SUPPORTING INFORMATION

Sustainable base-mediated chemical upcycling of waste polycarbonates to fine chemicals

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1. General Information

Unless stated otherwise, all reactions were carried out under argon in a Schlenk line tecnique. Anhydrous grade solvents were used as such received from the Spectrochem. All the reactions were monitored by analytical thin layer chromatography (TLC) using commercial aluminium sheets precoated with silica gel. Column chromatography was conducted on silica gel (Merck, 100-200 mesh). All other chemicals were received and used as such from the commercial sources. All acids were purchased from Spectrochem Pvt Limited (Purity-99%(GC)). PPC polymer was purchased from Sigma Aldrich. Solvents were purchased from Spectrochem Pvt. Ltd. NMR Solvents are purchased from Sigma-Aldrich. NMR spectra were recorded on Bruker Avance 400, 500 MHz instruments. NMR data have been reported as follows: chemical shift (δ) in ppm, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, and m = multiplet), coupling constant (J) in Hz. Mass spectra were recorded on Thermo Scientific QExactive mass spectrometer, the column specification is Hypersil gold C18 column 150 × 4.6 mm diameter 8 µm particle size mobile phase used in acetonitrile and methanol. OMNISEC RESOLVE and OMNISEC REVEAL of Malvern Panalytical Instrument were used to determine the number average molecular weight (Mn), weight average molecular weights (Mw), and polydispersities (Mw/Mn). OMNISEC RESOLVE is a combined pump, degasser, autosampler and column oven for mobile phase delivery and sample injection. OMNISEC REVEAL is an integrated multi-detector. The Columns were eluted with THF at 30 °C at 1.0mL/min, column T6000 M General Mixed. The calibration curve was obtained using 12 monodisperse polystyrene standards. X-ray diffraction (WXRD) measurements were performed on a Rigaku powder diffractometer (Rigaku, Japan) with Cu KR radiation. The tube voltage was 45 kV, and the current was 40 mA. The XRD diffraction patterns were taken over 2 h in a range of 10-90° at a scan speed of 2°/min. HRMS were recorded on Thermo Scientific Q-Exactive mass spectrometer, the column specification is Hypersil gold C18 column 150 × 4.6 mm diameter 8 µm particle size, Accela 1250 pump, mobile phase used is methanol. The required sample for the TGA analysis is 3-4 mg. TGA analysis was performed using a Diamond TGA instrument. Approximately 2.5–3 mg of the sample was heated from 30 to 700 °C at a rate of 10 °C/min under a nitrogen atmosphere with a flow rate of 20 mL/min.

2. Preparation of waste PC-BPA samples for experiment

The used PC-BPAs were obtained from compact discs, safety goggles, a sunroof, a helmet, a scooty light panel, a mixer lid, and an LED Bulb. All samples were first cleaned of any external contamination by washing the surface thoroughly with soap and water, followed by acetone. The Compact disc was then cut into small pieces with scissors. Other waste PC-BPA samples were also followed the same procedure to remove impurities and additives.

3. General procedure for waste PC-BPA to esters

An oven-dried Schlenk tube equipped with a Teflon-coated magnetic stir bar was charged under an argon atmosphere with waste PC-BPA (334 mg, 1.3 mmol, 2 equiv. based on monomer unit molecular weight of 254), acid (100 mg, 0.65 mmol, 1 equiv.), and dimethyl

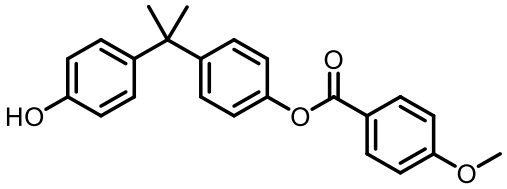
aminopyridine (DMAP) (80 mg, 0.65 mmol, 1 equiv.), followed by DMSO (2 mL). The Schlenk tube was sealed and placed in a preheated oil bath at 140 °C. After the reaction, the solvent was evaporated under reduced pressure, and the crude reaction mixture was purified by flash column chromatography (20-25 % EtOAc: petether) on silica gel, yielding di-aryl ester as the major product and di-aryl diester as the minor product.

4. General procedure for PPC to esters

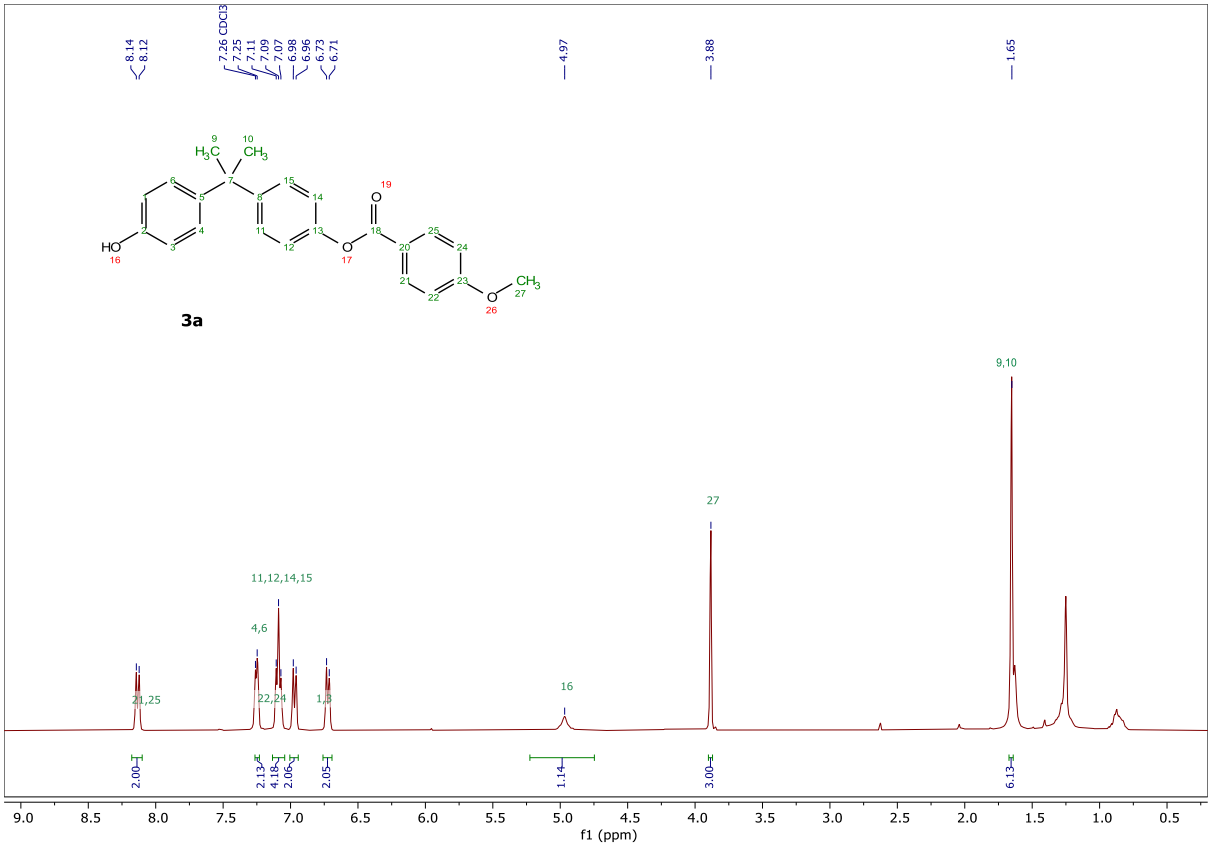
An oven-dried Schlenk tube equipped with a Teflon-coated magnetic stir bar was charged under an argon atmosphere with PPC (132 mg, 1.3 mmol, 2 equiv. based on monomer unit molecular weight of 102), acid (100 mg, 0.65 mmol, 1 equiv.), and dimethyl aminopyridine (DMAP) (80 mg, 0.65 mmol, 1 equiv.), followed by DMSO (2 mL). The Schlenk tube was sealed and placed in a preheated oil bath at 140 °C. After the reaction, the solvent was evaporated under reduced pressure, and the crude reaction mixture was purified by flash column chromatography (20% EtOAc:petether) on silica gel, yielding di-aryl ester as the major product and di-aryl di-ester as the minor product.

5. Analytical data of esters

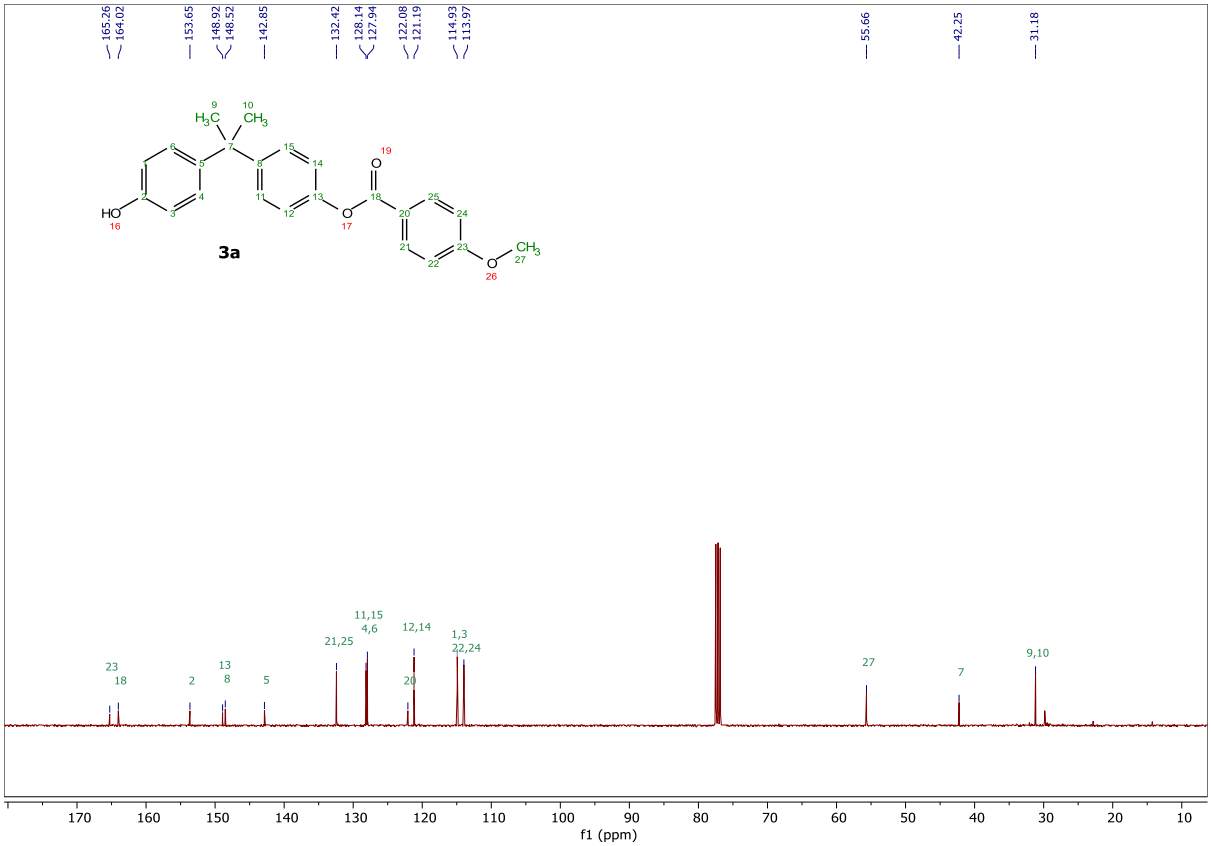
4-(2-(4-hydroxyphenyl)propan-2-yl)phenyl 4-methoxybenzoate (3a): Compound **3a** was



prepared according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 80% yield (191 mg).**^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.13 (d, *J* = 8.4 Hz, 2H), 7.26 – 7.23 (m, 2H), 7.09 (t, *J* = 6.9 Hz, 4H), 6.97 (d, *J* = 8.3 Hz, 2H), 6.72 (d, *J* = 8.0 Hz, 2H), 4.97 (s, 1H), 3.88 (s, 3H), 1.65 (s, 6H).

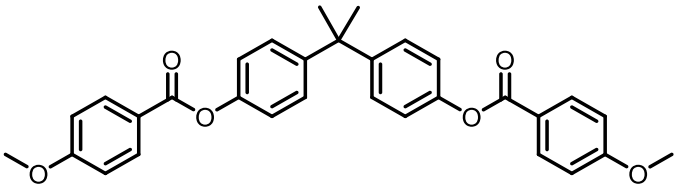


^{13}C NMR (101 MHz, $CDCl_3$) δ 165.26, 164.02, 153.65, 148.92, 148.52, 142.85, 128.14, 127.94, 122.08, 121.19, 115.97, 114.93, 113.97, 55.66, 42.25, 31.18.

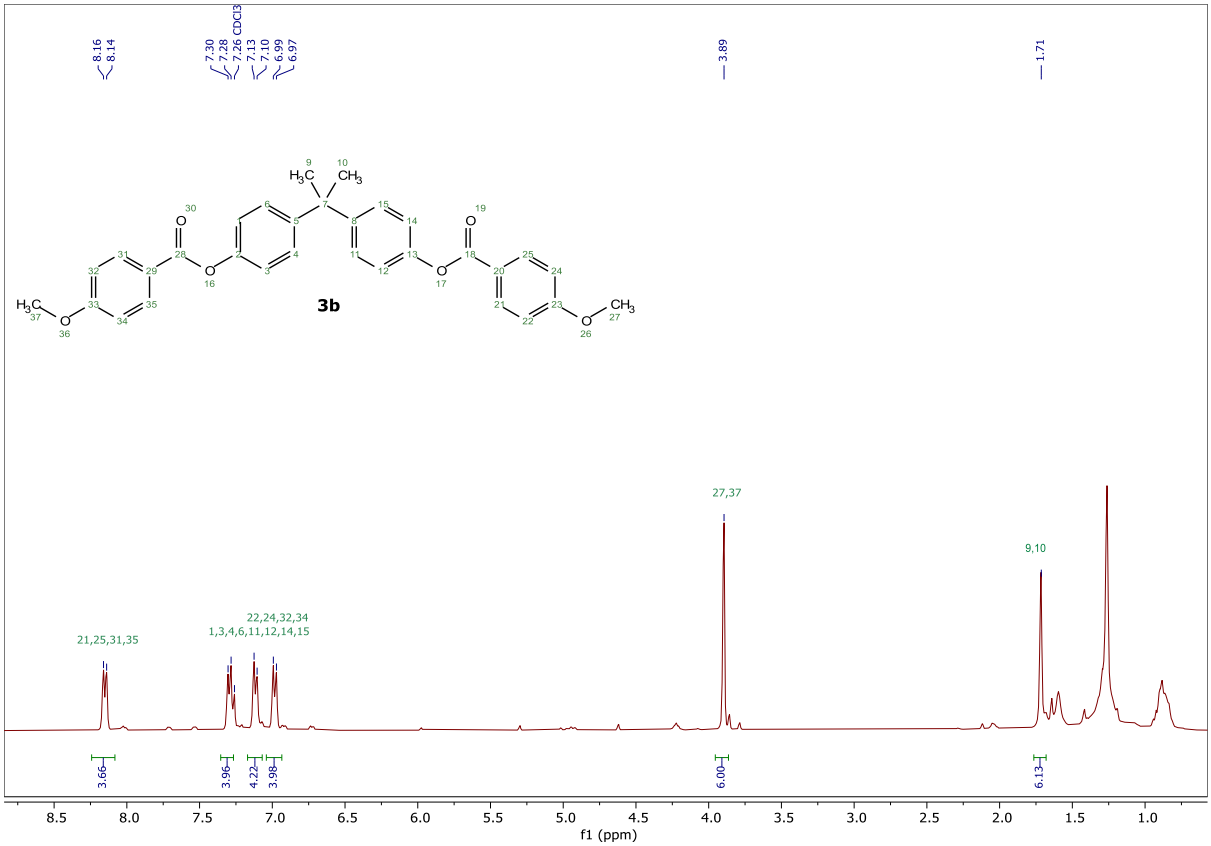


HRMS: m/z (ESI) Calculated for $C_{23}H_{23}O_4$ $[M+H]^+$: 363.1596; found; 363.1591.

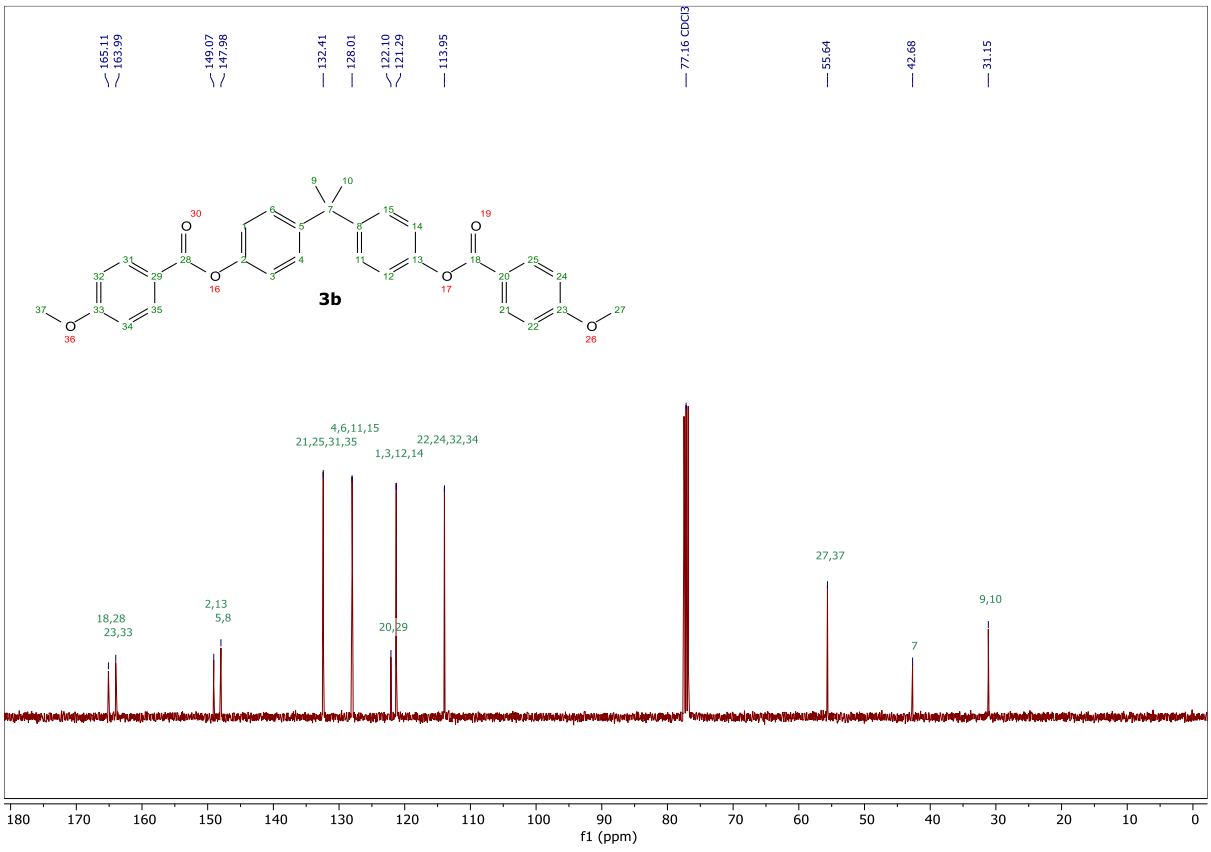
propane-2,2-diylbis(4,1-phenylene) bis(4-methoxybenzoate) (3b): Compound **3b** was



prepared according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid, in 18 % yield (59 mg). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.15 (d, *J* = 8.6 Hz, 4H), 7.29 (d, *J* = 8.5 Hz, 4H), 7.11 (d, *J* = 8.3 Hz, 4H), 6.98 (d, *J* = 8.5 Hz, 4H), 3.89 (s, 6H), 1.72 (s, 6H).

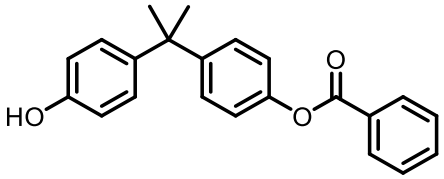


^{13}C NMR (101 MHz, $CDCl_3$) δ 165.11, 163.99, 149.07, 147.98, 132.41, 128.01, 122.10, 121.29, 113.95, 55.64, 42.68, 31.15.



HRMS: m/z (ESI) Calculated for $C_{31}H_{29}O_6$ $[M+H]^+$: 497.1964; found; 497.1959.

4-(2-(4-hydroxyphenyl)propan-2-yl)phenyl benzoate (4a): Compound **4a** was prepared

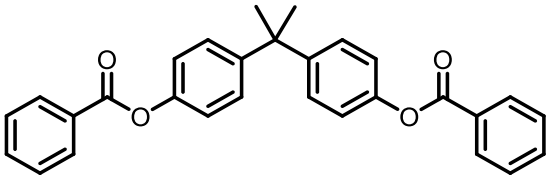


according to the general procedure (3) and purified by flash column chromatography (25% EtOAc/petether), affording a white solid in 78% yield (213 mg). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.17 (d, *J* = 7.4 Hz, 2H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 7.7 Hz, 2H), 7.24 (t, *J* = 5.8 Hz, 2H), 7.08 (d, *J* = 8.6 Hz, 4H), 6.71 (d, *J* = 8.6 Hz, 2H), 5.03 (s, 1H), 1.64 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.59, 153.68, 148.81, 148.79, 142.77, 133.71, 130.30, 129.76, 128.70, 128.12, 128.00, 121.10, 114.96, 42.26, 31.17.

HRMS: m/z (ESI) Calculated for $C_{22}H_{21}O_3$[M+H]$^+$: 333.1491; found; 333.1485.

propane-2,2-diylbis(4,1-phenylene) dibenzoate (4b): Compound **4b** was prepared according to

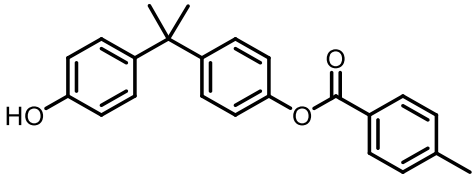


the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 17% yield (61 mg). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.21 (dd, *J* = 5.2, 3.3 Hz, 4H), 7.68 – 7.60 (m, 2H), 7.52 (t, *J* = 7.7 Hz, 4H), 7.36 – 7.28 (m, 4H), 7.19 – 7.10 (m, 4H), 1.73 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.39, 148.99, 148.14, 133.68, 130.30, 129.78, 128.69, 128.07, 121.24, 42.71, 31.14.

HRMS: m/z (ESI) Calculated for $C_{29}H_{25}O_4$ $[M+H]^+$: 437.1753; found; 437.1747.

4-(2-(4-hydroxyphenyl)propan-2-yl)phenyl 4-methylbenzoate (5a): Compound **5a** was

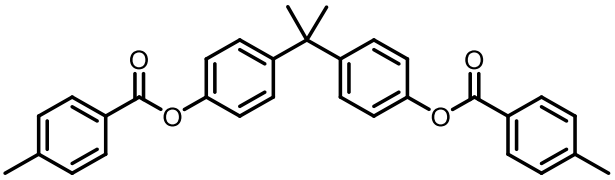


prepared according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 74% yield (184 mg).**^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.07 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.29 – 7.25 (m, 2H), 7.11 (d, *J* = 6.4 Hz, 2H), 7.09 (d, *J* = 6.3 Hz, 2H), 6.73 (d, *J* = 8.6 Hz, 2H), 4.73 (s, 1H), 2.45 (s, 3H), 1.66 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.55, 153.58, 148.90, 148.56, 144.51, 142.93, 130.34, 129.42, 128.16, 127.96, 127.03, 121.16, 114.93, 42.27, 31.18, 21.90.

HRMS: m/z (ESI) Calculated for $C_{23}H_{23}O_3$ $[M+H]^+$: 347.1647; found; 347.1642.

propane-2,2-diylbis(4,1-phenylene) bis(4-methylbenzoate) (5b): Compound **5b** was prepared according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 15 % yield (52 mg).

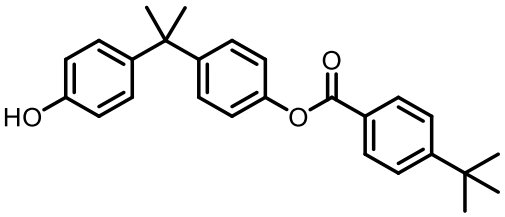


^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.1 Hz, 4H), 7.31 (d, J= 8.3, 4H), 7.29 (d, *J* = 2.1 Hz, 4H), 7.12 (d, *J* = 8.6 Hz, 4H), 2.45 (s, 6H), 1.72 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.46, 149.06, 148.05, 144.49, 130.35, 129.41, 128.05, 127.05, 121.27, 42.71, 31.16, 21.90.

HRMS: m/z (ESI) Calculated for $C_{31}H_{29}O_4$ $[M+H]^+$: 465.2066; found; 465.2060.

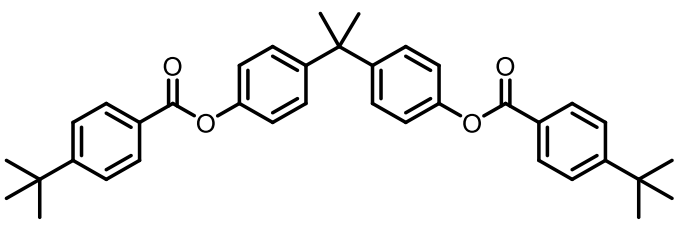
4-(2-(4-hydroxyphenyl)propan-2-yl)phenyl 4-(*tert*-butyl)benzoate (6a): Compound **(6a)** was prepared according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 74% yield (162 mg). **^{1}H NMR (400 MHz, CDCl3)** δ 8.12 (d, *J* = 8.5 Hz, 2H), 7.51 (d, *J* = 8.5 Hz, 2H), 7.29 – 7.24 (m, 2H), 7.08 (d, *J* = 8.8 Hz, 4H), 6.76 – 6.66 (m, 2H), 5.40 (s, 1H), 1.65 (s, 6H), 1.36 (s, 9H).



^{13}C NMR (101 MHz, $CDCl_3$) δ 165.56, 157.53, 153.66, 148.88, 148.61, 142.82, 130.21, 128.13, 127.97, 126.95, 125.70, 121.15, 114.94, 42.26, 35.33, 31.25, 31.18.

HRMS: m/z (ESI) Calculated for $C_{26}H_{29}O_3$ $[M+H]^+$: 389.2177; found; 389.2111.

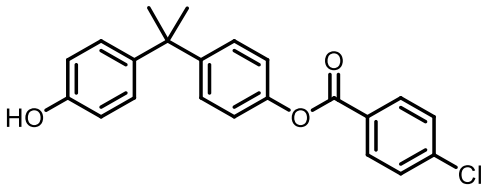
propane-2,2-diylbis(4,1-phenylene) bis(4-(*tert*-butyl)benzoate) (6b): Compound **6b** was prepared according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 14% yield (44 mg). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.13 (d, *J* = 8.4 Hz, 4H), 7.53 (d, *J* = 8.4 Hz, 4H), 7.30 (d, *J* = 8.6 Hz, 4H), 7.12 (d, *J* = 8.6 Hz, 4H), 1.72 (s, 6H), 1.37 (s, 18H).



^{13}C NMR (101 MHz, $CDCl_3$) δ 165.40, 157.49, 149.07, 148.06, 130.22, 128.04, 127.00, 125.69, 121.29, 42.71, 35.34, 31.27, 31.16.

HRMS: m/z (ESI) Calculated for $C_{37}H_{41}O_3$ $[M+H]^+$: 549.3005; found; 549.3001.

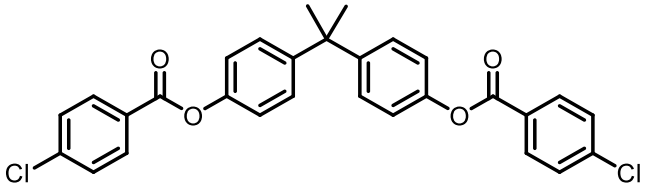
4-(2-(4-hydroxyphenyl)propan-2-yl)phenyl 4-chlorobenzoate (7a): Compound **7a** was prepared according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 68% yield (160 mg). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.12 (d, *J* = 8.3 Hz, 2H), 7.47 (d, *J* = 8.3 Hz, 2H), 7.27 (d, *J* = 8.6 Hz, 2H), 7.15 – 7.03 (m, 4H), 6.73 (d, *J* = 8.4 Hz, 2H), 5.03 (s, 1H), 1.66 (s, 6H).



^{13}C NMR (101 MHz, $CDCl_3$) δ 164.70, 153.67, 148.93, 148.62, 142.73, 140.25, 131.67, 129.08, 128.20, 128.12, 128.04, 121.00, 114.96, 42.27, 31.15.

HRMS: m/z (ESI) Calculated for $C_{22}H_{20}ClO_3$ $[M+H]^+$: 367.1101; found; 367.1095.

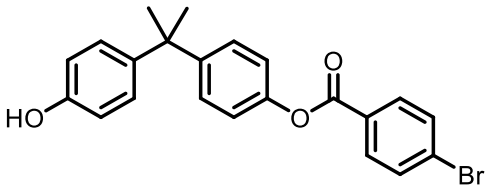
propane-2,2-diylbis(4,1-phenylene) bis(4-chlorobenzoate) (7b) : Compound **7b** was prepared according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 43% yield (42 mg). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.13 (d, *J* = 8.5 Hz, 4H), 7.49 (d, *J* = 8.5 Hz, 4H), 7.30 (d, *J* = 8.7 Hz, 4H), 7.12 (d, *J* = 8.7 Hz, 4H), 1.72 (s, 6H).



^{13}C NMR (101 MHz, $CDCl_3$) δ 164.56, 148.83, 148.28, 140.25, 131.68, 129.09, 128.23, 128.11, 121.17, 42.75, 31.13.

HRMS: m/z (ESI) Calculated for $C_{29}H_{23}Cl_2O_4$ $[M+H]^+$: 505.0973; found; 505.0967.

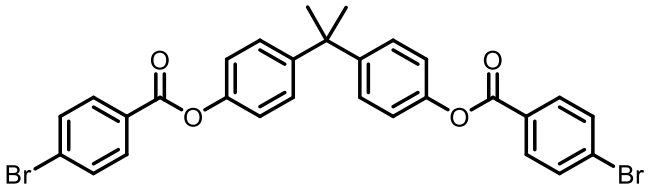
4-(2-(4-hydroxyphenyl)propan-2-yl)phenyl 4-bromobenzoate (8a): Compound **8a** was prepared according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 73% yield (149 mg). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.02 (d, *J* = 8.6 Hz, 2H), 7.62 (d, *J* = 8.6 Hz, 2H), 7.23 (d, *J* = 2.4 Hz, 2H), 7.08 (d, *J* = 2.2 Hz, 2H), 7.06 (d, *J* = 2.2 Hz, 2H), 6.75 – 6.67 (m, 2H), 5.01 (s, 1H), 1.64 (s, 6H).



^{13}C NMR (101 MHz, $CDCl_3$) δ 164.86, 153.66, 148.95, 148.60, 142.71, 132.08, 131.78, 128.96, 128.65, 128.11, 128.04, 120.98, 114.96, 42.27, 31.15.

HRMS: m/z (ESI) Calculated for $C_{22}H_{20}BrO_3$ $[M+H]^+$: 411.0596; found; 411.0591.

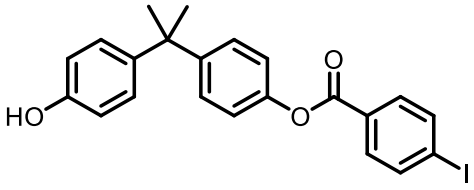
propane-2,2-diylbis(4,1-phenylene) bis(4-bromobenzoate) (8b): Compound **8b** was prepared according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 14% yield (42 mg). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.05 (d, *J* = 8.5 Hz, 4H), 7.65 (d, *J* = 8.5 Hz, 4H), 7.30 (d, *J* = 8.7 Hz, 4H), 7.12 (d, *J* = 8.7 Hz, 4H), 1.72 (s, 6H).



^{13}C NMR (101 MHz, $CDCl_3$) δ 164.70, 163.92, 148.82, 148.28, 132.09, 131.79, 128.94, 128.69, 128.11, 42.75, 31.13.

HRMS: m/z (ESI) Calculated for $C_{29}H_{23}Br_2O_4$ $[M+H]^+$: 592.9963; found; 592.9958.

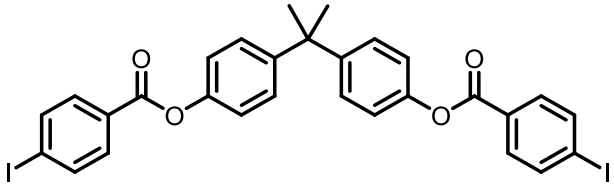
4-(2-(4-hydroxyphenyl)propan-2-yl)phenyl 4-iodobenzoate (9a): Compound **9a** was prepared according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 75% yield (139mg). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.93 – 7.84 (m, 4H), 7.26 (s, 2H), 7.10 (t, *J* = 8.8 Hz, 4H), 6.74 (d, *J* = 8.6 Hz, 2H), 4.70 (s, 1H), 1.67 (s, 6H).



^{13}C NMR (101 MHz, $CDCl_3$) δ 165.11, 153.62, 148.92, 148.59, 142.74, 138.09, 131.65, 129.21, 128.11, 128.04, 120.98, 114.95, 101.72, 42.26, 31.15.

HRMS: m/z (ESI) Calculated for $C_{22}H_{20}IO_3$ $[M+H]^+$: 459.0457; found; 459.0452.

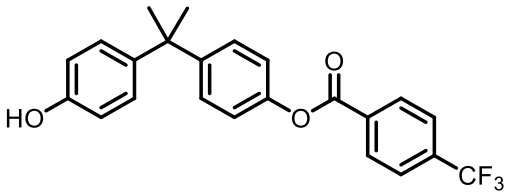
propane-2,2-diylbis(4,1-phenylene) bis(4-iodobenzoate) (9b): Compound **9b** was prepared according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 13% yield (37 mg). **^{1}H NMR (400 MHz, CDCl3)** δ 7.92 – 7.85 (m, 8H), 7.32 – 7.27 (m, 4H), 7.14 – 7.09 (m, 4H), 1.72 (s, 6H).



^{13}C NMR (101 MHz, $CDCl_3$) δ 164.94, 148.81, 148.28, 138.10, 131.67, 129.26, 128.11, 121.15, 101.68, 42.74, 31.13.

HRMS: m/z (ESI) Calculated for $C_{29}H_{23}I_2O_4$ $[M+H]^+$: 688.9686; found; 688.9680.

4-(2-(4-hydroxyphenyl)propan-2-yl)phenyl 4-(trifluoromethyl)benzoate (10a): Compound

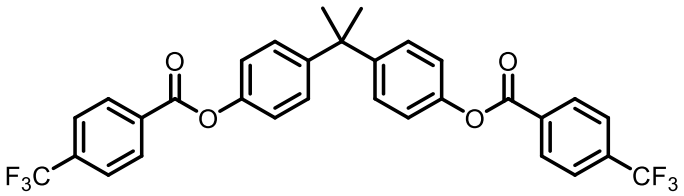


10a was prepared according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 67% yield (142 mg). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.31 (d, *J* = 8.0 Hz, 2H), 7.78 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.5 Hz, 2H), 7.12 (d, *J* = 8.4 Hz, 4H), 6.75 (d, *J* = 8.4 Hz, 2H), 4.81 (s, 1H), 1.68 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.30, 153.63, 149.12, 148.54, 142.77, 135.31, 134.99, 133.04, 130.70, 128.14, 128.11, 125.74, 120.94, 114.97, 77.16, 42.30, 31.15.**^{19}F NMR (376 MHz, $CDCl_3$)** δ -63.14 (s).

HRMS: m/z (ESI) Calculated for $C_{23}H_{20}F_3O_3$ $[M+H]^+$: 401.1365; found; 401.1359.

propane-2,2-diylbis(4,1-phenylene) bis(4-(trifluoromethyl)benzoate) (10b): Compound **10b**

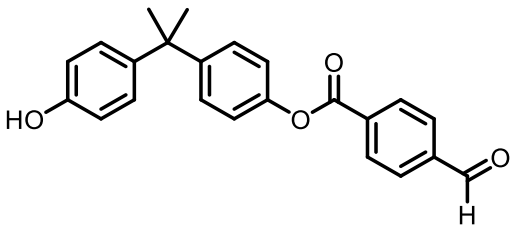


was prepared according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 11% yield (34 mg). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.32 (d, *J* = 8.1 Hz, 4H), 7.78 (d, *J* = 8.2 Hz, 4H), 7.32 (d, *J* = 8.7 Hz, 4H), 7.15 (d, *J* = 8.7 Hz, 4H), 1.73 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.21, 148.75, 148.45, 135.01, 134.52, 133.04, 130.71, 128.18, 125.75, 121.12, 77.16, 42.79, 31.12.**^{19}F NMR (376 MHz, $CDCl_3$)** δ -63.16. (s)

HRMS: m/z (ESI) Calculated for $C_{31}H_{23}F_6O_4$ $[M+H]^+$: 573.1501; found; 573.1496.

4-(2-(4-hydroxyphenyl)propan-2-yl)phenyl 4-formylbenzoate (11a): Compound **11a** was

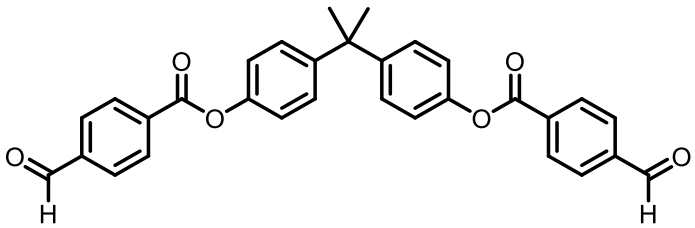


prepared according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in yield 71% (171 mg). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 10.14 (s, 1H), 8.35 (d, *J* = 7.7 Hz, 2H), 8.02 (d, *J* = 7.6 Hz, 2H), 7.29 (d, *J* = 8.1 Hz, 2H), 7.12 (d, *J* = 7.7 Hz, 4H), 6.75 (d, *J* = 8.0 Hz, 2H), 4.86 (s, 1H), 1.67 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 191.62, 164.31, 153.53, 148.98, 148.44, 142.62, 139.54, 134.64, 130.77, 129.66, 128.01, 127.97, 120.79, 114.84, 42.17, 31.03.

HRMS: m/z (ESI) Calculated for $C_{23}H_{21}O_4$ $[M+H]^+$: 361.1440; found; 361.1434.

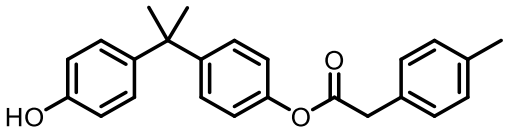
propane-2,2-diylbis(4,1-phenylene) bis(4-formylbenzoate) (11b): Compound **11b** was prepared according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 12% yield (40 mg). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 10.15 (s, 2H), 8.36 (d, *J* = 8.1 Hz, 4H), 8.02 (d, *J* = 8.1 Hz, 4H), 7.33 (d, *J* = 8.6 Hz, 4H), 7.15 (d, *J* = 8.5 Hz, 4H), 1.73 (s, 6H).



^{13}C NMR (101 MHz, $CDCl_3$) δ 191.57, 164.28, 148.66, 148.33, 139.60, 134.62, 130.79, 129.67, 128.06, 120.99, 42.68, 31.01.

HRMS: m/z (ESI) Calculated for $C_{31}H_{25}O_6$ $[M+H]^+$: 493.1651; found; 493.1646

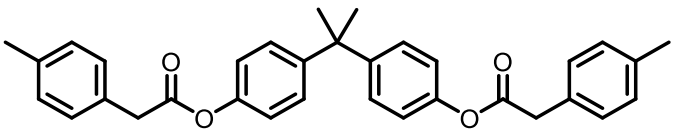
4-(2-(4-hydroxyphenyl)propan-2-yl)phenyl 2-(*p*-tolyl)acetate (12a): Compound **12a** was prepared according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 62% yield (149 mg). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.26 – 7.22 (m, 2H), 7.16 (t, *J* = 9.2 Hz, 4H), 7.05 (d, *J* = 8.6 Hz, 2H), 6.93 (d, *J* = 8.6 Hz, 2H), 6.69 (d, *J* = 8.6 Hz, 2H), 4.77 (s, 1H), 3.79 (s, 2H), 2.33 (s, 3H), 1.61 (s, 6H).



^{13}C NMR (101 MHz, $CDCl_3$) δ 170.56, 153.57, 148.66, 148.60, 142.82, 137.09, 130.57, 129.53, 129.29, 128.09, 127.85, 120.84, 114.90, 42.20, 41.19, 31.12, 21.23.

HRMS: m/z (ESI) Calculated for $C_{24}H_{24}O_3$ $[M]^+$: 360.1725; found; 360.1798.

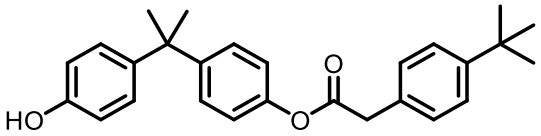
propane-2,2-diylbis(4,1-phenylene) bis(2-(*p*-tolyl)acetate) (12b): Compound **12b** was prepared according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 10% yield (34 mg). **^{1}H NMR (400 MHz, CDCl3)** δ 7.27 – 7.23 (m, 4H), 7.19 – 7.13 (m, 8H), 6.97 – 6.90 (m, 4H), 3.79 (s, 4H), 2.34 (s, 6H), 1.63 (s, 6H).



^{13}C NMR (101 MHz, $CDCl_3$) δ 170.40, 148.81, 148.00, 137.08, 130.57, 129.52, 129.28, 127.88, 120.93, 42.59, 41.17, 31.05, 21.23.

HRMS: m/z (ESI) Calculated for $C_{33}H_{33}O_4$ $[M+H]^+$: 493.2379; found; 493.2373

4-(2-(4-hydroxyphenyl)propan-2-yl)phenyl 2-(4-(*tert*-butyl)phenyl)acetate (13a):

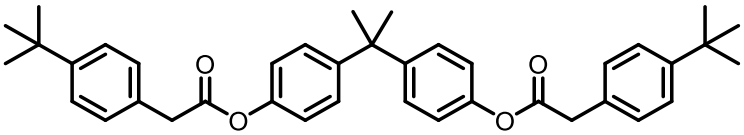


Compound **13a** was prepared according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 60% yield (126 mg). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.38 (d, *J* = 7.7 Hz, 2H), 7.31 (d, *J* = 7.6 Hz, 2H), 7.19 (d, *J* = 8.3 Hz, 2H), 7.06 (d, *J* = 8.1 Hz, 2H), 6.96 (d, *J* = 8.1 Hz, 2H), 6.71 (d, *J* = 7.9 Hz, 2H), 4.83 (s, 1H), 3.81 (s, 2H), 1.63 (s, 6H), 1.32 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.52, 153.59, 150.34, 148.68, 148.59, 142.82, 130.58, 129.07, 128.10, 127.84, 125.78, 120.86, 114.90, 42.21, 41.07, 34.63, 31.47, 31.12.

HRMS: m/z (ESI) Calculated for $C_{27}H_{31}O_3$ $[M+H]^+$: 403.2273; found; 403.2268.

propane-2,2-diylbis(4,1-phenylene) bis(2-(4-(tert-butyl)phenyl)acetate) (13b): Compound

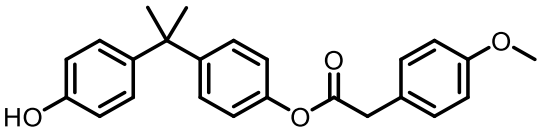


13b was prepared according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 13% yield (40 mg). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.37 (d, *J* = 8.1 Hz, 4H), 7.30 (d, *J* = 8.0 Hz, 4H), 7.18 (d, *J* = 8.5 Hz, 4H), 6.96 (d, *J* = 8.5 Hz, 4H), 3.81 (s, 4H), 1.63 (s, 6H), 1.32 (s, 18H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.39, 150.33, 148.82, 148.02, 130.58, 129.07, 127.88, 125.78, 120.96, 42.61, 41.06, 34.64, 31.48, 31.06.

HRMS: m/z (ESI) Calculated for $C_{39}H_{45}O_4$ $[M+H]^+$: 577.3318; found; 577.3319.

4-(2-(4-hydroxyphenyl)propan-2-yl)phenyl 4-(4-methoxybenzyl)benzoate (14a): Compound

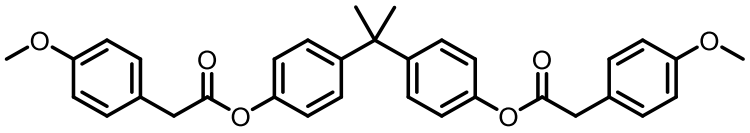


14a was prepared according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 68% yield (155 mg). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.29 (d, *J* = 8.3 Hz, 2H), 7.19 (d, *J* = 8.3 Hz, 2H), 7.06 (d, *J* = 8.0 Hz, 2H), 6.94 (d, *J* = 8.3 Hz, 2H), 6.89 (d, *J* = 8.2 Hz, 2H), 6.71 (d, *J* = 7.8 Hz, 2H), 4.91 (s, 1H), 3.81 (s, 3H), 3.78 (s, 2H), 1.62 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.66, 158.98, 153.62, 148.66, 148.62, 142.77, 130.49, 128.08, 127.85, 125.70, 120.83, 114.90, 114.26, 55.43, 42.20, 40.72, 31.12.

HRMS: m/z (ESI) Calculated for $C_{24}H_{25}O_4$ $[M+H]^+$: 377.1753; found; 377.1747

propane-2,2-diylbis(4,1-phenylene) bis(4-(4-methoxybenzyl)benzoate) (14b): Compound

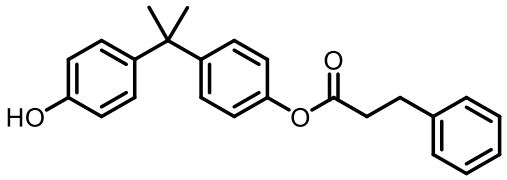


14b was prepared according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 11% yield (36 mg). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.29 (d, *J* = 8.6 Hz, 4H), 7.17 (d, *J* = 8.7 Hz, 4H), 6.94 (d, *J* = 8.7 Hz, 4H), 6.89 (d, *J* = 8.6 Hz, 4H), 3.81 (s, 6H), 3.78 (s, 4H), 1.63 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.55, 159.00, 148.81, 148.02, 130.49, 127.89, 125.69, 120.94, 114.27, 55.43, 42.60, 40.71, 31.05.

HRMS: m/z (ESI) Calculated for $C_{33}H_{33}O_6$ $[M+H]^+$: 525.2277; found; 525.2272.

4-(2-(4-hydroxyphenyl)propan-2-yl)phenyl 3-phenylpropanoate (15a): Compound **15a** was

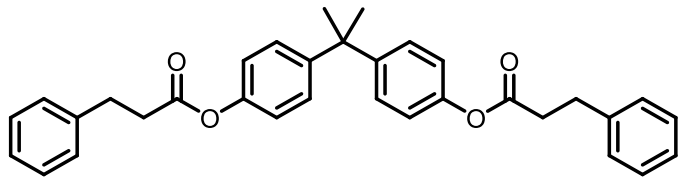


prepared according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 59% yield (142 mg).**^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.38 – 7.32 (m, 2H), 7.31 – 7.26 (m, 3H), 7.23 (d, *J* = 8.6 Hz, 2H), 7.11 (d, *J* = 8.6 Hz, 2H), 6.92 (d, *J* = 8.5 Hz, 2H), 6.75 (d, *J* = 8.3 Hz, 2H), 4.76 (s, 1H), 3.10 (t, *J* = 7.6 Hz, 2H), 2.90 (t, *J* = 7.6 Hz, 2H), 1.66 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.77, 153.57, 148.58, 148.52, 142.84, 140.27, 128.72, 128.55, 128.12, 127.89, 126.58, 120.92, 114.91, 42.21, 36.14, 31.13, 31.11.

HRMS: m/z (ESI) Calculated for $C_{24}H_{24}O_3$ $[M]^+$: 360.1725; found; 360.1798.

propane-2,2-diylbis(4,1-phenylene) bis(3-phenylpropanoate) (15b): Compound **15b** was

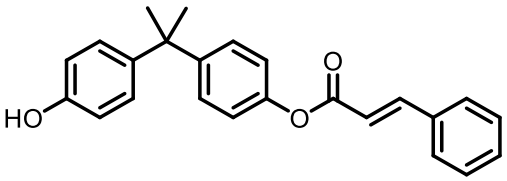


prepared according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 11% yield (37 mg). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.38 – 7.32 (m, 4H), 7.29 (d, *J* = 8.1 Hz, 5H), 7.27 – 7.20 (m, 5H), 6.93 (d, *J* = 8.6 Hz, 4H), 3.10 (t, *J* = 7.6 Hz, 4H), 2.90 (t, *J* = 7.6 Hz, 4H), 1.68 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.63, 148.67, 147.98, 140.28, 128.72, 128.55, 127.93, 126.58, 121.03, 42.60, 36.14, 31.11, 31.06.

HRMS: m/z (ESI) Calculated for $C_{33}H_{33}O_4$ $[M+H]^+$: 493.2379; found; 493.2373.

4-(2-(4-hydroxyphenyl)propan-2-yl)phenyl cinnamate (16a): Compound **16a** was prepared

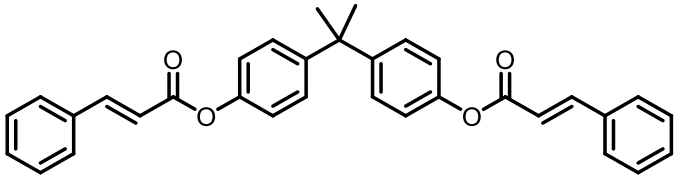


according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 65% yield (158 mg). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.87 (d, *J* = 16.0 Hz, 1H), 7.58 (dd, *J* = 6.5, 2.8 Hz, 2H), 7.47 – 7.37 (m, 3H), 7.25 (d, *J* = 8.8 Hz, 2H), 7.07 (t, *J* = 8.6 Hz, 4H), 6.71 (d, *J* = 8.6 Hz, 2H), 6.63 (d, *J* = 16.0 Hz, 1H), 5.49 (s, 1H), 1.65 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.91, 153.73, 148.66, 148.59, 146.77, 142.63, 134.28, 130.84, 129.11, 128.45, 128.07, 127.94, 120.98, 117.44, 114.95, 42.21, 31.14.

