Electronic Supplementary Material (ESI) for ChemComm.


# N-Heterocyclic Carbene/Photo-Cocatalyzed Oxidative Smiles Rearrangement: Synthesis of Aryl Salicylates from *O*-Aryl Salicylaldehydes

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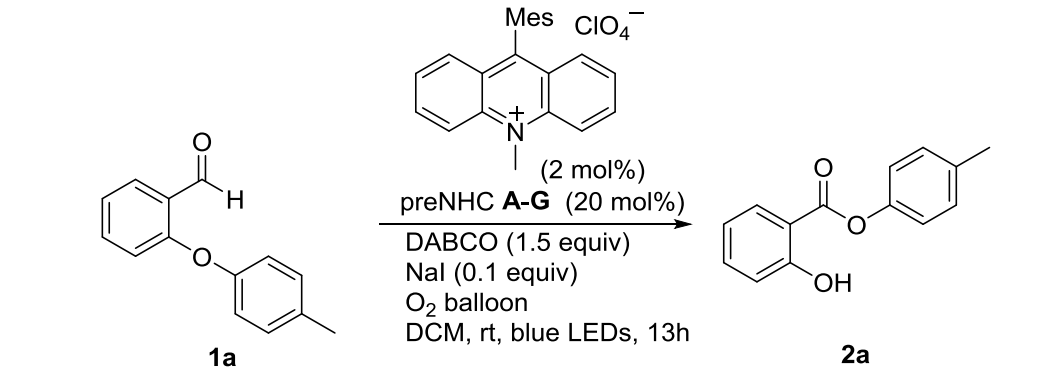
# Part I Experimental Part

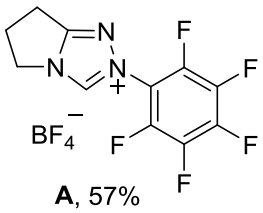
## 1. General Information

Unless otherwise indicated, all reactions were carried out under $O_2$ with the balloon at room temperature with magnetic stirring. Anhydrous 1,4-dioxane was distilled from sodium and benzophenone. Anhydrous $CH_2Cl_2$ and acetonitrile were distilled from $CaH_2$. Pre-NHCs **A**-**G** were prepared according to literatures.[1] Photocatalysts *fac*-Ir(ppy)$_3$,[2] 2-(aryloxy)benzaldehyde[3] were prepared according to literatures. Ru(bpy)$_3$Cl$_2$ was purchased from Aldrich. Mes-Acr-Me$^+$ClO$_4^-$ was purchased from TCI. All $^1$H NMR (400 and 500 MHz), $^{13}$C NMR (100 and 125 MHz) spectra were recorded on a Bruker Avance 400 and Bruker Avance 500 spectrometer in $CDCl_3$, with tetramethylsilane as an internal standard and reported in parts per million (ppm, δ). $^1$H NMR Spectroscopy splitting patterns were designated as singlet (s), doublet (d), triplet (t), quartet (q). Splitting patterns that could not be interpreted or easily visualized were designated as multiplet (m) or broad (br). Infrared spectra were recorded on a JASCO FT/IR-480 spectrophotometer and reported as wave number (cm$^{-1}$). HRMS were obtained on an ESI-Orbitrap mass analyzer or ESI-ICR mass analyzer. Experiments upon visible-light irradiation were carried out using household blue LED lamps (JDY-THDGY, $\lambda_{max}$ = 455 nm, 18 × 1W). Irradiation occurred from the bottom of each vial at a distance of 3 cm. Column chromatography was carried out on silica gel (200-300 mesh).

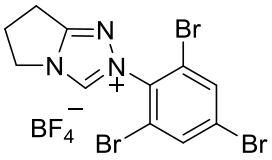
## 2. Screening of NHC precursors (Scheme S1)



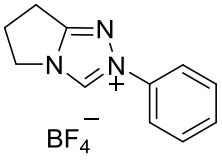

Yield of **2a**



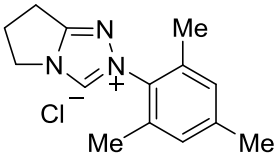
**A**, 57%



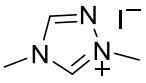
**B**, 34%



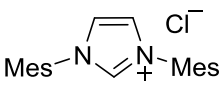
**C,** trace



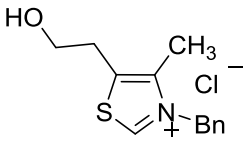
**D**, trace



**E**, 0%

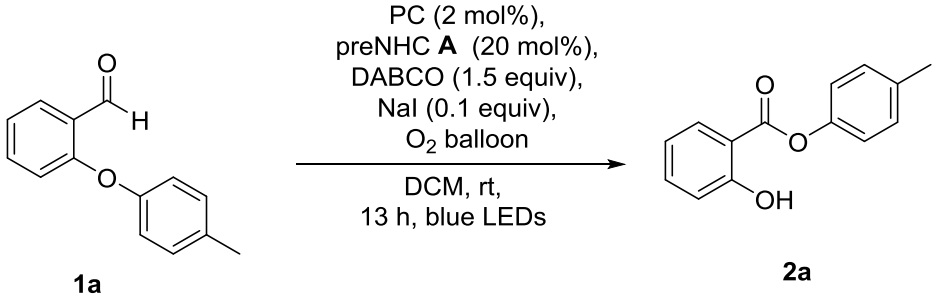


**F**, 0%



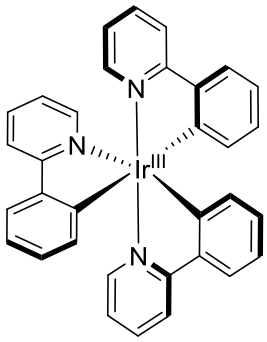
**G**, 0%

## 3. Screening of photocatalysts (Scheme S2)



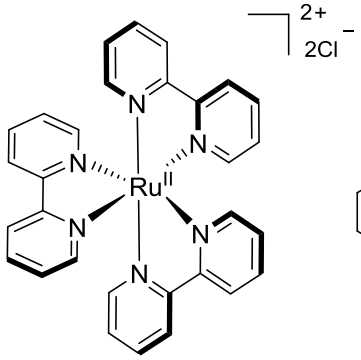

**1a** **2a**

Yield of **2a** under different photocatalysts:



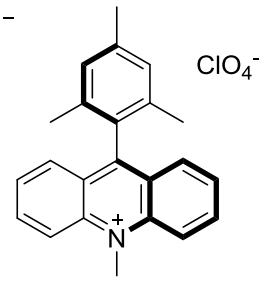

*fac*-Ir(ppy)$_3$

No reaction



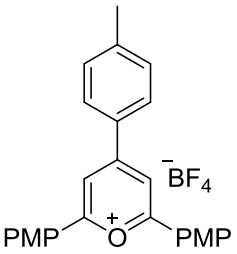

$Ru(bpy)_3Cl_2$

No reaction

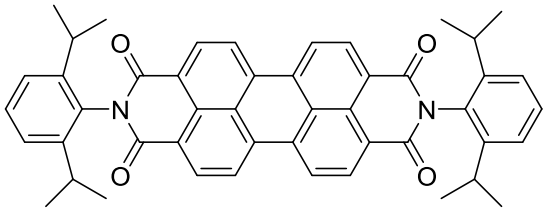



Mes-Acr-Me$^+$ $Cl\bar{O}_4$

57%

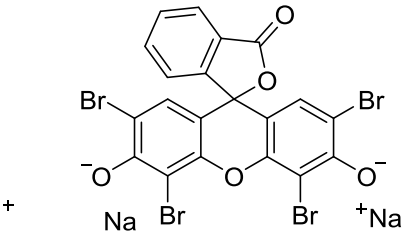



No reaction



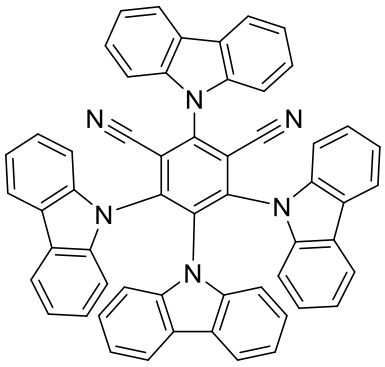

PDI

50%




Eosin Y

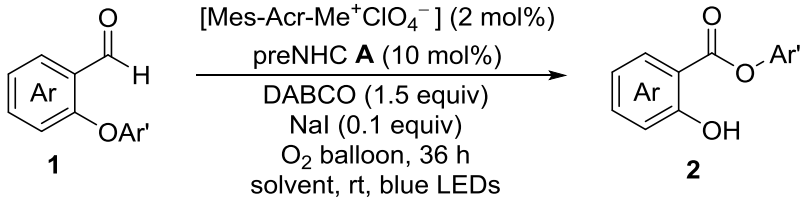
No reaction



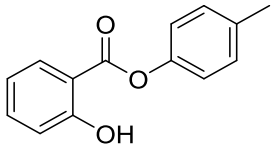

4CZIPN

No reaction

## 4. Typical procedure for the synthesis of compounds 2 (Scheme 2)




To a 10 mL Schlenk-tube equipped with a rubber septum, magnetic stir bar and $O_2$ balloon was charged with 2-(aryloxy)benzaldehyde **1** (0.3 mmol), preNHC **A** (10.9 mg, 10 mmol% ), DABCO (50.4 mg, 0.45 mmol), Mes-Acr-$Me^+ClO_4^-$ (2.5 mg, 2.0 mol%), NaI (4.5 mg, 10 mmol%). The tube was evacuated and backfilled with $O_2$ for three times. DCM (3.0 mL) was added with a syringe. The mixture was stirred under the irradiation of 18 W blue LEDs for 36 h. The reaction mixture was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether/EtOAc as the eluent, typically 80:1 to 50:1) to furnish the desired products **2**.



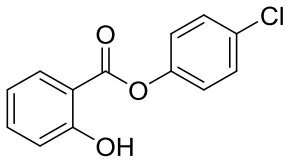

**2a** (837A, experiment# in record book, the same below**)**

***p*-tolyl 2-hydroxybenzoate**[4]

54 mg. 79% yield. Colorless oil. $R_f$ = 0.47 (petroleum ether/ethyl acetate 20:1);

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 10.54 (s, 1H), 8.07 (d, *J* = 8.0 Hz, 1H), 7.55-7.50 (m, 1H), 7.24 (d, *J* = 8.0 Hz, 2H), 7.08 (d, *J* = 8.0 Hz, 2H), 7.03 (d, *J* = 8.0 Hz, 1H), 6.96 (t, *J* = 8.0 Hz, 1H), 2.38 (s, 3H); **$^{13}$C NMR** (125 MHz, $CDCl_3$) δ 169.2, 162.2, 147.9,

136.4, 136.2, 130.4, 130.2, 121.3, 119.5, 117.8, 112.0, 20.9;

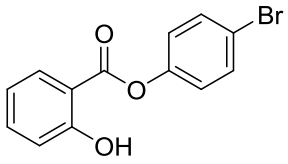



**2b** (849A**)**

**4-chlorophenyl 2-hydroxybenzoate**[4]

51 mg. 69% yield. White solid. $R_f$ = 0.45 (petroleum ether/ethyl acetate 20:1);

**$^1$H NMR** (500 MHz, $CDCl_3$) δ 10.39 (s, 1H), 8.05 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.57-7.53 (m, 1H), 7.41 (d, *J* = 9.0 Hz, 2H), 7.16 (d, *J* = 9.0 Hz, 2H), 7.05-7.03 (m, 1H), 6.99-6.95 (m, 1H); **$^{13}$C NMR** (125 MHz, $CDCl_3$) δ 168.7, 162.3, 148.6, 136.7, 131.9, 130.3, 129.7, 123.1, 119.6, 117.9, 111.6;

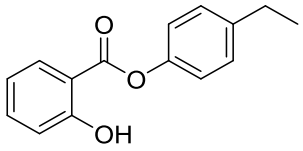



**2c** (851A**)**

**4-bromophenyl 2-hydroxybenzoate**[4]

45 mg. 51% yield. White solid. $R_f$ = 0.43 (petroleum ether/ethyl acetate 20:1);

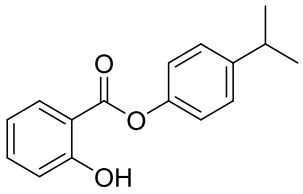
**$^1$H NMR** (400 MHz, $CDCl_3$) δ 10.39 (s, 1H), 8.05 (d, *J* = 8.0 Hz, 1H), 7.58-7.56 (m, 3H), 7.13-7.10 (m, 2H), 7.05 (d, *J* = 8.4 Hz, 1H), 7.00-6.96 (m, 1H); **$^{13}$C NMR** (100 MHz, $CDCl_3$) δ 168.6, 162.3, 149.1, 136.7, 132.7, 130.3, 123.5, 119.6, 118.0, 111.6;



**2d** (871B**)**

**4-ethylphenyl 2-hydroxybenzoate**

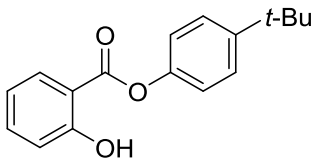
51 mg. 70% yield. Colorless oil. $R_f$ = 0.50 (petroleum ether/ethyl acetate 20:1); **$^1$H NMR** (500 MHz, $CDCl_3$) δ 10.54 (s, 1H), 8.07 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.54-7.51 (m, 1H), 7.27-7.24 (m, 2H), 7.11 (d, *J* = 8.5 Hz, 2H), 7.04-7.02 (m, 1H), 6.98-6.94 (m, 1H), 2.68 (q, *J* = 7.6 Hz, 2H), 1.26 (t, *J* = 7.6 Hz, 3H); **$^{13}$C NMR** (125 MHz, $CDCl_3$) δ 168.1, 161.2, 146.9, 141.4, 135.4, 129.3, 127.9, 120.3, 118.4, 116.8, 110.9, 27.3, 14.5. IR (KBr) 3221, 1694, 1191, 757 $cm^{-1}$. HRMS (ESI) calcd for $C_{15}H_{13}O_3$ $[M-H]^-$ 241.0870, found 241.0870.



**2e** (869B**)**

**4-isopropylphenyl 2-hydroxybenzoate**

63 mg. 82% yield. Colorless oil. $R_f$ = 0.59 (petroleum ether/ethyl acetate 20:1); **$^1$H NMR** (400 MHz, $CDCl_3$) δ 10.56 (s, 1H), 8.08 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.56-7.52 (m, 1H), 7.31 (d, *J* = 8.4 Hz, 2H), 7.14 (d, *J* = 8.4 Hz, 2H), 7.05 (d, *J* = 8.4 Hz, 1H), 7.00-6.96 (m, 1H), 3.00-2.93 (m, 1H), 1.29 (d, *J* = 6.8 Hz, 6H); **$^{13}$C NMR** (100 MHz, $CDCl_3$) δ 169.2, 162.2, 148.0, 147.1, 136.4, 130.4, 127.6, 121.3, 119.5, 117.8, 112.0, 33.7, 24.1. IR (KBr) 3221, 1695, 1196, 757 $cm^{-1}$. HRMS (ESI) calcd for $C_{16}H_{15}O_3$ $[M-H]^-$ 255.1027, found 255.1028.

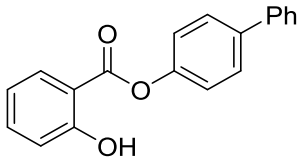



**2f** (851B**)**

**4-(tert-butyl)phenyl 2-hydroxybenzoate**[4]

60 mg. 74% yield. White solid. $R_f$ = 0.57 (petroleum ether/ethyl acetate 20:1);

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 10.57 (s, 1H), 8.10 (d, *J* = 8.0 Hz, 1H), 7.55 (t, *J* = 8.0, 1H), 7.49 – 7.47 (m, 2H), 7.16-7.14 (m, 2H), 7.05 (d, *J* = 8.4 Hz, 1H), 6.98 (t, *J* = 7.6 Hz, 1H), 1.37 (s, 9H); **$^{13}$C NMR** (100 MHz, $CDCl_3$) δ 169.2, 162.2, 149.4, 147.8, 136.4, 126.6, 121.0, 119.5, 117.9, 112.0, 34.6, 31.4.

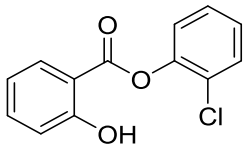



**2g** (850A**)**

**[1,1'-biphenyl]-4-yl 2-hydroxybenzoate**[4]

58 mg. 67% yield. White solid. $R_f$ = 0.27 (petroleum ether/ethyl acetate 20:1);

**$^1$H NMR** (500 MHz, $CDCl_3$) δ 10.53 (s, 1H), 8.12 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.67 (d, *J* = 8.5 Hz, 2H), 7.61 (d, *J* = 8.5 Hz, 2H), 7.58-7.55 (m, 1H), 7.47 (t, *J* = 8.0 Hz, 2H), 7.39 (t, *J* = 7.5 Hz, 1H), 7.30 (d, *J* = 9.0 Hz, 2H), 7.07 (d, *J* = 8.5 Hz, 1H), 7.00 (t, *J* = 7.5 Hz, 1H) ; **$^{13}$C NMR** (125 MHz, $CDCl_3$) δ 168.0, 161.2, 148.5, 139.2, 138.6, 135.5, 129.4, 127.8, 127.3, 126.5, 126.1, 120.9, 118.5, 116.9, 110.8;

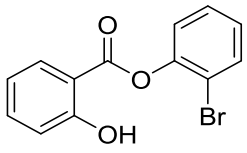



**2h** (872C**)**

**2-chlorophenyl 2-hydroxybenzoate**[4]

36 mg. 48% yield. White solid. $R_f$ = 0.48 (petroleum ether/ethyl acetate 20:1);

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 10.30 (s, 1H), 8.14 (d, *J* = 8.0 Hz, 1H), 7.58-7.50 (m, 2H), 7.38-7.34 (m, 1H), 7.29-7.25 (m, 2H), 7.06 (d, *J* = 8.4 Hz, 1H), 7.00 (t, *J* = 7.6 Hz, 1H); **$^{13}$C NMR** (100 MHz, $CDCl_3$) δ 168.0, 162.3, 146.5, 136.8, 130.6, 130.5, 127.9, 127.6, 127.1, 123.8, 119.7, 117.9, 111.4.

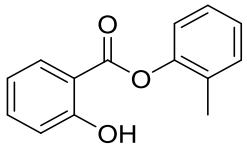



**2i** (875A**)**

**2-bromophenyl 2-hydroxybenzoate[4]**

30 mg. 34% yield. White solid. $R_f$ = 0.42 (petroleum ether/ethyl acetate 20:1);

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 10.30 (s, 1H), 8.15 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.68 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.59-7.54 (m, 1H), 7.43-7.39 (m, 1H), 7.28 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.23-7.18 (m, 1H), 7.06 (d, *J* = 8.4 Hz, 1H), 7.02-6.98 (m, 1H); **$^{13}$C NMR** (100 MHz, $CDCl_3$) δ 168.0, 162.3, 147.7, 136.8, 133.6, 130.6, 128.6, 127.8, 123.8, 119.7, 117.9, 116.2, 111.5.



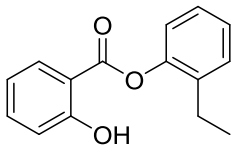

**2j** (856A**)**

***o*-tolyl 2-hydroxybenzoate[4]**

46 mg. 67% yield. Colorless oil. $R_f$ = 0.40 (petroleum ether/ethyl acetate 20:1);

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 10.54 (s, 1H), 8.11 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.56-7.52 (m, 1H), 7.30-7.21 (m, 3H), 7.13 (d, *J* = 8.0 Hz, 1H), 7.05 (d, *J* = 8.4 Hz, 1H), 6.98 (t,

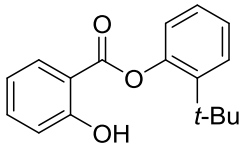
*J* = 7.6 Hz, 1H), 2.24 (s, 3H); **$^{13}$C NMR** (100 MHz, $CDCl_3$) δ 168.7, 162.3, 148.8, 136.5, 131.4, 130.34, 130.32, 127.1, 126.6, 121.9, 119.5, 117.9, 111.8, 16.2;




**2k** (917)

**2-ethylphenyl 2-hydroxybenzoate**

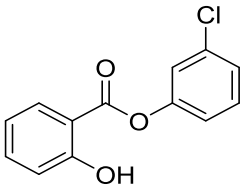
55mg. 76% yield. Colorless oil. $R_f$ = 0.45 (petroleum ether/ethyl acetate 20:1); **$^1$H NMR** (500 MHz, $CDCl_3$) δ 10.55 (s, 1H), 8.09 (dd, *J* = 7.5, 2.0 Hz, 1H), 7.56-7.53 (m, 1H), 7.34-7.32 (m, 1H), 7.28-7.26 (m, 2H), 7.14-7.12 (m, 1H), 7.05 (d, *J* = 8.5 Hz, 1H), 7.00-6.97 (m, 1H), 2.61 (q, *J* = 7.6 Hz, 2H), 1.22 (t, *J* = 7.5 Hz, 3H); **$^{13}$C NMR** (100 MHz, $CDCl_3$) δ 169.0, 162.3, 148.3, 136.5, 136.0, 130.3, 129.7, 127.1, 126.8, 122.2, 119.6, 117.9, 111.8, 23.3, 14.3; IR (KBr) 3446, 1687, 1170, 753 $cm^{-1}$. HRMS (ESI) calcd for $C_{15}H_{13}O_3$ $[M-H]^-$ 241.0870, found 241.0867.




**2l** (870B**)**

**2-(tert-butyl)phenyl 2-hydroxybenzoate**[4]

59 mg. 73% yield. Colorless oil. $R_f$ = 0.48 (petroleum ether/ethyl acetate 20:1); **$^1$H NMR** (400 MHz, $CDCl_3$) δ 10.64 (s, 1H), 8.09 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.57-7.53 (m, 1H), 7.47 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.29-7.24 (m, 2H), 7.09-7.05 (m, 2H), 7.02-6.98 (m, 1H), 1.38 (s, 9H); **$^{13}$C NMR** (100 MHz, $CDCl_3$) δ 169.3, 162.4, 148.6, 141.5, 136.5, 130.3, 127.6, 127.0, 126.4, 124.0, 119.7, 118.0, 112.2, 34.6, 30.4.

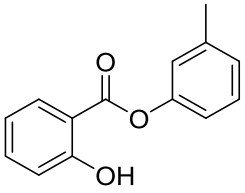



**2m** (880**)**

**3-chlorophenyl 2-hydroxybenzoate**[5]

25 mg. 34% yield. Colorless oil. $R_f$ = 0.47 (petroleum ether/ethyl acetate 20:1);

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 10.37 (s, 1H), 8.04 (d, *J* = 8.0 Hz, 1H), 7.59-7.53 (m, 1H), 7.38 (t, *J* = 8.0 Hz, 1H), 7.31- 7.26 (m, 2H), 7.13 (d, *J* = 8.0 Hz, 1H ), 7.05 (d, *J* = 8.4 Hz, 1H), 6.98 (t, *J* = 8.0 Hz, 1H); **$^{13}$C NMR** (100 MHz, $CDCl_3$) δ 168.5, 162.3, 150.6, 136.8, 135.0, 130.4, 130.3, 126.7, 122.4, 120.1, 119.6, 118.0, 111.5.

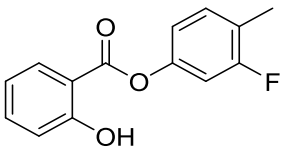



**2n** (866A**)**

**m-tolyl 2-hydroxybenzoate**[4]

40 mg. 58% yield. White solid. $R_f$ = 0.47 (petroleum ether/ethyl acetate 20:1);

**$^1$H NMR** (500 MHz, $CDCl_3$) δ 10.55 (s, 1H), 8.08 (d, *J* = 8.0 Hz, 1H), 7.55 (t, *J* = 8.0, Hz, 1H), 7.34 (t, *J* = 8.0 Hz, 1H), 7.14 (d, *J* = 7.5 Hz, 1H), 7.06-6.97 (m, 4H), 2.42 (s, 3H); **$^{13}$C NMR** (100 MHz, $CDCl_3$) δ 169.1, 162.2, 150.1, 140.0, 136.5, 130.4, 129.4, 127.2, 122.2, 119.5, 118.6, 117.9, 111.9, 21.4.

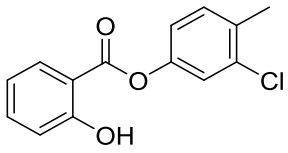



**2o** (914B)

**3-fluoro-4-methylphenyl 2-hydroxybenzoate**

48 mg. 65% yield. Yellow solid. m.p. = 76- 77 $^{o}$C. $R_f$ = 0.50 (petroleum ether/ethyl acetate 20:1);

**$^{1}$H NMR** (500 MHz, $CDCl_3$) δ 10.42 (d, *J* = 2.0 Hz, 1H), 8.04 (d, *J* = 8.0 Hz, 1H), 7.54 (t, *J* = 8.0 Hz, 1H), 7.26-7.23 (m, 1H), 7.04 (d, *J* = 8.0 Hz, 1H), 6.99-6.91 (m, 3H), 2.30 (s, 3H); **$^{13}$C NMR** (125 MHz, $CDCl_3$) δ 168.7, 162.3, 161.1 (d, *J* = 245.0 Hz), 148.5 (d, *J* = 11.3 Hz), 136.6, 131.6 (d, *J* = 6.3 Hz), 130.3, 123.1 (d, *J* = 16.3 Hz), 119.5, 117.9, 117.1 (d, *J* = 3.8 Hz), 111.6, 109.4 (d, *J* = 25.0 Hz), 14.2 (d, *J* = 3.8 Hz). IR (KBr) 3446, 1635, 606 cm$^{-1}$. HRMS (ESI) calcd for $C_{14}H_{10}FO_3$ $[M-H]^-$ 245.0620, found 245.0617.

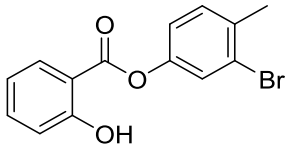



**2p** (885A**)**

**3-chloro-4-methylphenyl 2-hydroxybenzoate**

49 mg. 62% yield. Yellow solid. m.p. = 70- 71 $^{o}$C. $R_f$ = 0.48 (petroleum ether/ethyl acetate 20:1);

**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 10.40 (s, 1H), 8.05 (d, *J* = 8.4 Hz, 1H), 7.54 (t, *J* = 8.4 Hz, 1H), 7.31-7.25 (m, 2H), 7.04 (d, *J* = 8.4 Hz, 2H), 6.97 (t, *J* = 8.0 Hz, 1H), 2.40 (s, 3H); **$^{13}$C NMR** (125 MHz, $CDCl_3$) δ 168.7, 162.3, 148.3, 136.7, 134.7, 134.4, 131.4, 130.3, 122.5, 120.0, 119.6, 117.9, 111.6, 19.6. IR (KBr) 3220, 1691, 1181, 756 cm$^{-1}$. HRMS (ESI) calcd for $C_{14}H_{10}ClO_3$ $[M-H]^-$ 261.0324, found 261.0323.

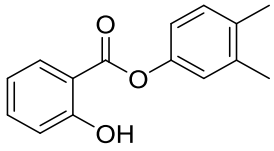



**2q** (912B)

**3-bromo-4-methylphenyl 2-hydroxybenzoate**

53 mg. 58% yield. Yellow solid. m.p. = 52- 53 $^{o}$C. $R_f$ = 0.48 (petroleum ether/ethyl acetate 20:1);

**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 10.40 (s, 1H), 8.03 (d, *J* = 8.0 Hz, 1H), 7.54 (t, *J* = 8.0 Hz, 1H), 7.43 (s, 1H), 7.30 (d, *J* = 8.0 Hz, 1H), 7.08 (d, *J* = 8.4 Hz, 1H), 7.04 (d, *J* = 8.4 Hz, 1H), 6.97 (t, *J* = 8.4 Hz, 1H), 2.40 (s, 3H); **$^{13}$C NMR** (125 MHz, $CDCl_3$) δ 168.7, 162.3, 148.2, 136.7, 136.2, 131.1, 130.3, 125.6, 124.7, 120.6, 119.6, 117.9, 111.6, 22.4. IR (KBr) 3450, 1685, 1052 $cm^{-1}$. HRMS (ESI) calcd for $C_{14}H_{10}BrO_3$ $[M-H]^-$ 304.9819, found 304.9818.

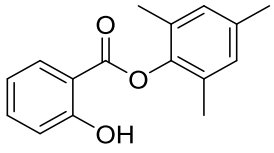



**2r** (856B)

**3,4-dimethylphenyl 2-hydroxybenzoate**

43 mg. 59% yield. Colorless oil. $R_f$ = 0.40 (petroleum ether/ethyl acetate 20:1);

**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 10.58 (s, 1H), 8.08 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.56-7.52 (m, 1H), 7.21 (d, *J* = 8.4 Hz, 1H), 7.05 (d, *J* = 8.4 Hz, 1H), 7.00-6.94 (m, 3H), 2.31 (s, 3H), 2.30 (s, 3H); **$^{13}$C NMR** (100 MHz, $CDCl_3$) δ 169.3, 162.2, 148.0, 138.2, 136.4, 134.8, 130.6, 130.4, 122.5, 119.4, 118.7, 117.8, 112.0, 19.9, 19.3. IR (KBr) 3217, 1688, 1158, 757 $cm^{-1}$. HRMS (ESI) calcd for $C_{15}H_{13}O_3$ $[M-H]^-$ 241.0870, found 241.0870.

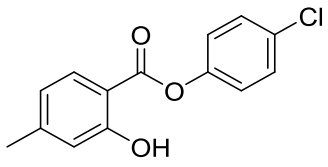



**2s** (872B**)**

**mesityl 2-hydroxybenzoate**

63 mg. 82% yield. Colorless oil. $R_f$ = 0.48 (petroleum ether/ethyl acetate 20:1);

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 10.61 (s, 1H), 8.15 (d, *J* = 8.0 Hz, 1H), 7.56 (t, *J* = 8.0 Hz, 1H), 7.07 (d, *J* = 8.4 Hz, 1H), 7.00 (t, *J* = 7.6 Hz, 1H), 6.94 (s, 2H), 2.31 (s, 3H), 2.17 (s, 6H); **$^{13}$C NMR** (100 MHz, $CDCl_3$) δ 168.5, 162.3, 145.4, 136.4, 135.9, 130.3, 129.8, 129.4, 119.5, 117.9, 111.7, 20.8, 16.3. IR (KBr) 3213, 1688, 1189, 758 $cm^{-1}$. HRMS (ESI) calcd for $C_{16}H_{15}O_3$ $[M-H]^-$ 255.1027, found 255.1028.

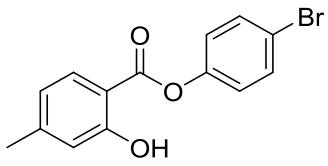



**2t** (887A**)**

**4-chlorophenyl 2-hydroxy-4-methylbenzoate**

53 mg. 67% yield. White solid. m.p. = 98- 99 $^oC$. $R_f$ = 0.45 (petroleum ether/ethyl acetate 20:1);

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 10.34 (s, 1H), 7.92 (d, *J* = 8.0, 1H), 7.41 (d, *J* = 8.4 Hz, 2H), 7.16 (d, *J* = 8.4 Hz, 2H), 6.86 (s, 1H), 6.79 (d, *J* = 8.0 Hz, 1H), 2.39 (s, 3H); **$^{13}$C NMR** (100 MHz, $CDCl_3$) δ 168.6, 162.3, 148.6, 148.3, 131.8, 130.1, 129.7, 123.1, 120.9, 118.0, 109.0, 22.0. IR (KBr) 3675, 2920, 1688, 765 $cm^{-1}$. HRMS (ESI) calcd for $C_{14}H_{10}ClO_3$ $[M-H]^-$ 261.0324, found 261.0325.

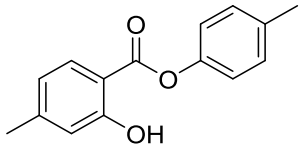



**2u** (874A**)**

**4-bromophenyl 2-hydroxy-4-methylbenzoate**

55 mg. 60% yield. White solid. m.p. = 101- 102 $^{o}$C. $R_f$ = 0.45 (petroleum ether/ethyl acetate 10:1);

**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 10.33 (s, 1H), 7.92 (d, *J* = 8.0 Hz, 1H), 7.56 (d, *J* = 8.8 Hz, 2H), 7.10 (d, *J* = 8.8 Hz, 2H), 6.86 (s, 1H), 6.79 (d, *J* = 8.4 Hz, 1H), 2.39 (s, 3H); **$^{13}$C NMR** (100 MHz, $CDCl_3$) δ 168.5, 162.3, 149.2, 148.3, 132.7, 130.1, 123.5, 120.9, 119.5, 118.0, 109.0, 22.0. IR (KBr) 3447, 1688, 1198, 766 $cm^{-1}$. HRMS (ESI) calcd for $C_{14}H_{10}BrO_3$ $[M-H]^-$ 304.9819, found 304.9821.

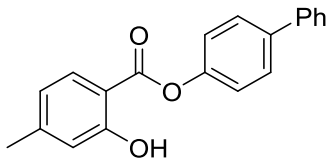



**2v** (866B**)**

**p-tolyl 2-hydroxy-4-methylbenzoate**[5]

56 mg. 77% yield. White solid. $R_f$ = 0.42 (petroleum ether/ethyl acetate 20:1);

**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 10.48 (s, 1H), 7.94 (d, *J* = 8.0, 1H), 7.23 (d, *J* = 8.4 Hz, 2H), 7.08 (d, *J* = 8.4 Hz, 2H), 6.84 (s, 1H), 6.78 (d, *J* = 8.0 Hz, 1H), 2.38 (s, 6H); **$^{13}$C NMR** (100 MHz, $CDCl_3$) δ 169.1, 162.2, 147.9, 136.0, 130.14, 130.12, 121.4, 120.8, 117.9, 109.4, 22.0, 20.9.

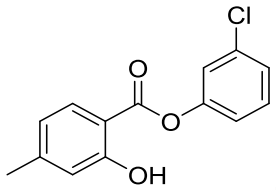



**2w** (914A)

**[1,1'-biphenyl]-4-yl 2-hydroxy-4-methylbenzoate**

67 mg. 73% yield. White solid. m.p. = 115-116 $^{o}$C. $R_f$ = 0.37 (petroleum ether/ethyl acetate 20:1);

**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 10.46 (s, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.64 (d, *J* = 8.8 Hz, 2H), 7.61 (d, *J* = 7.6 Hz, 2H), 7.44 (t, *J* = 8.0 Hz, 2H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.26 (d, *J* = 8.4 Hz, 2H), 6.86 (s, 1H), 6.78 (d, *J* = 8.4 Hz, 1H), 2.38 (s, 3H); **$^{13}$C NMR** (100 MHz, $CDCl_3$) δ 169.0, 162.3, 149.6, 148.1, 140.3, 139.5, 130.2, 128.9, 128.4, 127.5, 127.2, 122.0, 120.9, 118.0, 109.3, 22.0. IR (KBr) 3446, 1640, 759 cm$^{-1}$. HRMS (ESI) calcd for $C_{20}H_{15}O_3$ $[M-H]^-$ 303.1027, found 303.1026.



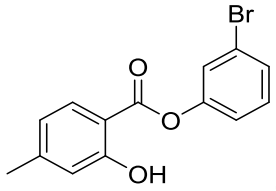

**2x** (916B)

**3-chlorophenyl 2-hydroxy-4-methylbenzoate**

26 mg. 33% yield. White solid. m.p. = 61-62 $^{o}$C. $R_f$ = 0.45 (petroleum ether/ethyl acetate 20:1);

**$^{1}$H NMR** (500 MHz, $CDCl_3$) δ 10.31 (s, 1H), 7.91 (d, *J* = 7.0 Hz, 1H), 7.37 (t, *J* = 7.5 Hz, 1H), 7.30-7.25 (m, 2H), 7.12 (d, *J* = 7.5 Hz, 1H), 6.85 (s, 1H), 6.79 (d, *J* = 7.5 Hz, 1H), 2.39 (s, 3H); **$^{13}$C NMR** (125 MHz, $CDCl_3$) δ 168.5, 162.3, 150.6, 148.4, 134.9, 130.3, 130.1, 126.6, 122.5, 120.9, 120.2, 118.0, 108.9, 22.0. IR (KBr) 3446, 1635, 612

$cm^{-1}$. HRMS (ESI) calcd for $C_{14}H_{10}ClO_3$ $[M-H]^-$ 261.0324, found 261.0324.

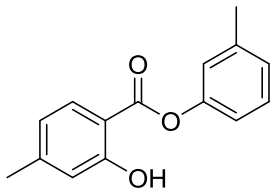



**2y** (919)

**3-bromophenyl 2-hydroxy-4-methylbenzoate**

30 mg. 33% yield. Yellow oil. $R_f$ = 0.47 (petroleum ether/ethyl acetate 20:1);

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 10.31 (s, 1H), 7.90 (d, *J* = 8.4 Hz, 1H), 7.45-7.41 (m, 2H), 7.31 (t, *J* = 8.4 Hz, 1H), 7.18-7.16 (m, 1H), 6.85 (s, 1H), 6.78 (d, *J* = 8.4 Hz, 1H), 2.39 (s, 3H); **$^{13}$C NMR** (100 MHz, $CDCl_3$) δ 168.5, 162.3, 150.7, 148.4, 130.6, 130.1, 129.5, 125.3, 122.6, 120.9, 120.6, 118.0, 108.9, 22.0. IR (KBr) 3442, 1637, 1052 $cm^{-1}$. HRMS (ESI) calcd for $C_{14}H_{10}BrO_3$ $[M-H]^-$ 304.9819, found 304.9817.

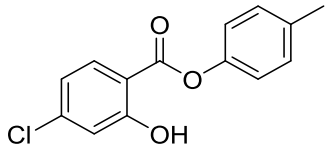



**2z** (916A)

***m*-tolyl 2-hydroxy-4-methylbenzoate**

37 mg. 51% yield. Yellow oil. $R_f$ = 0.43 (petroleum ether/ethyl acetate 20:1);

**$^1$H NMR** (500 MHz, $CDCl_3$) δ 10.47 (s, 1H), 7.93 (d, *J* = 8.0 Hz, 1H), 7.33-7.30 (m, 1H), 7.10 (d, *J* = 7.5 Hz, 1H), 7.01-6.98 (m, 2H), 6.84 (s, 1H), 6.77 (d, *J* = 8.0 Hz, 1H), 2.39-2.38 (m, 6H); **$^{13}$C NMR** (125 MHz, $CDCl_3$) δ 169.1, 162.2, 150.1, 148.0, 139.9, 130.2, 129.3, 127.1, 122.3, 120.8, 118.7, 117.9, 109.4, 22.0, 21.4. IR (KBr) 3446, 1635, 612 $cm^{-1}$. HRMS (ESI) calcd for $C_{15}H_{13}O_3$ $[M-H]^-$ 241.0870, found 241.0869.

