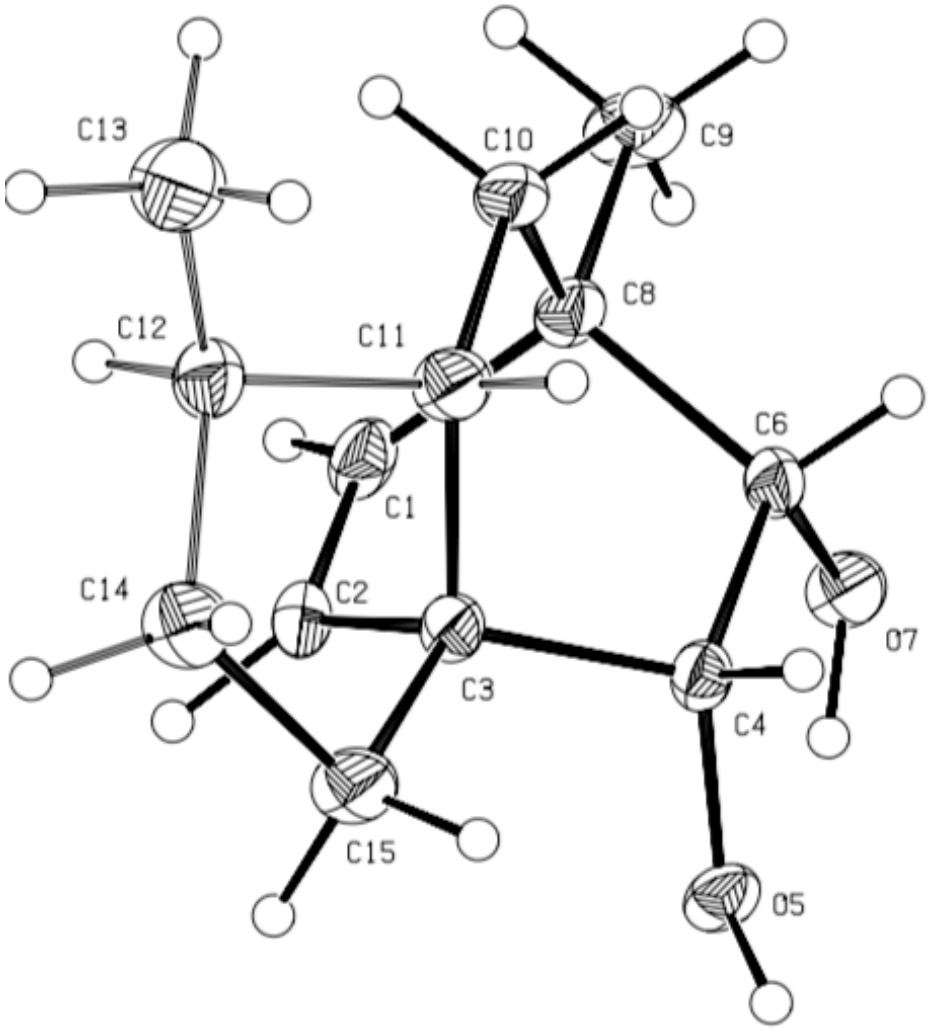


Figure S8: Plot arising from the single-crystal X-ray analysis of compound **40** – thermal ellipsoids at 30% probability (crystal grown by slow evaporation of a sample dissolved in hexane/ethyl acetate) (CCDC 2082653).

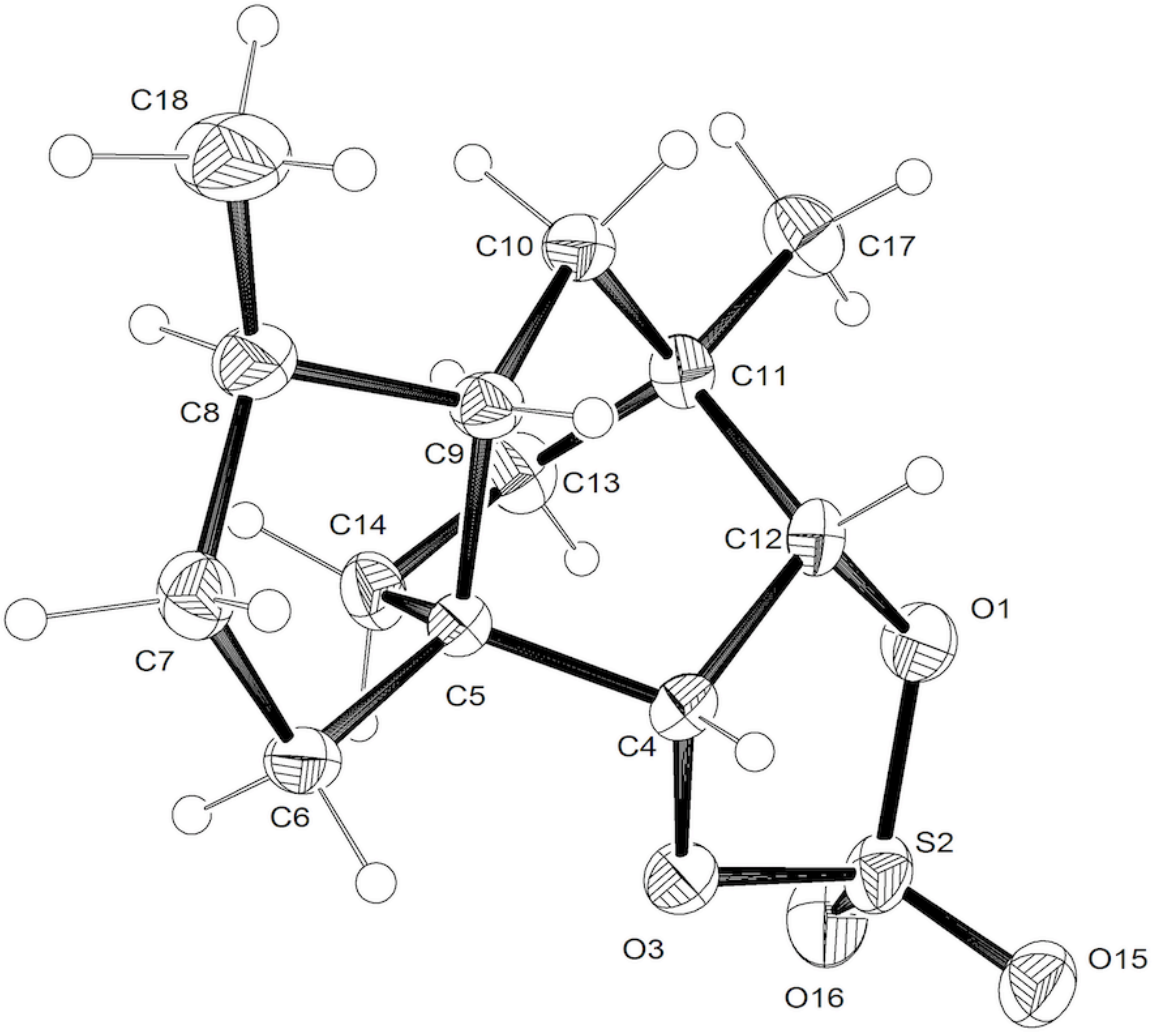
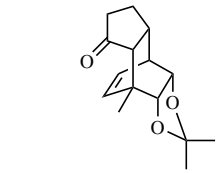
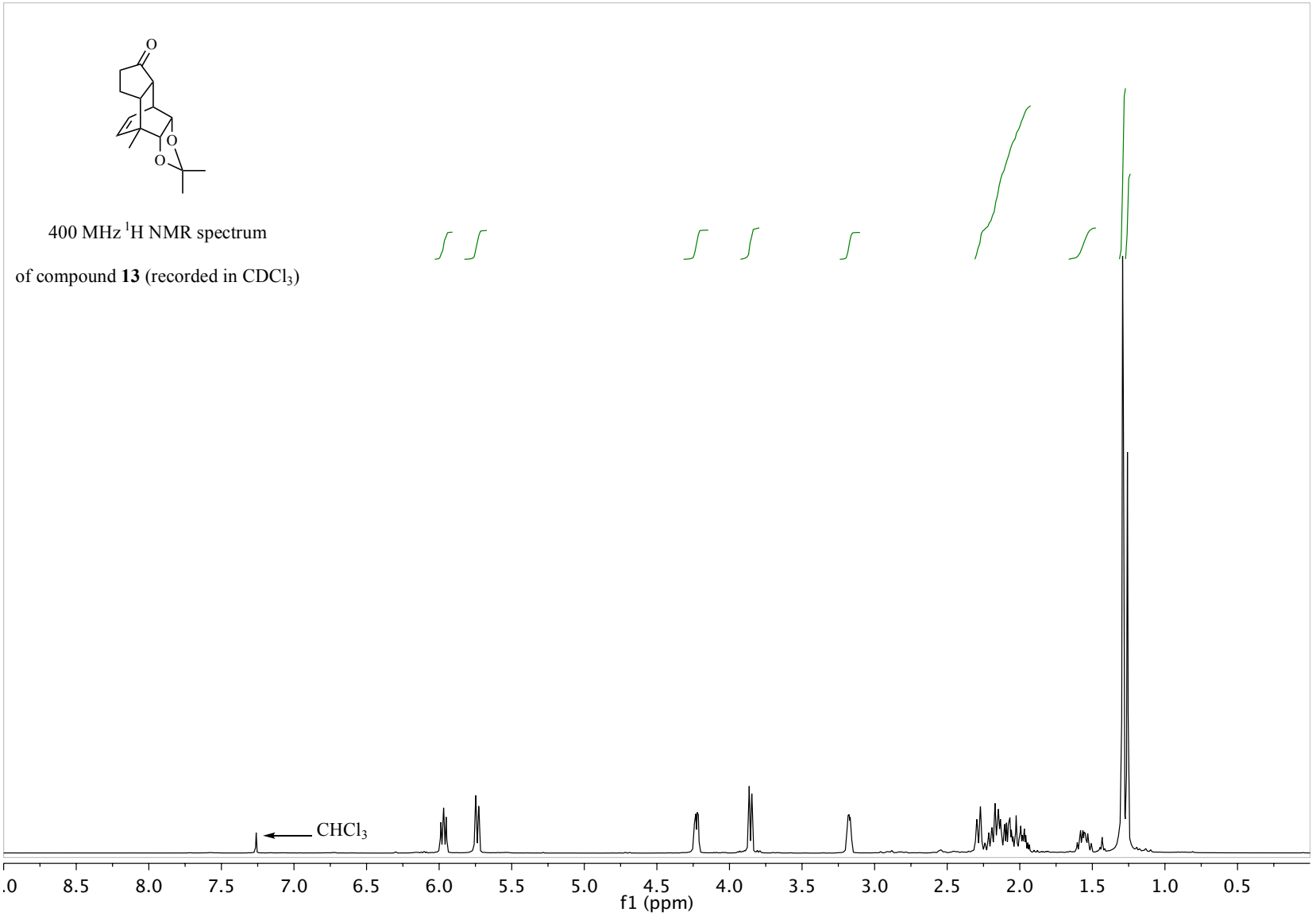


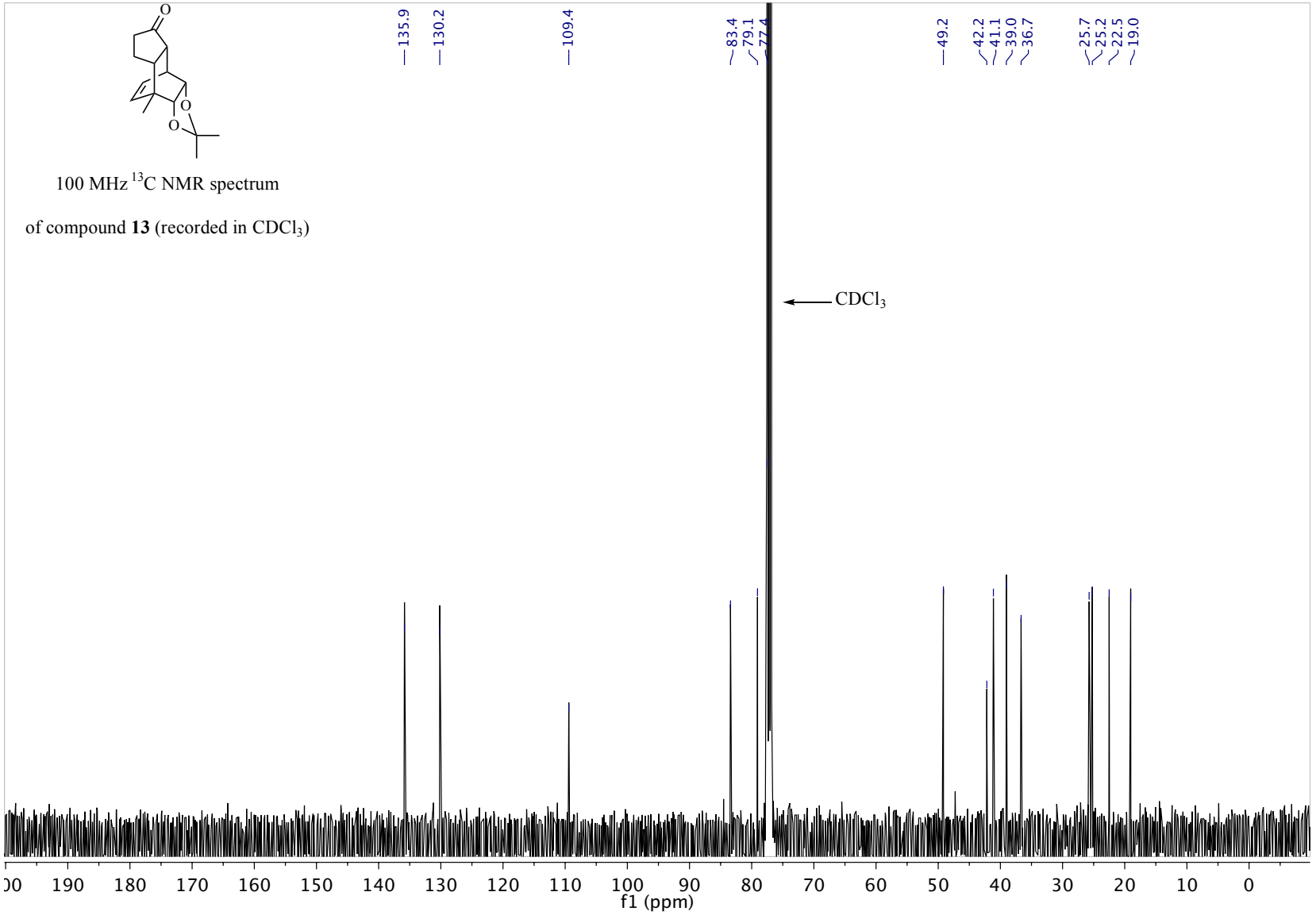
Figure S9: Plot arising from the single-crystal X-ray analysis of compound **42** – thermal ellipsoids at 50% probability (crystal grown by slow evaporation of a sample dissolved in dichloromethane/ hexane) (CCDC 2082654).



400 MHz ^{1}H NMR spectrum

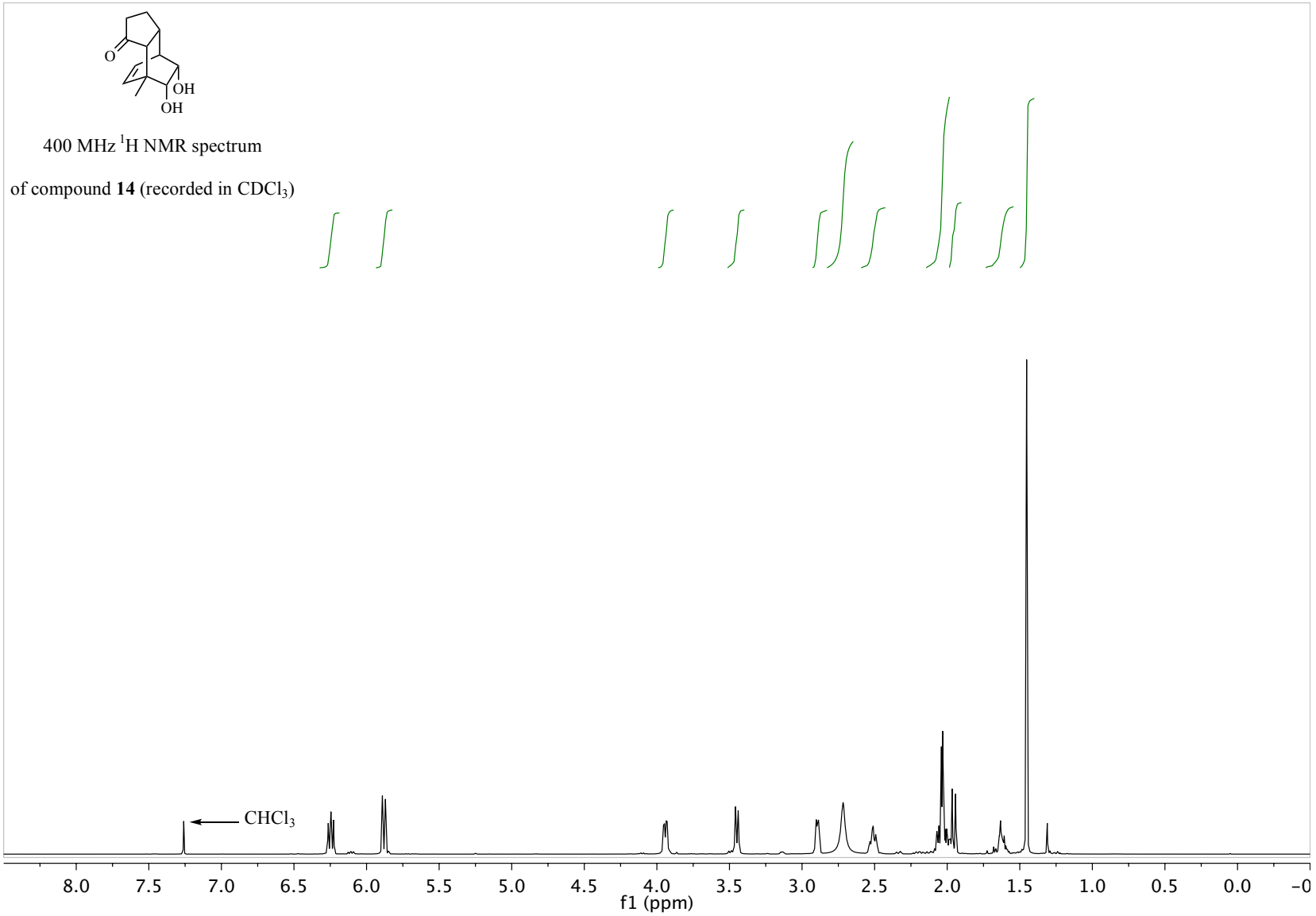
of compound **12** (recorded in $CDCl_3$)


O
O
O
400 MHz ^{1}H NMR spectrum
of compound **13** (recorded in $CDCl_3$)
$CHCl_3$
.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
f1 (ppm)



