Supporting Information

Metal-Free Synthesis of Ketonitriles via C-F Bond Cleavage

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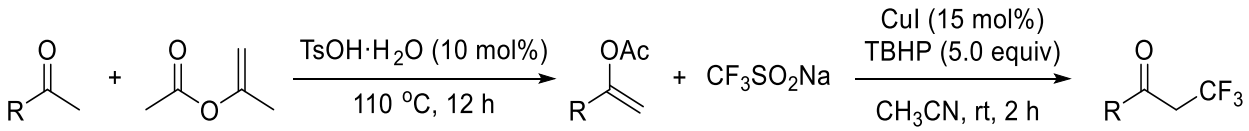
Contents

1. General information

^{1}H NMR spectra were recorded on Bruker 600 MHz spectrometer and the chemical shifts were reported in parts per million (δ) relative to internal standard TMS (0 ppm) for $CDCl_3$. The peak patterns are indicated as follows: s, singlet; d, doublet; dd, doublet of doublet; t, triplet; m, multiplet; q, quartet. The coupling constants, *J*, are reported in Hertz (Hz). ^{13}C NMR spectra were obtained at Bruker 150 MHz and referenced to the internal solvent signals (central peak is 77.0 ppm in $CDCl_3$). ^{19}F NMR spectra were obtained at Bruker 564 MHz. $CDCl_3$ was used as the NMR solvent. High-resolution mass spectra (HRMS) were acquired on Thermo Q-Exactive instrument (quadrupole mass analyzer) using electrospray ionization mode (ESI). Flash column chromatography was performed over silica gel 200-300. All reagents were weighed and handled in air at room temperature. All chemical reagents were purchased from Alfa, Aldrich, TCI, and J&K and used without further purification.

2. Synthesis of the substrates 1

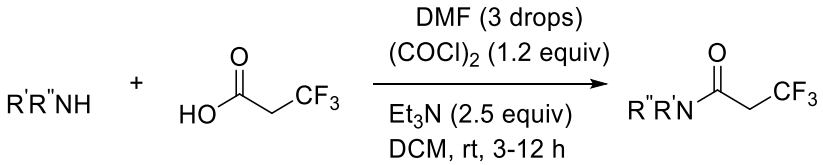
Method A: For synthesis of **1a-1k.**[1]



Step 1: The substrates α-CF_3 ketones (**1a-1k**) were synthesized according to the literature. To a mixture of the ketone (5.0 mmol) and isopropenyl acetate (25.0 mmol) was added *p*-TsOH·H_2O (0.5 mmol). The resulting mixture was refluxed overnight. The acetone formed was continuously distilled off. The reaction mixture was cooled to room temperature and diluted with ethyl acetate (20.0 mL) and water (30.0 mL). The aqueous layer was extracted with ethyl acetate (2 x 20.0 mL). The combined organic layers were dried over Na_2SO_4 and the solvent was evaporated in vacuo. The resulting crude mixture was purified by column chromatography using silica gel (200-300 mesh size) and petroleum ether/EtOAc (30:1 to 2:1) as the eluent.

Step 2: A flame-dried reaction vessel with a magnetic stirring bar was charged with CF_3SO_2Na (124.8 mg, 0.8 mmol, 4.0 equiv.), CuI (5.7 mg, 0.03 mmol, 0.15 equiv.), enol acetates (0.2 mmol, 1.0 equiv.) and MeCN (1.0 mL) in sequence. After the reaction mixture was cooled to 0 °C using an ice bath, an aqueous solution of TBHP (70% solution in water, 1.0 mmol, 5.0 equiv.) was slowly added dropwise with stirring. The mixture was stirred in the air at room temperature and the progress of the reaction was monitored by TLC (2-12 h). The resulting mixture was concentrated under reduced pressure. After evaporation, the residue was purified by column chromatography using silica gel (200-300 mesh size) and *n*-hexane/CH_2Cl_2 as the eluent.

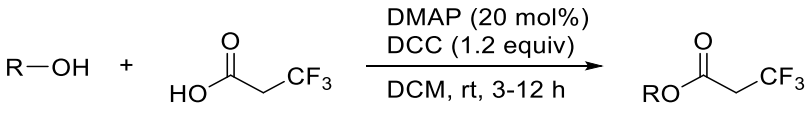
Method B: For synthesis of **1m-1r.**[2]



To a stirred suspension of 3,3,3-trifluoropropionic acid (1.3 equiv) in dichloromethane (4.0 mL) was added oxalyl chloride (1.2 equiv) followed by three drops of DMF at 0 °C. The reaction mixture was

stirred at room temperature for 3 h. To this solution was added a solution of anilines (1.0 mmol) in dichloromethane (2.0 mL) followed by triethylamine (2.5 equiv) at 0 °C. The reaction mixture was stirred for 12-24 h and then washed with water (3.0 mL) and 1 N HCl (3.0 mL). The organic layer was dried over Na_2SO_4 and evaporated to afford a residue, which was purified by flash column chromatography (petroleum ether/ethyl acetate) to afford trifluoropropanamides.

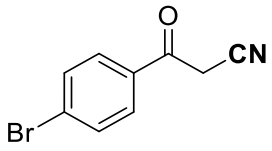
Method C: For synthesis of **1s-1w.**[3]



3,3,3-Trifluoropropanoates (**1s-1w**) were synthesized according to the reported literature. To a stirred solution of alcohol in anhydrous CH_2Cl_2 (3.0 mL/mmol) was added 3,3,3-trifluoropropanic acid (1.5 equiv), and DMAP (0.2 equiv). The reaction mixture was cooled to 0 ºC and DCC (1.2 equiv) was added. After stirring at 0 ºC for 0.5 h, the mixture was warmed to 25 ºC and the progress of the reaction was monitored by TLC (3-12 h). After the reaction finished, the mixture was filtered and the filtrate was evaporated in vacuo. The residue was purified by flash chromatography on silica gel to deliver the corresponding α-CF_3 ester as gum.

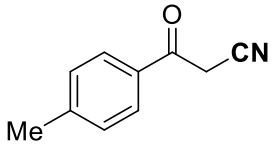
3. Synthesis and characterization for the products 3

To a Schlenk tube were added α-CF_3 Carbonyls **1** (0.2 mmol), K_2CO_3 (0.5 equiv) and MeCN (1.0 mL) in air at room temperature. Subsequently, aqueous ammonia **2a** (160. 0 μL, 2.0 mmol) was added to the mixture, and the resulting mixture was stirred at 50 ºC for 12 h. The organic phase was evaporated under vacuo. The residue was purified by flash column chromatography on silica gel to give the desired products **3**.

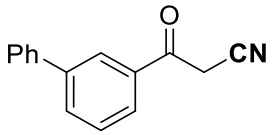


3-(4-Bromophenyl)-3-oxopropanenitrile (3a).[4] (42 mg, 95%). Isolated by column chromatography on silica gel (petroleum ether/ethyl acetate = 3:1, R_f = 0.5); ^{1}H NMR (600 MHz, $CDCl_3$, ppm) δ 7.79 (d, J = 8.6 Hz, 2H), 7.67 (d, J = 8.6 Hz, 2H), 4.05 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm) δ 186.2, 133.0, 132.6, 130.3, 129.9, 113.4, 29.4; HRMS (ESI) calcd for $C_9H_6BrNNaO$ [M + Na^+], 245.9525;

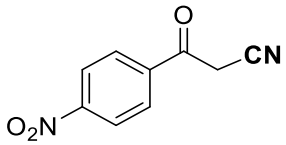
found: 245.9522.



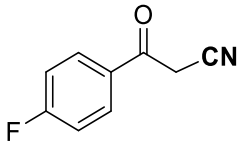
3-Oxo-3-(*p*-tolyl)propanenitrile (3b).[4] (18 mg, 56%). Isolated by column chromatography on silica gel (petroleum ether/ethyl acetate = 3:1, R_f = 0.4); ^{1}H NMR (600 MHz, $CDCl_3$, ppm) δ 7.82 (d, J = 8.2 Hz, 2H), 7.32 (t, J = 8.2 Hz, 2H), 4.05 (s, 2H), 2.44 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm) δ 186.6, 146.0, 131.8, 129.8, 128.6, 113.9, 29.2, 21.8; HRMS (ESI) calcd for $C_{10}H_9NNaO$ [M + Na^+], 182.0576; found: 182.0577.



3-([1,1'-Biphenyl]-3-yl)-3-oxopropanenitrile (3c).[5] (31 mg, 70%). Isolated by column chromatography on silica gel (petroleum ether/ethyl acetate = 3:1, R_f = 0.5); ^{1}H NMR (600 MHz, $CDCl_3$, ppm) δ 7.92 (d, J = 8.4 Hz, 2H), 7.67 (d, J = 8.4 Hz, 2H), 7.56 (d, J = 7.6 Hz, 2H), 7.42 (t, J = 7.2 Hz, 2H), 7.37 (d, J = 7.6 Hz, 1H), 4.03 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm) δ 185.6, 146.5, 138.2, 131.9, 128.1, 127.7, 126.7, 126.3, 112.8, 28.4; HRMS (ESI) calcd for $C_{15}H_{11}NNaO$ [M + Na^+], 244.0733; found: 244.0732.

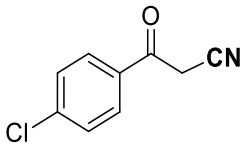


3-(4-Nitrophenyl)-3-oxopropanenitrile (3d).[4] (19 mg, 51%). Isolated by column chromatography on silica gel (petroleum ether/ethyl acetate = 3:1, R_f = 0.4); ^{1}H NMR (600 MHz, $CDCl_3$, ppm) δ 8.38 (d, J = 8.8 Hz, 2H), 8.12 (t, J = 8.8 Hz, 2H), 4.15 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm) δ 185.9, 151.2, 138.4, 129.6, 124.4, 112.8, 29.9; HRMS (ESI) calcd for $C_9H_6N_2NaO_3$ [M + Na^+], 213.0270; found: 213.0268.

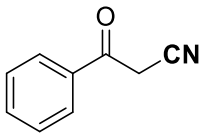


3-(4-Fluorophenyl)-3-oxopropanenitrile (3e).[4] (30 mg, 91%). Isolated by column chromatography on silica gel (petroleum ether/ethyl acetate = 3:1, R_f = 0.5); ^{1}H NMR (600 MHz, $CDCl_3$, ppm) δ 7.98-

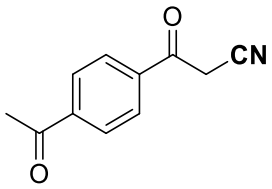
7.96 (m, 2H), 7.21 (t, J = 8.4 Hz, 2H), 4.09 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm) δ 185.7, 166.2 (d, $J_{C\text{-}F}$ = 258.2Hz), 131.3 (d, $J_{C\text{-}F}$ = 9.8Hz), 130.7 (d, $J_{C\text{-}F}$ = 3.2Hz), 116.5 (d, $J_{C\text{-}F}$ = 22.0Hz), 113.7, 29.4; ^{19}F NMR (565 MHz, $CDCl_3$, ppm) δ -101.6 (s, 1F); HRMS (ESI) calcd for C_9H_6FNNaO [M + Na^+], 186.0325; found: 186.0324.



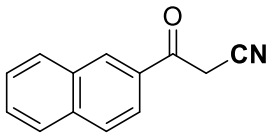
3-(4-Chlorophenyl)-3-oxopropanenitrile (3f).[4] (29 mg, 82%). Isolated by column chromatography on silica gel (petroleum ether/ethyl acetate = 3:1, R_f = 0.5); ^{1}H NMR (600 MHz, $CDCl_3$, ppm) δ 7.87 (d, J = 8.4 Hz, 2H), 7.51 (d, J = 8.6 Hz, 2H), 4.06 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm) δ 185.9, 141.5, 132.5, 129.8, 129.5, 113.4, 29.4; HRMS (ESI) calcd for C_9H_7ClNO [M + H^+], 180.0210; found: 180.0210.



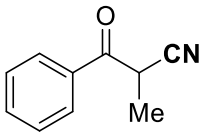
3-Oxo-3-phenylpropanenitrile (3g).[4] (28 mg, 95%). Isolated by column chromatography on silica gel (petroleum ether/ethyl acetate = 3:1, R_f = 0.4); ^{1}H NMR (600 MHz, $CDCl_3$, ppm) δ 7.92 (d, J = 7.6 Hz, 2H), 7.67 (t, J = 7.6 Hz,1H), 7.53 (t, J = 8.0 Hz, 2H), 4.11 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm) δ 187.2, 134.7, 134.2, 129.1, 128.4, 113.8, 29.4; HRMS (ESI) calcd for C_9H_7NNaO [M + Na^+], 168.0420; found:168.0419.



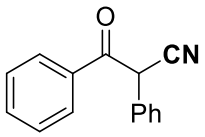
3-(4-Acetylphenyl)-3-oxopropanenitrile (3h).[4] (19 mg, 51%). Isolated by column chromatography on silica gel (petroleum ether/ethyl acetate = 3:1, R_f = 0.5); ^{1}H NMR (600 MHz, $CDCl_3$, ppm) δ 8.08 (d, J = 8.6 Hz, 2H), 8.01 (d, J = 8.6 Hz, 2H), 4.14 (s, 2H), 2.67 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm) δ 197.1, 186.8, 141.3, 137.2, 128.9, 128.8, 113.4, 29.8, 27.0; $C_{11}H_9NNaO_2$ [M + Na^+], 210.0525; found: 210.0524.



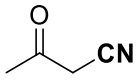
3-(Naphthalen-2-yl)-3-oxopropanenitrile (3i).[4] (36 mg, 92%). Isolated by column chromatography on silica gel (petroleum ether/ethyl acetate = 3:1, R_f = 0.5); ^{1}H NMR (600 MHz, $CDCl_3$, ppm) δ 8.37 (s, 1H), 7.96-7.87 (m, 4H), 7.65 (t, J = 7.2 Hz, 1H), 7.59 (t, J = 7.6 Hz, 1H), 4.20 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm) δ 187.0, 136.0, 132.2, 131.5, 130.6, 129.7, 129.4, 129.1, 127.8, 127.3, 123.3, 114.0, 29.4; HRMS (ESI) calcd for $C_{13}H_9NNaO$ [M + Na^+], 218.0576; found: 218.0580.



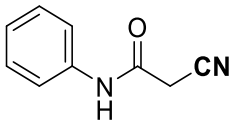
2-Methyl-3-oxo-3-phenylpropanenitrile (3j).[5] (25 mg, 77%). Isolated by column chromatography on silica gel (petroleum ether/ethyl acetate = 3:1, R_f = 0.5); ^{1}H NMR (600 MHz, $CDCl_3$, ppm) δ 7.99 (d, J = 7.6 Hz, 2H), 7.66 (t, J = 7.8 Hz, 1H), 7.53 (d, J = 8.0 Hz, 2H), 4.40 (m, 1H), 1.65 (d, J = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm) δ 190.7, 134.5, 133.7, 129.1, 128.8, 118.1, 33.7, 14.9; HRMS (ESI) calcd for $C_{10}H_{10}NO$ [M + H^+], 160.0756; found: 160.0756.



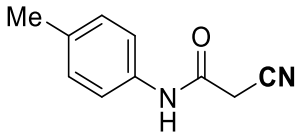
3-Oxo-2,3-diphenylpropanenitrile (3k).[5] (18 mg, 40%). Isolated by column chromatography on silica gel (petroleum ether/ethyl acetate = 3:1, R_f = 0.5); ^{1}H NMR (600 MHz, $CDCl_3$, ppm) δ 7.95 (d, J = 7.4 Hz, 2H), 7.60 (d, J = 7.4 Hz, 1H), 7.48-7.44 (m, 4H), 7.40 (t, J = 7.2 Hz, 2H), 7.2 (m, 1H), 5.60 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm) δ 188.9, 134.4, 133.6, 130.4, 129.7, 129.3, 129.2, 129.0, 128.3, 116.5, 46.7; HRMS (ESI) calcd for $C_{15}H_{11}NNaO$ [M + Na^+], 244.0733; found: 244.0730.



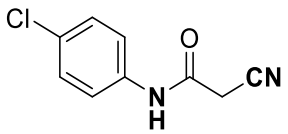
3-Oxobutanenitrile (3l).[6] (7 mg, 41%). Isolated by column chromatography on silica gel (petroleum ether/ethyl acetate = 3:1, R_f = 0.5); ^{1}H NMR (600 MHz, $CDCl_3$, ppm) δ 3.54 (s, 2H), 2.35 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm) δ 195.4, 113.9, 32.8, 29.3; HRMS (ESI) calcd for C_4H_5NNaO [M + Na^+], 106.0263; found: 106.0265.



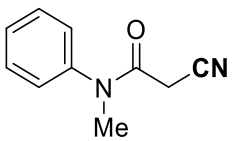
2-Cyano-*N*-phenylacetamide (3m).[7] (30 mg, 92%). Isolated by column chromatography on silica gel (petroleum ether/ethyl acetate = 2:1, R_f = 0.4); ^{1}H NMR (600 MHz, DMSO-*d*^{6}, ppm) δ 10.30 (s, 1H), 7.54 (d, *J* = 8.4 Hz, 2H), 7.34 (t, *J* = 7.8 Hz, 2H), 7.10 (t, *J* = 8.0 Hz, 1H), 3.39 (s, 2H); ^{13}C NMR (150 MHz, DMSO-*d*^{6}, ppm) δ 166.2, 143.6, 134.2, 129.2, 124.5, 121.1, 31.9; HRMS (ESI) calcd for $C_9H_8N_2NaO$ [M + Na^+], 183.0529; found: 183.0530.



***2*-Cyano-*N*-(*p*-tolyl)acetamide (3n)**.[8] (32 mg, 93%). Isolated by column chromatography on silica gel (petroleum ether/ethyl acetate = 2:1, R_f = 0.4); ^{1}H NMR (600 MHz, DMSO-*d*^{6}, ppm) δ 10.21 (s, 1H), 7.43 (t, *J* = 8.2 Hz, 2H), 7.13 (d, *J* = 8.0 Hz, 2H), 3.87 (s, 2H), 2.26 (s, 3H); ^{13}C NMR (150 MHz, DMSO-*d*^{6}, ppm) δ 161.2, 136.3, 133.4, 129.7, 119.7, 116.4, 27.1, 20.9; HRMS (ESI) calcd for $C_{10}H_{10}N_2NaO$ [M + Na^+], 197.0685; found: 197.0686.

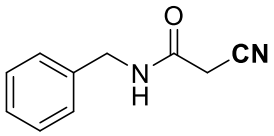


***N*-(4-Chlorophenyl)-2-cyanoacetamide (3o)**.[8] (36 mg, 94%). Isolated by column chromatography on silica gel (petroleum ether/ethyl acetate = 2:1, R_f = 0.4); ^{1}H NMR (600 MHz, DMSO-*d*^{6}, ppm) δ 10.43 (s, 1H), 7.57 d, *J* = 8.8 Hz, 2H), 7.39 (d, *J* = 8.8 Hz, 2H), 3.91 (s, 2H); ^{13}C NMR (150 MHz, DMSO-*d*^{6}, ppm) δ 161.7, 137.8, 129.3, 128.0, 121.3, 116.3, 27.2; HRMS (ESI) calcd for $C_9H_7ClN_2NaO$ [M + Na^+], 217.0139; found: : 217.0138.

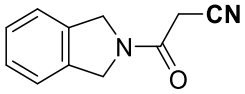


2-Cyano-*N*-methyl-*N*-phenylacetamide (3p).[7] (33 mg, 96%). Isolated by column chromatography on silica gel (petroleum ether/ethyl acetate = 2:1, R_f = 0.4); ^{1}H NMR (600 MHz, $CDCl_3$, ppm) δ 7.49 (t, *J* = 7.8 Hz, 2H), 7.43 (d, *J* = 6.8 Hz, 1H), 7.25(d, *J* = 7.4 Hz, 2H), 3.32 (s, 3H), 3.25 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm) δ 161.6, 142.3, 130.4, 128.9, 126.9, 114.1, 37.8, 25.3; HRMS (ESI)

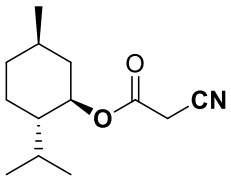
calcd for $C_{10}H_{10}N_2NaO$ [M + Na^+], 197.0685; found: 197.0685.



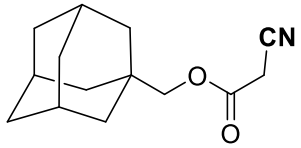
***N*-Benzyl-2-cyanoacetamide (3q)**.[7] (33 mg, 95%). Isolated by column chromatography on silica gel (petroleum ether/ethyl acetate = 2:1, R_f = 0.4); ^{1}H NMR (600 MHz, $CDCl_3$, ppm) δ 7.36 (t, J = 7.2 Hz, 2H), 7.31 (d, J = 7.2 Hz, 1H), 7.28 (d, J = 7.2 Hz, 2H), 6.44 (s, 1H), 4.47 (d, J = 5.6 Hz, 2H), 3.39 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm) δ 160.7, 136.8, 129.0, 128.1, 128.0, 114.6, 44.4, 25.8; HRMS (ESI) calcd for $C_{10}H_{10}N_2NaO$ [M + Na^+], 197.0685; found: 197.0685.



3-(Isoindolin-2-yl)-3-oxopropanenitrile (3r).[9] (34 mg, 93%). Isolated by column chromatography on silica gel (petroleum ether/ethyl acetate = 2:1, R_f = 0.4); ^{1}H NMR (600 MHz, DMSO-d^6, ppm) δ 8.01 (d, J = 8.0 Hz, 1H), 7.26 (d, J = 7.2 Hz, 1H), 7.19 (t, J = 7.8 Hz, 1H), 7.05 (t, J = 7.2 Hz, 1H), 4.18 (s, 2H), 4.05 (t, J = 8.2 Hz, 2H), 3.16 (t, J = 8.4 Hz, 2H); ^{13}C NMR (150 MHz, DMSO-d^6, ppm) δ 161.8, 142.7, 132.4, 127.6, 125.5, 124.5, 116.4, 116.2, 47.9, 27.8, 27.5; HRMS (ESI) calcd for $C_{11}H_{10}N_2NaO_3$ [M + Na^+], 209.0685; found: 209.0682.

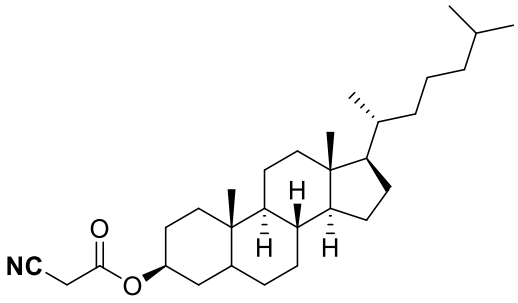


(1*R*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl 2-cyanoacetate (3s).[10] (41 mg, 91%). Isolated by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1, R_f = 0.5); ^{1}H NMR (600 MHz, $CDCl_3$, ppm) δ 4.79-4.75 (m, 1H), 3.44 (d, J = 1.2 Hz, 2H), 2.03-2.00 (m, 1H), 1.88-1.83 (m, 1H), 1.72-1.69 (m, 2H), 1.52-1.42 (m, 2H), 1.10-1.03 (m, 2H), 0.92 (t, J = 6.6 Hz, 7H), 0.77 (t, J = 7.0 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm) δ 162.5, 113.2, 77.5, 46.7, 40.5, 34.0, 31.4, 26.3, 25.0, 23.3, 21.9, 20.7, 16.2; HRMS (ESI) calcd for $C_{13}H_{21}NNaO_2$ [M + Na^+], 246.1465; found: 246.1463.

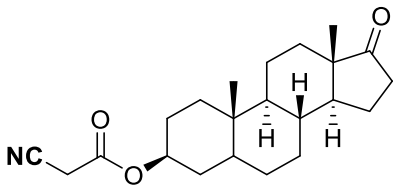


((3*r*,5*r*,7*r*)Adamantan-1-yl)methyl 2-cyanoacetate (3t). (45 mg, 97%). Isolated by column

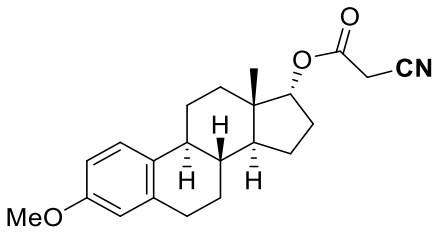
chromatography on silica gel (petroleum ether/ethyl acetate = 5:1, R_f = 0.5); ^{1}H NMR (600 MHz, $CDCl_3$, ppm) δ 3.80 (s, 2H), 3.48 (s, 2H), 2.00 (s, 3H), 1.73 (d, J = 12.6 Hz, 3H), 1.65 (d, J = 12.4 Hz, 3H), 1.55 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm) δ 163.0, 113.0, 76.2, 38.9, 36.7, 33.2, 29.6, 27.8, 24.6; HRMS (ESI) calcd for $C_{14}H_{20}NO_2$ [M + H^+], 234.1489; found: 234.1476.



(3*S*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-10,13-Dimethyl-17-(*R*)-6-methylheptan-2-yl)hexadecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl 2-cyanoacetate (3u). (88 mg, 97%). Isolated by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1, R_f = 0.5); ^{1}H NMR (600 MHz, $CDCl_3$, ppm) δ 4.81-4.76 (m, 1H), 3.42(s, 2H), 1.98-1.95(m, 1H), 1.85-1.74 (m, 3H), 1.67-1.40 (m, 8H), 1.37-1.19 (m, 9H), 1.17-0.96 (m, 10H), 0.89 (d, J = 6.6 Hz, 3H), 0.87-0.85 (m, 6H), 0.83 (s, 3H), 0.67 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm) δ 162.4, 113.2, 56.4, 56.3, 54.2, 44.6, 42.6, 40.0, 39.5, 36.6, 36.2, 35.8, 35.5, 35.4, 33.7, 31.9, 28.5, 28.2, 28.0, 27.2, 25.1, 24.2, 23.8, 22.8, 22.6, 21.2, 18.7, 12.2, 12.1; HRMS (ESI) calcd for $C_{30}H_{49}NNaO_2$ [M + Na^+], 478.3656; found: 478.3655.



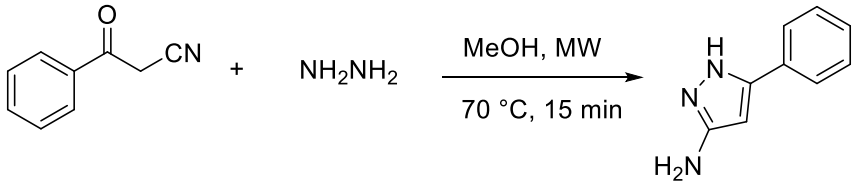
(3*S*,8*R*,9*S*,10*S*,13*S*,14*S*)-10,13-Dimethyl-17-oxohexadecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl 2-cyanoacetate. **(3v)** (69 mg, 97%). Isolated by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1, R_f = 0.5); ^{1}H NMR (600 MHz, $CDCl_3$, ppm) δ 4.82-4.76 (m, 1H), 3.44(s, 2H), 2.46-2.41(m, 1H), 2.10-2.04 (m, 1H), 1.95-1.86 (m, 2H), 1.82-1.76 (m, 3H), 1.68-1.63 (m, 2H), 1.60-1.42 (m, 4H),1.37-1.18 (m, 6H), 1.08-1.02 (m, 2H), 0.86 (s, 6H), 0.74-0.70 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm) δ 162.3, 113.1, 76.5, 54.1, 51.2, 47.7, 44.5, 36.4, 35.7, 35.5, 34.9, 33.5, 31.4, 30.6, 28.1, 27.0, 25.0, 21.7, 20.4, 13.7, 12.1; HRMS (ESI) calcd for $C_{22}H_{31}NNaO_3$ [M + Na^+], 380.2196; found: 380.2192.



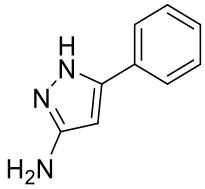
(8*R*,9*S*,13*S*,14*S*,17*R*)-3-Methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[*a*]phenanthren-17-yl 2-cyanoacetate (3w). (68 mg, 96%). Isolated by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1, R_f = 0.5); ^{1}H NMR (600 MHz, $CDCl_3$, ppm) δ 7.19 (d, J = 8.4 Hz, 1H), 6.73-6.70 (m, 1H), 6.63 (s, 1H), 4.77 (t, J = 8.6 Hz, 1H), 3.78 (s, 3H), 3.46 (s, 2H), 2.88-2.84 (m, 2H), 2.32-2.19 (s, 3H), 1.92-1.88 (m, 2H), 1.78-1.76 (m, 1H), 1.64-1.60 (m, 2H), 1.44-1.18 (m, 5H), 0.80 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm) δ 162.9, 157.5, 137.8, 132.2, 126.4, 113.9, 113.1, 111.5, 85.5, 55.2, 49.6, 43.7, 43.2, 38.5, 36.8, 29.7, 27.4, 27.2, 26.1, 24.9, 23.2, 12.0; HRMS (ESI) calcd for $C_{22}H_{27}NNaO_3$ [M + Na^+], 376.1883; found: 376.1867.

4. Synthesis and characterization for the products 4-6.

Method D: For synthesis of **4.**[11]



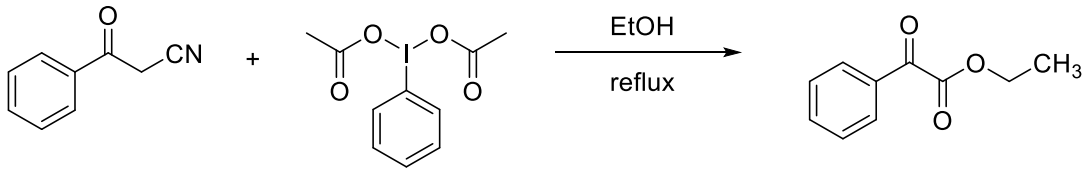
5-Phenyl-1*H*-pyrazol-3-amine **4** were synthesized according to the reported literature. Benzoylacetonitrile (2.0 mmol, 1.0 equiv), hydrazine (2.6 mmol, 1.3 equiv), MeOH (1.0 mL) were heated under microwave conditions (100 W, 70 °C) for 15 min. After the reaction was completed (monitored by TLC), the reaction mixture was concentrated under vacuum. The residue was purified by chromatography on silica gel to give the product **4**.



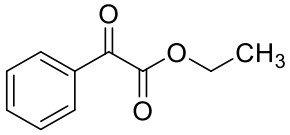
5-Phenyl-1*H*-pyrazol-3-amine (4).[11] (30 mg, 94%). Isolated by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1, R_f = 0.6); ^{1}H NMR (600 MHz, DMSO-d^6, ppm) δ 7.67 (d, J = 7.6 Hz, 2H), 7.37 (t, J = 7.4 Hz, 2H), 7.26 (t, J = 7.2 Hz, 1H), 5.79 (s, 1H); ^{13}C NMR (150 MHz, DMSO-d^6, ppm) δ 153.6, 145.9, 132.5, 129.1, 127.7, 125.2, 87.8; HRMS (ESI) calcd for $C_9H_{10}N_3$ [M + H^+],

160.0869; found: 160.0886.