HRMS: m/z (ESI) Calculated for $C_{24}H_{23}O_3$ $[M+H]^+$: 359.1647; found; 359.1642

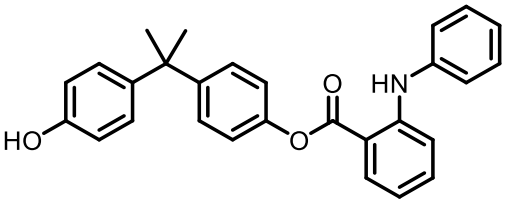
propane-2,2-diylbis(4,1-phenylene) (2*E*,2'*E*)-bis(3-phenylacrylate) (16b): Compound **16b**



was prepared according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 28% yield (25 mg). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.79 (d, *J* = 16.0 Hz, 2H), 7.51 (dd, *J* = 6.5, 2.8 Hz, 4H), 7.47 -7.35 (m, 6H), 7.20 (d, *J* = 8.3 Hz, 4H), 7.01 (d, *J* = 8.3 Hz, 4H), 6.56 (d, *J* = 16.0 Hz, 2H), 1.63 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.59, 148.82, 147.99, 146.60, 134.35, 130.80, 129.12, 128.43, 128.00, 121.12, 117.55, 42.66, 31.12.
HRMS: m/z (ESI) Calculated for $C_{33}H_{29}O_4$ $[M+H]^+$: 489.2066; found; 489.2060.

4-(2-(4-hydroxyphenyl)propan-2-yl)phenyl 2-(phenylamino)benzoate (17a): Compound **17a**

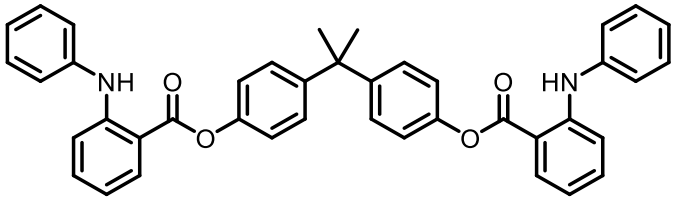


was prepared according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 48% yield (96 mg).**^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.47 (s, 1H), 8.22 (d, *J* = 7.4 Hz, 1H), 7.35 (dd, *J* = 22.2, 7.4 Hz, 4H), 7.27 (d, *J* = 7.4 Hz, 4H), 7.14 (d, *J* = 7.4 Hz, 4H), 6.95 – 6.76 (m, 2H), 6.77 (d, *J* = 6.8 Hz, 2H), 4.78 (s, 1H), 1.71 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 167.61, 148.92, 148.80, 148.57, 142.84, 140.52, 135.03, 132.19, 129.53, 128.15, 128.04, 123.97, 122.79, 121.36, 120.69, 117.32, 114.94, 114.16, 110.90, 42.28, 31.18.

HRMS: m/z (ESI) Calculated for $C_{28}H_{26}NO_3$ $[M+H]^+$: 424.1913; found; 424.1907.

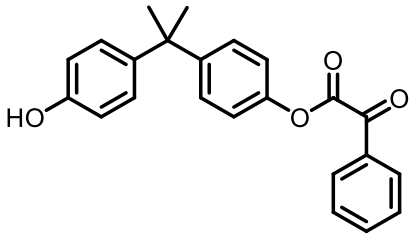
propane-2,2-diylbis(4,1-phenylene) bis(2-(phenylamino)benzoate) (17b): Compound **17b** was prepared according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 8% yield (24 mg). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.41 (s, 2H), 8.16 (dd, *J* = 8.1, 1.5 Hz, 2H), 7.38 – 7.27 (m, 12H), 7.23 – 7.19 (m, 4H), 7.10 (dd, *J* = 6.8, 4.7 Hz, 4H), 7.06 (t, *J* = 5.1 Hz, 2H), 6.80 – 6.74 (m, 2H), 1.70 (s, 6H).



^{13}C NMR (101 MHz, $CDCl_3$) δ 167.56, 148.94, 148.75, 148.23, 140.54, 135.04, 132.20, 129.54, 128.13, 123.98, 122.81, 121.52, 117.32, 114.16, 110.89, 77.16, 42.76, 31.17.

HRMS: m/z (ESI) Calculated for $C_{41}H_{35}N_2O_4$ $[M+H]^+$: 619.2597; found; 619.2591.

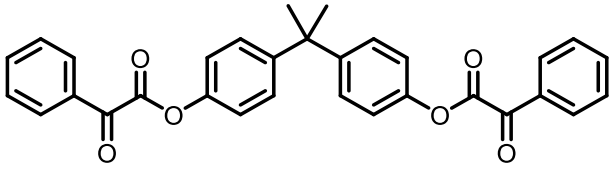
4-(2-(4-hydroxyphenyl)propan-2-yl)phenyl 2-oxo-2-phenylacetate (18a): Compound **18a** was prepared according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 60% yield (145 mg). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.06 (d, *J* = 7.8 Hz, 2H), 7.66 (t, *J* = 7.4 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 2H), 7.23 (d, *J* = 9.7 Hz, 2H), 7.12 (d, *J* = 8.4 Hz, 2H), 7.06 (d, *J* = 8.3 Hz, 2H), 6.71 (d, *J* = 8.4 Hz, 2H), 4.73 (s, 1H), 1.62 (s, 6H).



^{13}C NMR (101 MHz, $CDCl_3$) δ 185.55, 162.10, 153.66, 149.70, 147.82, 142.62, 135.37, 132.47, 130.31, 129.20, 128.20, 128.13, 120.65, 115.00, 42.34, 31.13.

HRMS: m/z (ESI) Calculated for $C_{23}H_{21}O_4$ $[M+H]^+$: 361.1440; found; 361.1435.

propane-2,2-diylbis(4,1-phenylene) bis(2-oxo-2-phenylacetate) (18b): Compound **18b** was prepared according to the general procedure (3) and purified by flash column



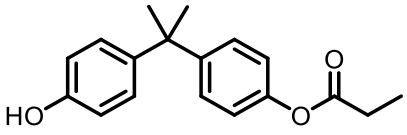
chromatography (EtOAc/petether), affording a white solid in 11% yield (37 mg).

^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.19 (d, *J* = 7.7 Hz, 2H), 7.62 (d, *J* = 7.3 Hz, 1H), 7.51 (t, *J* = 7.5 Hz, 2H), 7.27 (d, *J* = 9.2 Hz, 2H), 7.17 – 7.07 (m, 6H), 6.85 (d, *J* = 8.3 Hz, 1H), 6.73 (t, *J* = 7.4 Hz, 4H), 1.67 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) *δ* 165.52, 153.64, 148.72, 142.83, 133.70, 130.30, 128.71, 128.00, 121.11, 114.95, 42.27, 31.18.

HRMS: m/z (ESI) Calculated for $C_{31}H_{25}O_6$ $[M+H]^+$: 493.1651; found; 493.1645.

4-(2-(4-hydroxyphenyl)propan-2-yl)phenyl propionate (19a): Compound **19a** was prepared

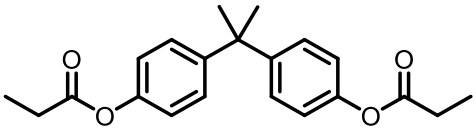


according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 55% yield (212 mg). **^{1}H NMR (400 MHz, $CDCl_3$)** *δ* 7.21 (d, *J* = 8.4 Hz, 2H), 7.08 (d, *J* = 8.2 Hz, 2H), 6.97 (d, *J* = 8.4 Hz, 2H), 6.71 (d, *J* = 8.1 Hz, 2H), 4.82 (s, 1H), 2.58 (dd, *J* = 14.9, 7.4 Hz, 2H), 1.64 (s, 6H), 1.26 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 173.39, 153.59, 148.63, 148.49, 142.84, 128.11, 127.88, 120.94, 114.90, 42.21, 31.14, 27.92, 9.23.

HRMS: m/z (ESI) Calculated for $C_{18}H_{21}O_3$ $[M+H]^+$: 285.1491; found; 285.1485.

propane-2,2-diylbis(4,1-phenylene) dipropionate (19b): Compound **19b** was prepared



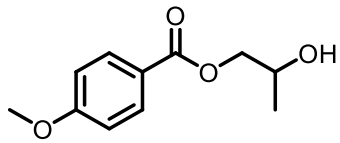
according to the general procedure (3) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 11% yield (51 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 (d, *J* = 8.6 Hz, 4H), 6.98 (d, *J* = 8.6 Hz, 4H), 2.57 (q, *J* = 7.5 Hz, 4H), 1.67 (s, 6H), 1.26 (t, *J* = 7.5 Hz, 6H).

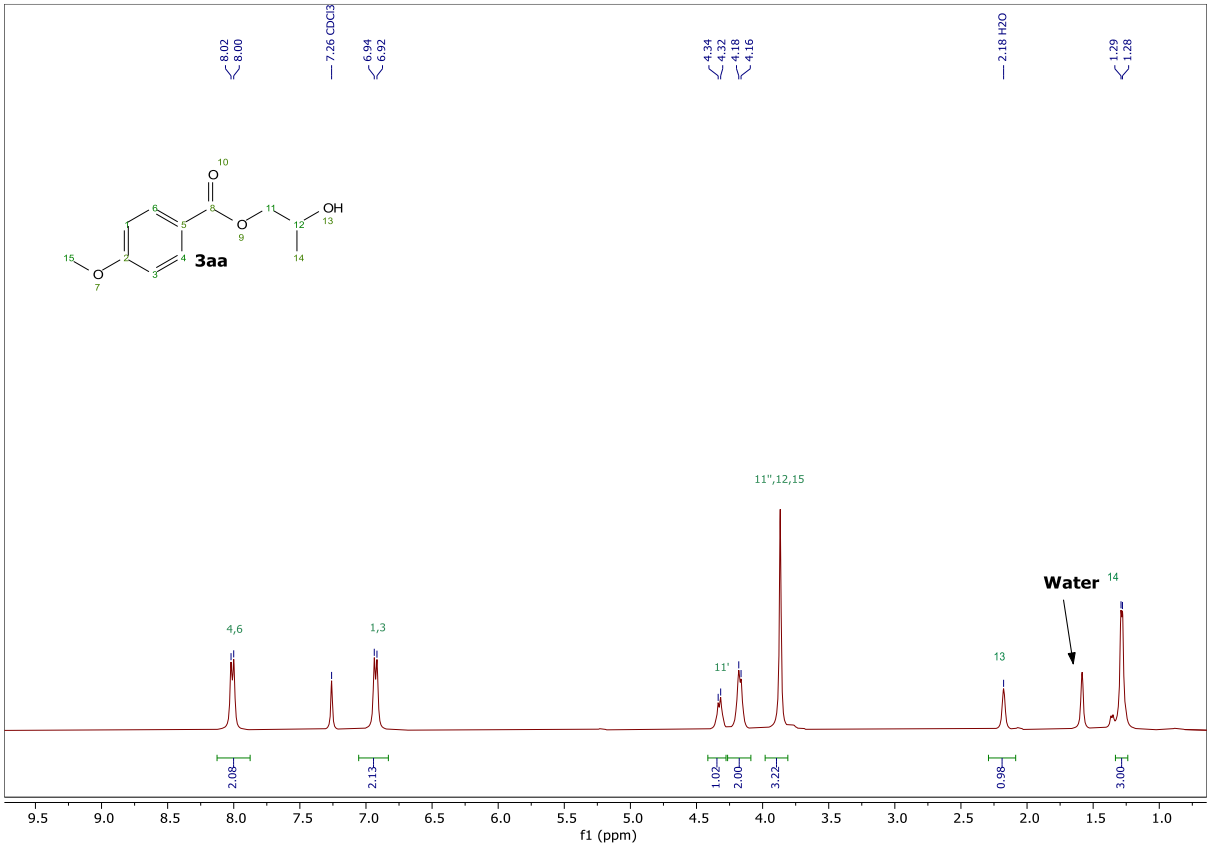
^{13}C NMR (101 MHz, $CDCl_3$) δ 173.17, 148.79, 147.91, 127.93, 121.04, 42.60, 31.09, 27.90, 9.23.

HRMS: m/z (ESI) Calculated for $C_{21}H_{25}O_4$ $[M+H]^+$: 341.1753; found; 341.1748.

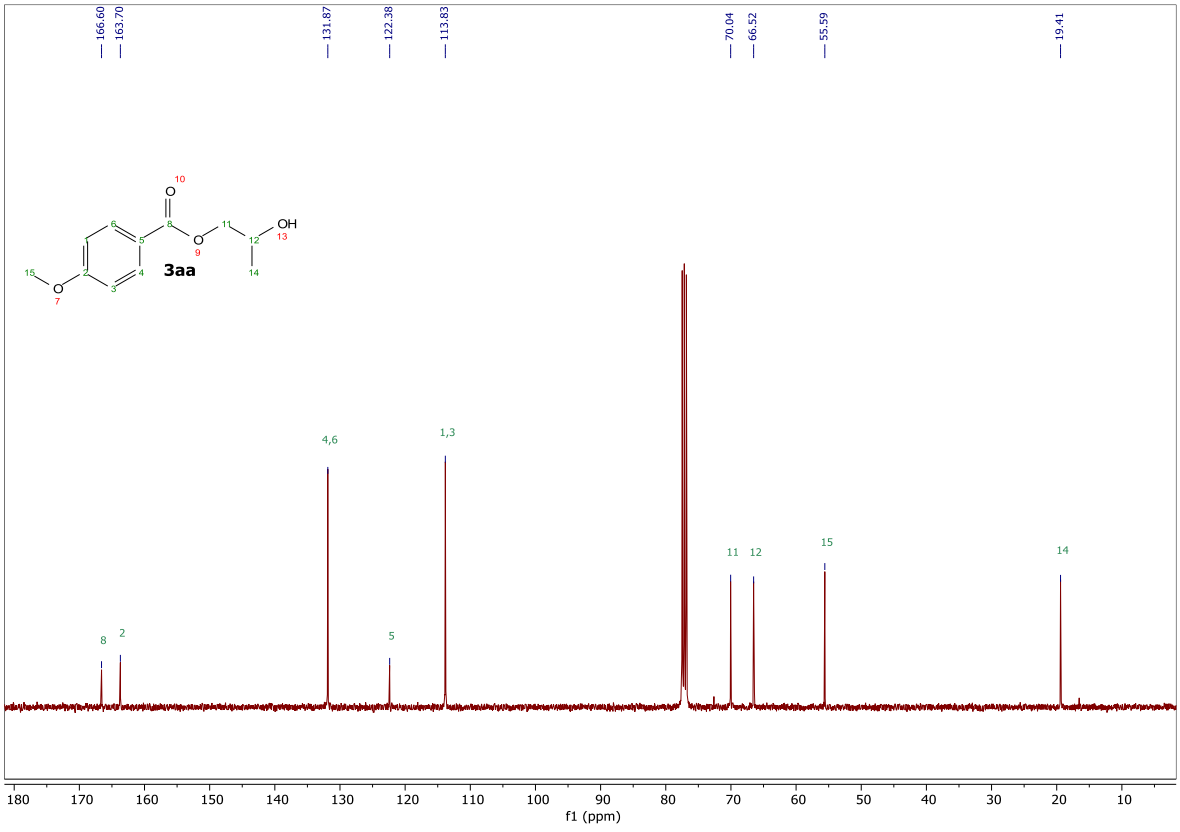
2-hydroxypropyl 4-methoxybenzoate (3aa): Compound **3aa** was prepared according to the



general procedure (4) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 78% yield (101 mg). **^{1}H NMR (400 MHz, $CDCl_3$)** *δ* 8.01 (d, *J* = 8.1 Hz, 2H), 6.93 (d, *J* = 8.1 Hz, 2H), 4.33 (d, *J* = 7.5 Hz, 1H), 4.17 (d, *J* = 6.9 Hz, 2H), 3.87 (s, 3H), 2.18 (s, 1H), 1.28 (d, *J* = 4.4 Hz, 3H).

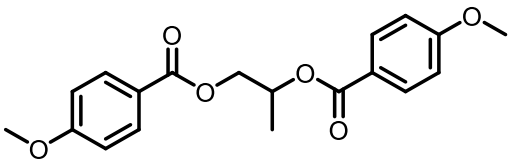


^{13}C NMR (101 MHz, $CDCl_3$) δ 166.60, 163.70, 131.87, 122.38, 113.83, 70.04, 66.52, 55.59, 19.41.

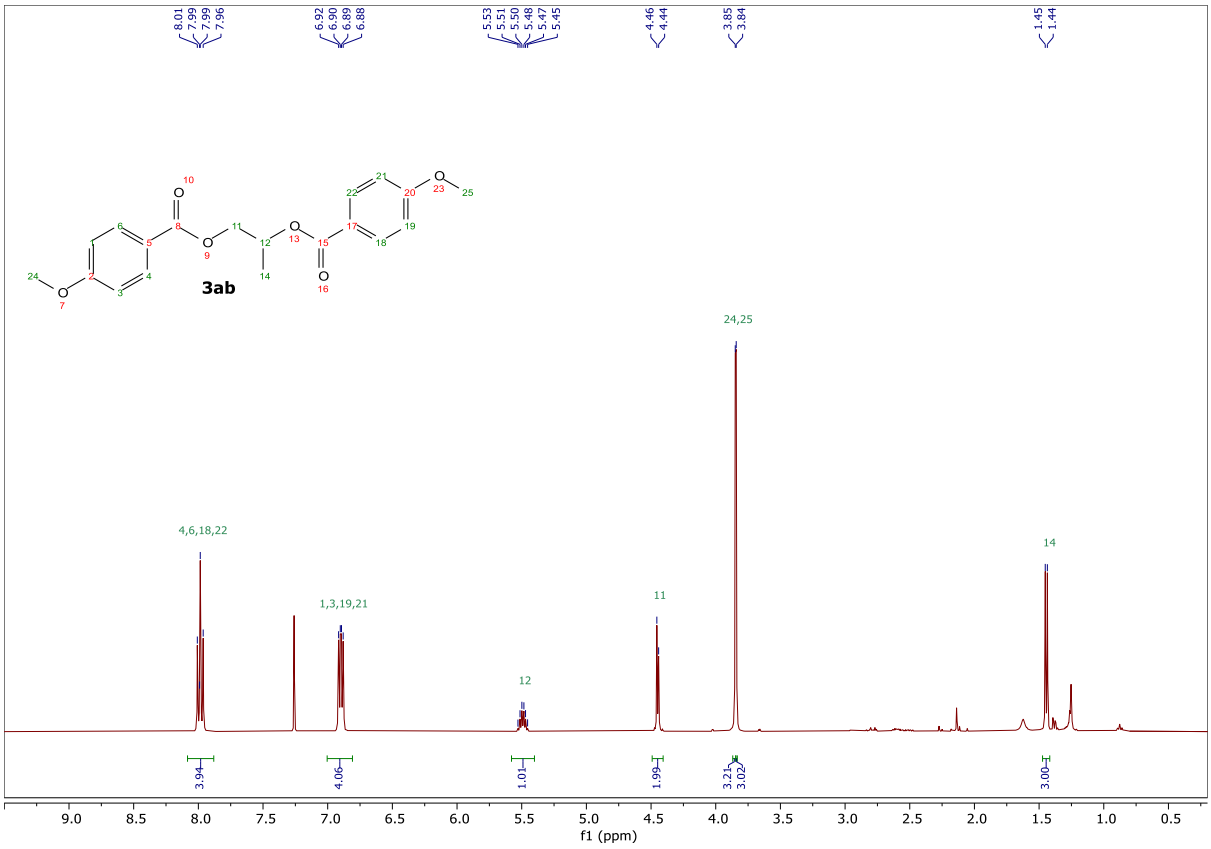


HRMS: m/z (ESI) Calculated for $C_{11}H_{15}O_4[M+H]^+$: 211.0970; found; 211.0964.

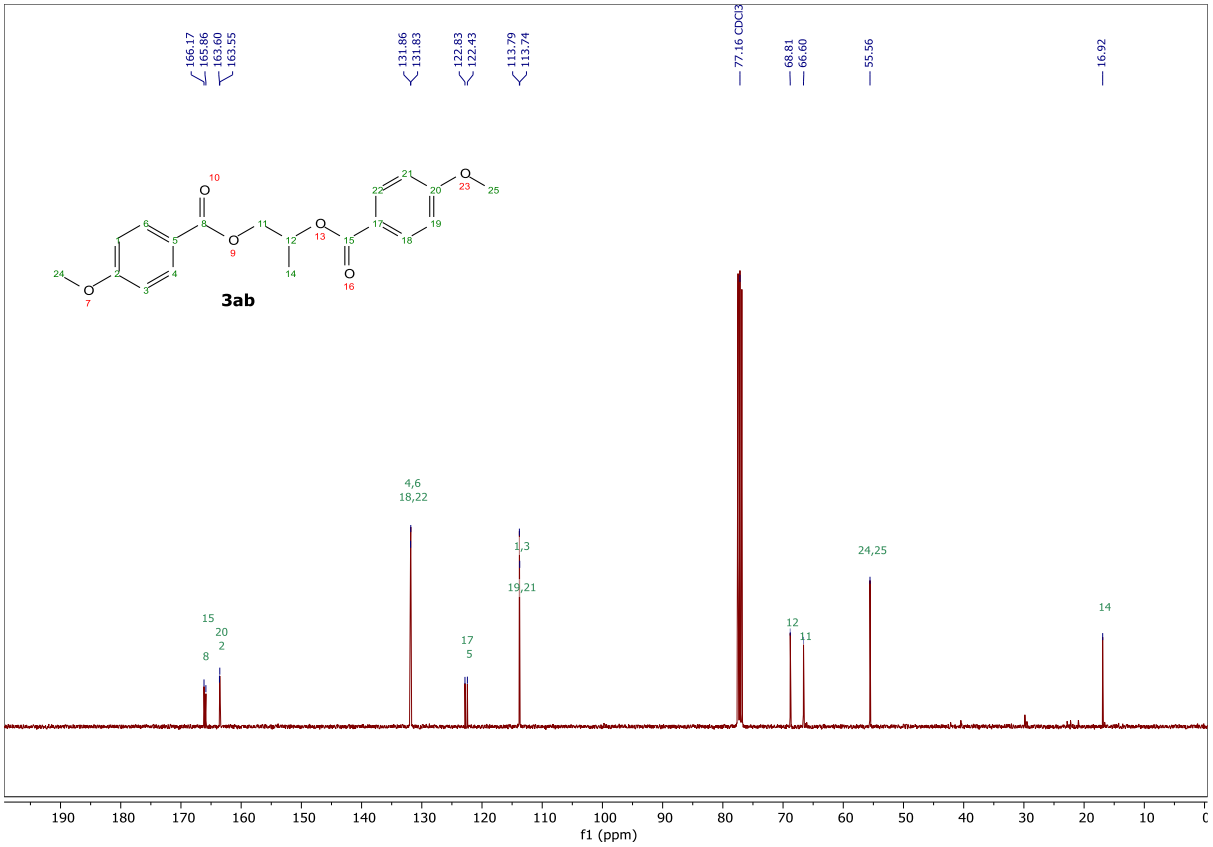
propane-1,2-diyl bis(4-methoxybenzoate) (3ab): Compound **3ab** was prepared according to



the general procedure (4) and purified by flash column chromatography (EtOAc/petether), affording a white solid in 15% yield (34 mg). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.99 (dd, *J* = 10.1, 8.0 Hz, 4H), 6.90 (dd, *J* = 8.9, 5.2 Hz, 4H), 5.58 – 5.40 (m, 1H), 4.45 (d, *J* = 5.5 Hz, 2H), 3.85 (s, 3H), 3.84 (s, 3H), 1.44 (d, *J* = 6.5 Hz, 3H).

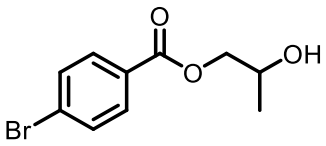


^{13}C NMR (101 MHz, $CDCl_3$) δ 166.04, 165.73, 163.47, 163.42, 131.73, 131.70, 122.70, 122.30, 113.66, 113.61, 68.68, 66.47, 55.43, 16.79.



HRMS: m/z (ESI) Calculated for $C_{19}H_{21}O_6[M+H]^+$: 345.1338; found; 345.1332.

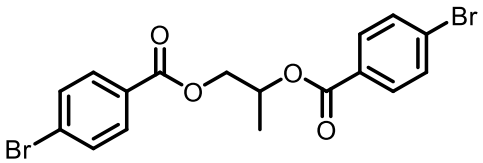
2-hydroxypropyl 4-bromobenzoate (8aa): Compound **8aa** was prepared according to the general procedure (4) and purified by flash column chromatography (14% EtOAc/petether), affording a white solid in 67% yield (86 mg). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.91 (d, J = 7.4 Hz, 2H), 7.59 (d, J = 7.3 Hz, 2H), 4.33 (d, J = 8.2 Hz, 1H), 4.19 (d, J = 7.4 Hz, 2H), 2.15 (s, 1H), 1.29 (s, 3H).



^{13}C NMR (101 MHz, $CDCl_3$) δ 166.09, 131.94, 131.32, 128.90, 128.49, 70.40, 66.34, 19.48.

HRMS: m/z (ESI) Calculated for $C_{10}H_{12}BrO_3$ $[M+H]^+$: 258.9970; found; 258.9964.

propane-1,2-diyl bis(4-bromobenzoate) (8ab): Compound **8ab** was prepared according to the general procedure (4) and purified by flash column chromatography (14% EtOAc/petether), affording a white solid in 10% yield (22 mg). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.88 (d, J = 9.1 Hz, 2H), 7.86 (d, J = 9.3 Hz, 2H), 7.58 (d, J = 4.4 Hz, 2H), 7.56



(d, *J* = 4.5 Hz, 2H), 5.52 (dd, *J* = 10.1, 6.3 Hz, 1H), 4.49 (d, *J* = 3.5 Hz, 2H), 1.46 (d, *J* = 6.4 Hz, 3H).

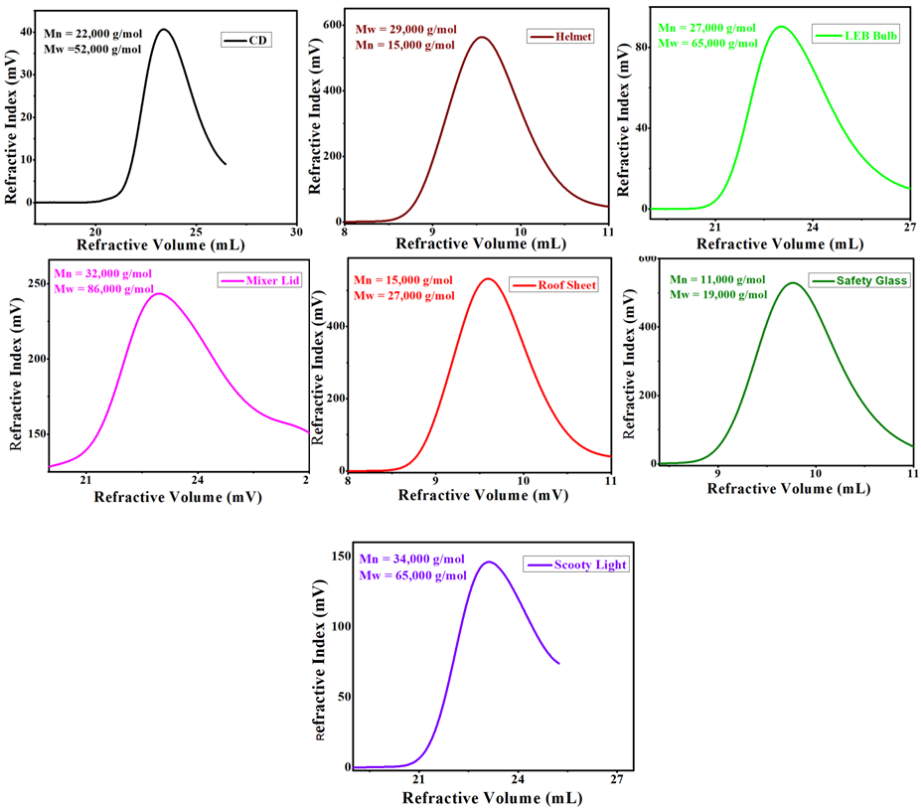
^{13}C NMR (101 MHz, $CDCl_3$) δ 165.66, 165.38, 131.96, 131.91, 131.31, 129.15, 128.77, 128.51, 128.40, 69.33, 66.91, 16.77.

HRMS: m/z (ESI) Calculated for $C_{17}H_{15}Br_2O_4$ $[M+H]^+$: 440.9337; found; 440.9332.

6. GPC data for the real-life polycarbonates

Figure S1: Waste PC-BPA samples CD, helmet, LED bulb, mixer Lid, roof sheet, safety glass, scooty light.

Before depolymerization:



After depolymerization:

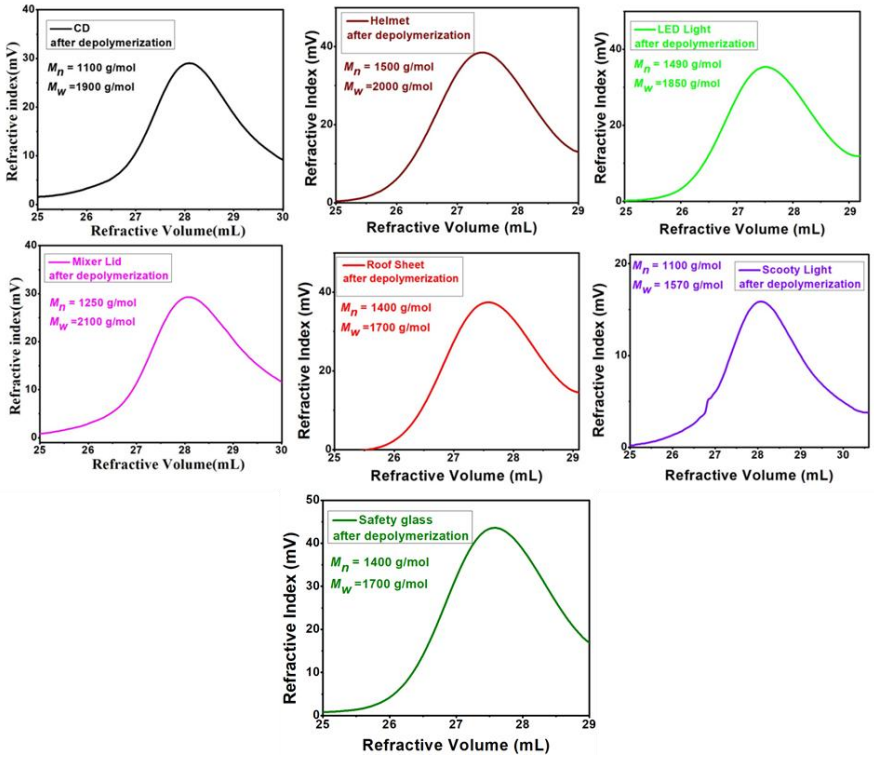


Figure S2: a) GPC of real life samples (CD, helmet, LED bulb, mixer Lid, roof sheet, safety glass, scooty light).

7. GPC analysis of PC-BPA before and after reaction

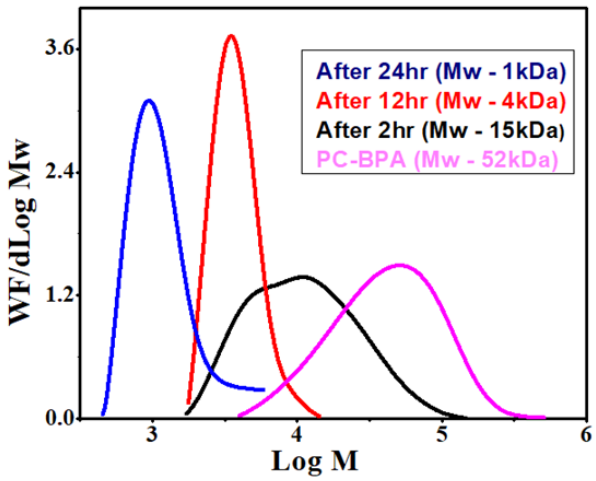


Figure S3: GPC of recovered PC-BPA before and after the reaction.

8. TGA analysis of PCBPA before and after the reaction

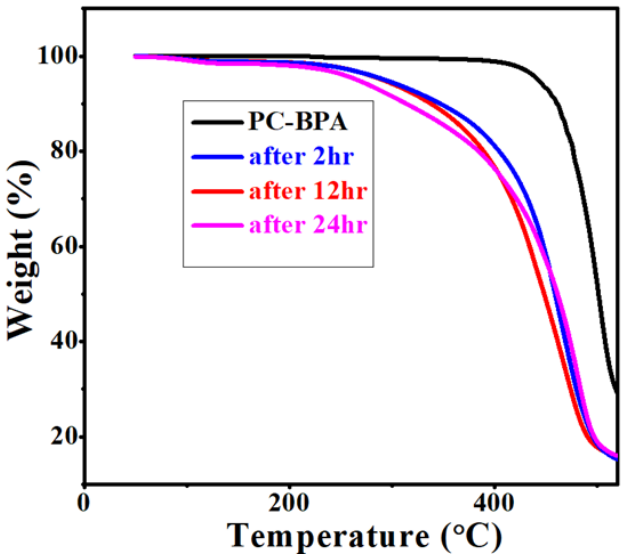


Figure S4: TGA of recovered PC-BPA before and after the reaction.

9. WAXD analysis of PCBPA before and after the reaction

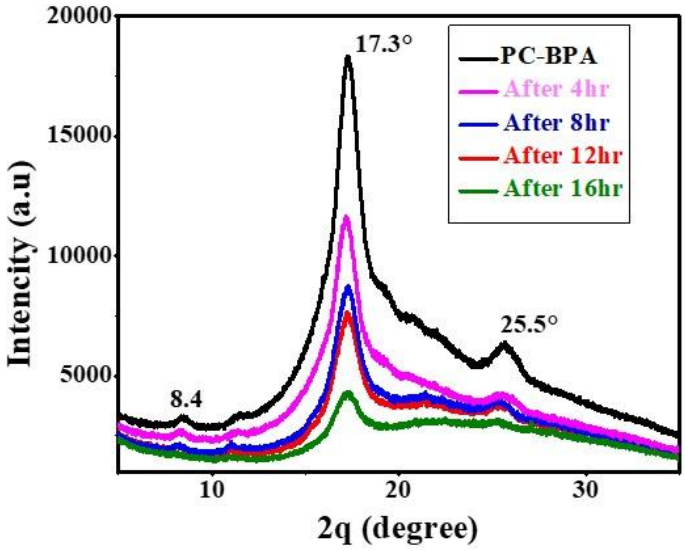
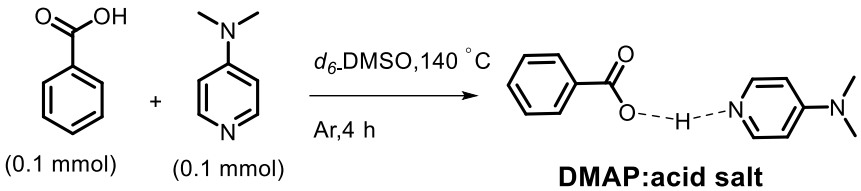


Figure S5: WAXD of recovered PC-BPA before and after the reaction.

10. Control experiments

Experiments (a & b) were carried out in an oven-dried NMR tube under the Schlenk line technique.

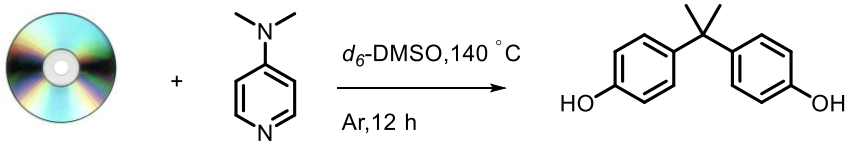
a) **DMAP reaction with acid**



(0.1 mmol) (0.1 mmol)

DMAP:acid salt

b) **DMAP reaction with PC**

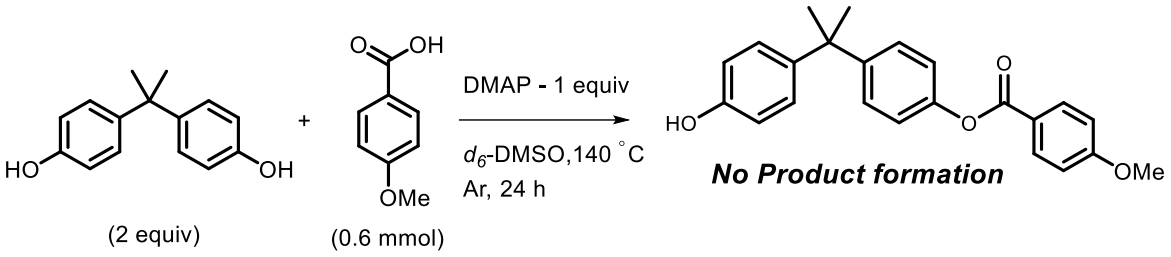


(0.2 mmol) (0.1 mmol)

Not observed

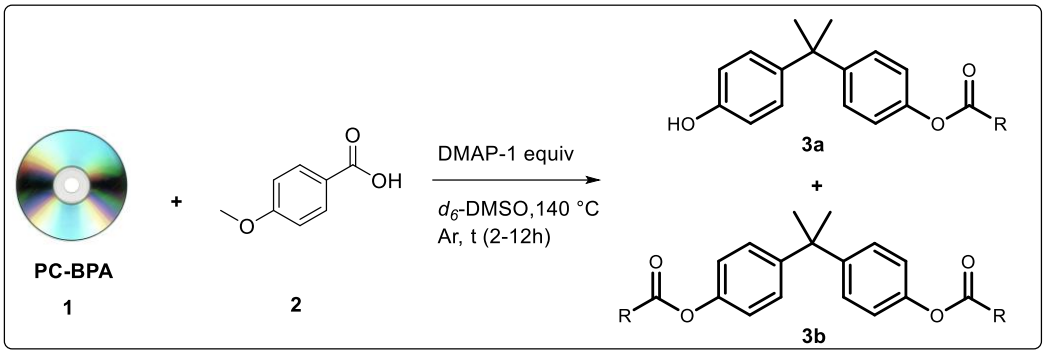
Reaction condition: a) DMAP (0.2 mmol, 1 equiv, 24.4 mg), acid (0.2 mmol,1 equiv, 30.4 mg), d_6-DMSO-0.5 mL, 140 °C, Ar, 4 h**; b)** PC-BPA (0.1 mmol, 1 equiv, 25 mg), base (0.1 mmol,1 equiv, 12 mg), d_6-DMSO(0.5 mL), Ar, 12 h.

c) **Esterification reaction with BPA**



An oven-dried Schlenk tube was charged with acid (0.6 mmol, 1 equiv, 91 mg), BPA (1.2 mmol, 2 equiv, 273 mg), and d_6-DMSO (2 mL) under an argon atmosphere. The tube was then placed in a preheated oil bath and stirred at 140 °C for 24 hours. After completion, thin-layer chromatography (TLC) was performed to analyze the reaction mixture. No formation of compounds 3a or 3b was observed by TLC, indicating that BPA does not act as an intermediate in the reaction pathway.

d) Time screening experiment



An oven-dried Schlenk tube equipped with a Teflon-coated magnetic stir bar was charged under an argon atmosphere with waste PC-BPA (334 mg, 1.3 mmol, 2 equiv. based on monomer unit molecular weight of 254), acid (100 mg, 0.65 mmol, 1 equiv.), and dimethyl aminopyridine (DMAP) (80 mg, 0.65 mmol, 1 equiv.), followed by d_6-DMSO (2 mL). The Schlenk tube was sealed and placed in a preheated oil bath at 140 °C. The crude ^{1}H NMR spectra were analysed at various times to observe the product formation.^{1}H NMR analysis revealed slow conversion of polycarbonate to the desired product up to 8 hours, with maximum conversion observed at 12 hours.

Sr. No.	Time (h)	% of PC-BPA Conversion
1	2	36
2	4	44
3	6-8	47
4	12	71

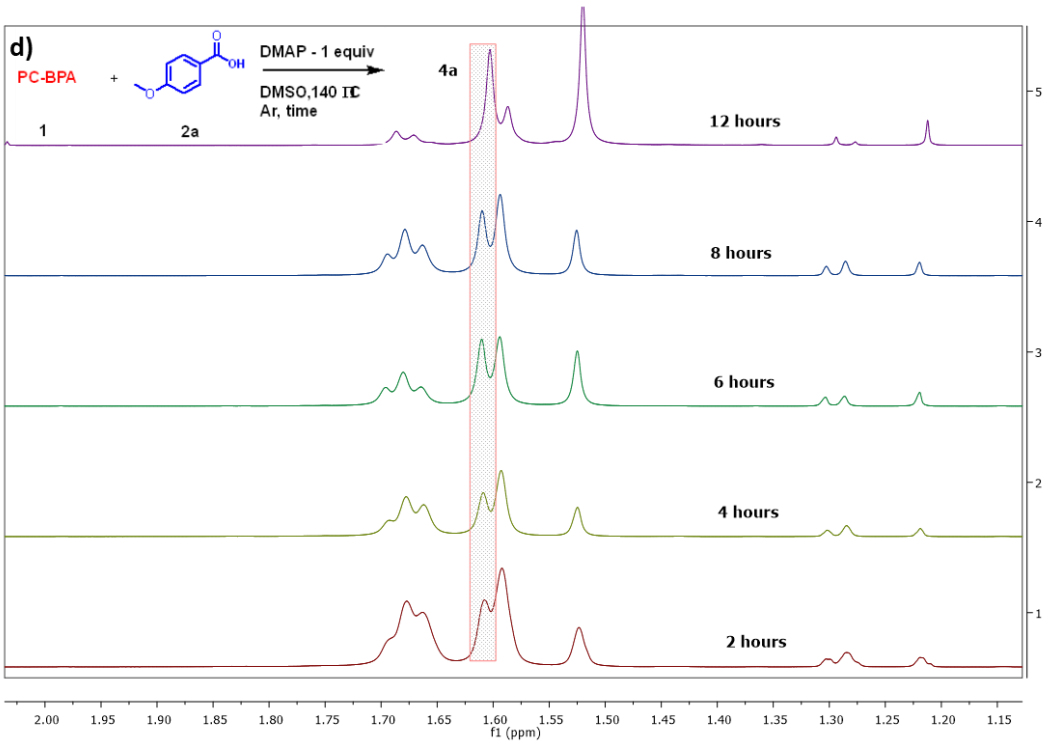
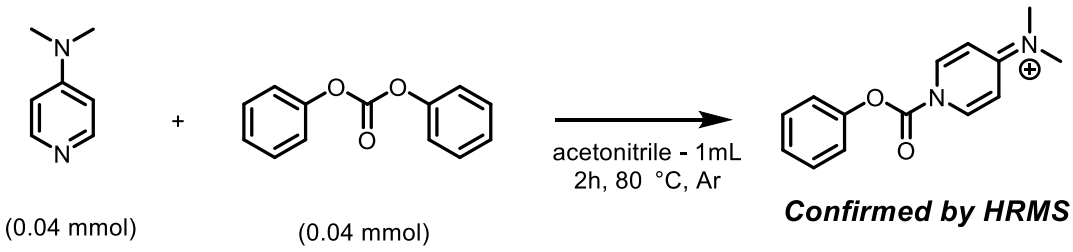


Figure S6: ^{1}H NMR study of depolymerization of PC-BPA into esters in d_6-DMSO at 140 °C.

e) **DMAP and diphenylcarbonate reaction**



An oven-dried Schlenk tube was charged with DMAP (0.04 mmol, 1 equiv, 6.1 mg), diphenyl carbonate (0.04 mmol, 1 equiv, 8.56 mg) and dry acetonitrile (1 mL) under an argon atmosphere. The tube was then placed in a preheated oil bath at 80 °C for 2 hours. The reaction mixture prepared for HRMS under argon. The HRMS was measure immediately without any delay assuming the formed intermediate is unstable.

f) **Detection of CO2 from the reaction**

As envisioned in the proposed mechanism, we attempted to monitor CO_2 formation during the standard reaction. Gas-phase GC analysis confirmed the evolution of CO_2, which was further validated by comparison with a reference CO_2 sample.

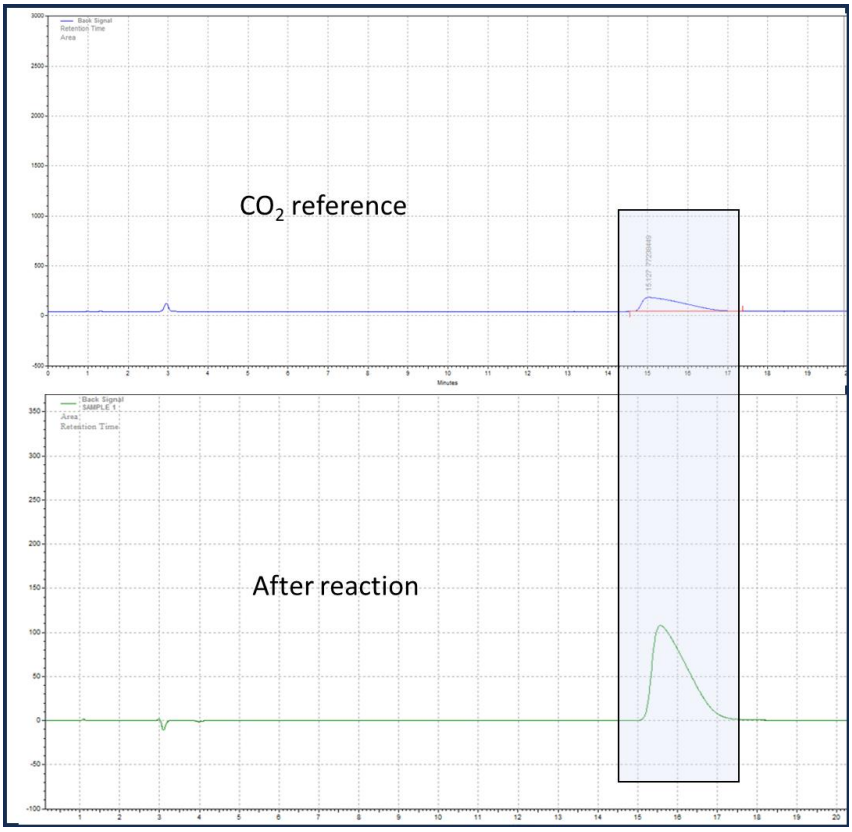
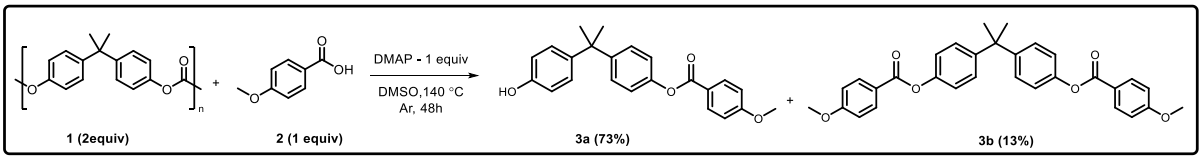


Figure S7: Gas phase analysis of CO_2 and its comparison with reference CO_2.

11. Gram scale reaction

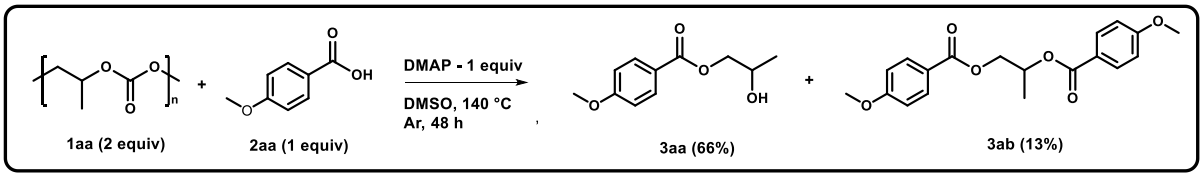
General procedure for PC-BPA to valuable ester

An oven-dried Schlenk flask equipped with a Teflon-coated magnetic stir bar was charged under an argon atmosphere with waste PC-BPA (3340 mg, 13.15 mmol, 2 equiv. based on monomer unit molecular weight of 254), acid (1000mg, 6.57 mmol, 1 equiv.), and dimethyl aminopyridine (DMAP) (801 mg, 6.57 mmol, 1 equiv.), followed by DMSO (12 mL). The Schlenk flask was sealed and placed in a preheated oil bath at 140 °C. After the reaction, the solvent was evaporated under reduced pressure, and the crude reaction mixture was purified by flash column chromatography (20% EtOAc:petether) on silica gel, yielding di-aryl Ester (**3a**) 1.7 g the major product and di-aryl diester (**3b**) 430 mg as the minor product.

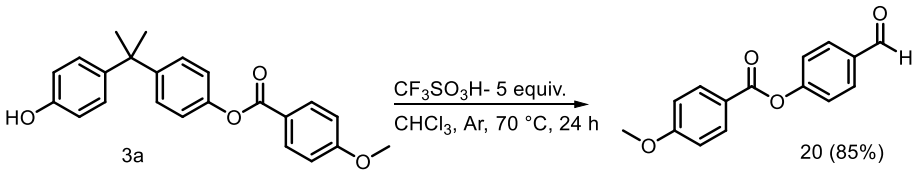


General procedure for PPC to valuable ester

An oven-dried Schlenk flask equipped with a Teflon-coated magnetic stir bar was charged under an argon atmosphere with waste PC-BPA (1341 mg, 13.15 mmol, 2 equiv. based on monomer unit molecular weight of 102), acid (1000mg, 6.57 mmol, 1 equiv.), and dimethyl aminopyridine (DMAP) (801 mg, 6.57 mmol, 1 equiv.), followed by DMSO (2 mL). The Schlenk flask was sealed and placed in a preheated oil bath at 140 °C. After the reaction, the solvent was evaporated under reduced pressure, and the crude reaction mixture was purified by flash column chromatography (20% EtOAc: petether) on silica gel, yielding **3aa** (905 mg) as a major product and **3ab** (302 mg) as a minor product.



