Electronic Supplementary Material (ESI) for RSC Advances.

Ring opening 1,3-arylboration of non-activated cyclopropanes mediated by BCl_3

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Supporting Information

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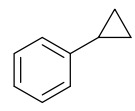
1. General

Melting points were measured by BÜCHI B-545 and all melting points were uncorrected. ^{1}H-NMR and ^{13}C-NMR spectra were measured by JEOL JNM-ECS 400, JEOL ECS 300 or JEOL JNM-LA 500 spectrometers with tetramethylsilane as an internal standard. IR spectra were recorded by Shimadzu FTIR 8400 (ATR). High resolution mass spectra and elemental analysis were performed by the Elemental Analysis Section of Osaka University. Column chromatography was performed with SiO_2 (Merck Silica Gel 60 (230-400 mesh) or Kanto Chemical Silicagel 60 (spherical, 63-210 μm). Unless otherwise noted, materials were purchased from Aldrich Inc., Tokyo Chemical Industry, Kanto Kagaku, Wako Chemicals, and other commercial suppliers and were used without purification.

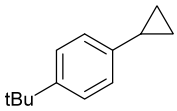
2. Preparation of arylcyclopropanes

1a is commercially available. **1b**, **1c**, **1e**, and **1f** were prepared according to the literature procedure.[1]

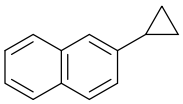
1d was prepared form 1-phenoxy-4-vinylbenzene.



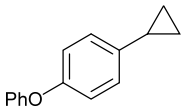
1a



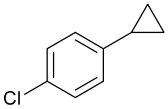
1b



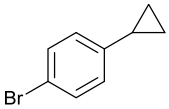
1c



1d

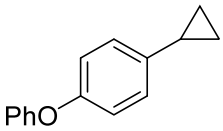


1e



1f

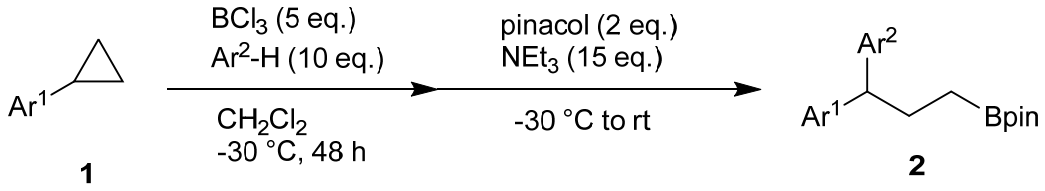
Preparation of 1d



To a solution of 1-phenoxy-4-vinylbenzene[2] (2.0 g, 10.2 mmol) and CH_2I_2 (2.7 ml, 33.5 mmol) in CH_2Cl_2 (0.5 M, 20 ml) was added Et_3Al (1 M in hexane solution, 34.0 ml, 34.0 mmol) at room temperature and the resulting solution was stirred at 30 ºC for 24 h. After completion of the reaction, the mixture was neutralized by 10% NaOH *aq*, and extracted with AcOEt. The organic layer was dried over Na_2SO_4, and the solvent was removed under reduced pressure. The residue was purified by SiO_2 column chromatography (Hexane to Hexane/AcOEt= 100/1) to give compound **1d** (1.43 g, 67%) as a colorless oil.

^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.35-7.27 (m, 2H), 7.10-6.88 (m, 7H), 1.94-1.83 (m, 1H), 0.98-0.90 (m, 2H), 0.69-0.62 (m, 2H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 157.8, 154.7, 138.9, 129.6, 126.9, 122.8, 119.1, 118.3, 14.8, 8.9; HRMS (MALDI-TOF) calcd for $C_{15}H_{14}O$ $[M]^+$: 210.1039, found 210.1035.

3. Ring-opening 1,3-arylboration (Table 2)

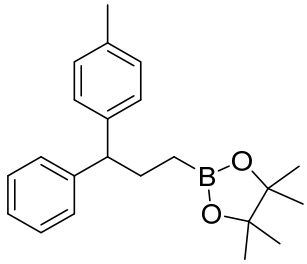


1 **2**

General procedure

To a solution of arylcyclopropane **1** (0.2 mmol) and arene (10 eq.) in CH_2Cl_2 (1 M) was added BCl_3 (5 eq., 1 M in CH_2Cl_2 solution) at -30℃. After the mixture was stirred at -30 °C for 48 h, pinacol (2 eq.) and Et_3N (15 eq.) solution in CH_2Cl_2 (1.0 mL) was added to the mixture and the reaction mixture was then stirred 6 h at rt. The resulting solution was diluted with AcOEt and filtrated through a short pad of celite. The filtrate was concentrated under reduced pressure, and the residue was purified by SiO_2 column chromatography to give **2**. Some product were obtained as inseparable o:p mixture or α:β, and ^1H and ^{13}C NMR spectrum of major isomer was reported.

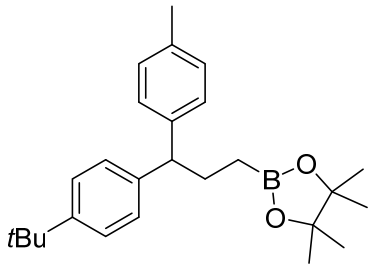
Compound 2a



Reaction was carried out according to the general procedure with **1a** (23.4 mg, 0.198 mmol), toluene (0.21 ml, 2.0 mmol), BCl_3 (1.0 ml, 1.0 mmol, 1 M in CH_2Cl_2 solution), pinacol (47.3 mg, 0.40 mmol), Et_3N (0.42 ml, 3.0 mmol), and CH_2Cl_2 (0.2 + 1.0 mL) to give compound **2a** (54.1 mg, 81%, >20:1) as colorless oil. SiO_2 Column chromatography: Hexane/AcOEt= 40/1.

^1H-NMR (300 MHz, $CDCl_3$): δ 7.28-7.20 (m, 4H), 7.17-7.03 (m, 5H), 3.80 (t, J = 7.7 Hz, 1H), 2.29 (s, 3H), 2.17-2.06 (m, 2H), 1.22 (s, 12H), 0.73 (t, J = 8.1 Hz, 2H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 145.2, 142.0, 135.2, 128.9, 128.2, 127.9, 127.8, 125.8, 82.8, 53.2, 30.0, 24.7, 20.9; HRMS (MALDI-TOF): calcd for $C_{22}H_{29}BO_2Na$ $[M+Na]^+$: 359.2153, found 359.2153.

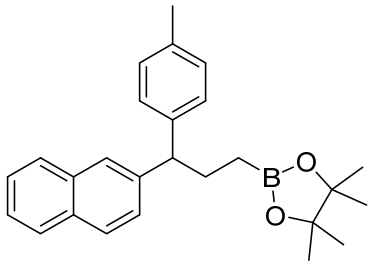
Compound 2b



Reaction was carried out according to the general procedure with **1b** (35.4 mg, 0.203 mmol), toluene (0.21 ml, 2.0 mmol), BCl_3 (1.0 ml, 1.0 mmol, 1 M in CH_2Cl_2 solution), pinacol (48.0 mg, 0.42 mmol), Et_3N (0.42 ml, 3.0 mmol), and CH_2Cl_2 (0.2 + 1.0 mL) to give compound **2b** (70.9 mg, 90%, >20:1) as colorless oil. SiO_2 Column chromatography: Hexane/AcOEt= 40/1.

^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.27-7.23 (m, 2H), 7.17-7.11 (m, 4H), 7.06 (d, J = 7.9 Hz, 2H), 3.76 (t, J = 7.7 Hz, 1H), 2.27 (s, 3H), 2.11 (q, J = 8.0 Hz, 2H), 1.26 (s, 9H), 1.21 (s, 12H), 0.73 (t, J = 8.1 Hz, 2H); ^{13}C-NMR (125 MHz, $CDCl_3$) δ 148.4, 142.24, 142.20, 135.2, 128.9, 127.9, 127.4, 125.1, 82.8, 52.8, 34.2, 31.4, 30.1, 24.8, 21.0; HRMS (MALDI-TOF) calcd for $C_{26}H_{37}BO_2Na$ $[M+Na]^+$: 415.2779, found 415.2793.

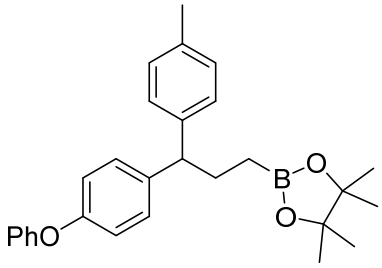
Compound 2c



Reaction was carried out according to the general procedure with **1c** (33.9 mg, 0.201 mmol), toluene (0.21 ml, 2.0 mmol), BCl_3 (1.0 ml, 1.0 mmol, 1 M in CH_2Cl_2 solution), pinacol (47.0 mg, 0.40 mmol), Et_3N (0.42 ml, 3.0 mmol), and CH_2Cl_2 (0.2 + 1.0 mL) to give compound **2c** (38.3 mg, 49%, >20:1) as colorless oil. SiO_2 Column chromatography: Hexane/AcOEt= 40/1.

^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.78 (d, J = 7.5 Hz, 1H), 7.75 (d, J = 7.5 Hz, 1H), 7.72-7.69 (m, 2H), 7.44-7.37 (m, 2H), 7.32 (dd, J = 8.5, 1.5 Hz, 1H), 7.16 (d, J = 8.0 Hz, 2H), 7.07 (d, J = 8.0 Hz, 2H), 3.97 (t, J = 7.5 Hz, 1H), 2.28 (s, 3H), 2.27-2.18 (m, 2H), 1.22 (s, 12H), 0.78 (t, J = 8.0 Hz, 2H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 142.7, 141.9, 135.4, 133.5, 132.1, 129.0, 128.0, 127.9, 127.7, 127.5, 127.0, 126.0, 125.7, 125.2, 82.9, 53.2, 29.7, 24.8, 21.0; HRMS (MALDI-TOF) calcd for $C_{26}H_{31}BO_2Na$ $[M+Na]^+$: 409.2309, found 409.2320.