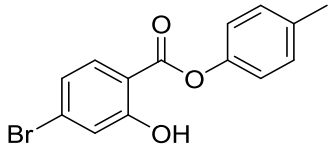



**2aa** (913B)

***p*-tolyl 4-chloro-2-hydroxybenzoate**

42 mg. 53% yield. Yellow solid. m.p. = 68-69 $^{o}$C. $R_f$ = 0.53 (petroleum ether/ethyl acetate 20:1);

**$^{1}$H NMR** (500 MHz, $CDCl_3$) δ 10.63 (s, 1H), 7.98 (d, *J* = 8.5, 1H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.08-7.05 (m, 3H), 6.94 (d, *J* = 8.5 Hz, 1H), 2.38 (s, 3H); **$^{13}$C NMR** (125 MHz, $CDCl_3$) δ 168.6, 162.7, 147.7, 142.3, 136.3, 131.4, 130.2, 121.2, 120.2, 118.0, 110.6, 20.9. IR (KBr) 3446, 1635, 1192 $cm^{-1}$. HRMS (ESI) calcd for $C_{14}H_{10}ClO_3$ $[M-H]^-$ 261.0324, found 261.0322.

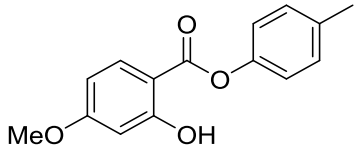



**2ab** (872A**)**

***p*-tolyl 4-bromo-2-hydroxybenzoate**

62 mg. 67% yield. White solid. m.p. = 71-72 $^{o}$C. $R_f$ = 0.51 (petroleum ether/ethyl acetate 10:1);

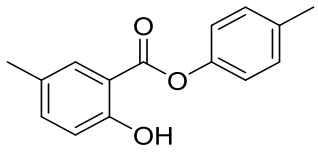
**$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 10.60 (s, 1H), 7.91 (d, *J* = 8.4, 1H), 7.25-7.23 (m, 3H), 7.11-7.06 (m, 3H), 2.38 (s, 3H); **$^{13}$C NMR** (100 MHz, $CDCl_3$) δ 168.7, 162.5, 147.7, 136.3, 131.3, 130.8, 130.2, 123.1, 121.2, 121.1, 111.0, 20.9. IR (KBr) 2919, 1684 , 1189, 799 $cm^{-1}$. HRMS (ESI) calcd for $C_{14}H_{10}BrO_3$ $[M-H]^-$ 304.9819, found 304.9822.




**2ac** (868B**)**

***p*-tolyl 2-hydroxy-4-methoxybenzoate**

41 mg. 53% yield. White solid. $R_f$ = 0.30 (petroleum ether/ethyl acetate 20:1); **$^1$H NMR** (500 MHz, $CDCl_3$) δ 10.75 (s, 1H), 7.97 (d, *J* = 8.5 Hz, 1H), 7.23 (d, *J* = 8.5 Hz, 2H), 7.07 (d, *J* = 8.5 Hz, 2H), 6.53-6.49 (m, 2H), 3.86 (s, 3H), 2.38 (s, 3H); **$^{13}$C NMR** (125 MHz, $CDCl_3$) δ 169.0, 166.2, 164.5, 148.0, 135.9, 131.7, 130.1, 121.4, 108.0, 104.9, 100.8, 55.6, 20.9. IR (KBr) 3395, 1667, 1167, 767 $cm^{-1}$. HRMS (ESI) calcd for $C_{15}H_{13}O_4$ $[M-H]^-$ 257.0819, found 257.0822.



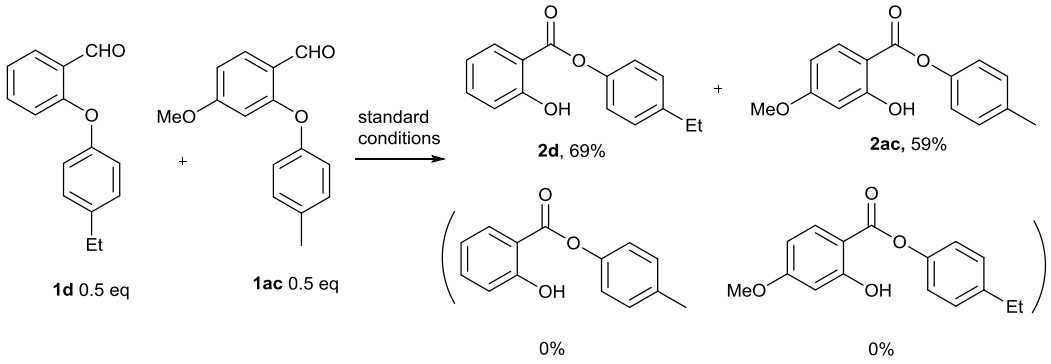

**2ad** (912A)

***p*-tolyl 2-hydroxy-5-methylbenzoate**

52 mg. 72% yield. Colorless oil. $R_f$ = 0.48 (petroleum ether/ethyl acetate 20:1); **$^1$H NMR** (500 MHz, $CDCl_3$) δ 10.34 (s, 1H), 7.86 (d, *J* = 1.5 Hz, 1H), 7.34 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.24 (d, *J* = 8.5 Hz, 2H), 7.08 (d, *J* = 8.5 Hz, 2H), 6.93 (d, *J* = 8.5 Hz, 1H), 2.38 (s, 3H), 2.33 (s, 3H); **$^{13}$C NMR** (125 MHz, $CDCl_3$) δ 169.2, 160.2, 147.9, 137.5, 136.1, 130.2, 130.0, 128.7, 121.4, 117.6, 111.5, 20.9, 20.4. IR (KBr) 3446, 1634, 1189, 574 $cm^{-1}$. HRMS (ESI) calcd for $C_{15}H_{13}O_3$ $[M-H]^-$ 241.0870, found 241.0868.

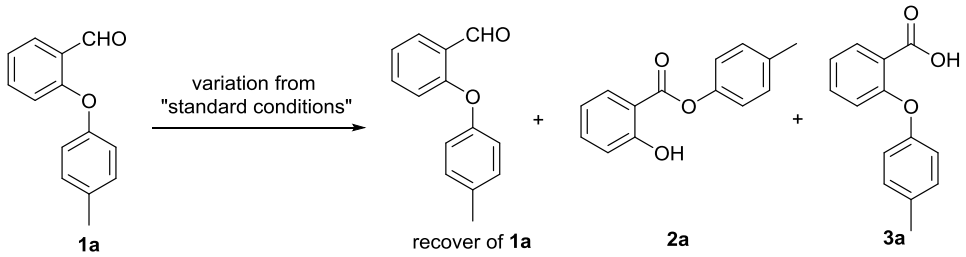
## 5. Investigation on mechanism (Scheme 4)

### (a) Crossover experiments (Scheme 4a)




To a 10 mL Schlenk-tube equipped with a rubber septum, magnetic stir bar and $O_2$ balloon was charged with **1d** (0.15 mmol), **1ac** (0.15 mmol), preNHC **A** (10.9 mg, 10 mmol% ), DABCO (50.4 mg, 0.45 mmol), Mes-Acr-$Me^{+}ClO_4^{-}$ (2.5 mg, 2.0 mol%), NaI (4.5 mg, 10 mmol%). The tube was evacuated and backfilled with $O_2$ for three times. DCM (3.0 mL) was added with a syringe. The mixture was stirred under the irradiation of 18 W blue LEDs for 36 h. The reaction mixture was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 100/0 - 50/1) to furnish the desired products **2d** (25mg, 69% yield) and **2ac** (23mg, 59% yield).

### (b) Control experiments (Scheme 4b)

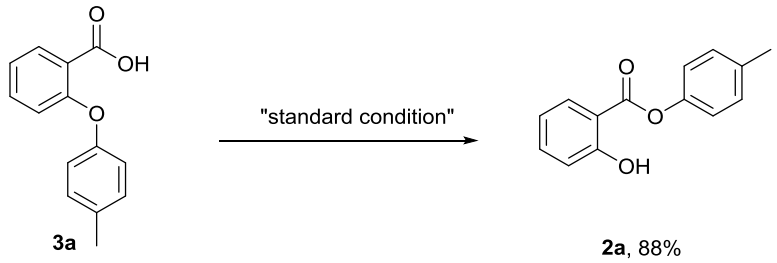



| | recover of **1a** | **2a** | **3a** |
|---|---|---|---|
| (1) without preNHC | 83% | 0% | 0% |
| (2) without Mes-Acr$^{+}$ | 75% | 0% | 0% |

Reaction (1): To a 10 mL Schlenk-tube equipped with a rubber septum, magnetic stir bar and $O_2$ balloon was charged with 2-(aryloxy)benzaldehyde **1a** (63.6 mg, 0.3 mmol), DABCO (50.4 mg, 0.45 mmol), Mes-Acr-$Me^+ClO_4^-$ (2.5 mg, 2.0 mol%), NaI (4.5 mg, 10 mmol%). The tube was evacuated and backfilled with $O_2$ for three times. DCM (3.0 mL) was added with a syringe. The mixture was stirred under the irradiation of 18 W blue LEDs for 36 h. The reaction mixture was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether/EtOAc as the eluent = 80:1 to 50:1) to recover **1a** (53mg, 83% yield).

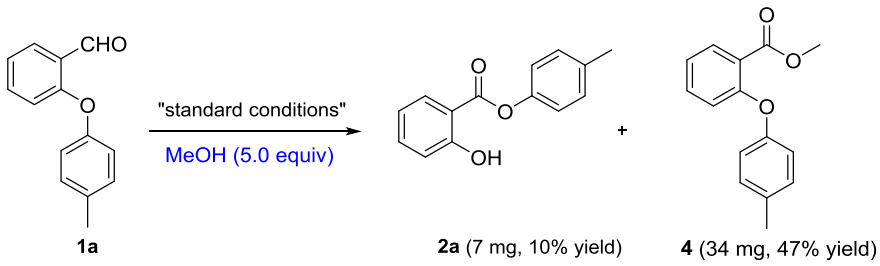
Reaction (2): To a 10 mL Schlenk-tube equipped with a rubber septum, magnetic stir bar and O2 balloon was charged with 2-(aryloxy)benzaldehyde **1a** (63.6 mg, 0.3 mmol), preNHC **A** (10.9 mg, 10 mmol% ), DABCO (50.4 mg, 0.45 mmol), NaI (4.5 mg, 10 mmol%). The tube was evacuated and backfilled with $O_2$ for three times. DCM (3.0 mL) was added with a syringe. The mixture was stirred under the irradiation of 18 W blue LEDs for 36 h. The reaction mixture was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether/EtOAc as the eluent = 80:1 to 50:1) to recover **1a** (48 mg, 75% yield).

**(c) Smiles rearrangement of O-toyl salicylic acid (Scheme 4c)**




To a 10 mL Schlenk-tube equipped with a rubber septum, magnetic stir bar and $O_2$ balloon was charged with **3a** (0.3 mmol), preNHC **A** (10.9 mg, 10 mmol% ), DABCO (50.4 mg, 0.45 mmol), Mes-Acr-$Me^{+}ClO_4^{-}$ (2.5 mg, 2.0 mol%), NaI (4.5 mg, 10 mmol%). The tube was evacuated and backfilled with $O_2$ for three times. DCM (3.0 mL) was added with a syringe under oxygen. The mixture was stirred under the irradiation of 18 W blue LEDs for 36 h. the reaction mixture was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 80/1) to furnish the desired products **2a** (60 mg, 88% yield).

**(d) Trap the acylazolium intermediate by the addition of MeOH**




To a 10 mL Schlenk-tube equipped with a rubber septum, magnetic stir bar and $O_2$ balloon was charged with 2-(aryloxy)benzaldehyde **1a** (63.6 mg, 0.3 mmol), preNHC **A** (10.9 mg, 10 mmol% ), DABCO (50.4 mg, 0.45 mmol), Mes-Acr-$Me^{+}ClO_4^{-}$ (2.5 mg, 2.0 mol%), NaI (4.5 mg, 10 mmol%). The tube was evacuated and backfilled

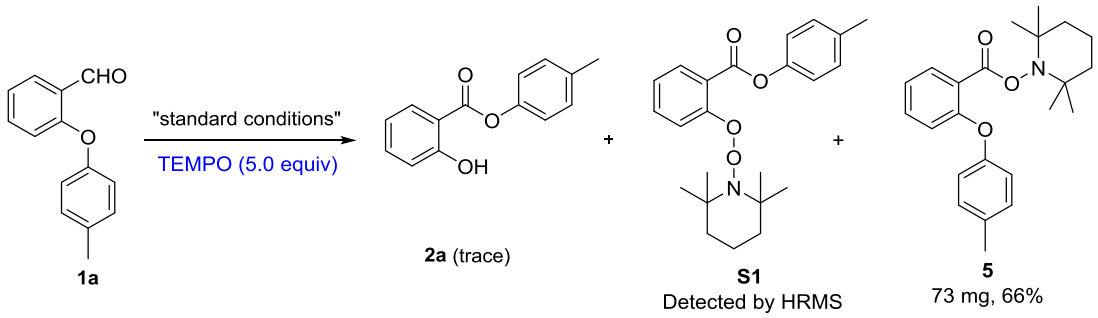
with $O_2$ for three times. MeOH (1.5 mmol, 5.0 equiv) and DCM (3.0 mL) was added with a syringe. The mixture was stirred under the irradiation of 18 W blue LEDs for 13 h. The reaction mixture was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether/EtOAc as the eluent = 60:1 to 20:1) to furnish the desired products **2a** (7 mg, 10% yield) and methyl ester **4** (34 mg, 47% yield).

**methyl 2-(*p*-tolyloxy)benzoate** (**4**, 938A)

34mg. 47% yield. Yellow oil. $R_f$ = 0.33 (petroleum ether/ethyl acetate 20:1);

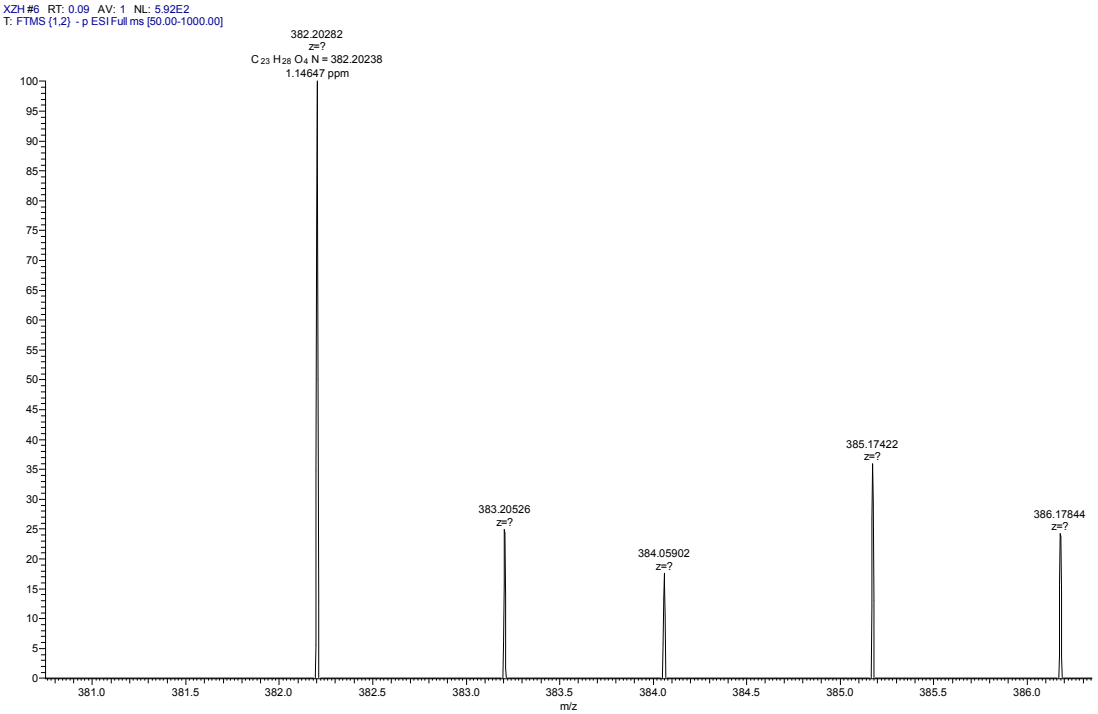
**$^1$H NMR** (500 MHz, $CDCl_3$) δ 7.89 (d, *J* = 7.5 Hz, 1H), 7.44-7.40 (m, 1H), 7.15-7.11 (m, 3H), 6.93 (d, *J* = 8.0 Hz, 1H), 6.88-6.86 (m, 2H), 3.82 (s, 3H), 2.32 (s, 3H); **$^{13}$C NMR** (125 MHz, $CDCl_3$) δ 166.4, 156.8, 155.1, 133.5, 132.8, 131.8, 130.2, 123.0, 122.8, 120.2, 118.5, 52.2, 20.7.

### (e) Trap the radical intermediate by the addition of TEMPO

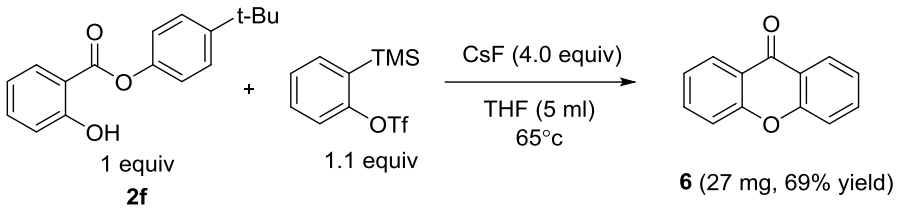



To a 10 mL Schlenk-tube equipped with a rubber septum, magnetic stir bar and $O_2$ balloon was charged with 2-(aryloxy)benzaldehyde **1** (0.3 mmol), preNHC **A** (10.9 mg, 10 mmol% ), DABCO (50.4 mg, 0.45 mmol), Mes-Acr-$Me^+ClO_4^-$ (2.5 mg, 2.0 mol%), NaI (4.5 mg, 10 mmol%) and TEMPO (234 mg, 1.5 mmol). The tube was

evacuated and backfilled with $O_2$ for three times. DCM (3.0 mL) was added with a syringe. The mixture was stirred under the irradiation of 18 W blue LEDs for 36 h. A sample of the reaction mixture was collected for HRMS, which confirmed the formation of compound S1 via the coupling of TEMPO with the radical intermediate. the The reaction mixture was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether/EtOAc as the eluent = 60:1 to 20:1) to furnish the products **5** (73 mg, 66% yield). **$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 7.6 Hz, 1H), 7.39 (t, *J* = 8.0 Hz, 1H), 7.15-7.13 (m, 3H), 6.93-6.91 (m, 3H), 2.34 (s, 3H), 1.78-1.34 (m, 6H), 1.23-1.11 (m, 12H); **$^{13}$C NMR** (100 MHz, $CDCl_3$) δ 167.2, 156.5, 154.7, 133.1, 132.9, 131.7, 130.3, 123.0, 122.8, 119.2, 119.1, 60.3, 39.2, 31.9, 20.8, 20.7, 17.0. HRMS (ESI) calcd for $C_{23}H_{30}O_3N$ $[M+H]^+$ 368.2220, found 368.2223.



## 6. Further chemical transformation




To a 50 mL Schlenk-tube equipped with a rubber septum and magnetic stir bar was charged with **2f** (0.2 mmol, 54.0 mg), silylaryl triflate (0.22 mmol, 65.6 mg), CsF (0.8 mmol, 121.6 mg) in 5 mL of anhydrous THF. The mixture was stirred at 65℃ for 19h. The reaction mixture was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 50/1) to furnish the desired xanthone **6** (27mg, 69% yield).[6] **$^{1}$H NMR** (400 MHz, $CDCl_3$) δ 8.35 (d, *J* = 7.6 Hz, 2H), 7.73 (t, *J* = 8.0 Hz, 2H), 7.49 (d, *J* = 8.4 Hz, 2H), 7.38 (t, *J* = 8.0 Hz, 2H); **$^{13}$C NMR** (100 MHz, $CDCl_3$) δ 177.2, 156.2, 134.8, 126.8, 123.9, 121.9, 118.0.

## 7. References

1 D. M. Flanigan, F. Romanov-Michailidis, N. A. White and T. Rovis, *Chem. Rev.*, 2015, **115**, 9307.

2 S. Aoki, Y. Matsuo, S. Ogura, H. Ohwada, Y. Hisamatsu, S. Moromizato, M. Shiro and M. Kitamura, *Inorg. Chem.*, 2011, **50**, 806.

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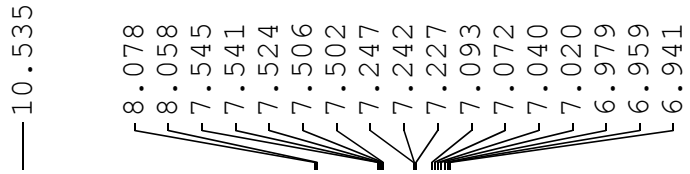
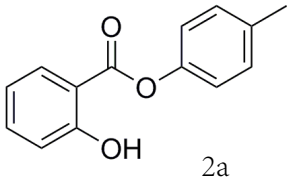
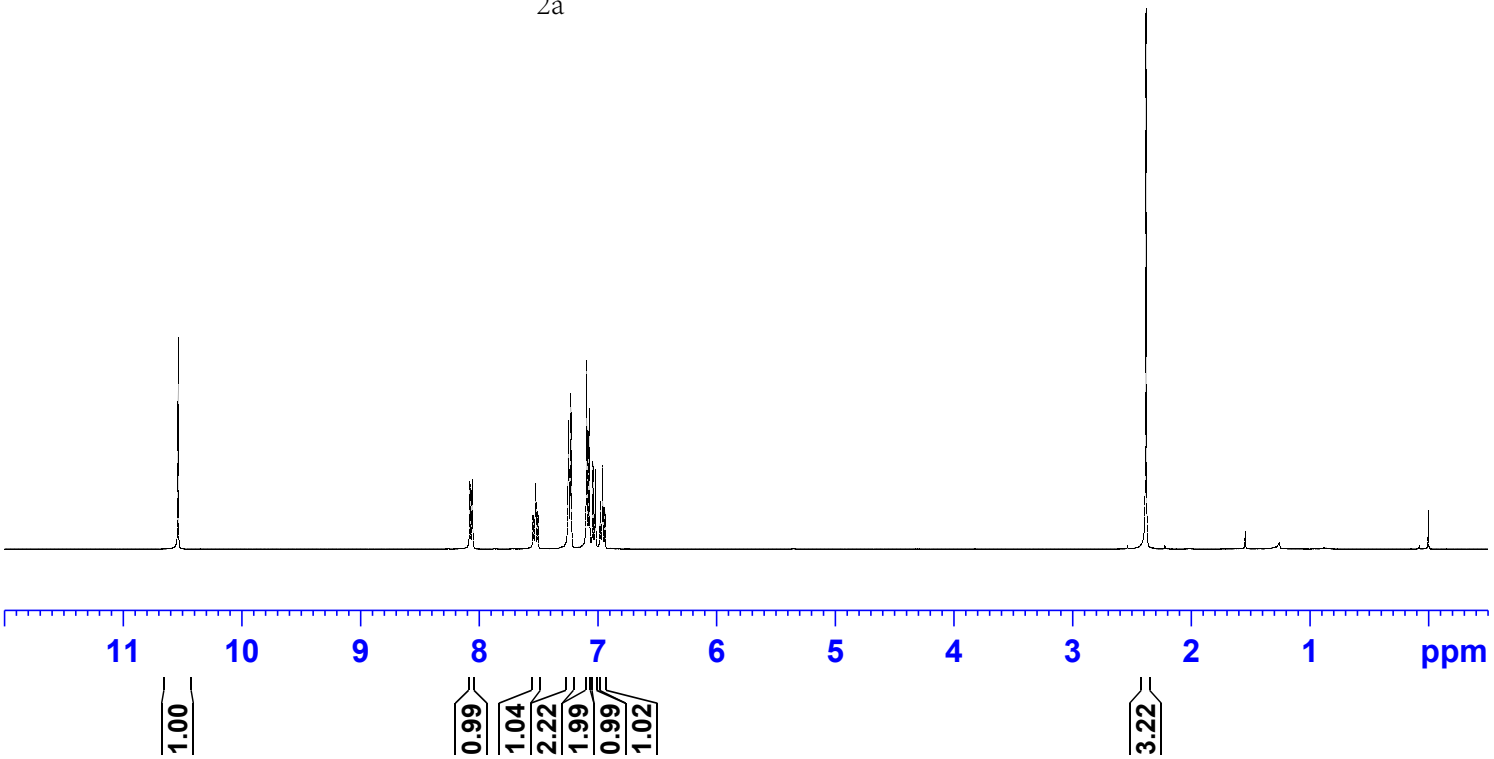
837-A




2a

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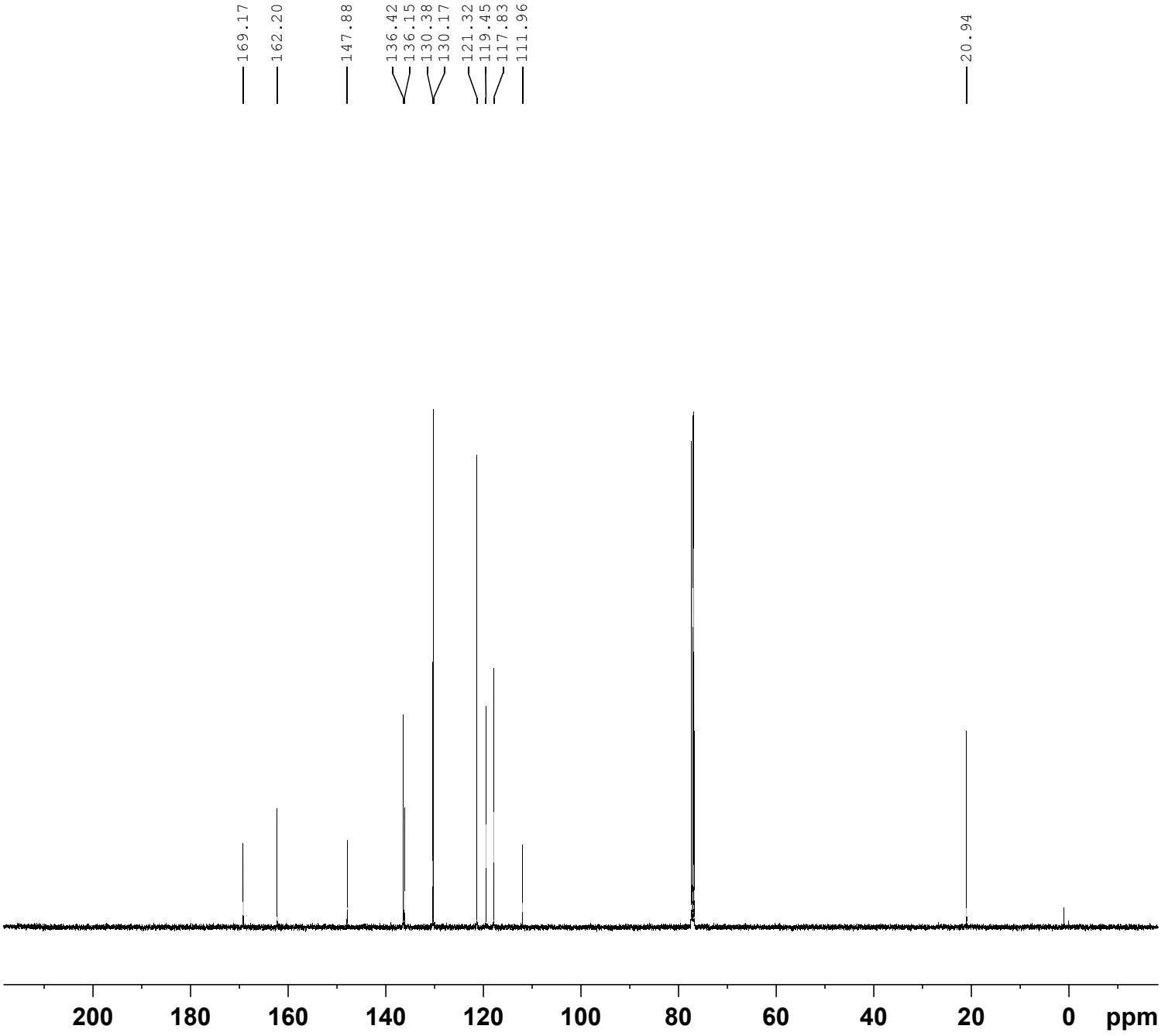
837-A

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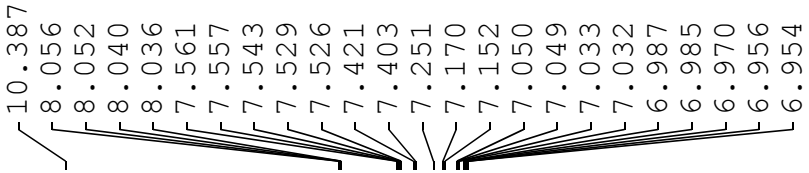
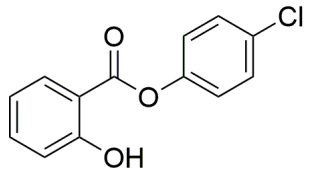
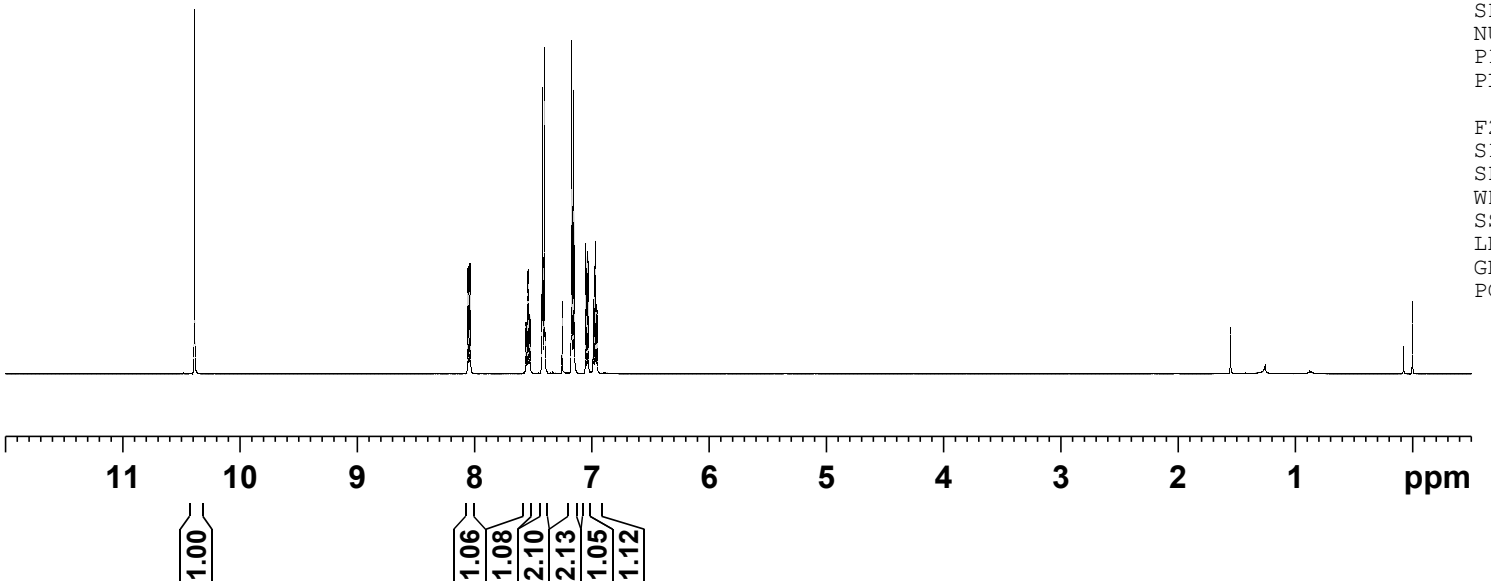
849-A




2b

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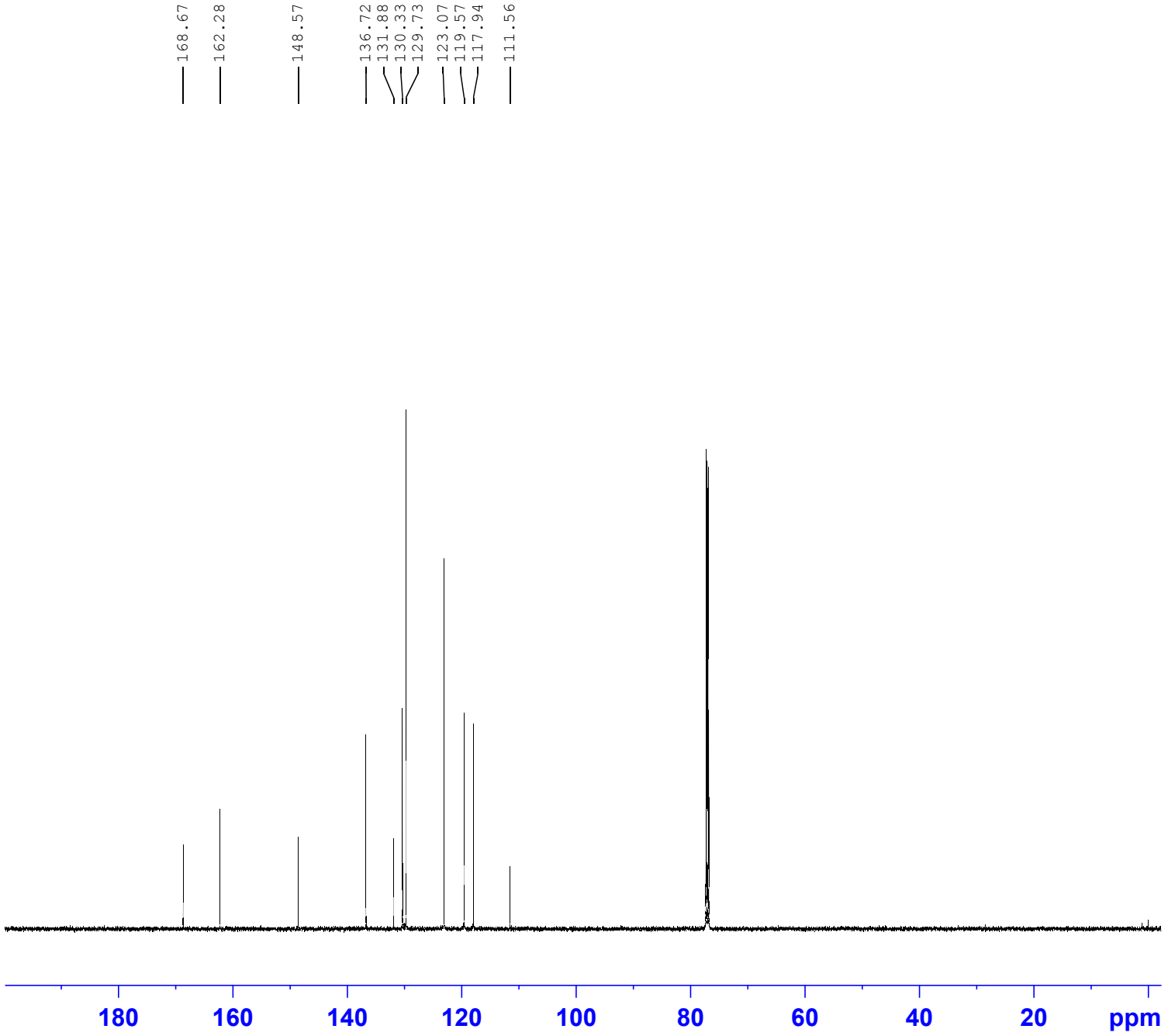
849-A

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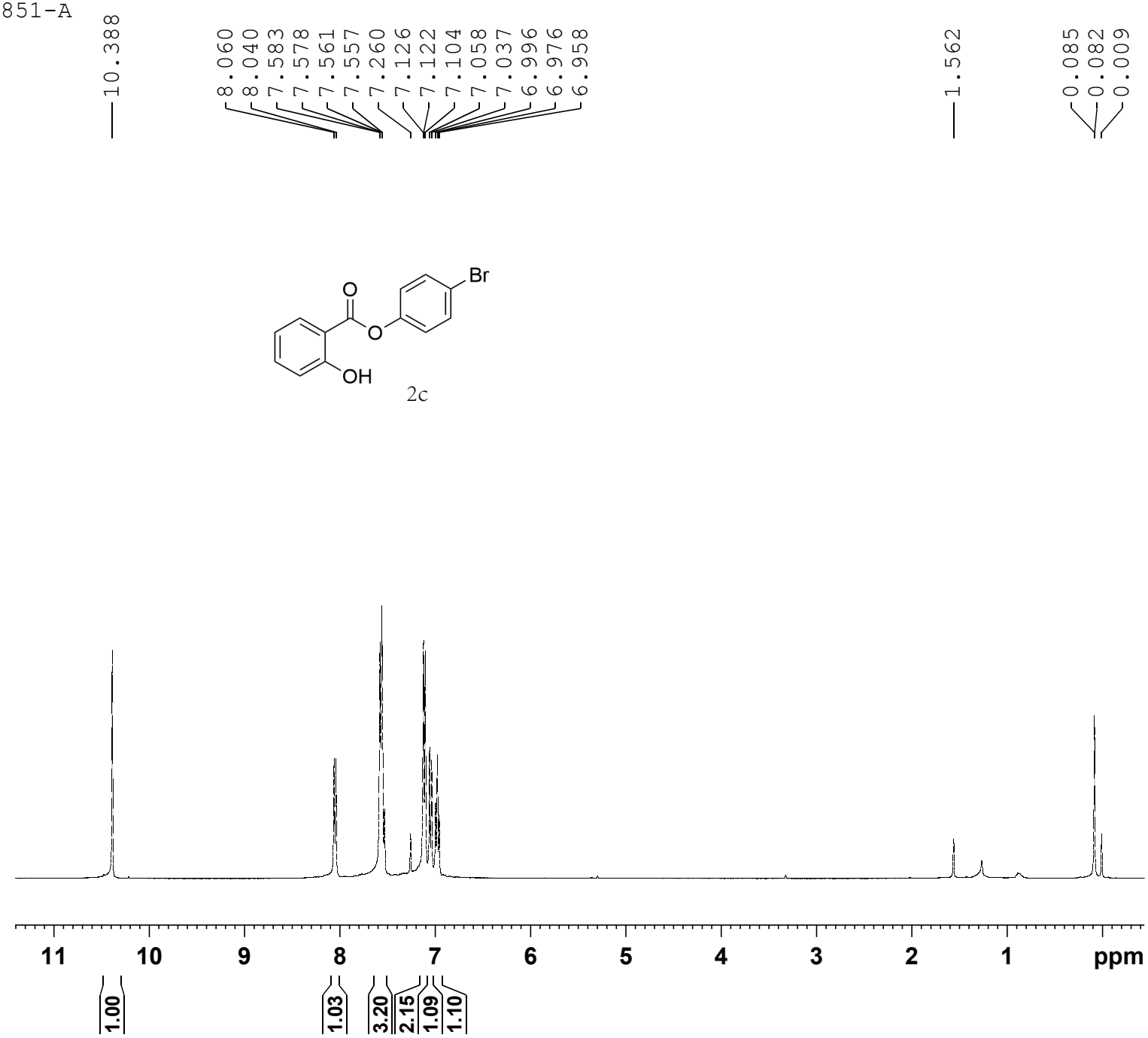
851-A