12. Derivatization of esters (A) (4-formylphenyl 4-methoxybenzoate (20))

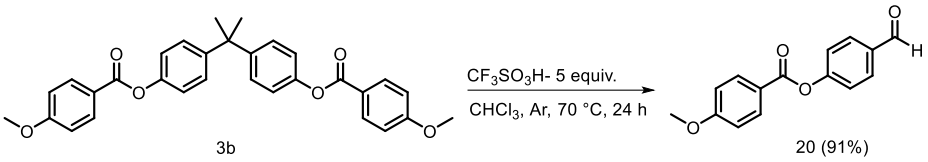


Procedure: An oven-dried Schlenk tube equipped with a Teflon-coated magnetic stir bar was charged under an argon atmosphere with compound 3a (0.27 mmol, 100 mg) and $CHCl_3$ (2 mL). Trifluoromethanesulfonic acid (1.38 mmol, 207 mg, 5 equiv.) was slowly added to the flask. The reaction mixture was stirred for 24 hours at 70 °C. After the reaction time, the Schlenk tube was cooled and ice water was added. The resulting mixture was made basic with a $NaHCO_3$ solution, then extracted with $CHCl_3$. The organic extracts were washed with brine. The solution was purified by flash column chromatography (petether:EtOAc-25%), affording ester as a light brown solid in 85% yield (60 mg).

^{1}H NMR (400 MHz, DMSO) δ 10.32 (s, 1H), 7.69 (d, J = 8.6 Hz, 2H), 7.62 (d, J = 8.5 Hz, 2H), 7.06 (d, J = 8.6 Hz, 2H), 6.89 (d, J = 8.5 Hz, 2H), 3.85 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ 193.11, 162.33, 161.48, 132.15, 131.69, 130.31, 128.52, 115.10, 113.68, 55.48. **HRMS:** m/z (ESI) Calculated for $C_{15}H_{13}O_4$ $[M+H]^+$: 257.0814; found; 257.0809.

Derivatization of Esters (B): (4-formylphenyl 4-methoxybenzoate (20))



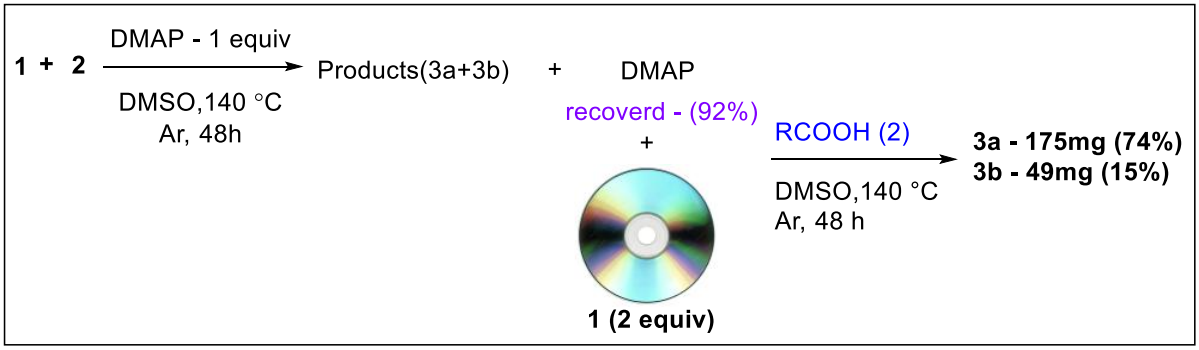
Procedure: An oven-dried Schlenk tube equipped with a Teflon-coated magnetic stir bar was charged under an argon atmosphere with compound 3b (0.2 mmol, 100 mg) and $CHCl_3$ (2 mL). trifluoromethanesulfonic acid (1 mmol, 151 mg, 5 equiv.) was slowly added to the flask. The reaction mixture was stirred for 24 hours at 70 °C. After the reaction time, the Schlenk tube was cooled, and ice water was added. The resulting mixture was made basic with a $NaHCO_3$ solution, then extracted with $CHCl_3$. The organic extracts were washed with brine. The solution was purified by flash column chromatography (petether: EtOAc-25%), yielding ester as a light brown solid in 91% yield (45 mg).

^{1}H NMR (400 MHz, DMSO) δ 10.32 (s, 1H), 7.69 (d, J = 8.6 Hz, 2H), 7.62 (d, J = 8.5 Hz, 2H), 7.06 (d, J = 8.6 Hz, 2H), 6.89 (d, J = 8.5 Hz, 2H), 3.85 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ 193.11, 162.33, 161.48, 132.15, 131.69, 130.31, 128.52, 115.10, 113.68, 55.48.

HRMS: m/z (ESI) Calculated for $C_{15}H_{13}O_4$ $[M+H]^+$: 257.0814; found; 257.0809.

13. Base recyclability experiment



An oven-dried Schlenk tube equipped with a Teflon-coated magnetic stir bar was charged under an argon atmosphere with waste PC-BPA (334 mg, 1.3 mmol, 2 equiv. based on monomer unit molecular weight of 254), acid (100mg, 0.65 mmol, 1 equiv.), and dimethyl aminopyridine (DMAP) (80 mg, 0.65 mmol, 1 equiv.), followed by DMSO (2 mL). The Schlenk tube was sealed and heated in a preheated oil bath at 140 °C for 48 hours. After the reaction time measured the 1H NMR of crude reaction mixture and observed the presence of regenerated base (Figure S8). Later isolated the regenerated base from the crude reaction

mixture through coloumn chromatography which afforded the DMAP in 92%. The isolated base was reused for the standard reaction, which furnished the products 3a (74%) and 3b (14%), comparable to those obtained under the standard conditions.

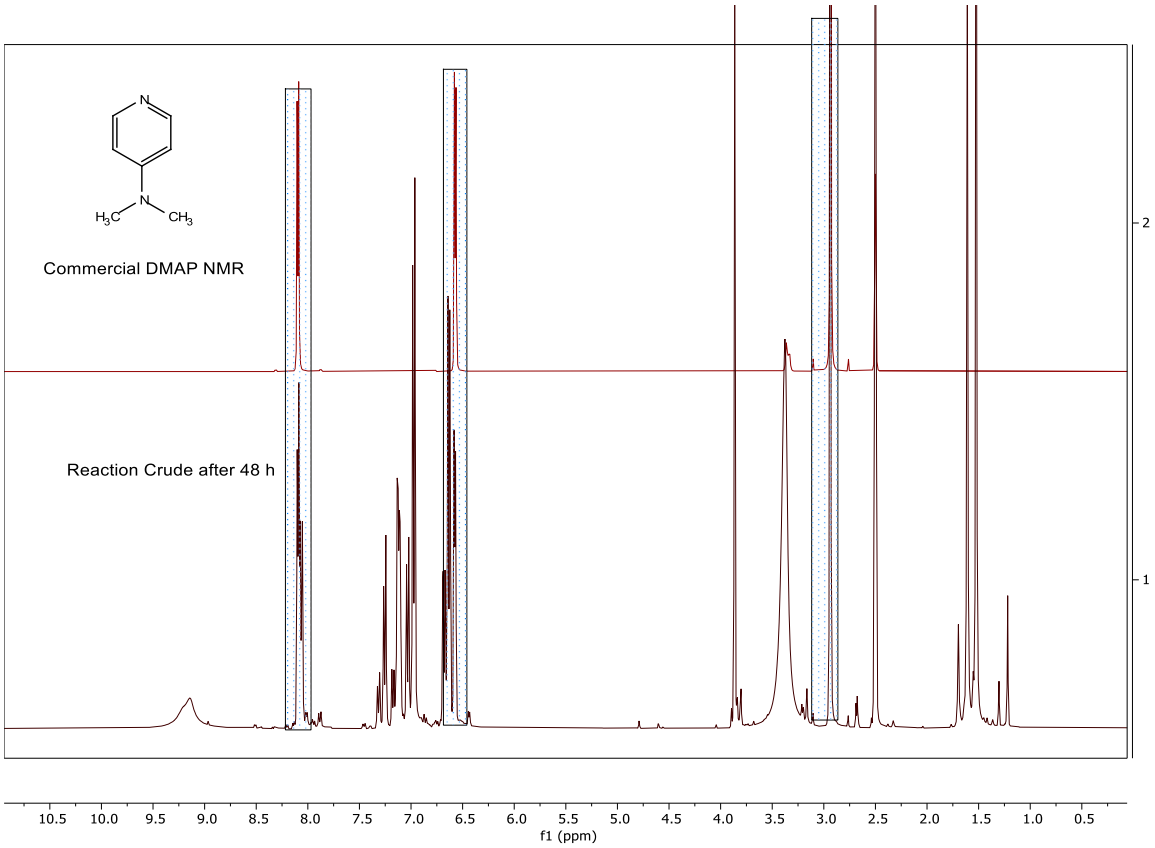
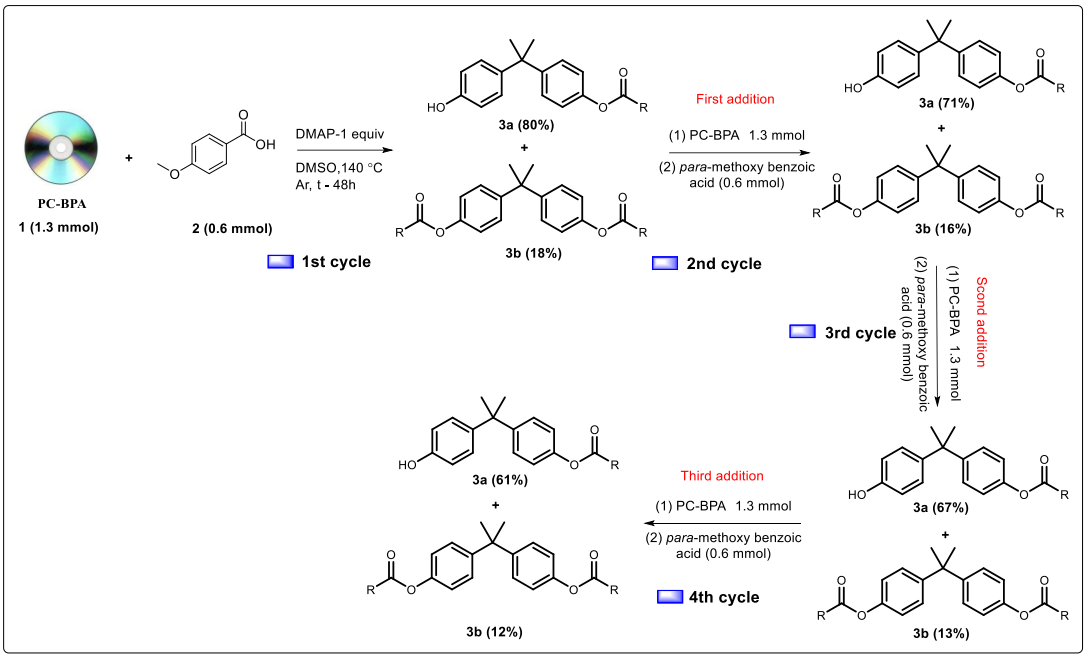


Figure S8: ^{1}H NMR of crude reaction mixture and the commercial DMAP.

14. Base activity experiment

An oven-dried Schlenk tube equipped with a Teflon-coated magnetic stir bar was charged under an argon atmosphere with waste PC-BPA (334 mg, 1.3 mmol, 2 equiv. based on monomer unit molecular weight of 254), acid (100mg, 0.65 mmol, 1 equiv.), and dimethyl aminopyridine (DMAP) (80 mg, 0.65 mmol, 1 equiv.), followed by DMSO (2 mL). The Schlenk tube was sealed and heated in a preheated oil bath at 140 °C for 48 hours. For the second cycle, fresh starting materials were added, and the tube was returned to the oil bath under the same conditions. As shown in the reaction scheme below, fresh starting materials were added at 48-hour intervals for up to four consecutive cycles. After completion of the final cycle, the solvent was removed under reduced pressure, and the crude mixture was purified by flash column chromatography (20% EtOAc/petroleum ether) on silica gel, affording the di-aryl ester (3a) as the major product and the di-aryl diester (3b) as the minor product.



15. Computational studies

Density Functional Theory (DFT) calculations were performed using the Gaussian 09[1] program package. Geometry optimizations and frequency calculations for all reported structures were carried out using the B3LYP[2] functional and the 6-31+G(d) basis set[3] for all atoms. Dispersion interactions were included through the Grimme DFT-D3[4] formalism, while solvent effects for DMSO were considered using the SMD solvation model[5]. Harmonic frequency calculations were performed for all stationary points to confirm their nature as either minima or transition states. Energy changes are reported as Gibbs free energies (T = 413.15 K, P = 1 atm).

To investigate the plausible mechanism of depolymerization of **PC-BPA** with *p*-anisic acid (**S**) in the presence of **DMAP**, all calculations were performed on the truncated system **R** (Figure S9) to reduce computational cost. The truncated system **R** reacts with *p*-anisic acid (**S**) in the presence of **DMAP** via two possible pathways:

(i) DMAP acts solely as a base (see Figure S10 for the detailed mechanism)

(ii) DMAP acts as a base as well as an active participant in the reaction via the $\mathbf{D_1}$ cation (see Figure S11 for the detailed mechanism).

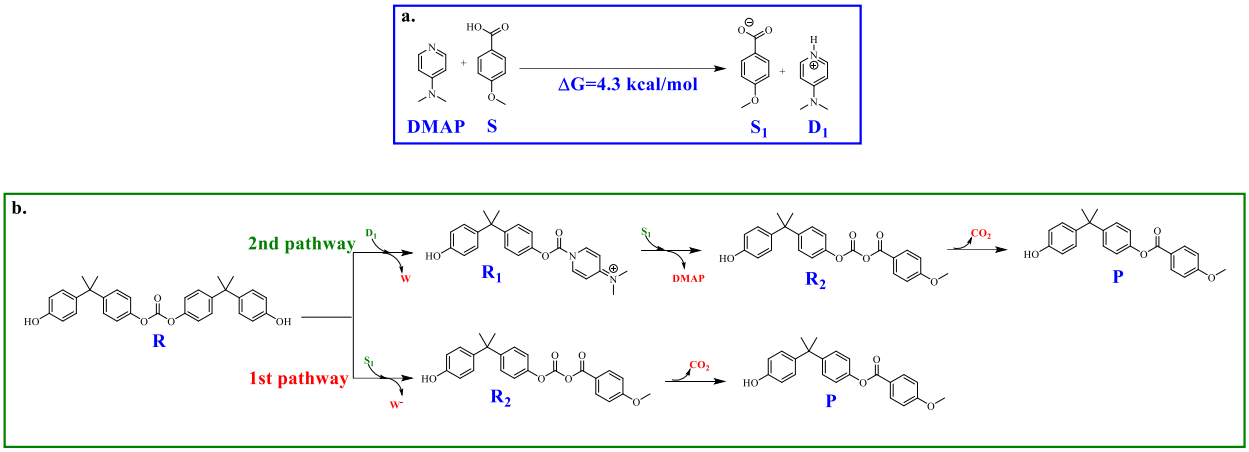


Figure S9: (a) Free energy value of reaction DMAP and *p*-anisic acid (**S**), (b) Two possible pathways of depolymerization of **PC-BPA**.

(i) First pathway: DMAP acts solely as a base

In this pathway, **S** first reacts with **DMAP** to form $\mathbf{D_1}$ and $\mathbf{S_1}$ (ΔG = 4.3 kcal/mol). In the second step (see Fig. S2), $\mathbf{S_1}$ acts as a nucleophile and reacts with **R** to form $\mathbf{R_2}$ and $\mathbf{W^-}$. This step is highly endothermic (ΔG = 15.7 kcal/mol) which is difficult to occur at even high temperature (140 °C). The final step is highly exothermic (ΔG = –26.8 kcal/mol), involving CO_2 elimination from $\mathbf{R_2}$ to yield the product **P**.

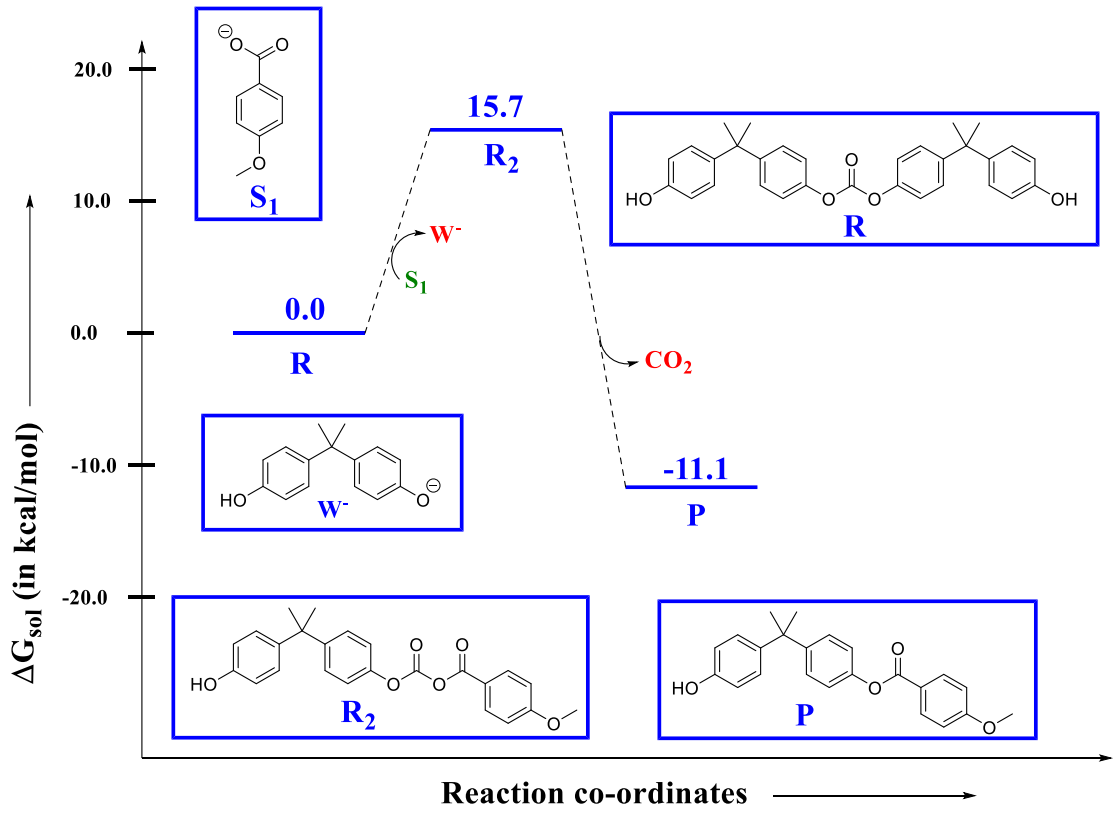


Figure S10:- Reaction pathway where DMAP acts solely as a base.

(ii) Second pathway: DMAP Acts as a Base and Actively Participates via the **D_1** Cation

In this pathway, the first step is the same as before, where **S** reacts with **DMAP** to form **D_1** and **S_1** (ΔG = 4.3 kcal/mol). In the second step (see Fig. S3), **D_1** (instead of **S_1**) acts as a nucleophile and reacts with **R** to form **R_1** and **W** (ΔG = 8.4 kcal/mol). **R_1** is more stable than **R_2** (from the first pathway) due to better delocalization of the negative charge in **R_1**. In the next step, **S_1** reacts with **R_1** to form **R_2**, and **DMAP** is regenerated (ΔG = –5.3 kcal/mol). The final step, which is also highly exothermic (ΔG = –26.8 kcal/mol), involves CO_2 elimination from **R_2** to produce **P**.

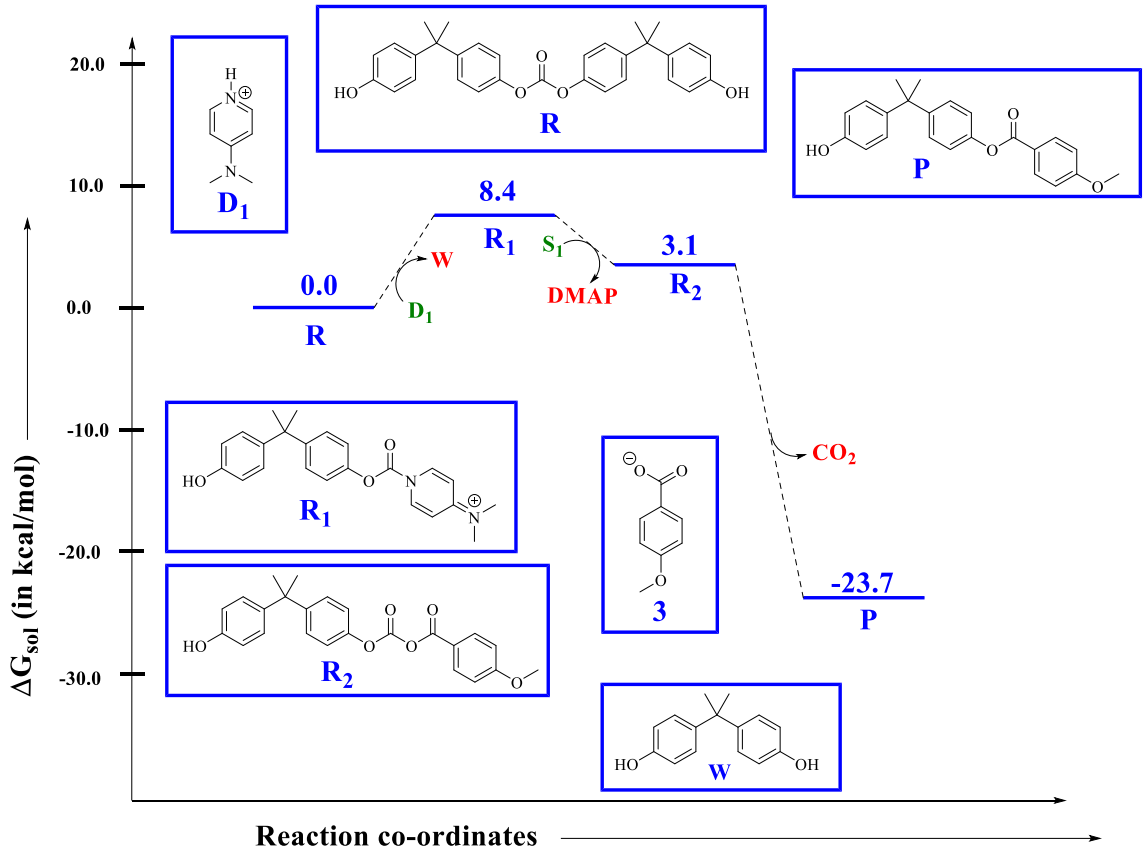


Figure 11: Reaction pathway where **DMAP** acts as a base and actively participates via the **D_1** cation.

From the DFT calculations, it is clear that the formation of **R_2** from **R** is more thermodynamically feasible in the second pathway (ΔG = 3.1 kcal/mol) compared to the first pathway (ΔG = 15.7 kcal/mol). Overall, the second pathway is more exothermic (ΔG = –23.7

kcal/mol) than the first pathway (ΔG = –11.1 kcal/mol). Therefore, the DFT results indicate that the reaction is more likely to proceed via the second pathway.

XYZ Co-ordinates

DMAP

E (in Hartree) = -382.297853468

C	0.433157	-0.614350	0.459067
C	1.809230	-0.437409	0.520226
C	2.426483	0.553660	-0.291052
C	1.547020	1.300800	-1.121546
C	0.184826	1.031744	-1.095245
N	-0.402771	0.092814	-0.327121
H	-0.029488	-1.376731	1.084265
H	2.387700	-1.064012	1.188689
H	1.913269	2.081070	-1.778157
H	-0.480109	1.610440	-1.734871
N	3.771793	0.772879	-0.273881
C	4.359529	1.793240	-1.135885
H	3.972346	2.792947	-0.896318
H	5.440525	1.801243	-0.992124
H	4.156010	1.587574	-2.195360
C	4.631429	-0.011545	0.606656
H	4.588359	-1.081399	0.361159
H	5.662171	0.325142	0.490417
H	4.346398	0.114051	1.659822

D_1

E (in Hartree) = -382.7664956

C	0.457482	-0.615937	0.507687
C	1.813803	-0.429568	0.542523
C	2.428460	0.564791	-0.285521

C	1.552187	1.325209	-1.125986
C	0.203610	1.087360	-1.113220
N	-0.327790	0.132430	-0.308086
H	-0.048836	-1.354723	1.117351
H	2.396058	-1.049346	1.210602
H	1.927421	2.095001	-1.786356
H	-0.494894	1.637003	-1.732762
N	3.755827	0.773329	-0.274261
C	4.351784	1.813359	-1.118536
H	3.934658	2.798017	-0.877577
H	5.425793	1.840370	-0.938628
H	4.179559	1.601824	-2.180572
C	4.627825	-0.036237	0.582261
H	4.536593	-1.100749	0.337025
H	5.661277	0.267590	0.420196
H	4.381654	0.109472	1.640817
H	-1.331865	-0.024658	-0.315977

S

E (in Hartree) = -535.398875838

C	-0.250256	-0.747957	-0.121667
C	1.115502	-0.598461	-0.351771
C	1.636206	0.682940	-0.607217
C	0.775443	1.797349	-0.627692
C	-0.582188	1.635198	-0.397001
C	-1.115875	0.356030	-0.139913
H	-0.652986	-1.736796	0.075557
H	1.757015	-1.471774	-0.330727
H	1.193369	2.780026	-0.826399
H	-1.232851	2.503008	-0.416014
O	2.943816	0.945236	-0.843791

C	3.880704	-0.143166	-0.838387
H	3.637215	-0.875334	-1.617491
H	4.852337	0.306891	-1.048967
H	3.906863	-0.634341	0.141605
C	-2.554088	0.136759	0.110972
O	-3.073774	-0.947665	0.338767
O	-3.288376	1.277891	0.068141
H	-4.219686	1.036007	0.244110

S_1

E (in Hartree) = -534.927151229

C	-0.253502	-0.730208	-0.123546
C	1.120461	-0.587594	-0.353970
C	1.647475	0.687554	-0.609449
C	0.787897	1.799568	-0.629756
C	-0.574858	1.633169	-0.397795
C	-1.125950	0.365034	-0.139580
H	-0.662014	-1.717050	0.074268
H	1.758932	-1.464313	-0.331940
H	1.206863	2.783048	-0.828718
H	-1.236341	2.494379	-0.414169
O	2.967277	0.947583	-0.847638
C	3.888368	-0.147698	-0.839019
H	3.640926	-0.881988	-1.616250
H	4.867673	0.287504	-1.048906
H	3.910599	-0.641375	0.140922
C	-2.628269	0.189220	0.115095
O	-3.032091	-0.988980	0.338377
O	-3.335367	1.237981	0.080081

R

E (in Hartree) =

C	-2.955468	-0.918351	0.513581
C	-4.076965	-0.106282	0.676251
C	-4.412866	0.885369	-0.264056
C	-3.585041	1.032746	-1.385548
C	-2.457564	0.222430	-1.568850
C	-2.158132	-0.737587	-0.612902
H	-2.702521	-1.681741	1.243838
H	-4.708710	-0.254073	1.548001
H	-3.804900	1.777919	-2.141787
H	-1.822208	0.339061	-2.442398
C	-5.652118	1.765537	-0.008549
C	-6.880560	0.854007	0.178244
C	-7.188360	-0.094323	-0.812747
C	-7.741343	0.932388	1.281948
C	-8.302933	-0.927220	-0.716670
H	-6.539910	-0.193211	-1.680103
C	-8.863501	0.104202	1.396969
H	-7.552574	1.642634	2.080336
C	-9.147518	-0.827623	0.396817
H	-8.513644	-1.653316	-1.499968
H	-9.517904	0.177072	2.261725
C	-5.362876	2.631878	1.239058
H	-4.457702	3.225423	1.067742
H	-6.187614	3.326653	1.436581
H	-5.203049	2.023920	2.135799
C	-5.946475	2.727234	-1.182147
H	-6.850585	3.304215	-0.957373
H	-5.123877	3.436896	-1.331526
H	-6.115082	2.190607	-2.122001

O	-10.258791	-1.617779	0.555399
H	-10.343835	-2.221012	-0.204569
O	-1.065932	-1.604889	-0.819300
C	0.144436	-1.169767	-0.419854
O	0.391723	-0.113338	0.114425
C	2.378803	-1.896714	-0.414114
C	2.890885	-2.368701	0.785293
C	3.183827	-1.246388	-1.345524
C	4.250754	-2.178582	1.063226
H	2.240604	-2.872768	1.494742
C	4.533363	-1.062616	-1.049746
H	2.757499	-0.886258	-2.277640
C	5.094148	-1.522856	0.156437
H	4.634409	-2.550269	2.006804
H	5.161123	-0.543015	-1.768730
C	6.598617	-1.305282	0.410342
C	7.376474	-2.180924	-0.599221
H	7.170144	-1.897369	-1.636812
H	8.457661	-2.112038	-0.430940
H	7.083756	-3.229302	-0.471493
C	7.027102	-1.741865	1.829918
H	8.094218	-1.532435	1.964687
H	6.477452	-1.203453	2.609417
H	6.874944	-2.817539	1.979452
C	6.916202	0.194692	0.258492
C	6.190066	1.131992	1.017227
C	7.918568	0.689228	-0.584270
C	6.448347	2.498760	0.943898
H	5.396692	0.786645	1.676009
C	8.192841	2.060686	-0.672193
H	8.508919	0.015014	-1.195858

C	7.457077	2.968196	0.092915
H	5.874296	3.206970	1.535752
H	8.977098	2.416973	-1.337906
O	7.672617	4.323111	0.051733
H	8.392255	4.522138	-0.573796
O	1.025920	-2.140847	-0.726424

R_2

E (in Hartree) = -1379.28769135

C	-1.465172	-0.467442	0.743609
C	-2.774096	0.010057	0.792588
C	-3.222482	1.025730	-0.072415
C	-2.310925	1.546941	-1.000638
C	-0.992918	1.078039	-1.067695
C	-0.592025	0.081924	-0.190220
H	-1.125348	-1.251185	1.414672
H	-3.462300	-0.422251	1.514121
H	-2.609716	2.326115	-1.693093
H	-0.291080	1.483912	-1.790758
C	-4.670731	1.534631	0.060390
C	-5.636271	0.338413	-0.042602
C	-5.556264	-0.517186	-1.154913
C	-6.629527	0.065143	0.908228
C	-6.424980	-1.596030	-1.319985
H	-4.793663	-0.344878	-1.910777
C	-7.509158	-1.013105	0.761057
H	-6.736875	0.689698	1.788951
C	-7.409435	-1.846323	-0.354755
H	-6.336116	-2.241864	-2.192002
H	-8.271480	-1.211128	1.510075

C	-4.781882	2.270218	1.416206
H	-4.046574	3.082040	1.451131
H	-5.776305	2.713287	1.544801
H	-4.588767	1.602954	2.262926
C	-5.044963	2.544651	-1.048623
H	-6.091450	2.845082	-0.924538
H	-4.427327	3.448787	-0.989812
H	-4.934252	2.115094	-2.050194
O	-8.294562	-2.890784	-0.454042
H	-8.120773	-3.391705	-1.271079
O	0.717413	-0.439802	-0.295065
C	1.670696	0.160096	0.435667
O	1.528203	1.069089	1.213333
O	2.854198	-0.409785	0.079929
C	3.893021	-0.496667	1.031490
O	3.645267	-0.702215	2.197493
C	5.212454	-0.382030	0.408501
C	6.348239	-0.600684	1.208202
C	5.386963	-0.047523	-0.951368
C	7.629930	-0.490809	0.680781
H	6.222476	-0.860514	2.254881
C	6.659342	0.066376	-1.486101
H	4.525384	0.127163	-1.586447
C	7.791765	-0.152702	-0.676580
H	8.485944	-0.667413	1.321432
H	6.802748	0.327739	-2.530323
O	8.986959	-0.014880	-1.290584
C	10.189999	-0.201055	-0.525793
H	10.251020	-1.222778	-0.133770

H	11.008844	-0.026629	-1.225501
H	10.246312	0.521523	0.296595

W$^-$

E (in Hartree) = -731.265292125

C	-0.094665	-0.688966	1.190975
C	1.223743	-0.367967	0.878199
C	1.564043	0.711000	0.035352
C	0.488726	1.453905	-0.480890
C	-0.843263	1.149903	-0.179437
C	-1.216455	0.057203	0.676670
H	-0.306681	-1.530841	1.850828
H	2.023153	-0.969269	1.312532
H	0.679296	2.301613	-1.135273
H	-1.643112	1.758987	-0.601660
C	3.043645	0.998320	-0.282296
C	3.827271	1.167907	1.035394
C	3.376522	2.097294	1.989924
C	4.997020	0.457605	1.341153
C	4.054913	2.315405	3.188994
H	2.465064	2.658503	1.798732
C	5.689777	0.657725	2.541747
H	5.392280	-0.276431	0.646568
C	5.220329	1.589248	3.468627
H	3.678539	3.040932	3.908562
H	6.591529	0.091566	2.761175
C	3.599730	-0.162663	-1.140205
H	2.998217	-0.258075	-2.051662
H	4.639459	0.015715	-1.443314

H	3.556810	-1.120386	-0.609480
C	3.226897	2.297794	-1.102392
H	4.294887	2.476699	-1.275209
H	2.737656	2.222036	-2.081136
H	2.819270	3.172428	-0.583433
O	5.931597	1.752550	4.632822
H	5.497307	2.422532	5.190367
O	-2.438863	-0.231389	0.963507

CO_2

E (in Hartree) = -188.592651110

C	-1.938246	-0.621930	-0.521943
O	-2.995470	-0.621930	-1.021597
O	-0.881021	-0.621930	-0.022289

P

E (in Hartree) = -1190.71266912

C	-0.229087	-0.344597	0.538752
C	1.150401	-0.162002	0.459246
C	1.713912	0.904867	-0.265976
C	0.839881	1.790367	-0.910309
C	-0.549381	1.622011	-0.839967
C	-1.067477	0.555660	-0.117302
H	-0.654235	-1.169624	1.103614
H	1.801494	-0.858212	0.981661
H	1.223310	2.632607	-1.475714
H	-1.220456	2.315651	-1.339060
C	3.248195	1.039592	-0.327502
C	3.798363	1.099606	1.110765

C	3.307941	2.078220	1.993041
C	4.788328	0.234491	1.597000
C	3.780002	2.196067	3.300153
H	2.532031	2.762352	1.657441
C	5.273071	0.335739	2.906029
H	5.200903	-0.543356	0.962976
C	4.769910	1.318143	3.760887
H	3.380091	2.963058	3.961066
H	6.038421	-0.346785	3.266327
C	3.796827	-0.168861	-1.120359
H	3.346336	-0.182996	-2.119331
H	4.884020	-0.099464	-1.243432
H	3.565946	-1.121968	-0.633094
C	3.699201	2.320443	-1.066195
H	4.793457	2.378739	-1.053331
H	3.375790	2.311348	-2.114078
H	3.308683	3.227665	-0.592959
O	5.274926	1.377853	5.035888
H	4.843829	2.100543	5.526308
O	-2.457423	0.434072	0.018776
C	-3.115651	-0.428684	-0.815395
O	-2.543723	-1.073711	-1.677309
C	-5.375328	-1.315077	-1.328857
C	-5.171046	0.297630	0.465463
C	-6.741800	-1.389471	-1.112233
H	-4.918426	-1.913204	-2.111242
C	-6.545208	0.232447	0.693130
H	-4.567728	0.954915	1.082521
C	-7.339490	-0.614969	-0.098406

H	-7.368330	-2.040340	-1.715352
H	-6.981615	0.837882	1.478874
C	-4.567308	-0.469619	-0.542907
O	-8.680220	-0.754607	0.036237
C	-9.358322	0.008785	1.045906
H	-8.989859	-0.246946	2.046414
H	-9.243662	1.084627	0.868125
H	-10.411020	-0.266536	0.962100

R_1

E (in Hartree) = -1226.65479269

C	-0.715316	-0.116517	-0.903835
C	-2.072294	-0.434799	-0.871662
C	-2.641792	-1.131573	0.210285
C	-1.802519	-1.498006	1.271564
C	-0.438020	-1.183267	1.262650
C	0.077339	-0.501464	0.171655
H	-0.281306	0.423911	-1.740111
H	-2.701069	-0.124127	-1.701520
H	-2.195907	-2.029221	2.130870
H	0.206811	-1.462695	2.090934
C	-4.146433	-1.463033	0.174373
C	-4.934887	-0.149924	0.003073
C	-4.740620	0.893068	0.925544
C	-5.863641	0.065716	-1.024508
C	-5.439048	2.096985	0.835621
H	-4.021788	0.769497	1.732318
C	-6.572572	1.267441	-1.132184
H	-6.052437	-0.701553	-1.768227

C	-6.362271	2.286275	-0.201103
H	-5.266442	2.887410	1.563945
H	-7.286907	1.417306	-1.937516
C	-4.384349	-2.452973	-0.989123
H	-3.773077	-3.349311	-0.834711
H	-5.434307	-2.765266	-1.030015
H	-4.115096	-2.024274	-1.959976
C	-4.631369	-2.149562	1.471468
H	-5.708644	-2.336565	1.399059
H	-4.132340	-3.114425	1.622446
H	-4.457081	-1.529010	2.356789
O	-7.080040	3.446665	-0.348765
H	-6.842612	4.072273	0.359009
O	1.438994	-0.106264	0.180239
C	2.350921	-1.005055	-0.200609
O	2.148329	-2.133837	-0.575988
N	3.665995	-0.445952	-0.113617
C	4.732266	-1.240786	-0.475266
C	3.901391	0.847923	0.303802
C	6.010575	-0.780316	-0.438953
H	4.486333	-2.246400	-0.788537
C	5.160371	1.358694	0.356063
H	3.037120	1.431656	0.585692
C	6.295191	0.565217	-0.024916
H	6.797377	-1.459321	-0.738386
H	5.271821	2.379640	0.695198
N	7.536677	1.049843	0.002939
C	8.679509	0.204675	-0.371841
H	8.601109	-0.104826	-1.419735

H	9.597437	0.775339	-0.240778
H	8.725684	-0.684091	0.266171
C	7.786764	2.440385	0.408157
H	7.498628	2.594418	1.453799
H	8.849049	2.652818	0.300687
H	7.225510	3.132445	-0.228098

W

E (in Hartree) = -731.750506204

C	-0.085250	-0.681962	1.209075
C	1.235267	-0.355697	0.900331
C	1.557438	0.715987	0.049279
C	0.491391	1.454731	-0.482814
C	-0.840121	1.144549	-0.182968
C	-1.131569	0.073908	0.664090
H	-0.302900	-1.516788	1.873260
H	2.033124	-0.947645	1.342550
H	0.679137	2.295096	-1.142891
H	-1.652872	1.731726	-0.602773
C	3.035999	1.004591	-0.275553
C	3.819125	1.170111	1.041356
C	3.377927	2.106769	1.992473
C	4.982104	0.448289	1.344291
C	4.060194	2.319933	3.190217
H	2.473961	2.680099	1.800954
C	5.679280	0.646071	2.541740
H	5.368091	-0.290621	0.649894
C	5.219585	1.583846	3.468001
H	3.692410	3.051217	3.908133

H	6.577339	0.073822	2.759912
C	3.570283	-0.165578	-1.134064
H	2.957465	-0.262253	-2.037543
H	4.605592	0.012014	-1.448995
H	3.532222	-1.120082	-0.597824
C	3.214518	2.300877	-1.099909
H	4.282470	2.478173	-1.270827
H	2.727479	2.220206	-2.079126
H	2.806421	3.176447	-0.583275
O	5.935196	1.742415	4.628836
H	5.511932	2.420262	5.185550
O	-2.451862	-0.191866	0.930410
H	-2.518459	-0.956162	1.530409

16. References

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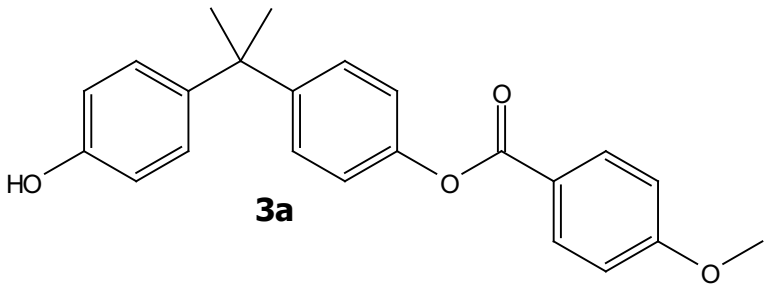
17. NMR Spectra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O
O
O

3a

8.14
8.12
7.26
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7.11
7.09
7.07
6.98
6.96
6.73
6.71
4.97
3.88
1.65
2.00
2.13
4.18
2.06
2.05
1.14
3.00
6.13
9.0
8.5
8.0
7.5
7.0
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3.0
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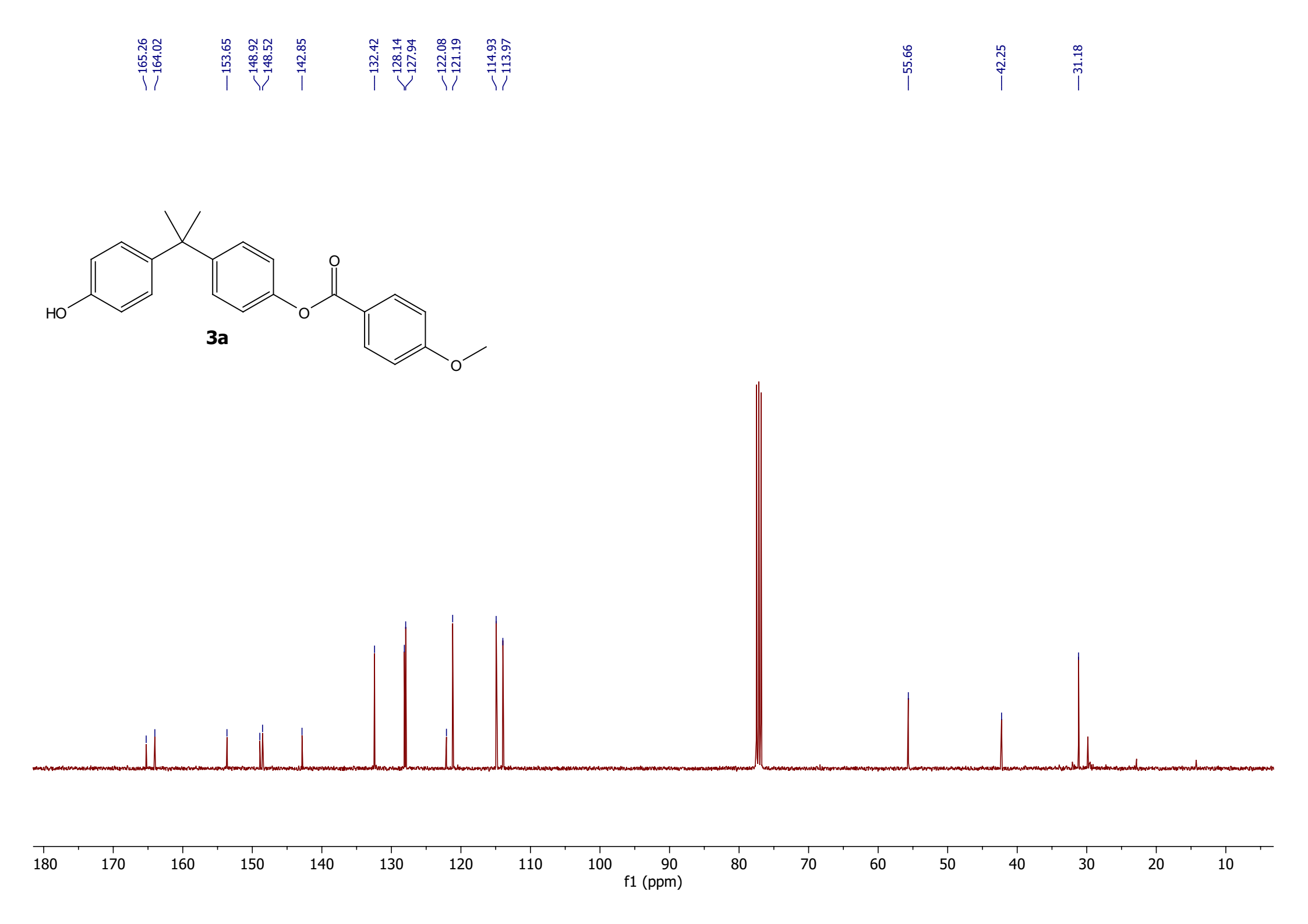
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164.02
153.65
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148.52
142.85
132.42
128.14
127.94
122.08
121.19
114.93
113.97
55.66
42.25
31.18
HO
O
O
O
3a
180
170
160
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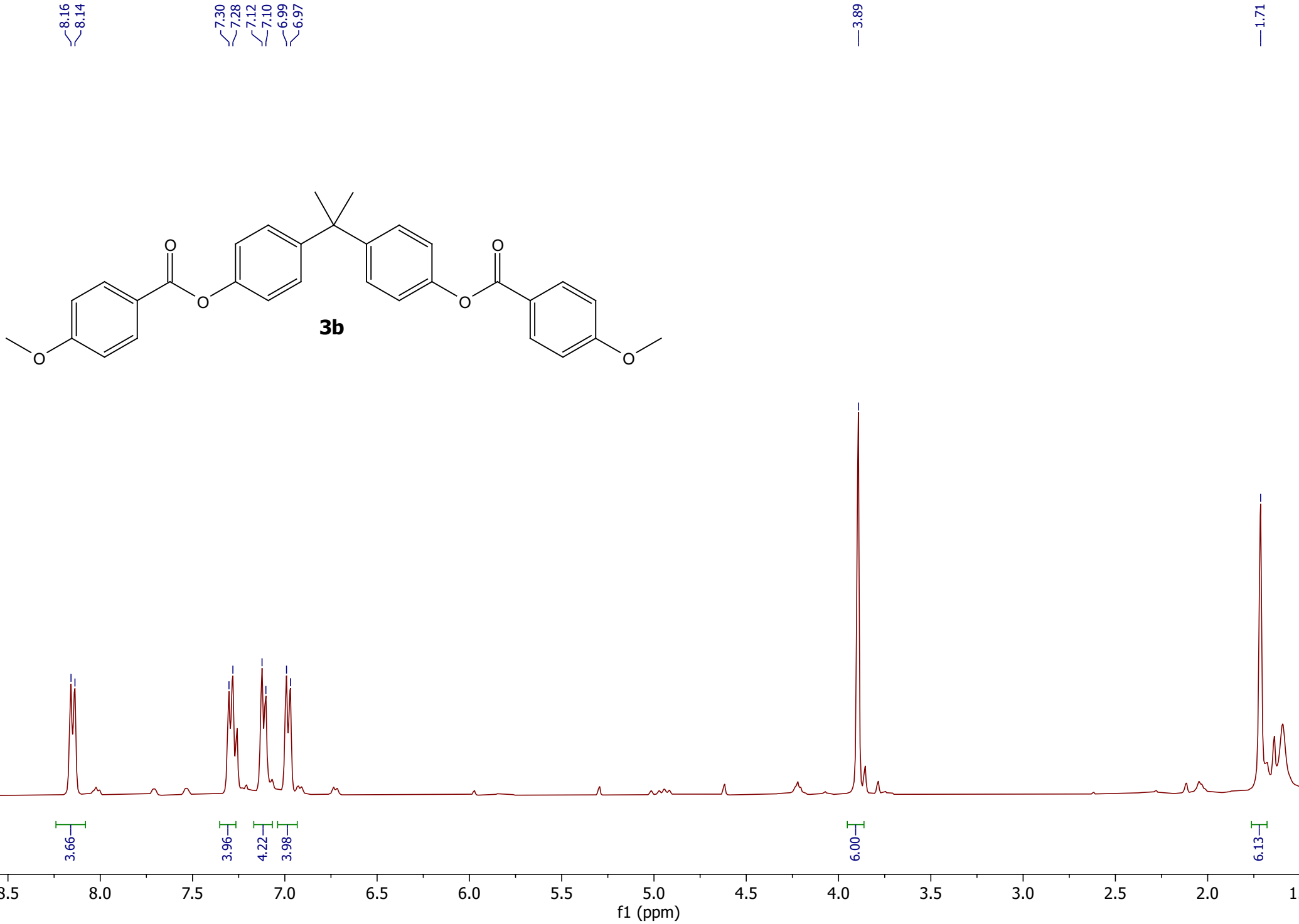
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.10
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6.97
3.89
1.71
O
O
O
O
O
O
3b
3.66
3.96
4.22
3.98
6.00
6.13
8.5
8.0
7.5
7.0
6.5
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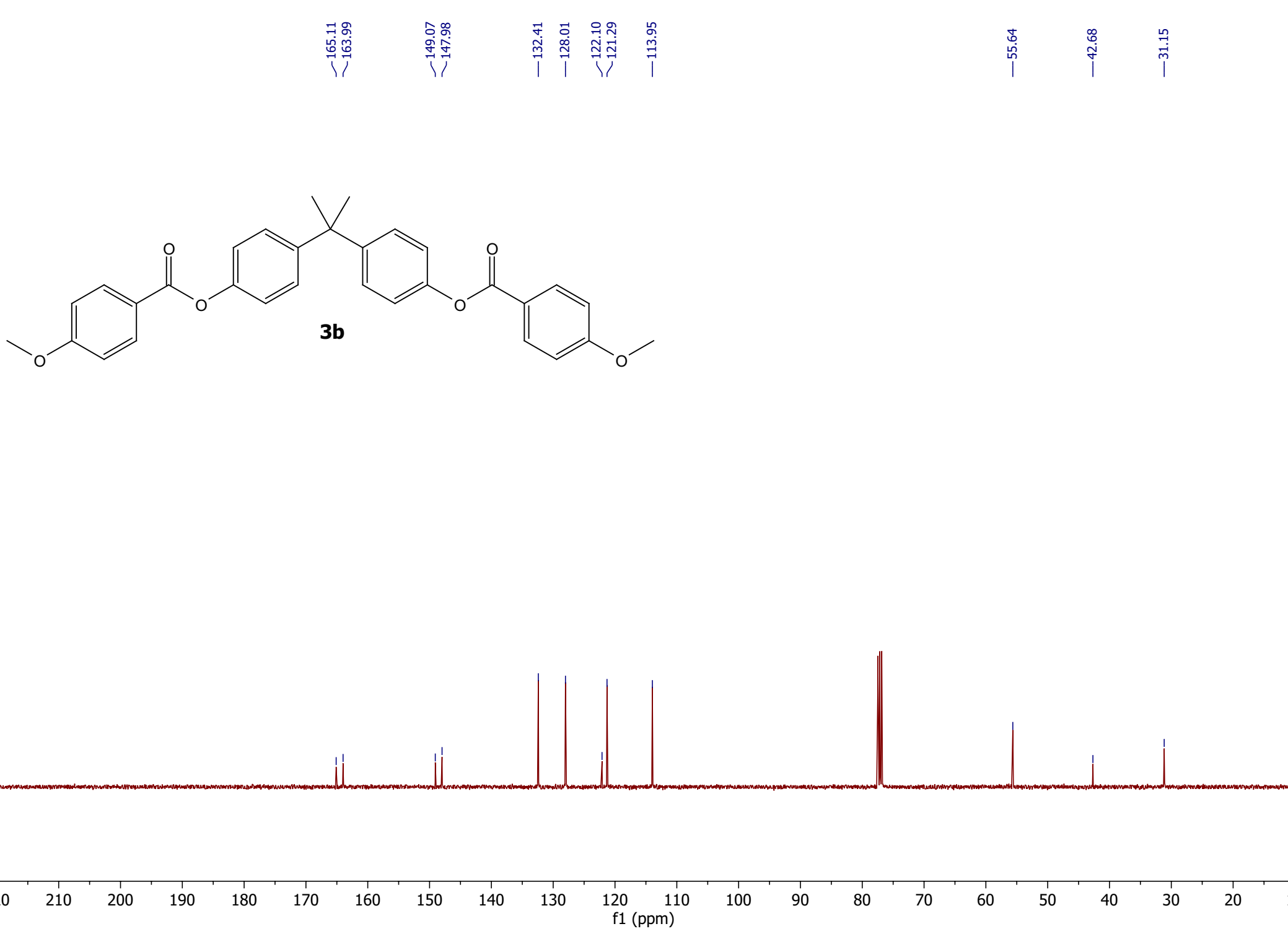
1.5
f1 (ppm)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121.29
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42.68
31.15
O
O
O
O
O
O
3b
220
210
200
190
180
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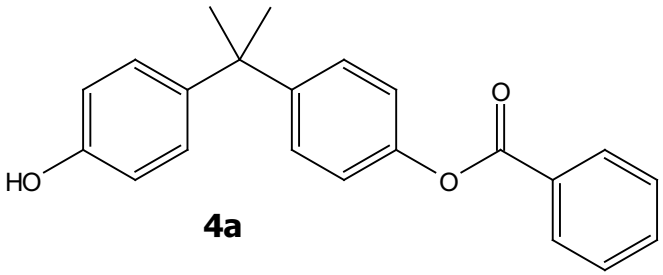
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


