Supporting Information for:

Chemical Synthesis Study Establishes the Correct Structure of the Potent Anti-Inflammatory Agent Myrsinoic Acid F

Jiri Mikusek,[a] Jeremy Nugent,[a] Ping Lan,[b,c] and Martin G. Banwell,*[,a,b]

[a]*Research School of Chemistry, Institute of Advanced Studies, The Australian National University, Canberra, ACT 2601, Australia*

[b]*Institute of Advanced and Applied Chemical Synthesis, Jinan University, Zhuhai, 519070, China*

[c]*Department of Food Science and Engineering, Jinan University, Guangzhou, 510632, China*

CONTENTS PAGE

Biological Evaluations

Anti-inflammatory Test. The TPA-induced mouse ear edema assay inflammatory tests used in this study were modifications of a protocol defined by Gschwendt[1] and employed in the original evaluation of myrsinoic acid F.[2] Specifically, 20 μL solutions of each of compounds **3**, **7**, **8, 12** and **13** in acetone at concentrations of 1.4 or 0.56 μmol were applied to the outer surface of right ears of the mice by means of an automatic microliter pipet. After 0.5 h, 12-*O*-tetradecanoylphorbol-13-acetate (TPA) (0.5 μg in 20 μL of acetone) was applied to the right ears of each animal. Blank controls received acetone alone while indometacin served as the positive control. After a further 7 h the animals were sacrificed and both ears removed. Plugs of 0.8 cm in diameter were then obtained from the tips of both the right and left ears with the aid of a punch and these were weighed to the nearest 0.1 mg. The extent of the edema was determined from the mean difference in weight of right and left ear-plugs (Δweight) and taken to represent the degree of swelling. The inhibition rate (in % terms) was determined using the following equation:

$$\text{Inhibition rate (\%)} = \frac{\Delta\text{weight of control} - \Delta\text{weight of sample}}{\Delta\text{weight of control}} \times 100\%$$

Table S1. The Anti-inflammatory Activities of Compounds 3, **7**, **8, 12 and 13 in a Mouse Ear Inflammation Test**

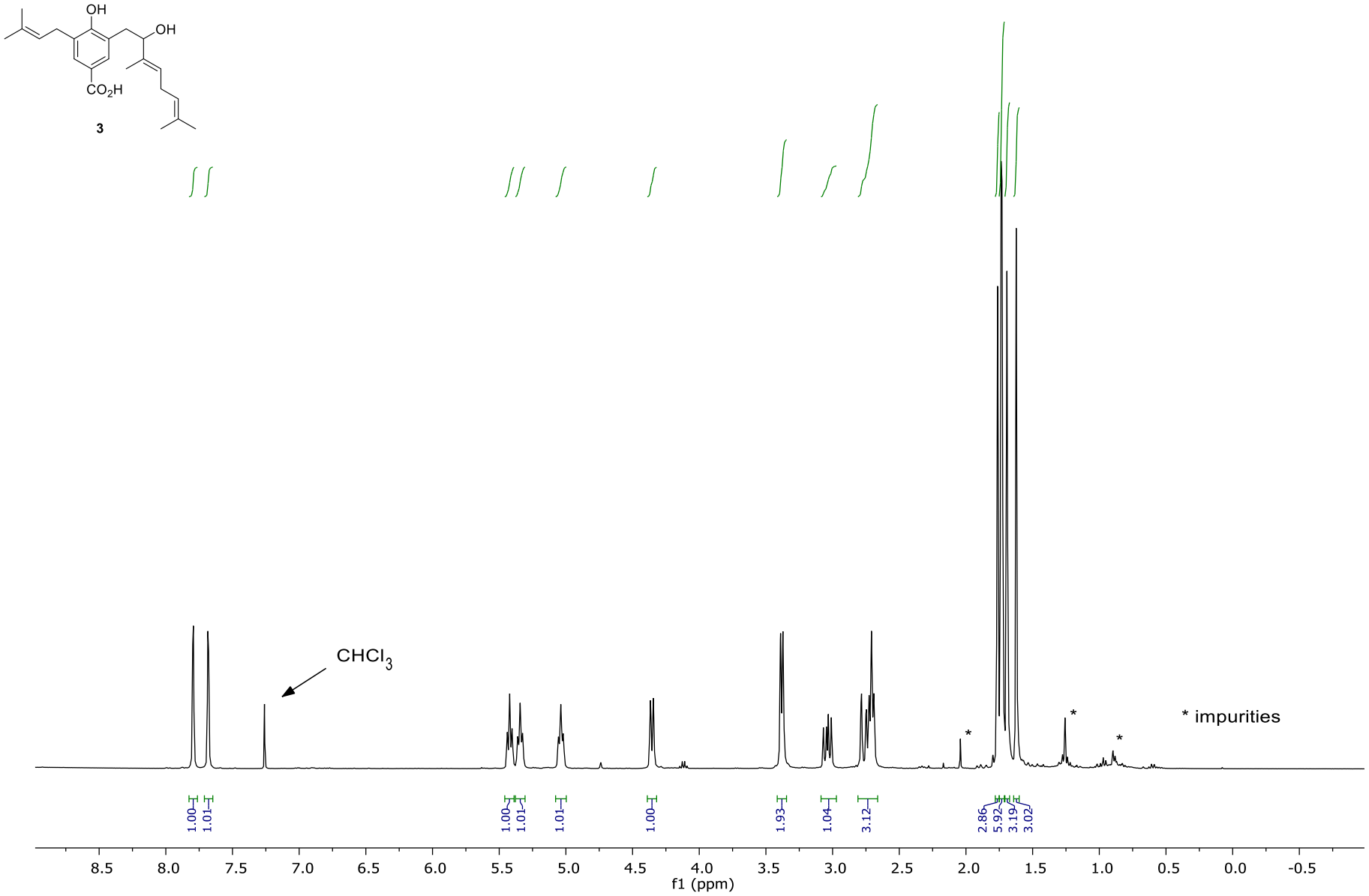
Sample	Concentration	Swelling degree	Inhibition rate (%)
Blank	–	0.0222±0.0058	–
Indomethacin	1.4 μmol	0.0155±0.0031*	30
	0.6 μmol	0.0152±0.0025*	32
3	1.4 μmol	0.0069±0.0024*	69
	0.6 μmol	0.0100±0.0042*	55
7	1.4 μmol	0.0152±0.0026*	32
	0.6 μmol	0.0161±0.0044*	27
8	1.4 μmol	0.0155±0.0026*	32
	0.6 μmol	0.0142±0.0024*	36
12	1.4 μmol	0.0153±0.0014*	31
	0.6 μmol	0.013±0.0024*	41
13	1.4 μmol	0.0137±0.0018*	38
	0.6 μmol	0.0125±0.0042*	44