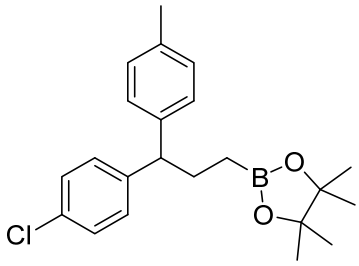
Compound 2d



Reaction was carried out according to the general procedure with **1d** (46.6 mg, 0.222 mmol), toluene (0.23 ml, 2.2 mmol), BCl_3 (1.1 ml, 1.1 mmol, 1M in CH_2Cl_2 solution), pinacol (51.7 mg, 0.44 mmol), Et_3N (0.48 ml, 3.4 mmol), and CH_2Cl_2 (0.22 + 1.0 mL) to give compound **1d** (15.3 mg, 16%, >20:1) as pale yellow oil. SiO_2 Column chromatography: Hexane/AcOEt= 40/1.

^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.33-7.28 (m, 2H), 7.21-7.17 (m, 2H), 7.16-7.04 (m, 5H), 6.99-6.95 (m, 2H), 6.93-6.87 (m, 2H), 3.79 (t, J = 8.0 Hz, 1H), 2.30 (s, 3H), 2.11 (td, J = 8.0, 8.0 Hz, 2H), 1.24 (s, 12H), 0.74 (t, J = 8.0 Hz, 2H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 157.5, 155.1, 142.1, 140.3, 135.4, 129.6, 129.1, 129.0, 127.8, 122.9, 118.8, 118.6, 82.9, 52.6, 30.2, 24.8, 21.0; HRMS (MALDI-TOF) calcd for $C_{28}H_{33}BO_3Na$ $[M+Na]^+$: 451.2415, found 451.2424.

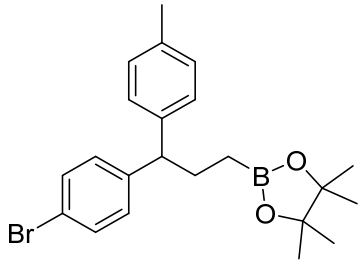
Compound 2e



Reaction was carried out according to the general procedure with **1e** (30.8 mg, 0.201 mmol), toluene (0.21 ml, 2.0 mmol), BCl_3 (1.0 ml, 1.0 mmol, 1 M in CH_2Cl_2 solution), pinacol (47.0 mg, 0.41 mmol), Et_3N (0.42 ml, 3.0 mmol), and CH_2Cl_2 (0.2 + 1.0 mL) to give compound **2e** (52.9 mg, 71%, >20:1) as colorless oil. SiO_2 Column chromatography: Hexane/AcOEt= 40/1.

^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.23-7.19 (m, 2H), 7.17-7.13 (m, 2H), 7.08 (bs, 4H), 3.77 (t, J = 7.8 Hz, 1H), 2.29 (s, 3H), 2.08 (td, J = 8.2, 5.6 Hz, 2H), 1.22 (s, 12H), 0.71 (dd, J = 9.4, 7.0 Hz, 2H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 143.8, 141.5, 135.6, 131.5, 129.3, 129.1, 128.4, 127.8, 83.0, 52.5, 29.9, 24.8, 21.0; HRMS (MALDI-TOF) calcd for $C_{22}H_{28}BClO_2Na$ $[M+Na]^+$: 393.1763, found 393.1756

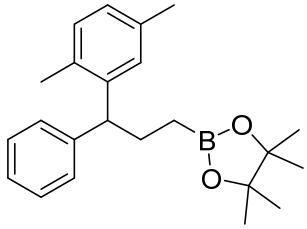
Compound 2f



Reaction was carried out according to the general procedure with **1f** (43.2 mg, 0.219 mmol), toluene (0.23 ml, 2.2 mmol), BCl_3 (1.1 ml, 1.1 mmol, 1M in CH_2Cl_2 solution), pinacol (52.3 mg, 0.44 mmol), Et_3N (0.46 ml, 3.3 mmol), and CH_2Cl_2 (0.22 + 1.0 mL) to give compound **2f** (74.1 mg, 81%, 13:1) as colorless oil. SiO_2 Column chromatography: Hexane/AcOEt= 40/1.

^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.38-7.33 (m, 2H), 7.12-7.06 (m, 6H), 3.76 (t, J = 7.7 Hz, 1H), 2.29 (s, 3H), 2.13-2.03 (m, 2H), 1.22 (s, 12H), 0.75-0.68 (m, 2H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 144.4, 141.4, 135.7, 131.3, 129.8, 129.1, 127.8, 119.6, 83.0, 52.6, 29.8, 24.9, 21.0; HRMS (MALDI-TOF) calcd for $C_{22}H_{28}BBrO_2Na$ $[M+Na]^+$: 437.1258, found 437.1251.

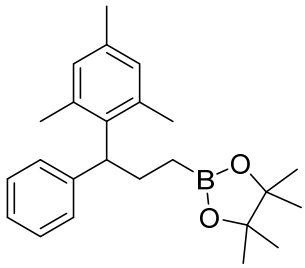
Compound 2g



Reaction was carried out according to the general procedure with **1a** (23.5 mg, 0.199 mmol), *p*-xylene (0.25 ml, 2.0 mmol), BCl_3 (1.0 ml, 1.0 mmol, 1M in CH_2Cl_2 solution), pinacol (47.3 mg, 0.40 mmol), Et_3N (0.42 ml, 3.0 mmol), and CH_2Cl_2 (0.2 + 1.0 mL) to give compound **2g** (50.8 mg, 73%) as pale yellow oil. SiO_2 Column chromatography: Hexane/AcOEt= 30/1.

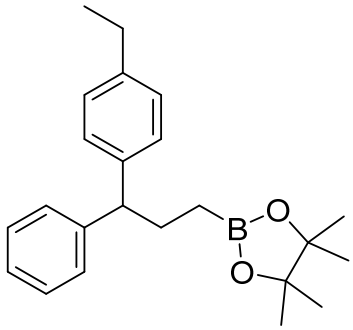
^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.25-7.18 (m, 6H), 7.16-7.11 (m, 2H), 4.03 (t, J = 7.90 Hz, 1H), 2.32 (s, 3H), 2.22 (s, 3H), 2.11 (td, J = 7.9, 7.9 Hz, 2H), 1.24 (s, 12H), 0.78 (t, J = 7.9 Hz, 2H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 144.7, 142.7, 135.1, 133.2, 130.2, 128.4, 128.1, 127.4, 126.5, 125.7, 82.9, 49.0, 30.2, 24.8, 21.3, 19.5; HRMS (MALDI-TOF) calcd for $C_{23}H_{31}BO_2Na$ $[M+Na]^+$: 373.2309, found 373.2320.

Compound 2h



Reaction was carried out according to the general procedure with **1a** (23.5 mg, 0.199 mmol), mesitylene (0.28 ml, 2.0 mmol), BCl_3 (1.0 ml, 1.0 mmol, 1M in CH_2Cl_2 solution), pinacol (47.1 mg, 0.40 mmol), Et_3N (0.42 ml, 3.0 mmol), and CH_2Cl_2 (0.2 + 1.0 mL) to give compound **2h** (63.3 mg, 87%) as pale yellow oil. ^{1}H-NMR (500 MHz, $CDCl_3$, 60 °C) δ 7.24-7.15 (m, 4H), 7.11-7.08 (m, 1H), 6.77 (s, 2H), 4.45 (dd, *J* = 9.0, 6.5 Hz, 1H), 2.45-2.08 (m, 11H), 1.21 (s, 12H), 0.85-0.67 (m, 2H); ^{13}C-NMR (125 MHz, $CDCl_3$, 60 °C) *δ* 144.9, 138.3, 137.2, 135.2, 130.0, 128.0, 127.5, 125.2, 83.0, 45.9, 25.7, 24.90, 24.87, 21.4, 20.7; HRMS (MALDI-TOF) calcd for $C_{24}H_{33}BO_2Na$ $[M+Na]^+$: 387.2466, found 387.2430.

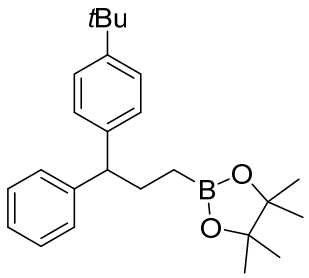
Compound 2i



Reaction was carried out according to the general procedure with **1a** (23.5 mg, 0.199 mmol), ethylbenzene (0.25 ml, 2.0 mmol), BCl_3 (1.0 ml, 1.0 mmol, 1M in CH_2Cl_2 solution), pinacol (47.2 mg, 0.40 mmol), Et_3N (0.42 ml, 3.0 mmol), and CH_2Cl_2 (0.2 + 1.0 mL) to give compound **2i** (53.2 mg, 76%, >20:1) as pale yellow oil. SiO_2 Column chromatography: Hexane/AcOEt= 40/1.

^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.26-7.06 (m, 9H), 3.80 (t, *J* = 7.8 Hz, 1H), 2.58 (q, *J* = 7.5 Hz, 2H), 2.08-2.16 (m, 2H), 1.27-1.16 (m, 15H), 0.73 (t, *J* = 8.3 Hz, 2H), ^{13}C-NMR (125 MHz, $CDCl_3$) δ 145.3, 142.3, 141.7, 128.2, 128.0, 127.9, 127.7, 125.8, 82.9, 53.3, 30.0, 28.3, 24.8, 15.5; HRMS (MALDI-TOF) calcd for $C_{23}H_{30}BO_2$ $[M–H]^+$:349.2333, found 349.2339.

