Supporting Information for:

$Bi(OTf)_3$-Catalysed Synthesis of Substituted Indanes by a Double Hydroarylation of Unactivated 1,3-Dienes

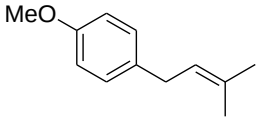
Bastien Cacciuttolo, Pierrick Ondet, Sophie Poulain-Martini, Gilles Lemière and Elisabet Duñach*

General remarks:

Reactions were carried out under an anhydrous atmosphere of Nitrogen. Glassware was oven-dried prior to use. Anhydrous Anhydrous $MeNO_2$ was obtained by drying over $CaCl_2$. Other commercially available reagents were used as received unless stated otherwise. Column chromatography was carried out on silica gel (spherical. neutral. 63-200 µm. Geduran Si 60. Merck KGaA). GC/MS analyses were performed with a Shimadzu QP2010S-MS chromatograph (EI. 70 eV) equipped with a SLB-5ms capillary column (thickness: 0.25 mm. length: 30 m. inside diameter: 0.25 mm). Analytical thin-layer chromatography (TLC) was performed on 0.2 mm precoated plate Kieselgel 60 F254 (Merck). NMR spectra (^1H, ^{13}C, DEPT, COSY ^1H–^1H and ^1H–^{13}C, nOe) were recorded on a BRUKER AC 200 spectrometer. ^1H NMR spectra are referenced at 7.26 ppm for $CDCl_3$. ^{13}C NMR spectra are referenced at 77.00 ppm for $CDCl_3$. Chemical shifts are given in ppm.
High resolution mass spectroscopy (HRMS) were performed on a LTQ/Orbitrap Thermo Fisher.

1-methoxy-4-(3-methylbut-2-enyl)benzene *p*-3a and 1-methoxy-2-(3-methylbut-2-enyl)benzene *o*-3a

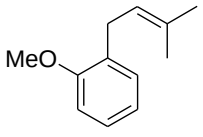
$Bi(OTf)_3$ (7 mg , 0.01 mmol) was added to a mixture of anisole **1a** (2.2 mL, 20 mmol) and isoprene **2a** (320 µL, 2 mmol). The solution was stirred at room temperature for 1h. After complete consumption of the diene (GC monitoring), the reaction mixture was quenched with a saturated aqueous solution of $NaHCO_3$, extracted thrice with diethyl ether, washed with a saturated aqueous solution of NaCl, dried over anhydrous $MgSO_4$ and concentrated under reduced pressure. The residue was purified by column chromatography (pentane) to afford the *o*-**3a** (63 mg), o-**3a** and *p*-**3a** (204 mg, *o:p* = 25:75) and *p*-**3a** (63 mg) as colorless oil (overall yield: 94%).



Chemical Formula: $C_{12}H_{16}O$
Molecular Weight: 176,25

p-**3a**

^{1}H NMR *(200 MHz, $CDCl_3$)* 7.17-7.08 (m, 2H), 6.90-6.80 (m, 2H), 5.33 (bt, *J* = 7.3 Hz, 1H), 3.80 (s, 3H), 3.31 (d, *J* = 7.4 Hz, 2H), 1.77 (bs, 3H), 1.74 (bs, 3H).
^{13}C NMR *(50 MHz, $CDCl_3$)* 158.1, 133.9, 132.1, 129.2, 123.6, 113.8 , 55.3, 33.4, 25.8, 17.7.
MS *(m/z)* 176(52) [$M^{+\cdot}$], 161(100), 146(17), 121(38), 115(25), 108 (16), 91(95), 77(72), 65(50), 51 (44).
Spectral data were in accordance with those reported in literature[1]



Chemical Formula: $C_{12}H_{16}O$
Molecular Weight: 176,25

o-**3a**

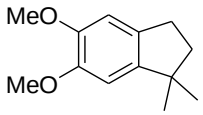
^{1}H NMR *(200 MHz, $CDCl_3$)* 7.25-7.09 (m, 2H), 6.98-6.78 (m, 2H), 5.33 (bt, *J* = 7.3 Hz, 1H), 3.85 (s, 3H), 3.34 (d, *J* = 7.4 Hz, 2H), 1.76 (bs, 3H), 1.73 (bs, 3H).
^{13}C NMR *(50 MHz, $CDCl_3$)* 157.7, 133.9, 131.4, 129.0, 127.7, 123.5, 120.3, 110.1, 55.3, 33.3, 25.6, 17.6.
MS *(m/z)* 176(22) [$M^{+\cdot}$], 161 (27), 121 (17), 107(10), 91 (100), 77 (39), 65 (35).
Spectral data were in accordance with those reported in literature [2]

[1] Y. Yang and S. L. Buchwald, *J. Am. Chem. Soc.*, 2013, **135**, 10642-10645.

General procedure for the formation of indanes from 1,3-dienes:

To a solution of 1,2-dimethoxybenzene **1b** (127 µL, 1.0 mmol) and $Bi(OTf)_3$ (33 mg, 0.05 mmol) in nitromethane (1 mL) was slowly added isoprene **2a** (150 µL, 1.5 mmol) in nitromethane (1 mL) over 1 hour at room temperature using a syringe pump. After the addition, the solution was stirred for 1h. After complete consumption of the aromatic compound (GC monitoring), the reaction mixture was quenched with a saturated aqueous solution of $NaHCO_3$, extracted thrice with diethyl ether, washed with a saturated aqueous solution of NaCl, dried over anhydrous $MgSO_4$ and concentrated under reduced pressure. The residue was purified by column chromatography (pentane/Et2O: 100/0 to 90/10) to afford the indane compound **4a** (163 mg, 79 %) as a colorless oil.

5,6-dimethoxy-1,1-dimethyl-2,3-dihydro-1*H*-indene 4a

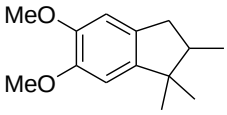


Chemical Formula: $C_{13}H_{18}O_2$
Molecular Weight: 206,28

Indane **4a** was obtained as a colorless oil (163 mg, 79%) following the General Procedure from 1,2-dimethoxybenzene **1b** (127 µL, 1.0 mmol), isoprene **2a** (150 µL, 1.5 mmol) and $Bi(OTf)_3$ (33 mg, 0.05 mmol).

^{1}H NMR *(200 MHz, $CDCl_3$)* 6.75 (s, 1H), 6.68 (s,1H), 3.89 (s, 3H), 3.86 (s, 3H), 2.84 (t, J = 7.0 Hz, 2H), 1.93 (t, J= 7.0 Hz,2H), 1.25 (s, 6H)
^{13}C NMR *(50 MHz, $CDCl_3$)* 148.0, 147.8, 144.2, 134.0, 107.7, 105.4, 56.0, 55.9, 44.0, 29.8, 28.6 (2C)
MS *(m/z)* 206 (21) [$M^{+\cdot}$], 192 (15), 191 (100), 161 (8), 160 (27), 115 (12), 103 (9), 91 (12), 77 (14), 51 (8)
HRMS (ESI$^+$) Calculated for $[C_{13}H_{19}O_2]^+$: 207.1380; Found: 207.1377.
Spectral data were in accordance with those reported in literature [3]

5,6-dimethoxy-1,1,2-trimethyl-2,3-dihydro-1*H*-indene 4b

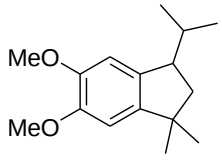


Chemical Formula: $C_{14}H_{20}O_2$
Molecular Weight: 220,31

Indane **4b** was obtained as a colorless oil (209 mg, 95%) following the General Procedure from 1,2-dimethoxybenzene **1b** (127 µL, 1.0 mmol), 2,3-dimethyl-1,3-butadiene **2b** (170 µL, 1.5 mmol) and $Bi(OTf)_3$ (33 mg, 0.05 mmol).

^{1}H NMR *(200 MHz, $CDCl_3$)* 6.73 (s, 1H), 6.67 (s, 1H), 3.88 (s, 3H), 3.85 (s, 3H), 2.86 (dd, ^{3}J = 7.5 Hz , ^{2}J= 15.1 Hz, 1H), 2.48 (dd, ^{3}J = 7.5 Hz , ^{2}J= 15.1 Hz, 1H), 2.13 (m, 1H), 1.25 (s, 3H), 1.04 (d, 3J = 7.0 Hz, 3H), 0.94 (s, 3H)
^{13}C NMR *(50 MHz, $CDCl_3$)* 148.0, 147.7, 145.1, 133.2, 107.7, 105.8, 56.1, 56.0, 45.9, 45.4, 38.3, 26.8, 23.1, 14.0
MS *(m/z)* 220 (25) [$M^{+\cdot}$], 206 (19), 205 (100), 145 (14), 105 (14), 81 (18), 57 (69), 55 (13), 44 (17), 41 (35)
HRMS (ESI$^+$) Calculated for $[C_{14}H_{21}O_2]^+$: 221.1536; Found: 221.1535.

3-isopropyl-5,6-dimethoxy-1,1-dimethyl-2,3-dihydro-1*H*-indene 4c



Chemical Formula: $C_{16}H_{24}O_2$
Molecular Weight: 248,36

Indane **4c** was obtained as a colorless oil (176 mg, 71%) following the General Procedure from 1,2-dimethoxybenzene **1b** (127 µL, 1.0 mmol), 2,5-dimethyl-2,4-hexadiene **2c** (213 µL, 1.5 mmol) and $Bi(OTf)_3$ (33 mg, 0.05 mmol).

^{1}H NMR *(200 MHz, $CDCl_3$)* 6.67 (s, 1H), 6.64 (s,1H), 3.88 (s, 3H), 3.86 (s, 3H), 3.16 (m, 1H), 2.21 (m, 1H), 1.87 (m, 1H), 1.65 (m, 1H), 1.32 (s, 3H), 1.15 (s, 3H), 1.03 (d, J = 7Hz, 3H), 0.75 (d, J = 7 Hz, 3H)

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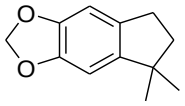
[2] J. L. Farmer, H. N. Hunter and M. G. Organ, *J. Am. Chem. Soc.*, 2012, **134**, 17470-17473.

[3] H. Lebel, C. Ladjel and L. Bréthous, *J. Am. Chem. Soc.*, 2007, **129**, 13321-13326.

^{13}C NMR *(50 MHz, $CDCl_3$)* 184.1, 147.9, 144.8, 136.3, 107.0, 105.2, 56.0, 55.9, 47.8, 42.3, 42.1, 29.9, 29.2, 21.4, 17.0
MS *(m/z)* 248 (14) [$M^{+\cdot}$], 233 (7), 206 (14), 205 (100), 190 (7), 175 (7), 174 (20), 115 (6), 91 (7), 41 (7)
HRMS (ESI$^+$) Calculated for $[C_{16}H_{25}O_2]^+$: 249.1849; Found: 249.1847.

5,5-dimethyl-6,7-dihydro-5H-indeno[5,6-d][1,3]dioxole 4d

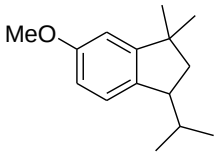


Chemical Formula: $C_{12}H_{14}O_2$
Molecular Weight: 190,24

Indane **4d** was obtained as a colorless oil (173 mg, 91%) following the General Procedure from 1,3-benzodioxole **1c** (115 µL, 1.0 mmol), isoprene **2a** (150 µL, 1.5 mmol) and $Bi(OTf)_3$ (33 mg, 0.05 mmol).

^{1}H NMR *(200 MHz, $CDCl_3$)* 6.65 (s, 1H), 6.61 (s, 1H), 5.90 (s, 2H), 2.78 (t, J = 7 Hz, 2H), 1.92 (t, J = 7 Hz, 2H), 1.21 (s, 3H)
^{13}C NMR *(50 MHz, $CDCl_3$)* 146.4, 146.2, 145.6, 135.2, 105.0, 102.8, 100.8, 43.7, 41.8, 30.0, 28.7 (2C)
MS *(m/z)* 190 (26) [$M^{+\cdot}$], 176 (10), 175 (100), 146 (7), 145 (50), 117 (30), 115 (23), 91 (12), 77 (8), 51 (12)
Spectral data were in accordance with those reported in literature [4]

3-isopropyl-6-methoxy-1,1-dimethyl-2,3-dihydro-1H-indene 4e

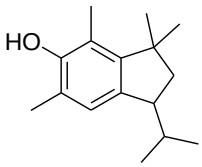


Chemical Formula: $C_{15}H_{22}O$
Molecular Weight: 218,33

Indane **4e** was obtained as a colorless oil (172 mg, 79%) following the General Procedure from anisole **1a** (109 µL, 1.0 mmol), 2,5-dimethyl-2,4-hexadiene **2c** (213 µL, 1.5 mmol) and $Bi(OTf)_3$ (33 mg, 0.05 mmol).) The temperature was increased to reflux after total consumption of the diene.

^{1}H NMR *(200 MHz, $CDCl_3$)* 7.04 – 6.66 (m, 3H), 3.80 (s, 3H), 3.14 (m, 1H), 2.16 (m,1H), 1.24 (m,1H), 1.71 (m, 1H), 1.33 (s, 3H), 1.16 (s, 3H), 1.04 (d, J = 7 Hz, 3H), 0.74 (d, J = 7 Hz, 3H)
^{13}C NMR *(50 MHz, $CDCl_3$)* 158.8, 154.6, 137.0, 124.36, 111.7, 107.6, 53.3, 47.3, 42.6, 42.35, 29.7, 29.2, 28.8, 21.4, 17.2
MS *(m/z)* 218 (7) [$M^{+\cdot}$], 176 (13), 175 (100), 160 (13), 145 (12), 128 (13), 117 (10), 115 (20), 91 (17), 43 (25), 41 (29)

1-isopropyl-3,3,4,6-tetramethyl-2,3-dihydro-1*H*-inden-5-ol 4f



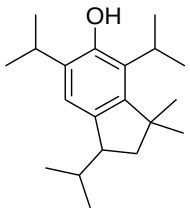
Chemical Formula: $C_{16}H_{24}O$
Molecular Weight: 232,36

Indane **4f** was obtained as a colorless oil (216 mg, 93%) following the General Procedure from 2,6-dimethylphenol **1d** (122 mg, 1.0 mmol), 2,5-dimethyl-2,4-hexadiene **2c** (213 µL, 1.5 mmol) and $Bi(OTf)_3$ (33 mg, 0.05 mmol).) The temperature was increased to reflux after total consumption of the diene.