HO
O
O

4a

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7.23
7.09
7.07
6.72
6.70
5.03
1.64
1.92
1.00
2.00
2.31
4.06
2.00
1.01
6.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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3.0
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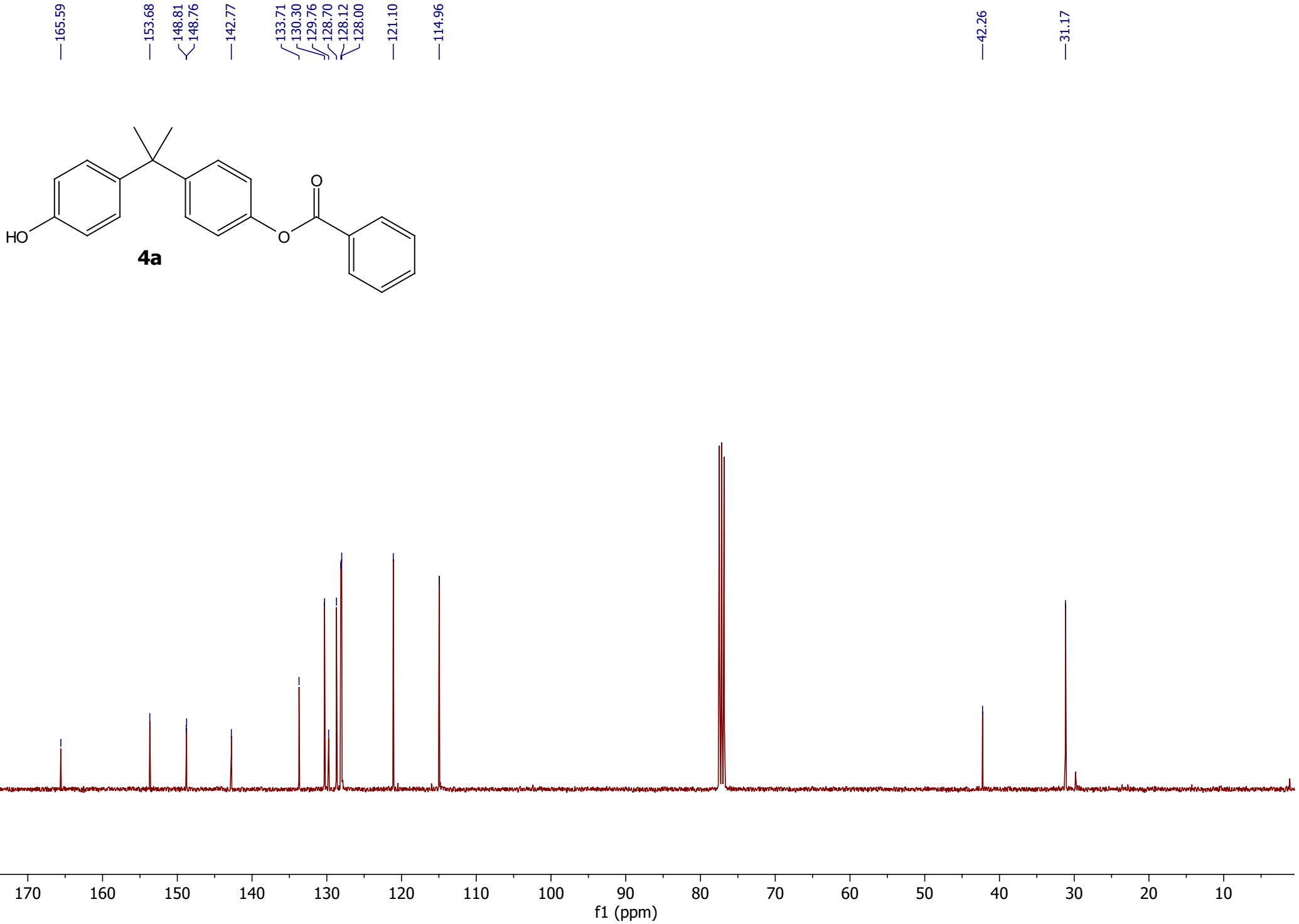
f1 (ppm)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31.17
HO
O
O
4a
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130
120
110
100
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80
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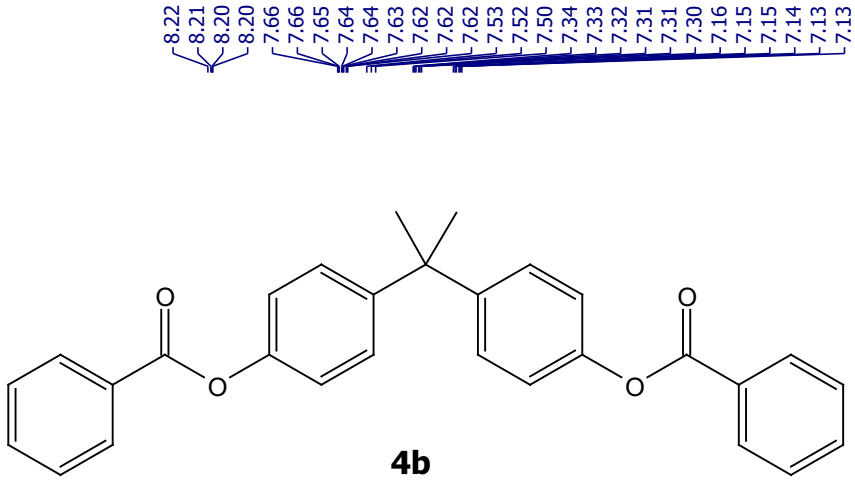
60
50
40
30
20
10
f1 (ppm)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7.64
7.64
7.63
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7.62
7.62
7.53
7.52
7.50
7.34
7.33
7.32
7.31
7.31
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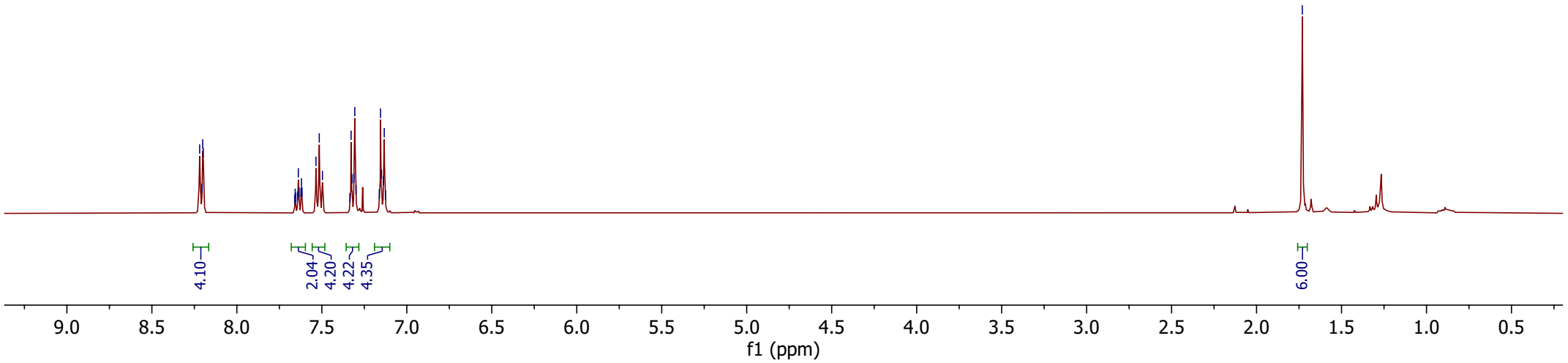
7.16
7.15
7.15
7.14
7.13
7.13
1.73
O
O
O
O
4b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8.5
8.0
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7.0
6.5
6.0
5.5
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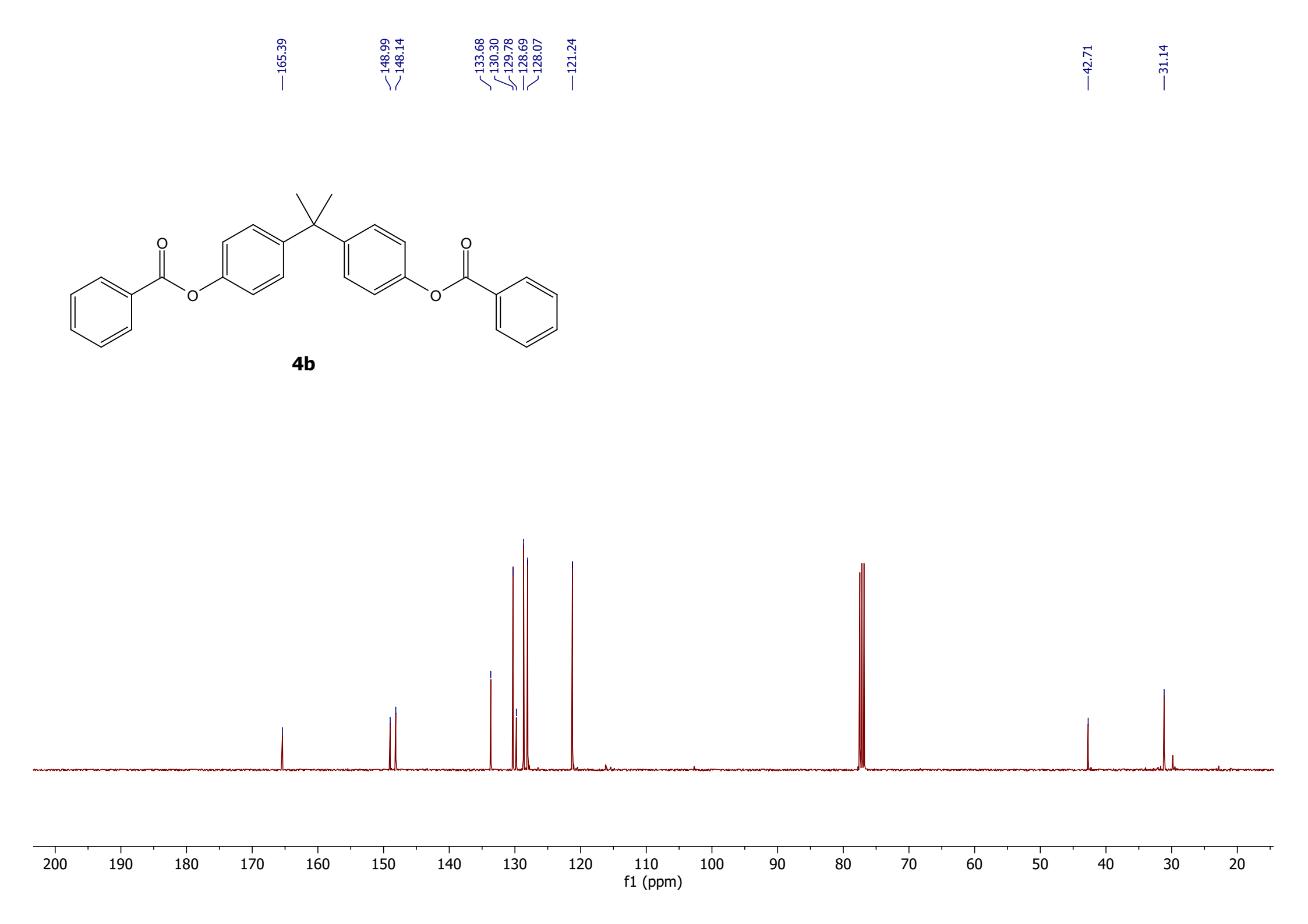
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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31.14
O
O
O
O
4b
200
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180
170
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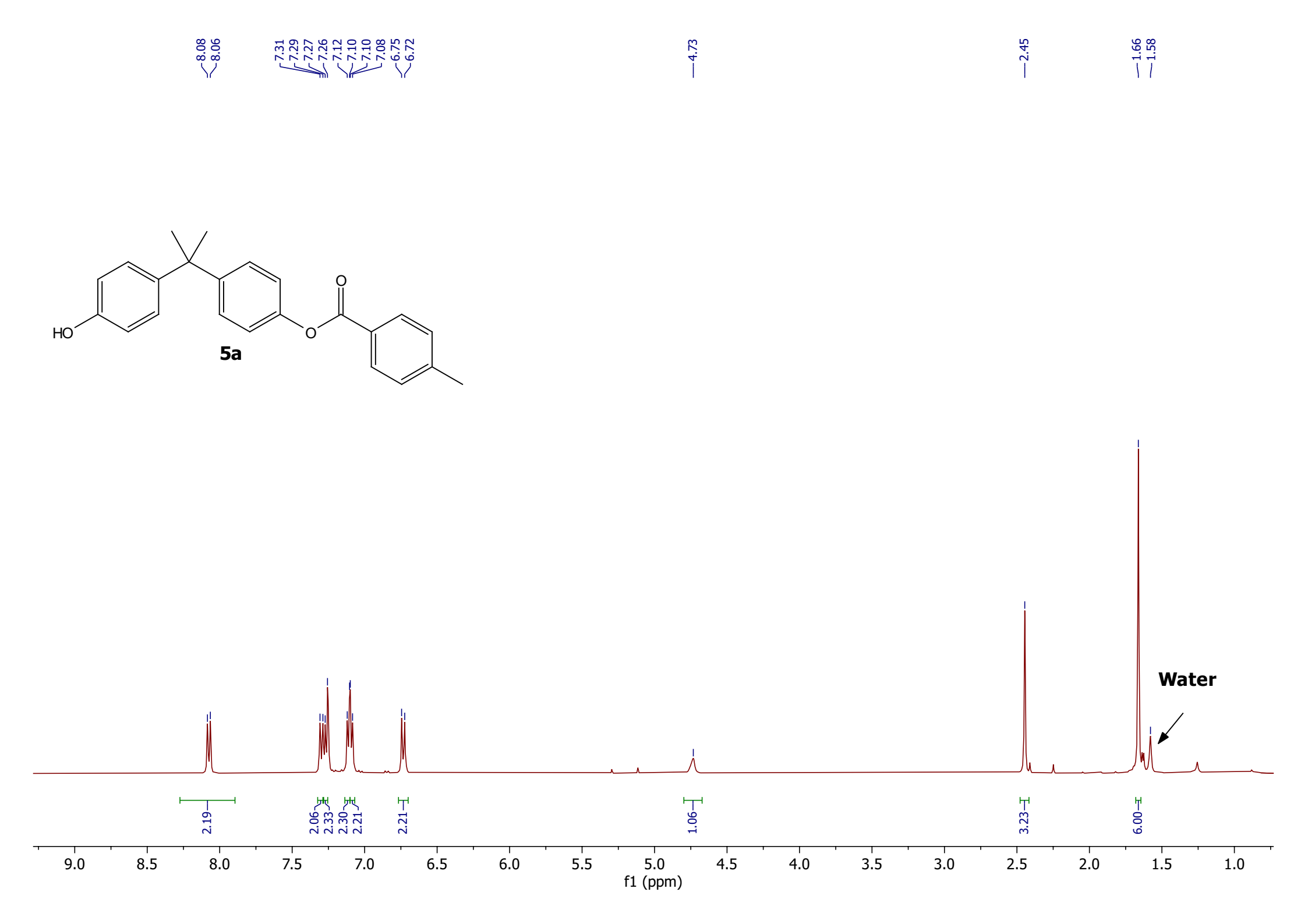
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)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2.45
1.66
1.58
HO
O
O
5a
Water
2.19
2.06
2.33
2.30
2.21
2.21
1.06
3.23
6.00
9.0
8.5
8.0
7.5
7.0
6.5
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5.5
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4.5
4.0
3.5
3.0
2.5
2.0
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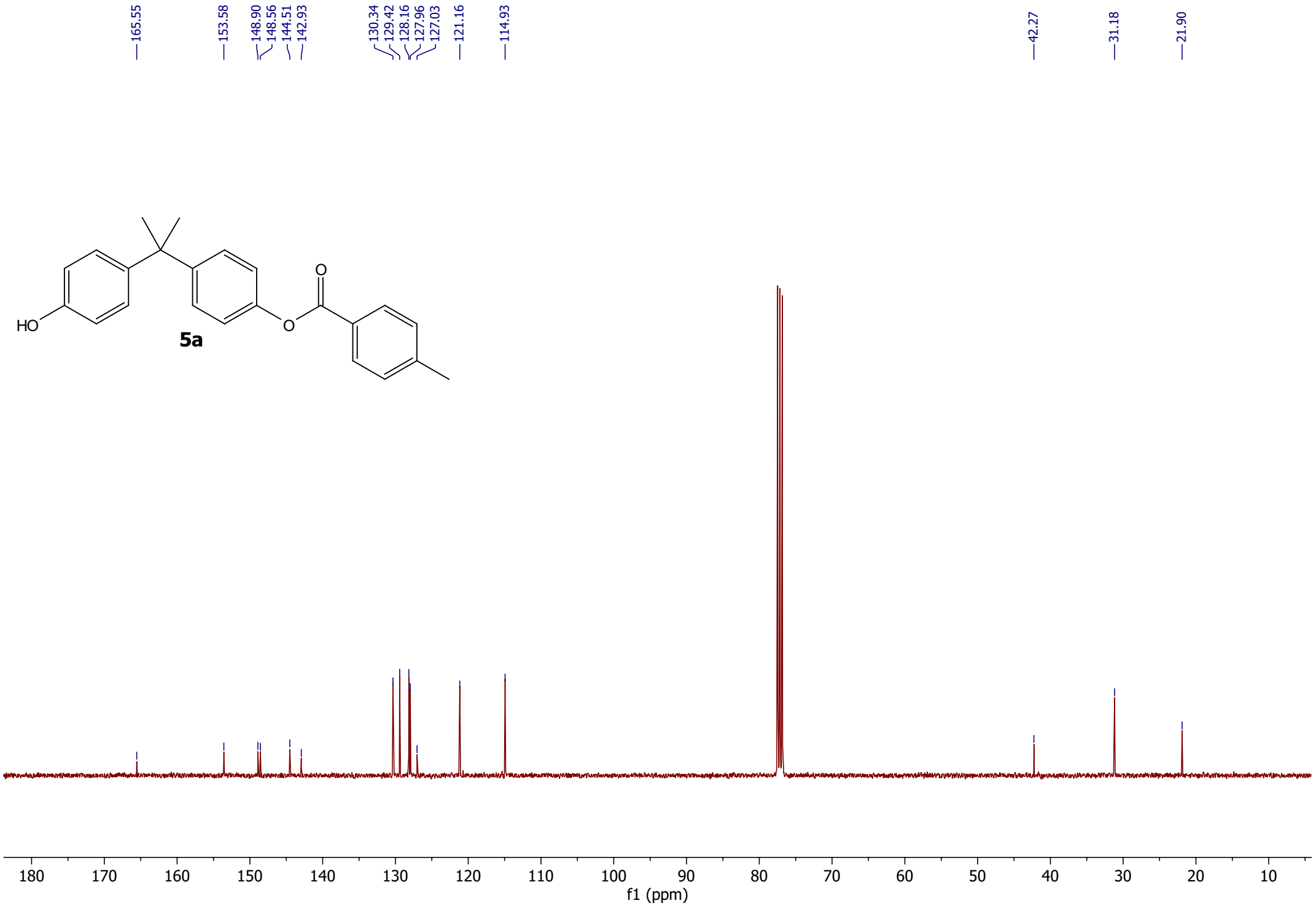
1.0
f1 (ppm)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127.03
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114.93
42.27
31.18
21.90
HO
O
O
5a
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120
110
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50
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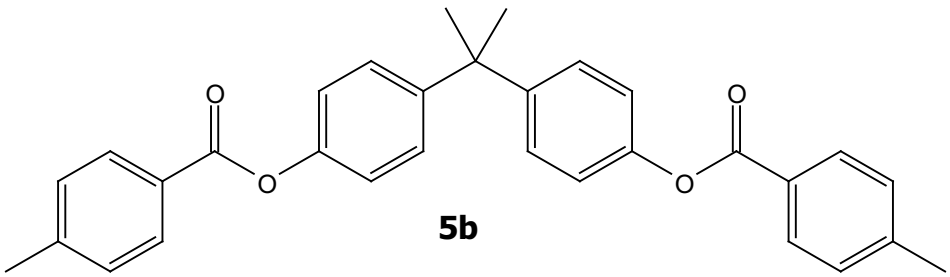
30
20
10
f1 (ppm)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O
O

5b

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7.29
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4.27
4.01
4.03
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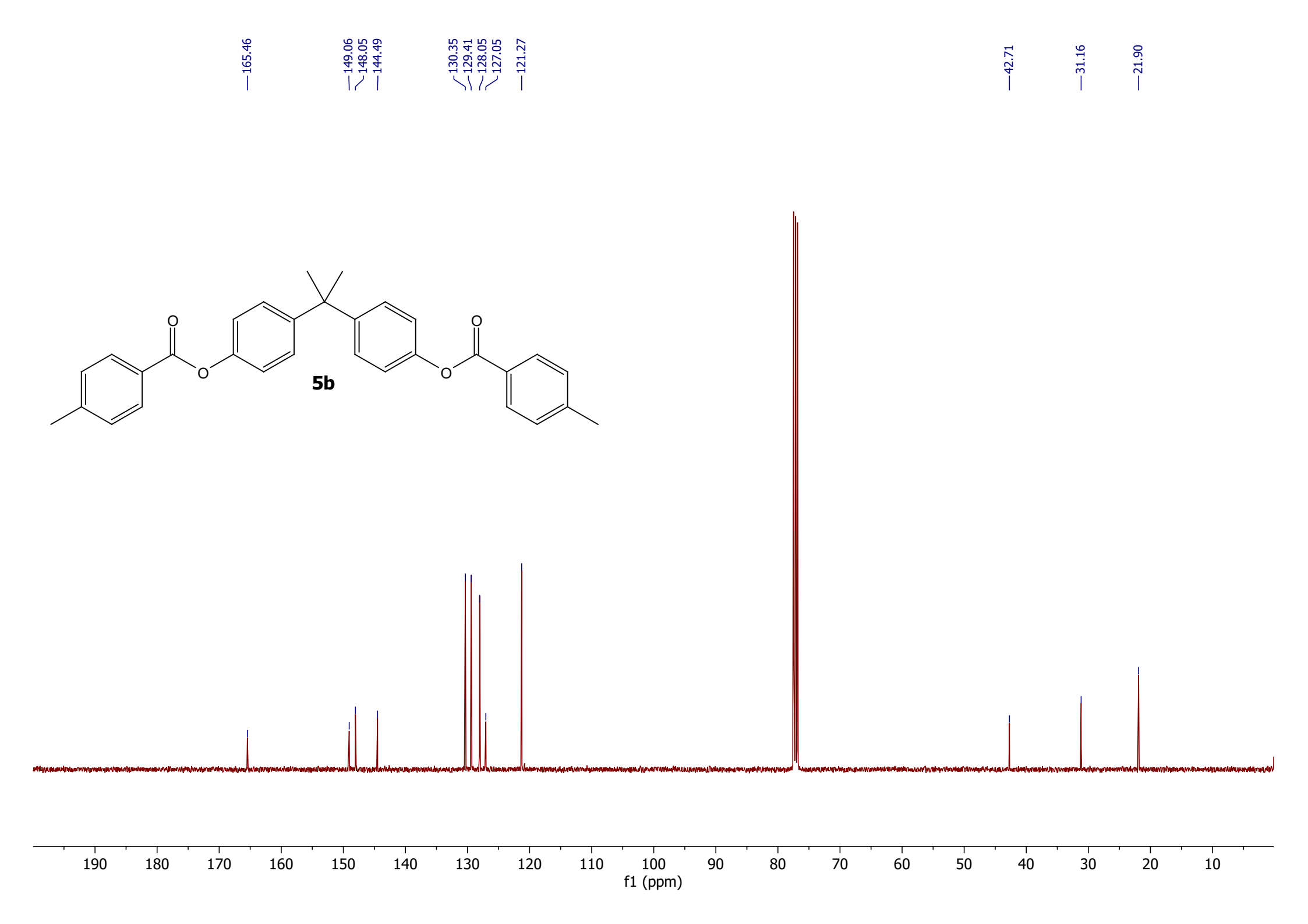
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O
O
5b
190
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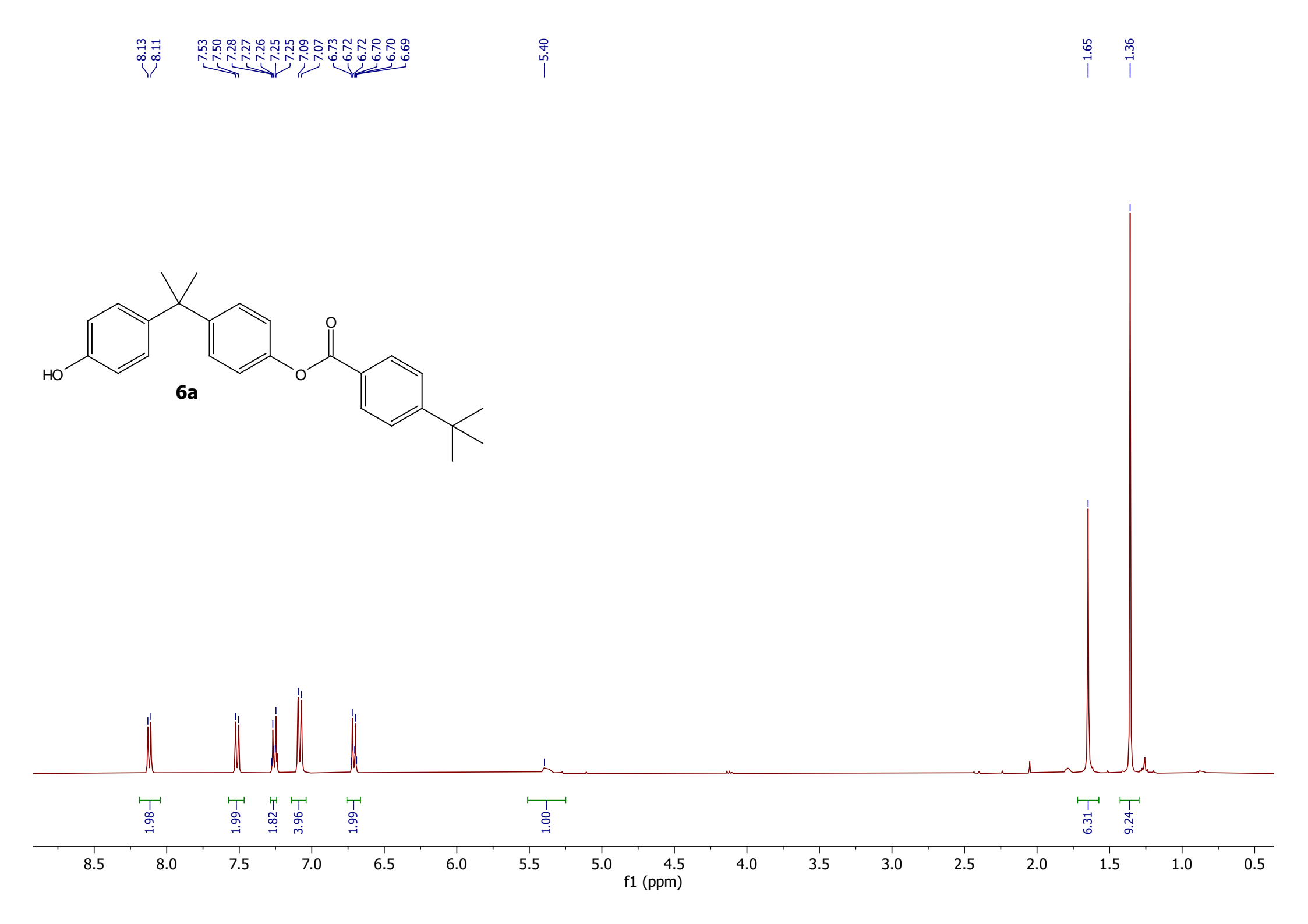
f1 (ppm)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HO
O
O
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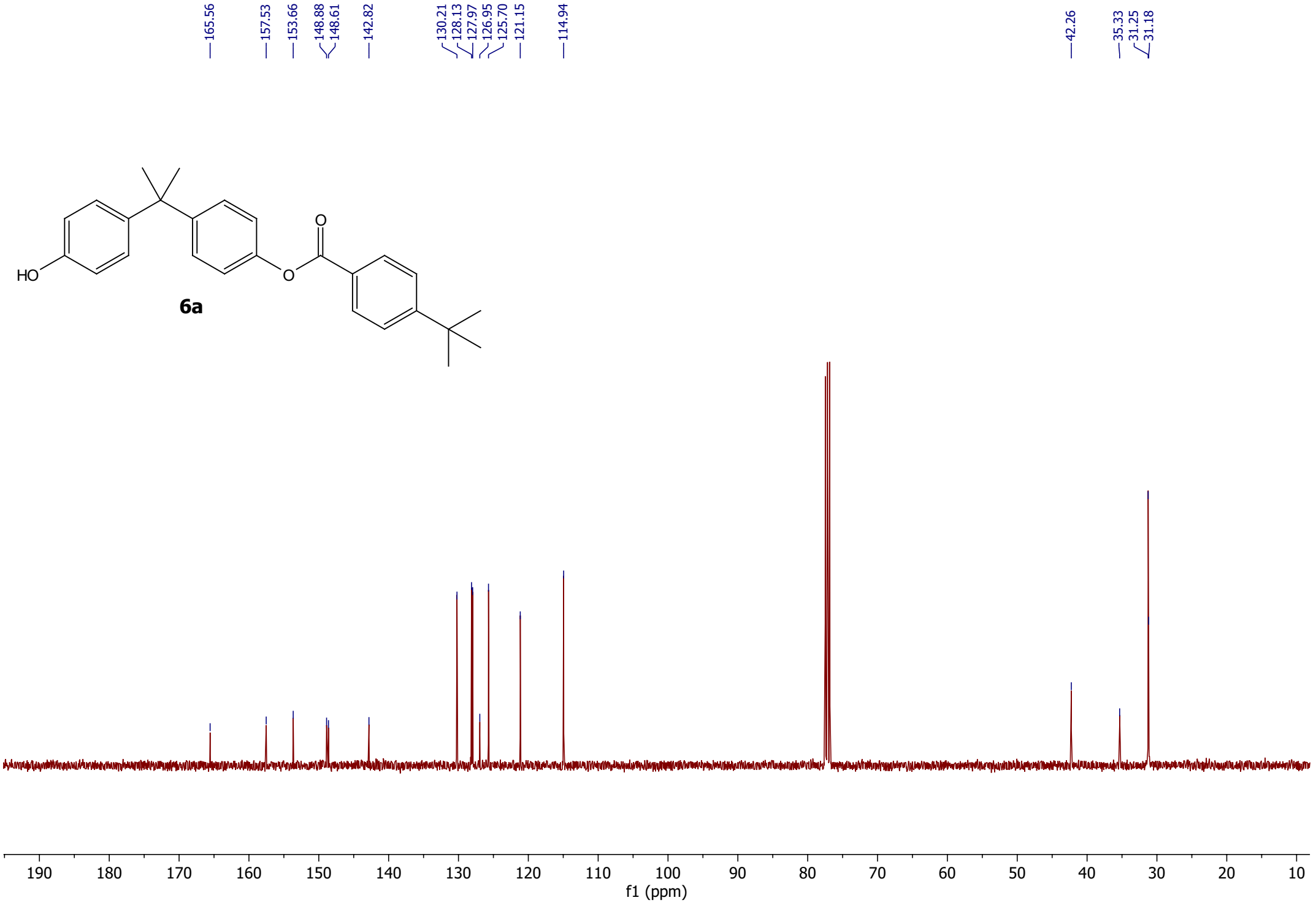
f1 (ppm)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31.18
HO
O
O
6a
190
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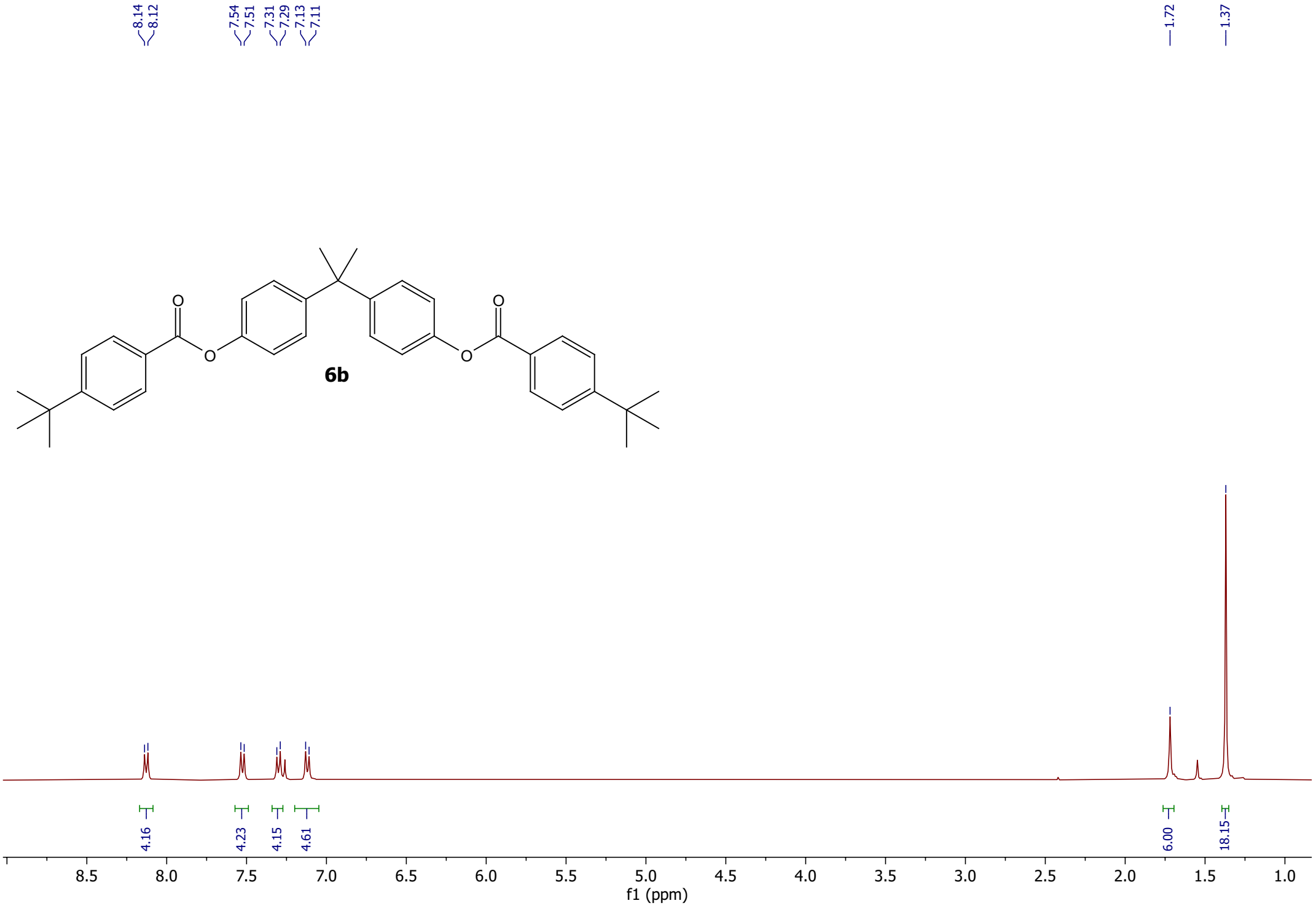
f1 (ppm)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O
6b
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4.23
4.15
4.61
6.00
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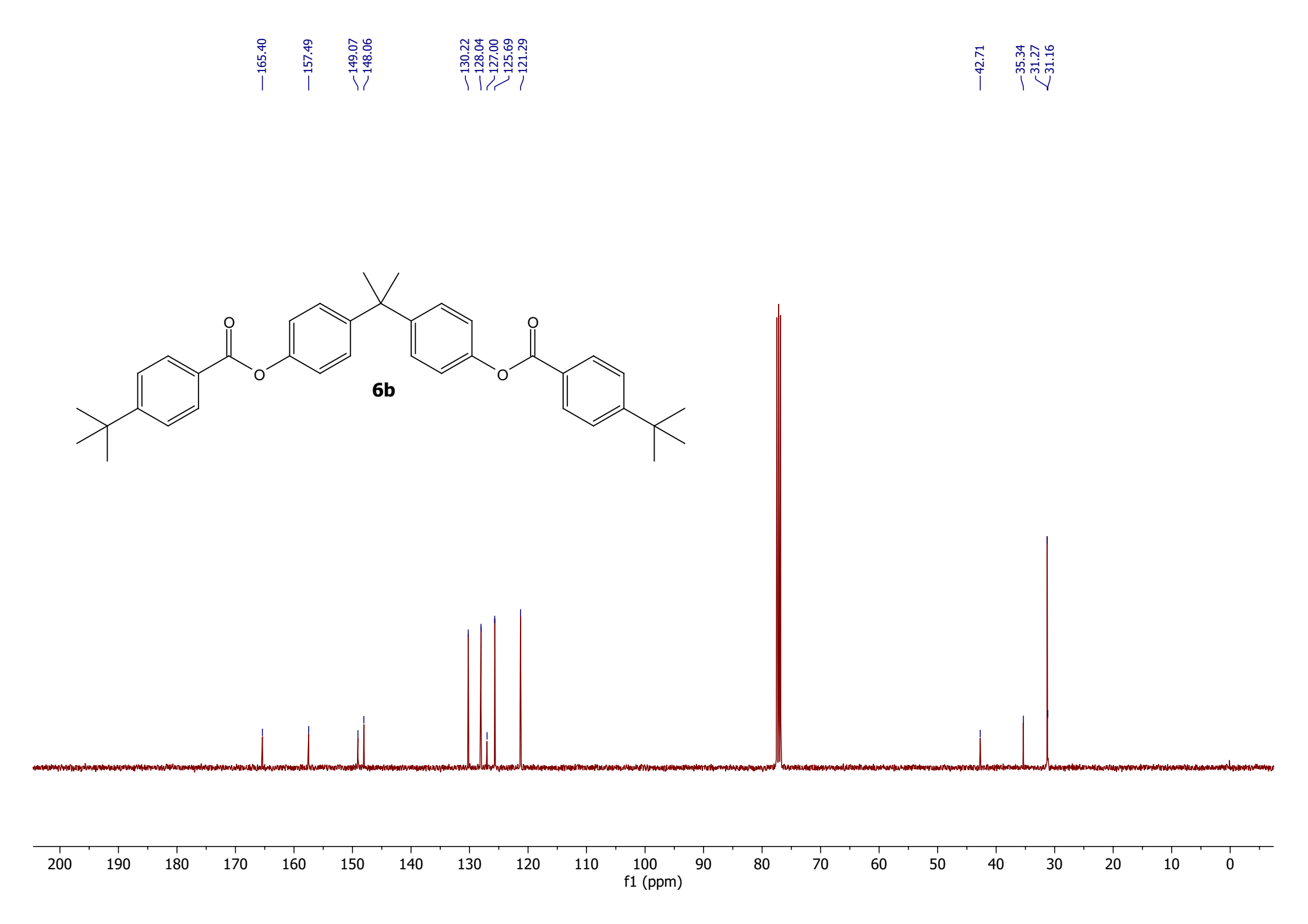
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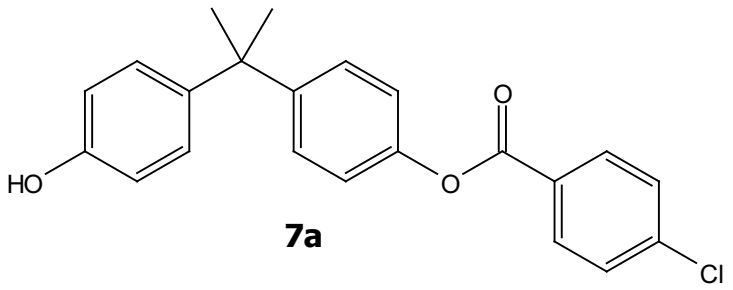
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7a

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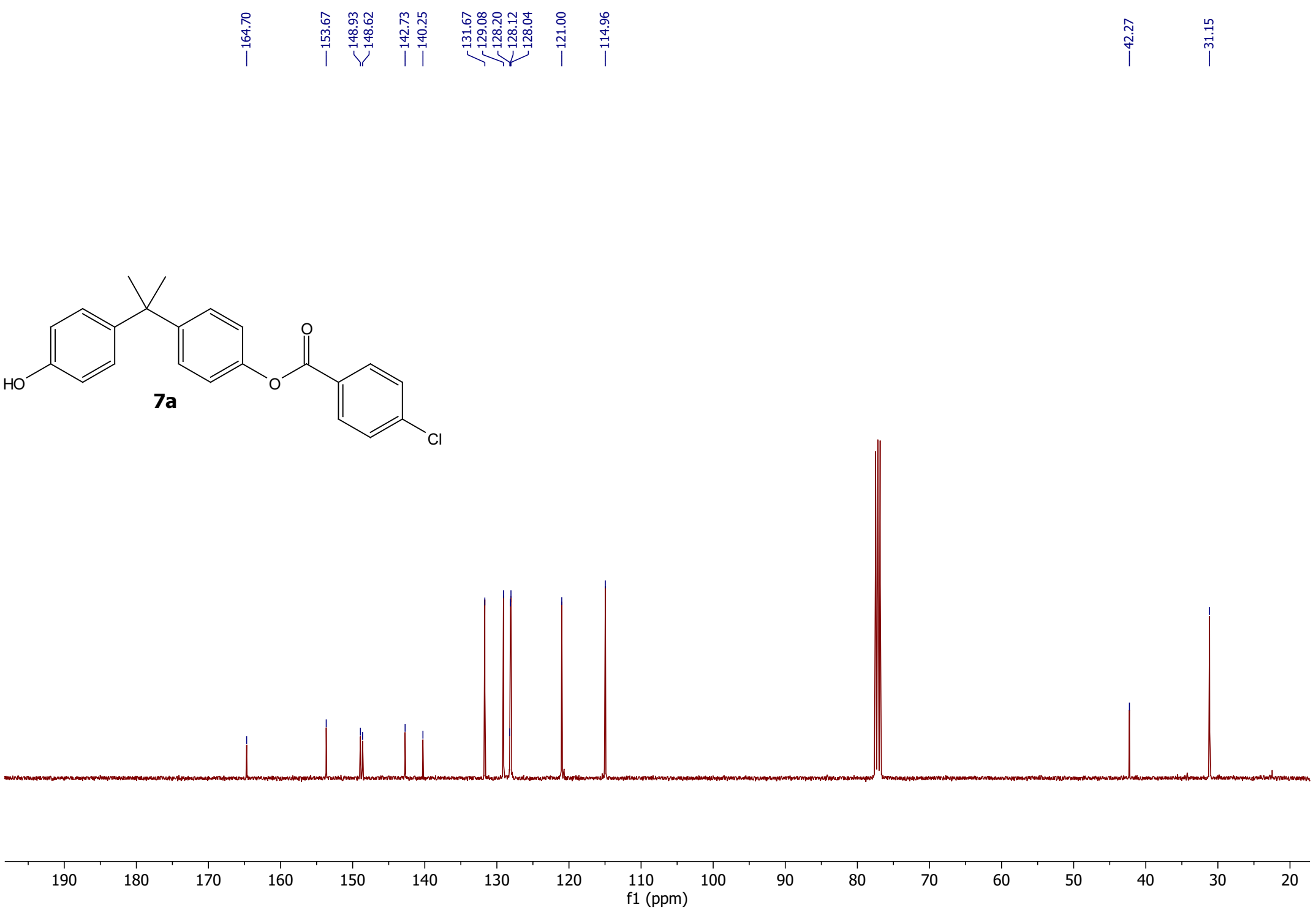
2.0
1.5
1.0
f1 (ppm)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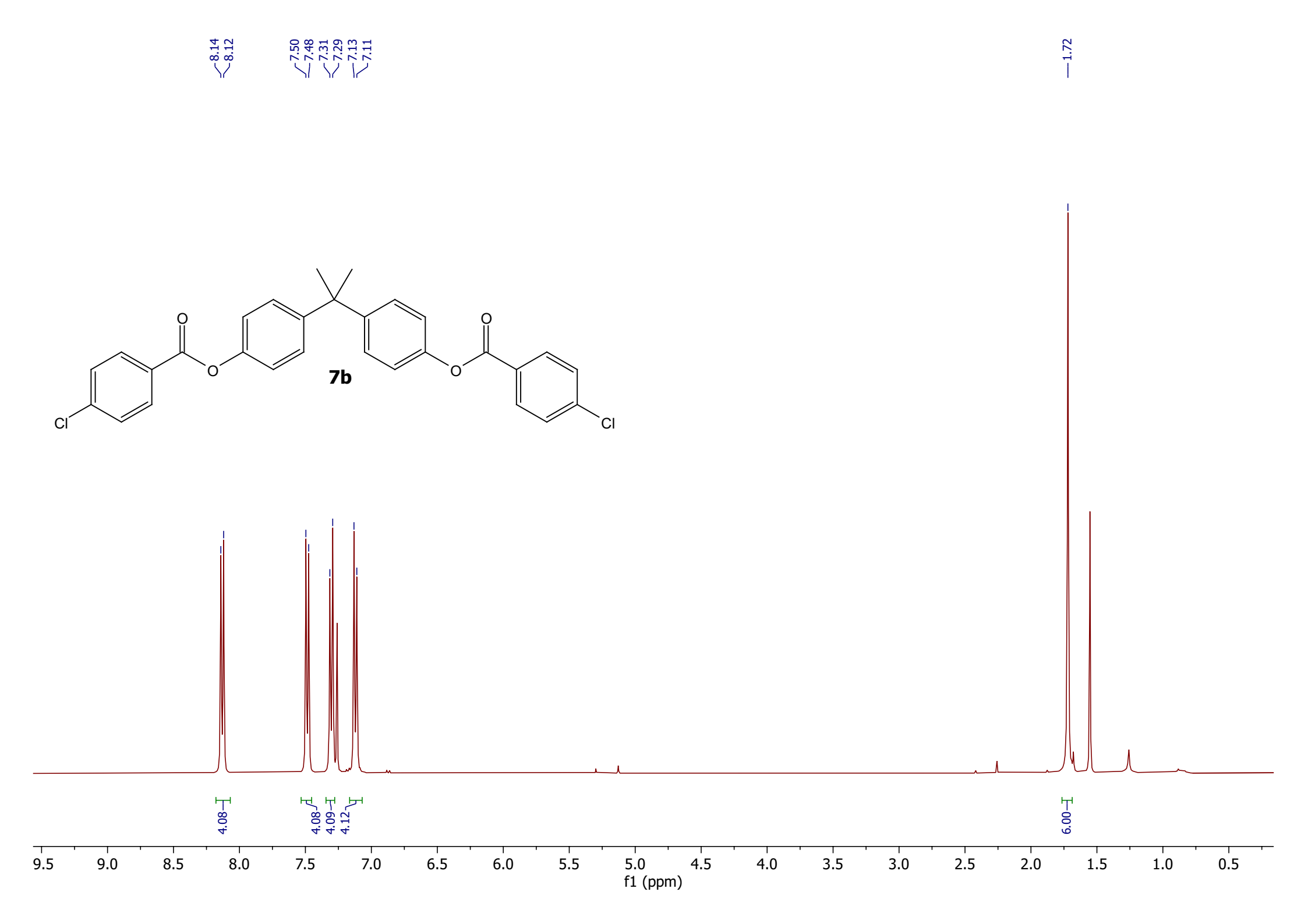
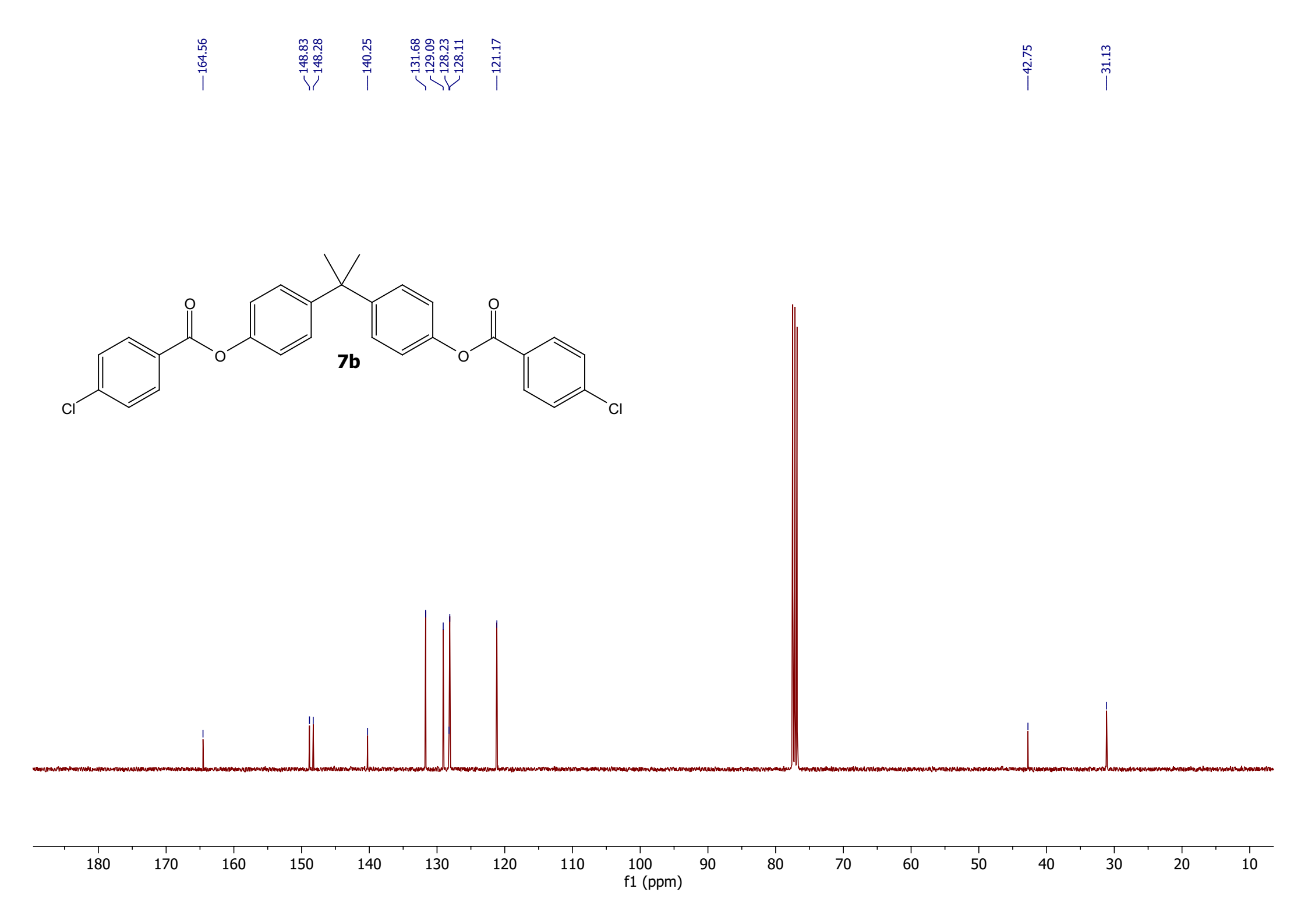
153.67
148.93
148.62
142.73
140.25
131.67
129.08
128.20
128.12
128.04
121.00
114.96
42.27
31.15
HO
O
O
Cl
7a
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)