2c

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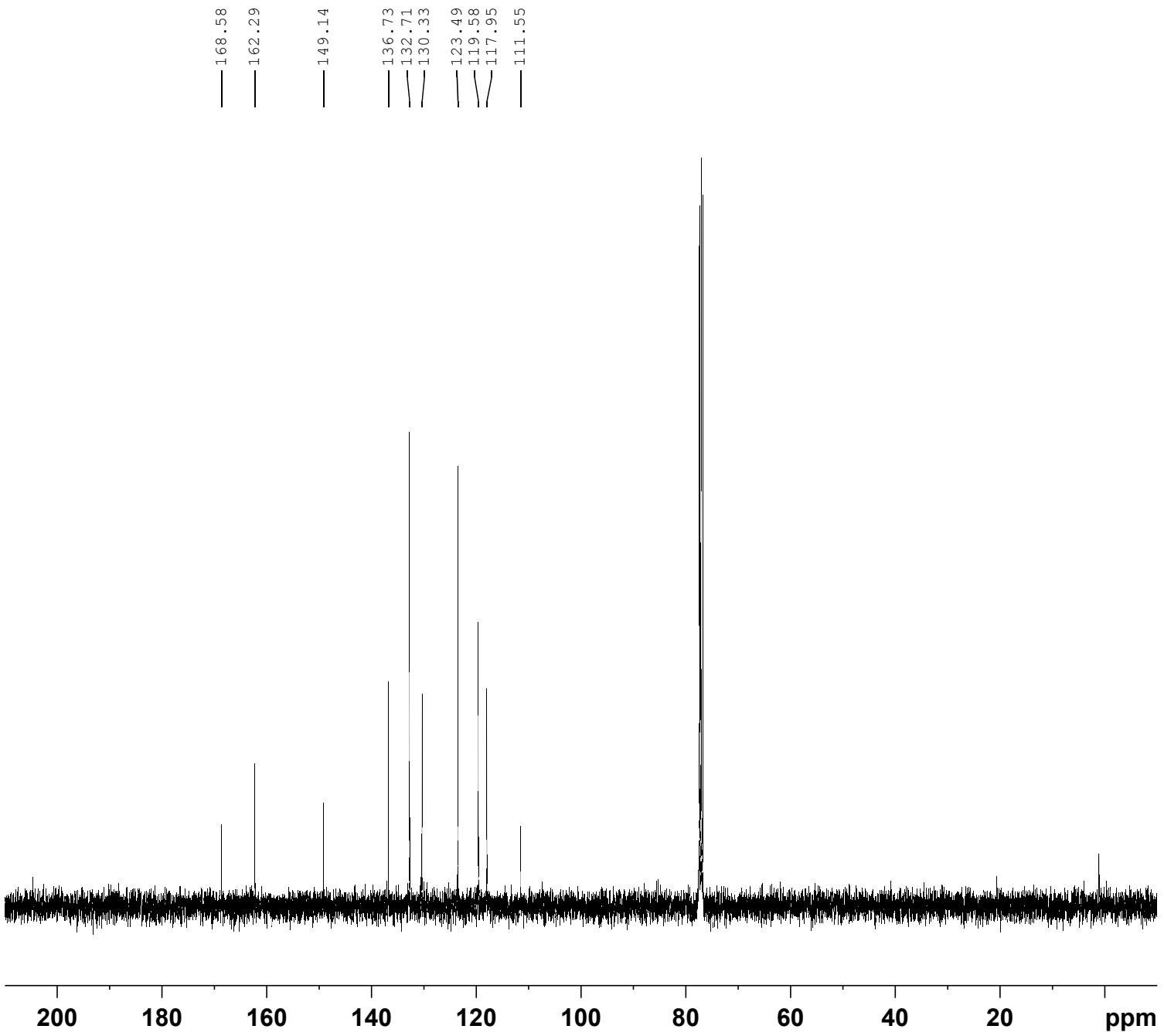
851-A

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871- B

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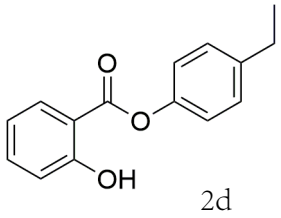


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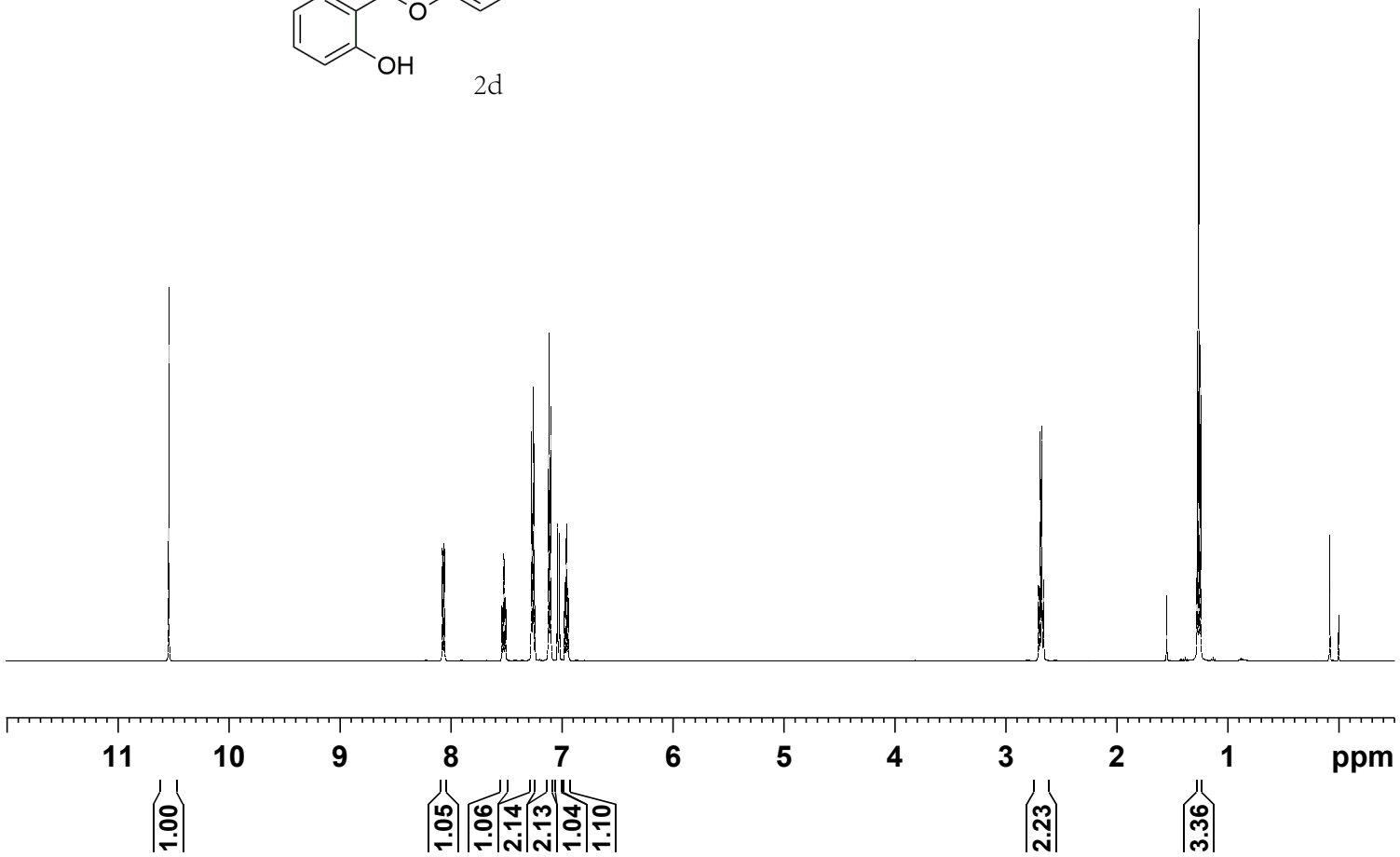


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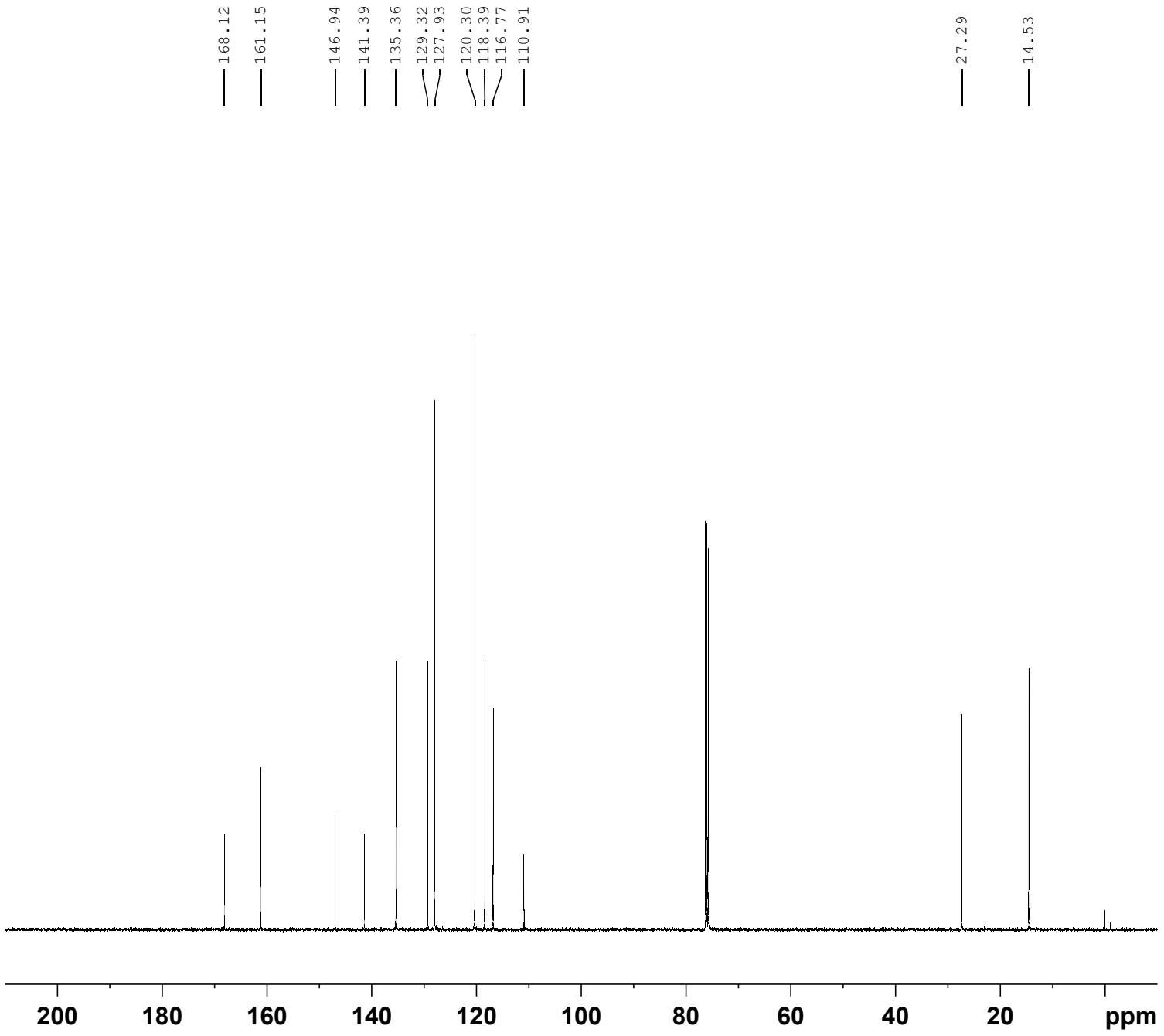
871- B

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TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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PLW13 0.22898000 W

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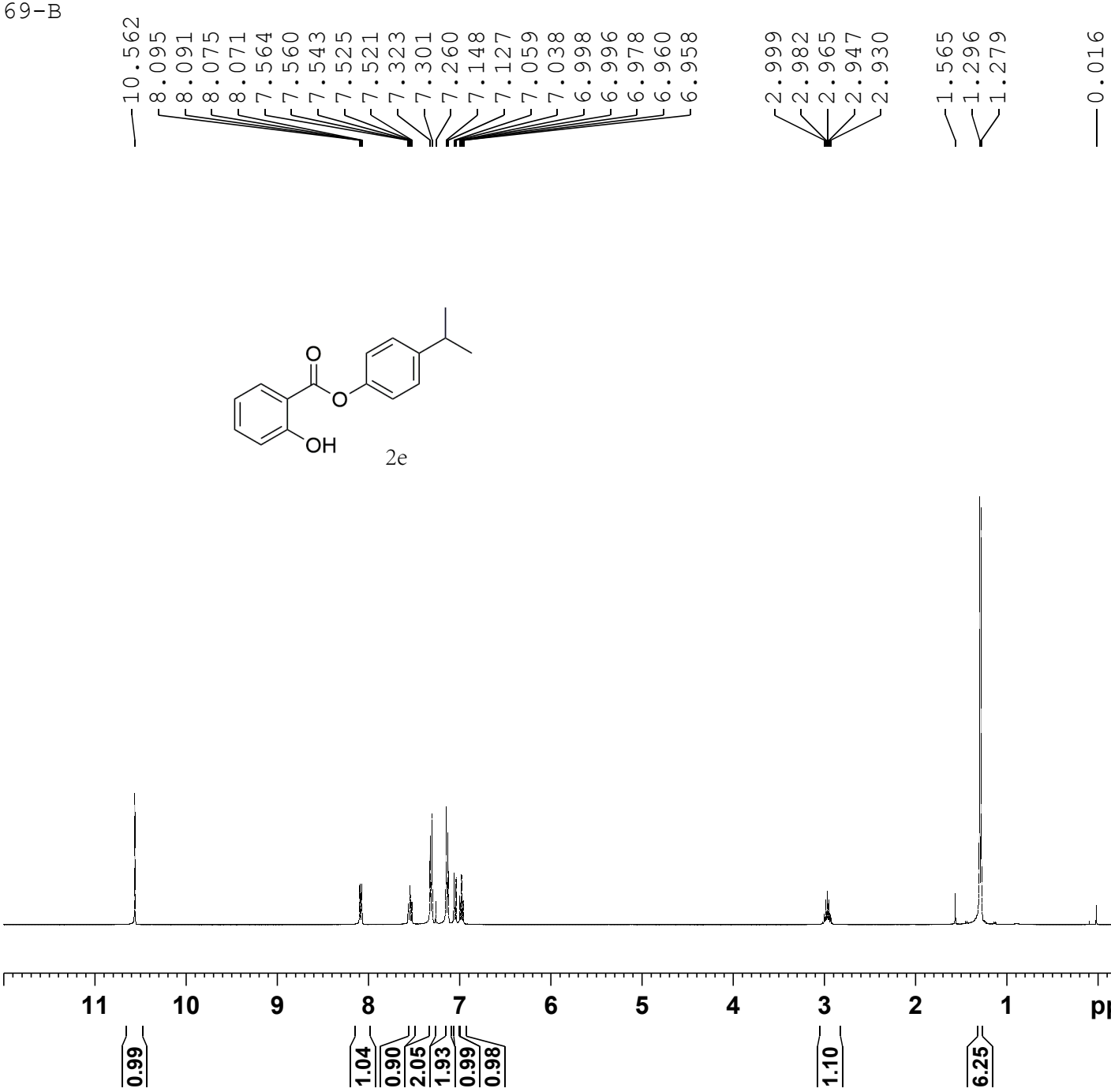
GB 0
PC 1.40

869-B



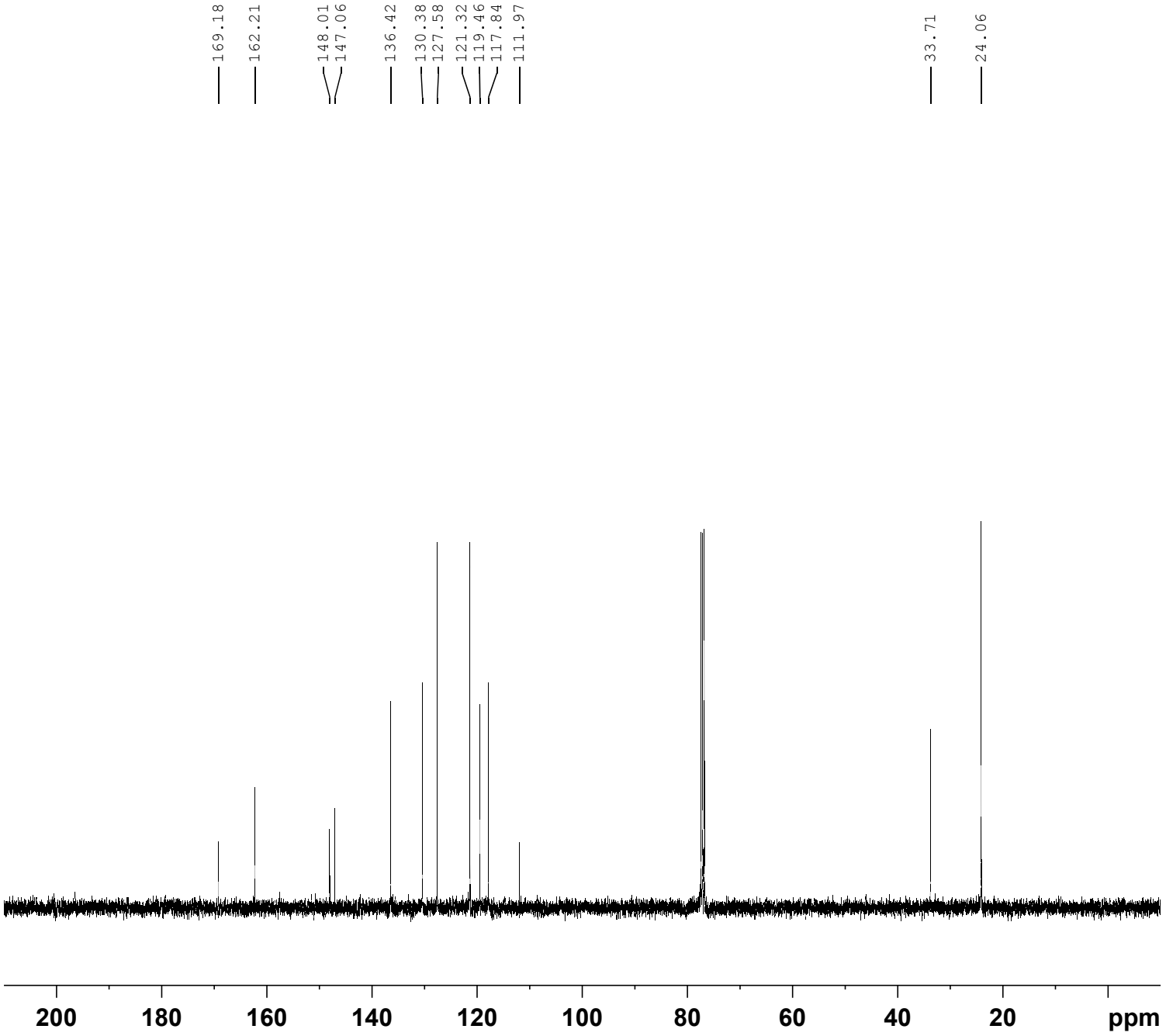

Current Data Parameters
NAME xzh-400
EXPNO 73
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190605
Time 14.46
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 73.9
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.2424716 MHz
NUC1 1H
P1 14.30 usec
PLW1 12.00000000 W

F2 - Processing parameters
SI 65536
SF 400.2400099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

869-B




Current Data Parameters
NAME xzh-400
EXPNO 74
PROCNO 1

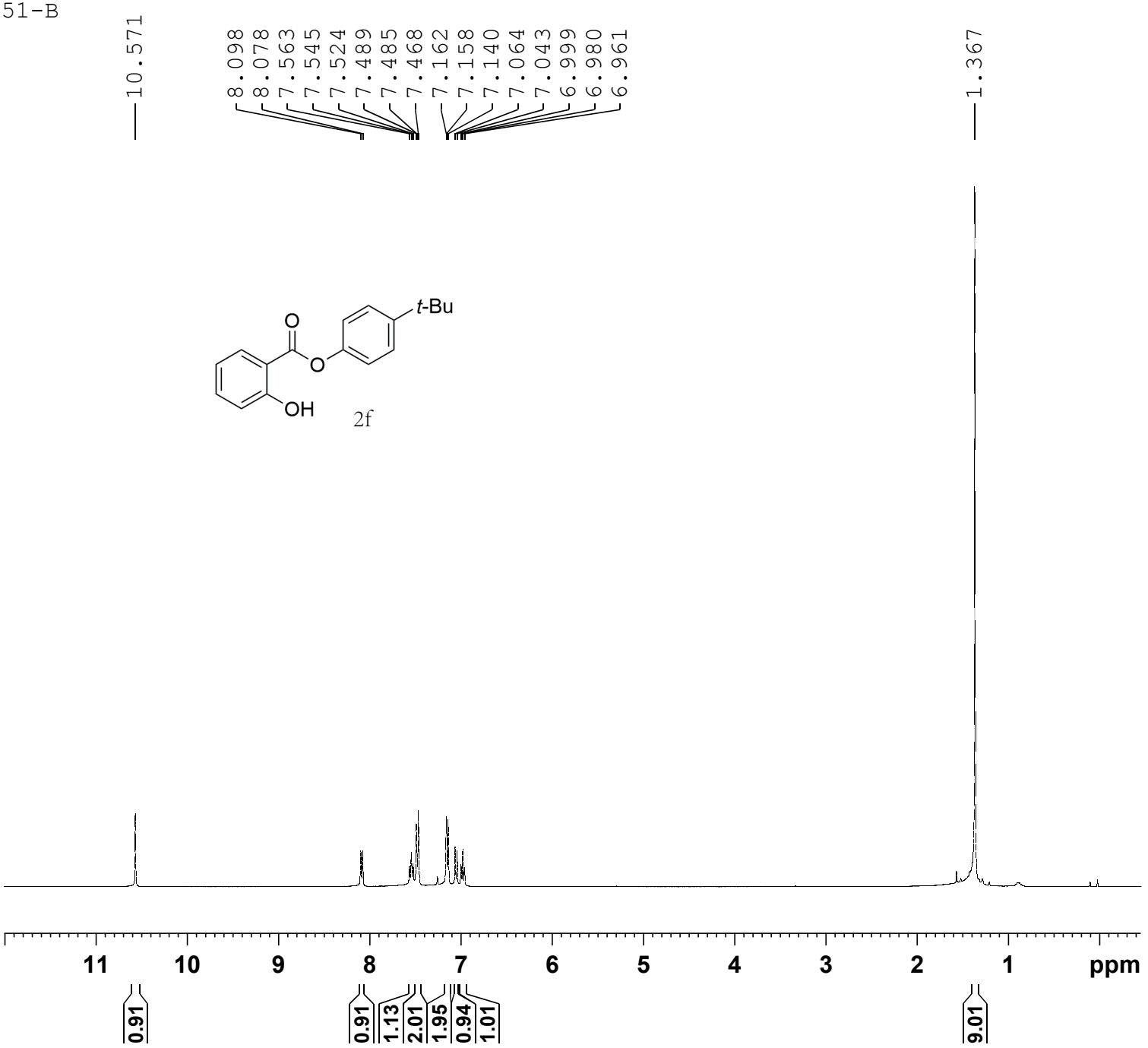
F2 - Acquisition Parameters
Date_ 20190605
Time 14.49
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 35
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 206.33
DW 20.800 usec
DE 6.50 usec
TE 298.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6504916 MHz
NUC1 13C
P1 10.00 usec
PLW1 54.00000000 W

======== CHANNEL f2 ========
SFO2 400.2416010 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.30294999 W
PLW13 0.24539000 W

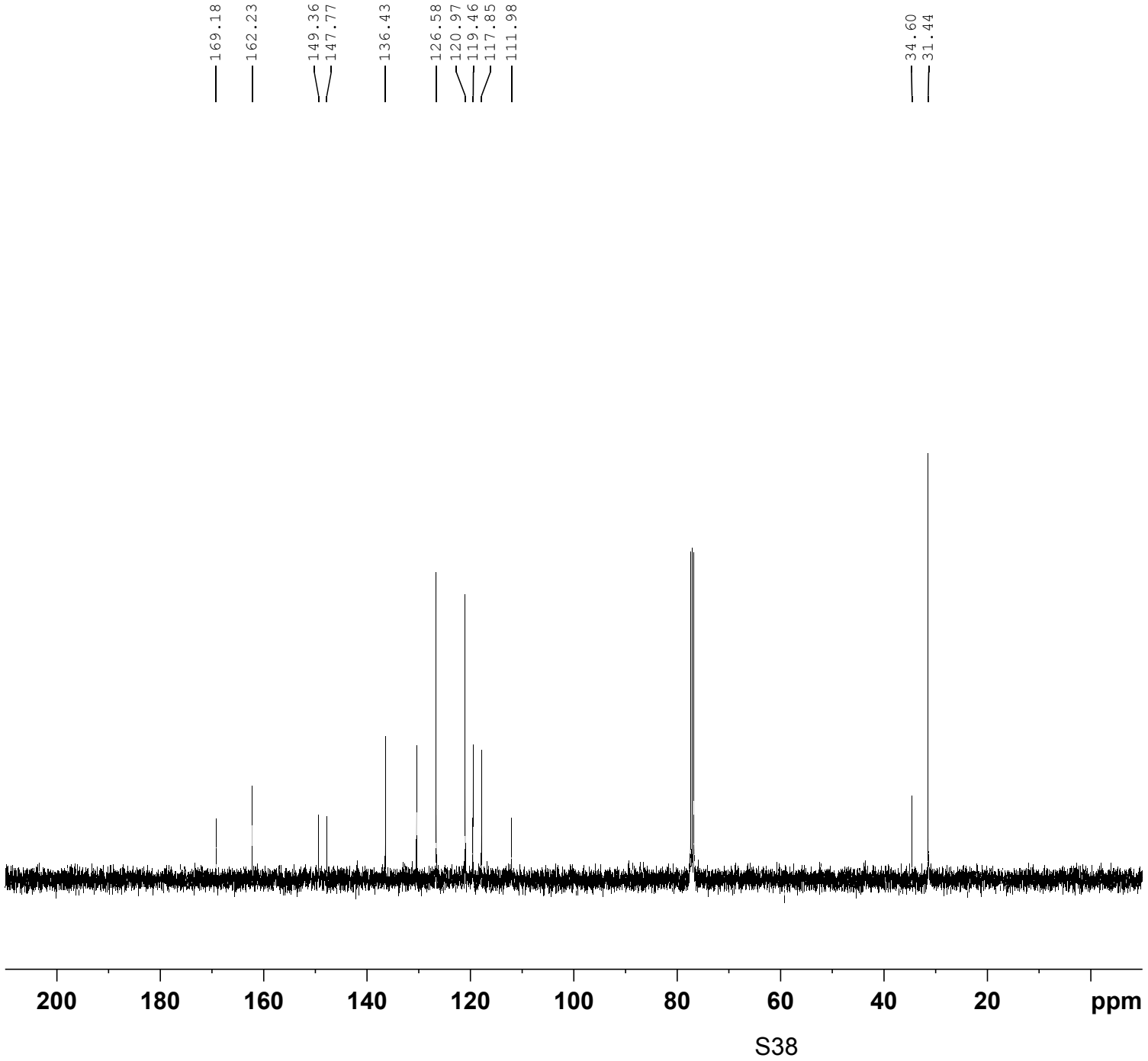
F2 - Processing parameters
SI 32768
SF 100.6404280 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

851-B




```
Current Data Parameters
NAME                  xzh-400
EXPNO                      57
PROCNO                      1

F2 - Acquisition Parameters
Date_               20190510
Time                   12.39
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                        16
DS                         0
SWH                 8012.820 Hz
FIDRES              0.244532 Hz
AQ                2.0447233 sec
RG                      73.9
DW                    62.400 usec
DE                     6.50 usec
TE                    298.6 K
D1                2.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1            400.2424716 MHz
NUC1                       1H
P1                    14.30 usec
PLW1           12.00000000 W

F2 - Processing parameters
SI                         65536
SF              400.2400107 MHz
WDW                        EM
SSB         0
LB                     0.30 Hz
GB          0
PC                     1.00
```

851-B




Current Data Parameters
NAME xzh-400
EXPNO 58
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190510
Time 12.41
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 21
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 206.33
DW 20.800 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6504916 MHz
NUC1 13C
P1 10.00 usec
PLW1 54.00000000 W

======== CHANNEL f2 ========
SFO2 400.2416010 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.30294999 W
PLW13 0.24539000 W

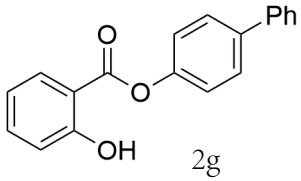
F2 - Processing parameters
SI 32768
SF 100.6404280 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

850-A

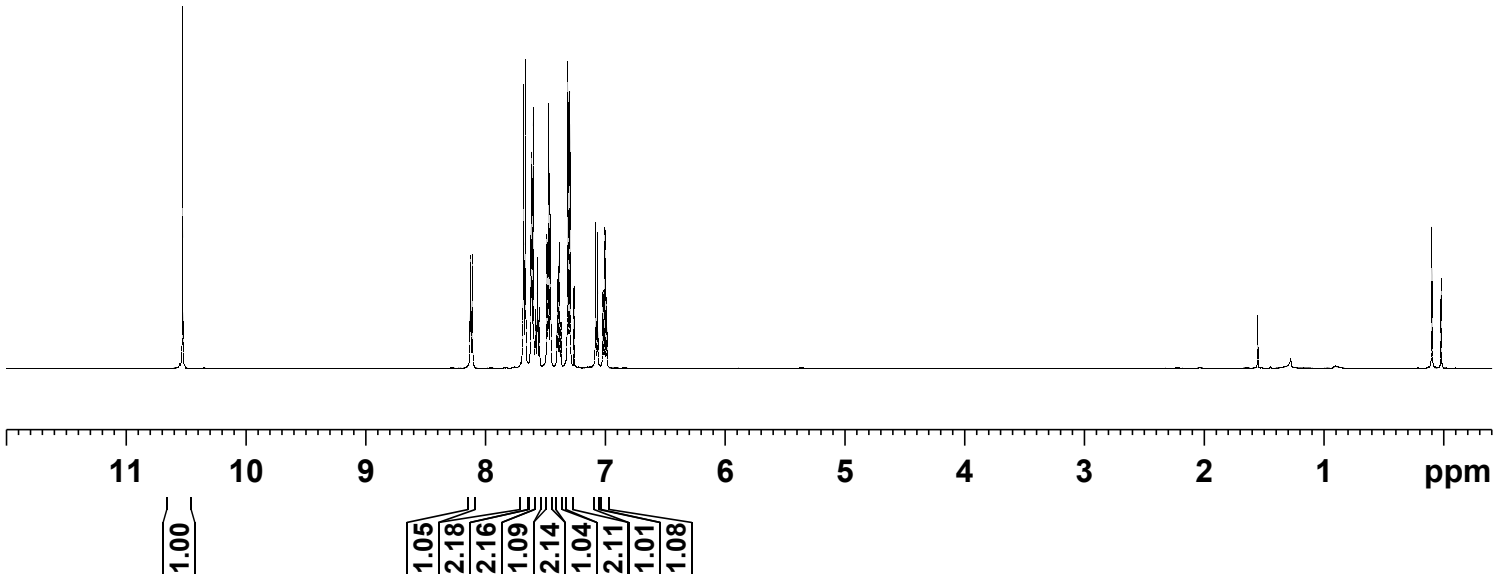
10.529
8.127
8.124
8.111
8.108
7.683
7.666
7.616
7.601
7.583
7.580
7.566
7.552
7.549
7.487
7.472
7.456
7.399
7.385
7.370
7.312
7.294
7.260
7.080
7.063
7.017
7.003
6.987