^{1}H NMR *(200 MHz, $CDCl_3$)* 6.75 (s, 1H), 4.52 (s, 1H), 3.03 (m, 1H), 2.26 (s, 3H), 2.22 (s, 3H), 1.75 (m,3H), 1.44 (s, 3H), 1.24 (s, 3H), 1.01 (d, J = 7Hz, 3H), 0.75 (d, J = 7 Hz, 3H)
^{13}C NMR *(125 MHz, $CDCl_3$)* 150.9, 148.6, 137.2, 123.1, 120.8, 119.1, 46.6, 44.0, 43.5, 29.2, 28.7, 27.1, 21.5, 16.7, 16.4, 11.4
MS *(m/z)* 287 (22), 286 (100) [$M^{+\cdot}$], 271 (53), 232 (23), 231 (89), 215 (78), 201 (24), 44 (27), 43 (28), 41 (42)
HRMS (ESI$^+$) Calculated for $[C_{16}H_{25}O]^+$: 233.1900; Found: 233.1899.

[4] S. A. Bonderoff, F. G. West and M. Tremblay, *Tetrahedron Lett.*, 2012, **53**, 4600-4603.

1,4,6-triisopropyl-3,3-dimethyl-2,3-dihydro-1H-inden-5-ol 4g

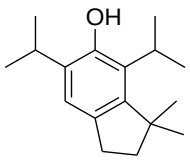


Chemical Formula: $C_{20}H_{32}O$
Molecular Weight: 288,47

Indane **4g** was obtained as a colorless oil (271 mg, 94%) following the General Procedure from 2,6-diisopropylphenol **1e** (185 µL, 1.0 mmol), 2,5-dimethyl-2,4-hexadiene **2c** (213 µL, 1.5 mmol) and $Bi(OTf)_3$ (33 mg, 0.05 mmol).

^{1}H NMR *(200 MHz, $CDCl_3$)* 6.78 (s, 1H), 4.60 (s, 1H), 3.42 (dt, J = 14.3, 7.2 Hz, 1H), 3.21 – 2.86 (m, 2H), 2.33 – 2.11 (m, 1H), 1.78 (dd, J = 12.4, 7.9 Hz, 2H), 1.48 – 1.31 (m, 10H), 1.25 (dd, J = 6.8, 4.0 Hz, 10H), 1.02 (d, J = 6.8 Hz, 4H), 0.76 (d, J = 6.8 Hz, 3H)
^{13}C NMR *(50 MHz, $CDCl_3$)* 151.0, 147.3, 137.4, 132.3, 129.7, 118.3, 46.6, 44.5, 43.7, 30.3, 28.8, 28.1, 27.8, 27.0, 23.0, 22.8, 21.5, 20.8, 20.8, 16.8
MS *(m/z)* 288 (20) [$M^{+\cdot}$], 245 (17), 231 (100), 192 (8), 147 (53), 137 (17), 128 (4), 100 (12), 43 (20), 41 (10)

4,6-diisopropyl-3,3-dimethyl-2,3-dihydro-1H-inden-5-ol 4h

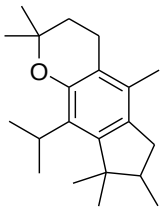


Chemical Formula: $C_{17}H_{26}O$
Molecular Weight: 246,39

Indane **4h** was obtained as a colorless oil (202 mg, 82%) following the General Procedure from 2,6-diisopropylphenol **1e** (185 µL, 1.0 mmol), isoprene **2a** (150 µL, 1.5 mmol) and $Bi(OTf)_3$ (33 mg, 0.05 mmol).

^{1}H NMR *(200 MHz, $CDCl_3$)* 6.86 (s, 1H), 4.61 (s, 1H), 3.56 – 3.32 (m, 1H), 3.02 (m, 1H), 2.73 (t, J = 7.4 Hz, 2H), 1.88 (t, J = 7.4 Hz, 2H), 1.40 (d, J = 7.2 Hz, 6H), 1.36 (s, 6H), 1.25 (d, *J* = 7.2 Hz, 6H)
^{13}C NMR *(50 MHz, $CDCl_3$)* 151.1, 146.8, 135.2, 132.5, 130.1, 119.1, 45.8, 43.9, 29.3, 28.6 (2C), 27.9, 26.9, 22.8 (2C), 20.8 (2C)
MS *(m/z)* 246 (29) [$M^{+\cdot}$], 232 (17), 231 (100), 189 (8), 147 (53), 129 (12), 128 (9), 100 (15), 43 (17), 41 (13)
Synthesis of this compound has already been reported [5]

9-isopropyl-2,2,5,6,6,7-hexamethyl-2,3,4,6,7,8-hexahydrocyclopenta[*g*]chromene 4i



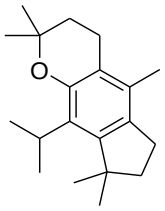
Chemical Formula: $C_{21}H_{32}O$
Molecular Weight: 300,48

Indane **4i** was obtained as a colorless oil (291 mg, 97%) following the General Procedure from the corresponding chromane derivative **1f** (218 mg, 1.0 mmol), 2,3-dimethyl-1,3-butadiene **2b** (170 µL, 1.5 mmol) and $Bi(OTf)_3$ (33 mg, 0.05 mmol). The temperature was increased to reflux after total consumption of the diene.

^{1}H NMR *(200 MHz, $CDCl_3$)* 3.36 (dt, *J* = 13.9, 7.0 Hz, 1H), 2.84 (dd, *J* = 14.8, 7.7 Hz, 1H), 2.62 (td, *J* = 6.8, 2.3 Hz, 2H), 2.30 (dd, *J* = 14.8, 11.2 Hz, 1H), 2.08 (s, 3H), 2.05 – 1.92 (m, 1H), 1.76 (t, *J* = 6.9 Hz, 2H), 1.42 – 1.29 (m, 15H), 1.03 (d, *J* = 8.1 Hz, 3H), 1.01 (s, 3H)
^{13}C NMR *(50 MHz, $CDCl_3$)* 135.7, 133.5, 132.0, 131.3, 128.6, 128.0, 127.1, 126.4, 44.5, 33.6, 31.7, 25.9, 20.9, 19.9, 18.2
MS *(m/z)* 300 (48) [$M^{+\cdot}$], 286 (14), 140 (21), 93 (14), 77 (10), 55 (36), 51 (14), 44 (76), 43 (100), 41 (87)

[5] T. F. Wood and G. H. Goodwin, *GE Patent 1801662*, 1977

9-isopropyl-2,2,5,6,6-pentamethyl-2,3,4,6,7,8-hexahydrocyclopenta[*g*]chromene 4j

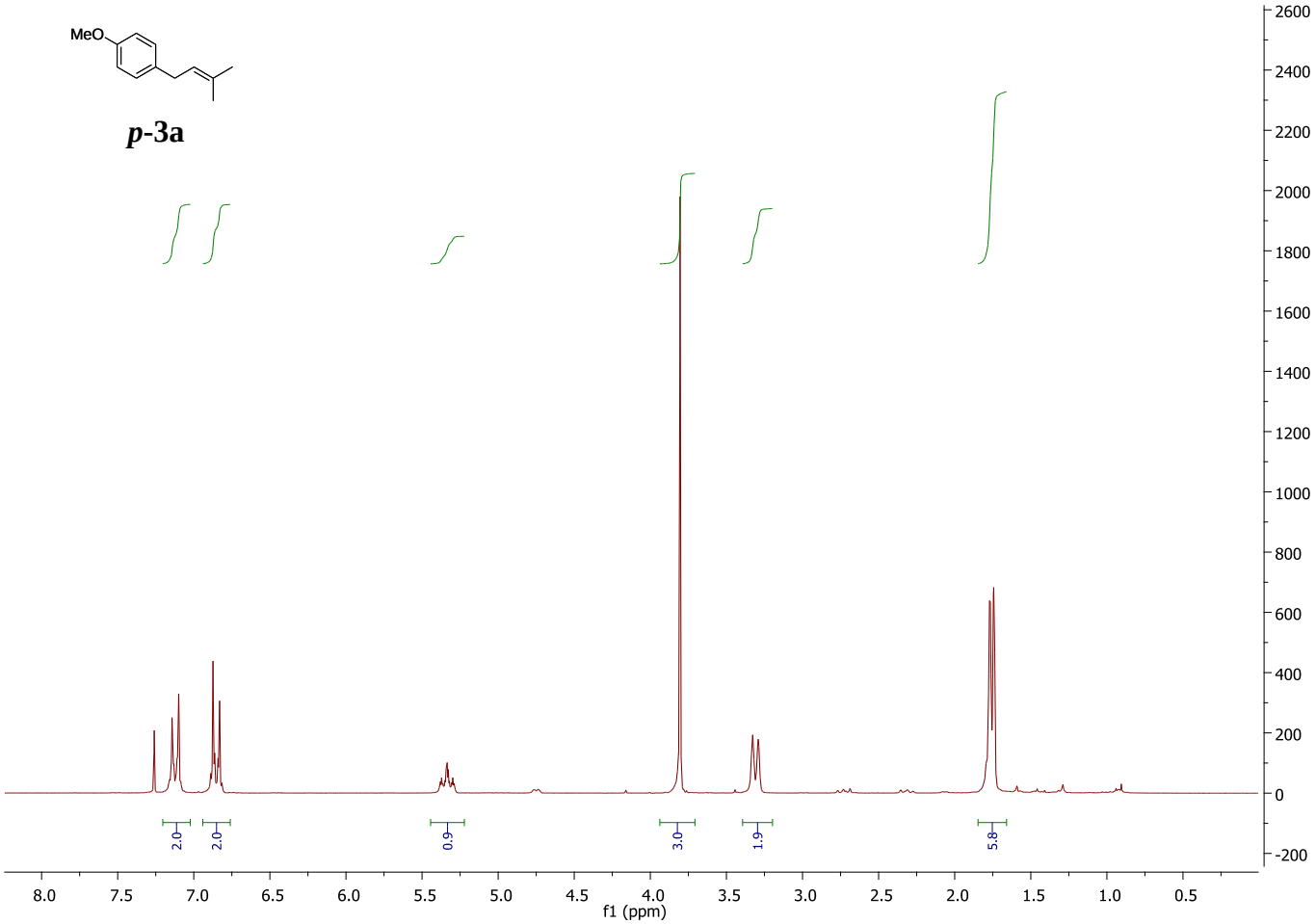


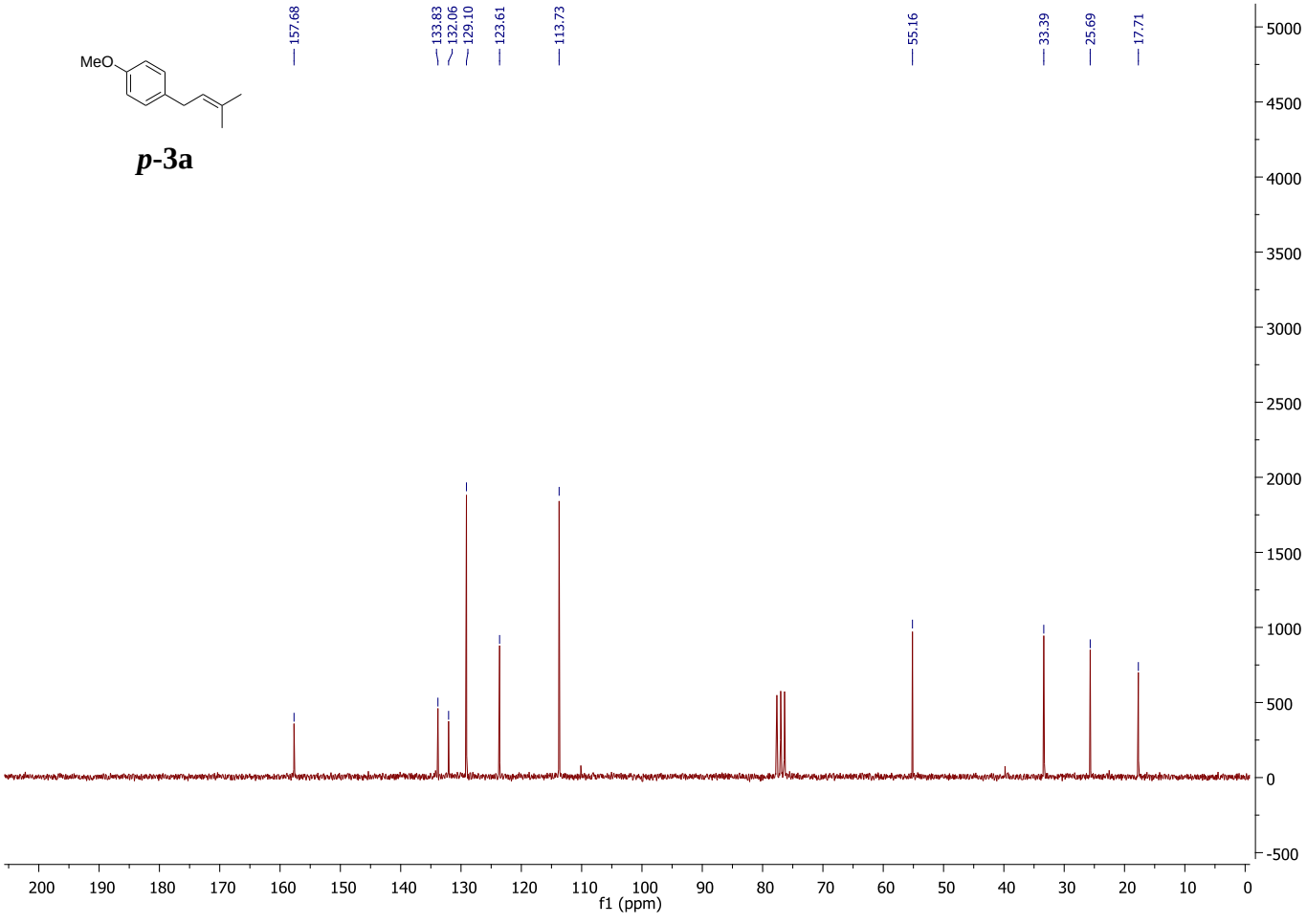
Chemical Formula: $C_{20}H_{30}O$
Molecular Weight: 286,45