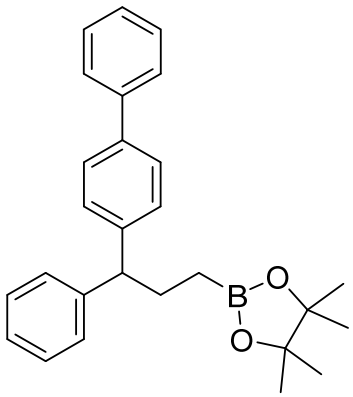
Compound 2j



Reaction was carried out according to the general procedure with **1a** (24.1 mg, 0.204 mmol), *t*-butylbenzene (0.31 ml, 2.0 mmol), BCl_3 (1.0 ml, 1.0 mmol, 1M in CH_2Cl_2 solution), pinacol (48.2 mg, 0.41 mmol), Et_3N (0.42 ml, 3.0 mmol), and CH_2Cl_2 (0.2 + 1.0 mL) to give compound **2j** (55.4 mg, 72%, >20:1) as colorless oil. SiO_2 Column chromatography: Hexane/AcOEt= 40/1.

^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.30-7.24 (m, 6H), 7.20-7.13 (m, 3H), 3.82 (t, J = 8.0 Hz, 1H), 2.19-2.10 (m, 2H), 1.29 (s, 9H), 1.24 (s, 12H), 0.75 (t, J = 8.0 Hz, 2H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 148.5, 145.2, 142.0, 128.2, 128.1, 127.5, 125.9, 125.1, 82.9, 53.3, 34.3, 31.4, 30.1, 24.8; HRMS (MALDI-TOF) calcd for $C_{25}H_{35}BO_2Na$ $[M+Na]^+$: 401.2622, found 401.2627.

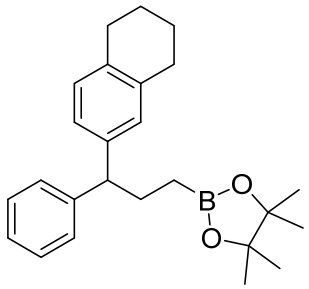
Compound 2k



Reaction was carried out according to the general procedure with **1a** (23.6 mg, 0.200 mmol), biphenyl (308.4 mg, 2.0 mmol), BCl_3 (1.0 ml, 1.0 mmol, 1M in CH_2Cl_2 solution), pinacol (47.4 mg, 0.40 mmol), Et_3N (0.42 ml, 3.0 mmol), and CH_2Cl_2 (0.2 + 1.0 mL) to give compound **2k** (46.2 mg, 58%, >20:1) as pale yellow oil. SiO_2 Column chromatography: Hexane/AcOEt= 40/1.

^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.57-7.46 (m, 4H), 7.43-7.37 (m, 2H), 7.33-7.24 (m, 7H), 7.19-7.14 (m, 1H), 3.88 (t, J = 7.8 Hz, 1H), 2.22-2.14 (m, 2H), 1.23 (s, 12H), 0.78 (t, J = 8.2 Hz, 2H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 144.9, 144.2, 141.0, 138.8, 128.6, 128.4, 128.3, 128.0, 127.0, 126.96, 126.93, 126.0, 83.0, 53.3, 30.0, 24.8; HRMS (MALDI-TOF) calcd for $C_{27}H_{31}BO_2Na$ $[M+Na]^+$:421.2309, found 421.2307.

Compound 2l

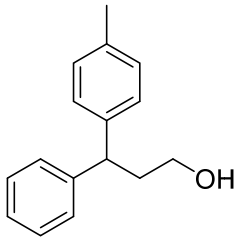


Reaction was carried out according to the general procedure with **1a** (24.4 mg, 0.206 mmol), tetrahydronaphthalene (0.27 ml, 2.0 mmol), BCl_3 (1.0 ml, 1.0 mmol, 1M in CH_2Cl_2 solution), pinacol (47.4 mg, 0.40 mmol), Et_3N (0.42 ml, 3.0 mmol), and CH_2Cl_2 (0.2 + 1.0 mL) to give compound **2l** (64.3 mg, 83%, 14:1) as pale yellow oil. SiO_2 Column chromatography: Hexane/AcOEt= 40/1.

^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.26-7.23 (m, 5H), 7.17-7.12 (m, 1H), 6.96-6.94 (m, 2H), 6.93 (s, 1H), 3.76 (t, J = 8.0 Hz, 1H), 2.74-2.67 (m, 4H), 2.12 (td, J = 8.0, 8.0 Hz, 2H), 1.78-1.73 (m, 4H), 1.23 (s, 12H), 0.74 (t, J = 8.0 Hz, 2H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 145.3, 142.1, 136.8, 134.6, 129.0, 128.6, 128.2, 128.0, 125.8, 125.0, 82.9, 53.4, 30.0, 29.5, 29.0, 24.8, 23.3, 23.2; HRMS (MALDI-TOF) calcd for $C_{25}H_{33}BO_2Na$ $[M+Na]^+$: 399.2466, found 399.2473.

4. Synthesis of 4 and 5 (Scheme 2)

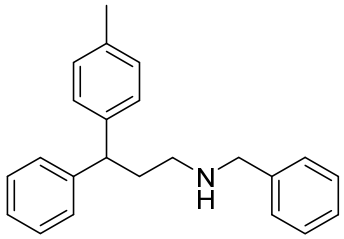
Compound 4[3]



To a solution of aryl cyclopropane **1a** (23.6 mg, 0.200 mmol) and toluene (0.21 ml. 2.0 mmol) in CH_2Cl_2 (0.2 ml, 1 M) was added BCl_3 (1 M in CH_2Cl_2 solution, 1.0 ml, 1.0 mmol) at -30 °C. After the mixture was stirred at -30 °C for 48 h, a solution of 2 M NaOH/30% H_2O_2 (1.5 mL, 1:1 v/v) was added to a mixture at -30 °C. The reaction mixture was allowed to warm to 0 °C and further stirred for 3 h. After the completion of the reaction, the resulting mixture was diluted with AcOEt and extracted with AcOEt. The organic layer was washed with brine, dried over Na_2SO_4, and concentrated in vacuo. The residue was purified by SiO_2 column chromatography (Hexane/AcOEt= 10/1 to 3/1) to give **4** as a colorless oil (39.8 mg, 88%, 20:1).

^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.30-7.06 (m, 9H), 4.09 (t, J = 7.8 Hz, 1H), 3.60 (t, J = 6.4 Hz, 2H), 2.35-2.27 (m, 5H), 1.48-1.37 (1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 144.7, 141.4, 135.8, 129.2, 128.5, 127.8, 127.7, 126.2, 61.1, 46.9, 38.2, 21.0. The spectrum was consistent with the reported data in reference 3.

Compound 5

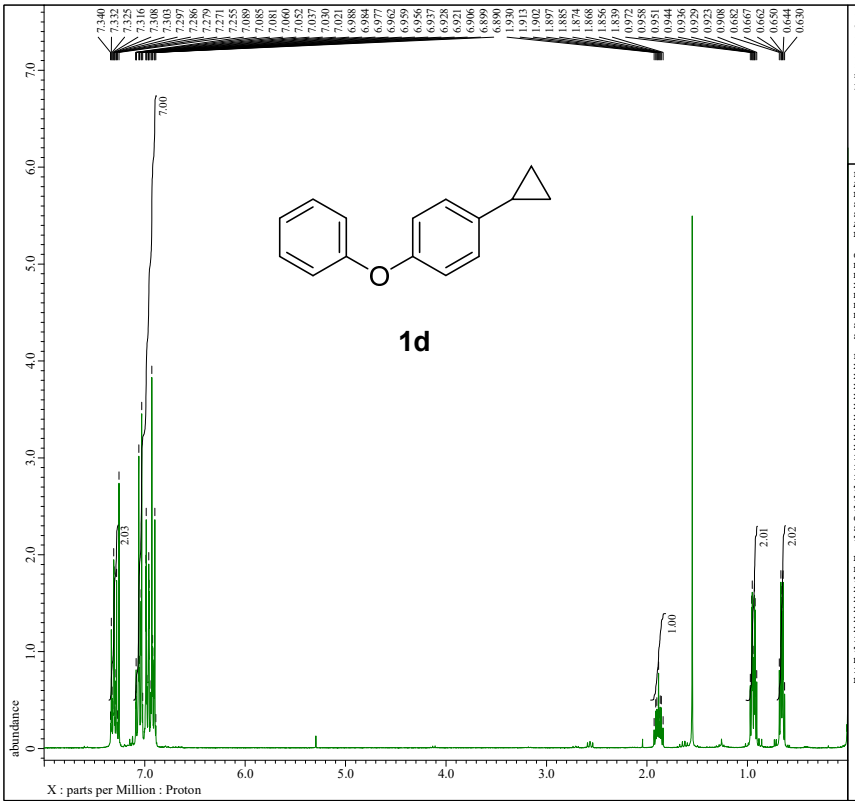


To a solution of aryl cyclopropane **1a** (23.6 mg, 0.20 mmol) and toluene (0.21 ml. 2.0 mmol) in CH_2Cl_2 (0.2 ml, 1 M) was added BCl_3 (1 M in CH_2Cl_2 solution, 1.0 ml, 1.0 mmol) at -30 ℃. After the mixture was stirred at -30 °C for 48 h, the volatile was removed in vacuo. To the residue, benzyl azide (53.4 mg, 0.40 mmol, 2.0 eq.) in CH_2Cl_2 (1.5 ml) was added dropwise slowly at room temperature and the mixture was stirred for 2 h. After the completion of the reaction, 10% NaOH aq. was added to the resulting mixture and the resulting mixture was extracted with CH_2Cl_2. The organic layer was dried over Na_2SO_4, and concentrated in vacuo. The residue was purified by SiO_2 column chromatography (Hexane/AcOEt= 4/1 with 5% Et_3N to AcOEt with 5% Et_3N) to give **5** as a pale yellow oil (40.3 mg, 64%, >20:1).

