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Supporting Information

Substrate Controlled, Regioselective Carbopalladation for the One-pot Synthesis of C4-Substituted Tetrahydroisoquinoline Analogues.

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Materials and methods:

All reactions were carried out in oven-dried glassware with magnetic stirring. All reactions were carried out under nitrogen atmosphere. Cesium carbonate was purchased from Merck. Silica gel 200-400 (code 5699D00500) mesh size was purchased from Loba Chemie Pvt Ltd. Melting points were uncorrected. ^{1}H NMR was recorded Bruker model 300 MHz and $^{13}C\{1H\}$ 75 MHz spectrometer using TMS as an internal standard and $CDCl_3$ as a solvent. High resolution mass spectra were obtained using Q-TOF mass spectrometer or Thermofisher Exactive Orbitrap mass spectrometer.

General procedure for synthesis of Tertiary amine 1:

Substituted cinnamaldehyde (2.0 mmol, 1 equiv.) and amine (4.0 mmol, 2 equiv.) were dissolved in methanol (5 mL) taken in a 25 mL sealed tube and anhydrous magnesium sulphate (4.0 mmol, 480 mg) was added. The reaction mixture was stirred at 50 ^{o}C for 10 hours in an oil bath. After complete consumption of the starting material, the reaction mixture was cooled to 0 ^{o}C and sodium borohydride (4.0 mmol, 152 mg) was added to the reaction mixture and stirred for 2 hours. Then, the reaction mixture was quenched with saturated ammonium chloride solution (3 mL). Then contents were poured into a separating funnel (60 mL) and extracted with ethyl acetate (1 × 5 mL) and the organic layer was extracted. The aqueous layer was further extracted with ethyl acetate (2 × 5 mL) and the combined organic extracts were washed with water (1 × 10 mL), brine (1 × 10 mL), dried over anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The crude residue was used for next step without further purification.

In a 25 mL sealed reaction tube, 2-bromobenzyl bromide (1.0 mmol, 250 mg) and amine (1.0 mmol, 1.0 equiv.) were dissolved in DMF (5 mL) and K_2CO_3 (2.0 mmol, 276 mg)

were added and heated to 90 ºC for 10 hours in an oil bath. After complete consumption of the starting material, the reaction mixture was cooled to room temperature and water (1 × 10 mL) was added to the reaction mixture. Then contents were poured into a separating funnel (60 mL) and extracted with ethyl acetate (1 × 5 mL) and the organic layer was separated .The aqueous layer was further extracted with ethyl acetate (2 × 5 mL) and the combined organic extracts were washed with brine solution (1 × 10 mL). Finally the organic layer was dried over anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The crude compound was purified by column chromatography (eluent 5% EtOAc hexane).

[(2-bromophenyl)methyl](butyl)[(2*E*)-3-phenylprop-2-en-1-yl]amine (1a): : Yellow color liquid: 545 mg (95 %). ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.59 (d, *J* = 7.5 Hz, 1H), 7.51 (dd, *J* = 6 Hz, 1.2 Hz , 1H), 7.38-7.18 (m, 6 H), 7.08 (td, *J* = 7.8 Hz, 1.8 Hz, 1H), 6.53 (d, *J* = 15.9 Hz, 1H), 6.29 (dt, *J* = 15.9 Hz, 6.6 Hz, 1H), 3.70 (s, 2H), 3.27 (dd, *J* = 6.3 Hz, 0.9 Hz, 2H), 2.53 (t, *J* = 7.2 Hz, 2H), 1.55-1.46 (m, 2H) 1.38-1.25(m, 2H) 0.88 (t, *J* = 7.2 Hz, 3H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 142.0, 139.2, 137.2, 132.1, 130.2, 128.5, 128.4, 128.0, 127.8, 127.2, 126.2, 100.1, 62.7, 56.3, 53.6, 29.3, 20.5, 14.0. HRMS (ESI, *m/z*): calcd for $C_{20}H_{25}NBr$ $[M+H]^+$ 358.1165; found, 358.1166.

[(2-bromophenyl)methyl](ethyl)[(2*E*)-3-phenylprop-2-en-1-yl]amine (1b): Yellow color liquid: 187 mg (71%). ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.59 (dd, *J* = 9 Hz, 1.5 Hz, 1H), 7.51 (dd, *J* = 6 Hz, 1.2 Hz, 1H), 7.38-7.19 (m, 6H), 7.08 (td, *J* = 7.8 Hz, 3.0 Hz, 1H), 6.54 (d, *J* =15 Hz, 1H), 6.29 (dt, *J* = 15.9 Hz, 9 Hz, 1H), 3.70 (s, 2H), 3.29 (dd, *J* = 6, 1.2 Hz, 2H), 2.62 (q, *J* = 7.2 Hz, 2H), 1.10 (t, *J* = 7.2 Hz, 3H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 142.0, 139.3, 137.3, 132.2, 130.3, 128.6, 128.5, 128.1, 127.8, 127.3, 126.3, 100.2 62.2, 55.9, 47.7, 12.0. HRMS (ESI, *m/z*): calcd for $C_{18}H_{21}BrN^+$ $[M+H]^+$ 330.0852; found, 330.0853.

[(2-bromophenyl)methyl](*tert*-butyl)[(2*E*)-3-phenylprop-2-en-1-yl]amine (1c):

Yellow color liquid: 194 mg (68 %).^{1}H-NMR (300 MHz, CDCl3): δ 7.74 (d, *J* = 7.8 Hz, 1H), 7.70 (d, *J* = 8.1 Hz, 1H), 7.34-7.14 (m, 6H), 6.86 (t, *J* = 7.8 Hz, 1H), 6.37 (d, *J* = 15.9 Hz, 1H), 6.15 (dt, *J* = 15.9 Hz, 6.6 Hz, 1H), 3.71 (s, 2H), 3.41 (d, *J* = 6.6 Hz, 2H) 1.16(s, 9H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 143.2, 137.7, 136.4, 129.5, 129.2, 129.1, 127.3, 126.9, 126.7, 125.9, 125.1, 97.9, 56.8, 54.2, 51.6, 26.6. HRMS (ESI, *m/z*): calcd for $C_{20}H_{25}BrN^{+}$ $[M+H]^{+}$ 358.1165; found, 358.1166.

[(2-bromophenyl)methyl](ethyl)[(2*E*)-3-(4-methoxyphenyl)prop-2-en-1-yl]amine (1d):

Yellow color liquid: 334 mg (74 %).^{1}H-NMR (300 MHz, $CDCl_3$): 7.58 (dd, *J* = 7.8 Hz, 1.5 Hz 1H), 7.51 (dd, *J* = 7.8 Hz, 1.2 Hz 1H), 7.32-7.26 (m, 3H), 7.08 (td, *J* = 7.8 Hz, 1.8 Hz,1H), 6.84 (d, *J* = 9.0 Hz, 2H) , 6.48 (d, *J* = 15.9 Hz, 1H), 6.15 (dt, *J* = 15.6 Hz, 6.6 Hz, 1H), 3.80 (s, 3H), 3.69 (s, 2H), 3.27 (dd, *J* = 6.6 Hz, 1.2 Hz, 2H), 2.61 (q, *J* = 6.9 Hz, 2H), 1.09 (t, *J* = 7.2 Hz, 3H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 159.0, 139.3, 132.6, 131.7, 130.7, 130.1, 128.1, 127.5, 127.2 , 125.5, 124.3, 114.0, 57.2 , 56.1, 55.3, 47.7, 12.1. HRMS (ESI, *m/z*): calcd for $C_{19}H_{23}BrNO^{+}$ $[M+H]^{+}$ 360.0958; found 360.0969.

[(2-bromophenyl)methyl](butyl)[(2*E*)-3-(4-methoxyphenyl)prop-2-en-1-yl]amine (1e):

Yellow color liquid: 484 mg (60 %). ^{1}H-NMR (300 MHz, CDCl3): δ 7.60 -7.55 (m, 1H), 7.50 (dd, *J* = 6.9 Hz, 1.2 Hz, 1H), 7.31-7.28 (m, 3H), 7.07 (td, *J* = 7.8 Hz, 1.5 Hz, 1H), 6.83 (d, *J* = 8.7 Hz, 2H) 6.47 (d, *J* = 15.9 Hz, 1H), 6.14 (dt, *J* = 15.9 Hz, 6.3 Hz, 1H), 3.79 (s, 3H), 3.68 (s, 2H) , 3.24(d, *J* = 6.6 Hz, 2H), 2.52 (t, *J* =7.5 Hz, 2H) , 1.55-1.45 (m, 2H) 1.37-1.25 (m, 2H) 0.87 (t , *J* =7.2 Hz, 3H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$ δ 159.0, 139.4, 132.6,

131.7, 130.6, 130.1, 128.1, 127.4, 127.2, 125.6, 124.3, 114.0, 57.7, 56.4, 55.3, 53.7, 29.4, 20.6, 14.1. HRMS (ESI, *m/z*): calcd for $C_{21}H_{27}ONBr$ $[M+H]^+$ 388.1271; found 388.1263.

[(2-bromophenyl)methyl](tert-butyl)[(2*E*)-3-(4-methoxyphenyl)prop-2-en-1-yl]amine (1f):

Yellow color liquid:448 mg (85%). ^{1}H-NMR (300 MHz, $CDCl_3$): δ 7.79 (d, *J* = 7.8 Hz, 1H), 7.41 (dd, *J* = 8.1 Hz, 0.9 Hz, 1H), 7.29-7.24(m, 1H), 7.2(d, *J* = 8.7 Hz, 2H), 7.06 (td, *J* = 7.8 Hz, 1.8 Hz, 1H), 6.77 (d, *J* = 8.7 Hz, 2H) 6.31 (d, *J* = 15.9 Hz, 1H), 6.01 (dt, *J* = 15.6 Hz, 6.9 Hz, 1H), 3.80 (s, 2H), 3.77(s, 3H) 3.38 (d, *J* = 6.6 Hz, 2H), 1.15(s, 9H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 158.8, 141.9, 132.1, 130.5, 130.4, 130.0, 127.9, 127.5, 127.3, 126.9, 123.0, 113.8, 55.3, 55.2, 52.7, 52.4, 27.6. HRMS (ESI, *m/z*): calcd for $C_{21}H_{27}ONBr$ $[M+H]^+$ 388.1271; found, 388.1264.

Benzyl [(2-iodophenyl) methyl][(2*E*)-3-(4-methoxyphenyl)prop-2-en-1-yl]amine (1g):

Yellow color liquid: 710 mg (72 %). ^{1}H-NMR (300 MHz, $CDCl_3$): δ 7.80 (d, *J* = 7.8 Hz, 1H), 7.61 (d, *J* = 6.9 Hz, 1H), 7.41-7.20 (m, 8H), 6.93 (td, *J* = 8.1 Hz, 1.5 Hz, 1H) 6.84 (d, *J* = 8.7 Hz, 2H), 6.47 (d, *J* = 15.9 Hz, 1H), 6.18 (dt, *J* = 15.6 Hz, 6.6 Hz, 1H), 3.80 (s, 3H), 3.67(s, 4H) 3.24 (d, *J* = 6.6 Hz, 2H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$): δ 159.0, 141.8, 139.5, 139.4, 132.2, 130.3, 130.0, 128.8, 128.6 , 128.3, 128.1, 127.5, 126.9, 125.0, 113.9, 100.2, 62.2, 58.0, 55.9, 55.3. HRMS (ESI, *m/z*): calcd for $C_{24}H_{25}ONI$ $[M+H]^+$ 470.0975; found, 470.0974.

[(2-iodophenyl)methyl][(4-methoxyphenyl)methyl][(2*E*)-3-phenylprop-2-en-1-yl]amine (1h) :

Yellow color liquid: 486 mg (74 %).^{1}H-NMR (300 MHz, $CDCl_3$): δ 7.80 (dd, *J* = 7.8 Hz, 0.9 Hz, 1H), 7.60 (dd, *J* = 7.5 Hz, 1.2 Hz, 1H), 7.38-7.19(m, 8H) 6.92 (td, *J* = 7.8 Hz, 1.5 Hz, 1H) 6.85 (d, *J* = 8.4 Hz, 2H) 6.53 (d, *J* = 15.9 Hz, 1H), 6.31 (dt, *J* = 15.9 Hz, 6.3 Hz, 1H), 3.80 (s, 3H), 3.66 (s, 2H), 3.62 (s, 2H), 3.24 (d, *J* = 6.3 Hz, 2H). ^{13}C{1H} NMR (75 MHz,

$CDCl_3$) δ 158.7, 141.9, 139.4, 137.3, 132.7, 131.4, 130.4, 130.1, 128.7 , 128.6, 128.2, 127.5, 127.4, 126.4, 113.8, 100.4, 62.2, 57.4, 55.7, 55.3. HRMS (ESI, *m/z*): calcd for $C_{24}H_{25}ONI$ $[M+H]^+$ 470.0975; found, 470.0975.

1*N*-[(2-bromophenyl)methyl]-4-methyl-*N*-[(2*E*)-3-phenylprop-2-en-1-yl]aniline (1i):Yellow color liquid: 160 mg (68 %). ^{1}H-NMR (300 MHz, $CDCl_3$): δ 7.86 (d, *J* = 7.8 Hz, 1H), 7.37-7.24 (m, 5H), 7.21-7.16 (m, 2H), 7.02-6.94 (m, 3H), 6.59 (d, *J* = 8.7 Hz, 2H), 6.52-6.43 (m, 1H), 6.29 (dt, *J* =15.9, 5.1 Hz, 1H), 4.43 (s, 2H), 4.16 (d, *J* = 4.8 Hz, 2H), 2.23(s, 3H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 146.3, 139.9, 139.5, 136.9, 131.5, 129.8, 128.7, 128.6, 128.4, 127.8, 127.5, 126.4, 126.0, 125.5. 112.4, 97.8, 60.1, 52.9, 20.3. HRMS (ESI, *m/z*): calcd for $C_{23}H_{23}BrN^+$ $[M+H]^+$ 392.1008; found, 392.1014.

***N*-[(2-bromophenyl)methyl]-4-methyl-*N*-(prop-2-en-1-yl)aniline (1j):** Yellow color liquid: 520 mg (95 %). ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.57 (dd, *J* = 7.8 Hz, 0.6 Hz 1H), 7.21-7.15 (m, 2 H), 7.14-7.08 (m, 1 H), 7.00 (d, *J* = 8.4 Hz, 2H), 6.54 (d, *J* = 8.7 Hz, 2H), 5.96-5.84 (m, 1 H), 5.25-5.17 (m, 2H) 4.50 (s, 2H) 4.01 (d, *J* =4.8 Hz, 2H), 2.23 (s, 3H), ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 146.3, 137.4, 133.6, 132.8, 129.7, 128.3, 128.0, 127.5, 125.8, 122.7, 116.4, 112.2, 55.0, 53.4, 20.2. HRMS (ESI, *m/z*): calcd for $C_{17}H_{19}BrN^+$ $[M+H]^+$ 316.0695; found, 316.0706.

[(2-bromophenyl)methyl]bis(prop-2-en-1-yl)amine (1k):

Yellow color liquid: 176 mg (60 %). ^{1}HNMR: δ 7.56 (d, *J* = 7.5 Hz, 1H), 7.51 (d, *J* = 8.1 Hz, 1H), 7.28 (t, *J* = 7.5 Hz, 1H), 7.08 (t, *J* = 7.5 Hz, 1H), 5.95-5.82 (m , 2H) 5.24-5.12 (m, 4H), 3.65 (s, 2H), 3.12 (d, *J* = 6.3 Hz, 4H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 139.0, 135.8,

132.6, 130.5, 128.2, 127.3, 124.3, 117.5, 57.0, 56.8. HRMS (ESI, *m/z*): calcd for $C_{13}H_{17}BrN^+$ $[M+H]^+$ 266.0539; found, 266.0540.

[(2-bromophenyl)methyl](octyl)(prop-2-en-1-yl]amine:(1l).

Yellow color liquid: 131 mg (58 %). ^{1}HNMR: δ 7.56 (d, *J* = 7.5 Hz, 1H), 7.51 (d, *J* = 8.1 Hz, 1H), 7.30-7.26 (m, 1H), 7.08 (t, *J* = 6.3 Hz, 1H), 5.96-5.83 (m, 1H), 5.22-5.10 (m, 2H), 3.64 (s, 2H), 3.11 (d, *J* = 6.3 Hz, 2H), 2.46 (t, *J* = 7.2 Hz, 2H), 1.50-1.43 (m, 2H), 1.25 (br s, 10H), 0.87 (t, *J* = 6.3 Hz, 3H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 139.4, 136.1, 132.5, 130.5, 128.0, 127.2, 124.2, 117.1, 57.6, 57.2, 53.9, 31.9, 29.5, 29.3, 27.4, 27.1, 22.6, 14.1. HRMS (ESI, *m/z*): calcd for $C_{18}H_{29}BrN^+$ $[M+H]^+$ 338.1478; found, 338.1493.

[(2-bromophenyl)methyl][(2*E*)-3-phenylprop-2-en-1-yl](prop-2-en-1-yl)amine (1m):

Yellow color liquid: 256 mg (75 %). ^{1}H NMR: δ 7.59 (d, *J* = 7.8 Hz, 1H), 7.51 (dd, *J* = 7.8 Hz, 0.9 Hz, 1H), 7.38-7.19 (m, 6H), 7.01 (td, *J* = 7.8 Hz, 1.8 Hz 1H),6.54 (d, *J* =15.9 Hz, 1H*)* 6.28 (dt, *J* = 15.9 Hz, 6.6 Hz, 1H) 5.99-5.86 (m, 1H) 5.30-5.04 (m, 2H), 3.71. (s, 2H), 3.28 (d, *J* = 6.3 Hz, 2H) 3.18 (d, *J* = 6.3 Hz, 2H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 139.0, 137.2, 135.8, 132.7, 132.6, 130.6, 128.6, 128.3, 127.6, 127.4, 127.3, 126.4, 124.4, 117.7, 57.2, 57.0, 56.3. HRMS (ESI, *m/z*): calcd for $C_{19}H_{21}BrN^+$ $[M+H]^+$ 342.0852; found, 342.0847.

[(2-iodophenyl)methyl][(2*E*)-3-(4-methoxyphenyl)prop-2-en-1-yl](prop-2-en-1-yl)amine (1n):

Yellow color liquid: 656 mg (89 %). ^{1}HNMR: δ 7.80 (d, *J* = 7.8 Hz, 1H), 7.54 (d, *J* = 7.5 Hz, 1H), 7.35-7.29 (m, 3H), 6.93 (t ,*J* = 7.8 Hz, 1H), 6.84 (d, *J* = 8.7 Hz, 2H), 6.47 (d, *J* =

15.9 Hz, 1H), 6.13 (dt, *J* = 15.9 Hz, 6.3 Hz ,1H),5.99-5.86 (m, 1H) 5.26-5.14 (m, 2H), 3.80 (s, 3H), 3.64 (s, 2H), 3.26 (d, *J* = 6.3 Hz, 2H), 3.17 (d, *J* = 6.3 Hz, 2H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 159.0, 141.8, 139.3, 135.8, 132.0, 130.2, 130.0, 128.5, 128.1, 127.5, 125.2, 117.5, 113.9, 100.2, 62.0, 56.8, 56.1, 55.3. HRMS (ESI, *m/z*): calcd for $C_{20}H_{23}INO^+$ $[M+H]^+$ 420.0819; found, 420.0820.

[(2-bromophenyl)methyl][(2*E*)-2-methylbut-2-en-1-yl][(2*E*)-3-phenylprop-2-en-1-yl]amine:(1o). Yellow color liquid: 225 mg (76 %). ^{1}HNMR: δ 7.63 (d, *J* = 7.5 Hz, 1H), 7.50 (d, *J* =7.8 Hz, 1H), 7.34-7.18(m, 6H) 7.09-7.04 (m, 1H,) 6.52 (d, *J* = 15.9 Hz, 1H) 6.32-6.22 (m, 1H) 5.45-5.41 (m, 1H) 3.63 (s, 2H), 3.18 (d, *J* = 6.3 Hz,2H), 3.00 (s, 2H), 1.65 (s, 3H) 1.60 (d, *J* = 6.6 Hz, 3H), ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 142.2, 139.3, 137.3, 134.0, 132.3, 130.2, 128.5, 128.4, 128.0, 127.8, 127.3, 126.3, 122.0, 100.1, 62.8, 62.1, 55.9, 14.8, 13.4. . HRMS (ESI, *m/z*): calcd for $C_{21}H_{25}BrN^+$ $[M+H]^+$ 370.1165; found, 370.1176.

[(2-bromophenyl)methyl][(2*E*)-2-methylbut-2-en-1-yl] (prop-2-en-1-yl)amine (1p): Yellow color liquid: 479 mg (68%) ^{1}H NMR: δ 7.79 (d, *J* = 7.8 Hz, 1H), 7.54 (d, *J* = 6.6 Hz, 1H), 7.31 (t, *J* = 6.9 Hz, 1H) 6.91(t, *J* = 7.5Hz 1H) 5.96-5.83 (m, 1H) 5.43-5.39 (m, 1H,) 5.22-5.10 (m, 2H) 3.52 (s, 2H), 3.03 (d, *J* = 6.3 Hz,2H), 2.94 (s, 2H), 1.62 (s, 3H) 1.59 (d, *J* = 6.9 Hz, 3H), ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 142.2, 139.2, 136.0, 134.0, 130.1, 128.3, 128.0, 121.9, 117.2, 100.1, 62.5, 62.0, 56.5, 14.7, 13.3. HRMS (ESI, *m/z*): calcd for $C_{15}H_{21}BrN^+$ $[M+H]^+$ 294.0852; found, 294.0850.

***N*-[(2-bromophenyl)methyl]-4-methyl-N-[(2*E*)-2-methylbut-2-en-1-yl]aniline (1q)**: White color solid: 162mg (65%). MP: 70-75 ^{o}C. ^{1}HNMR: δ 7.58-7.55 (m, 1H), 7.22-7.08 (m, 3H), 6.98 (d, *J* = 8.7 Hz, 2H) 6.50 (d, *J* = 8.7 Hz, 2H) 5.39-5.33 (m, 1H) 4.48 (s, 2H), 3.87 (s, 2H), 2.22 (s, 3H), 1.63(brs, 6H).^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 146.6, 137.4, 132.9,

130.6, 129.7, 128.2, 128.0, 127.5, 125.4, 122.8, 119.0, 112.1, 58.0, 54.7, 20.3, 14.2, 13.2. HRMS (ESI, *m/z*): calcd for $C_{19}H_{23}BrN^+$ $[M+H]^+$ 344.1008; found, 344.1005.

[(2-bromophenyl)methyl][(2*E*)-2,3-diphenylprop-2-en-1-yl]ethylamine (1r): Yellow color liquid: 370 mg (72%) ^{1}HNMR: δ 7.48-7.47 (m, 1H) 7.46-6.96 (m, 13H), 6.69 (s, 1H), 3.71 (s, 2H), 3.44 (s, 2H) 2.62 (q, *J* = 7.2 Hz, 2H), 1.04 (t, *J* = 6.9 Hz, 3H) **.** ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 140.7, 140.6, 139.3, 137.1, 132.4, 130.5., 129.3, 128.9, 128.4, 128.2, 127.9, 127.2, 127.0.,126.5, 124.1, 62.6., 57.2, 47.7, 12.1. HRMS (ESI, *m/z*): calcd for $C_{24}H_{25}BrN^+$ $[M+H]^+$ 406.1165; found, 406.1160.

[(2-bromophenyl)methyl][(2*E*)-3-(4-methoxyphenyl)prop-2-en-1-yl][(2*E*)-3-(4-nitrophenyl)prop-2-en-1-yl]amine.(1s): yellow color liquid: 316 mg (60%) ^{1}HNMR: δ 8.15 (d, *J* = 9 Hz, 2H), 7.60 (dd, *J* = 7.5, 1.2 Hz, 1H), 7.52 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.45 (d, *J* = 8.7 Hz, 2H) 7.33-7.29 (m, 3H) 7.10 (dt, *J* = 7.5,1.5 Hz, 1H) 6.85 (d, *J* = 8.7 Hz, 2H), 6.62 (d, *J* = 16.2 Hz, 1H), 6.53-6.43 (m, 2H), 6.17 (td, *J* = 15.9,6.6 Hz, 1H) 3.80 (s, 3H), 3.76 (s, 2H), 3.37 (d, *J* = 6.0 Hz, 2H), 3.33 (d, *J* = 6.3 Hz, 2H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 159.1, 146.7, 143.6, 138.6, 133.3, 132.7, 132.4, 130.6, 130.2, 129.7, 128.4, 127.4, 127.3, 126.7, 124.7, 124.4, 124.0, 114.0, 57.5, 56.8, 56.2, 55.3. HRMS (ESI, *m/z*): calcd for $C_{26}H_{26}BrN_2O_3^+$ $[M+H]^+$ 493.1121; found, 493.1120.

General procedure for synthesis C4-substituted Tetrahydroisoquinoline 3:

In 5 mL glass vial containing aryl halide (0.1 mmol, 1.0 equiv.) in toluene (3 mL), Cs_2CO_3 (0.2 mmol, 65 mg) was added. Then reaction mass was purged with nitrogen before and after addition of $Pd(OAc)_2$ (0.01 mmol, 2.24 mg) and PPh_3 (0.02 mmol, 5.24 mg). Then the reaction mass was stirred for 24 h at 110 ^{o}C in an oil bath. After complete consumption of

the starting material, the reaction mixture was cooled to room temperature. Then the reaction vessel was opened and the contents were poured into a separating funnel (60 ml). Water (5 mL) and ethyl acetate (5 mL) were added into the separating funnel, extracted and the organic layer was isolated. The aqueous layer was further extracted with ethyl acetate (2×5 mL) and the combined organic extracts were washed with brine solution (1 × 10 mL). Finally the organic layer was dried over anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The obtained crude mixture was purified on neutral alumina column with 2% ethyl acetate in hexanes to afford the pure product.

(4*Z*)-2-butyl-4-(phenylmethylidene)-1, 2, 3, 4-tetrahydroisoquinoline (3a):

(Reaction performed with 0.08 mmol (30 mg) scale of **1a**).Yellow color liquid: 22 mg (95%). ^{1}H-NMR (300 MHz, $CDCl_3$) . δ 7.78-7.75 (m, 1H), 7.41-7.36 (m, 2H), 7.31-7.26 (m, 3H), 7.24-7.20 (m, 3H), 7.10-7.08 (m, 1H), 3.74 (s, 2H), 3.66 (s, 2H), 2.48 (t, *J* = 7.5 Hz, 2H), 1.52-1.42 (m, 2H) 1.35-1.23 (m, 2H) 0.87 (t, *J* = 7.2 Hz, 3H).). ^{13}C{1H} NMR (75 MHz $CDCl_3$) δ 137.4, 135.2, 133.4, 133.4, 129.4, 128.2, 127.5, 127.0, 126.8, 126.7, 123.4, 123.3, 57.4, 56.3, 54.0, 29.3, 20.7, 14.0. HRMS (ESI, *m/z*): calcd for $C_{20}H_{24}N^+$ $[M+H]^+$ 278.1903; found,278.1907.

(4*Z*)-2-ethyl-4-(phenylmethylidene)-1,2,3,4-tetrahydroisoquinoline (3b):

(Reaction performed with 0.15 mmol (50 mg) scale of **1b**).Yellow color liquid: 33 mg, (87 %). ^{1}H-NMR (300 MHz, $CDCl_3$) :δ 7.78-7.75 (m, 1H), 7.40-7.35 (m, 2H), 7.32-7.19 (m, 6H), 7.12-7.09 (m, 1H), 3.74 (s, 2H), 3.67 (s, 2H), 2.56 (q, *J* = 7.2 Hz, 2H), 1.09 (t, *J* = 7.2 Hz, 3H). ^{13}C{1H} NMR (75 MHz $CDCl_3$) δ 137.4, 135.1, 133.4, 133.3, 129.4, 128.3, 127.5, 127.0, 126.8, 126.8, 123.4, 123.3, 55.9, 53.6, 51.3, 12.4. HRMS (ESI, *m/z*): calcd for $C_{18}H_{20}N^+$.[$M+H]^+$ 250.1590; found, 250.1596.

(4*Z*)-2-*tert*-butyl-4-(phenylmethylidene)-1,2,3,4-tetrahydroisoquinoline (3c):

(Reaction performed with 0.14 mmol (50 mg) scale of **1c**).Yellow color liquid: 30 mg (78%). ^{1}H-NMR (300 MHz, $CDCl_3$): δ 7.77-7.72 (m, 1H), 7.41-7.28 (m, 5H), 7.22-7.16(m, 3H), 7.12-7.09 (m, 1H), 3.86 (s, 2H), 3.67 (s, 2H), 1.12(s, 9H). ^{13}C{1H} NMR (75 MHz $CDCl_3$) **δ** 137.6, 136.5, 135.1, 133.6, 129.2, 128.2, 127.4, 127.1, 126.7, 126.5, 123.5, 122.6, 54.2, 49.8, 46.9, 25.9. HRMS (ESI, *m/z*): calcd for $C_{20}H_{24}N^+$ $[M+H]^+$ 278.1903; found, 278.1904.

(4*Z*)-2-ethyl-4-[(4-methoxyphenyl)methylidene]-1,2,3,4-tetrahydroisoquinoline:(3d)

(Reaction performed with 0.14 mmol (50 mg) scale of **1d**).Yellow color liquid: 33 mg, (86%) . ^{1}H-NMR (300 MHz, $CDCl_3$): δ 7.75-7.72 (m, 1H), 7.26-7.13 (m, 5H), 7.10-7.07 (m, 1H), 6.94-6.89 (m, 2H), 3.84 (s, 3H), 3.73 (s, 2H), 3.67(s, 2H), 2.56 (q, *J* = 7.5 Hz, 2H), 1.10 (t, *J* = 7.3 Hz, 3H). ^{13}C{1H} NMR (75 MHz $CDCl_3$) δ 158.5, 134.8, 133.7, 131.8, 130.6, 130.0, 127.2, 127.0, 126.7, 123.2, 123.1, 113.7, 55.8, 55.3, 53.7, 51.3, 12.4. HRMS (ESI, *m/z*): calcd for $C_{19}H_{22}NO^+$ $[M+H]^+$ 280.1696; found 280.1702.

(4*Z*)-2-butyl-4-[(4-methoxyphenyl)methylidene]-1,2,3,4-tetrahydroisoquinoline.:(3e).

(Reaction performed with 0.13 mmol (50 mg) scale of **1e**).Yellow color liquid: 35 mg (89%). ^{1}H-NMR (300 MHz, $CDCl_3$): δ 7.75-7.72 (m, 1H), 7.25-7.14 (m, 5H), 7.09-7.06 (m, 1H), 6.94-6.90 (m, 2H), 3.84 (s, 3H), 3.73 (s, 2H), 3.66(s, 2H), 2.48 (t, *J* = 7.5 Hz, 2H), 1.53-1.40 (m, 2H) 1.33-1.26 (m, 2H) 0.88 (t, *J* = 7.2 Hz, 3H). ^{13}C{1H} NMR (75 MHz $CDCl_3$) δ 158.4, 134.9, 133.7, 131.9, 130.6, 130.0, 127.2, 126.9, 126.7, 123.2, 123.0, 113.7, 57.4, 56.3, 55.3, 54.1, 29.3, 20.7, 14.0. HRMS (ESI, *m/z*): calcd for $C_{21}H_{26}NO^+$ $[M+H]^+$ 308.2009; found 308.2003.

(4*Z*)-2-tert-butyl-4-[(4-methoxyphenyl)methylidene]-1,2,3,4-tetrahydroIsoquinoline (3f):

(Reaction performed with 0.11 mmol (40 mg) scale of **1f**).Yellow color liquid: 30 mg (85%). ^{1}H-NMR (300 MHz, $CDCl_3$): δ 7.73-7.70 (m, 1H), 7.26-7.17 (m, 4H), 7.09 (br s, 2H), 6.91 (d, *J* = 9 Hz, 2H), 3.84-3.85 (two singlets merged, 5H), 3.67 (s, 2H), 1.13 (s, 9H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 158.3, 136.3, 133.8, 133.7, 130.5, 130.2, 127.1, 127.0, 126.5, 123.3, 122.3, 113.7, 55.3, 54.2, 49.8, 46.9, 25.9 HRMS (ESI, *m/z*): calcd for $C_{21}H_{26}NO^{+}$ $[M+H]^{+}$ 308.2009; found 308.2004.

(4*Z*)-2-benzyl-4-[(4-methoxyphenyl)methylidene]-1,2,3,4-tetrahydroisoquinoline (3g): (Reaction performed with 0.25 mmol (120 mg) scale of **1g**).White color solid: 68 mg(78%), MP =85 ^{o}C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ 7.75 (d, *J* = 7.5 Hz, 1H), 7.29-7.16 (m, 10H), 7.00 (d, *J* = 7.5 Hz, 1H), 6.86 (d, *J* = 8.7 Hz, 2H), 3.82 (s, 3H), 3.74 (s, 2H), 3.71 (s, 2H), 3.65 (s, 2H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 158.4, 137.9, 134.7, 133.7, 131.7, 130.6, 129.9, 129.3, 128.3, 127.2, 127.2, 127.0, 126.7, 123.3, 123.2, 113.7, 61.7, 55.7, 55.3, 53.9. HRMS (ESI, *m/z*): calcd for $C_{24}H_{24}ON$ $[M+H]^{+}$ 342.1852; found, 342.1843.

(4*Z*)-2-[(4-methoxyphenyl)methyl]-4-(phenylmethylidene)-1,2,3,4-tetrahydroisoquinoline (3h): (Reaction performed with 0.42 mmol (200 mg) scale of **1h**).Yellow color liquid: 114 mg (78%). ^{1}H-NMR (300 MHz, $CDCl_3$): δ 7.77 (d, *J* = 7.5 Hz, 1H), 7.35-7.30 (m, 2H), 7.25-7.18 (m, 8H), 7.02 (d, *J* = 6.9 Hz, 1H), 6.79 (d, *J* = 8.4 Hz, 2H),
3.77 (s, 3H), 3.70 (s, 2H merged with the 3.69 peak), 3.69 (s, 2H), 3.58 (s, 2H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 158.8, 137.4, 135.0, 133.5, 133.2, 130.6, 129.8, 129.4, 128.3, 127.6, 127.1, 126.8, 123.6, 123.3, 113.7, 60.9, 55.6, 55.3, 53.5.HRMS (ESI, *m/z*): calcd for $C_{24}H_{24}ON$ $[M+H]^{+}$ 342.1852; found, 342.1851.

(4*Z*)-2-(4-methylphenyl)-4-(phenylmethylidene)-1,2,3,4-tetrahydroisoquinoline (3i): (Reaction performed with 0.25 mmol (100 mg) scale of **1i**).Yellow color liquid: 57 mg (81%).(As per starting material recovery). ^{1}H-NMR (300 MHz, $CDCl_3$): δ 7.76-7.73 (m, 1H), 7.43-7.38 (m, 2H), 7.33-7.16 (m, 7H), 7.00 (d, *J* = 8.4 Hz, 2H), 6.77 (d, *J* = 8.7 Hz, 2H), 4.45

(s, 2H), 4.39 (s, 2H), 2.22 (s, 3H), . $^{13}C\{1H\}$ NMR (75 MHz, $CDCl_3$) δ 148.0, 137.2, 134.7, 133.8, 132.7, 129.7, 129.3, 129.1, 128.4, 127.7, 127.1, 126.9, 126.7, 124.2, 123.8, 116.8, 52.9, 50.6, 20.4. HRMS (ESI, *m/z*): calcd for $C_{23}H_{21}N$ $[M]^+$ 311.1674; found, 311.1679.

4-methylidene-2-(4-methylphenyl)-1,2,3,4-tetrahydroisoquinoline (3j): (Reaction performed with 0.094 mmol (30 mg) scale of **1j**).Yellow color liquid: 18 mg (80%). ^1H-NMR (300 MHz, $CDCl_3$) . δ 7.69-7.65 (m, 1H), 7.24-7.20 (m, 2H), 7.18-7.14 (m, 1H), 7.07 (d, *J* =8.1 Hz, 2H), 6.93 (d, *J* =8.7 Hz, 2H), 5.63 (s, 1H), 5.10 (s, 1H), 4.42 (s, 2H), 4.10 (s, 2H), 2.26 (s, 3H). $^{13}C\{1H\}$ NMR (75 MHz. $CDCl_3$) δ 148.2, 138.9, 134.4, 132.5, 129.7, 129.3, 128.0, 126.8, 126.7, 123.8, 117.0,108.4, 55.4, 53.3, 20.4. HRMS (ESI, *m/z*): calcd for $C_{17}H_{16}N$ $[M-H]^+$ 234.1277; found, 234.1278.

4-methylidene-2-(prop-2-en-1-yl)-1,2,3,4-tetrahydroisoquinoline (3k):

(Reaction performed with 0.19 mmol (50 mg) scale of **1k**). Yellow color liquid: 26 mg (75%). ^1H-NMR (300 MHz, $CDCl_3$): δ 7.69-7.66 (m, 1H), 7.21-7.18 (m, 2H), 7.08-7.05 (m, 1H) ,6.01-5.88 (m, 1H), 5.61,(s, 1H), 5.28-5.19 (m, 2H), 5.01 (s, 1H), 3.73 (s, 2H), 3.39 (s, 2H), 3.17 (d, *J* = 6.6 Hz, 2H)): $^{13}C\{1H\}$ NMR 75 MHz, $CDCl_3$) δ 139.3, 135.1, 134.6, 132.2, 127.9, 126.9, 126.6, 123.4, 118.2, 108.0, 60.3, 58.0 , 56.4. HRMS (ESI, *m/z*): calcd for $C_{13}H_{16}N$ $[M+H]^+$ 186.1277; found, 186.1279.

4-methylidene-2-octyl-1,2,3,4-tetrahydroisoquinoline (3l): (Reaction performed with 0.30 mmol (100 mg) scale of **1l**).Pale yellow color liquid: 60 mg (79 %). ^1H-NMR (300 MHz, $CDCl_3$): δ 7.68-7.64 (m, 1H), 7.21-7.17 (m , 2H) 7.08-7.05 (m, 1H) 5.60 ,(s, 1H), 5.01 (s, 1H) 3.72 (s, 2H), 3.38 (s, 2H), 2.49 (t, *J* = 7.5 Hz, 2H), 1.61- 1.53 (m, 2H), 1.31-1.27 (m, 10H) 0.88(t, *J* = 6 Hz, 3H). $^{13}C\{1H\}$ NMR (75 MHz, $CDCl_3$) δ 139.5, 134.9, 132.2, 127.8, 126.9, 126.5, 123.4, 107.8, 58.5, 57.4, 56.8, 31.9, 29.6, 29.3, 27.6, 27.3, 22.7, 14.1. HRMS (ESI, *m/z*): calcd for $C_{18}H_{28}N$ $[M+H]^+$ 258.2216; found, 258.2209.

4-methylidene-2[(2*E*)-3-phenylprop-2-en-1-yl]-1,2,3,4-tetrahydroisoquinoline (3m): (Reaction performed with 0.15 mmol (50 mg) scale of **1m**).Yellow color liquid 31mg (79 %). ^{1}H-NMR (300 MHz, $CDCl_3$): δ 7.70-7.67 (m, 1H), 7.42-7.40 (m, 2H), 7.32 (t, *J* = 6.9 Hz, 2H) ,7.27-7.24 (m, 1H), 7.22-7.19 (m, 2H) , 7.08-7.05(m, 1H), 6.58 (d, *J* = 15.9 Hz, 1H) , 6.35 (dt, *J* = 15.9 Hz, 6.6Hz, 1H) 5.63,(s, 1H), 5.02 (s, 1H), 3.79 (s, 2H), 3.45 (s, 2H), 3.34 (d, *J* = 6.6 Hz, 2H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 139.2, 136.9, 134.5, 133.1, 132.2, 128.6, 127.9, 127.6, 126.9, 126.6, 126.4, 123.5, 108.1, 59.6, 58.2, 56.5. HRMS (ESI, *m/z*): calcd for $C_{19}H_{20}N$ $[M+H]^+$ 262.1590; found, 262.1583.

2-[(2*E*)-3-(4-methoxyphenyl)prop-2-en-1-yl]-4-methylidene-1,2,3,4-tetrahydroisoquinoline (3n): (Reaction performed with 0.17 mmol (70 mg) scale of **1n**).Pale yellow color solid: 38 mg (79%). MP =105-110 ºC. ^{1}H-NMR (300 MHz, $CDCl_3$): δ 7.70-7.67 (m, 1H), 7.34 (d , *J* = 8.7 Hz, 2H), 7.22-7.18 (m, 2H) ,7.08-7.05 (m, 1H), 6.87 (d, *J* = 8.7 Hz, 2H) 6.52 (d, *J* = 15.9 Hz, 1H), 6.20 (dt, *J* = 15.9 Hz, 6.6 Hz, 1H) 5.63, (s, 1H), 5.02 (s, 1H), 3.82 (s, 3H), 3.78 (s, 2H), 3.44 (s, 2H), 3.31 (d, *J* = 6.6 Hz, 2H): ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 159.2, 139.3, 134.7, 132.6, 132.2, 129.8, 127.9, 127.6, 126.9, 126.6, 124.4, 123.5, 114.0, 108.0, 59.8, 58.2, 56.5, 55.3.. HRMS (ESI, *m/z*): calcd for $C_{20}H_{22}NO$ $[M+H]^+$ 292.1696; found, 292.1688.

(4*Z*)-2-(2-methylbut-2-en-1-yl)-4-(phenylmethylidene-1,2,3,4-tetrahydroisoquinoline (3o): (Reaction performed with 0.22 mmol (80 mg) scale of **1o**).Yellow color liquid: 43 mg (70%). ^{1}H-NMR (300 MHz, $CDCl_3$): δ 7.79-7.74 (m, 1H), 7.39-7.33 (m, 3H), 7.30-7.19 (m, 5H), 7.10-7.07 (m, 1H), 5.36-5.29 (m, 1H), 3.66 (s, 2H), 3.61 (s, 2H), 2.97 (s, 2H), 1.64 (s, 3H), 1.51 (d, *J* = 7.8 Hz, 3H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 137.5, 135.3, 133.6, 133.4, 132.7, 129.3, 128.1, 127.5, 127.0, 126.7, 126.6, 123.4, 123.3, 122.7, 66.0, 55.9, 53.3, 14.7, 13.2. HRMS (ESI, *m/z*): calcd for $C_{21}H_{22}N$ $[M-H]^+$ 288.1746; found, 288.1740.

2-[(2E)-2-methylbut-2-en-1-yl]-4-methylidene-1,2,3,4-tetrahydroisoquinoline:(3p)

(Reaction performed with 0.18 mmol (60 mg) scale of 1p).Yellow color liquid: 29 mg (77%). ^{1}H-NMR (300 MHz, $CDCl_3$): δ 7.69-7.66 (m, 1H), 7.20-7.17(m, 2H), 7.07-7.04 (m, 1H), 5.60 (s, 1H), 5.44-5.39 (m, 1H), 4.99 (s, 1H), 3.63 (s, 2H), 3.29 (s, 2H), 3.00 (s, 2H) , 1.68 (s, 3H) ,1.65(d, *J* =6.6 Hz, 3H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$): δ 139.6, 135.1, 132.9, 132.3, 127.8, 126.9, 126.4, 123.4, 122.4, 107.6, 66.0, 57.9, 56.4, 14.7, 13.3. HRMS (ESI, *m/z*): calcd for $C_{15}H_{20}N$ $[M+H]^+$ 214.1590; found, 214.1586.