8.14
8.12
7.50
7.48
7.31
7.29
7.13
7.11
1.72
O
O
O
O
Cl
Cl
7b
4.08
4.08
4.09
4.12
6.00
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
f1 (ppm)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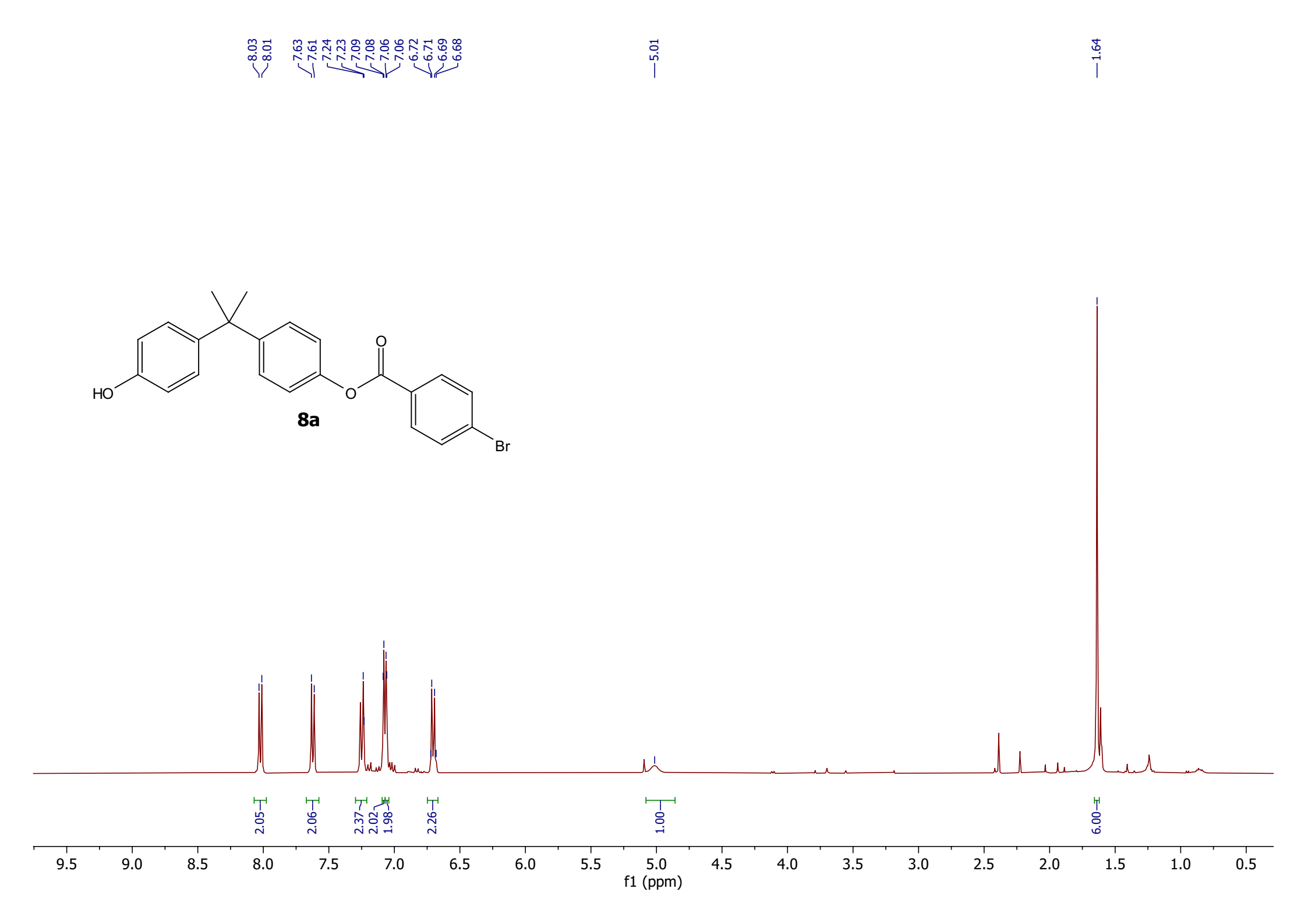
131.68
129.09
128.23
128.11
121.17
42.75
31.13
O
O
O
O
Cl
Cl
7b
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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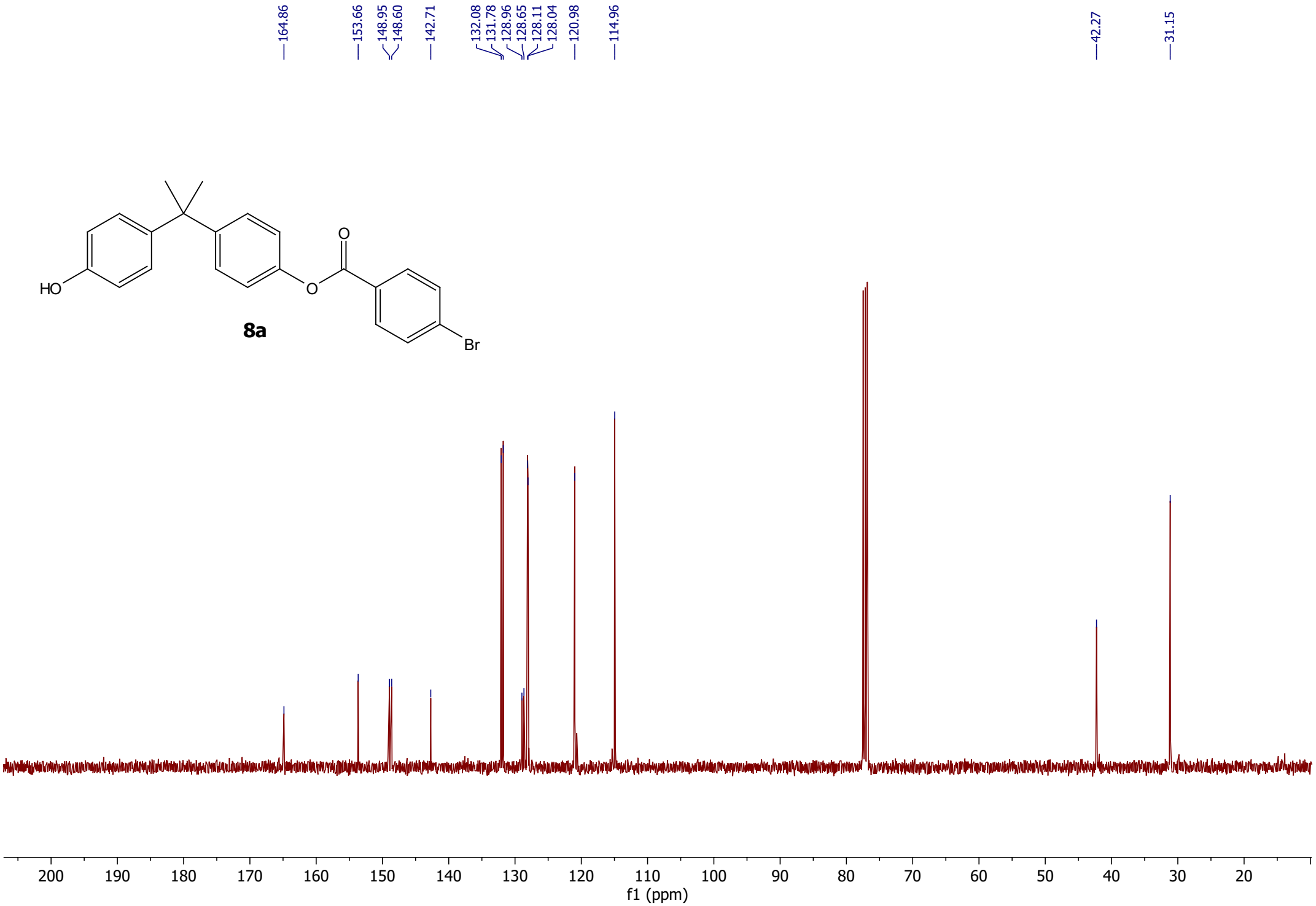
8.01
7.63
7.61
7.24
7.23
7.09
7.08
7.06
7.06
6.72
6.71
6.69
6.68
5.01
1.64
HO
O
O
Br
8a
2.05
2.06
2.37
2.02
1.98
2.26
1.00
6.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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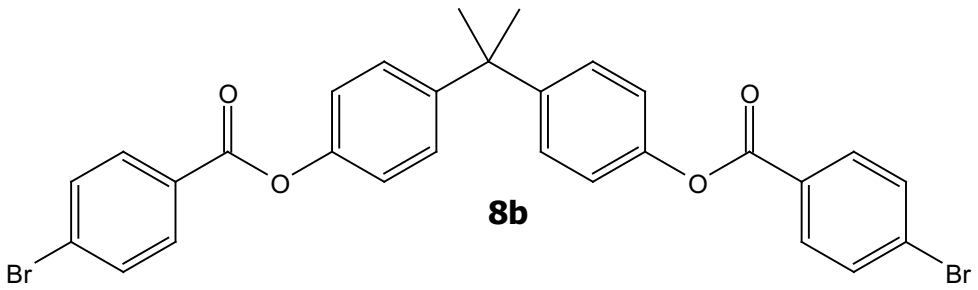
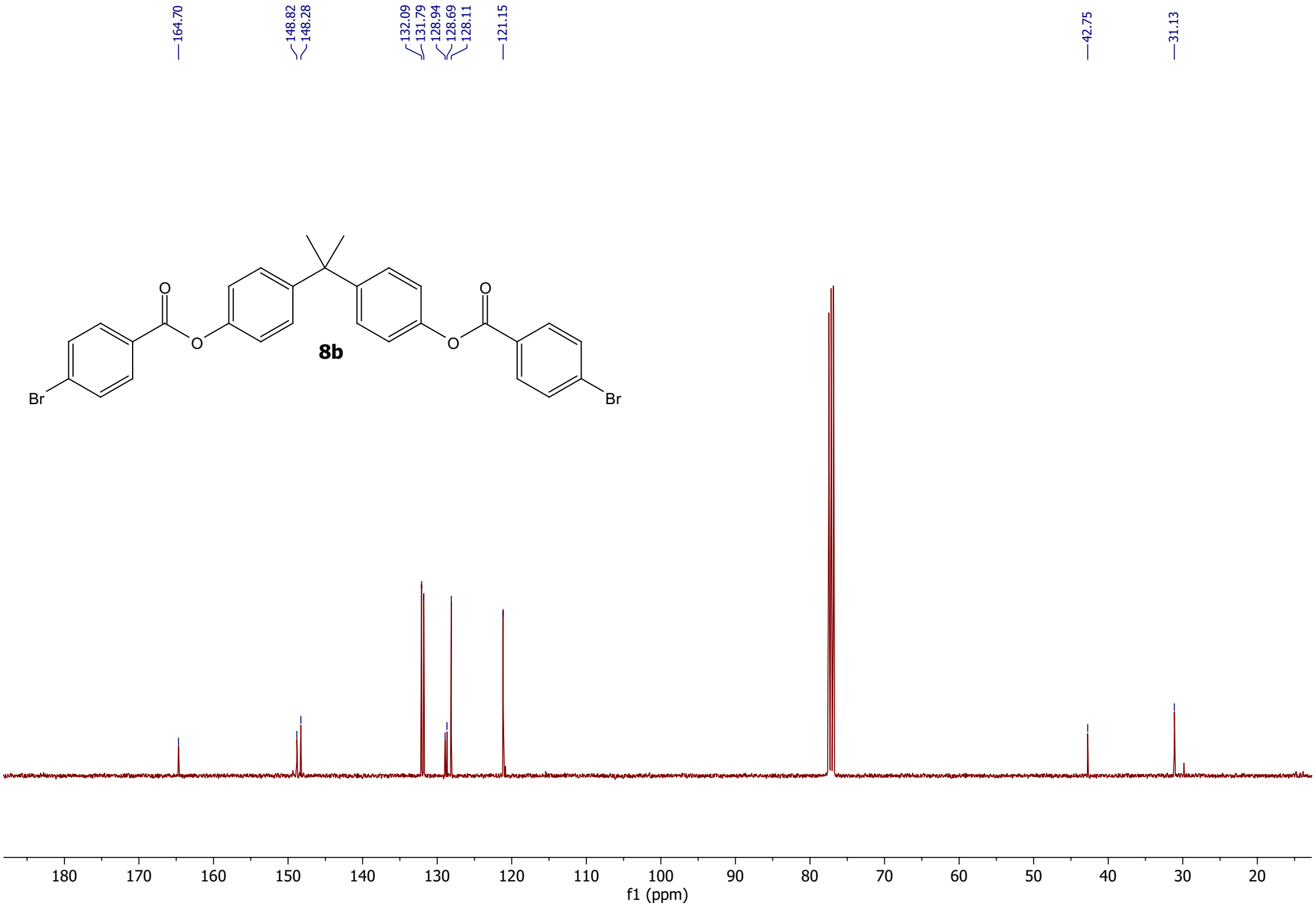
148.60
142.71
132.08
131.78
128.96
128.65
128.11
128.04
120.98
114.96
42.27
31.15
HO
O
O
Br
8a
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)


O
O
O
O
Br
Br

8b

8.06
8.04
7.66
7.64
7.31
7.29
7.13
7.11
1.72
4.35
4.30
4.27
4.27
6.00
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
f1 (ppm)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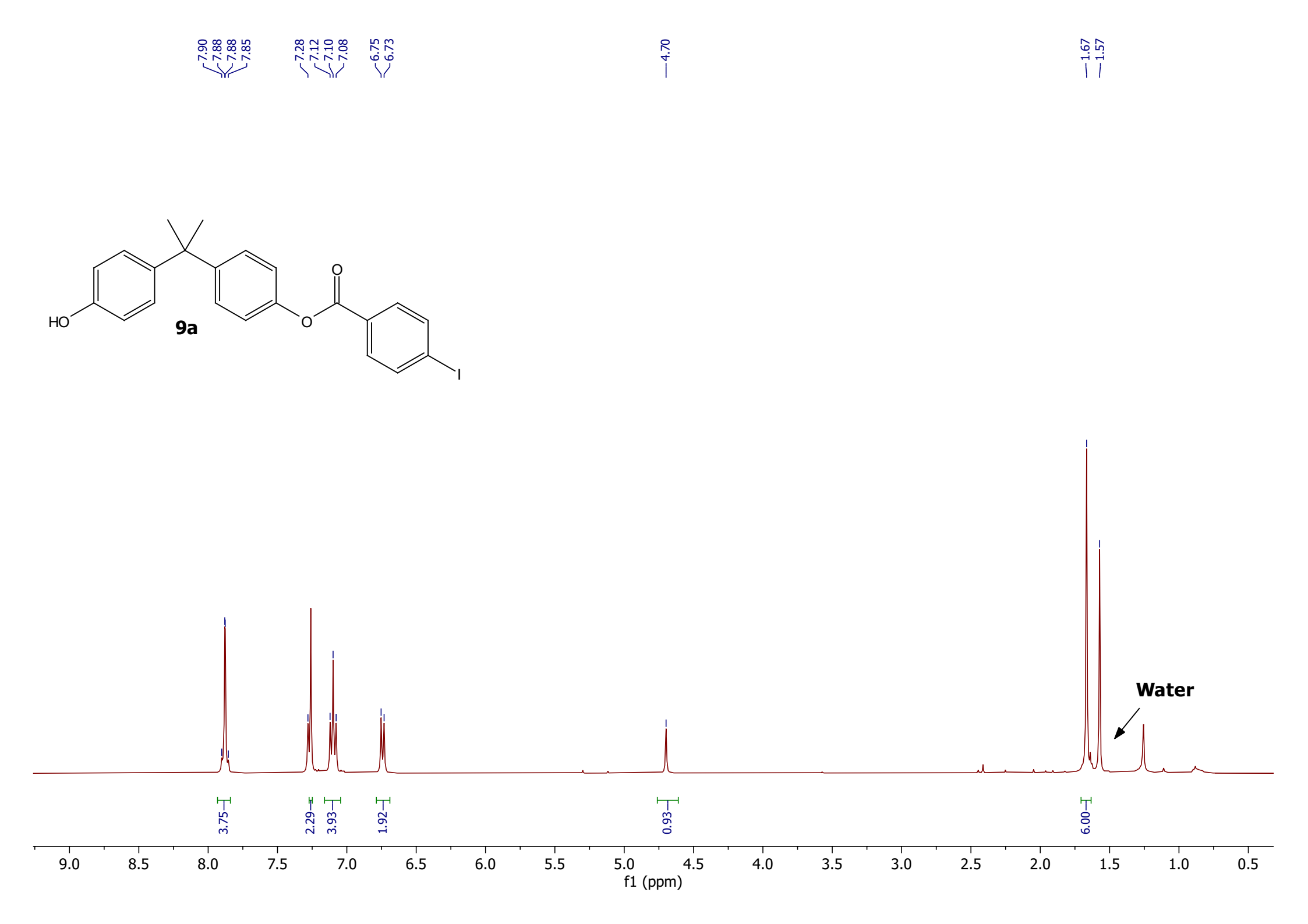
148.82
148.28
132.09
131.79
128.94
128.69
128.11
121.15
42.75
31.13
O
O
O
O
Br
Br
8b
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)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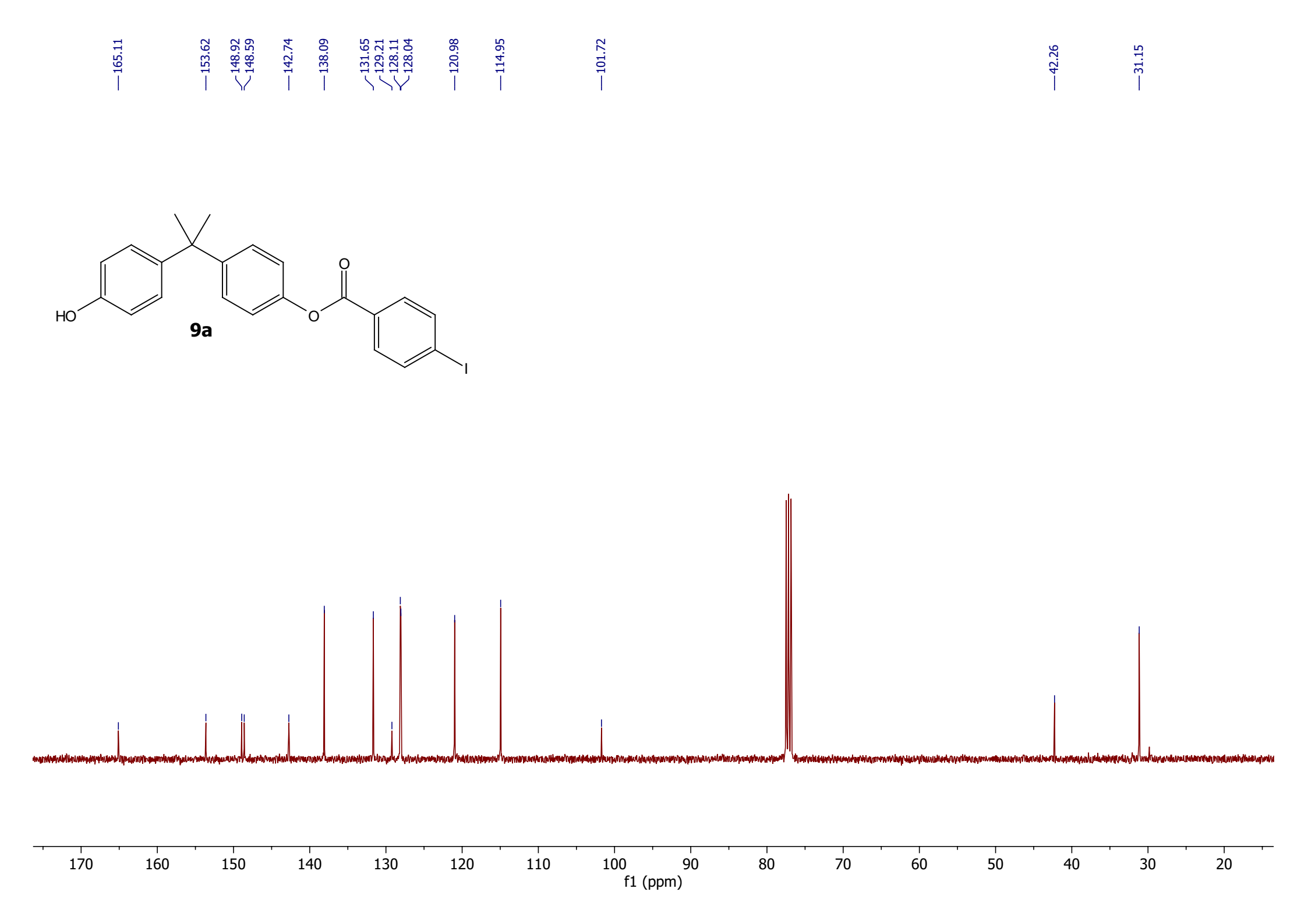
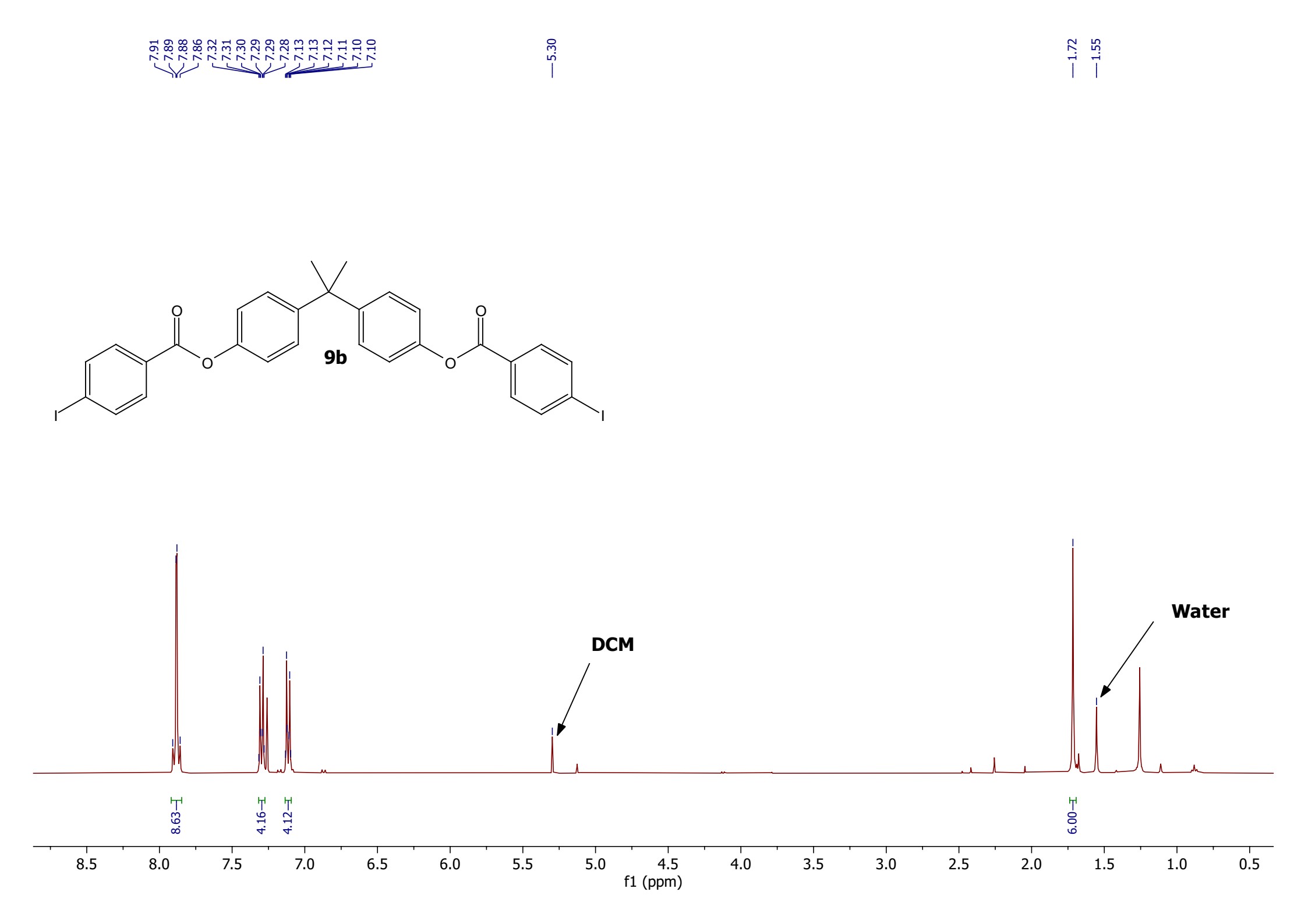
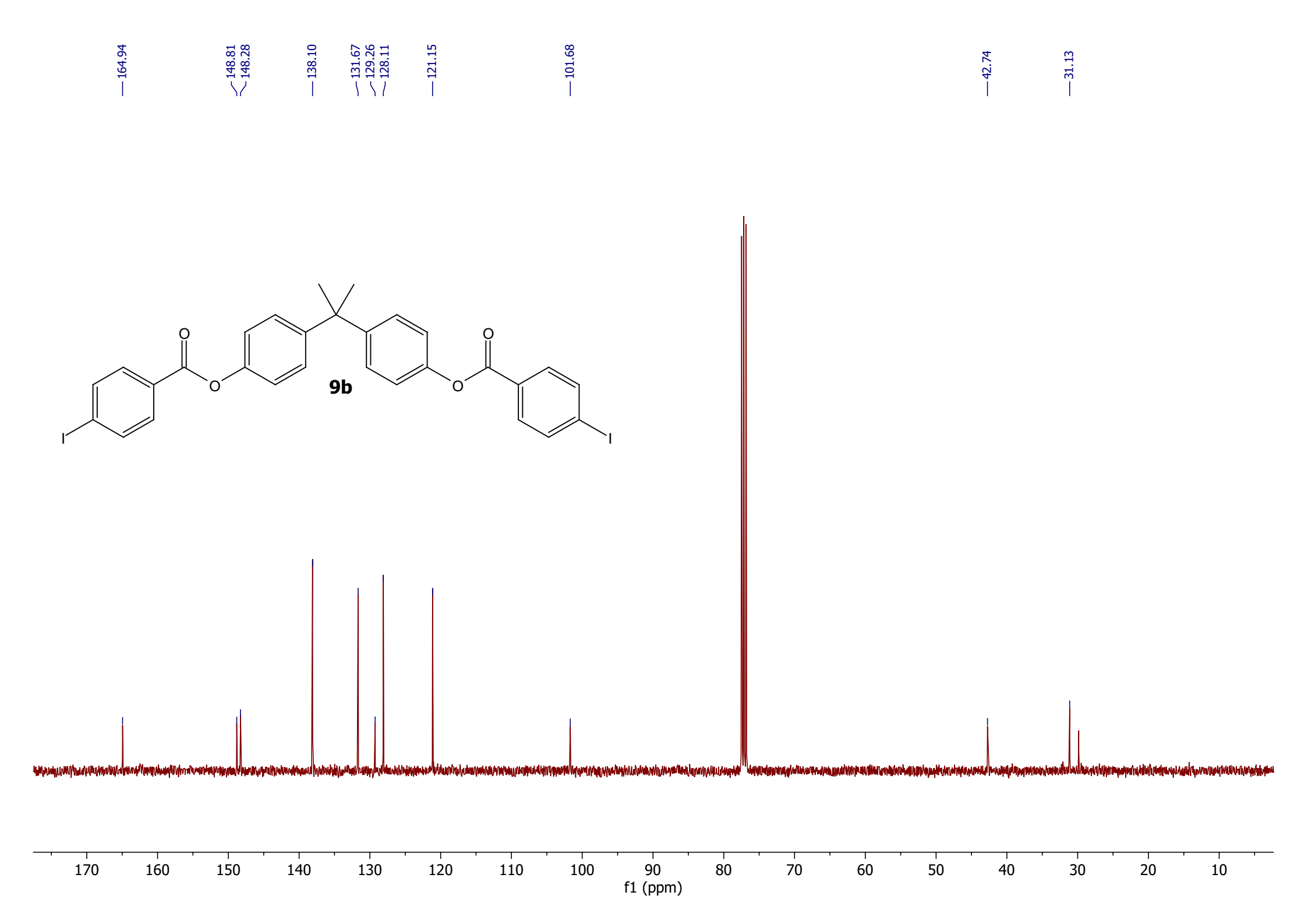
7.88
7.88
7.85
7.28
7.12
7.10
7.08
6.75
6.73
4.70
1.67
1.57
HO
O
O
I
9a
Water
3.75
2.29
3.93
1.92
0.93
6.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


165.11
153.62
148.92
148.59
142.74
138.09
131.65
129.21
128.11
128.04
120.98
114.95
101.72
42.26
31.15
HO
O
O
I
9a
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)


7.91
7.89
7.88
7.86
7.32
7.31
7.30
7.29
7.29
7.28
7.13
7.13
7.12
7.11
7.10
7.10
5.30
1.72
1.55
9b
O
O
O
O
I
I
DCM
Water
8.63
4.16
4.12
6.00
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)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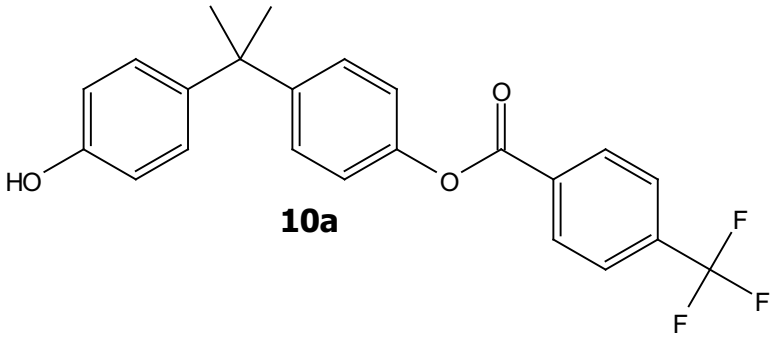
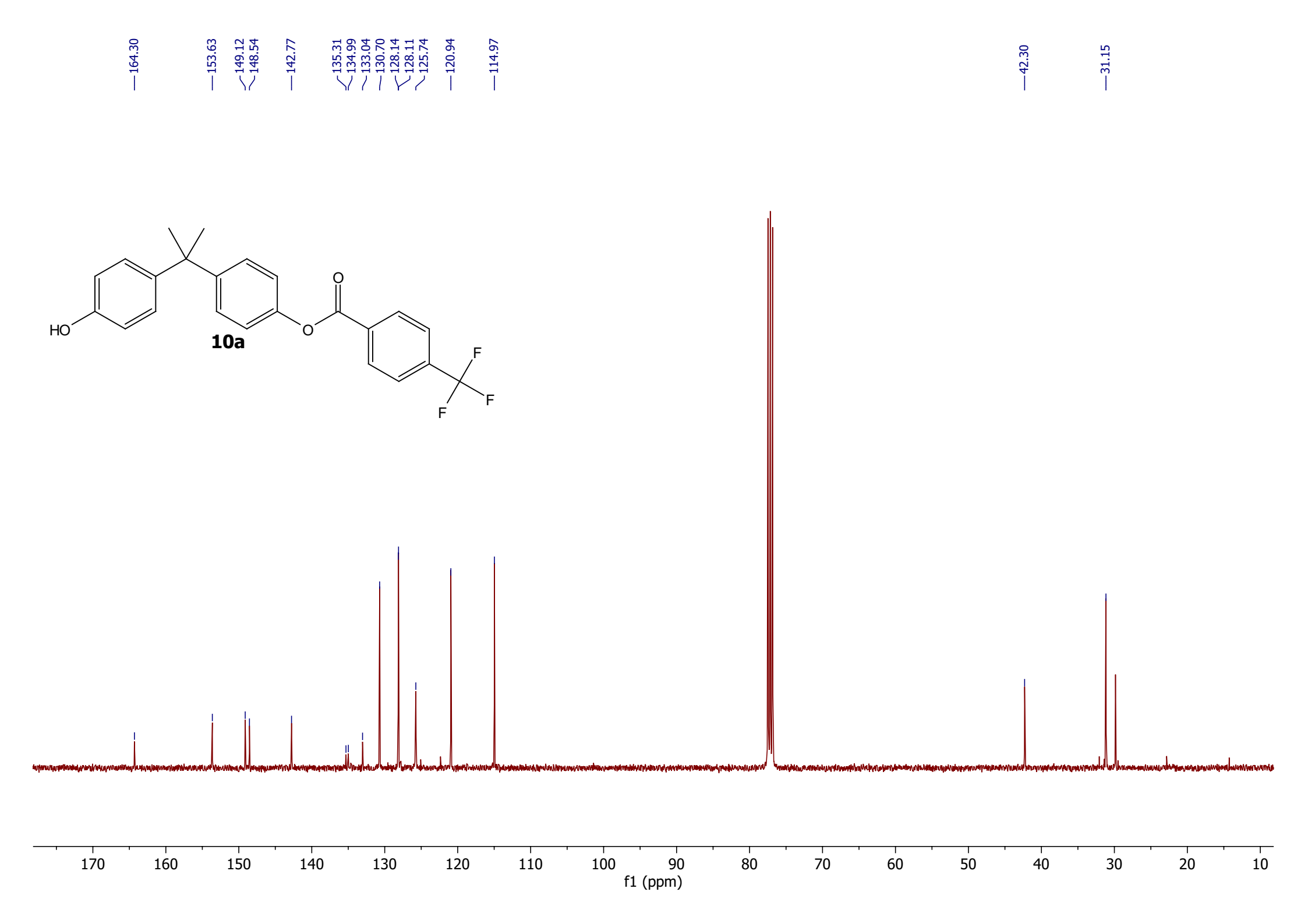
148.81
148.28
138.10
131.67
129.26
128.11
121.15
101.68
42.74
31.13
O
O
O
O
I
I
9b
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


HO
O
O
F
F
F

10a

8.32
8.30
7.79
7.77
7.30
7.28
7.13
7.11
6.76
6.73
4.81
1.68
2.03
2.02
2.07
4.26
2.09
1.07
6.00
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
f1 (ppm)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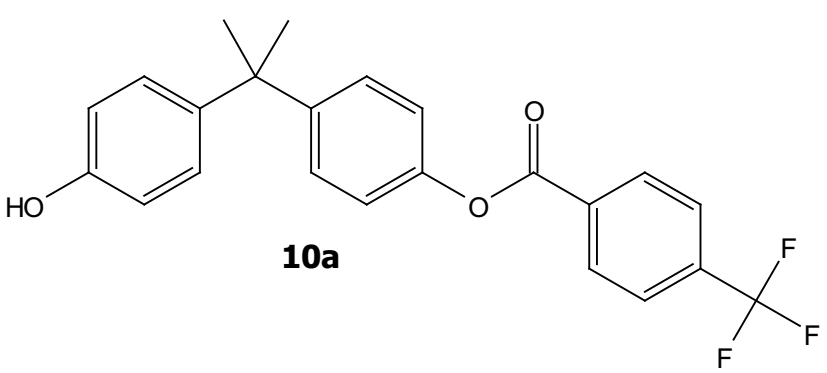
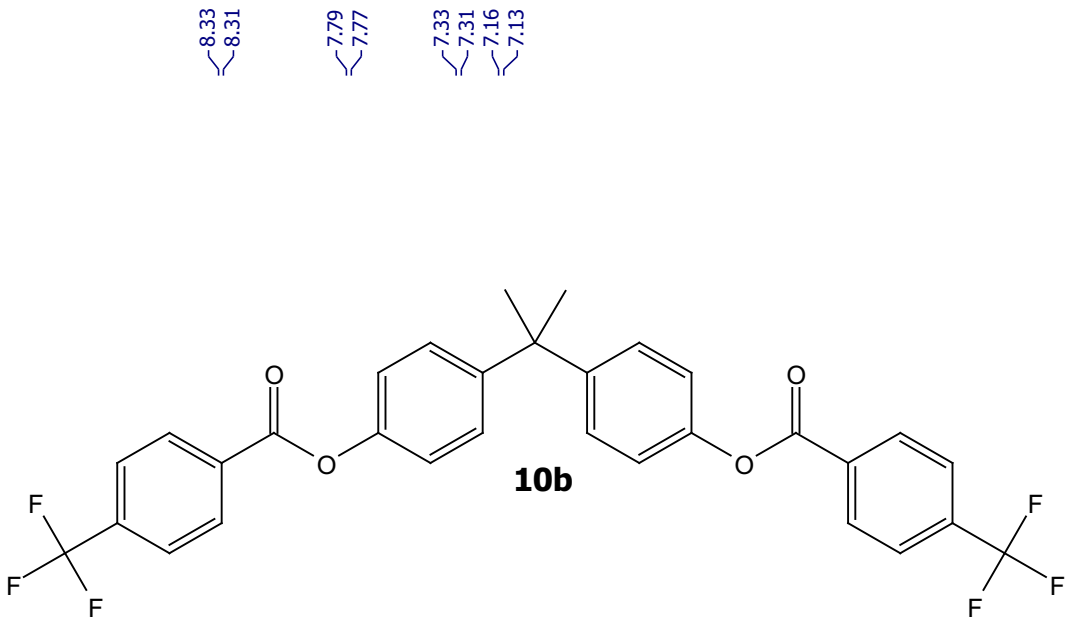
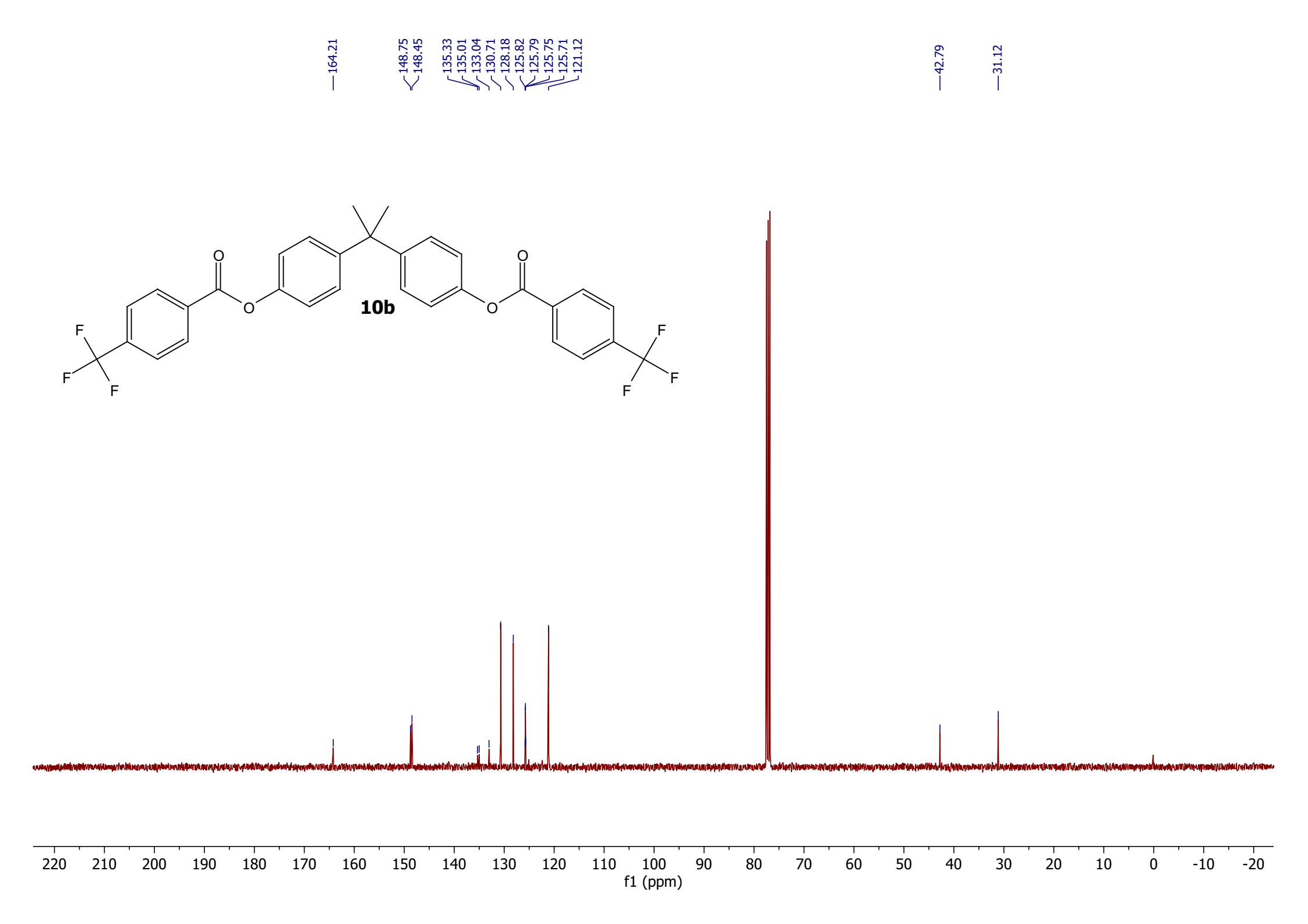
148.54
142.77
135.31
134.99
133.04
130.70
128.14
128.11
125.74
120.94
114.97
42.30
31.15
HO
O
O
F
F
F
10a
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


HO
O
O
F
F
F

10a

-63.14
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115
-120
f1 (ppm)


8.33
8.31
7.79
7.77
7.33
7.31
7.16
7.13
1.73
O
O
O
O
F
F
F
F
F
F
10b
Water
4.19
4.20
4.12
4.20
6.00
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
f1 (ppm)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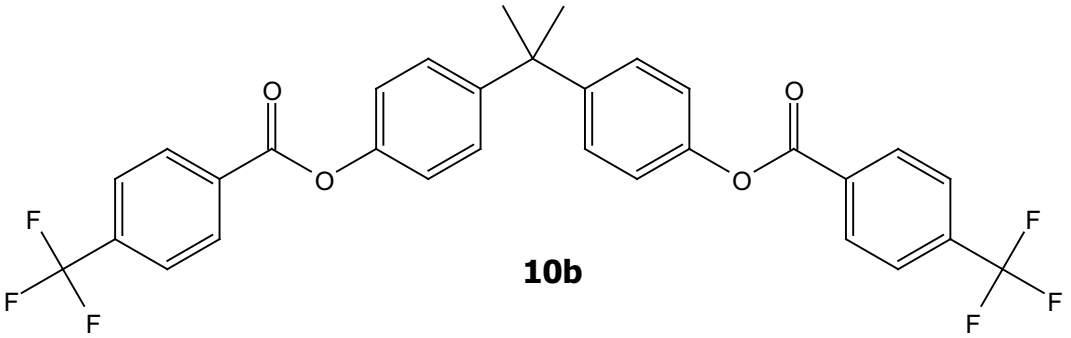
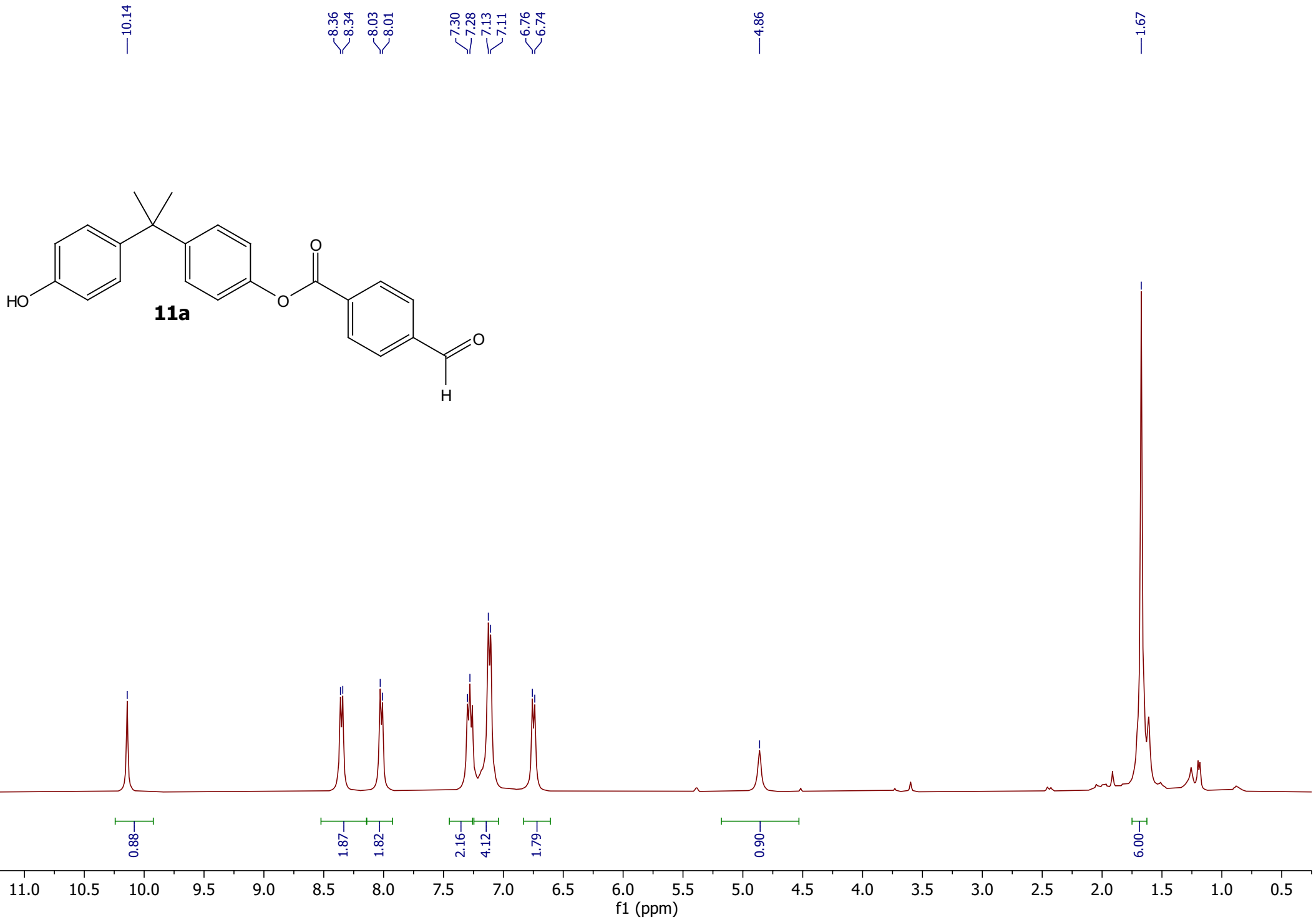
148.45
135.33
135.01
133.04
130.71
128.18
125.82
125.79
125.75
125.71
121.12
42.79
31.12
10b
O
O
O
O
F
F
F
F
F
F
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)