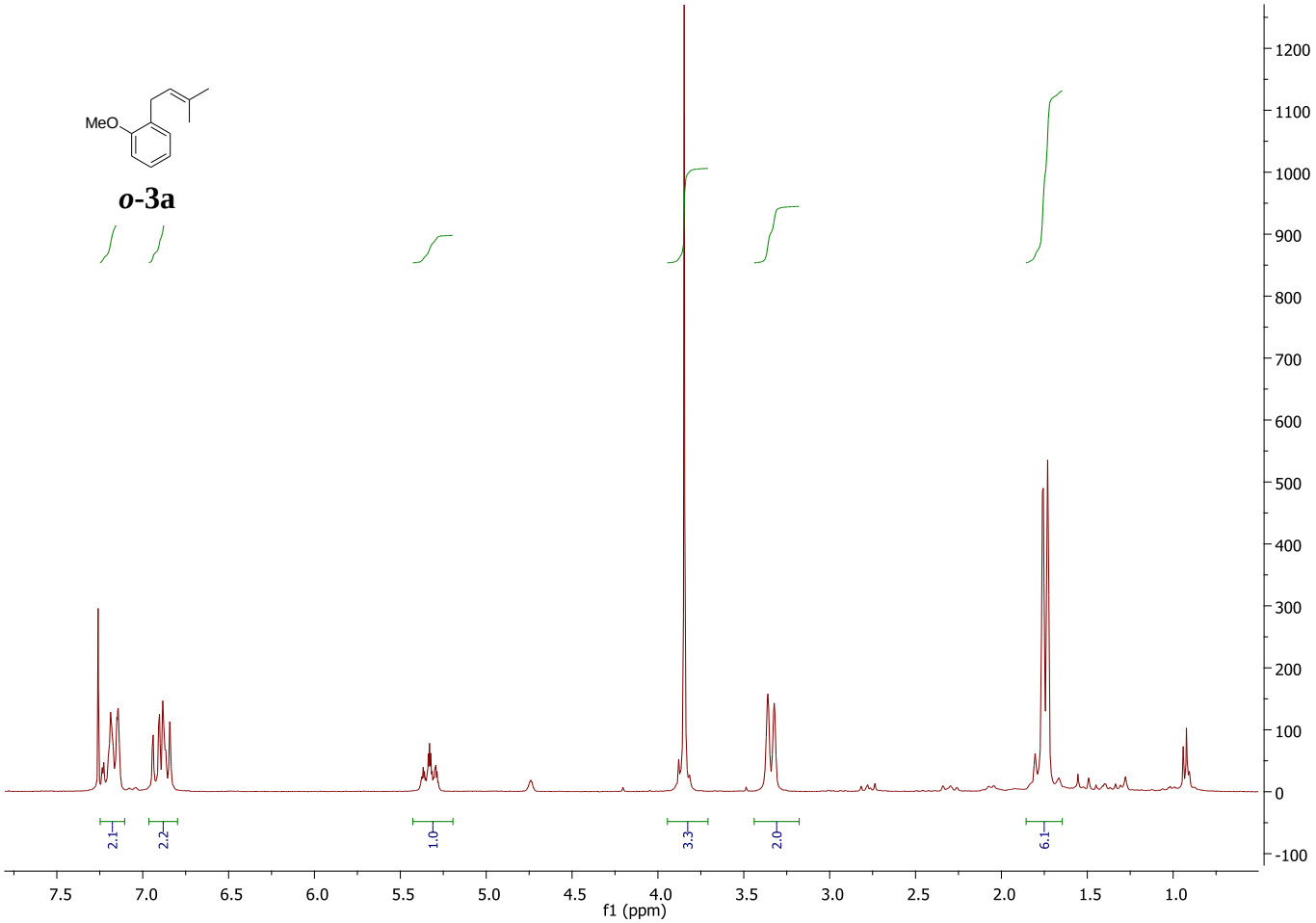
To a solution of thymol **1g** (150 mg, 1.0 mmol) and $Bi(OTf)_3$ (33 mg, 0.05 mmol) in 1,2-dichloroethane (1 mL) was slowly added isoprene **2a** (300 µL, 3.0 mmol) in 1,2-dichloroethane (1 mL) over 1 hour at room temperature using a syringe pump. After the addition, the solution was stirred for 1h at 50 °C. After complete consumption of the aromatic compound (GC monitoring), the reaction mixture was quenched with a saturated aqueous solution of $NaHCO_3$, extracted thrice with diethyl ether, washed with a saturated aqueous solution of NaCl, dried over anhydrous $MgSO_4$ and concentrated under reduced pressure. The residue was purified by column chromatography to afford the indane compound **4j** (263 mg, 92 %) as a colorless oil.

^{1}H NMR *(200 MHz, $CDCl_3$)* 3.32 (dt, *J* = 14.0, 6.9 Hz, 1H), 2.71 (t, *J* = 7.4 Hz, 2H), 2.62 (t, *J* = 6.9 Hz, 2H), 2.08 (s, 2H), 1.93 – 1.81 (m, 2H), 1.80 (s, 2H), 1.33 (m, 15H)
^{13}C NMR *(50 MHz, $CDCl_3$)* 152.0, 147.7, 131.8, 129.8, 129.0, 117.6, 72.4, 46.9, 45.5, 36.6, 32.8, 28.0, 27.9, 27.1, 26.3, 21.4, 20.9, 20.8, 15.3, 13.6
MS *(m/z)* 287 (21), 286 (94) [$M^{+\cdot}$], 271 (68), 232 (18), 231 (100), 215 (70), 187 (18), 173 (19), 43 (21), 41 (30)
HRMS (ESI$^+$) Calculated for $[C_{13}H_{19}O_2]^+$: 287.2369; Found: 287.2368.

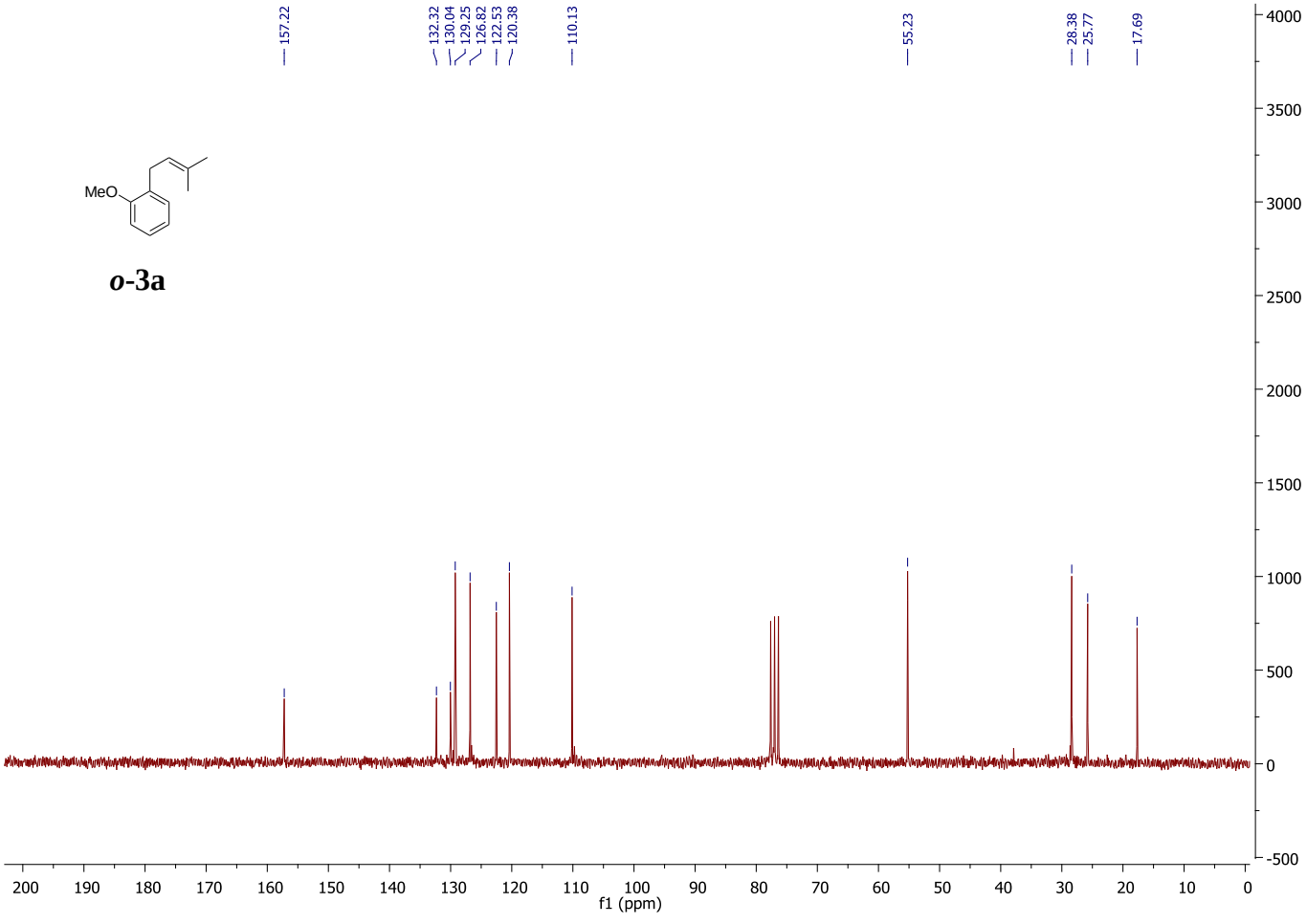
NMR SPECTRA


MeO
p-3a
2.0
2.0
0.9
3.0
1.9
5.8
f1 (ppm)

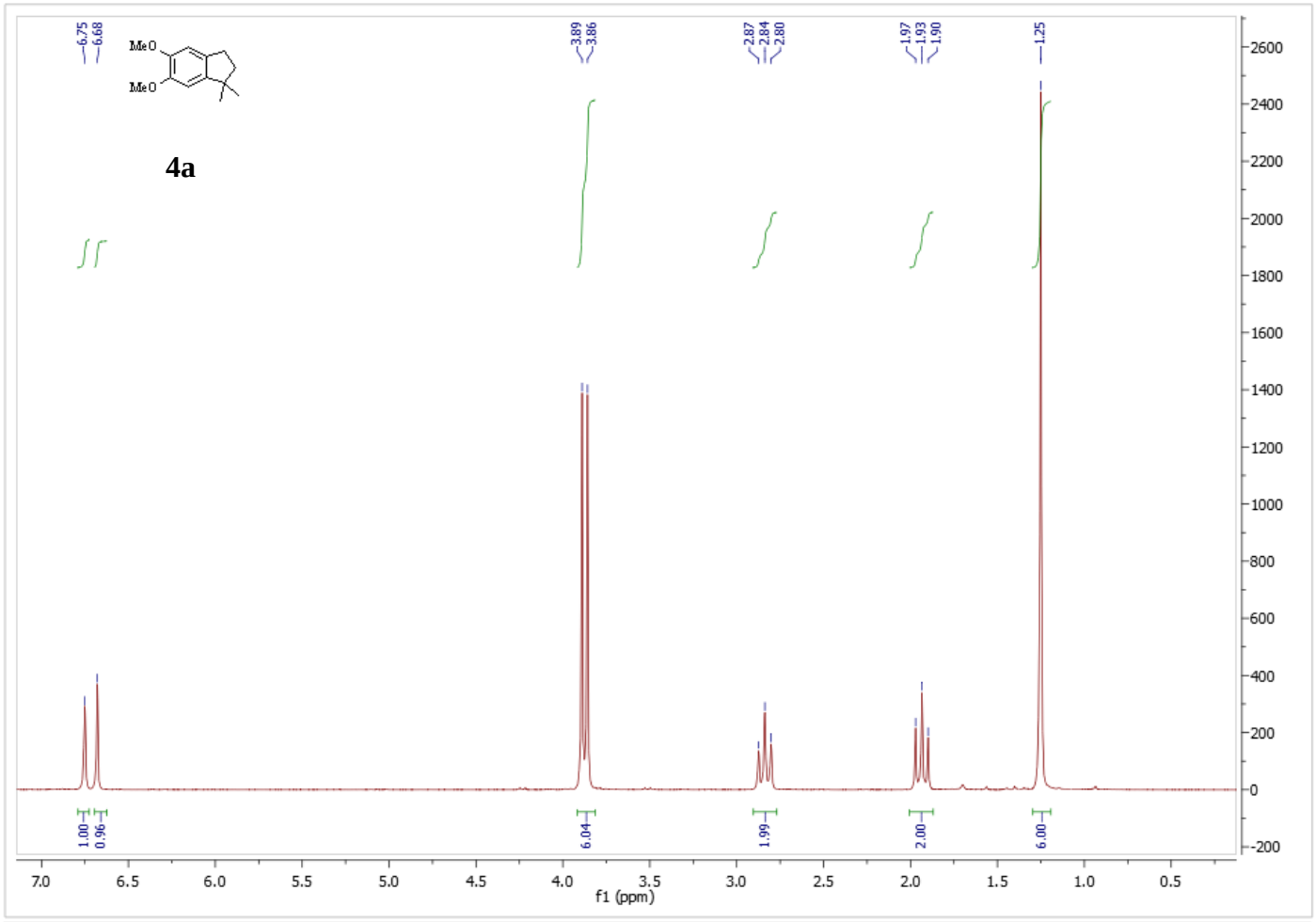

MeO
p-3a
157.68
133.83
132.06
129.10
123.61
113.73
55.16
33.39
25.69
17.71
f1 (ppm)

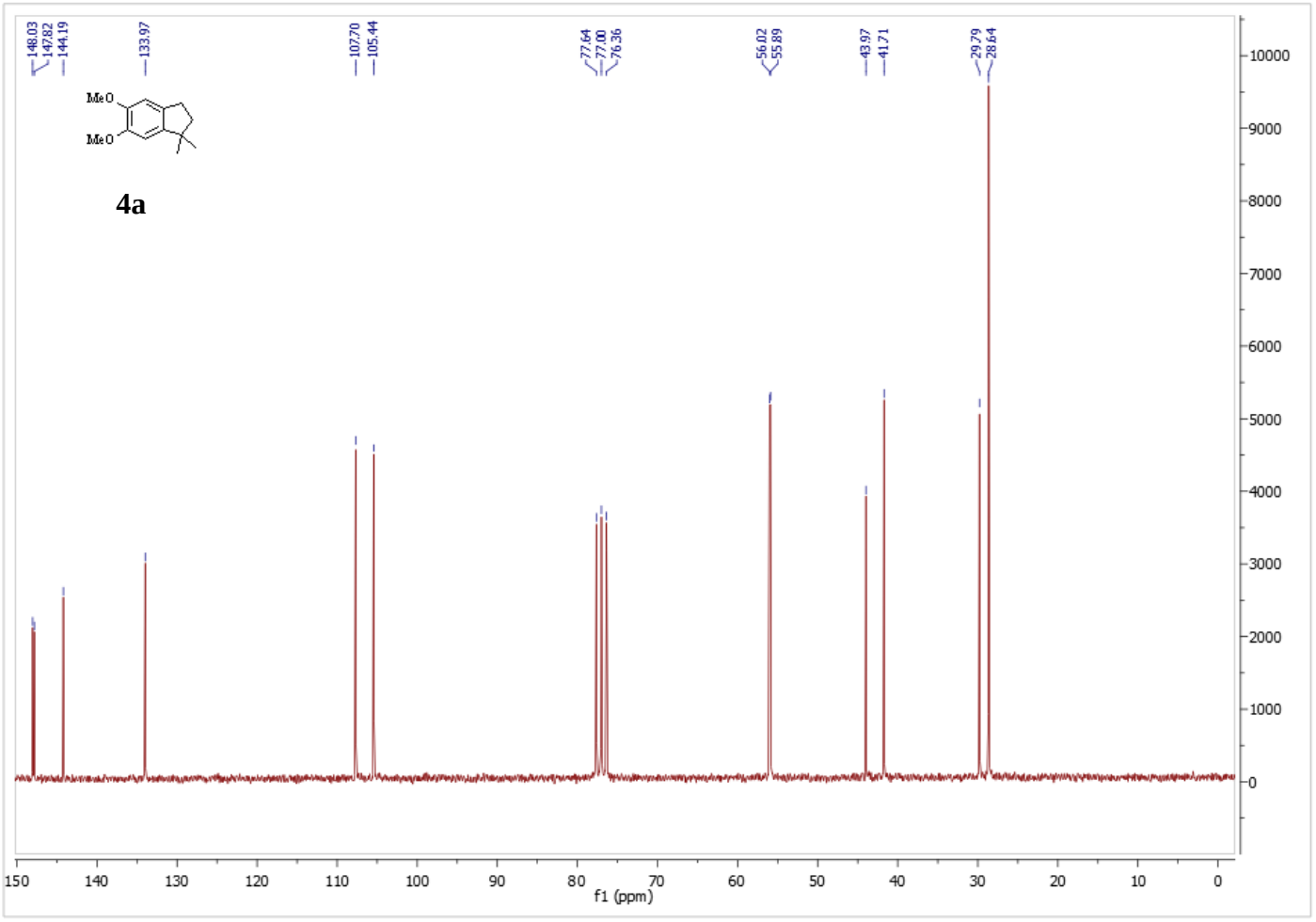

MeO
2.1
2.2
1.0
3.3
2.0
6.1
f1 (ppm)