Method E: For synthesis of **5.** [12]

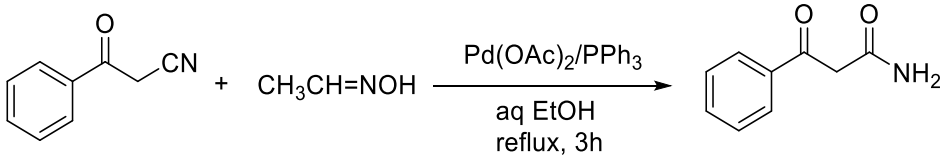


Methyl 2-oxo-2-phenylacetate **5** were synthesized according to the reported literature. Benzoylacetonitrile (1.0 mmol) and PIDA (2.2 mmol) were dissolved in EtOH (8.0 mL) and stirred under refluxing for 1 h. After the reaction was completed (monitored by TLC), the reaction mixture was concentrated under vacuum. The residue was purified by chromatography on silica gel (20:1 petroleum ether/EtOAc) to give the product **5**.

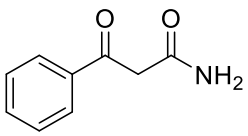


Methyl 2-oxo-2-phenylacetate (5).[12] (30 mg, 86%). Isolated by column chromatography on silica gel (petroleum ether/ethyl acetate = 10:1, R_f = 0.5); ^{1}H NMR (600 MHz, $CDCl_3$, ppm) δ 8.01 (t, J = 7.4 Hz, 2H), 7.65 (t, J = 7.2 Hz, 1H), 7.51 (t, J = 8.0 Hz, 2H), 4.47-4.43 (m, 2H), 1.41 (t, J = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm) δ 186.5, 163.9, 134.9, 132.5, 130.0, 128.9, 62.3, 14.1; HRMS (ESI) calcd for $C_{10}H_{10}NaO_3$ [M + Na^+], 201.0522; found: 201.0521.

Method F: For synthesis of **6.**[13]



3-Oxo-3-phenylpropanamide **6** were synthesized according to the reported literature. Benzoylacetonitrile (1.0 mmol), acetaldoxime (2.0 mmol), $Pd(OAc)_2$, (10 mol %) and PPh_3 (20 mol %) were dissolved in H_2O/EtOH (1:4), and stirred under refluxing for 3 h. After the reaction was completed (monitored by TLC), the reaction mixture was concentrated under vacuum. The residue was purified by chromatography on silica gel to give the product **6**.



3-Oxo-3-phenylpropanamide (6)[13] (25 mg, 77%). Isolated by column chromatography on silica gel (petroleum ether/ethyl acetate = 1:1, R_f = 0.3); ^{1}H NMR (600 MHz, $CDCl_3$, ppm) δ 7.99 (d, J = 7.6 Hz, 2H), 7.63 (t, J = 7.2 Hz, 1H), 7.50 (t, J = 7.8 Hz, 2H), 3.98 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm) δ 195.7, 168.1, 136.1, 134.2, 128.9, 128.6, 45.1; HRMS (ESI) calcd for $C_9H_{10}NO_2$ [M + H^+], 164.0706; found: 164.0702.

5. References

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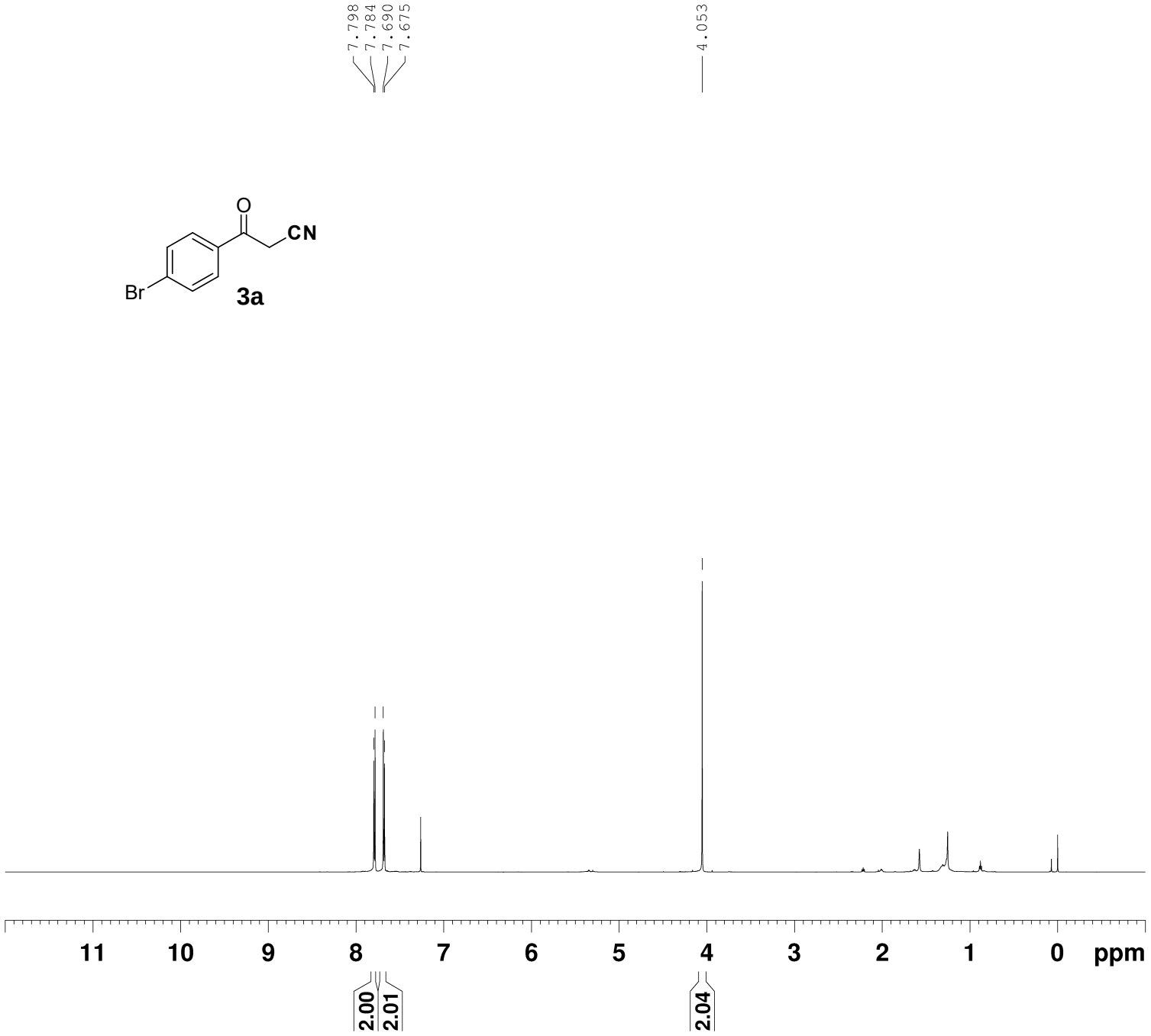
6. Copies of ^{1}H NMR and ^{13}C NMR spectra for all compounds.

3a



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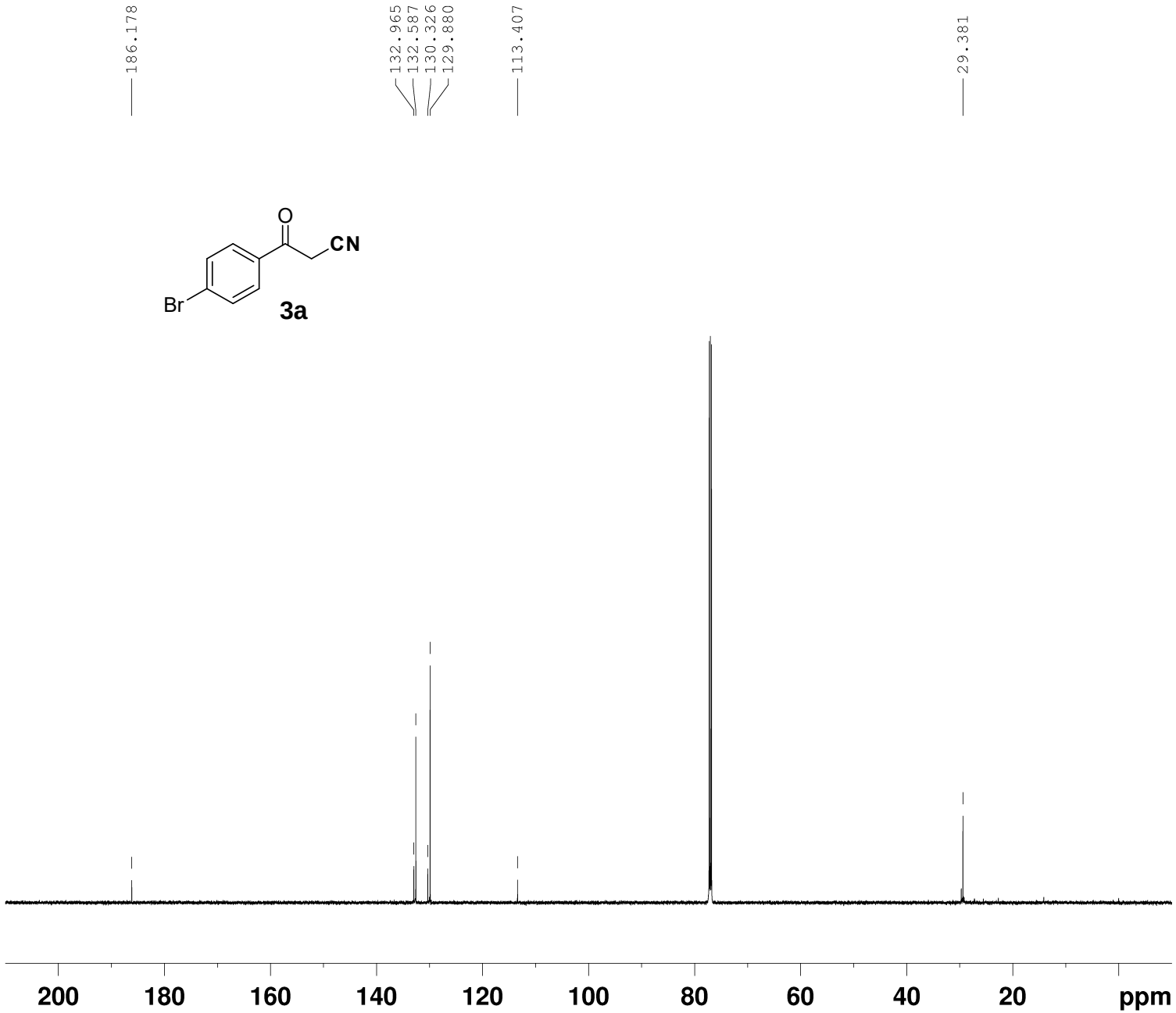

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TD0	1
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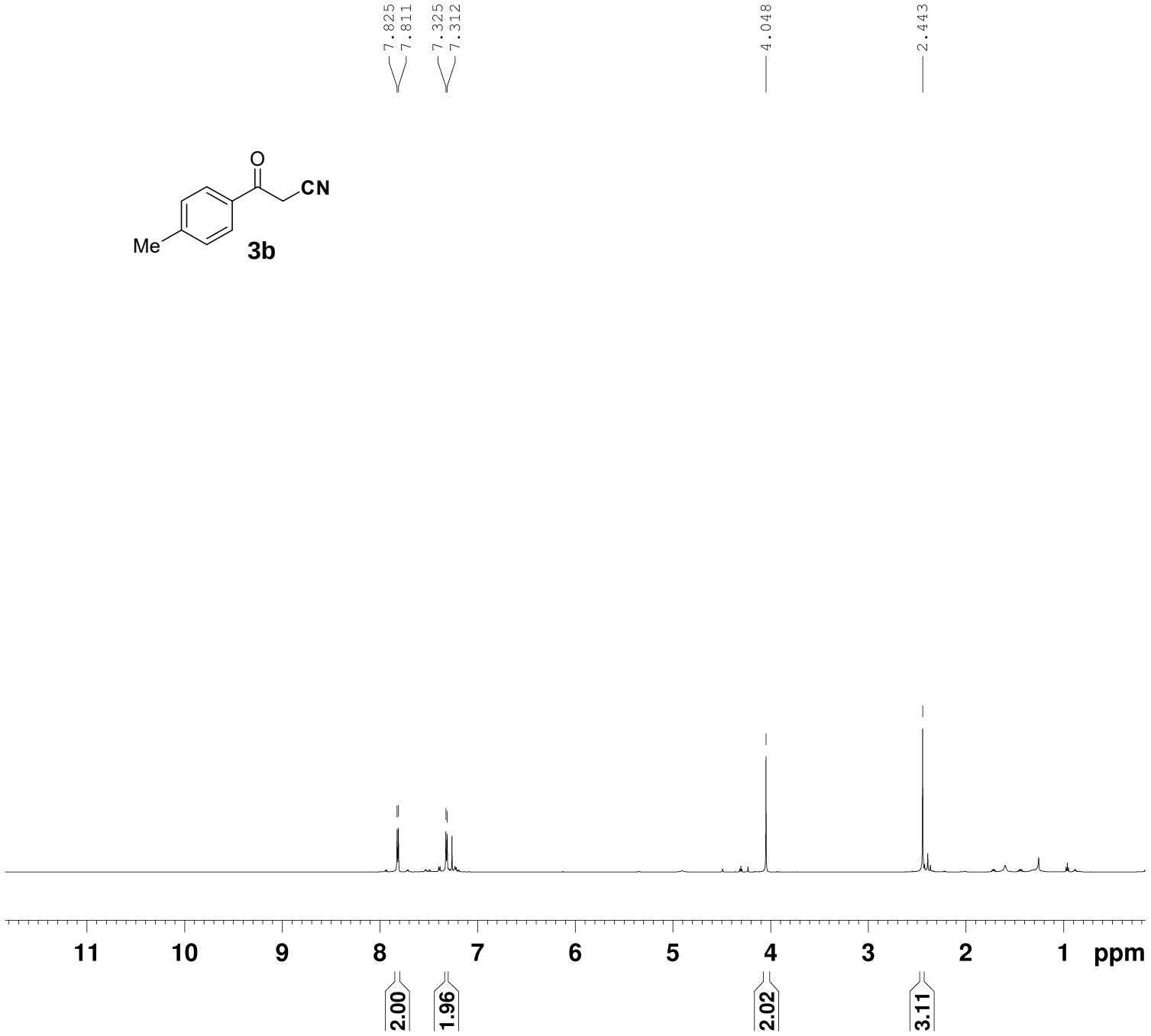
3b



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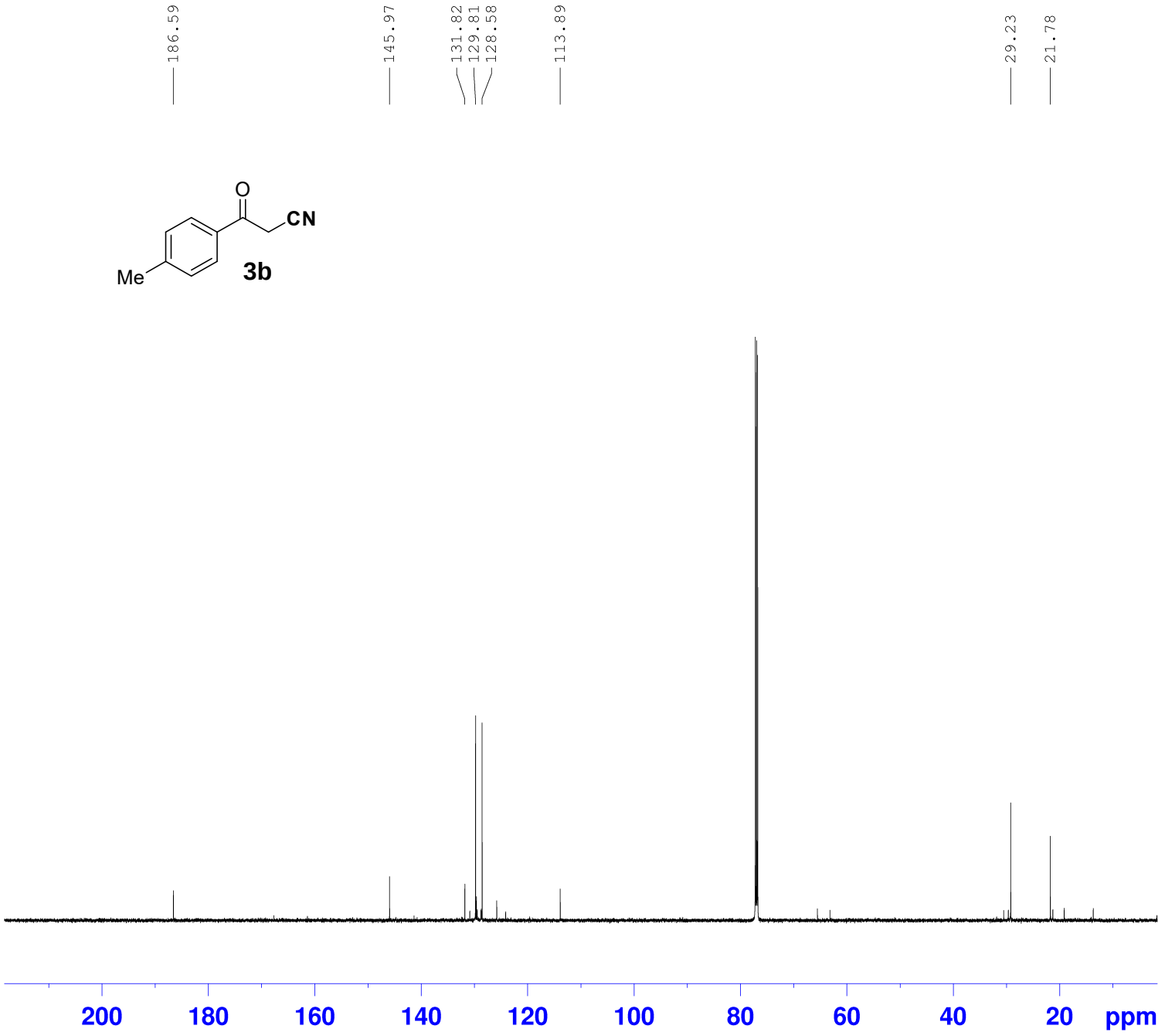

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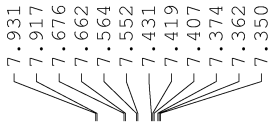

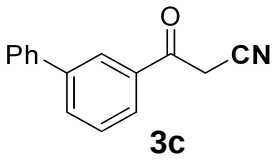

3c

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DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
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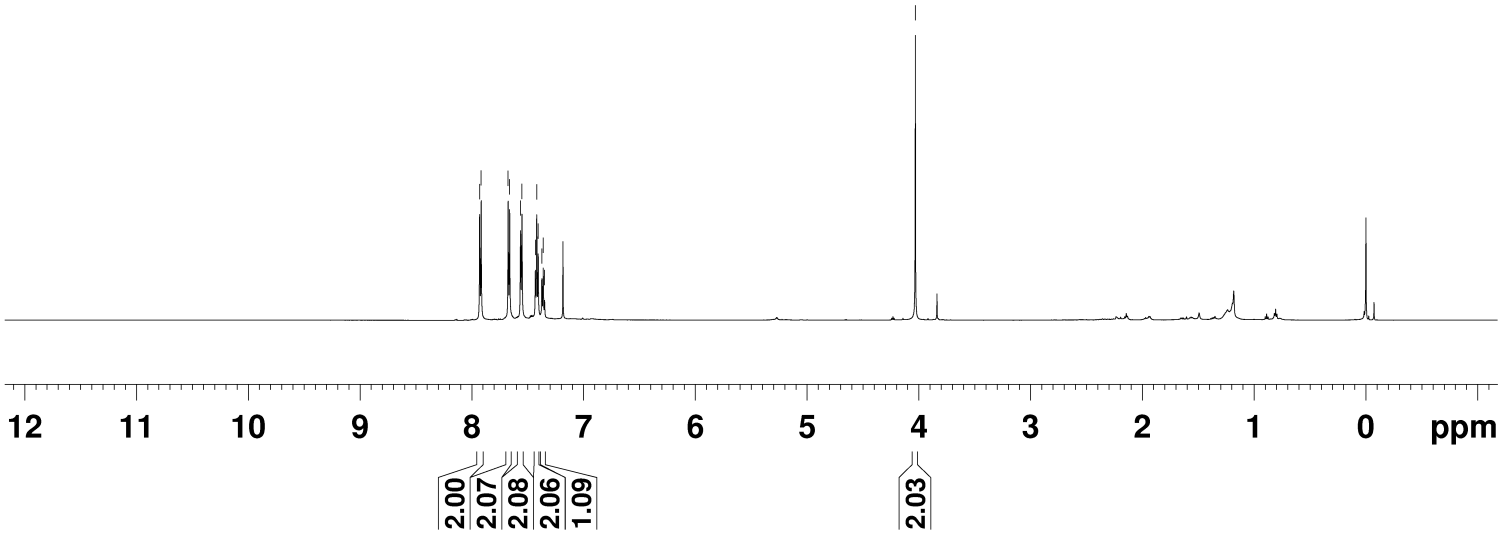
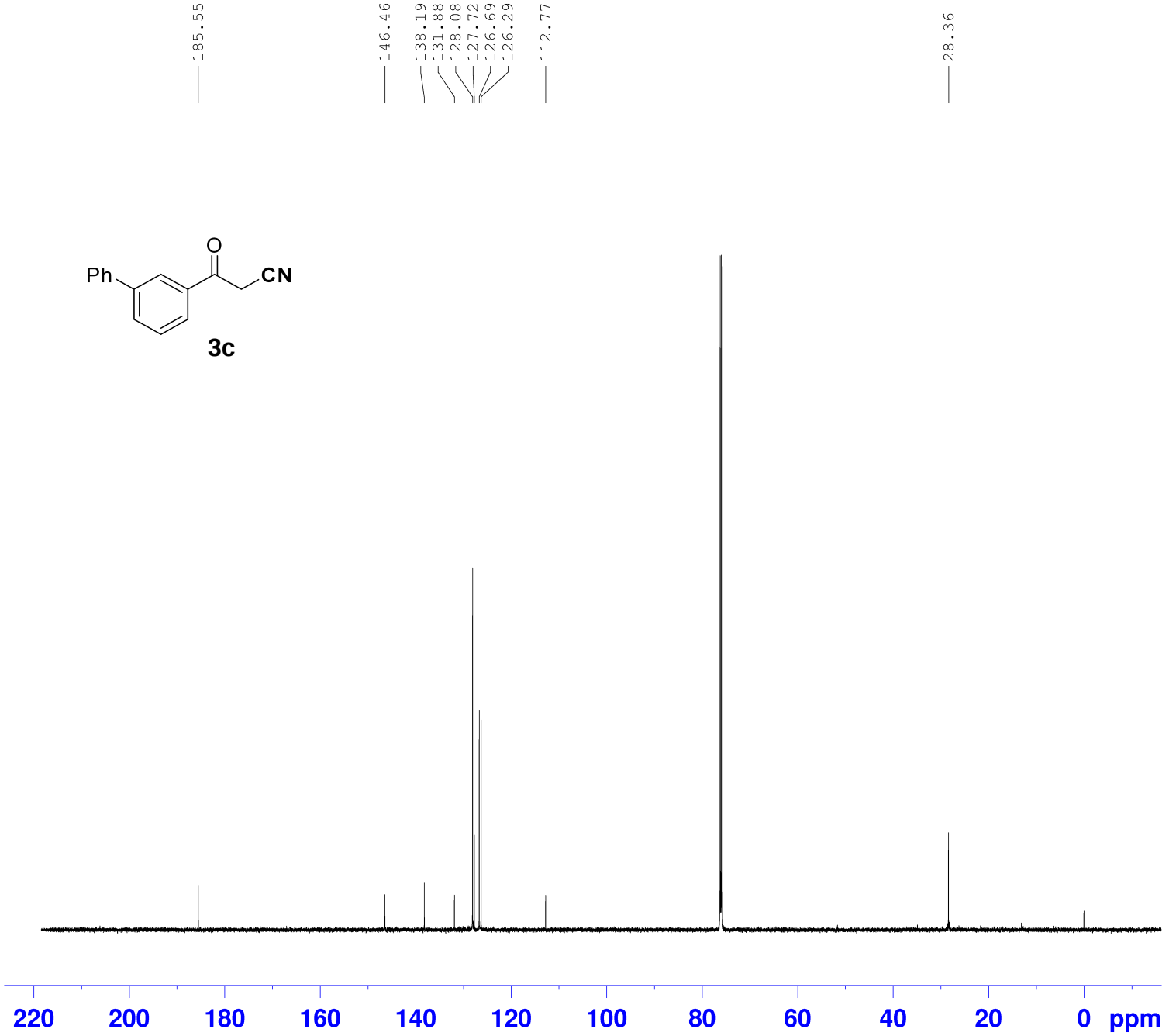
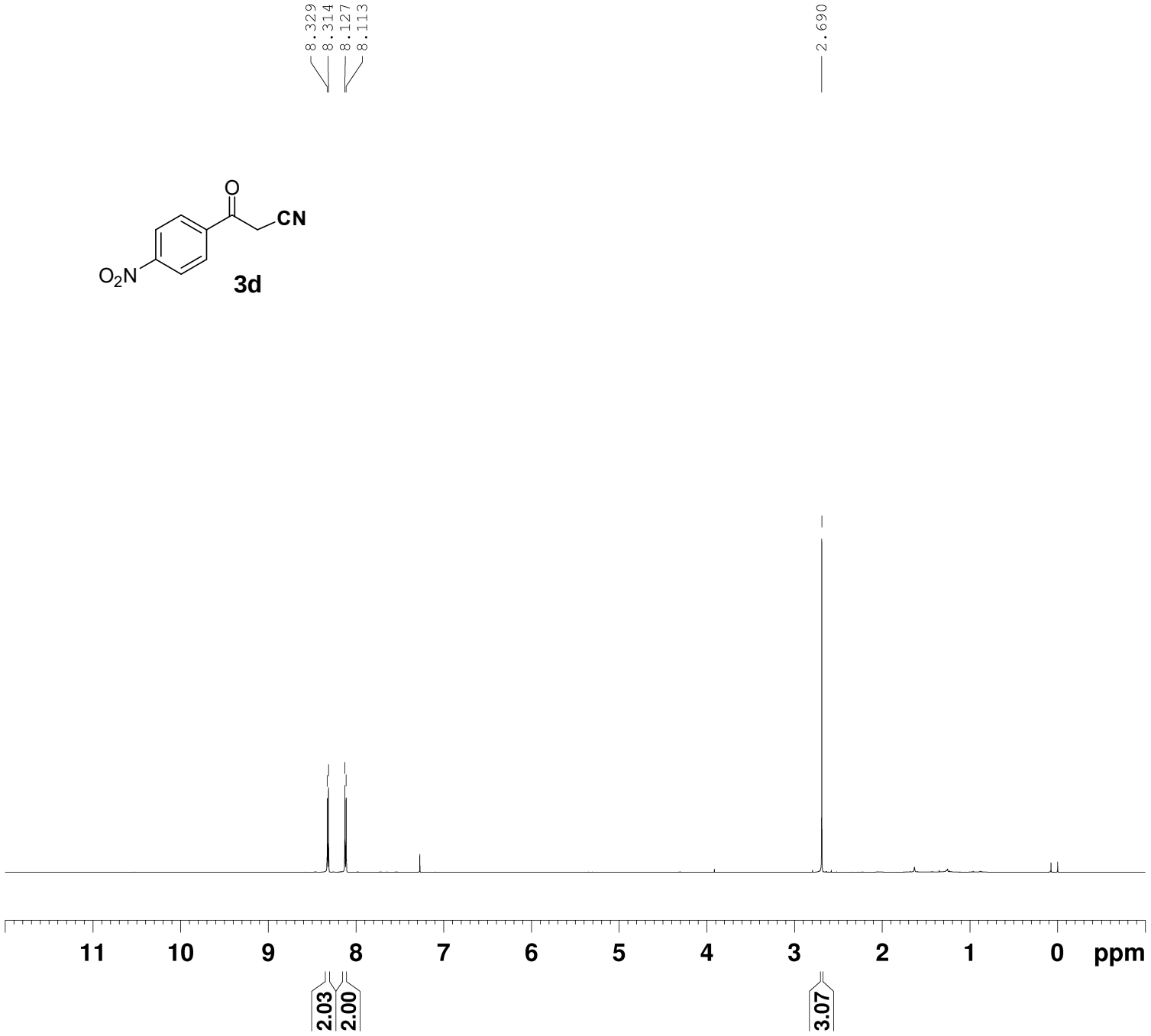
SI	65536
SF	600.1700595 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



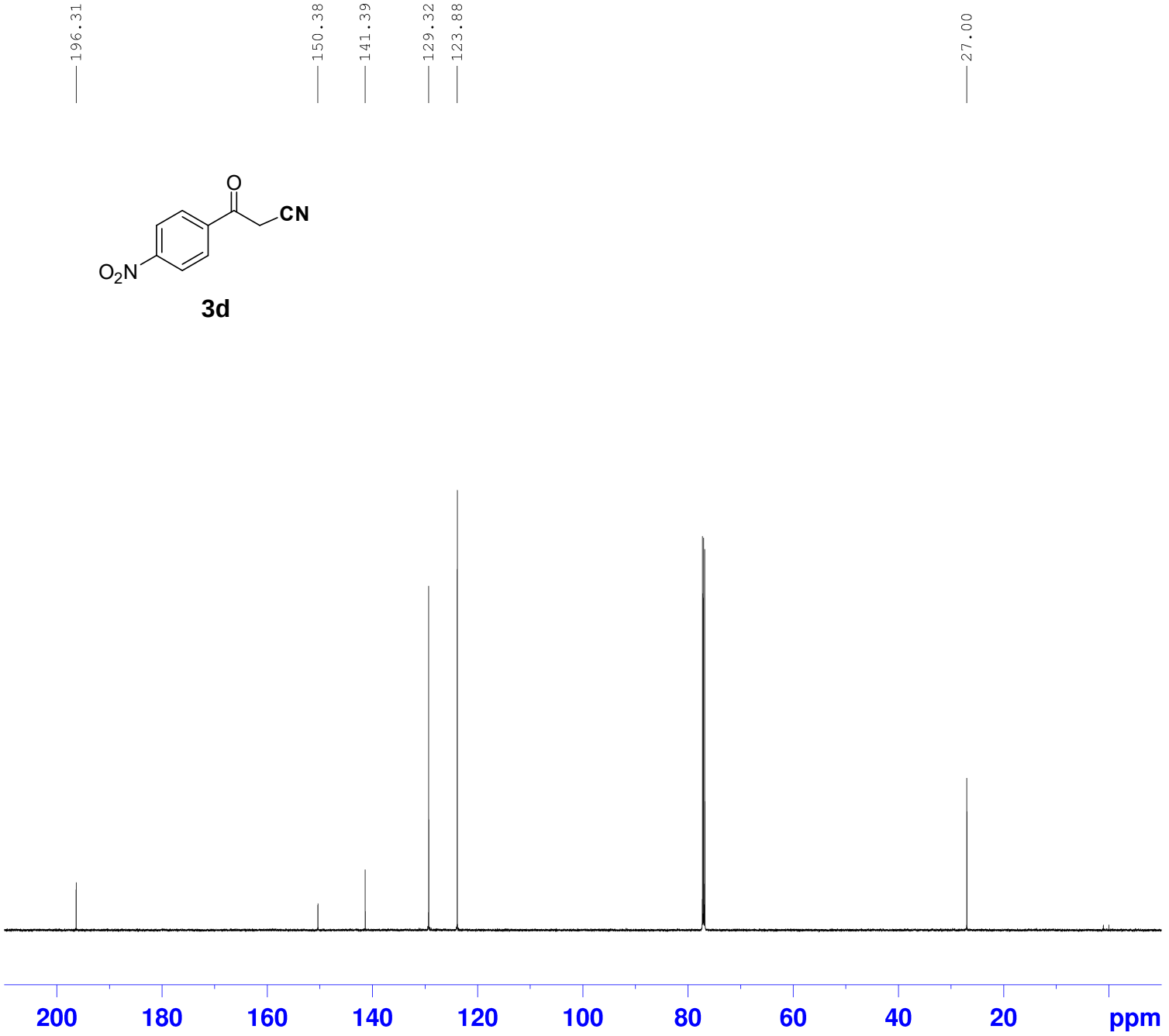


NAME	GG-591P-20230203
EXPNO	2
PROCNO	1
Date_	20230203
Time	17.28
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	190.02
DW	13.867 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	150.9279571 MHz
NUC1	13C
P1	11.90 usec
SI	32768
SF	150.9130239 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