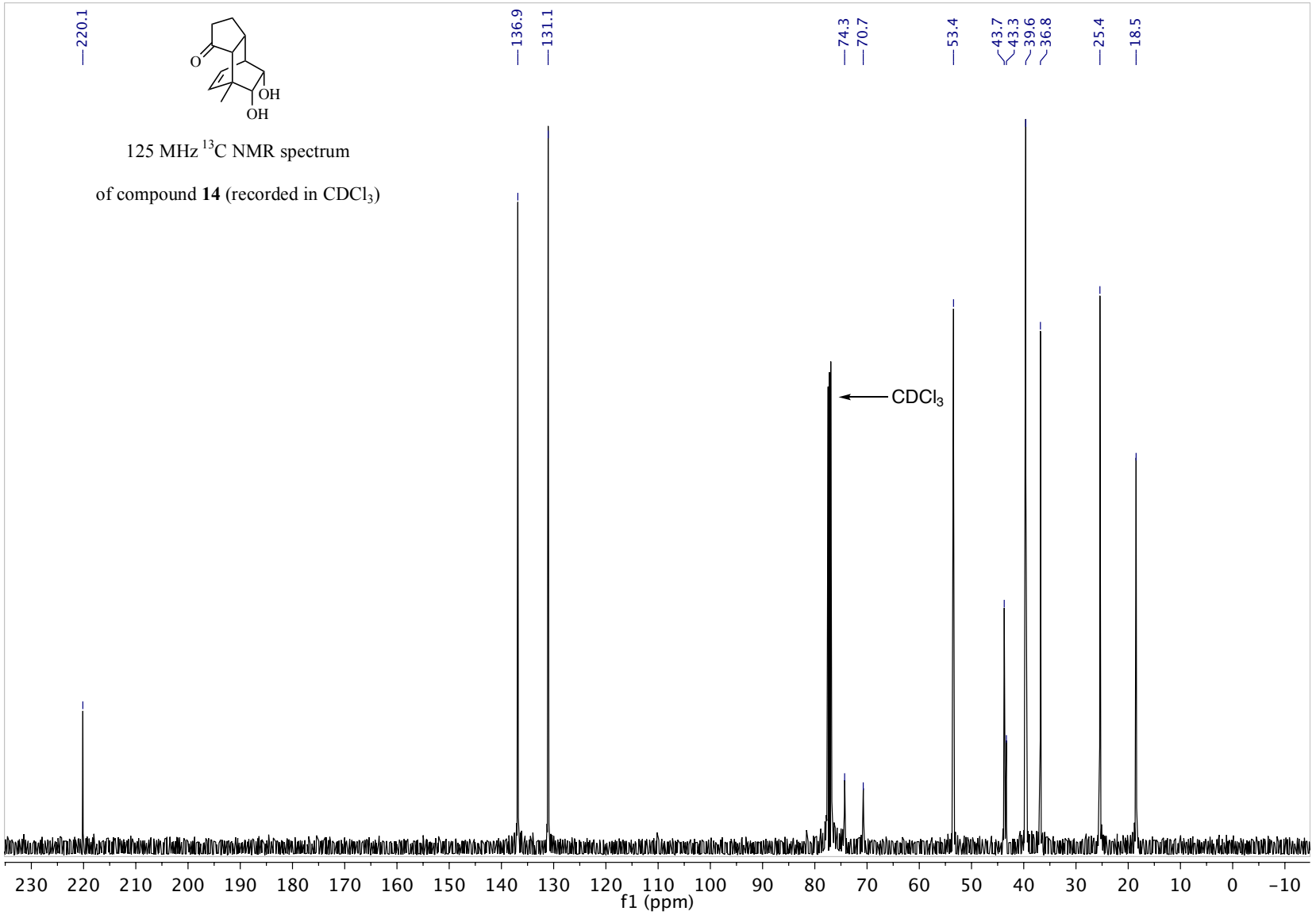
100 MHz ^{13}C NMR spectrum

of compound **13** (recorded in $CDCl_3$)



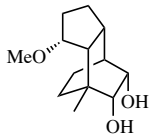
400 MHz ^{1}H NMR spectrum

of compound **14** (recorded in $CDCl_3$)



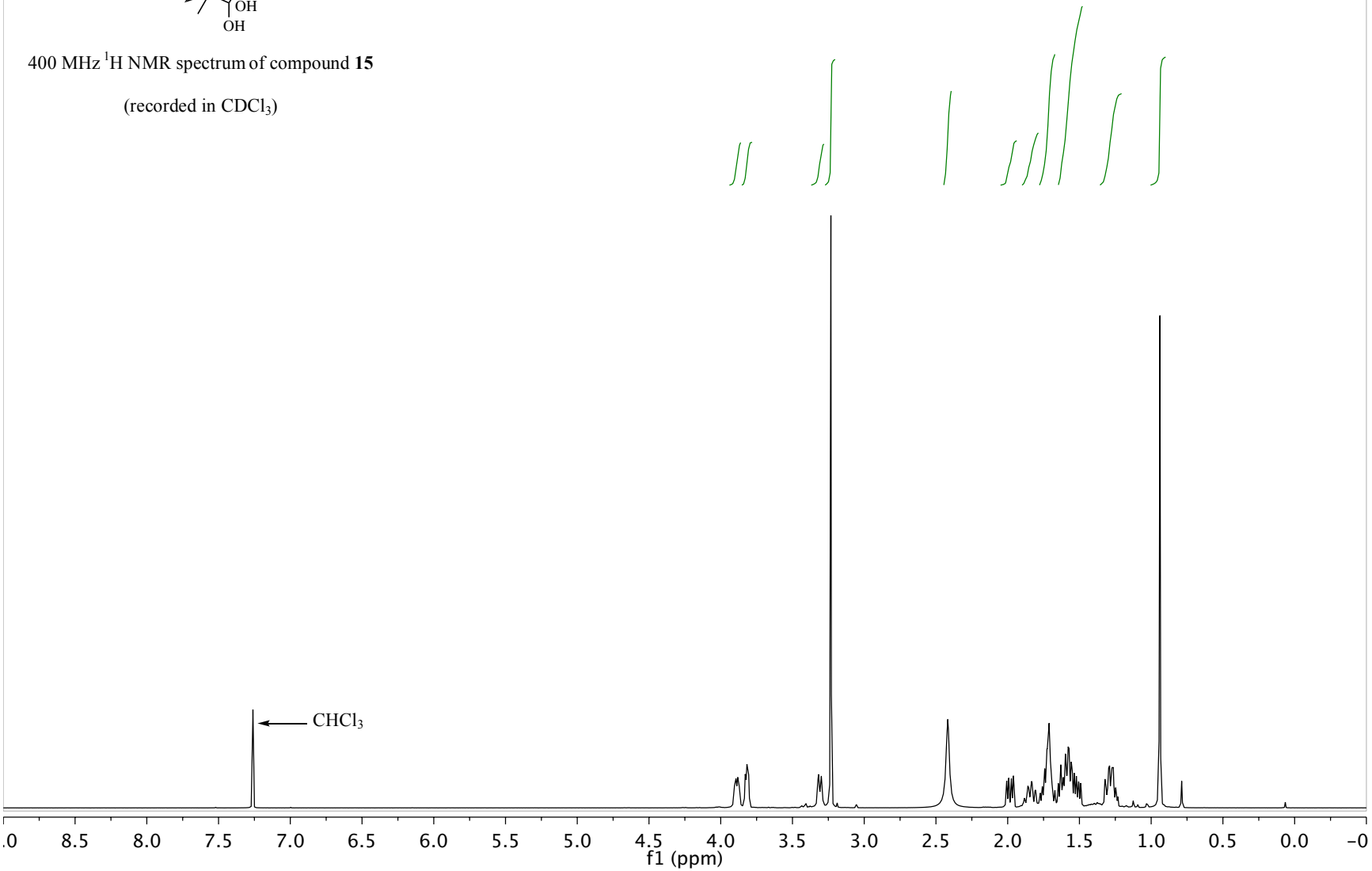
125 MHz ^{13}C NMR spectrum

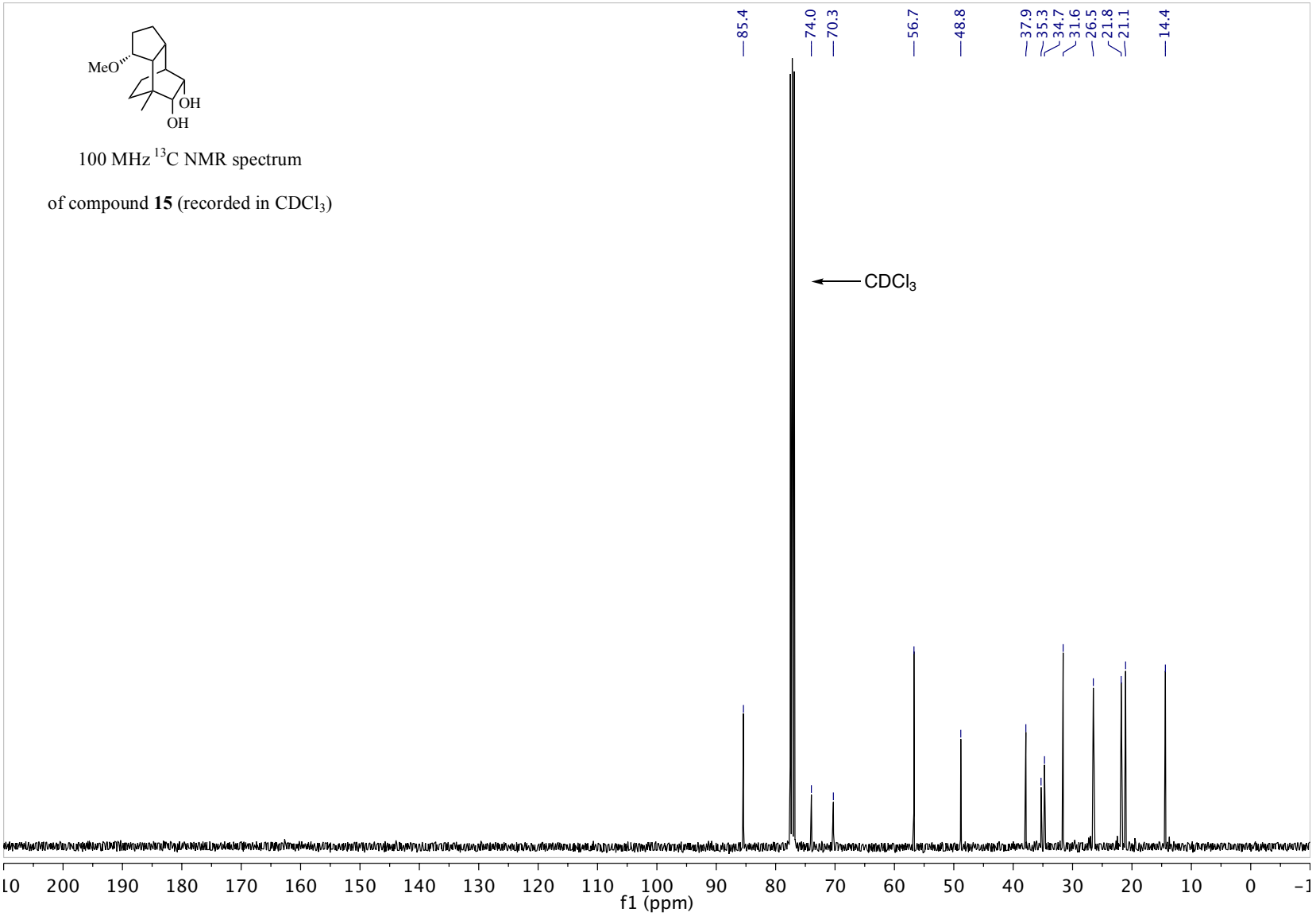
of compound **14** (recorded in $CDCl_3$)

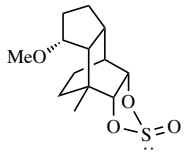


400 MHz ^{1}H NMR spectrum of compound **15**

(recorded in $CDCl_3$)

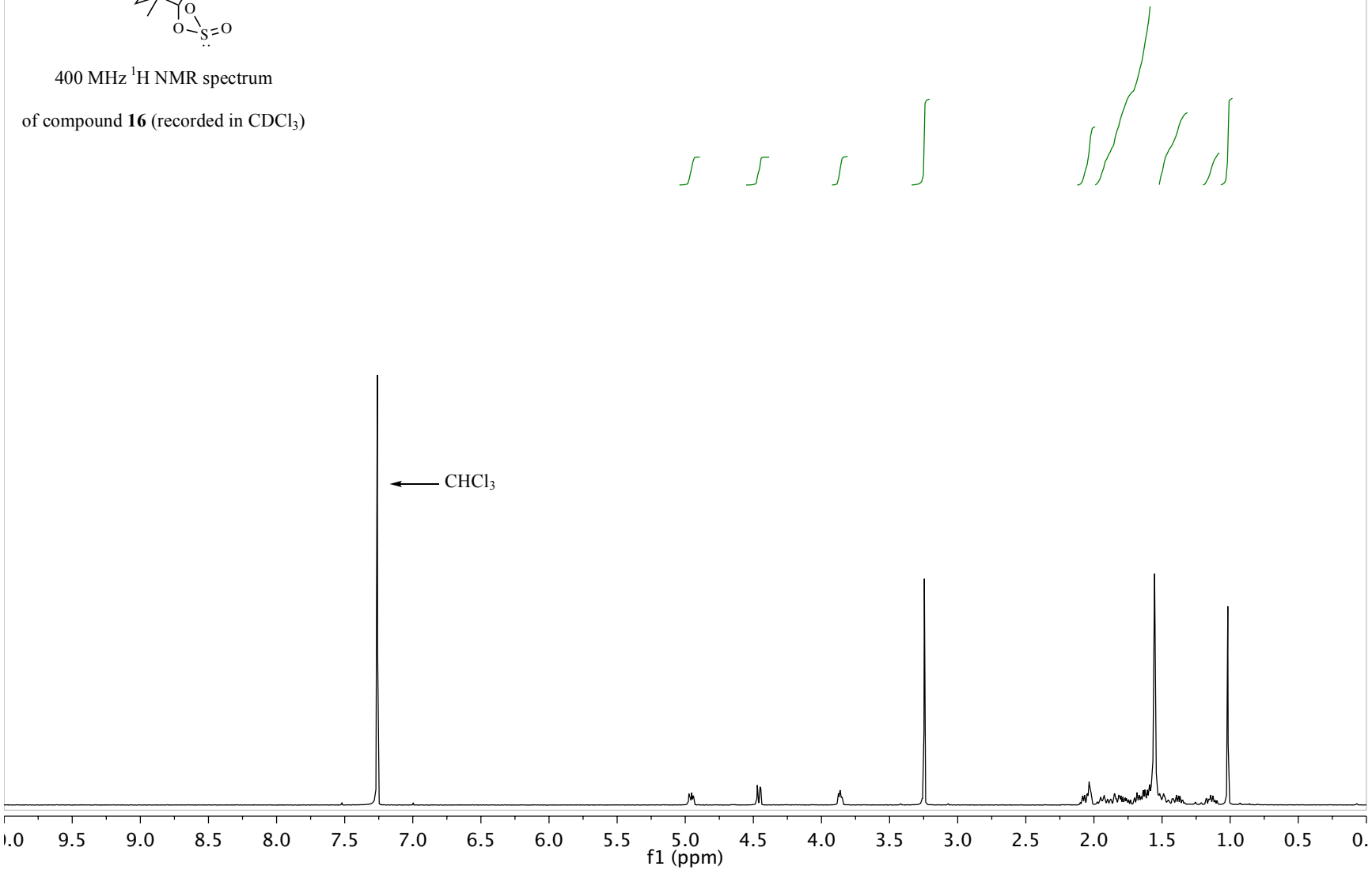


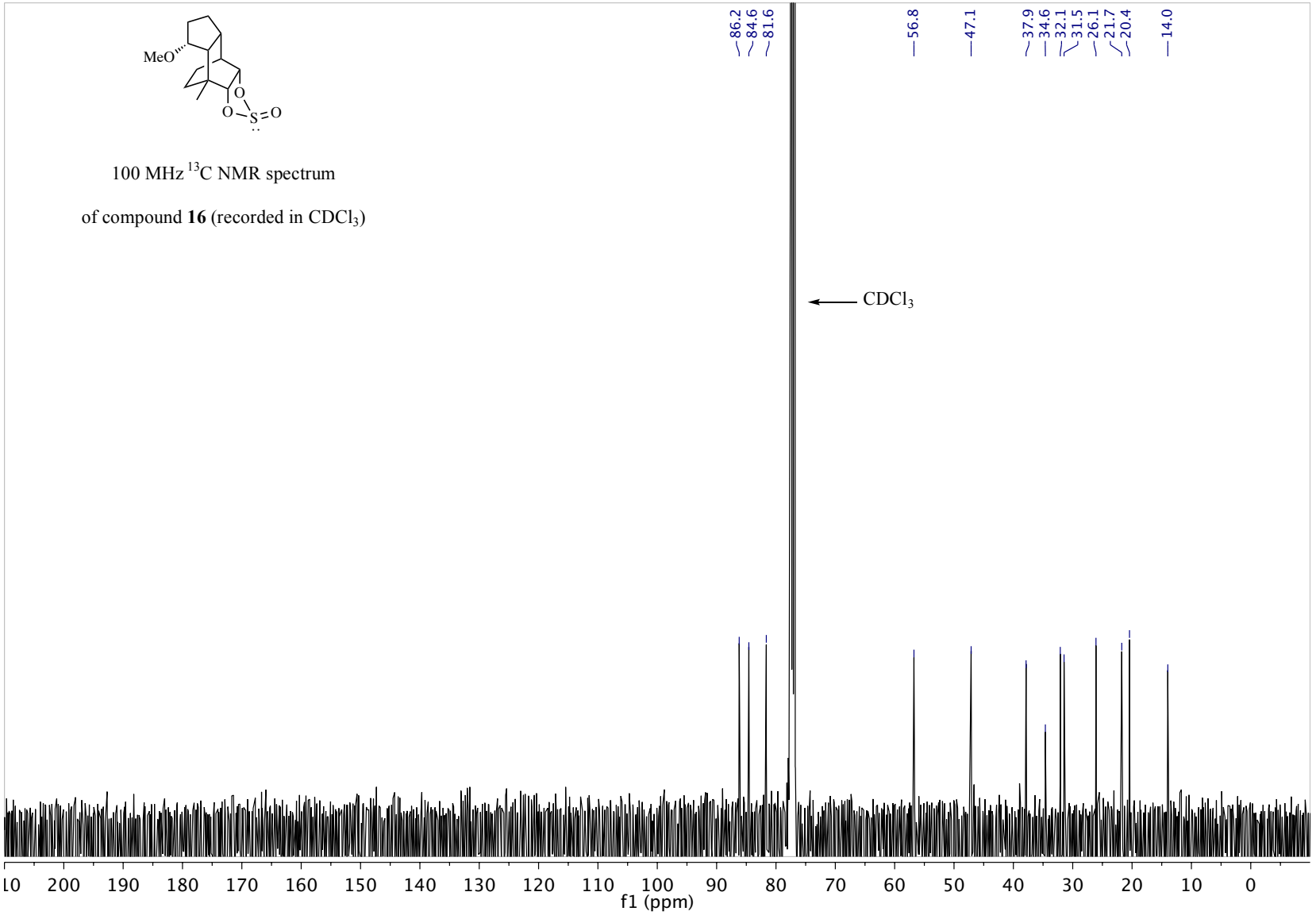

MeO
OH
OH
100 MHz ^{13}C NMR spectrum
of compound **15** (recorded in $CDCl_3$)
85.4
74.0
70.3
56.7
48.8
37.9
35.3
34.7
31.6
26.5
21.8
21.1
14.4
$CDCl_3$
f1 (ppm)



400 MHz ^{1}H NMR spectrum

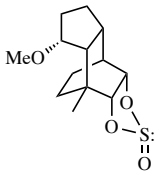
of compound **16** (recorded in $CDCl_3$)