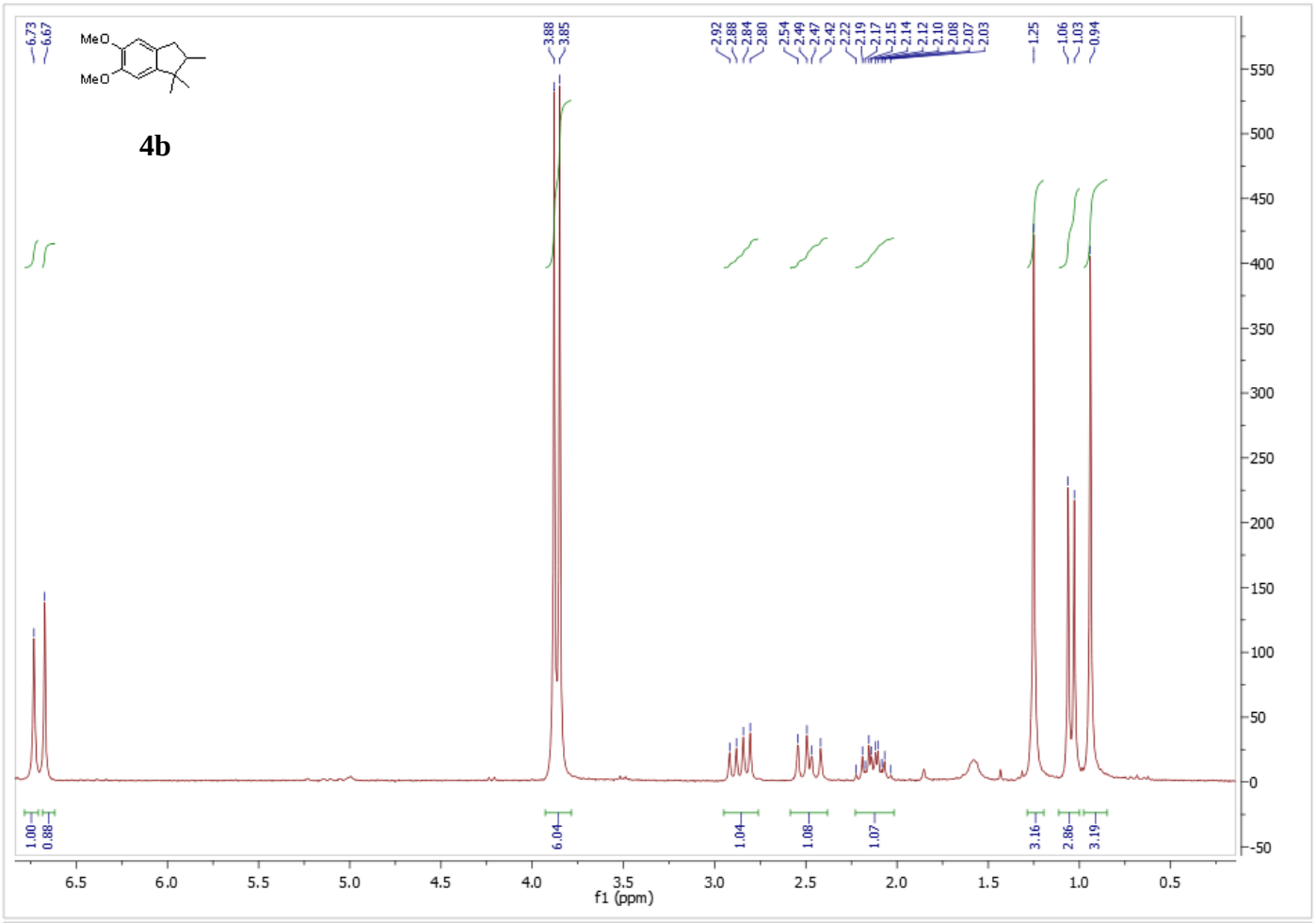
***o*-3a**

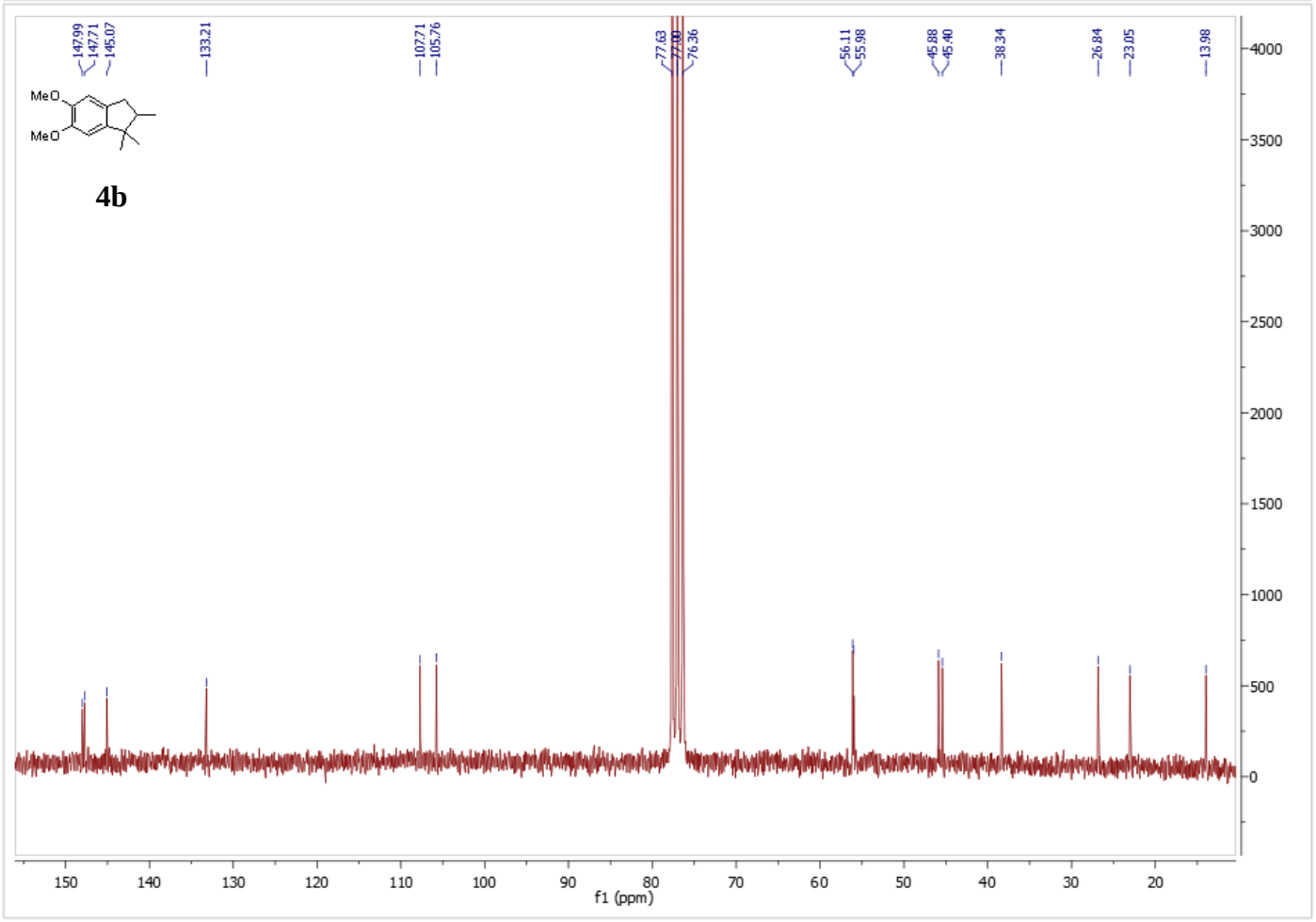

157.22
132.32
130.04
129.25
126.82
122.53
120.38
110.13
55.23
28.38
25.77
17.69
MeO
f1 (ppm)

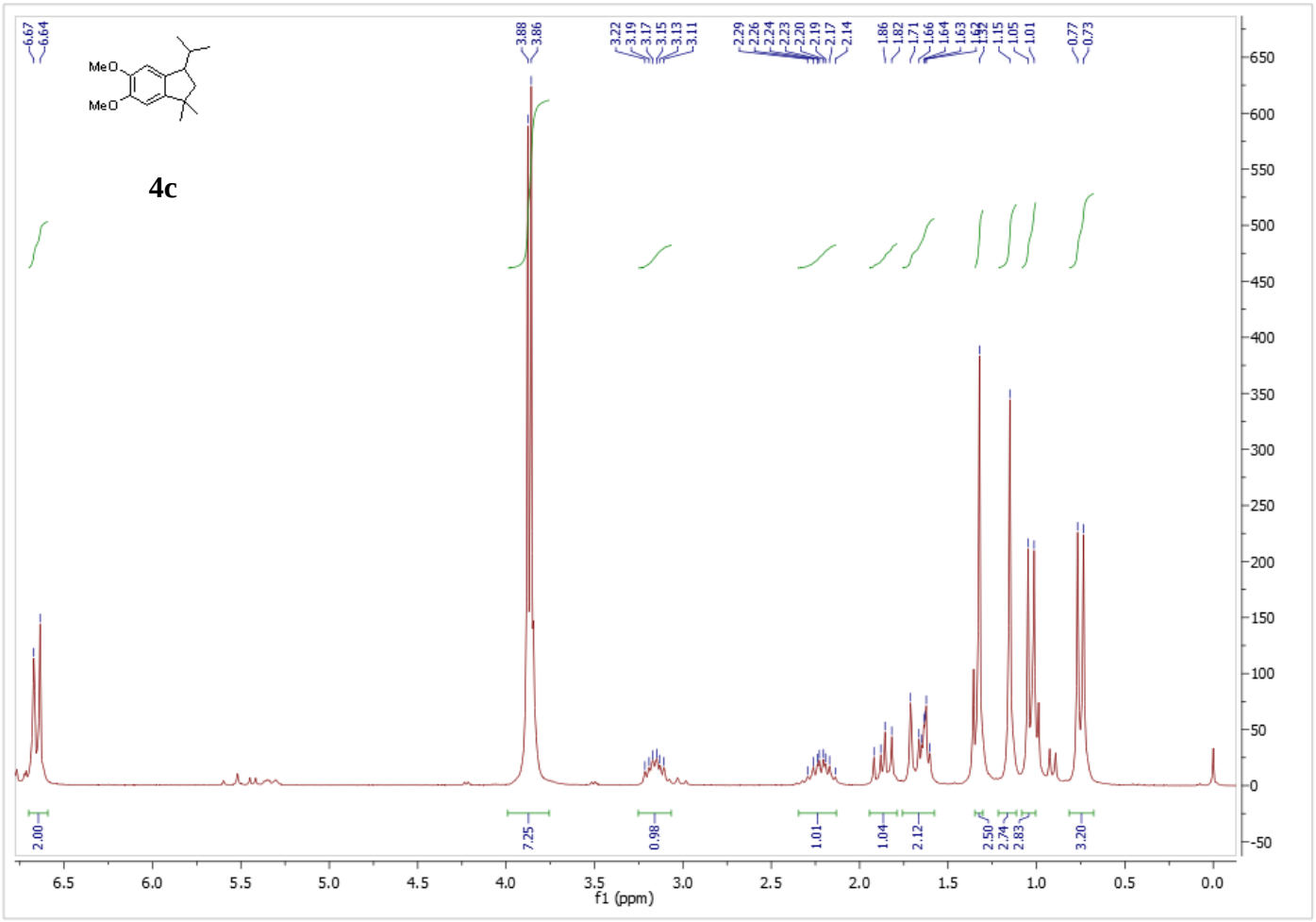
***o*-3a**

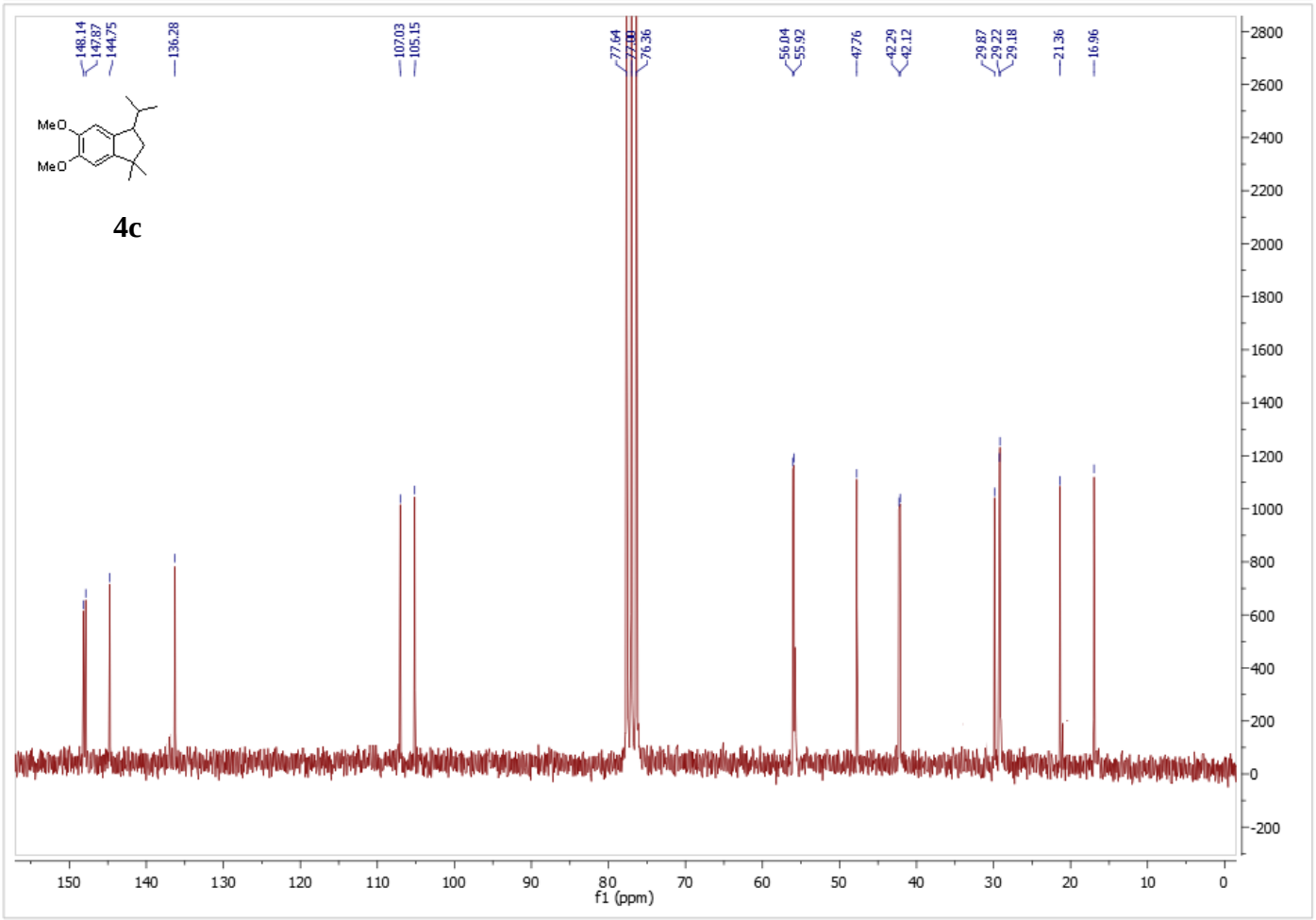

6.75
6.68
3.89
3.86
2.87
2.84
2.80
1.97
1.93
1.90
1.25
MeO
MeO
4a
1.00
0.96
6.04
1.99
2.00
6.00
f1 (ppm)