1.552

0.020

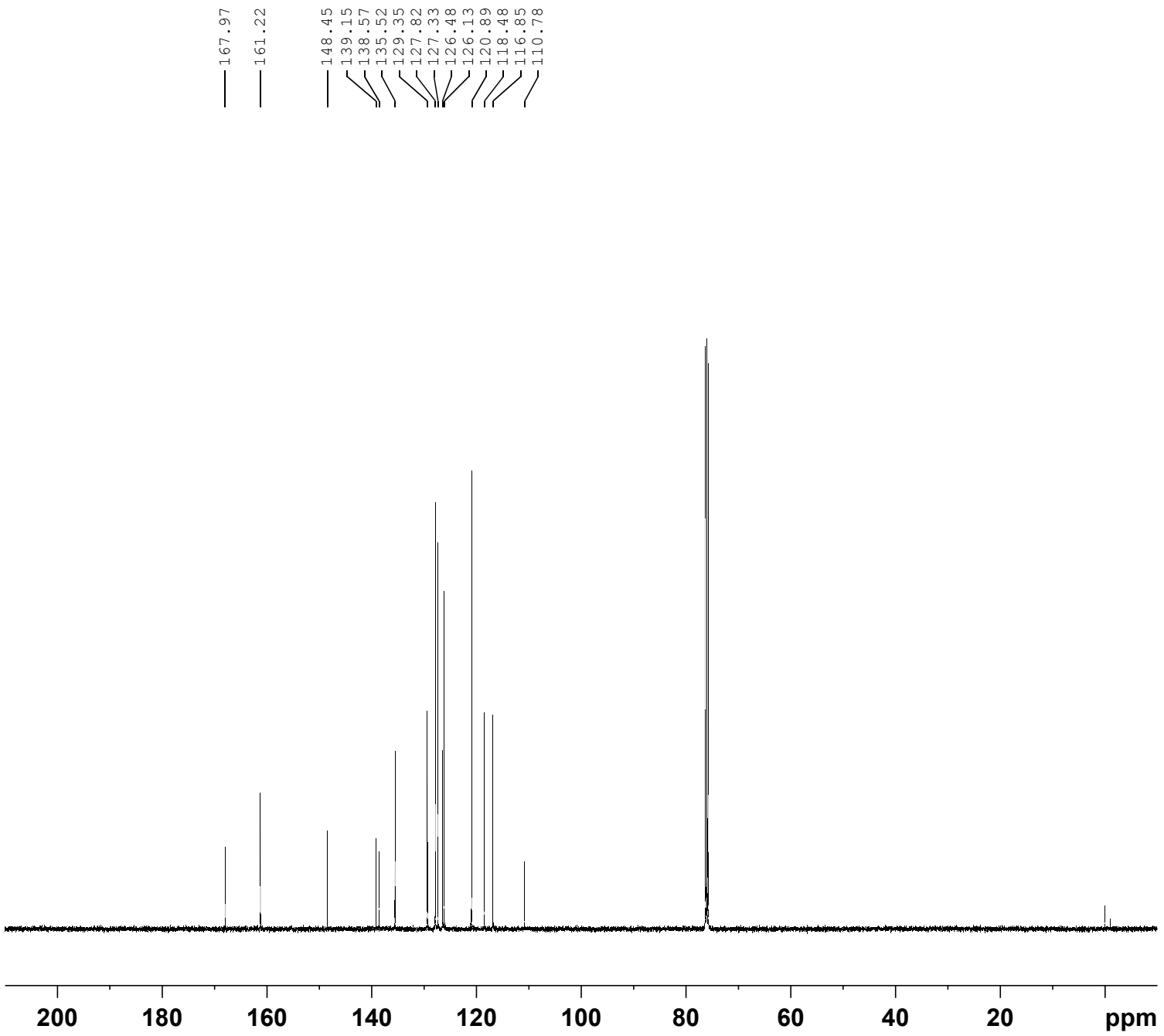



2g




```
Current Data Parameters
NAME                  xzh
EXPNO                  92
PROCNO                  1

F2 - Acquisition Parameters
Date_           20190509
Time               14.18
INSTRUM            spect
PROBHD   5 mm CPPBBO BB
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES         0.152588 Hz
AQ            3.2767999 sec
RG                 31.72
DW                50.000 usec
DE                 6.50 usec
TE                 298.1 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.1330885 MHz
NUC1                   1H
P1                 11.50 usec
PLW1         20.00000000 W

F2 - Processing parameters
SI                 65536
SF           500.1300121 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

850-A




Current Data Parameters
NAME xzh
EXPNO 93
PROCNO 1

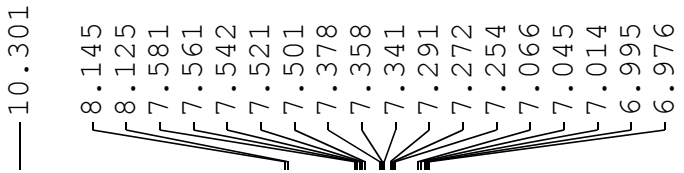
F2 - Acquisition Parameters
Date_ 20190509
Time 14.22
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 71
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 192.89
DW 16.800 usec
DE 18.00 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

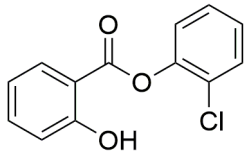
======== CHANNEL f1 ========
SFO1 125.7703637 MHz
NUC1 13C
P1 9.80 usec
PLW1 57.00000000 W

======== CHANNEL f2 ========
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 20.00000000 W
PLW12 0.35778001 W
PLW13 0.22898000 W

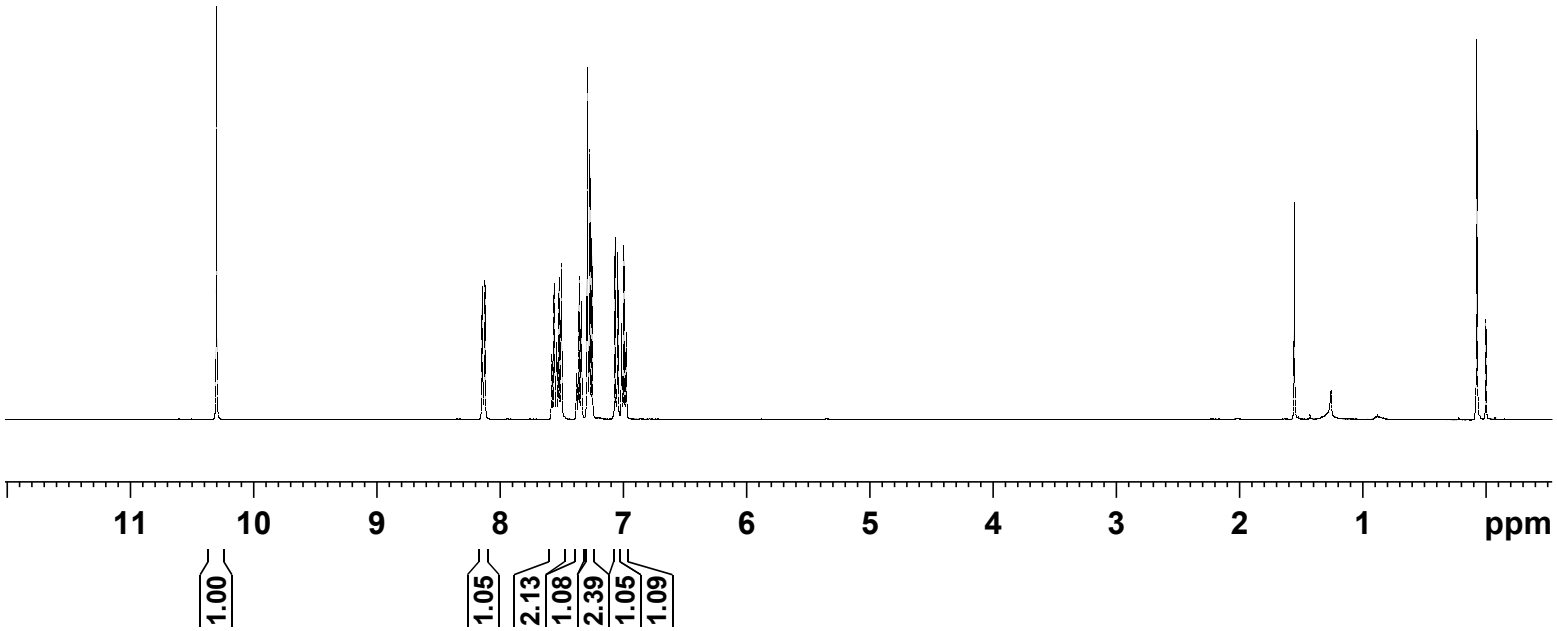
F2 - Processing parameters
SI 32768
SF 125.7579224 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

872-C



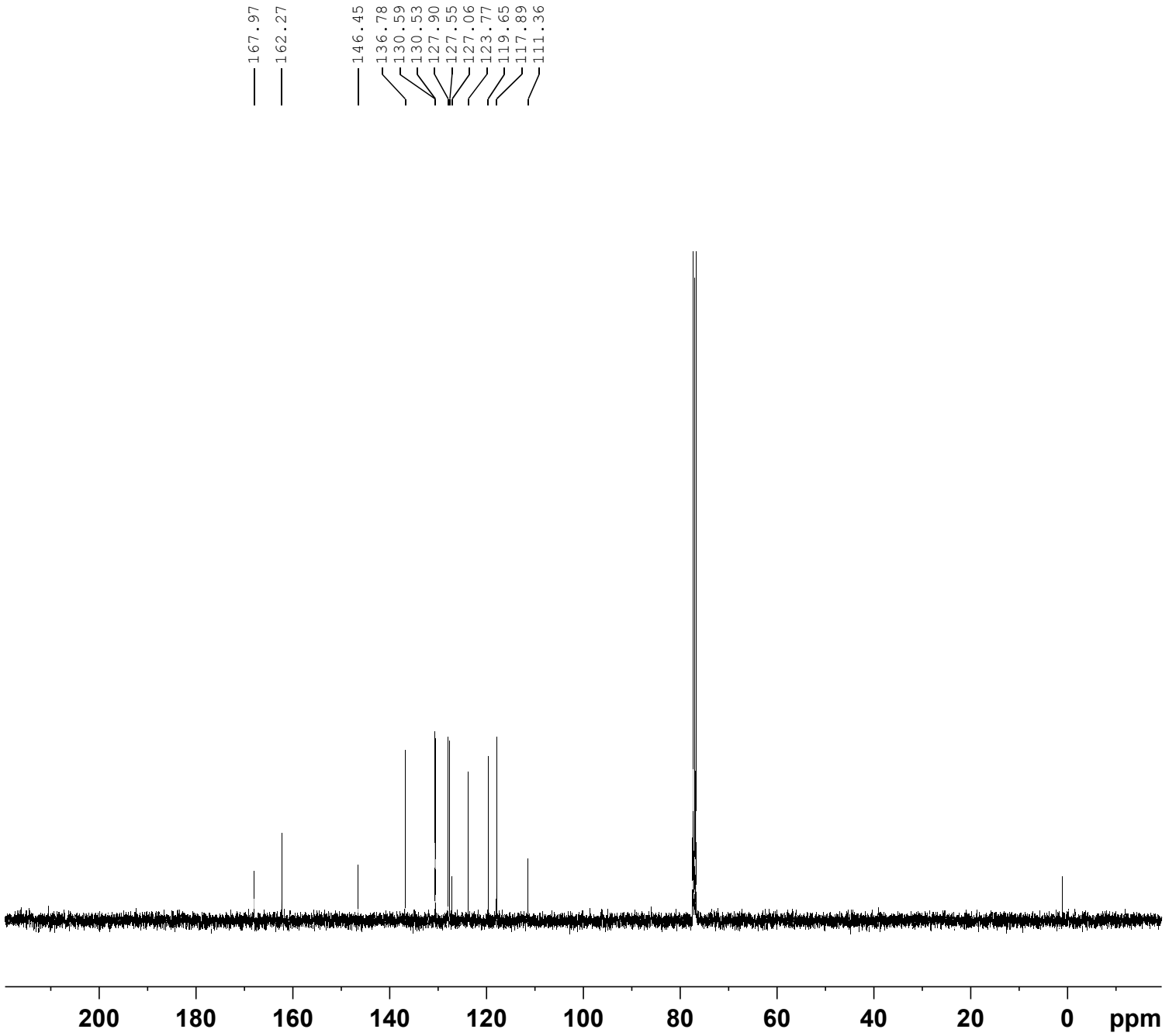




2h



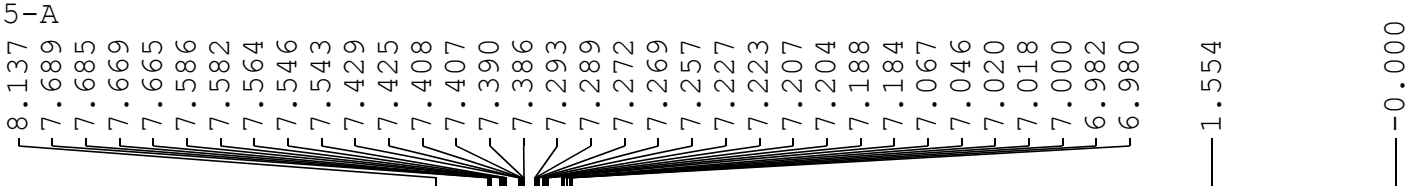

```
Current Data Parameters
NAME                  xzh-400
EXPNO                      86
PROCNO                      1

F2 - Acquisition Parameters
Date_                20190613
Time                    14.26
INSTRUM                 spect
PROBHD    5 mm PABBO BB/
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                        16
DS                         0
SWH                 8012.820 Hz
FIDRES              0.244532 Hz
AQ                2.0447233 sec
RG                   206.33
DW                   62.400 usec
DE                    6.50 usec
TE                   299.0 K
D1                2.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1             400.2424716 MHz
NUC1                       1H
P1                      14.30 usec
PLW1             12.00000000 W

F2 - Processing parameters
SI                         65536
SF               400.2400119 MHz
WDW                        EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```

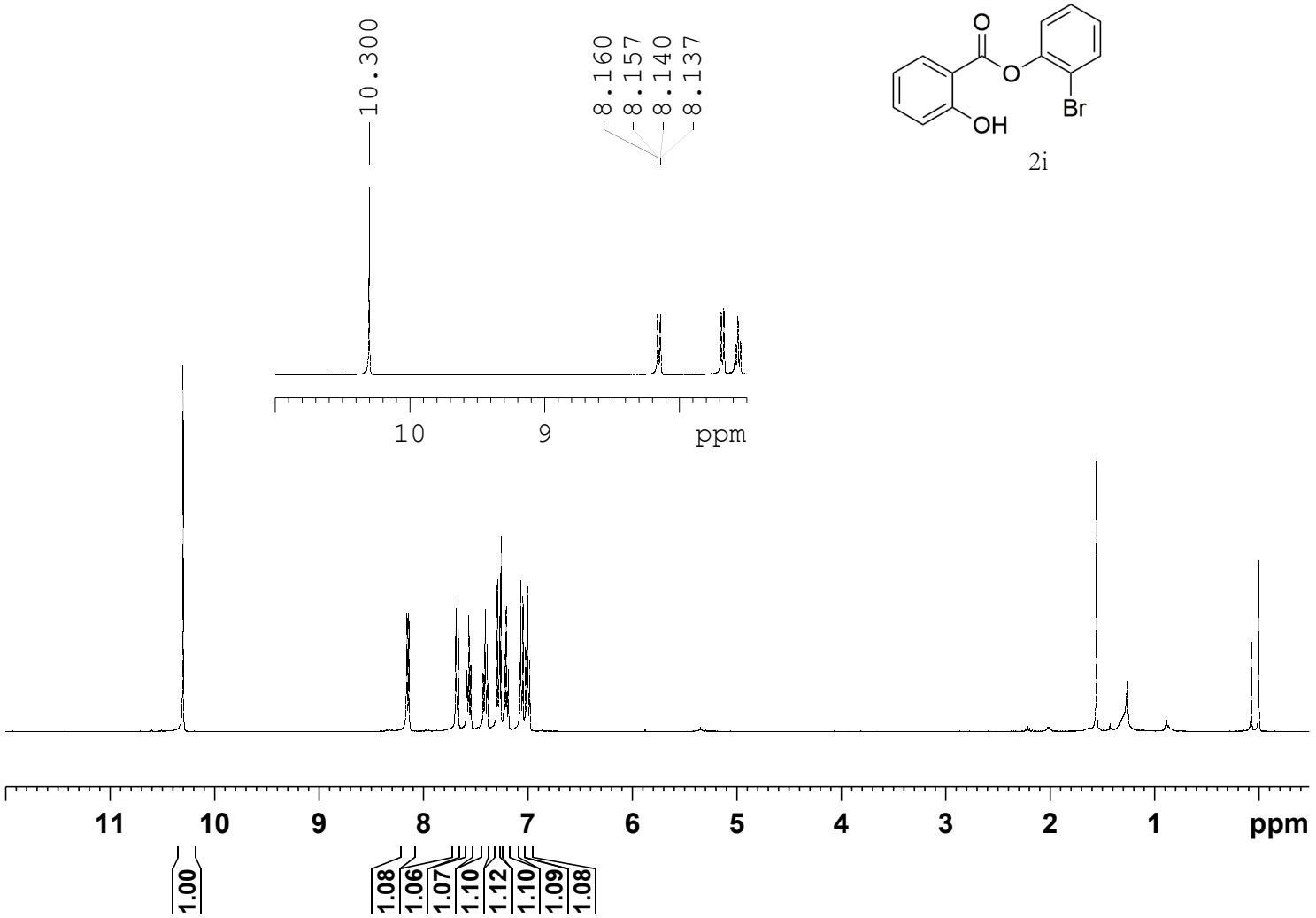
872-C




```
Current Data Parameters
NAME                 xzh-400
EXPNO                     87
PROCNO                     1

F2 - Acquisition Parameters
Date_               20190613
Time                   14.30
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       100
DS                         4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                     206.33
DW                     20.800 usec
DE                      6.50 usec
TE                     299.7 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1               100.6504916 MHz
NUC1                       13C
P1                      10.00 usec
PLW1               54.00000000 W

======== CHANNEL f2 ========
SFO2               400.2416010 MHz
NUC2                       1H
CPDPRG[2                waltz16
PCPD2                   90.00 usec
PLW2               12.00000000 W
PLW12               0.30294999 W
PLW13               0.24539000 W

F2 - Processing parameters
SI                         32768
SF                 100.6404280 MHz
WDW                           EM
SSB           0
LB                      1.00 Hz
GB            0
PC                      1.40
```

875-A







2i

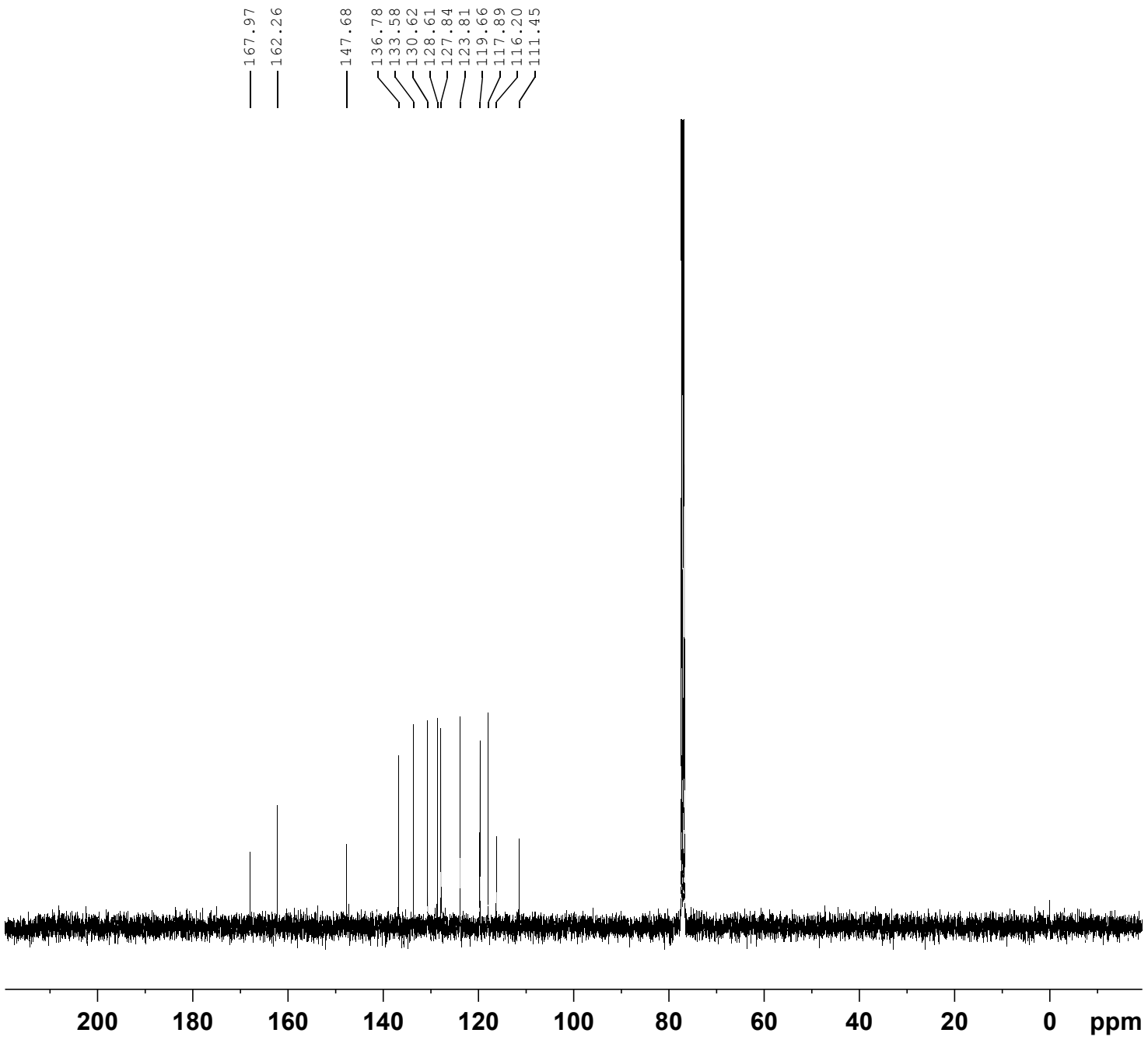
Current Data Parameters
NAME xzh-400
EXPNO 90
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190617
Time 8.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 206.33
DW 62.400 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.2424716 MHz
NUC1 1H
P1 14.30 usec
PLW1 12.00000000 W

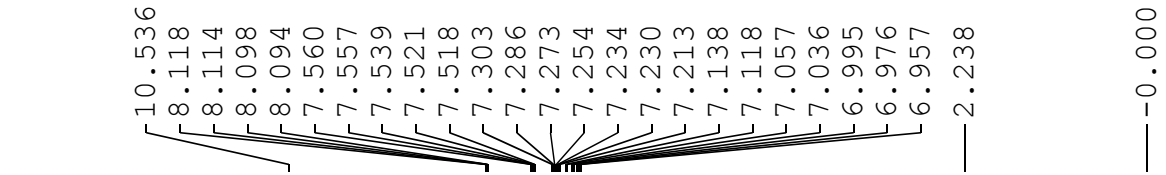
F2 - Processing parameters
SI 65536
SF 400.2400111 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

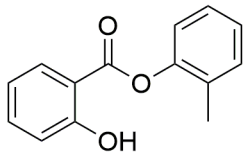
875-A




```
Current Data Parameters
NAME                  xzh-400
EXPNO                      91
PROCNO                      1

F2 - Acquisition Parameters
Date_                20190617
Time                     8.41
INSTRUM                 spect
PROBHD    5 mm PABBO BB/
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                        300
DS                          4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                     206.33
DW                     20.800 usec
DE                      6.50 usec
TE                     299.1 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1             100.6504916 MHz
NUC1                     13C
P1                     10.00 usec
PLW1            54.00000000 W

======== CHANNEL f2 ========
SFO2             400.2416010 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                  90.00 usec
PLW2            12.00000000 W
PLW12            0.30294999 W
PLW13            0.24539000 W

F2 - Processing parameters
SI                      32768
SF               100.6404280 MHz
WDW                        EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```

856-A




2j



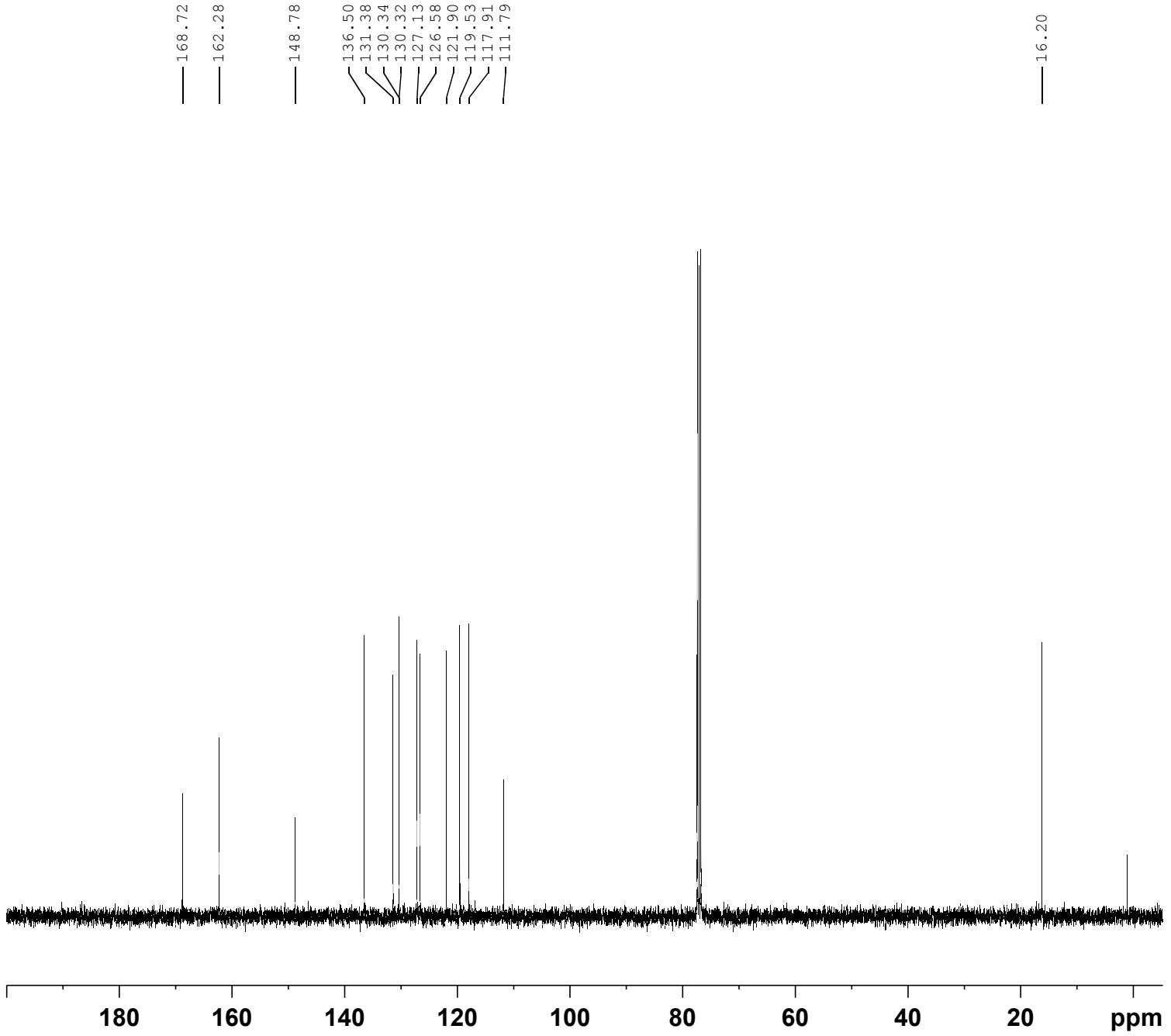

Current Data Parameters
NAME xzh-400
EXPNO 67
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190516
Time 16.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 80.72
DW 62.400 usec
DE 6.50 usec
TE 298.8 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.2424716 MHz
NUC1 1H
P1 14.30 usec
PLW1 12.00000000 W

F2 - Processing parameters
SI 65536
SF 400.2400194 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

856-A



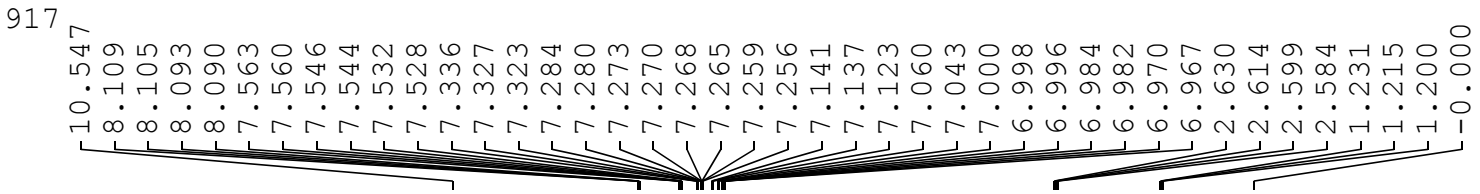

Current Data Parameters
NAME xzh
EXPNO 68
PROCNO 1

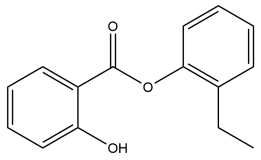
F2 - Acquisition Parameters
Date_ 20190516
Time 16.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 88
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 206.33
DW 20.800 usec
DE 6.50 usec
TE 299.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6504916 MHz
NUC1 13C
P1 10.00 usec
PLW1 54.00000000 W

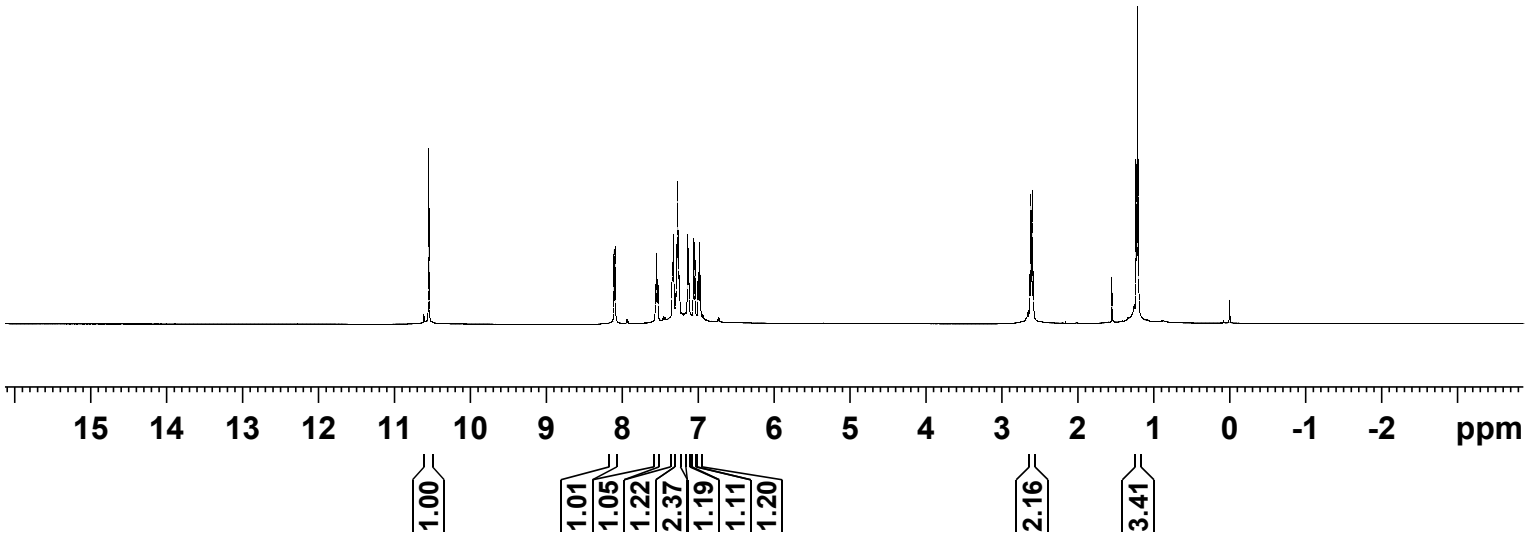
======== CHANNEL f2 ========
SFO2 400.2416010 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.30294999 W
PLW13 0.24539000 W

F2 - Processing parameters
SI 32768
SF 100.6404280 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



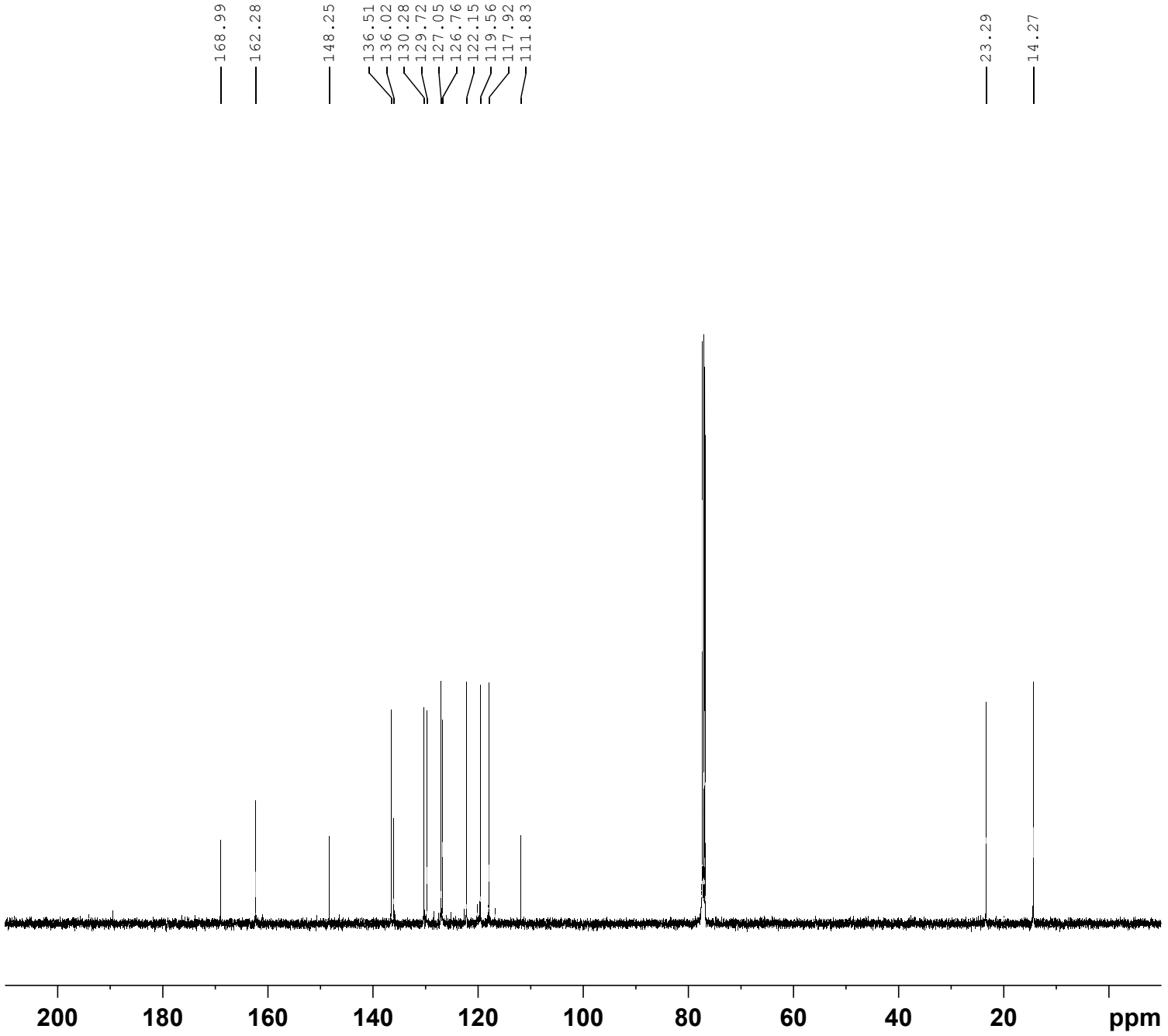




2k




```
Current Data Parameters
NAME                  500
EXPNO                 155
PROCNO                  1

F2 - Acquisition Parameters
Date_            20190829
Time                15.58
INSTRUM             spect
PROBHD   5 mm CPPBBO BB
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH             10000.000 Hz
FIDRES          0.152588 Hz
AQ              3.2767999 sec
RG                  31.72
DW                 50.000 usec
DE                  6.50 usec
TE                 298.2 K
D1            1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          500.1330885 MHz
NUC1                   1H
P1                  11.50 usec
PLW1         20.00000000 W

F2 - Processing parameters
SI                  65536
SF            500.1300221 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

917




Current Data Parameters
NAME 500
EXPNO 156
PROCNO 1

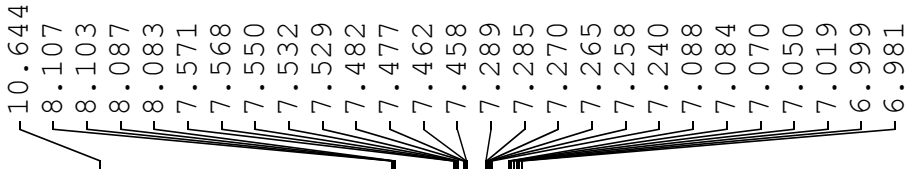
F2 - Acquisition Parameters
Date_ 20190829
Time 15.59
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 29
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 192.89
DW 16.800 usec
DE 18.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

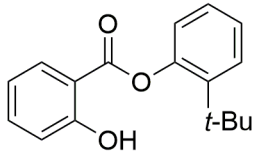
======== CHANNEL f1 ========
SFO1 125.7703637 MHz
NUC1 13C
P1 9.80 usec
PLW1 57.00000000 W

======== CHANNEL f2 ========
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 20.00000000 W
PLW12 0.35778001 W
PLW13 0.22898000 W

F2 - Processing parameters
SI 32768
SF 125.7577885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