4-ethenyl-4methyl-2-(4-methylphenyl)-1, 2, 3, 4-tetrahydroisoquinoline :(3q)

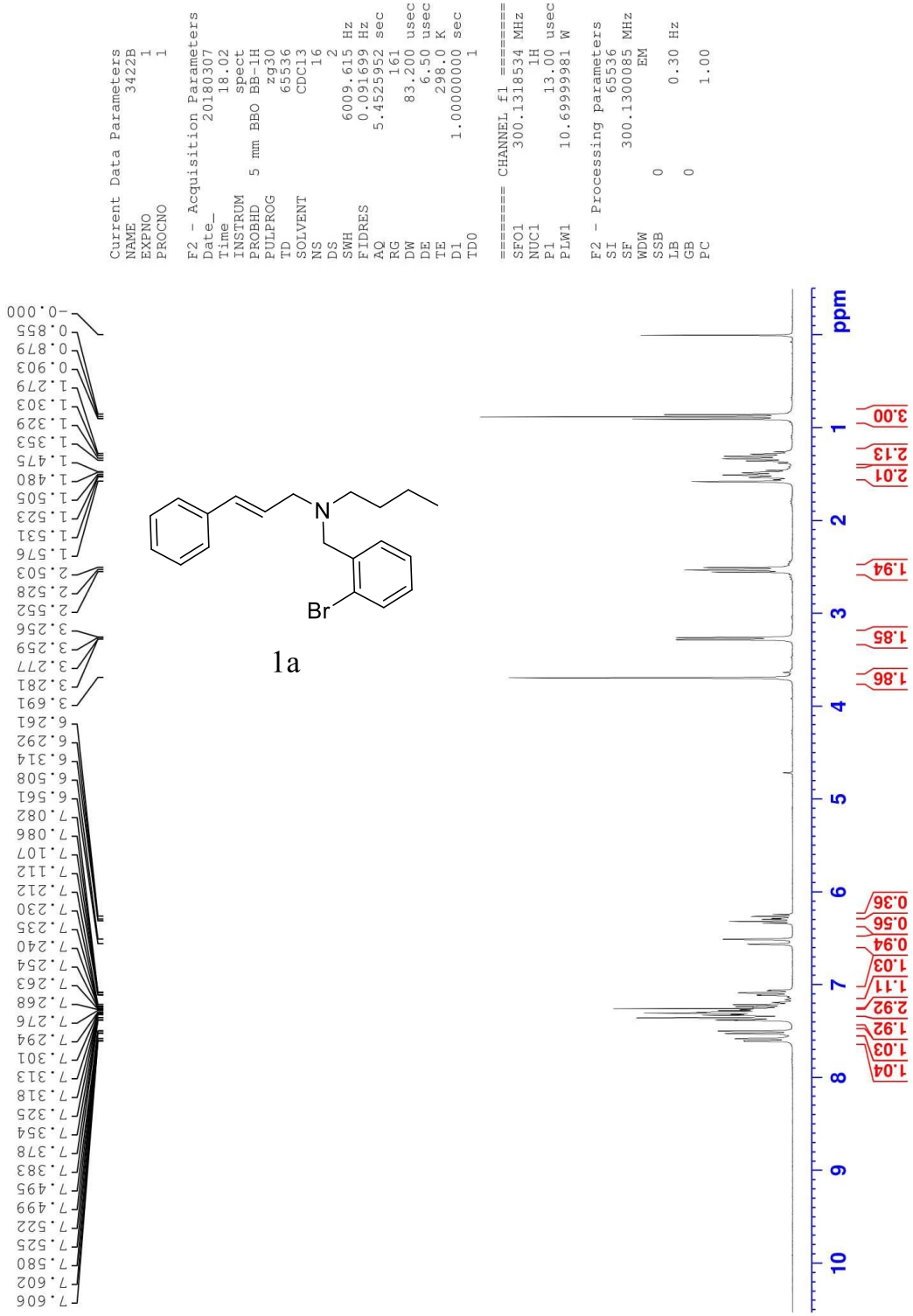
(Reaction performed with 0.14 mmol (50 mg) scale of **1q**). Yellow color liquid: 30 mg (78%). 1H-NMR (300 MHz, CDCl3): δ 7.27-7.23 (m, 1H), 7.22-7.14 (m, 3H), 7.11 (d, J = 8.1 Hz, 2H), 6.89 (d, J = 8.7 Hz, 2H), 6.05 (dd, J = 17.1, 10.8 Hz, 1H), 5.16 (brs, 1H), 5.12 (dd, J =7.2, 1.2 Hz, 1H), 4.34 (dd, J = 20.7, 15 Hz ,2H), 3.30 (dd, J = 19.8, 12.3 Hz, 2H), 2.28 (s, 3H), 1.49 (s, 3H). ^{13}C{1H} NMR (75 MHz, CDCl3) δ 148.7, 145.0, 141.1, 133.8, 129.6, 128.1, 127.3, 126.52, 126.50, 126.2, 115.2, 113.5, 59.4, 51.4, 42.5, 24.7, 20.4. HRMS calcd for (ESI, m/z): calcd for $C_{19}H_{20}N$ $[M-H]^+$ 262.1590 found, 262.1591

$3S_1$ and $3S_2$ formed as 1:1 mixture

<u>Procedure for the gram scale preparation of compound: 3c:</u>

Compound **1c** (10 mmol, 3.58 g, 1.0 equiv.), Cs_2CO_3 (20 mmol, 6.4 g, 2.0 equiv.) and toluene (150 mL) were taken in a 500 mL two neck round bottomed flask fitted with reflux condenser. Then reaction mass was purged with nitrogen before and after the addition of $Pd(OAc)_2$ (1.0 mmol, 224 mg) and PPh_3 (2.0 mmol, 524 mg). The reaction mass was stirred for 20 h at 110 ^{o}C in an oil bath. After complete consumption of the starting material, the reaction mixture was cooled to room temperature. Then the reaction vessel was opened and the contents were poured into a separating funnel (500 ml). Water (50 mL) and ethyl acetate

(100 mL) were added into the separating funnel, extracted and the organic layer was isolated. The aqueous layer was further extracted with ethyl acetate (2×50 mL).) and the combined organic extracts were washed with brine solution (1 × 100 mL). Finally, the organic layer was dried over anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The obtained crude mixture was purified on neutral alumina column with 2% ethyl acetate in hexanes to afford the pure product. 2.05 g of pure compound of **3c** was isolated with (76% yield).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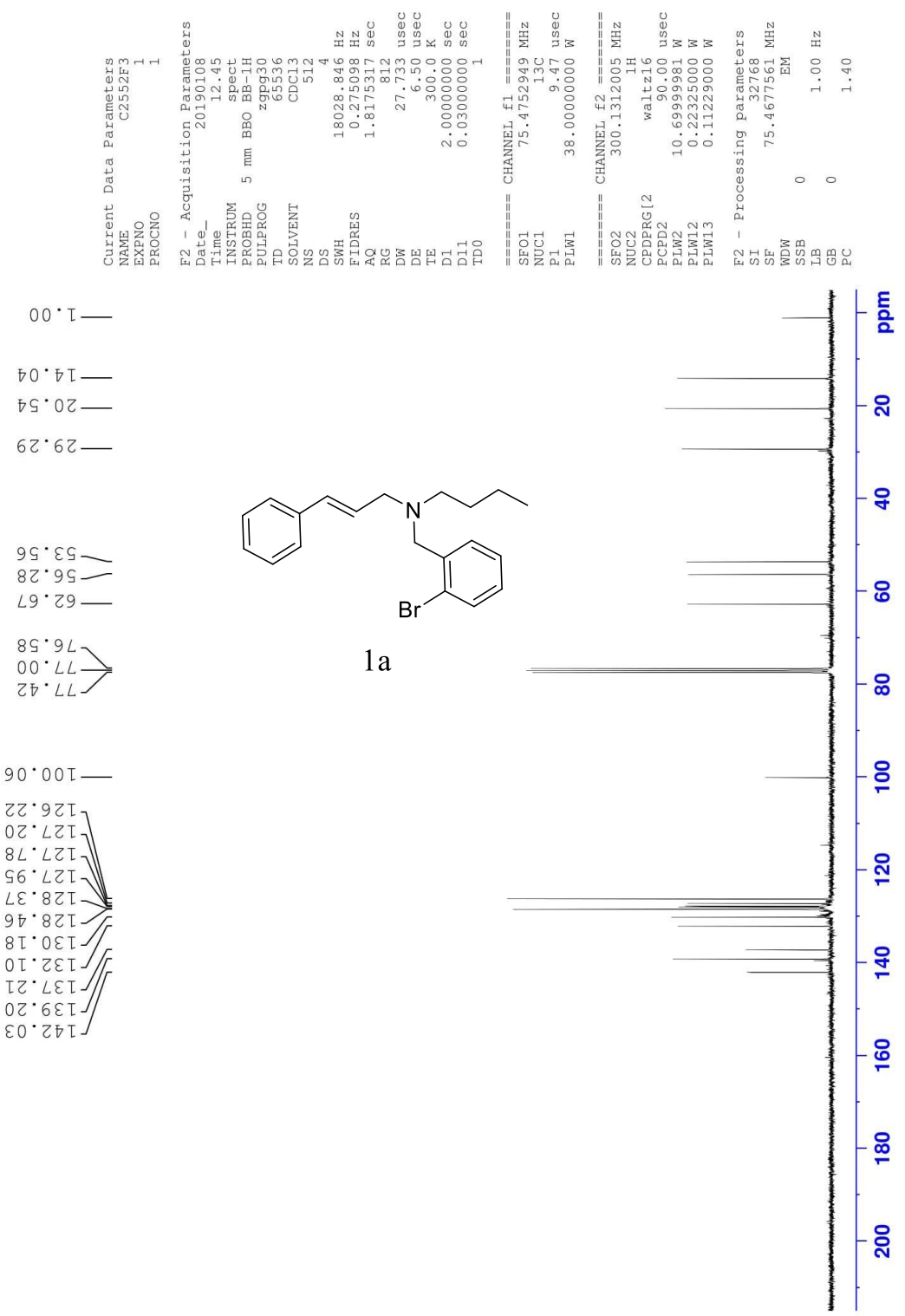
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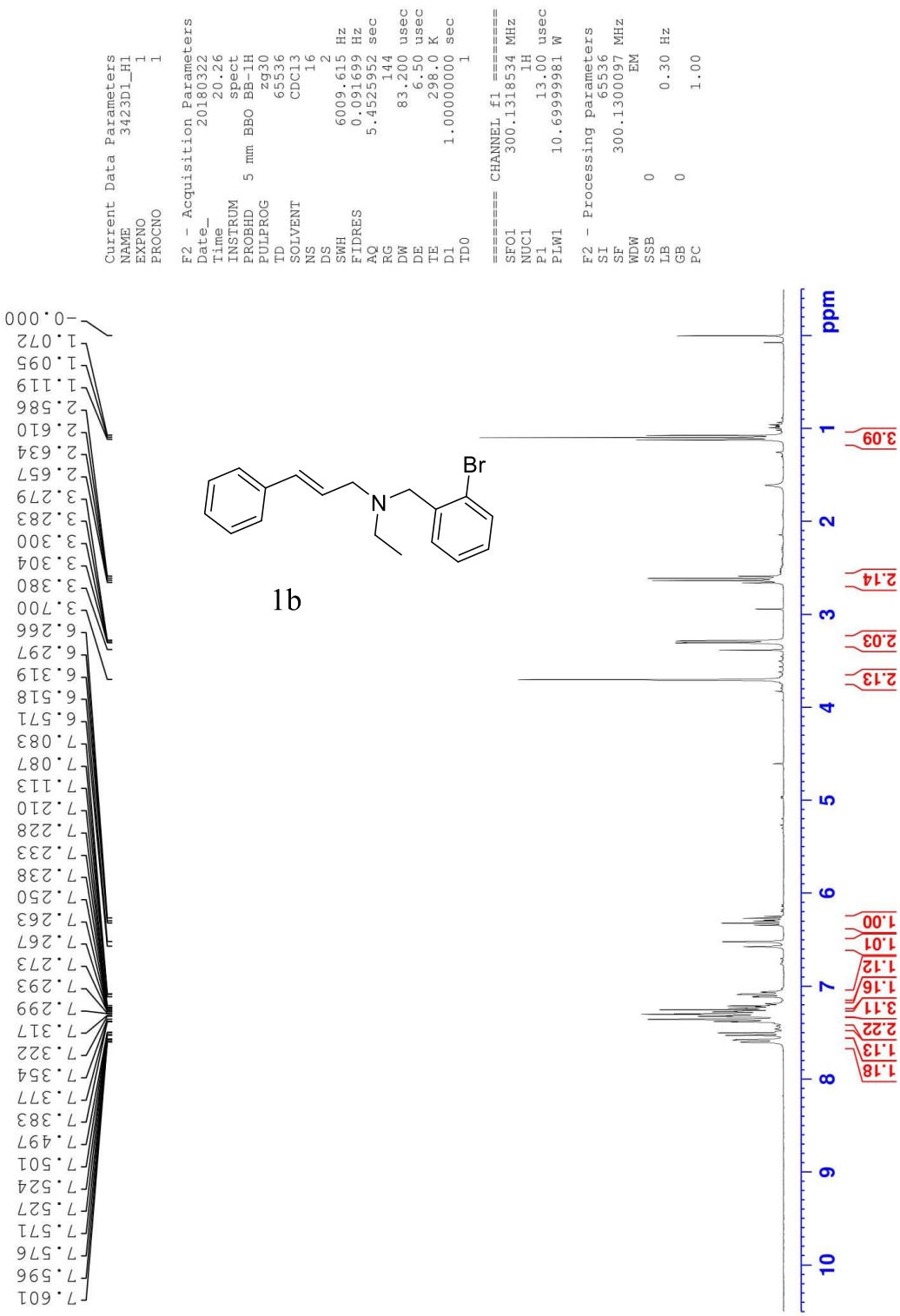
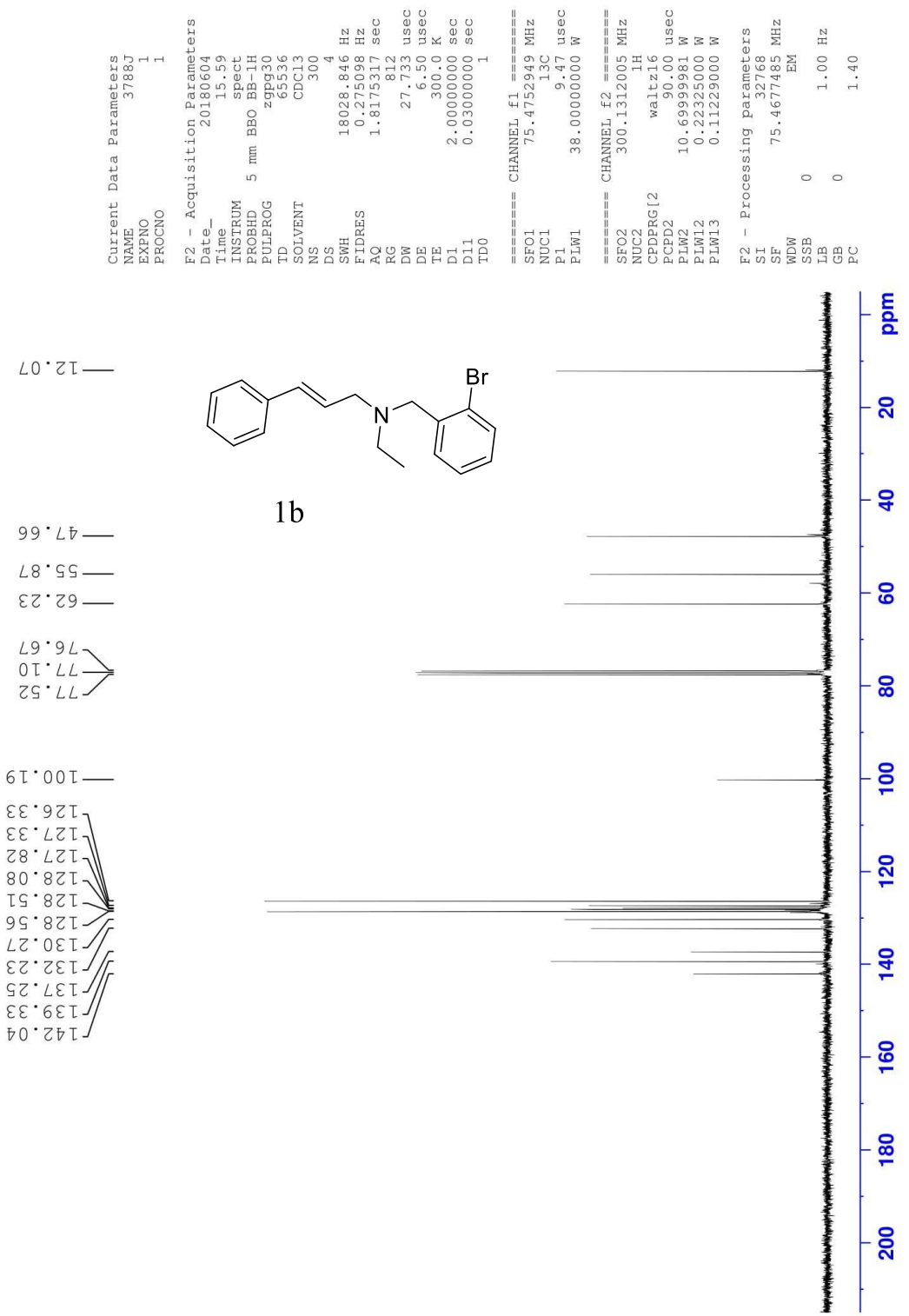
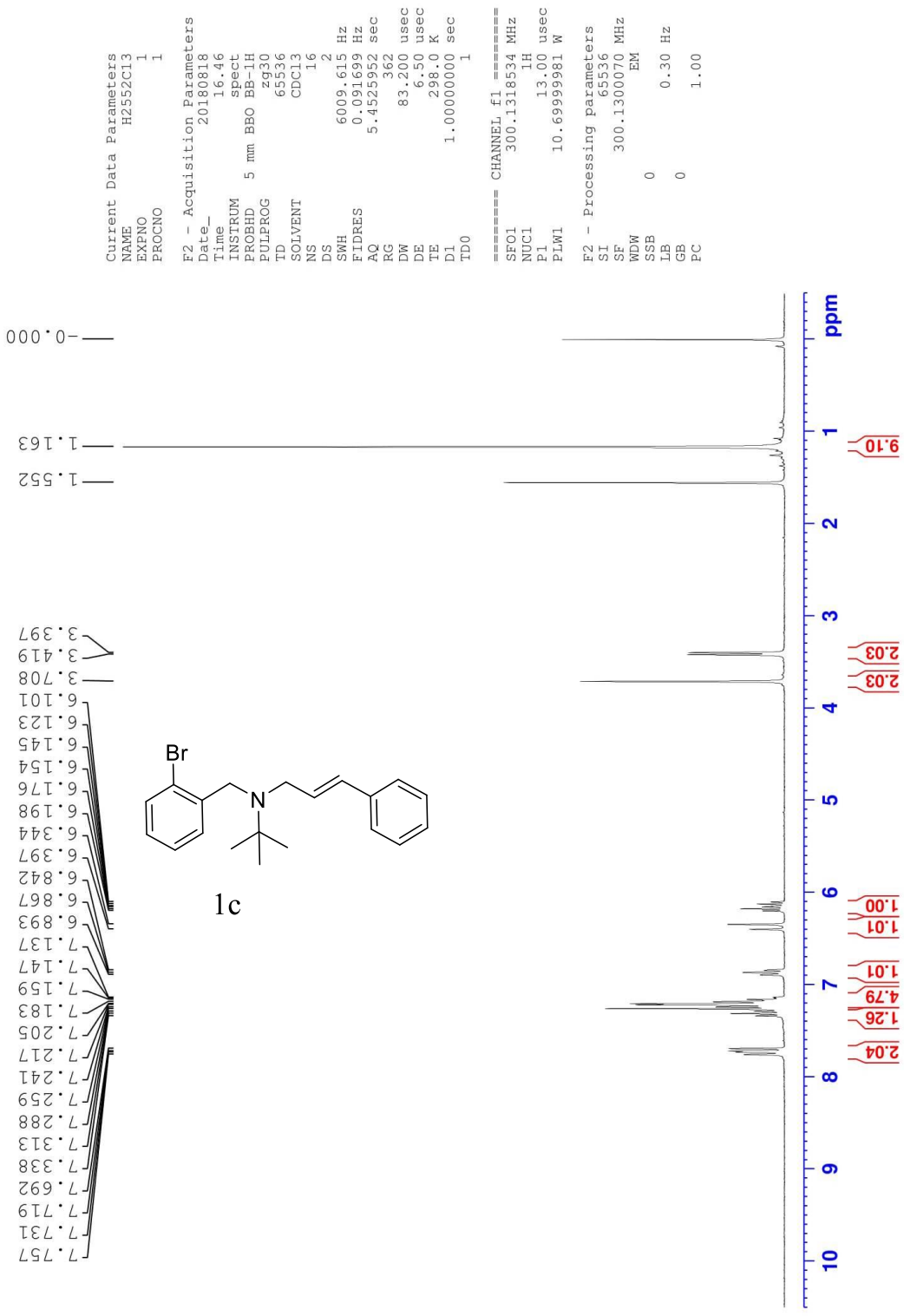
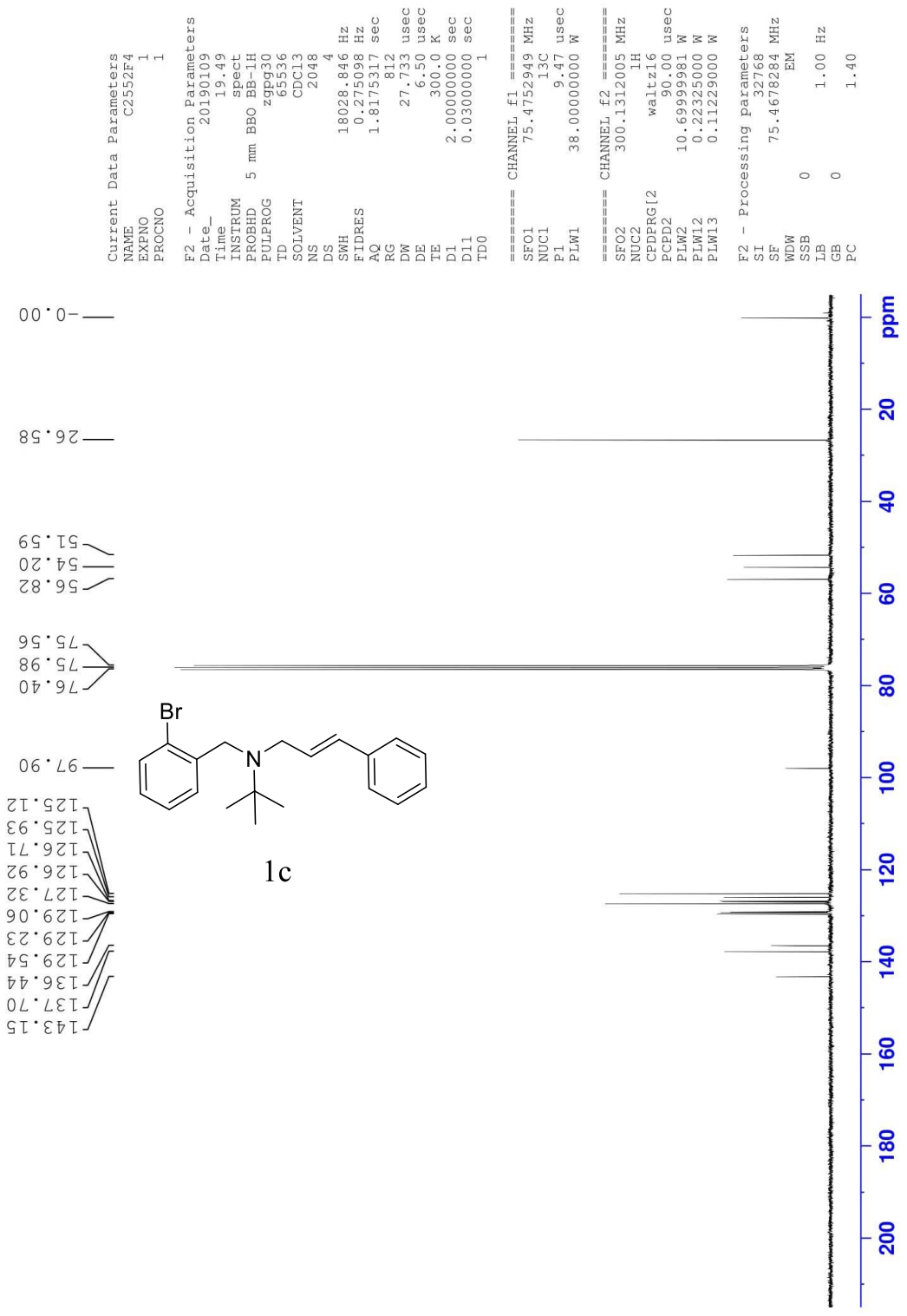
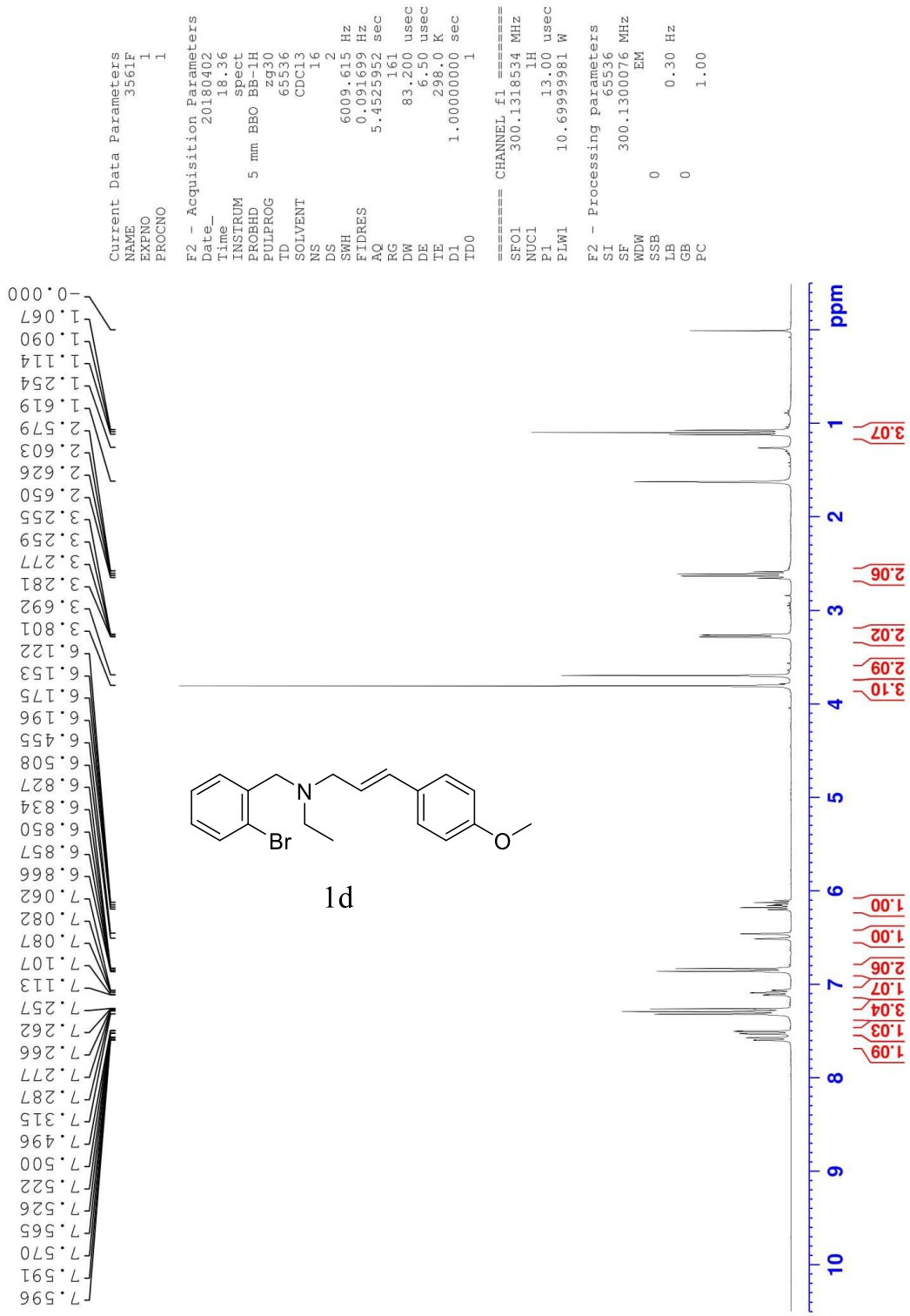
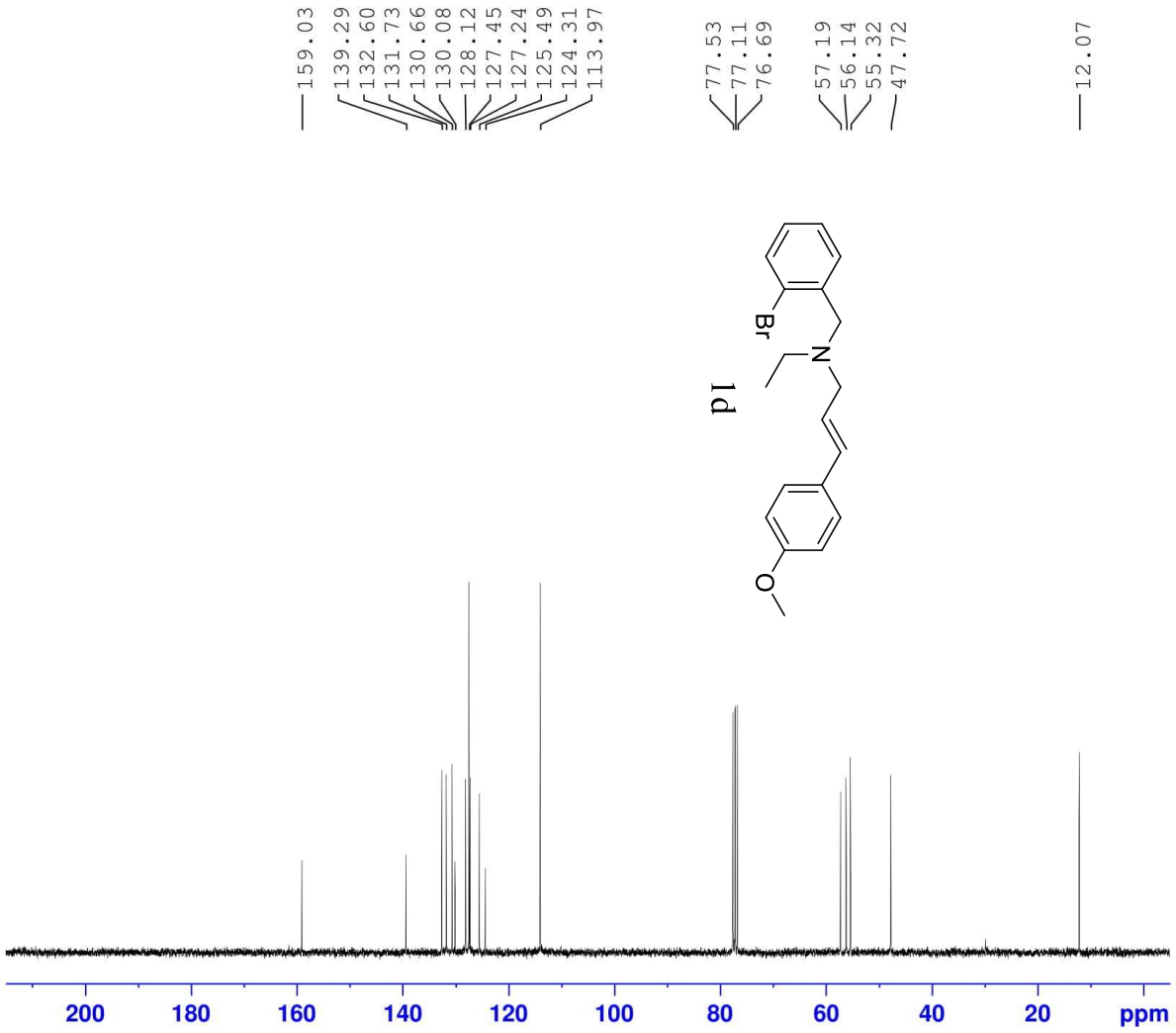

Current Data Parameters
NAME 3423D1_H1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180322
Time 20.26
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 144
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.69999981 W
F2 - Processing parameters
SI 65536
SF 300.1300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Br
N
1b
ppm
3.09
2.14
2.03
2.13
1.00
1.01
1.12
1.16
3.11
2.22
1.13
1.18


Current Data Parameters
NAME 3788J
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180604
Time 15.59
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 300
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 812
DW 27.733 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 75.4752949 MHz
NUC1 13C
P1 9.47 usec
PLW1 38.00000000 W
======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 10.69999981 W
PLW12 0.22325000 W
PLW13 0.11229000 W
F2 - Processing parameters
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Br
N
1b
12.07
47.66
55.87
62.23
76.67
77.10
77.52
100.19
126.33
127.33
127.82
128.08
128.51
128.56
130.27
132.23
137.25
139.33
142.04
ppm
200
180
160
140
120
100
80
60
40
20

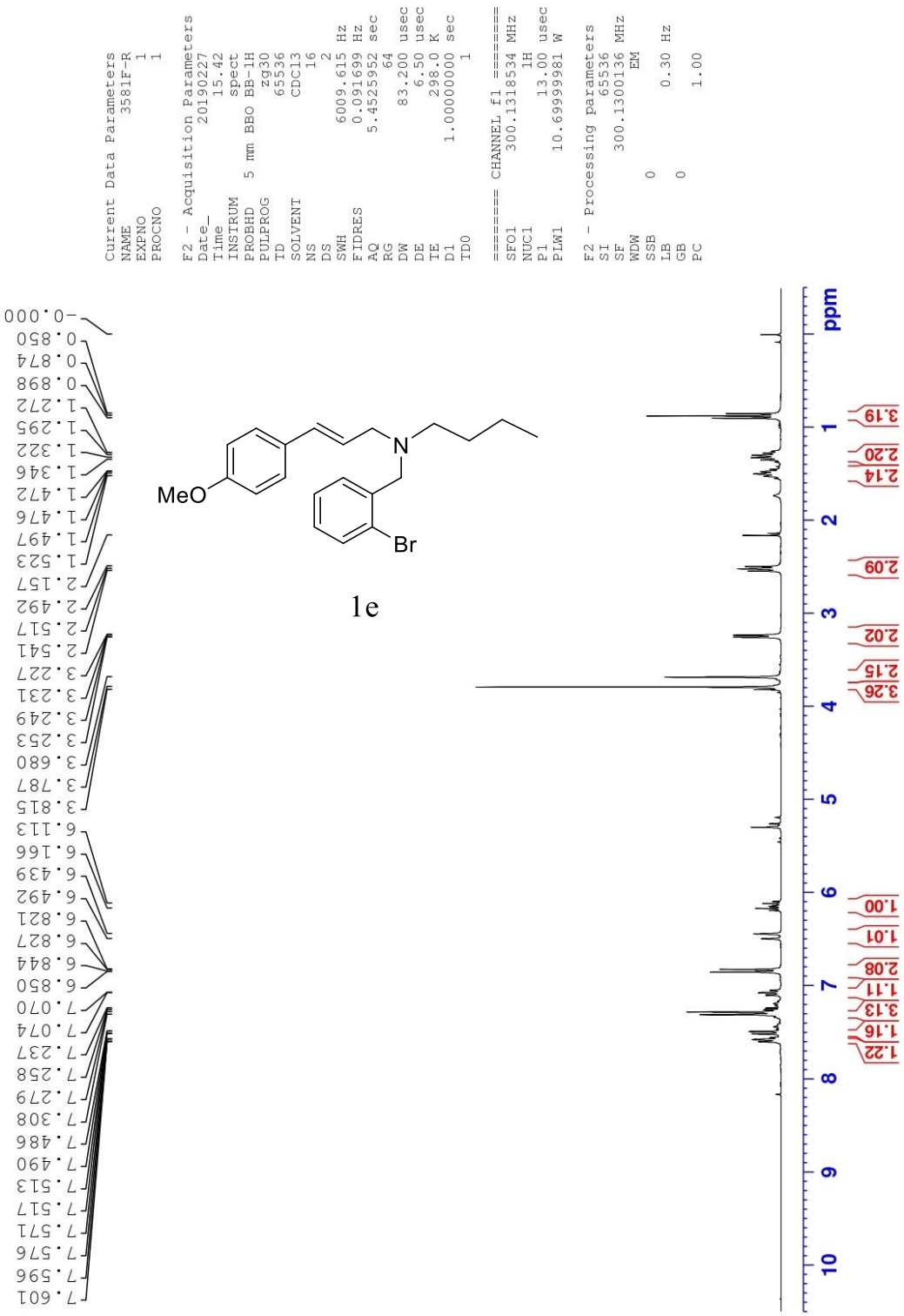

Current Data Parameters
NAME H2552C13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180818
Time 16.46
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 362
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.69999981 W
F2 - Processing parameters
SI 65536
SF 300.1300070 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
-0.000
1.163
1.552
3.397
3.419
3.708
6.101
6.123
6.145
6.154
6.176
6.198
6.344
6.397
6.842
6.867
6.893
7.137
7.147
7.159
7.183
7.205
7.217
7.241
7.259
7.288
7.313
7.338
7.692
7.719
7.731
7.757
Br
N
1c
ppm
9.10
2.03
2.03
1.00
1.01
1.01
4.79
1.26
2.04

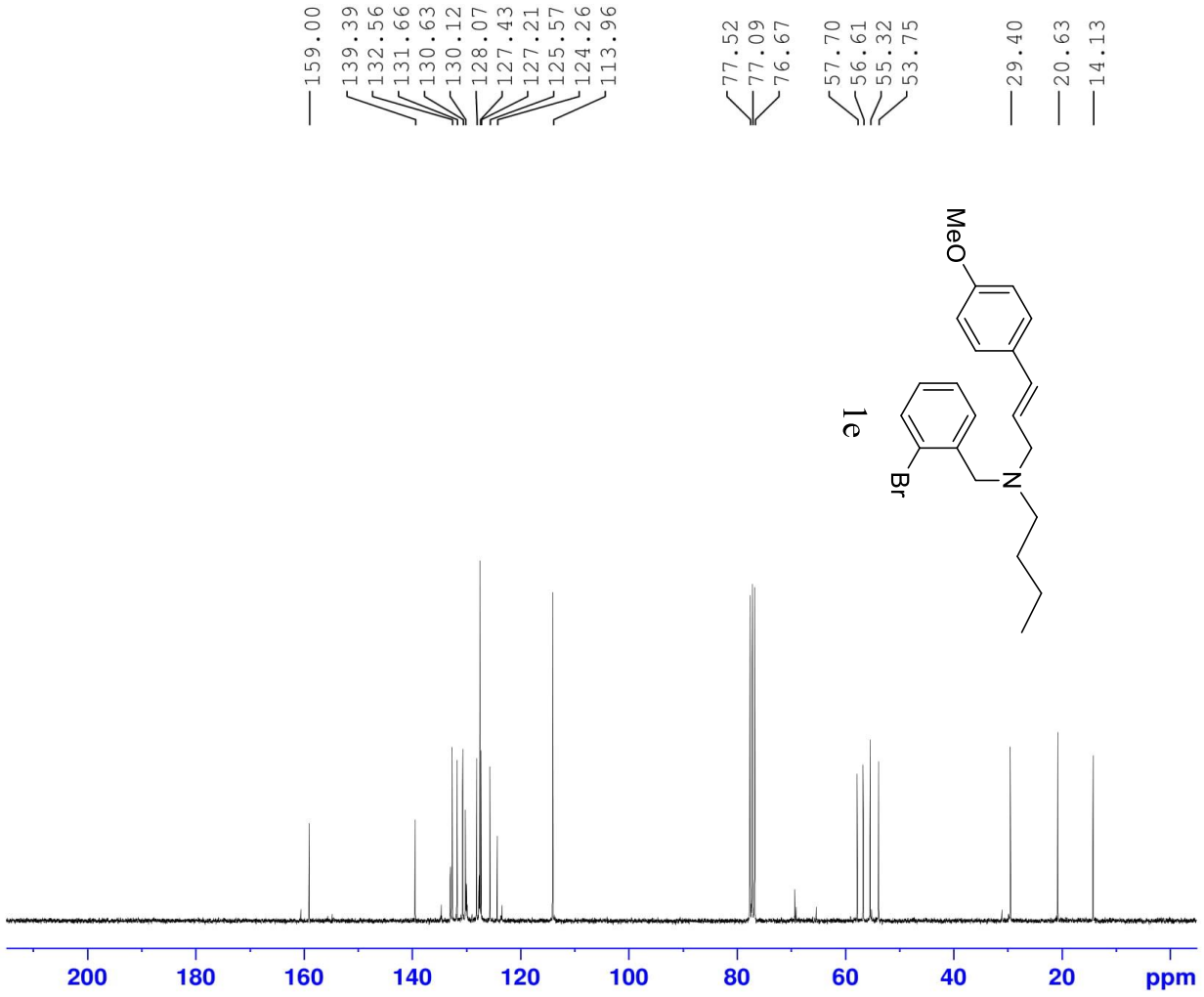

Current Data Parameters
NAME C2552F4
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190109
Time 19.49
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.81175317 sec
RG 812
DW 27.733 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 75.4752949 MHz
NUC1 13C
P1 9.47 usec
PLW1 38.00000000 W
======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 10.69999981 W
PLW12 0.22325000 W
PLW13 0.11229000 W
F2 - Processing parameters
SI 32768
SF 75.4678284 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
-0.00
26.58
51.59
54.20
56.82
75.56
75.98
76.40
97.90
125.12
125.93
126.71
126.92
127.32
129.06
129.23
129.54
136.44
137.70
143.15
Br
N
1c
ppm
200
180
160
140
120
100
80
60
40
20


Current Data Parameters
NAME 3561F
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180402
Time 18.36
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 161
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.69999981 W
F2 - Processing parameters
SI 65536
SF 300.1300076 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
ppm
3.07
2.06
2.02
2.09
3.10
1.09
1.03
3.04
1.07
2.06
1.00
1.00
N
Br
O
1d