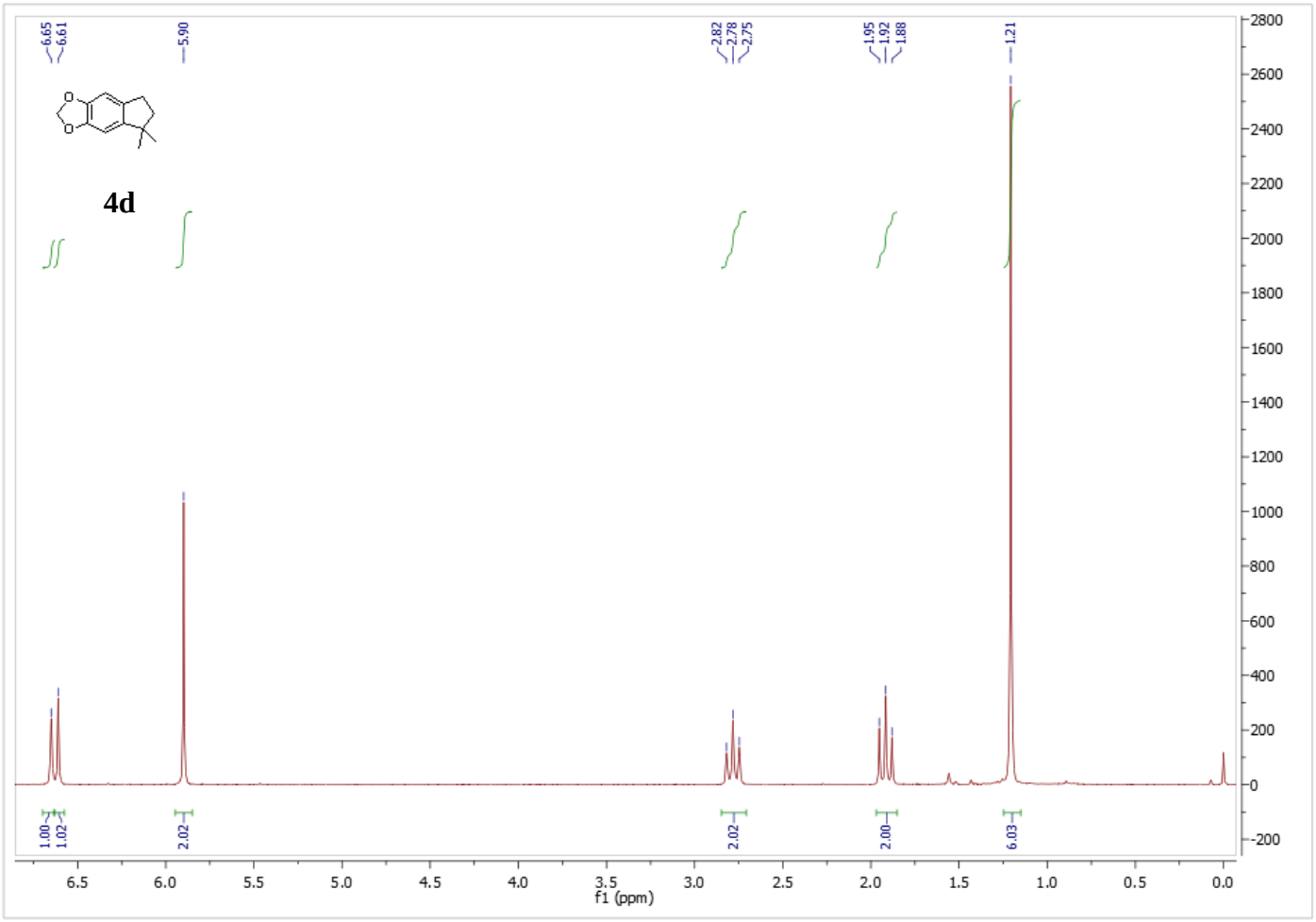

148.03
147.82
144.19
133.97
107.70
105.44
77.64
77.00
76.36
56.02
55.89
43.97
41.71
29.79
28.64
MeO
MeO
4a
f1 (ppm)

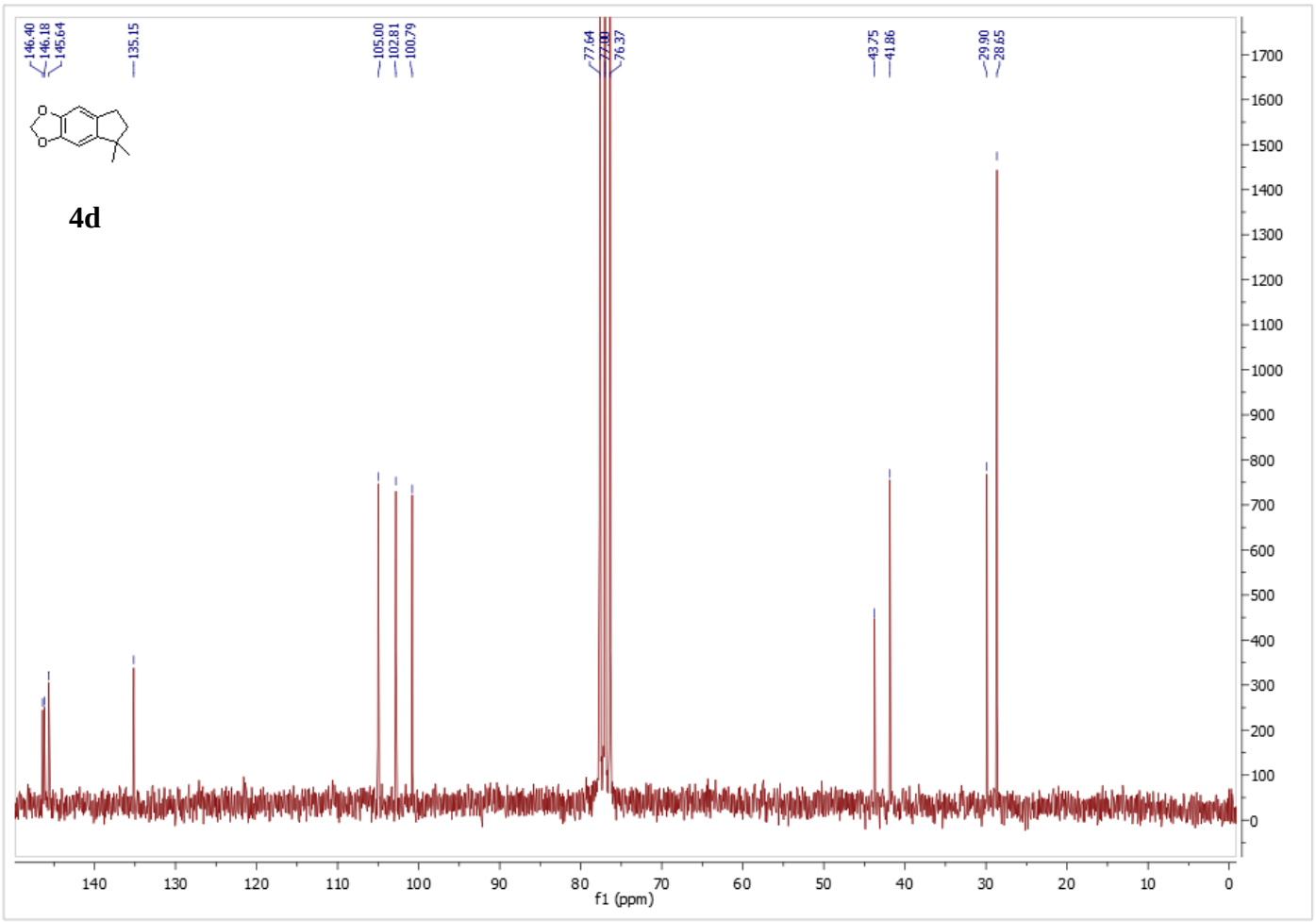

MeO
MeO
4b
6.73
6.67
3.88
3.85
2.92
2.88
2.84
2.80
2.54
2.49
2.47
2.42
2.22
2.19
2.17
2.15
2.14
2.12
2.10
2.08
2.07
2.03
1.25
1.06
1.03
0.94
1.00
0.88
6.04
1.04
1.08
1.07
3.16
2.86
3.19
f1 (ppm)

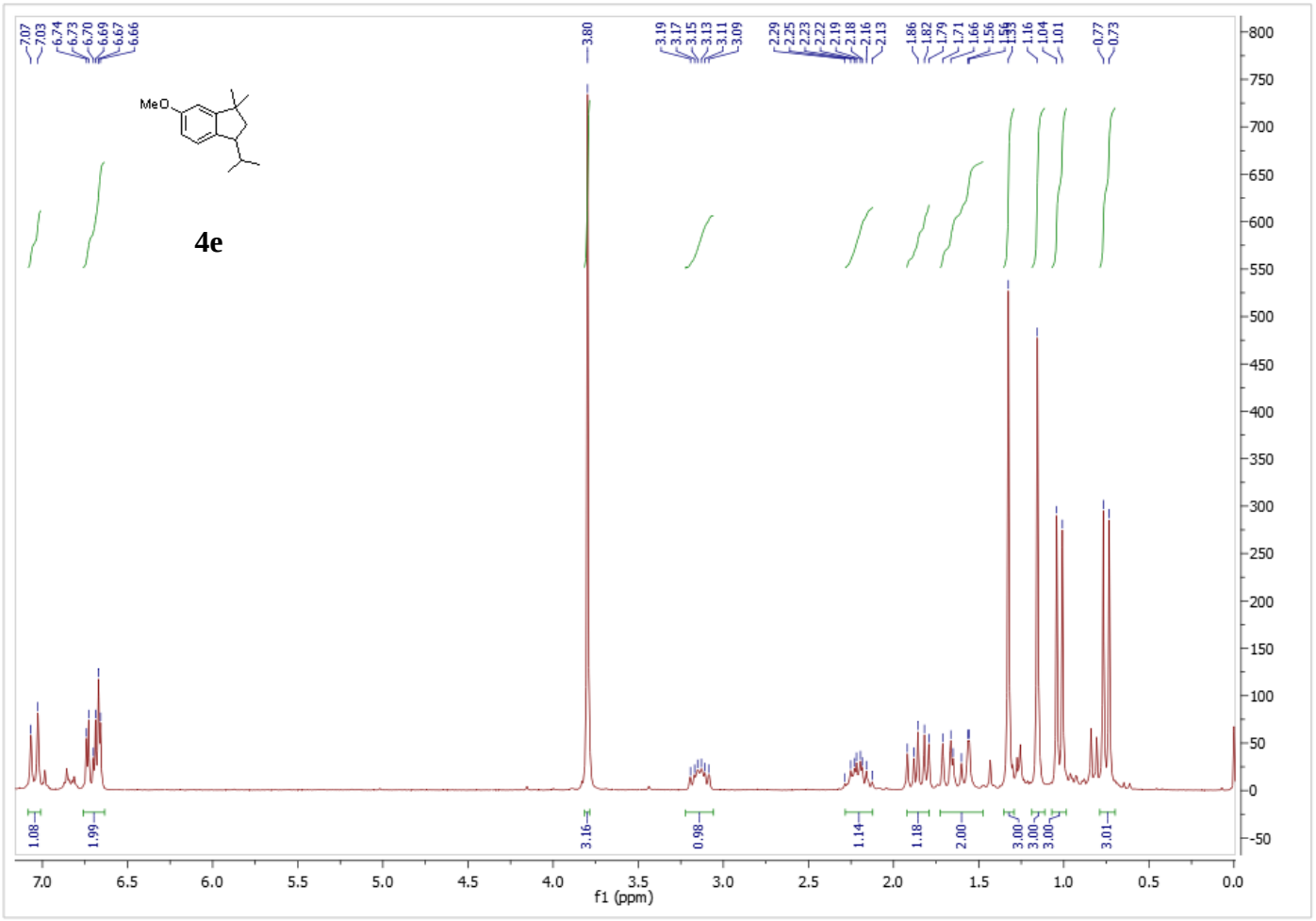

MeO
MeO
4b
147.99
147.71
145.07
133.21
107.71
105.76
77.63
77.00
76.36
56.11
55.98
45.88
45.40
38.34
26.84
23.05
13.98
f1 (ppm)