^{1}H-NMR (500 MHz, C_6D_6) δ 7.29-6.94 (m, 14H), 4.02 (t, J = 7.5 Hz, 1H), 3.51 (s, 2H), 2.46 (t, J = 6.8 Hz, 2H), 2.14-2.07 (m, 5H); ^{13}C-NMR (100 MHz, C_6D_6) δ 145.8, 142.5, 141.3, 135.6, 129.4, 128.7, 128.6, 128.5, 128.4, 128.3, 127.0, 126.3, 54.1, 48.7, 47.8, 36.4, 21.0; HRMS (MALDI-TOF) calcd for $C_{23}H_{26}N$ $[M+H]^+$: 316.2060, found 316.2063.

5. References

1) For **1b**, **1e**, **1f**, **1g**: M. H. Gieuw, Z. Ke, and Y. Y. Yeung, *Angew. Chem. Int. Ed.* 2018, **57**, 3782–3786.; For **1c**: D. Wang, X. Xue, K. N. Houk, and Z. Shi, *Angew. Chemie Int. Ed.* 2018, **57**, 16861–16865.
2) T. W. Butcher, E. J. Mcclain, T. G. Hamilton, T. M. Perrone, K. M. Kroner, G. C. Donohoe, N. G. Akhmedov, L. Petersen, and B. V Popp, *Org. Lett.* 2016, **18**, 6428–6431.
3) W. J. Jang, S. M. Song, Y. Park, and J. Yun, *J. Org. Chem.* 2019, **84**, 4429–4434.

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trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
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Author	= delta
Experiment	= proton.jxp
Sample_Id	= 0821 phoph cp
Solvent	= CHLOROFORM-D
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Revision_Time	= 25-AUG-2020 00:42:14
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X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 300
Spectrometer	= DELTA2_NMR
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X_Acq_Duration	= 2.90717696[s]
X_Domain	= 1H
X_Freq	= 300.52965592[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.34397631[Hz]
X_Sweep	= 5.63570784[kHz]
X_Sweep_Clipped	= 4.50856628[kHz]
Irr_Domain	= Proton
Irr_Freq	= 300.52965592[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 300.52965592[MHz]
Tri_Offset	= 5[ppm]
Clipped	= TRUE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 23.2[dC]
X_90_Width	= 11[us]
X_Acq_Time	= 2.90717696[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 5.5[us]
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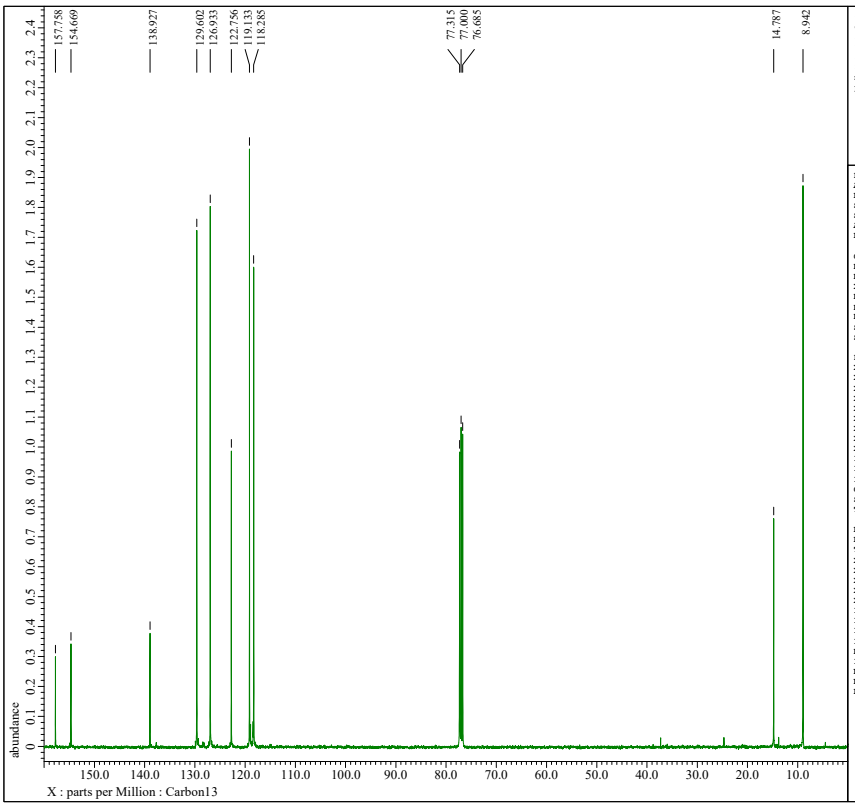
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 4.90717696[s]

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zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
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Author	= delta
Experiment	= carbon.jxp
Sample_Id	= KY Phoph cp
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 21-AUG-2020 21:07:52
Revision_Time	= 25-AUG-2020 00:43:48
Comment	= single pulse decoupled ga
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Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.52530333[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Clipped	= TRUE
Scans	= 1024
Total_Scans	= 1024
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Recvr_Gain	= 60
Temp_Get	= 21.1[dC]
X_90_Width	= 8.6[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 4.7[dB]
X_Pulse	= 2.86666667[us]
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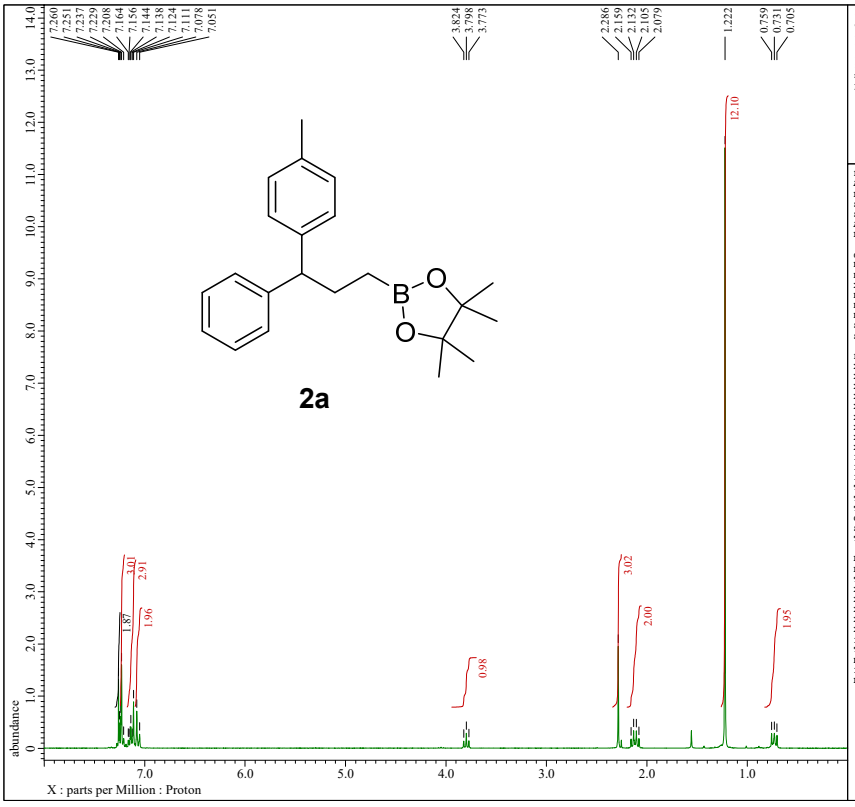
Irr_Atn_Noe	= 22.07[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.04333312[s]

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dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

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Filename          = 2aa 4 ph-tol _proton-1-3.
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 306 4
Solvent           = CHLOROFORM-D
Actual_Start_Time =  6-MAR-2020 17:04:25
Revision_Time     = 15-JUL-2020 20:08:20

Comment           = single_pulse
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Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECS 300
Spectrometer      = DELTA2_NMR

Field_Strength    = 7.0586013[T] (300[MHz])
X_Acq_Duration    = 2.90717696[s]
X_Domain          = 1H
X_Freq            = 300.52965592[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.34397631[Hz]
X_Sweep           = 5.63570784[kHz]
X_Sweep_Clipped   = 4.50856628[kHz]
Irr_Domain        = Proton
Irr_Freq          = 300.52965592[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 300.52965592[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 16
Total_Scans       = 16

Relaxation_Delay  = 2[s]
Recvr_Gain        = 42
Temp_Get          = 18.4[dC]
X_90_Width        = 11[us]
X_Acq_Time        = 2.90717696[s]
X_Angle           = 45[deg]
X_Atn             = 1[dB]
X_Pulse           = 5.5[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 4.90717696[s]
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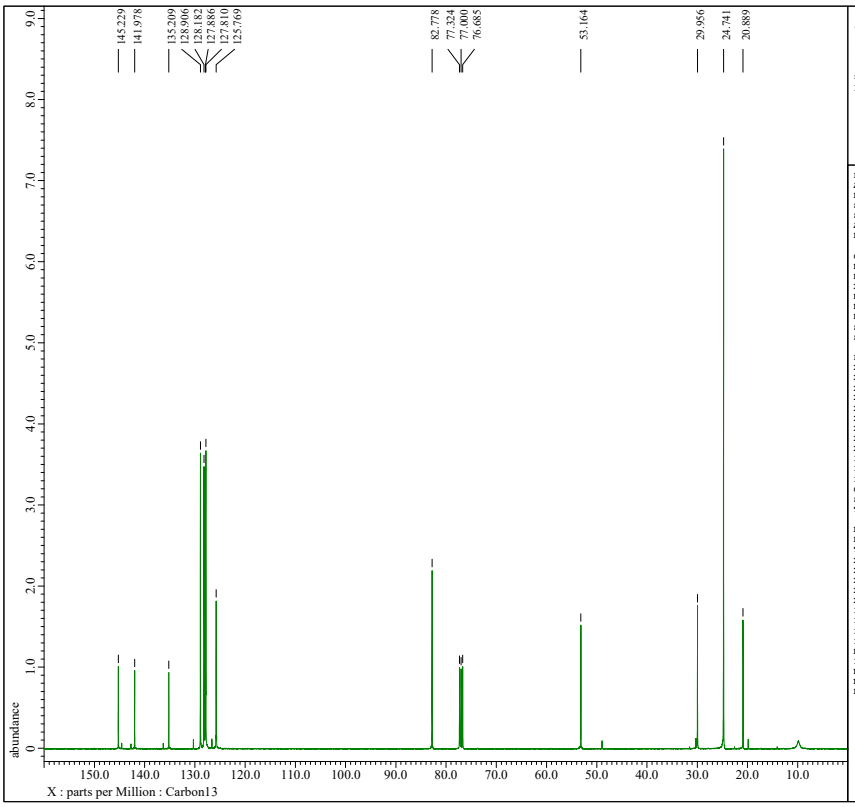