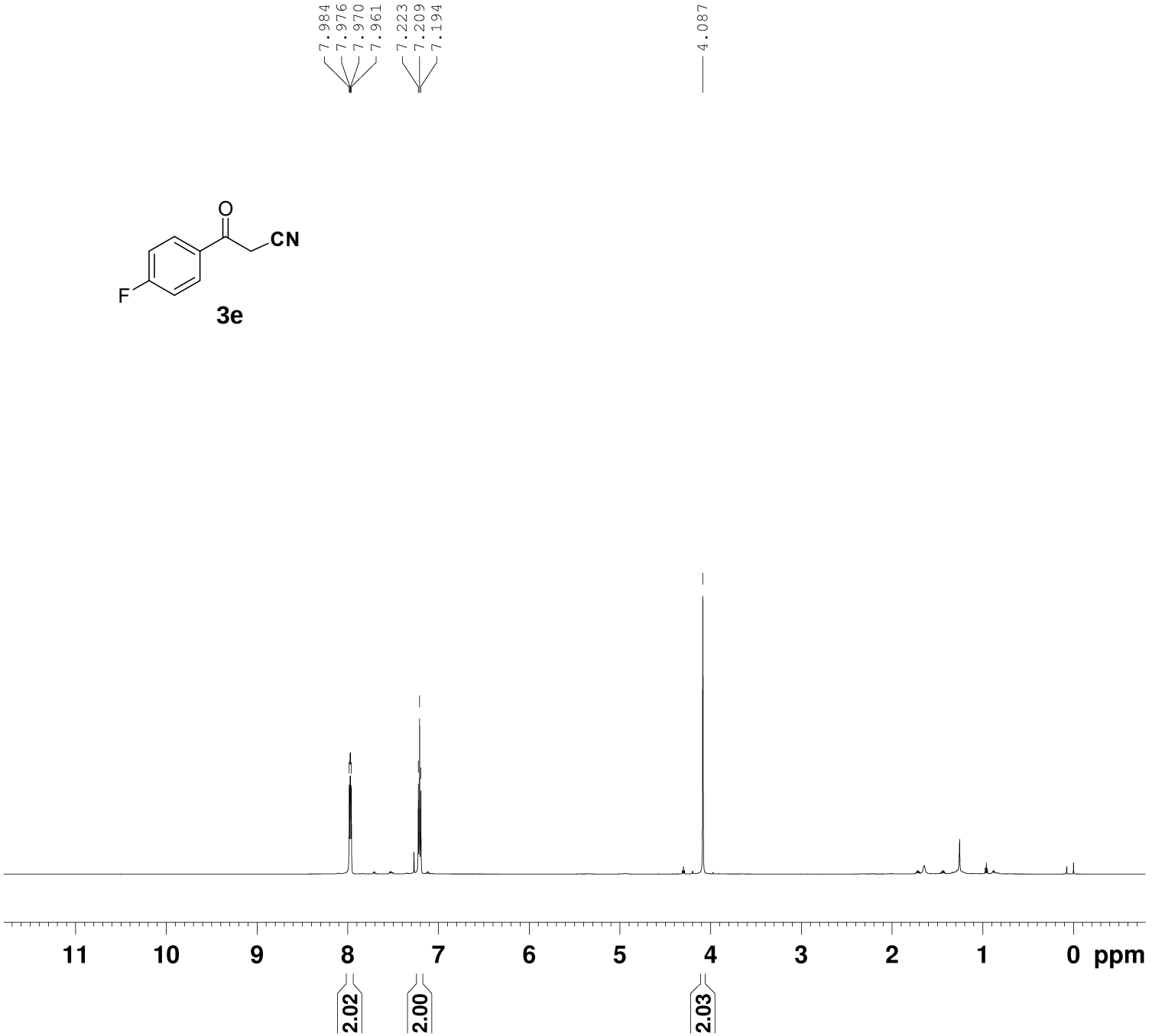


NAME	GG-694-1P-20221029
EXPNO	1
PROCNO	1
Date_	20221030
Time	4.07
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	0
SWH	9615.385 Hz
FIDRES	0.146719 Hz
AQ	3.4079220 sec
RG	76.92
DW	52.000 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1

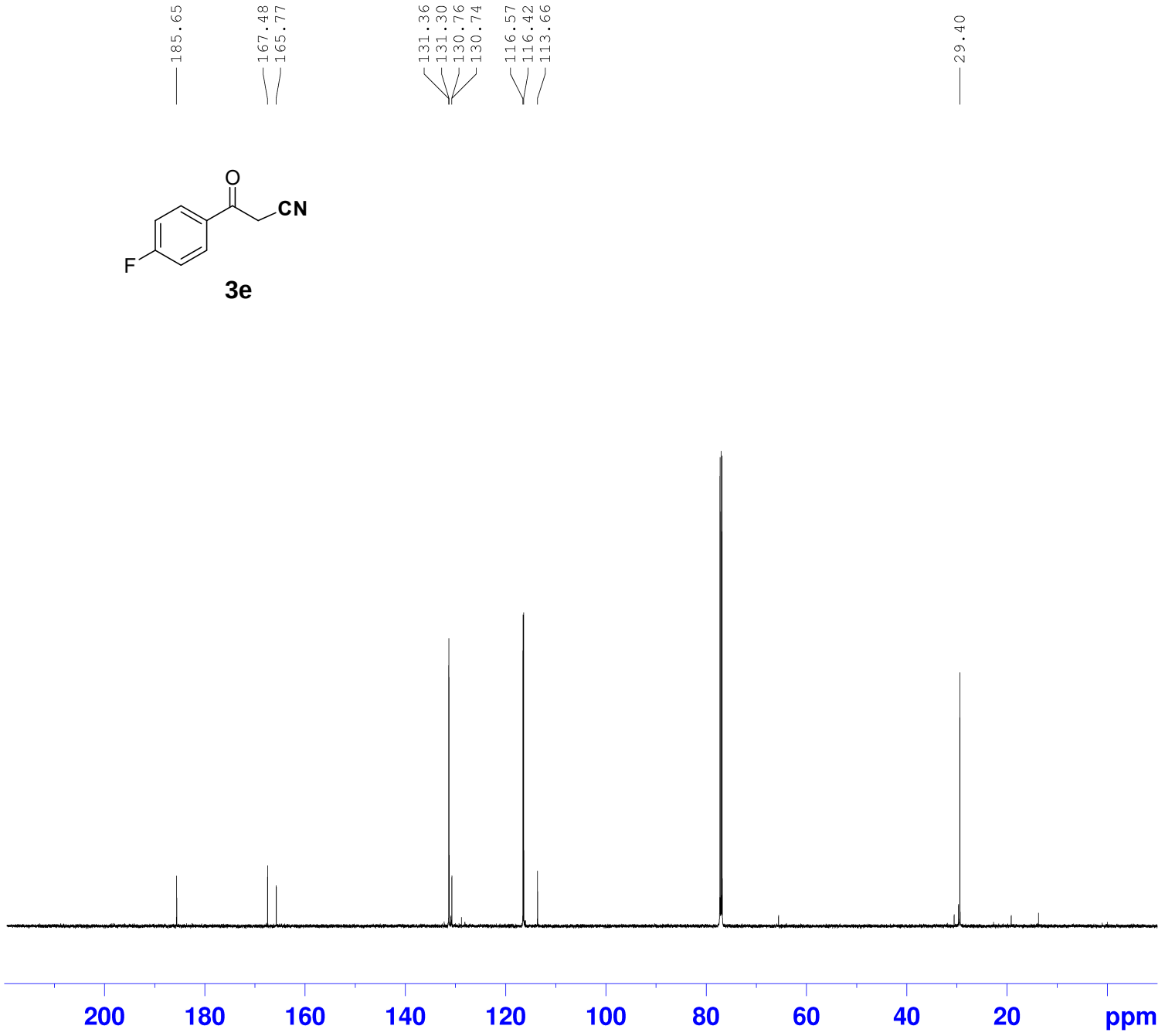
======== CHANNEL f1 ========	
SFO1	600.1739011 MHz
NUC1	1H
P1	9.96 usec
SI	65536
SF	600.1700064 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



NAME	GG-694-1P-20221029
EXPNO	2
PROCNO	1
Date_	20221030
Time	4.59
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	190.02
DW	13.867 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	150.9279571 MHz
NUC1	13C
P1	11.90 usec
SI	32768
SF	150.9128665 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

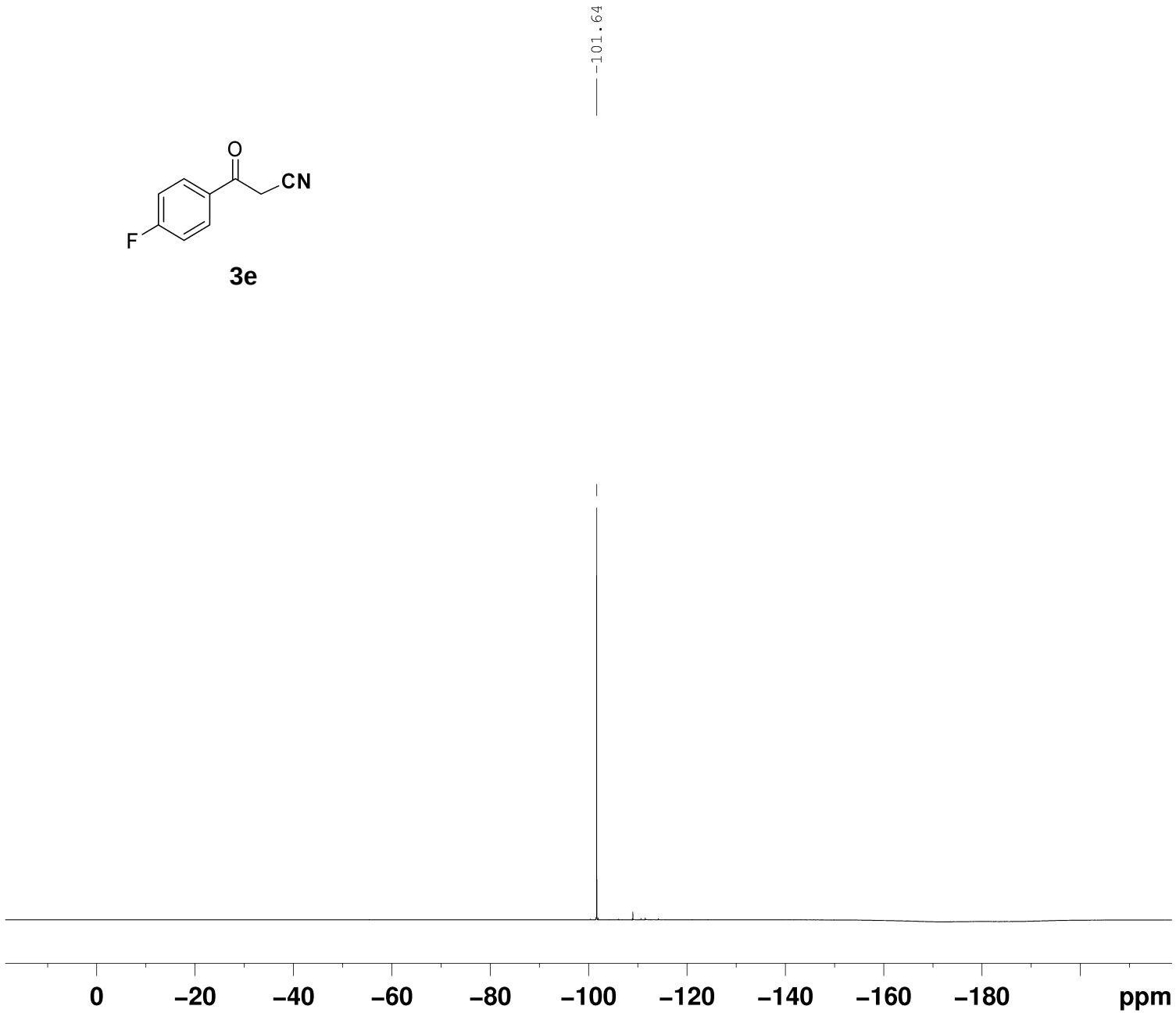


NAME	GG-646P-20220707
EXPNO	1
PROCNO	1
Date_	20220707
Time	12.44
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	0
SWH	9615.385 Hz
FIDRES	0.146719 Hz
AQ	3.4079220 sec
RG	76.92
DW	52.000 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	600.1739011 MHz
NUC1	1H
P1	9.96 usec
SI	65536
SF	600.1700081 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

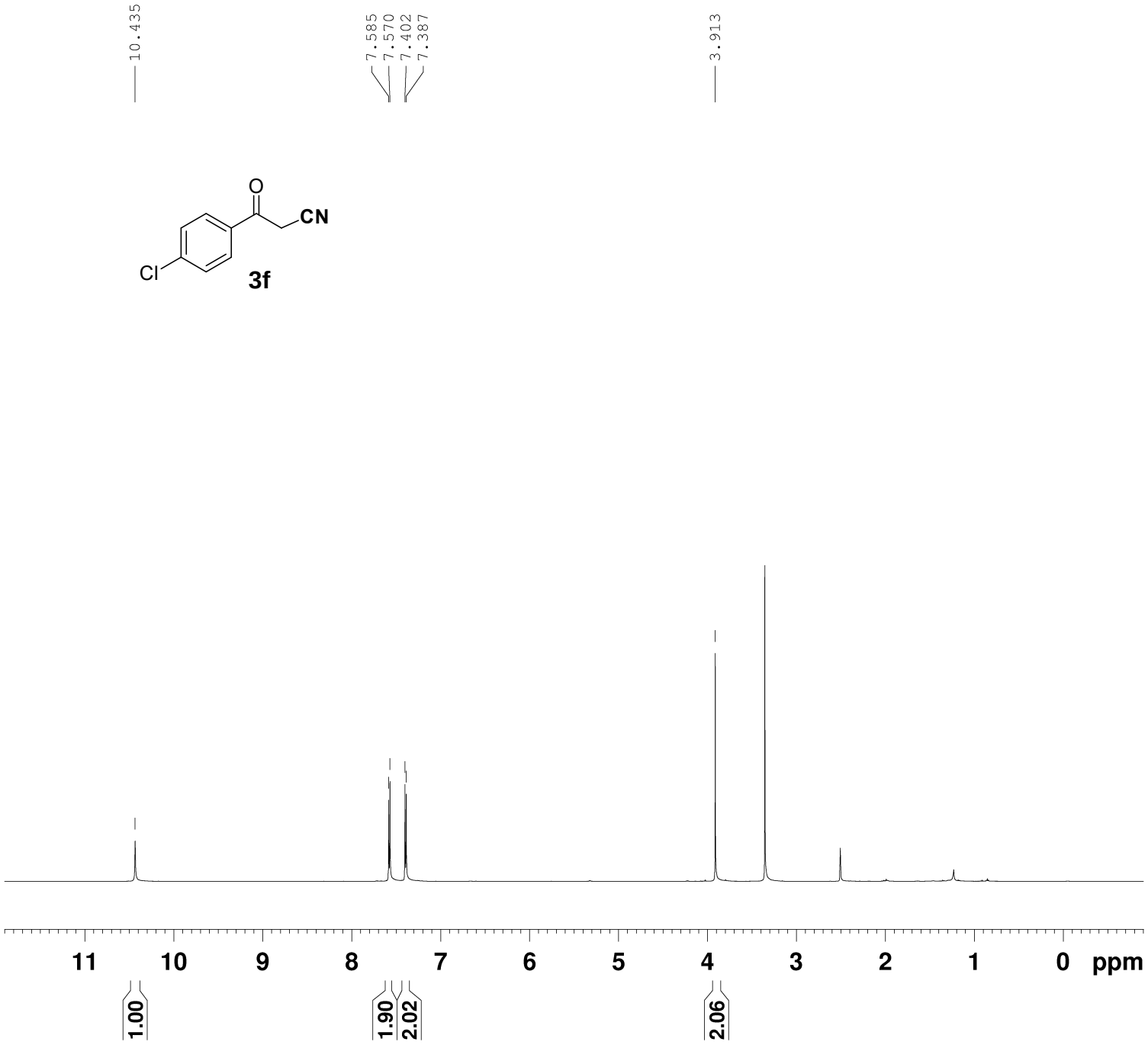


NAME	GG-646P-20220707
EXPNO	2
PROCNO	1
Date_	20220707
Time	13.35
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	190.02
DW	13.867 usec
DE	6.50 usec
TE	298.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	150.9279571 MHz
NUC1	13C
P1	11.90 usec
SI	32768
SF	150.9128665 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

3e

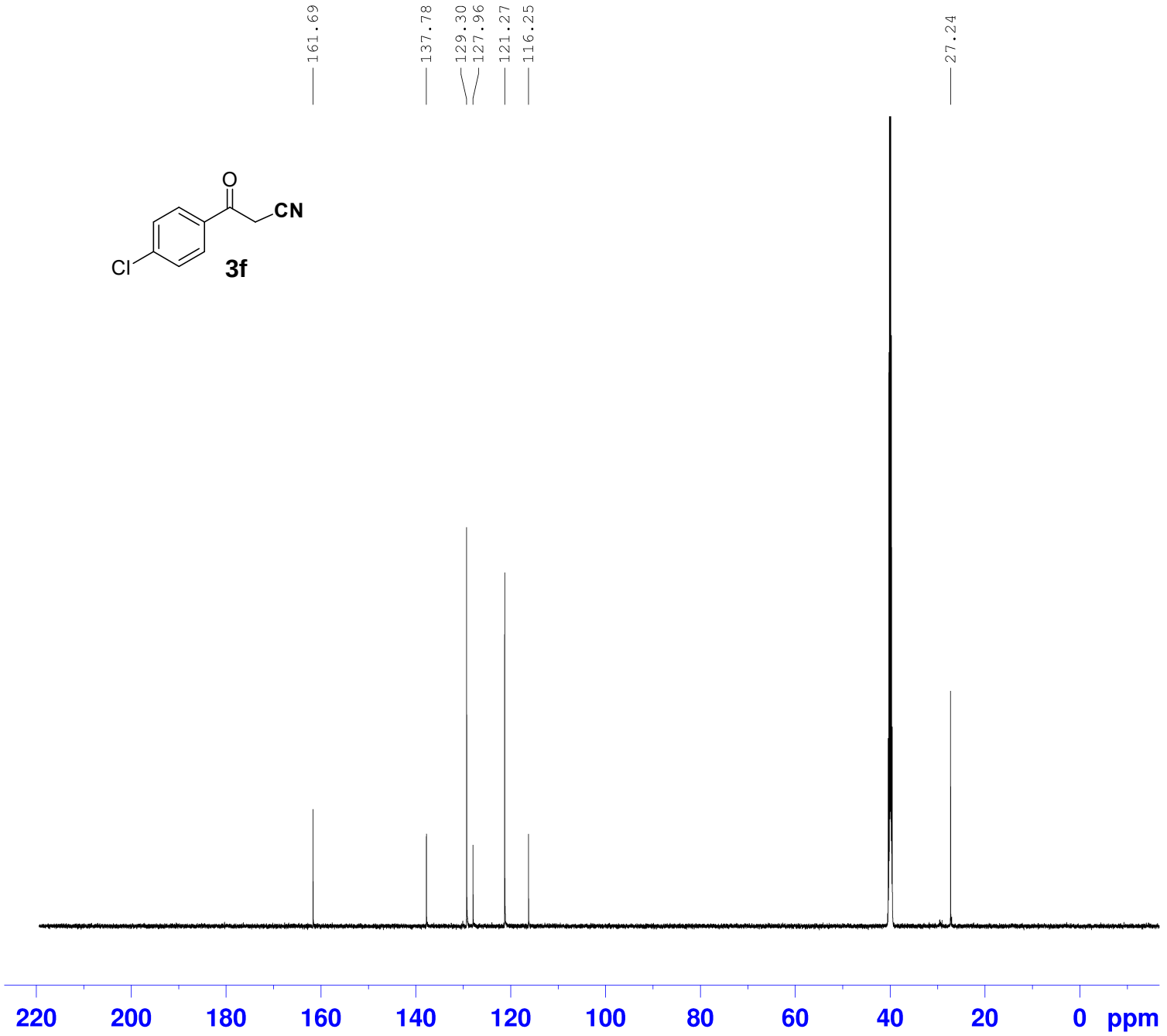


NAME	GG-786P-20230206
EXPNO	2
PROCNO	1
Date_	20230206
Time	20.38
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgflqn
TD	131072
SOLVENT	CDCl3
NS	16
DS	4
SWH	133928.578 Hz
FIDRES	1.021794 Hz
AQ	0.4893855 sec
RG	190.02
DW	3.733 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	564.6675534 MHz
NUC1	19F
P1	12.00 usec
SI	65536
SF	564.7240258 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

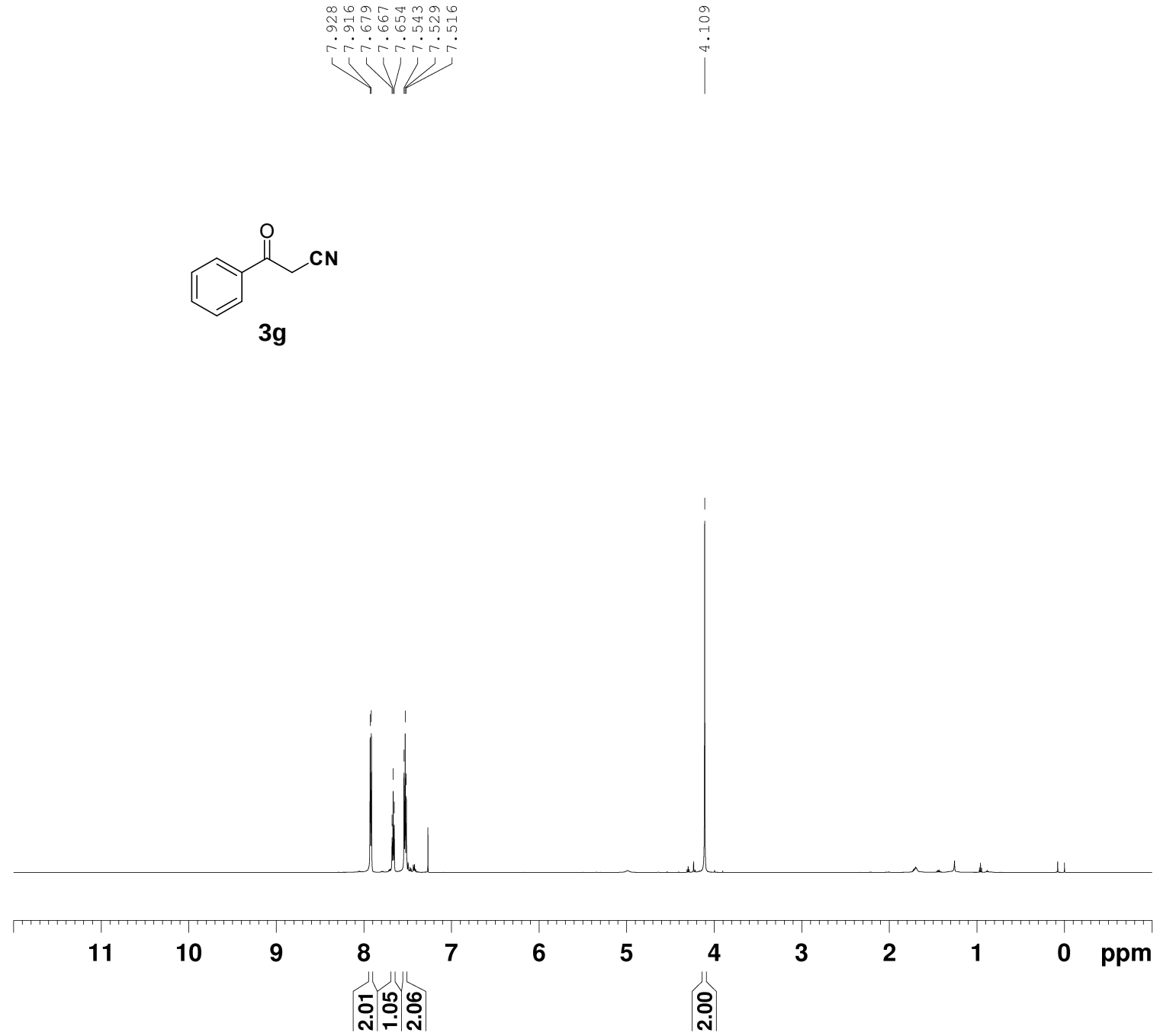


NAME	GG-669P-20220917
EXPNO	1
PROCNO	1
Date_	20220917
Time	12.30
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
DS	0
SWH	9615.385 Hz
FIDRES	0.146719 Hz
AQ	3.4079220 sec
RG	87.54
DW	52.000 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
SFO1	600.1739011 MHz
NUC1	1H
P1	9.96 usec
SI	65536
SF	600.1700000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

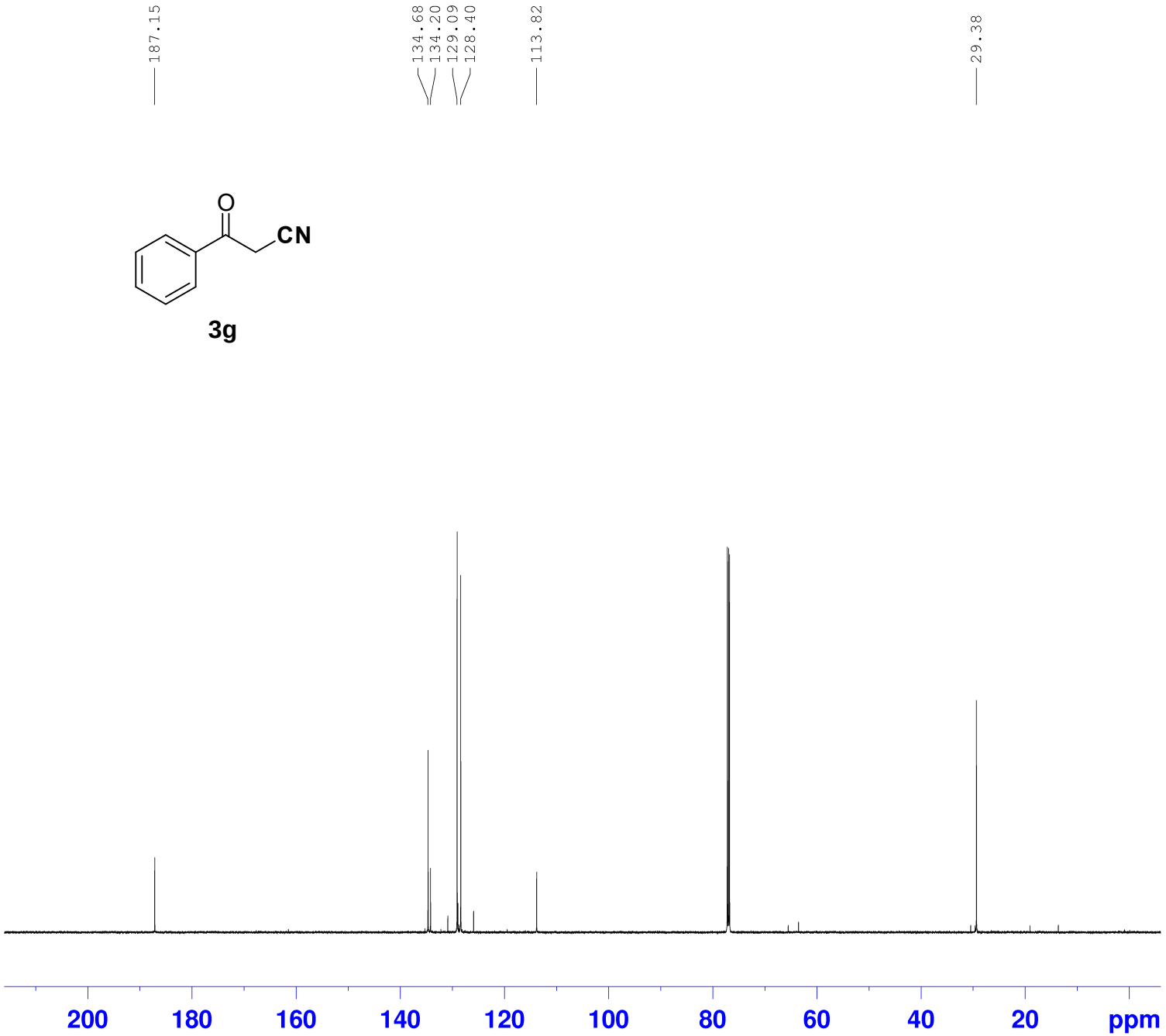


NAME	GG-669P-20220917
EXPNO	2
PROCNO	1
Date_	20220917
Time	13.22
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	1024
DS	4
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	190.02
DW	13.867 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	150.9279571 MHz
NUC1	13C
P1	11.90 usec
SI	32768
SF	150.9128665 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