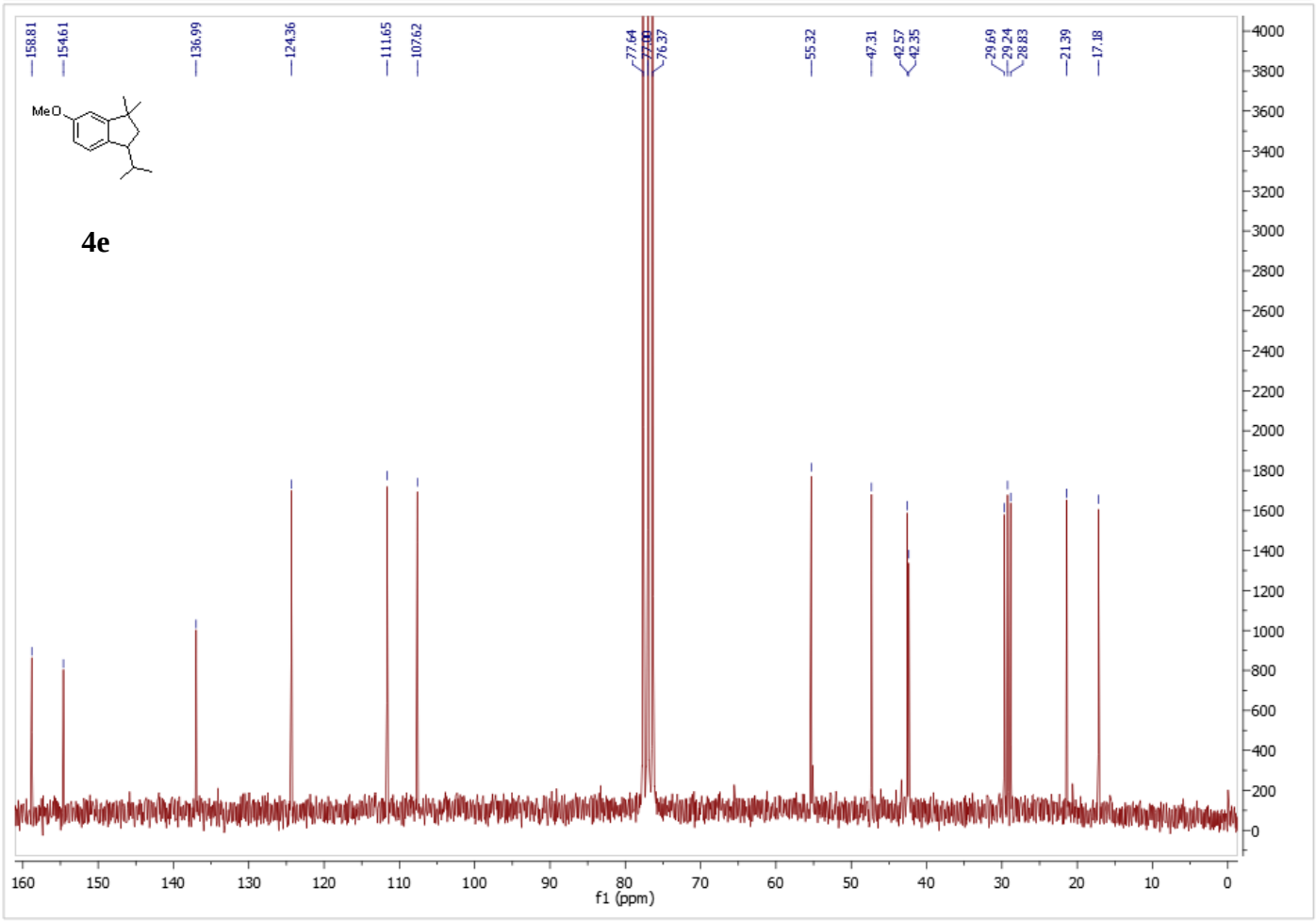

MeO
MeO
4c
6.67
6.64
3.88
3.86
3.22
3.19
3.17
3.15
3.13
3.11
2.29
2.26
2.24
2.23
2.20
2.19
2.17
2.14
1.86
1.82
1.71
1.66
1.64
1.63
1.32
1.15
1.05
1.01
0.77
0.73
2.00
7.25
0.98
1.01
1.04
2.12
2.50
2.74
2.83
3.20
f1 (ppm)

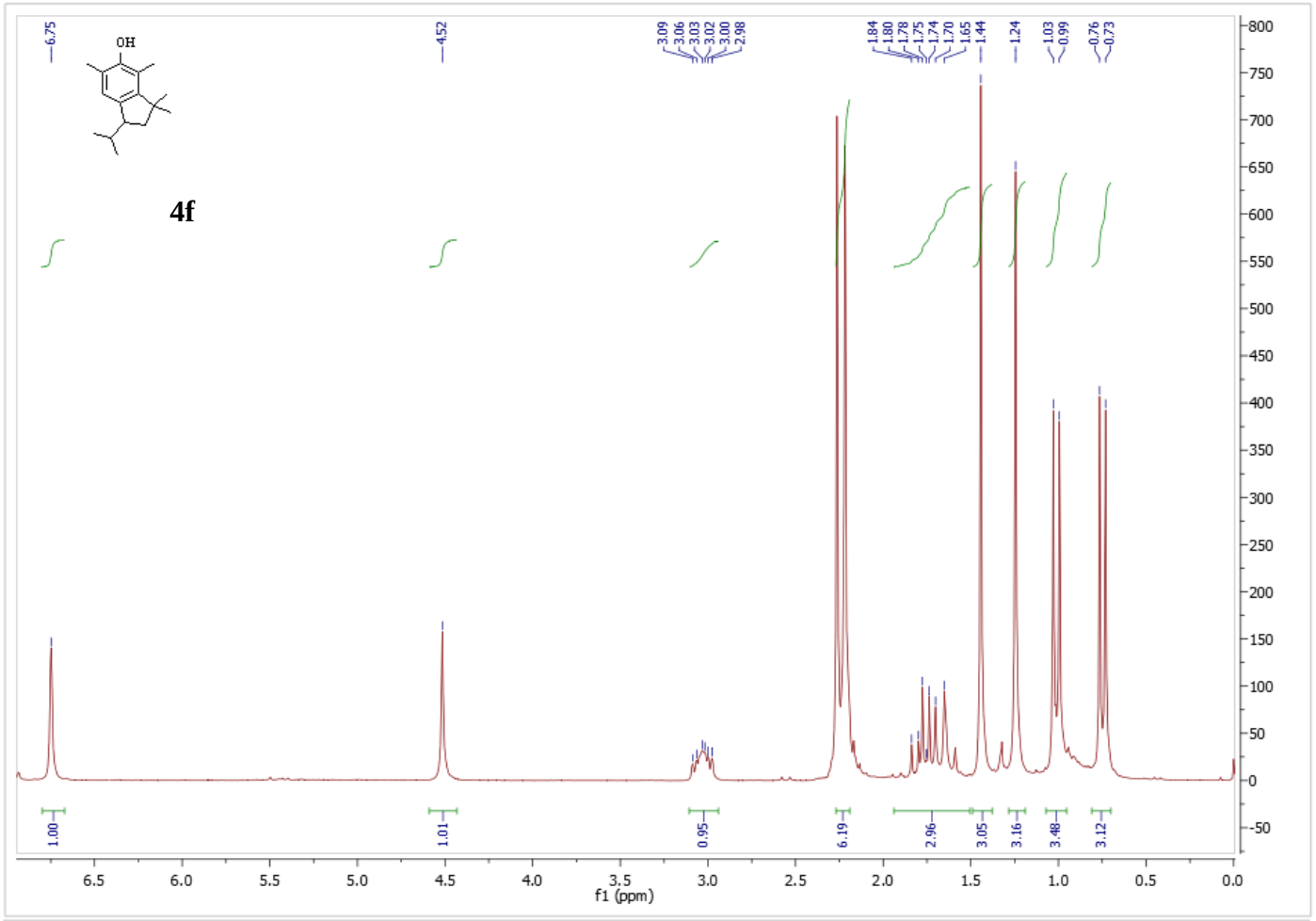

MeO
MeO
4c
148.14
147.87
144.75
136.28
107.03
105.15
77.64
77.00
76.36
56.04
55.92
47.76
42.29
42.12
29.87
29.22
29.18
21.36
16.96
f1 (ppm)

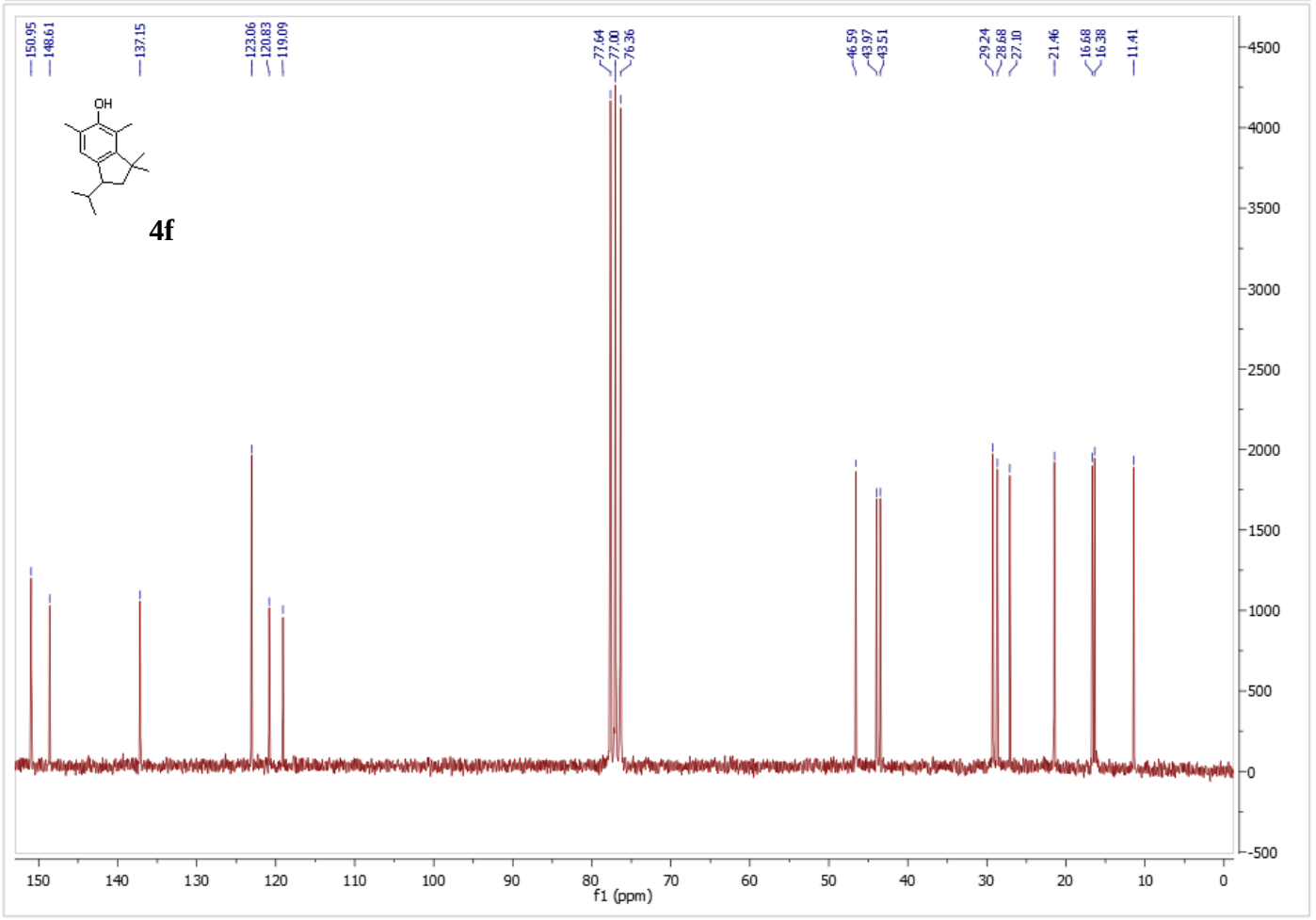

6.65
6.61
5.90
2.82
2.78
2.75
1.95
1.92
1.88
1.21
4d
1.00
1.02
2.02
2.02
2.00
6.03
f1 (ppm)

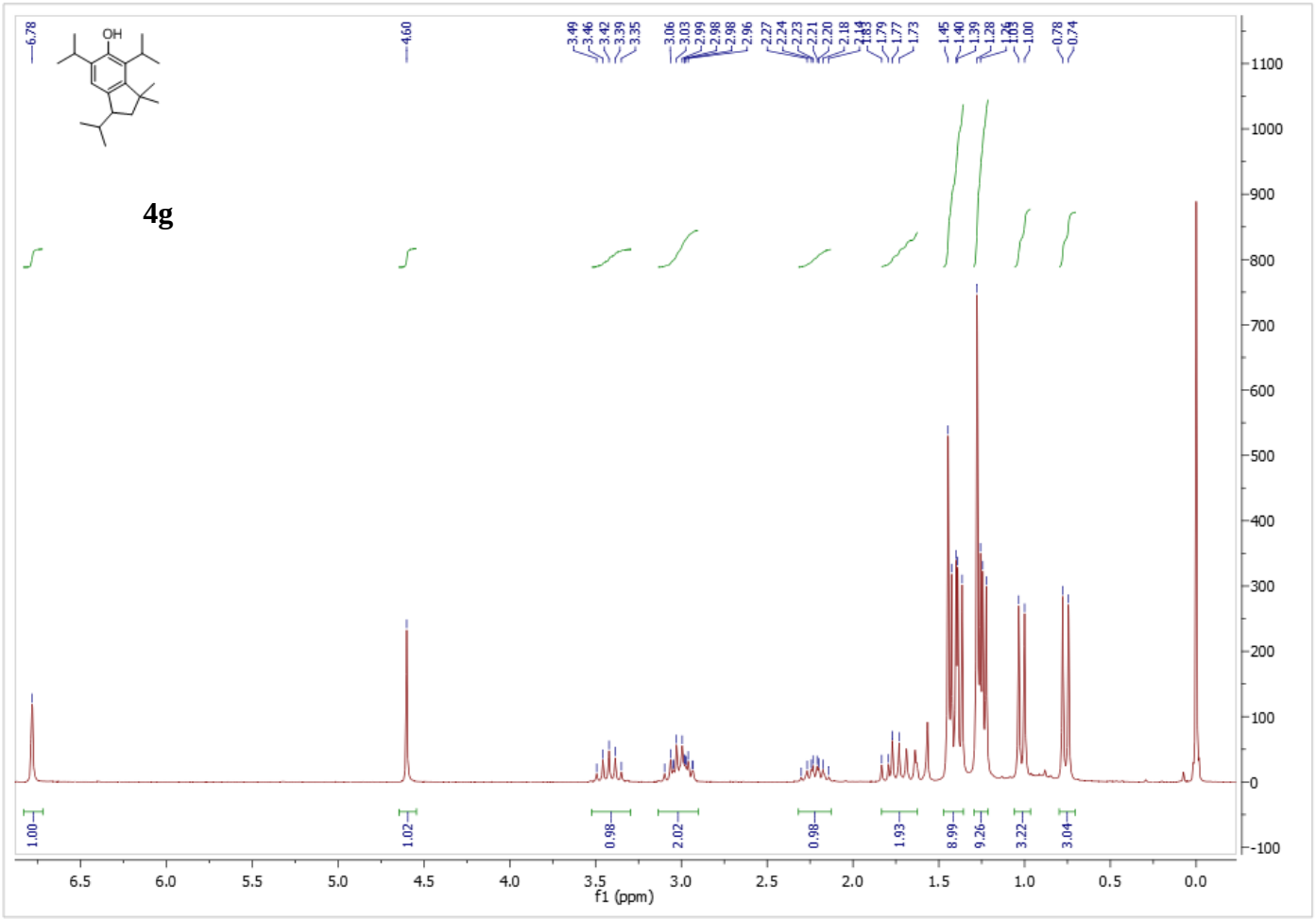

146.40
146.18
145.64
135.15
105.00
102.81
100.79
77.64
76.37
43.75
41.86
29.90
28.65
4d
f1 (ppm)