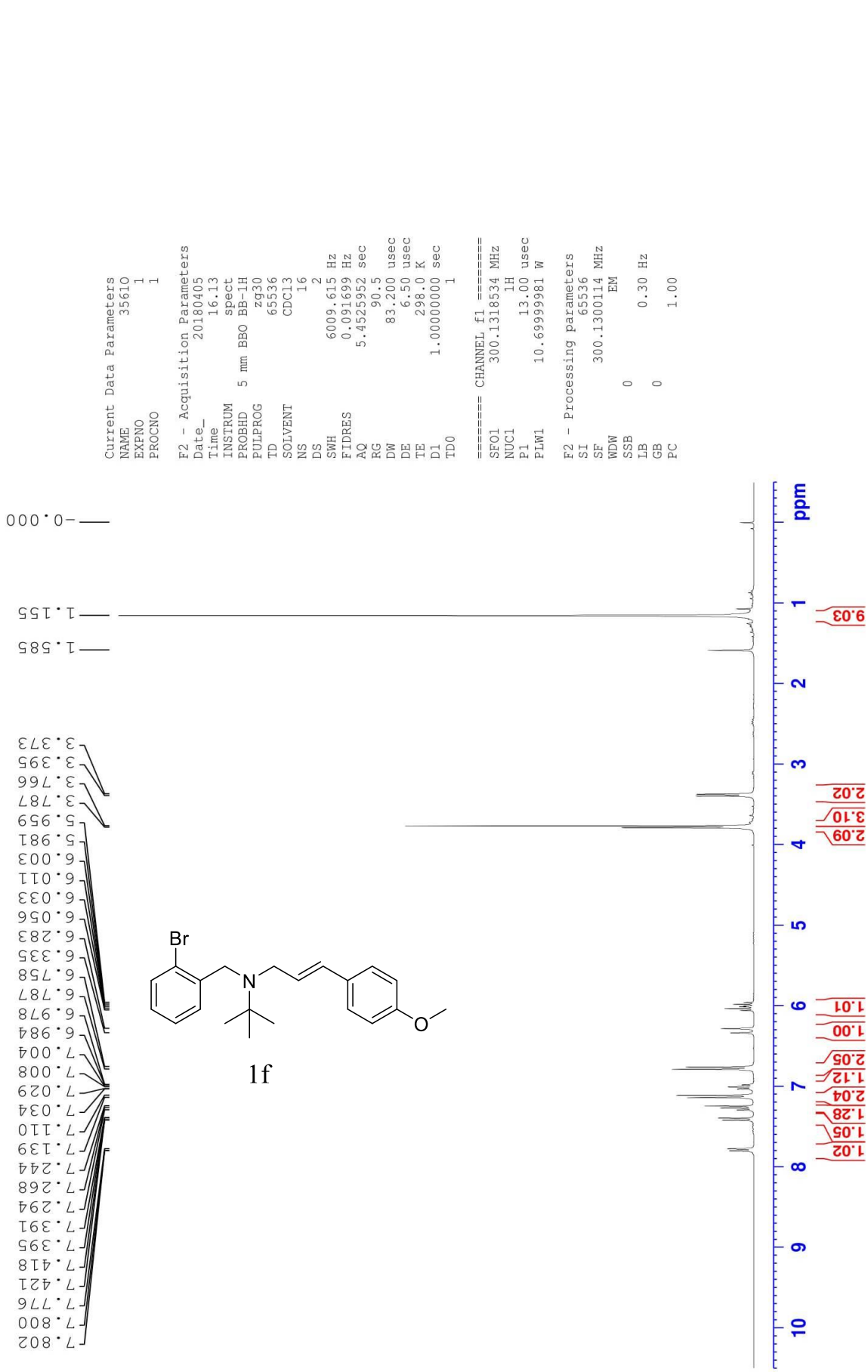



```
Current Data Parameters
NAME          3561KL_C13
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180405
Time               13.44
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  128
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175317 sec
RG                  812
DW               27.733 usec
DE                6.50 usec
TE                300.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         75.4752949 MHz
NUC1                13C
P1                 9.47 usec
PLW1        38.00000000 W

======== CHANNEL f2 ========
SFO2        300.1312005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2        10.69999981 W
PLW12        0.22325000 W
PLW13        0.11229000 W

F2 - Processing parameters
SI                 32768
SF          75.4677485 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

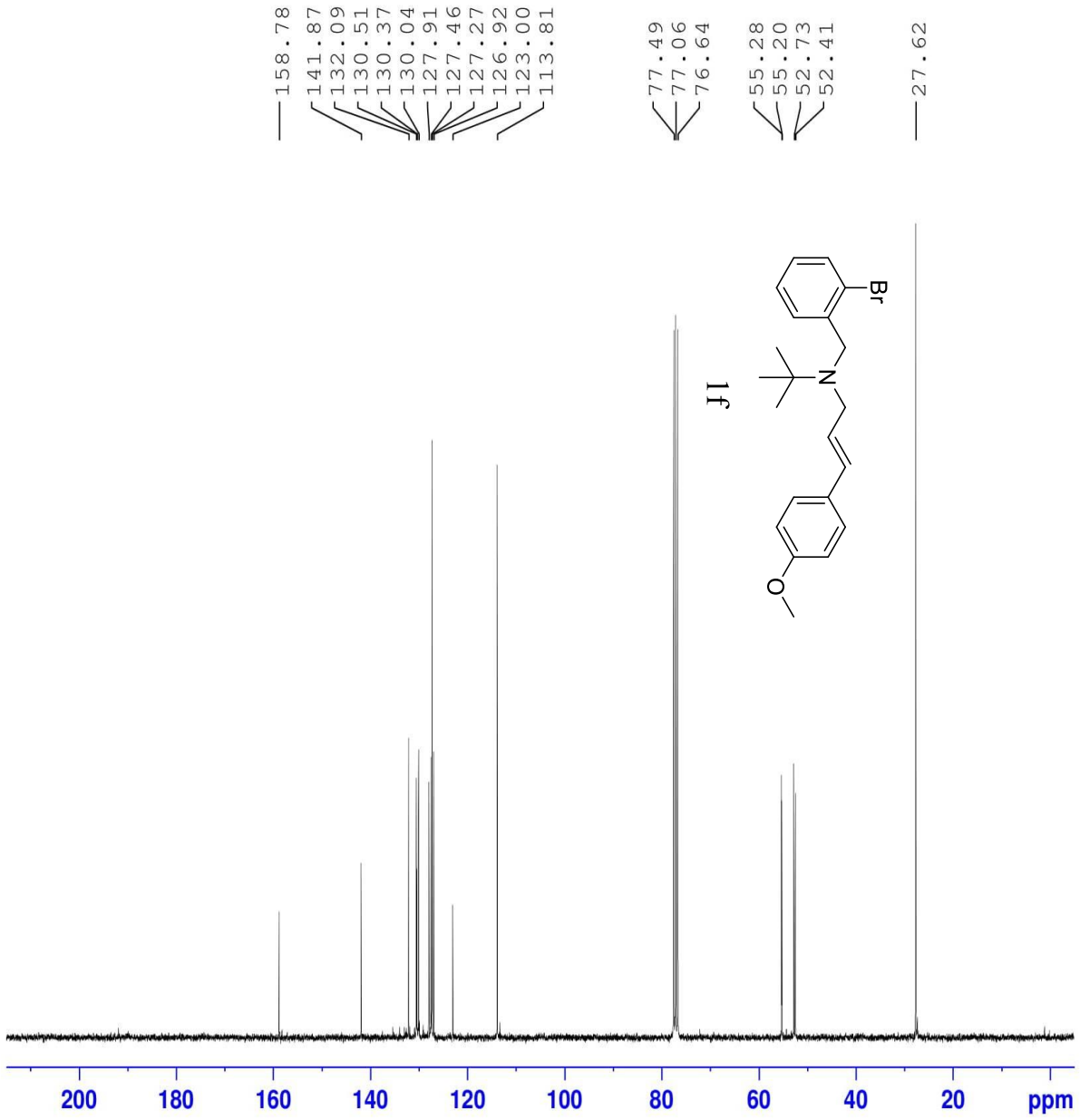

Current Data Parameters
NAME 3581F-R
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190227
Time 15.42
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 64
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.69999981 W
F2 - Processing parameters
SI 65536
SF 300.1300136 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
MeO
N
Br
1e
ppm
3.19
2.14
2.20
2.09
2.02
2.15
3.26
1.00
1.01
2.08
1.11
3.13
1.16
1.22



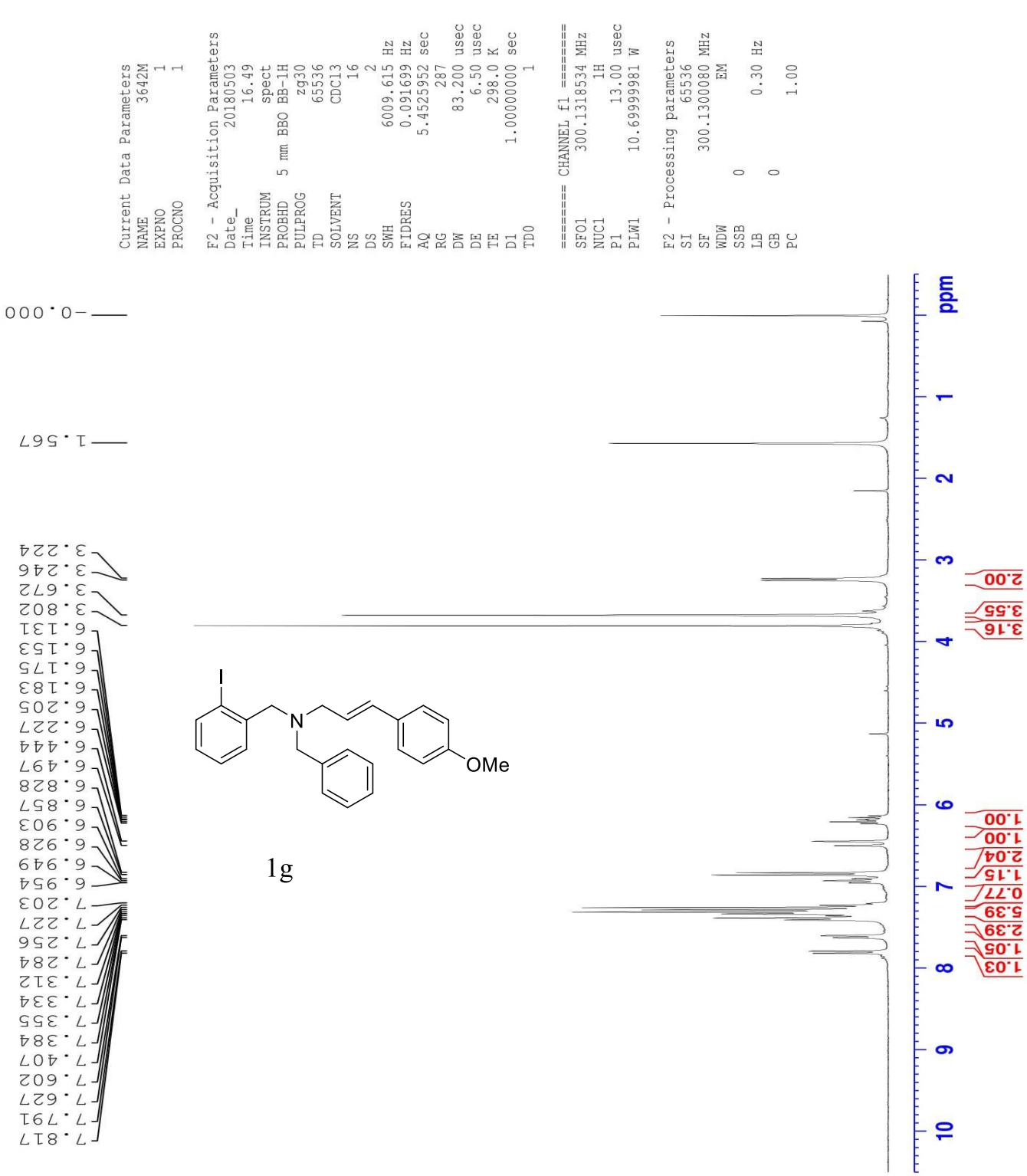

```
Current Data Parameters
NAME                  3581F-R
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_                20190304
Time                    16.23
INSTRUM                 spect
PROBHD    5 mm BBO BB-1H
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                        1024
DS                           4
SWH                 18028.846 Hz
FIDRES               0.275098 Hz
AQ                   1.8175317 sec
RG                         812
DW                      27.733 usec
DE                       6.50 usec
TE                      300.0 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1               75.4752949 MHz
NUC1                      13C
P1                       9.47 usec
PLW1               38.00000000 W

======== CHANNEL f2 ========
SFO2              300.1312005 MHz
NUC2                      1H
CPDPRG[2               waltz16
PCPD2                   90.00 usec
PLW2               10.69999981 W
PLW12               0.22325000 W
PLW13               0.11229000 W

F2 - Processing parameters
SI                       32768
SF                 75.4677485 MHz
WDW                         EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.40
```

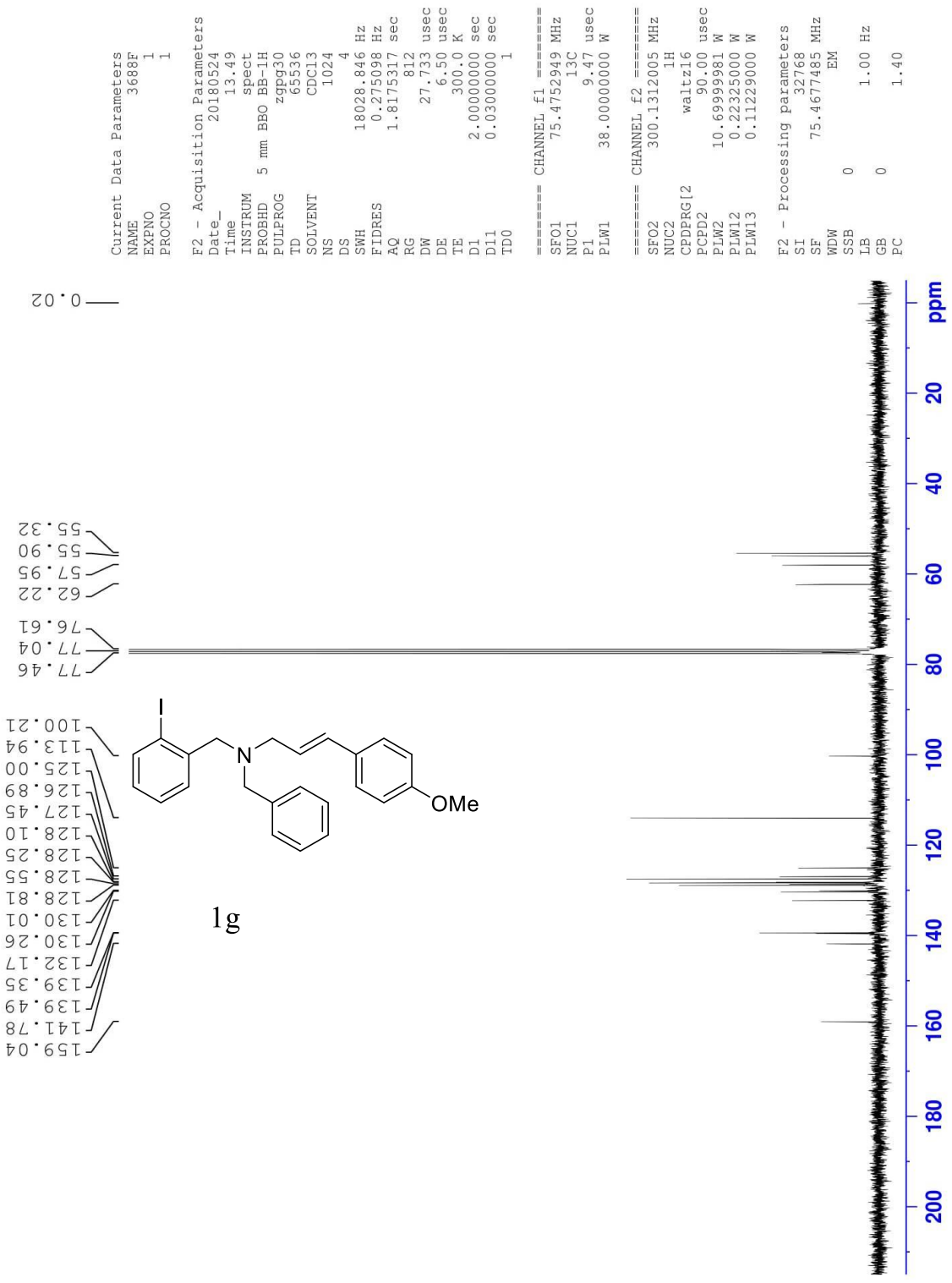

Current Data Parameters
NAME 35610
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180405
Time 16.13
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 90.5
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.69999981 W
F2 - Processing parameters
SI 65536
SF 300.1300114 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
ppm
9.03
2.02
3.10
2.09
1.01
1.00
2.05
1.12
2.04
1.28
1.05
1.02
1.155
1.585
0.000
3.373
3.395
3.766
3.787
5.959
5.981
6.003
6.011
6.033
6.056
6.283
6.335
6.758
6.787
6.978
6.984
7.004
7.008
7.029
7.034
7.110
7.139
7.244
7.268
7.294
7.391
7.395
7.418
7.421
7.776
7.800
7.802
Br
N
O

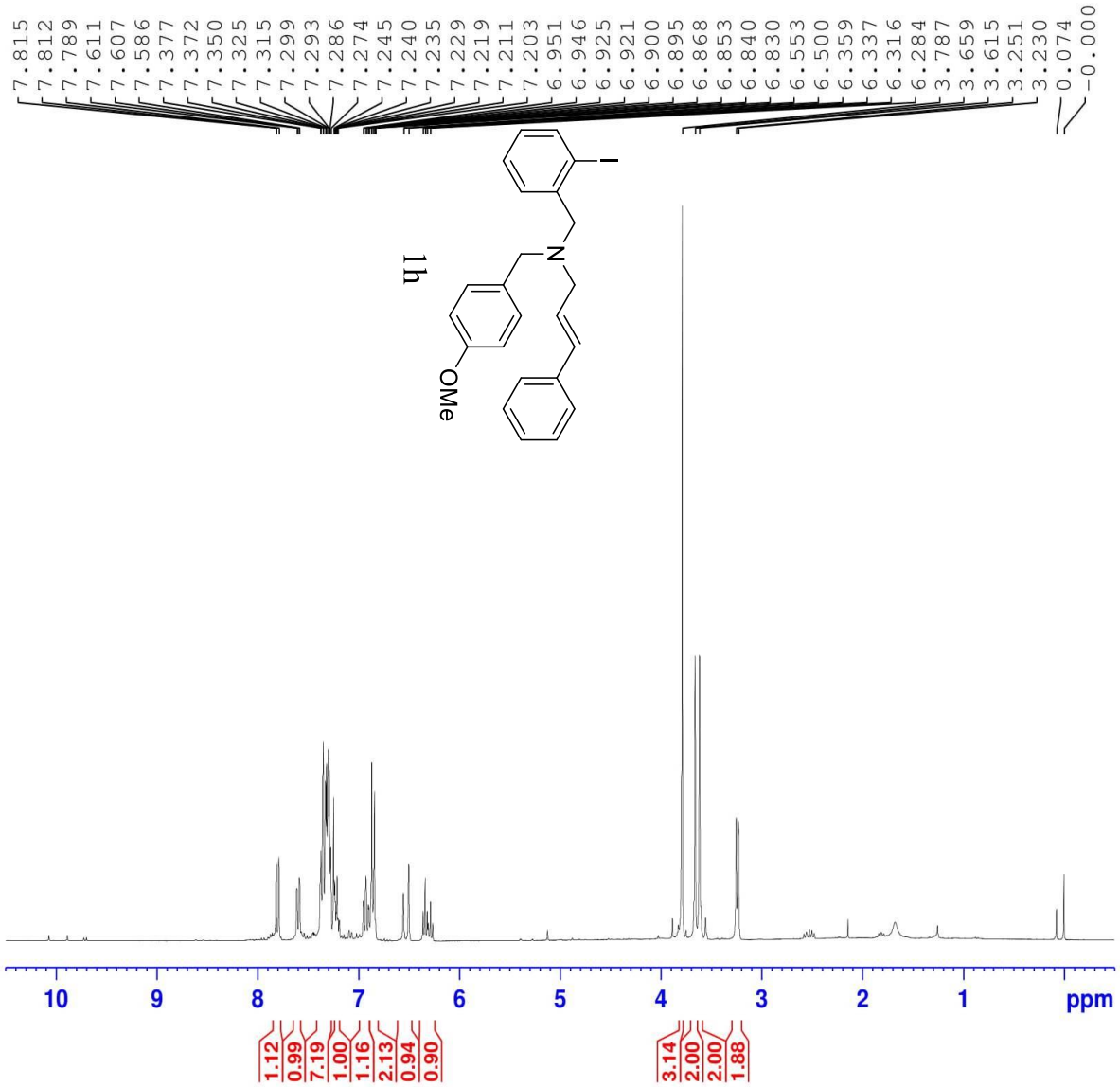
1f



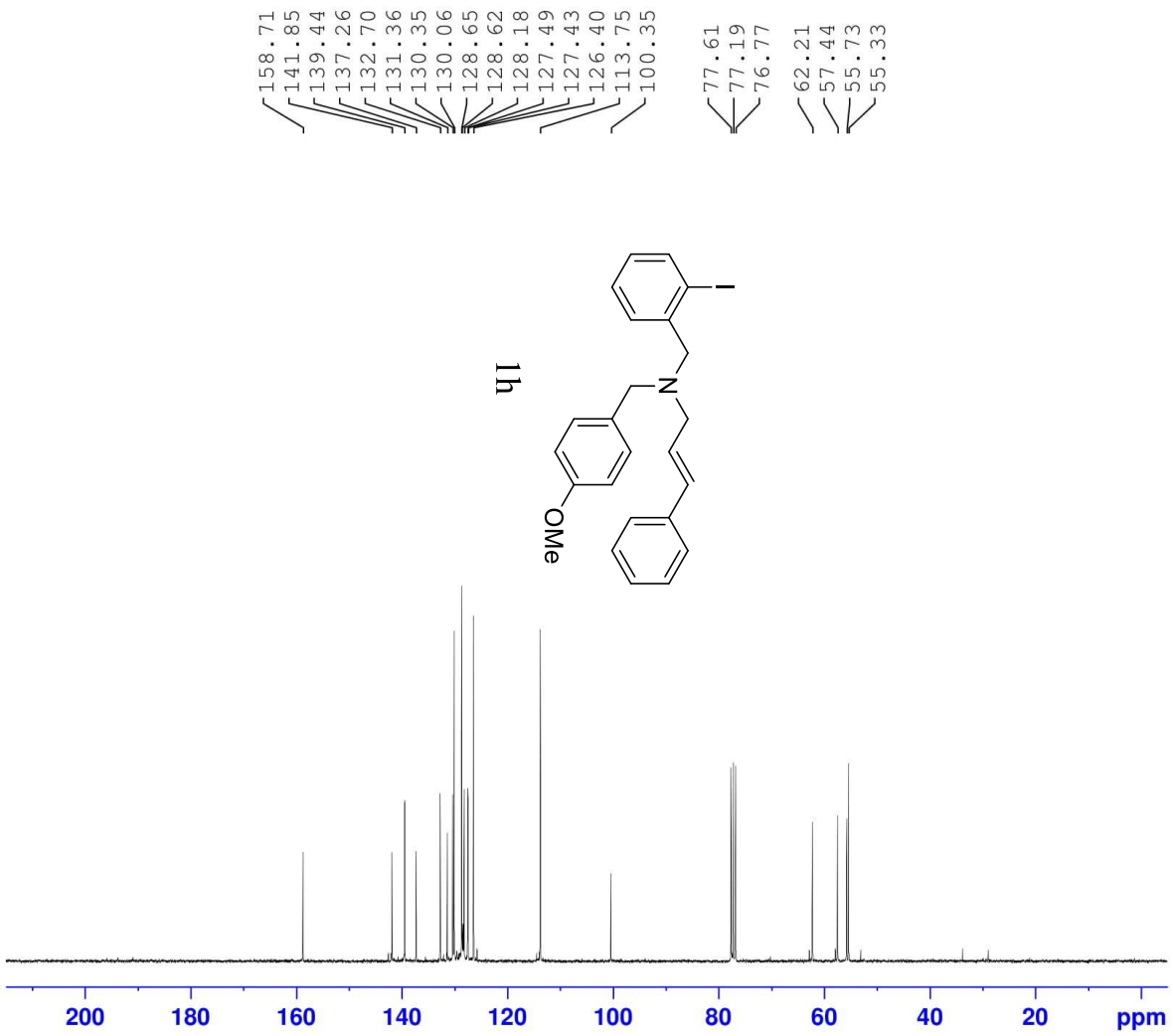

```
Current Data Parameters
NAME            C2552F8
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20190129
Time              11.57
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175317 sec
RG                 1290
DW               27.733 usec
DE                6.50 usec
TE               300.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         75.4752949 MHz
NUC1                13C
P1                 9.47 usec
PLW1        38.00000000 W

======== CHANNEL f2 ========
SFO2        300.1312005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        10.69999981 W
PLW12        0.22325000 W
PLW13        0.11229000 W

F2 - Processing parameters
SI                 32768
SF           75.4677485 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```


Current Data Parameters
NAME 3642M
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180503
Time 16.49
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 287
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.69999981 W
F2 - Processing parameters
SI 65536
SF 300.1300080 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
0.000
1.567
3.224
3.246
3.672
3.802
6.131
6.153
6.175
6.183
6.205
6.227
6.444
6.497
6.828
6.857
6.903
6.928
6.949
6.954
7.203
7.227
7.256
7.284
7.312
7.334
7.355
7.384
7.407
7.602
7.627
7.791
7.817
I
N
OMe
1g
ppm
1.03
1.05
2.39
5.39
0.77
1.15
2.04
1.00
1.00
2.00
3.16
3.55

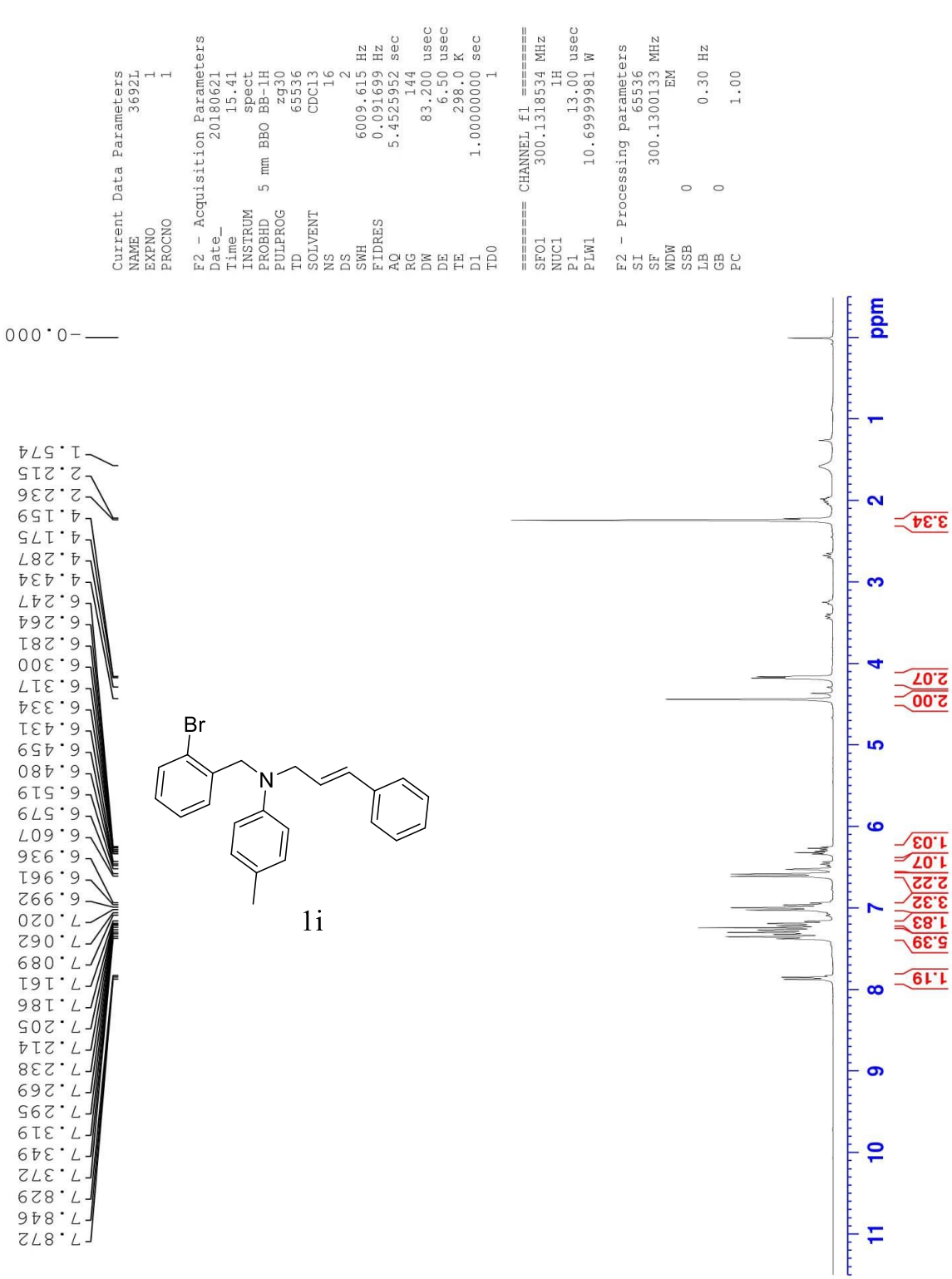

Current Data Parameters
NAME 3688F
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180524
Time 13.49
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 812
DW 27.733 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 75.4752949 MHz
NUC1 13C
P1 9.47 usec
PLW1 38.00000000 W
======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 10.69999981 W
PLW12 0.22325000 W
PLW13 0.11229000 W
F2 - Processing parameters
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
0.02
77.46
77.04
76.61
62.22
57.95
55.90
55.32
159.04
141.78
139.49
139.35
132.17
130.26
130.01
128.81
128.55
128.25
128.10
127.45
126.89
125.00
113.94
100.21
I
N
OMe
1g
ppm
200
180
160
140
120
100
80
60
40
20

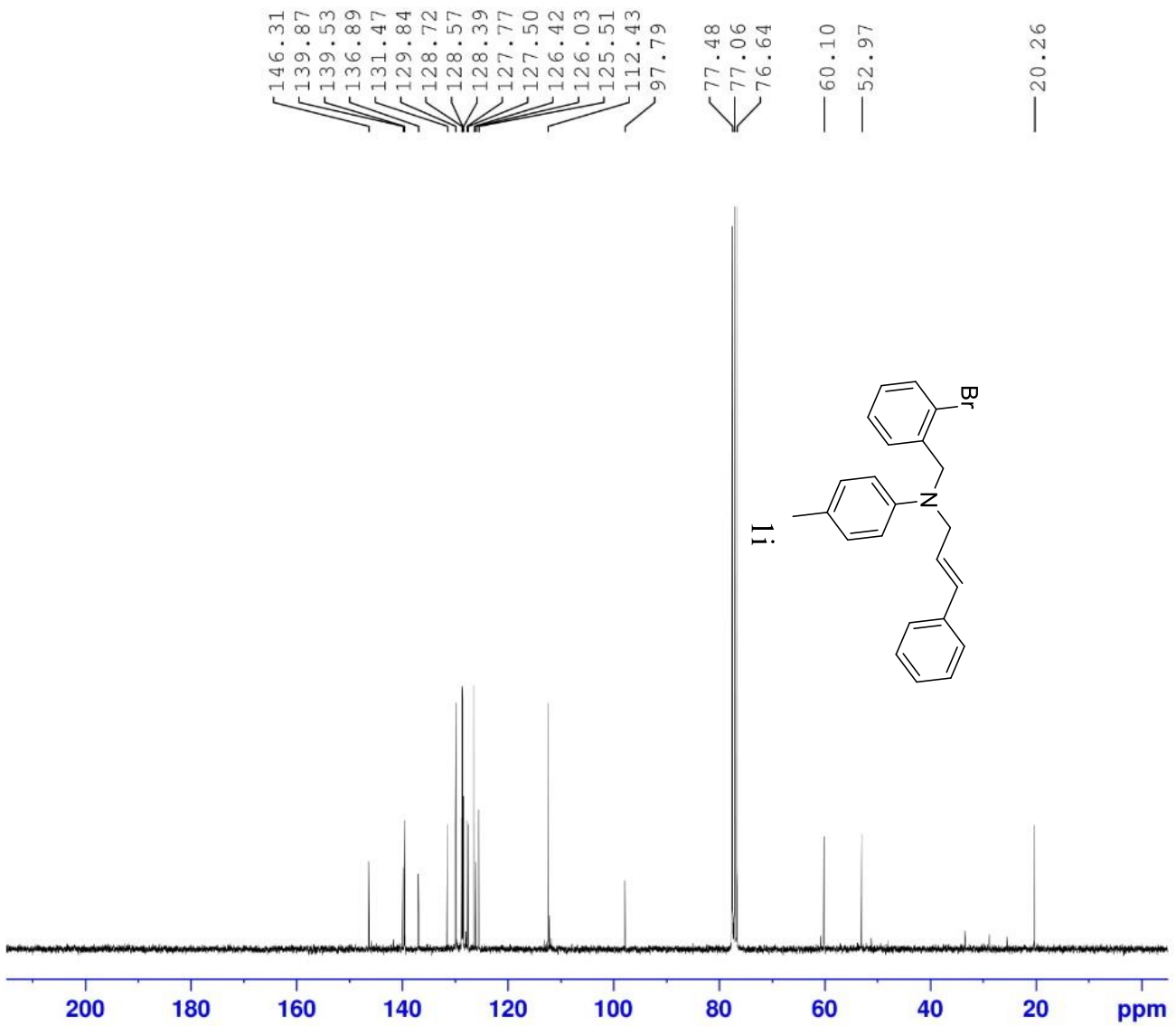



```
Current Data Parameters
NAME                  3679C
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20180518
Time                  12.25
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                6009.615 Hz
FIDRES            0.091699 Hz
AQ                5.4525952 sec
RG                      101
DW                   83.200 usec
DE                    6.50 usec
TE                   298.0 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           300.1318534 MHz
NUC1                    1H
P1                   13.00 usec
PLW1           10.69999981 W

F2 - Processing parameters
SI                    65536
SF             300.1300109 MHz
WDW                     EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

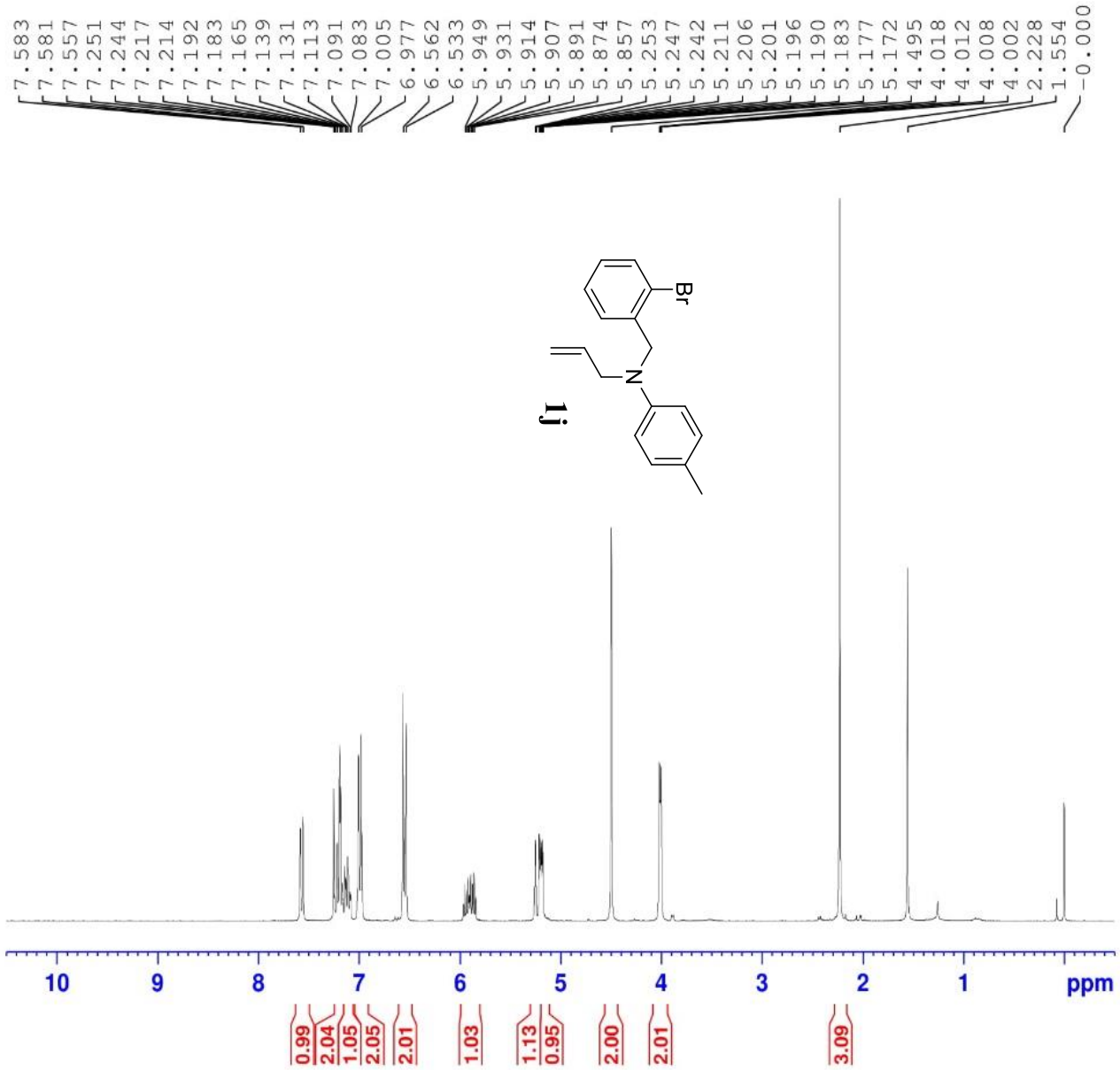



```
Current Data Parameters
NAME                 3788G
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20180524
Time                 16.26
INSTRUM              spect
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH              18028.846 Hz
FIDRES           0.275098 Hz
AQ               1.8175317 sec
RG                     812
DW                27.733 usec
DE                 6.50 usec
TE                 300.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           75.4752949 MHz
NUC1                  13C
P1                  9.47 usec
PLW1          38.00000000 W

======== CHANNEL f2 ========
SFO2           300.1312005 MHz
NUC2                  1H
CPDPRG[2           waltz16
PCPD2              90.00 usec
PLW2          10.69999981 W
PLW12          0.22325000 W
PLW13          0.11229000 W

F2 - Processing parameters
SI                   32768
SF             75.4677485 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

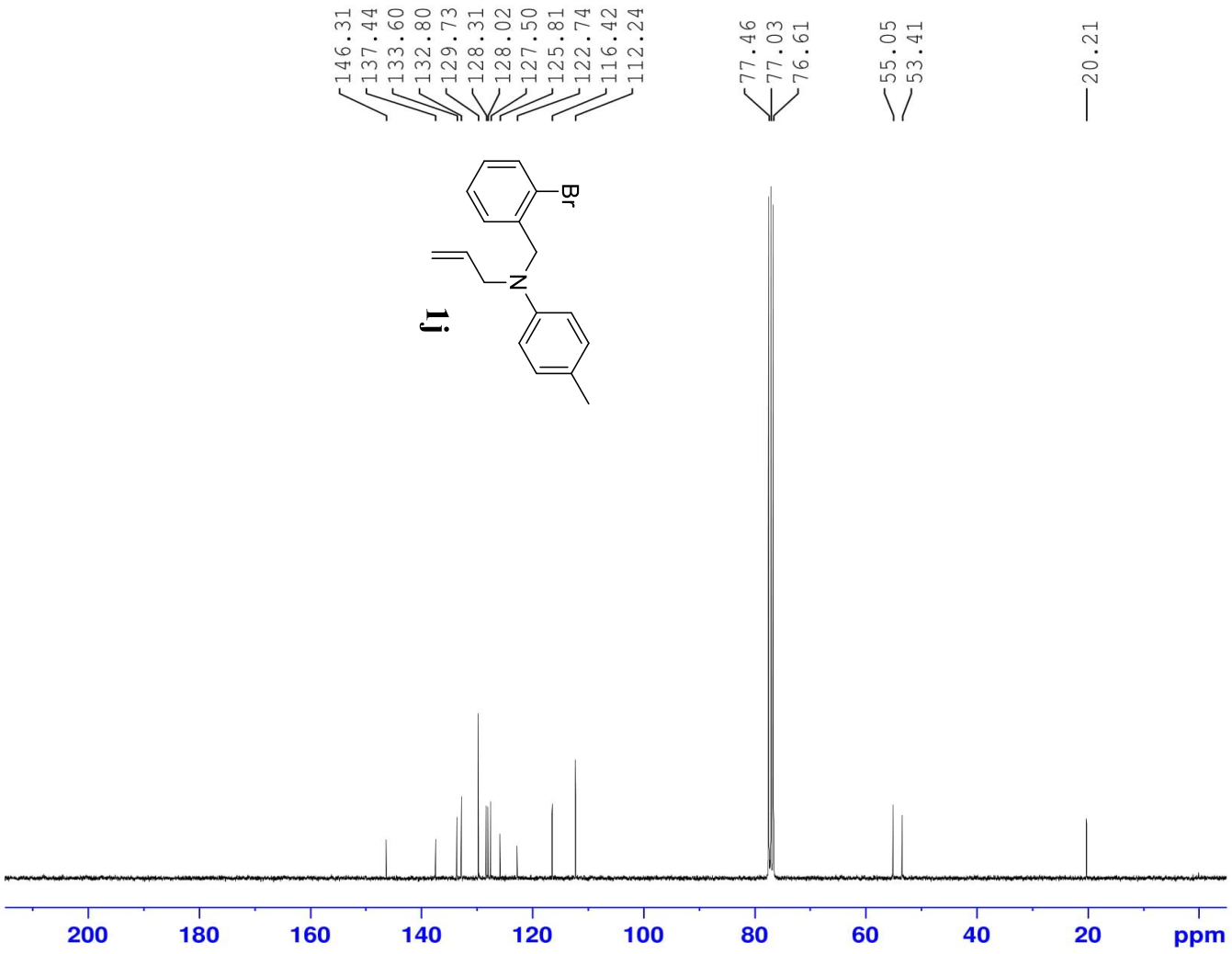

Current Data Parameters
NAME 3692L
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180621
Time 15.41
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 144
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.69999981 W
F2 - Processing parameters
SI 65536
SF 300.1300133 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Br
N
1i
ppm
3.34
2.07
2.00
1.03
1.07
2.22
3.32
1.83
5.39
1.19



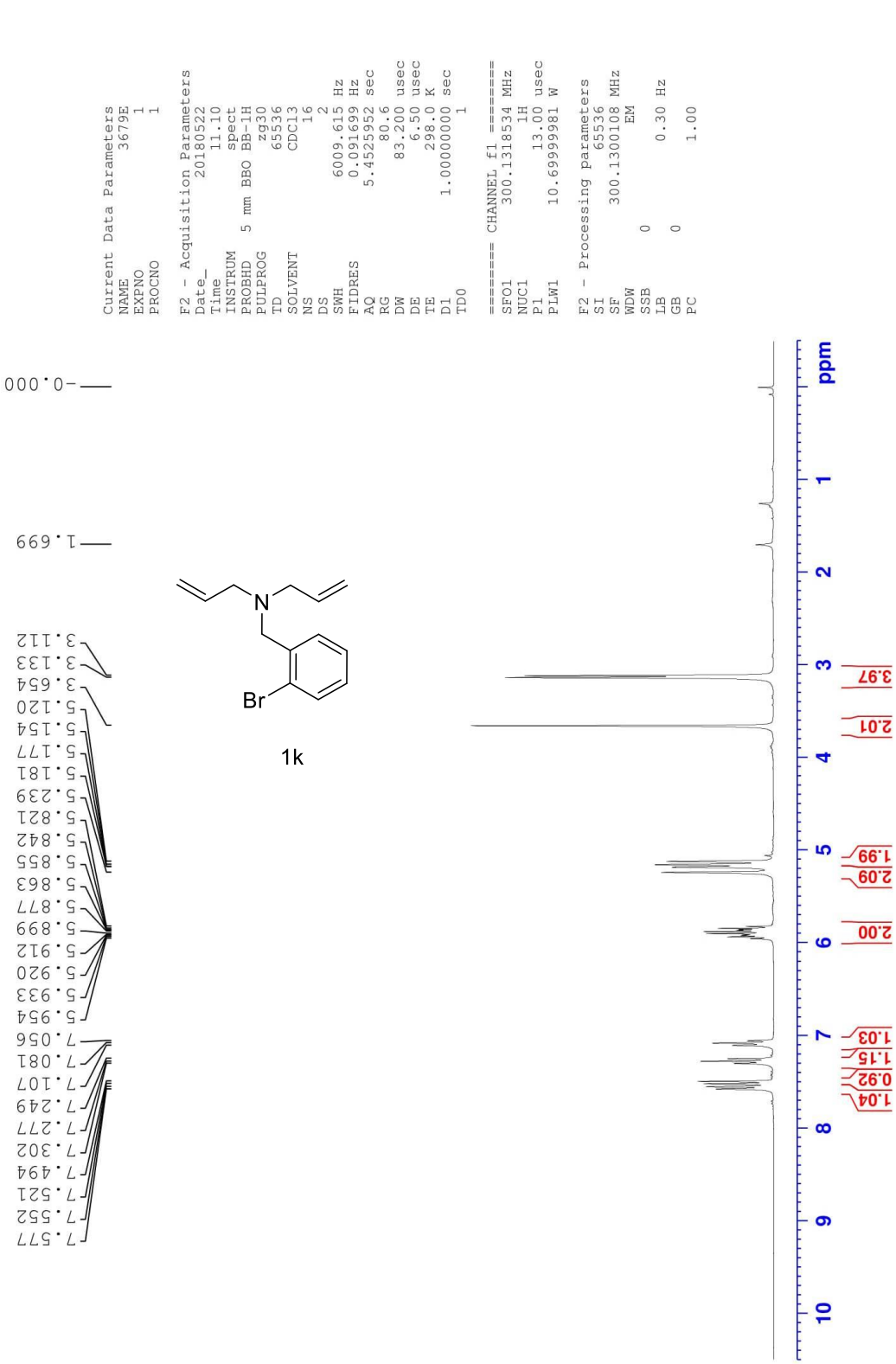

```
Current Data Parameters
NAME                  C2552B2
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20180630
Time                  13.04
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1112
DS                       4
SWH              18028.846 Hz
FIDRES            0.275098 Hz
AQ                1.8175317 sec
RG                     912
DW                  27.733 usec
DE                   6.50 usec
TE                  300.0 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1            75.4752949 MHz
NUC1                    13C
P1                    9.47 usec
PLW1           38.00000000 W

======== CHANNEL f2 ========
SFO2           300.1312005 MHz
NUC2                    1H
CPDPRG[2            waltz16
PCPD2                90.00 usec
PLW2           10.69999981 W
PLW12           0.22325000 W
PLW13           0.11229000 W

F2 - Processing parameters
SI                      32768
SF              75.4677485 MHz
WDW                        EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

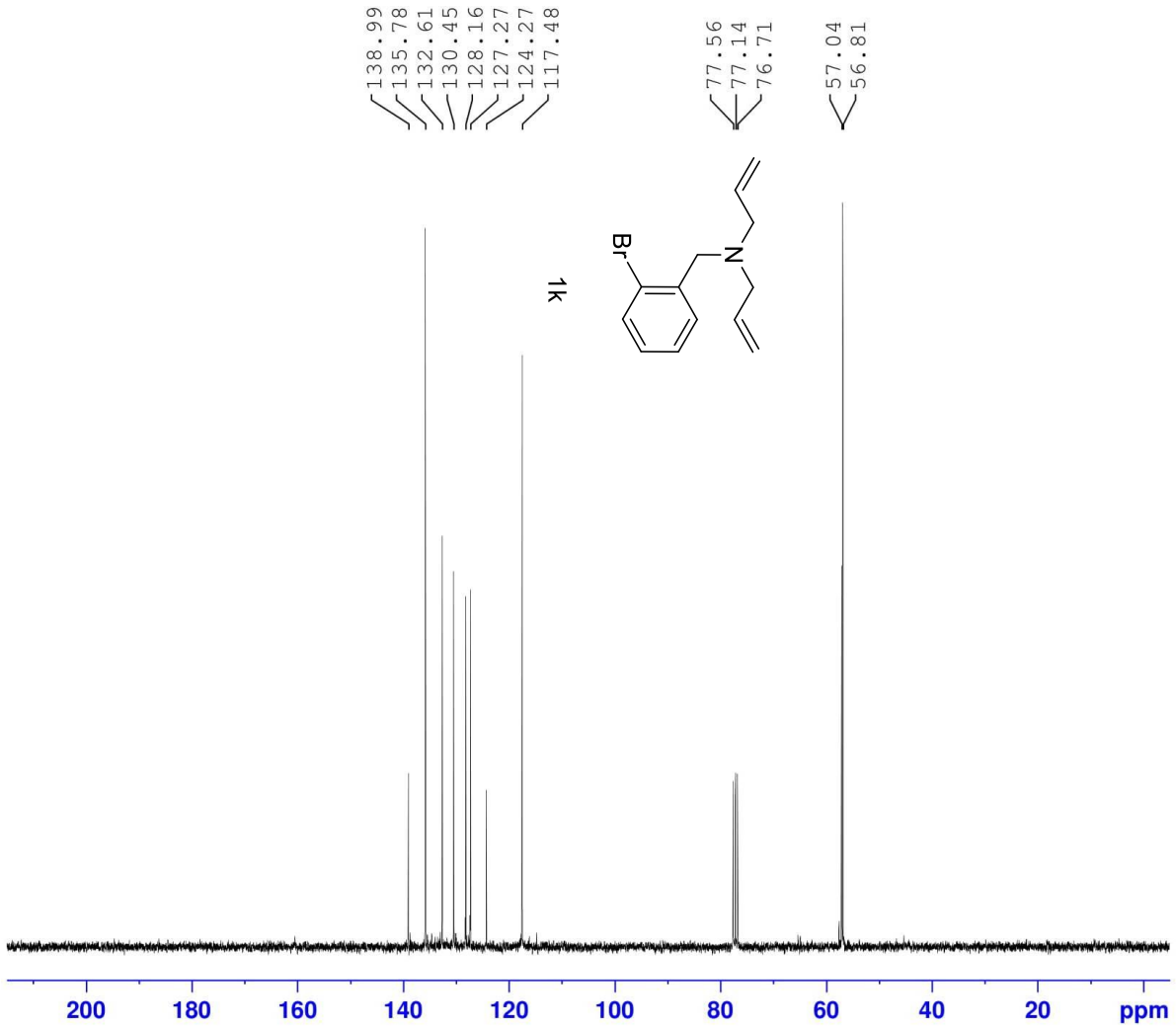



```
Current Data Parameters
NAME                 H3339D2
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_               20190621
Time                   12.35
INSTRUM                spect
PROBHD   5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                6009.615 Hz
FIDRES            0.091699 Hz
AQ                5.4525952 sec
RG                      181
DW                   83.200 usec
DE                    6.50 usec
TE                   298.0 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1            300.1318534 MHz
NUC1                    1H
P1                   13.00 usec
PLW1           10.69999981 W