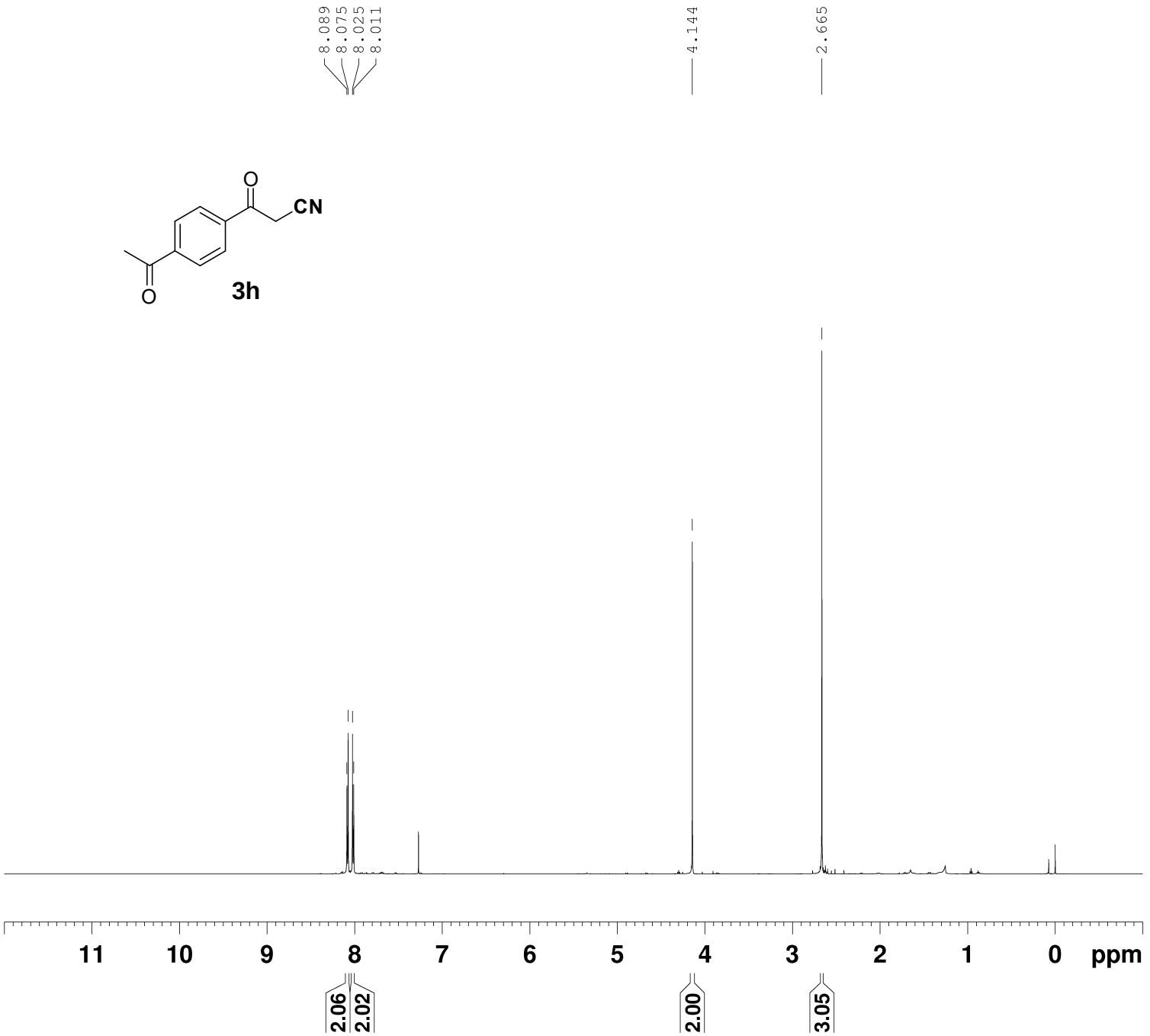


NAME	GG-586P-20220611
EXPNO	1
PROCNO	1
Date_	20220611
Time	12.47
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	0
SWH	9615.385 Hz
FIDRES	0.146719 Hz
AQ	3.4079220 sec
RG	62.22
DW	52.000 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1

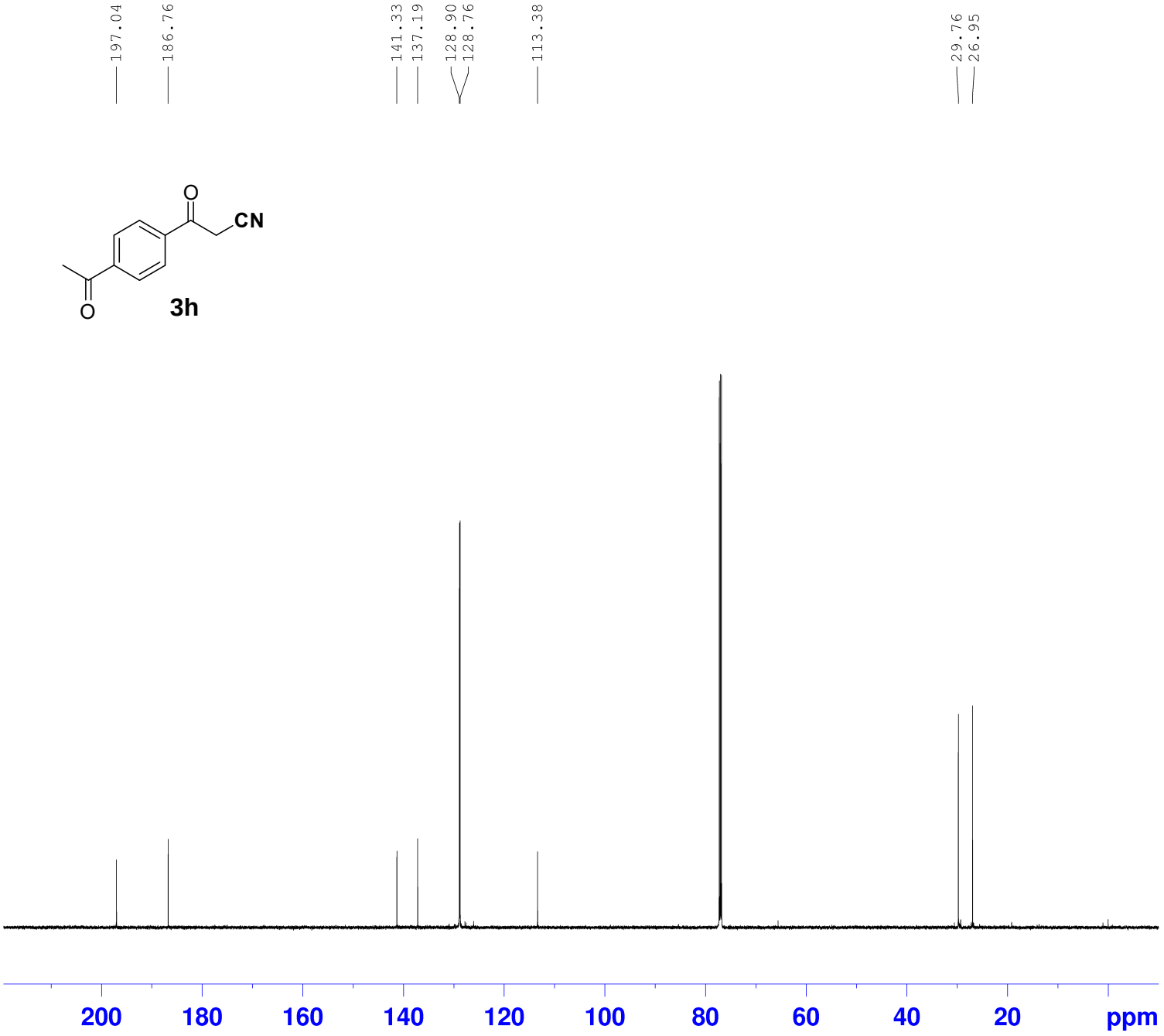
======== CHANNEL f1 ========	
SFO1	600.1739011 MHz
NUC1	1H
P1	9.96 usec
SI	65536
SF	600.1700125 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



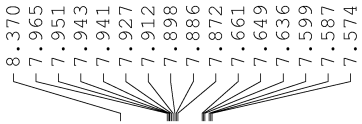
NAME	GG-586P-20220611
EXPNO	2
PROCNO	1
Date_	20220611
Time	13.39
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	190.02
DW	13.867 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	150.9279571 MHz
NUC1	13C
P1	11.90 usec
SI	32768
SF	150.9128799 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

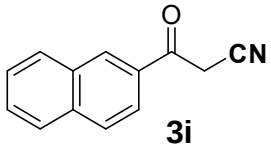


NAME	GG-692-2P-20221027
EXPNO	1
PROCNO	1
Date_	20221028
Time	2.14
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	0
SWH	9615.385 Hz
FIDRES	0.146719 Hz
AQ	3.4079220 sec
RG	76.92
DW	52.000 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	600.1739011 MHz
NUC1	1H
P1	9.96 usec
SI	65536
SF	600.1700080 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



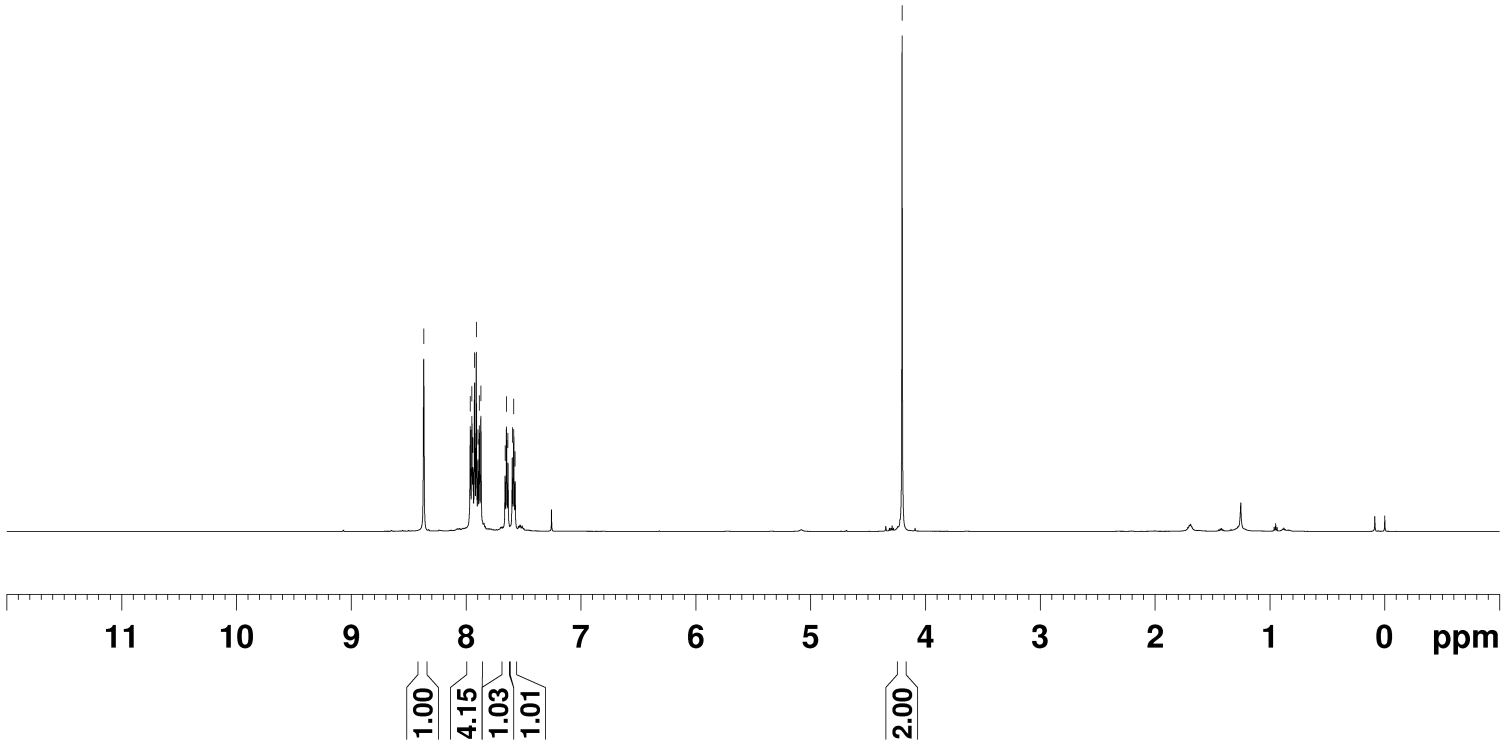
NAME	GG-692-2P-20221027
EXPNO	2
PROCNO	1
Date_	20221028
Time	3.06
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	190.02
DW	13.867 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	150.9279571 MHz
NUC1	13C
P1	11.90 usec
SI	32768
SF	150.9128665 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

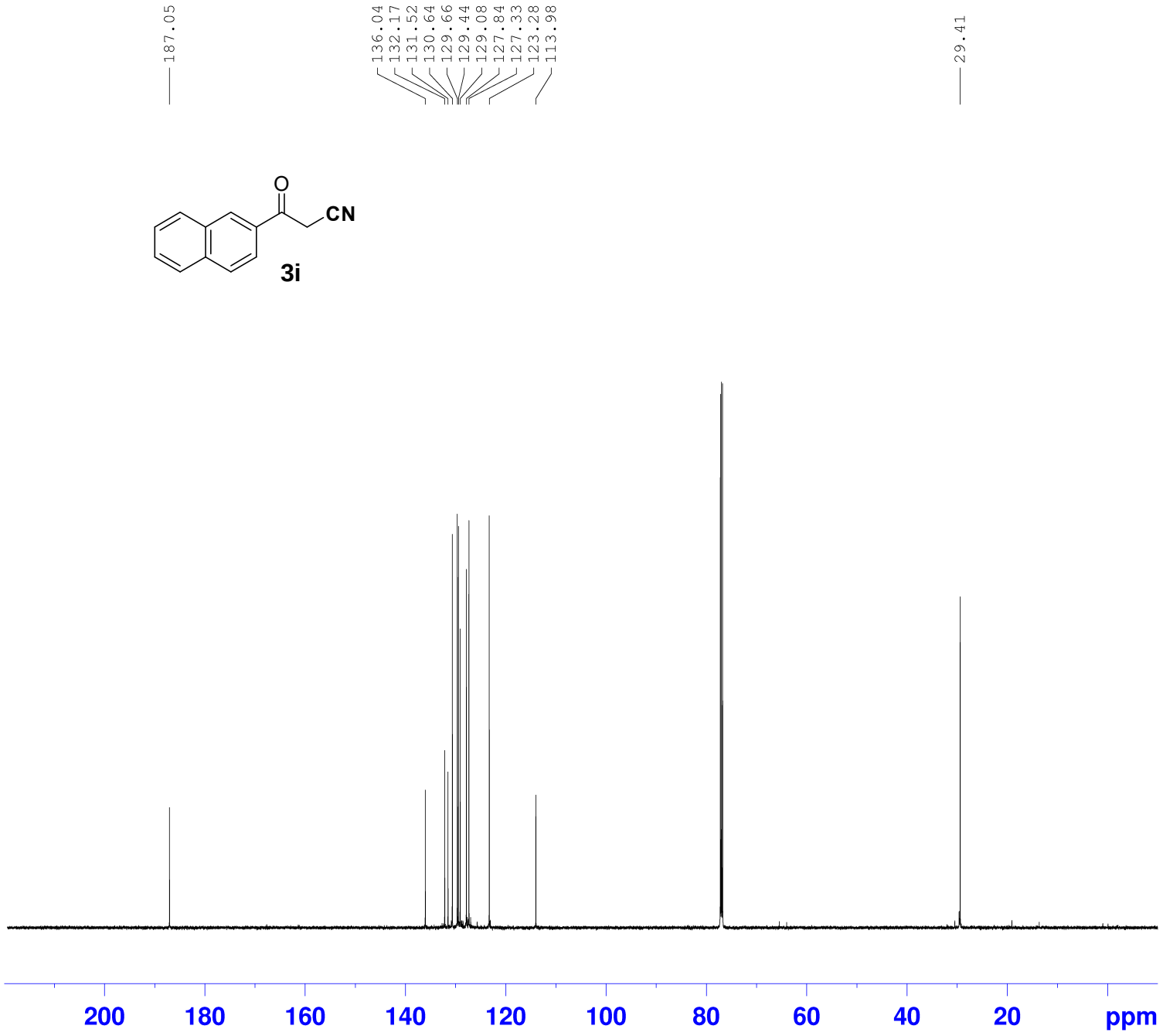




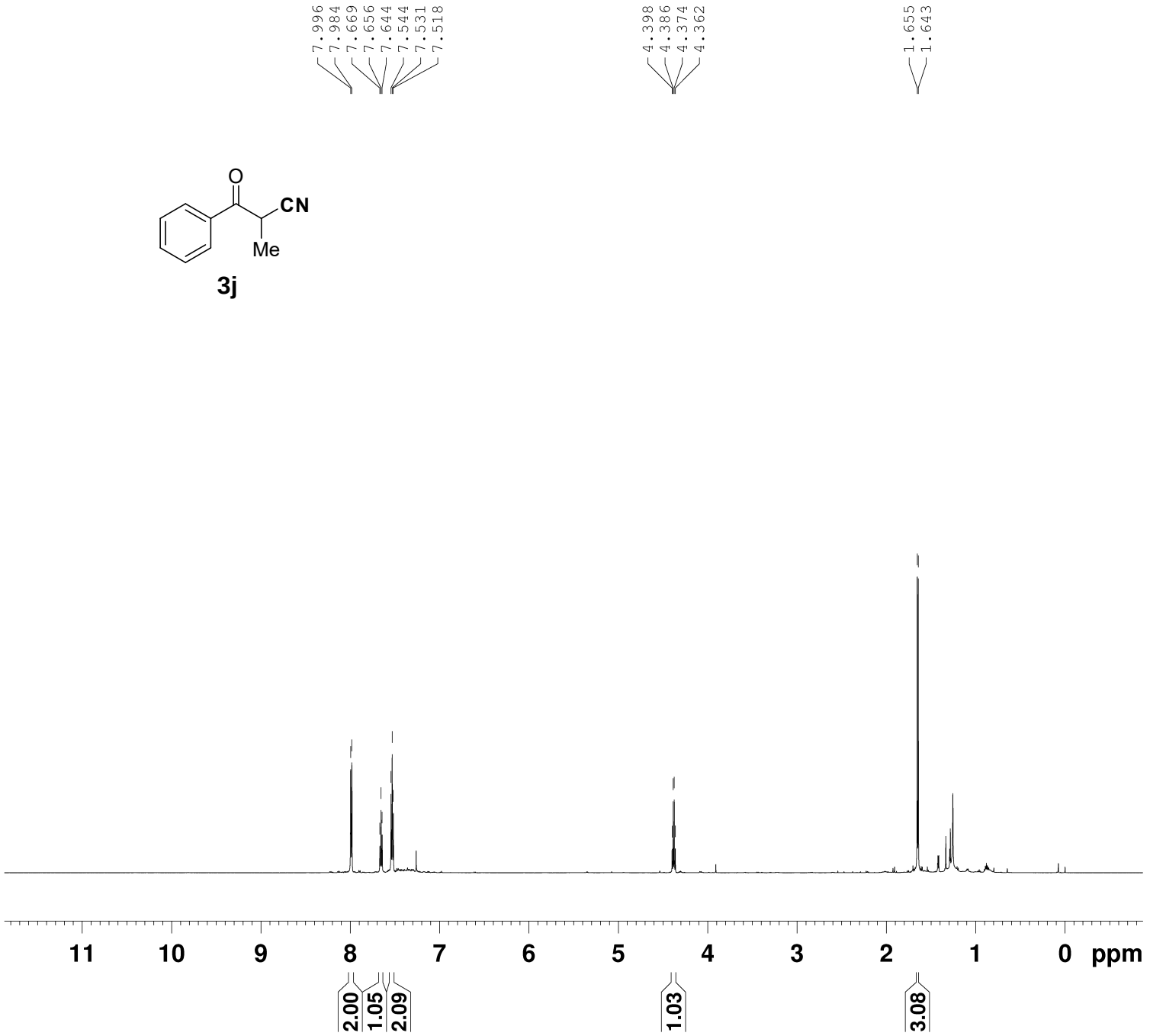
3i

```
NAME      GG-647P-20220707
EXPNO                    1
PROCNO                   1
Date_             20220707
Time                 11.54
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               9615.385 Hz
FIDRES            0.146719 Hz
AQ                3.4079220 sec
RG                   50.85
DW                  52.000 usec
DE                   6.50 usec
TE                  298.0 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          600.1739011 MHz
NUC1                    1H
P1                   9.96 usec
SI                  65536
SF            600.1700159 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

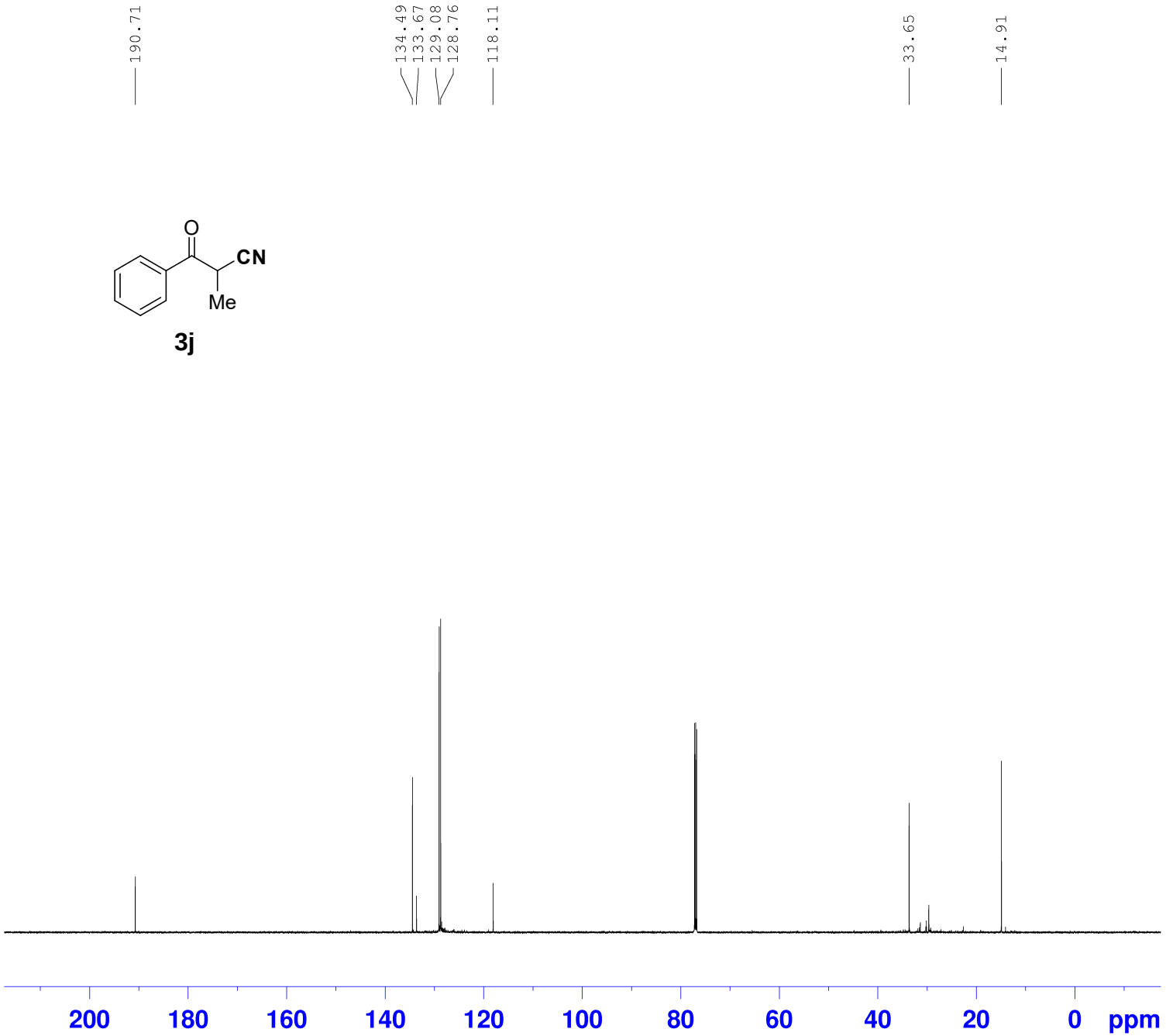




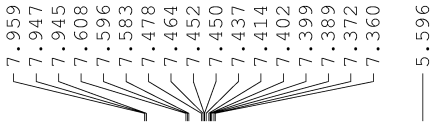
NAME	GG-647P-20220707
EXPNO	2
PROCNO	1
Date_	20220707
Time	12.35
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	800
DS	4
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	190.02
DW	13.867 usec
DE	6.50 usec
TE	298.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	150.9279571 MHz
NUC1	13C
P1	11.90 usec
SI	32768
SF	150.9128821 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

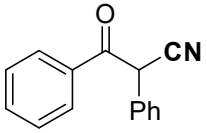


NAME	GG-679P-20220930
EXPNO	1
PROCNO	1
Date_	20220930
Time	10.52
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	0
SWH	9615.385 Hz
FIDRES	0.146719 Hz
AQ	3.4079220 sec
RG	62.22
DW	52.000 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	600.1739011 MHz
NUC1	1H
P1	9.96 usec
SI	65536
SF	600.1700124 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00




```
NAME      GG-679P-20220930
EXPNO                    2
PROCNO                   1
Date_             20220930
Time                 11.43
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH              36057.691 Hz
FIDRES            0.550197 Hz
AQ               0.9088159 sec
RG                   190.02
DW                   13.867 usec
DE                     6.50 usec
TE                    298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1          150.9279571 MHz
NUC1                    13C
P1                   11.90 usec
SI                   32768
SF            150.9128744 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

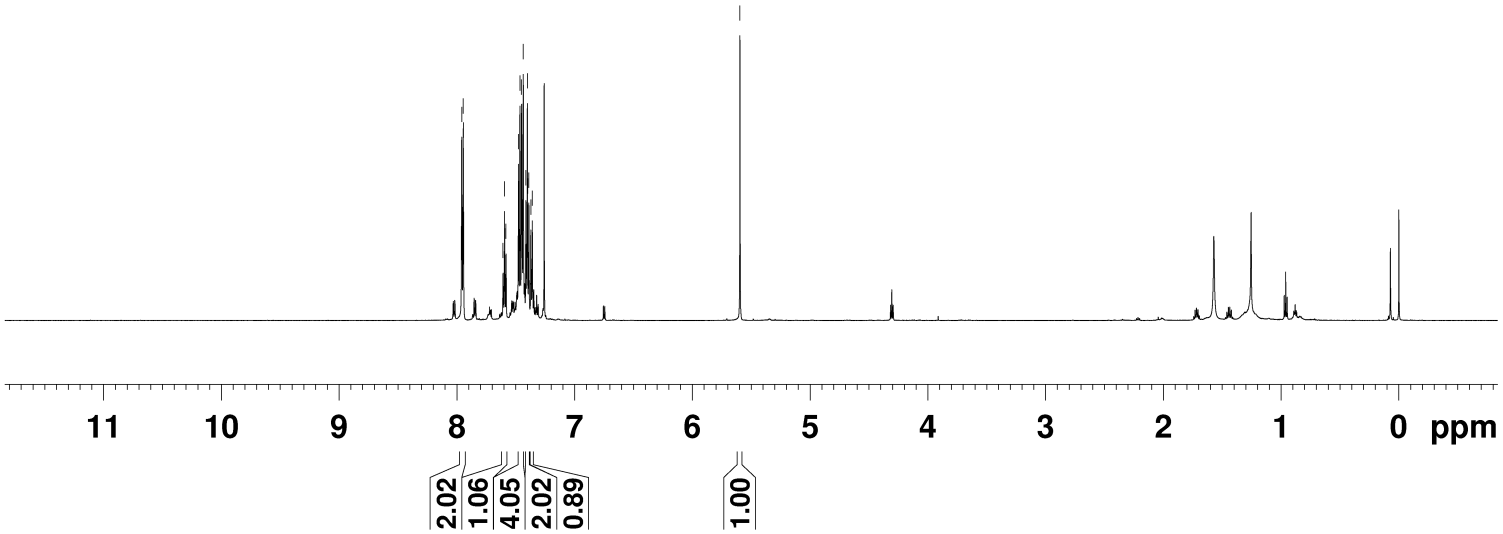


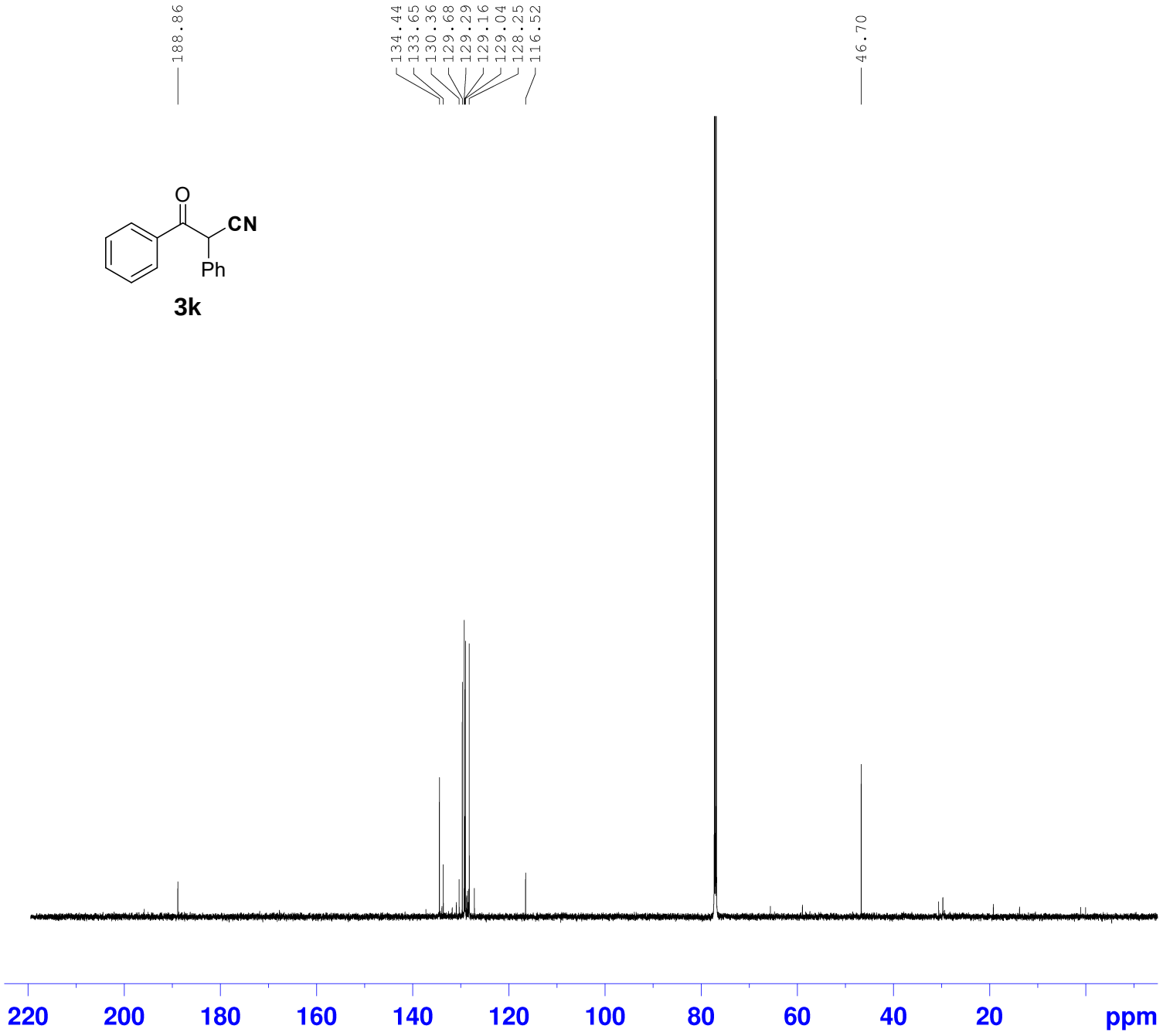


3k

NAME	GG-642P-20220710
EXPNO	1
PROCNO	1
Date_	20220711
Time	13.50
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	0
SWH	9615.385 Hz
FIDRES	0.146719 Hz
AQ	3.4079220 sec
RG	109.27
DW	52.000 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1