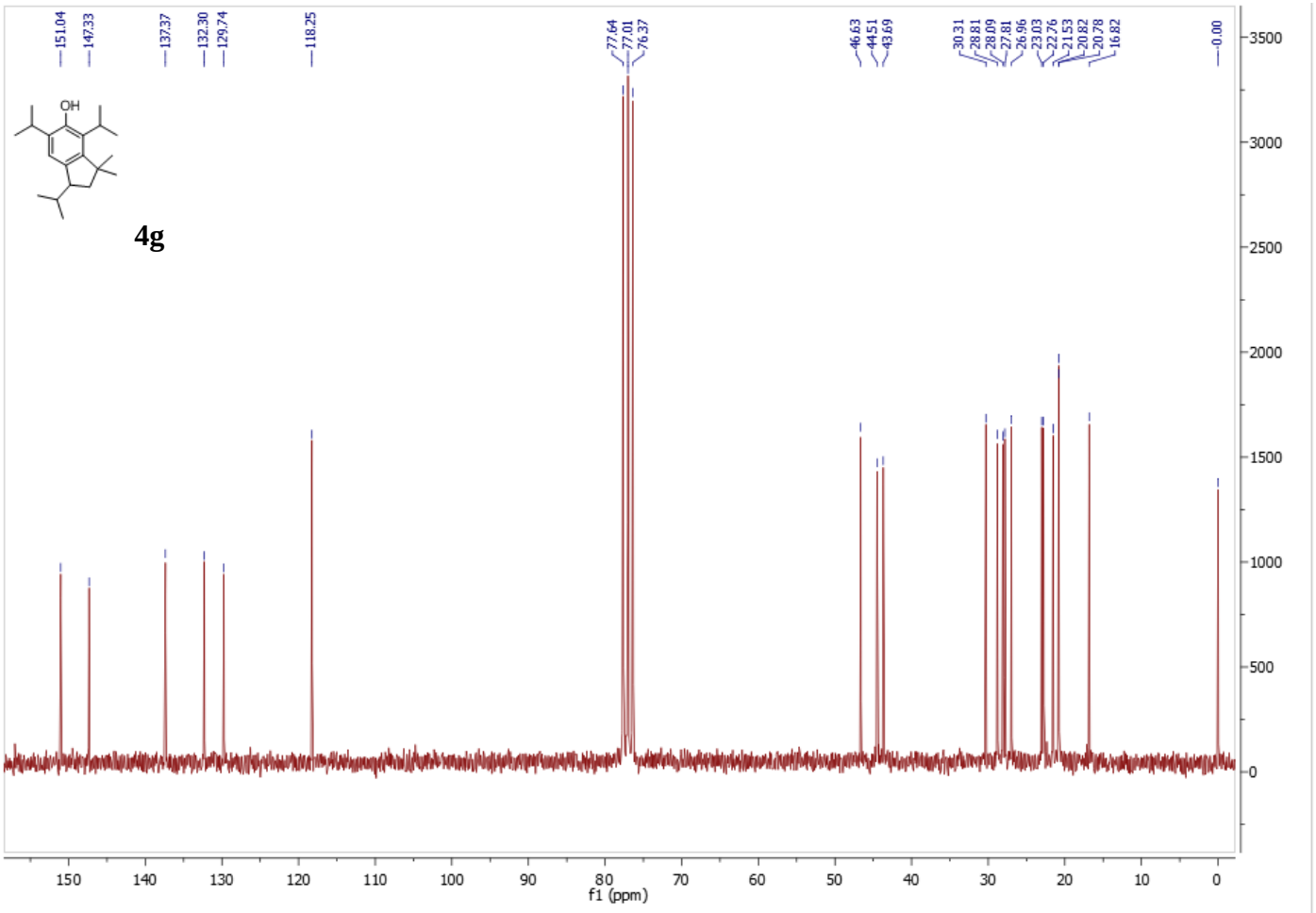

MeO
4e
7.07
7.03
6.74
6.73
6.70
6.69
6.67
6.66
3.80
3.19
3.17
3.15
3.13
3.11
3.09
2.29
2.25
2.23
2.22
2.19
2.18
2.16
2.13
1.86
1.82
1.79
1.71
1.66
1.56
1.16
1.04
1.01
0.77
0.73
1.08
1.99
3.16
0.98
1.14
1.18
2.00
3.00
3.00
3.00
3.01
f1 (ppm)

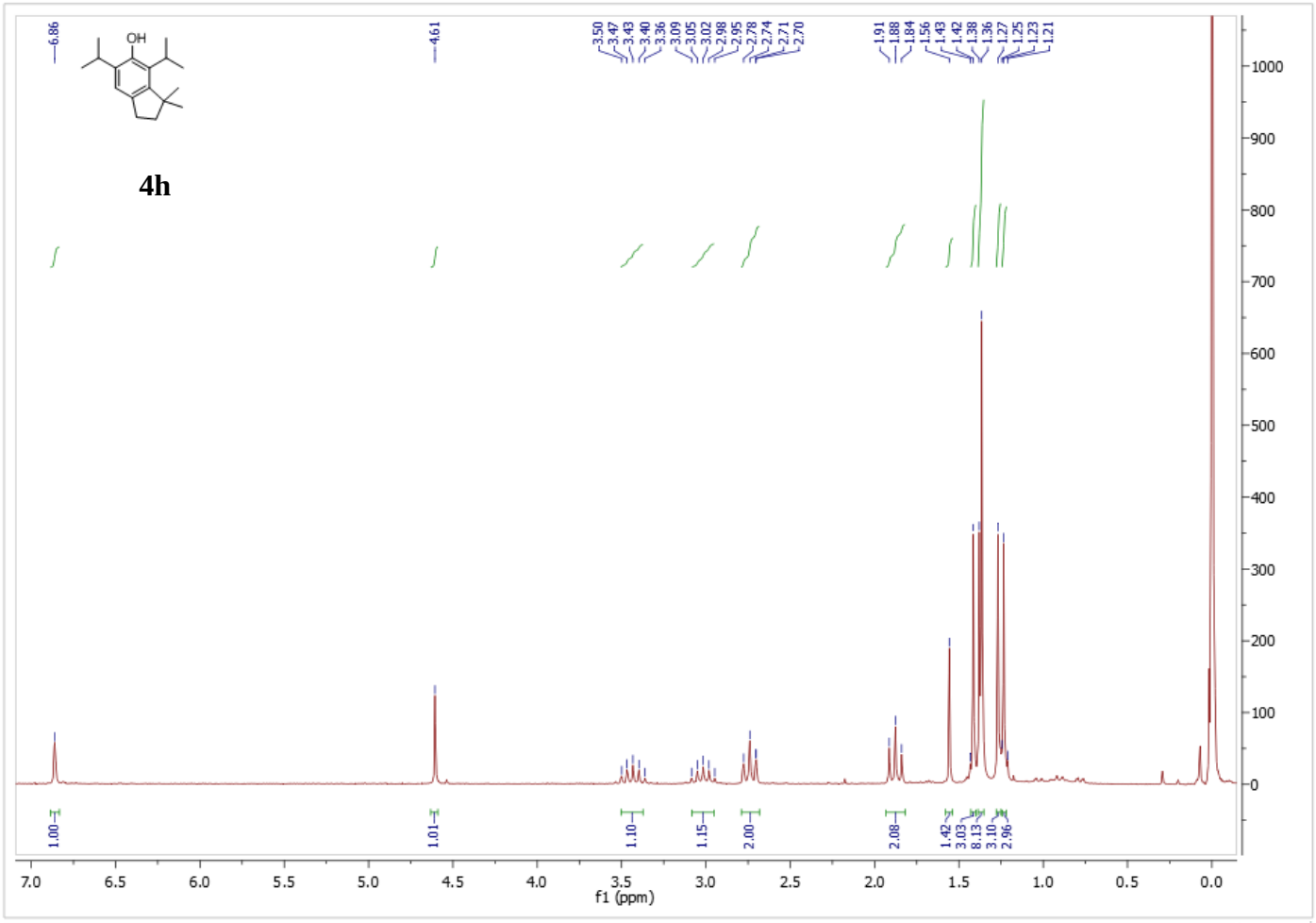

MeO
4e
158.81
154.61
136.99
124.36
111.65
107.62
77.64
77.00
76.37
55.32
47.31
42.57
42.35
29.69
29.24
28.83
21.39
17.18
f1 (ppm)


OH
4f
6.75
4.52
3.09
3.06
3.03
3.02
3.00
2.98
1.84
1.80
1.78
1.75
1.74
1.70
1.65
1.44
1.24
1.03
0.99
0.76
0.73
1.00
1.01
0.95
6.19
2.96
3.05
3.16
3.48
3.12
f1 (ppm)

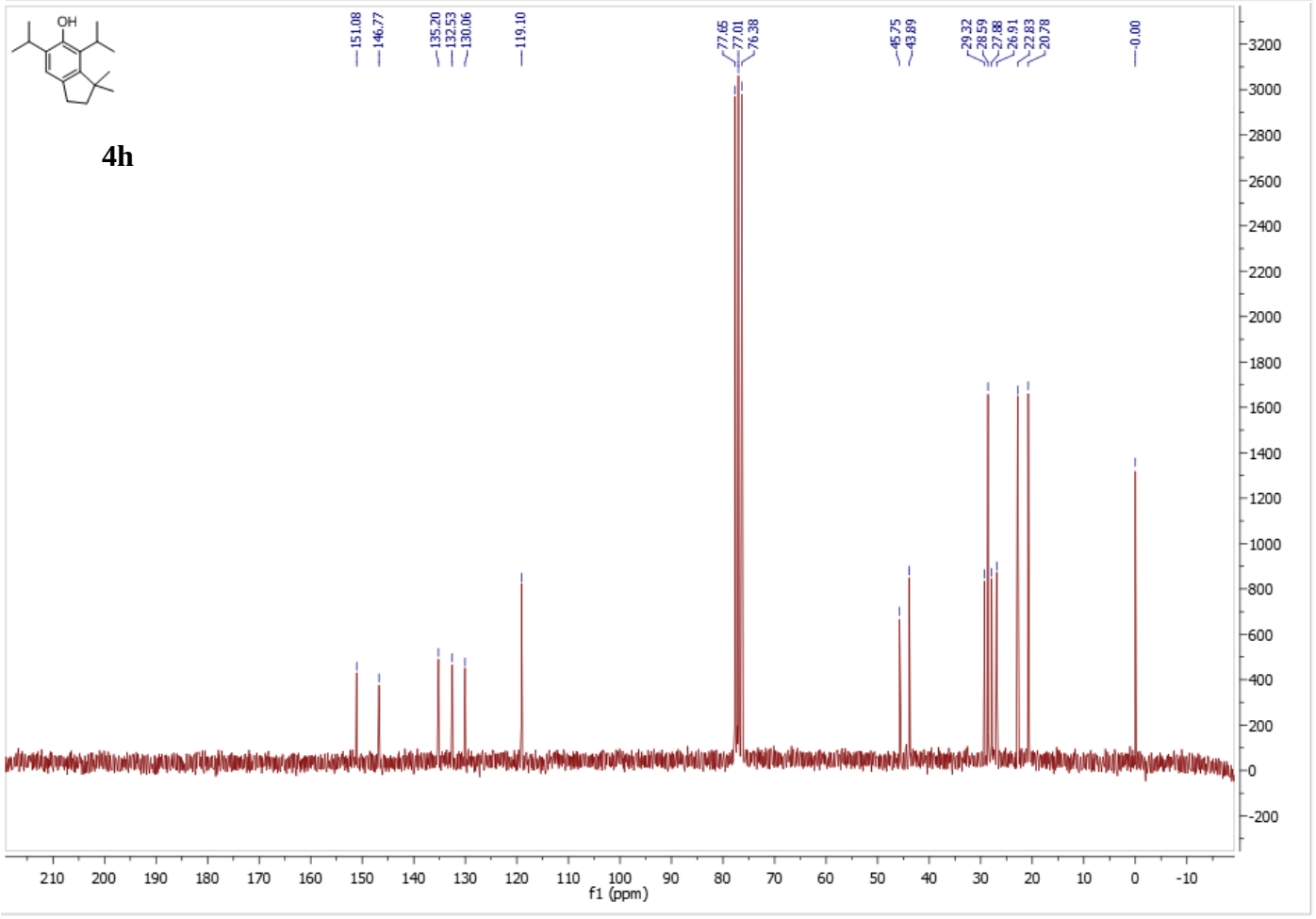

OH
4f
150.95
148.61
137.15
123.06
120.83
119.09
77.64
77.00
76.36
46.59
43.97
43.51
29.24
28.68
27.10
21.46
16.68
16.38
11.41
f1 (ppm)


OH
4g
f1 (ppm)


OH
4g
f1 (ppm)