O
O
O
O
F
F
F
F
F
F

10b

-63.16
320 300 280 260 240 220 200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280 -300 -320
f1 (ppm)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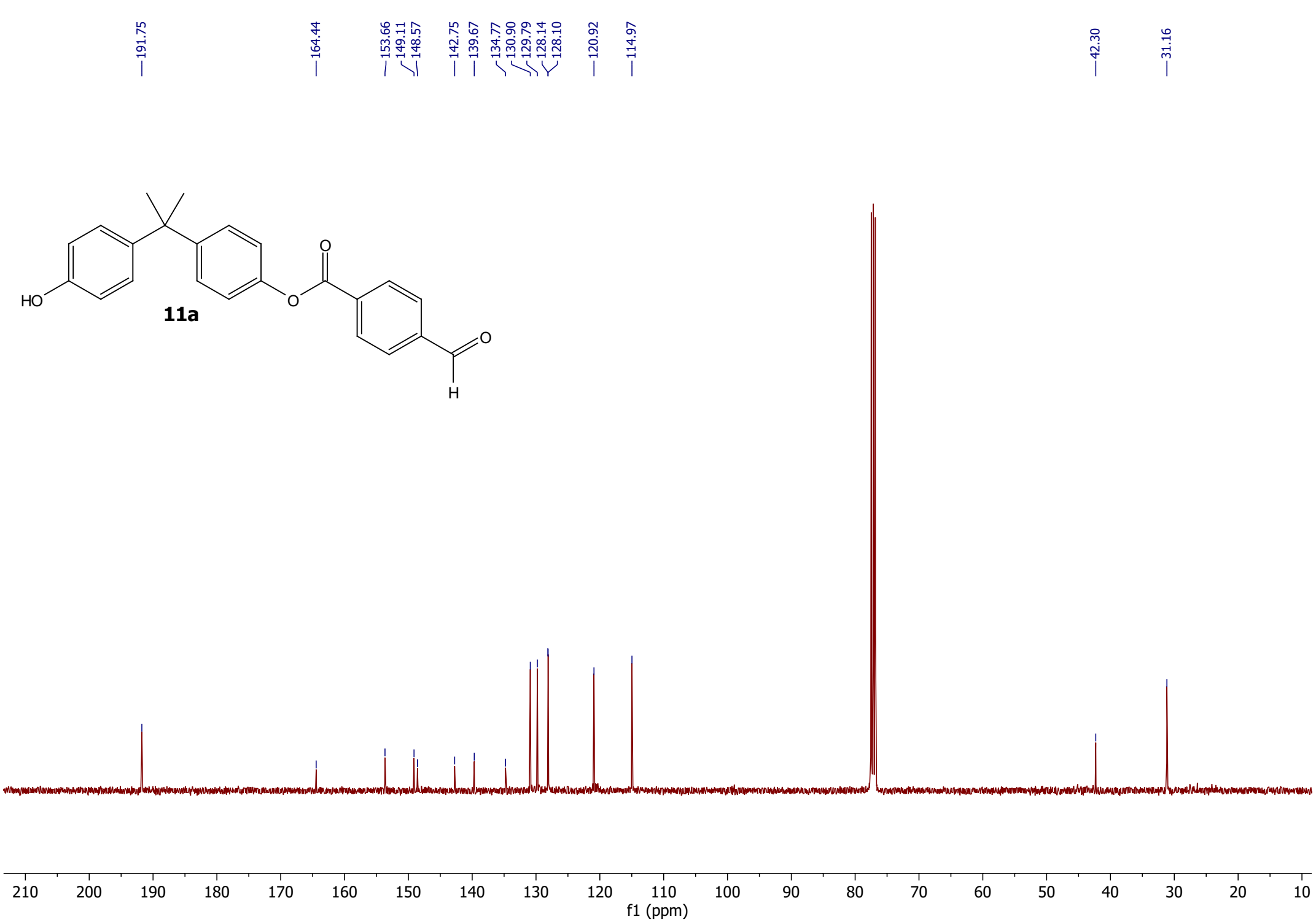
8.36
8.34
8.03
8.01
7.30
7.28
7.13
7.11
6.76
6.74
4.86
1.67
HO
O
O
O
H
11a
0.88
1.87
1.82
2.16
4.12
1.79
0.90
6.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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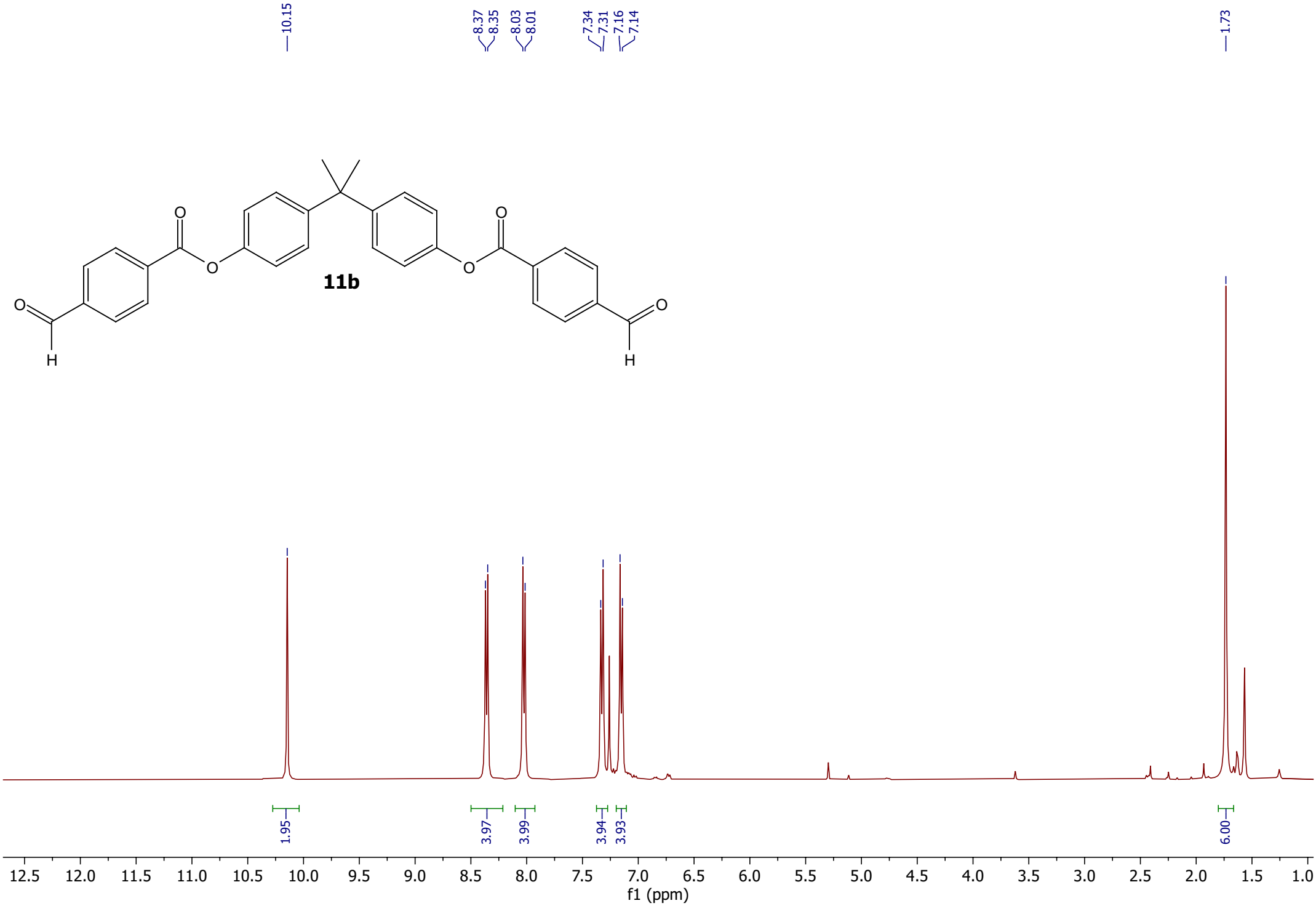
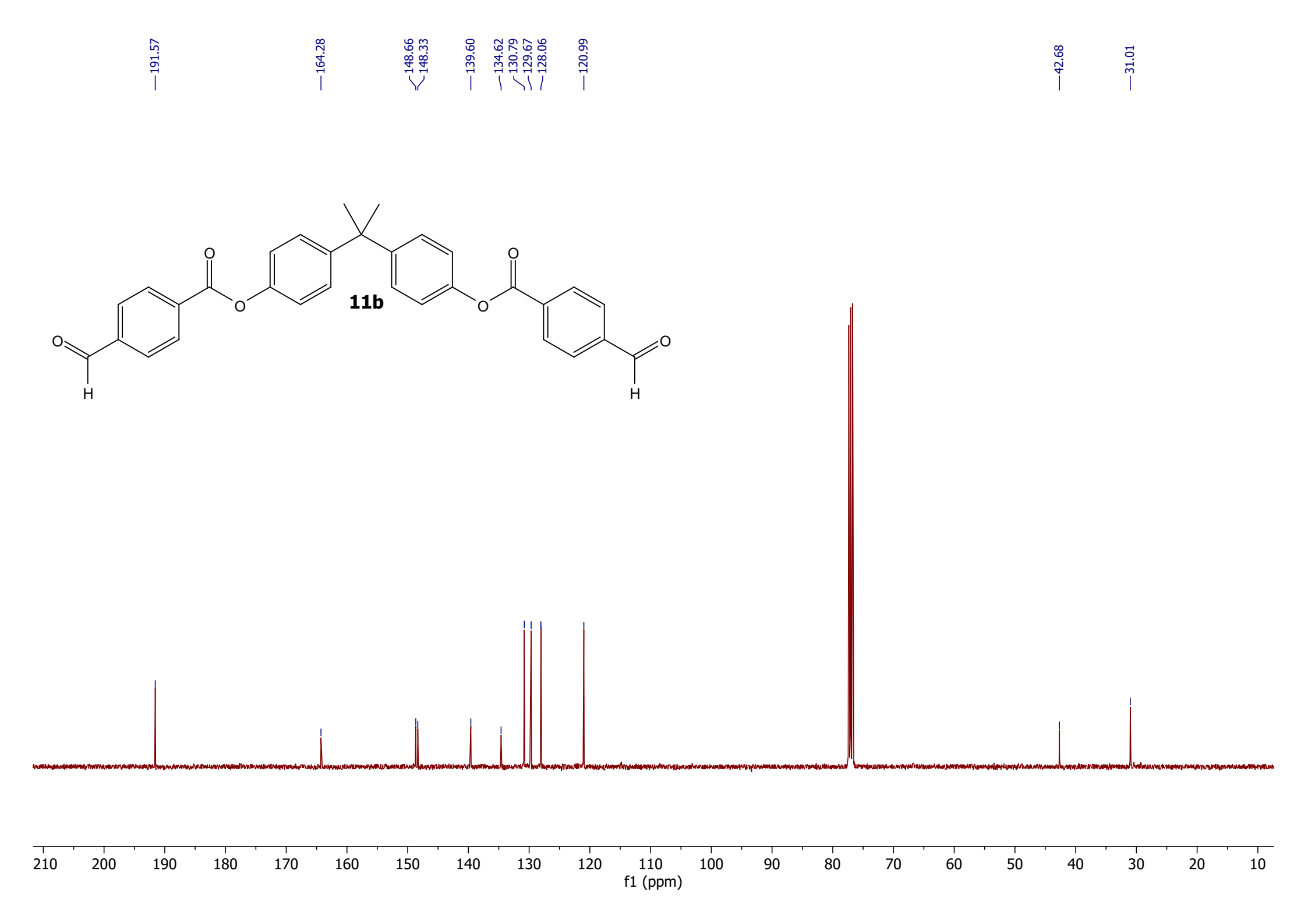
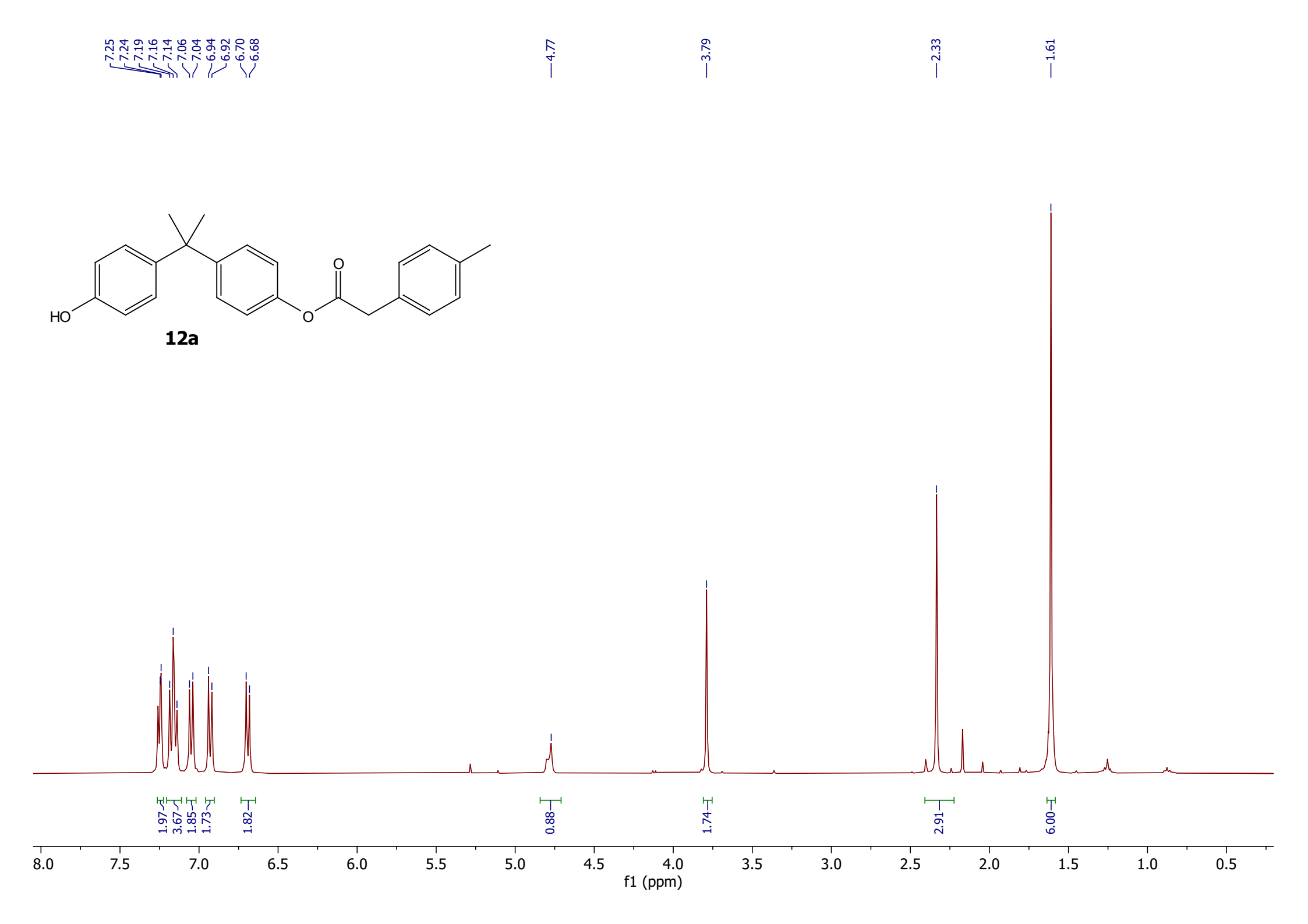
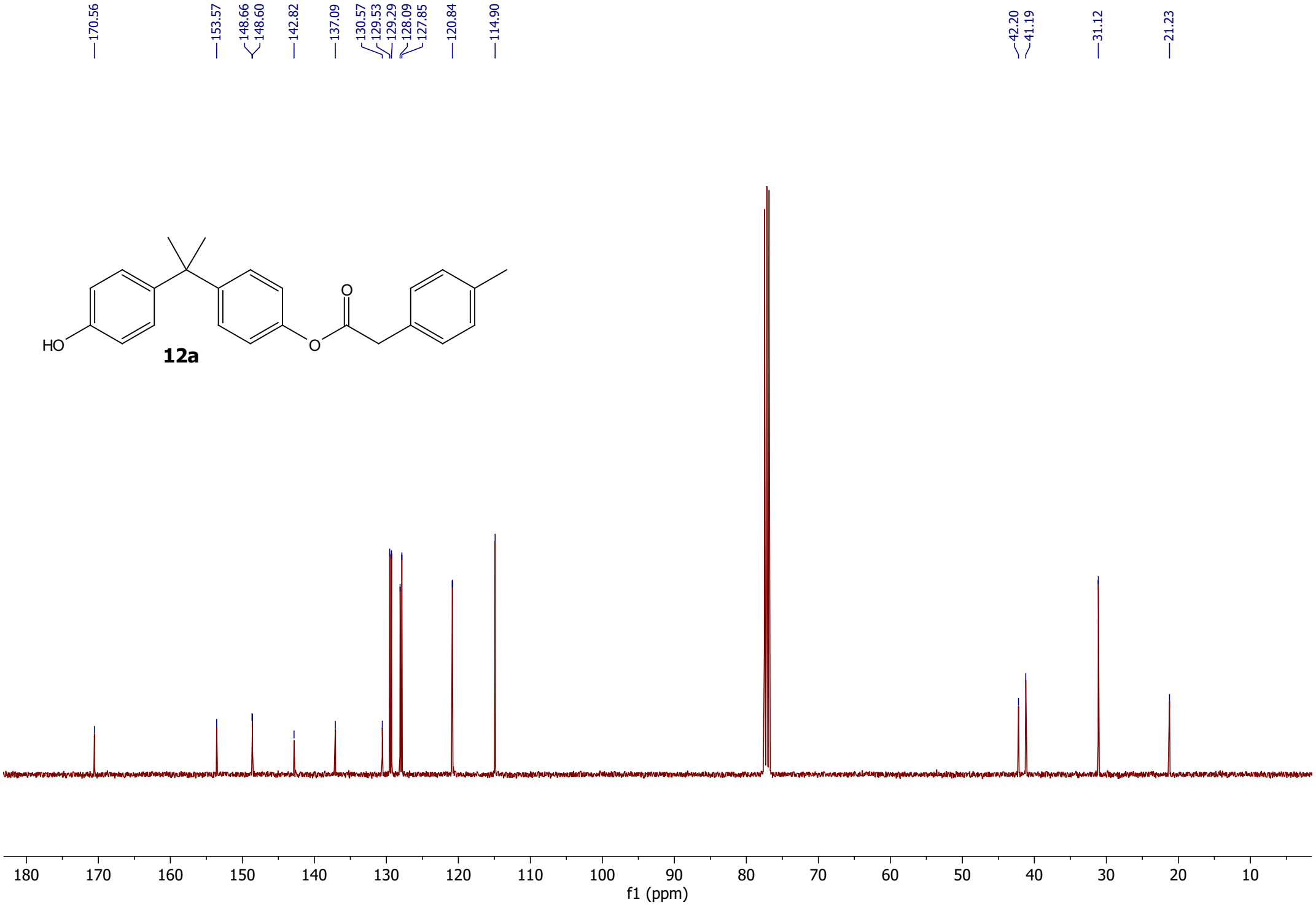
149.11
148.57
142.75
139.67
134.77
130.90
129.79
128.14
128.10
120.92
114.97
42.30
31.16
HO
O
O
O
H
11a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


10.15
8.37
8.35
8.03
8.01
7.34
7.31
7.16
7.14
1.73
11b
O
O
O
O
O
O
H
H
1.95
3.97
3.99
3.94
3.93
6.00
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
f1 (ppm)


191.57
164.28
148.66
148.33
139.60
134.62
130.79
129.67
128.06
120.99
42.68
31.01
11b
O
O
O
O
O
O
H
H
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.25
7.24
7.19
7.16
7.14
7.06
7.04
6.94
6.92
6.70
6.68
4.77
3.79
2.33
1.61
HO
O
O
12a
1.97
3.67
1.85
1.73
1.82
0.88
1.74
2.91
6.00
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)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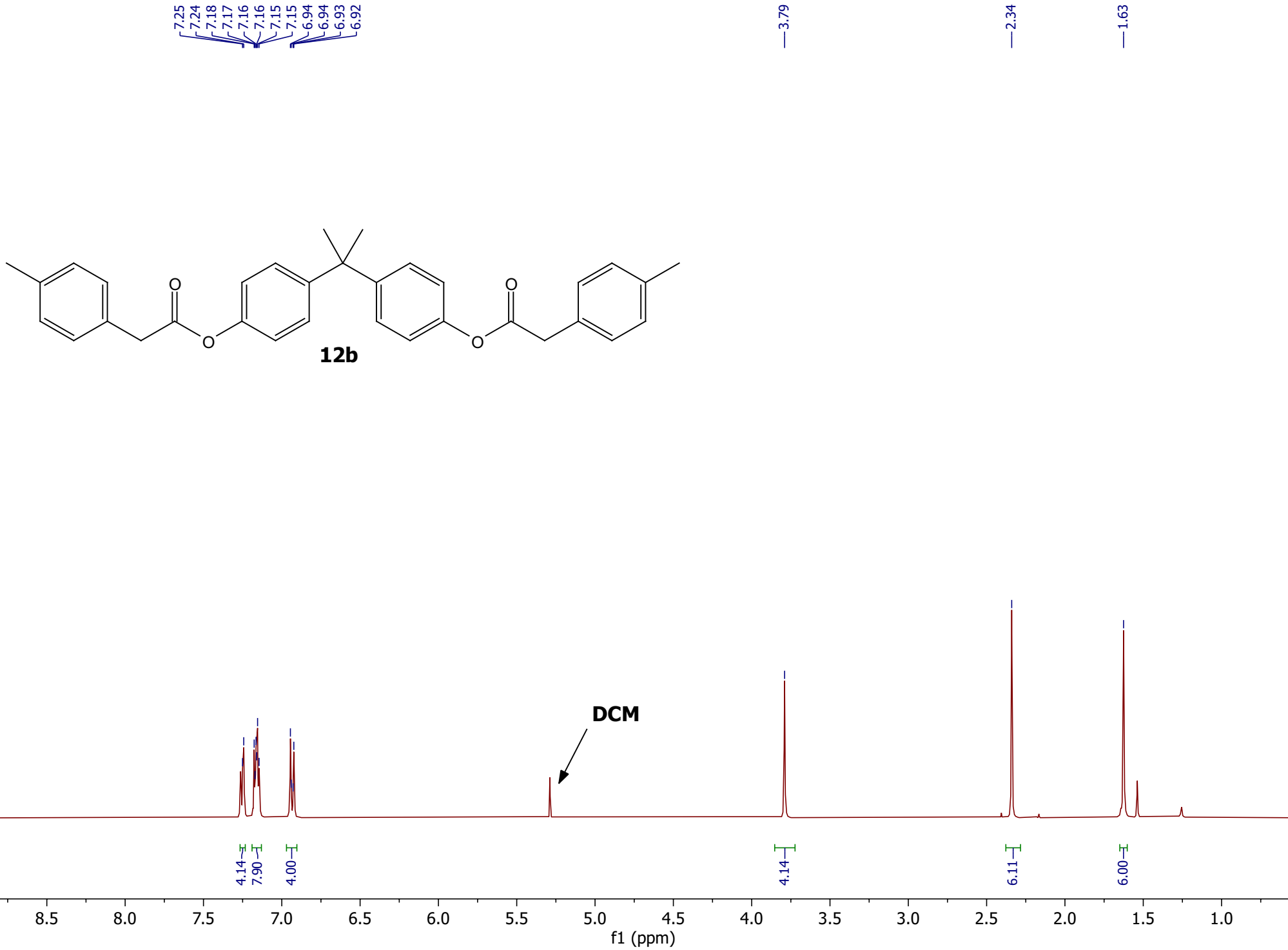
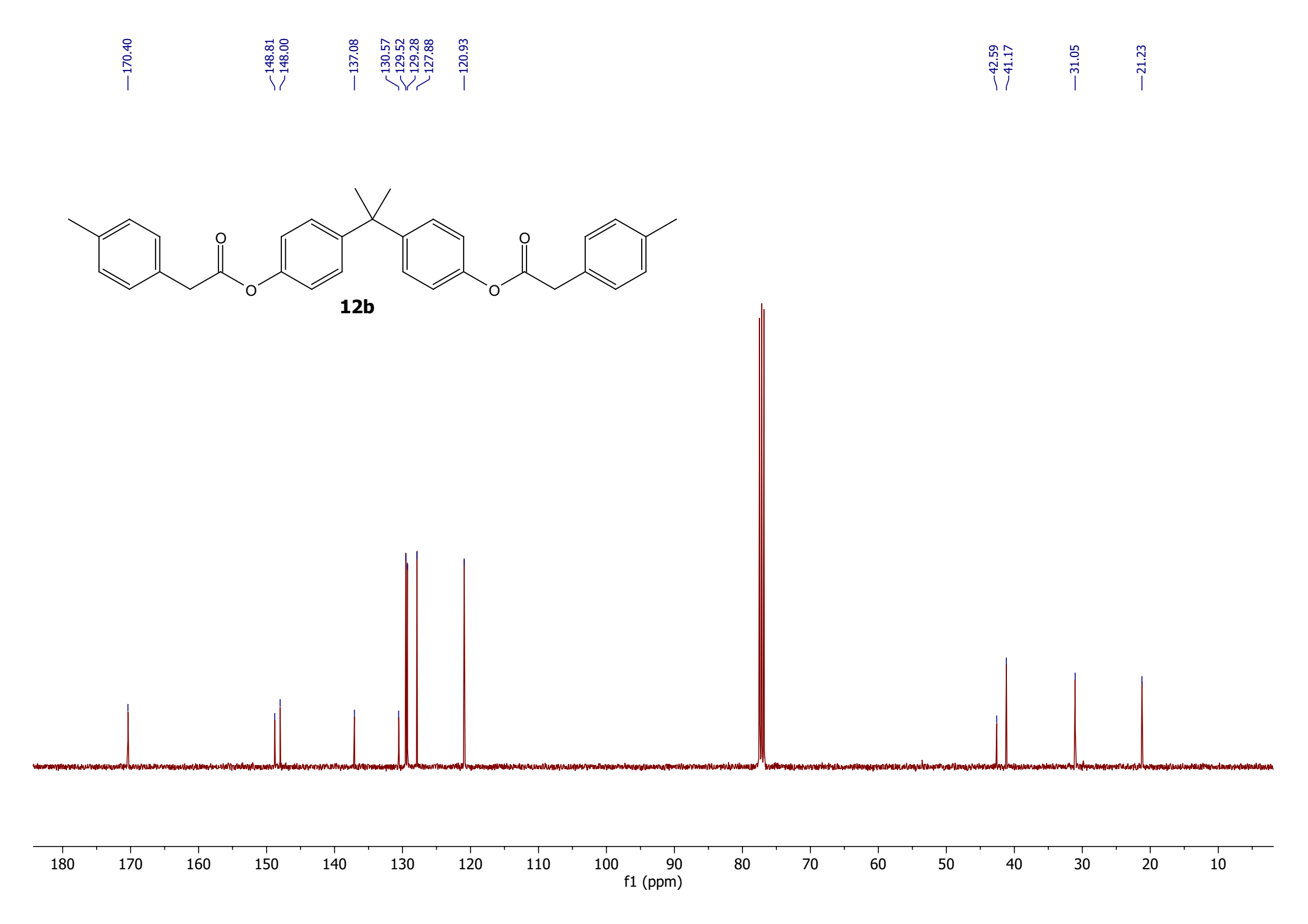
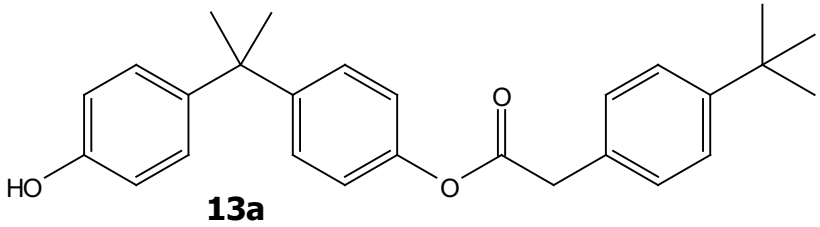
153.57
148.66
148.60
142.82
137.09
130.57
129.53
129.29
128.09
127.85
120.84
114.90
42.20
41.19
31.12
21.23
HO
O
O
12a
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

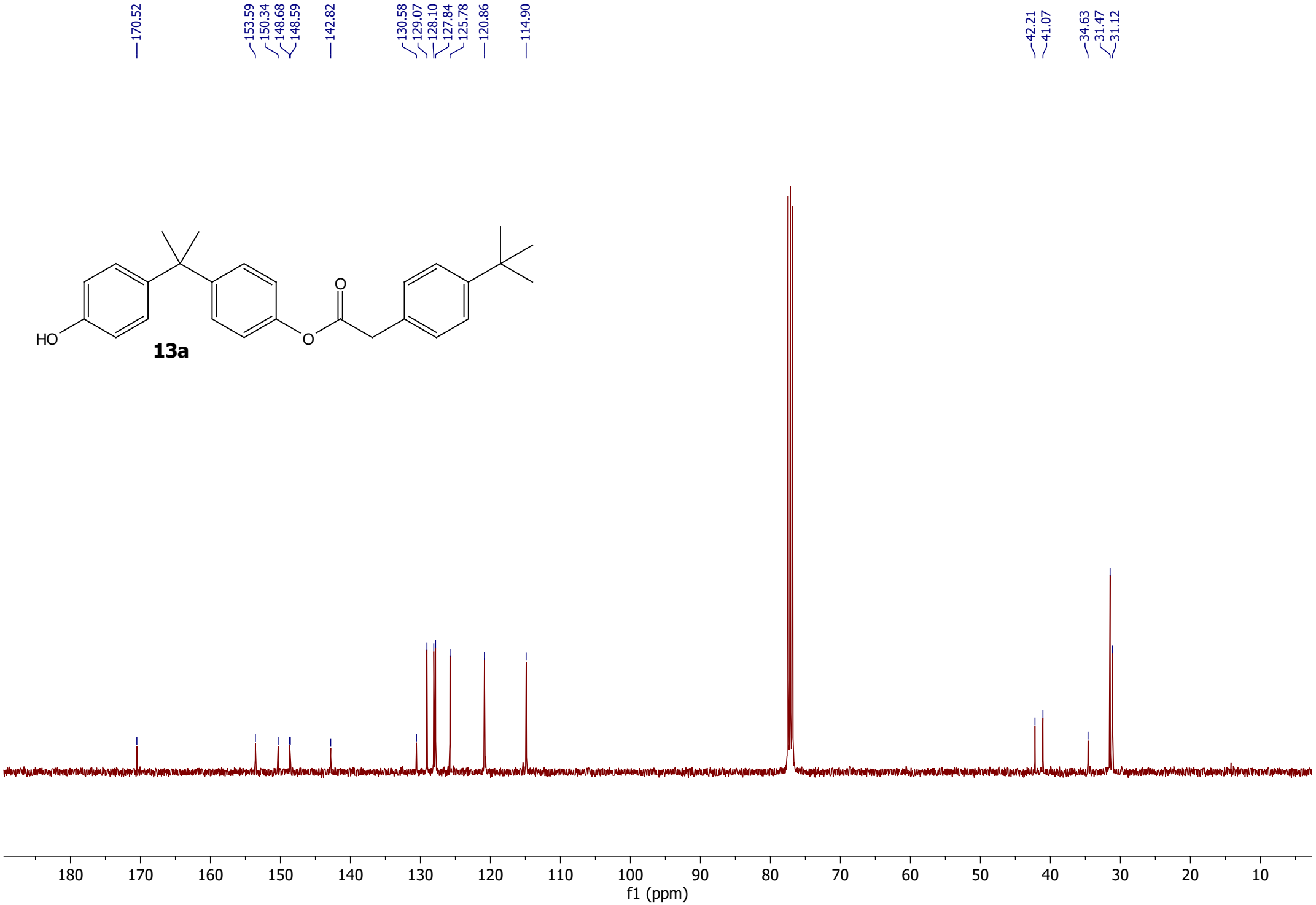

7.25
7.24
7.18
7.17
7.16
7.16
7.15
7.15
6.94
6.94
6.93
6.92
3.79
2.34
1.63
O
O
O
O
12b
DCM
4.14
7.90
4.00
4.14
6.11
6.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


170.40
148.81
148.00
137.08
130.57
129.52
129.28
127.88
120.93
42.59
41.17
31.05
21.23
O
O
O
O
12b
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


HO
O
O

13a

7.39
7.37
7.32
7.30
7.20
7.18
7.07
7.05
6.97
6.95
6.72
6.70
4.83
3.81
1.63
1.32
1.62
1.68
1.79
2.23
1.64
1.82
0.91
1.81
6.27
9.00
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)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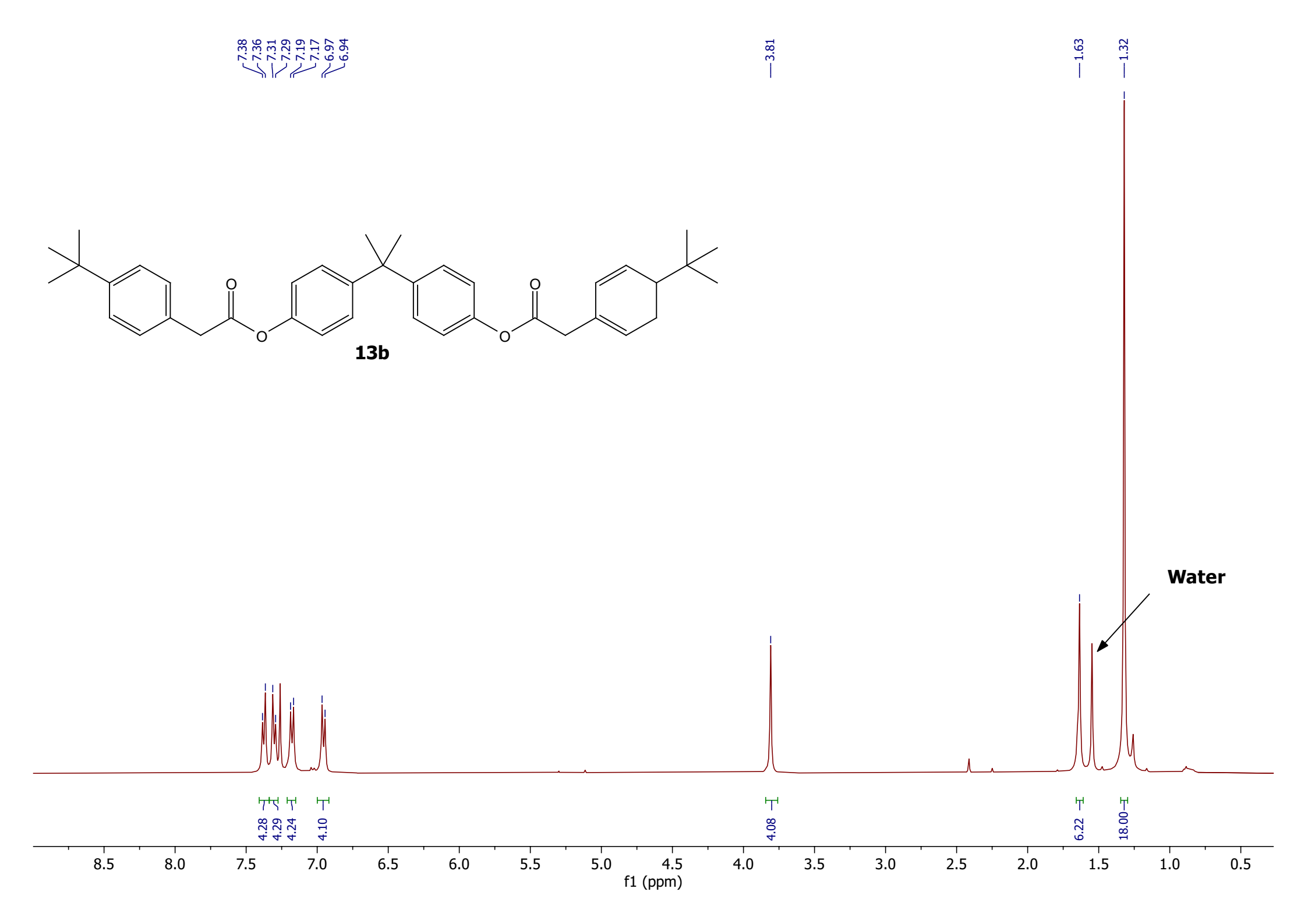
150.34
148.68
148.59
142.82
130.58
129.07
128.10
127.84
125.78
120.86
114.90
42.21
41.07
34.63
31.47
31.12
HO
O
O
13a
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.36
7.31
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7.17
6.97
6.94
3.81
1.63
1.32
13b
Water
4.28
4.29
4.24
4.10
4.08
6.22
18.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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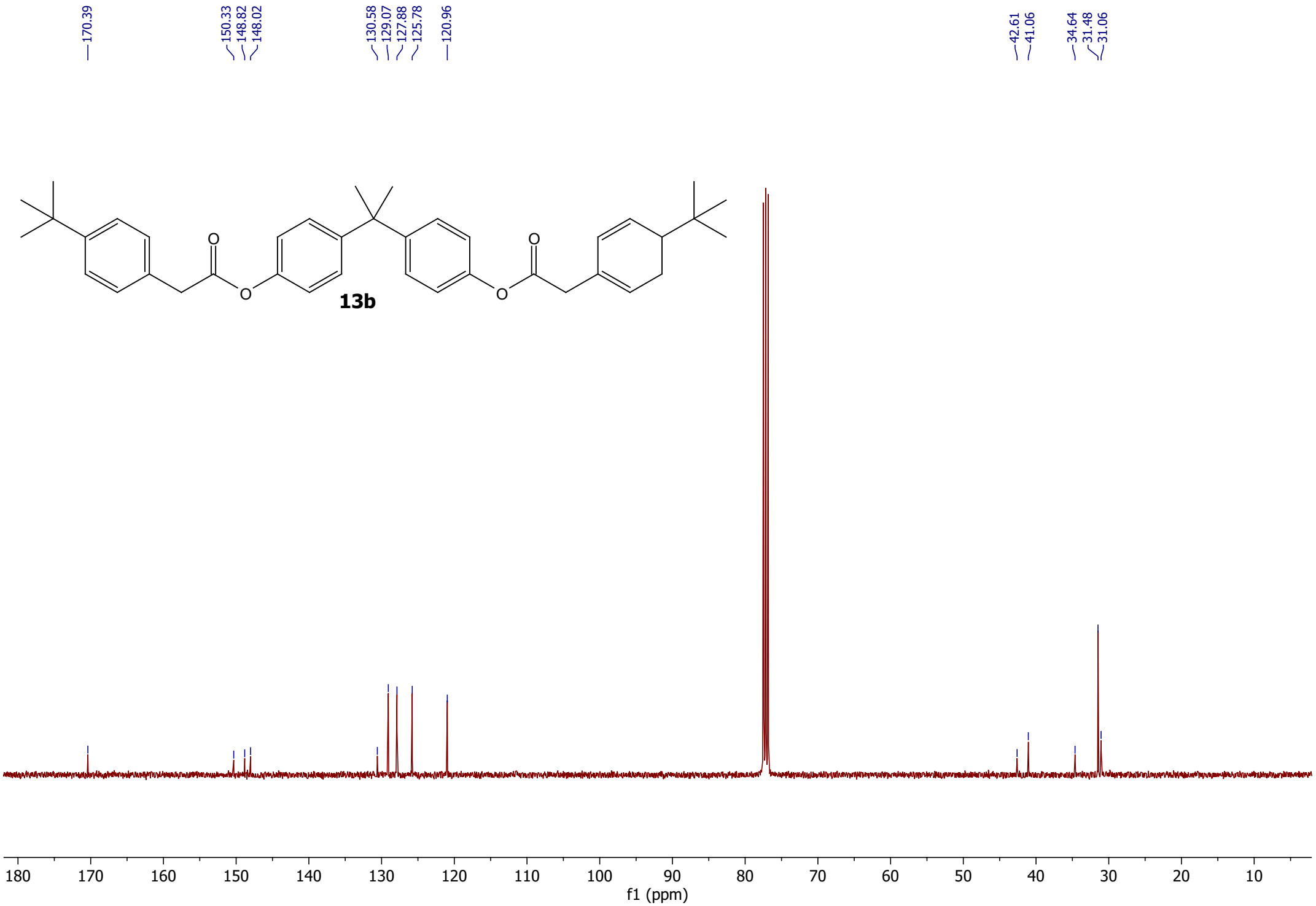
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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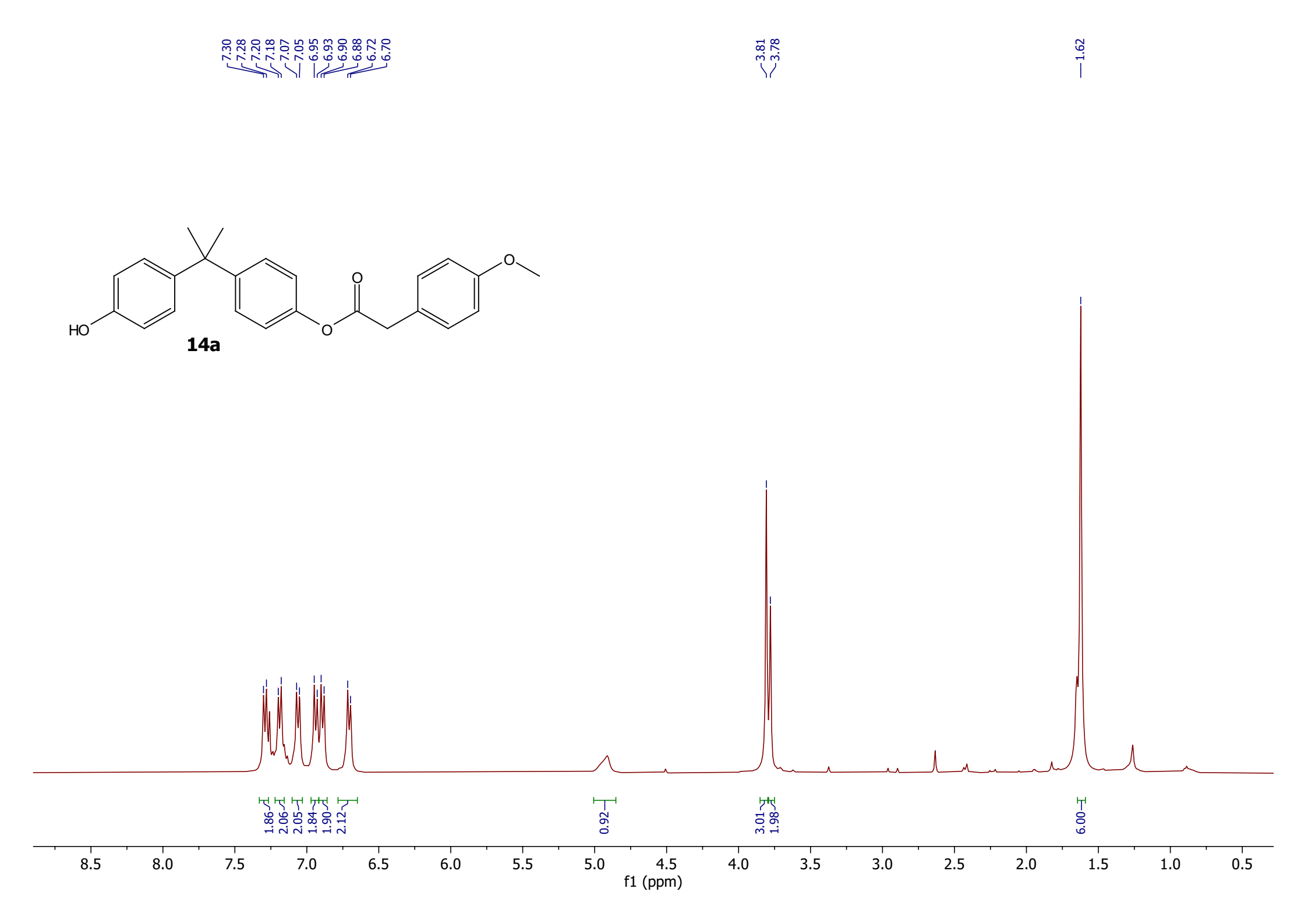
150.33
148.82
148.02
130.58
129.07
127.88
125.78
120.96
42.61
41.06
34.64
31.48
31.06
O
O
O
O
13b
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.28
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7.05
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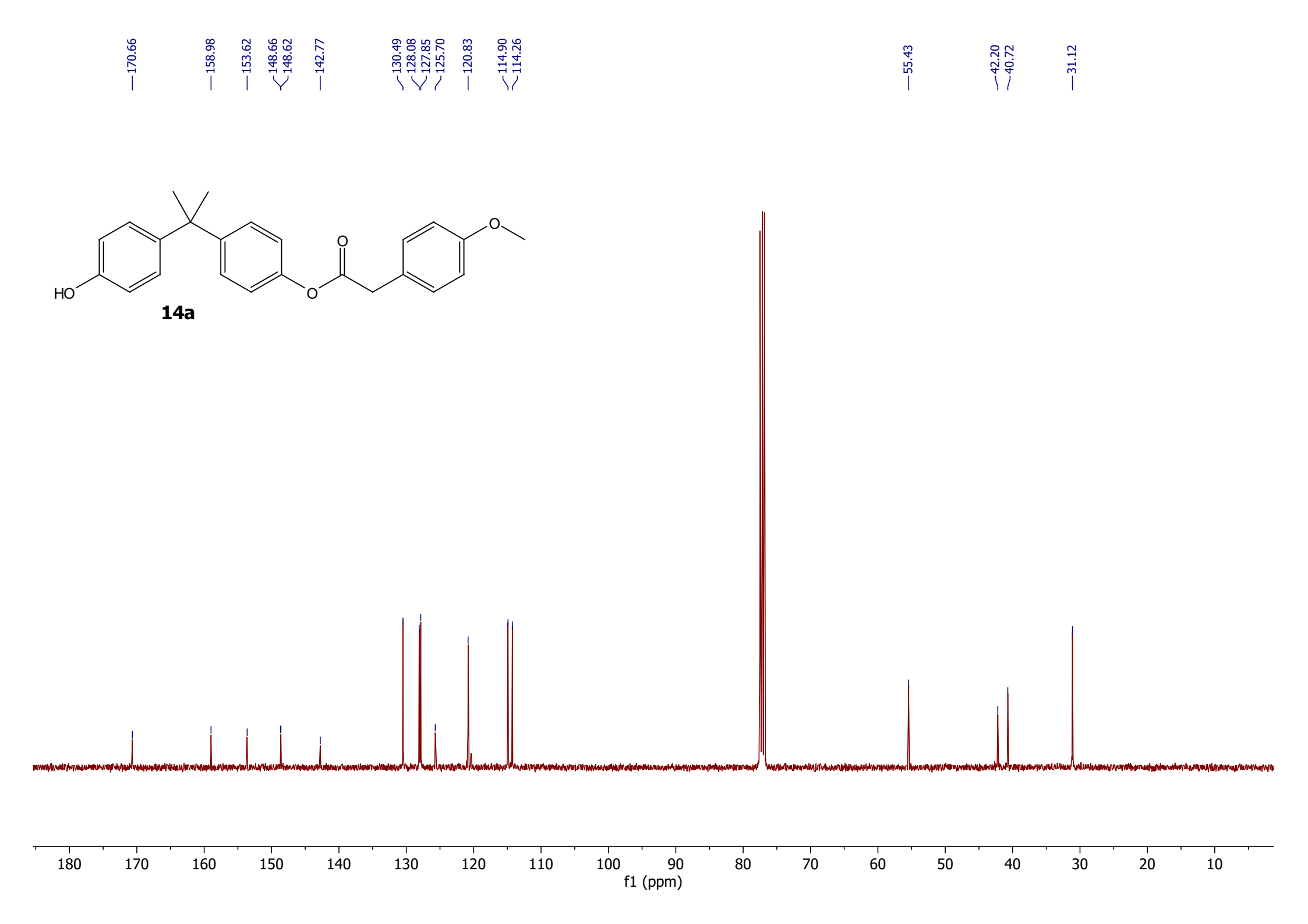
6.93
6.90
6.88
6.72
6.70
3.81
3.78
1.62
HO
O
O
O
14a
1.86
2.06
2.05
1.84
1.90
2.12
0.92
3.01
1.98
6.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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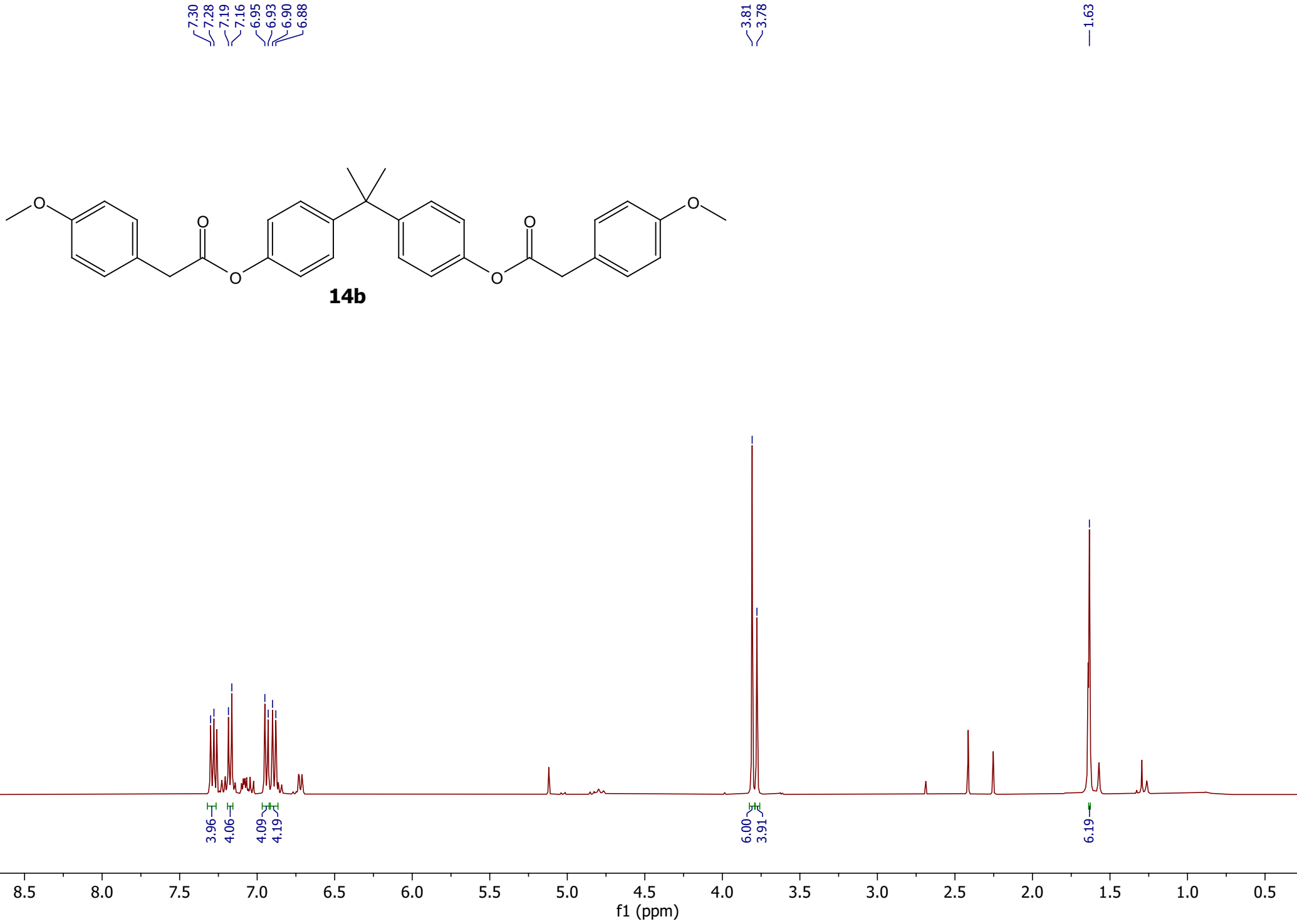
158.98
153.62
148.66
148.62
142.77
130.49
128.08
127.85
125.70
120.83
114.90
114.26
55.43
42.20
40.72
31.12
HO
O
O
O
14a
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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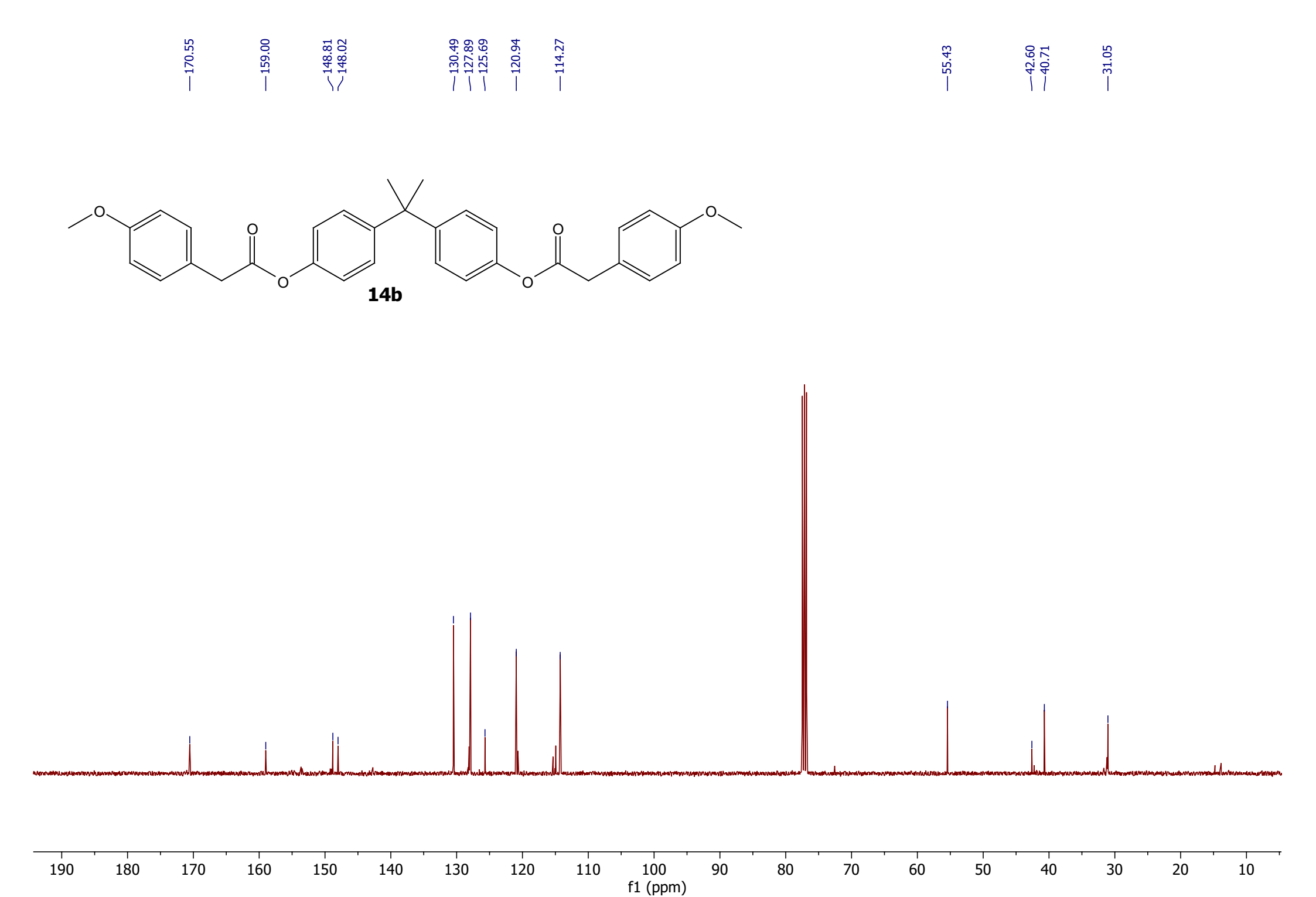
7.28
7.19
7.16
6.95
6.93
6.90
6.88
3.81
3.78
1.63
O
O
O
O
O
O
14b
3.96
4.06
4.09
4.19
6.00
3.91
6.19
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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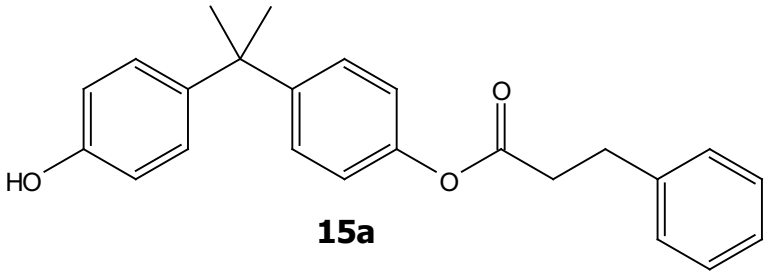
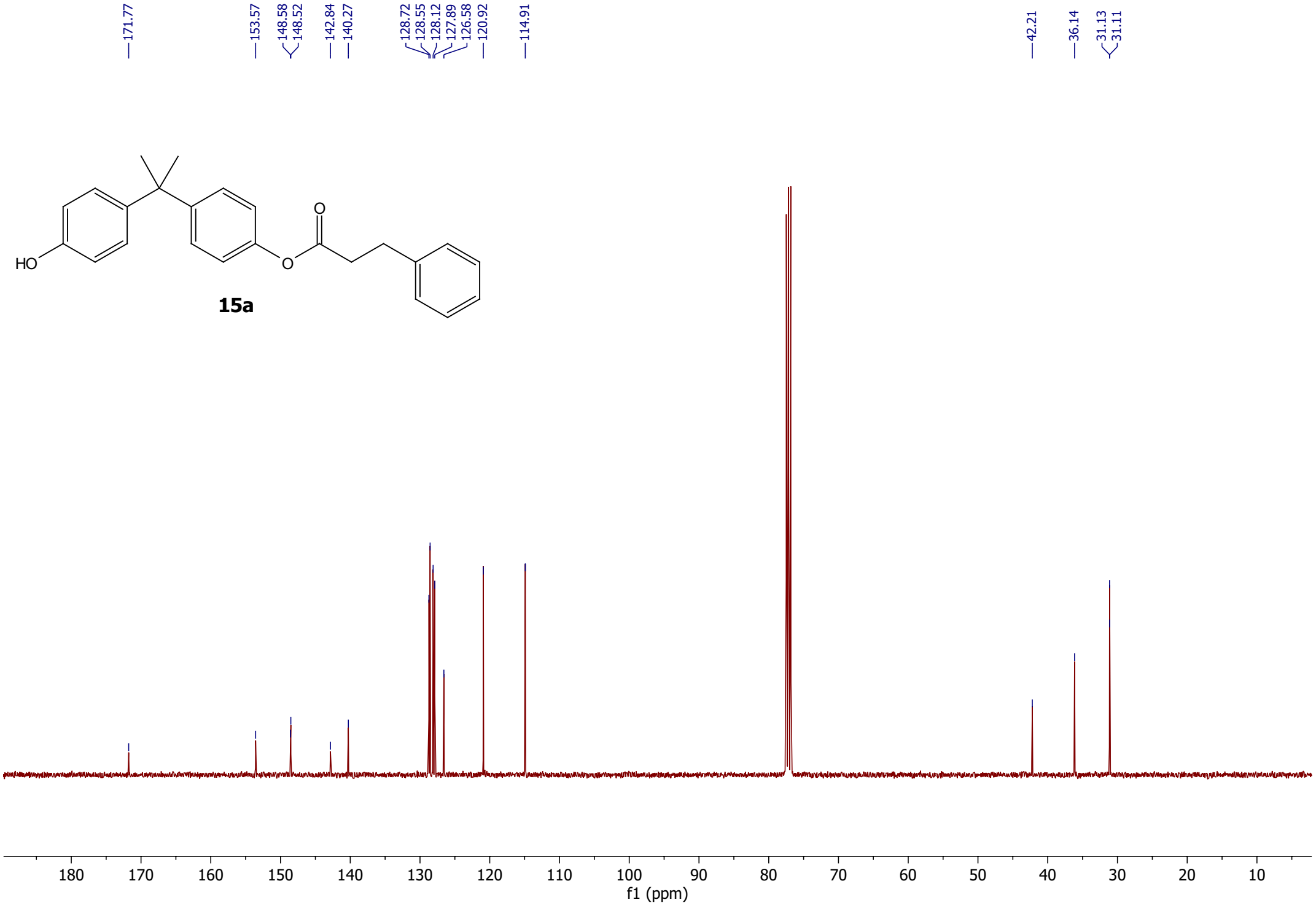
159.00
148.81
148.02
130.49
127.89
125.69
120.94
114.27
55.43
42.60
40.71
31.05
O
O
O
O
O
O
14b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