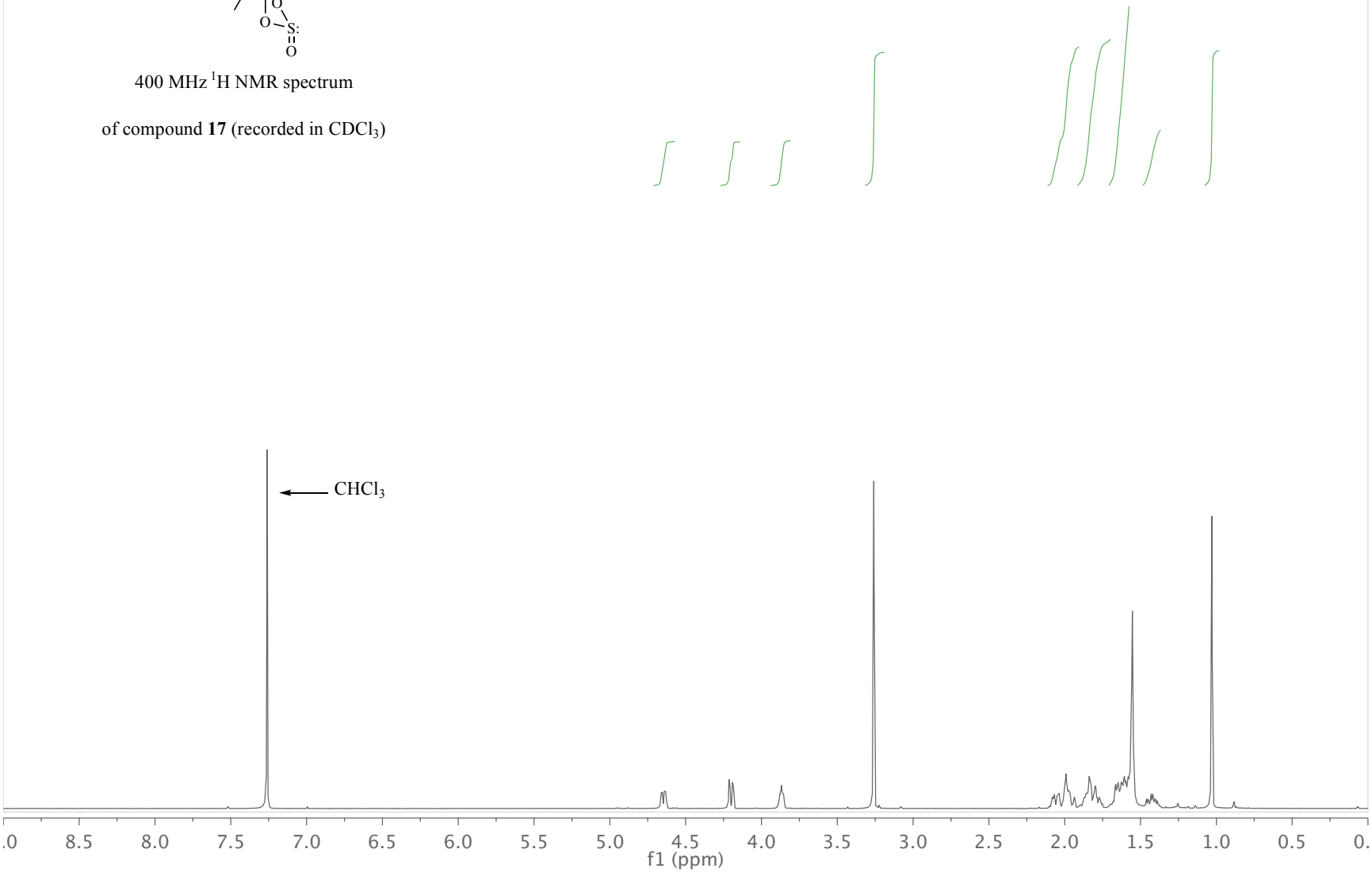
100 MHz ^{13}C NMR spectrum

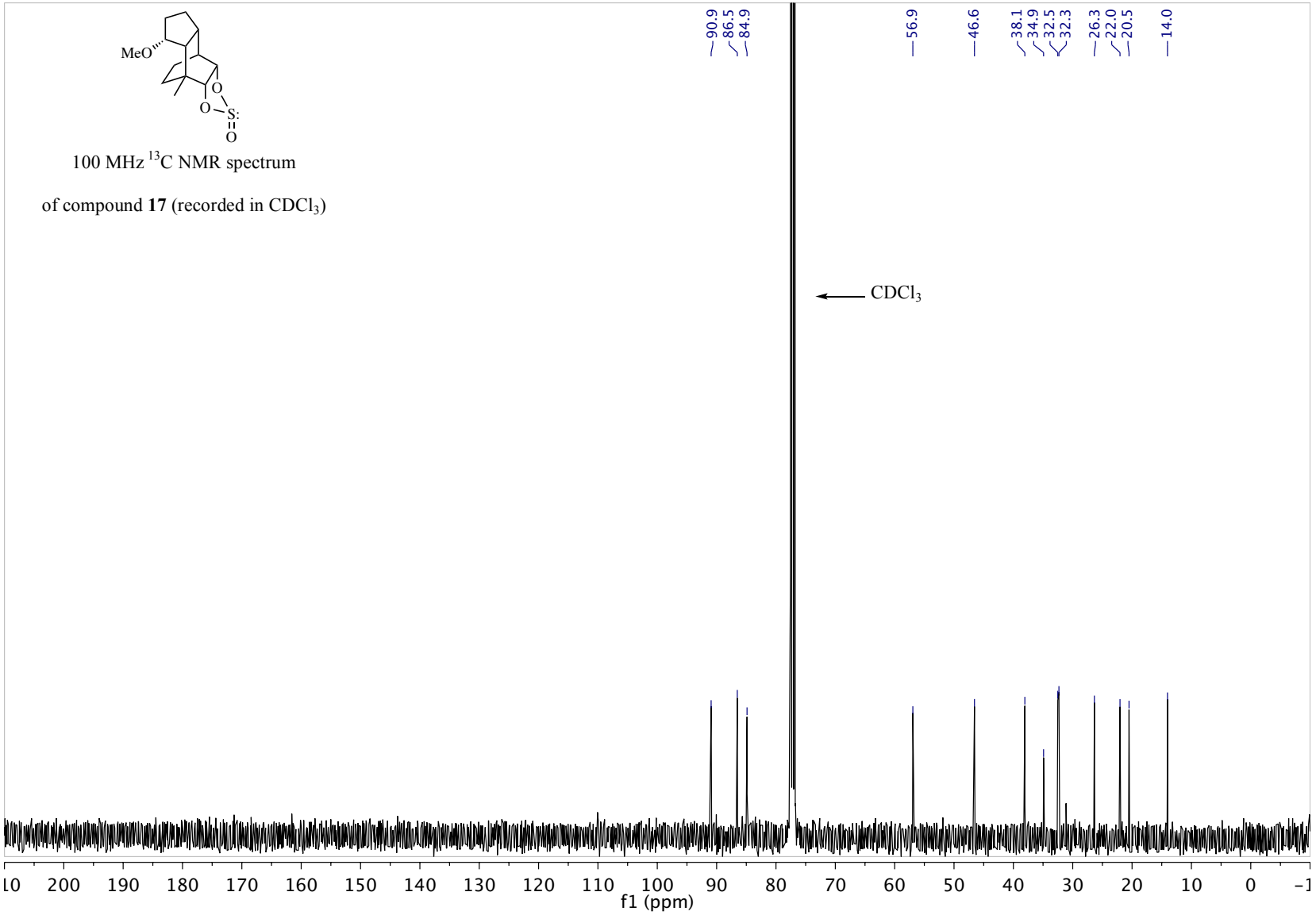
of compound **16** (recorded in $CDCl_3$)



400 MHz ^{1}H NMR spectrum

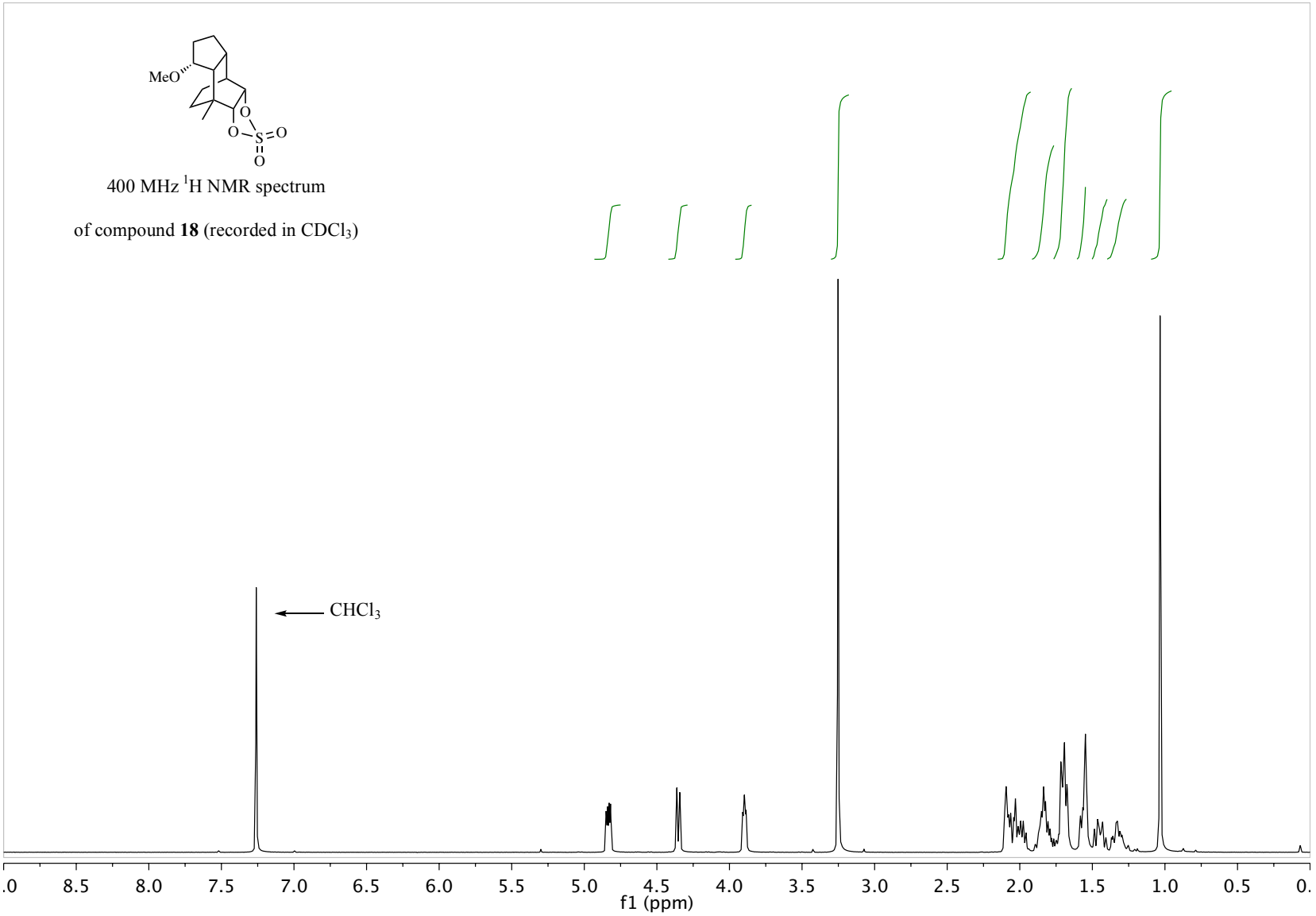
of compound **17** (recorded in $CDCl_3$)