*Significantly different, P<0.01.

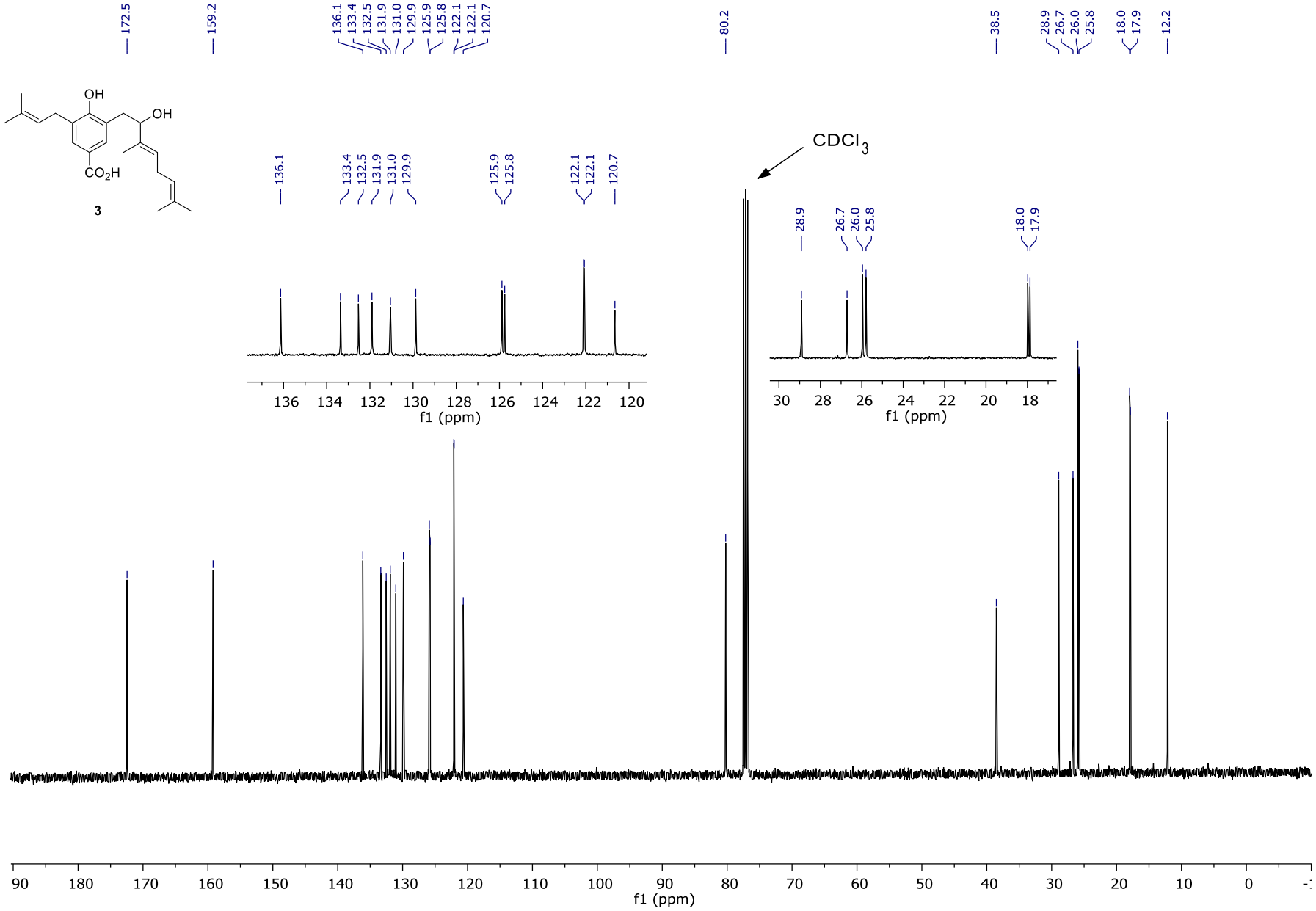
References

1. Gschwendt, M.; Kittstein, W.; Furstenberger, G.; Marks, F., *Cancer Letters*, **1984**, *25*, 177.
2. See ref. 1 of paper.