870-B



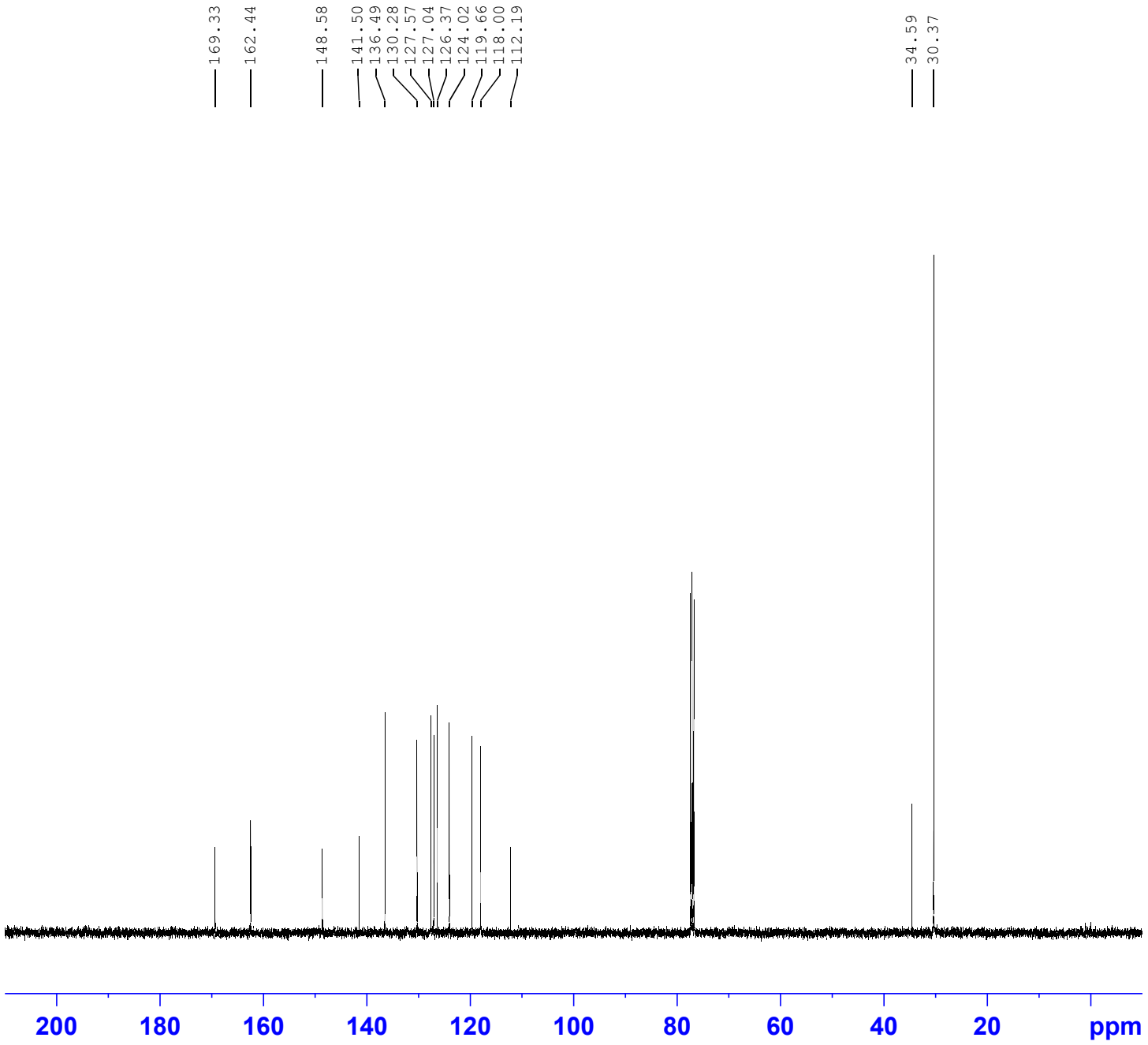




2l




```
Current Data Parameters
NAME            xzh-400
EXPNO                77
PROCNO                1

F2 - Acquisition Parameters
Date_          20190606
Time              16.18
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            8012.820 Hz
FIDRES         0.244532 Hz
AQ            2.0447233 sec
RG                65.71
DW               62.400 usec
DE                6.50 usec
TE               299.4 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.2424716 MHz
NUC1                 1H
P1                14.30 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                65536
SF           400.2400173 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

870-B



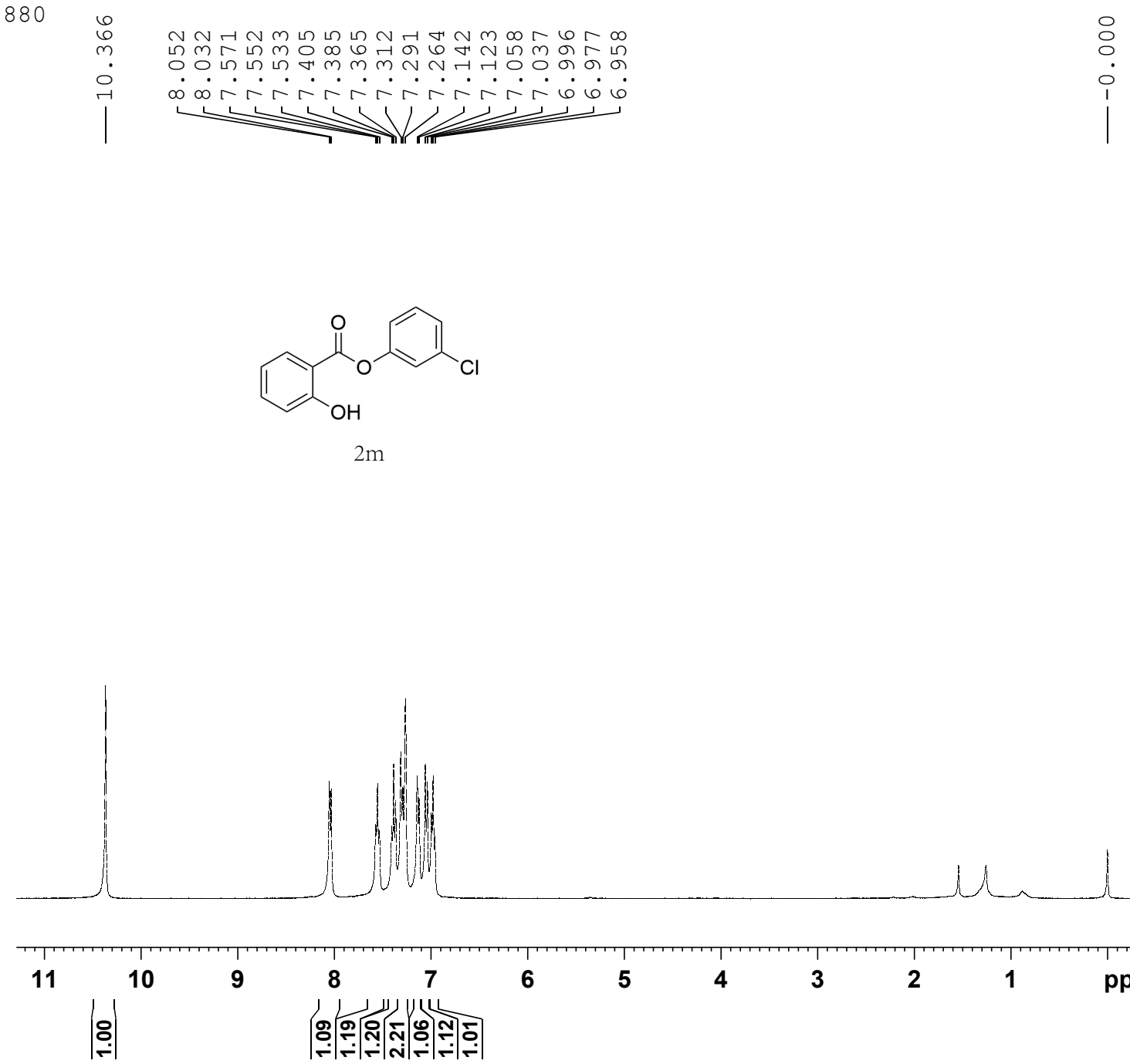

Current Data Parameters
NAME xzh-400
EXPNO 78
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190606
Time 16.20
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 80
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 206.33
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6504916 MHz
NUC1 13C
P1 10.00 usec
PLW1 54.00000000 W

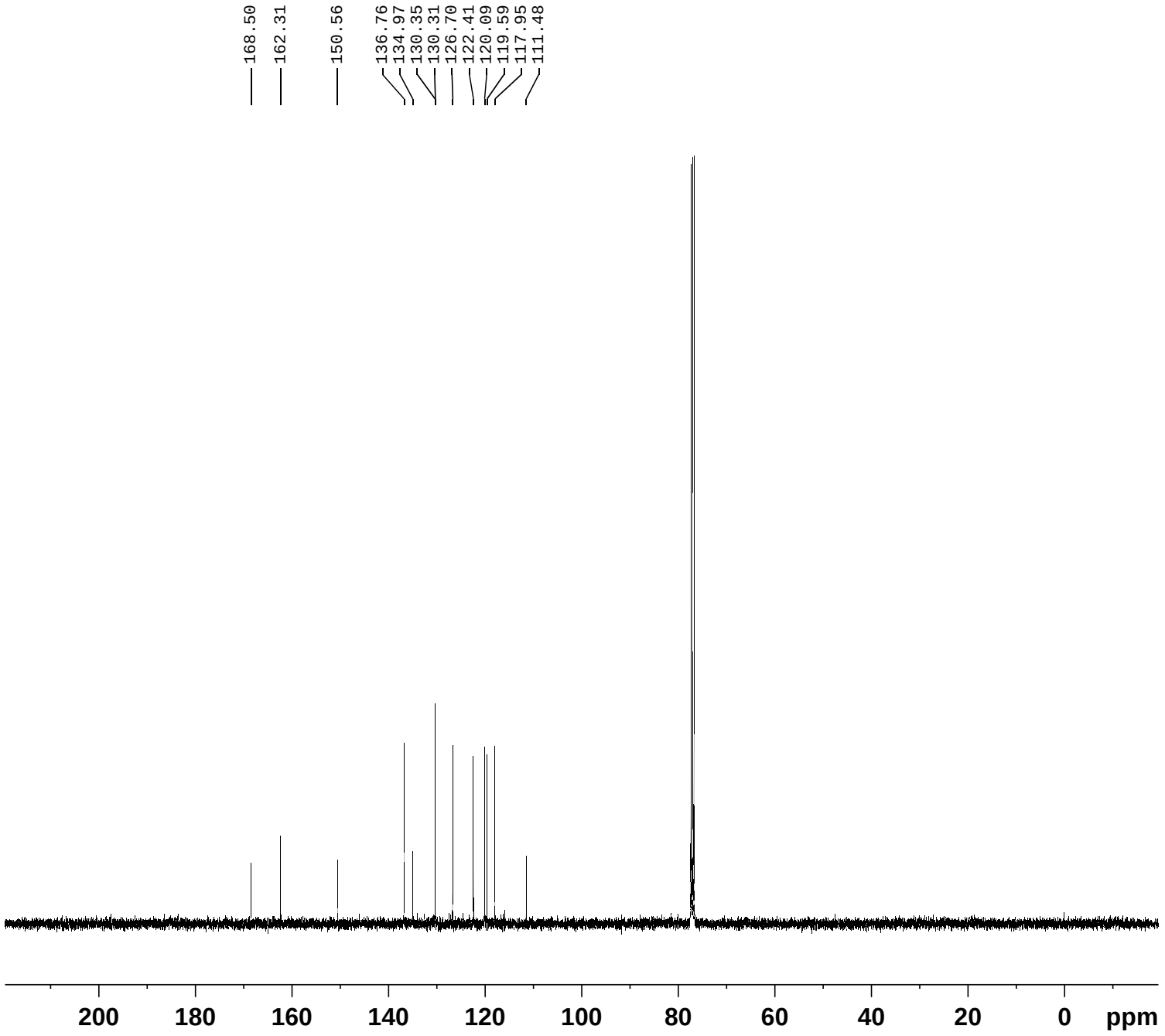
======== CHANNEL f2 ========
SFO2 400.2416010 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.30294999 W
PLW13 0.24539000 W

F2 - Processing parameters
SI 32768
SF 100.6404280 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40




```
Current Data Parameters
NAME                  review
EXPNO                     12
PROCNO                     1

F2 - Acquisition Parameters
Date_              20191212
Time                  16.33
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       16
DS                        0
SWH                8012.820 Hz
FIDRES             0.244532 Hz
AQ                2.0447233 sec
RG                   206.33
DW                   62.400 usec
DE                    6.50 usec
TE                   298.0 K
D1              2.00000000 sec
D11       0 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           400.2424716 MHz
NUC1                      1H
P1                    14.30 usec
PLW1           12.00000000 W

======== CHANNEL f2 ========
SFO2           400.2424716 MHz
NUC2                     off
CPDPRG[2
PCPD2      0 usec
PLW2       0 W
PLW12      0 W
PLW13      0 W

F2 - Processing parameters
SI                    65536
SF           400.2400118 MHz
WDW                      EM
SSB        0
LB                    0.30 Hz
GB         0
PC                    1.00
```

880




Current Data Parameters
NAME xzh-400
EXPNO 97
PROCNO 1

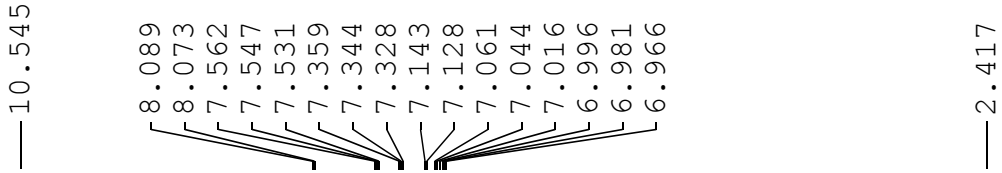
F2 - Acquisition Parameters
Date_ 20190620
Time 16.01
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 300
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 206.33
DW 20.800 usec
DE 6.50 usec
TE 300.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

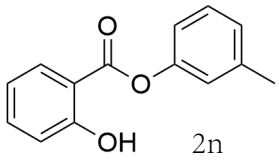
======== CHANNEL f1 ========
SFO1 100.6504916 MHz
NUC1 13C
P1 10.00 usec
PLW1 54.00000000 W

======== CHANNEL f2 ========
SFO2 400.2416010 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.30294999 W
PLW13 0.24539000 W

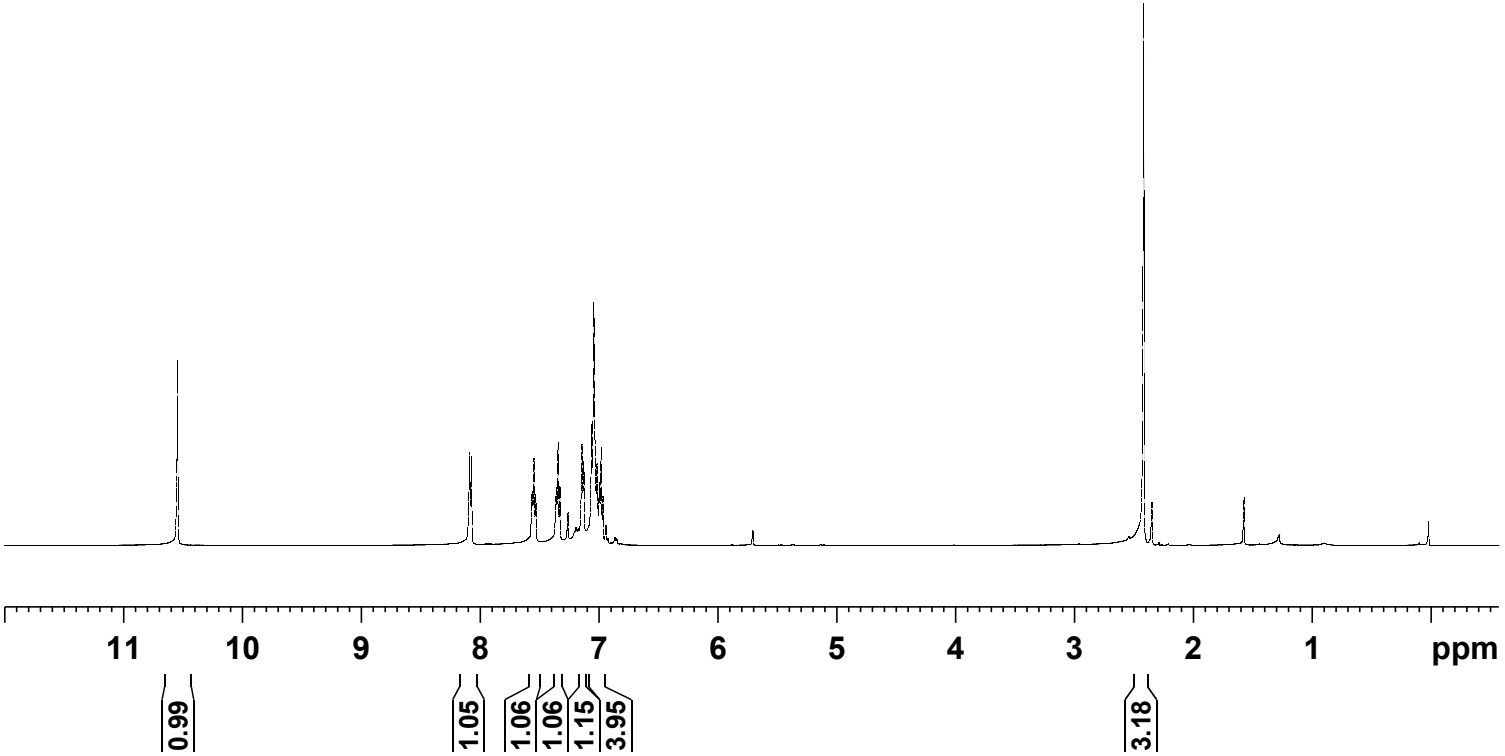
F2 - Processing parameters
SI 32768
SF 100.6404280 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

866-A



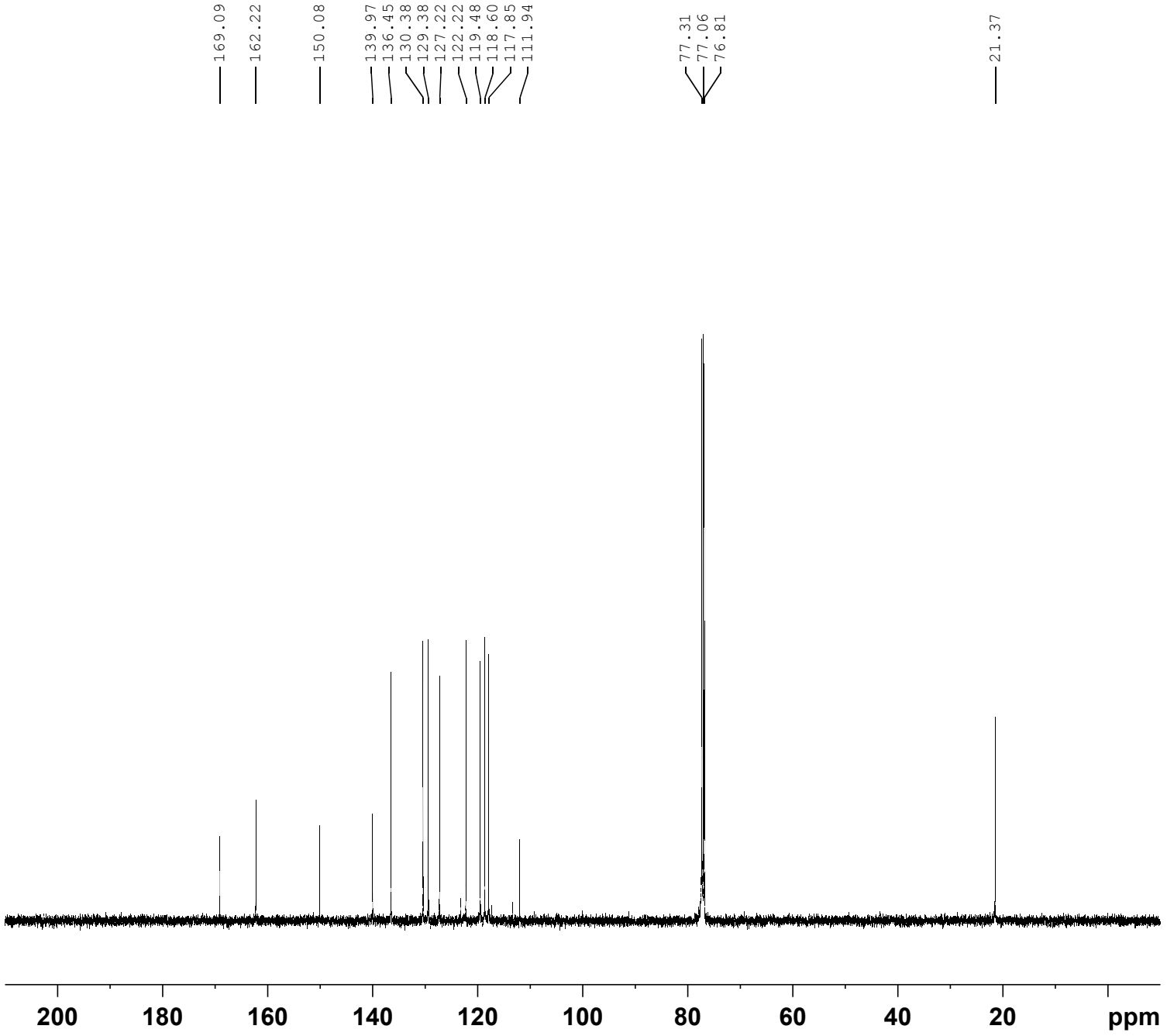




2n




```
Current Data Parameters
NAME                  xzh
EXPNO                 100
PROCNO                  1

F2 - Acquisition Parameters
Date_            20190603
Time                21.06
INSTRUM             spect
PROBHD   5 mm CPPBBO BB
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES         0.152588 Hz
AQ             3.2767999 sec
RG                 31.72
DW                50.000 usec
DE                 6.50 usec
TE                298.1 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.1330885 MHz
NUC1                1H
P1                 11.50 usec
PLW1        20.00000000 W

F2 - Processing parameters
SI                 65536
SF           500.1300116 MHz
WDW                  EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

866-A




Current Data Parameters
NAME xzh
EXPNO 101
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190603
Time 21.08
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 27
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 192.89
DW 16.800 usec
DE 18.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

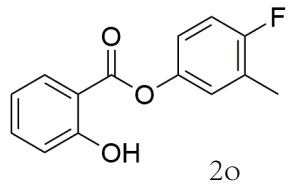
======== CHANNEL f1 ========
SFO1 125.7703637 MHz
NUC1 13C
P1 9.80 usec
PLW1 57.00000000 W

======== CHANNEL f2 ========
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 20.00000000 W
PLW12 0.35778001 W
PLW13 0.22898000 W

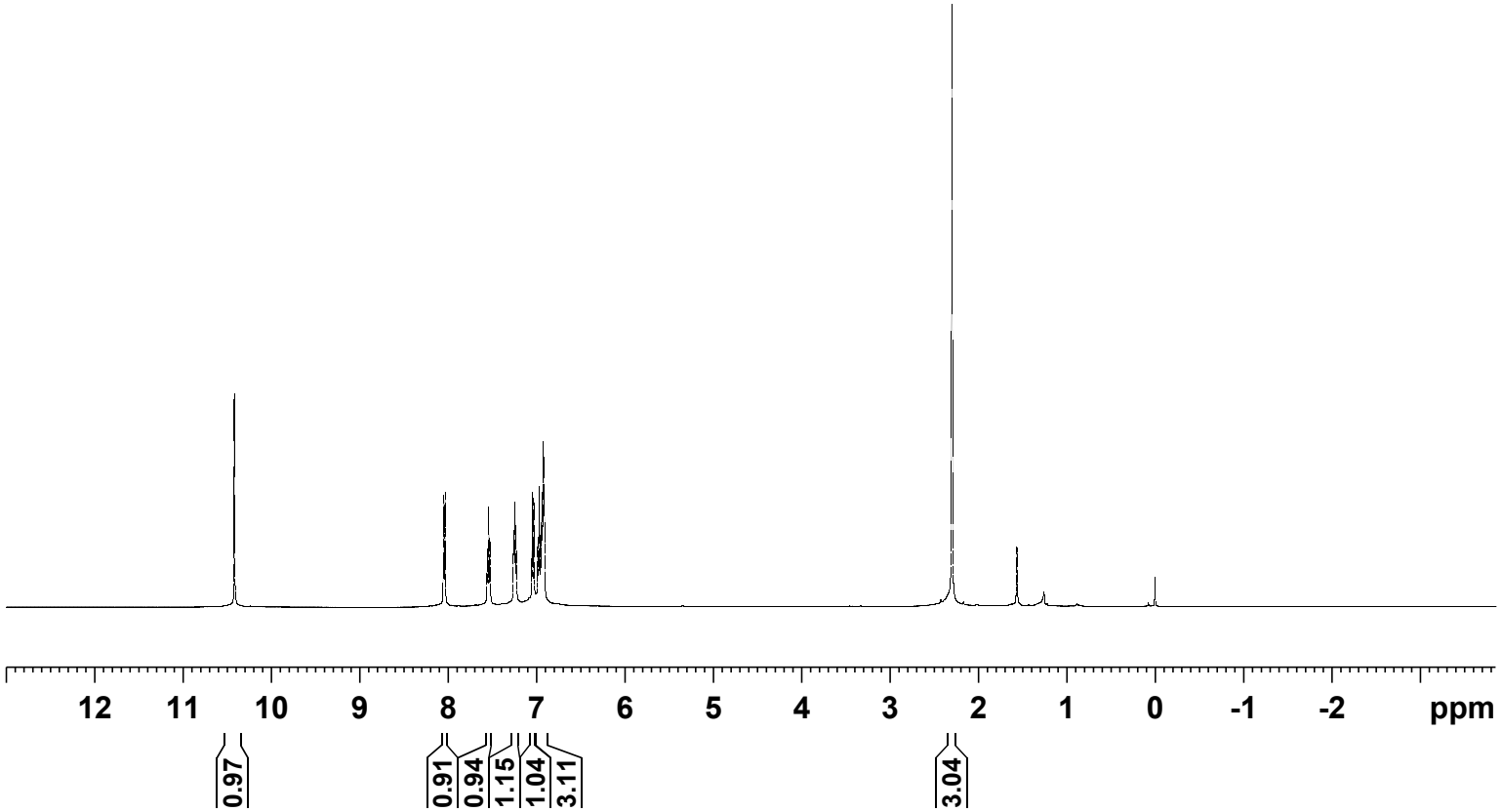
F2 - Processing parameters
SI 32768
SF 125.7577885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

914B

10.420
10.416
8.051
8.035
7.556
7.540
7.525
7.256
7.252
7.243
7.227
7.049
7.032
6.985
6.983
6.969
6.954
6.952
6.940
6.936
6.924
6.920
6.915
6.910
2.299
1.564
0.000

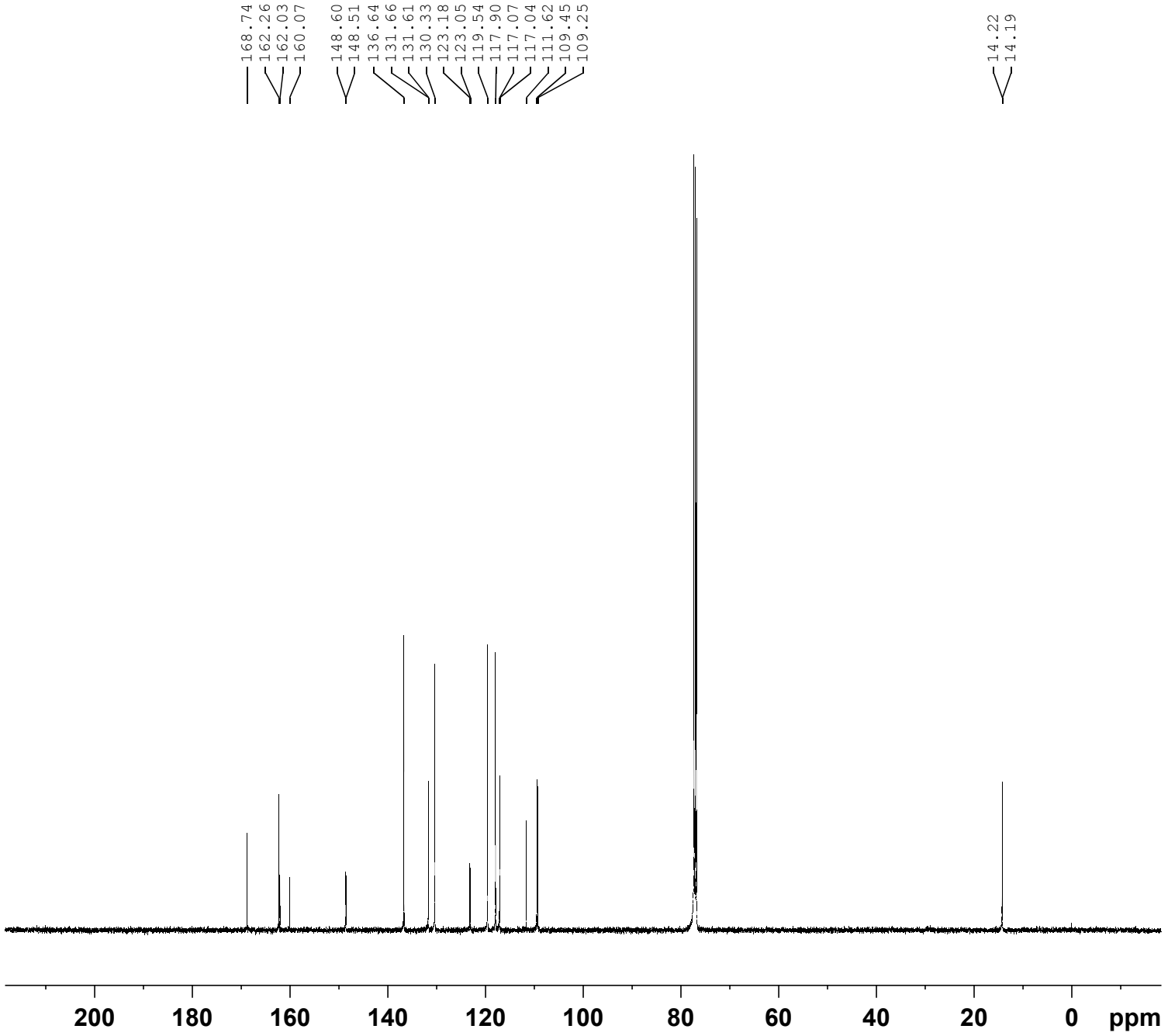



2o




```
Current Data Parameters
NAME                  500
EXPNO                 148
PROCNO                  1

F2 - Acquisition Parameters
Date_           20190826
Time                15.18
INSTRUM             spect
PROBHD   5 mm CPPBBO BB
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH           10000.000 Hz
FIDRES         0.152588 Hz
AQ             3.2767999 sec
RG                  31.72
DW                50.000 usec
DE                 6.50 usec
TE                298.2 K
D1           1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         500.1330885 MHz
NUC1                   1H
P1                 11.50 usec
PLW1         20.00000000 W

F2 - Processing parameters
SI                  65536
SF           500.1300153 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

914B




Current Data Parameters

| | |
|---|---|
| NAME | 500 |
| EXPNO | 149 |
| PROCNO | 1 |

F2 - Acquisition Parameters

| | |
|---|---|
| Date_ | 20190826 |
| Time | 15.21 |
| INSTRUM | spect |
| PROBHD | 5 mm CPPBBO BB |
| PULPROG | zgpg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 231 |
| DS | 4 |
| SWH | 29761.904 Hz |
| FIDRES | 0.454131 Hz |
| AQ | 1.1010048 sec |
| RG | 192.89 |
| DW | 16.800 usec |
| DE | 18.00 usec |
| TE | 298.2 K |
| D1 | 2.00000000 sec |
| D11 | 0.03000000 sec |
| TD0 | 1 |

======== CHANNEL f1 ========

| | |
|---|---|
| SFO1 | 125.7703637 MHz |
| NUC1 | 13C |
| P1 | 9.80 usec |
| PLW1 | 57.00000000 W |

======== CHANNEL f2 ========

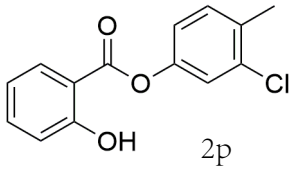
| | |
|---|---|
| SFO2 | 500.1320005 MHz |
| NUC2 | 1H |
| CPDPRG[2 | waltz16 |
| PCPD2 | 80.00 usec |
| PLW2 | 20.00000000 W |
| PLW12 | 0.35778001 W |
| PLW13 | 0.22898000 W |

F2 - Processing parameters

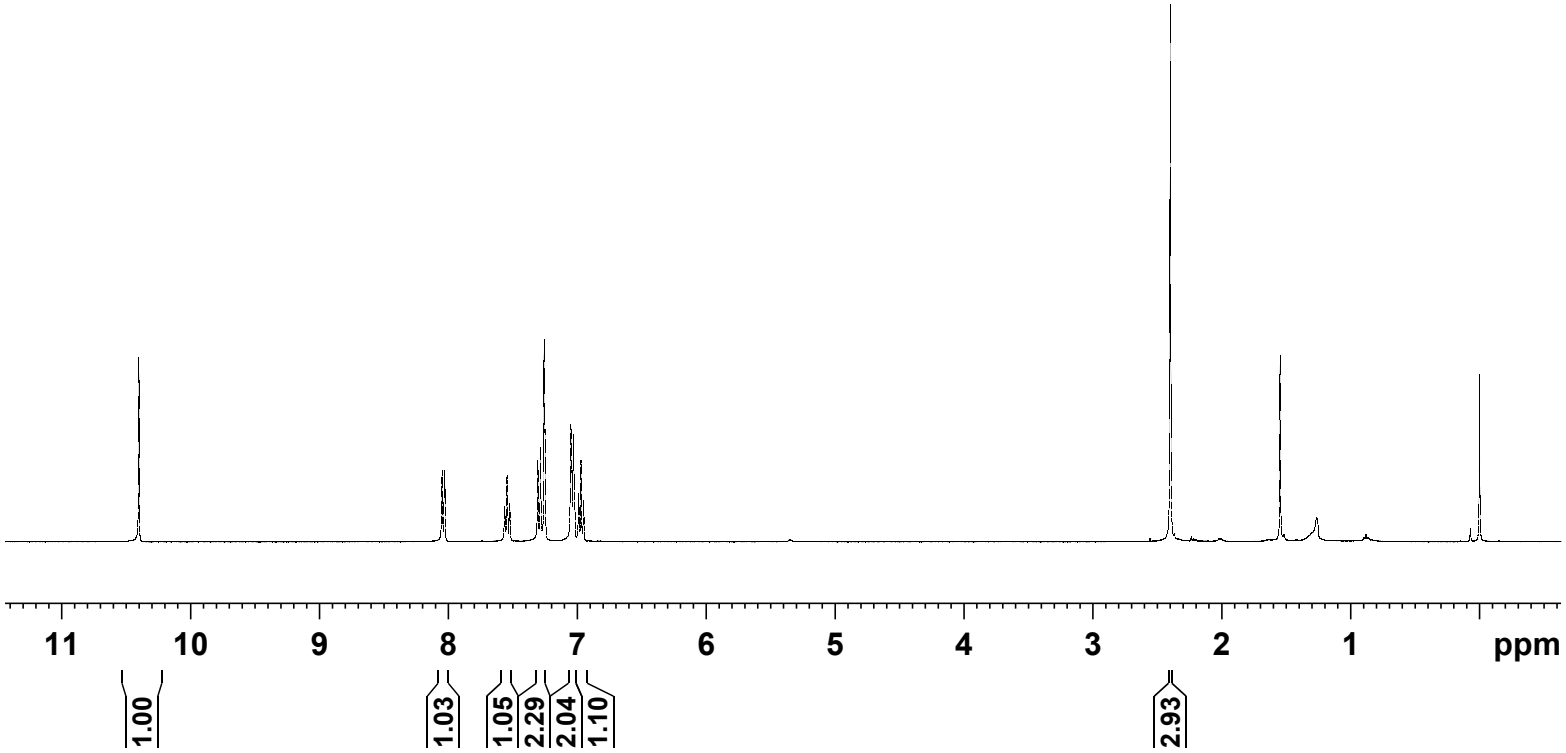
| | |
|---|---|
| SI | 32768 |
| SF | 125.7577885 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 1.00 Hz |
| GB | 0 |
| PC | 1.40 |

885-A

10.401
8.048
8.027
7.562
7.544
7.523
7.305
7.285
7.256
7.249
7.049
7.028
6.988
6.970
6.950
2.397
1.546
-0.000

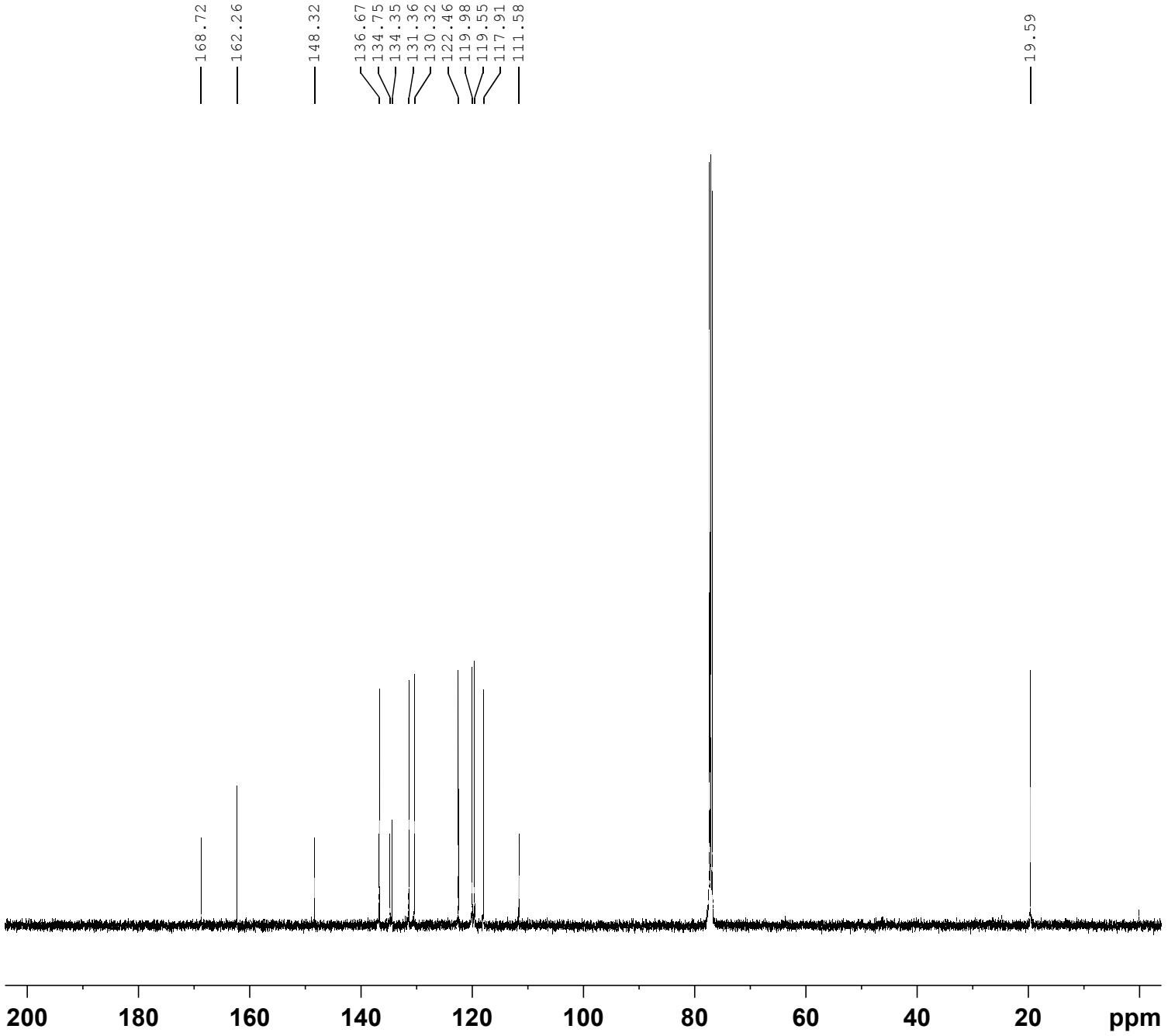



2p




```
Current Data Parameters
NAME                  xzh-400
EXPNO                     101
PROCNO                      1

F2 - Acquisition Parameters
Date_                20190624
Time                    15.07
INSTRUM                 spect
PROBHD    5 mm PABBO BB/
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                        16
DS                         0
SWH                 8012.820 Hz
FIDRES              0.244532 Hz
AQ                2.0447233 sec
RG                   206.33
DW                   62.400 usec
DE                    6.50 usec
TE                   299.6 K
D1                2.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1             400.2424716 MHz
NUC1                       1H
P1                      14.30 usec
PLW1             12.00000000 W

F2 - Processing parameters
SI                         65536
SF               400.2400109 MHz
WDW                        EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```

885-A




Current Data Parameters
NAME xzh
EXPNO 117
PROCNO 1

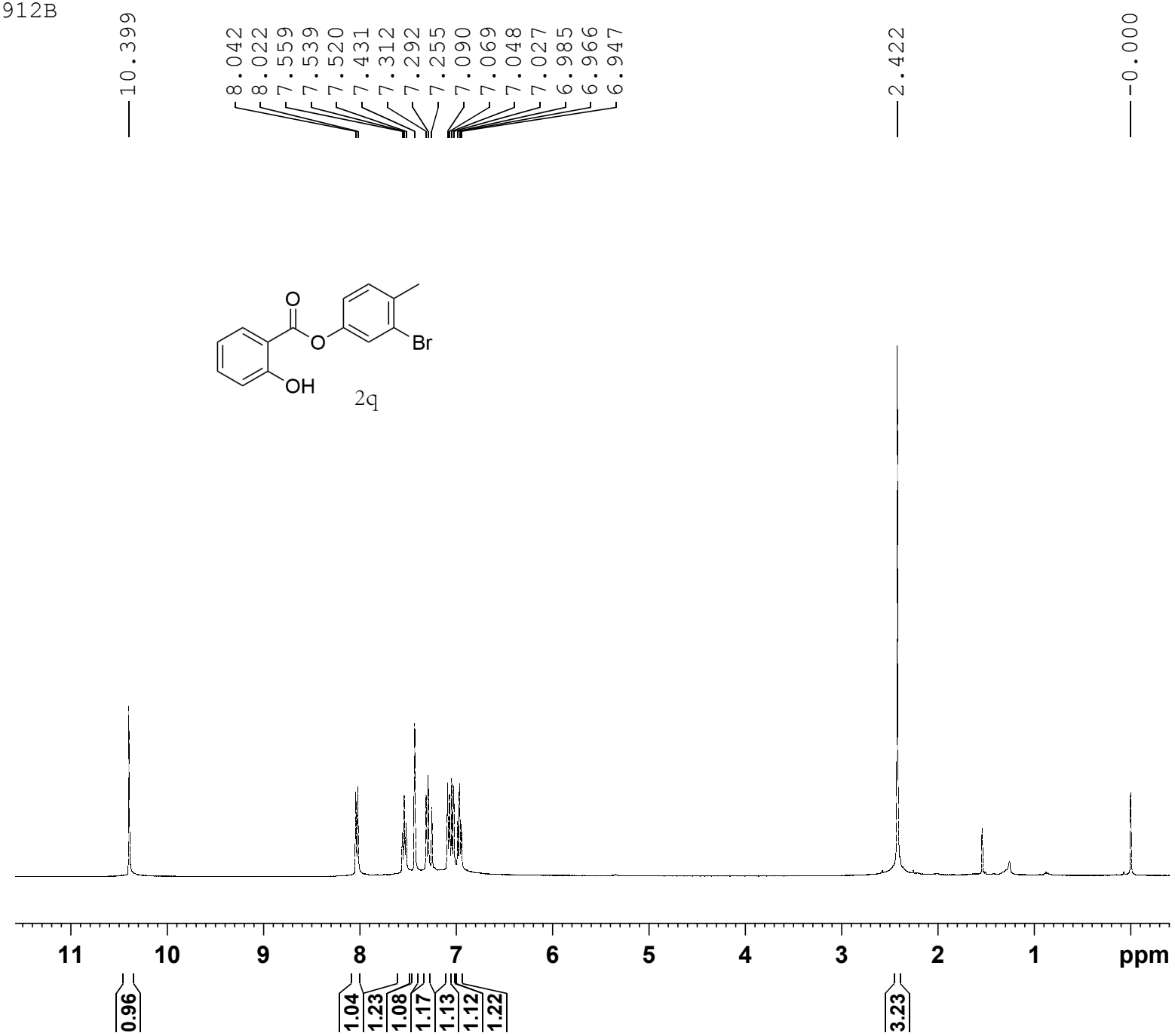
F2 - Acquisition Parameters
Date_ 20190624
Time 14.35
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 63
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 192.89
DW 16.800 usec
DE 18.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 125.7703637 MHz
NUC1 13C
P1 9.80 usec
PLW1 57.00000000 W