F2 - Processing parameters
SI                    65536
SF              300.1300093 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

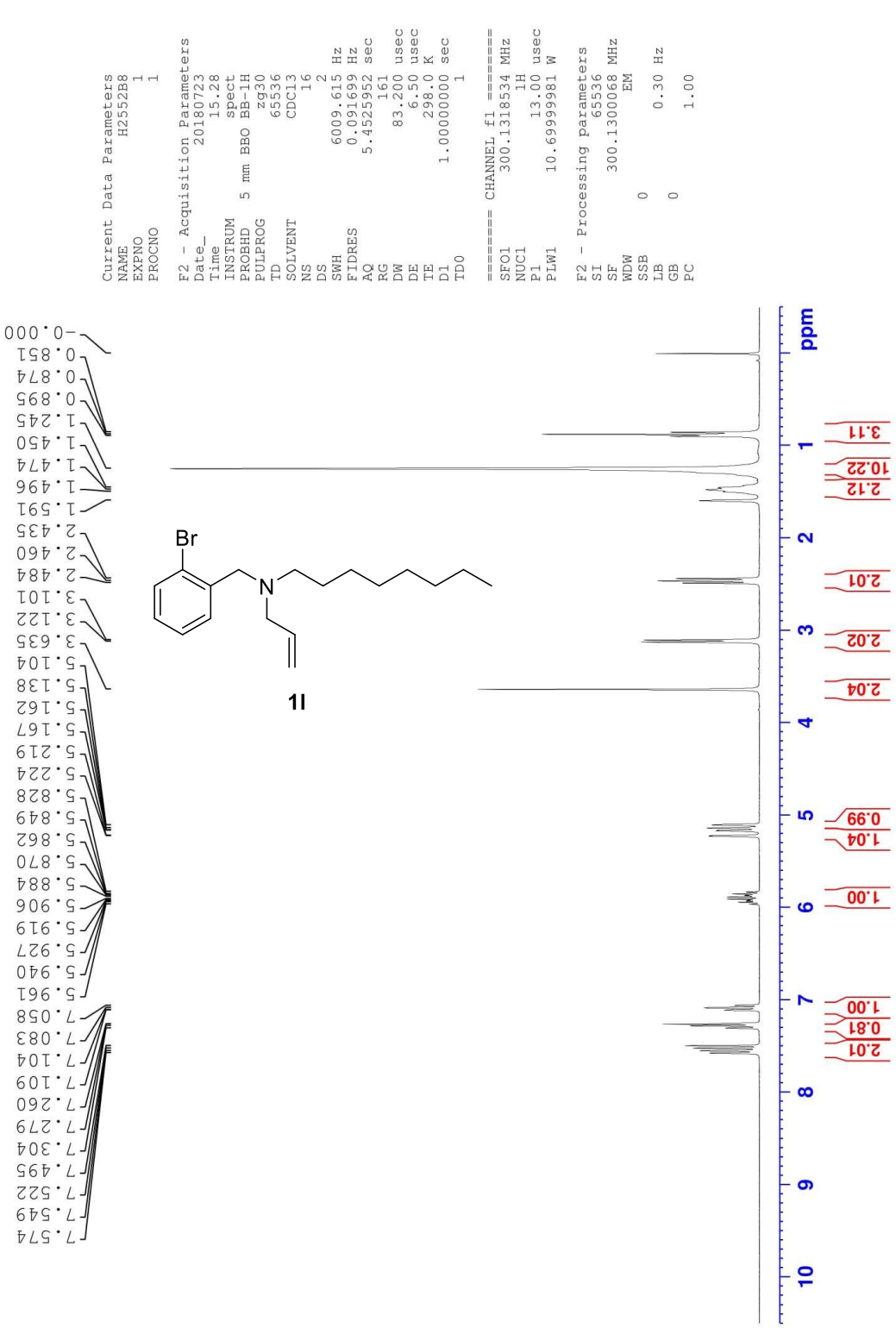


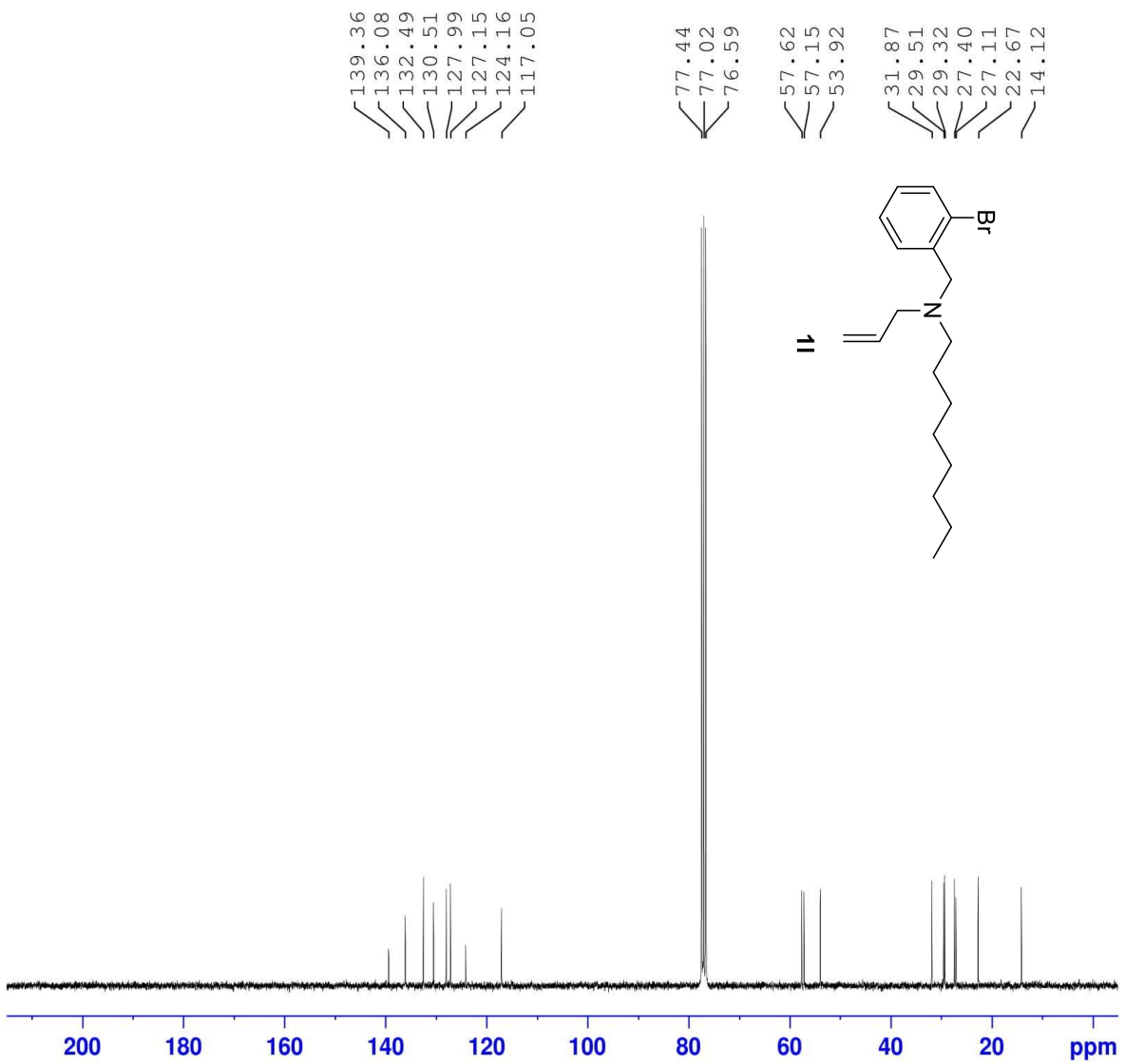

```
Current Data Parameters
NAME                  C3339B10
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                20190625
Time                    19.38
INSTRUM                 spect
PROBHD    5 mm BBO BB-1H
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                        2048
DS                           4
SWH                 18028.846 Hz
FIDRES               0.275098 Hz
AQ                   1.8175317 sec
RG                         724
DW                      27.733 usec
DE                        6.50 usec
TE                       300.0 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1                75.4752949 MHz
NUC1                       13C
P1                        9.47 usec
PLW1               38.00000000 W

======== CHANNEL f2 ========
SFO2               300.1312005 MHz
NUC2                       1H
CPDPRG[2                waltz16
PCPD2                    90.00 usec
PLW2               10.69999981 W
PLW12               0.22325000 W
PLW13               0.11229000 W

F2 - Processing parameters
SI                       32768
SF                  75.4677485 MHz
WDW                         EM
SSB          0
LB                        1.00 Hz
GB           0
PC                        1.40
```


Current Data Parameters
NAME 3679E
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180522
Time 11.10
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 80.6
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.69999981 W
F2 - Processing parameters
SI 65536
SF 300.1300108 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
-0.000
1.699
3.112
3.133
3.654
5.120
5.154
5.177
5.181
5.239
5.821
5.842
5.855
5.863
5.877
5.899
5.912
5.920
5.933
5.954
7.056
7.081
7.107
7.249
7.277
7.302
7.494
7.521
7.552
7.577
N
Br
1k
ppm
1
2
3
4
5
6
7
8
9
10
3.97
2.01
1.99
2.09
2.00
1.03
1.15
0.92
1.04

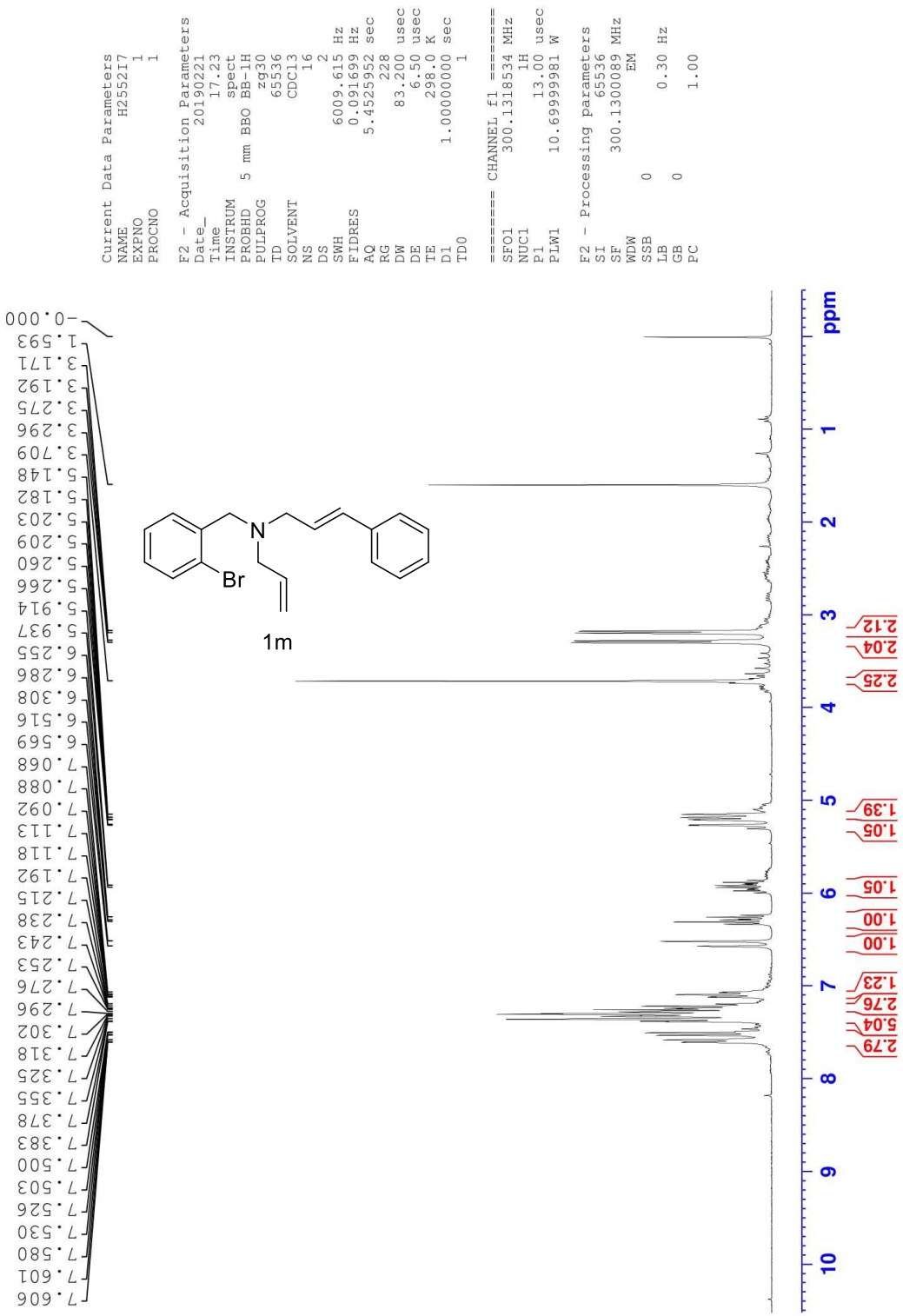


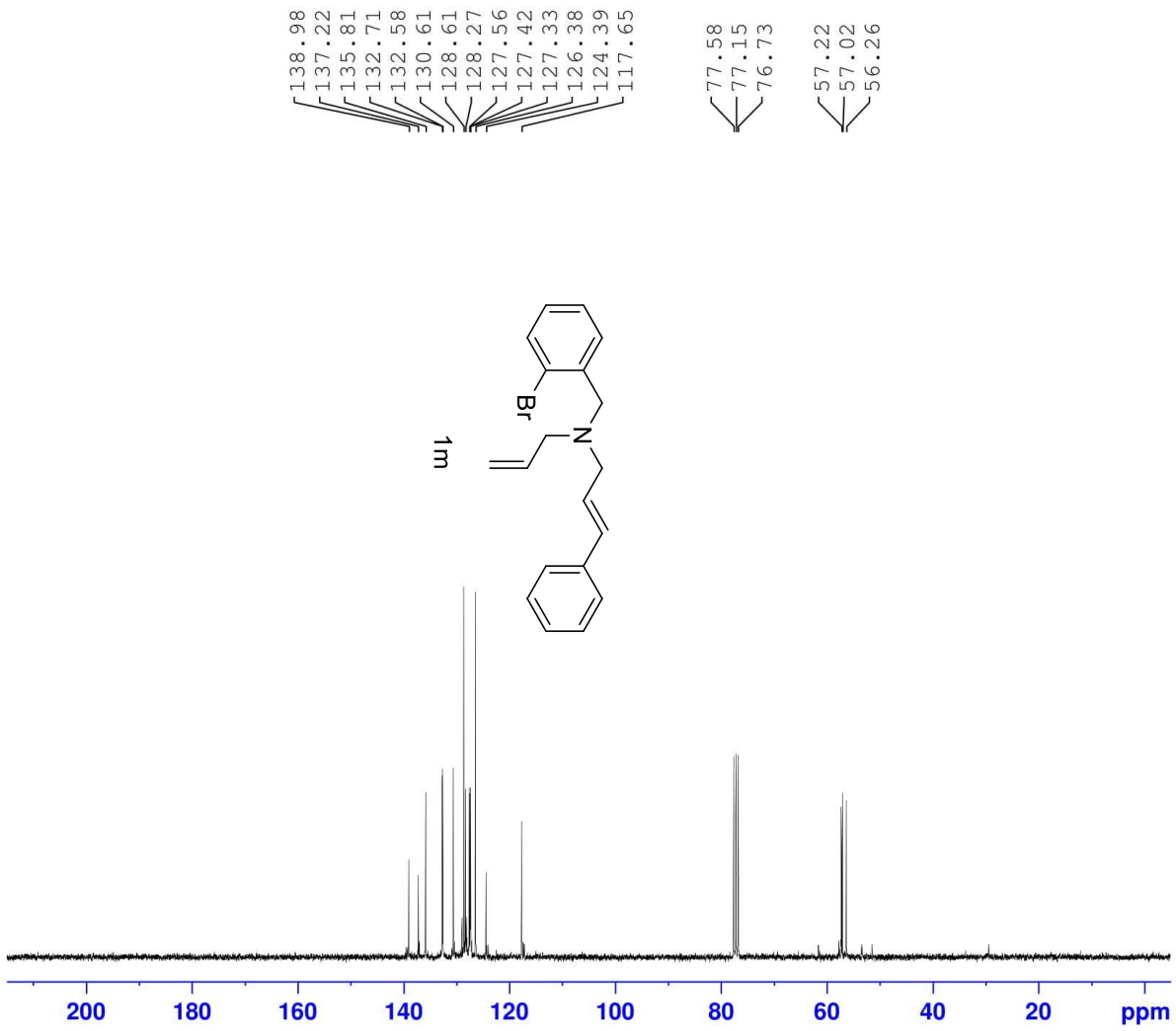

```
Current Data Parameters
NAME                  C2552F6
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_                20190117
Time                    13.10
INSTRUM                 spect
PROBHD    5 mm BBO BB-1H
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                         64
DS                          4
SWH                 18028.846 Hz
FIDRES              0.275098 Hz
AQ                  1.8175317 sec
RG                        912
DW                     27.733 usec
DE                      6.50 usec
TE                     300.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1               75.4752949 MHz
NUC1                      13C
P1                       9.47 usec
PLW1              38.00000000 W

======== CHANNEL f2 ========
SFO2               300.1312005 MHz
NUC2                      1H
CPDPRG[2               waltz16
PCPD2                   90.00 usec
PLW2              10.69999981 W
PLW12              0.22325000 W
PLW13              0.11229000 W

F2 - Processing parameters
SI                        32768
SF                 75.4677485 MHz
WDW                        EM
SSB           0
LB                      1.00 Hz
GB            0
PC                      1.40
```


Current Data Parameters
NAME H255288
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180723
Time 15.28
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 161
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.69999981 W
F2 - Processing parameters
SI 65536
SF 300.1300068 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Br
N
1l
ppm
3.11
10.22
2.12
2.01
2.02
2.04
0.99
1.04
1.00
1.00
0.81
2.01

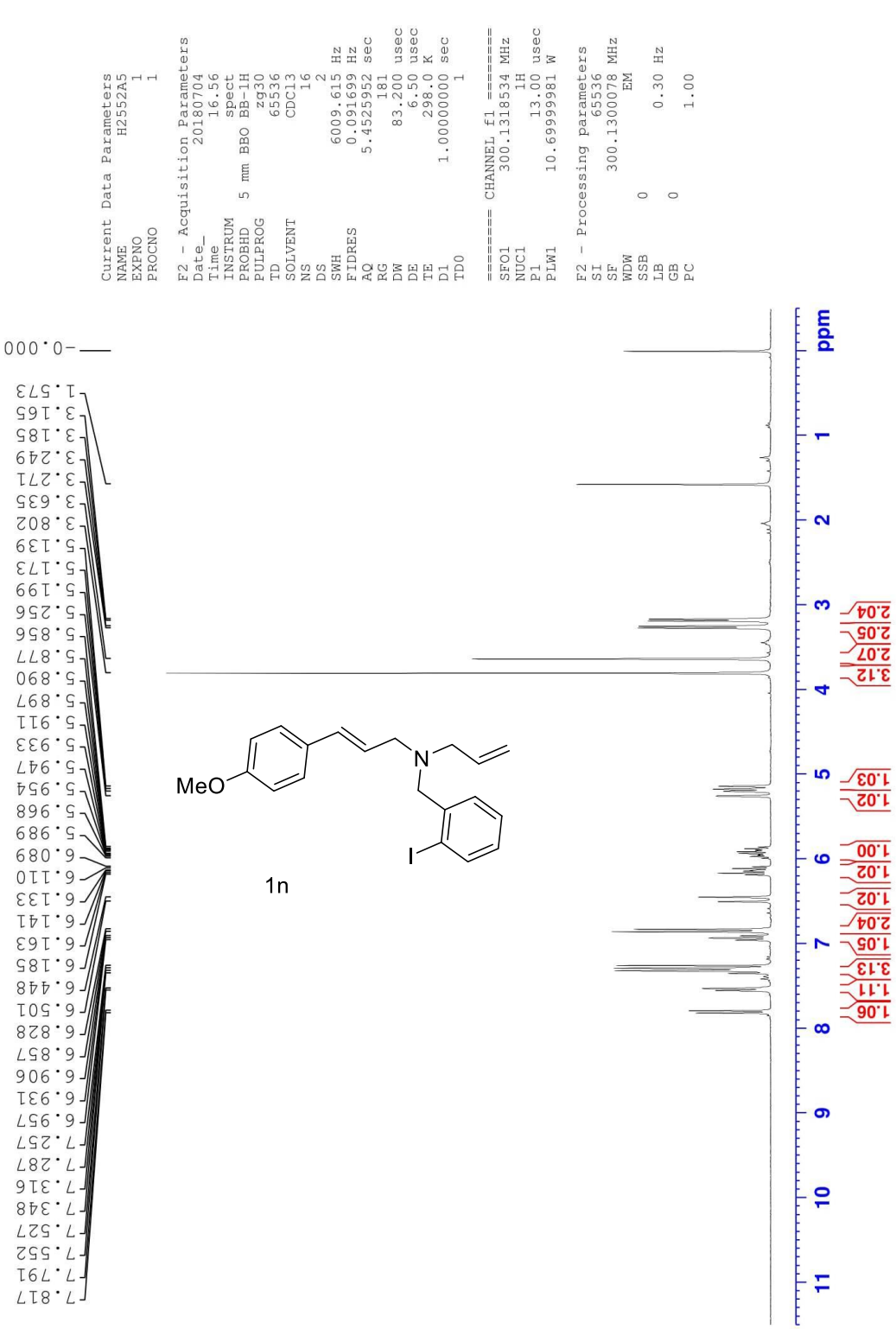


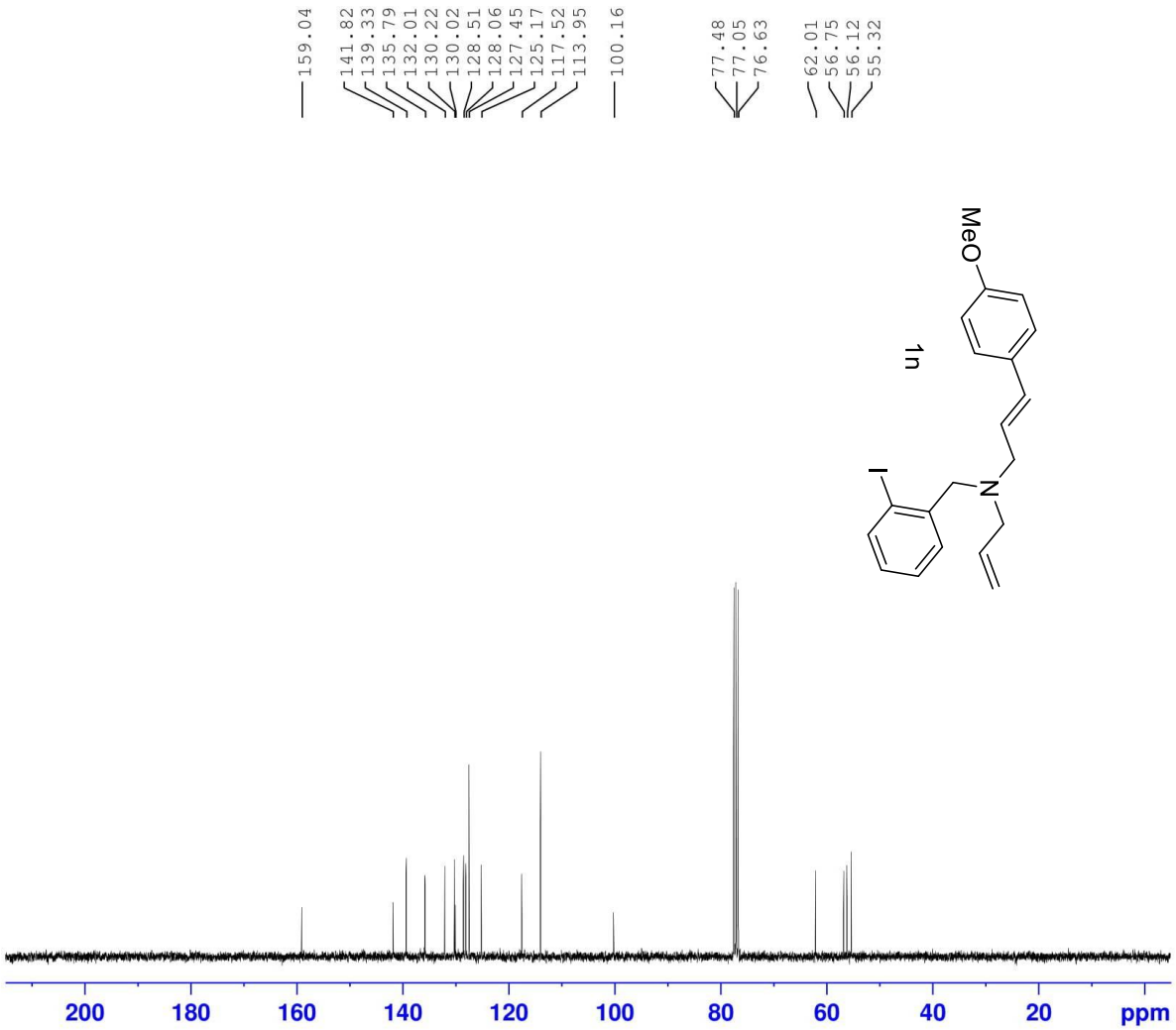

```
Current Data Parameters
NAME            C2552B10
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180724
Time               19.45
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 2048
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175317 sec
RG                  912
DW               27.733 usec
DE                6.50 usec
TE                300.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         75.4752949 MHz
NUC1                13C
P1                 9.47 usec
PLW1        38.00000000 W

======== CHANNEL f2 ========
SFO2        300.1312005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2        10.69999981 W
PLW12        0.22325000 W
PLW13        0.11229000 W

F2 - Processing parameters
SI                 32768
SF           75.4677485 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```


Current Data Parameters
NAME H2552I7
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190221
Time 17.23
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 228
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.69999981 W
F2 - Processing parameters
SI 65536
SF 300.1300089 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Br
N
1m
ppm
2.12
2.04
2.25
1.39
1.05
1.05
1.00
1.00
1.23
2.76
5.04
2.79

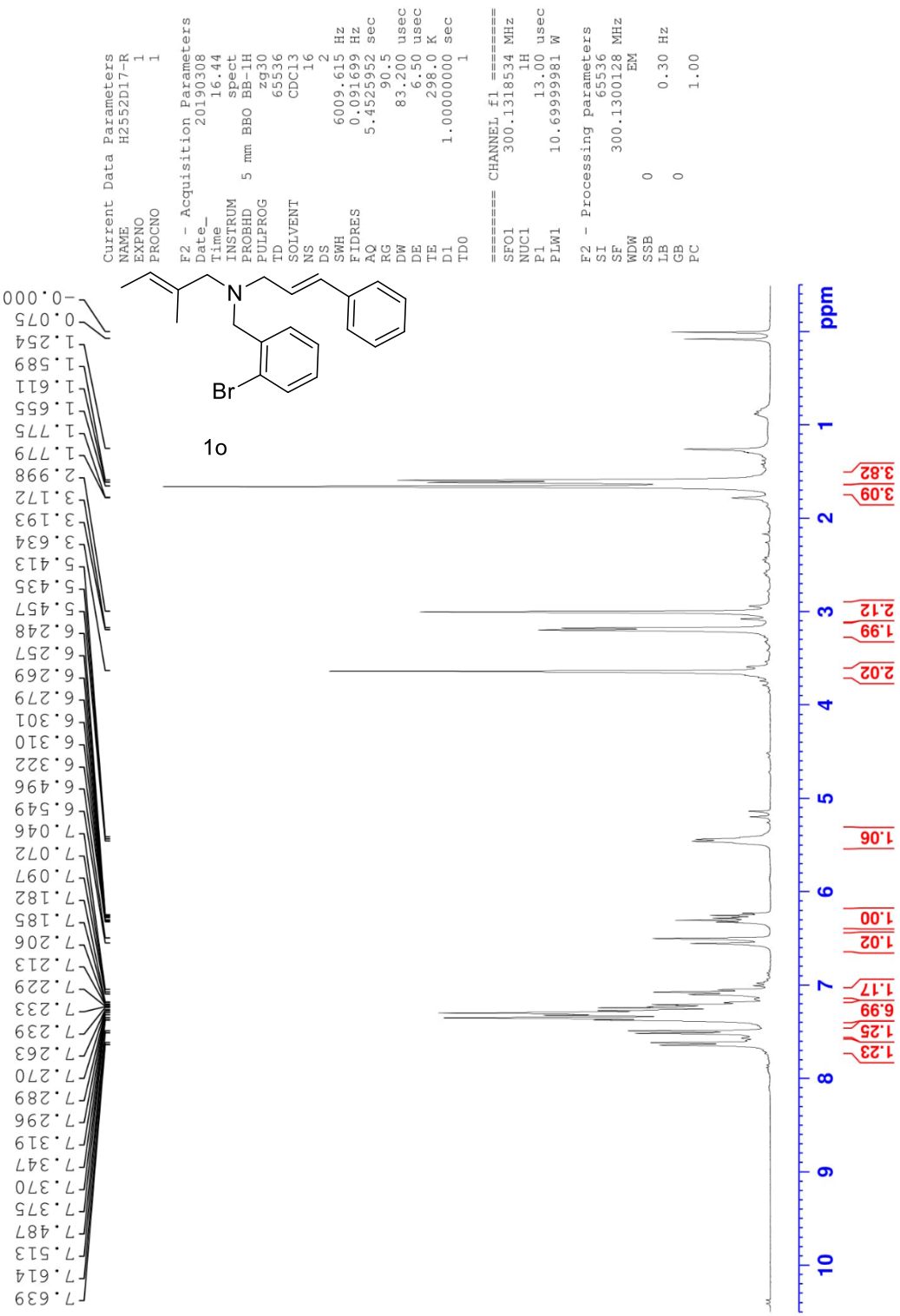


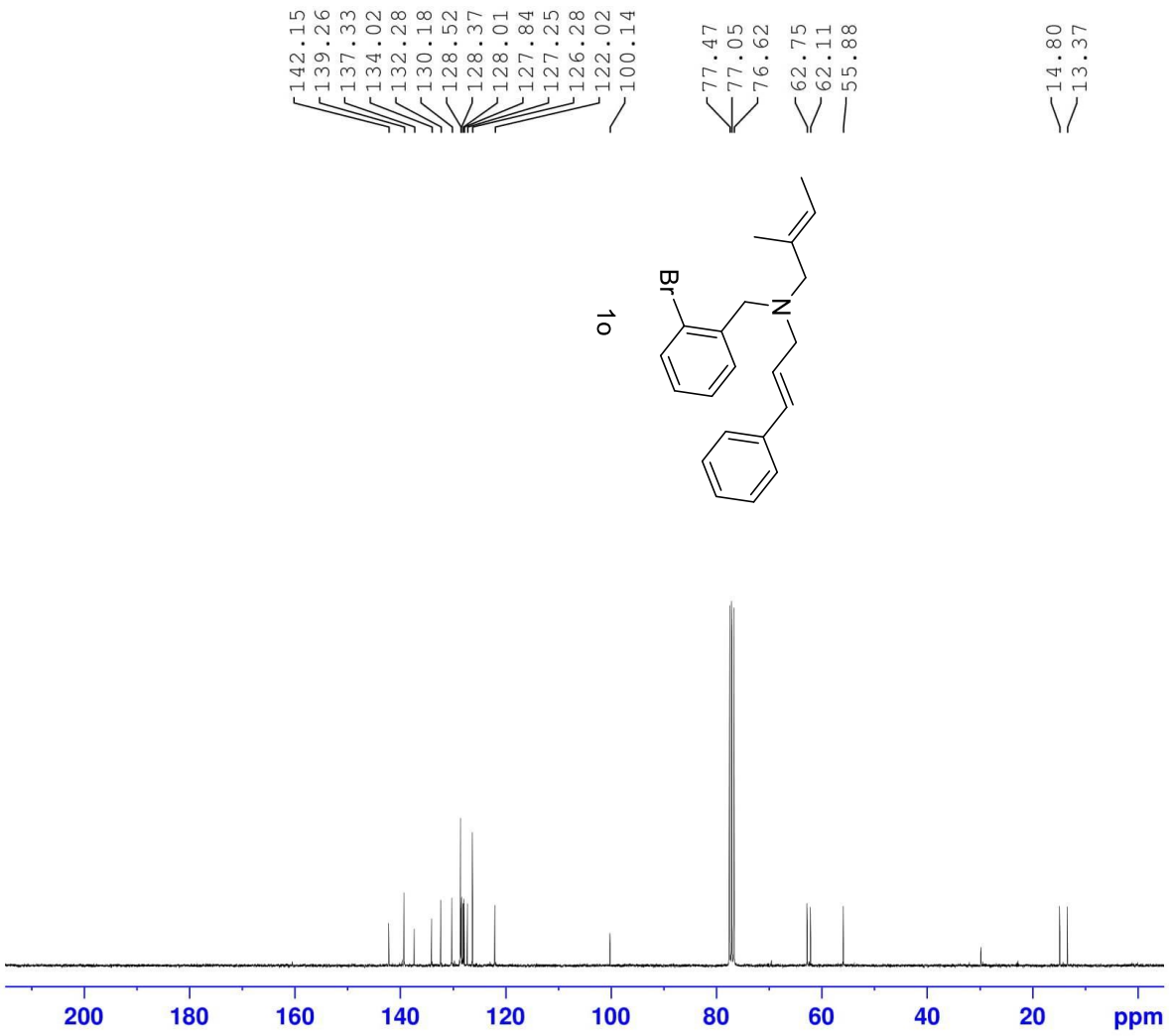

```
Current Data Parameters
NAME                  C3339A2
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_                20190222
Time                    11.04
INSTRUM                 spect
PROBHD    5 mm BBO BB-1H
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                        128
DS                          4
SWH                 18028.846 Hz
FIDRES                0.275098 Hz
AQ                  1.8175317 sec
RG                        724
DW                     27.733 usec
DE                      6.50 usec
TE                     300.0 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1               75.4752949 MHz
NUC1                      13C
P1                       9.47 usec
PLW1               38.00000000 W

======== CHANNEL f2 ========
SFO2               300.1312005 MHz
NUC2                      1H
CPDPRG[2               waltz16
PCPD2                   90.00 usec
PLW2               10.69999981 W
PLW12               0.22325000 W
PLW13               0.11229000 W

F2 - Processing parameters
SI                        32768
SF                 75.4677485 MHz
WDW                        EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```


Current Data Parameters
NAME H2552A5
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180704
Time 16.56
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 181
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.69999981 W
F2 - Processing parameters
SI 65536
SF 300.1300078 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
MeO
N
I
1n
ppm
2.04
2.05
2.07
3.12
1.02
1.03
1.00
1.02
1.02
2.04
1.05
3.13
1.11
1.06

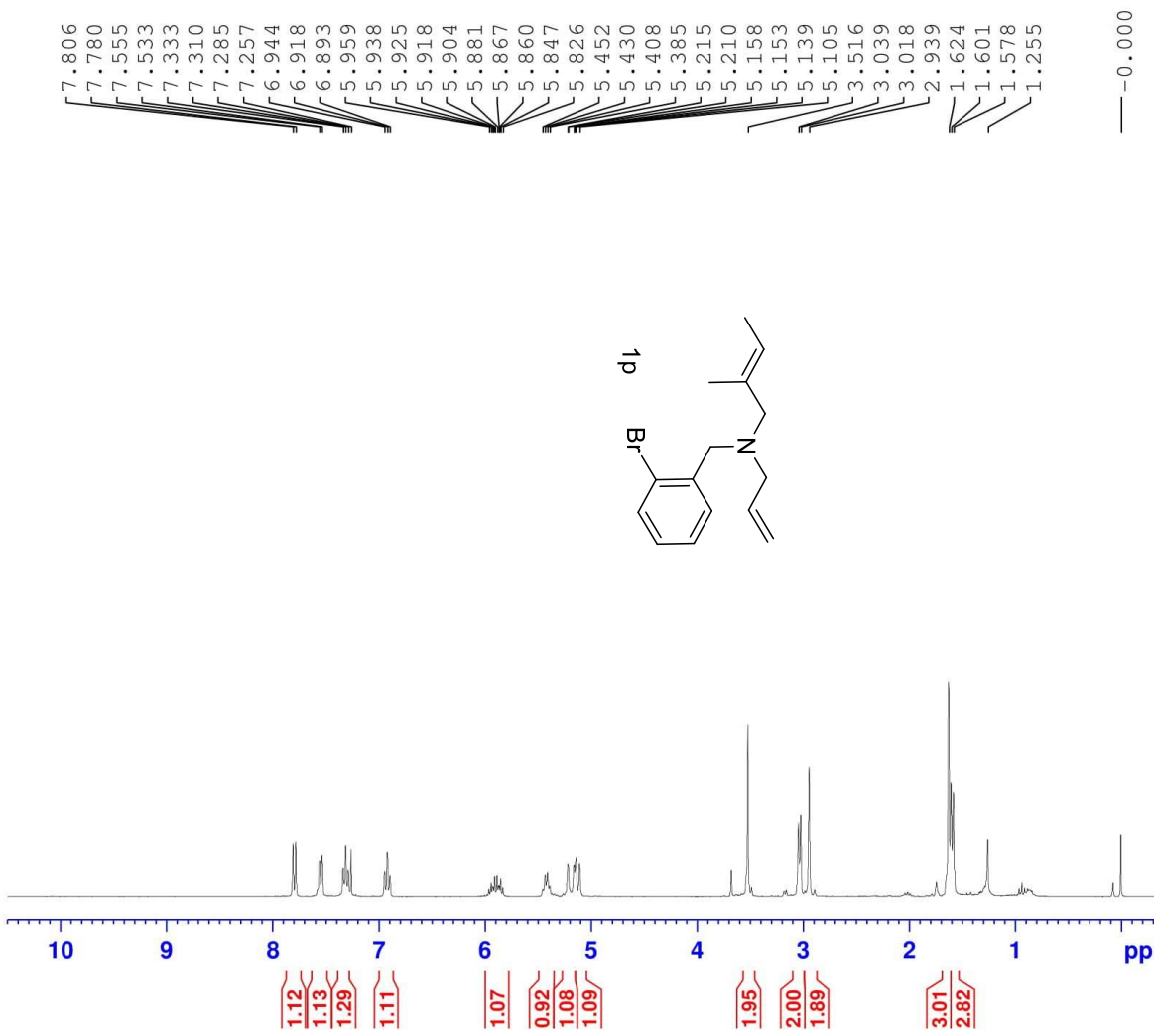



```
Current Data Parameters
NAME                  C2552B7
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20180705
Time                   17.36
INSTRUM                spect
PROBHD    5 mm BBO BB-1H
PULPROG              zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       136
DS                         4
SWH                18028.846 Hz
FIDRES             0.275098 Hz
AQ                 1.8175317 sec
RG                       812
DW                    27.733 usec
DE                     6.50 usec
TE                    300.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1               75.4752949 MHz
NUC1                      13C
P1                       9.47 usec
PLW1              38.00000000 W

======== CHANNEL f2 ========
SFO2              300.1312005 MHz
NUC2                      1H
CPDPRG[2               waltz16
PCPD2                   90.00 usec
PLW2              10.69999981 W
PLW12              0.22325000 W
PLW13              0.11229000 W

F2 - Processing parameters
SI                        32768
SF                 75.4677485 MHz
WDW                          EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.40
```

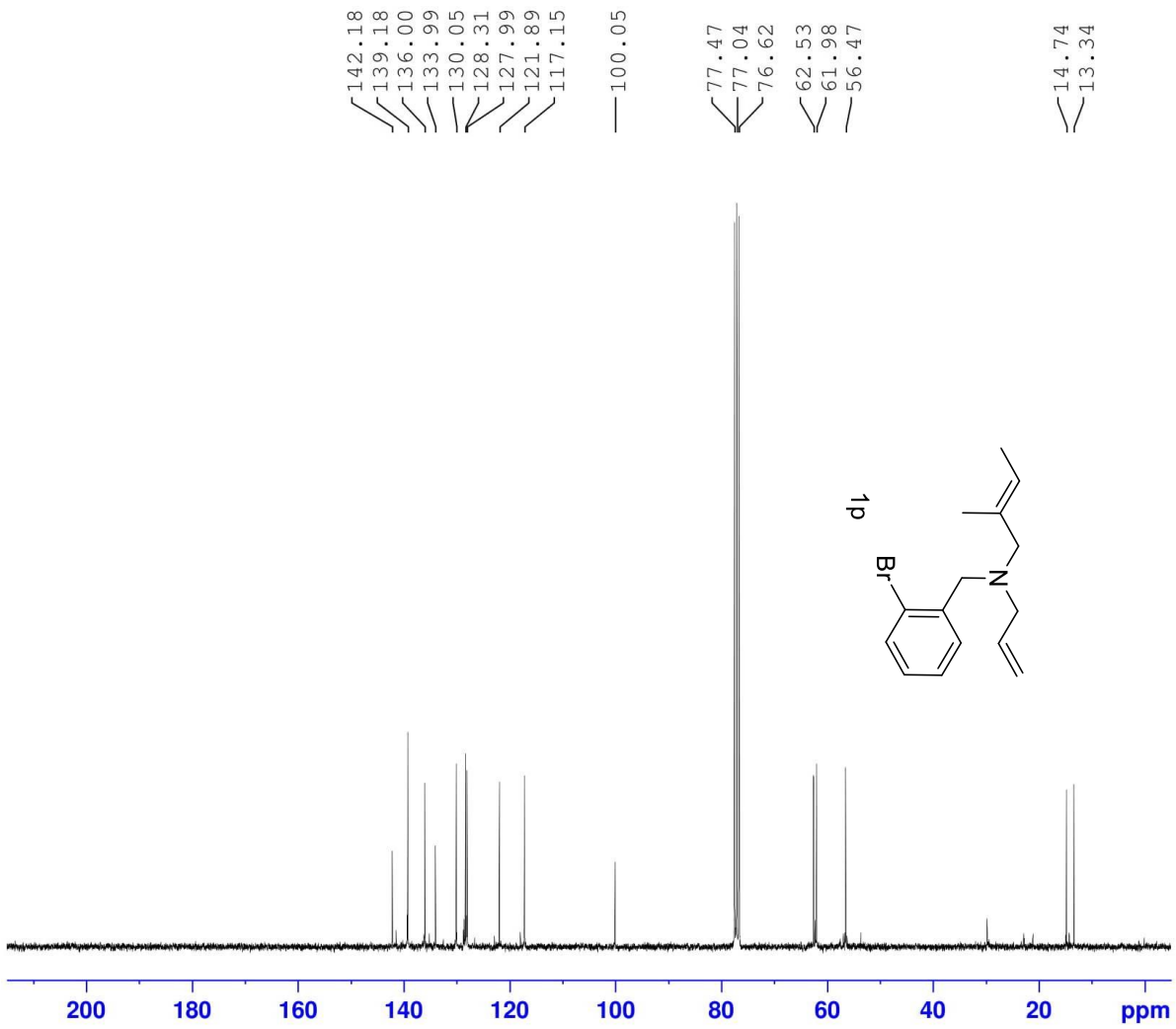

Current Data Parameters
NAME H2552D17-R
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190308
Time 16.44
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 90.5
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.69999981 W
F2 - Processing parameters
SI 65536
SF 300.1300128 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
N
Br
1o
ppm
3.82
3.09
2.12
1.99
2.02
1.06
1.00
1.02
1.17
6.99
1.25
1.23



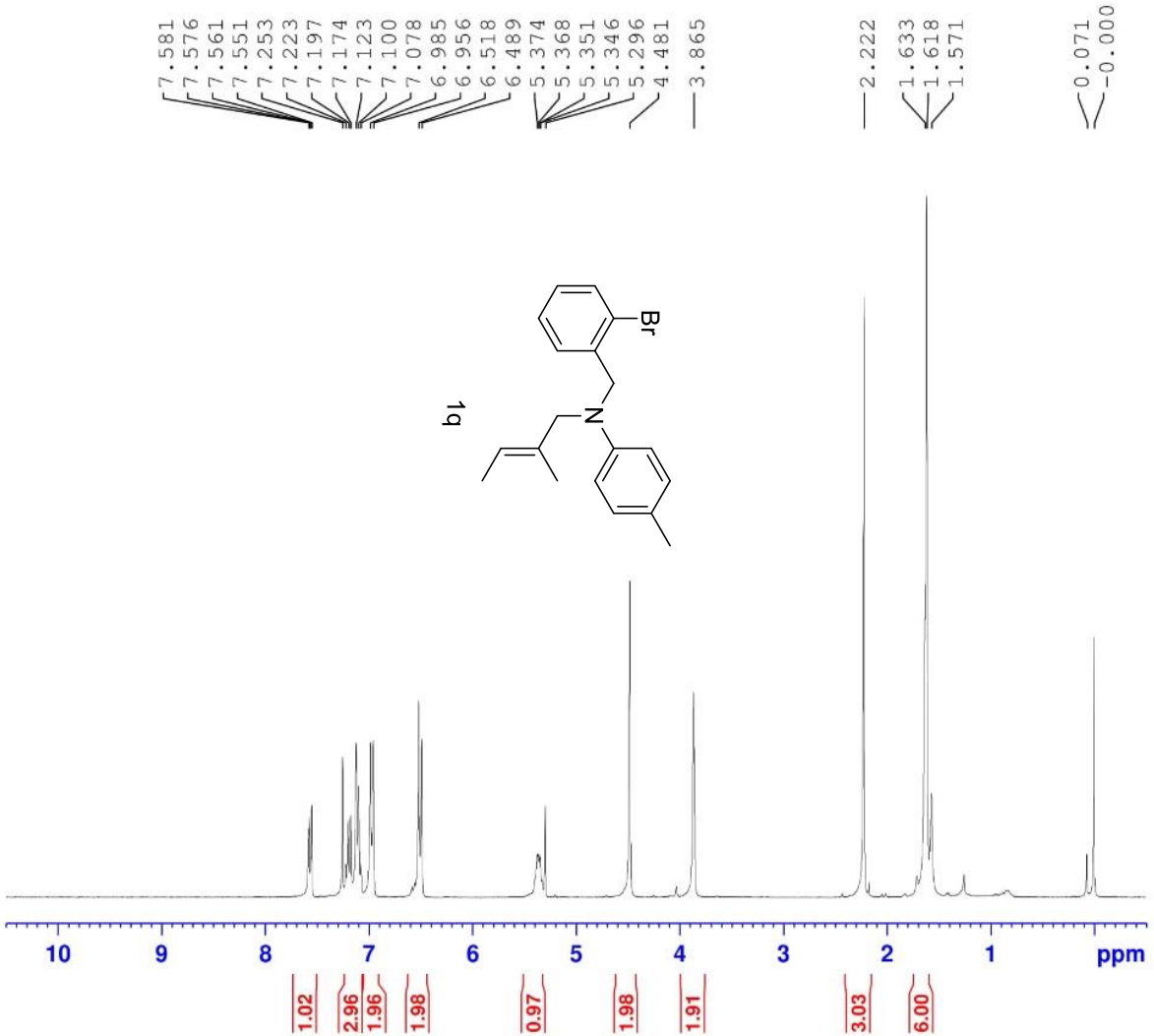

```
Current Data Parameters
NAME                  C2552D6
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_                20180915
Time                    14.37
INSTRUM                 spect
PROBHD    5 mm BBO BB-1H
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                       1565
DS                          4
SWH                 18028.846 Hz
FIDRES                0.275098 Hz
AQ                    1.8175317 sec
RG                        575
DW                     27.733 usec
DE                      6.50 usec
TE                      300.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1               75.4752949 MHz
NUC1                      13C
P1                      9.47 usec
PLW1               38.00000000 W

======== CHANNEL f2 ========
SFO2              300.1312005 MHz
NUC2                      1H
CPDPRG[2               waltz16
PCPD2                   90.00 usec
PLW2               10.69999981 W
PLW12               0.22325000 W
PLW13               0.11229000 W

F2 - Processing parameters
SI                        32768
SF                 75.4677485 MHz
WDW                        EM
SSB           0
LB                      1.00 Hz
GB            0
PC                      1.40
```