HO
O
O

15a

7.37
7.35
7.33
7.30
7.29
7.24
7.21
7.12
7.10
6.93
6.91
6.76
6.73
4.76
3.12
3.10
3.08
2.92
2.91
2.89
1.66
2.04
3.14
2.25
2.06
2.01
1.96
0.98
2.08
2.08
6.00
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
f1 (ppm)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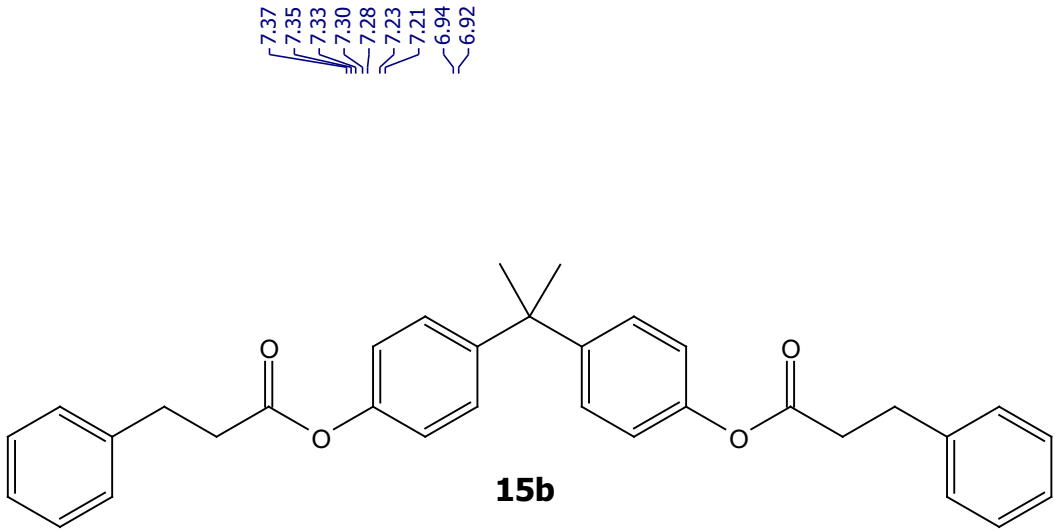
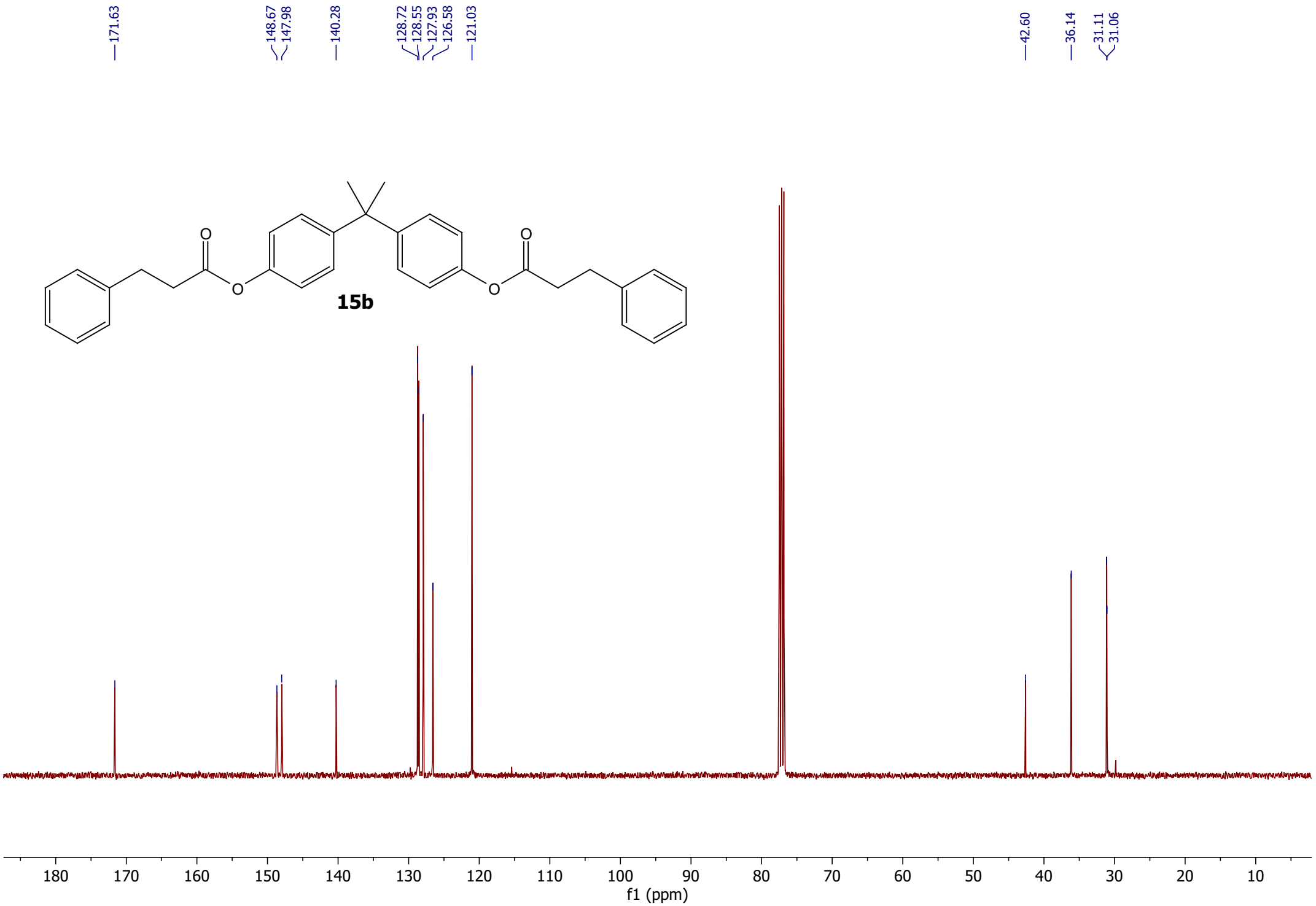
153.57
148.58
148.52
142.84
140.27
128.72
128.55
128.12
127.89
126.58
120.92
114.91
42.21
36.14
31.13
31.11
HO
O
O
15a
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.37
7.35
7.33
7.30
7.28
7.23
7.21
6.94
6.92
3.12
3.10
3.08
2.92
2.90
2.88
1.68
O
O
O
O
15b
3.84
5.09
5.18
3.75
3.95
3.94
6.00
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)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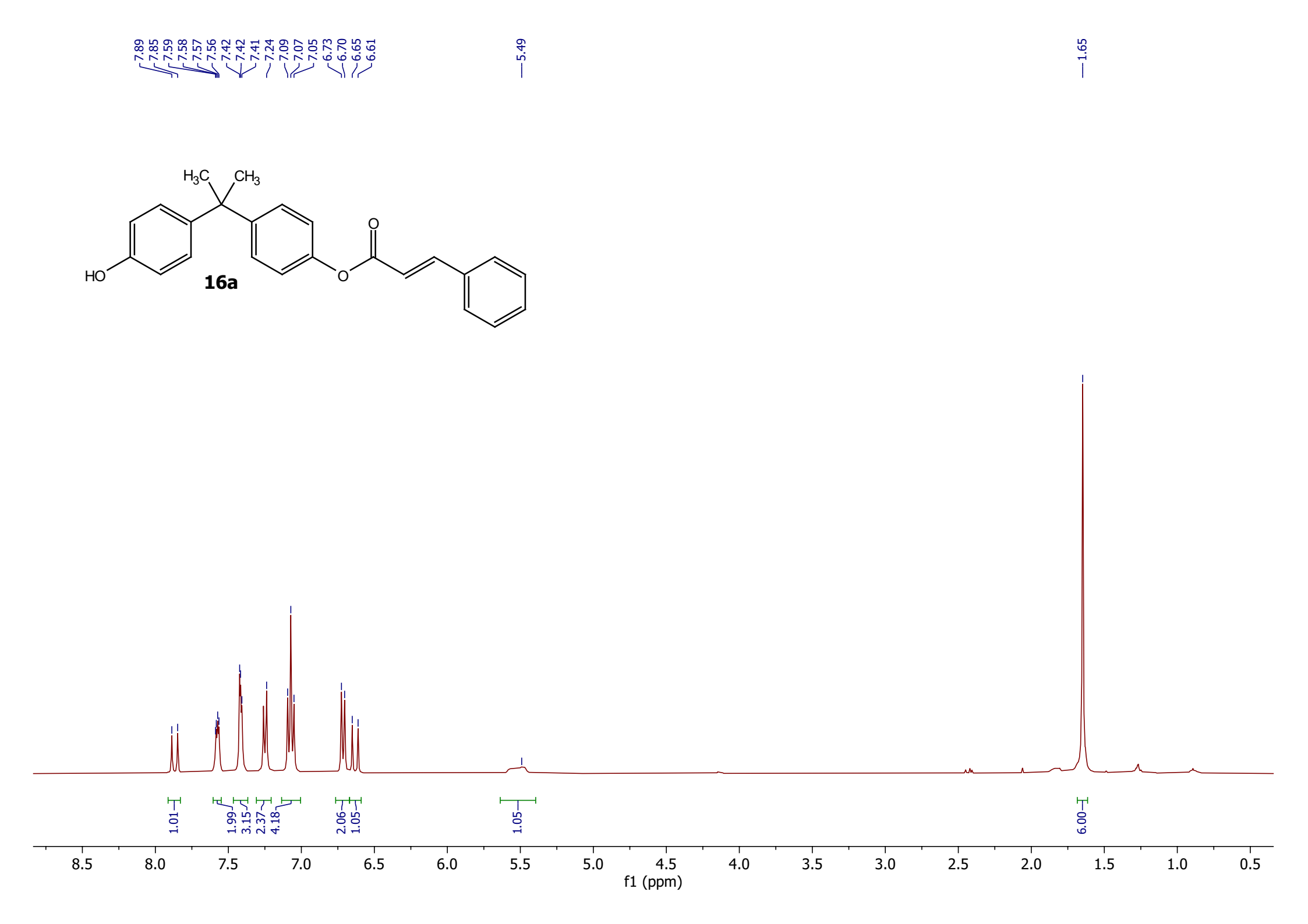
148.67
147.98
140.28
128.72
128.55
127.93
126.58
121.03
42.60
36.14
31.11
31.06
O
O
O
O
15b
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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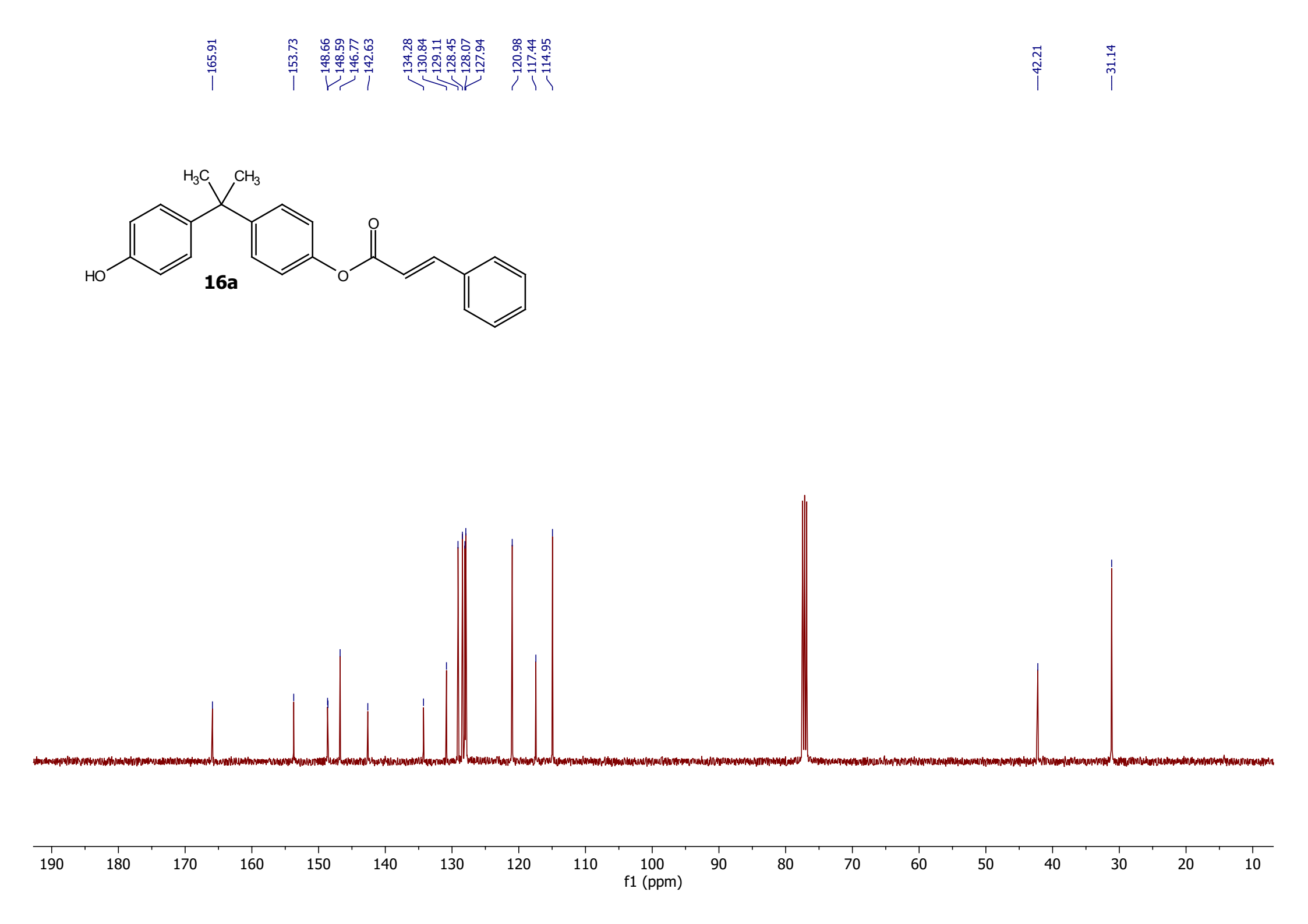
7.85
7.59
7.58
7.57
7.56
7.42
7.42
7.41
7.24
7.09
7.07
7.05
6.73
6.70
6.65
6.61
5.49
1.65
H3C
CH3
HO
O
O
16a
1.01
1.99
3.15
2.37
4.18
2.06
1.05
1.05
6.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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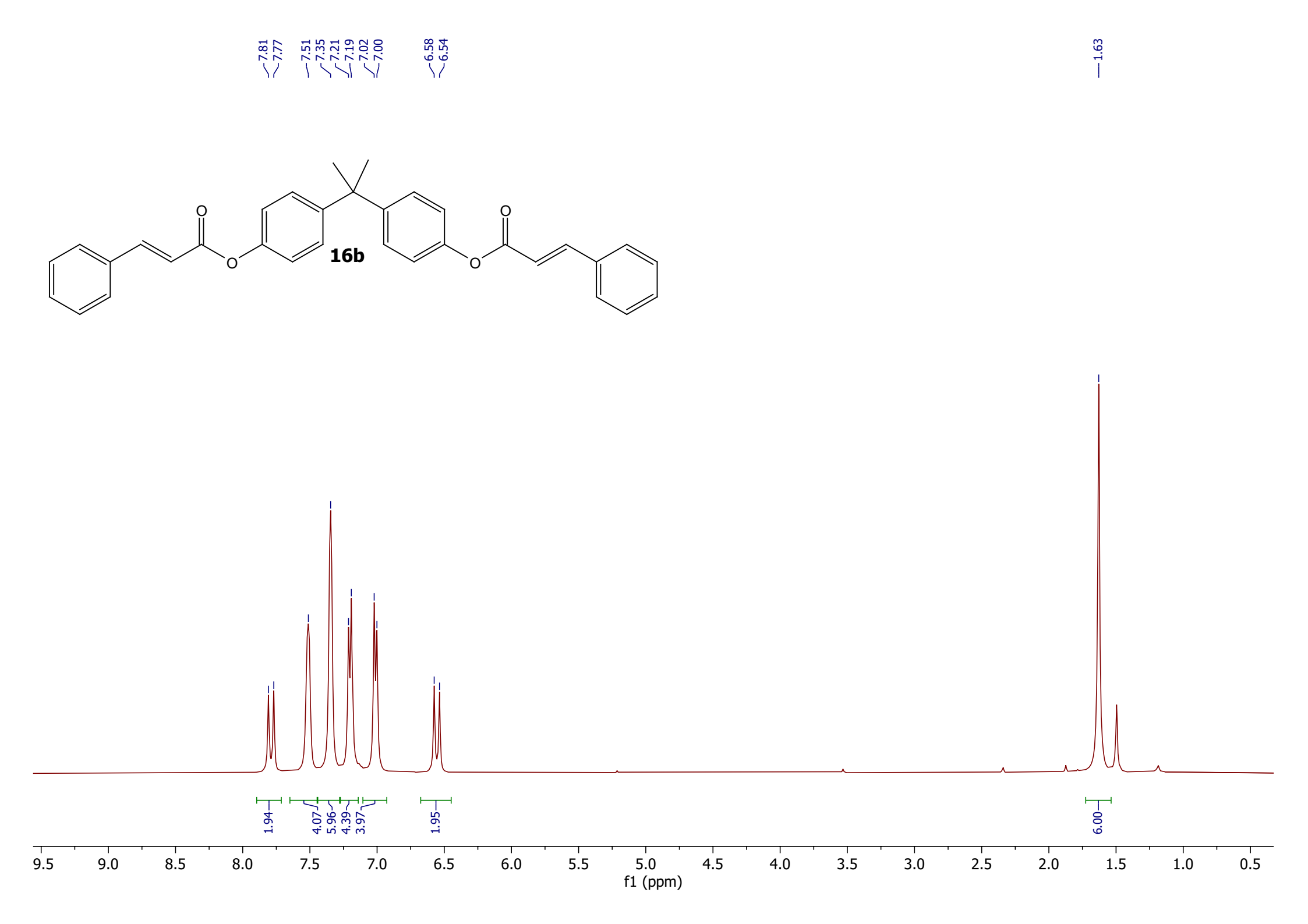
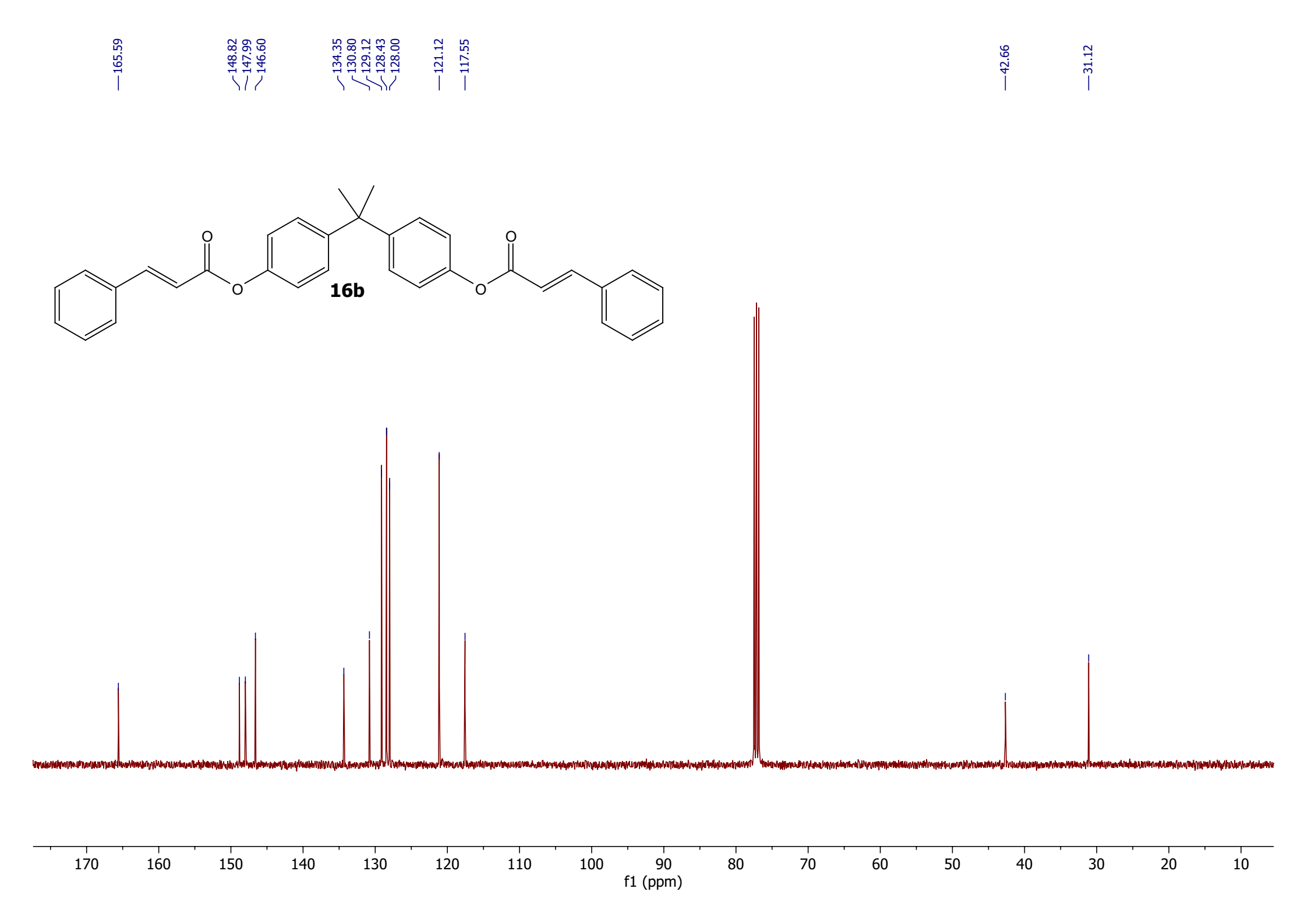
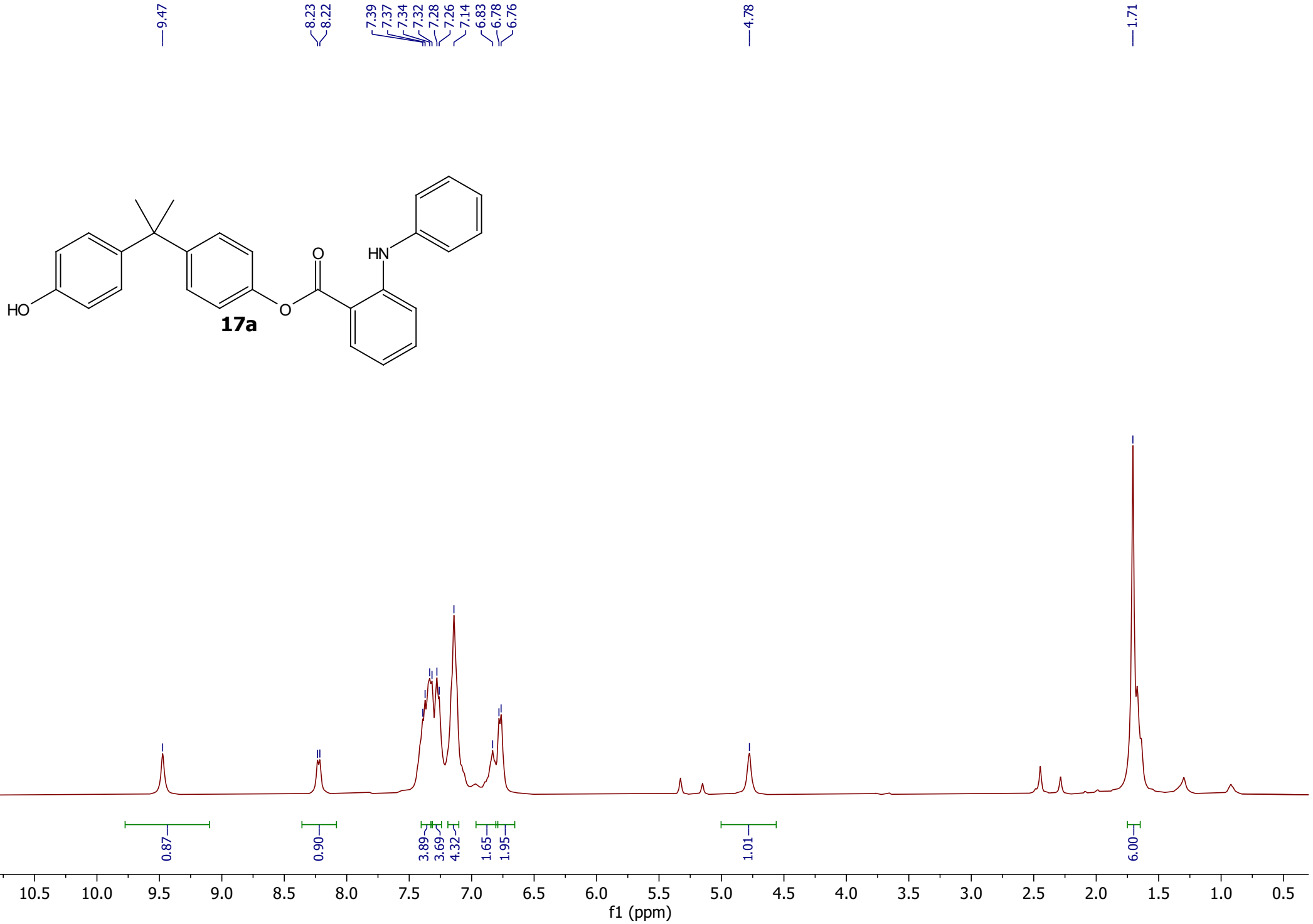
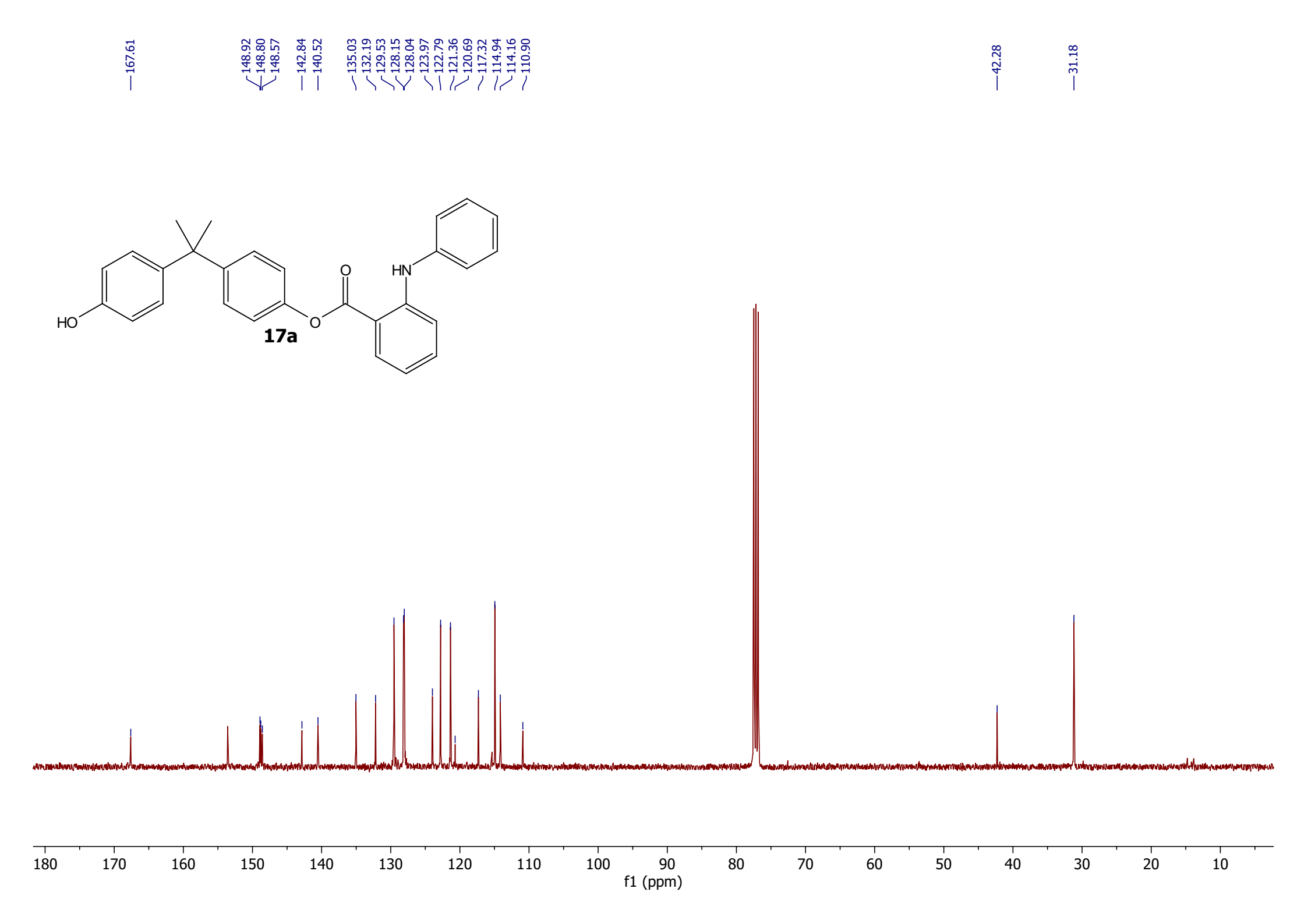
148.59
146.77
142.63
134.28
130.84
129.11
128.45
128.07
127.94
120.98
117.44
114.95
42.21
31.14
H3C
CH3
HO
O
O
16a
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.81
7.77
7.51
7.35
7.21
7.19
7.02
7.00
6.58
6.54
1.63
16b
O
O
O
O
1.94
4.07
5.96
4.39
3.97
1.95
6.00
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
f1 (ppm)


165.59
148.82
147.99
146.60
134.35
130.80
129.12
128.43
128.00
121.12
117.55
42.66
31.12
16b
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


9.47
8.23
8.22
7.39
7.37
7.34
7.32
7.28
7.26
7.14
6.83
6.78
6.76
4.78
1.71
HO
O
O
HN
17a
0.87
0.90
3.89
3.69
4.32
1.65
1.95
1.01
6.00
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
f1 (ppm)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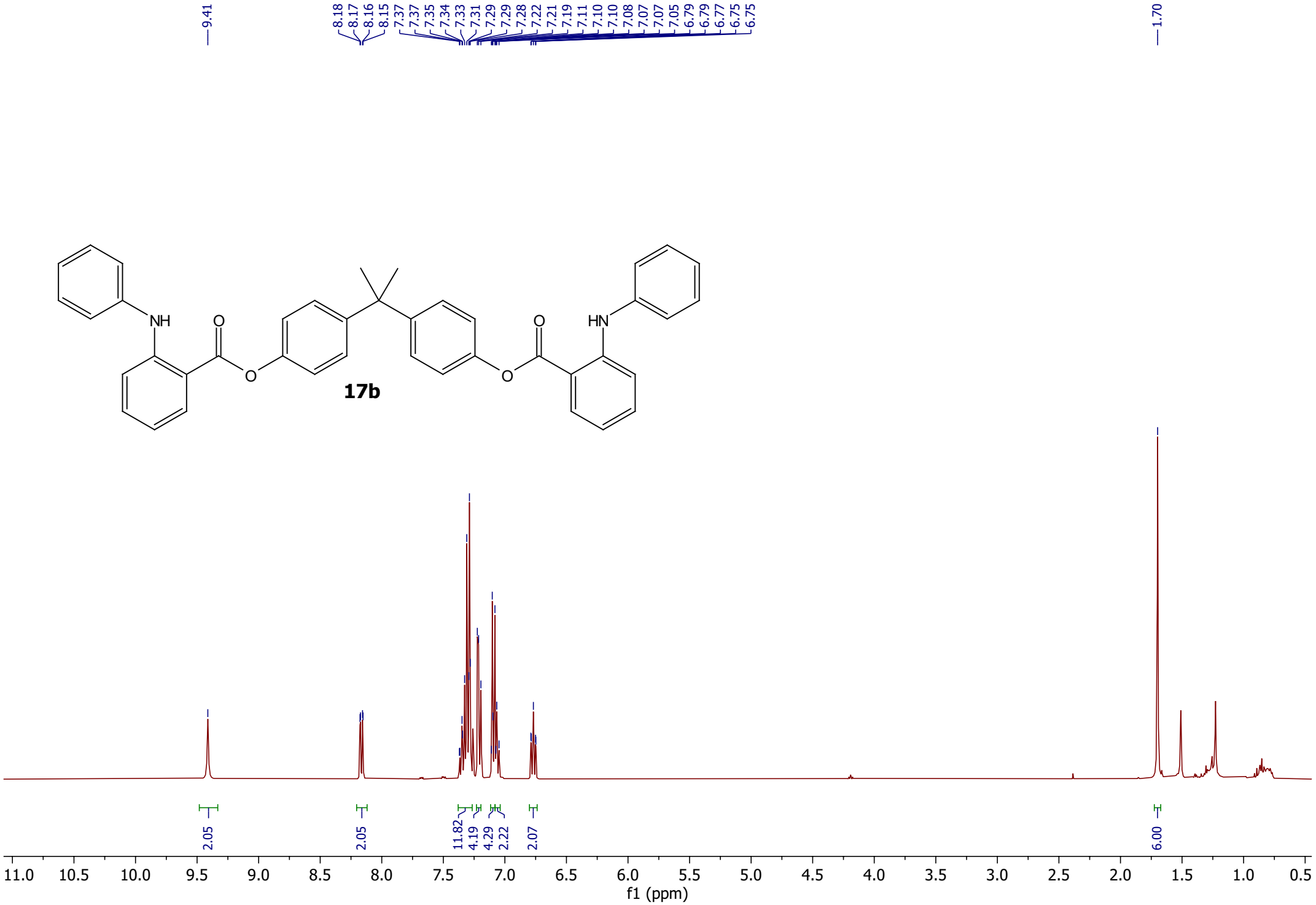
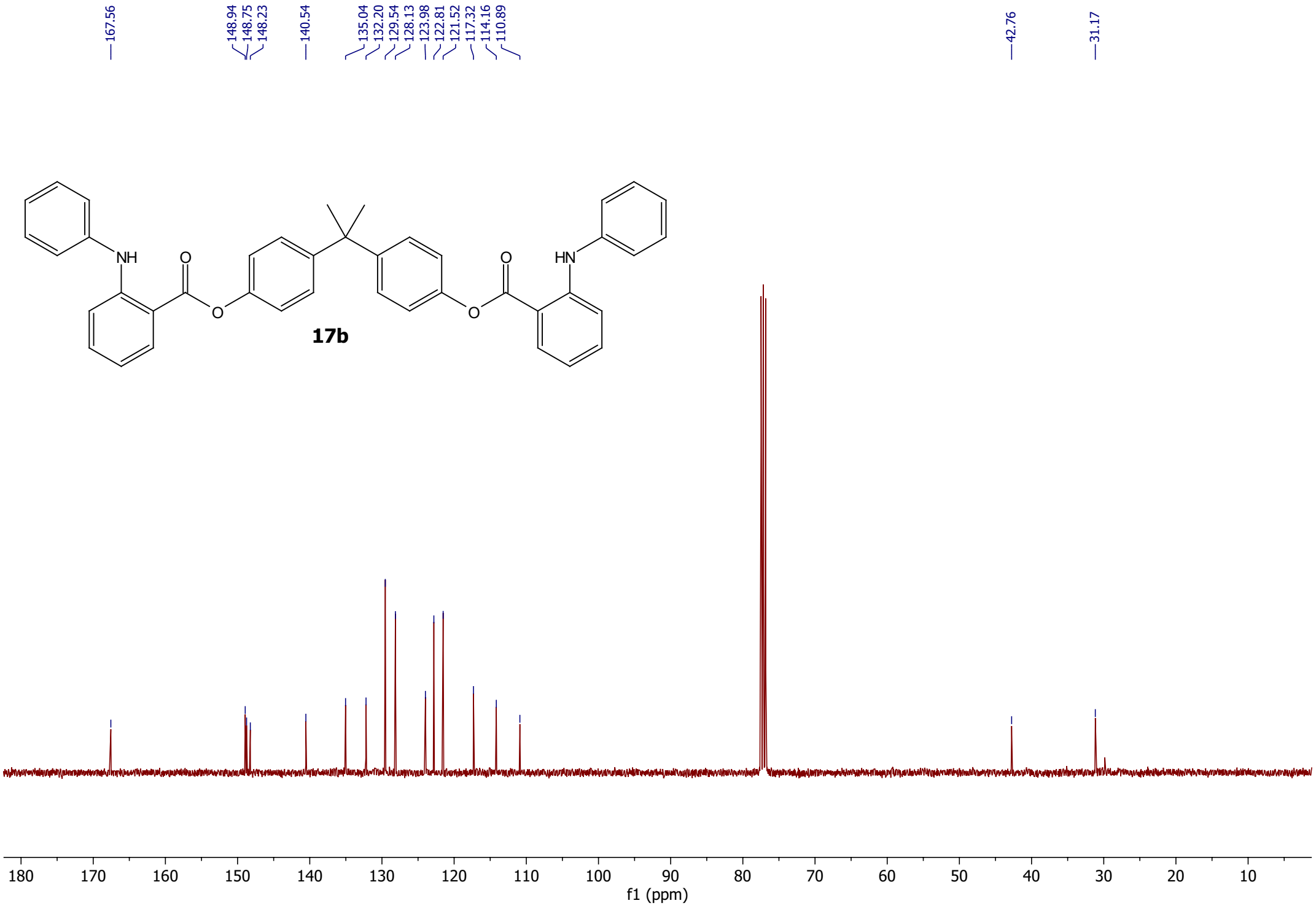
148.80
148.57
142.84
140.52
135.03
132.19
129.53
128.15
128.04
123.97
122.79
121.36
120.69
117.32
114.94
114.16
110.90
42.28
31.18
HO
O
O
HN
17a
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