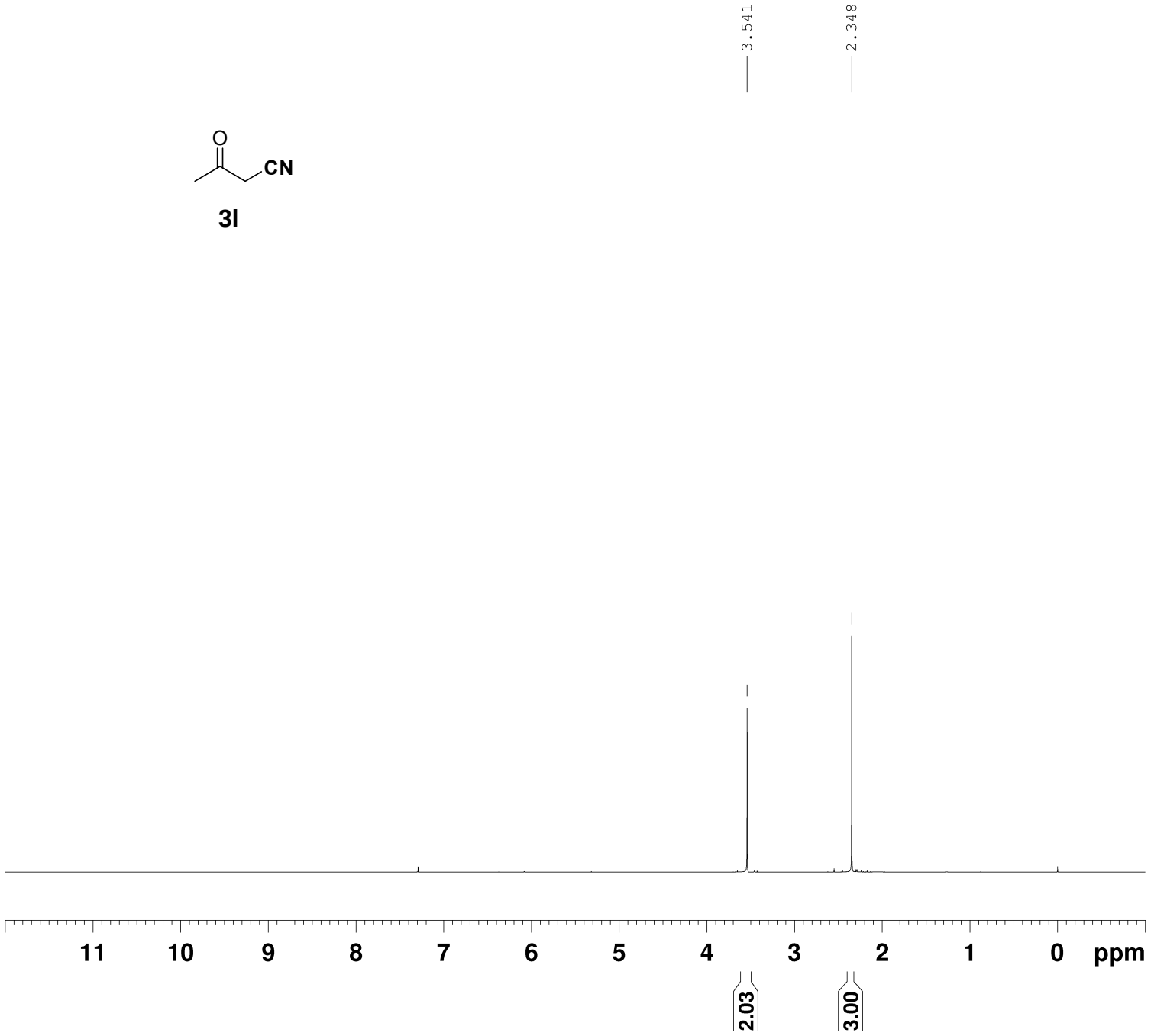
======== CHANNEL f1 ========	
SFO1	600.1739011 MHz
NUC1	1H
P1	9.96 usec
SI	65536
SF	600.1700152 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



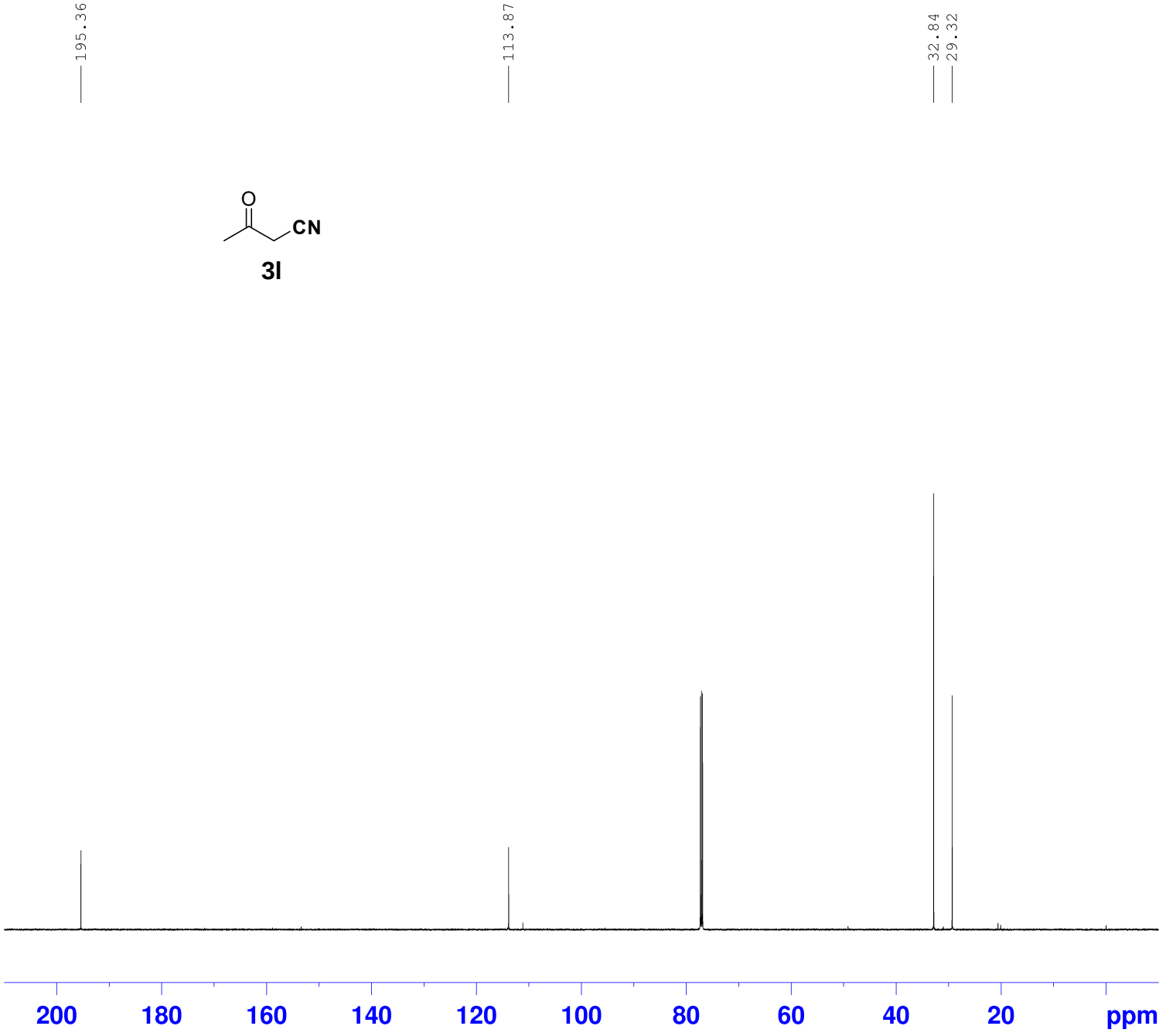


NAME	GG-642P-20220710
EXPNO	2
PROCNO	1
Date_	20220711
Time	14.42
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	190.02
DW	13.867 usec
DE	6.50 usec
TE	298.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	150.9279571 MHz
NUC1	13C
P1	11.90 usec
SI	32768
SF	150.9128665 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

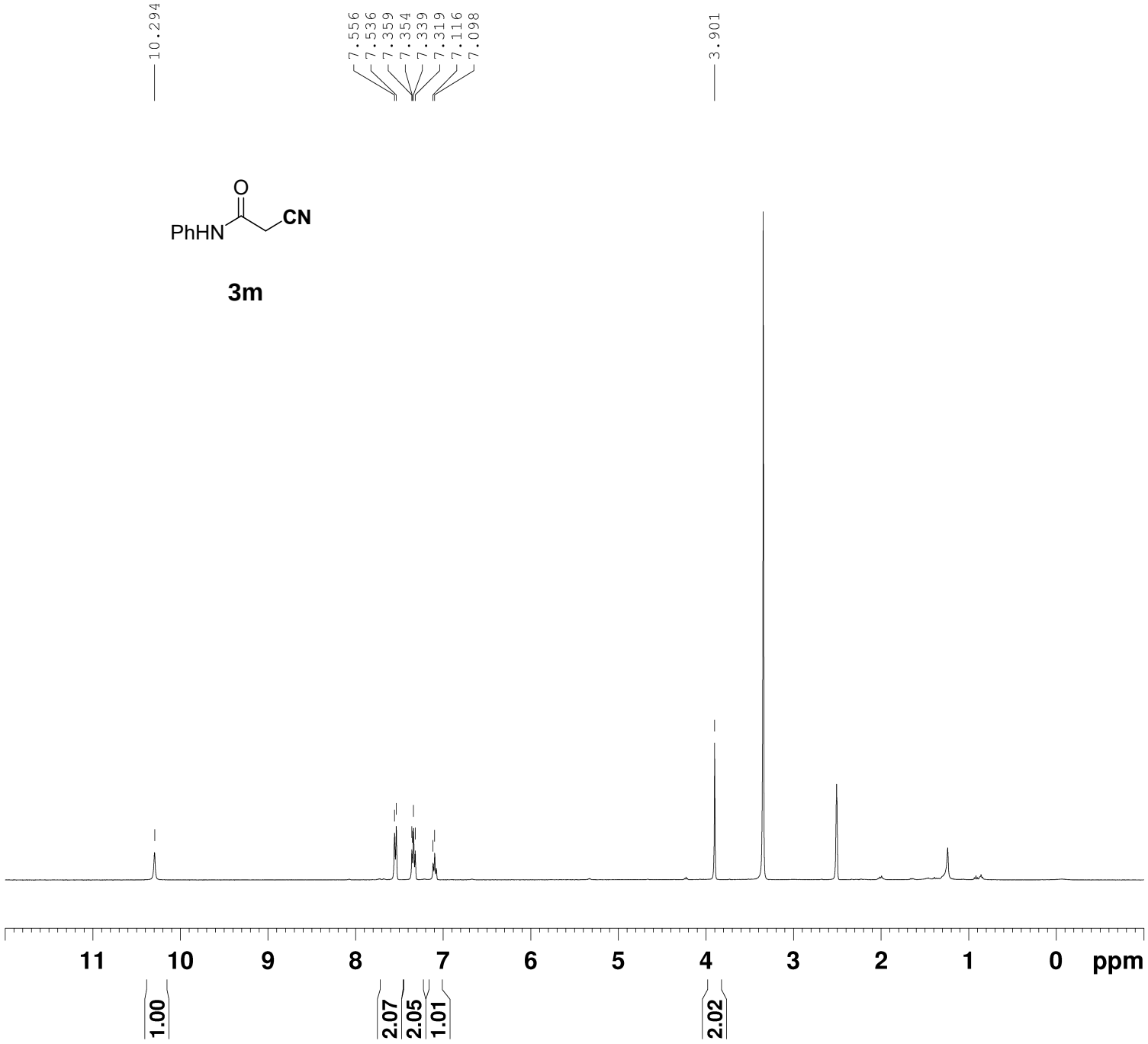
3l



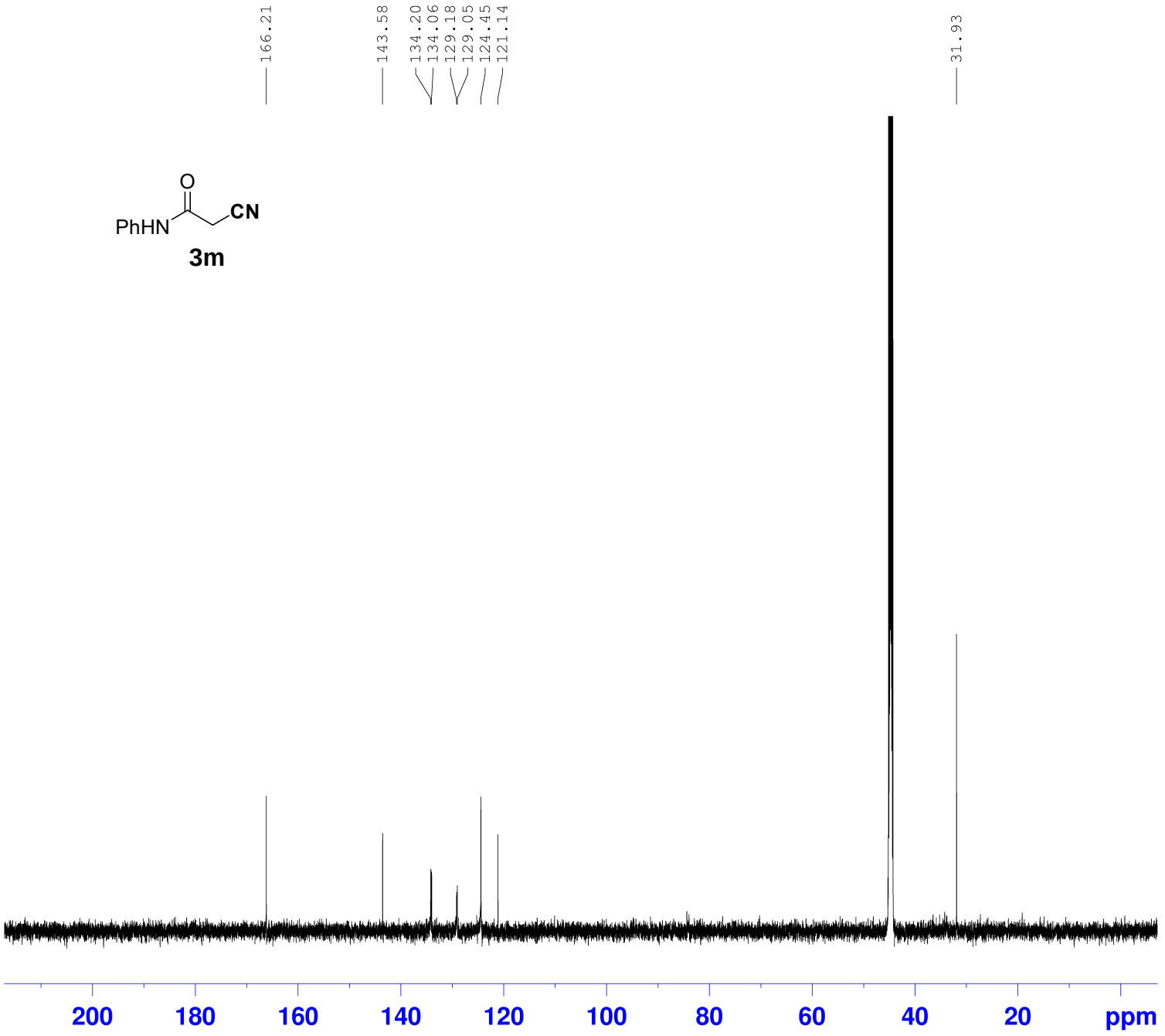
NAME	GG-703P-20221031
EXPNO	1
PROCNO	1
Date_	20221031
Time	22.37
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	0
SWH	9615.385 Hz
FIDRES	0.146719 Hz
AQ	3.4079220 sec
RG	56.75
DW	52.000 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	600.1739011 MHz
NUC1	1H
P1	9.96 usec
SI	65536
SF	600.1699952 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



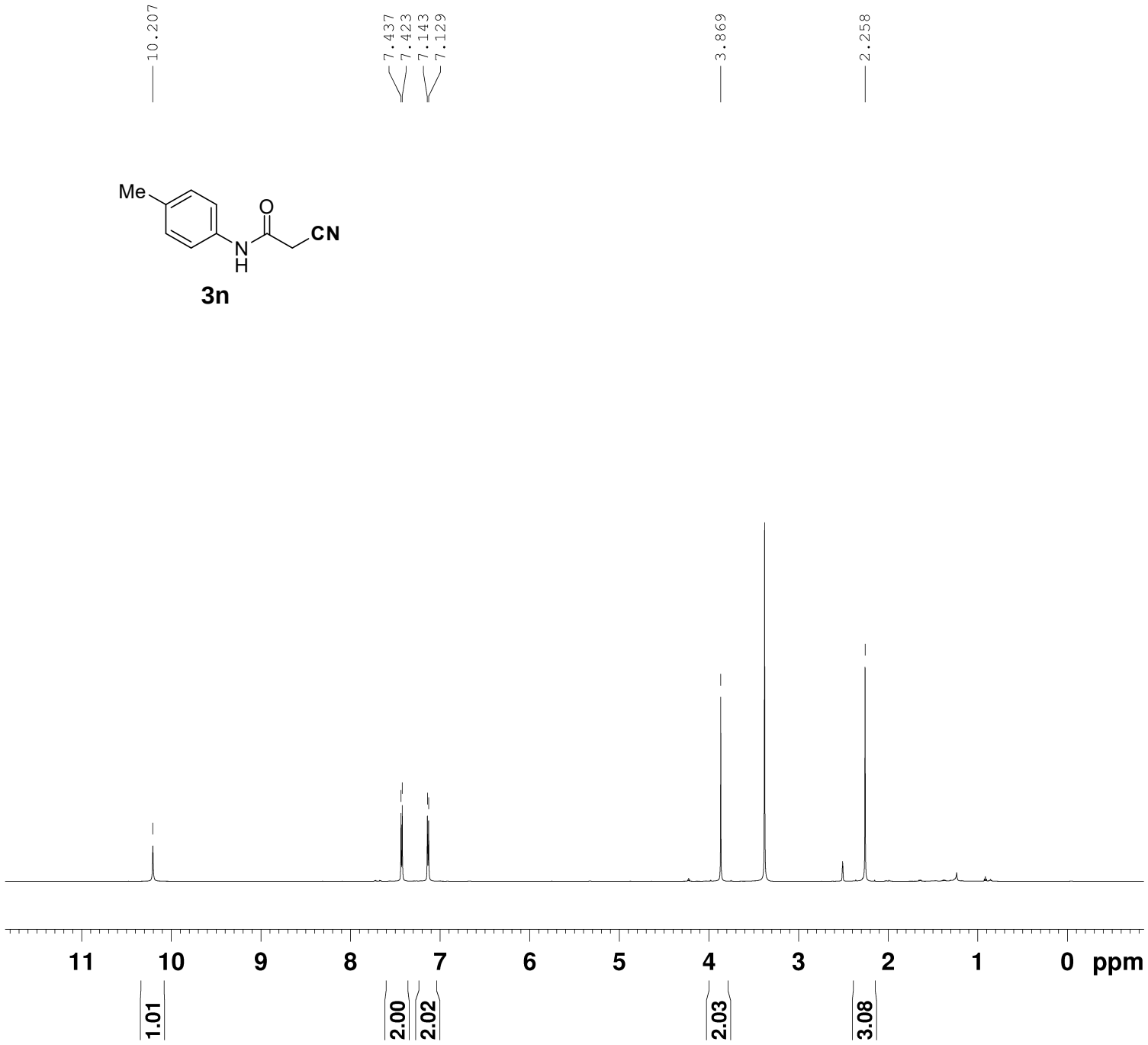
NAME	GG-703P-20221031
EXPNO	2
PROCNO	1
Date_	20221031
Time	23.18
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	800
DS	4
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	190.02
DW	13.867 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	150.9279571 MHz
NUC1	13C
P1	11.90 usec
SI	32768
SF	150.9128665 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



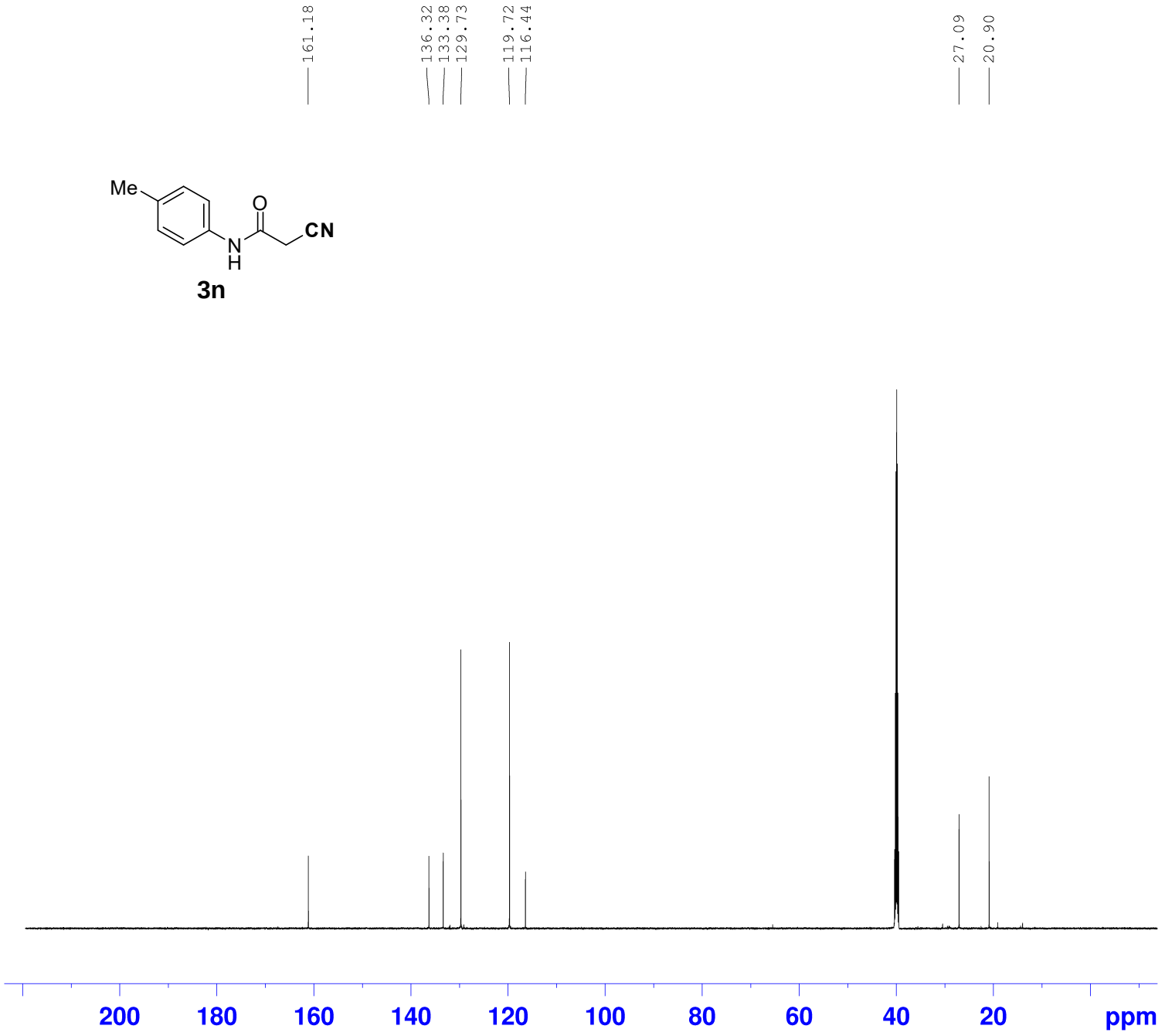
NAME	gg-569p-1-20220607
EXPNO	1
PROCNO	1
Date_	20220607
Time	22.04
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	32768
SOLVENT	DMSO
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	322
DW	78.200 usec
DE	6.50 usec
TE	296.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.40 usec
PL1	-1.00 dB
PL1W	17.01305389 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



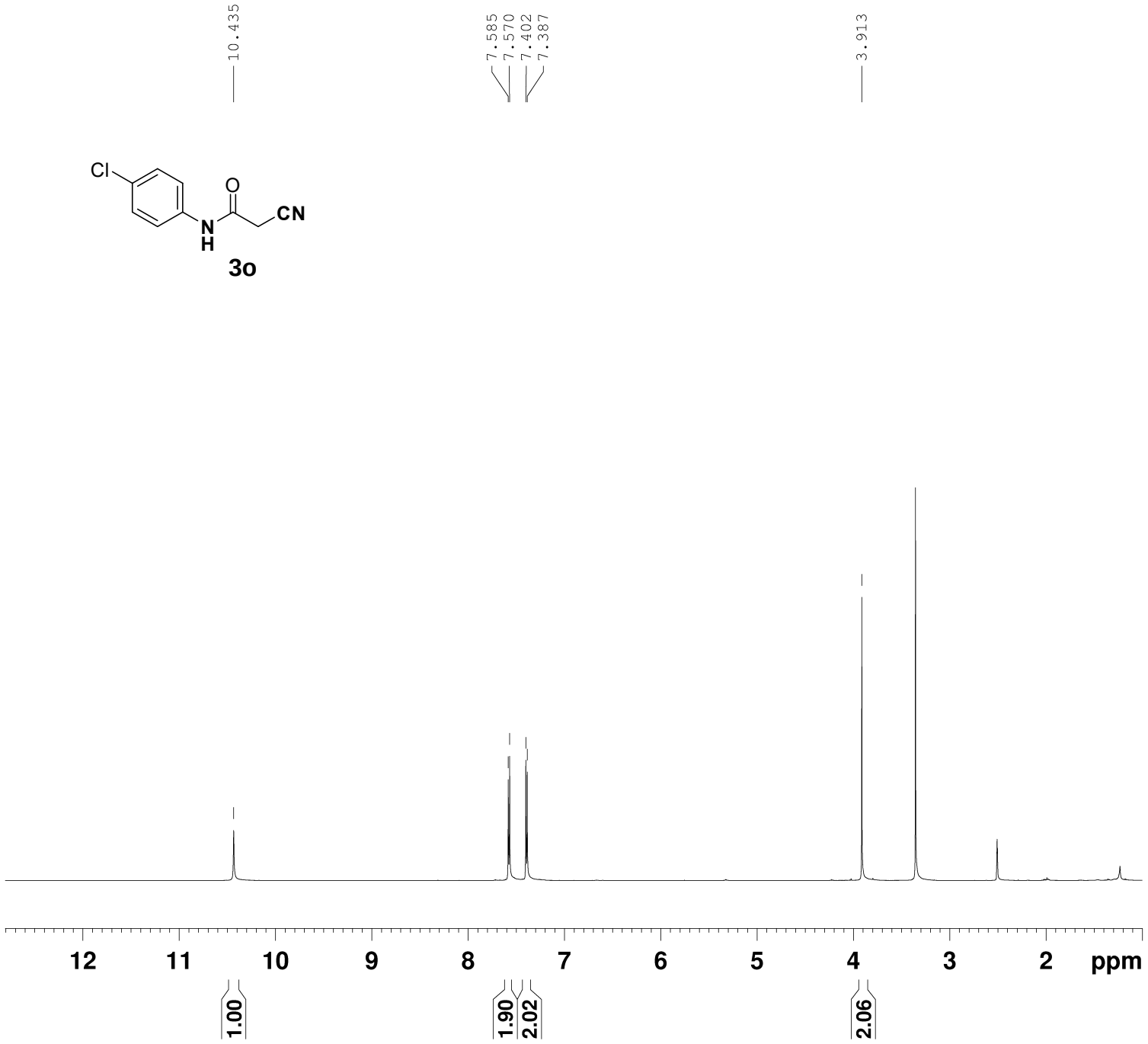
NAME	GG-569P-3-220607
EXPNO	2
PROCNO	1
Date_	20220608
Time	6.45
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	824
DS	4
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	190.02
DW	13.867 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	150.9279571 MHz
NUC1	13C
P1	11.90 usec
SI	32768
SF	150.9128665 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



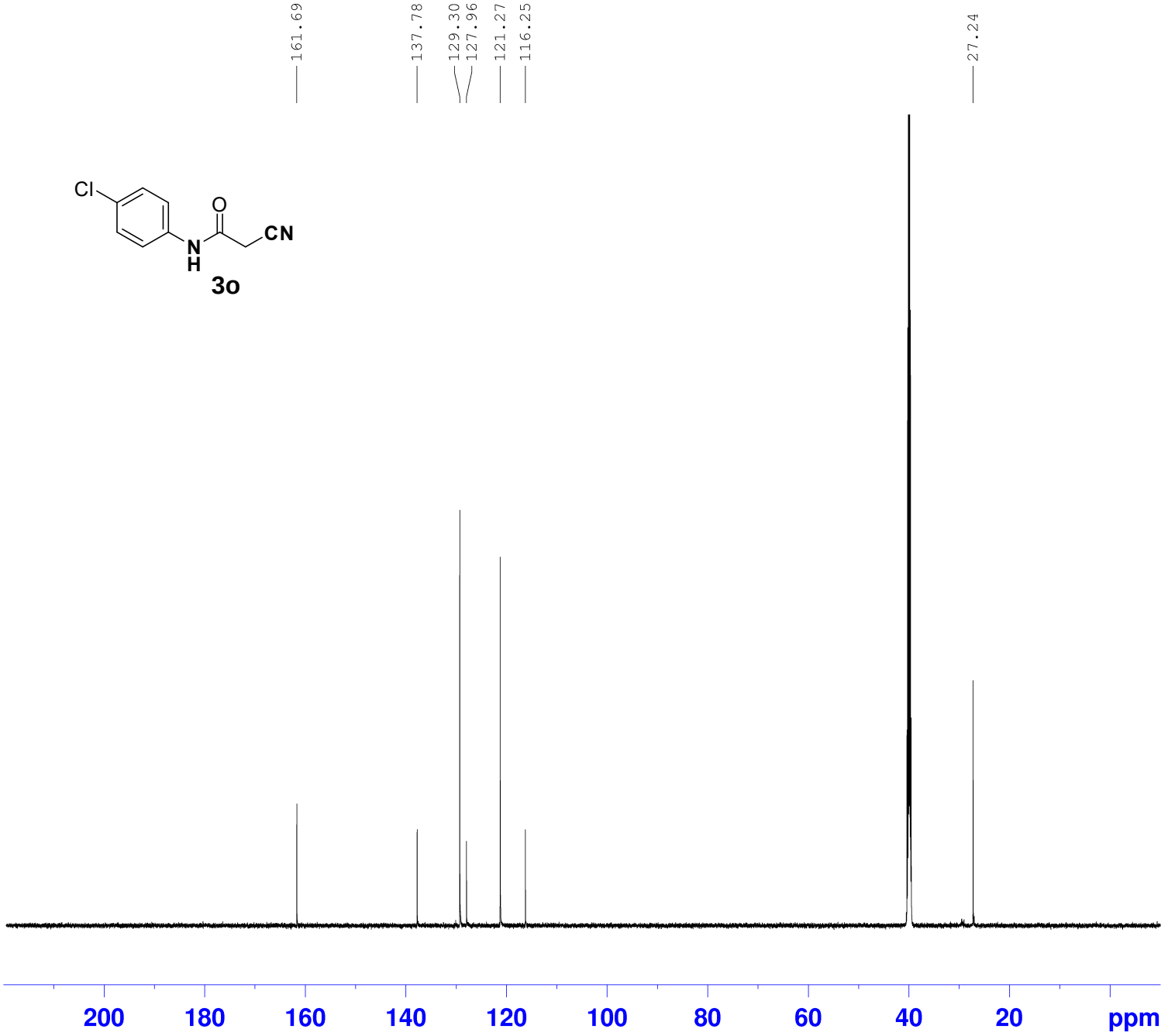

```
NAME      GG-615P-20220629
EXPNO                    1
PROCNO                   1
Date_             20220629
Time                 10.54
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        8
DS                        0
SWH               9615.385 Hz
FIDRES           0.146719 Hz
AQ               3.4079220 sec
RG                    56.75
DW                52.000 usec
DE                 6.50 usec
TE                 298.0 K
D1            1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1         600.1739011 MHz
NUC1                    1H
P1                   9.96 usec
SI                    65536
SF           600.1700000 MHz
WDW                     EM
SSB                      0
LB                  0.30 Hz
GB                       0
PC                    1.00
```