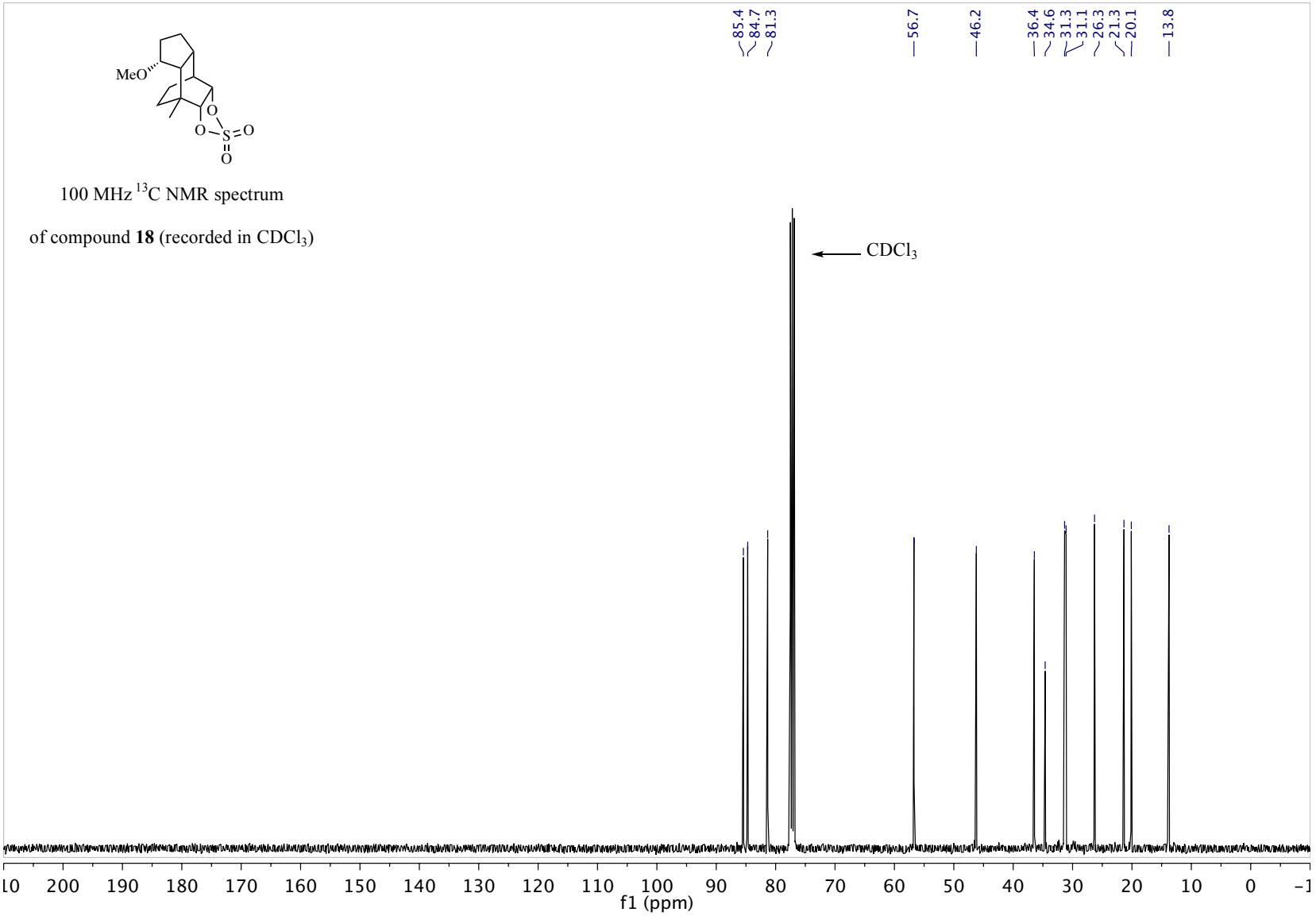


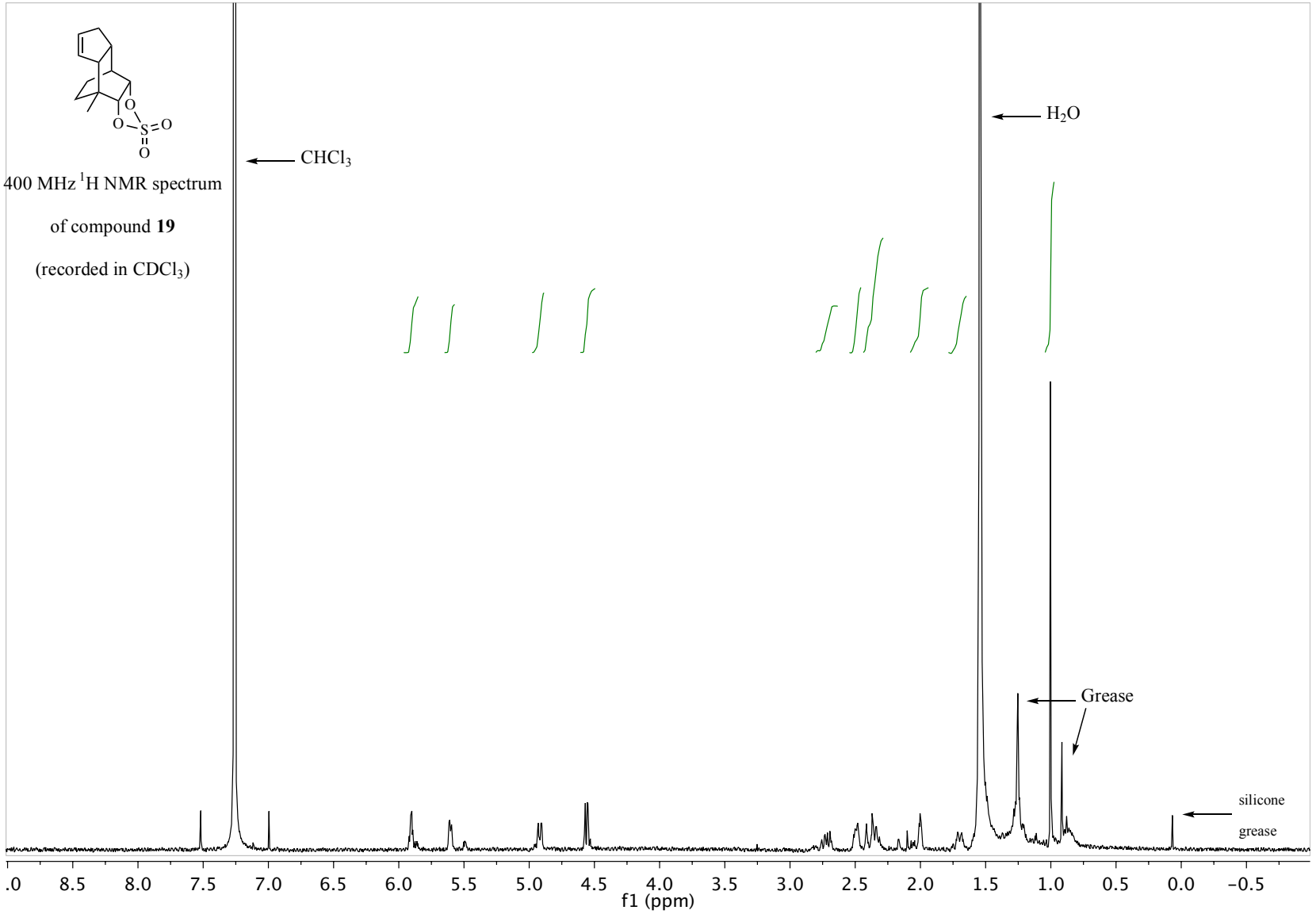


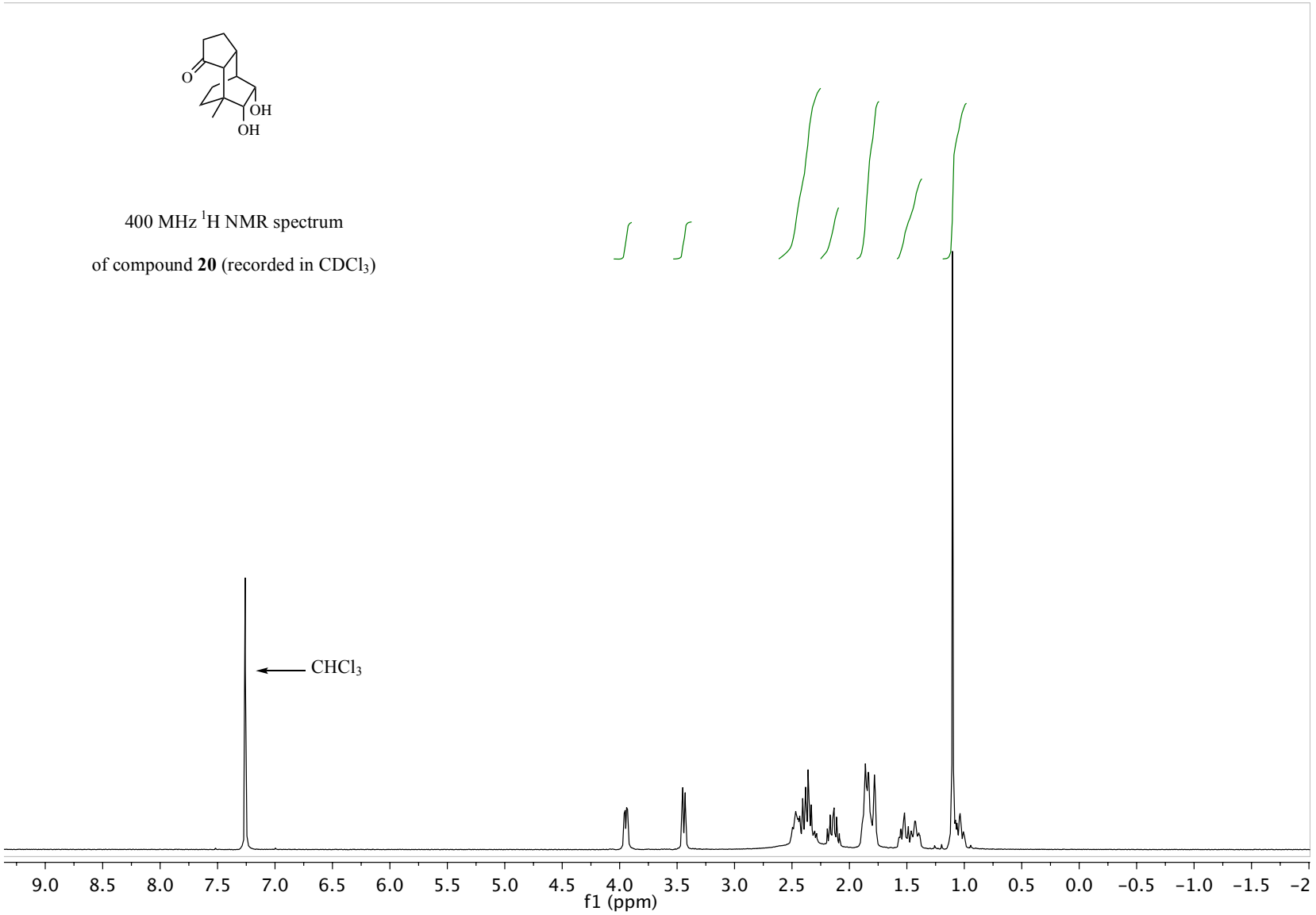
100 MHz ^{13}C NMR spectrum

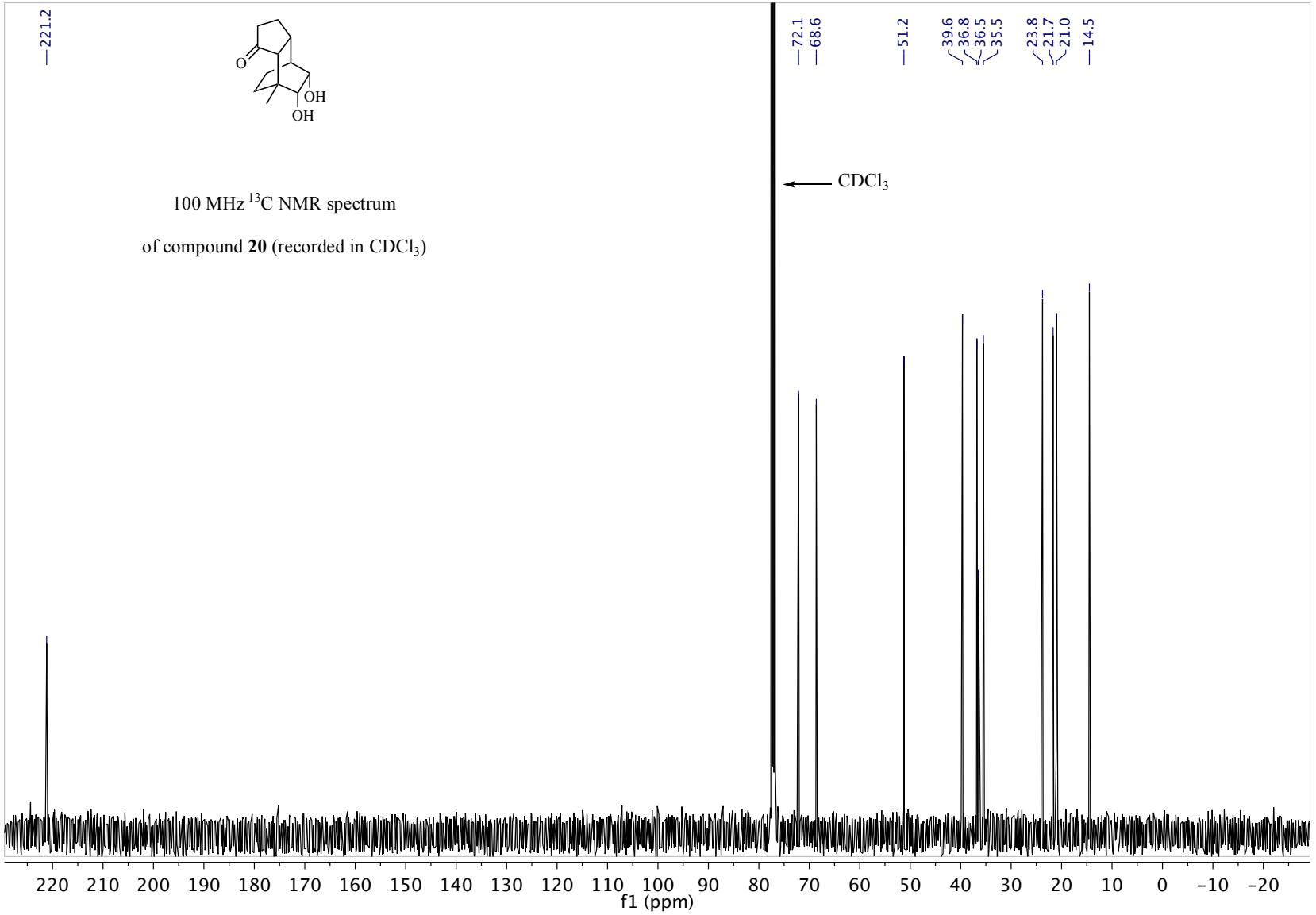
of compound **17** (recorded in $CDCl_3$)

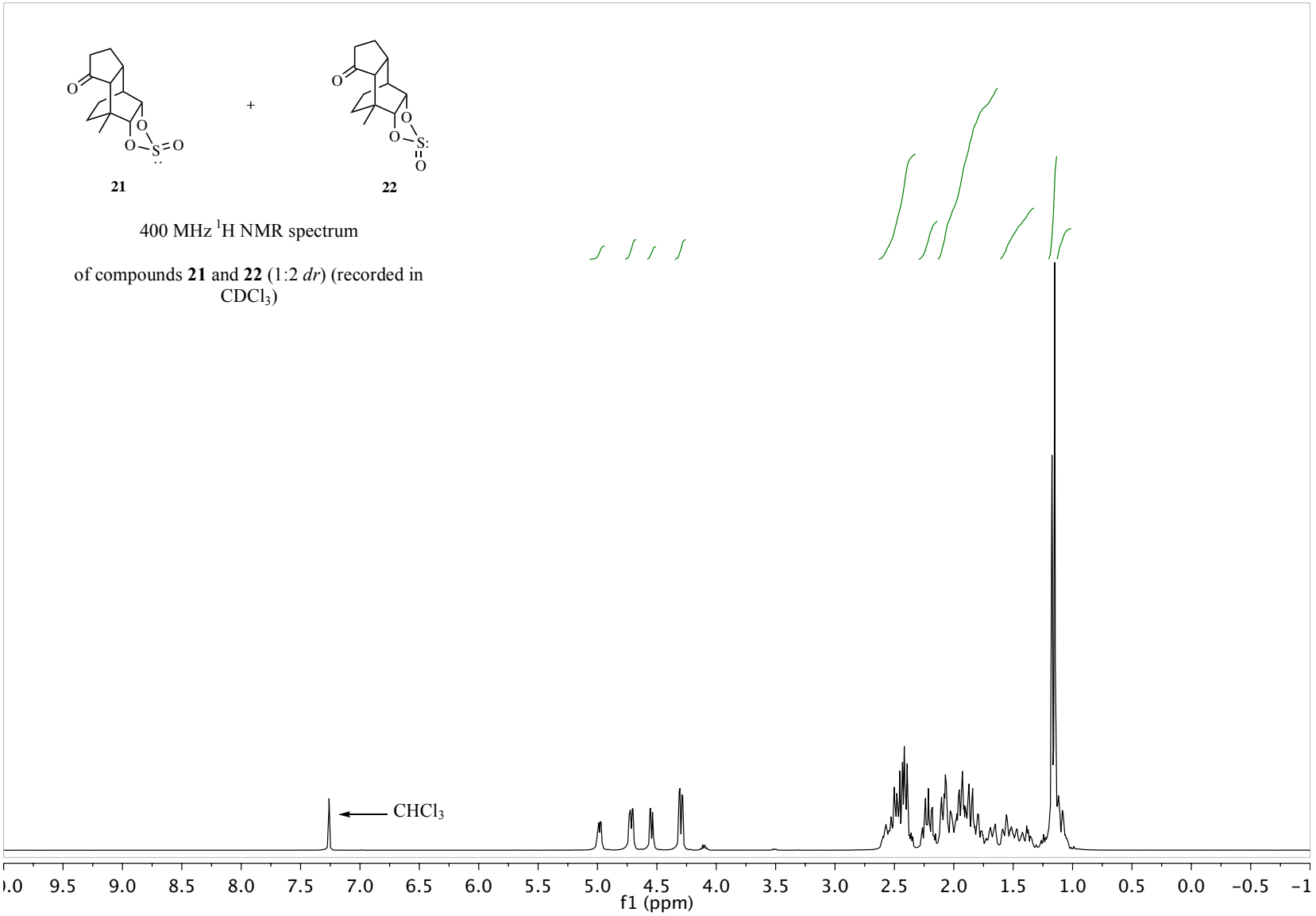

MeO
O
O
S
O
O
400 MHz ^{1}H NMR spectrum
of compound **18** (recorded in $CDCl_3$)
$CHCl_3$
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

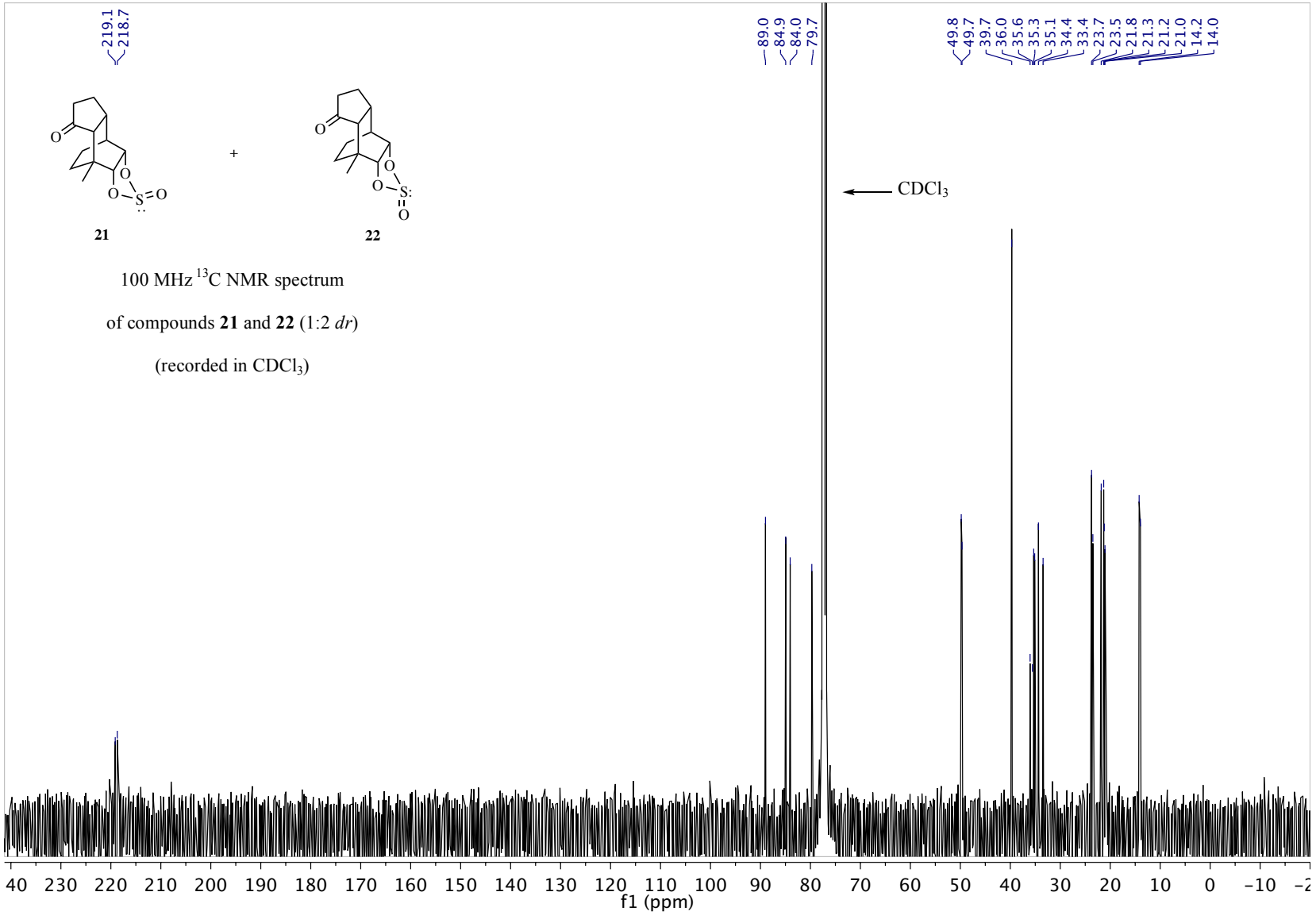

MeO
O
O
S
O
O
100 MHz 13C NMR spectrum
of compound 18 (recorded in CDCl3)
85.4
84.7
81.3
56.7
46.2
36.4
34.6
31.3
31.1
26.3
21.3
20.1
13.8
CDCl3
f1 (ppm)


400 MHz ^{1}H NMR spectrum
of compound **19**
(recorded in $CDCl_3$)
$CHCl_3$
H_2O
Grease
silicone
grease
f1 (ppm)


O
OH
OH
400 MHz ^{1}H NMR spectrum
of compound **20** (recorded in $CDCl_3$)
$CHCl_3$
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 -1.5 -2
f1 (ppm)


221.2
72.1
68.6
51.2
39.6
36.8
36.5
35.5
23.8
21.7
21.0
14.5
O
OH
OH
CDCl3
100 MHz 13C NMR spectrum
of compound 20 (recorded in CDCl3)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

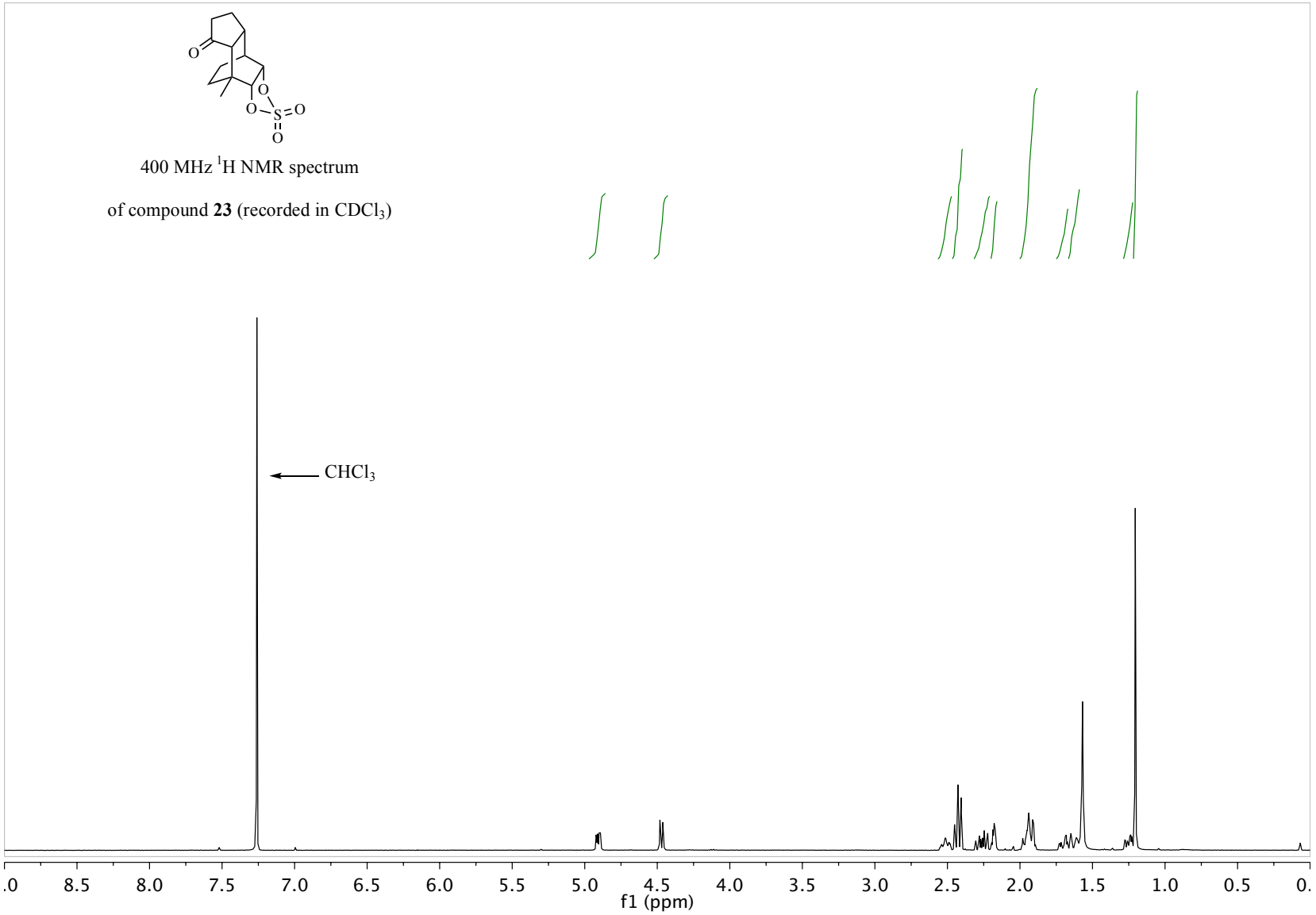

21
22
400 MHz ^{1}H NMR spectrum
of compounds **21** and **22** (1:2 *dr*) (recorded in $CDCl_3$)
$CHCl_3$
f1 (ppm)

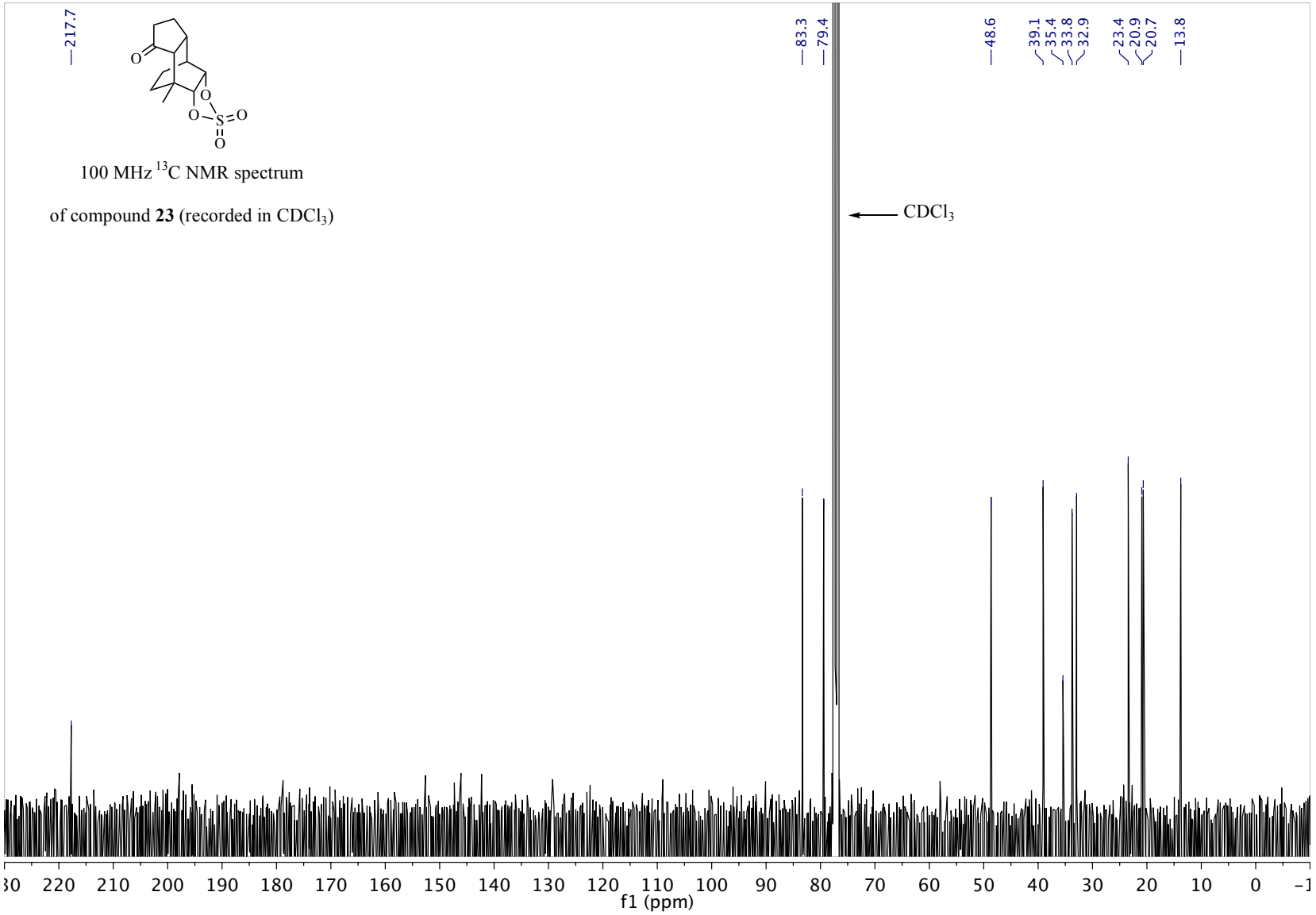


100 MHz ^{13}C NMR spectrum

of compounds **21** and **22** (1:2 *dr*)