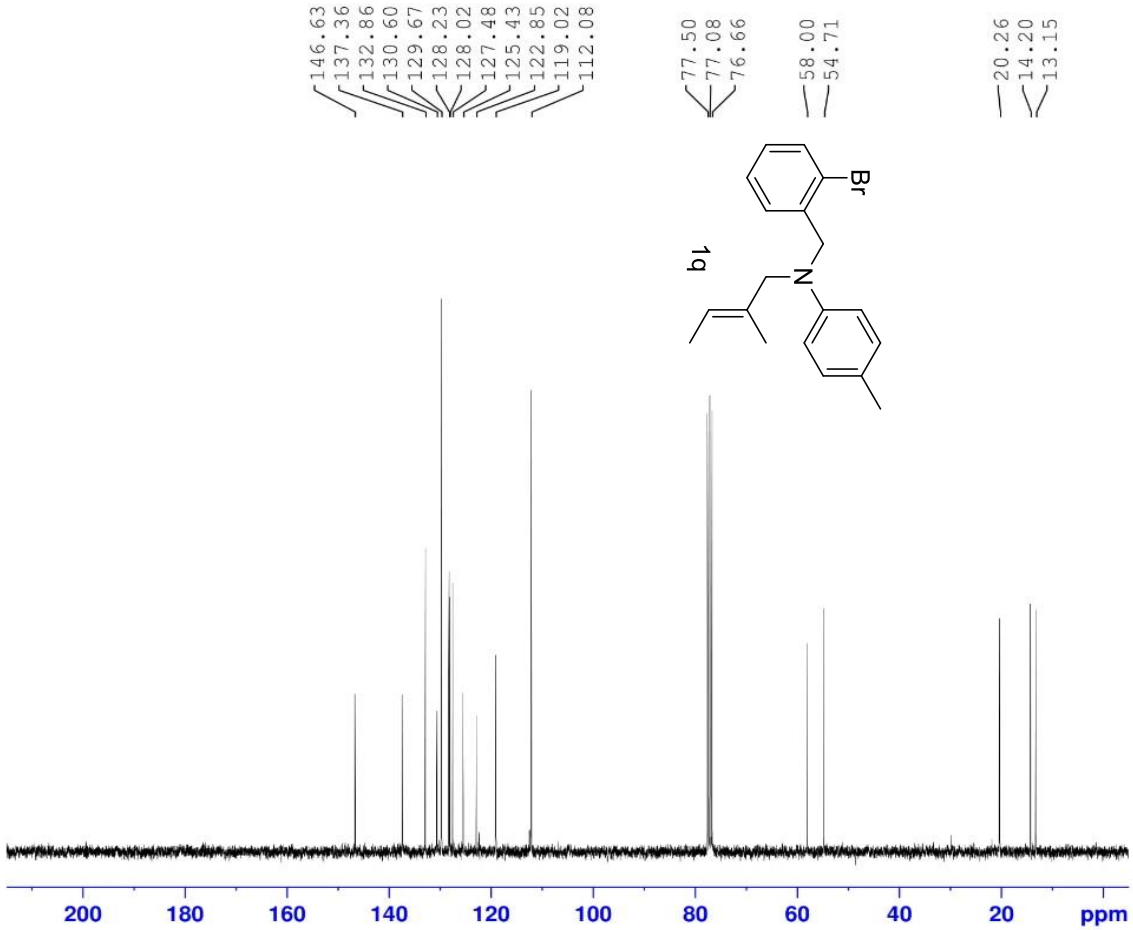

```
Current Data Parameters
NAME            H2552E18
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181009
Time               17.08
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6009.615 Hz
FIDRES          0.091699 Hz
AQ              5.4525952 sec
RG                   144
DW                83.200 usec
DE                 6.50 usec
TE                298.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         300.1318534 MHz
NUC1                 1H
P1                13.00 usec
PLW1         10.69999981 W

F2 - Processing parameters
SI                 65536
SF           300.1300076 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



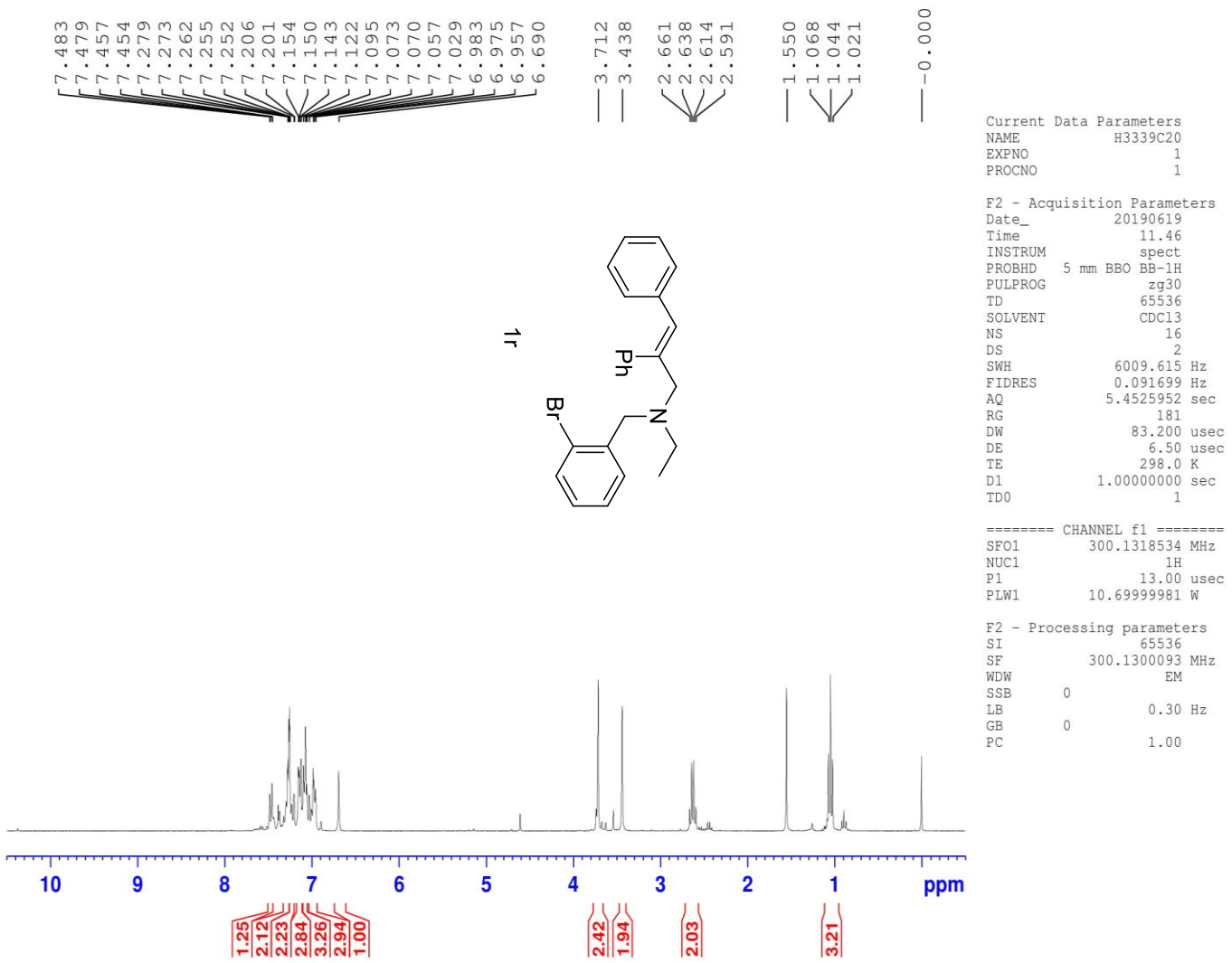

```
Current Data Parameters
NAME                  C2552E3
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20181010
Time                   13.46
INSTRUM                spect
PROBHD    5 mm BBO BB-1H
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                       1169
DS                          4
SWH                18028.846 Hz
FIDRES             0.275098 Hz
AQ                 1.8175317 sec
RG                        912
DW                    27.733 usec
DE                     6.50 usec
TE                     300.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1              75.4752949 MHz
NUC1                     13C
P1                     9.47 usec
PLW1             38.00000000 W

======== CHANNEL f2 ========
SFO2             300.1312005 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                  90.00 usec
PLW2             10.69999981 W
PLW12             0.22325000 W
PLW13             0.11229000 W

F2 - Processing parameters
SI                       32768
SF                75.4677485 MHz
WDW                        EM
SSB           0
LB                      1.00 Hz
GB            0
PC                      1.40
```




```
Current Data Parameters
NAME          H3339A11-R
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190404
Time               14.56
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6009.615 Hz
FIDRES          0.091699 Hz
AQ            5.4525952 sec
RG                   287
DW                83.200 usec
DE                 6.50 usec
TE                298.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         300.1318534 MHz
NUC1                   1H
P1                 13.00 usec
PLW1         10.69999981 W

F2 - Processing parameters
SI                 65536
SF           300.1300086 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



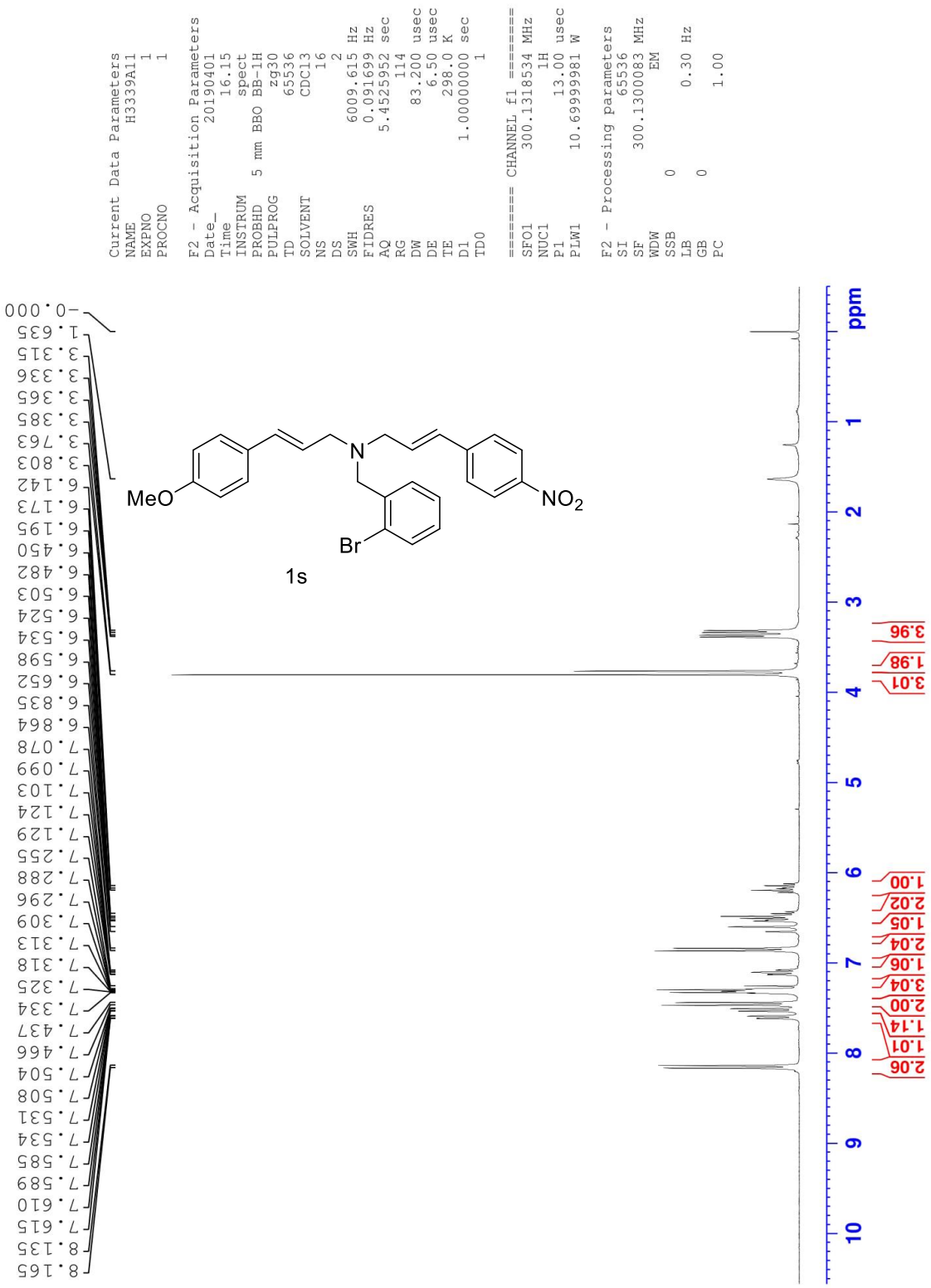

```
Current Data Parameters
NAME                  C3339B6
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_                20190508
Time                     9.43
INSTRUM                 spect
PROBHD    5 mm BBO BB-1H
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                        235
DS                          4
SWH                 18028.846 Hz
FIDRES                0.275098 Hz
AQ                    1.8175317 sec
RG                          645
DW                     27.733 usec
DE                      6.50 usec
TE                      300.0 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1                75.4752949 MHz
NUC1                       13C
P1                       9.47 usec
PLW1               38.00000000 W

======== CHANNEL f2 ========
SFO2               300.1312005 MHz
NUC2                       1H
CPDPRG[2                waltz16
PCPD2                   90.00 usec
PLW2               10.69999981 W
PLW12               0.22325000 W
PLW13               0.11229000 W

F2 - Processing parameters
SI                        32768
SF                  75.4677485 MHz
WDW                        EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.40
```

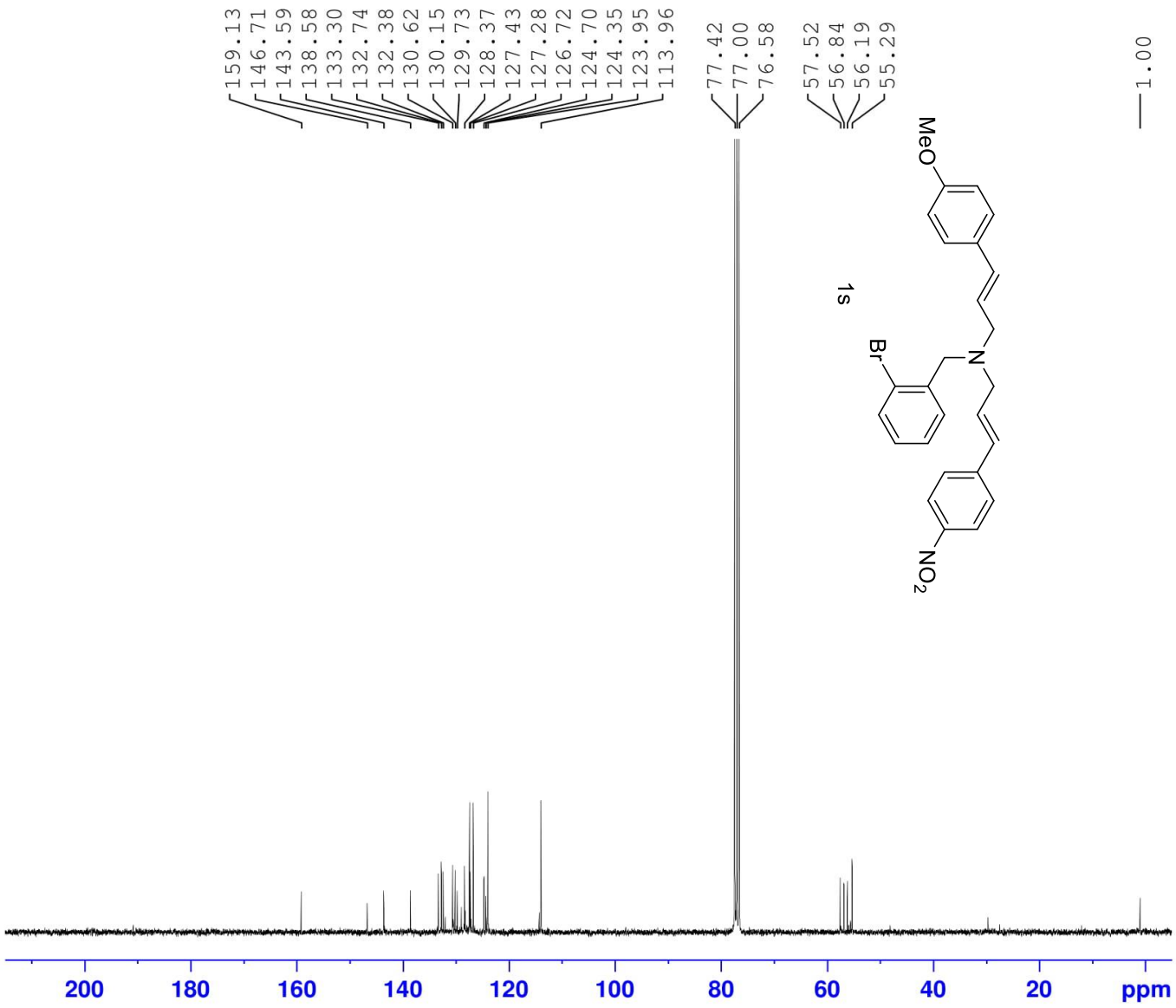



```
Current Data Parameters
NAME            H3339C20
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190619
Time               11.46
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6009.615 Hz
FIDRES          0.091699 Hz
AQ            5.4525952 sec
RG                   181
DW                83.200 usec
DE                 6.50 usec
TE                298.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         300.1318534 MHz
NUC1                   1H
P1                 13.00 usec
PLW1         10.69999981 W

F2 - Processing parameters
SI                 65536
SF           300.1300093 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

Current Data Parameters
NAME C3339B9
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190620
Time 12.26
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 111
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 456
DW 27.733 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 75.4752949 MHz
NUC1 13C
P1 9.47 usec
PLW1 38.00000000 W
======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 10.69999981 W
PLW12 0.22325000 W
PLW13 0.11229000 W
F2 - Processing parameters
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
N
Ph
Br
1r
12.05
47.68
57.20
62.62
76.71
77.14
77.56
124.07
126.55
126.99
127.20
127.95
128.24
128.37
128.91
129.32
130.50
132.38
137.12
139.26
140.59
140.66
ppm
200
180
160
140
120
100
80
60
40
20

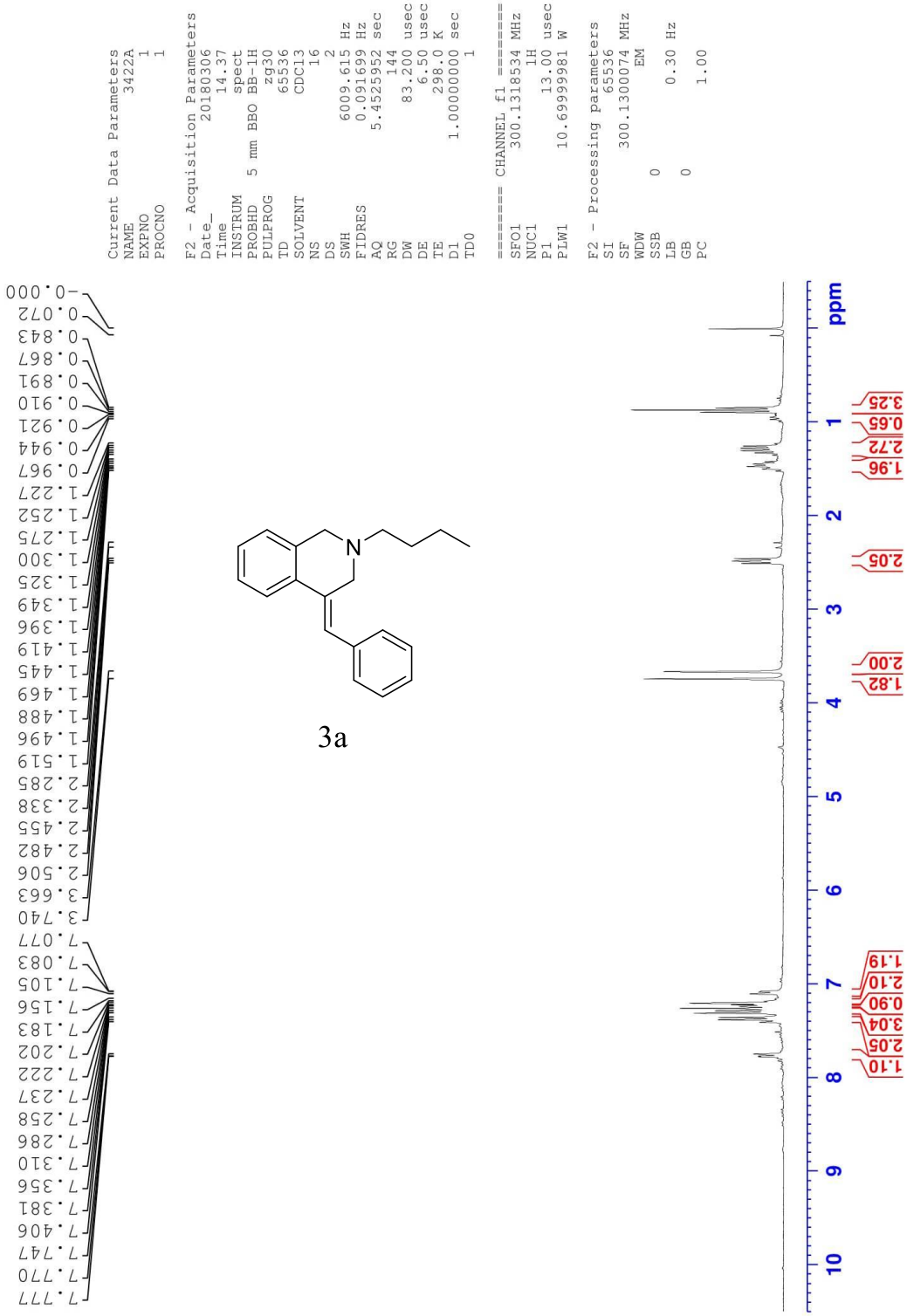
-

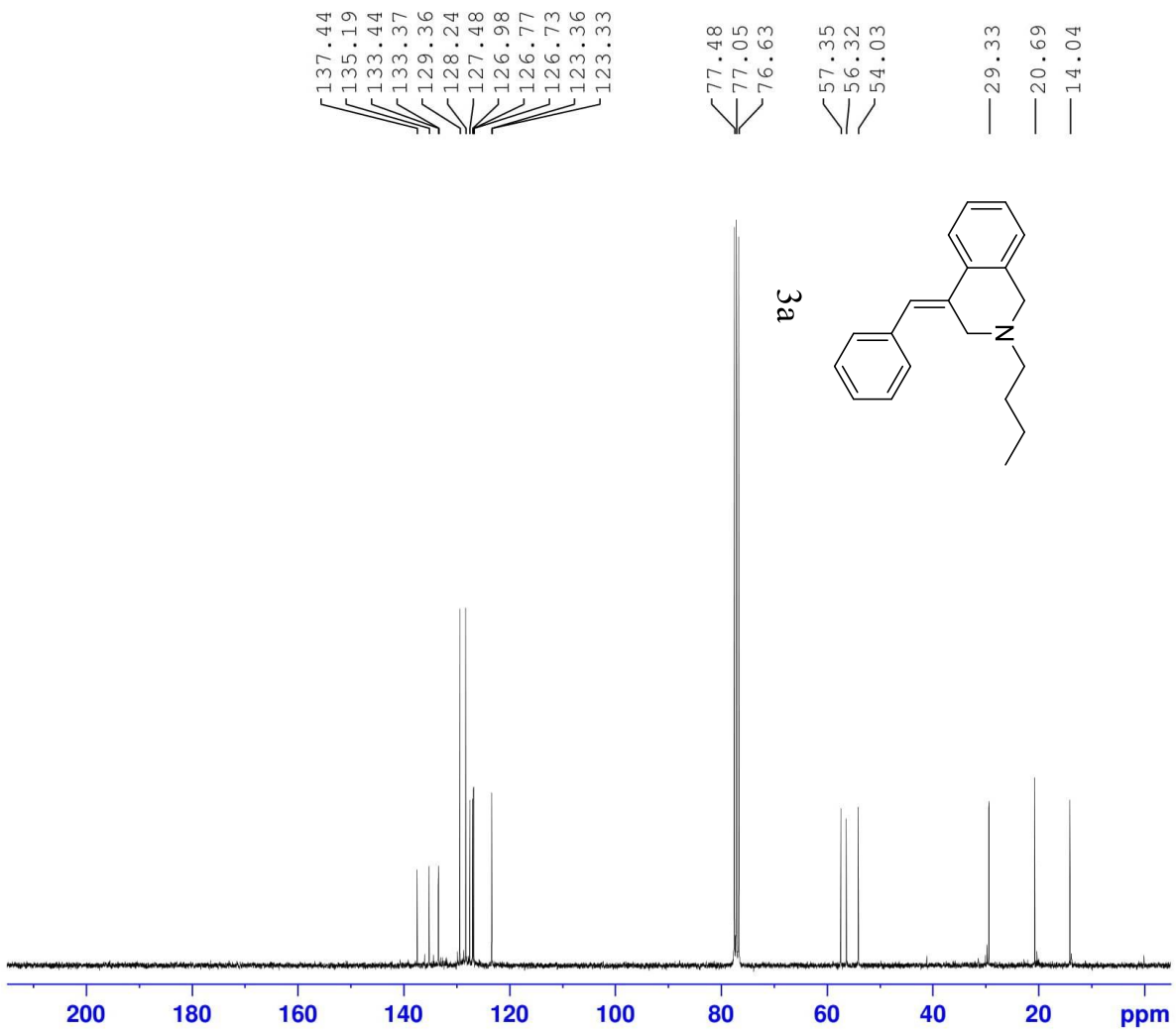

Current Data Parameters
NAME H3339A11
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190401
Time 16.15
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 114
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.69999981 W
F2 - Processing parameters
SI 65536
SF 300.1300083 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
MeO
N
NO2
Br
1s
ppm
3.96
1.98
3.01
1.00
2.02
1.05
2.04
1.06
3.04
2.00
1.14
1.01
2.06



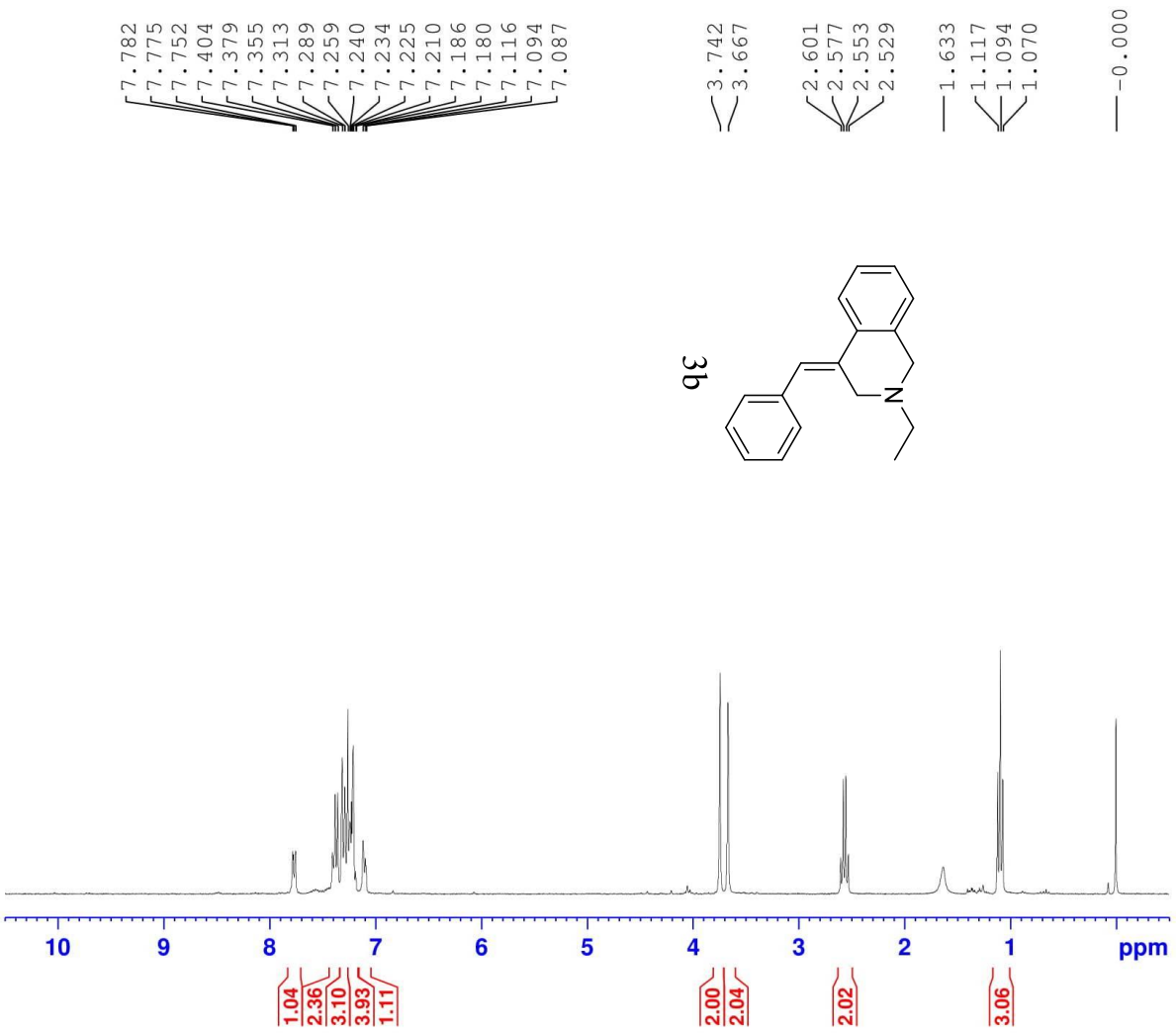

```
Current Data Parameters
NAME                 C3339C1
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_               20190626
Time                   19.39
INSTRUM                spect
PROBHD    5 mm BBO BB-1H
PULPROG                zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      2048
DS                         4
SWH                18028.846 Hz
FIDRES             0.275098 Hz
AQ                 1.8175317 sec
RG                       645
DW                    27.733 usec
DE                     6.50 usec
TE                     300.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1               75.4752949 MHz
NUC1                      13C
P1                        9.47 usec
PLW1              38.00000000 W

======== CHANNEL f2 ========
SFO2              300.1312005 MHz
NUC2                      1H
CPDPRG[2               waltz16
PCPD2                    90.00 usec
PLW2              10.69999981 W
PLW12              0.22325000 W
PLW13              0.11229000 W

F2 - Processing parameters
SI                       32768
SF                 75.4677516 MHz
WDW                         EM
SSB       0
LB                        1.00 Hz
GB        0
PC                        1.40
```

Cyclization



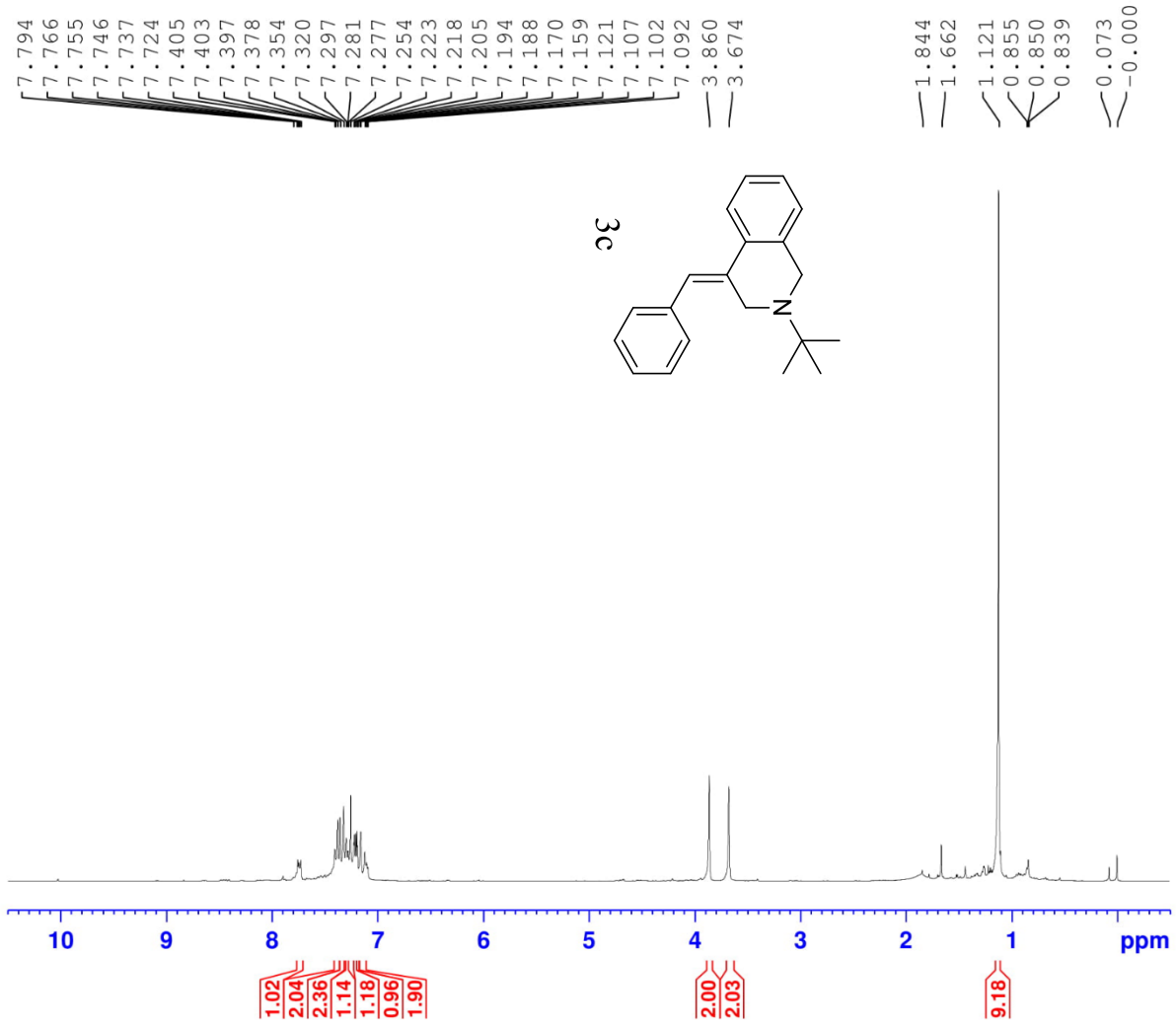



```
Current Data Parameters
NAME                  3423A
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20180307
Time                  21.22
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     2048
DS                        4
SWH               18028.846 Hz
FIDRES             0.275098 Hz
AQ                1.8175317 sec
RG                      912
DW                   27.733 usec
DE                    6.50 usec
TE                   300.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1            75.4752949 MHz
NUC1                   13C
P1                    9.47 usec
PLW1           38.00000000 W

======== CHANNEL f2 ========
SFO2           300.1312005 MHz
NUC2                   1H
CPDPRG[2            waltz16
PCPD2                90.00 usec
PLW2           10.69999981 W
PLW12           0.22325000 W
PLW13           0.11229000 W

F2 - Processing parameters
SI                    32768
SF              75.4677485 MHz
WDW                      EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

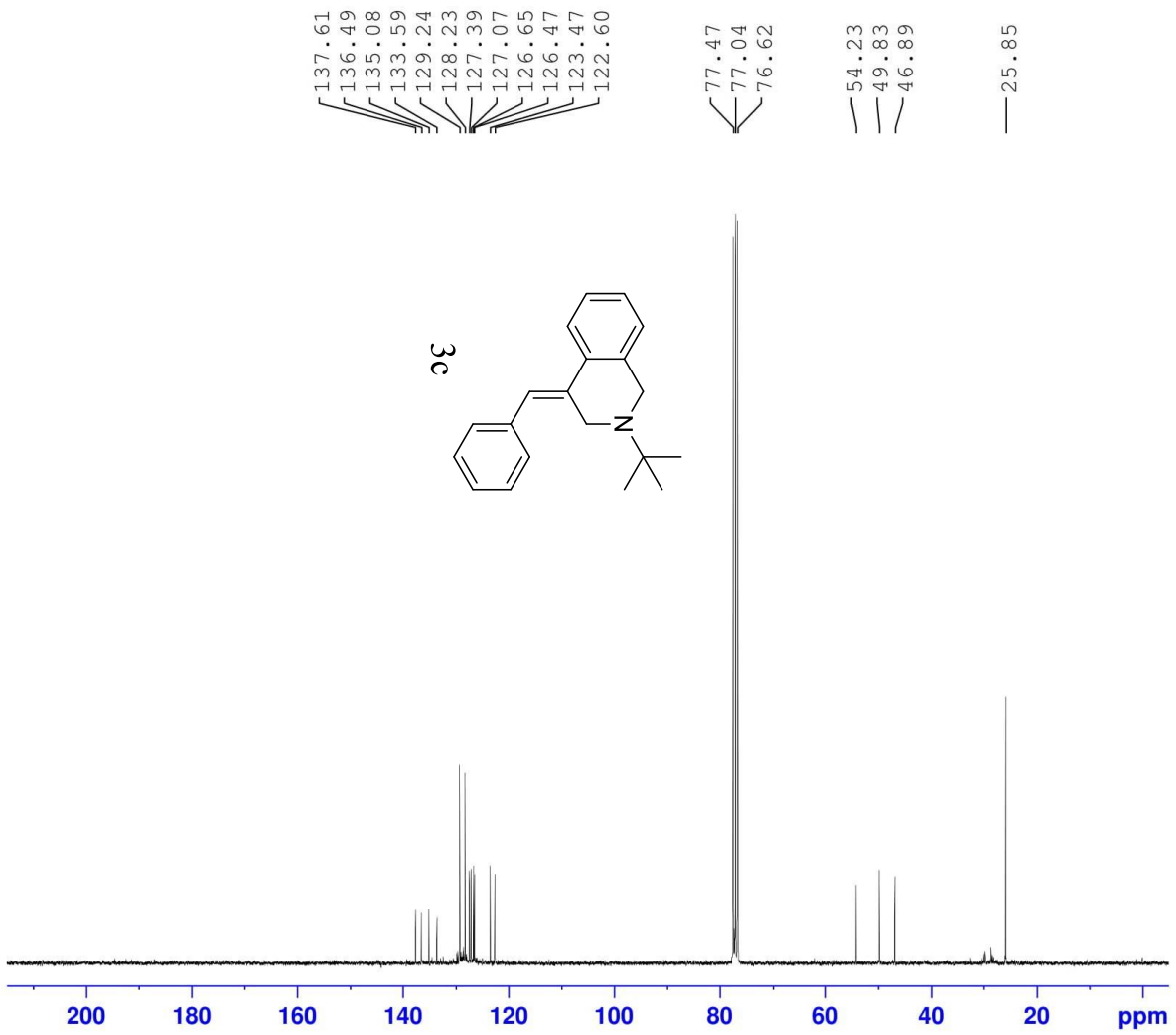



```
Current Data Parameters
NAME            H2552C12
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180818
Time               16.37
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6009.615 Hz
FIDRES          0.091699 Hz
AQ              5.4525952 sec
RG                   228
DW                83.200 usec
DE                 6.50 usec
TE                298.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         300.1318534 MHz
NUC1                   1H
P1                 13.00 usec
PLW1         10.69999981 W

F2 - Processing parameters
SI                 65536
SF           300.1300070 MHz
WDW                   EM
SSB      0
LB                 0.30 Hz
GB       0
PC                 1.00
```

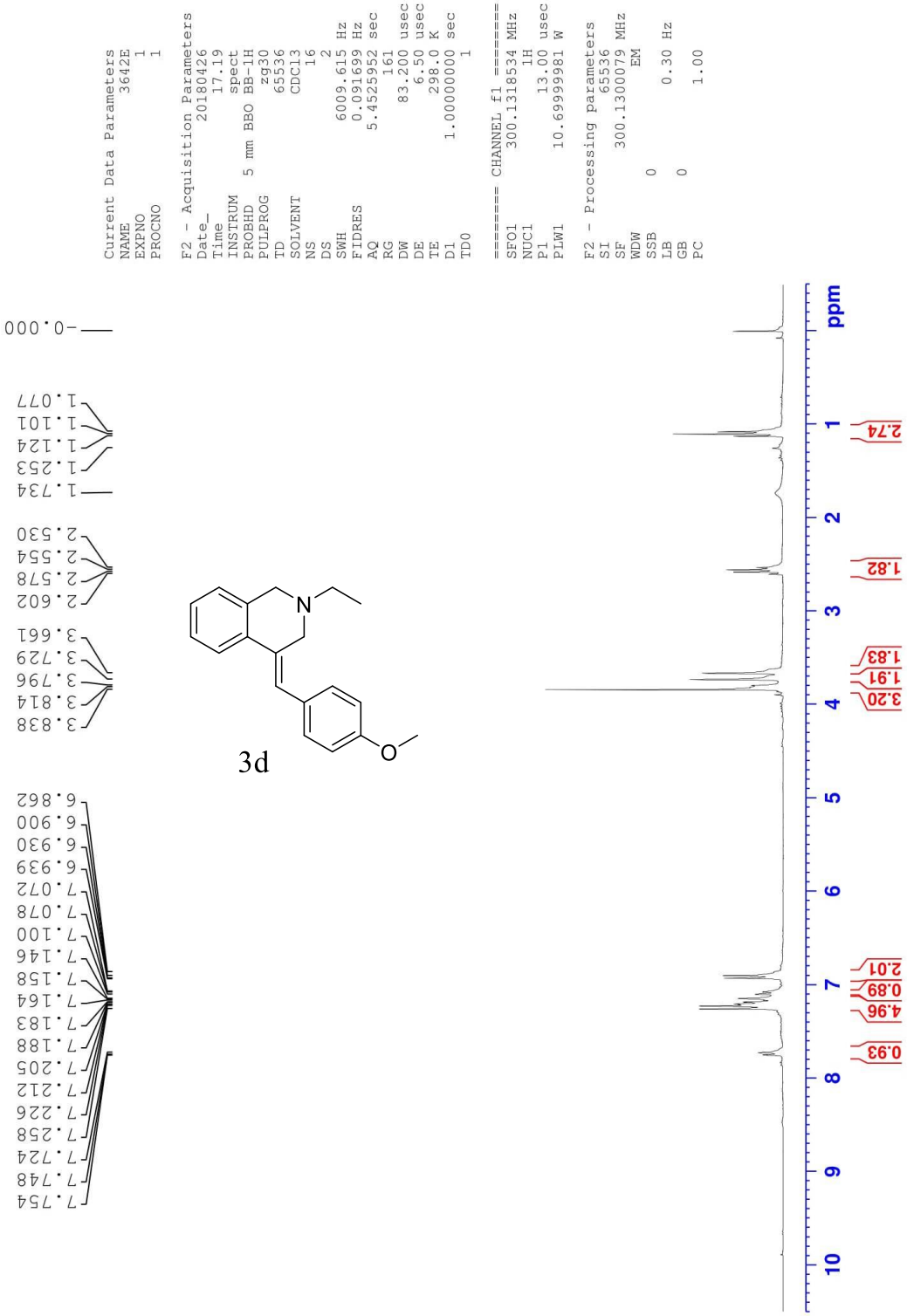

Current Data Parameters
NAME 3581A
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180412
Time 20.31
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3072
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 912
DW 27.733 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 75.4752949 MHz
NUC1 13C
P1 9.47 usec
PLW1 38.00000000 W
======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 10.69999981 W
PLW12 0.22325000 W
PLW13 0.11229000 W
F2 - Processing parameters
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
12.37
51.31
53.60
55.86
76.64
77.06
77.49
123.34
123.44
126.77
126.80
127.00
127.51
128.25
129.36
133.28
133.40
135.06
137.38
N
3b
ppm
200
180
160
140
120
100
80
60
40
20