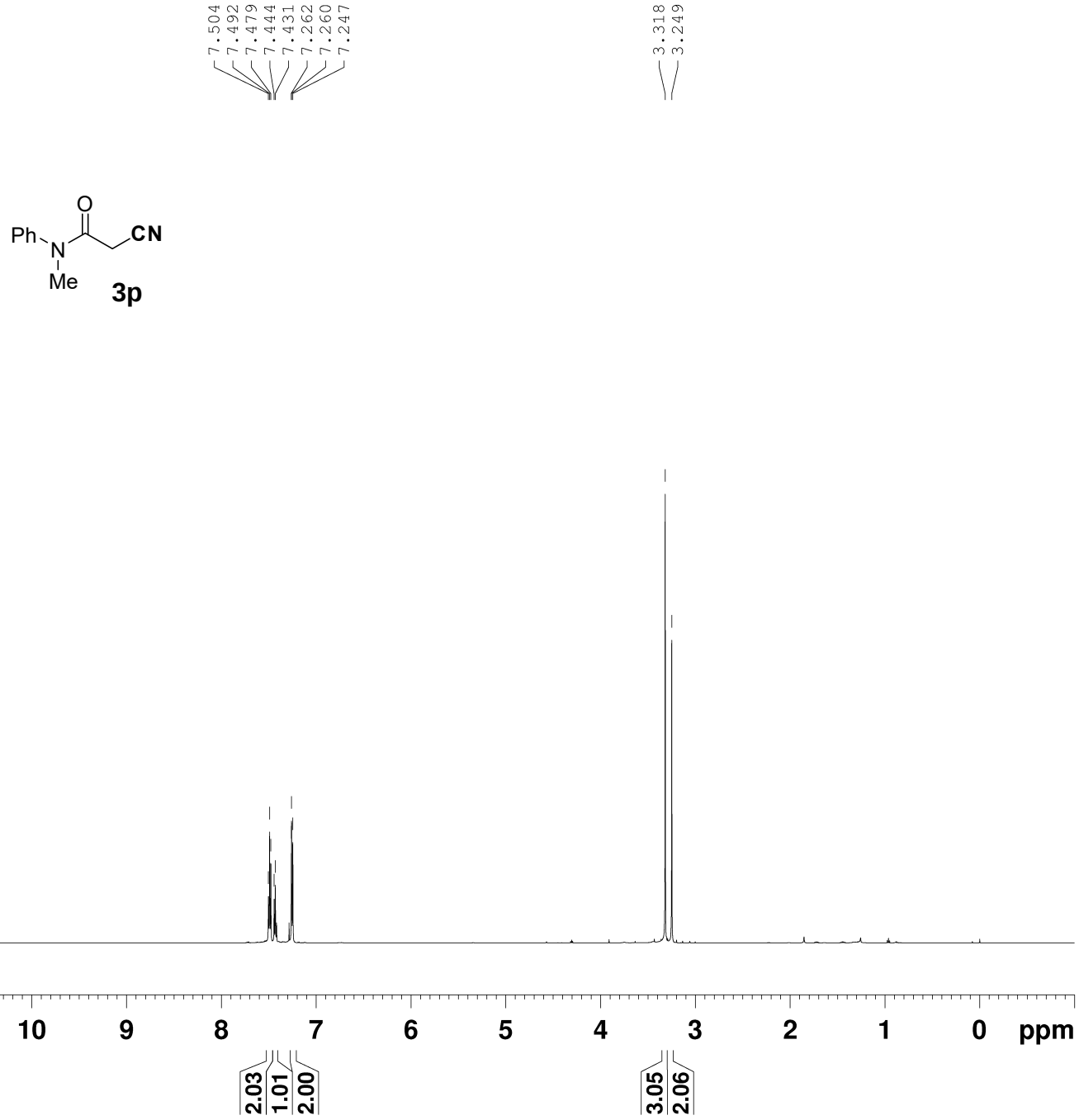
NAME	GG-615P-20220629
EXPNO	2
PROCNO	1
Date_	20220629
Time	11.47
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	1024
DS	4
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	190.02
DW	13.867 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	150.9279571 MHz
NUC1	13C
P1	11.90 usec
SI	32768
SF	150.9128665 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



NAME	GG-669P-20220917
EXPNO	1
PROCNO	1
Date_	20220917
Time	12.30
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
DS	0
SWH	9615.385 Hz
FIDRES	0.146719 Hz
AQ	3.4079220 sec
RG	87.54
DW	52.000 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	600.1739011 MHz
NUC1	1H
P1	9.96 usec
SI	65536
SF	600.1700000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

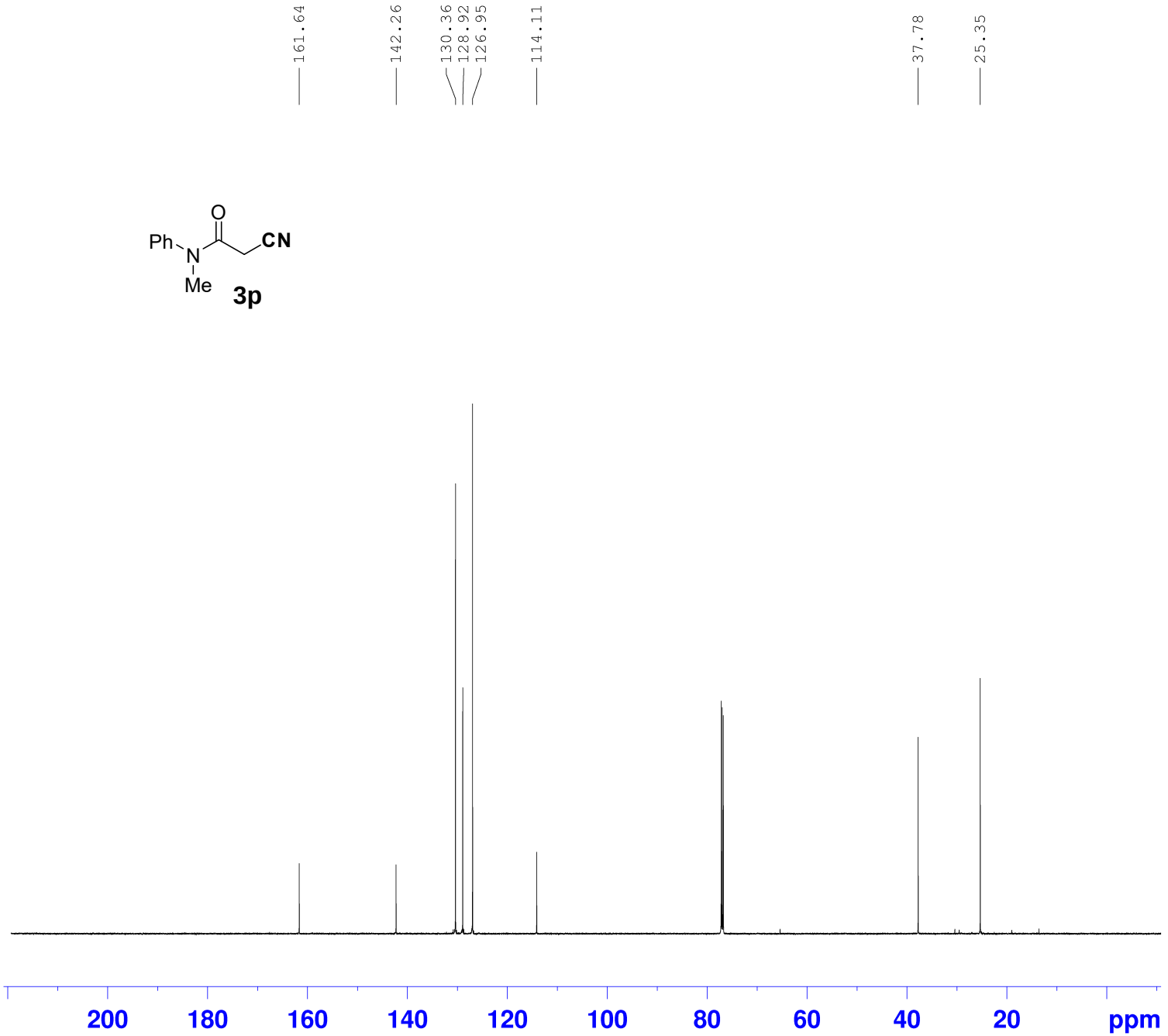


NAME	GG-669P-20220917
EXPNO	2
PROCNO	1
Date_	20220917
Time	13.22
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	1024
DS	4
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	190.02
DW	13.867 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	150.9279571 MHz
NUC1	13C
P1	11.90 usec
SI	32768
SF	150.9128665 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

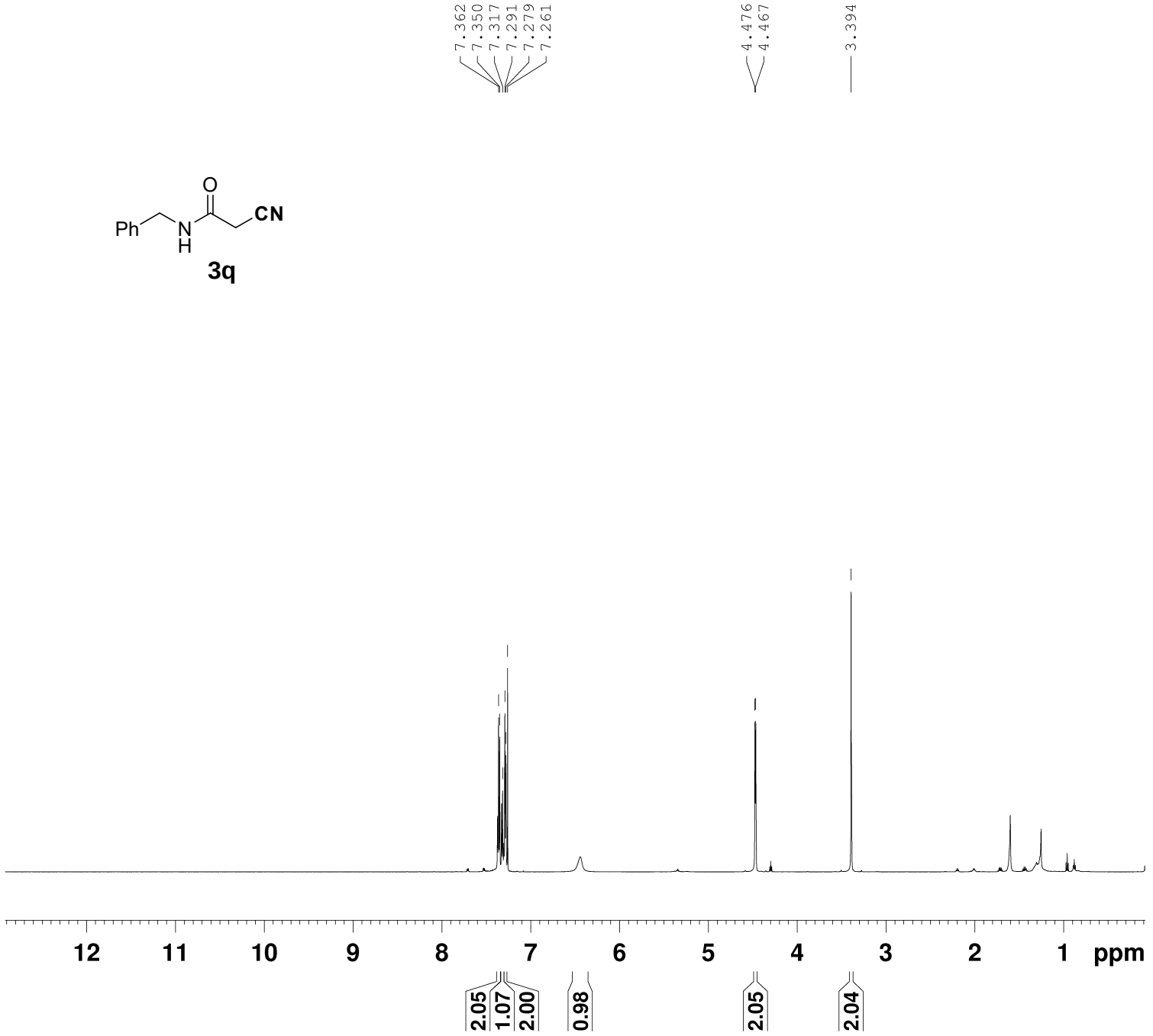


NAME	GG-572P-20220609
EXPNO	1
PROCNO	1
Date_	20220610
Time	4.10
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	0
SWH	9615.385 Hz
FIDRES	0.146719 Hz
AQ	3.4079220 sec
RG	44.5
DW	52.000 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
SFO1	600.1739011 MHz
NUC1	1H
P1	9.96 usec
SI	65536
SF	600.1699985 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

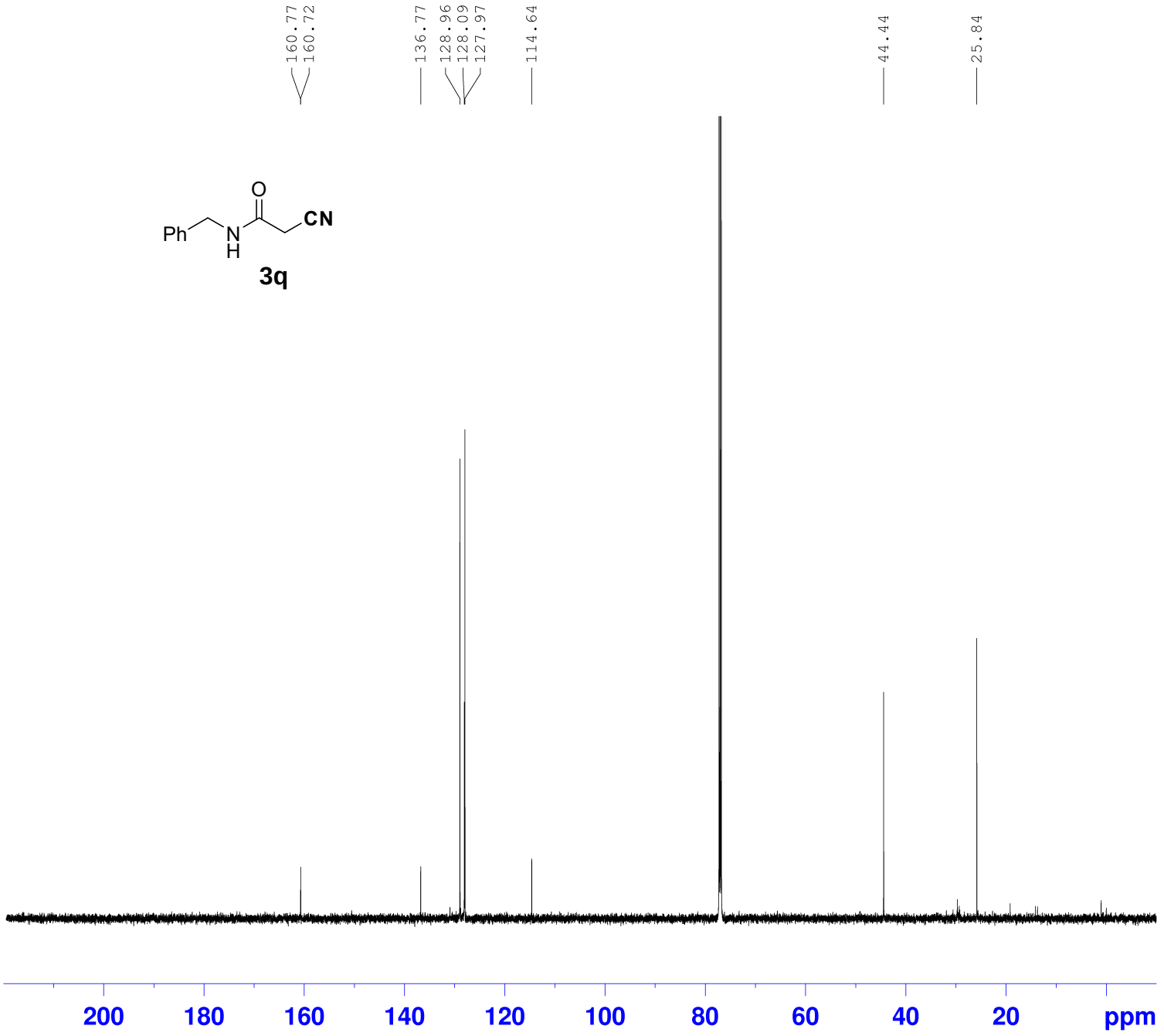


NAME	GG-572P-20220609
EXPNO	2
PROCNO	1
Date_	20220610
Time	5.02
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	190.02
DW	13.867 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	150.9279571 MHz
NUC1	13C
P1	11.90 usec
SI	32768
SF	150.9128863 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

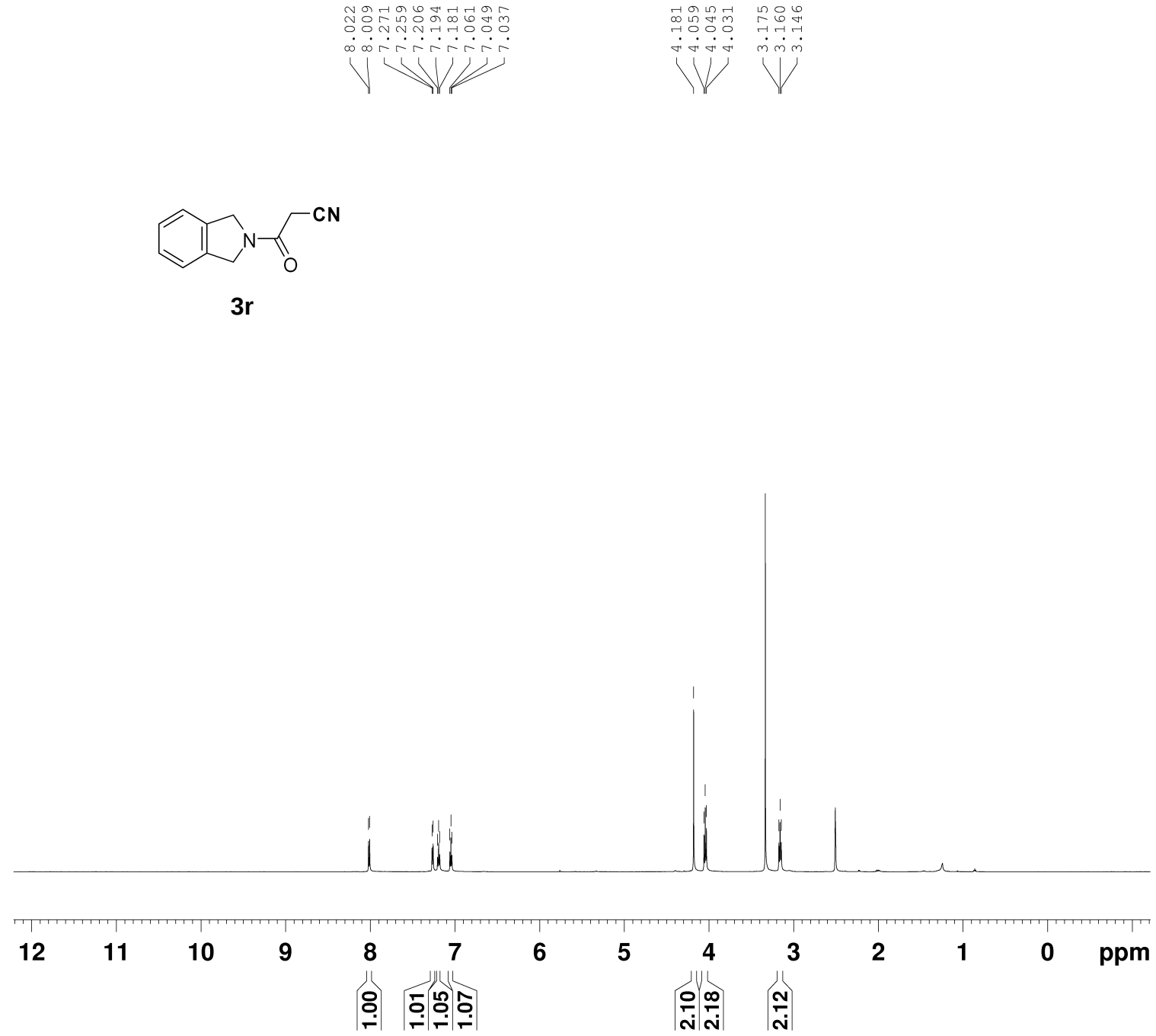


NAME	GG-584P-20220613
EXPNO	1
PROCNO	1
Date_	20220613
Time	21.17
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	0
SWH	9615.385 Hz
FIDRES	0.146719 Hz
AQ	3.4079220 sec
RG	109.27
DW	52.000 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
SFO1	600.1739011 MHz
NUC1	1H
P1	9.96 usec
SI	65536
SF	600.1700147 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

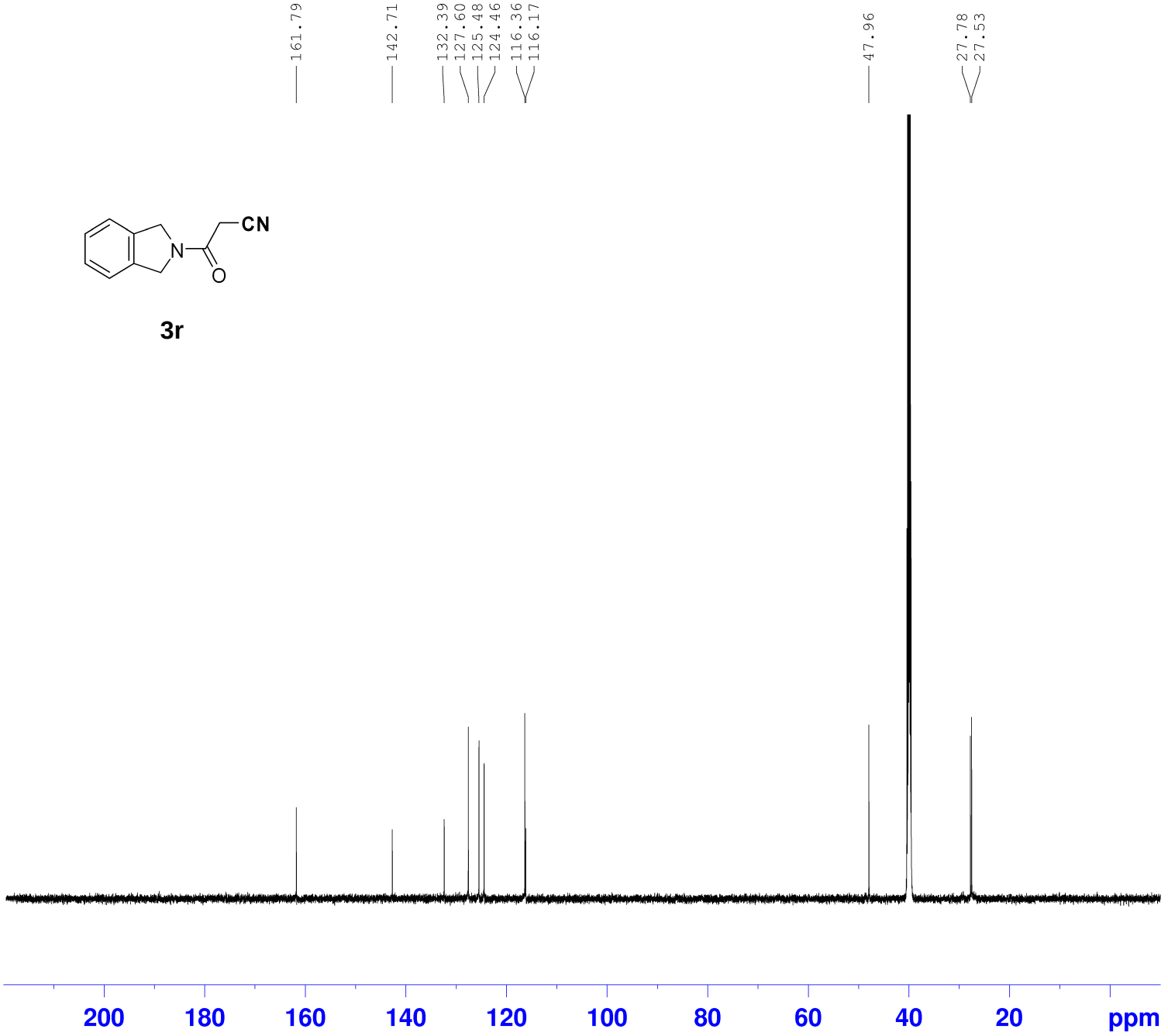


NAME	GG-584P-20220613
EXPNO	2
PROCNO	1
Date_	20220613
Time	22.09
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	190.02
DW	13.867 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	150.9279571 MHz
NUC1	13C
P1	11.90 usec
SI	32768
SF	150.9128665 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

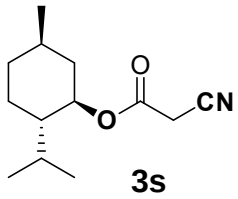


NAME	GG-610P-20230202
EXPNO	1
PROCNO	1
Date_	20230202
Time	17.22
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
DS	0
SWH	9615.385 Hz
FIDRES	0.146719 Hz
AQ	3.4079220 sec
RG	96.28
DW	52.000 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1

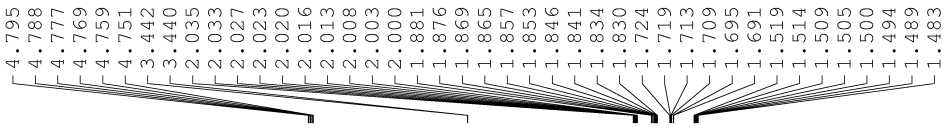
======== CHANNEL f1 ========	
SFO1	600.1739011 MHz
NUC1	1H
P1	9.96 usec
SI	65536
SF	600.1700000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

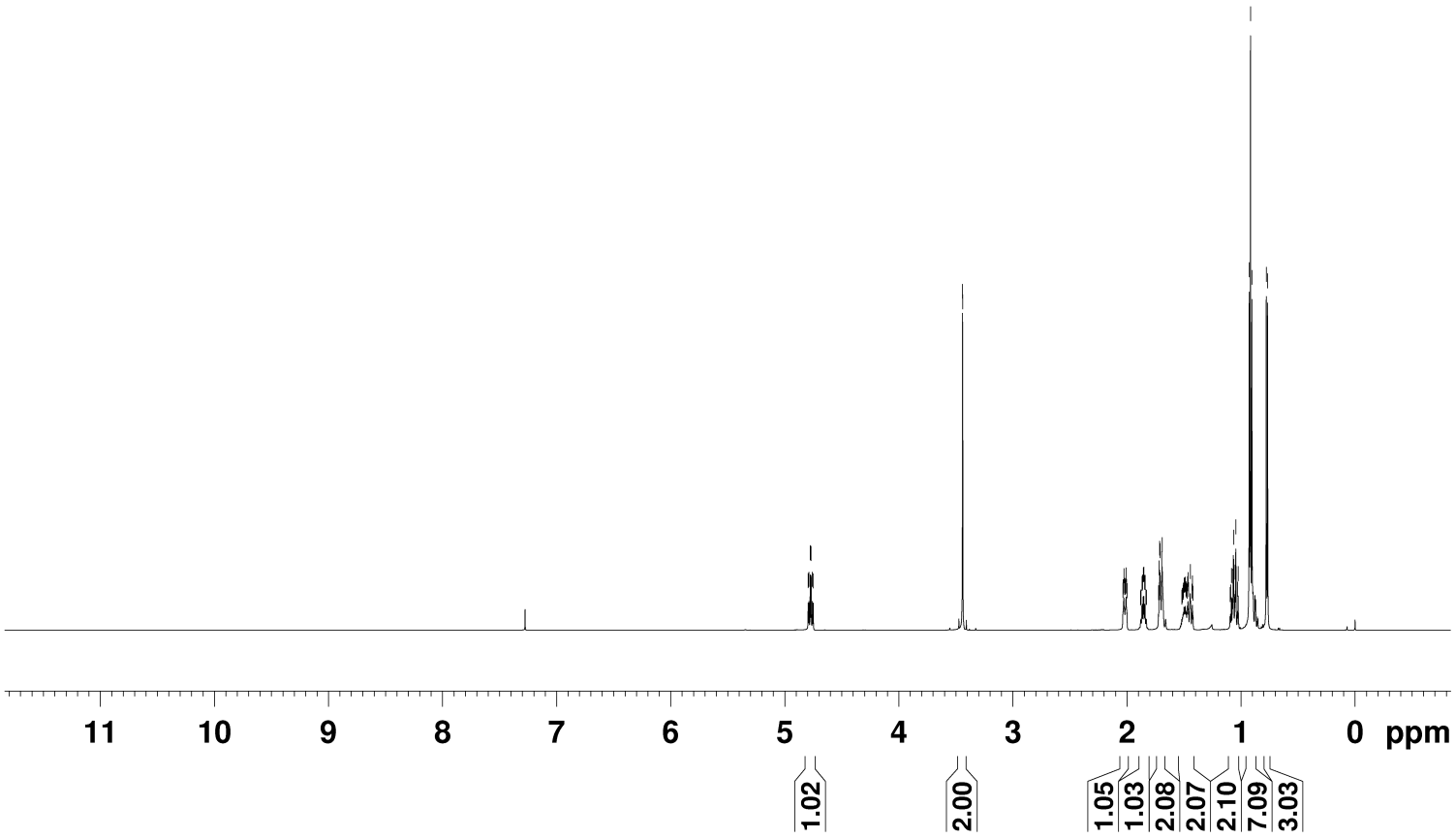


NAME	GG-610P-20230202
EXPNO	2
PROCNO	1
Date_	20230202
Time	18.14
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	1024
DS	4
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	190.02
DW	13.867 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	150.9279571 MHz
NUC1	13C
P1	11.90 usec
SI	32768
SF	150.9128665 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