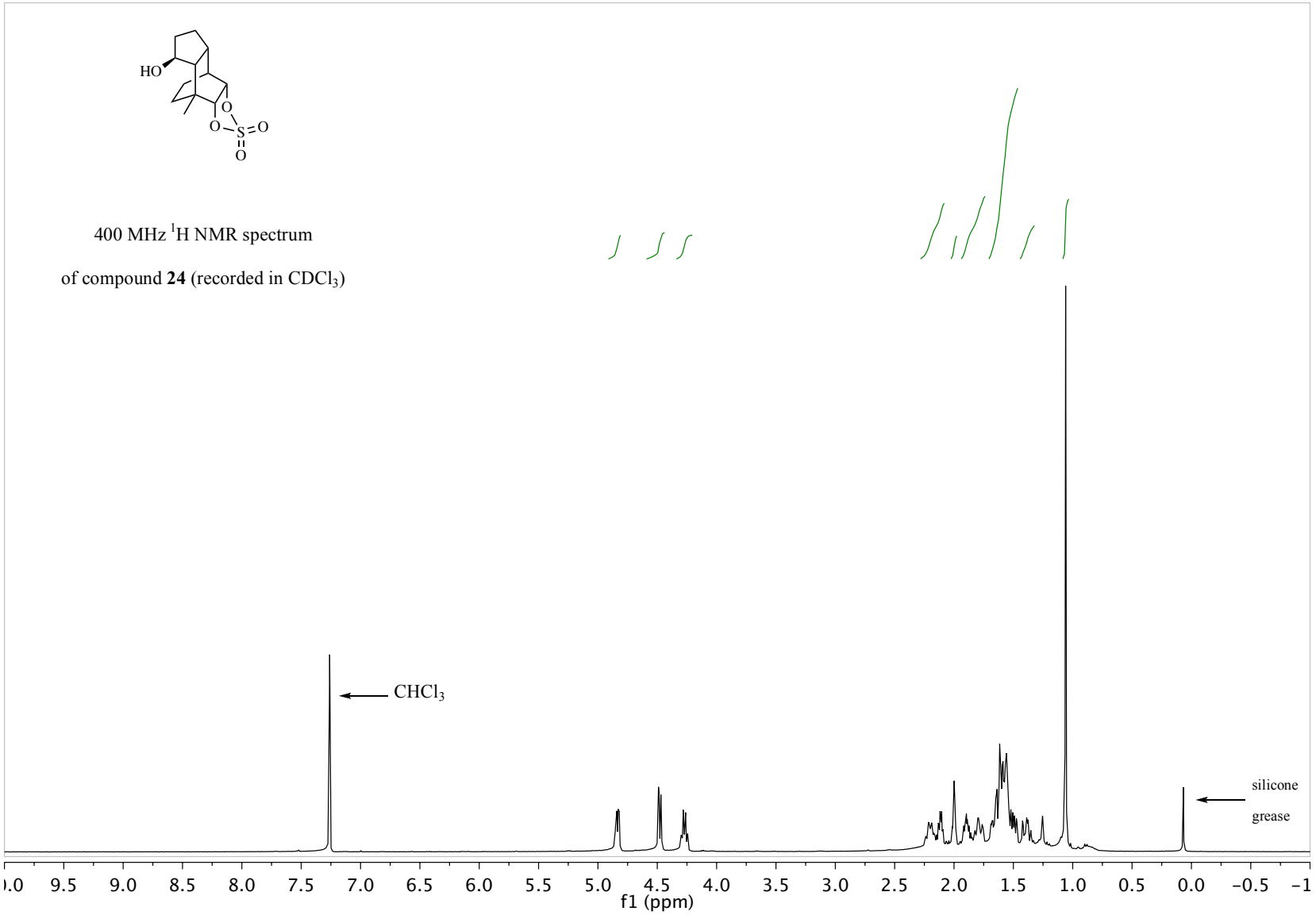
(recorded in $CDCl_3$)

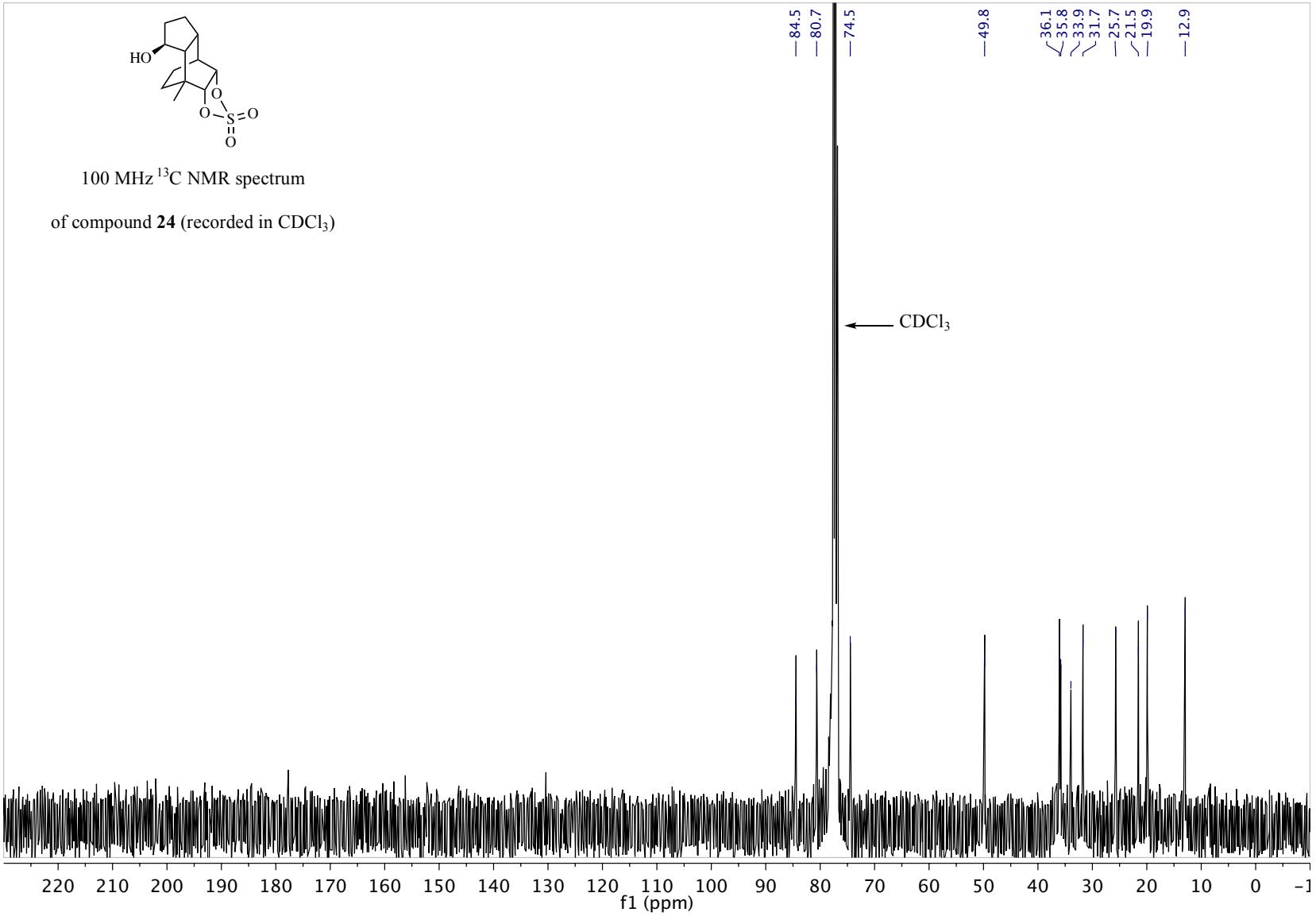

O
O
O
S
O
O
400 MHz ^{1}H NMR spectrum
of compound **23** (recorded in $CDCl_3$)
$CHCl_3$
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

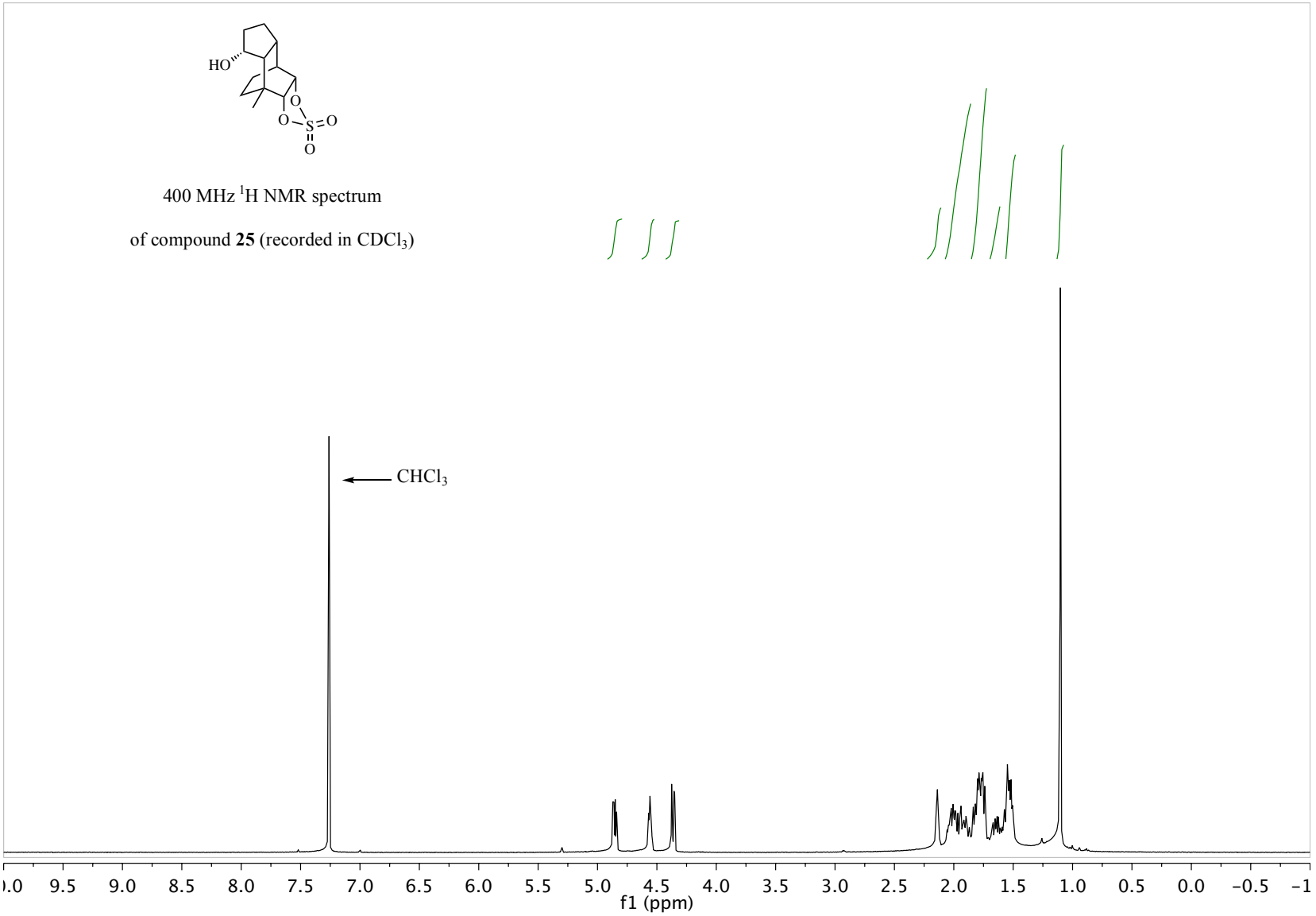


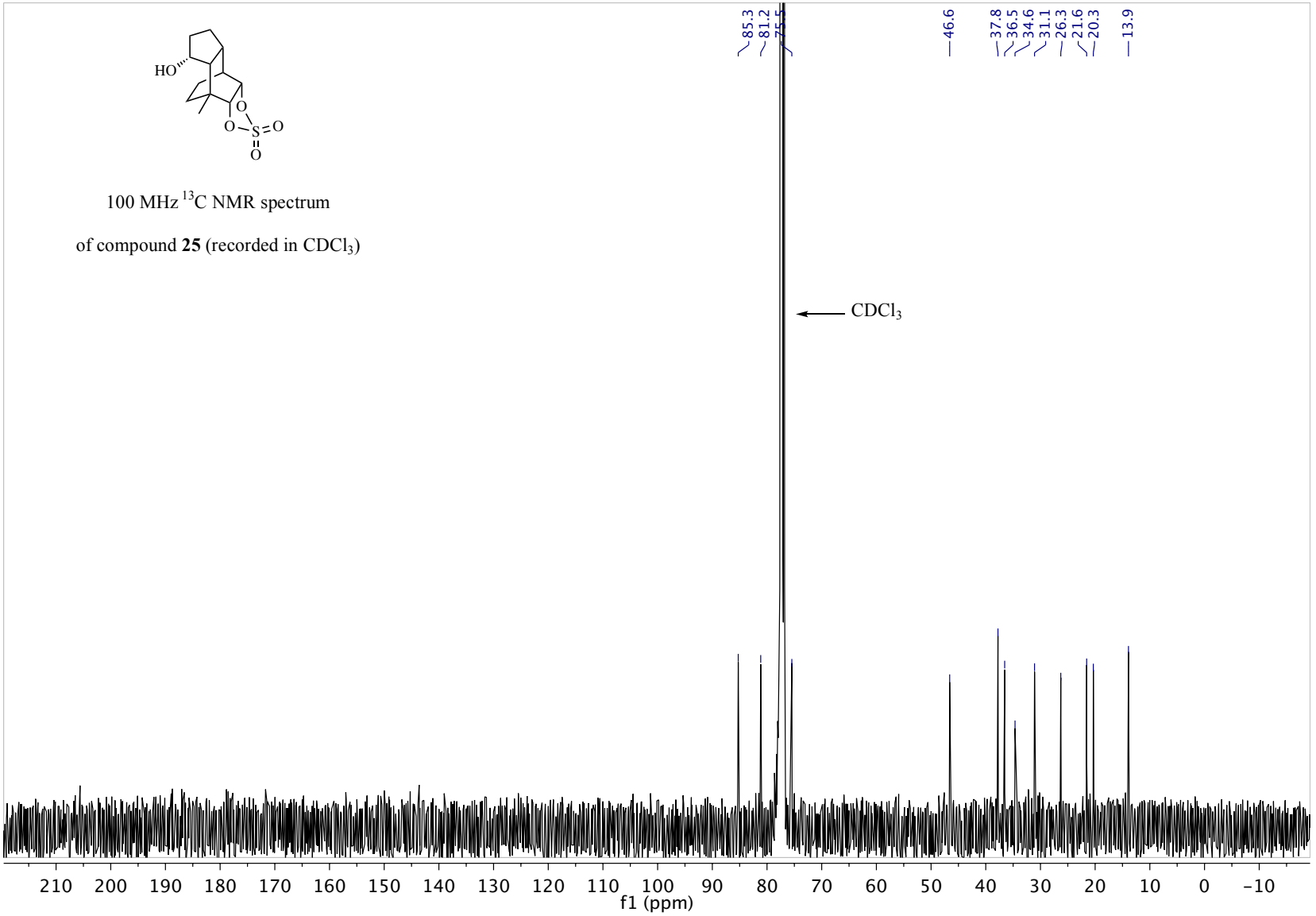
100 MHz ^{13}C NMR spectrum

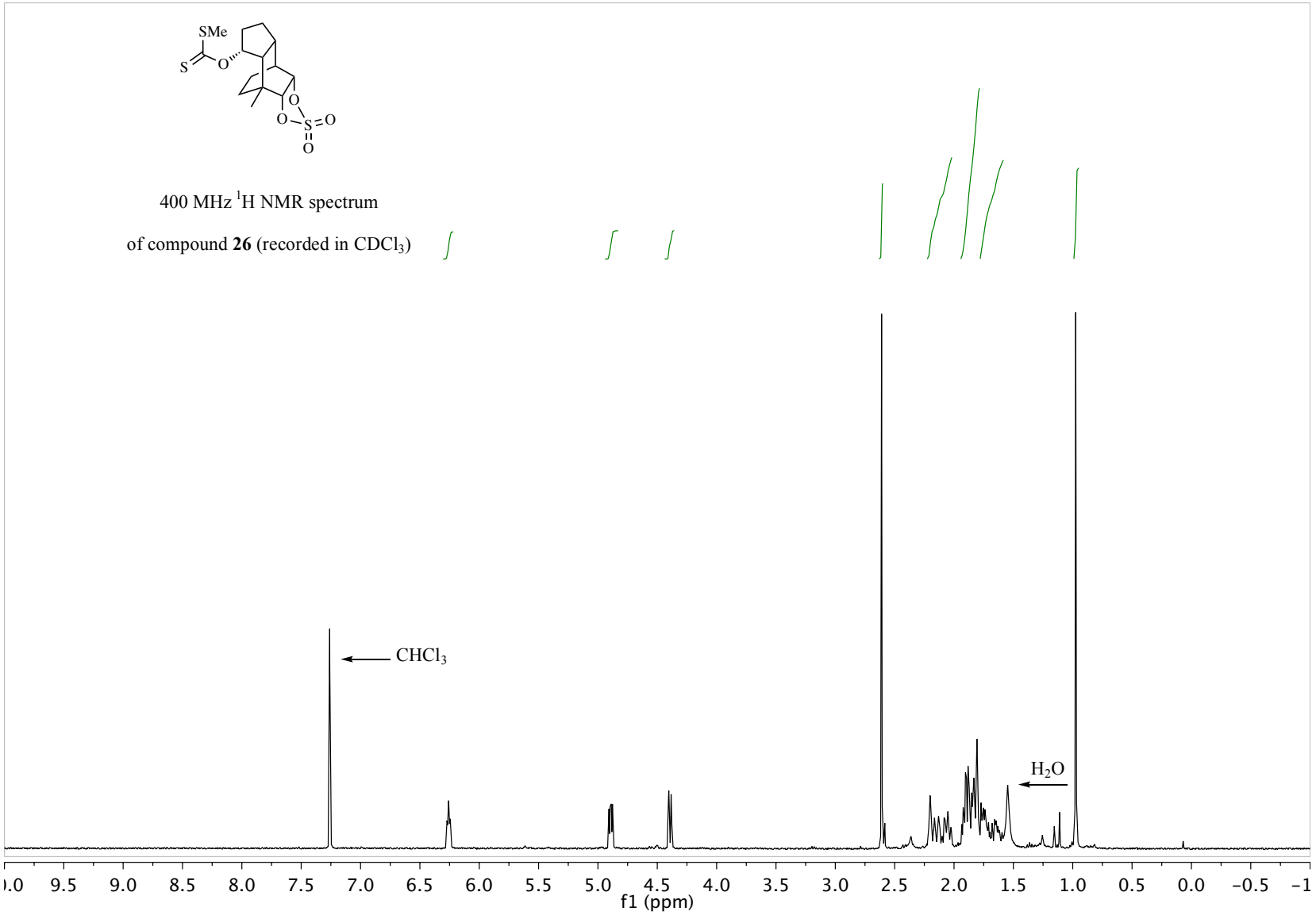
of compound **23** (recorded in $CDCl_3$)

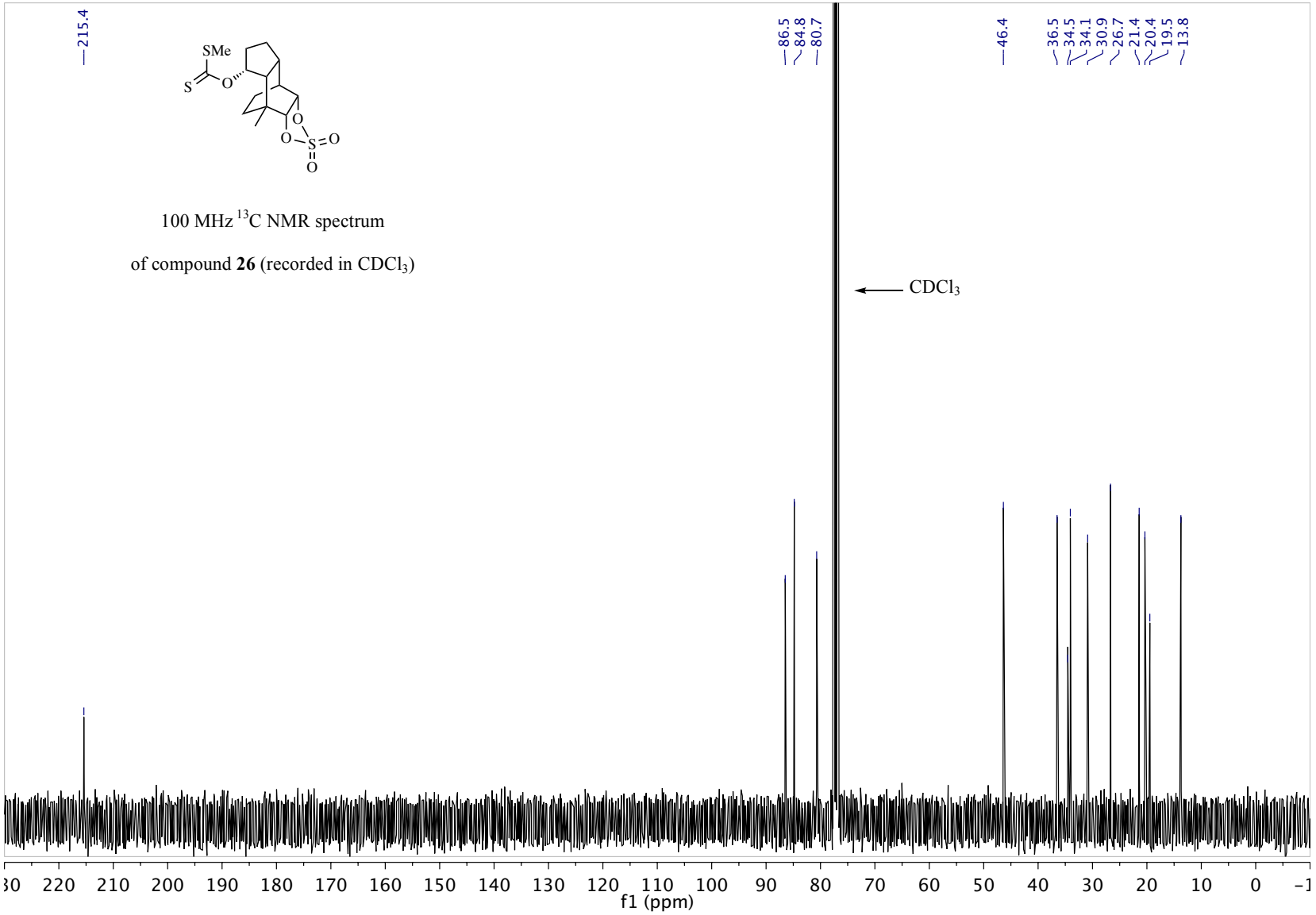

HO
O
O
S
O
O
400 MHz ^{1}H NMR spectrum
of compound **24** (recorded in $CDCl_3$)
$CHCl_3$
silicone
grease
f1 (ppm)