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---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
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Filename          = 2aa ph-tol_carbon-1-2.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 306 ph-tol
Solvent           = CHLOROFORM-D
Actual_Start_Time =  6-MAR-2020 18:54:05
Revision_Time     = 15-JUL-2020 20:10:48

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECS 400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

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Temp_Get          = 21[dC]
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X_Atn             = 4.5[dB]
X_Pulse           = 3.4[us]
Irr_Atn_Dec       = 21.137[dB]
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Irr_Noise         = WALTZ
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Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
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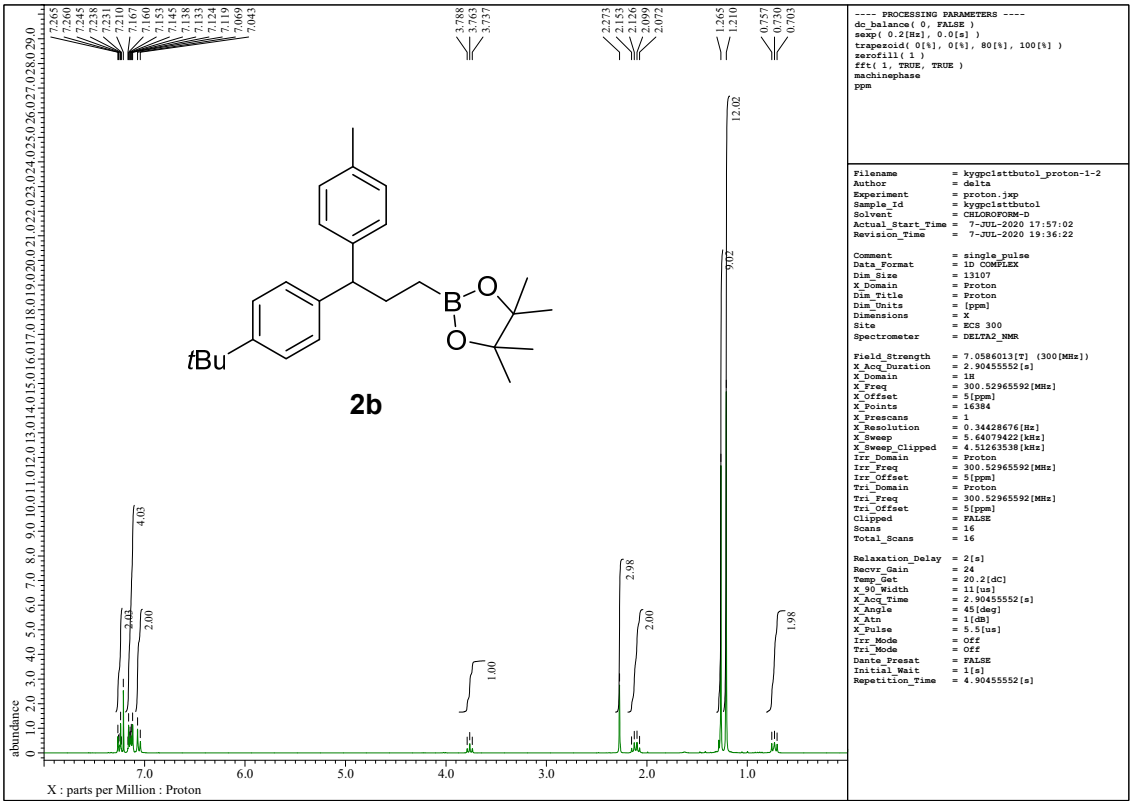


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sexp( 0.2[Hz], 0.0[s] )
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fft( 1, TRUE, TRUE )
machinephase
ppm
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Author            = delta
Experiment        = proton.jxp
Sample_Id         = kygpc1sttbutol
Solvent           = CHLOROFORM-D
Actual_Start_Time =  7-JUL-2020 17:57:02
Revision_Time     =  7-JUL-2020 19:36:22

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Dimensions        = X
Site              = ECS 300
Spectrometer      = DELTA2_NMR

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X_Resolution      = 0.34428676[Hz]
X_Sweep           = 5.64079422[kHz]
X_Sweep_Clipped   = 4.51263538[kHz]
Irr_Domain        = Proton
Irr_Freq          = 300.52965592[MHz]
Irr_Offset        = 5[ppm]
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Tri_Freq          = 300.52965592[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 16
Total_Scans       = 16

Relaxation_Delay  = 2[s]
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X_Angle           = 45[deg]
X_Atn             = 1[dB]
X_Pulse           = 5.5[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 4.90455552[s]
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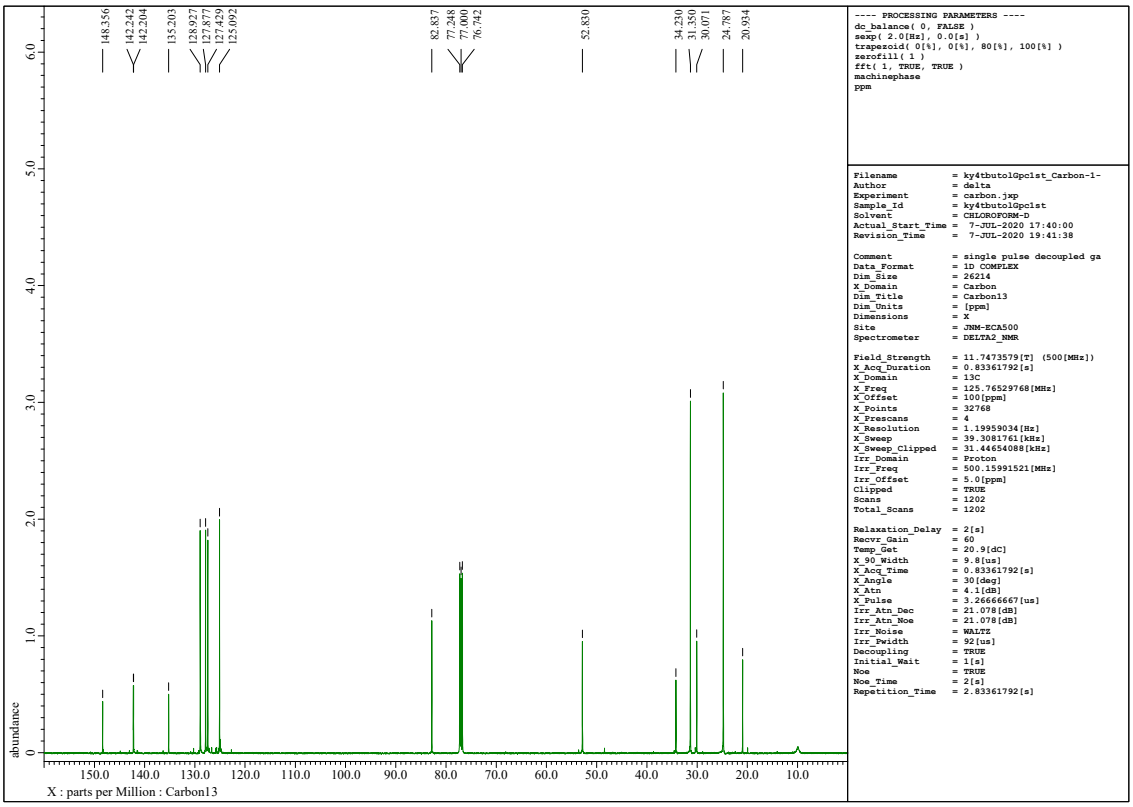


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sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

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Author            = delta
Experiment        = carbon.jxp
Sample_Id         = ky4tbutolGpc1st
Solvent           = CHLOROFORM-D
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Revision_Time     =  7-JUL-2020 19:41:38

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Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
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Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