9.41
8.18
8.17
8.16
8.15
7.37
7.37
7.35
7.34
7.33
7.31
7.29
7.29
7.28
7.22
7.21
7.19
7.11
7.10
7.10
7.08
7.07
7.07
7.05
6.79
6.79
6.77
6.75
6.75
1.70
NH
O
O
O
O
HN
17b
2.05
2.05
11.82
4.19
4.29
2.22
2.07
6.00
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
f1 (ppm)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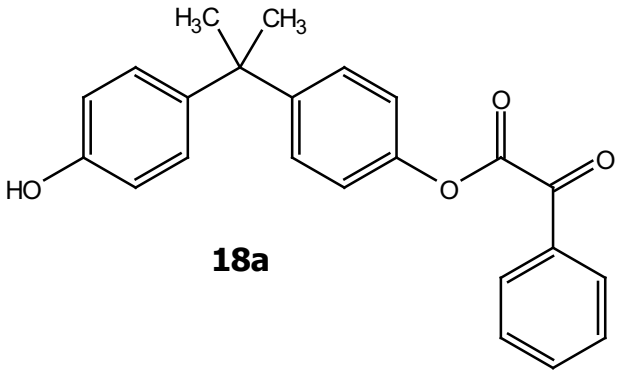
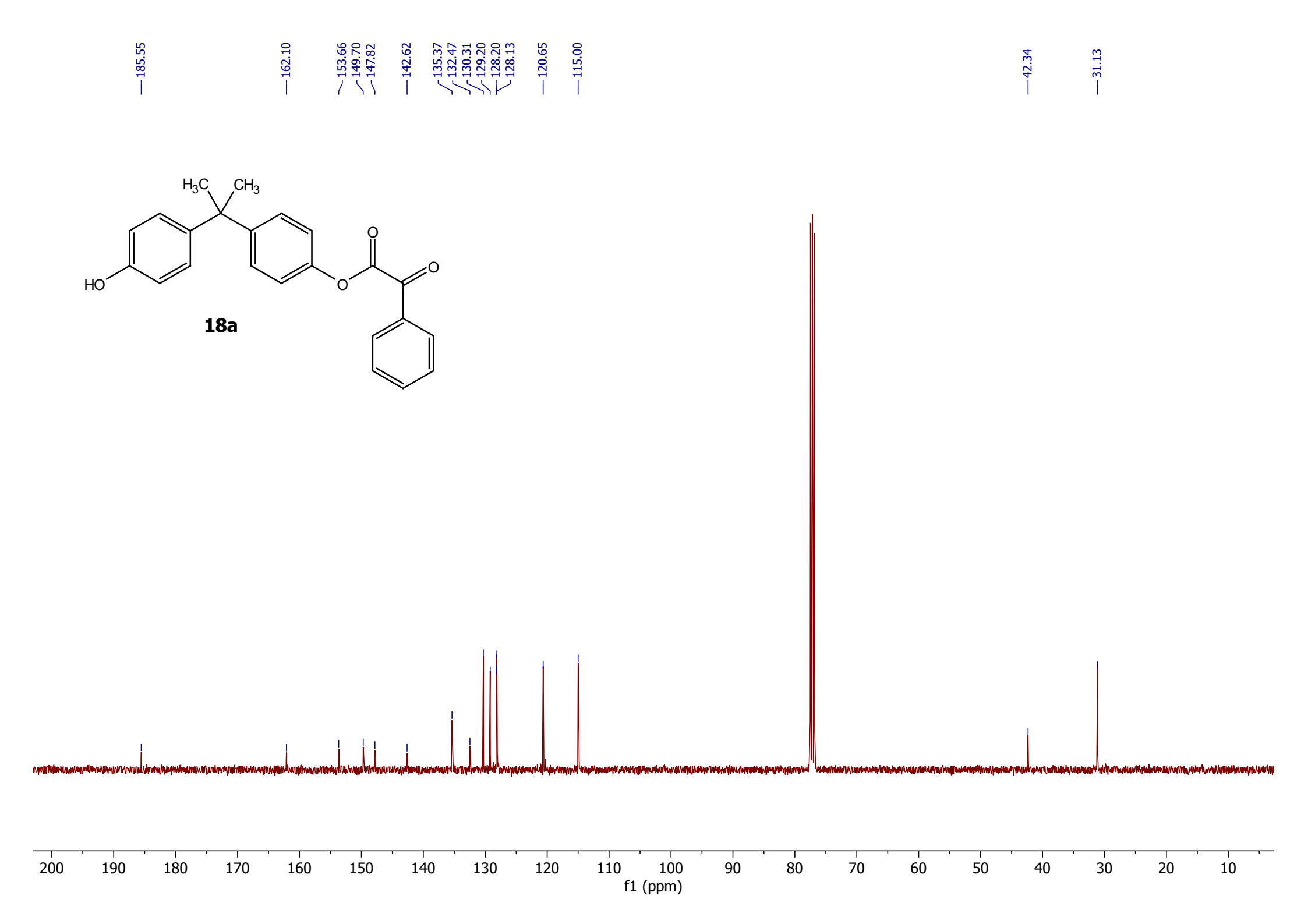
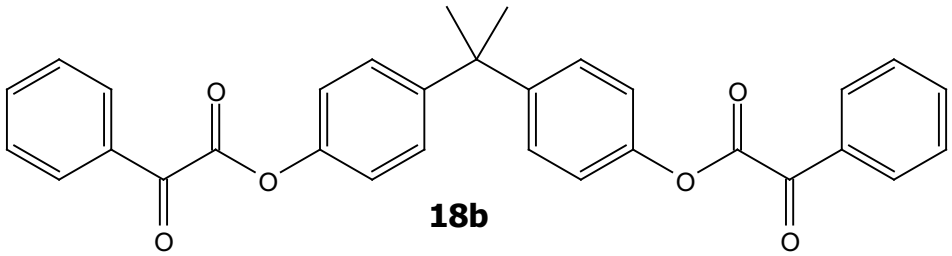
148.75
148.23
140.54
135.04
132.20
129.54
128.13
123.98
122.81
121.52
117.32
114.16
110.89
42.76
31.17
NH
O
O
O
HN
17b
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


H3C
CH3
HO
O
O
O

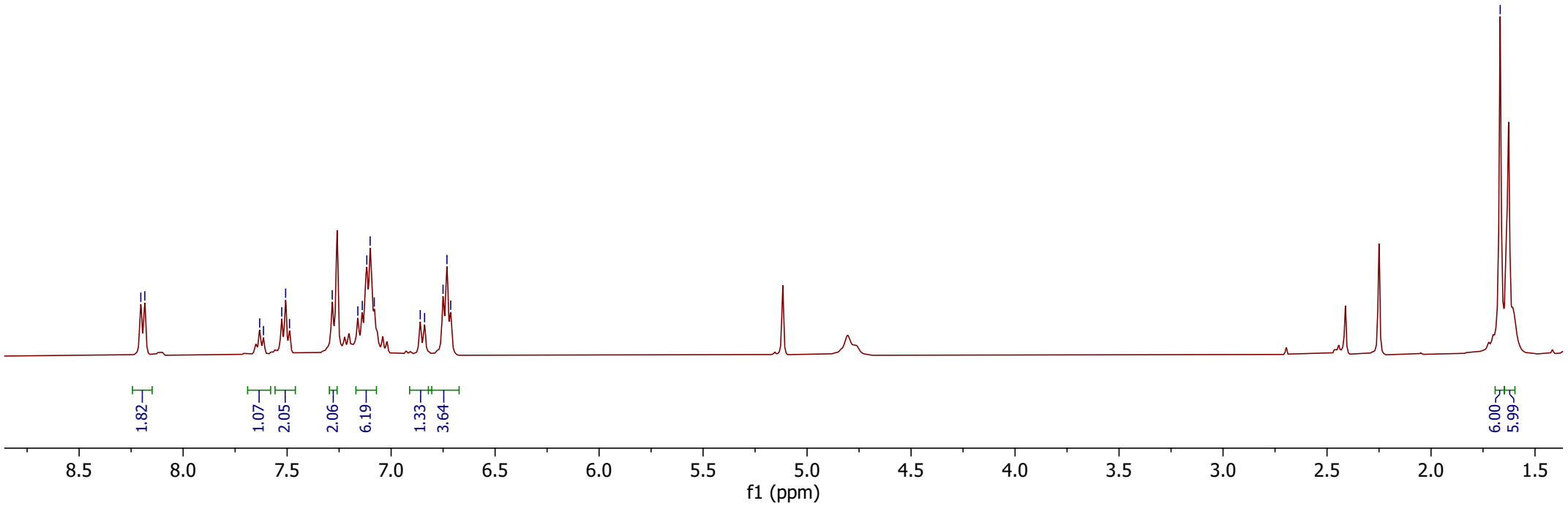
18a

8.07
8.05
7.68
7.66
7.64
7.53
7.51
7.49
7.24
7.21
7.13
7.10
7.07
7.05
6.72
6.70
4.73
1.62
1.65
0.96
1.73
1.98
2.17
2.11
1.97
0.93
6.00
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
f1 (ppm)


185.55
162.10
153.66
149.70
147.82
142.62
135.37
132.47
130.31
129.20
128.20
128.13
120.65
115.00
42.34
31.13
H3C
CH3
HO
O
O
O
18a
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


O
O
O
O
O

18b


8.20
8.18
7.63
7.61
7.53
7.51
7.49
7.28
7.16
7.14
7.12
7.10
7.08
6.86
6.84
6.75
6.73
6.71
1.67
1.82
1.07
2.05
2.06
6.19
1.33
3.64
6.00
5.99
8.5
8.0
7.5
7.0
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4.5
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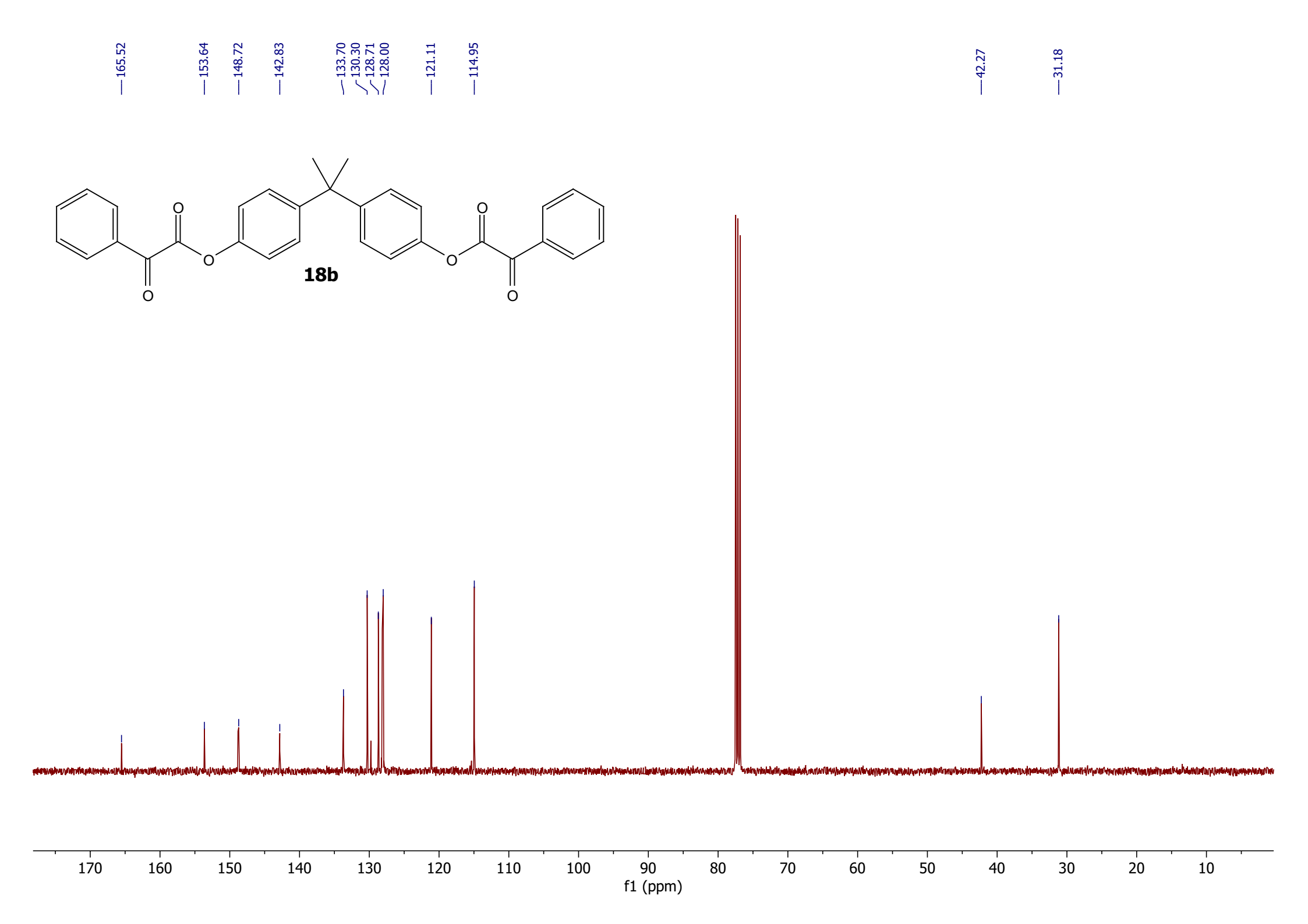
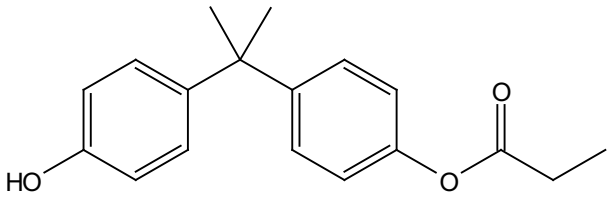
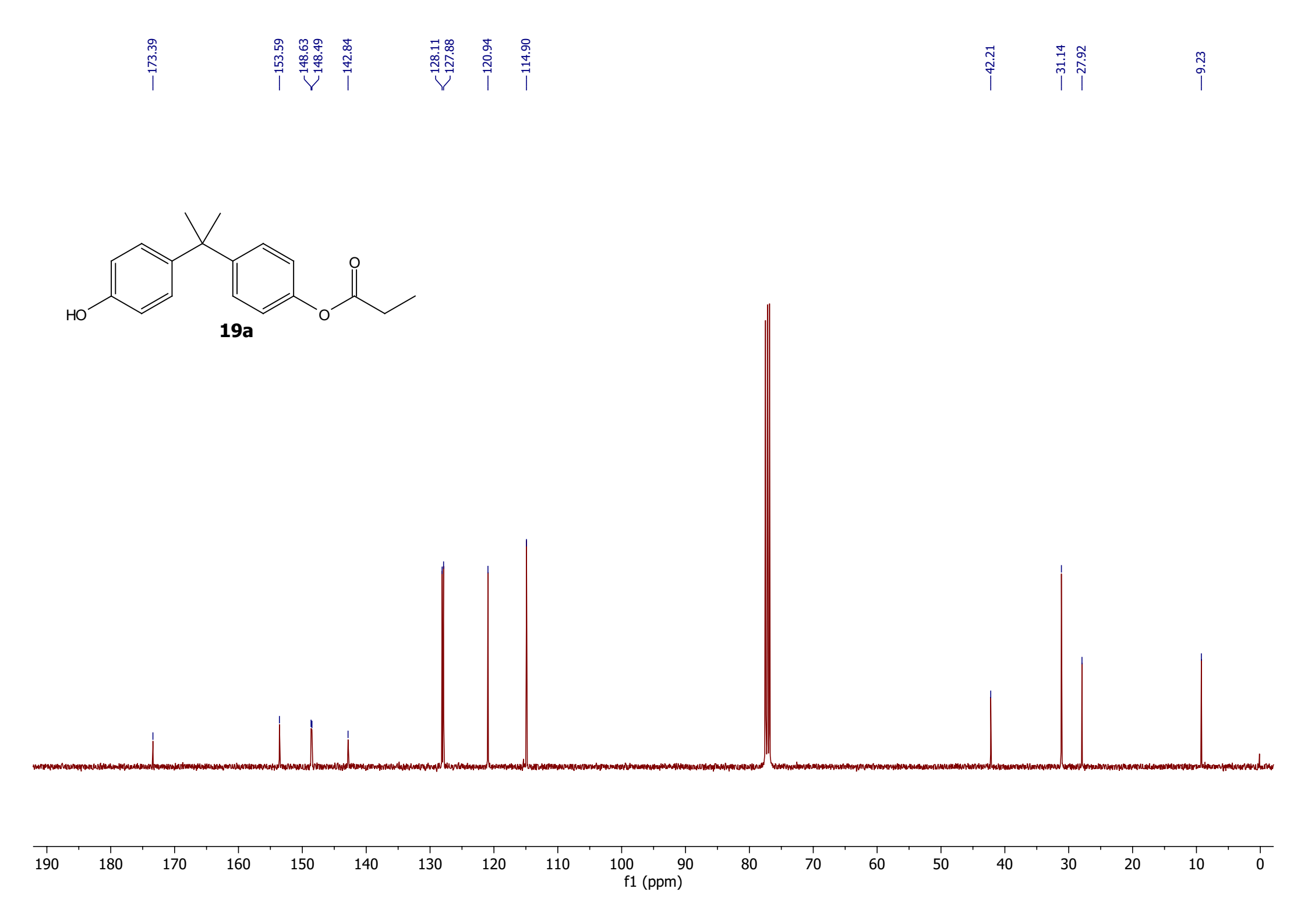
3.5
3.0
2.5
2.0
1.5
f1 (ppm)

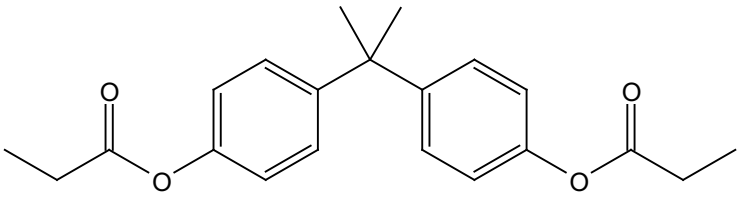

165.52
153.64
148.72
142.83
133.70
130.30
128.71
128.00
121.11
114.95
42.27
31.18
O
O
O
O
O
O
18b
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


HO
O
O

19a

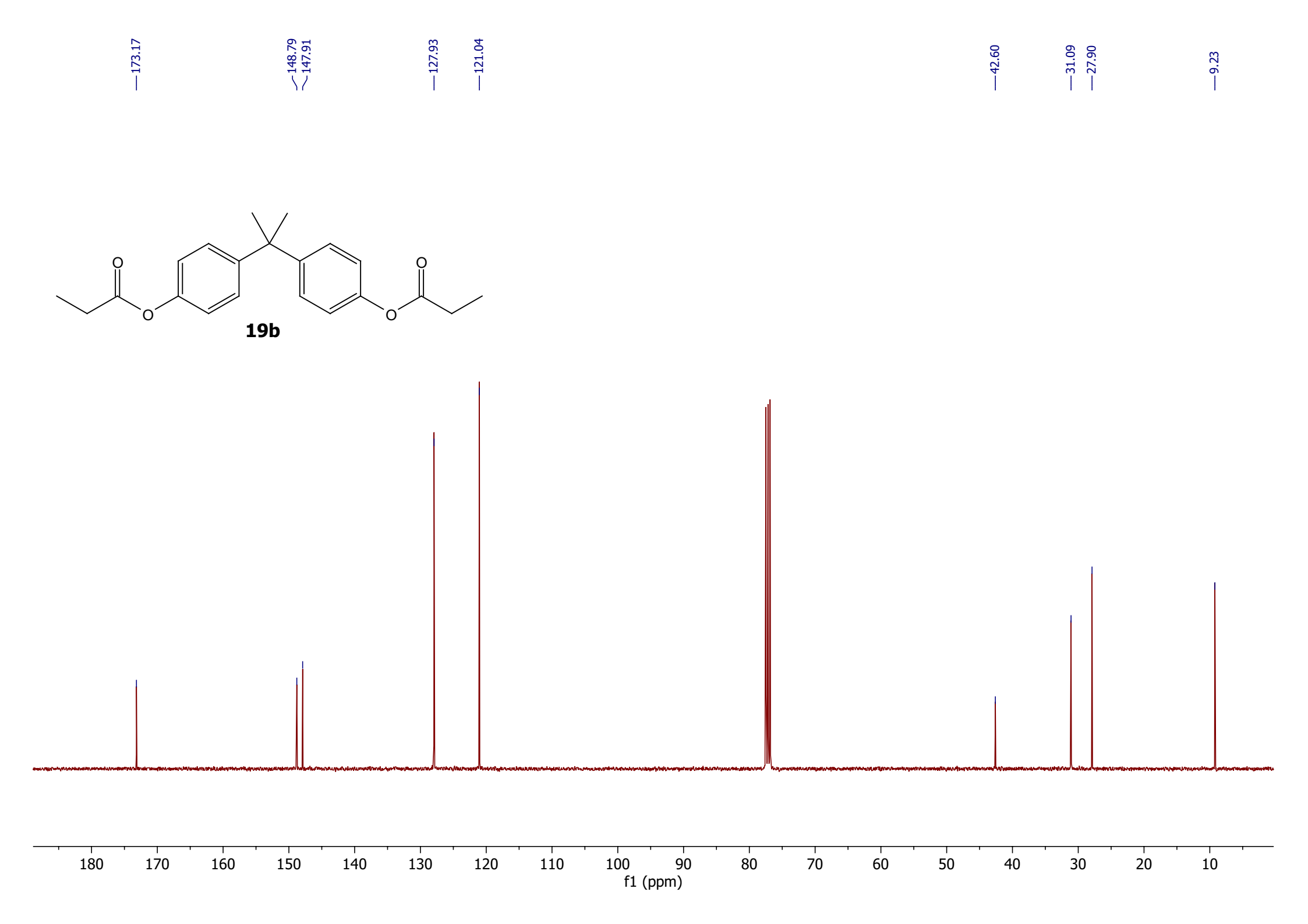
7.22
7.20
7.09
7.07
6.98
6.96
6.72
6.70
4.82
2.61
2.59
2.57
2.55
1.64
1.28
1.26
1.24
1.71
1.73
1.67
1.71
0.81
1.71
6.00
2.63
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

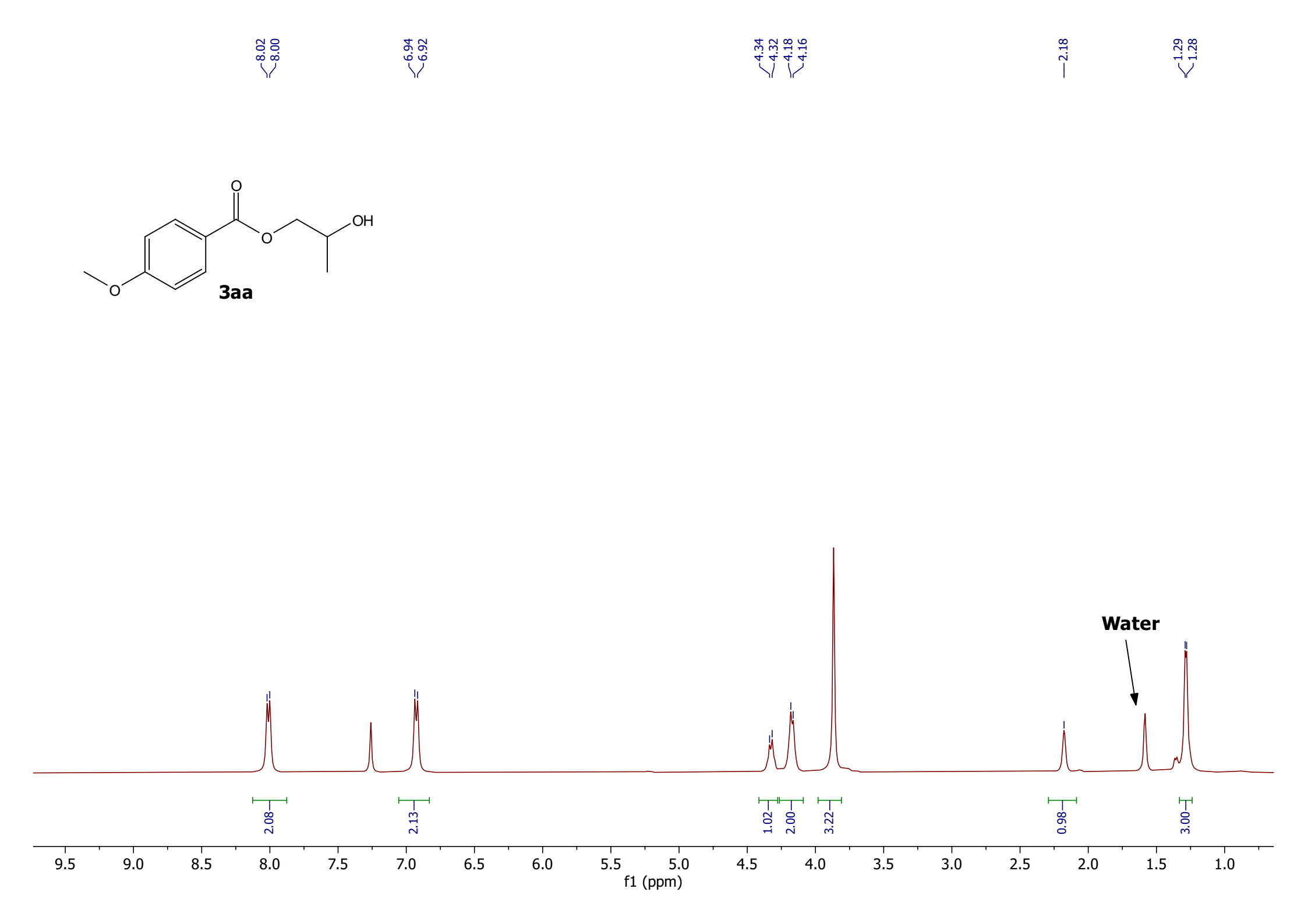

173.39
153.59
148.63
148.49
142.84
128.11
127.88
120.94
114.90
42.21
31.14
27.92
9.23
HO
O
O
19a
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

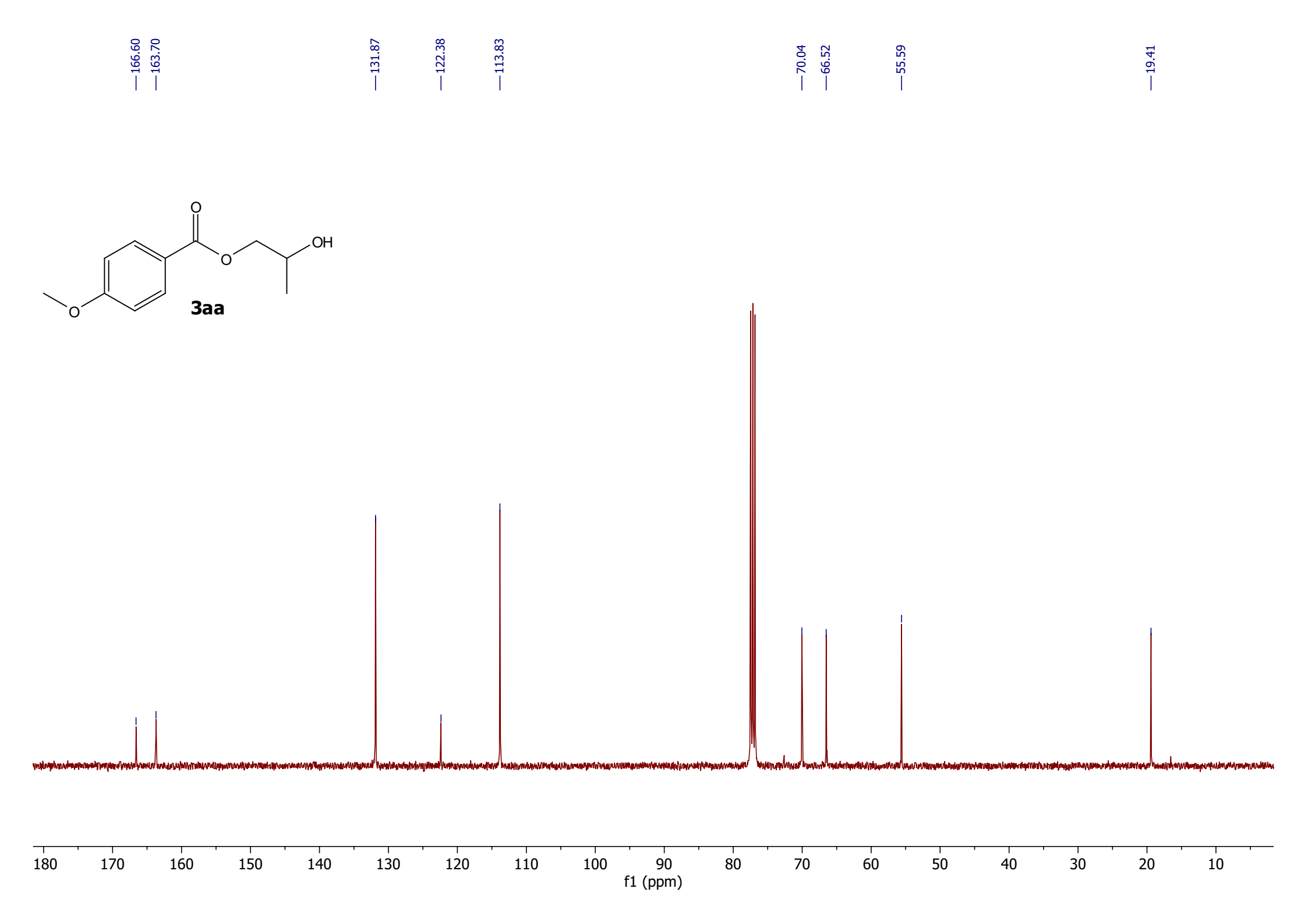


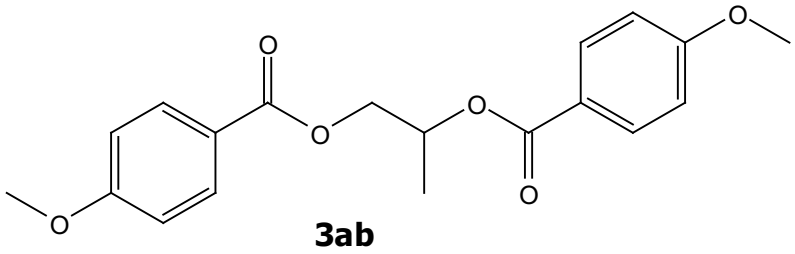
19b

7.23
7.21
6.99
6.97
2.60
2.58
2.56
2.55
1.67
1.28
1.26
1.24
3.87
3.78
3.96
6.00
6.03
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)


173.17
148.79
147.91
127.93
121.04
42.60
31.09
27.90
9.23
O
O
O
O
19b
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

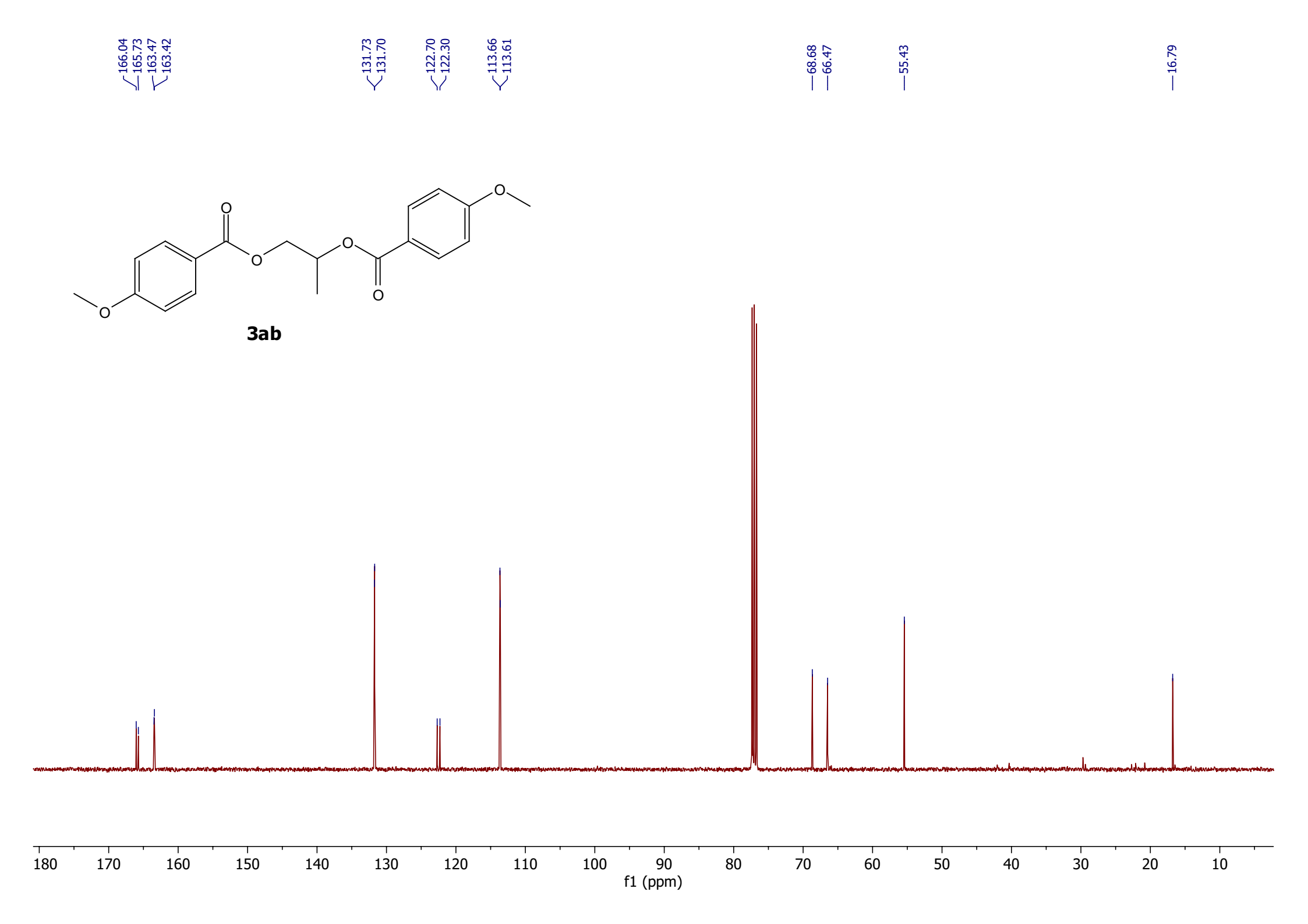

8.02
8.00
6.94
6.92
4.34
4.32
4.18
4.16
2.18
1.29
1.28
O
O
OH
O
3aa
Water
2.08
2.13
1.02
2.00
3.22
0.98
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)

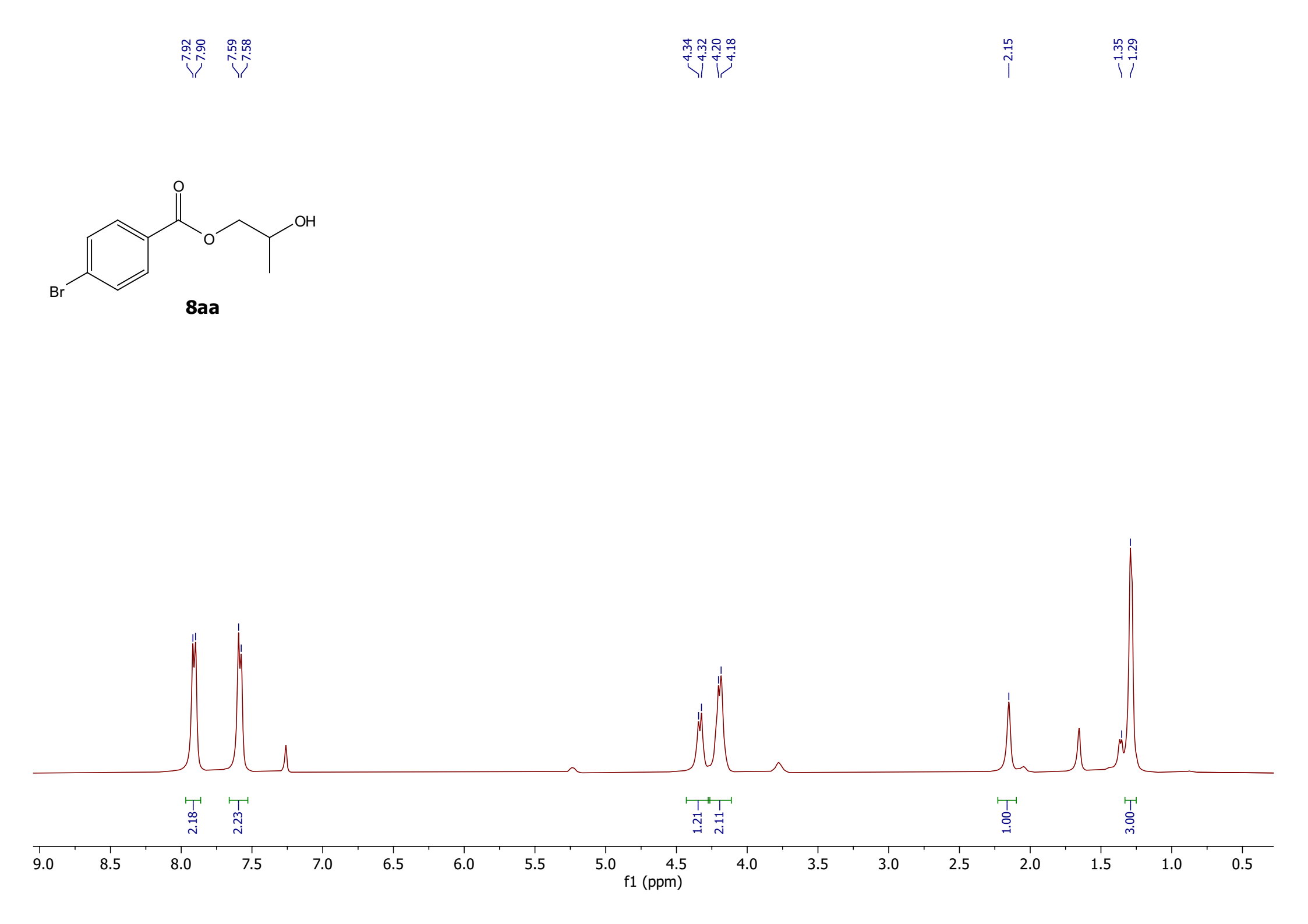

166.60
163.70
131.87
122.38
113.83
70.04
66.52
55.59
19.41
O
O
OH
O
3aa
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

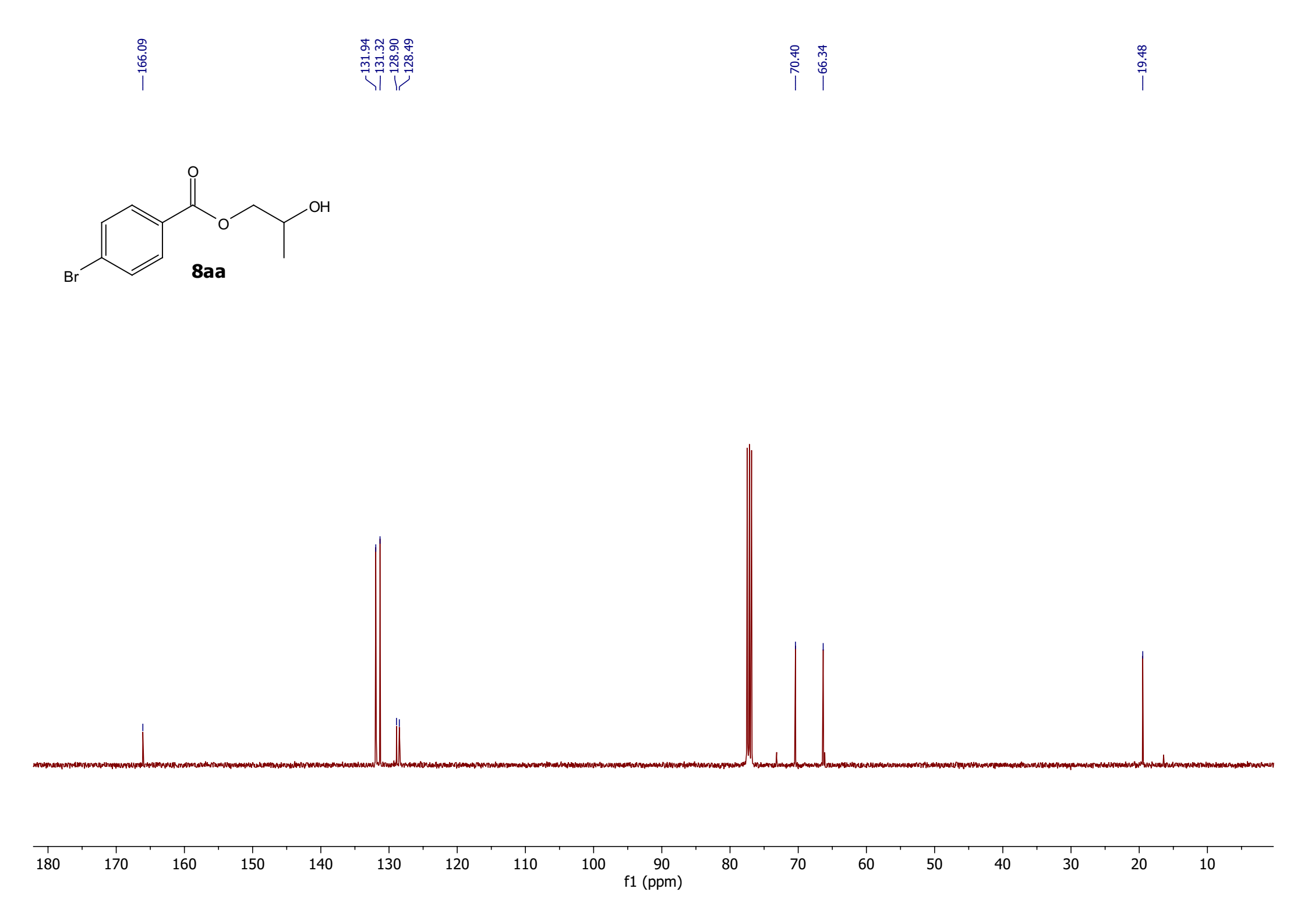


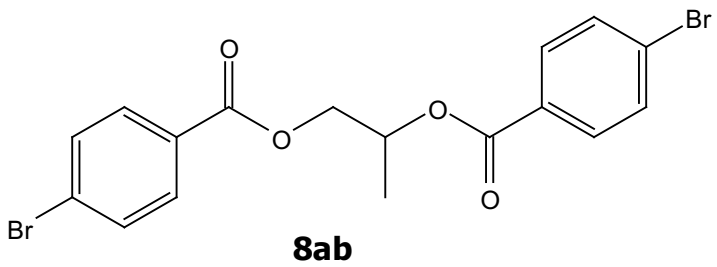
3ab

8.01
7.99
7.99
7.96
6.92
6.90
6.89
6.88
5.53
5.51
5.50
5.48
5.47
5.45
4.46
4.44
3.85
3.84
1.45
1.44
3.94
4.06
1.01
1.99
3.21
3.02
3.00
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
f1 (ppm)


166.04
165.73
163.47
163.42
131.73
131.70
122.70
122.30
113.66
113.61
68.68
66.47
55.43
16.79
O
O
O
O
O
O
3ab
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

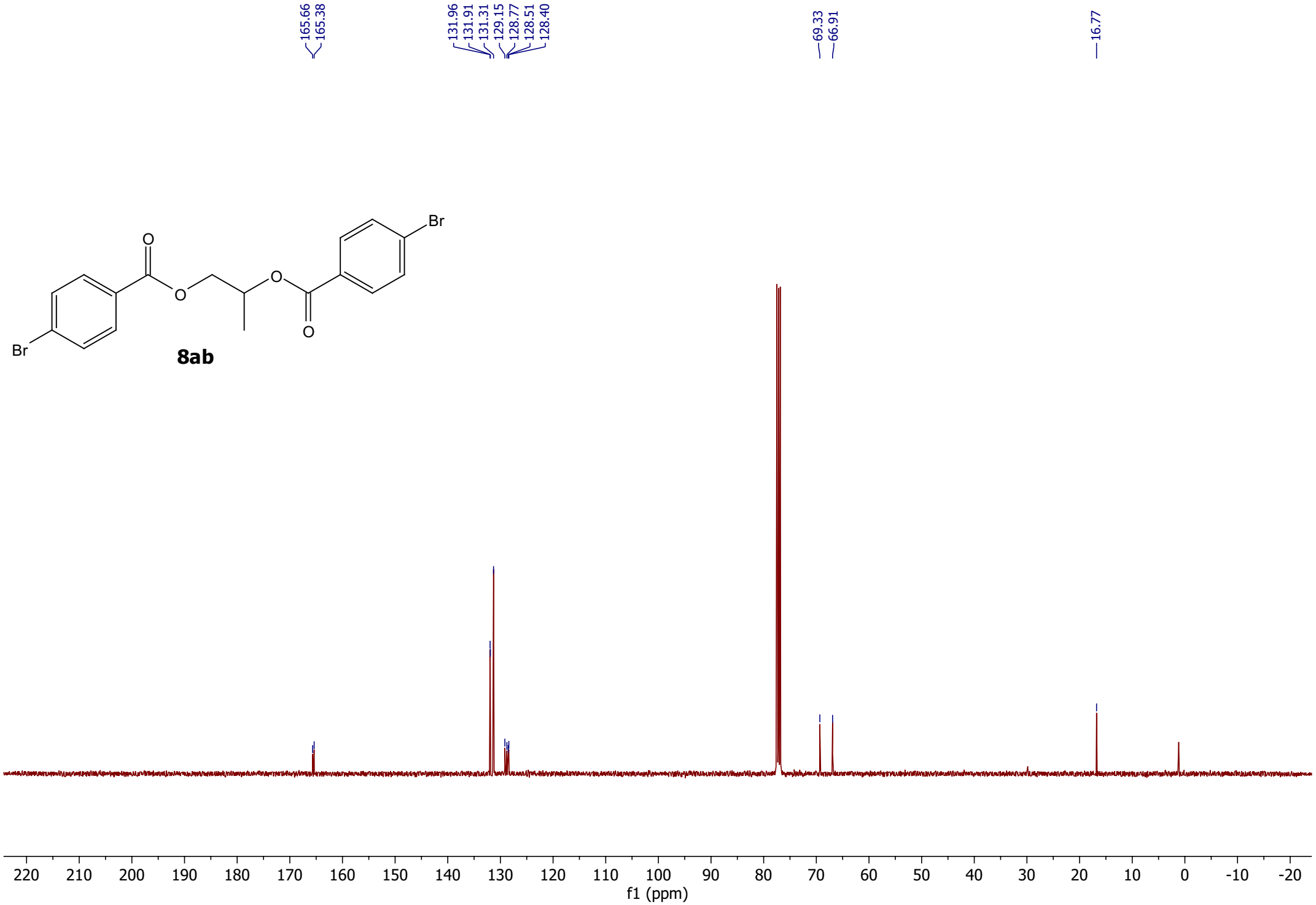

7.92
7.90
7.59
7.58
4.34
4.32
4.20
4.18
2.15
1.35
1.29
O
O
OH
Br
8aa
2.18
2.23
1.21
2.11
1.00
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

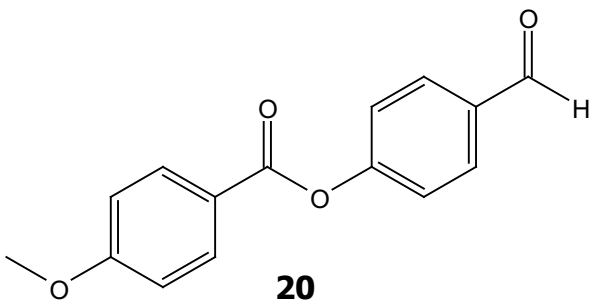

166.09
131.94
131.32
128.90
128.49
70.40
66.34
19.48
O
O
OH
Br
8aa
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


Br
O
O
O
O
Br

8ab

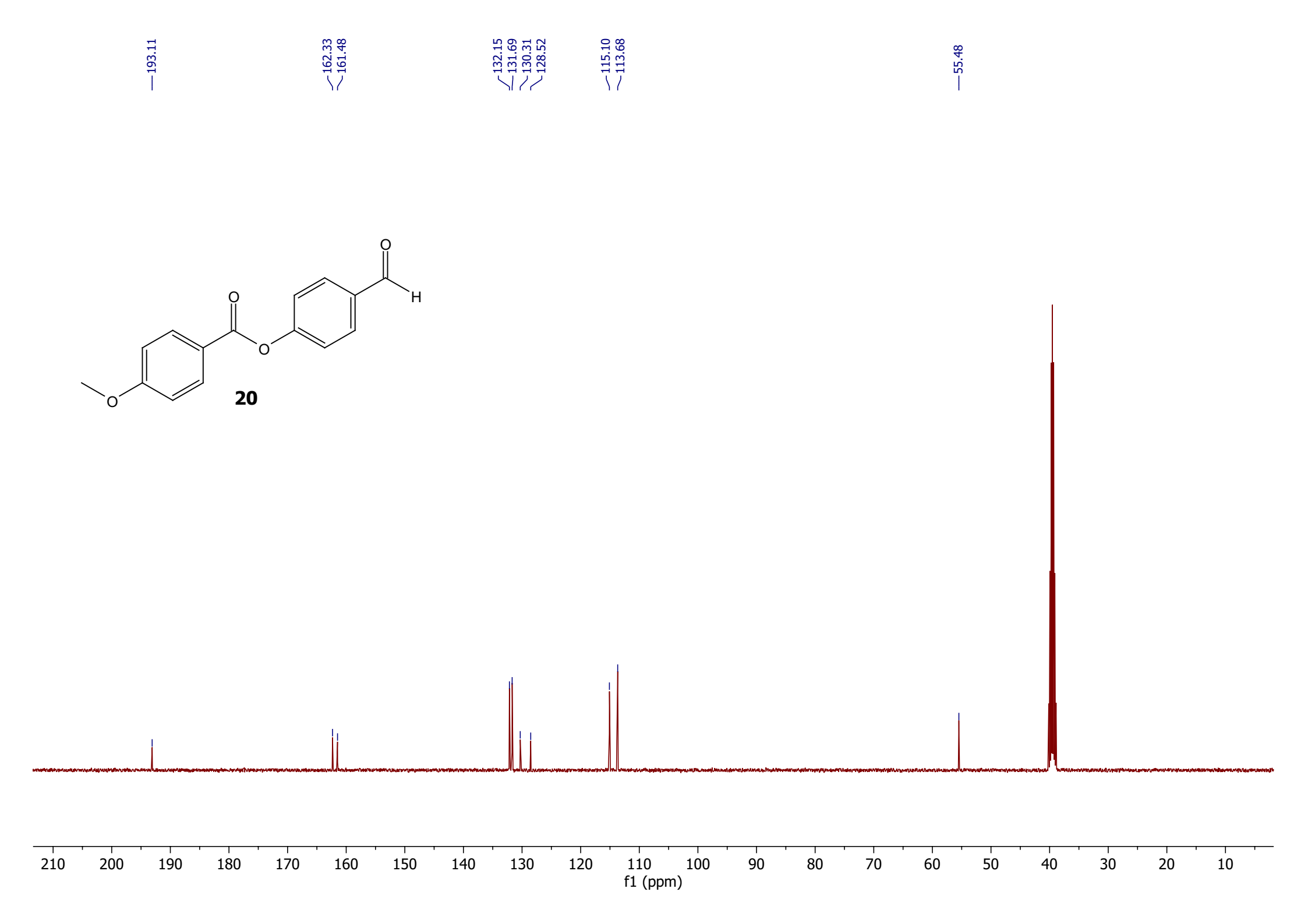
7.90
7.87
7.85
7.58
7.57
7.56
7.55
5.54
5.53
5.52
5.50
4.50
4.49
1.47
1.45
2.28
2.10
1.96
2.05
0.97
1.96
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


165.66
165.38
131.96
131.91
131.31
129.15
128.77
128.51
128.40
69.33
66.91
16.77
Br
O
O
O
O
Br
8ab
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)


O
H
O
O
O

20

10.32
7.70
7.68
7.63
7.61
7.08
7.05
6.90
6.87
3.85
0.99
2.03
2.03
2.04
2.05
3.00
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
f1 (ppm)


193.11
162.33
161.48
132.15
131.69
130.31
128.52
115.10
113.68
55.48
O
O
O
H
O
20
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)