HO
O
O
S
O
O
100 MHz 13C NMR spectrum
of compound 24 (recorded in CDCl3)
84.5
80.7
74.5
49.8
36.1
35.8
33.9
31.7
25.7
21.5
19.9
12.9
CDCl3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)


HO
O
O
S
O
O
400 MHz ^{1}H NMR spectrum
of compound **25** (recorded in $CDCl_3$)
$CHCl_3$
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
f1 (ppm)

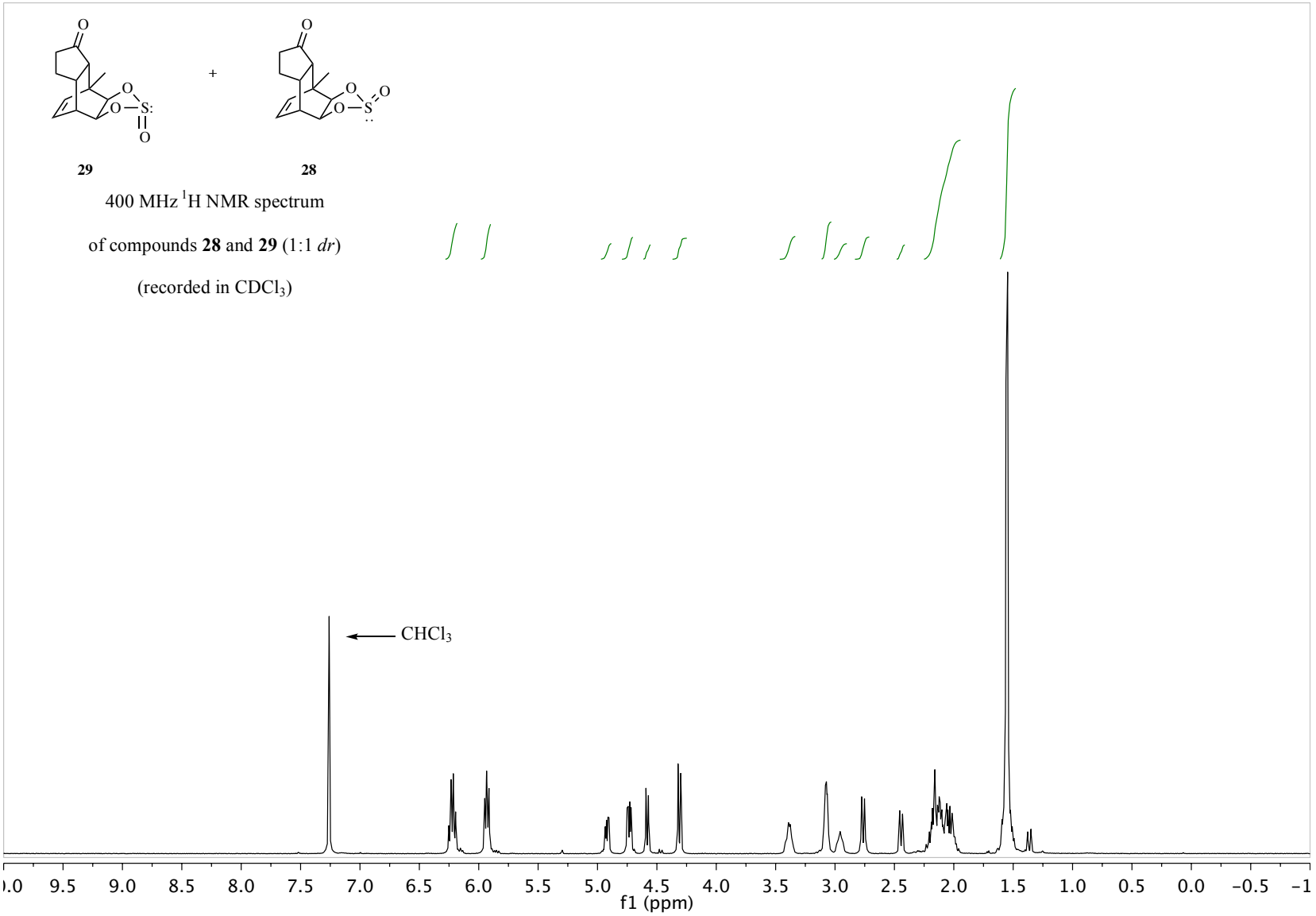

HO
O
O
S
O
O
100 MHz 13C NMR spectrum
of compound 25 (recorded in CDCl3)
85.3
81.2
75.5
46.6
37.8
36.5
34.6
31.1
26.3
21.6
20.3
13.9
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

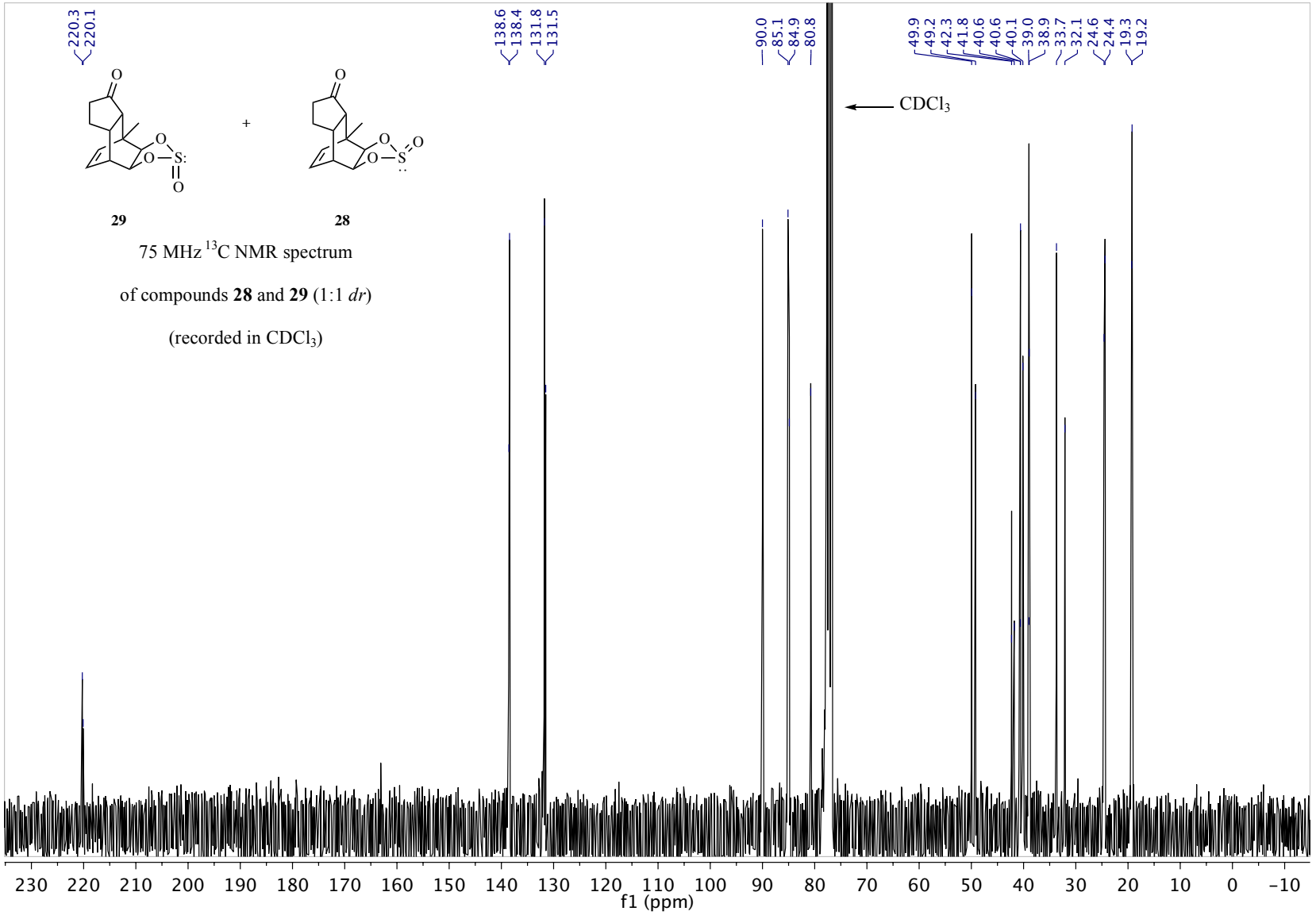

SMe
S
O
O
O
S
O
O
400 MHz ^{1}H NMR spectrum
of compound **26** (recorded in $CDCl_3$)
$CHCl_3$
H_2O
f1 (ppm)

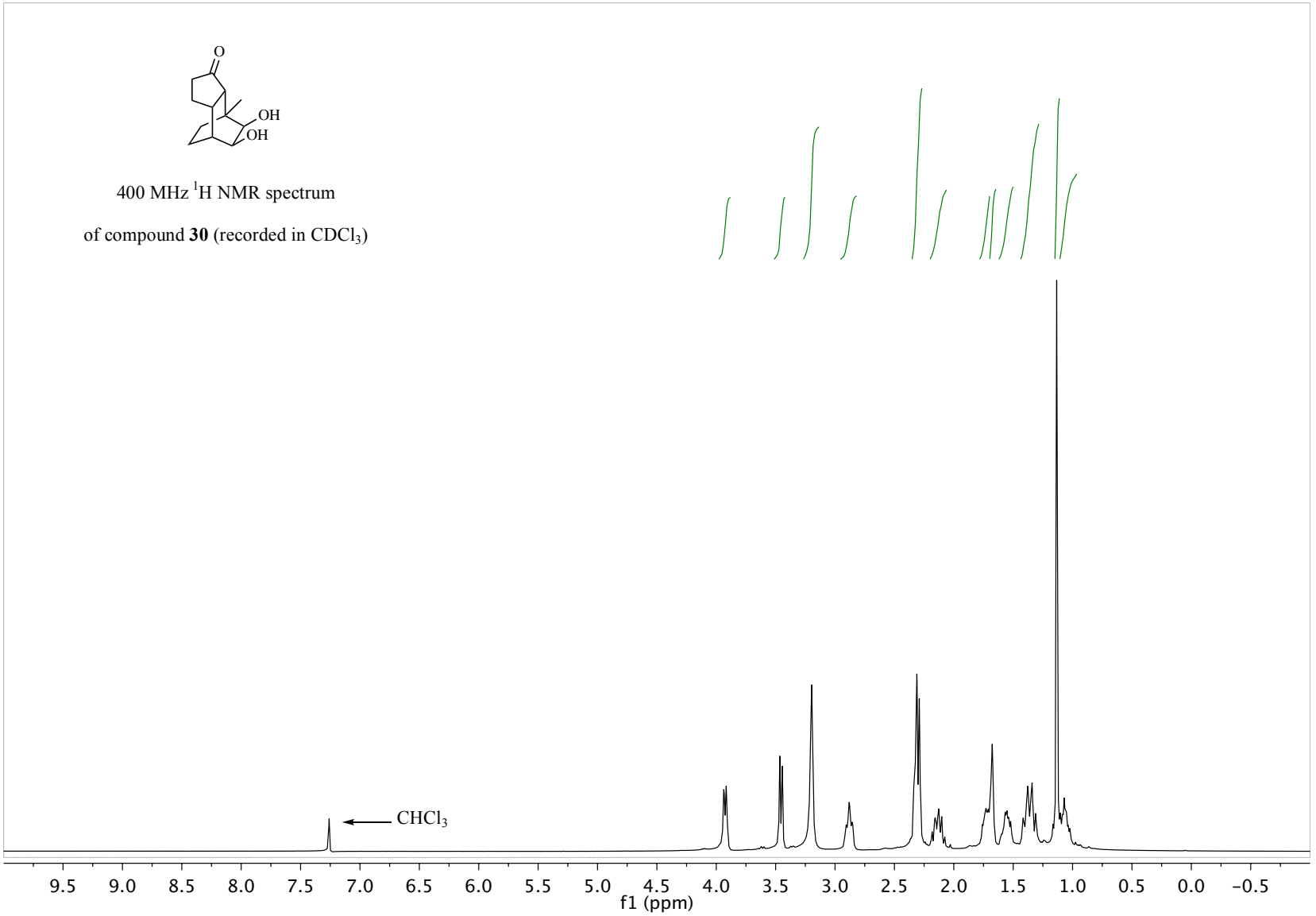


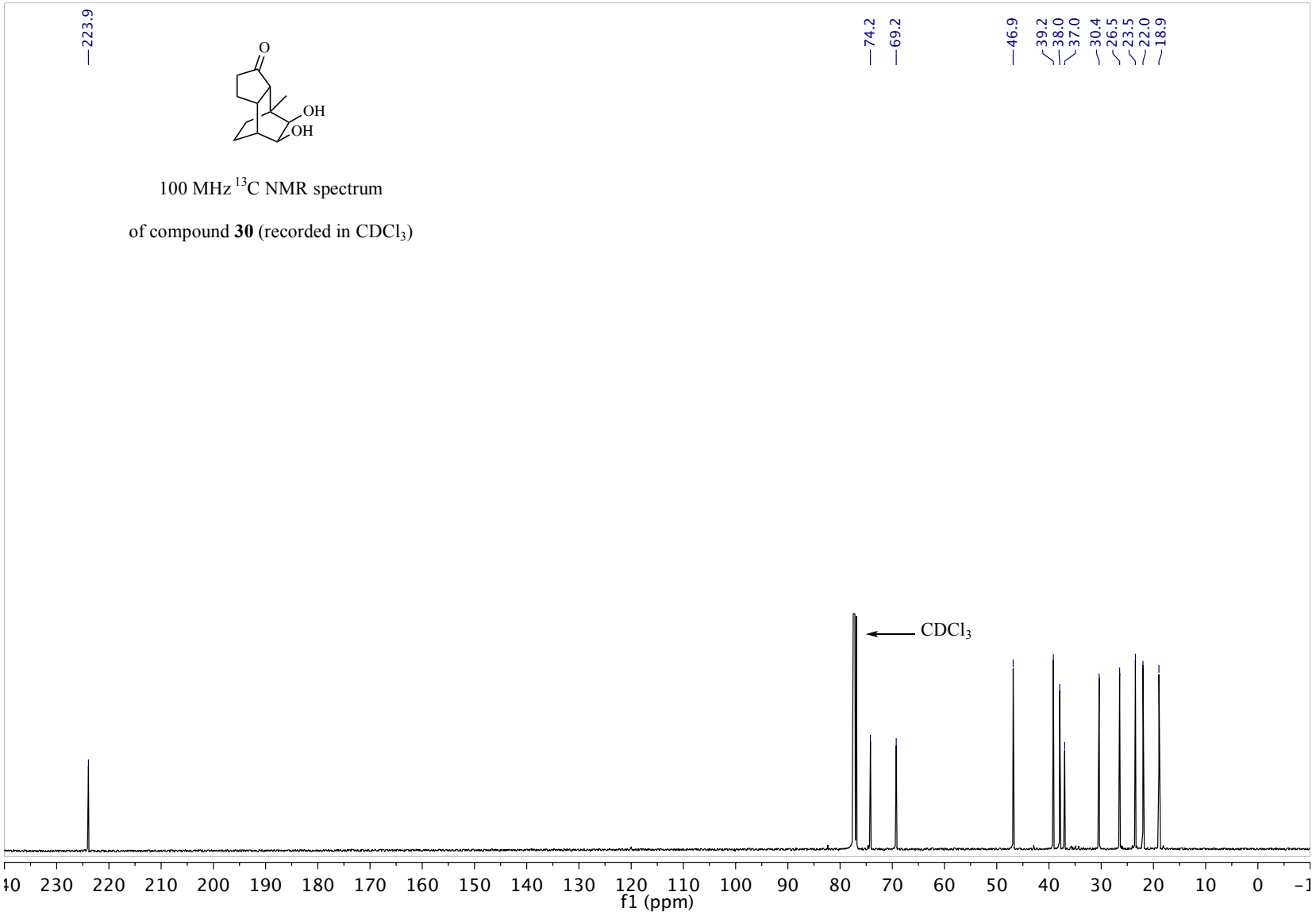
100 MHz ^{13}C NMR spectrum

of compound **26** (recorded in $CDCl_3$)


29
28
400 MHz ^{1}H NMR spectrum
of compounds **28** and **29** (1:1 *dr*)
(recorded in $CDCl_3$)
$CHCl_3$
f1 (ppm)

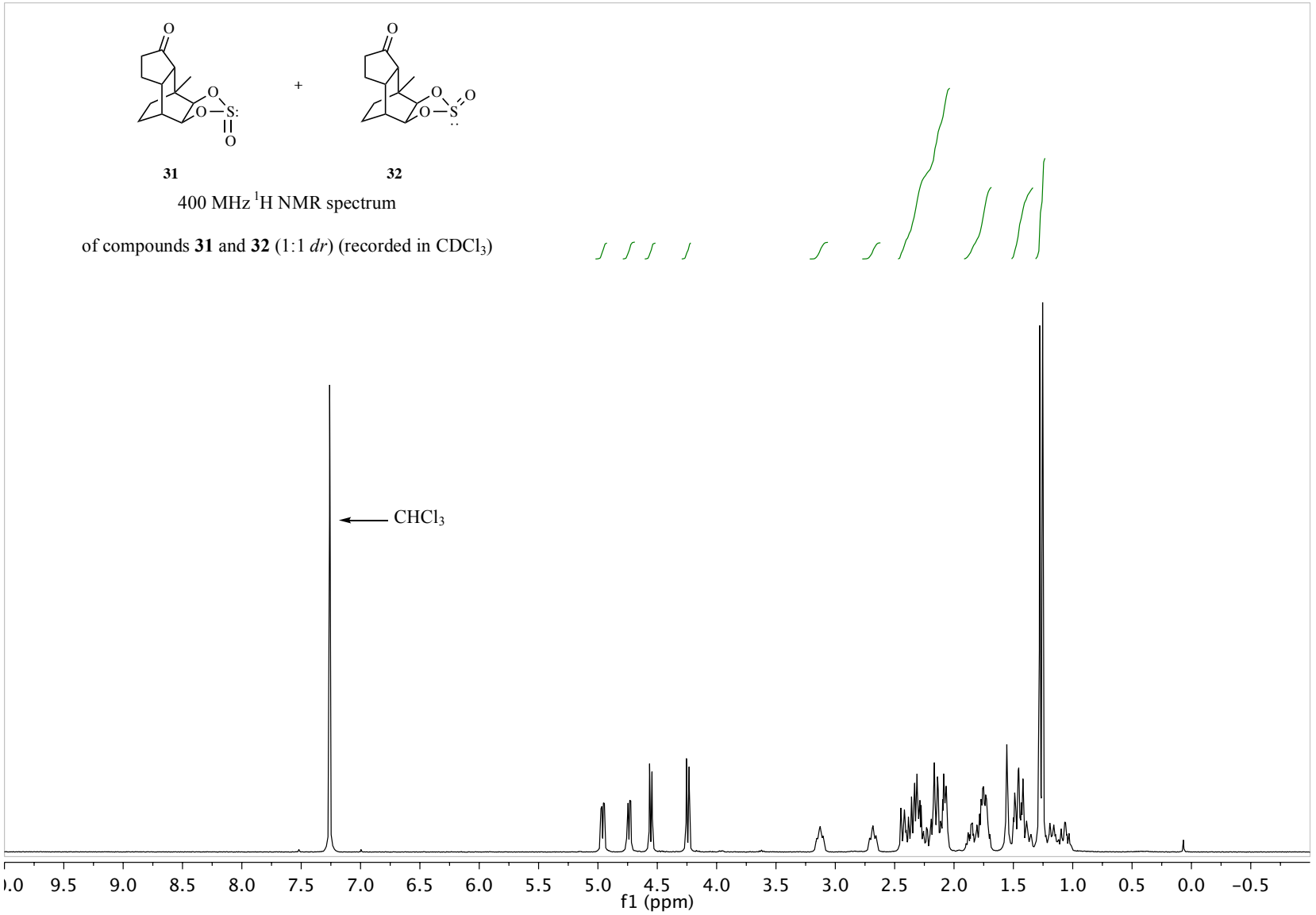

220.3
220.1
138.6
138.4
131.8
131.5
90.0
85.1
84.9
80.8
49.9
49.2
42.3
41.8
40.6
40.6
40.1
39.0
38.9
33.7
32.1
24.6
24.4
19.3
19.2
CDCl3
29
28
75 MHz 13C NMR spectrum
of compounds 28 and 29 (1:1 dr)
(recorded in CDCl3)
f1 (ppm)