======== CHANNEL f2 ========
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 20.00000000 W
PLW12 0.35778001 W
PLW13 0.22898000 W

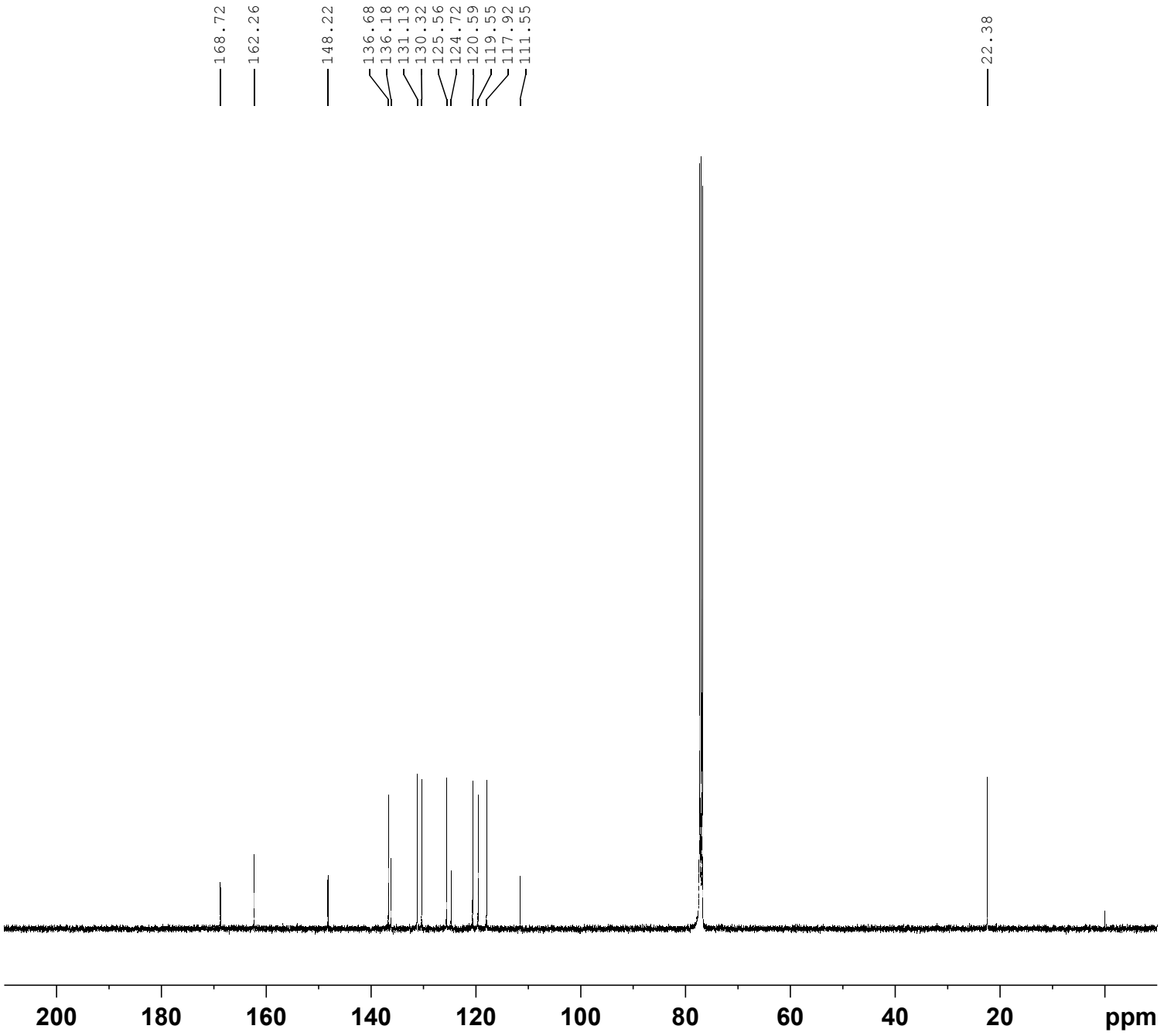
F2 - Processing parameters
SI 32768
SF 125.7577885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

912B



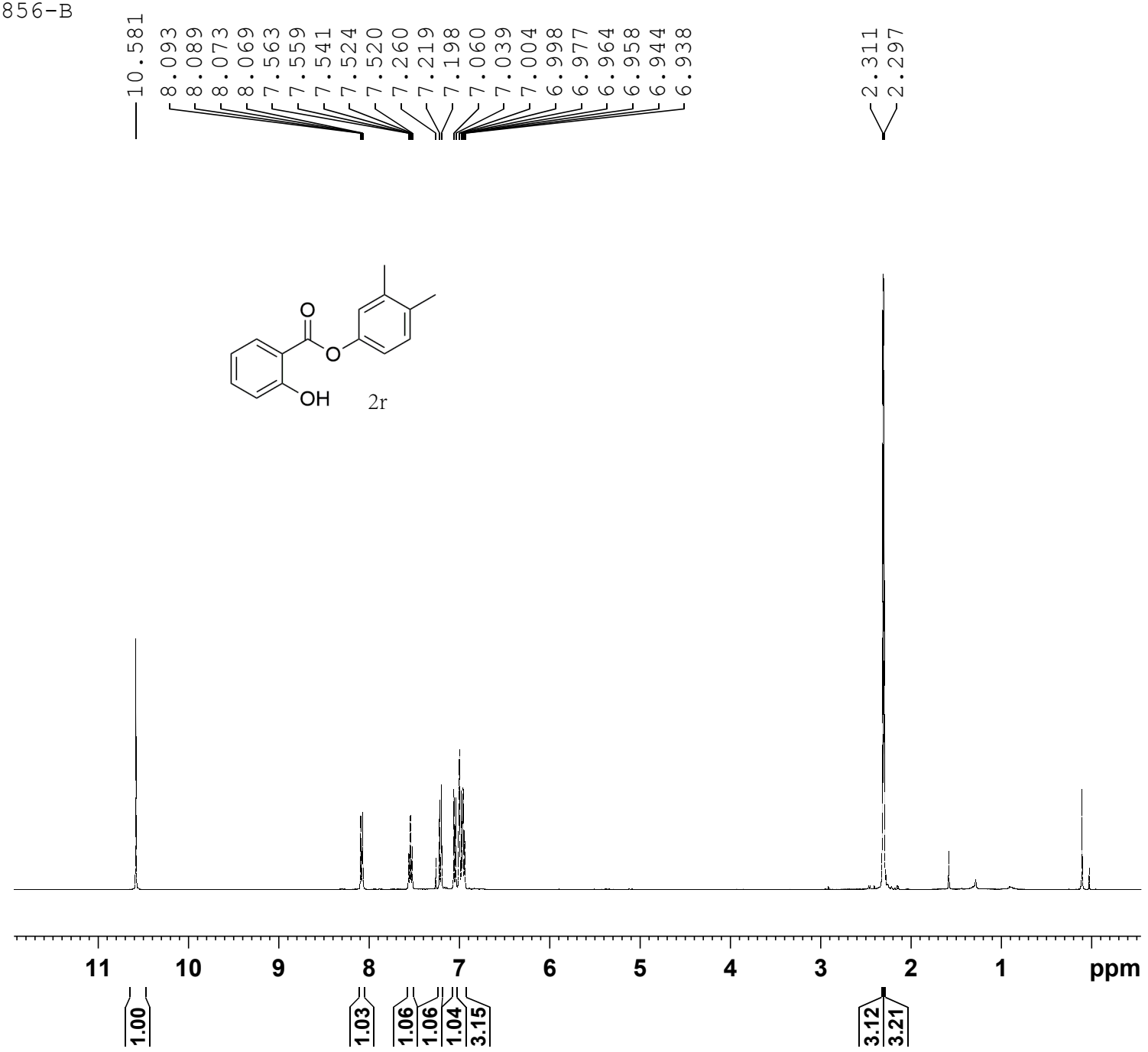

```
Current Data Parameters
NAME                  400
EXPNO                 124
PROCNO                  1

F2 - Acquisition Parameters
Date_            20190823
Time                18.18
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     16
DS                      0
SWH               8012.820 Hz
FIDRES            0.244532 Hz
AQ               2.0447233 sec
RG                  206.33
DW                  62.400 usec
DE                   6.50 usec
TE                  298.4 K
D1             2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          400.2424716 MHz
NUC1                   1H
P1                  14.30 usec
PLW1          12.00000000 W

F2 - Processing parameters
SI                  65536
SF            400.2400128 MHz
WDW                    EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```

912B




```
Current Data Parameters
NAME                  500
EXPNO                 146
PROCNO                  1

F2 - Acquisition Parameters
Date_            20190823
Time                18.42
INSTRUM             spect
PROBHD   5 mm CPPBBO BB
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   231
DS                     4
SWH            29761.904 Hz
FIDRES          0.454131 Hz
AQ             1.1010048 sec
RG                192.89
DW                16.800 usec
DE                18.00 usec
TE                298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         125.7703637 MHz
NUC1                  13C
P1                   9.80 usec
PLW1         57.00000000 W

======== CHANNEL f2 ========
SFO2         500.1320005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2               80.00 usec
PLW2         20.00000000 W
PLW12         0.35778001 W
PLW13         0.22898000 W

F2 - Processing parameters
SI                 32768
SF           125.7577885 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

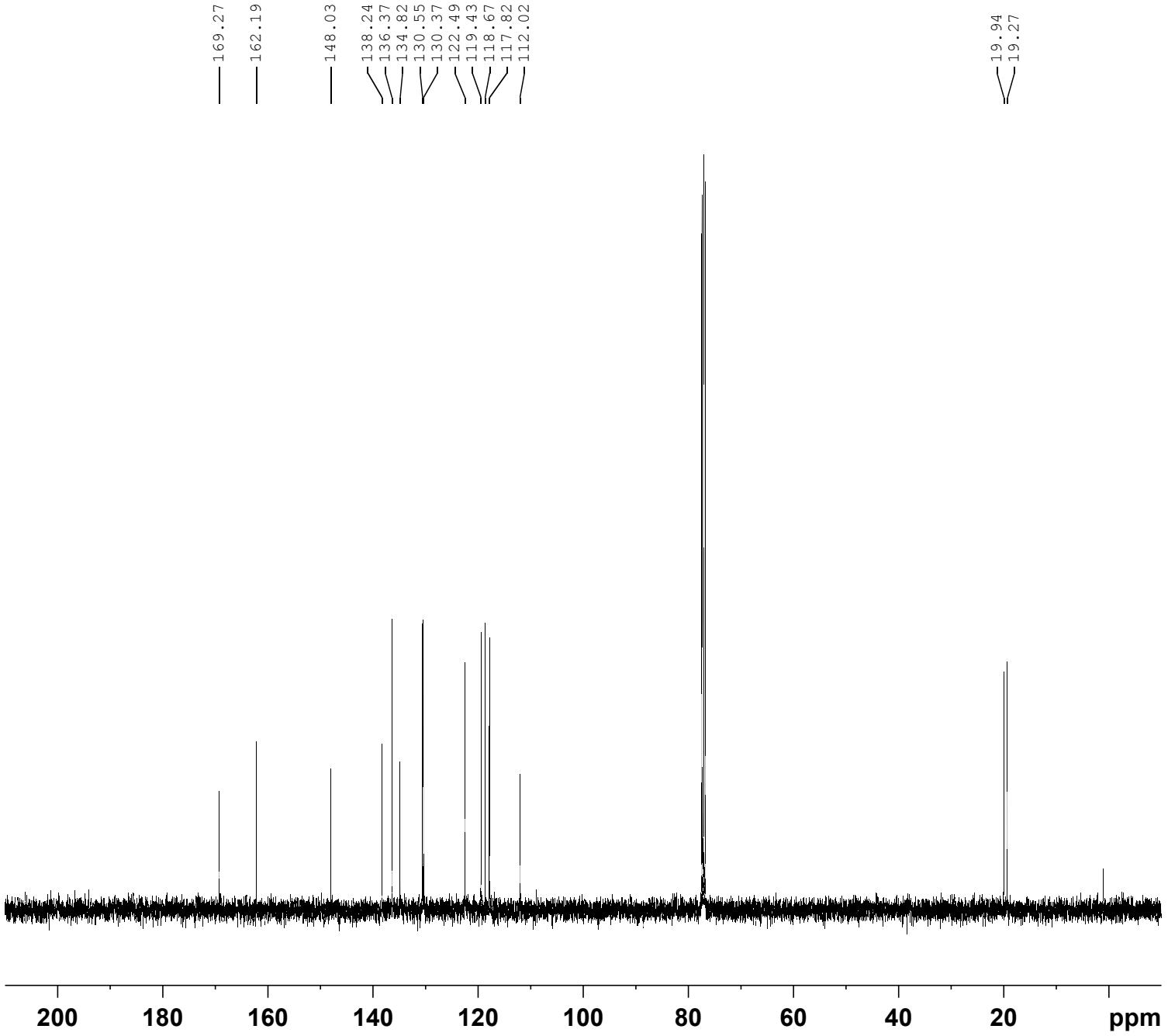
856-B




BRUKER

```
Current Data Parameters
NAME                  xzh-400
EXPNO                      69
PROCNO                      1

F2 - Acquisition Parameters
Date_               20190516
Time                   16.09
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                        16
DS                         0
SWH                 8012.820 Hz
FIDRES              0.244532 Hz
AQ                2.0447233 sec
RG                      73.9
DW                    62.400 usec
DE                     6.50 usec
TE                    298.8 K
D1                2.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1            400.2424716 MHz
NUC1                       1H
P1                    14.30 usec
PLW1            12.00000000 W

F2 - Processing parameters
SI                     65536
SF              400.2400095 MHz
WDW                       EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

856-B




Current Data Parameters
NAME xzh-400
EXPNO 70
PROCNO 1

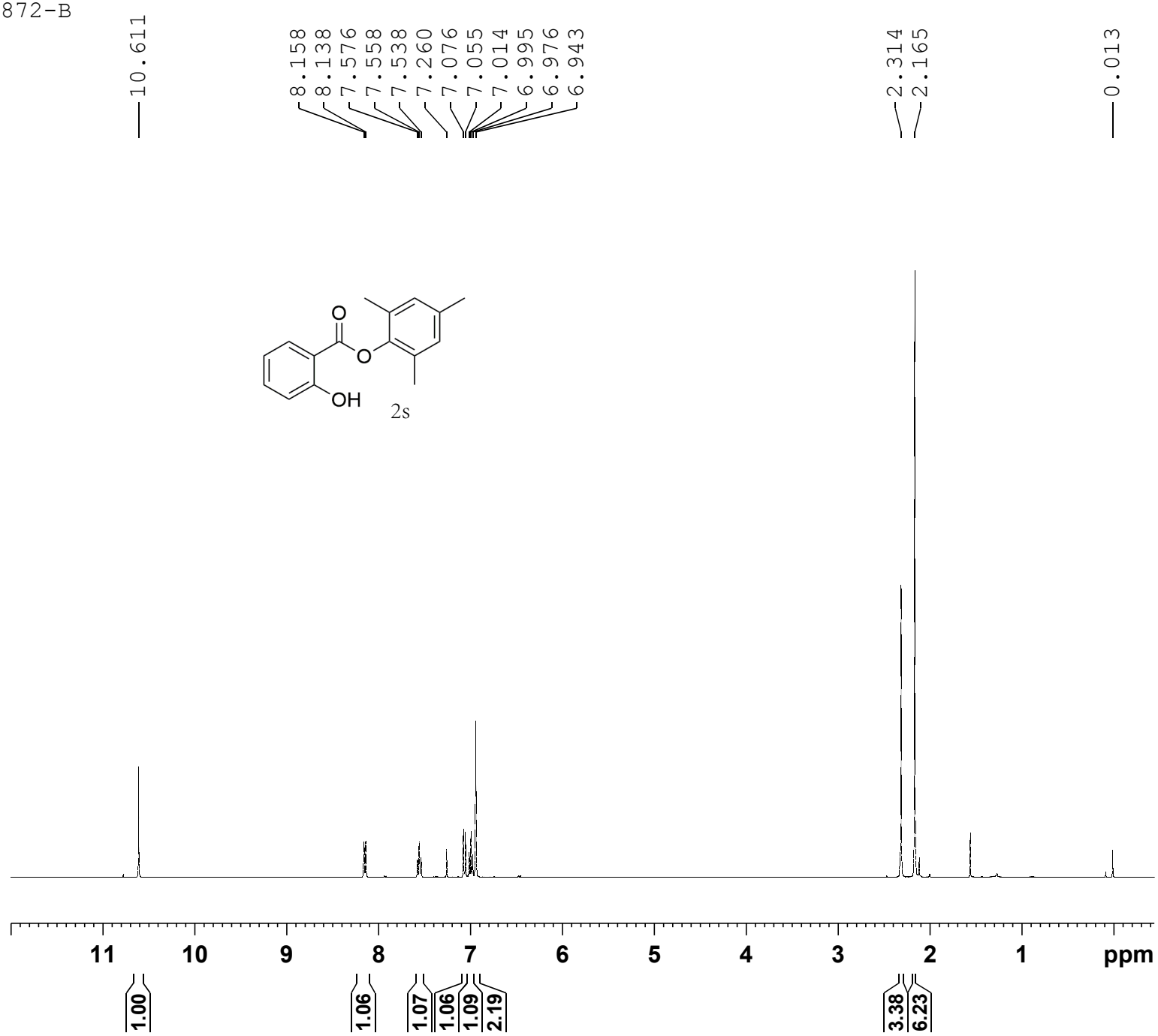
F2 - Acquisition Parameters
Date_ 20190516
Time 16.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 56
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 206.33
DW 20.800 usec
DE 6.50 usec
TE 299.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6504916 MHz
NUC1 13C
P1 10.00 usec
PLW1 54.00000000 W

======== CHANNEL f2 ========
SFO2 400.2416010 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.30294999 W
PLW13 0.24539000 W

F2 - Processing parameters
SI 32768
SF 100.6404280 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

872-B



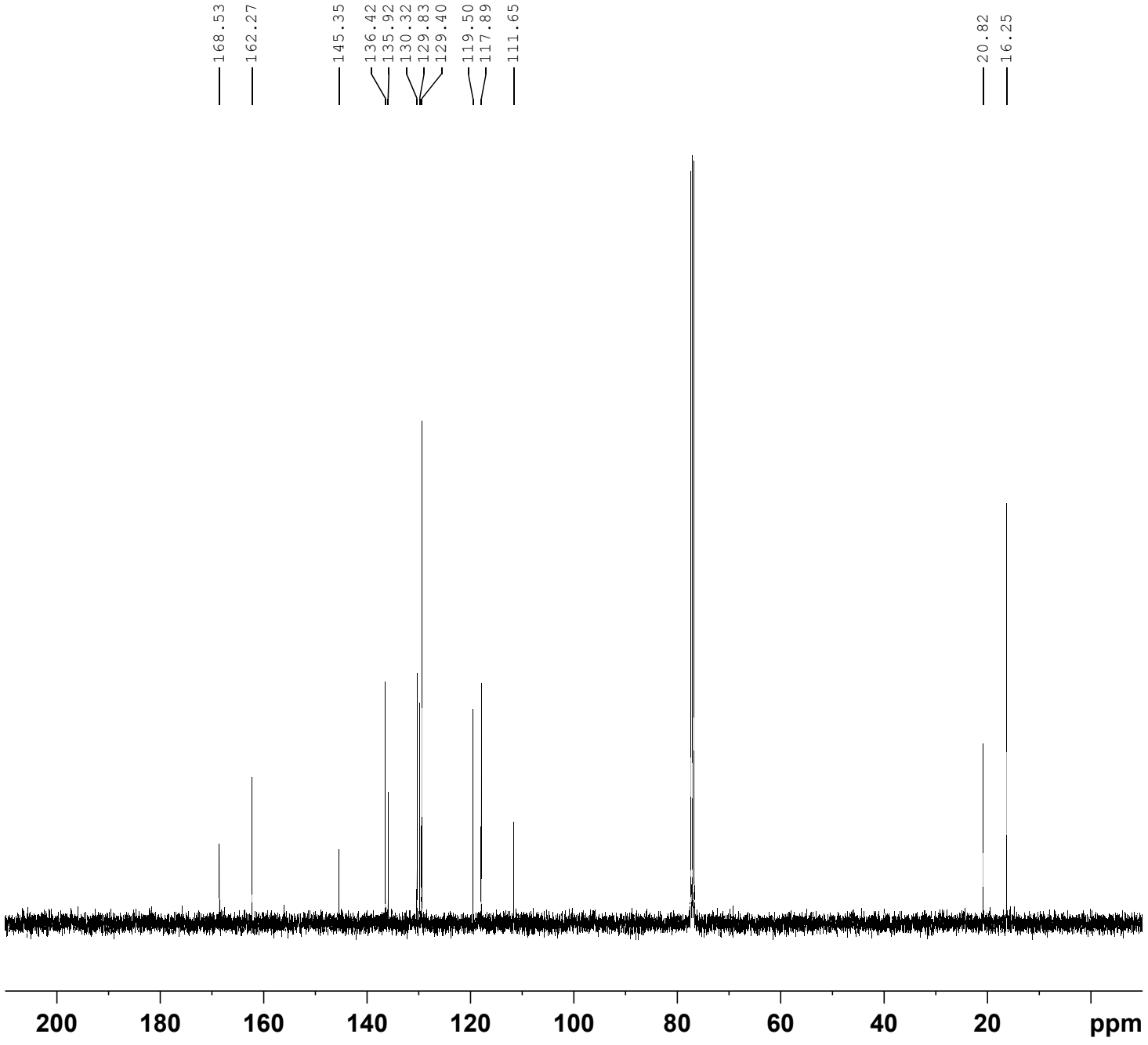

Current Data Parameters
NAME xzh-400
EXPNO 82
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190613
Time 14.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 162.77
DW 62.400 usec
DE 6.50 usec
TE 298.9 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.2424716 MHz
NUC1 1H
P1 14.30 usec
PLW1 12.00000000 W

F2 - Processing parameters
SI 65536
SF 400.2400097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

872-B




Current Data Parameters
NAME xzh-400
EXPNO 83
PROCNO 1

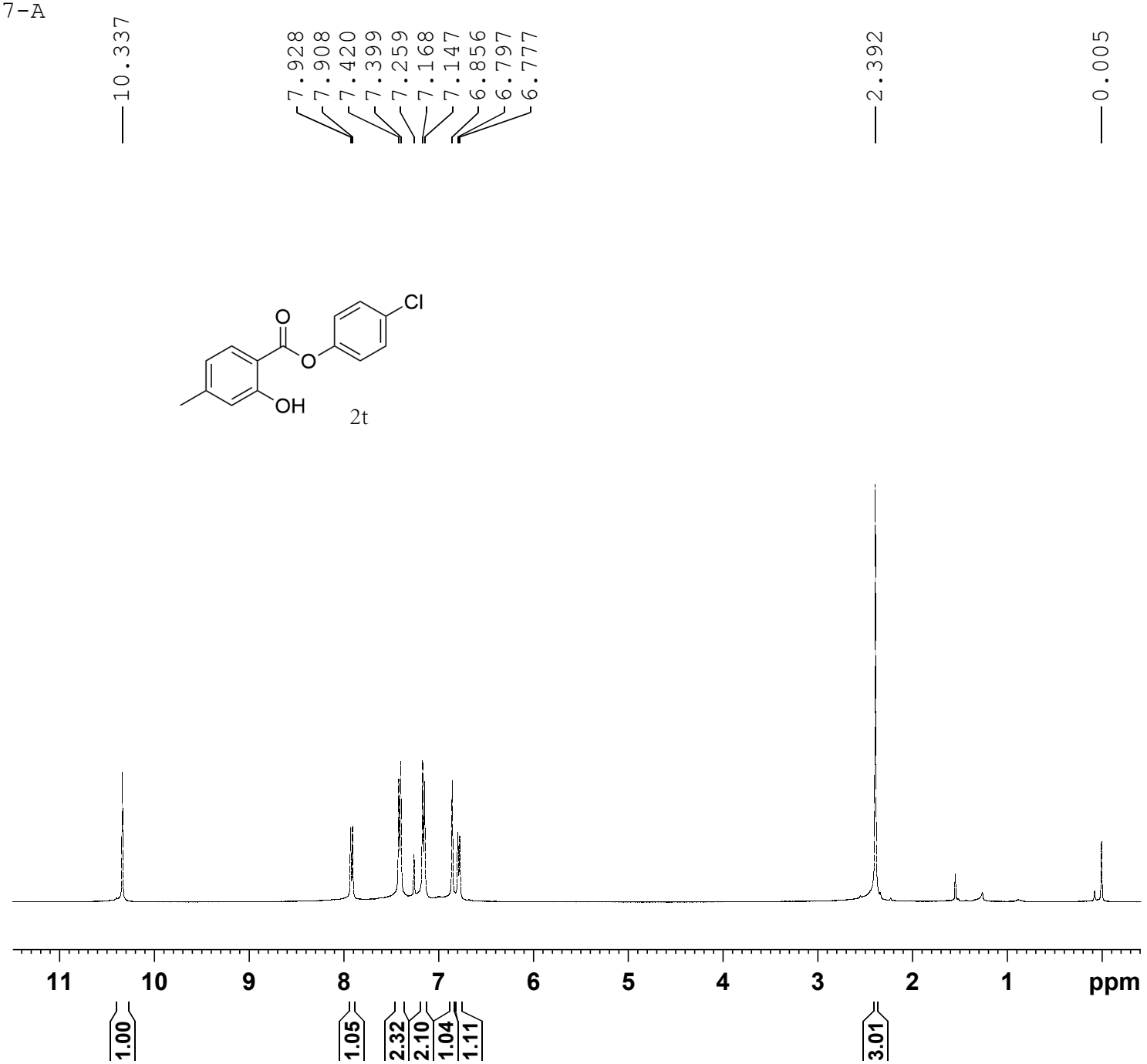
F2 - Acquisition Parameters
Date_ 20190613
Time 14.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 77
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 206.33
DW 20.800 usec
DE 6.50 usec
TE 299.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6504916 MHz
NUC1 13C
P1 10.00 usec
PLW1 54.00000000 W

======== CHANNEL f2 ========
SFO2 400.2416010 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.30294999 W
PLW13 0.24539000 W

F2 - Processing parameters
SI 32768
SF 100.6404280 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

887-A



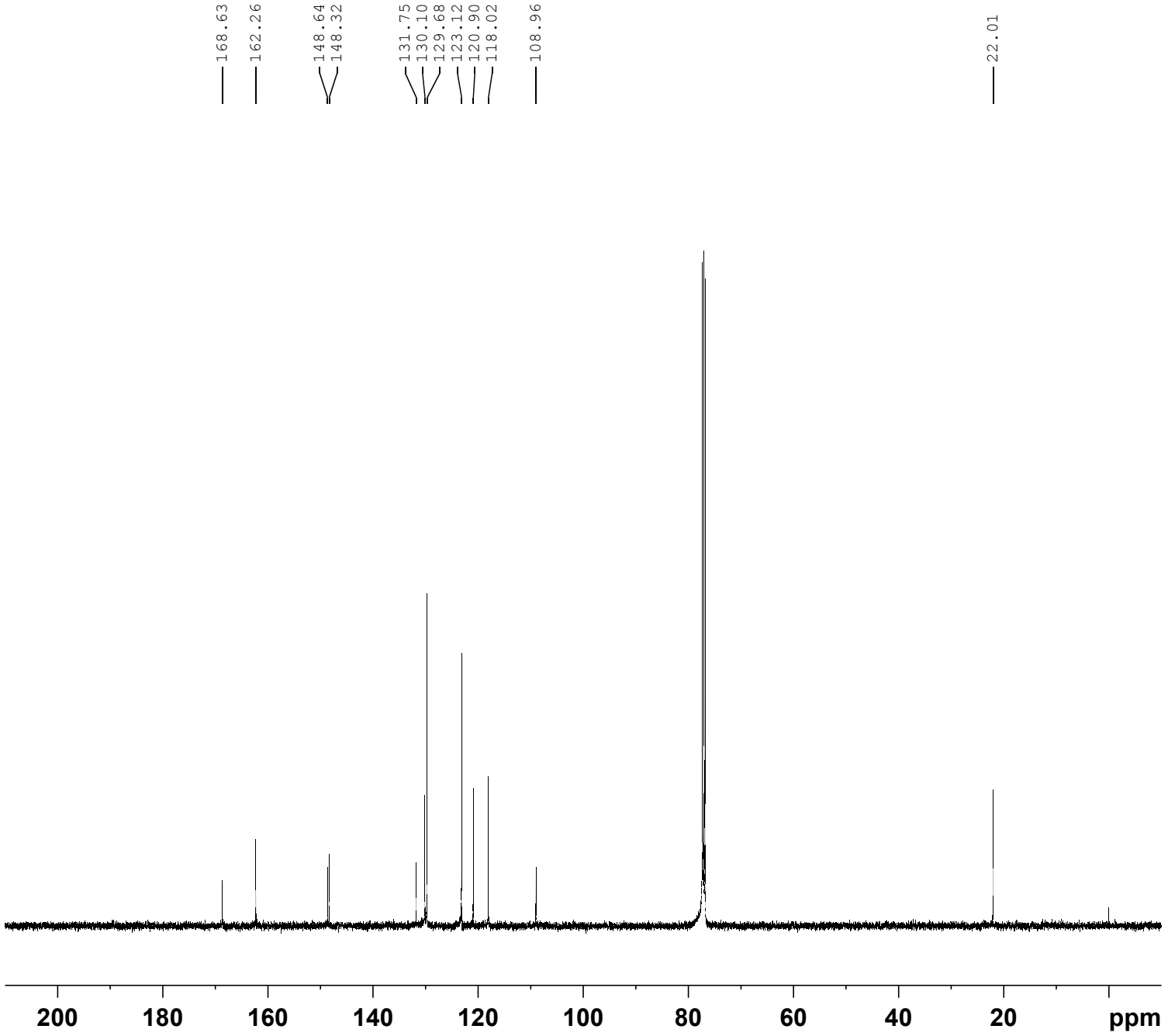

Current Data Parameters
NAME xzh-400
EXPNO 113
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190626
Time 16.44
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 206.33
DW 62.400 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.2424716 MHz
NUC1 1H
P1 14.30 usec
PLW1 12.00000000 W

F2 - Processing parameters
SI 65536
SF 400.2400101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

887-A




Current Data Parameters
NAME xzh
EXPNO 120
PROCNO 1

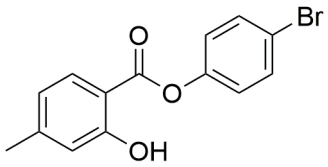
F2 - Acquisition Parameters
Date_ 20190626
Time 16.57
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 120
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 192.89
DW 16.800 usec
DE 18.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 125.7703637 MHz
NUC1 13C
P1 9.80 usec
PLW1 57.00000000 W

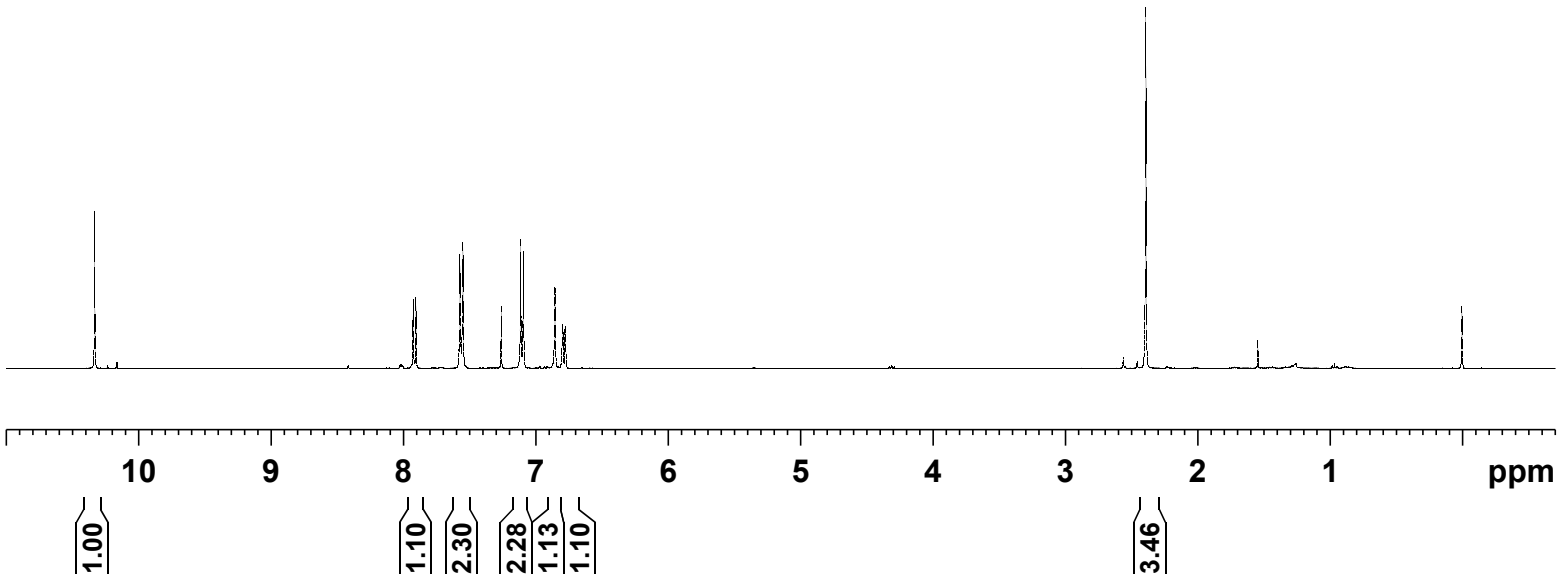
======== CHANNEL f2 ========
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 20.00000000 W
PLW12 0.35778001 W
PLW13 0.22898000 W

F2 - Processing parameters
SI 32768
SF 125.7577885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

874-A

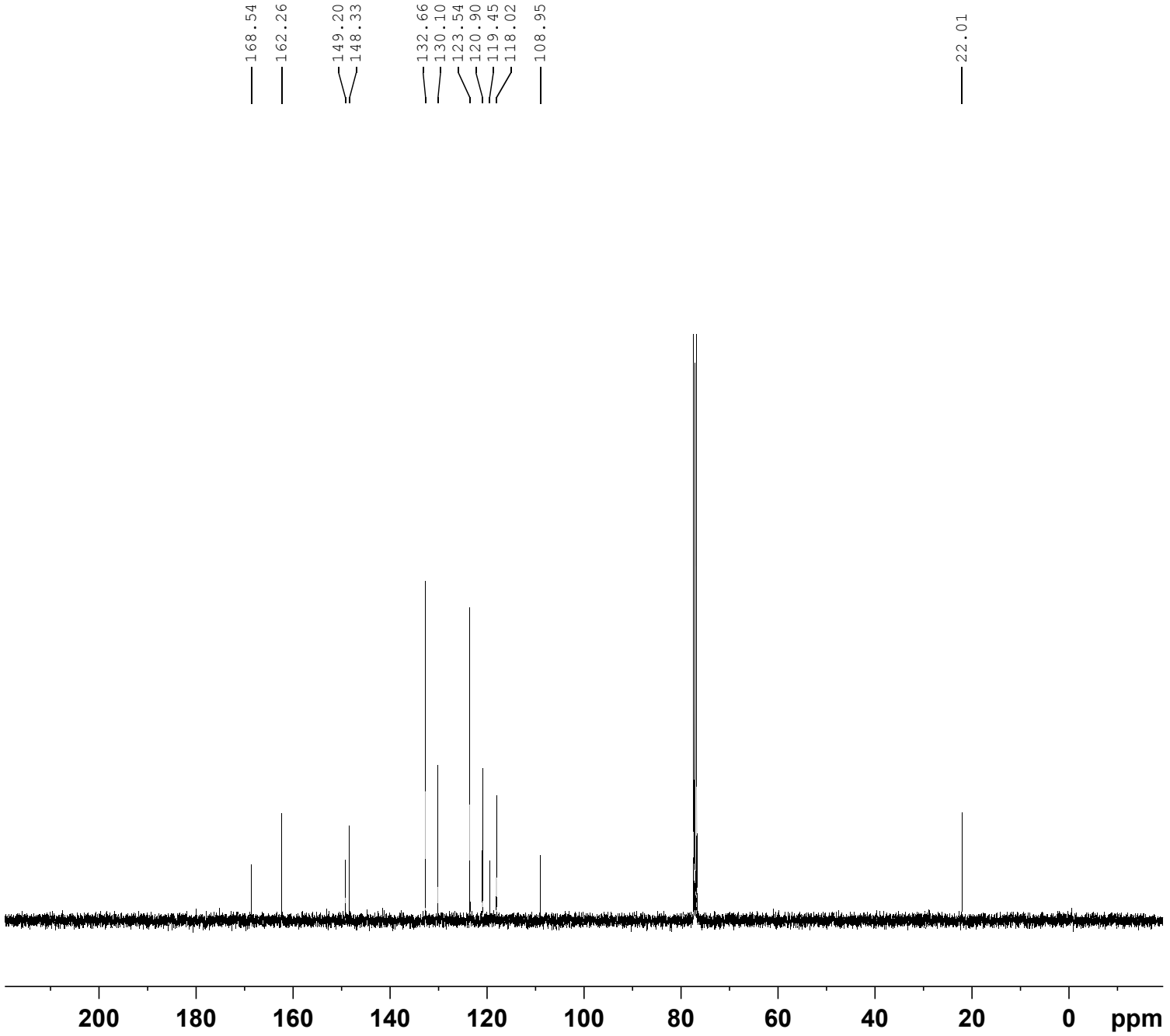




2u




```
Current Data Parameters
NAME                  review
EXPNO                     13
PROCNO                     1

F2 - Acquisition Parameters
Date_              20191213
Time                   8.54
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       16
DS                        0
SWH                8012.820 Hz
FIDRES             0.244532 Hz
AQ                 2.0447233 sec
RG                    206.33
DW                    62.400 usec
DE                     6.50 usec
TE                    298.0 K
D1              2.00000000 sec
D11       0 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           400.2424716 MHz
NUC1                     1H
P1                    14.30 usec
PLW1           12.00000000 W