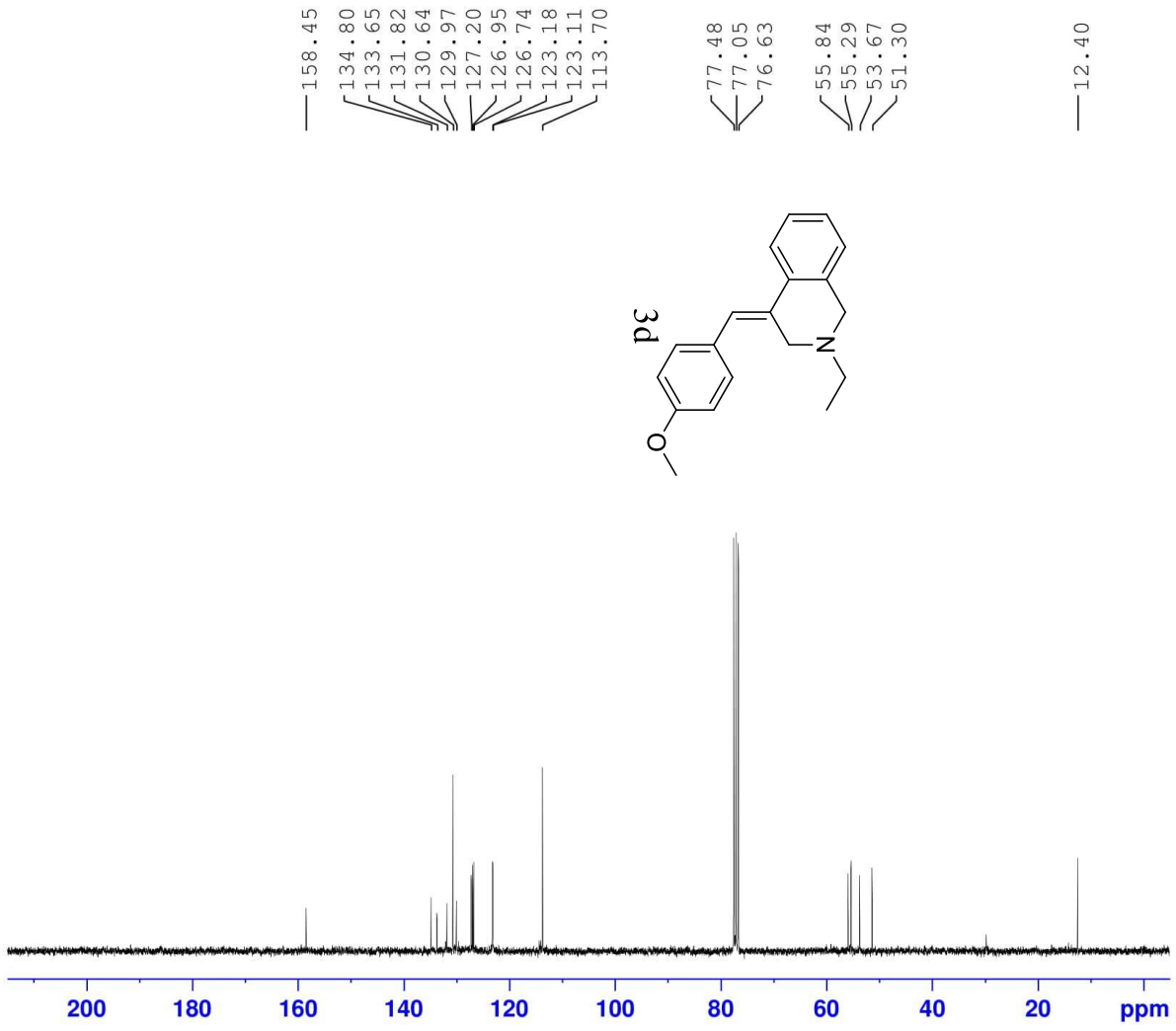



```
Current Data Parameters
NAME          3422B2_H1
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20180321
Time              15.24
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            6009.615 Hz
FIDRES        0.091699 Hz
AQ            5.4525952 sec
RG                  128
DW               83.200 usec
DE                6.50 usec
TE                298.0 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         300.1318534 MHz
NUC1                 1H
P1                13.00 usec
PLW1         10.69999981 W

F2 - Processing parameters
SI                65536
SF           300.1300082 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

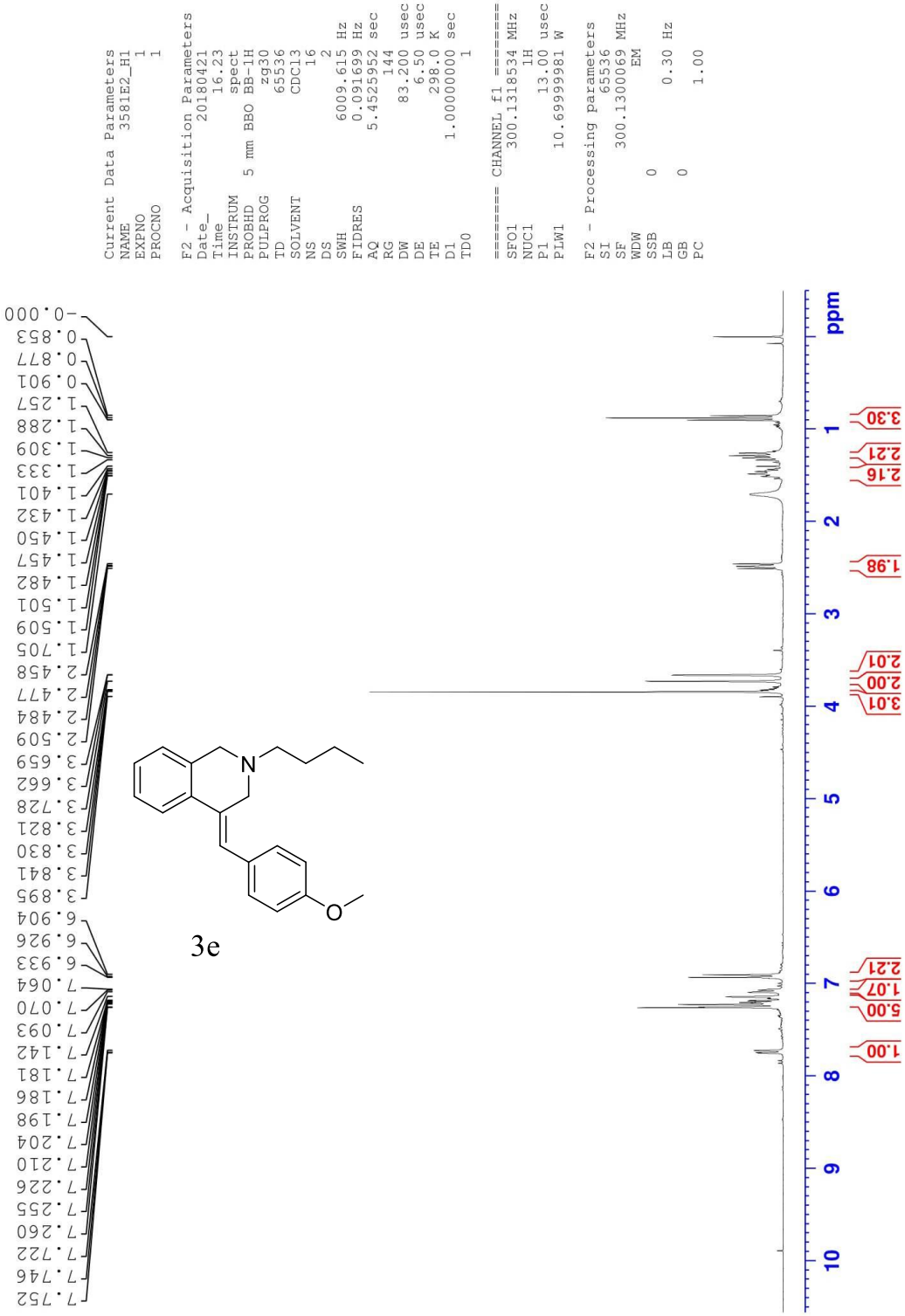


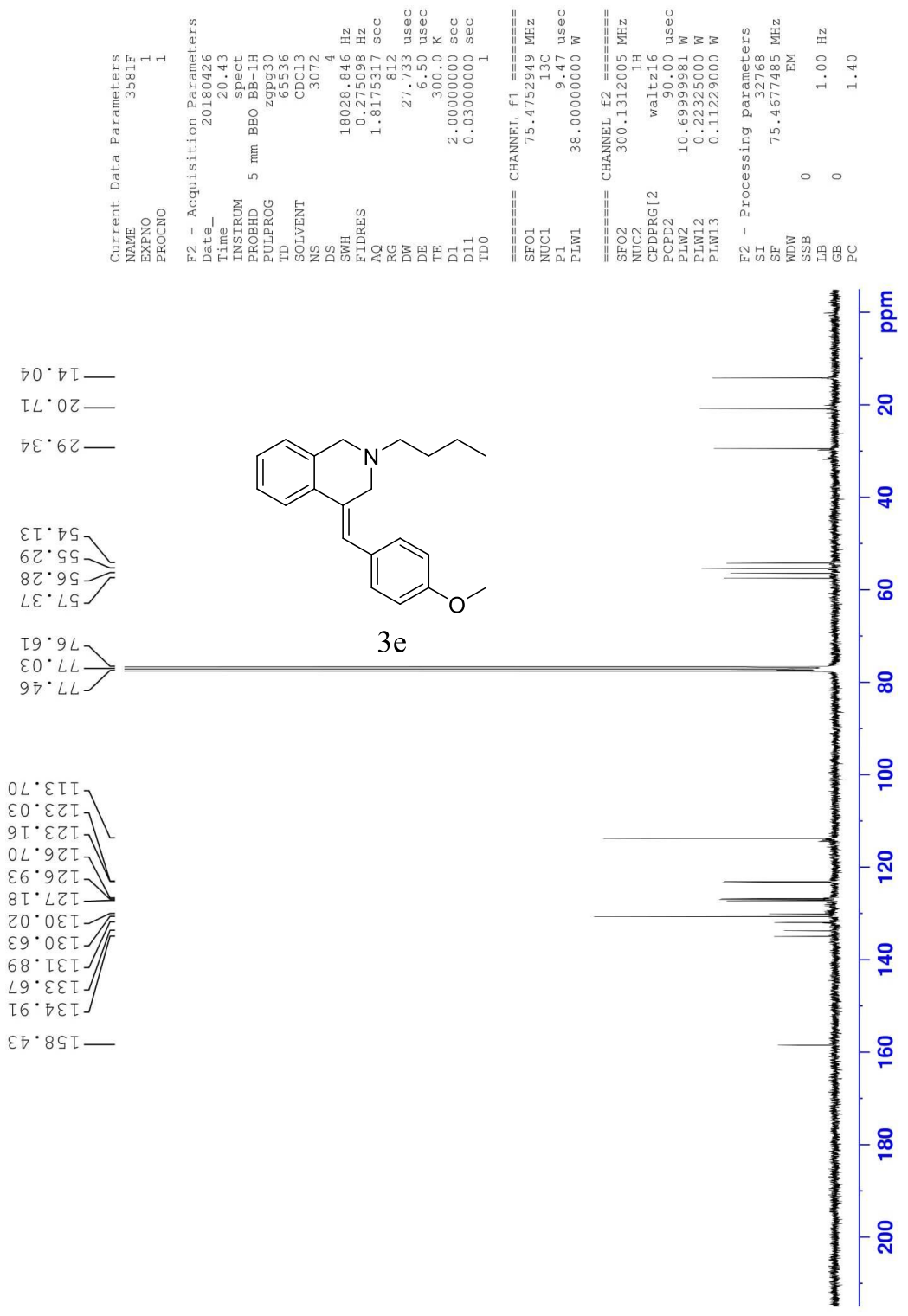

```
Current Data Parameters
NAME                  3423E
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20180323
Time      0
INSTRUM                spect
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                    65536
SOLVENT               CDC13
NS                     3072
DS                        4
SWH               18028.846 Hz
FIDRES                0.275098 Hz
AQ                 1.8175317 sec
RG                     1030
DW                    27.733 usec
DE                     6.50 usec
TE                    300.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1              75.4752949 MHz
NUC1                     13C
P1                     9.47 usec
PLW1             38.00000000 W

======== CHANNEL f2 ========
SFO2             300.1312005 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                 90.00 usec
PLW2             10.69999981 W
PLW12             0.22325000 W
PLW13             0.11229000 W

F2 - Processing parameters
SI                    32768
SF                75.4677485 MHz
WDW                      EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```

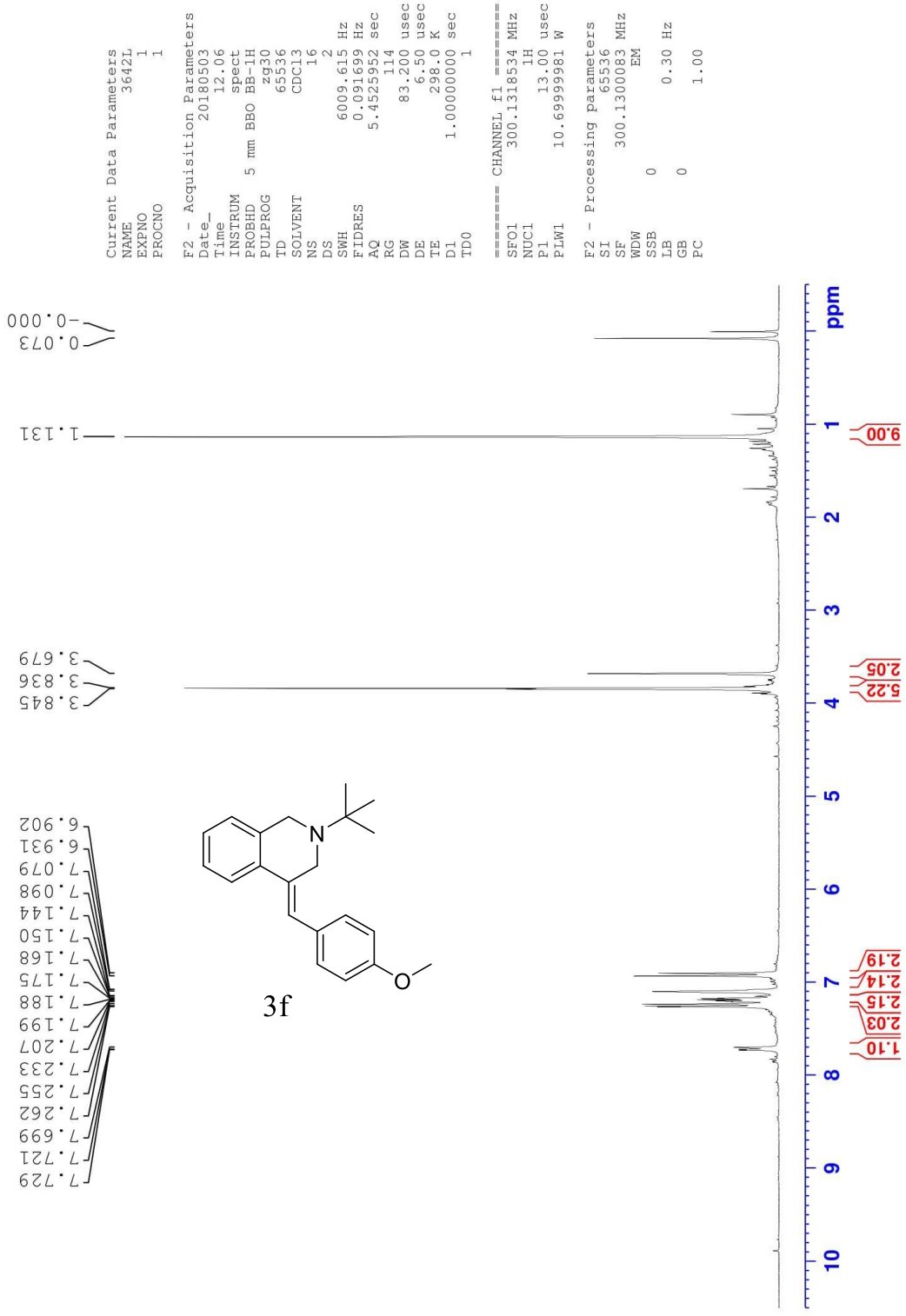

Current Data Parameters
NAME 3642E
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180426
Time 17.19
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 161
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.69999981 W
F2 - Processing parameters
SI 65536
SF 300.1300079 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
-0.000
1.077
1.101
1.124
1.253
1.734
2.530
2.554
2.578
2.602
3.661
3.729
3.796
3.814
3.838
6.862
6.900
6.930
6.939
7.072
7.078
7.100
7.146
7.158
7.164
7.183
7.188
7.205
7.212
7.226
7.258
7.724
7.748
7.754
N
O
3d
ppm
1
2
3
4
5
6
7
8
9
10
2.74
1.82
1.83
1.91
3.20
2.01
0.89
4.96
0.93

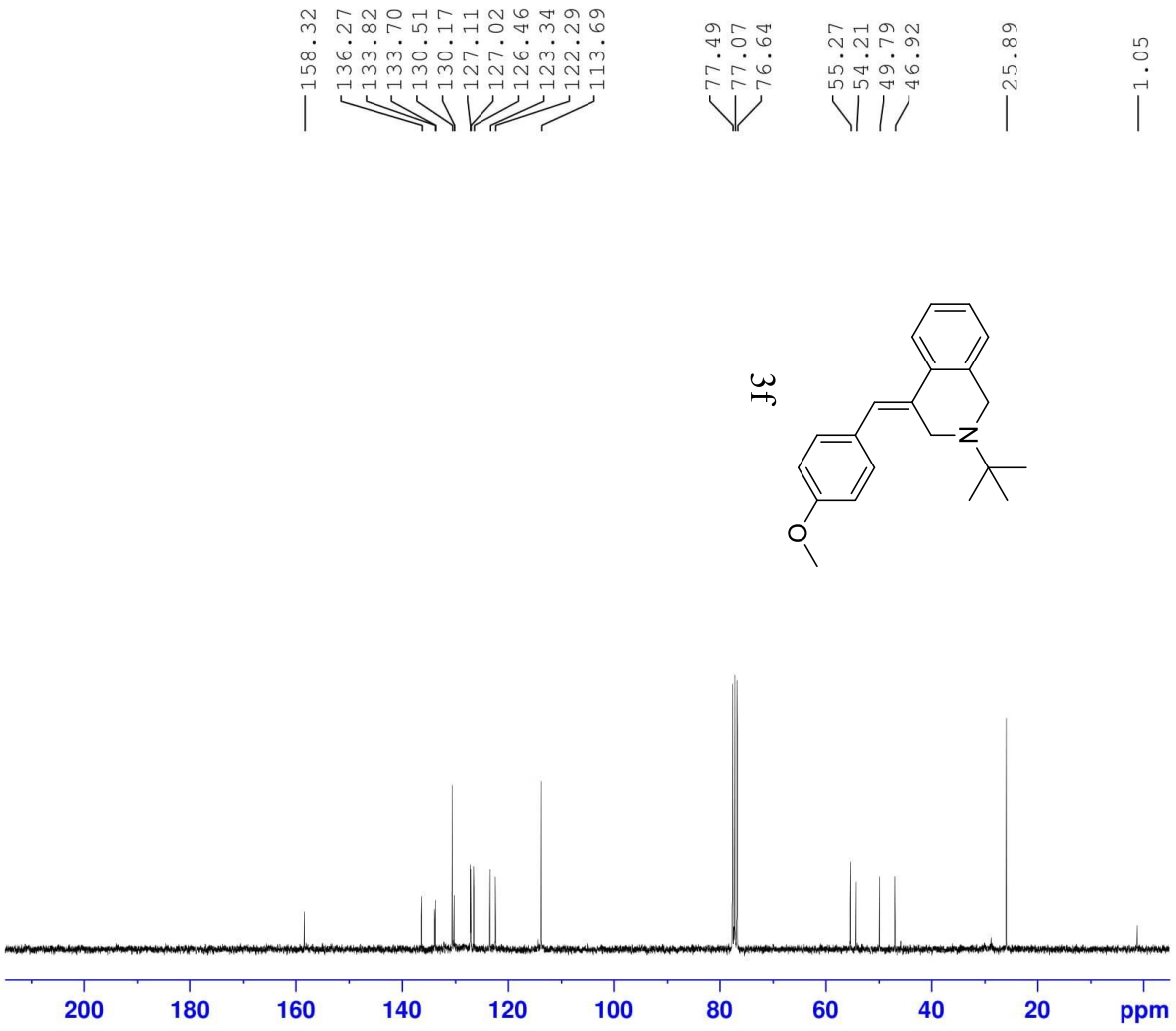



```
Current Data Parameters
NAME          3561MN_C13
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180405
Time               15.12
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  512
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175317 sec
RG                  812
DW               27.733 usec
DE                6.50 usec
TE                300.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         75.4752949 MHz
NUC1                13C
P1                 9.47 usec
PLW1        38.00000000 W

======== CHANNEL f2 ========
SFO2        300.1312005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2        10.69999981 W
PLW12        0.22325000 W
PLW13        0.11229000 W

F2 - Processing parameters
SI                 32768
SF           75.4677485 MHz
WDW                   EM
SSB      0
LB                 1.00 Hz
GB       0
PC                 1.40
```

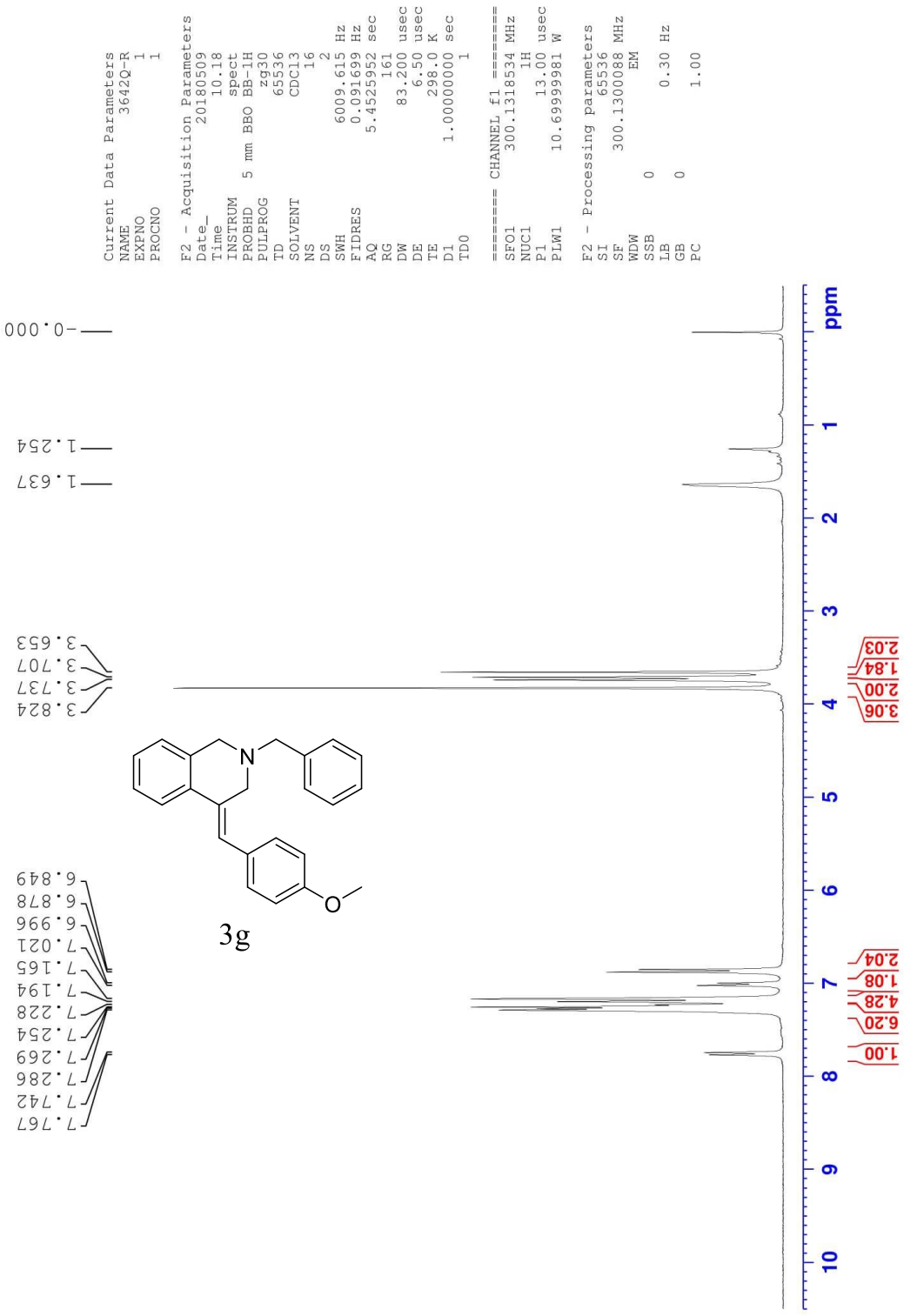

Current Data Parameters
NAME 3581E2_H1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180421
Time 16.23
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 144
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.69999981 W
F2 - Processing parameters
SI 65536
SF 300.1300069 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.752
7.746
7.722
7.260
7.255
7.226
7.210
7.204
7.198
7.186
7.181
7.142
7.093
7.070
7.064
6.933
6.926
6.904
3.895
3.841
3.830
3.821
3.728
3.662
3.659
2.509
2.484
2.477
2.458
1.705
1.509
1.501
1.482
1.457
1.450
1.432
1.401
1.333
1.309
1.288
1.257
0.901
0.877
0.853
0.000
N
O
3e
ppm
1
2
3
4
5
6
7
8
9
10
3.30
2.21
2.16
1.98
2.01
2.00
3.01
2.21
1.07
5.00
1.00

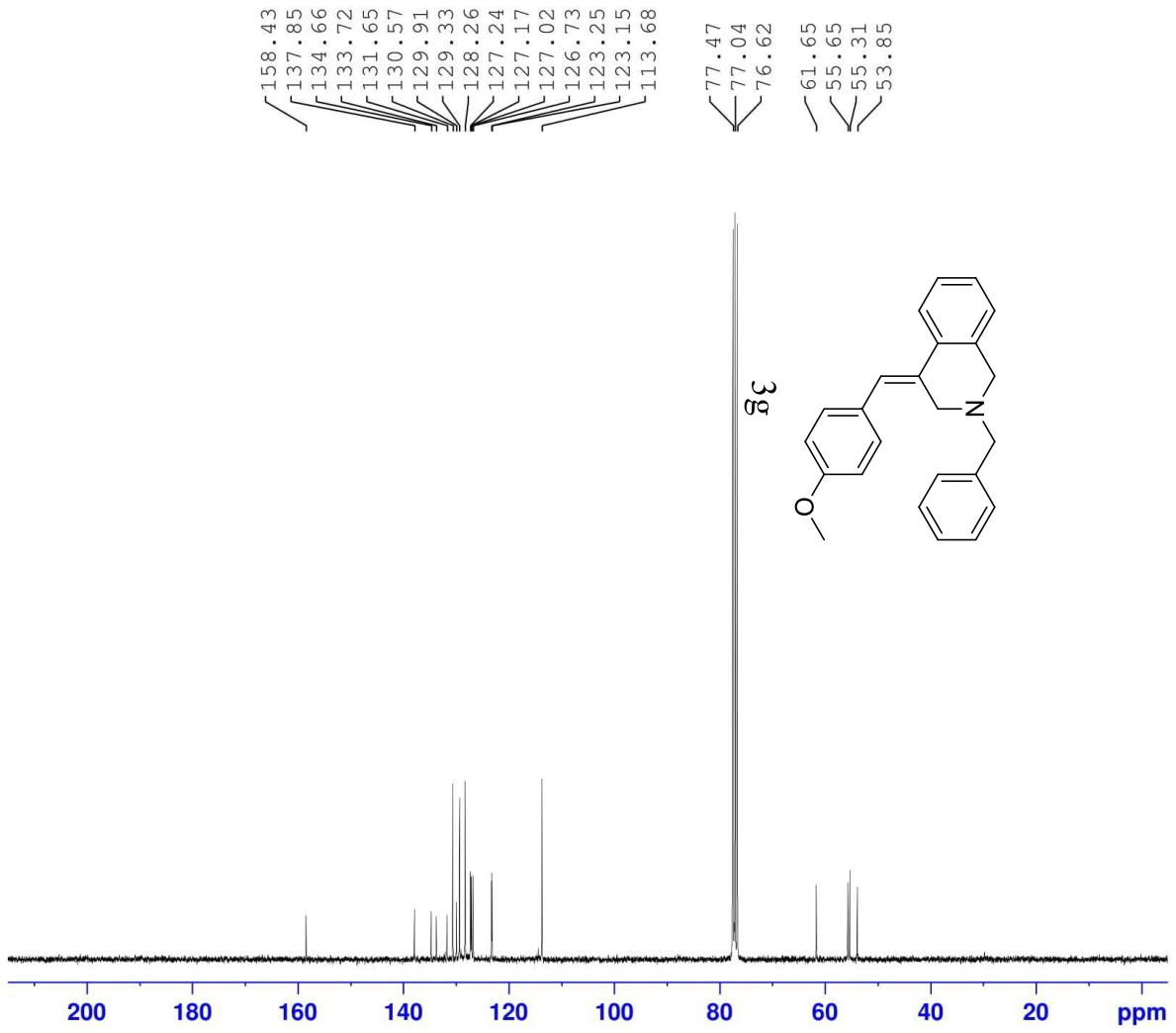

Current Data Parameters
NAME 3581F
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180426
Time 20.43
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3072
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 812
DW 27.733 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 75.4752949 MHz
NUC1 13C
P1 9.47 usec
PLW1 38.00000000 W
======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 10.69999981 W
PLW12 0.22325000 W
PLW13 0.11229000 W
F2 - Processing parameters
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
N
O
3e
14.04
20.71
29.34
54.13
55.29
56.28
57.37
76.61
77.03
77.46
113.70
123.03
123.16
126.70
126.93
127.18
130.02
130.63
131.89
133.67
134.91
158.43
ppm
200
180
160
140
120
100
80
60
40
20


Current Data Parameters
NAME 3642L
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180503
Time 12.06
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 114
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.69999981 W
F2 - Processing parameters
SI 65536
SF 300.1300083 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
0.073
-0.000
1.131
3.845
3.836
3.679
6.902
6.931
7.079
7.098
7.144
7.150
7.168
7.175
7.188
7.199
7.207
7.233
7.255
7.262
7.699
7.721
7.729
9.00
5.22
2.05
1.10
2.03
2.15
2.14
2.19
ppm
N
O
3f

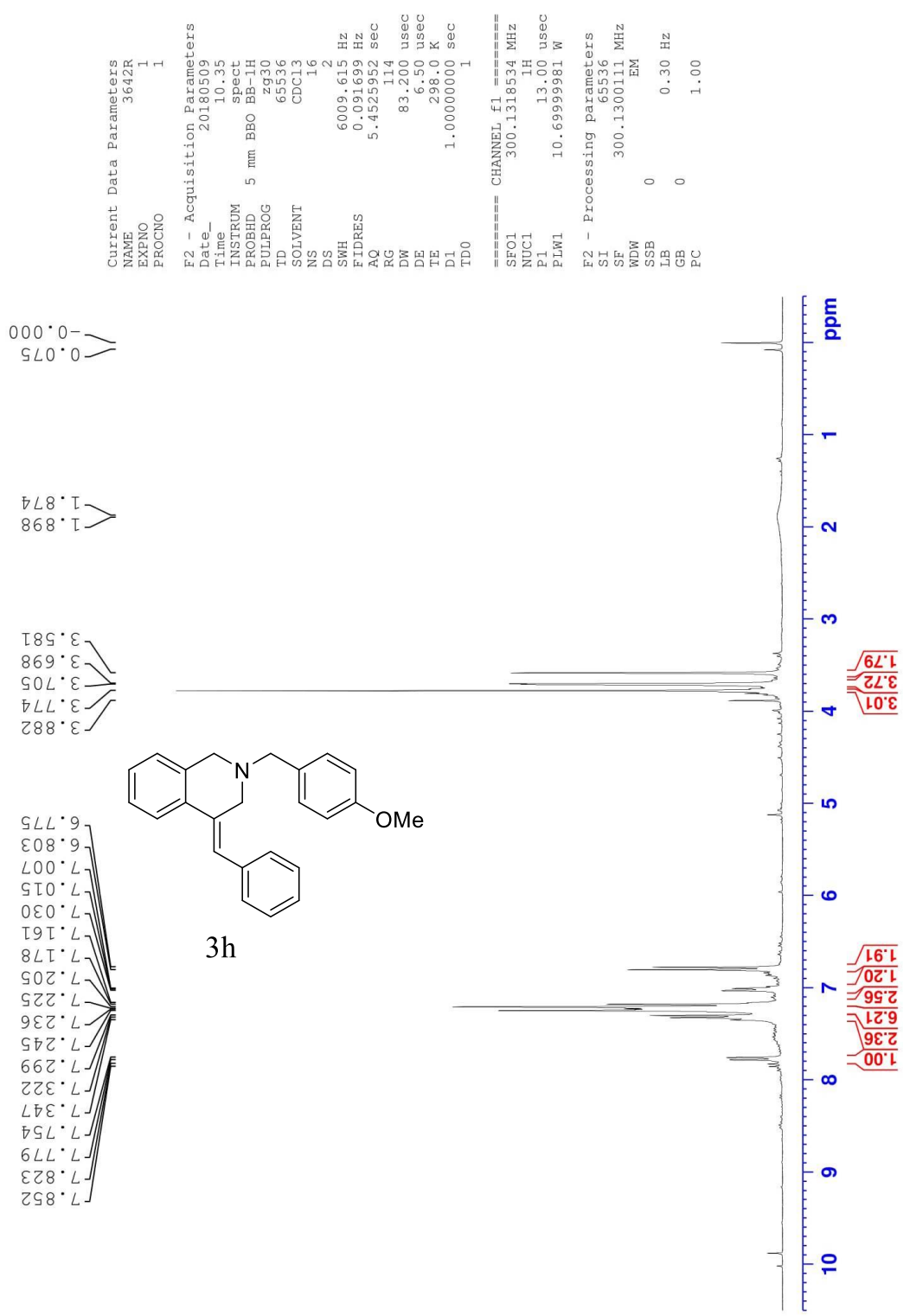


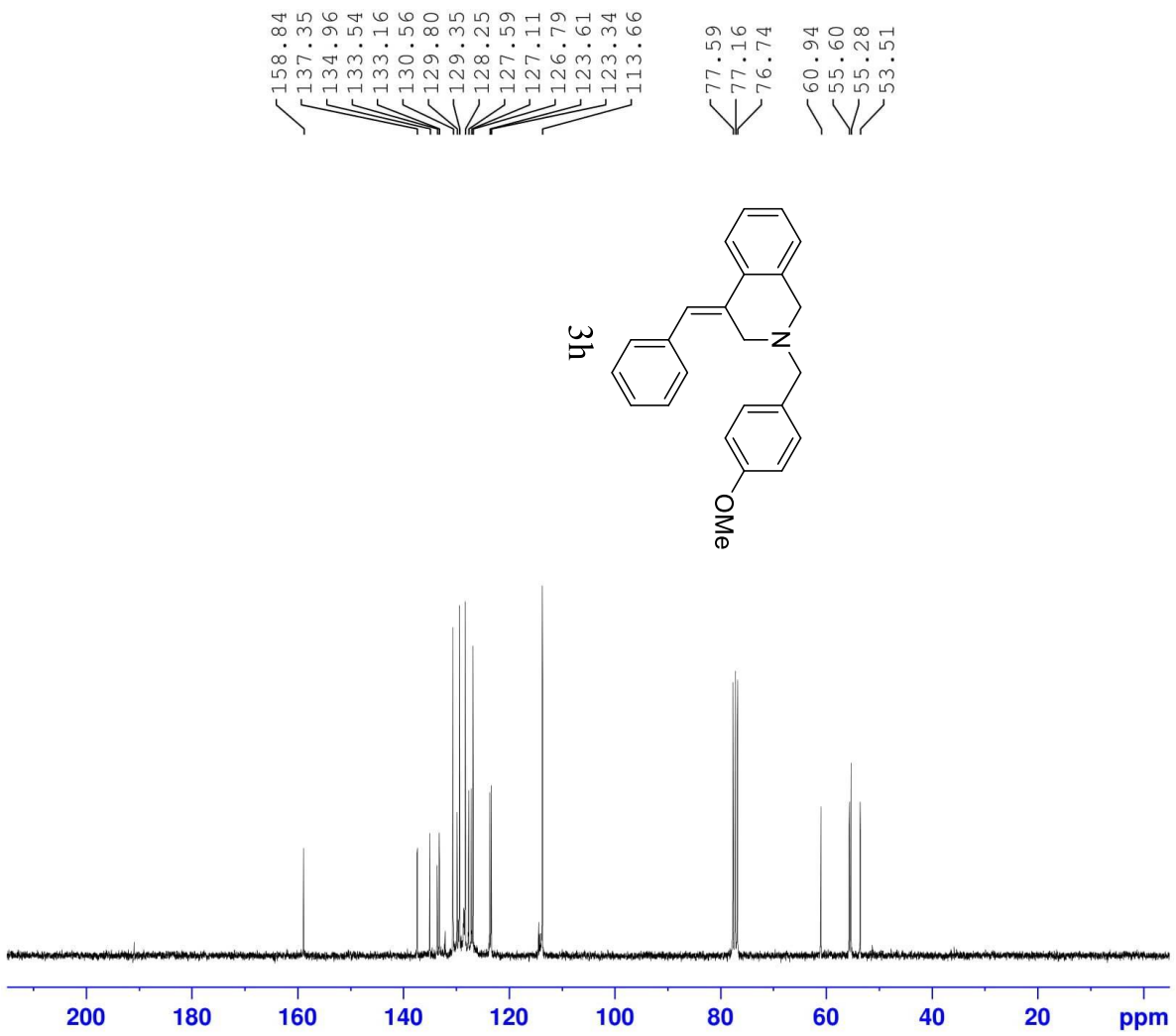

```
Current Data Parameters
NAME                  3688E
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20180524
Time                  12.35
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      356
DS                        4
SWH               18028.846 Hz
FIDRES             0.275098 Hz
AQ                1.8175317 sec
RG                      812
DW                   27.733 usec
DE                    6.50 usec
TE                   300.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1            75.4752949 MHz
NUC1                   13C
P1                    9.47 usec
PLW1           38.00000000 W

======== CHANNEL f2 ========
SFO2           300.1312005 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2                90.00 usec
PLW2           10.69999981 W
PLW12           0.22325000 W
PLW13           0.11229000 W

F2 - Processing parameters
SI                    32768
SF              75.4677485 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```


Current Data Parameters
NAME 36420-R
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180509
Time 10.18
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 161
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.69999981 W
F2 - Processing parameters
SI 65536
SF 300.1300088 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
-0.000
1.254
1.637
3.824
3.737
3.707
3.653
7.767
7.742
7.286
7.269
7.254
7.228
7.194
7.165
7.021
6.996
6.878
6.849
N
O
3g
1.00
6.20
4.28
1.08
2.04
3.06
2.00
1.84
2.03
ppm

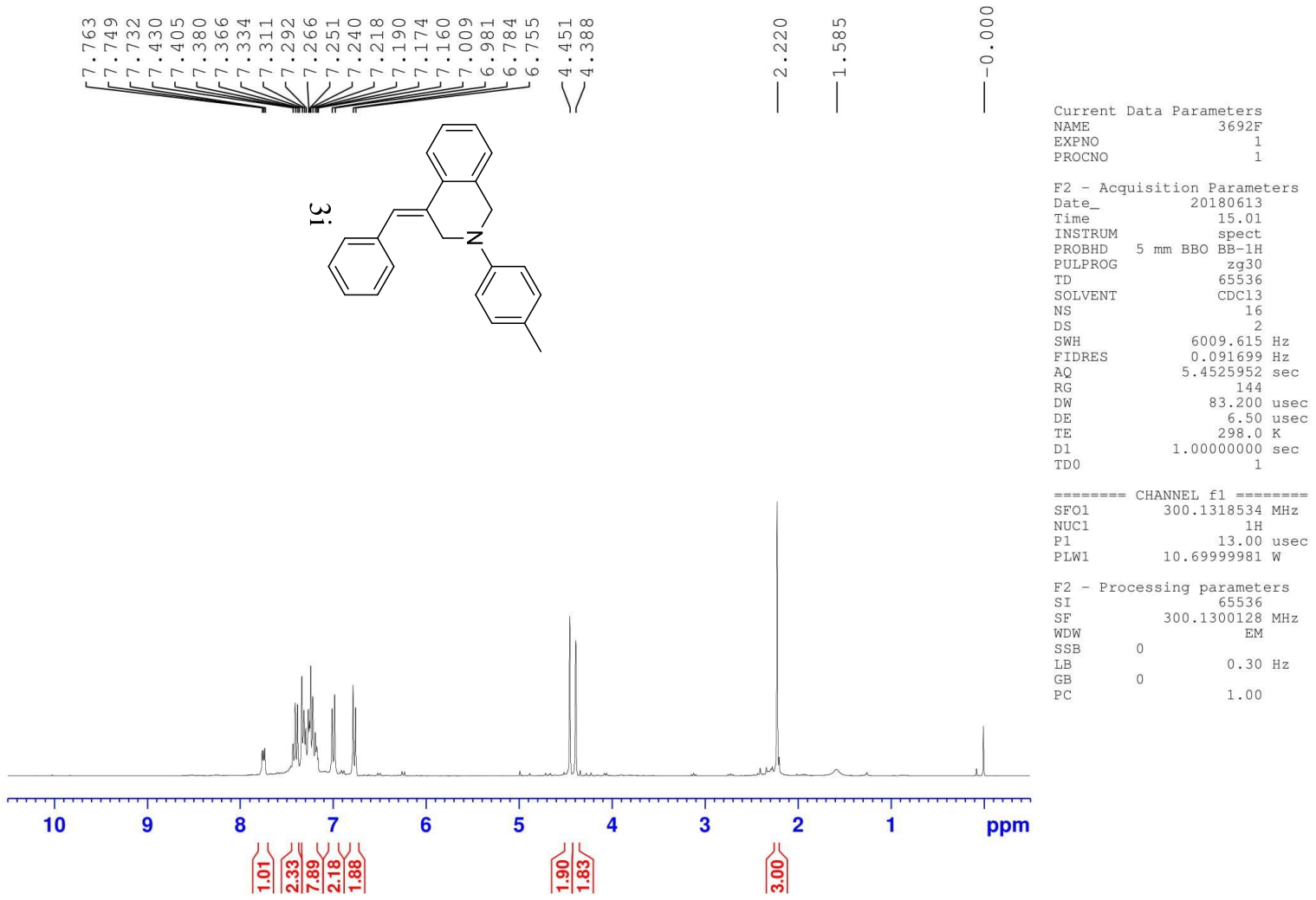



```
Current Data Parameters
NAME                 3688C
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20180523
Time                 20.42
INSTRUM              spect
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    3072
DS                       4
SWH              18028.846 Hz
FIDRES           0.275098 Hz
AQ               1.8175317 sec
RG                     912
DW                27.733 usec
DE                 6.50 usec
TE                 300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           75.4752949 MHz
NUC1                  13C
P1                  9.47 usec
PLW1          38.00000000 W

======== CHANNEL f2 ========
SFO2          300.1312005 MHz
NUC2                  1H
CPDPRG[2           waltz16
PCPD2               90.00 usec
PLW2          10.69999981 W
PLW12          0.22325000 W
PLW13          0.11229000 W

F2 - Processing parameters
SI                   32768
SF             75.4677485 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

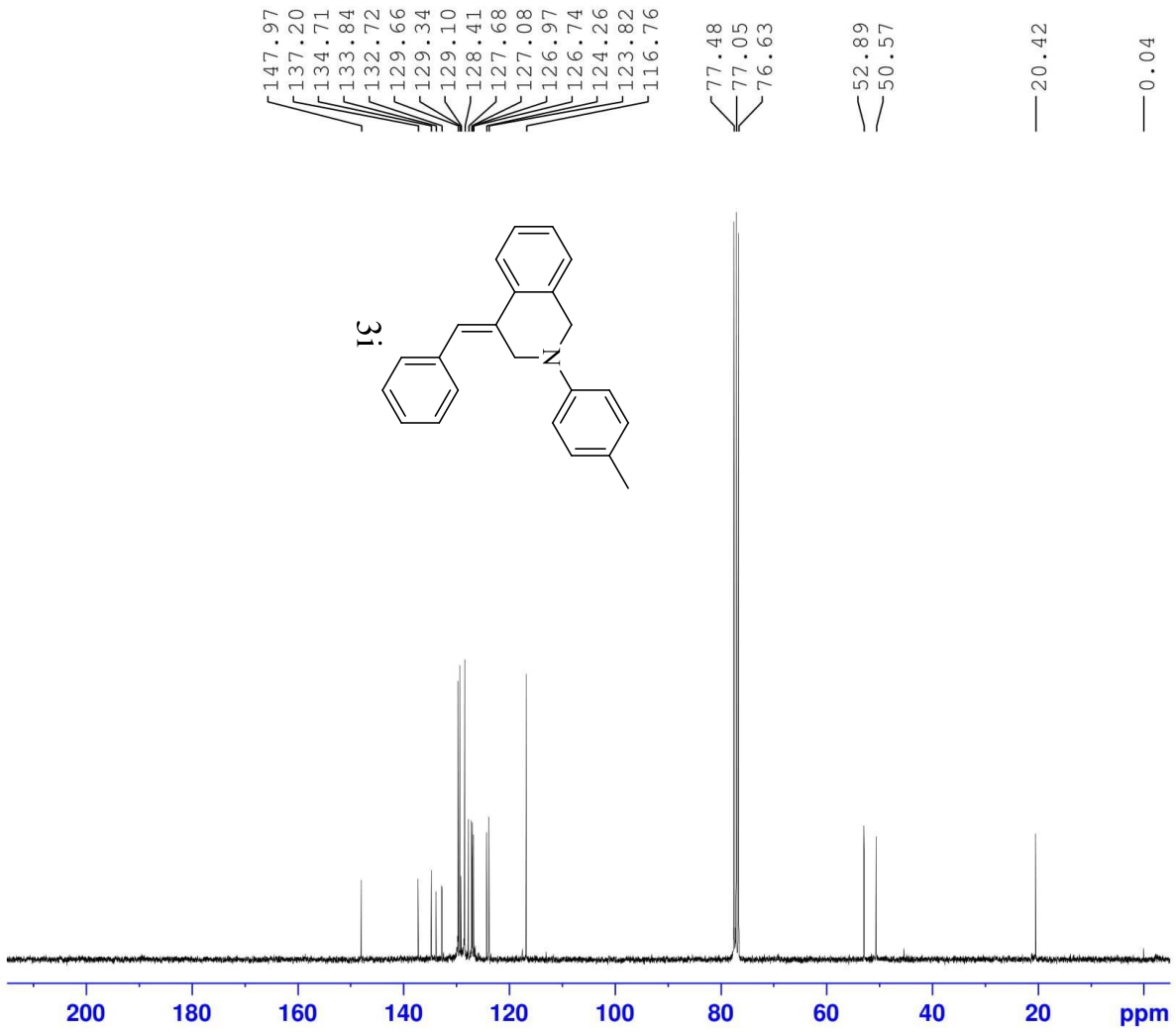

Current Data Parameters
NAME 3642R
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180509
Time 10.35
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 114
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.69999981 W
F2 - Processing parameters
SI 65536
SF 300.1300111 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
-0.000
0.075
1.874
1.898
3.581
3.698
3.705
3.774
3.882
6.775
6.803
7.007
7.015
7.030
7.161
7.178
7.205
7.225
7.236
7.245
7.299
7.322
7.347
7.754
7.779
7.823
7.852
1.00
2.36
6.21
2.56
1.20
1.91
3.01
3.72
1.79
ppm
OMe
3h