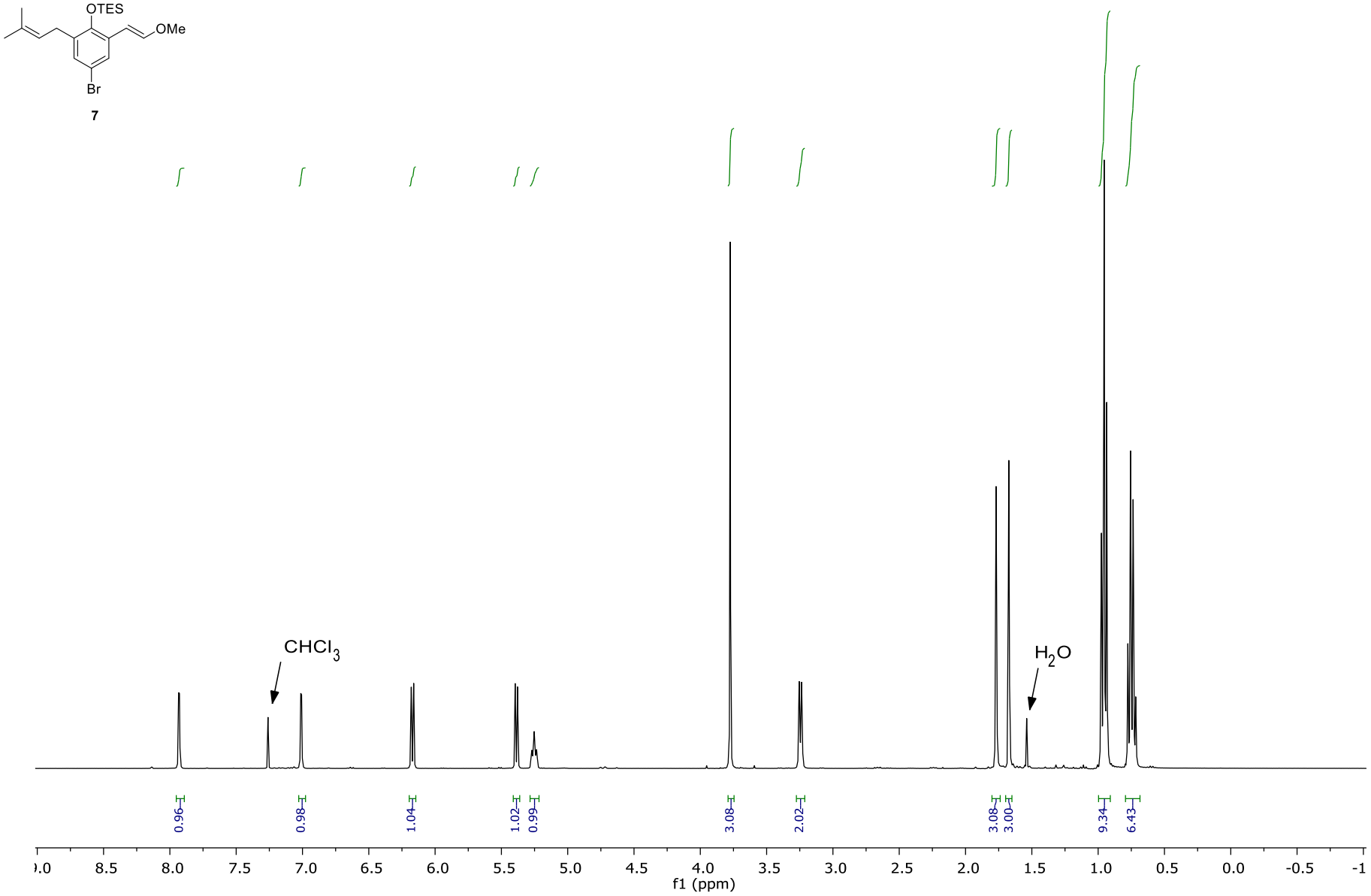
400 MHz ^{1}H NMR Spectrum of Compound **3** (recorded in $CDCl_3$)



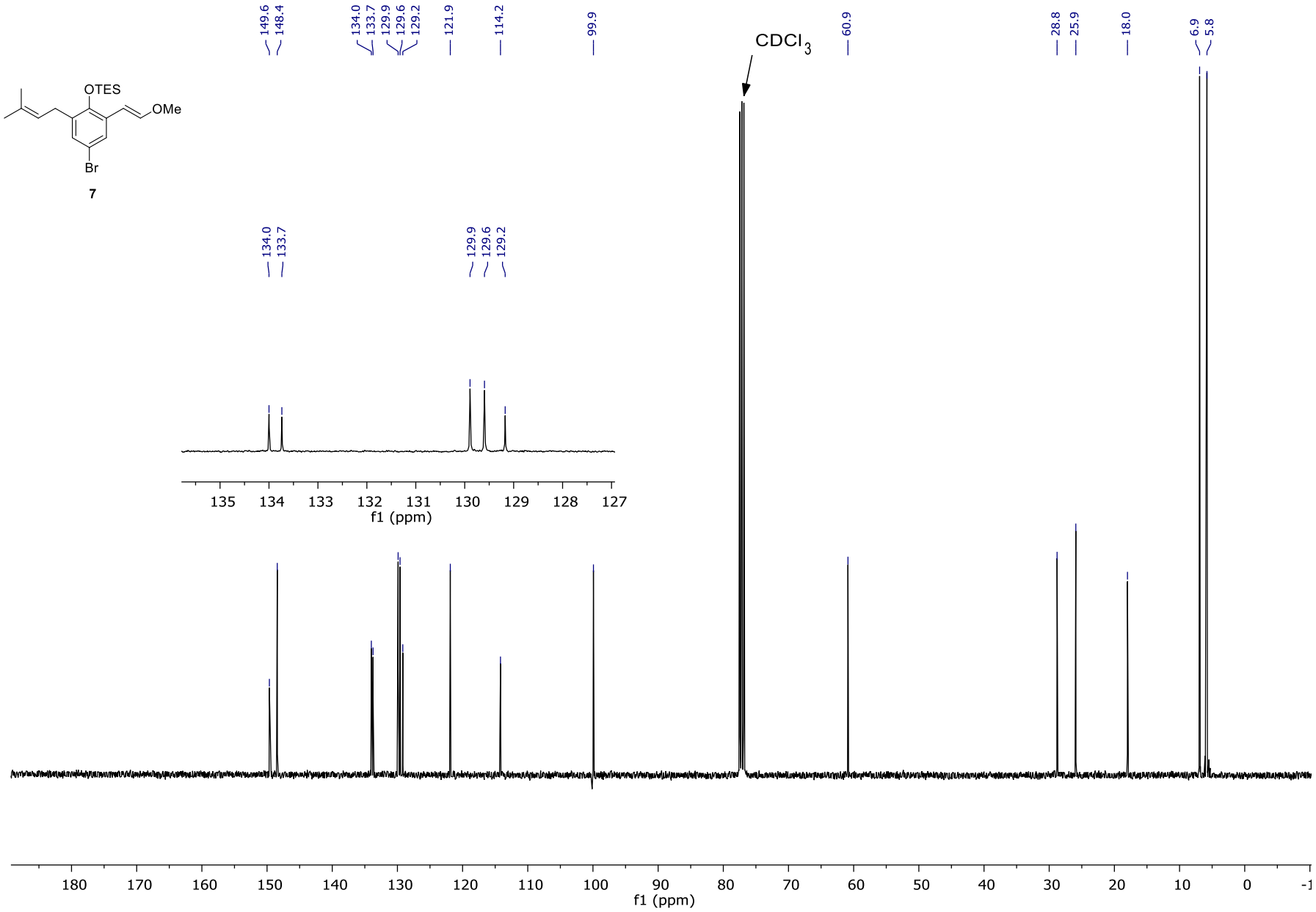
100 MHz ^{13}C NMR Spectrum of Compound **3** (recorded in $CDCl_3$)