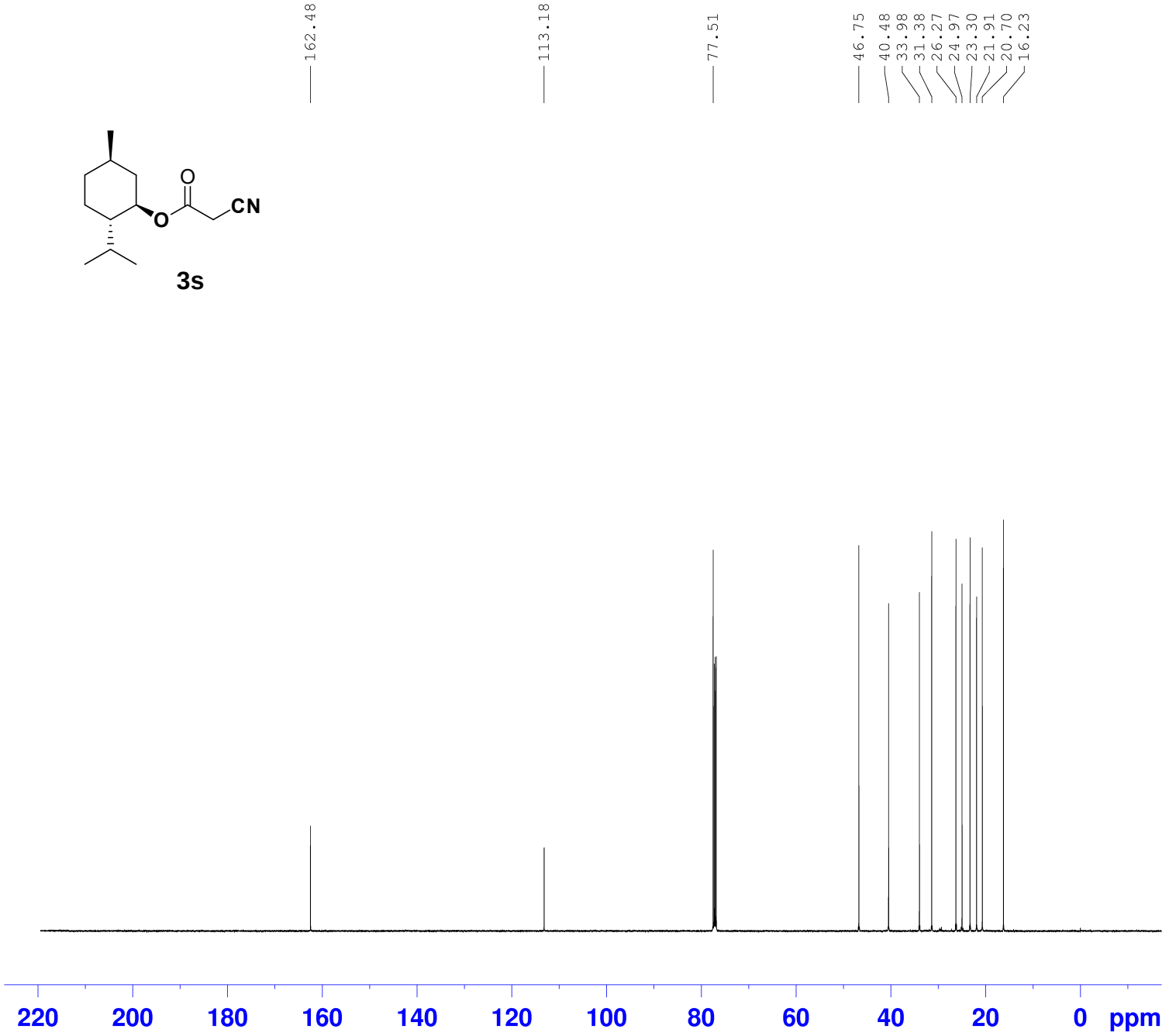


3s





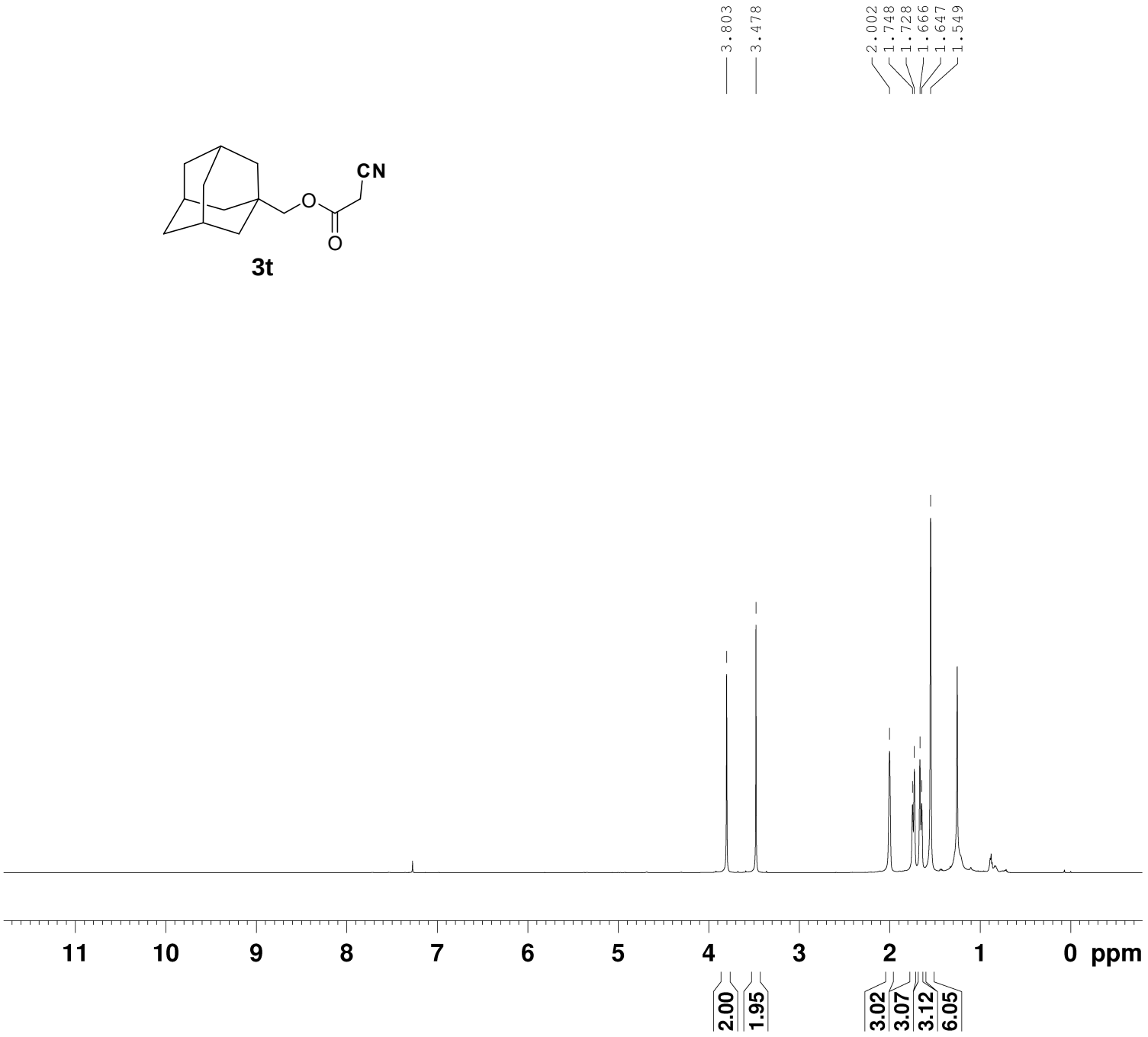
NAME	GG-682-1P-20221015
EXPNO	1
PROCNO	1
Date_	20221015
Time	15.38
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	0
SWH	9615.385 Hz
FIDRES	0.146719 Hz
AQ	3.4079220 sec
RG	15.49
DW	52.000 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	600.1739011 MHz
NUC1	1H
P1	9.96 usec
SI	65536
SF	600.1700043 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



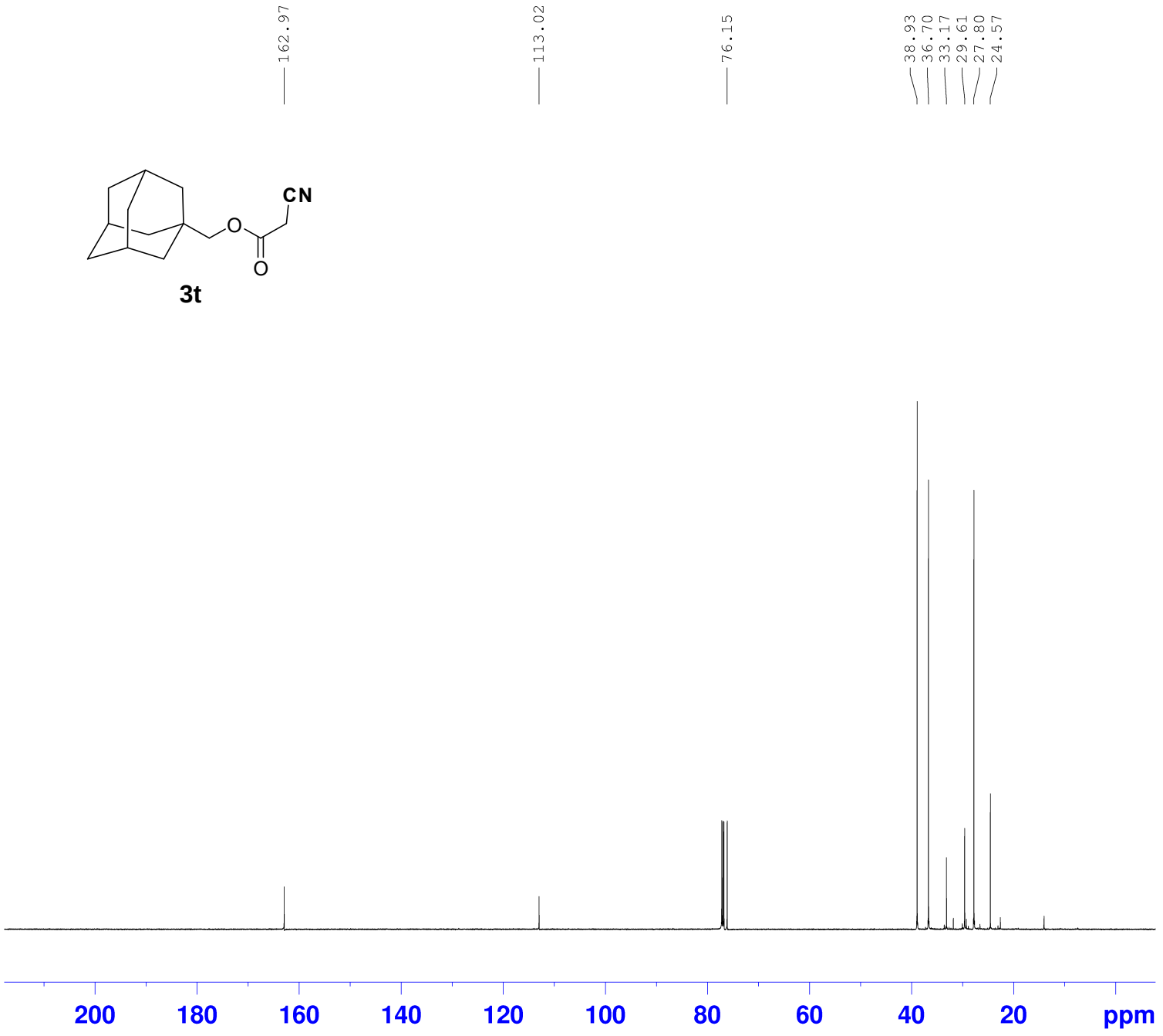
NAME	GG-682-1P-20221015
EXPNO	2
PROCNO	1
Date_	20221015
Time	16.30
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	190.02
DW	13.867 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1

======== CHANNEL f1 ========	
SFO1	150.9279571 MHz
NUC1	13C
P1	11.90 usec
SI	32768
SF	150.9128665 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

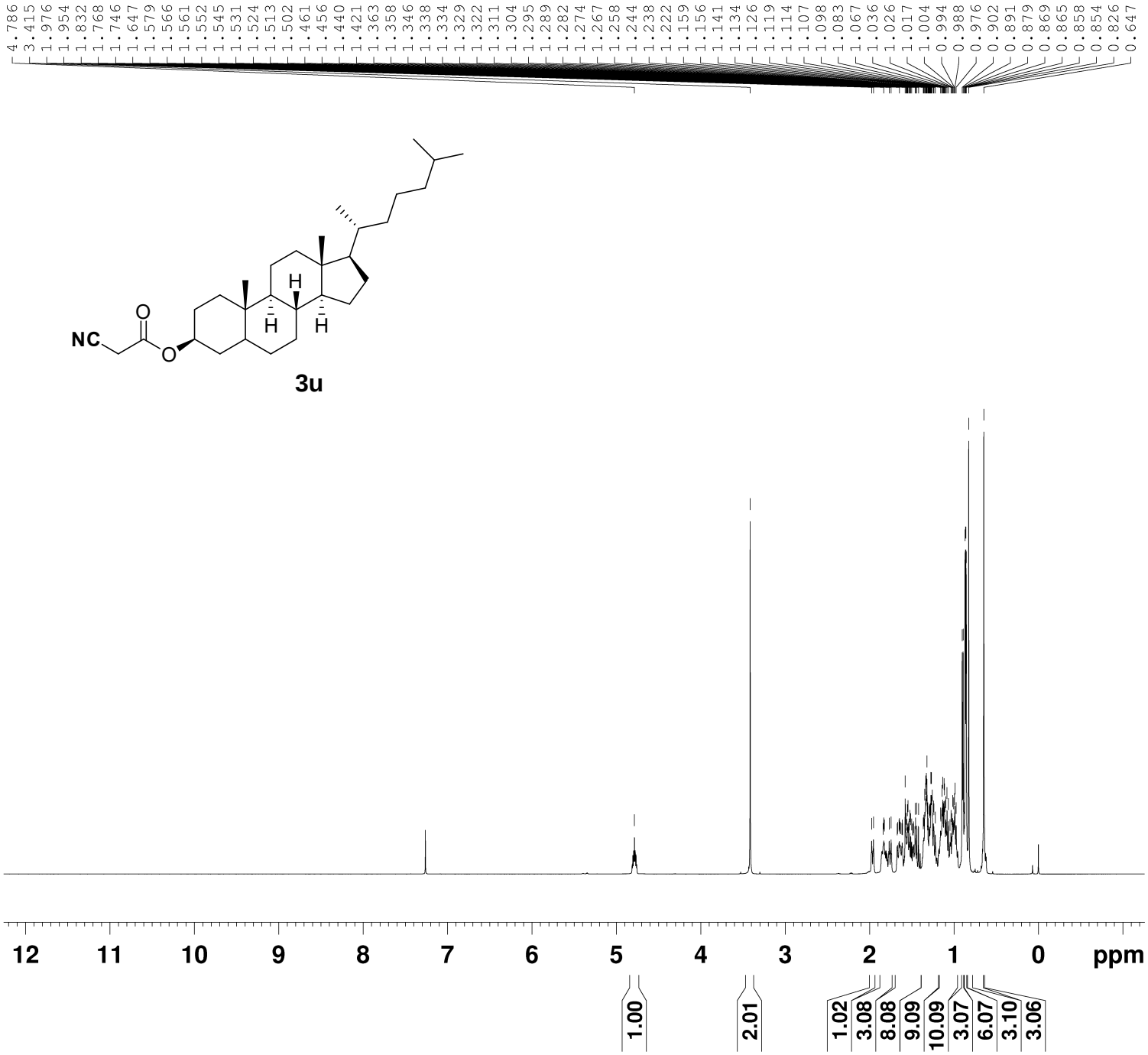
3t



NAME	GG-594P-20220616
EXPNO	1
PROCNO	1
Date_	20220616
Time	11.02
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	0
SWH	9615.385 Hz
FIDRES	0.146719 Hz
AQ	3.4079220 sec
RG	15.49
DW	52.000 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	600.1739011 MHz
NUC1	1H
P1	9.96 usec
SI	65536
SF	600.1700061 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

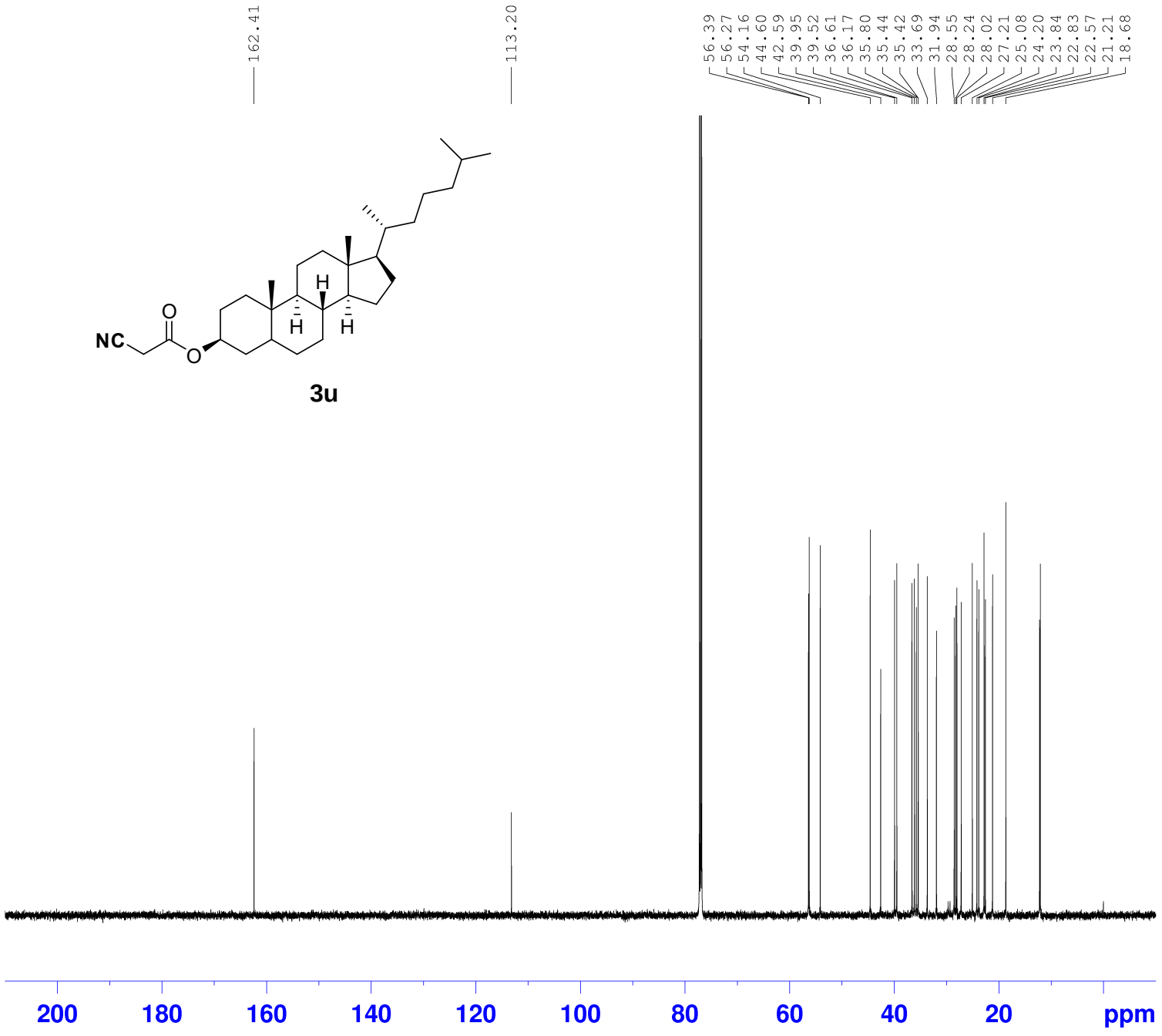


NAME	GG-594P-20220616
EXPNO	2
PROCNO	1
Date_	20220616
Time	11.54
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	190.02
DW	13.867 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	150.9279571 MHz
NUC1	13C
P1	11.90 usec
SI	32768
SF	150.9128796 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

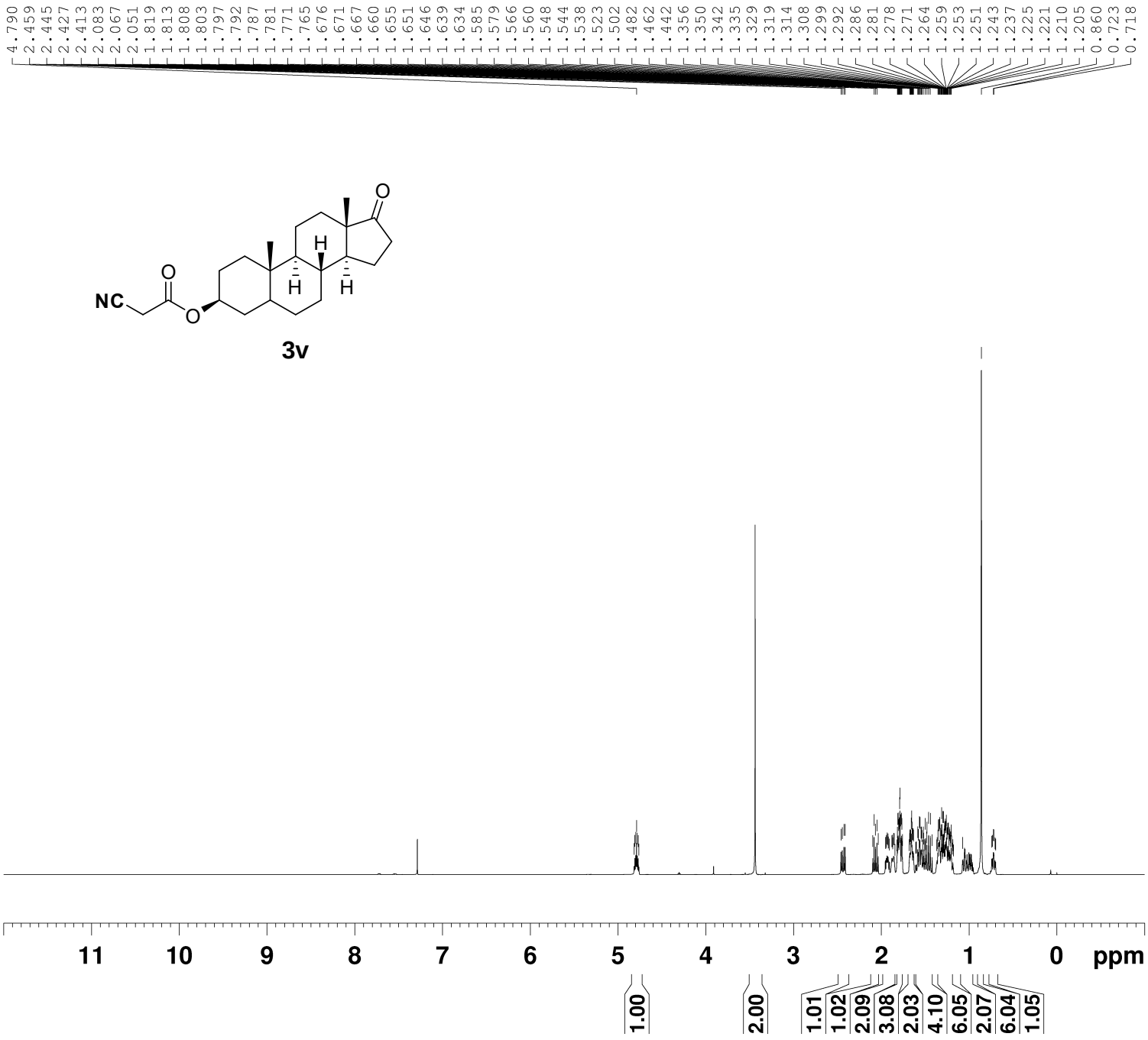


3u

NAME	GG-663-1P-20220916
EXPNO	1
PROCNO	1
Date_	20220916
Time	10.59
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	0
SWH	9615.385 Hz
FIDRES	0.146719 Hz
AQ	3.4079220 sec
RG	44.5
DW	52.000 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	600.1739011 MHz
NUC1	1H
P1	9.96 usec
SI	65536
SF	600.1700128 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

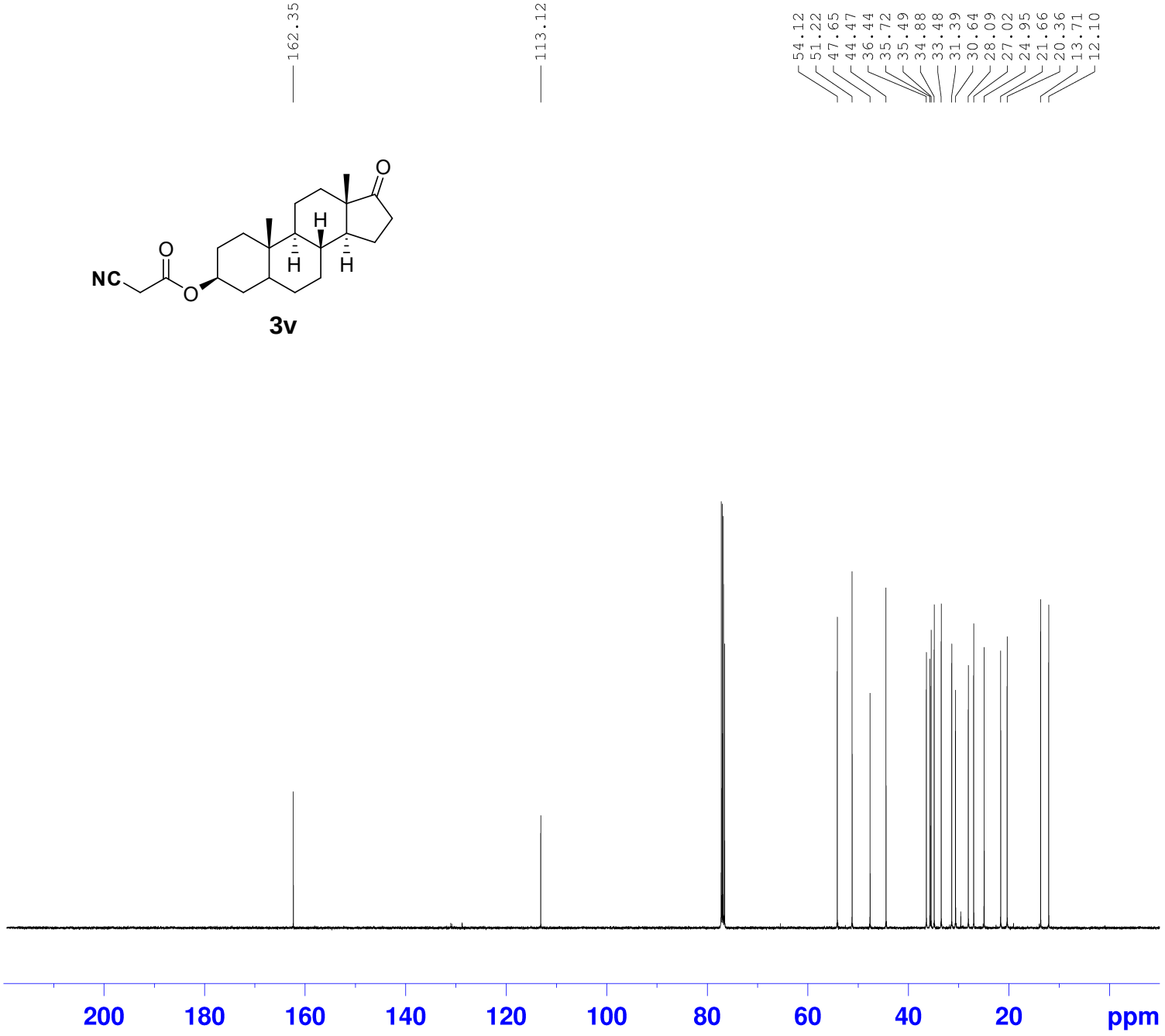


NAME	GG-663-1P-20220916
EXPNO	2
PROCNO	1
Date_	20220916
Time	11.51
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	190.02
DW	13.867 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	150.9279571 MHz
NUC1	13C
P1	11.90 usec
SI	32768
SF	150.9128665 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



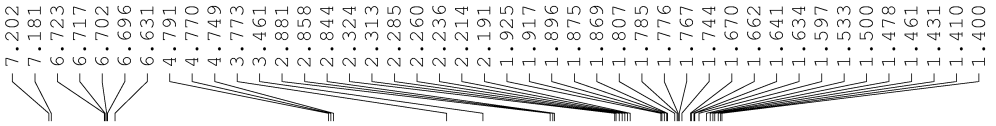
NAME	GG-608P-20220621
EXPNO	1
PROCNO	1
Date_	20220621
Time	21.42
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	0
SWH	9615.385 Hz
FIDRES	0.146719 Hz
AQ	3.4079220 sec
RG	28.69
DW	52.000 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	600.1739011 MHz
NUC1	1H
P1	9.96 usec
SI	65536
SF	600.1699974 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

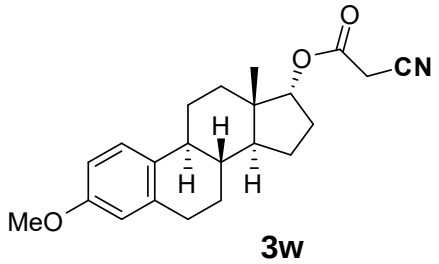
3v



NAME	GG-608P-20220621
EXPNO	2
PROCNO	1
Date_	20220621
Time	22.34
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	190.02
DW	13.867 usec
DE	6.50 usec
TE	298.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1

======== CHANNEL f1 ========	
SFO1	150.9279571 MHz
NUC1	13C
P1	11.90 usec
SI	32768
SF	150.9128811 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