======== CHANNEL f2 ========
SFO2           400.2424716 MHz
NUC2                    off
CPDPRG[2
PCPD2     0 usec
PLW2      0 W
PLW12     0 W
PLW13     0 W

F2 - Processing parameters
SI                     65536
SF             400.2400111 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

874-A




Current Data Parameters
NAME xzh-400
EXPNO 89
PROCNO 1

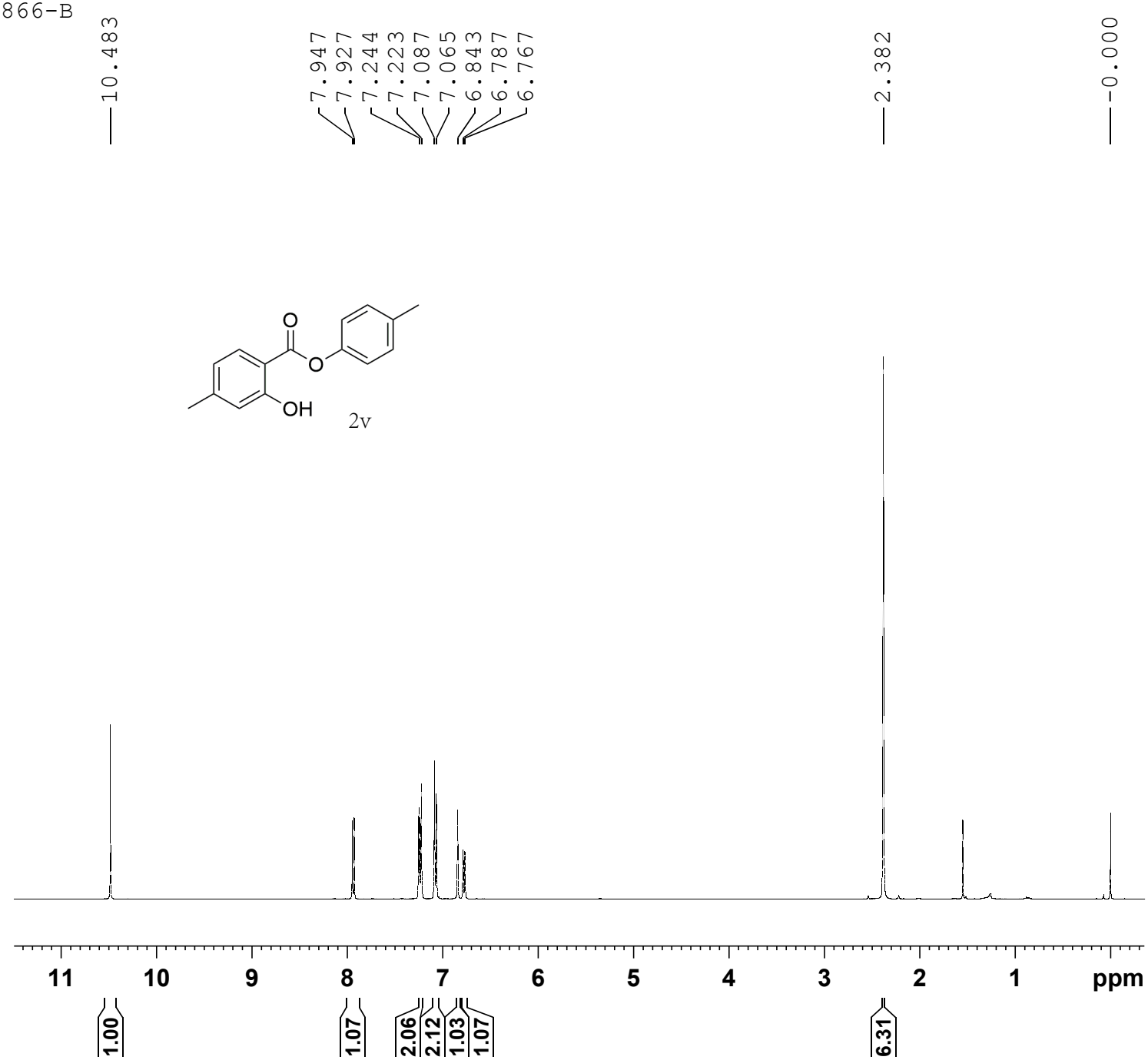
F2 - Acquisition Parameters
Date_ 20190617
Time 8.31
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 102
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 206.33
DW 20.800 usec
DE 6.50 usec
TE 298.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6504916 MHz
NUC1 13C
P1 10.00 usec
PLW1 54.00000000 W

======== CHANNEL f2 ========
SFO2 400.2416010 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.30294999 W
PLW13 0.24539000 W

F2 - Processing parameters
SI 32768
SF 100.6404280 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

866-B



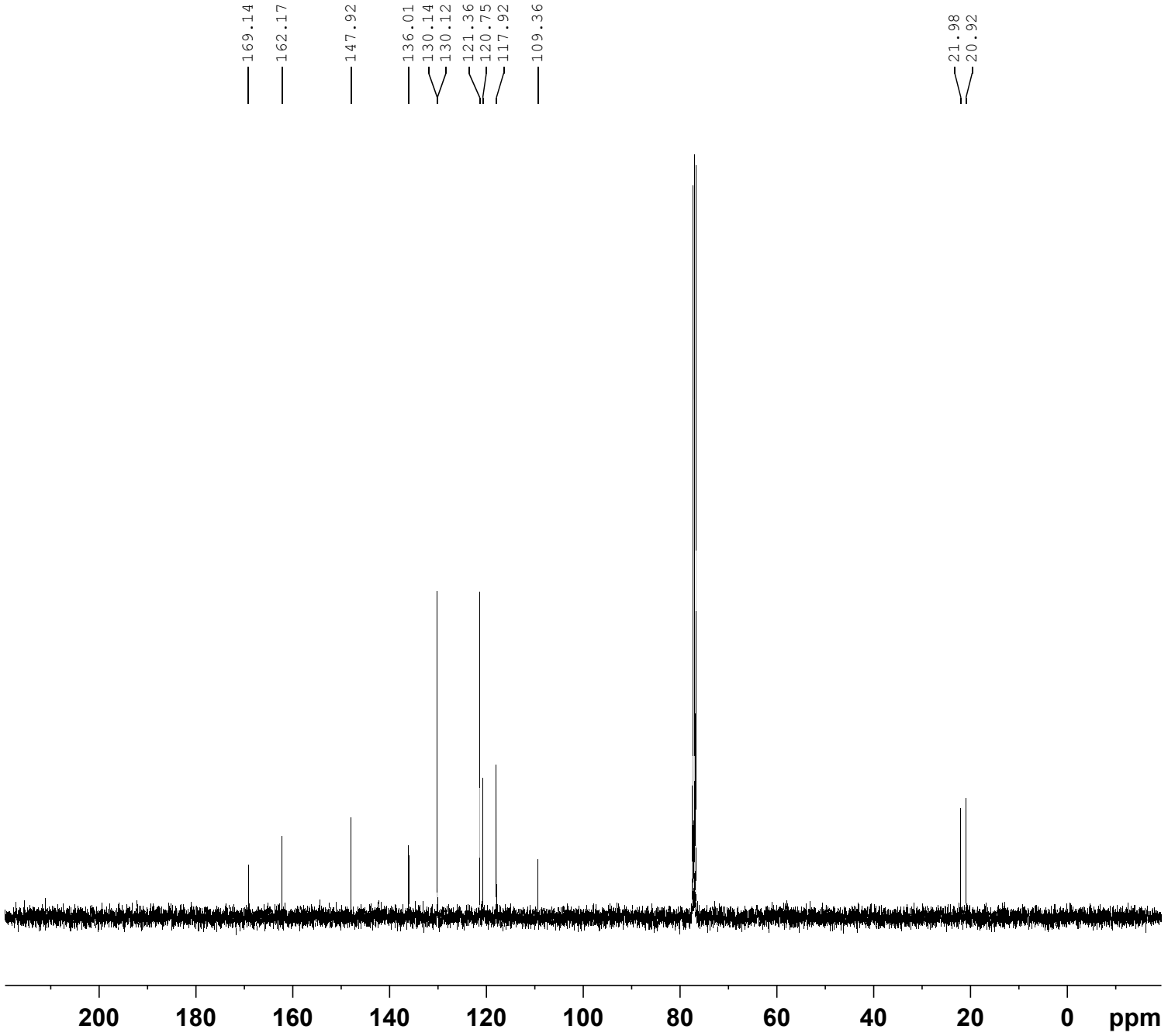

Current Data Parameters
NAME xzh-400
EXPNO 71
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190605
Time 14.38
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 206.33
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.2424716 MHz
NUC1 1H
P1 14.30 usec
PLW1 12.00000000 W

F2 - Processing parameters
SI 65536
SF 400.2400120 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

866-B




Current Data Parameters
NAME xzh-400
EXPNO 72
PROCNO 1

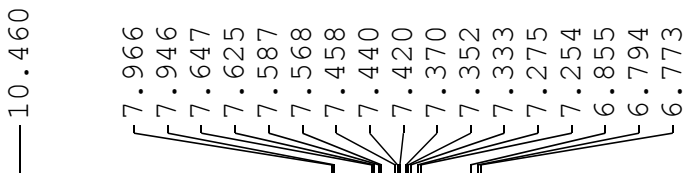
F2 - Acquisition Parameters
Date_ 20190605
Time 14.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 67
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 206.33
DW 20.800 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

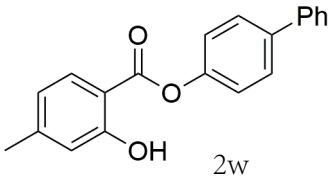
======== CHANNEL f1 ========
SFO1 100.6504916 MHz
NUC1 13C
P1 10.00 usec
PLW1 54.00000000 W

======== CHANNEL f2 ========
SFO2 400.2416010 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.30294999 W
PLW13 0.24539000 W

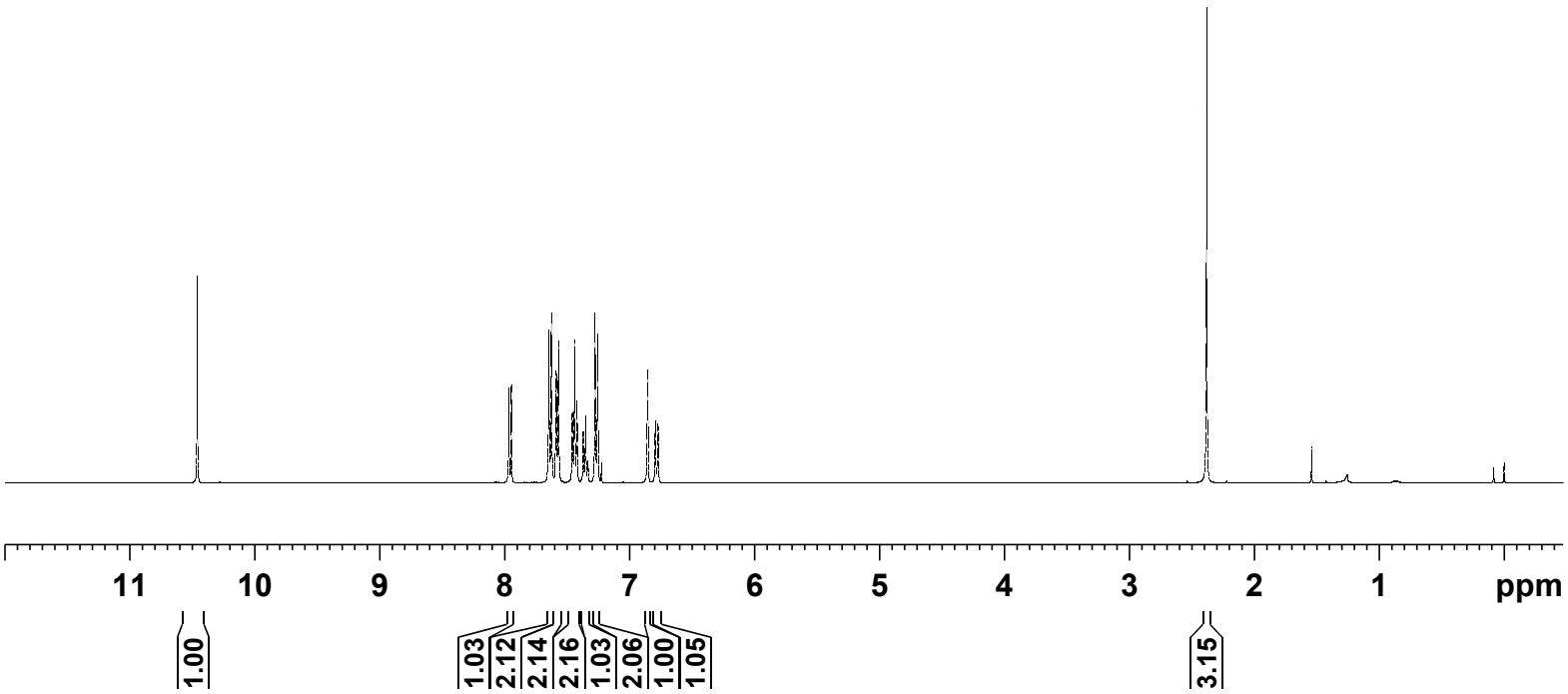
F2 - Processing parameters
SI 32768
SF 100.6404280 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

914A




2w



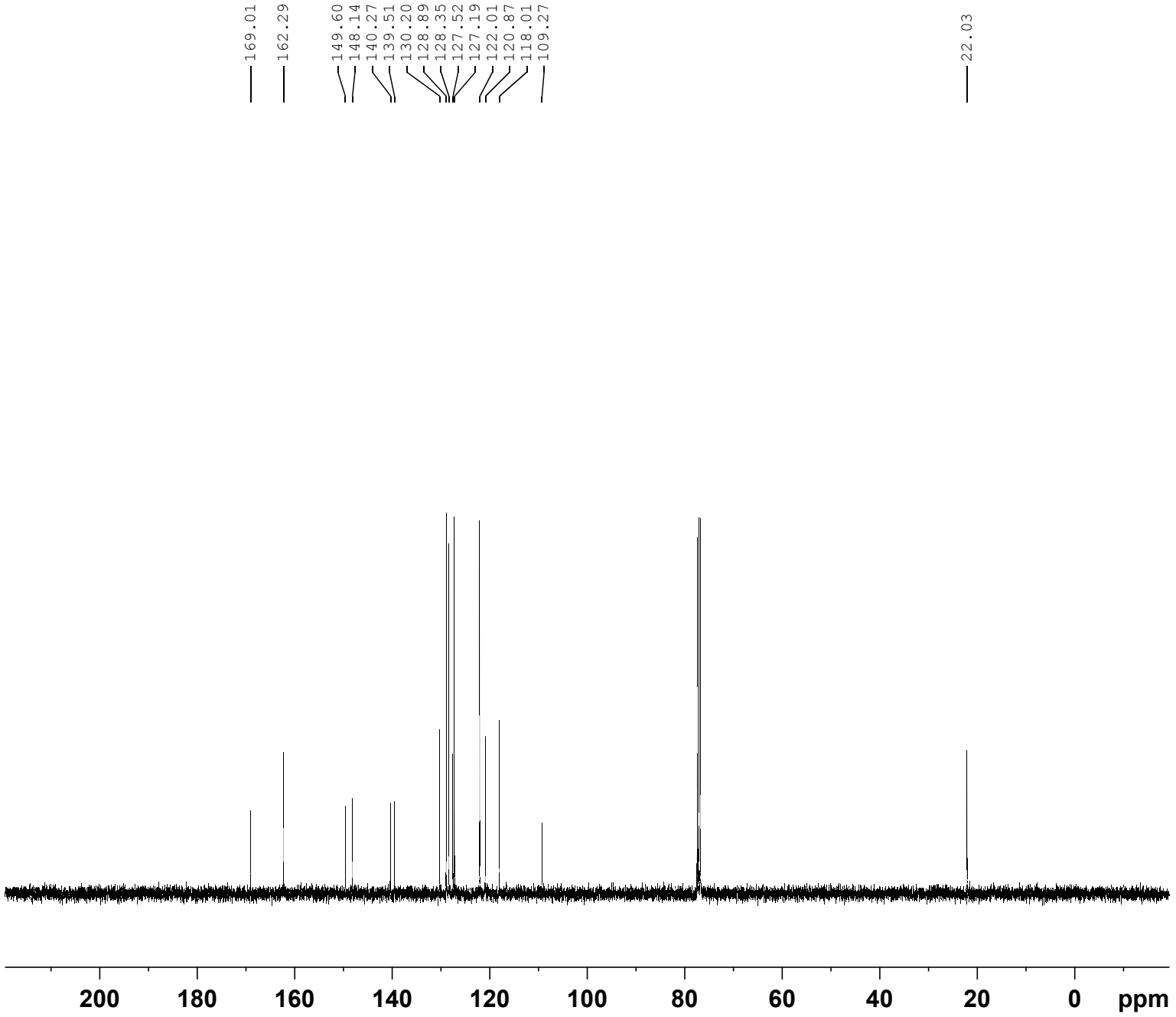

Current Data Parameters
NAME 400
EXPNO 133
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190824
Time 16.38
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 102.73
DW 62.400 usec
DE 6.50 usec
TE 298.6 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.2424716 MHz
NUC1 1H
P1 14.30 usec
PLW1 12.00000000 W

F2 - Processing parameters
SI 65536
SF 400.2400238 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

914A




Current Data Parameters
NAME 400
EXPNO 132
PROCNO 1

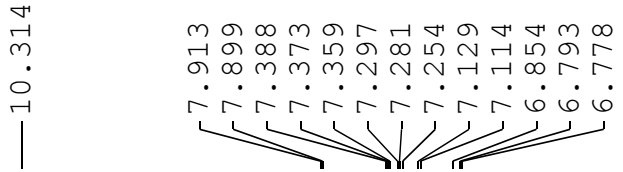
F2 - Acquisition Parameters
Date_ 20190824
Time 16.34
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 50
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 206.33
DW 20.800 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

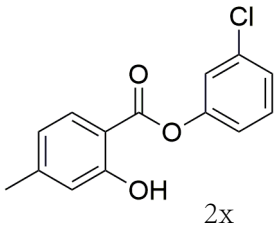
======== CHANNEL f1 ========
SFO1 100.6504916 MHz
NUC1 13C
P1 10.00 usec
PLW1 54.00000000 W

======== CHANNEL f2 ========
SFO2 400.2416010 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.30294999 W
PLW13 0.24539000 W

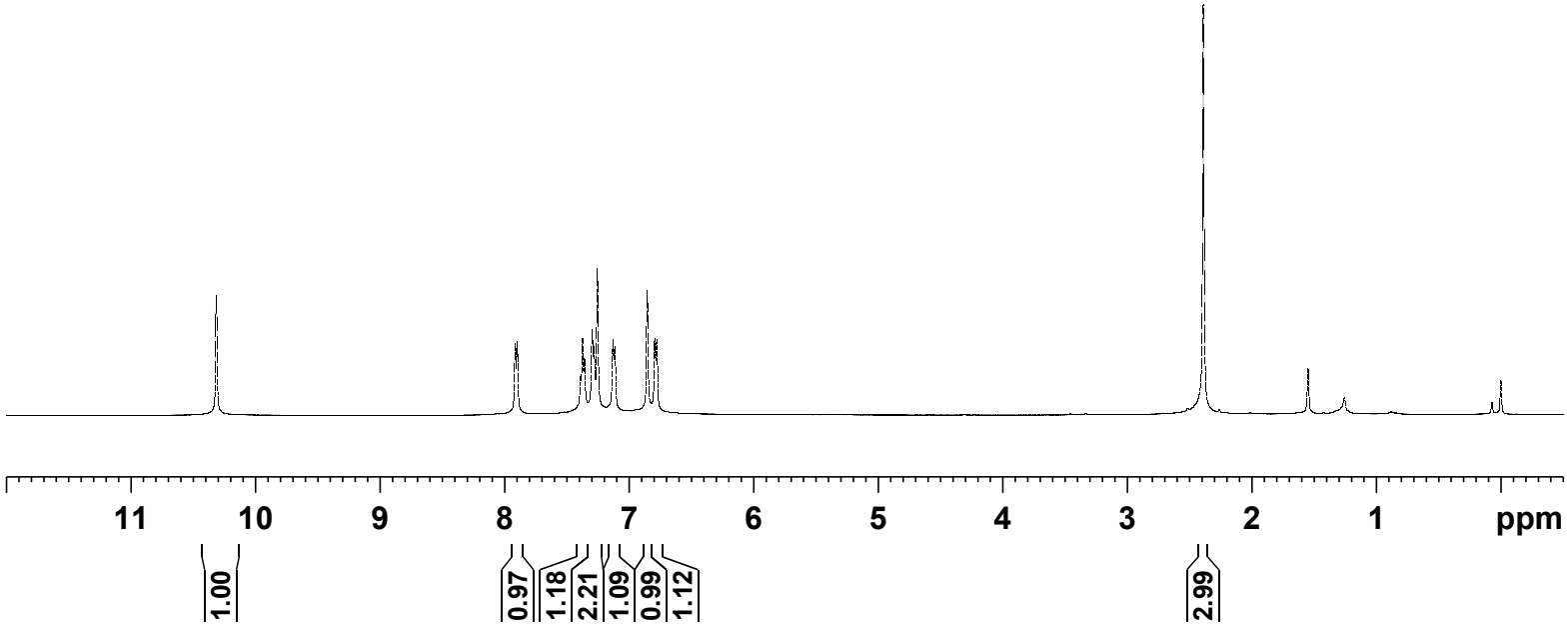
F2 - Processing parameters
SI 32768
SF 100.6404280 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

916B



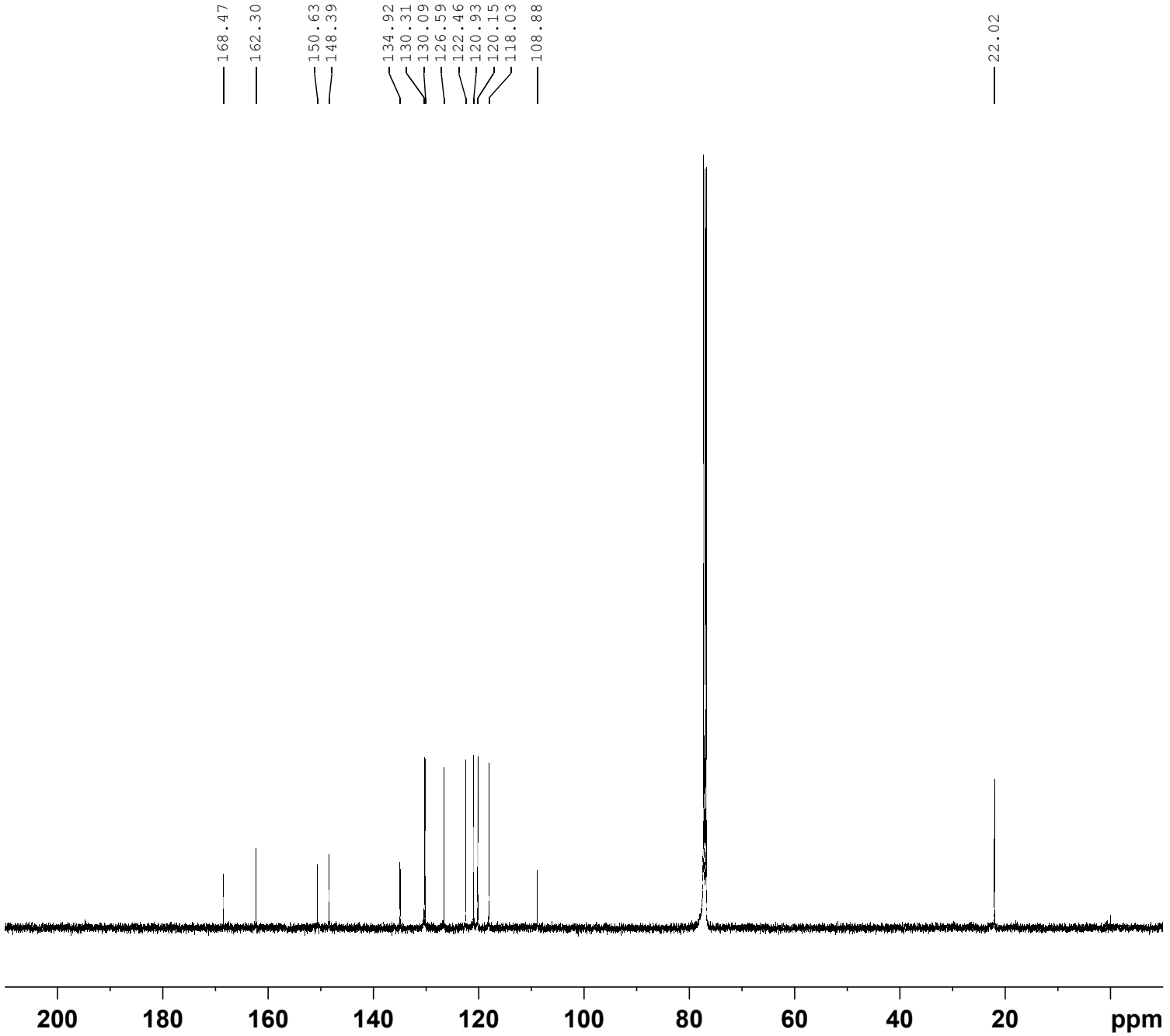




2x




```
Current Data Parameters
NAME                  500
EXPNO                 158
PROCNO                  1

F2 - Acquisition Parameters
Date_            20190829
Time                19.28
INSTRUM             spect
PROBHD   5 mm CPPBBO BB
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH             10000.000 Hz
FIDRES              0.152588 Hz
AQ              3.2767999 sec
RG                  31.72
DW                  50.000 usec
DE                   6.50 usec
TE                  298.2 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          500.1330885 MHz
NUC1                    1H
P1                  11.50 usec
PLW1          20.00000000 W

F2 - Processing parameters
SI                  65536
SF            500.1300163 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

916B




Current Data Parameters
NAME 500
EXPNO 159
PROCNO 1

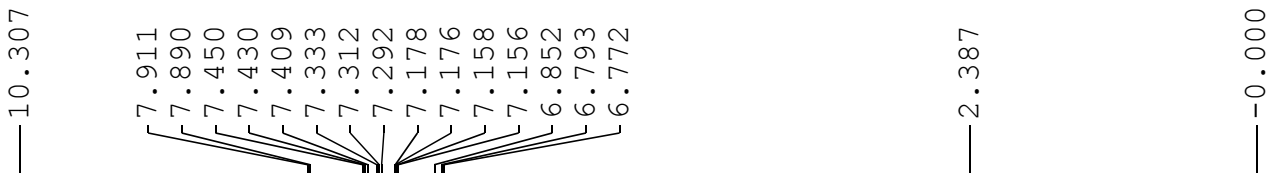
F2 - Acquisition Parameters
Date_ 20190829
Time 19.32
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 170
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 192.89
DW 16.800 usec
DE 18.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

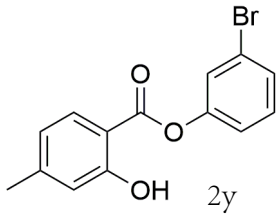
======== CHANNEL f1 ========
SFO1 125.7703637 MHz
NUC1 13C
P1 9.80 usec
PLW1 57.00000000 W

======== CHANNEL f2 ========
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 20.00000000 W
PLW12 0.35778001 W
PLW13 0.22898000 W

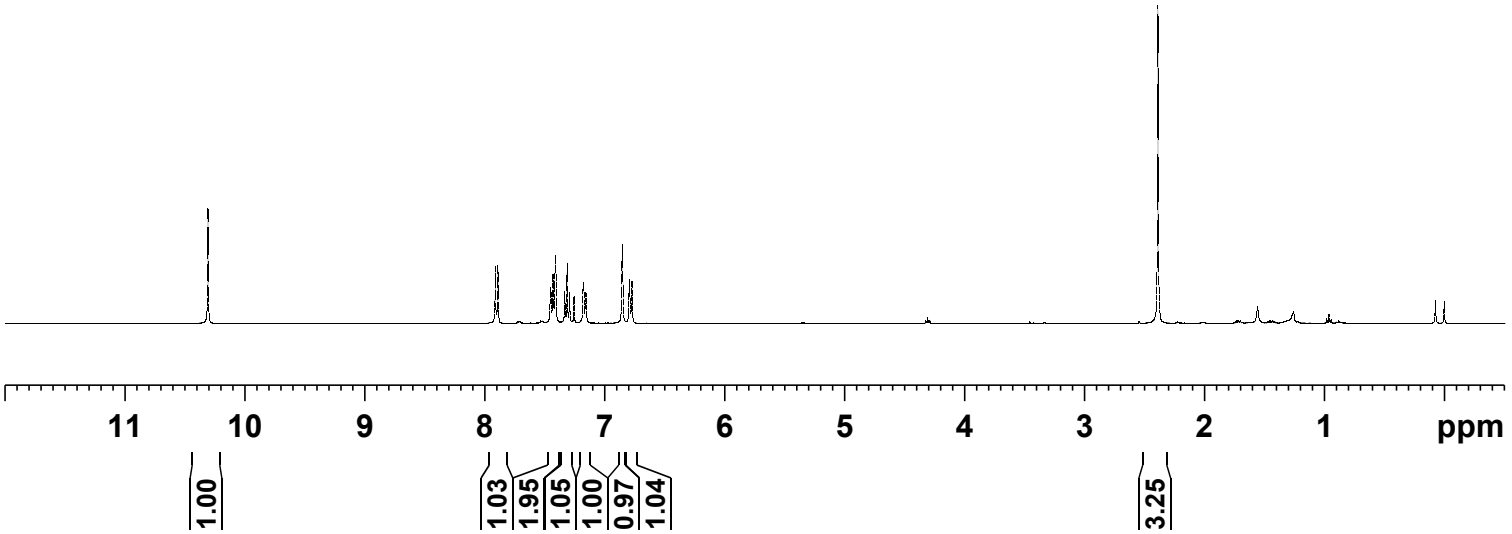
F2 - Processing parameters
SI 32768
SF 125.7577885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

919



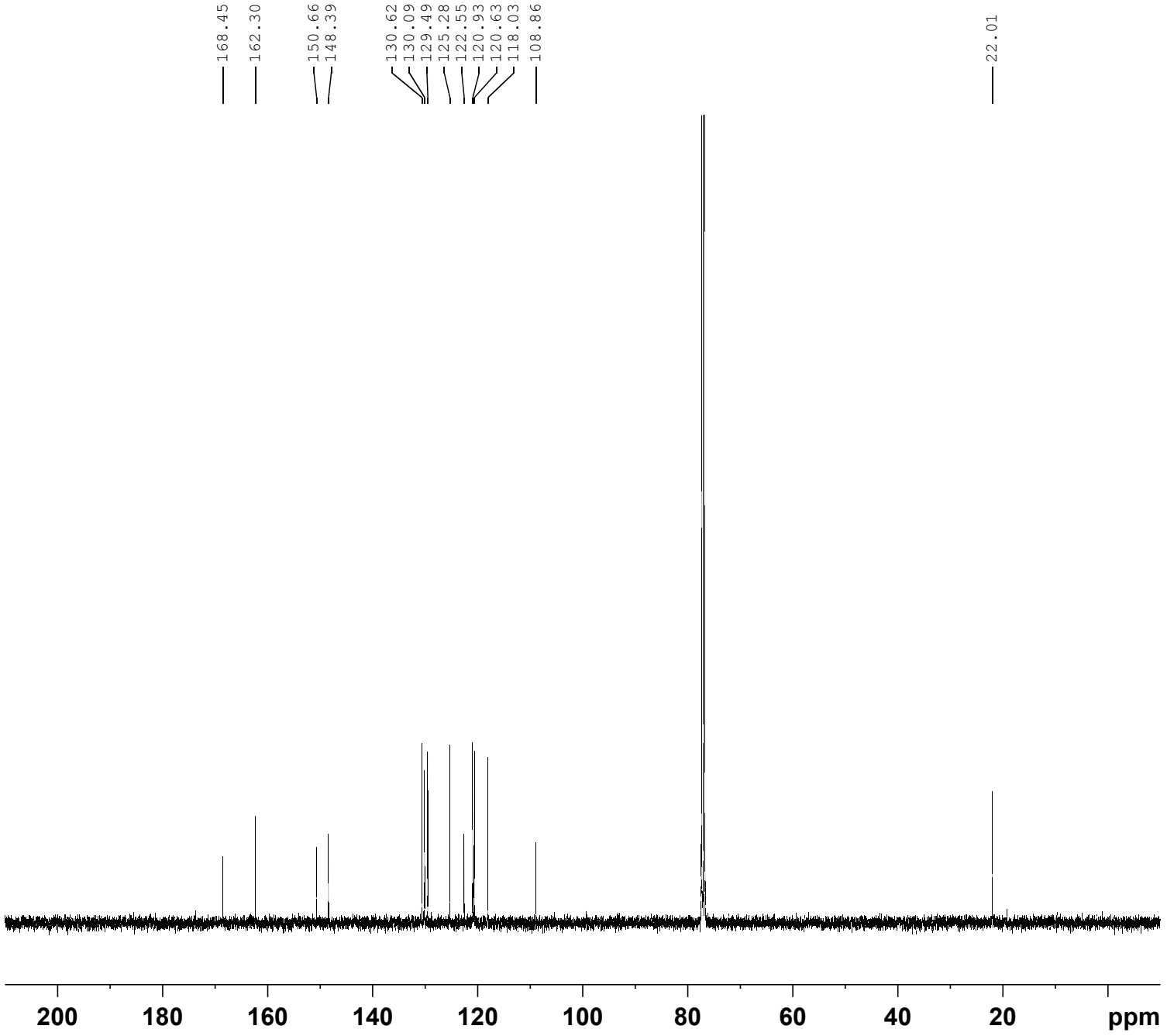




2y



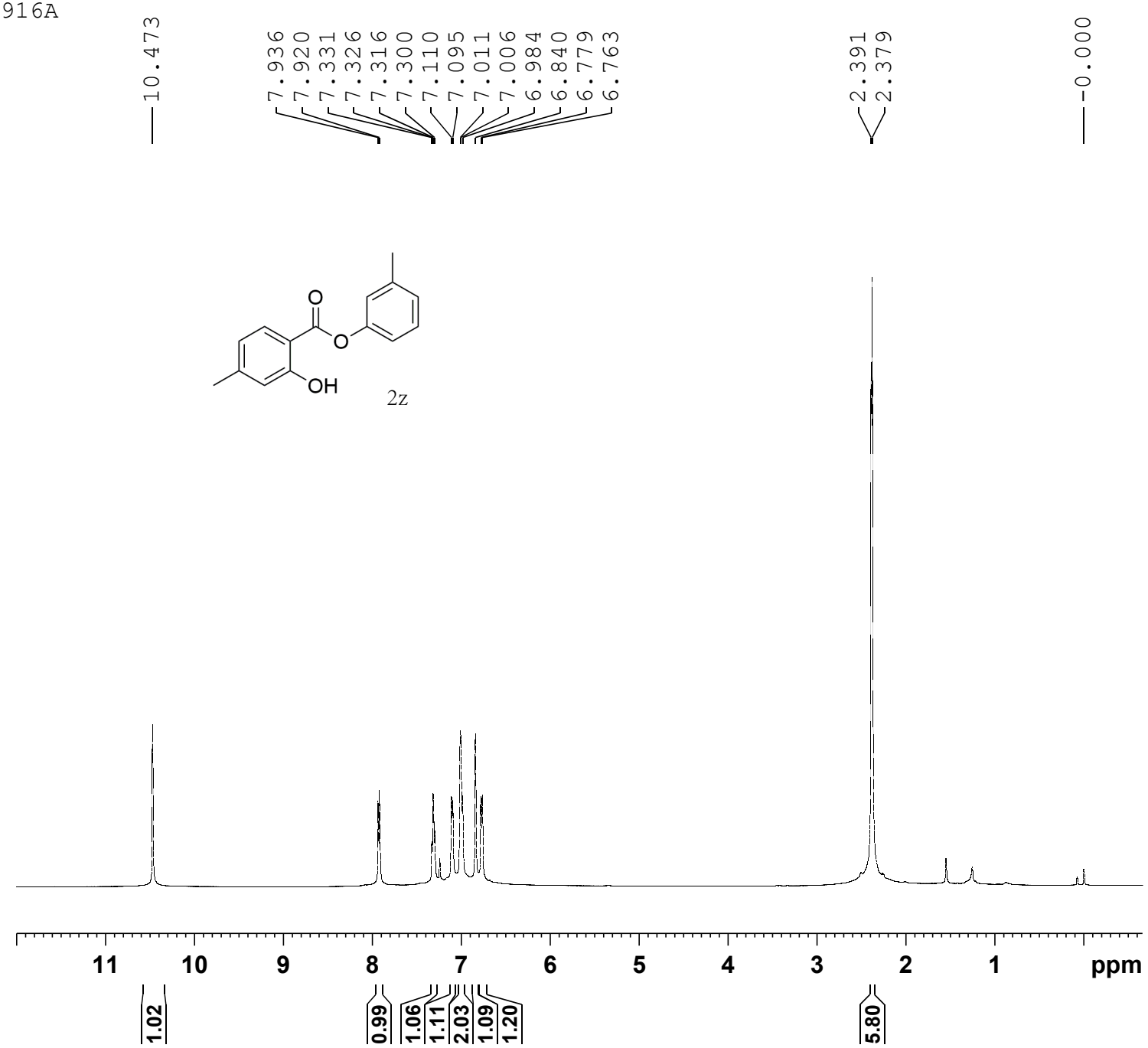

```
Current Data Parameters
NAME                  400
EXPNO                 136
PROCNO                  1

F2 - Acquisition Parameters
Date_            20190830
Time                16.46
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     16
DS                      0
SWH              8012.820 Hz
FIDRES           0.244532 Hz
AQ               2.0447233 sec
RG                 206.33
DW                 62.400 usec
DE                  6.50 usec
TE                 299.5 K
D1            2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          400.2424716 MHz
NUC1                   1H
P1                  14.30 usec
PLW1          12.00000000 W

F2 - Processing parameters
SI                  65536
SF            400.2400119 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