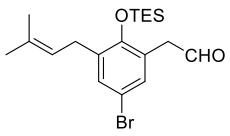
400 MHz ^{1}H NMR Spectrum of Compound **7** (recorded in $CDCl_3$)



100 MHz ^{13}C NMR Spectrum of Compound **7** (recorded in $CDCl_3$)

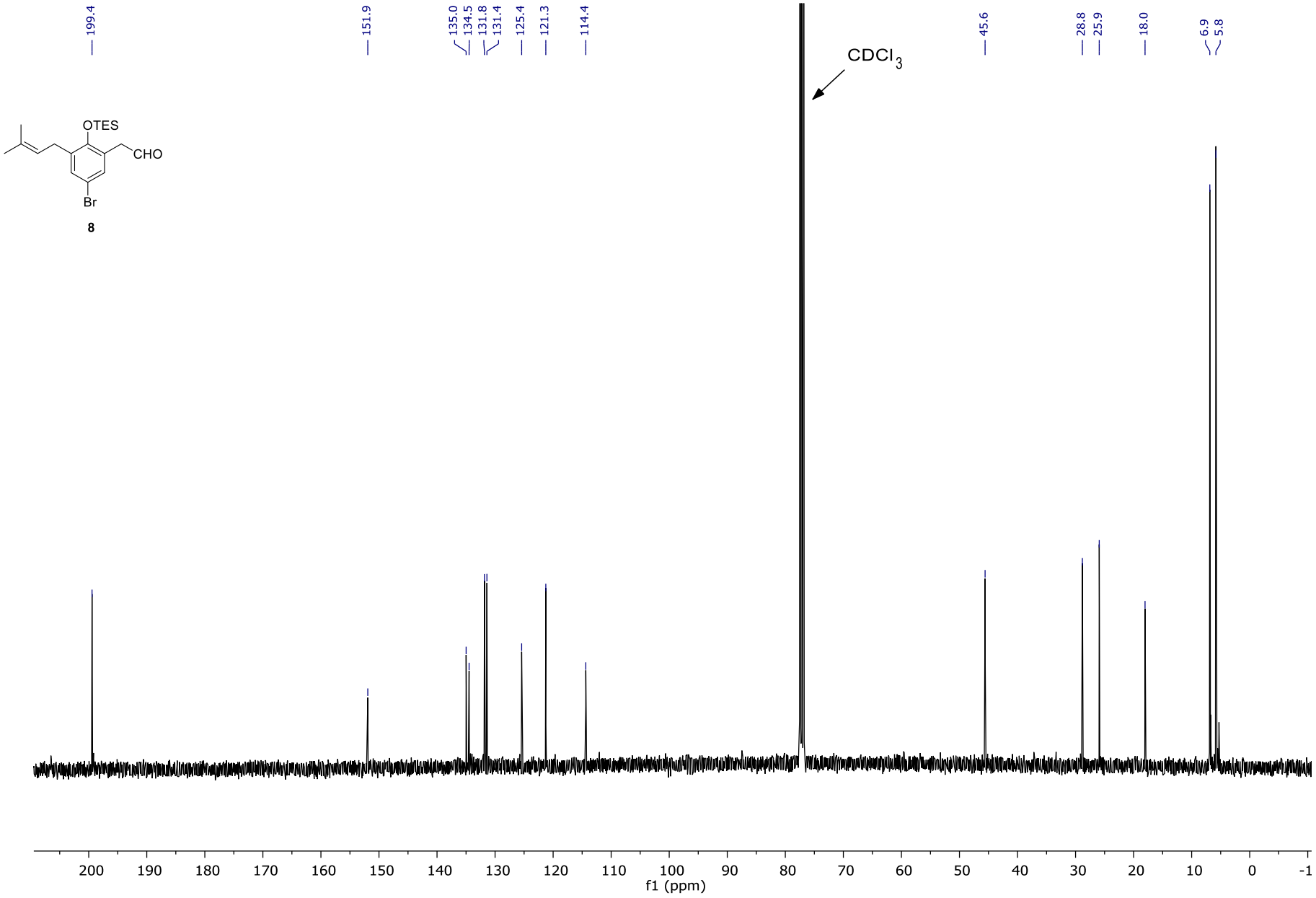