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X_Resolution      = 1.19959034[Hz]
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X_Sweep_Clipped   = 31.44654088[kHz]
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Recvr_Gain        = 60
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X_90_Width        = 9.8[us]
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Irr_Atn_Noe       = 21.078[dB]
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Irr_Pwidth        = 92[us]
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Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
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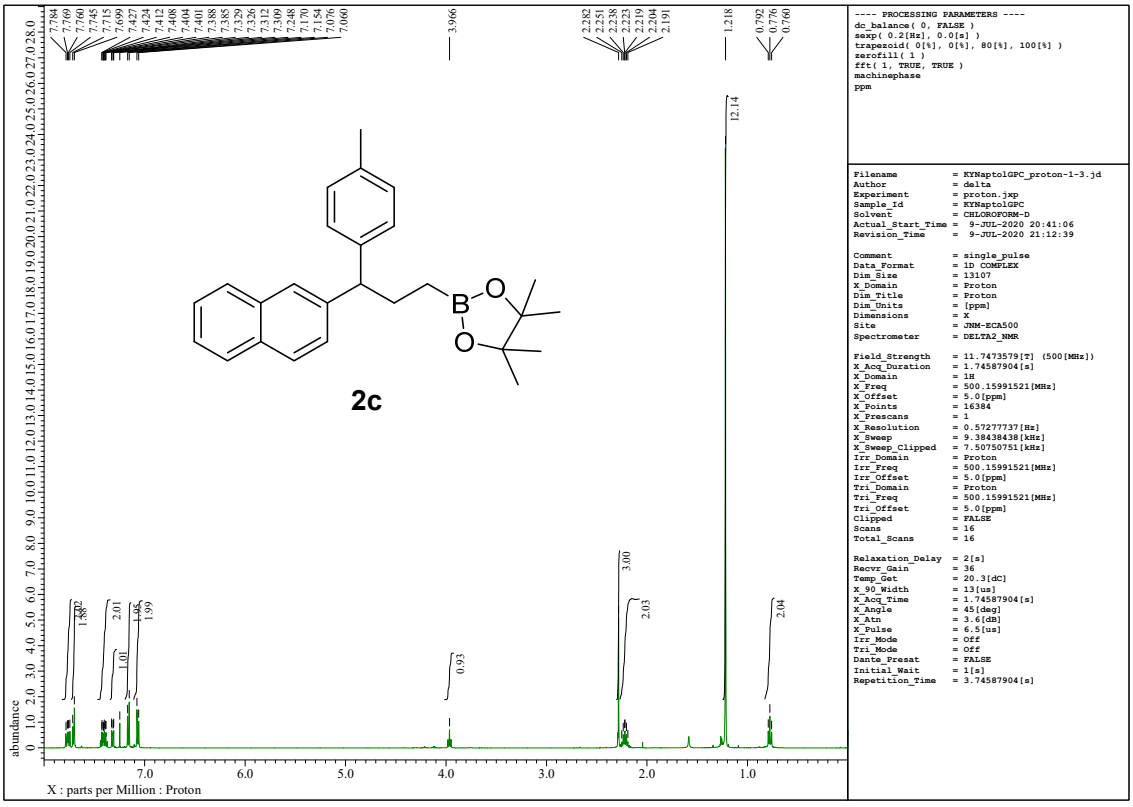


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fft( 1, TRUE, TRUE )
machinephase
ppm
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Author            = delta
Experiment        = proton.jxp
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Revision_Time     =  9-JUL-2020 21:12:39

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Dim_Size          = 13107
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Spectrometer      = DELTA2_NMR

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X_Resolution      = 0.57277737[Hz]
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X_Sweep_Clipped   = 7.50750751[kHz]
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Irr_Freq          = 500.15991521[MHz]
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Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
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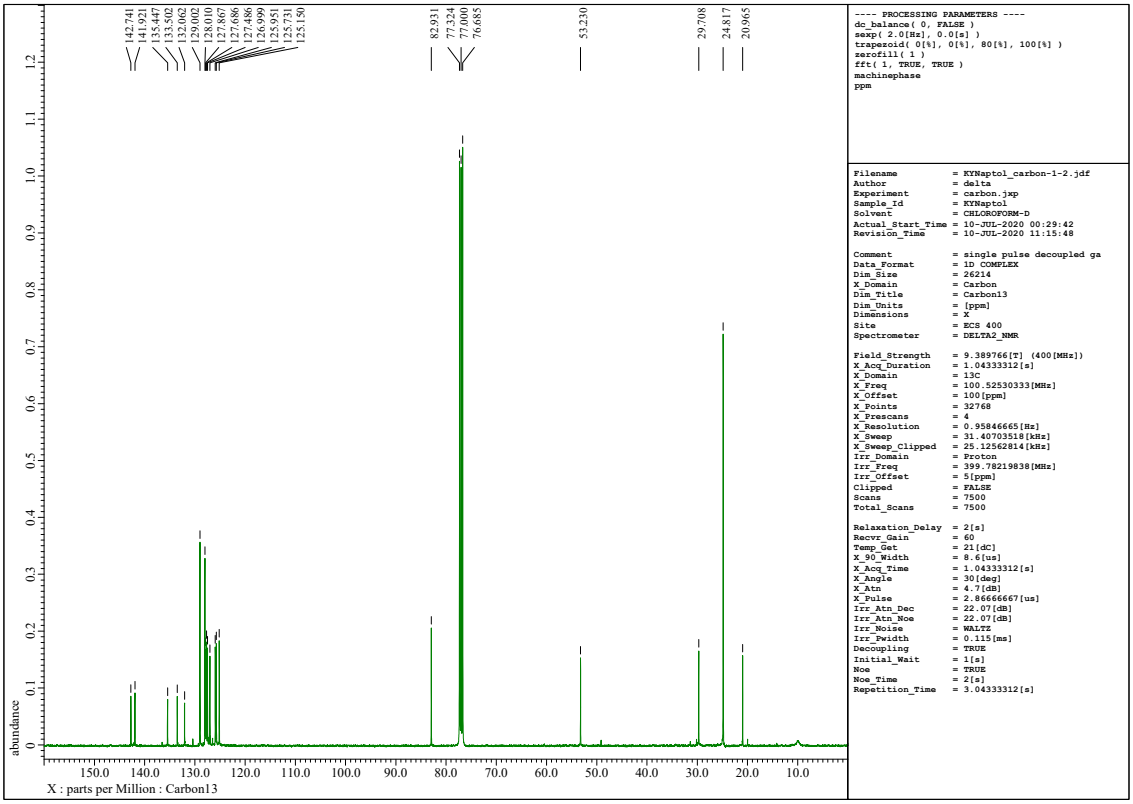
Relaxation_Delay  = 2[s]
Recvr_Gain        = 36
Temp_Get          = 20.3[dC]
X_90_Width        = 13[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 3.6[dB]
X_Pulse           = 6.5[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 3.74587904[s]
```



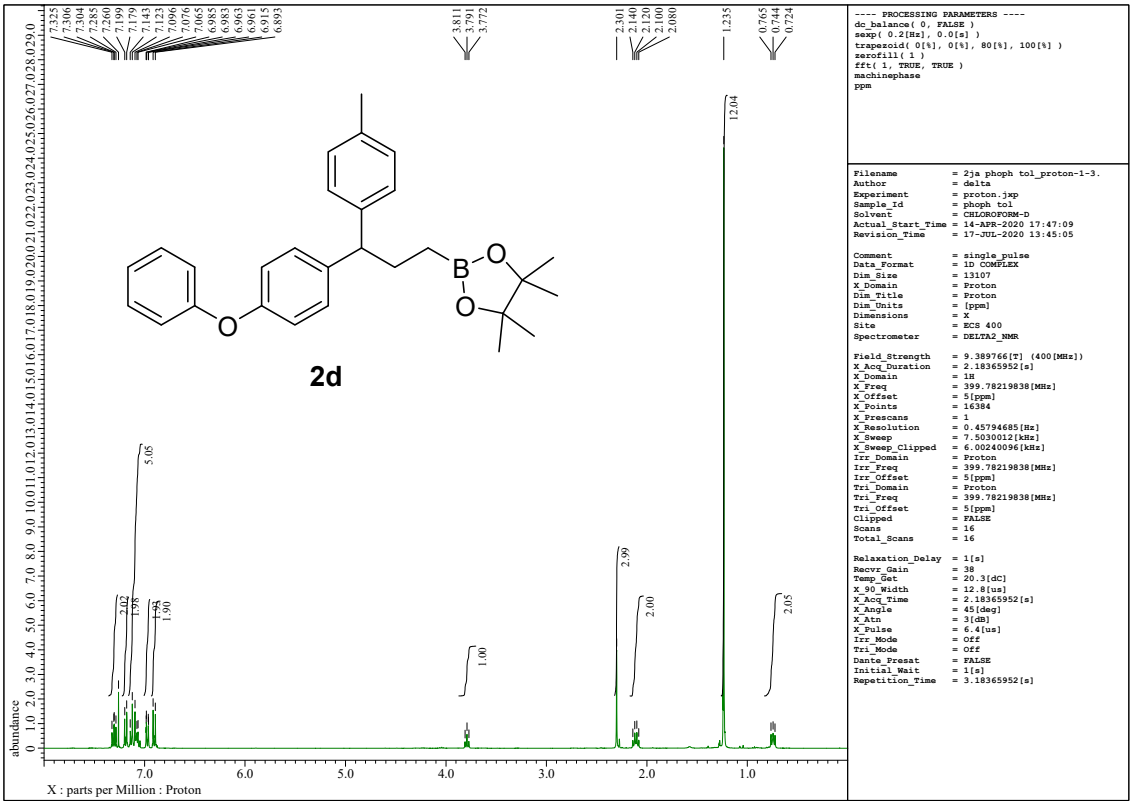

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = KYNaptol_carbon-1-2.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = KYNaptol
Solvent           = CHLOROFORM-D
Actual_Start_Time = 10-JUL-2020 00:29:42
Revision_Time     = 10-JUL-2020 11:15:48

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECS 400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 7500
Total_Scans       = 7500

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21[dC]
X_90_Width        = 8.6[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 4.7[dB]
X_Pulse           = 2.86666667[us]
Irr_Atn_Dec       = 22.07[dB]
Irr_Atn_Noe       = 22.07[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```



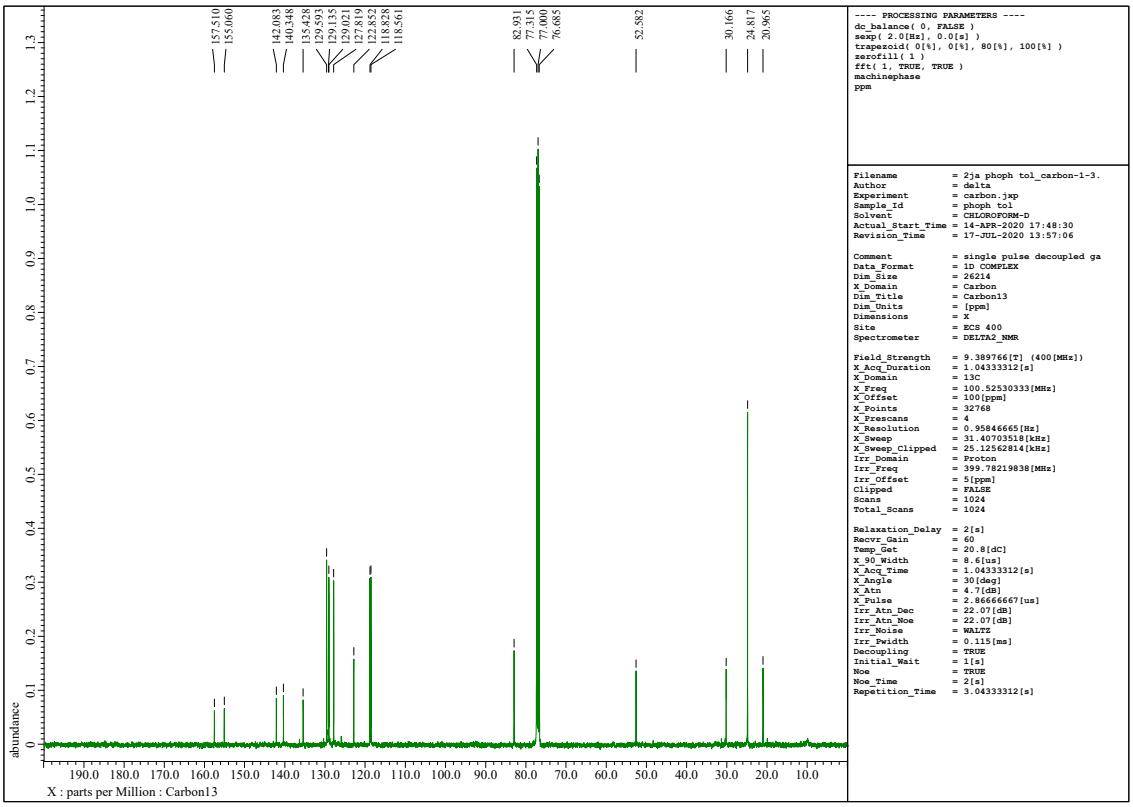

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = 2ja phoph tol_proton-1-3.
Author            = delta
Experiment        = proton.jxp
Sample_Id         = phoph tol
Solvent           = CHLOROFORM-D
Actual_Start_Time = 14-APR-2020 17:47:09
Revision_Time     = 17-JUL-2020 13:45:05

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECS 400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 16
Total_Scans       = 16

Relaxation_Delay  = 1[s]
Recvr_Gain        = 38
Temp_Get          = 20.3[dC]
X_90_Width        = 12.8[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 3[dB]
X_Pulse           = 6.4[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 3.18365952[s]
```