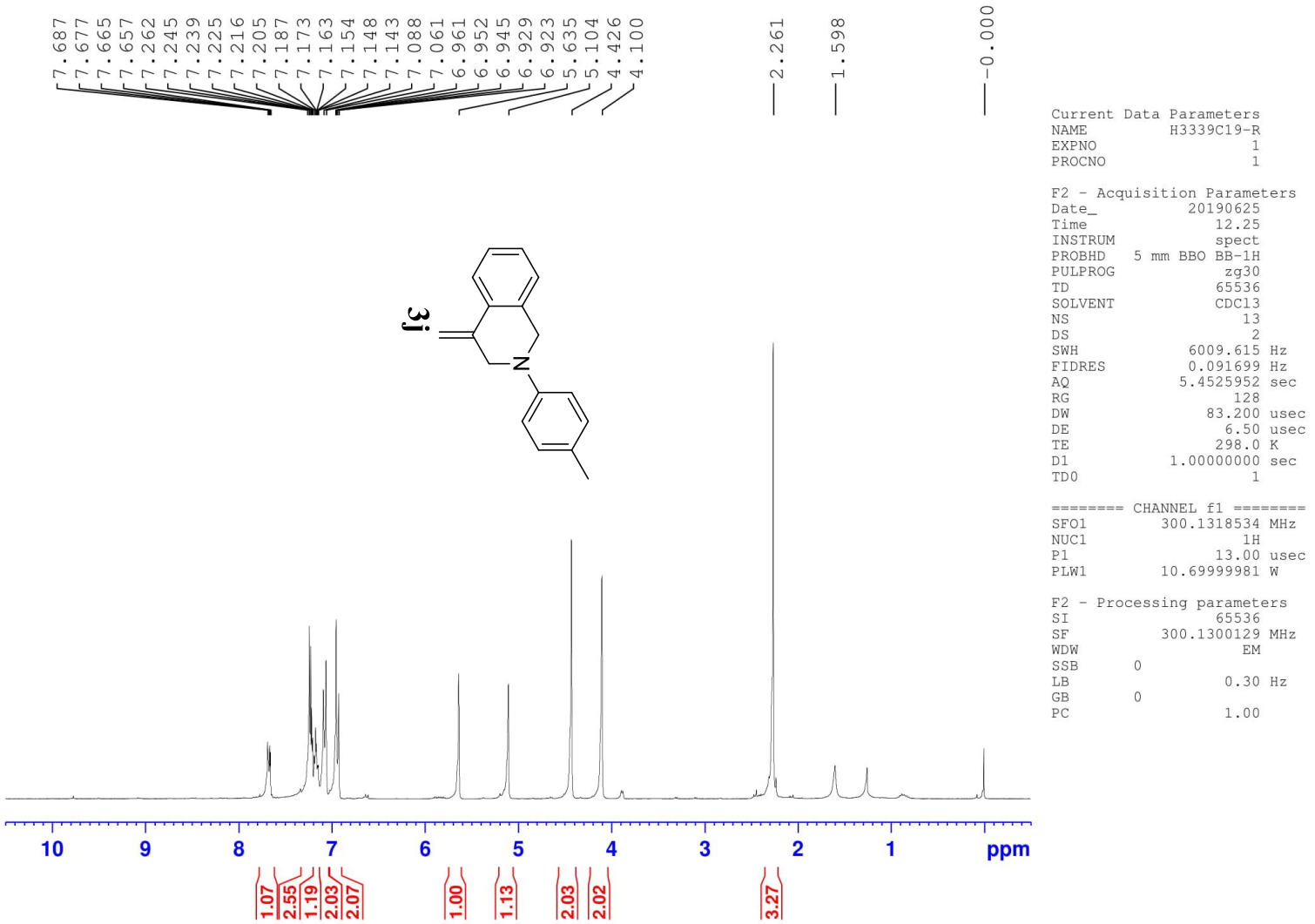

```
Current Data Parameters
NAME                 3688D
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20180524
Time                 11.47
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     426
DS                       4
SWH              18028.846 Hz
FIDRES           0.275098 Hz
AQ               1.8175317 sec
RG                     812
DW                27.733 usec
DE                 6.50 usec
TE                 300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          75.4752949 MHz
NUC1                 13C
P1                  9.47 usec
PLW1         38.00000000 W

======== CHANNEL f2 ========
SFO2         300.1312005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2         10.69999981 W
PLW12         0.22325000 W
PLW13         0.11229000 W

F2 - Processing parameters
SI                   32768
SF            75.4677485 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```



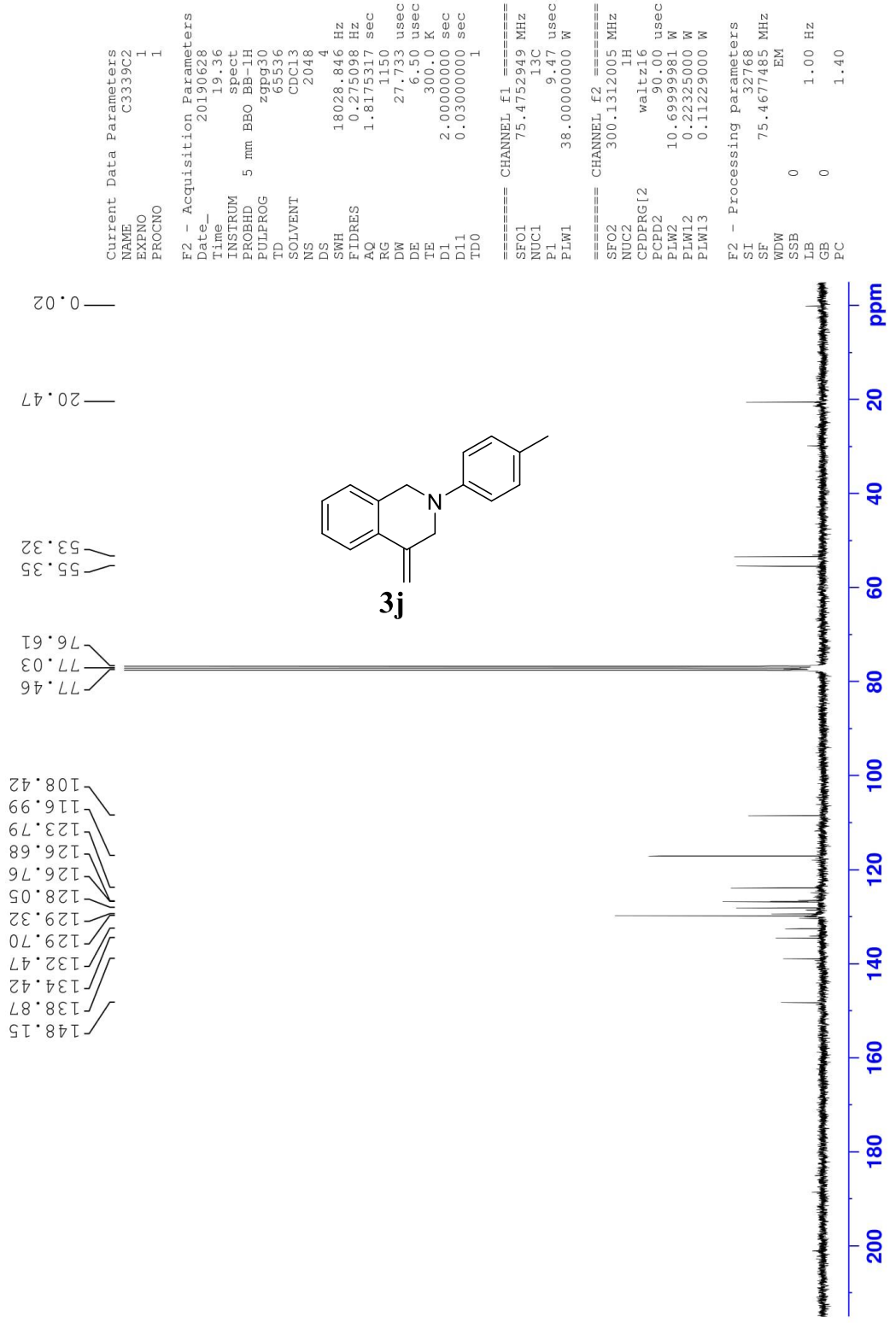

```
Current Data Parameters
NAME                  3692F
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20180613
Time                  15.01
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                6009.615 Hz
FIDRES            0.091699 Hz
AQ                5.4525952 sec
RG                      144
DW                   83.200 usec
DE                    6.50 usec
TE                   298.0 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1            300.1318534 MHz
NUC1                      1H
P1                    13.00 usec
PLW1           10.69999981 W

F2 - Processing parameters
SI                    65536
SF              300.1300128 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

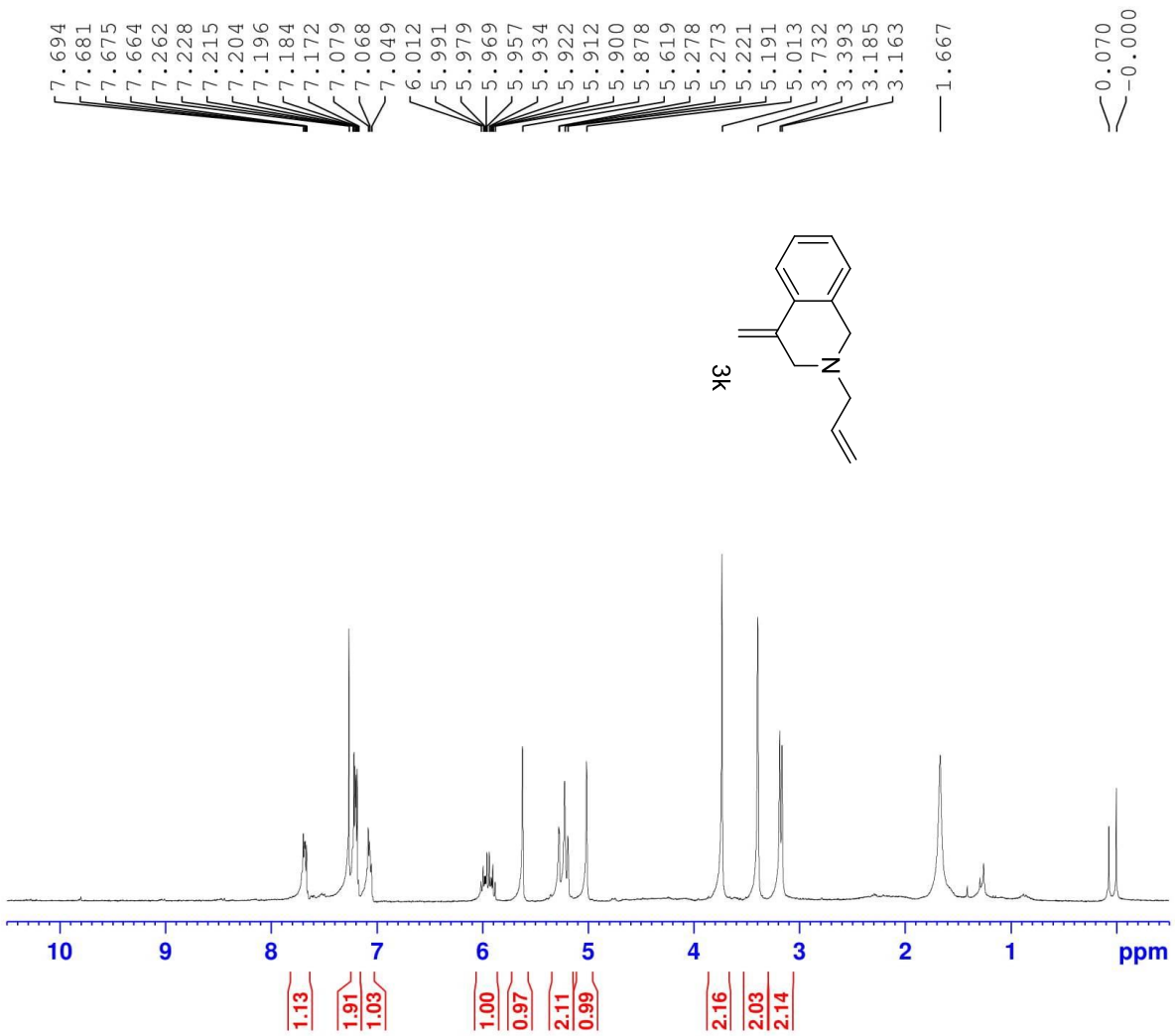



```
Current Data Parameters
NAME                 3688K
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20180614
Time                 19.30
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    2048
DS                       4
SWH              18028.846 Hz
FIDRES           0.275098 Hz
AQ               1.8175317 sec
RG                     912
DW                27.733 usec
DE                 6.50 usec
TE                 300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          75.4752949 MHz
NUC1                  13C
P1                  9.47 usec
PLW1         38.00000000 W

======== CHANNEL f2 ========
SFO2         300.1312005 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         10.69999981 W
PLW12         0.22325000 W
PLW13         0.11229000 W

F2 - Processing parameters
SI                   32768
SF            75.4677485 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

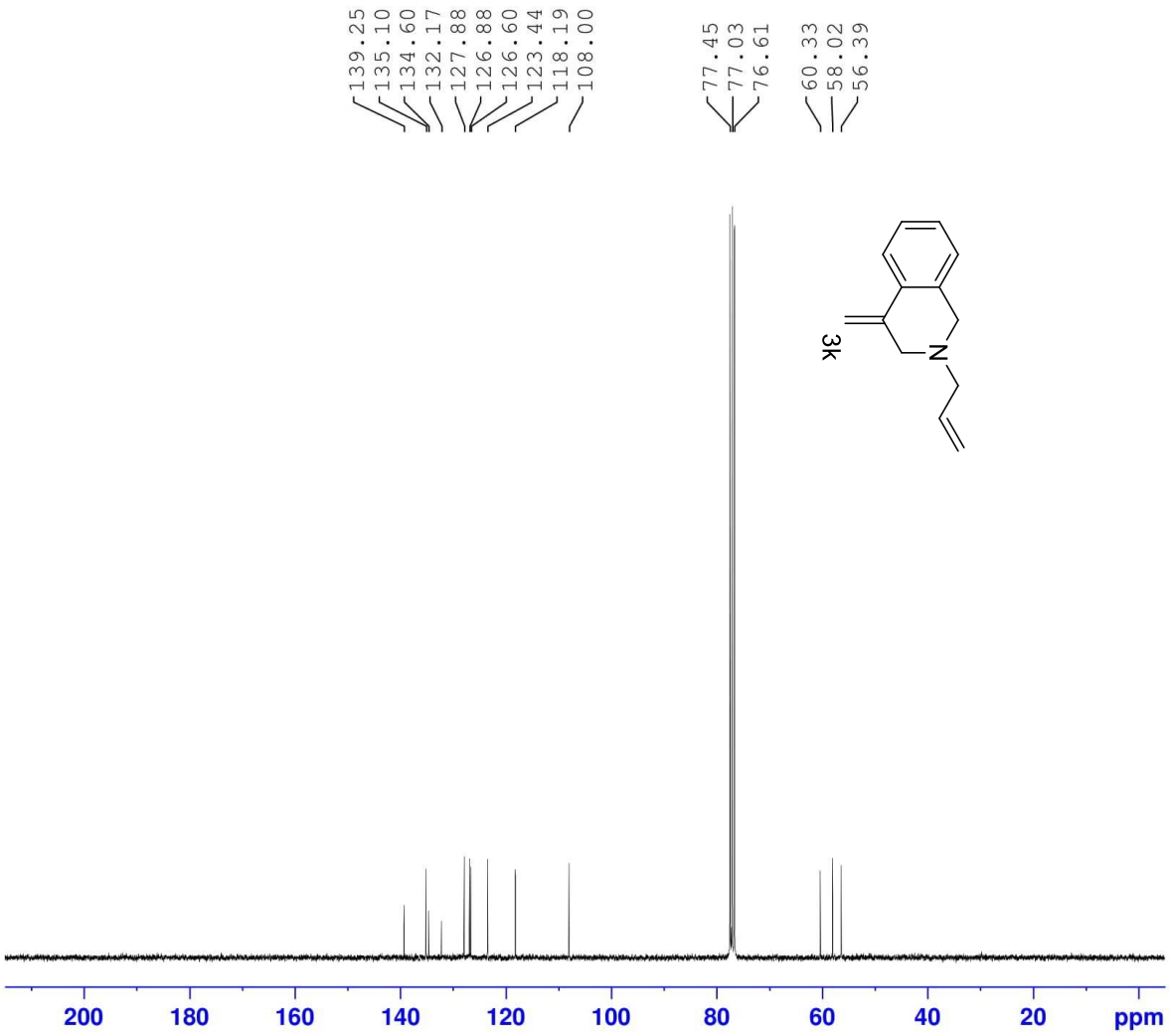



```
Current Data Parameters
NAME          H3339C19-R
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190625
Time               12.25
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    13
DS                     2
SWH             6009.615 Hz
FIDRES          0.091699 Hz
AQ              5.4525952 sec
RG                   128
DW                83.200 usec
DE                 6.50 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         300.1318534 MHz
NUC1                   1H
P1                 13.00 usec
PLW1         10.69999981 W

F2 - Processing parameters
SI                 65536
SF           300.1300129 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

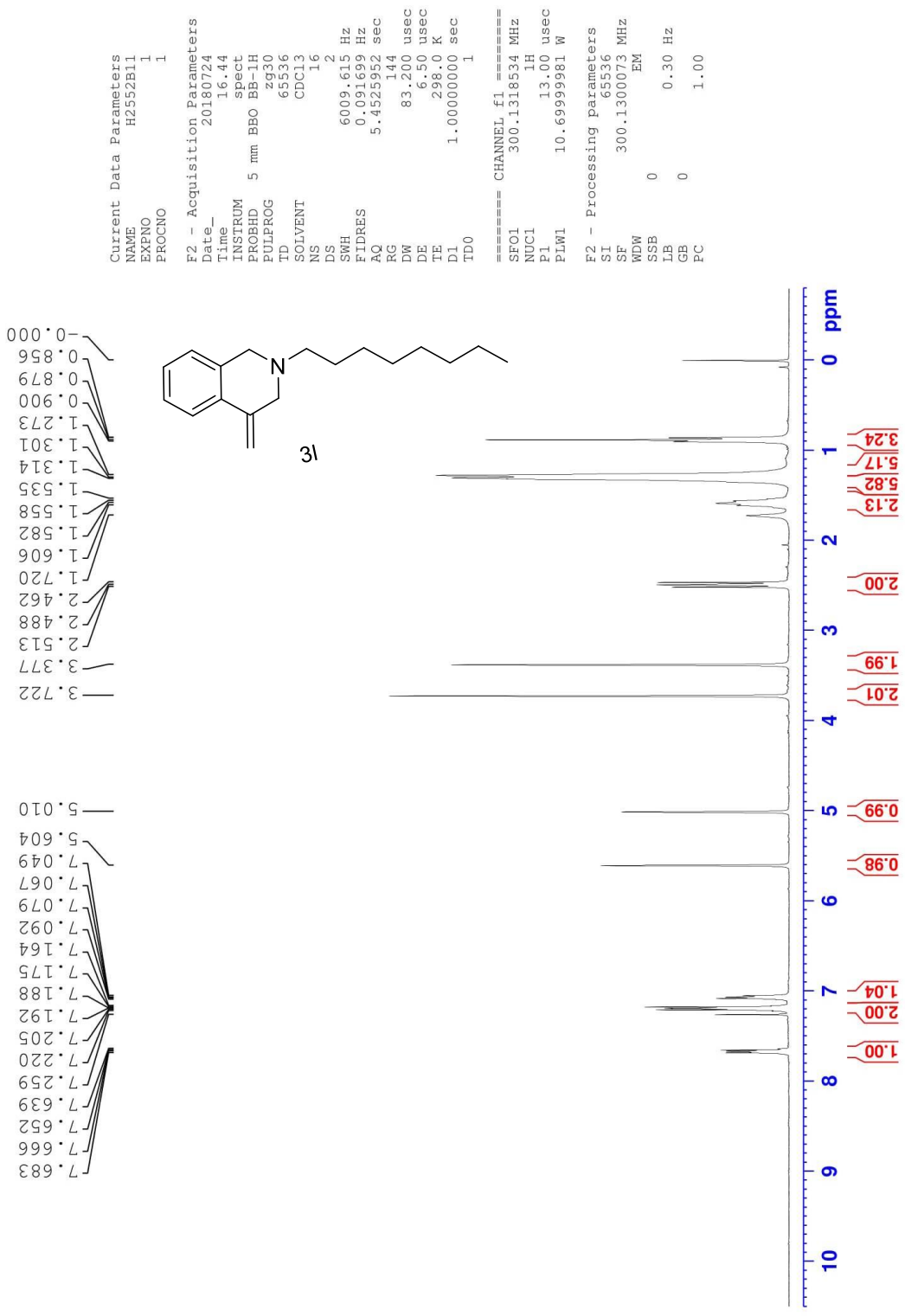

Current Data Parameters
NAME C3339C2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190628
Time 19.36
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.81753317 sec
RG 1150
DW 27.733 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 75.4752949 MHz
NUC1 13C
P1 9.47 usec
PLW1 38.00000000 W
======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 10.69999981 W
PLW12 0.22325000 W
PLW13 0.11229000 W
F2 - Processing parameters
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
0.02
20.47
53.32
55.35
76.61
77.03
77.46
108.42
116.99
123.79
126.68
126.76
128.05
129.32
129.70
132.47
134.42
138.87
148.15
N
3j
ppm
200
180
160
140
120
100
80
60
40
20

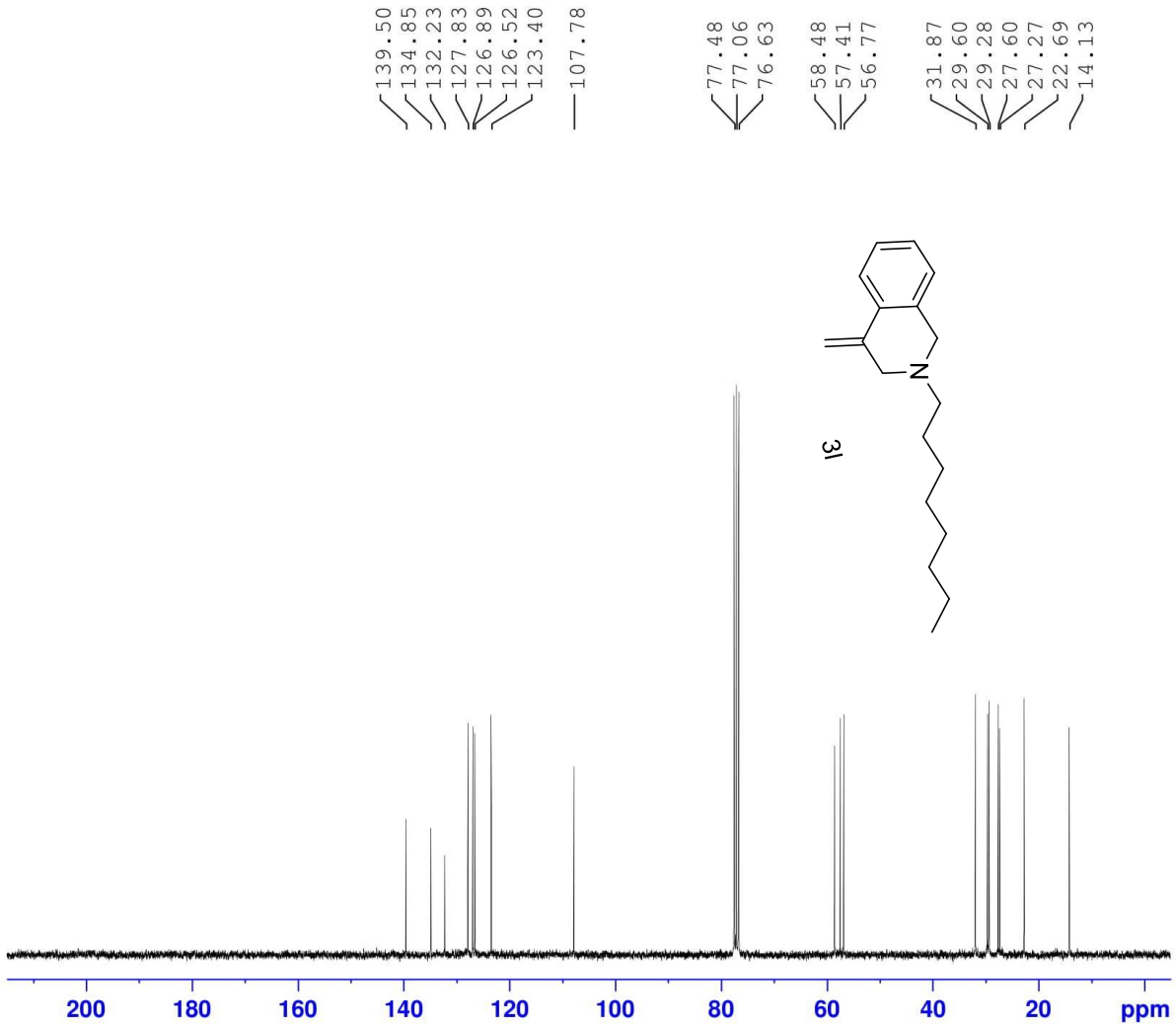



```
Current Data Parameters
NAME                  3692D
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20180612
Time                  16.58
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                6009.615 Hz
FIDRES            0.091699 Hz
AQ                5.4525952 sec
RG                      203
DW                   83.200 usec
DE                    6.50 usec
TE                   298.0 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1            300.1318534 MHz
NUC1                    1H
P1                   13.00 usec
PLW1           10.69999981 W

F2 - Processing parameters
SI                    65536
SF              300.1300060 MHz
WDW                     EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

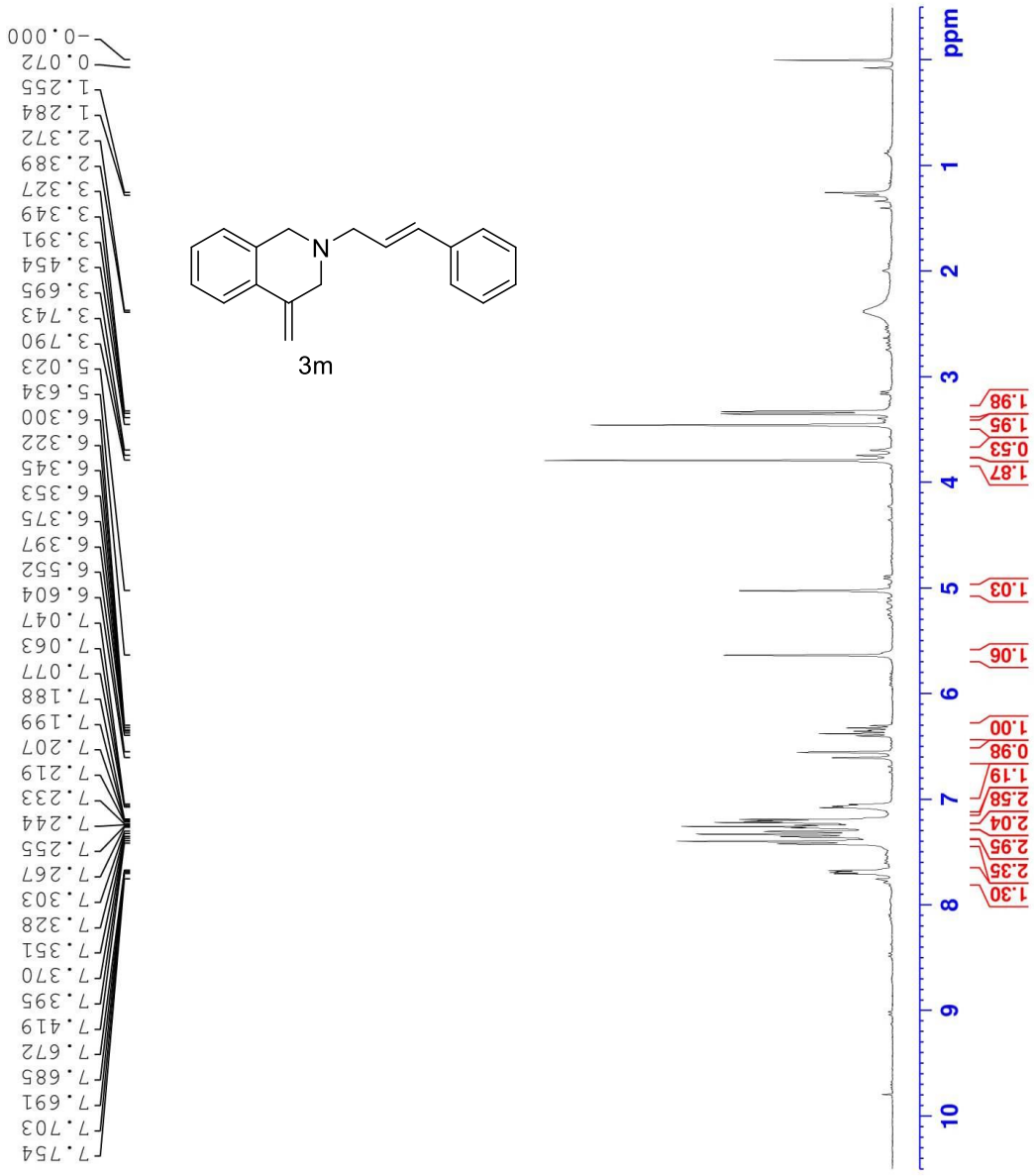



```
Current Data Parameters
NAME                  C2552B5
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_                20180703
Time                    19.29
INSTRUM                 spect
PROBHD    5 mm BBO BB-1H
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                        2048
DS                           4
SWH                  18028.846 Hz
FIDRES                0.275098 Hz
AQ                    1.8175317 sec
RG                         812
DW                      27.733 usec
DE                       6.50 usec
TE                      300.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1               75.4752949 MHz
NUC1                      13C
P1                       9.47 usec
PLW1               38.00000000 W

======== CHANNEL f2 ========
SFO2              300.1312005 MHz
NUC2                      1H
CPDPRG[2               waltz16
PCPD2                   90.00 usec
PLW2               10.69999981 W
PLW12               0.22325000 W
PLW13               0.11229000 W

F2 - Processing parameters
SI                       32768
SF                 75.4677485 MHz
WDW                         EM
SSB           0
LB                       1.00 Hz
GB            0
PC                       1.40
```

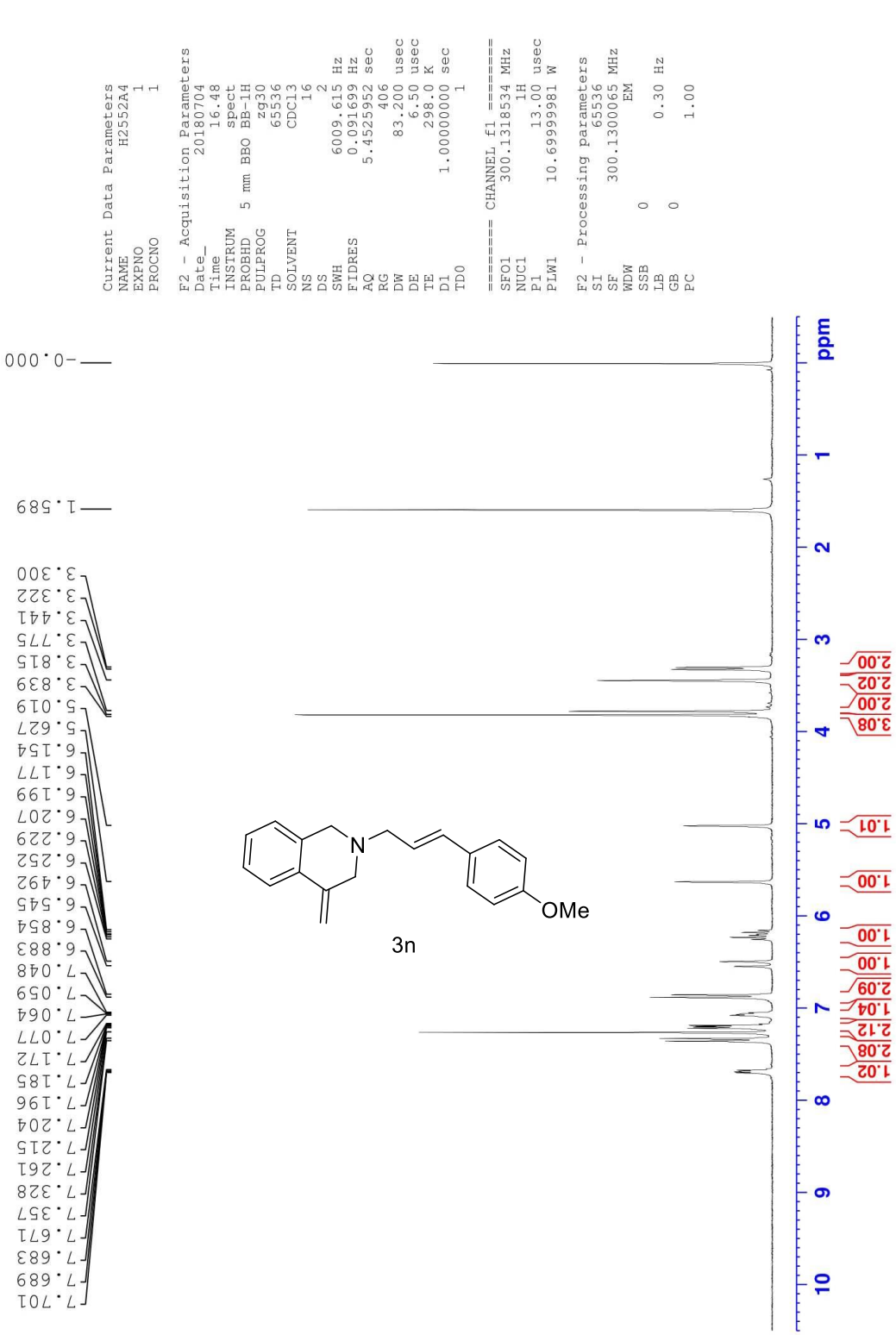

Current Data Parameters
NAME H2552B11
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180724
Time 16.44
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 144
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.69999981 W
F2 - Processing parameters
SI 65536
SF 300.1300073 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
3l
ppm
0
1
2
3
4
5
6
7
8
9
10
3.24
5.17
5.82
2.13
2.00
1.99
2.01
0.99
0.98
1.04
2.00
1.00
-0.000
0.856
0.879
0.900
1.273
1.301
1.314
1.535
1.558
1.582
1.606
1.720
2.462
2.488
2.513
3.377
3.722
5.010
5.604
7.049
7.067
7.079
7.092
7.164
7.175
7.188
7.192
7.205
7.220
7.259
7.639
7.652
7.666
7.683

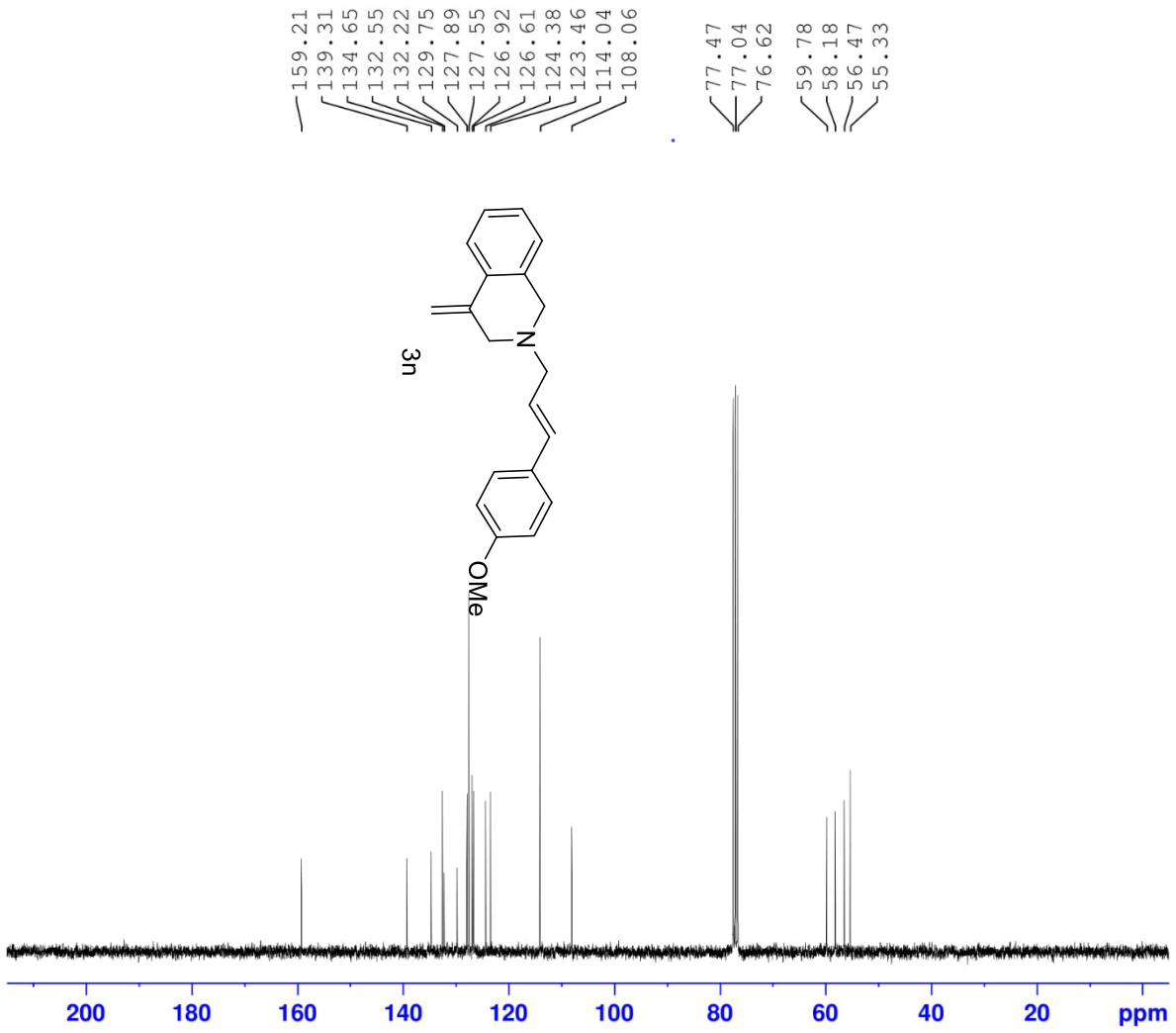



```
Current Data Parameters
NAME            C2552B11
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180725
Time               13.16
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   560
DS                     4
SWH            18028.846 Hz
FIDRES          0.275098 Hz
AQ             1.8175317 sec
RG                   912
DW                27.733 usec
DE                 6.50 usec
TE                300.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          75.4752949 MHz
NUC1                 13C
P1                  9.47 usec
PLW1        38.00000000 W

======== CHANNEL f2 ========
SFO2         300.1312005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2        10.69999981 W
PLW12        0.22325000 W
PLW13        0.11229000 W