400 MHz ^{1}H NMR Spectrum of Compound **8** (recorded in $CDCl_3$)

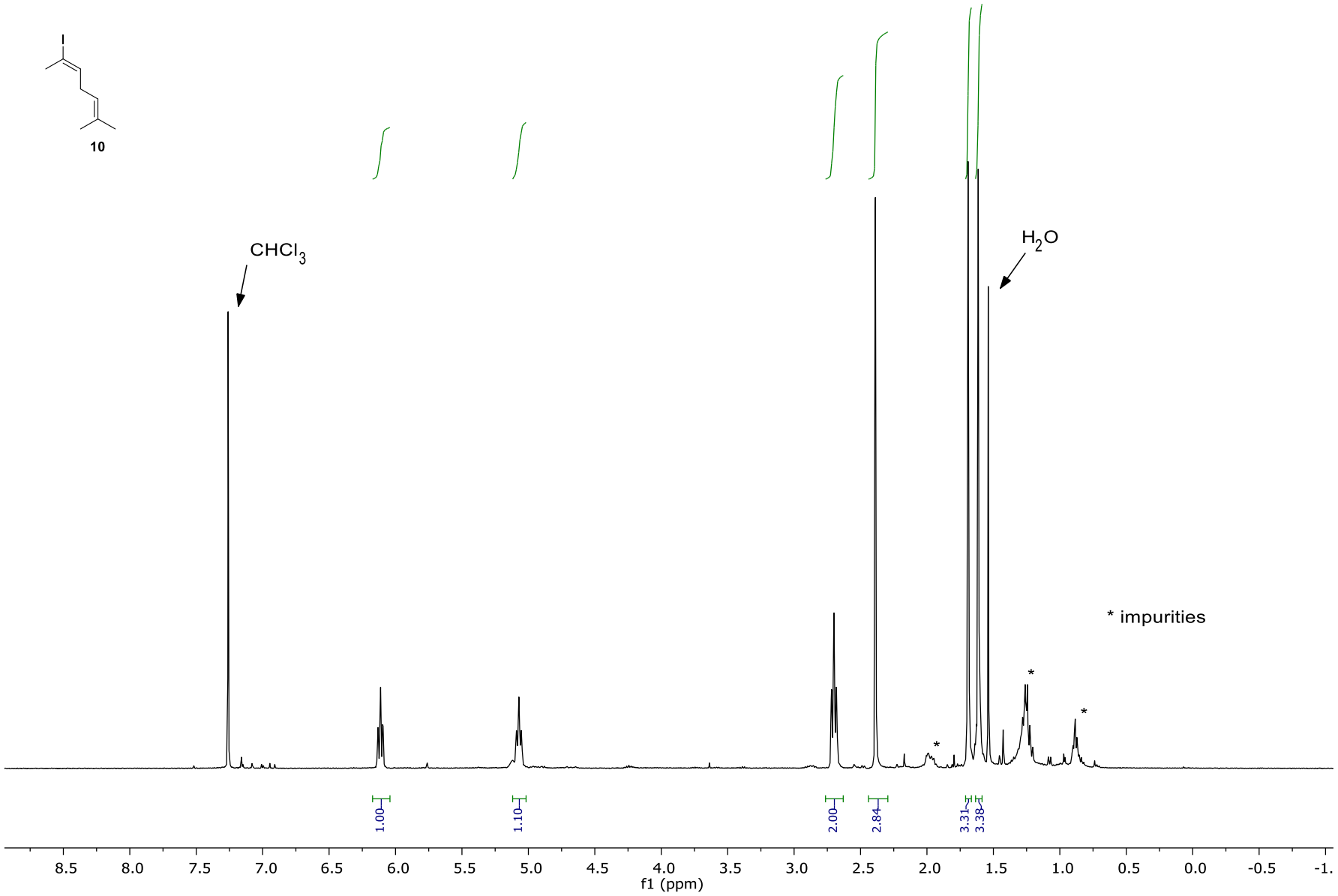


8

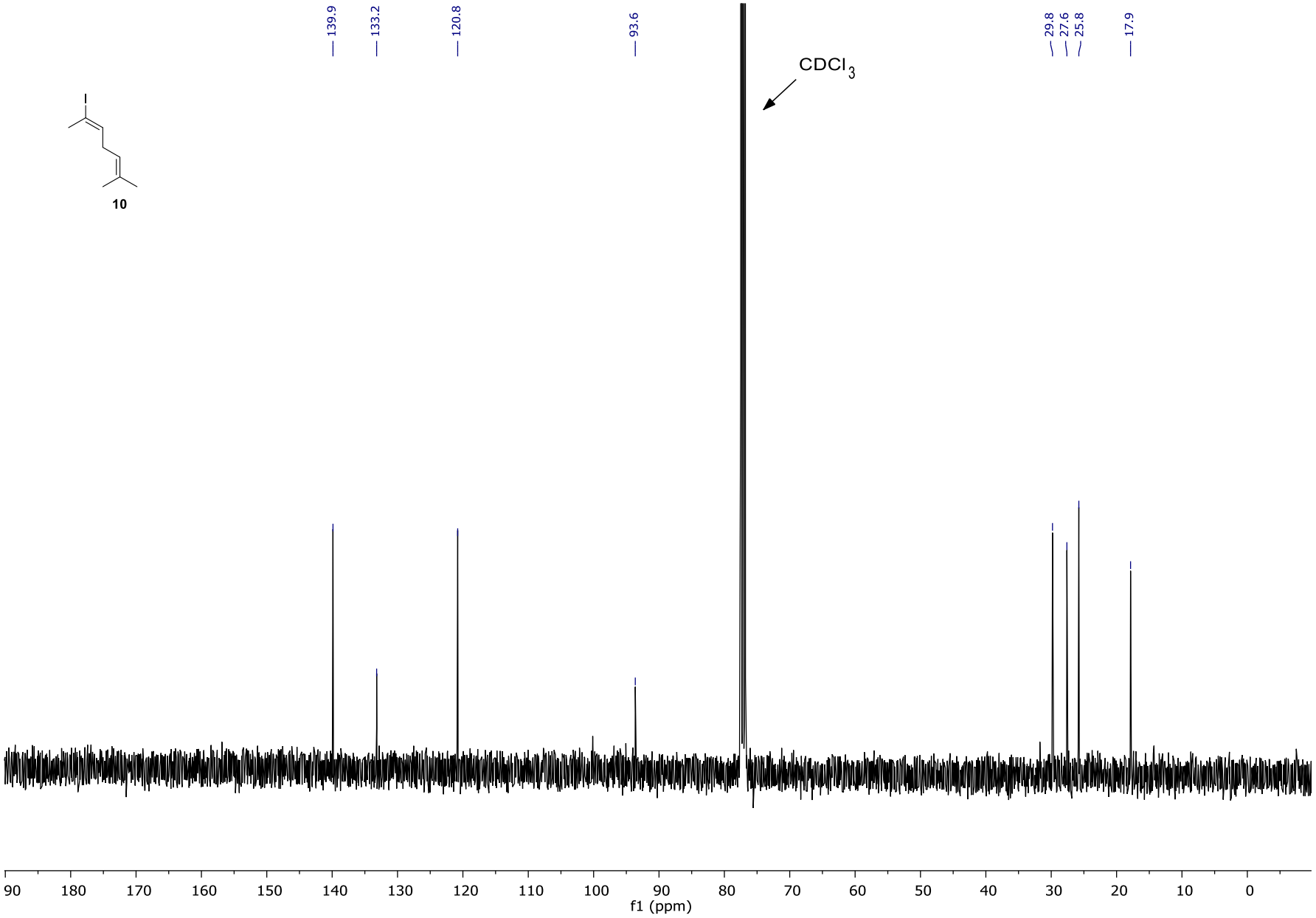
100 MHz ^{13}C NMR Spectrum of Compound **8** (recorded in $CDCl_3$)