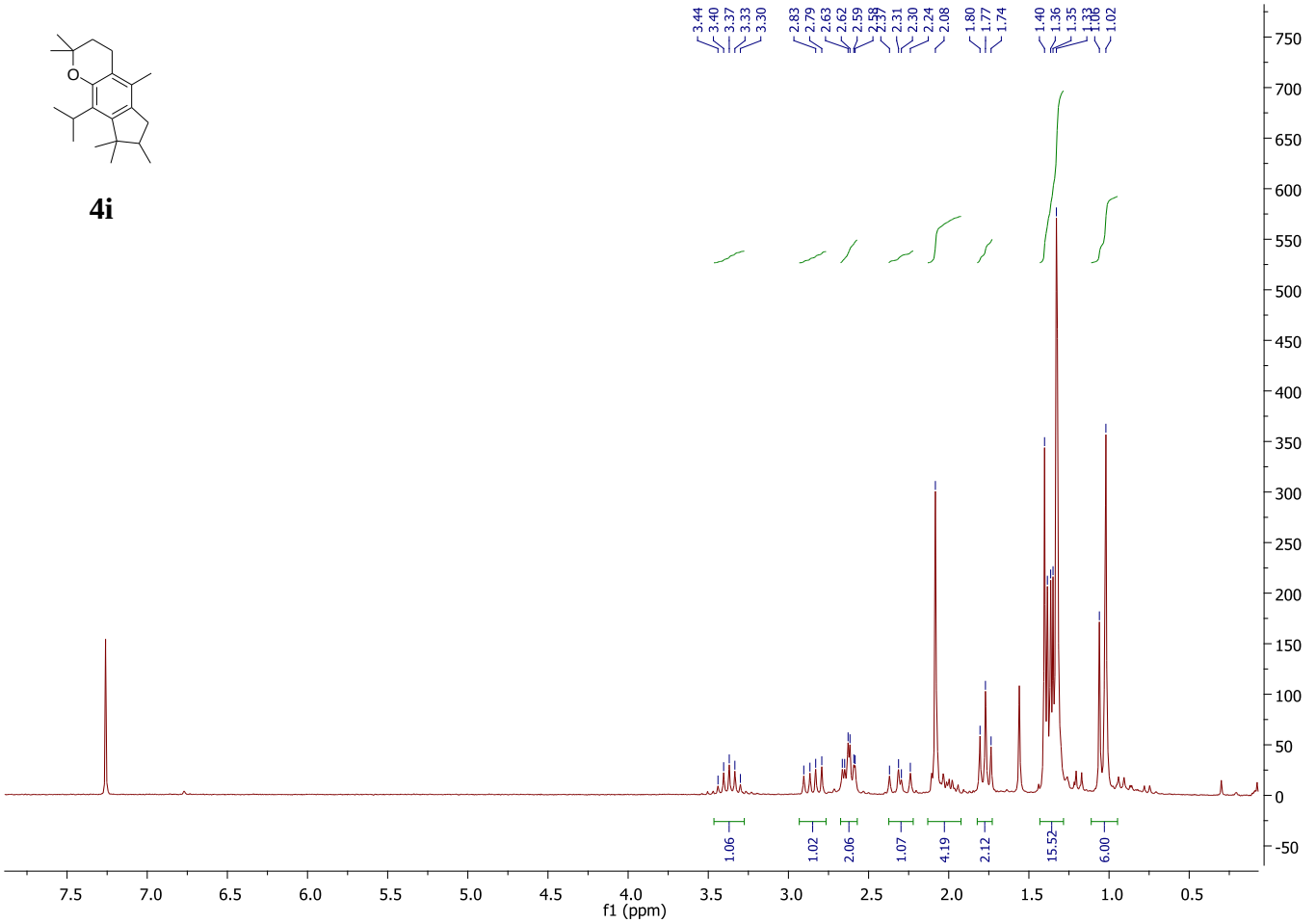

OH
6.86
4.61
3.50
3.47
3.43
3.40
3.36
3.09
3.05
3.02
2.98
2.95
2.78
2.74
2.71
2.70
1.91
1.88
1.84
1.56
1.43
1.42
1.38
1.36
1.27
1.25
1.23
1.21
1.00
1.01
1.10
1.15
2.00
2.08
1.42
3.03
8.13
3.10
2.96
f1 (ppm)

4h

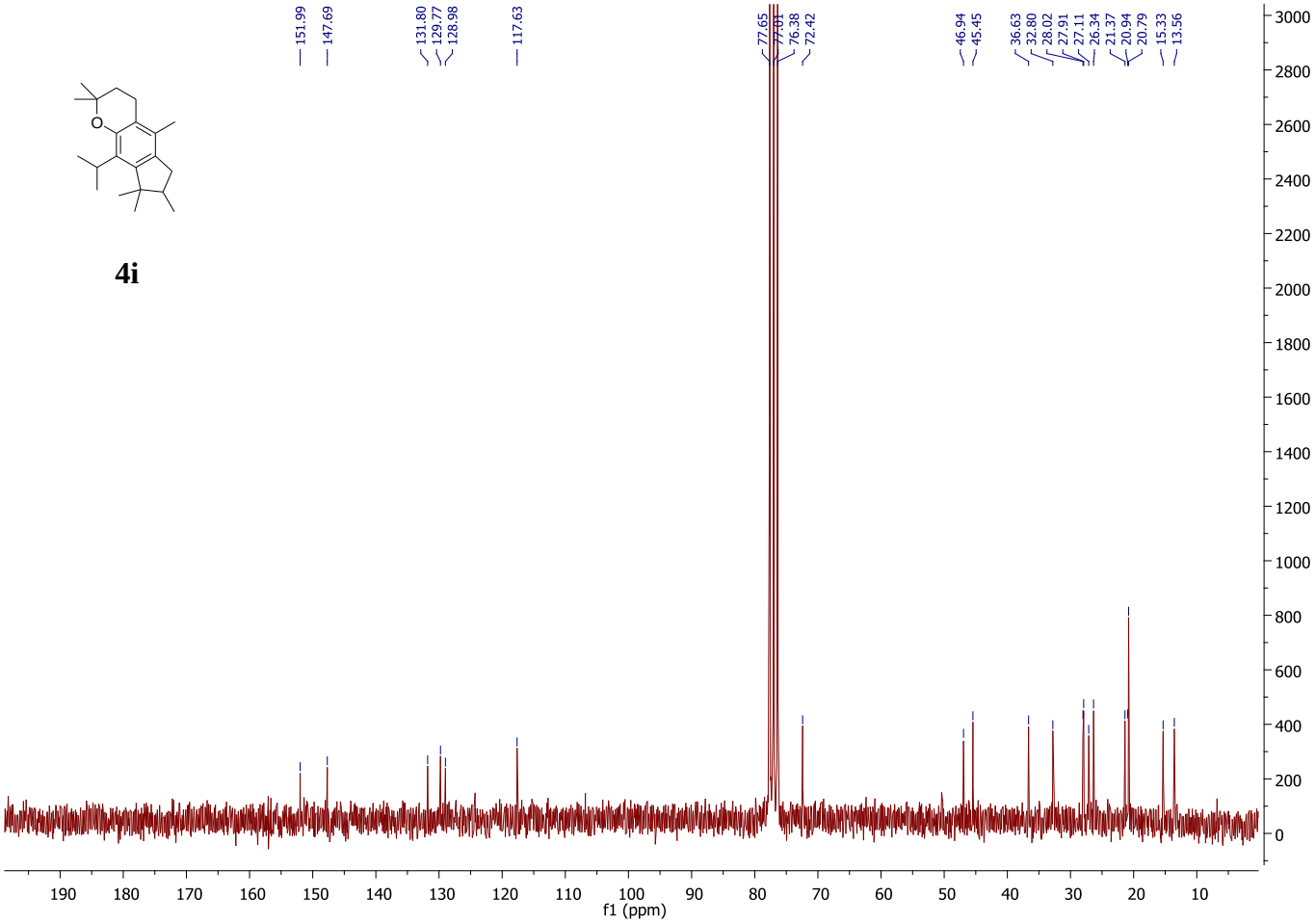

OH
151.08
146.77
135.20
132.53
130.06
119.10
77.65
77.01
76.38
45.75
43.89
29.32
28.59
27.88
26.91
22.83
20.78
0.00
f1 (ppm)

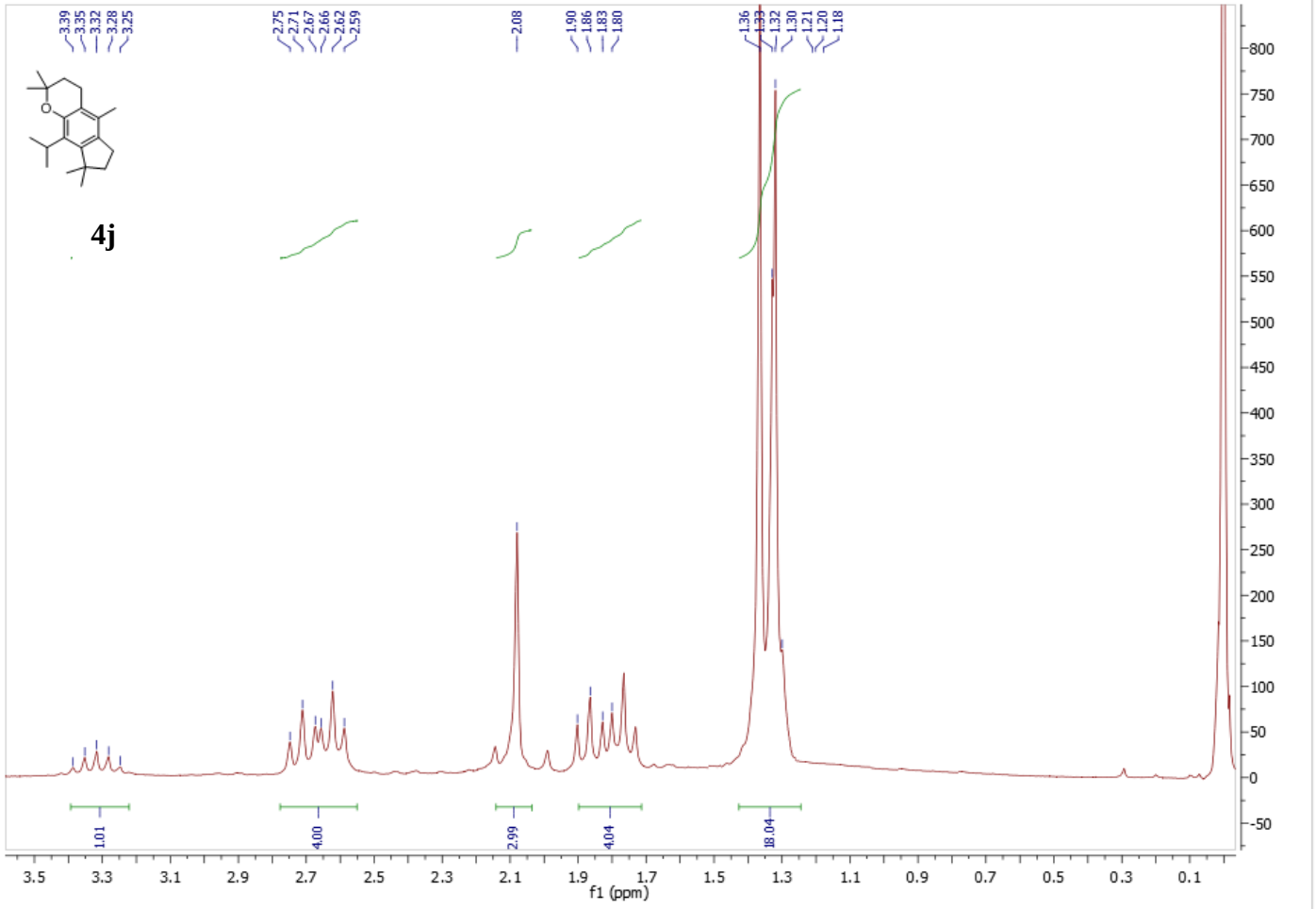
4h

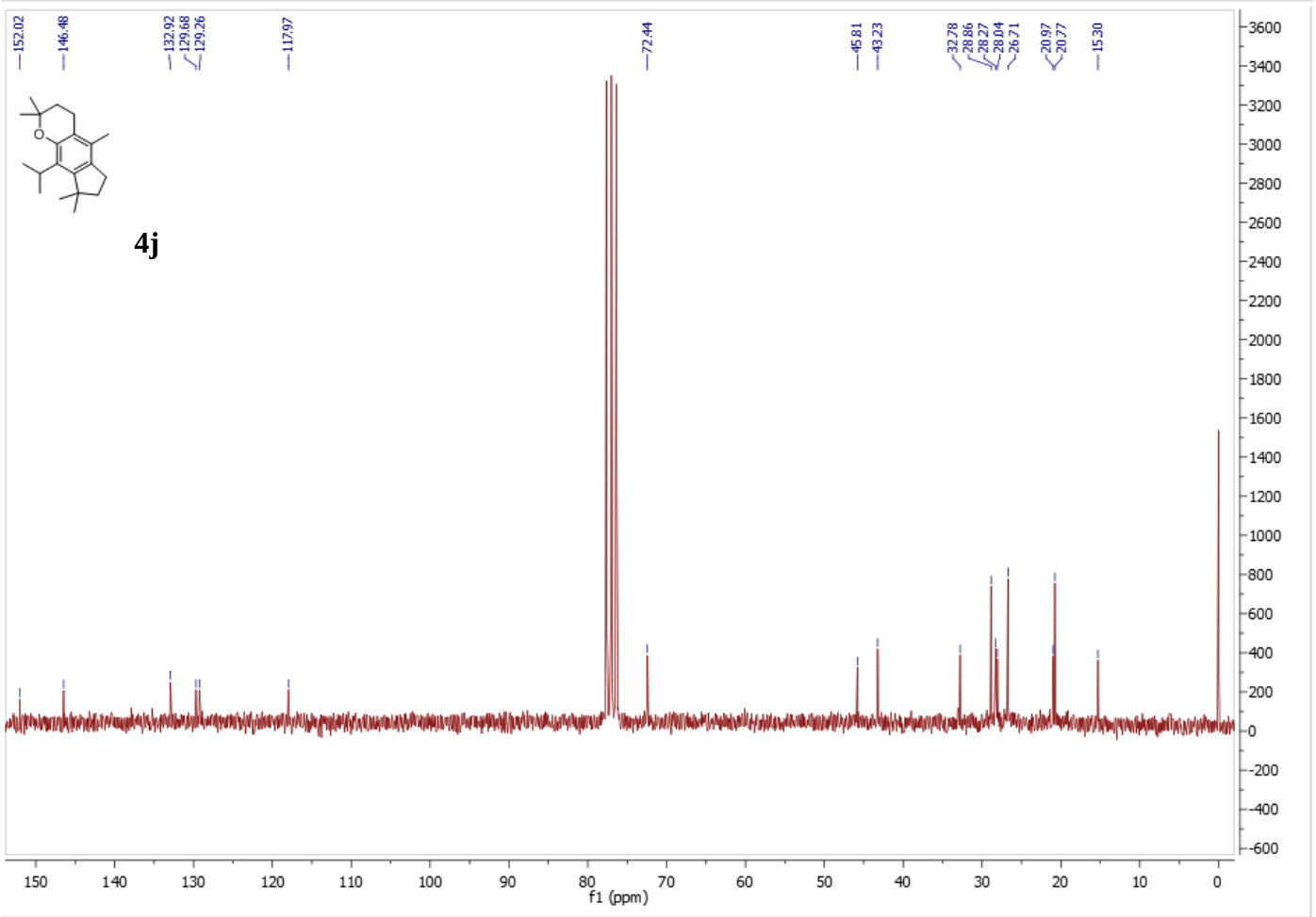
4i


3.44
3.40
3.37
3.33
3.30
2.83
2.79
2.63
2.62
2.59
2.31
2.30
2.24
2.08
1.80
1.77
1.74
1.40
1.36
1.35
1.33
1.08
1.02
1.06
1.02
2.06
1.07
4.19
2.12
15.52
6.00
f1 (ppm)

4i


151.99
147.69
131.80
129.77
128.98
117.63
77.65
77.01
76.38
72.42
46.94
45.45
36.63
32.80
28.02
27.91
27.11
26.34
21.37
20.94
20.79
15.33
13.56
f1 (ppm)


3.39
3.35
3.32
3.28
3.25
2.75
2.71
2.67
2.66
2.62
2.59
2.08
1.90
1.86
1.83
1.80
1.36
1.33
1.32
1.30
1.21
1.20
1.18
4j
1.01
4.00
2.99
4.04
18.04
f1 (ppm)


152.02
146.48
132.92
129.68
129.26
117.97
72.44
45.81
43.23
32.78
28.86
28.27
28.04
26.71
20.97
20.77
15.30
4j
f1 (ppm)