O
OH
OH
400 MHz ^{1}H NMR spectrum
of compound **30** (recorded in $CDCl_3$)
$CHCl_3$
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
f1 (ppm)



100 MHz ^{13}C NMR spectrum

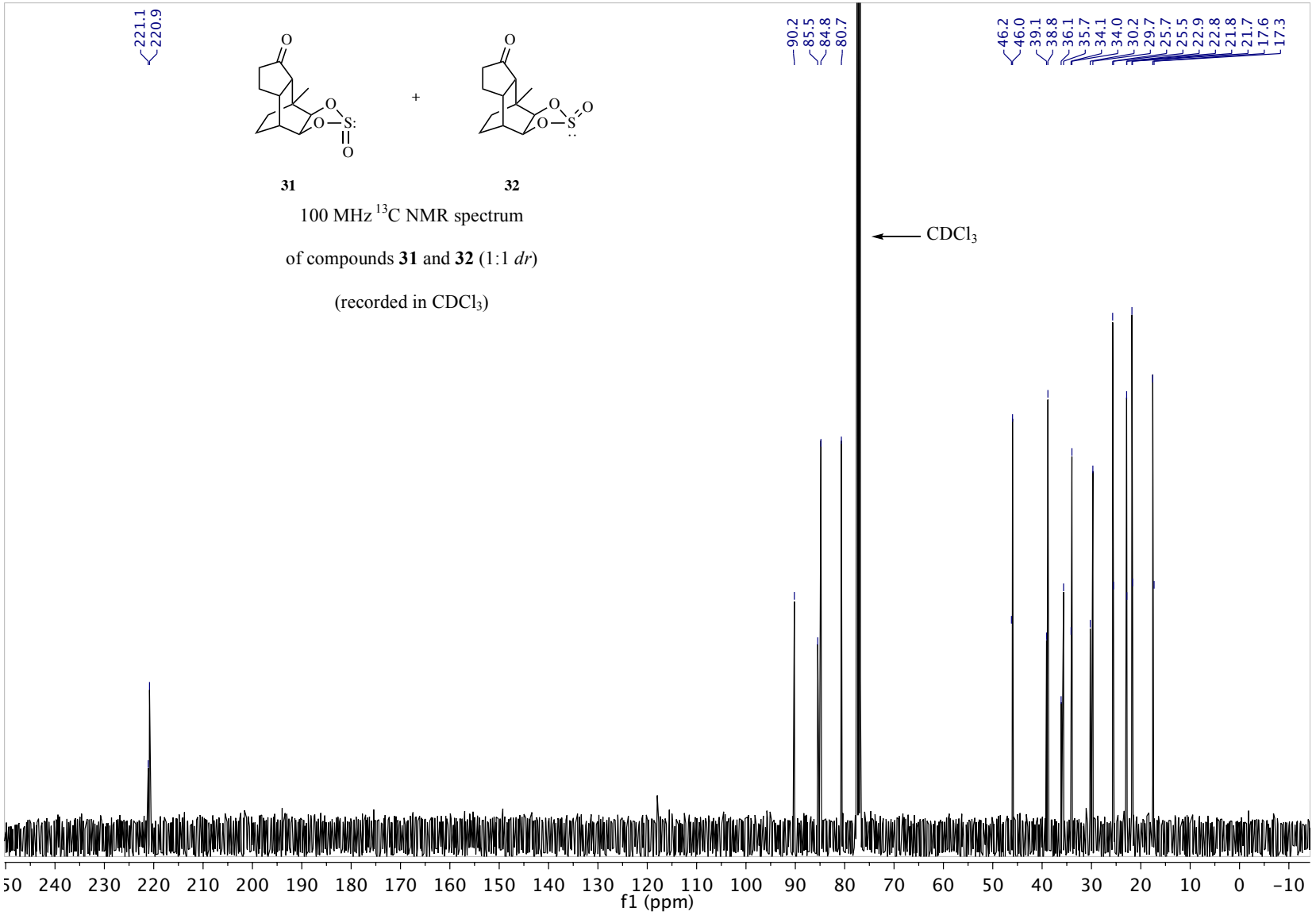
of compound **30** (recorded in $CDCl_3$)



31 **32**

400 MHz ^{1}H NMR spectrum

of compounds **31** and **32** (1:1 *dr*) (recorded in $CDCl_3$)

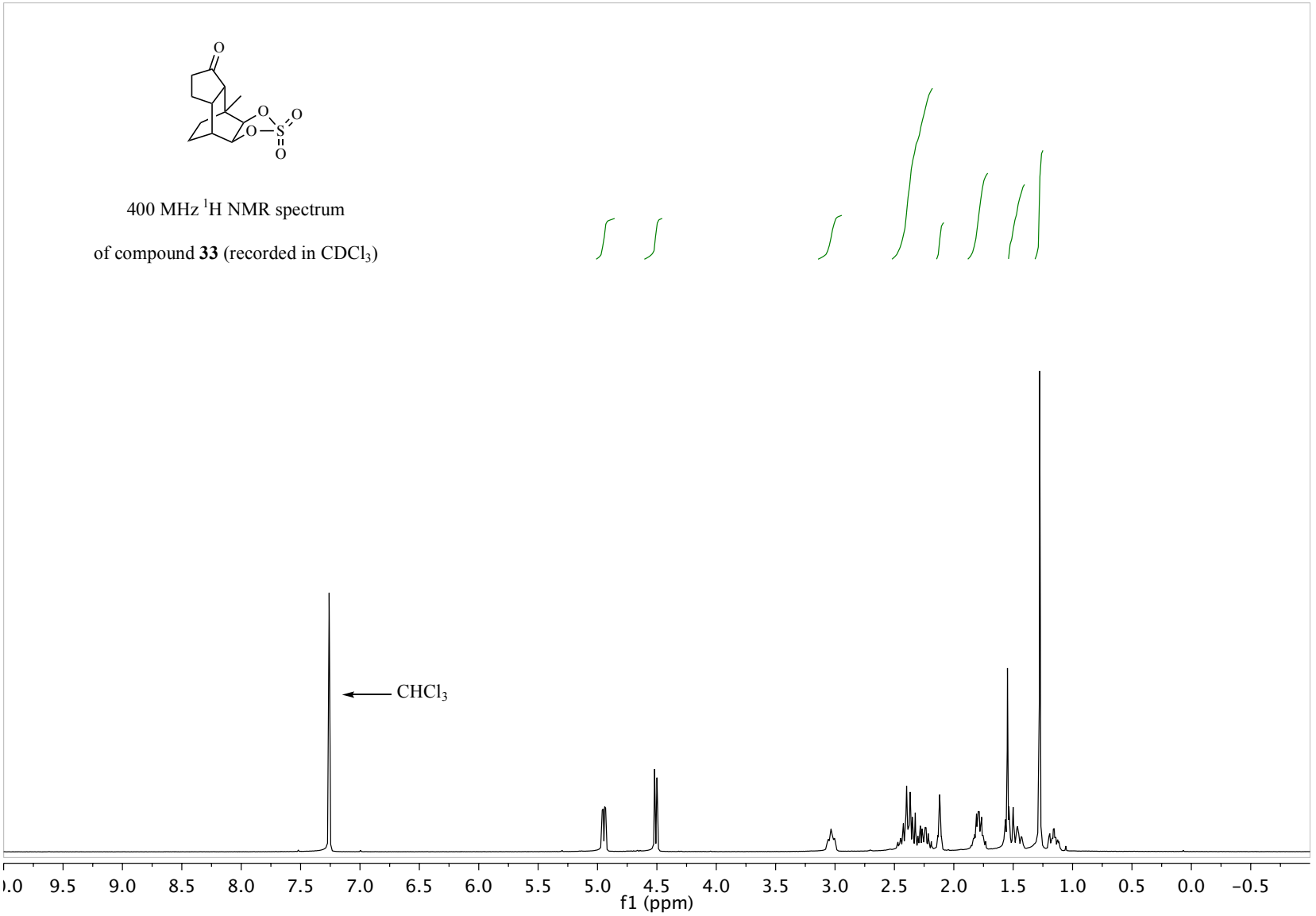


31 + **32**

100 MHz ^{13}C NMR spectrum

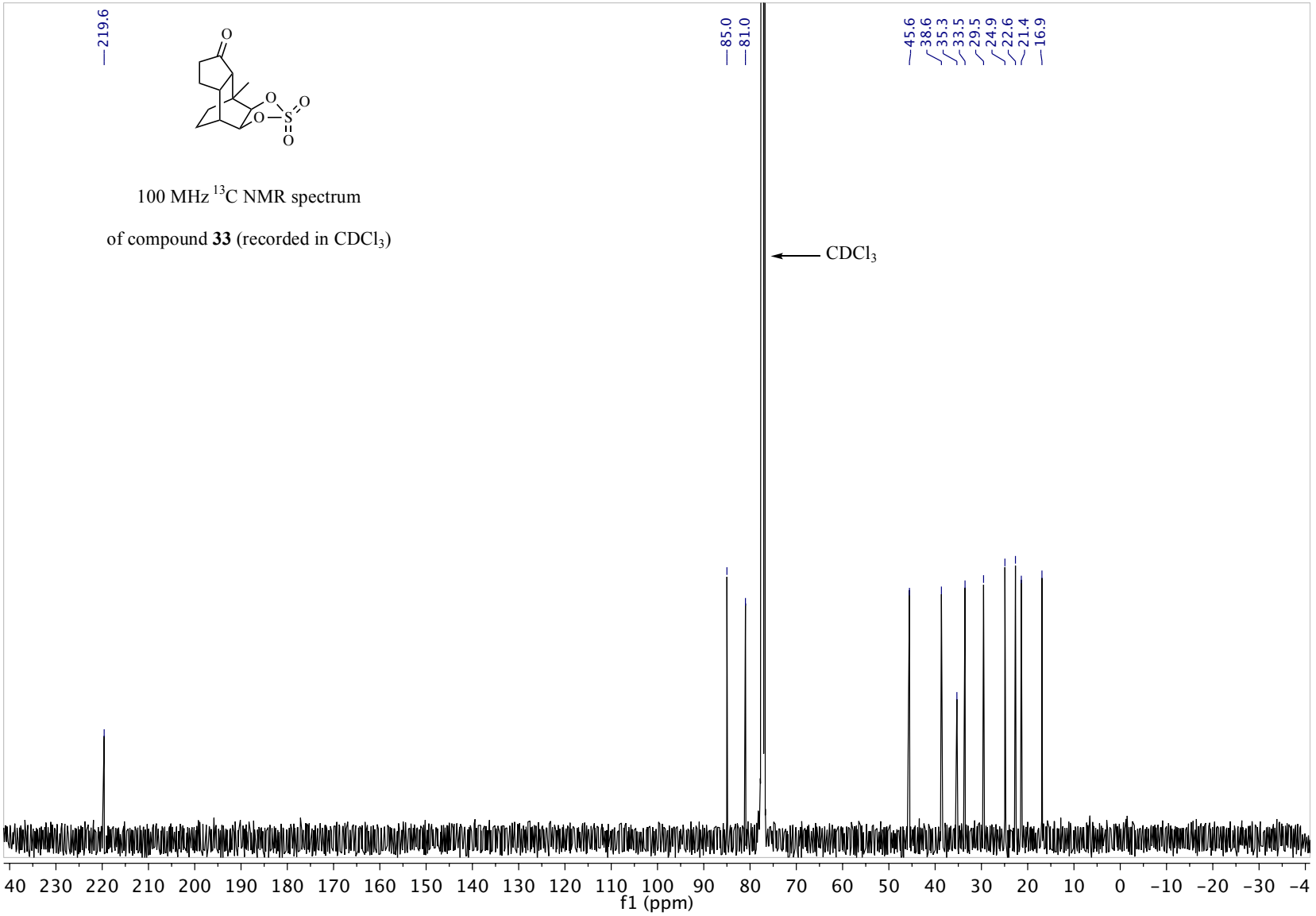
of compounds **31** and **32** (1:1 *dr*)

(recorded in $CDCl_3$)



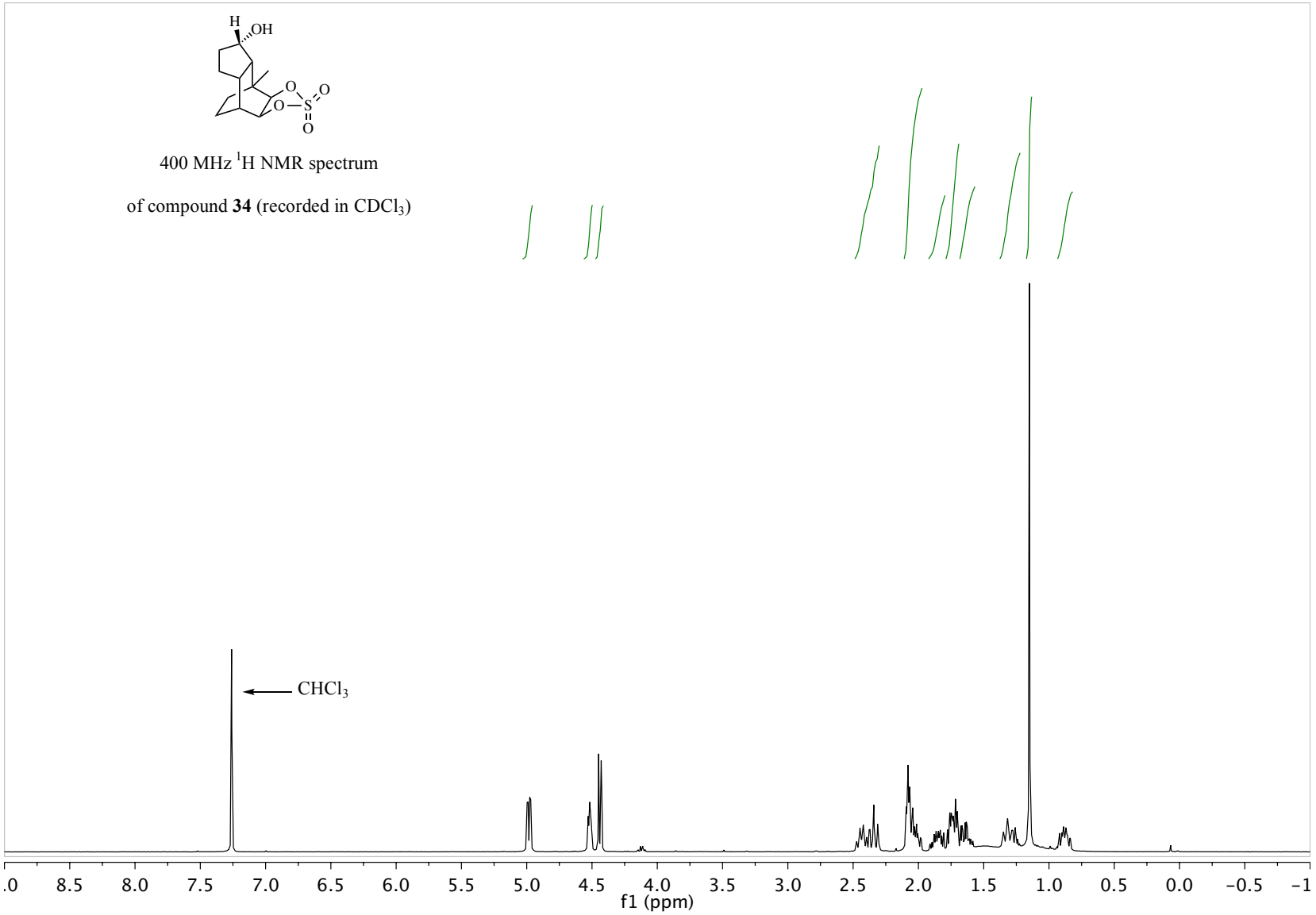
400 MHz ^{1}H NMR spectrum

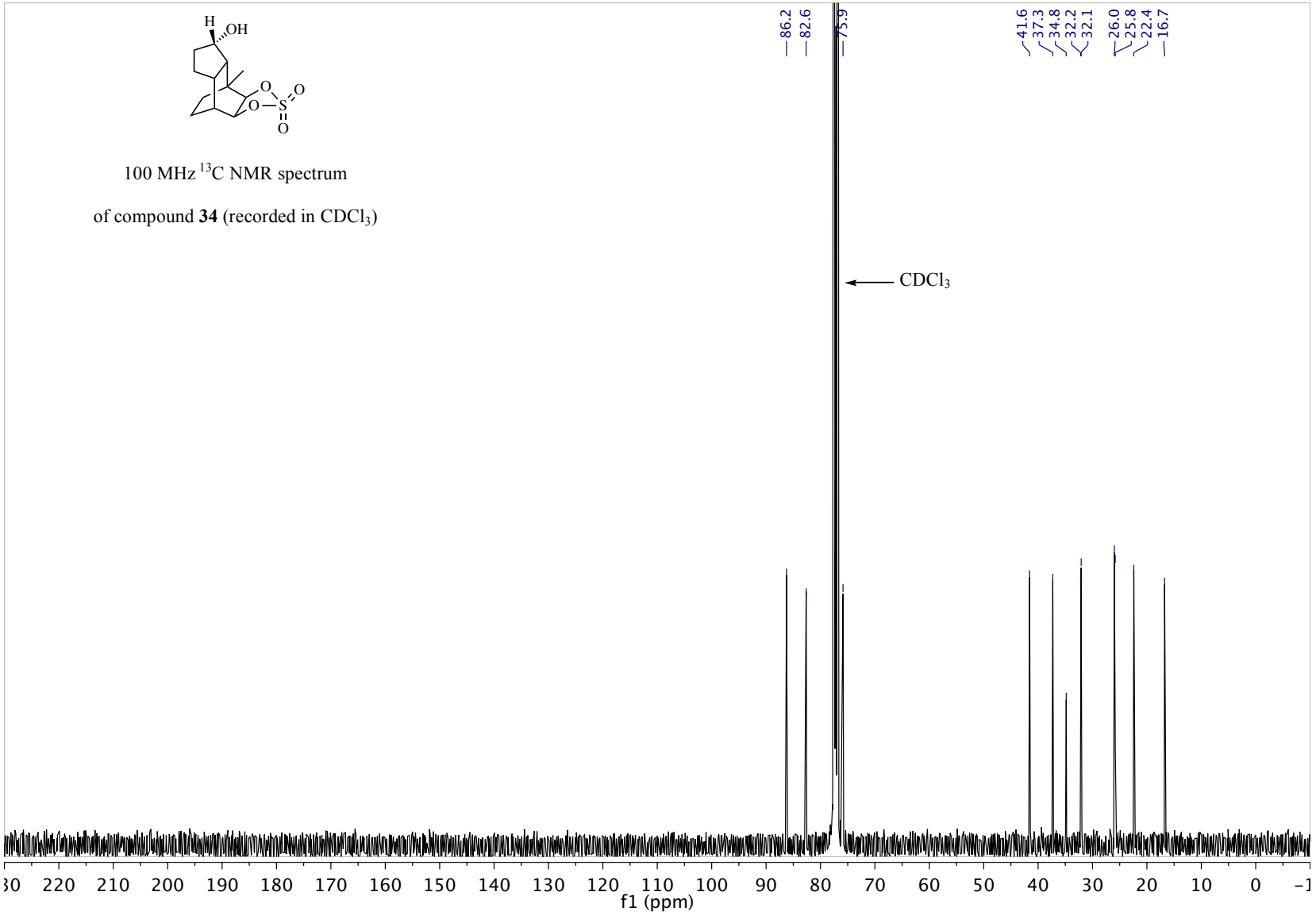
of compound **33** (recorded in $CDCl_3$)