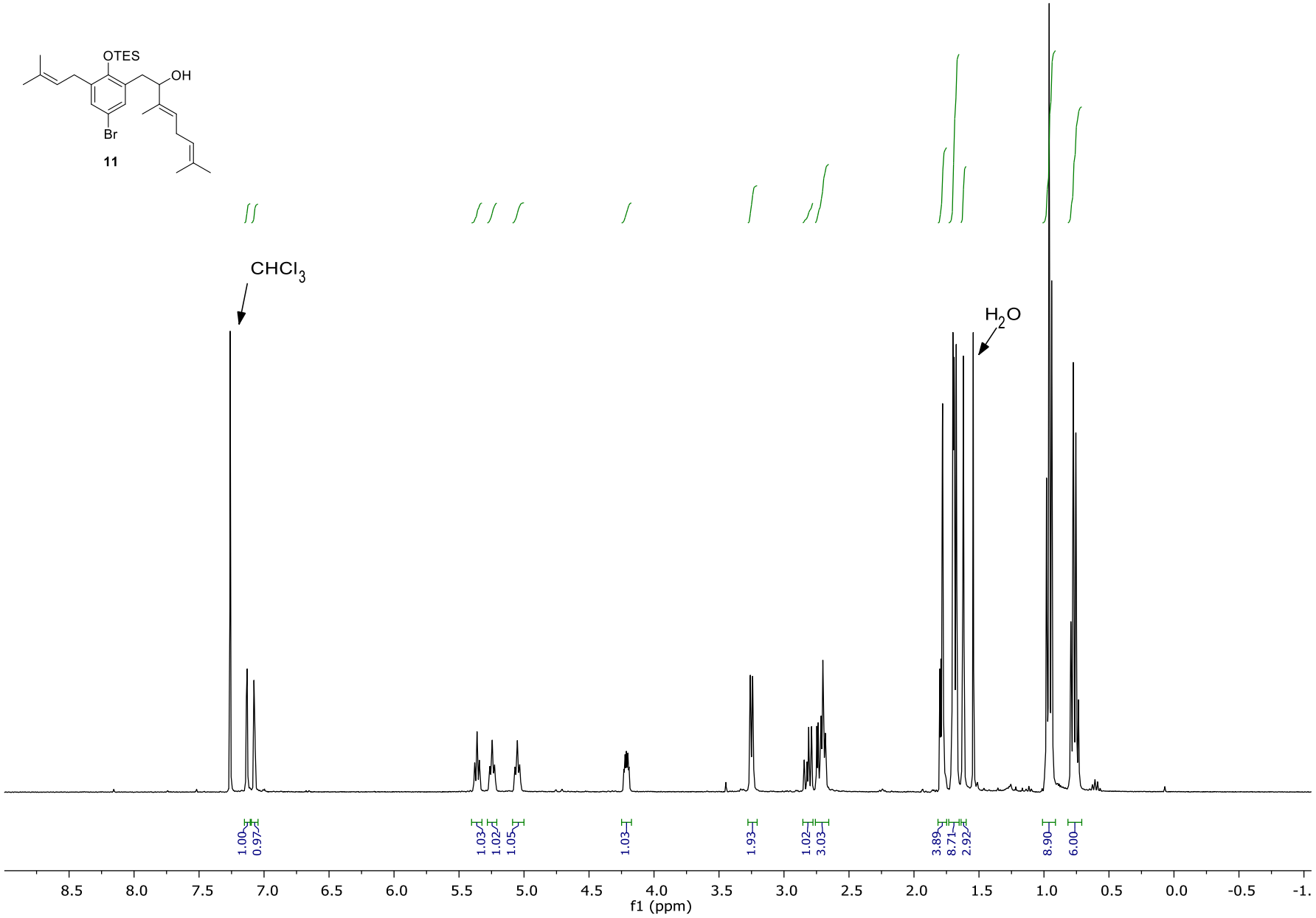
400 MHz ^{1}H NMR Spectrum of Compound **10** (recorded in $CDCl_3$)