F2 - Processing parameters
SI                 32768
SF            75.4677485 MHz
WDW                  EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.40
```


Current Data Parameters
NAME 3679P
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180606
Time 17.19
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 161
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.69999981 W
F2 - Processing parameters
SI 65536
SF 300.1300081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
N
3m
ppm
1.30
2.35
2.95
2.04
2.58
1.19
0.98
1.00
1.06
1.03
1.87
0.53
1.95
1.98


Current Data Parameters
NAME C2552B4
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180702
Time 18.18
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 912
DW 27.733 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 75.4752949 MHz
NUC1 13C
P1 9.47 usec
PLW1 38.00000000 W
======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 10.69999981 W
PLW12 0.22325000 W
PLW13 0.11229000 W
F2 - Processing parameters
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1.04
56.47
58.19
59.63
76.61
77.03
77.45
3m
108.14
123.46
126.39
126.64
126.92
127.58
127.92
128.61
132.18
133.11
134.53
136.91
139.20
ppm
200
180
160
140
120
100
80
60
40
20


Current Data Parameters
NAME H2552A4
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180704
Time 16.48
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 406
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.69999981 W
F2 - Processing parameters
SI 65536
SF 300.1300065 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
0.000
1.589
3.300
3.322
3.441
3.775
3.815
3.839
5.019
5.627
6.154
6.177
6.199
6.207
6.229
6.252
6.492
6.545
6.854
6.883
7.048
7.059
7.064
7.077
7.172
7.185
7.196
7.204
7.215
7.261
7.328
7.357
7.671
7.683
7.689
7.701
N
OMe
3n
ppm
1 2 3 4 5 6 7 8 9 10
2.00
2.02
2.00
3.08
1.01
1.00
1.00
1.00
2.09
1.04
2.12
2.08
1.02

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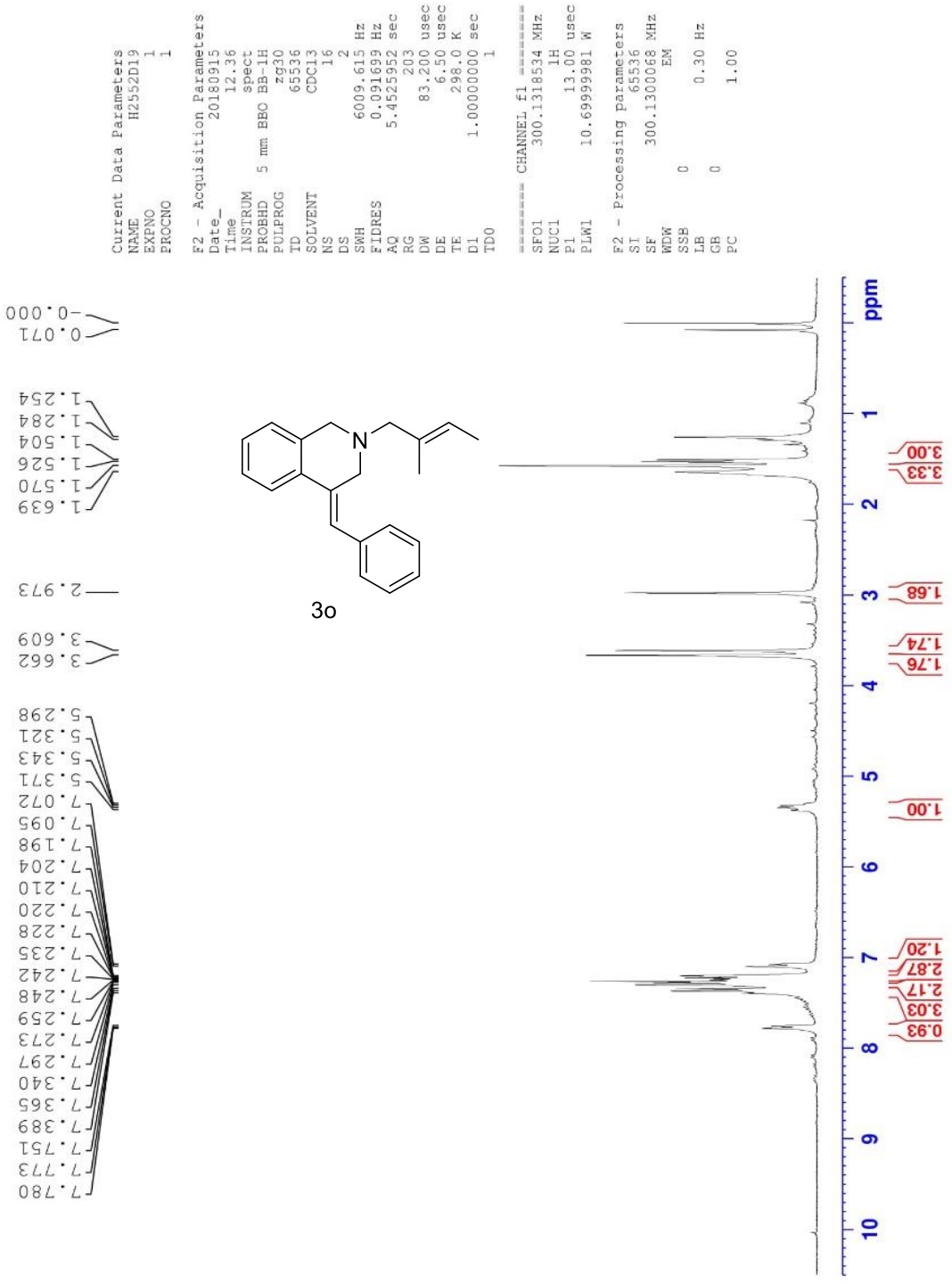
Current Data Parameters
NAME                 C2552B6
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_               20180705
Time                   17.22
INSTRUM                spect
PROBHD    5 mm BBO BB-1H
PULPROG                zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       400
DS                         4
SWH                18028.846 Hz
FIDRES             0.275098 Hz
AQ                 1.8175317 sec
RG                       912
DW                    27.733 usec
DE                     6.50 usec
TE                     300.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1              75.4752949 MHz
NUC1                     13C
P1                     9.47 usec
PLW1             38.00000000 W

======== CHANNEL f2 ========
SFO2             300.1312005 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                 90.00 usec
PLW2             10.69999981 W
PLW12             0.22325000 W
PLW13             0.11229000 W

F2 - Processing parameters
SI                       32768
SF                75.4677485 MHz
WDW                        EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```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EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180915
Time 12.36
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 203
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.69999981 W
F2 - Processing parameters
SI 65536
SF 300.1300068 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
-0.000
0.071
1.254
1.284
1.504
1.526
1.570
1.639
2.973
3.609
3.662
5.298
5.321
5.343
5.371
7.072
7.095
7.198
7.204
7.210
7.220
7.228
7.235
7.242
7.248
7.259
7.273
7.297
7.340
7.365
7.389
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7.773
7.780
N
3o
ppm
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2
3
4
5
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7
8
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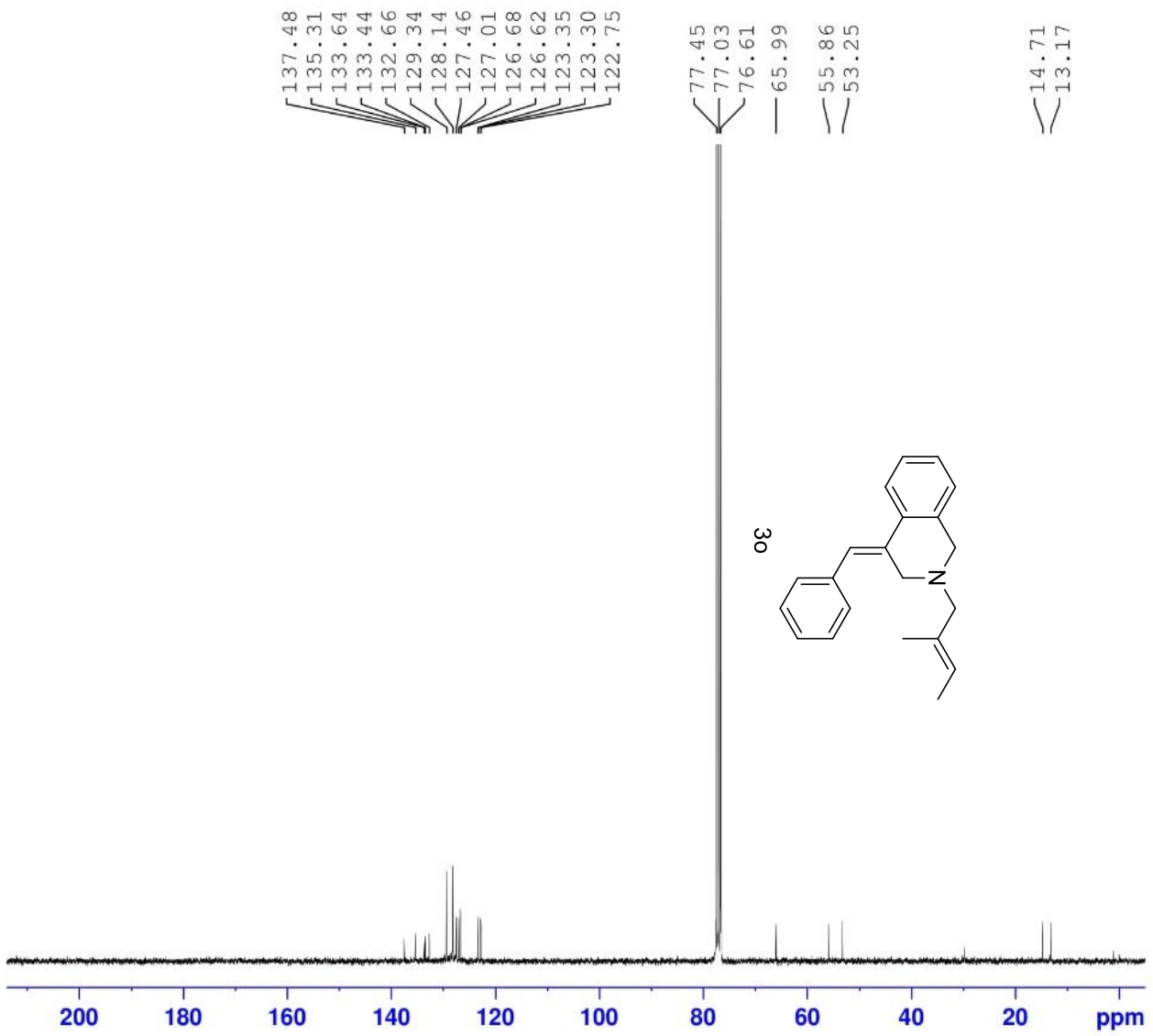
0.93

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Current Data Parameters
NAME                  C2552D7
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_                20180915
Time                    19.01
INSTRUM                 spect
PROBHD    5 mm BBO BB-1H
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                       3072
DS                          4
SWH                 18028.846 Hz
FIDRES              0.275098 Hz
AQ                  1.8175317 sec
RG                        812
DW                     27.733 usec
DE                      6.50 usec
TE                     300.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1               75.4752949 MHz
NUC1                      13C
P1                       9.47 usec
PLW1               38.00000000 W

======== CHANNEL f2 ========
SFO2              300.1312005 MHz
NUC2                       1H
CPDPRG[2               waltz16
PCPD2                   90.00 usec
PLW2               10.69999981 W
PLW12               0.22325000 W
PLW13               0.11229000 W

F2 - Processing parameters
SI                        32768
SF                 75.4677485 MHz
WDW                          EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.40
```

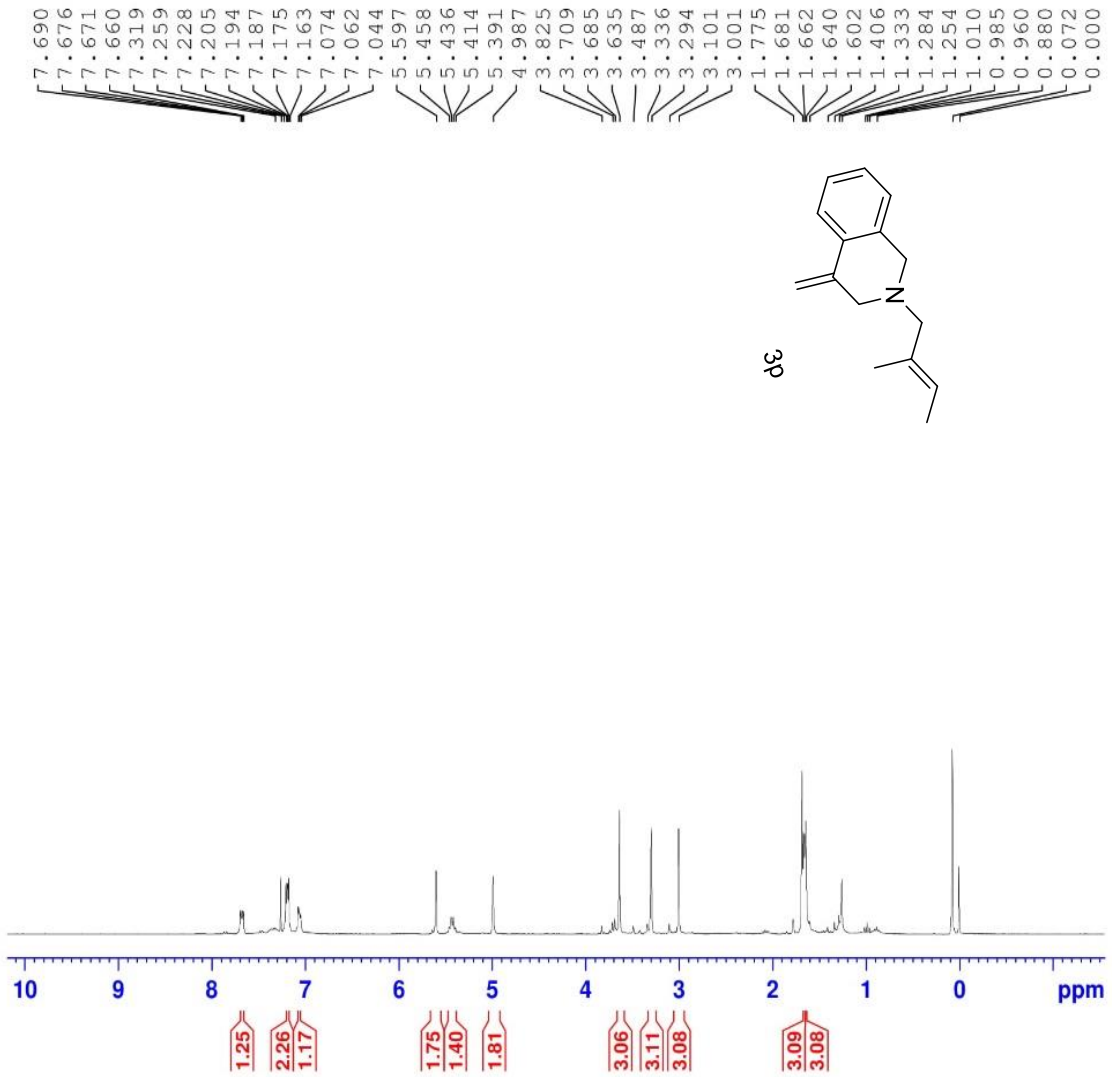


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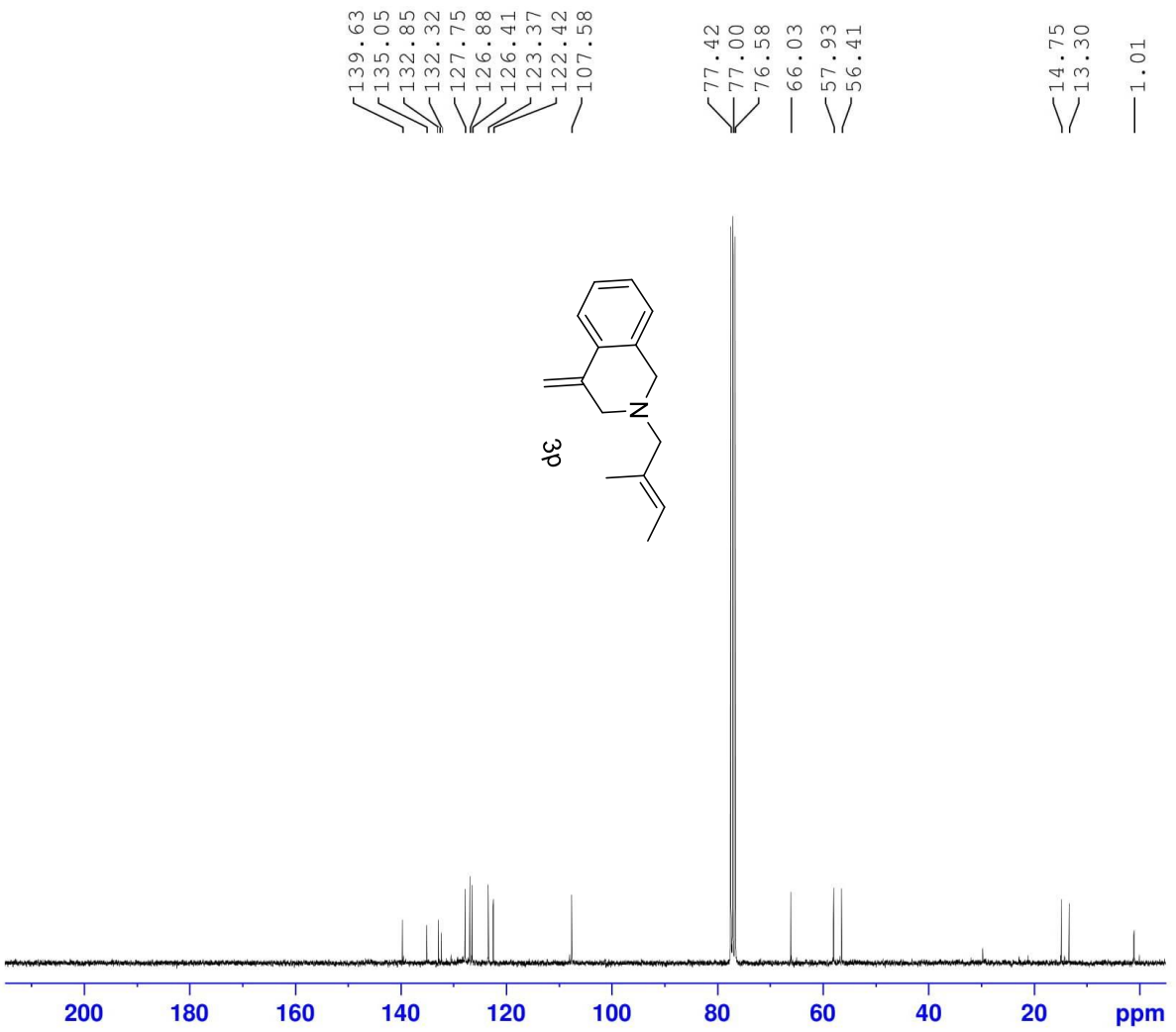
NAME                  H2552F1
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_                20181011
Time                    16.21
INSTRUM                 spect
PROBHD    5 mm BBO BB-1H
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                         16
DS                          2
SWH                  6009.615 Hz
FIDRES               0.091699 Hz
AQ                 5.4525952 sec
RG                        181
DW                     83.200 usec
DE                      6.50 usec
TE                     298.0 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1            300.1318534 MHz
NUC1                      1H
P1                     13.00 usec
PLW1             10.69999981 W

F2 - Processing parameters
SI                     65536
SF              300.1300071 MHz
WDW                       EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```

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EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_                20181012
Time                    12.12
INSTRUM                 spect
PROBHD   5 mm BBO BB-1H
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDC13
NS                        2048
DS                           4
SWH                  18028.846 Hz
FIDRES                0.275098 Hz
AQ                   1.8175317 sec
RG                         912
DW                      27.733 usec
DE                        6.50 usec
TE                       300.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1               75.4752949 MHz
NUC1                      13C
P1                       9.47 usec
PLW1               38.00000000 W

======== CHANNEL f2 ========
SFO2              300.1312005 MHz
NUC2                      1H
CPDPRG[2               waltz16
PCPD2                   90.00 usec
PLW2               10.69999981 W
PLW12               0.22325000 W
PLW13               0.11229000 W

F2 - Processing parameters
SI                       32768
SF                 75.4677509 MHz
WDW                         EM
SSB             0
LB                       1.00 Hz
GB              0
PC                       1.40
```

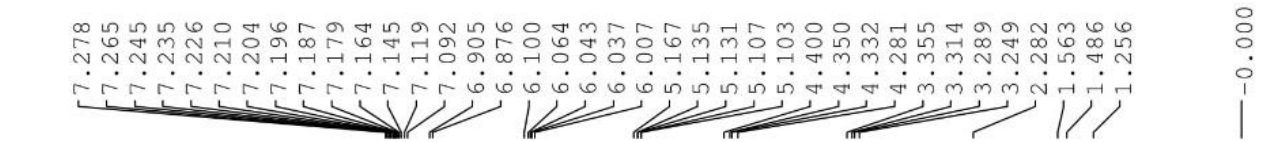

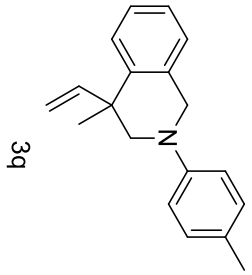

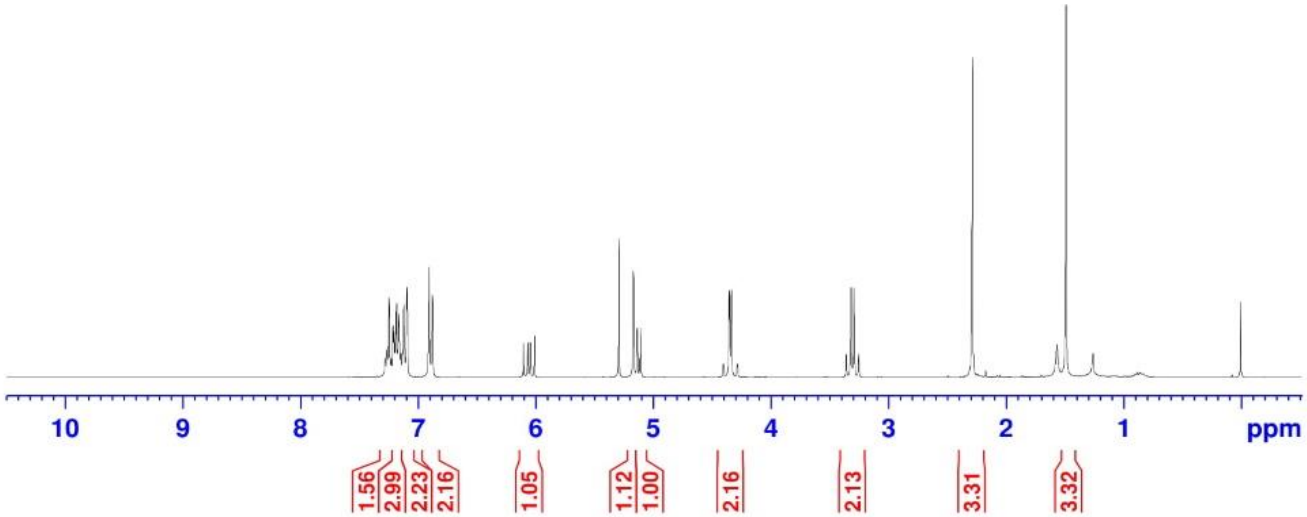


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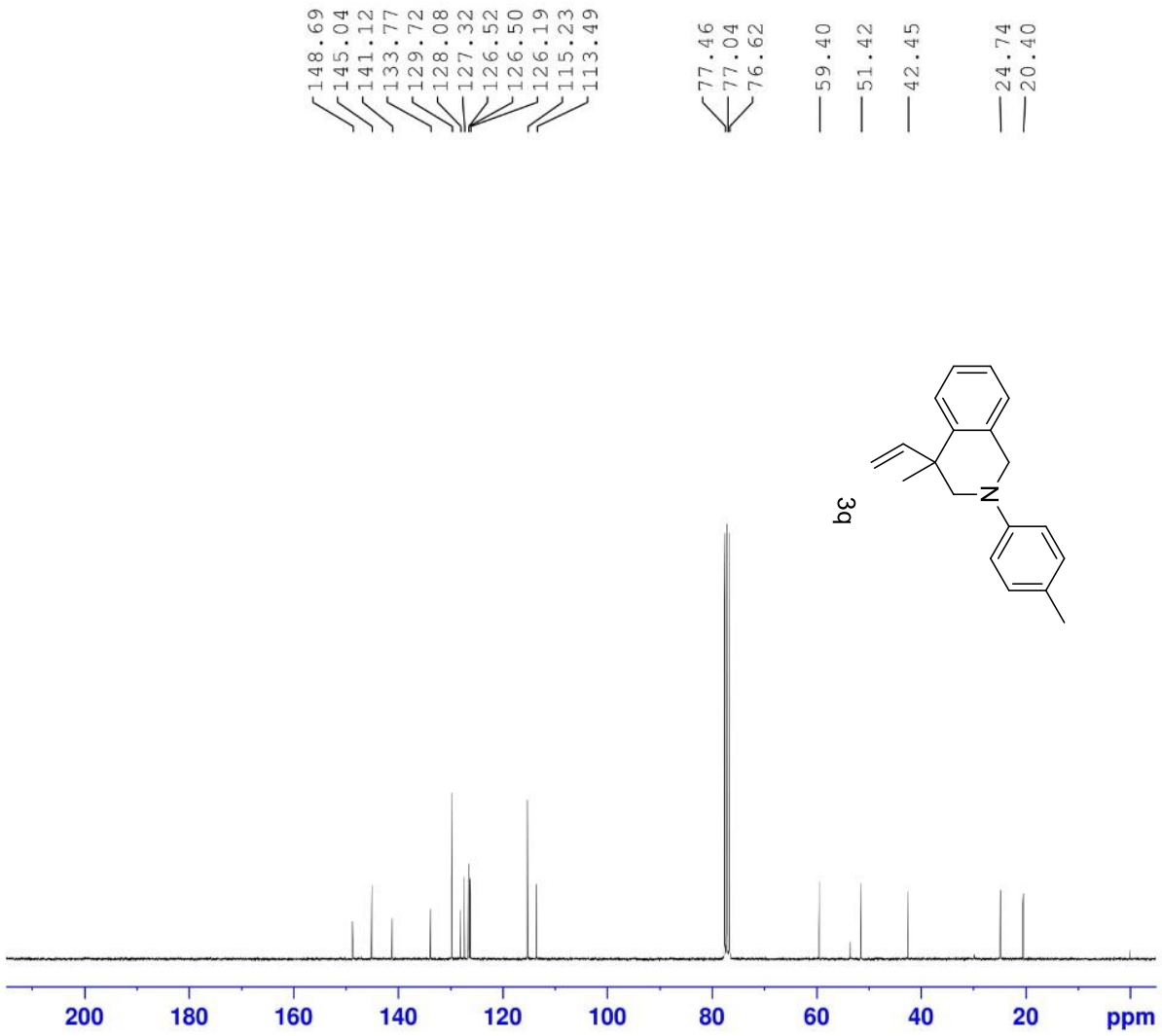
Current Data Parameters
NAME          H3339A12-R
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190415
Time               13.50
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6009.615 Hz
FIDRES          0.091699 Hz
AQ              5.4525952 sec
RG                   203
DW                83.200 usec
DE                 6.50 usec
TE                298.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         300.1318534 MHz
NUC1                   1H
P1                 13.00 usec
PLW1        10.69999981 W

F2 - Processing parameters
SI                 65536
SF           300.1300114 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

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Current Data Parameters
NAME                 C3339B4
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_               20190415
Time                   20.40
INSTRUM                spect
PROBHD    5 mm BBO BB-1H
PULPROG              zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      3072
DS                         4
SWH               18028.846 Hz
FIDRES             0.275098 Hz
AQ                1.8175317 sec
RG                       724
DW                  27.733 usec
DE                   6.50 usec
TE                   300.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1             75.4752949 MHz
NUC1                    13C
P1                   9.47 usec
PLW1            38.00000000 W

======== CHANNEL f2 ========
SFO2            300.1312005 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                90.00 usec
PLW2            10.69999981 W
PLW12            0.22325000 W
PLW13            0.11229000 W

F2 - Processing parameters
SI                     32768
SF               75.4677485 MHz
WDW                       EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```
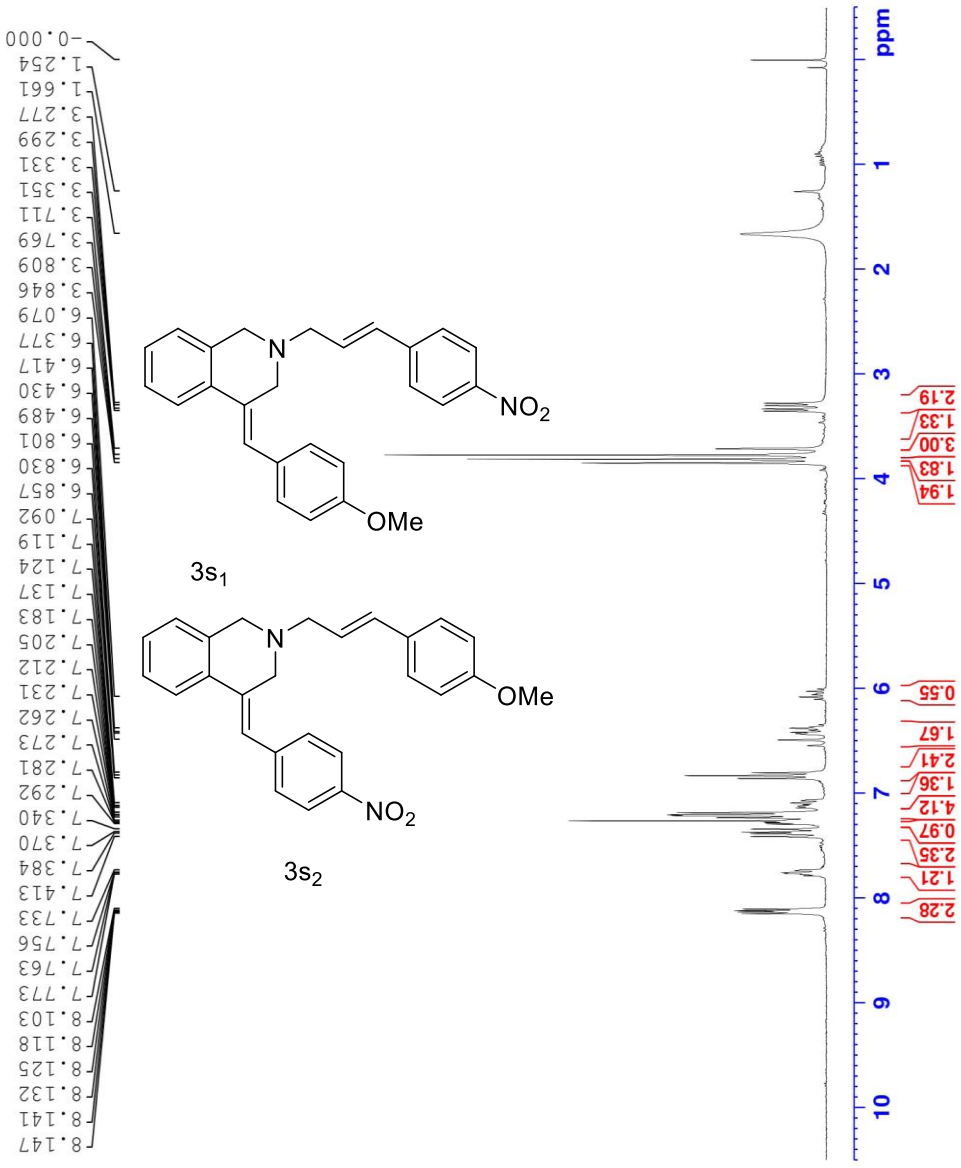
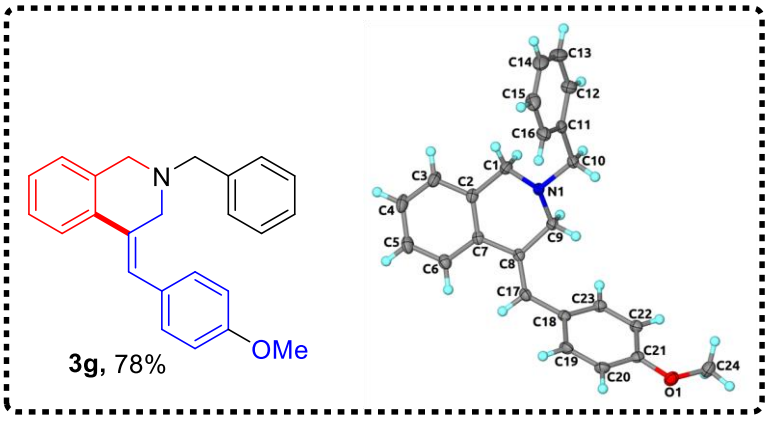


Current Data Parameters
NAME H3339b4
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190423
Time 12.20
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 181
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 13.00 usec
PLW1 10.69999981 W
F2 - Processing parameters
SI 65536
SF 300.1300062 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
ppm
1.94
1.83
3.00
1.33
2.19
0.55
1.67
2.41
1.36
4.12
0.97
2.35
1.21
2.28
3s1
3s2
N
OMe
NO2

1. Single crystal XRD analysis of compound 3g

Compound **3g** was dissolved in acetonitrile:ethanol (1:1 v/v) mixture and kept for solvent evaporation at room temperature. After three days, single crystals of **3g** were harvested and used for single crystal XRD studies.

X-ray data for the compound **3g** were collected at room temperature using a Bruker D8 Quest single crystal X-ray diffractometer equipped with microfocus Mo-Kα radiation (λ=0.71073Å) and Photon 100 detector. Preliminary lattice parameters and orientation matrices were obtained from four sets of frames. Unit cell dimensions were determined using 8290 reflections. Integration and scaling of intensity data were accomplished using SAINT program. The structure was solved using SHELXS-97 and refinement was carried out by full-matrix least-squares technique using SHELXL-2018/3. Anisotropic displacement parameters were included for all non-hydrogen atoms. All H atoms were positioned geometrically and treated as riding on their parent C atoms with C-H distances of 0.93--0.97 Å, and with $U_{iso}(H) = 1.2U_{eq}$ (C) or $1.5U_{eq}$ for methyl atoms. Crystal data and refinement parameters for compound **3g** are summarized in Table S1. CCDC 1912875 contains the supplementary crystallographic data for this paper which can be obtained free of charge at https://summary.ccdc.cam.ac.uk/structure-summary-form or from the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0) 1223 336 033; email: deposit@ccdc.cam.ac.uk.



X-ray crystal structure of **3g** compound. Displacement ellipsoids are drawn at the 30% probability level.

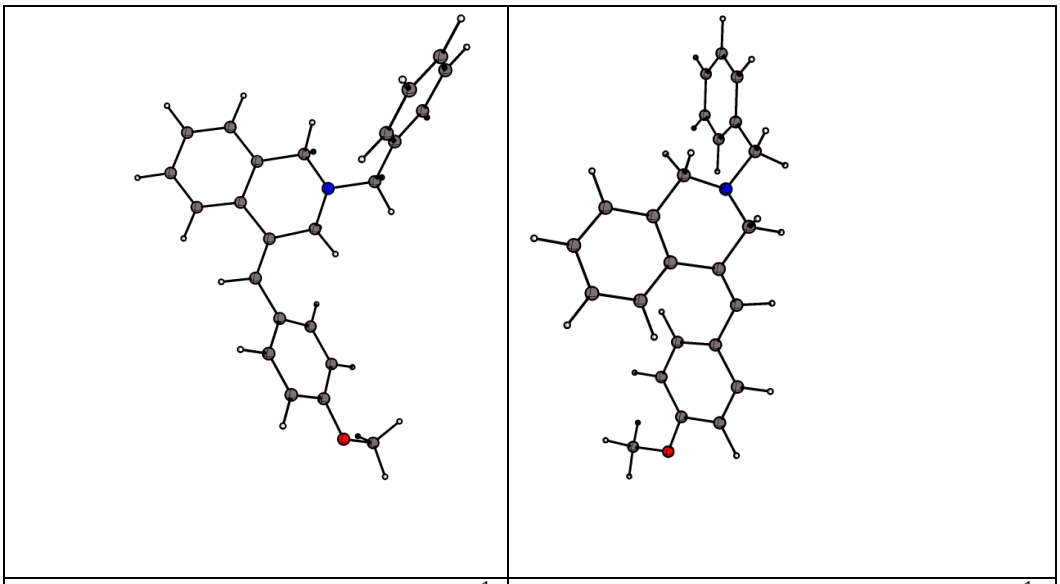
Table S1. Crystal Data Collection and Refinement Parameters for compound 3g.

Chemical formula	$C_{24}H_{23}NO$
Fw; *F*(000)	341.43; 364
T (K)	293(2)
wavelength (Å)	0.71073
Crystal system	Triclinic
space group	P-1
a (Å)	6.1269(7)
b (Å)	9.0770(12)
c (Å)	17.366(2)
α (deg)	79.554(4)
β (deg)	84.737(4)
γ (deg)	81.243(5)
Z	2
V (Å^3)	936.6(2)
ρ_{calcd} (g·cm^{-3})	1.211
μ (mm^{-1})	0.073
θ range (deg); completeness	2.304 – 27.496; 0.999
collected reflections; R_σ	20789; 0.0400
unique reflections; R_{int}	20789; 0.0473
R1[a]; wR2[b] [I > 2σ(I)]	0.0466; 0.1479
R1; wR2 [all data]	0.0681; 0.1672
GOF	1.158
largest diff peak and hole	0.170 and -0.196

2. Quantum chemical calculation.

All the quantum chemical calculation was carried using Gaussian09 program with B3LYP/6-311++G(d,p) level of theory. The X-ray geometries of compound **3g** were taken for structural optimization. The *trans* configuration of compound **3g** was modeled

using Gaussview from the *cis* conformer of the X-ray structure. The cis and trans conformers were fully optimized without any geometrical constraints followed by vibrational frequency calculation. The frequency calculation revealed that no negative frequency was obtained for *cis* and *trans* conformers. This is indicating that both conformers in the energy minima on their potential energy surface. It is also indicating that the cis conformer ((*Z*)-isomer) is found to be 2.6 kcal mol^{-1} more stable form than the corresponding trans conformer ((*E*)-isomer). The optimized structures of these conformers are depicted in Fig. S1.



***cis* conformer: -664297.3** kcal mol^{-1}	***trans* conformer: -664294.7** kcal mol^{-1}

Fig. S1. Optimized structures of cis and trans conformers of compound **3g**.

Coordinates for optimized trans conformer (compound 3g)

C	-2.550688000	2.676856000	1.053462000
C	-2.785183000	1.312611000	1.239296000
C	-1.716411000	0.434140000	1.342270000
C	-0.387123000	0.888014000	1.260616000
C	-0.158123000	2.270804000	1.120802000
C	-1.243698000	3.144797000	1.003741000
C	0.780324000	-0.008823000	1.414232000
C	2.008046000	0.711368000	1.929987000
N	2.288349000	1.848695000	1.049430000
C	1.238158000	2.854316000	1.157282000
C	0.866866000	-1.324777000	1.133759000
C	3.618308000	2.415491000	1.259069000
C	4.044284000	3.370133000	0.159312000

C	3.903763000	3.011230000	-1.186383000
C	4.329799000	3.869120000	-2.196723000
C	4.905366000	5.100166000	-1.878022000
C	5.048260000	5.466588000	-0.542207000
C	4.616721000	4.606044000	0.468084000
C	-0.083174000	-2.236671000	0.467358000
C	-0.779141000	-1.886541000	-0.694758000
C	-1.623316000	-2.786684000	-1.343497000
C	-1.786076000	-4.077944000	-0.833229000
C	-1.083790000	-4.455264000	0.317259000
C	-0.241594000	-3.550628000	0.944365000
O	-2.588340000	-5.035255000	-1.384493000
C	-3.325767000	-4.711612000	-2.555120000
H	-3.380493000	3.368803000	0.962394000
H	-3.800092000	0.937607000	1.310316000
H	-1.906491000	-0.618706000	1.501308000
H	-1.056003000	4.207388000	0.881317000
H	2.869586000	0.041967000	1.918889000
H	1.853831000	1.042979000	2.976418000
H	1.342635000	3.422255000	2.105612000
H	1.358378000	3.579791000	0.348123000
H	1.802485000	-1.805940000	1.415340000
H	4.325071000	1.579166000	1.294620000
H	3.692107000	2.932462000	2.234572000
H	3.446138000	2.059194000	-1.431075000
H	4.213938000	3.577857000	-3.235072000
H	5.236715000	5.767728000	-2.665623000
H	5.489472000	6.423064000	-0.284101000
H	4.724743000	4.900368000	1.507472000
H	-0.654798000	-0.893707000	-1.110111000
H	-2.135048000	-2.473343000	-2.243790000
H	-1.209250000	-5.462380000	0.696566000
H	0.301376000	-3.862340000	1.830860000
H	-3.891409000	-5.607076000	-2.807608000
H	-2.662159000	-4.455699000	-3.388339000
H	-4.019552000	-3.883312000	-2.374478000

Total energy: -1058.6207130 au

Number of imaginary frequency: 0

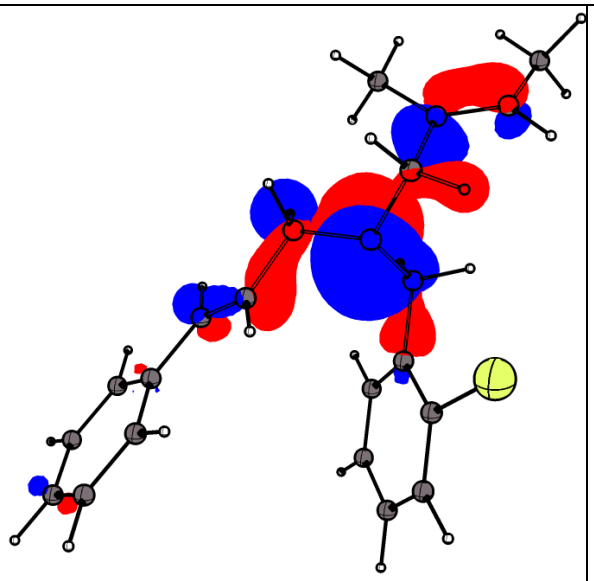
Coordinates for optimized cis conformer (compound 3g)

O	8.196154000	5.959044000	6.037727000
N	6.314354000	2.752951000	12.835661000
C	8.562340000	3.209714000	9.180835000
C	6.555344000	2.448207000	11.424615000
H	6.472292000	3.375929000	10.859438000
H	5.783596000	1.753621000	11.031172000
C	7.936840000	1.857038000	11.247206000
C	8.313069000	0.838225000	12.254364000
C	9.465610000	4.958253000	7.736137000
H	10.277338000	5.611212000	7.438466000
C	8.790787000	2.266960000	10.284397000
C	7.365367000	3.291506000	8.457398000
H	6.551305000	2.615556000	8.688853000
C	8.249614000	5.040142000	7.044821000
C	6.297221000	1.535930000	13.633623000
H	5.400928000	0.924185000	13.394763000
H	6.217049000	1.806045000	14.689117000
C	5.109435000	3.557936000	13.026282000
H	4.193297000	2.976970000	12.807661000
H	5.144513000	4.371808000	12.293826000
C	4.998372000	4.154282000	14.416644000
C	7.199609000	4.192751000	7.404776000
H	6.259511000	4.209917000	6.869658000
C	9.413217000	-0.023191000	12.083796000
H	10.001259000	0.033124000	11.176041000
C	7.530781000	0.691472000	13.416224000
C	9.615025000	4.054671000	8.773291000
H	10.564880000	4.003332000	9.295486000
C	7.876536000	-0.265030000	14.374335000
H	7.270734000	-0.356652000	15.270805000
C	3.801269000	4.080303000	15.132255000
H	2.952378000	3.558181000	14.701543000
C	6.085495000	4.822904000	14.991682000
H	7.021618000	4.870012000	14.446745000
C	8.979619000	-1.091992000	14.199880000
H	9.235264000	-1.827549000	14.954149000
C	9.748671000	-0.969762000	13.041329000
H	10.601370000	-1.620017000	12.880658000
C	3.684047000	4.666609000	16.393192000
H	2.746939000	4.598581000	16.934842000
C	6.991248000	6.083373000	5.294541000
H	7.172353000	6.869768000	4.563678000

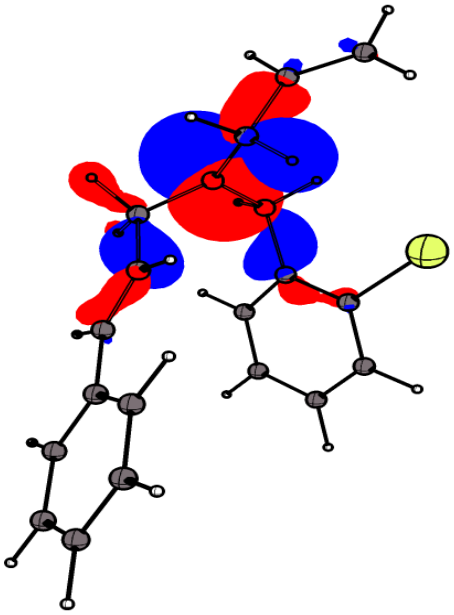
H	6.152850000	6.372242000	5.937732000
H	6.746086000	5.152511000	4.771672000
C	4.770810000	5.330518000	16.956525000
H	4.684583000	5.784499000	17.937460000
C	5.973061000	5.405158000	16.251379000
H	6.824223000	5.919184000	16.684641000
H	9.807640000	1.886468000	10.327276000

Total energy: -1058.6248977 au

Number of imaginary frequency: 0



Highest occupied molecular orbitals of **1o.**



Highest occupied molecular orbitals of **1m.**

Fig. S2. Highest occupied molecular orbitals of **1o** and **1m**

Coordinates for optimized structure of 1o

Br	-0.861792540	-1.349154505	-2.232591172
C	-2.290323013	-2.336275347	3.884725883
C	-1.388357262	-0.909706847	5.599018304
C	-2.531886104	-1.103810998	6.370174392
C	-3.432178808	-2.530219042	4.652249153
C	-0.013948254	-1.273336920	3.572498548
C	-3.561089211	-1.915597574	5.899846204
C	0.291223734	-1.728814892	2.352134599
C	4.227857921	-0.316347385	-1.840671960

C	-1.242492147	-1.518143253	4.341935619
C	1.612612187	-1.485201583	1.670942528
C	-2.274125405	1.548005863	1.180614011
C	-3.196929140	0.941205710	0.333189559
C	-2.754685273	0.074346535	-0.662929360
C	-0.918403076	1.274871481	1.030466973
C	-1.392545917	-0.182679786	-0.794668560
C	3.878630730	-0.896717096	-0.683707039
C	1.055441012	0.162178753	-0.088013855
C	-0.438964459	0.397990082	0.049845546
C	2.582496034	-1.696603528	-0.616742547
H	2.163903695	-0.705383335	2.226049912
H	2.207513669	-2.402183389	1.756347121
H	-0.403079440	-2.351106783	1.794366914
H	2.176559451	-1.785128273	-1.628402138
H	1.339171486	0.355634266	-1.124903659
H	1.574710105	0.920832587	0.520389121
H	0.715674954	-0.639118474	4.075032220
H	-4.227076692	-3.166266314	4.278167427
H	-4.452740149	-2.071435988	6.496468416
H	-2.617187169	-0.621803419	7.337922315
H	-0.590364374	-0.276540228	5.974121046
H	-2.212020867	-2.826782704	2.921708779
H	-2.607499976	2.225571049	1.957962208
H	-4.257248346	1.140463138	0.438206416
H	-3.459108580	-0.392929967	-1.339113356
H	3.547865659	-0.444933577	-2.682110015
H	2.802431052	-2.715135745	-0.277246218
N	1.501232659	-1.189794506	0.244269641
H	-0.200854754	1.743089829	1.696033155
C	5.450582445	0.498242960	-2.151096659
C	4.703230751	-0.836815490	0.578880857
H	6.002888286	0.061337756	-2.990660458
H	5.170831104	1.512615203	-2.458339790
H	6.136591056	0.586197055	-1.308093647
H	5.701494113	-0.432526019	0.410501276
H	4.222828753	-0.216903636	1.343330364
H	4.817707834	-1.836156004	1.012891743

Total energy: -3443.7649532 au

Number of imaginary frequency: 0

Coordinates for optimized structure of 1m

Br	-0.433432203	-0.855990223	-1.697191989
C	-1.865796619	-2.928972546	3.512753711
C	-2.345781768	-1.186203287	5.099335194
C	-3.489438093	-1.867154705	5.509483472
C	-3.007144027	-3.609227878	3.919436990
C	-0.316693798	-0.934093276	3.703799541
C	-3.826755479	-3.083216998	4.920476649
C	0.600865764	-1.256400496	2.785700441
C	3.603900476	-1.502620828	-1.968147791
C	-1.510222639	-1.699963264	4.094936894
C	1.833561072	-0.431793014	2.483457236
C	-1.843639787	2.184268235	1.590299275
C	-2.766674461	1.479214763	0.823218323
C	-2.317312360	0.572680159	-0.132208782
C	-0.483997759	1.960689265	1.405600815
C	-0.949567456	0.367455817	-0.297788669
C	3.638994564	-1.093733283	-0.702153983
C	1.523154594	0.864597539	0.356430041
C	0.007903550	1.034420779	0.474338693
C	2.597470157	-1.416972803	0.337612751
H	1.748282238	0.547786481	2.965878711
H	2.699289601	-0.924781323	2.948698850
H	0.510604732	-2.183282526	2.224356888
H	1.776377623	-1.981133907	-0.127072083
H	1.801468356	0.769992236	-0.694794202
H	1.960697594	1.806695516	0.711398440
H	-0.190118935	0.005947530	4.239507007
H	-3.261086077	-4.555469746	3.454195042
H	-4.715930857	-3.617198536	5.235877508
H	-4.115900182	-1.447274524	6.288848527
H	-2.090537614	-0.238706381	5.563389329
H	-1.247194516	-3.357133705	2.732777668
H	-2.179886187	2.906296047	2.325560254
H	-3.831020997	1.636486421	0.954223369
H	-3.022014898	0.033919247	-0.752338037
H	4.401233708	-1.266701270	-2.664086677
H	2.776249939	-2.090631861	-2.352494334
H	3.057029170	-2.087015405	1.075224711

N	2.164371536	-0.234252782	1.077448335
H	4.474151804	-0.492426954	-0.347894865
H	0.232539590	2.519699384	1.999212364

Total energy: -3365.1059389 au

Number of imaginary frequency: 0