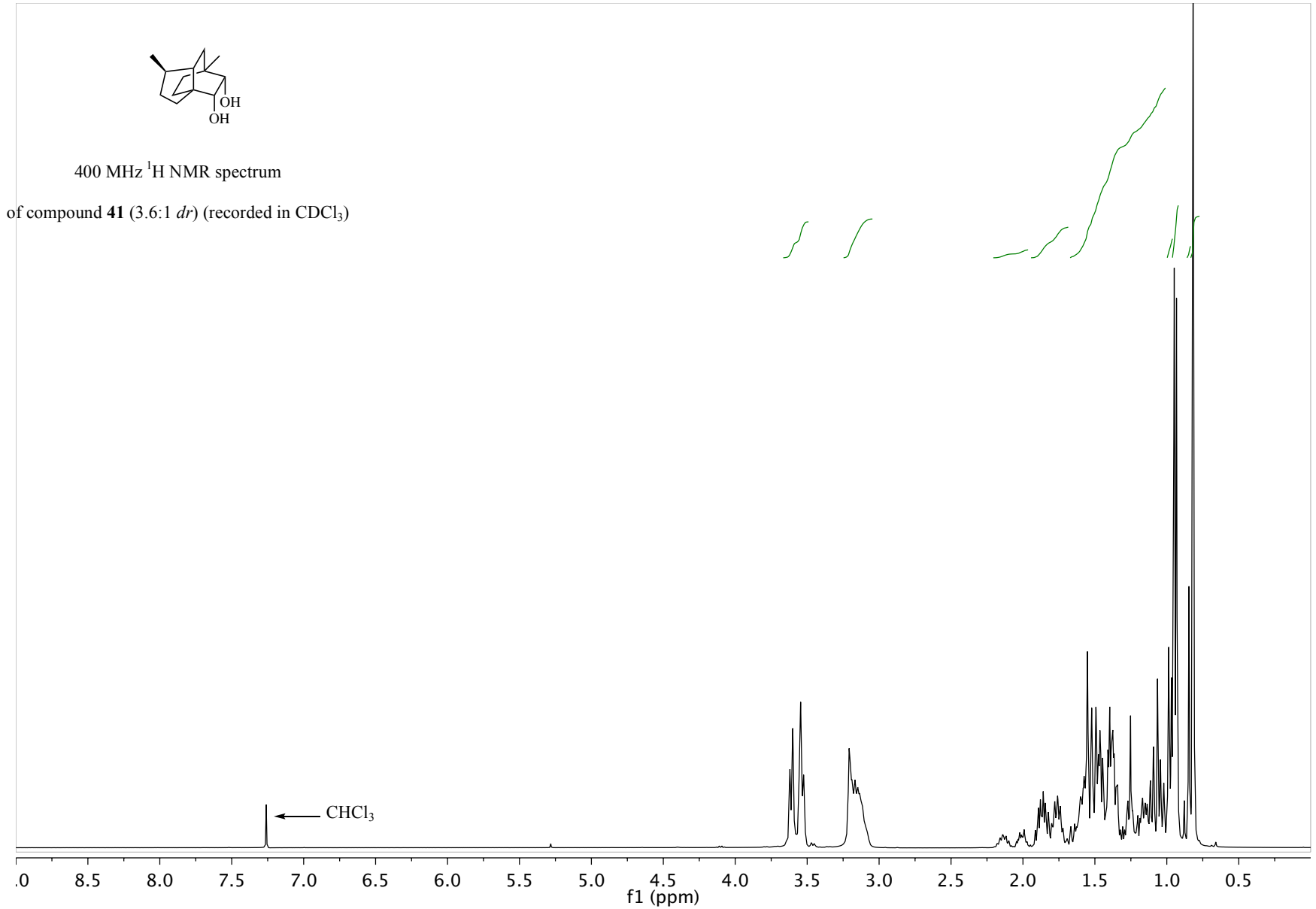


100 MHz ^{13}C NMR spectrum

of compound **33** (recorded in $CDCl_3$)

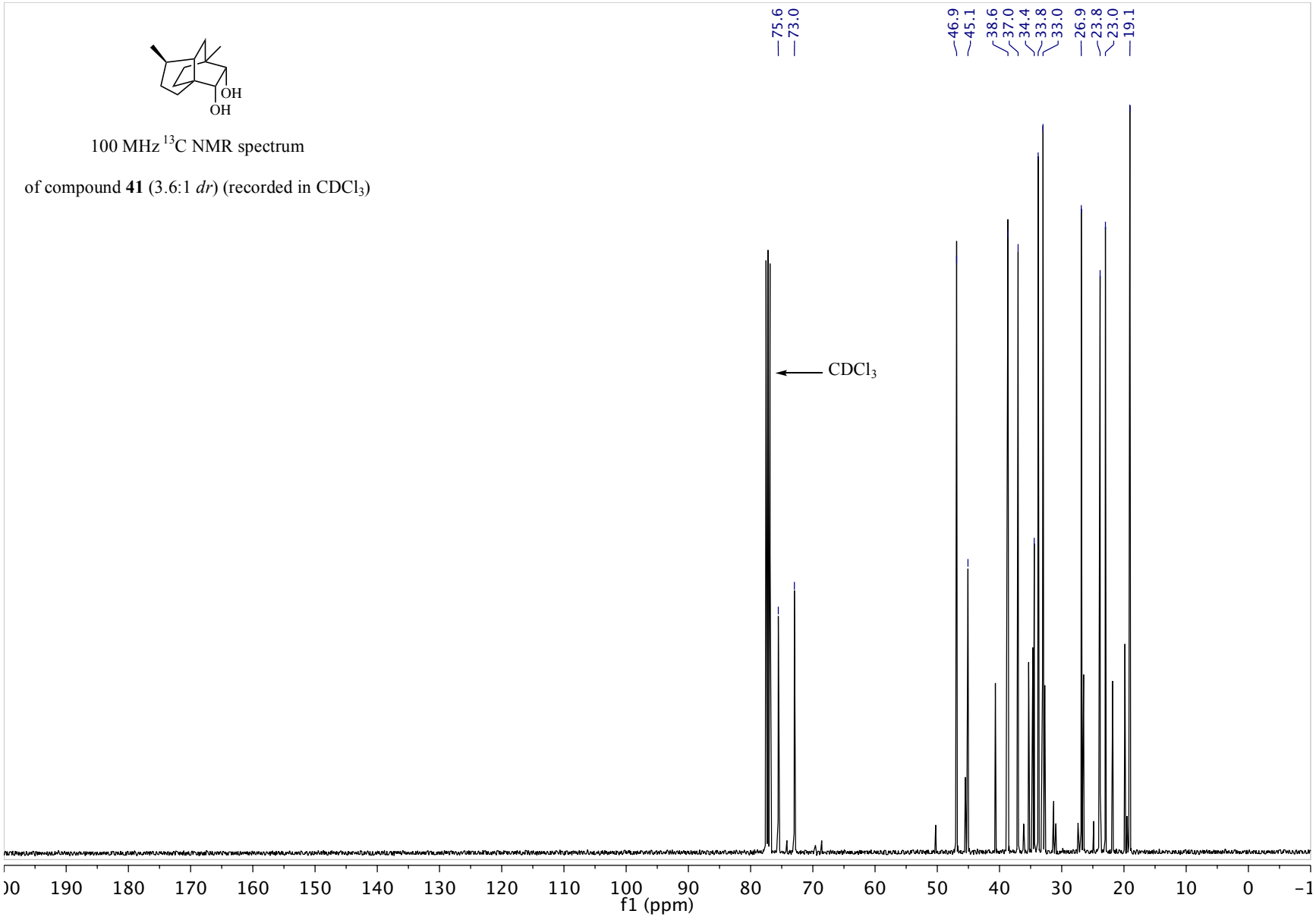

H
OH
O
O
S
O
O
400 MHz ^{1}H NMR spectrum
of compound **34** (recorded in $CDCl_3$)
$CHCl_3$
.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

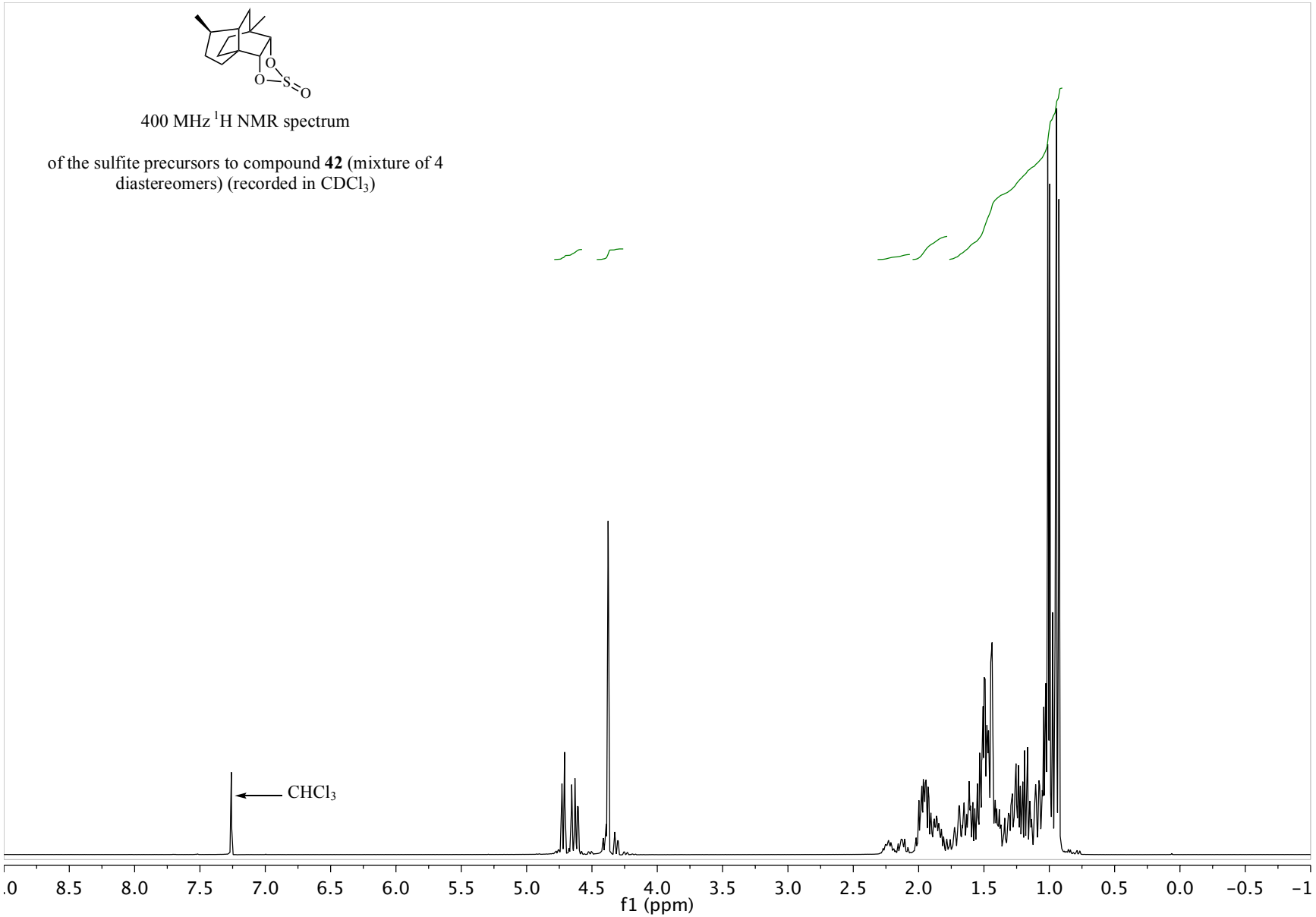

H
OH
O
O
S
O
O
100 MHz ^{13}C NMR spectrum
of compound **34** (recorded in $CDCl_3$)
86.2
82.6
77.9
41.6
37.3
34.8
32.2
32.1
26.0
25.8
22.4
16.7
$CDCl_3$
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



400 MHz ^{1}H NMR spectrum

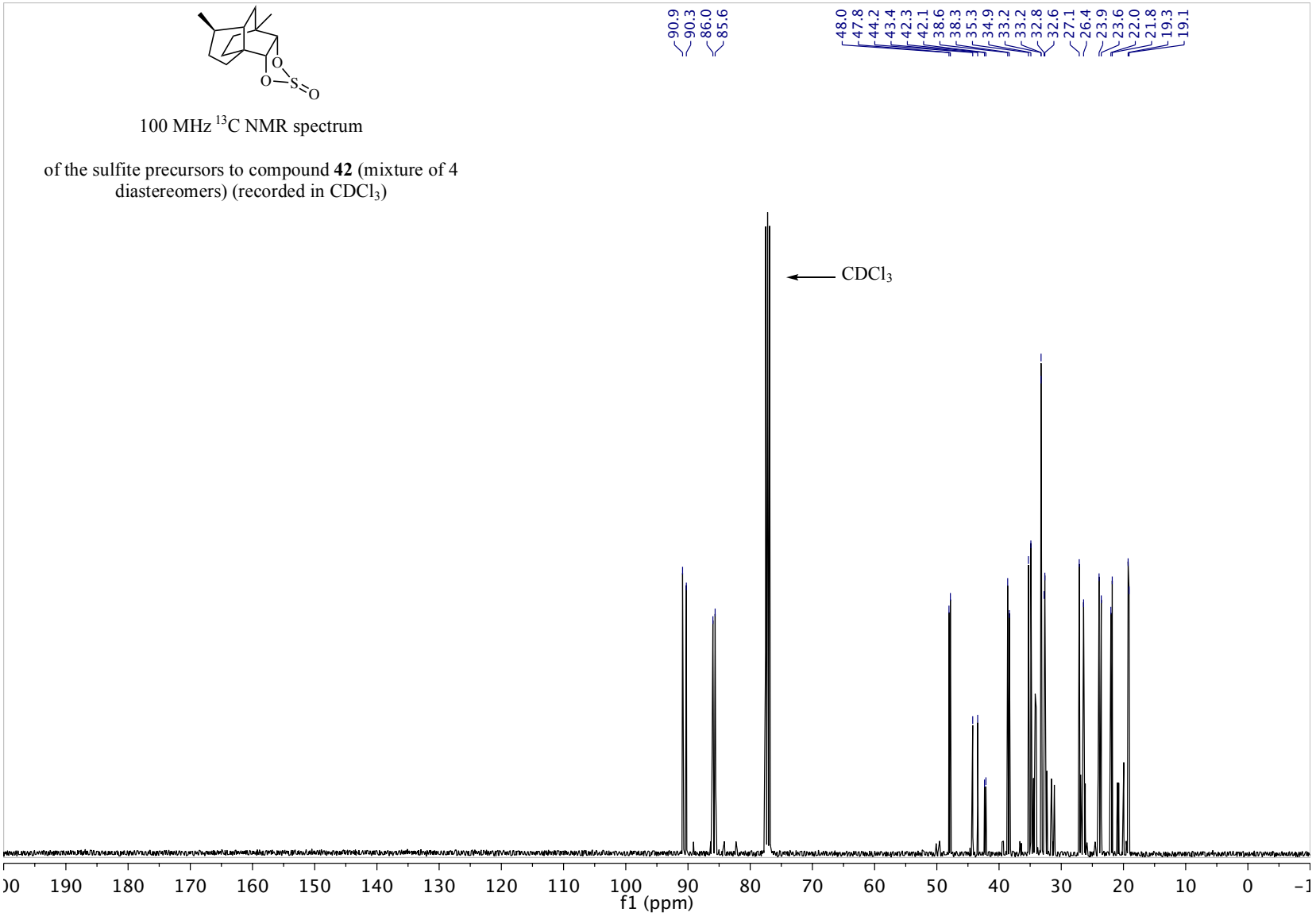
of compound **41** (3.6:1 *dr*) (recorded in $CDCl_3$)


OH
OH
100 MHz ^{13}C NMR spectrum
of compound **41** (3.6:1 *dr*) (recorded in $CDCl_3$)
75.6
73.0
46.9
45.1
38.6
37.0
34.4
33.8
33.0
26.9
23.8
23.0
19.1
$CDCl_3$
f1 (ppm)



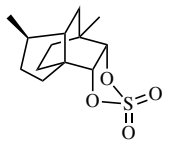
400 MHz ^{1}H NMR spectrum

of the sulfite precursors to compound **42** (mixture of 4 diastereomers) (recorded in $CDCl_3$)



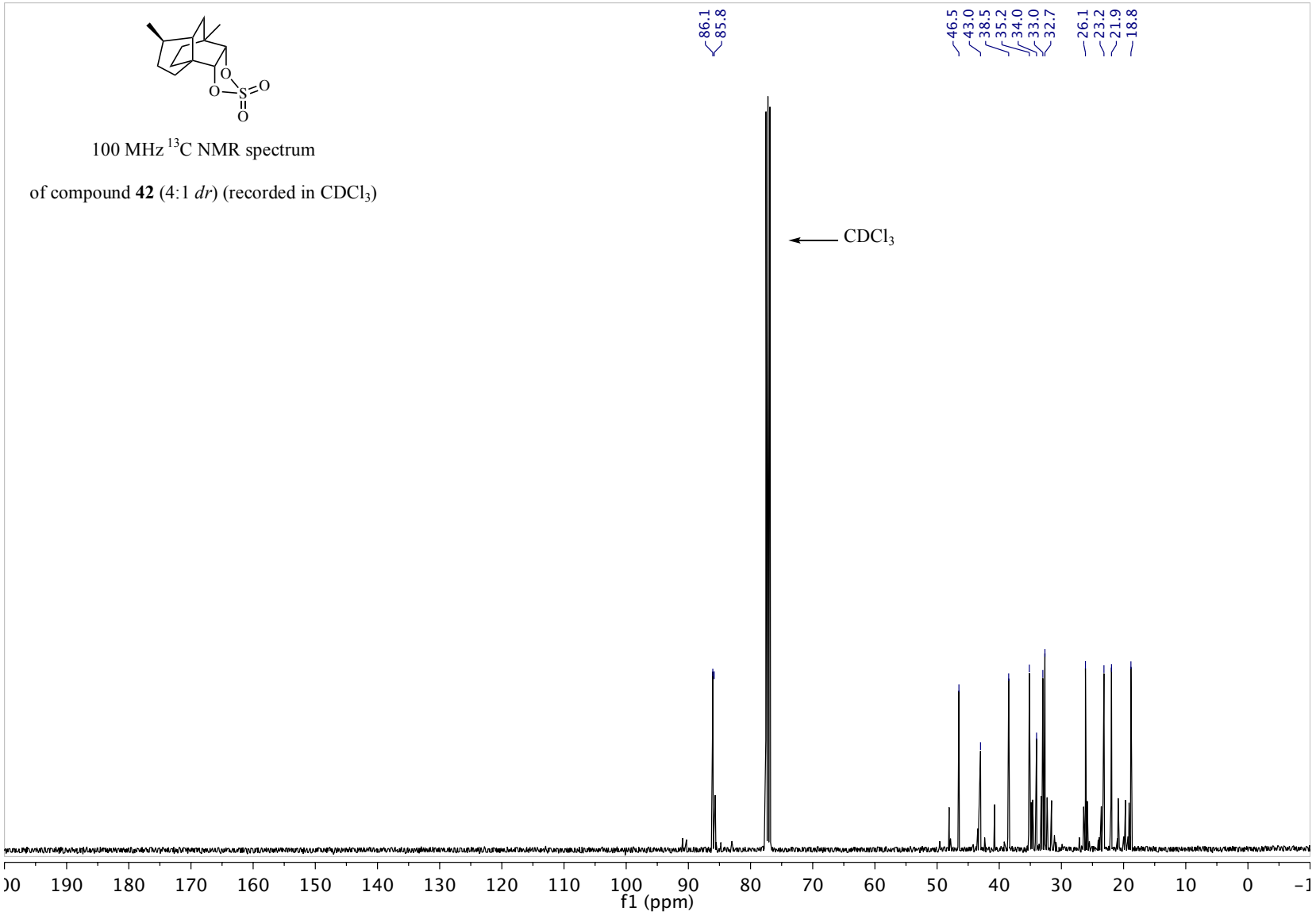
100 MHz ^{13}C NMR spectrum

of the sulfite precursors to compound **42** (mixture of 4 diastereomers) (recorded in $CDCl_3$)



400 MHz ^{1}H NMR spectrum

of compound **42** (4:1 *dr*) (recorded in $CDCl_3$)



100 MHz ^{13}C NMR spectrum

of compound **42** (4:1 *dr*) (recorded in $CDCl_3$)