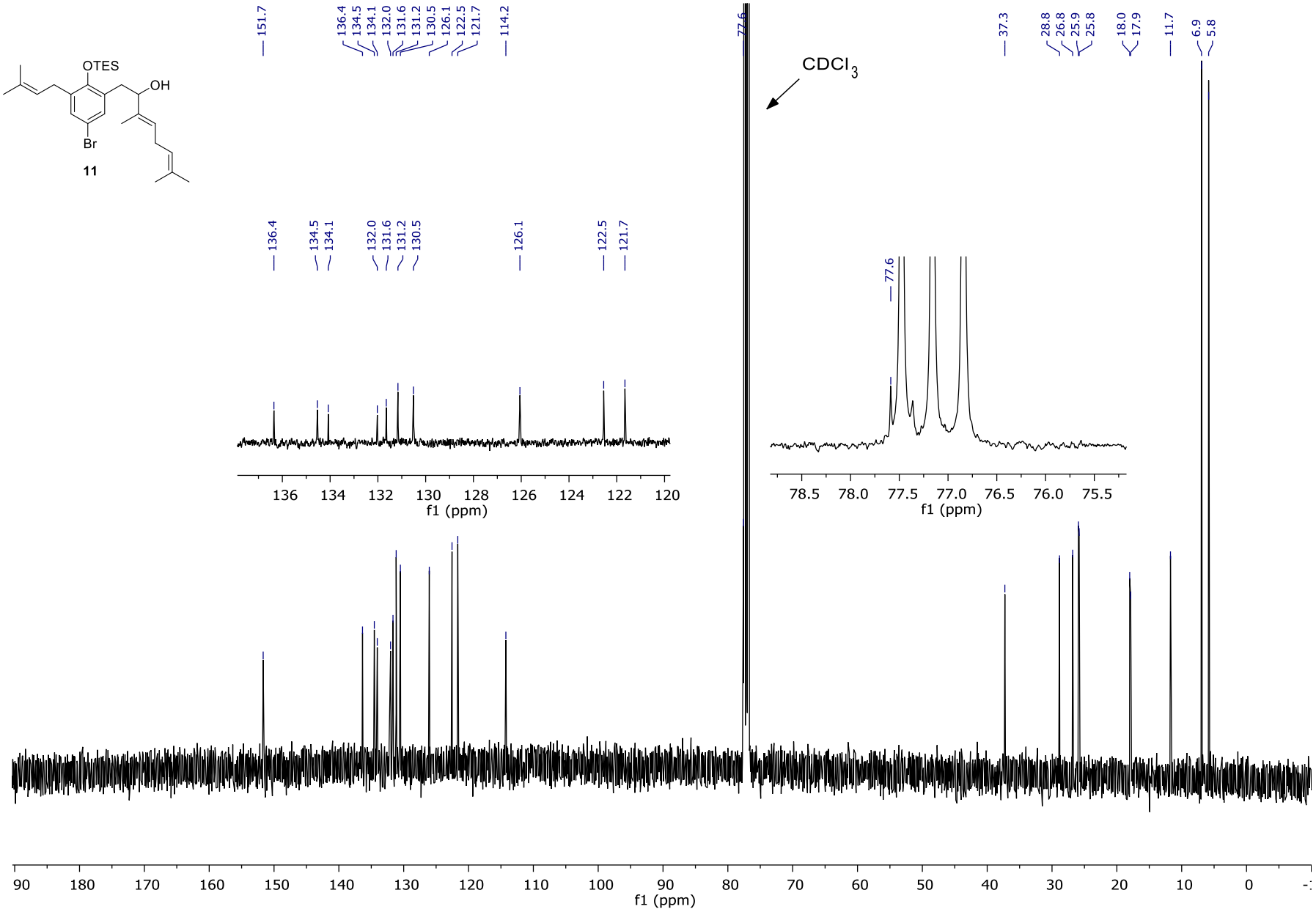
100 MHz ^{13}C NMR Spectrum of Compound **10** (recorded in $CDCl_3$)



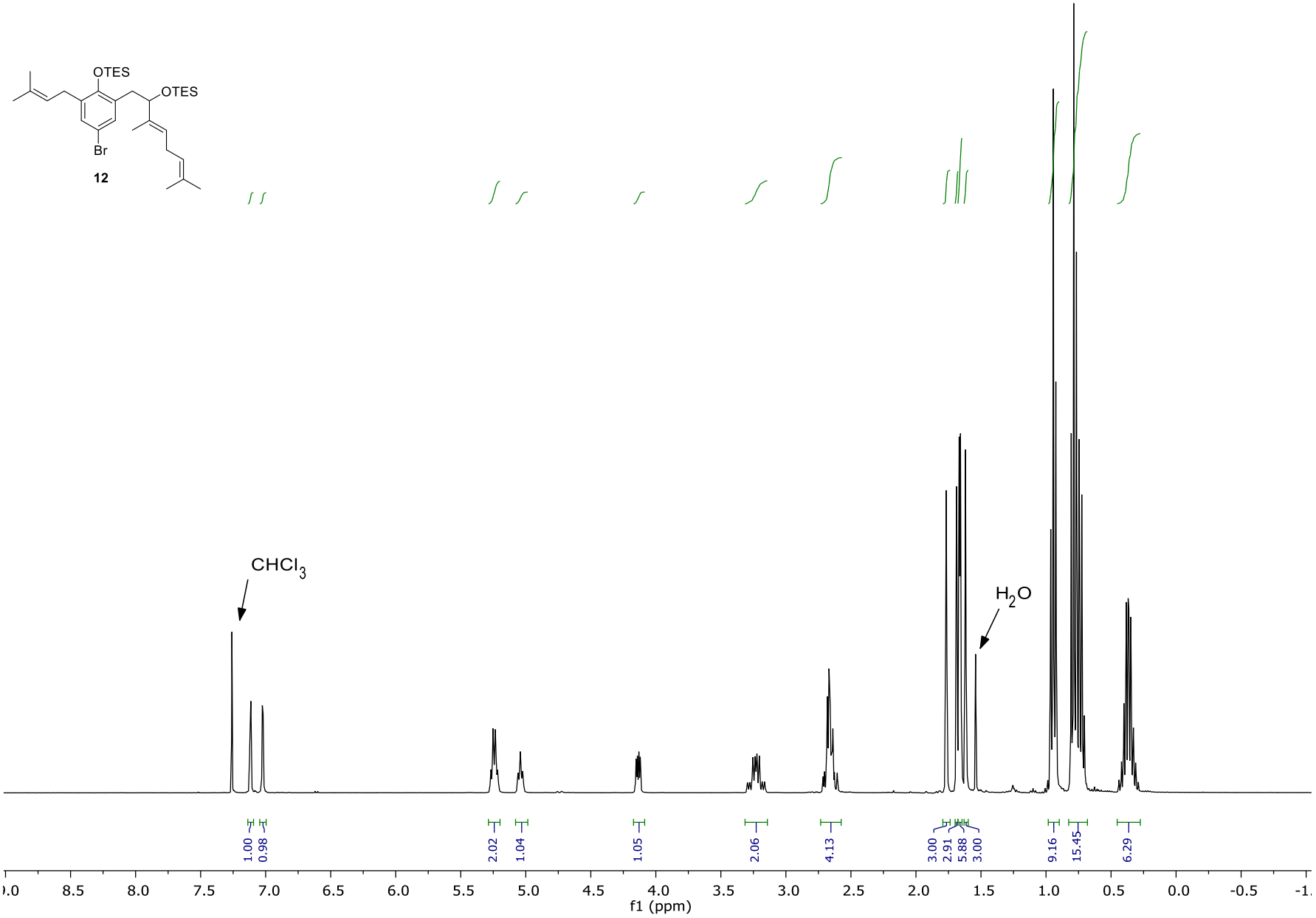
400 MHz ^{1}H NMR Spectrum of Compound **11** (recorded in $CDCl_3$)