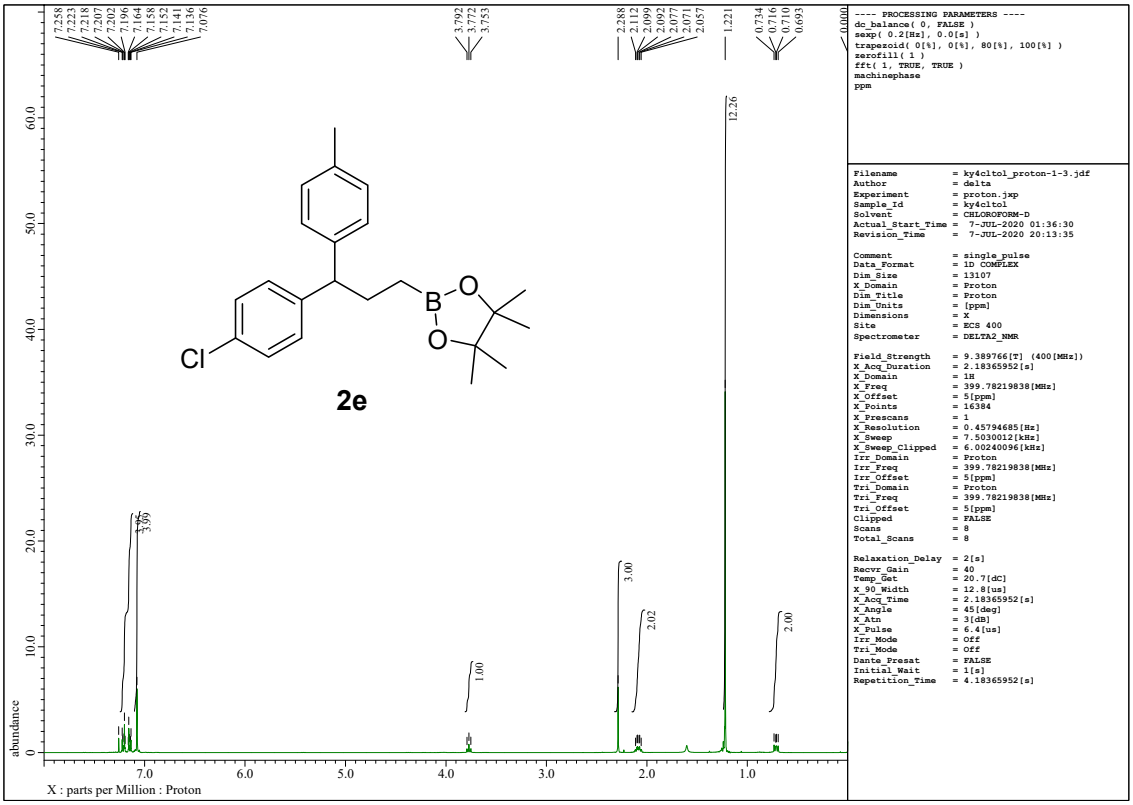

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = 2ja phoph tol_carbon-1-3.
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = phoph tol
Solvent           = CHLOROFORM-D
Actual_Start_Time = 14-APR-2020 17:48:30
Revision_Time     = 17-JUL-2020 13:57:06

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECS 400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 20.8[dC]
X_90_Width        = 8.6[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 4.7[dB]
X_Pulse           = 2.86666667[us]
Irr_Atn_Dec       = 22.07[dB]
Irr_Atn_Noe       = 22.07[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```



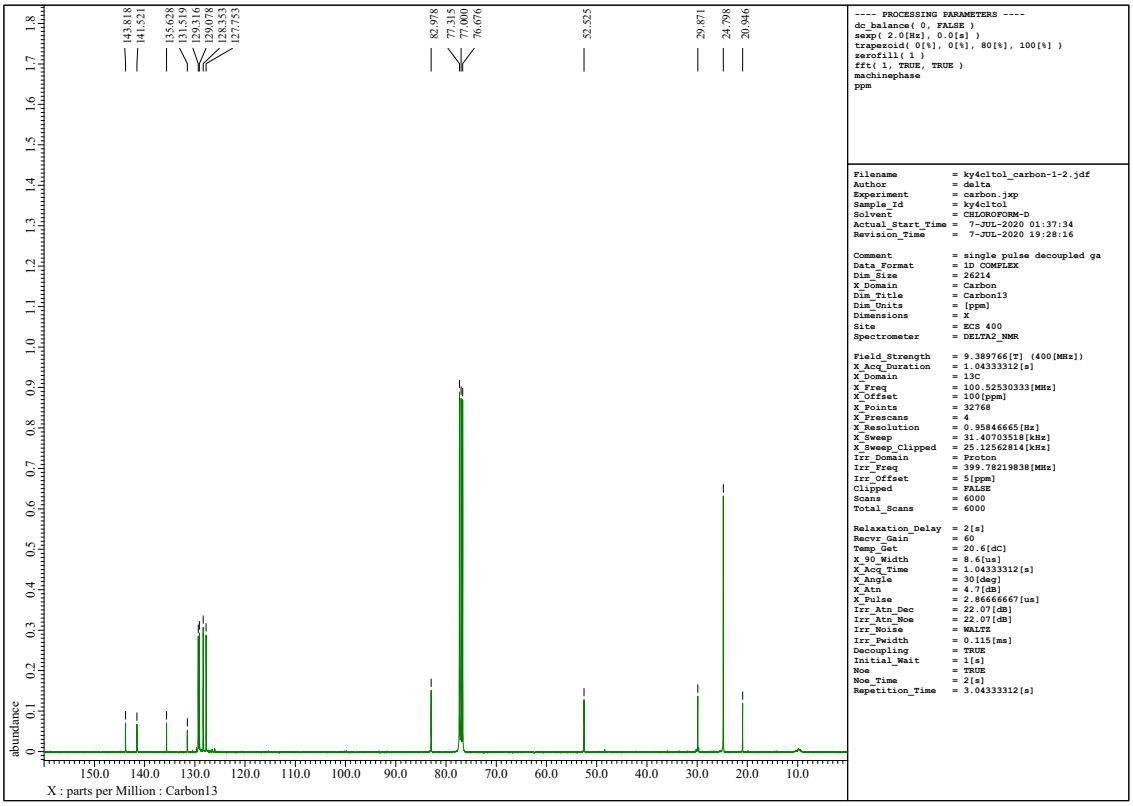

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = ky4cltol_proton-1-3.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = ky4cltol
Solvent           = CHLOROFORM-D
Actual_Start_Time =  7-JUL-2020 01:36:30
Revision_Time     =  7-JUL-2020 20:13:35