919




```
Current Data Parameters
NAME                   400
EXPNO                  137
PROCNO                   1

F2 - Acquisition Parameters
Date_           20190830
Time                17.04
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDC13
NS                   300
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                206.33
DW                20.800 usec
DE                 6.50 usec
TE                300.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6504916 MHz
NUC1                 13C
P1                10.00 usec
PLW1         54.00000000 W

======== CHANNEL f2 ========
SFO2         400.2416010 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         12.00000000 W
PLW12         0.30294999 W
PLW13         0.24539000 W

F2 - Processing parameters
SI                 32768
SF           100.6404280 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

916A



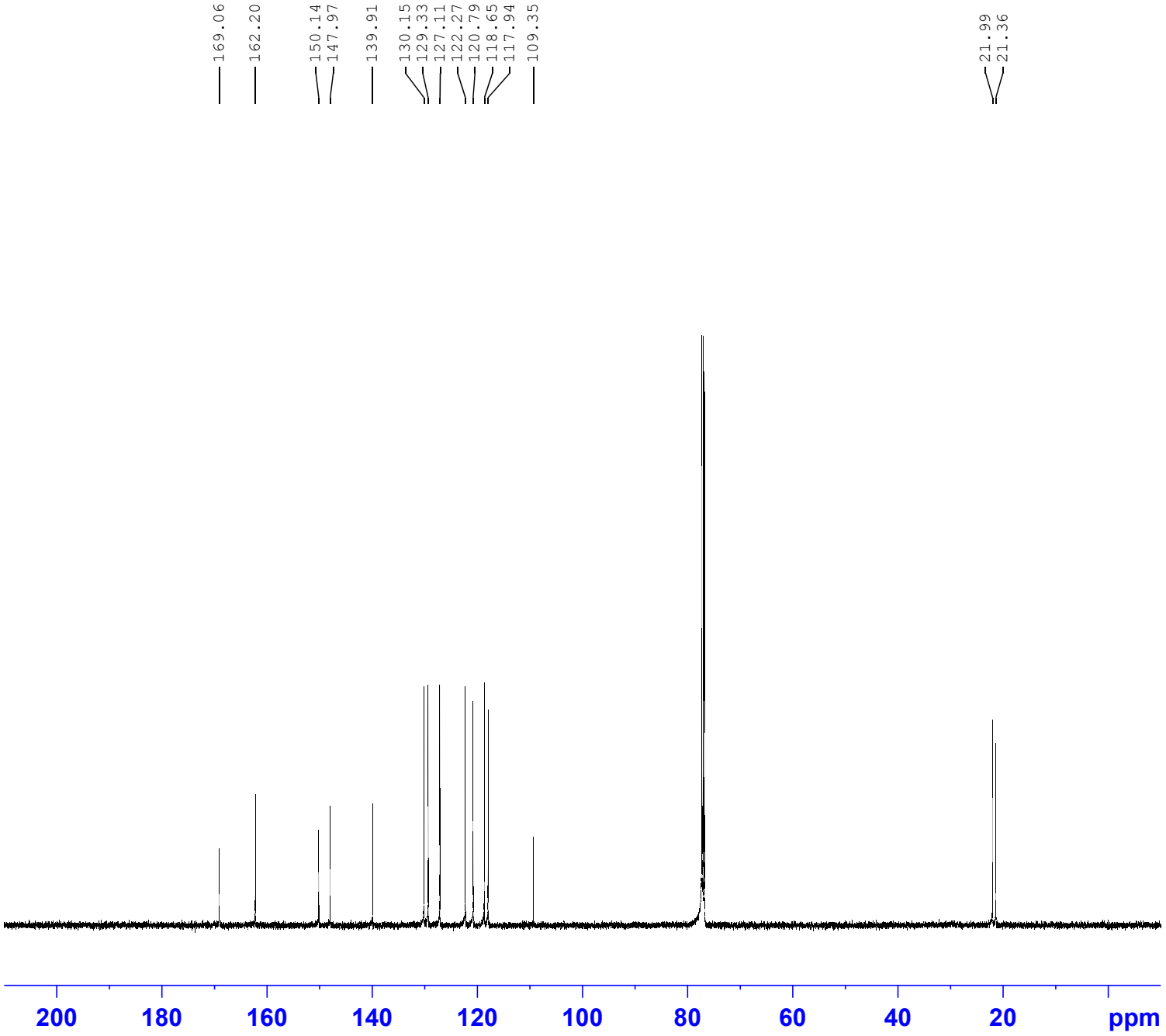

Current Data Parameters
NAME 500
EXPNO 152
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190829
Time 14.46
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 31.72
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 500.1330885 MHz
NUC1 1H
P1 11.50 usec
PLW1 20.00000000 W

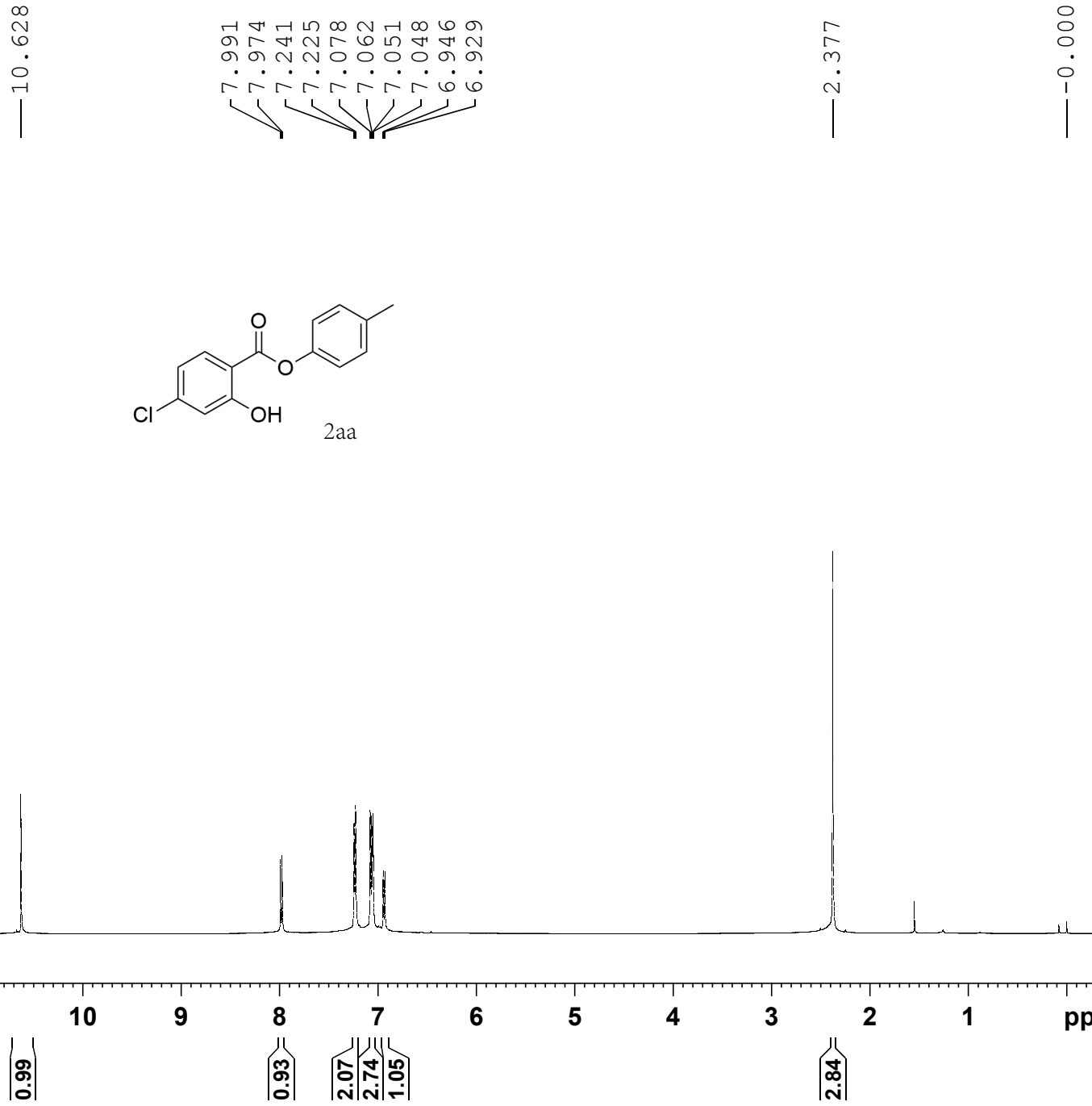
F2 - Processing parameters
SI 65536
SF 500.1300225 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

916A




```
Current Data Parameters
NAME                  500
EXPNO                 153
PROCNO                  1

F2 - Acquisition Parameters
Date_            20190829
Time                14.52
INSTRUM             spect
PROBHD   5 mm CPPBBO BB
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   150
DS                     4
SWH            29761.904 Hz
FIDRES          0.454131 Hz
AQ             1.1010048 sec
RG                192.89
DW                16.800 usec
DE                18.00 usec
TE                298.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         125.7703637 MHz
NUC1                 13C
P1                  9.80 usec
PLW1         57.00000000 W

======== CHANNEL f2 ========
SFO2         500.1320005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2               80.00 usec
PLW2         20.00000000 W
PLW12         0.35778001 W
PLW13         0.22898000 W

F2 - Processing parameters
SI                  32768
SF           125.7577885 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

913B



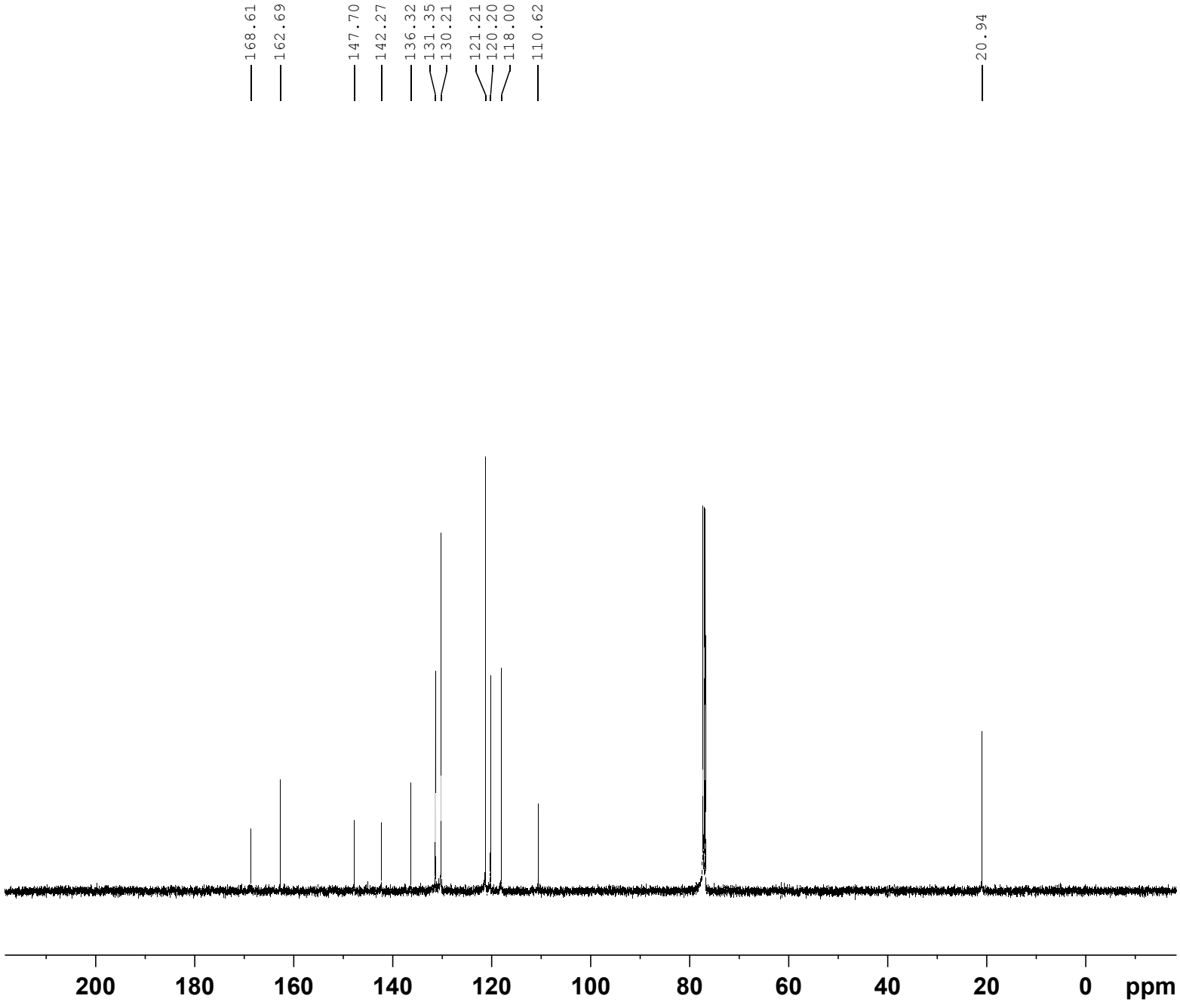

Current Data Parameters
NAME 500
EXPNO 143
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190823
Time 18.31
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 31.72
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 500.1330885 MHz
NUC1 1H
P1 11.50 usec
PLW1 20.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300223 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

913B




Current Data Parameters
NAME 500
EXPNO 144
PROCNO 1

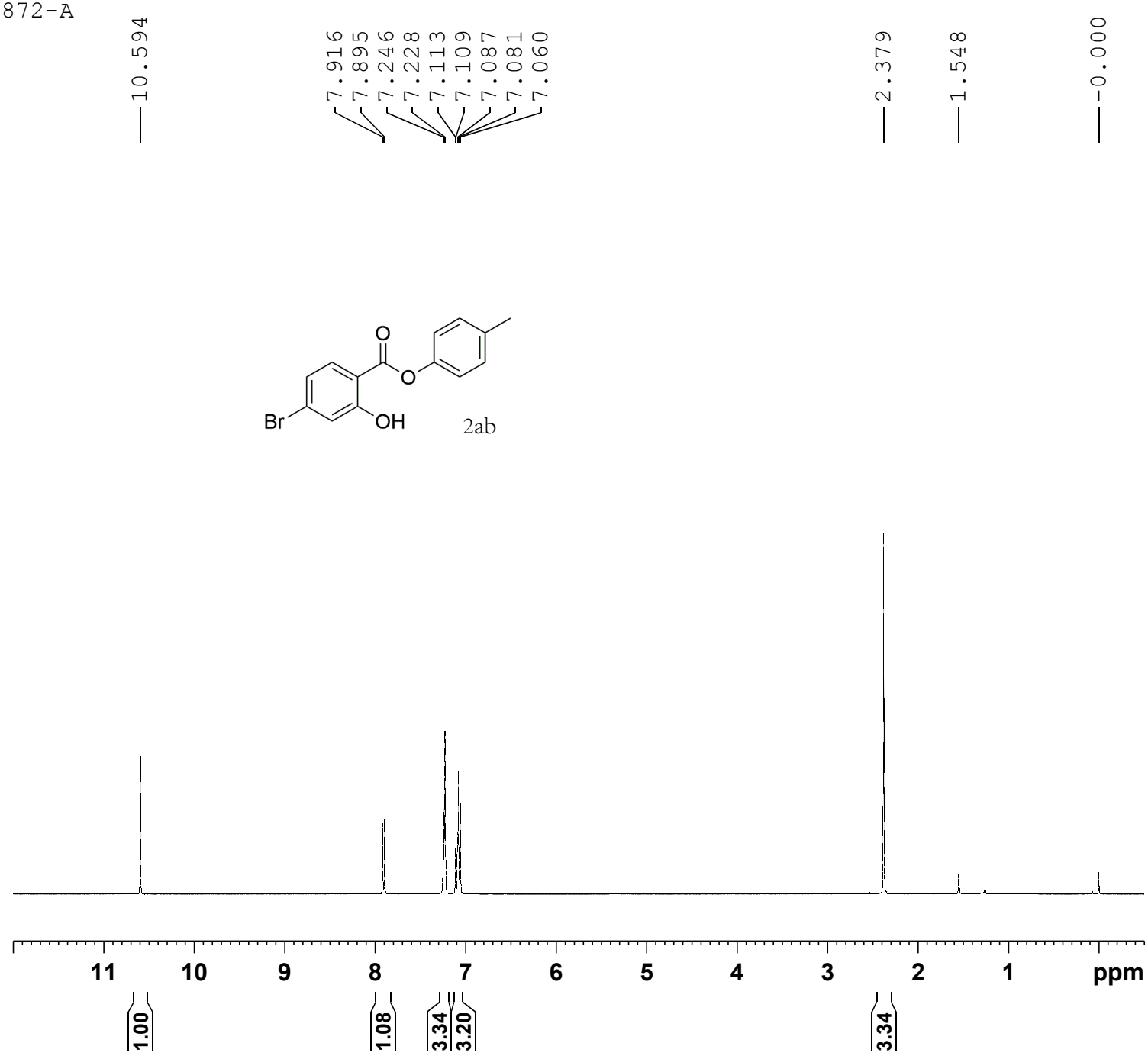
F2 - Acquisition Parameters
Date_ 20190823
Time 18.32
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 21
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 192.89
DW 16.800 usec
DE 18.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 125.7703637 MHz
NUC1 13C
P1 9.80 usec
PLW1 57.00000000 W

======== CHANNEL f2 ========
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 20.00000000 W
PLW12 0.35778001 W
PLW13 0.22898000 W

F2 - Processing parameters
SI 32768
SF 125.7577885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

872-A



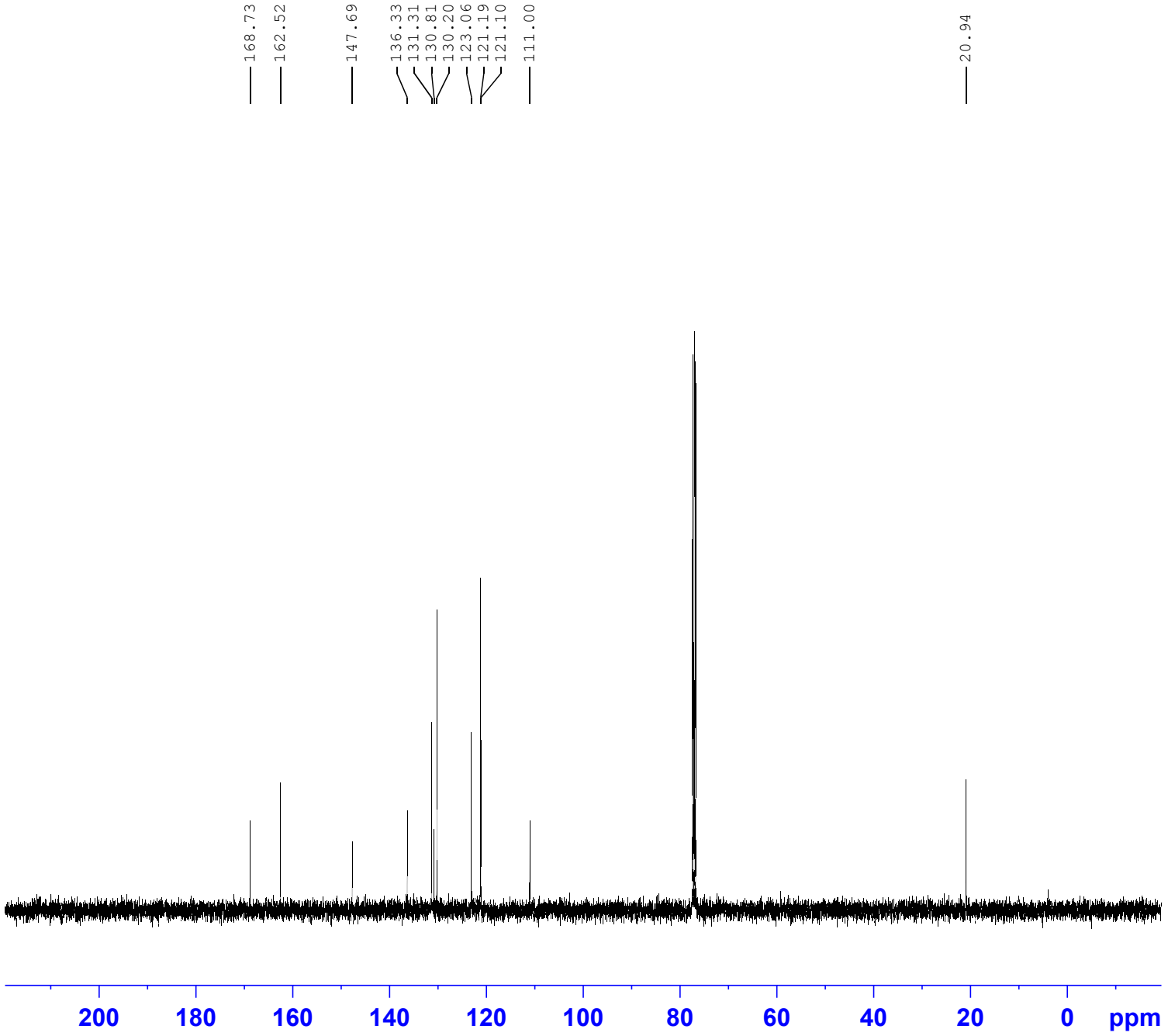

Current Data Parameters
NAME xzh-400
EXPNO 79
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190612
Time 14.01
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 140.59
DW 62.400 usec
DE 6.50 usec
TE 299.0 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.2424716 MHz
NUC1 1H
P1 14.30 usec
PLW1 12.00000000 W

F2 - Processing parameters
SI 65536
SF 400.2400149 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

872-A




Current Data Parameters
NAME xzh-400
EXPNO 81
PROCNO 1

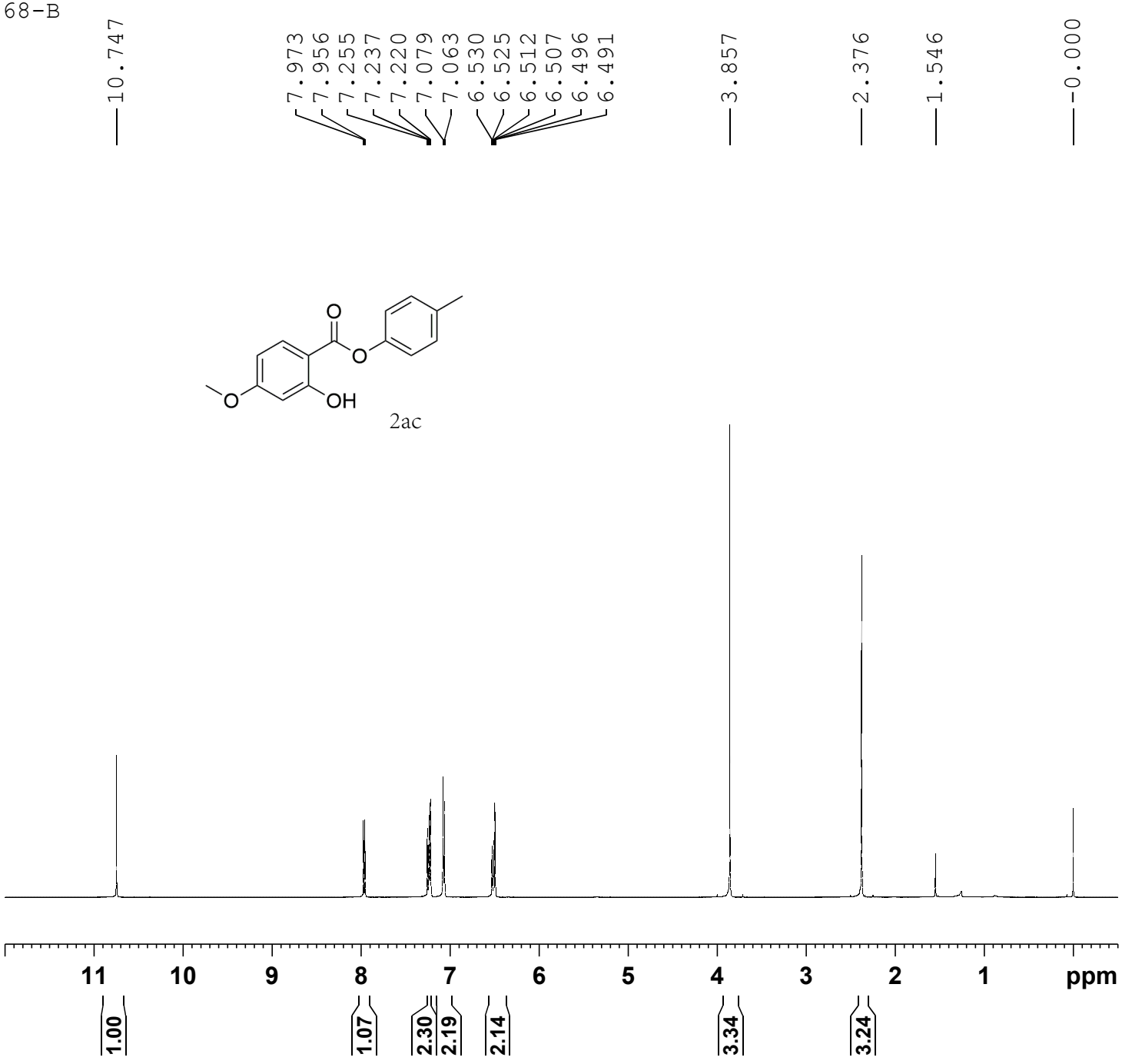
F2 - Acquisition Parameters
Date_ 20190612
Time 14.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 48
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 206.33
DW 20.800 usec
DE 6.50 usec
TE 299.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6504916 MHz
NUC1 13C
P1 10.00 usec
PLW1 54.00000000 W

======== CHANNEL f2 ========
SFO2 400.2416010 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.30294999 W
PLW13 0.24539000 W

F2 - Processing parameters
SI 32768
SF 100.6404280 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

868-B



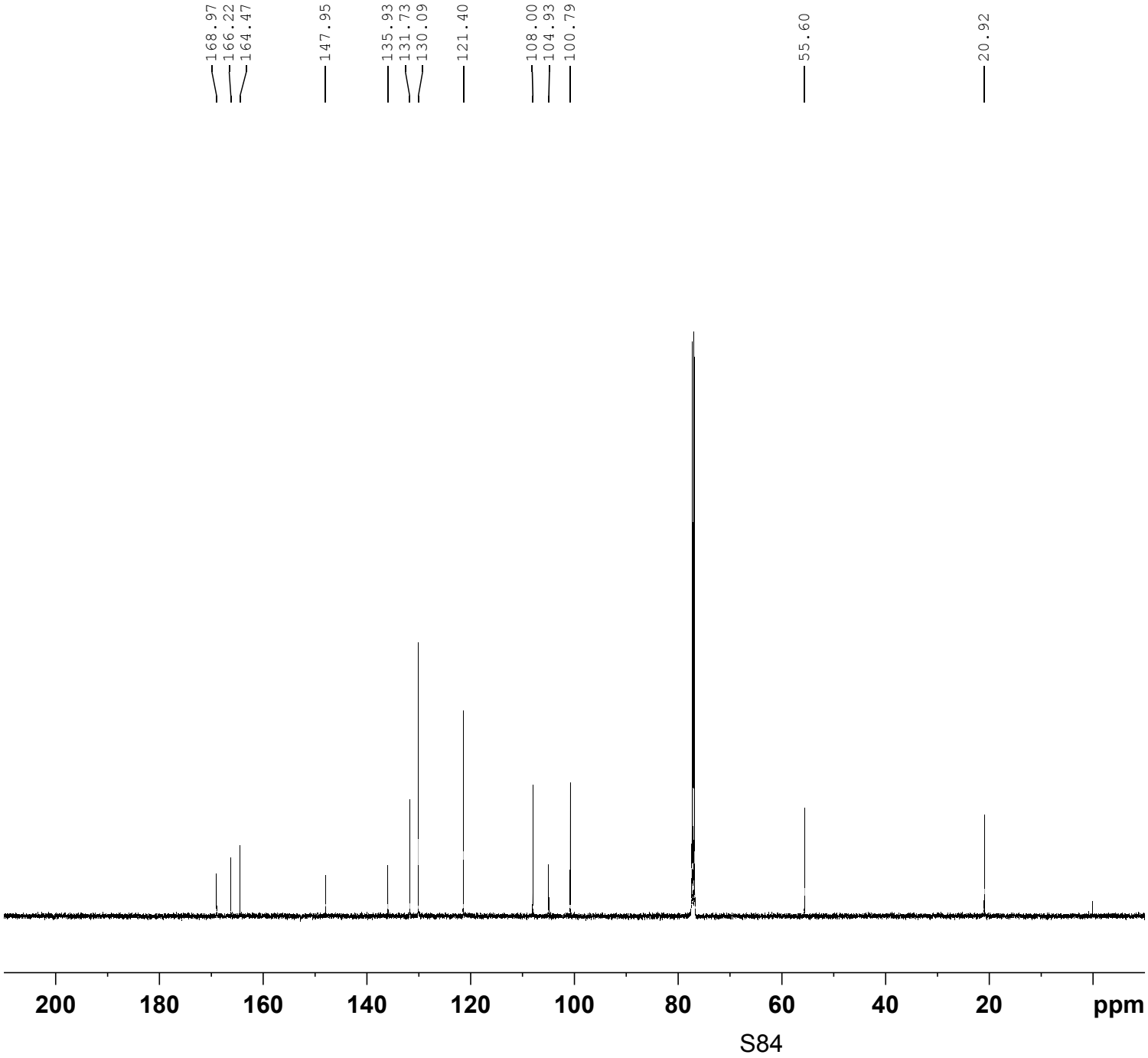

Current Data Parameters
NAME xzh
EXPNO 102
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190603
Time 21.12
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 31.72
DW 50.000 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 500.1330885 MHz
NUC1 1H
P1 11.50 usec
PLW1 20.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300150 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

868-B




Current Data Parameters
NAME xzh
EXPNO 103
PROCNO 1

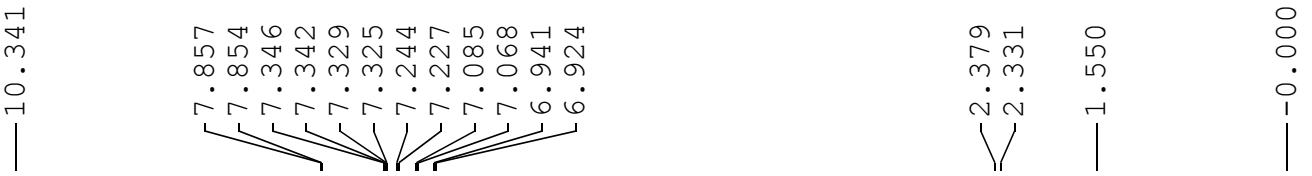
F2 - Acquisition Parameters
Date_ 20190603
Time 21.14
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 82
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 192.89
DW 16.800 usec
DE 18.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

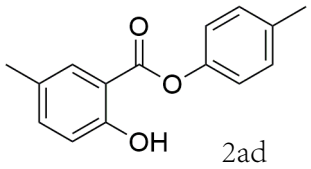
======== CHANNEL f1 ========
SFO1 125.7703637 MHz
NUC1 13C
P1 9.80 usec
PLW1 57.00000000 W

======== CHANNEL f2 ========
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 20.00000000 W
PLW12 0.35778001 W
PLW13 0.22898000 W

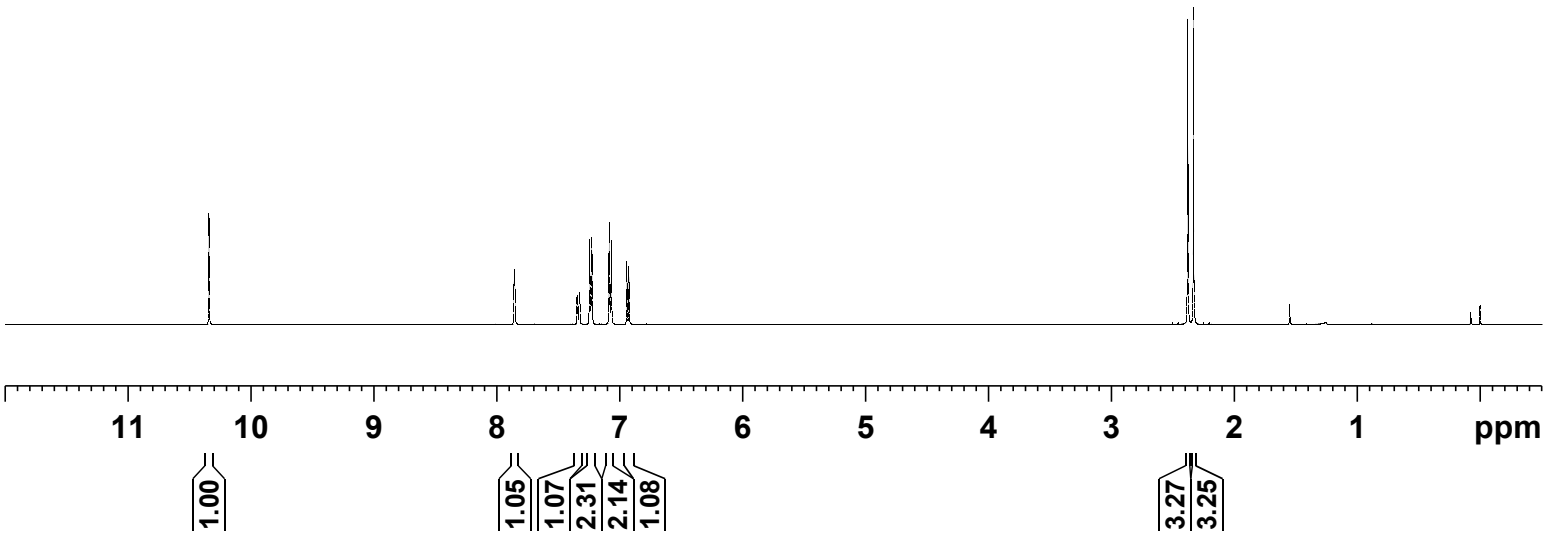
F2 - Processing parameters
SI 32768
SF 125.7577885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

912A



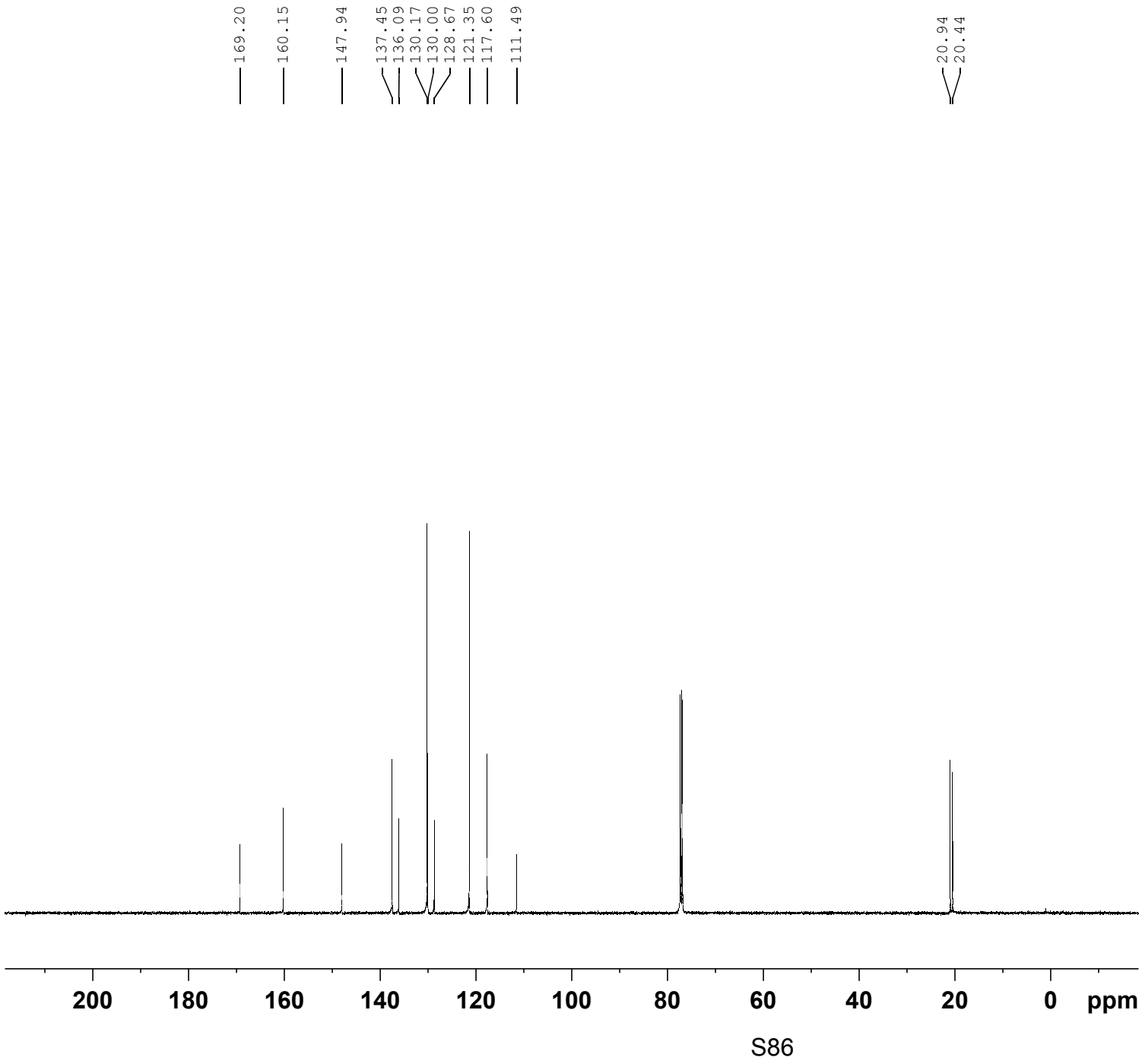




2ad




```
Current Data Parameters
NAME                  500
EXPNO                 137
PROCNO                  1

F2 - Acquisition Parameters
Date_            20190822
Time                14.25
INSTRUM             spect
PROBHD   5 mm CPPBBO BB
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH           10000.000 Hz
FIDRES         0.152588 Hz
AQ             3.2767999 sec
RG                 31.72
DW                50.000 usec
DE                 6.50 usec
TE                298.1 K
D1           1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         500.1330885 MHz
NUC1                   1H
P1                 11.50 usec
PLW1         20.00000000 W

F2 - Processing parameters
SI                  65536
SF           500.1300200 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

912a




Current Data Parameters
NAME 500
EXPNO 136
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190822
Time 10.42
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 68
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 192.89
DW 16.800 usec
DE 18.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 125.7703637 MHz
NUC1 13C
P1 9.80 usec
PLW1 57.00000000 W

======== CHANNEL f2 ========
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 20.00000000 W
PLW12 0.35778001 W
PLW13 0.22898000 W

F2 - Processing parameters
SI 32768
SF 125.7577885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40