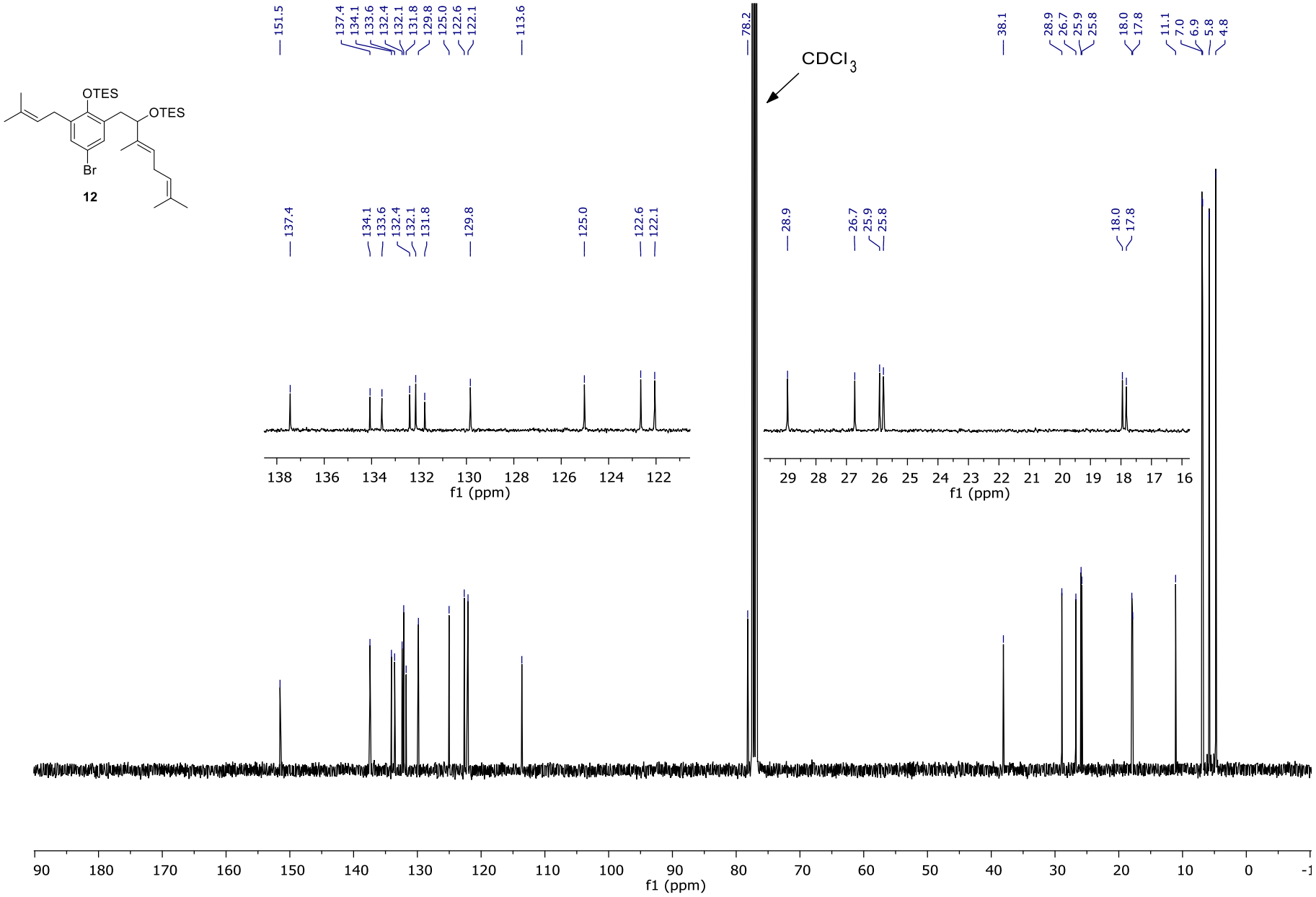
100 MHz ^{13}C NMR Spectrum of Compound **11** (recorded in $CDCl_3$)



400 MHz ^{1}H NMR Spectrum of Compound **12** (recorded in $CDCl_3$)



100 MHz ^{13}C NMR Spectrum of Compound **12** (recorded in $CDCl_3$)



400 MHz ^{1}H NMR Spectrum of Compound **13** (recorded in $CDCl_3$)