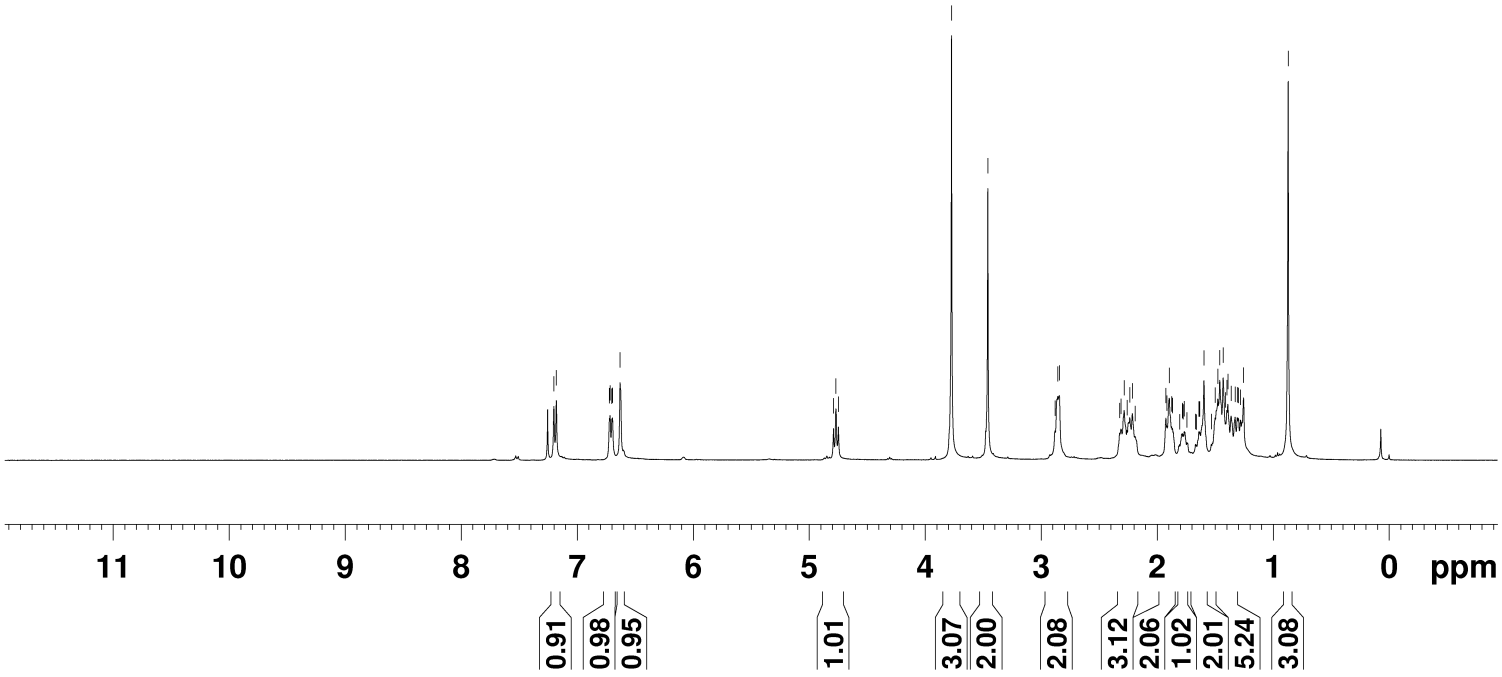


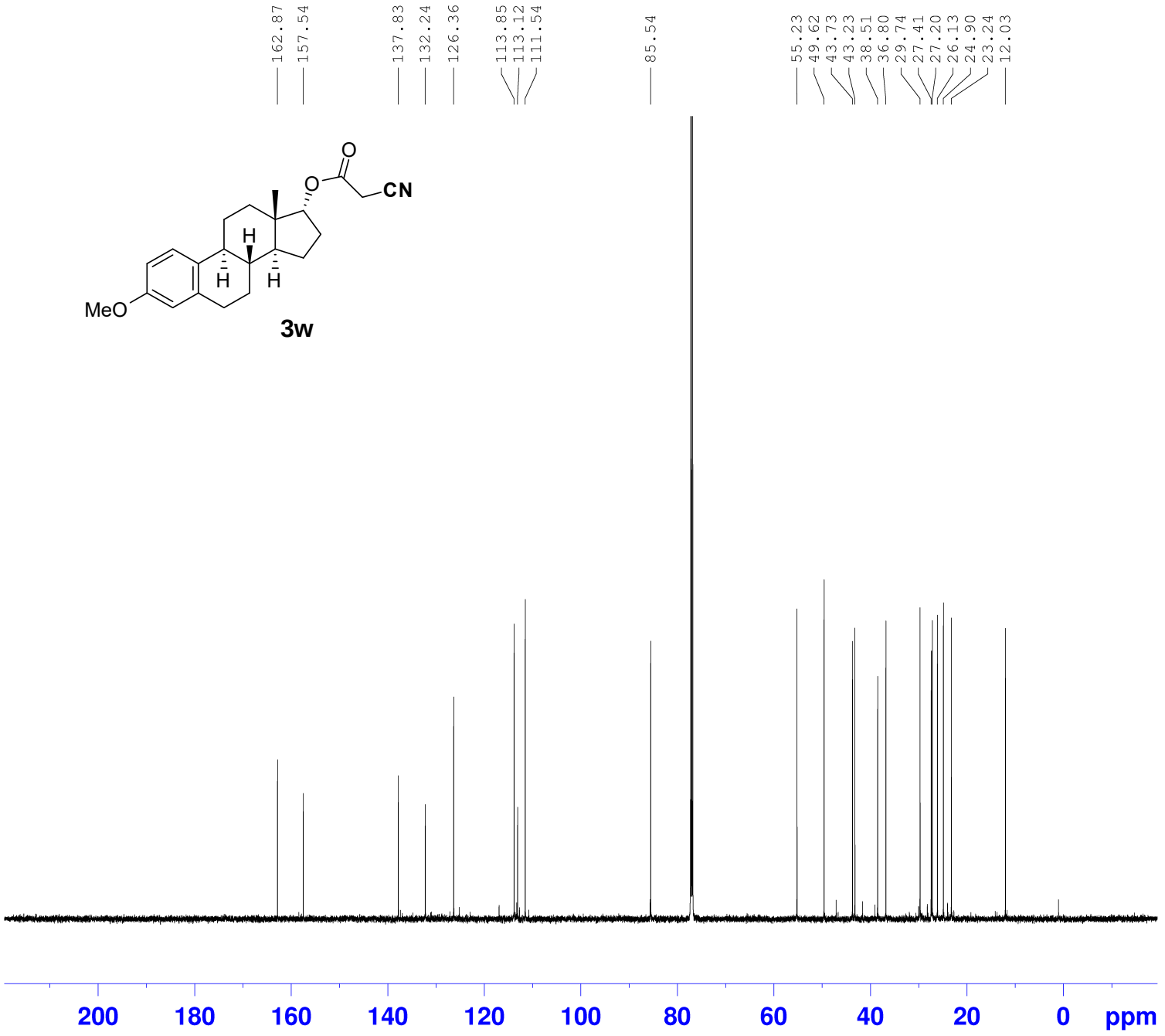


3w

NAME	gg-607-20220620
EXPNO	1
PROCNO	1
Date_	20220620
Time	20.59
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	203
DW	78.200 usec
DE	6.50 usec
TE	298.2 K
D1	1.00000000 sec
TD0	1

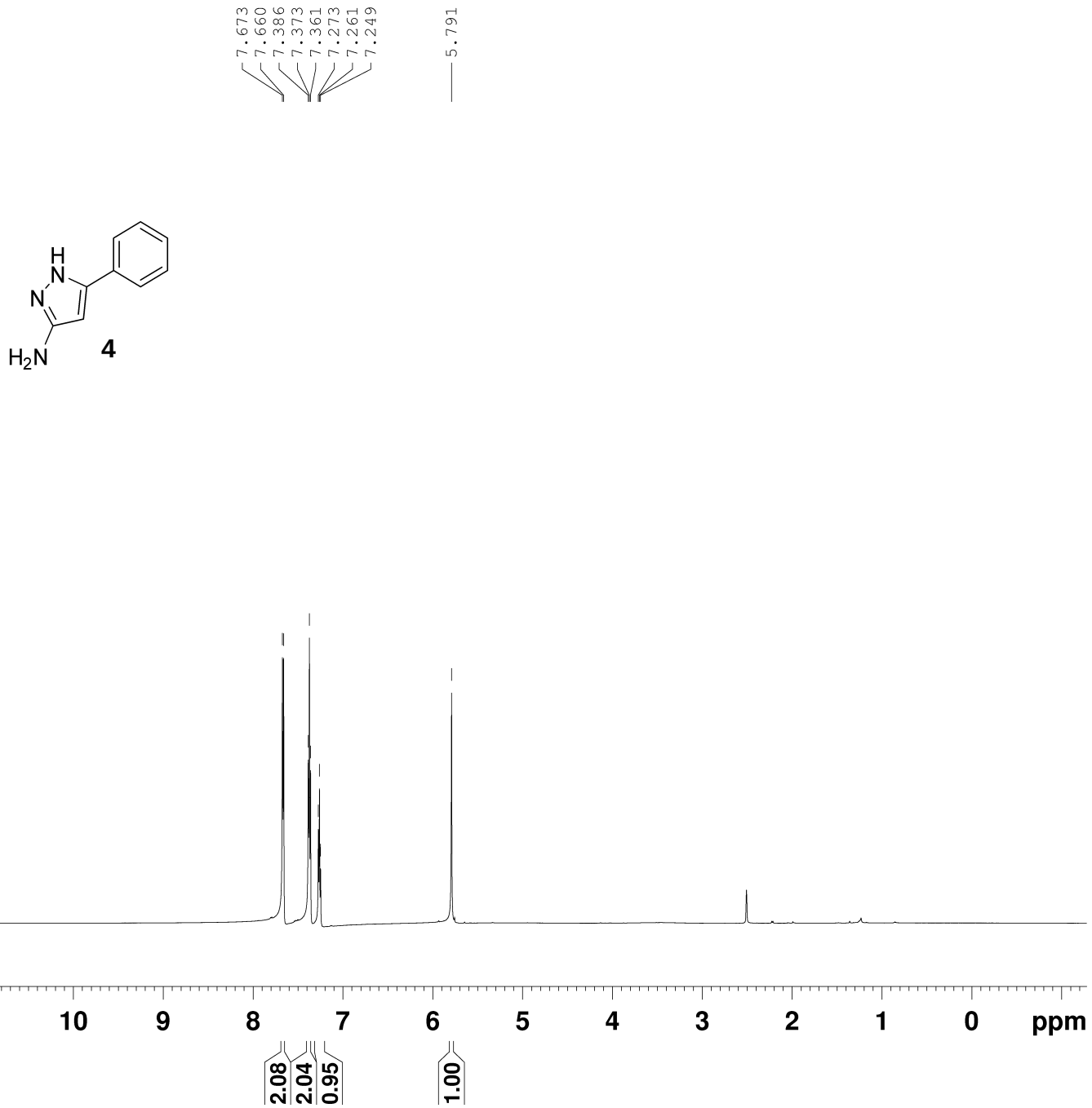
======== CHANNEL f1 ========	
NUC1	1H
P1	10.40 usec
PL1	-1.00 dB
PL1W	17.01305389 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300113 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00





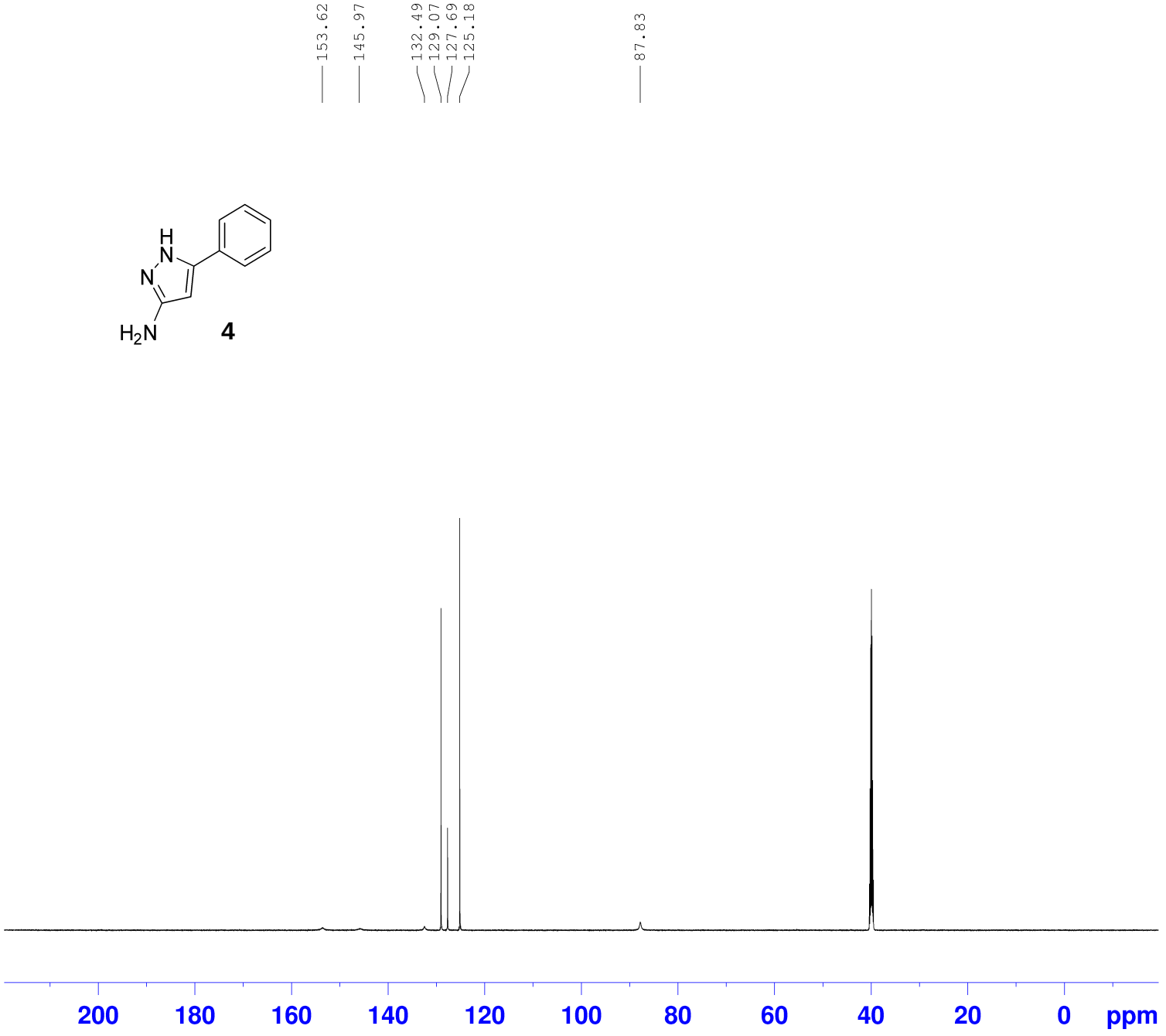
NAME	GG-607P-20220621
EXPNO	2
PROCNO	1
Date_	20220621
Time	23.34
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	190.02
DW	13.867 usec
DE	6.50 usec
TE	298.3 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1

======== CHANNEL f1 ========	
SFO1	150.9279571 MHz
NUC1	13C
P1	11.90 usec
SI	32768
SF	150.9128665 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

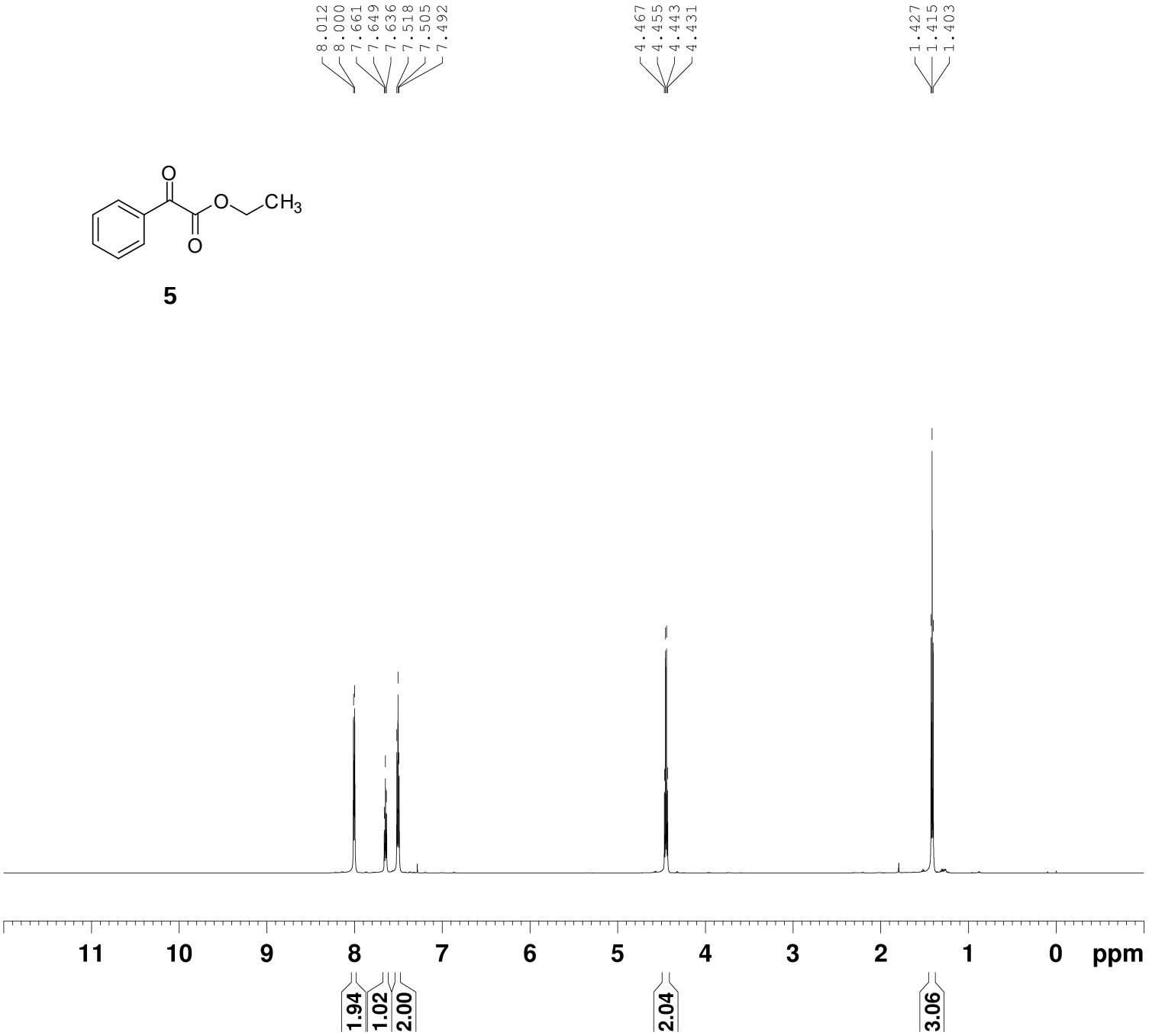


NAME	GG-711P-20230202
EXPNO	1
PROCNO	1
Date_	20230202
Time	16.21
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	8
DS	0
SWH	9615.385 Hz
FIDRES	0.146719 Hz
AQ	3.4079220 sec
RG	38.1
DW	52.000 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1

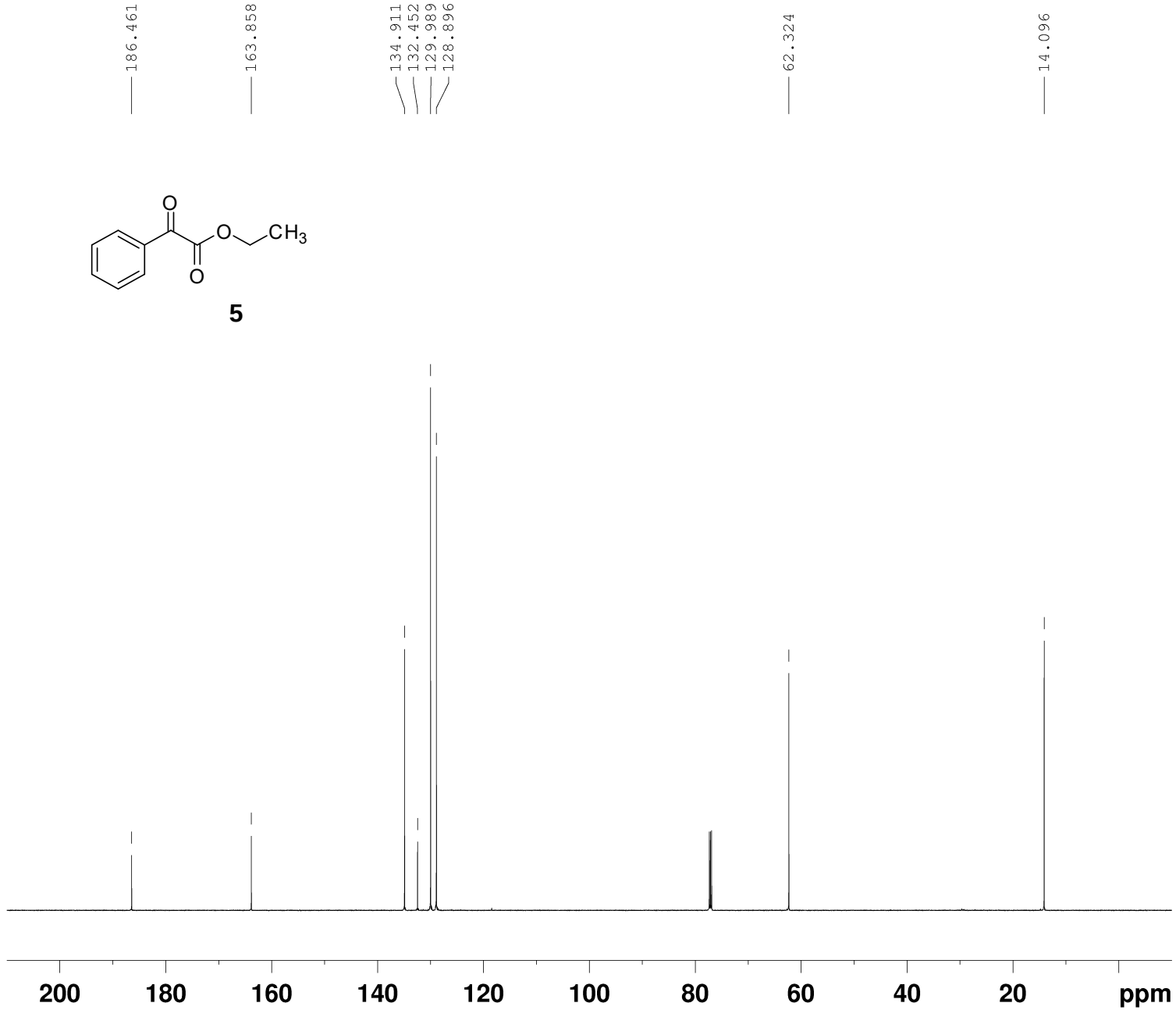
======== CHANNEL f1 ========	
SFO1	600.1739011 MHz
NUC1	1H
P1	9.96 usec
SI	65536
SF	600.1700000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



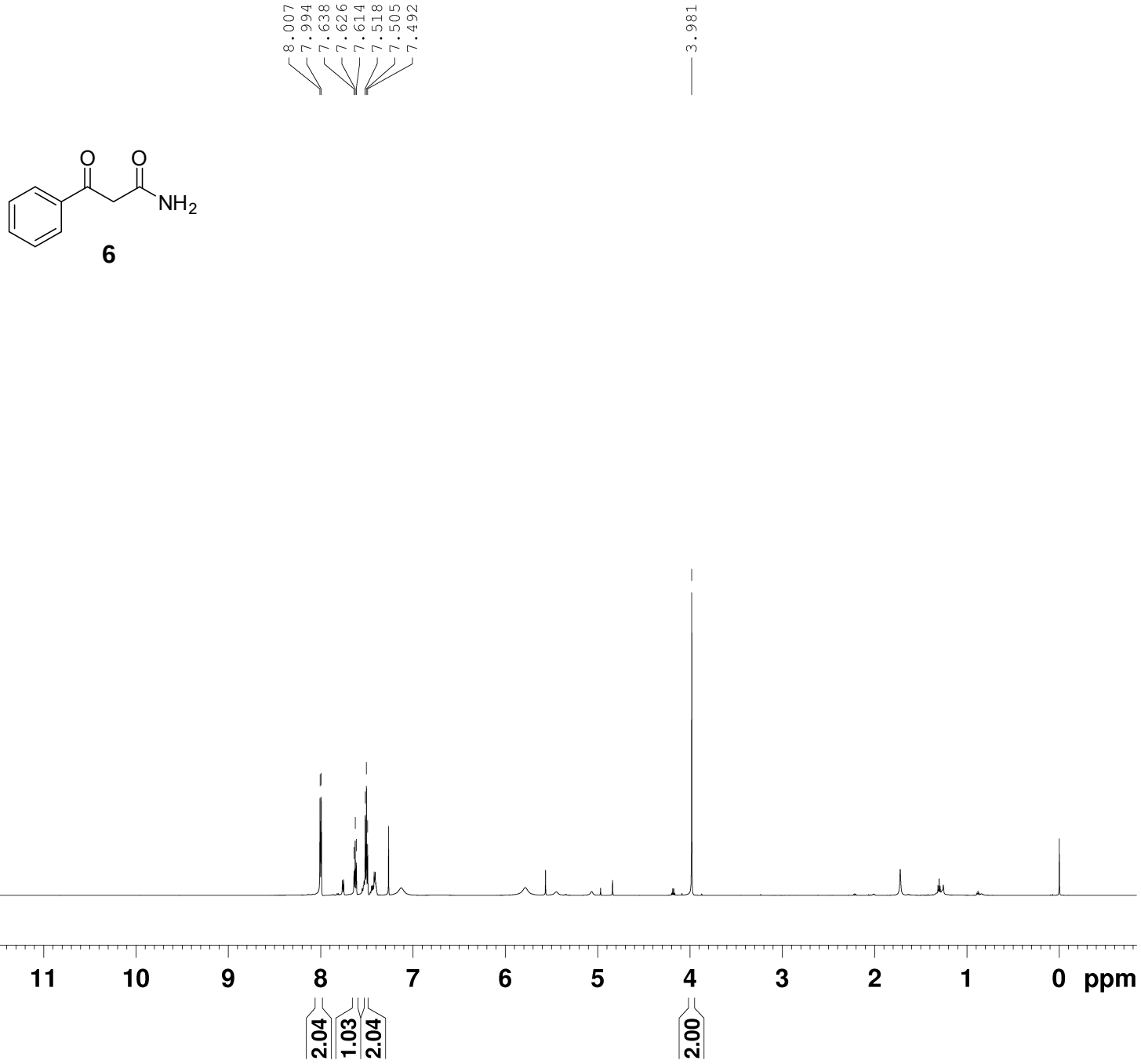
NAME	GG-711P-20230202
EXPNO	2
PROCNO	1
Date_	20230202
Time	17.14
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	1024
DS	4
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	190.02
DW	13.867 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
========	CHANNEL f1 ========
SFO1	150.9279571 MHz
NUC1	13C
P1	11.90 usec
SI	32768
SF	150.9128665 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



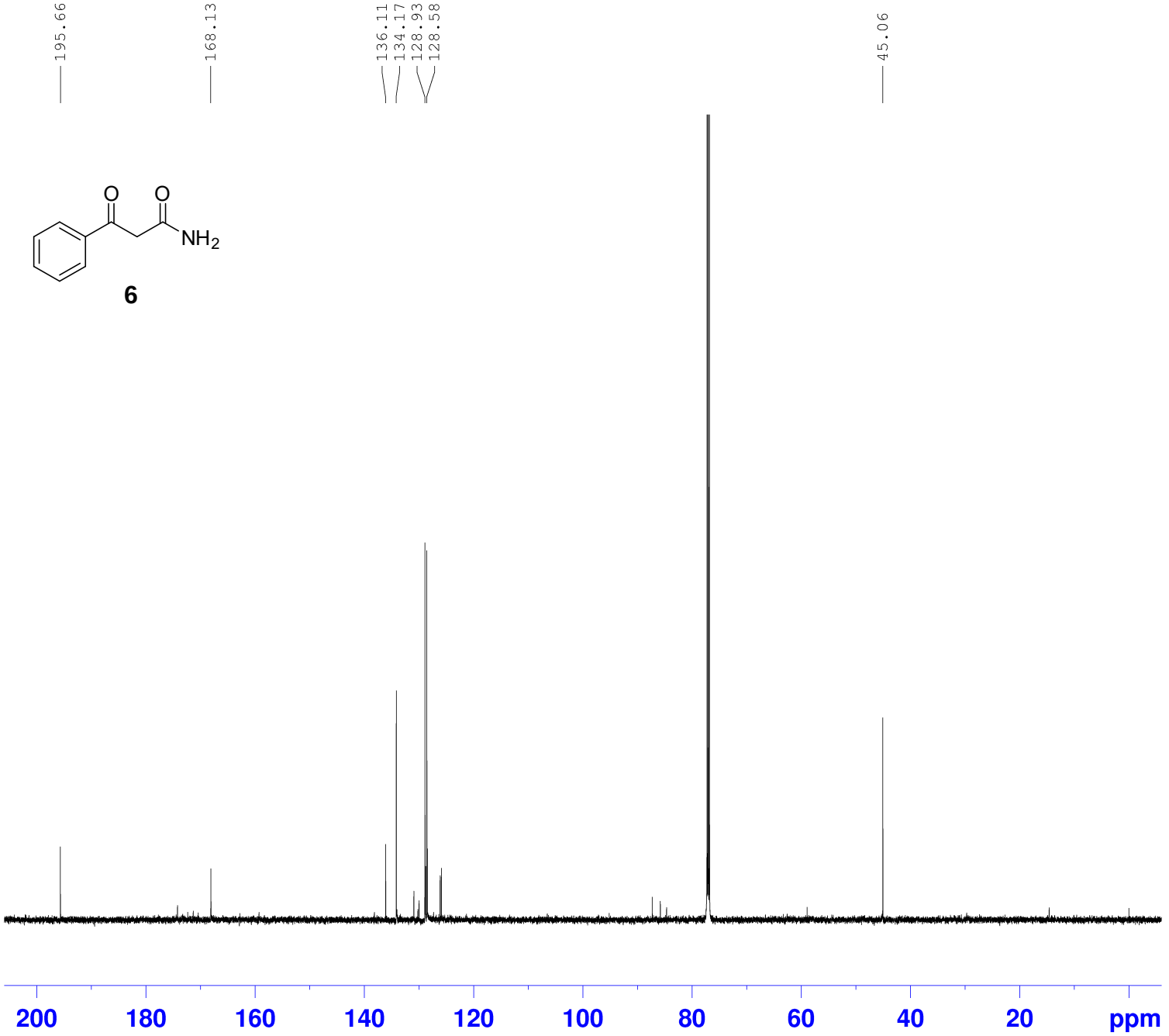
NAME	GG-713P-20221111
EXPNO	1
PROCNO	1
Date_	20221111
Time	17.31
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	0
SWH	9615.385 Hz
FIDRES	0.146719 Hz
AQ	3.4079220 sec
RG	15.49
DW	52.000 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
========	CHANNEL f1 ========
SFO1	600.1739011 MHz
NUC1	1H
P1	9.96 usec
SI	65536
SF	600.1699991 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



NAME	GG-713P-20221111
EXPNO	2
PROCNO	1
Date_	20221111
Time	18.11
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	800
DS	4
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	190.02
DW	13.867 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	150.9279571 MHz
NUC1	13C
P1	11.90 usec
SI	32768
SF	150.9128665 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



NAME	GG780P2--20221120
EXPNO	1
PROCNO	1
Date_	20221120
Time	17.59
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	0
SWH	9615.385 Hz
FIDRES	0.146719 Hz
AQ	3.4079220 sec
RG	96.28
DW	52.000 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
========	CHANNEL f1 ========
SFO1	600.1739011 MHz
NUC1	1H
P1	9.96 usec
SI	65536
SF	600.1700113 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00




```
NAME      GG780P2--20221120
EXPNO                     2
PROCNO                    1
Date_              20221120
Time                 18.40
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    800
DS                      4
SWH             36057.691 Hz
FIDRES           0.550197 Hz
AQ              0.9088159 sec
RG                  190.02
DW                13.867 usec
DE                 6.50 usec
TE                 298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         150.9279571 MHz
NUC1                  13C
P1                  11.90 usec
SI                  32768
SF           150.9128665 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```