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECS 400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 2[s]
Recvr_Gain        = 40
Temp_Get          = 20.7[dC]
X_90_Width        = 12.8[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 3[dB]
X_Pulse           = 6.4[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 4.18365952[s]
```



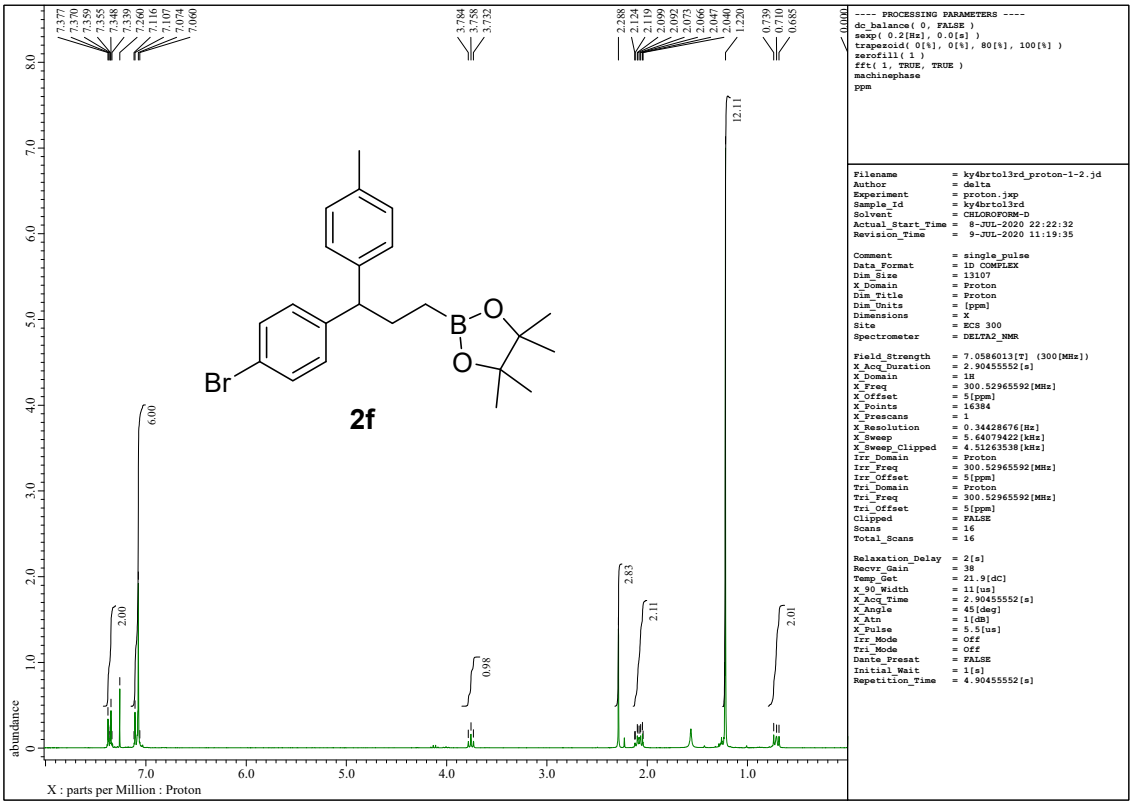

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = ky4cltol_carbon-1-2.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = ky4cltol
Solvent           = CHLOROFORM-D
Actual_Start_Time =  7-JUL-2020 01:37:34
Revision_Time     =  7-JUL-2020 19:28:16

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECS 400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 6000
Total_Scans       = 6000

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 20.6[dC]
X_90_Width        = 8.6[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 4.7[dB]
X_Pulse           = 2.86666667[us]
Irr_Atn_Dec       = 22.07[dB]
Irr_Atn_Noe       = 22.07[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```



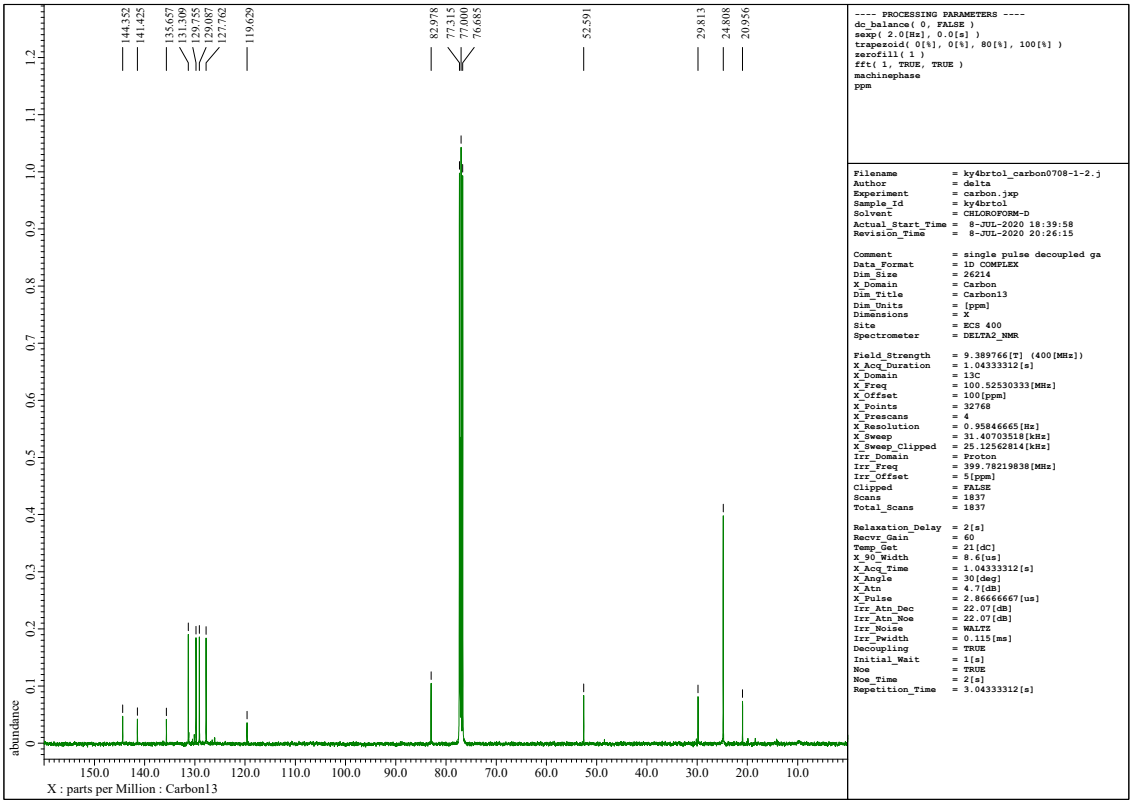

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = ky4brtol3rd_proton-1-2.jd
Author            = delta
Experiment        = proton.jxp
Sample_Id         = ky4brtol3rd
Solvent           = CHLOROFORM-D
Actual_Start_Time =  8-JUL-2020 22:22:32
Revision_Time     =  9-JUL-2020 11:19:35

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECS 300
Spectrometer      = DELTA2_NMR

Field_Strength    = 7.0586013[T] (300[MHz])
X_Acq_Duration    = 2.90455552[s]
X_Domain          = 1H
X_Freq            = 300.52965592[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.34428676[Hz]
X_Sweep           = 5.64079422[kHz]
X_Sweep_Clipped   = 4.51263538[kHz]
Irr_Domain        = Proton
Irr_Freq          = 300.52965592[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 300.52965592[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 16
Total_Scans       = 16

Relaxation_Delay  = 2[s]
Recvr_Gain        = 38
Temp_Get          = 21.9[dC]
X_90_Width        = 11[us]
X_Acq_Time        = 2.90455552[s]
X_Angle           = 45[deg]
X_Atn             = 1[dB]
X_Pulse           = 5.5[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 4.90455552[s]
```



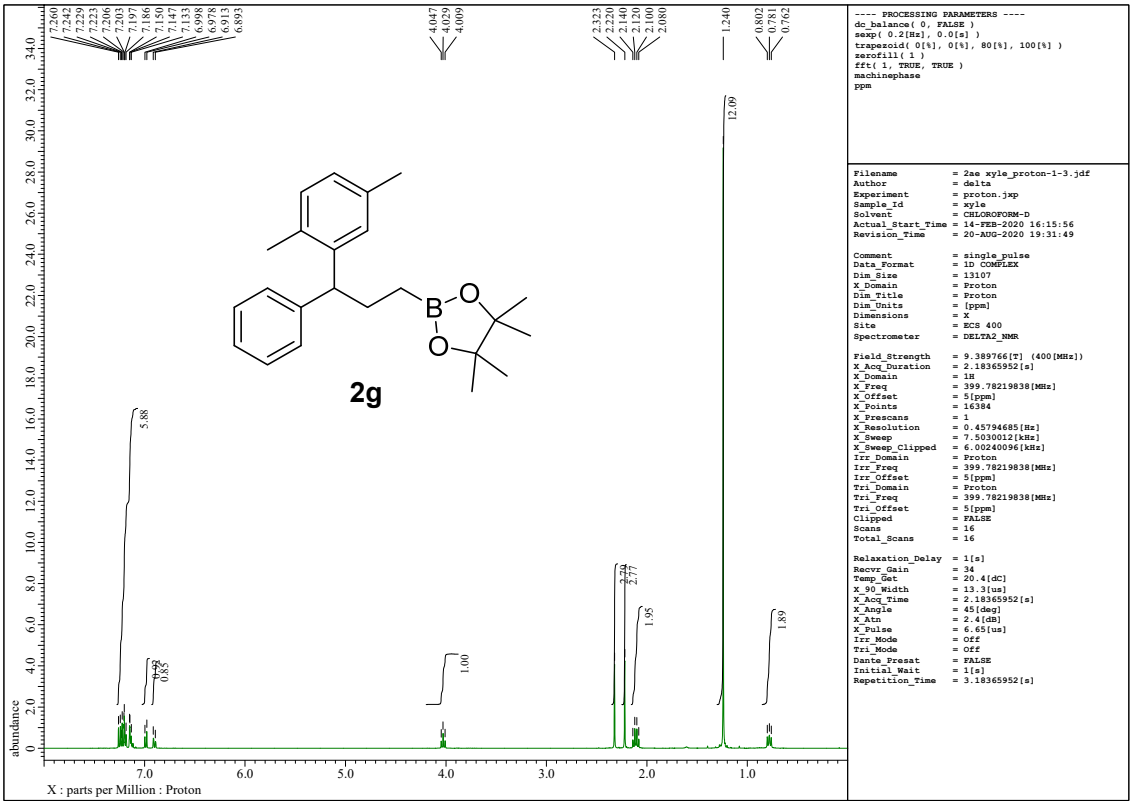

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

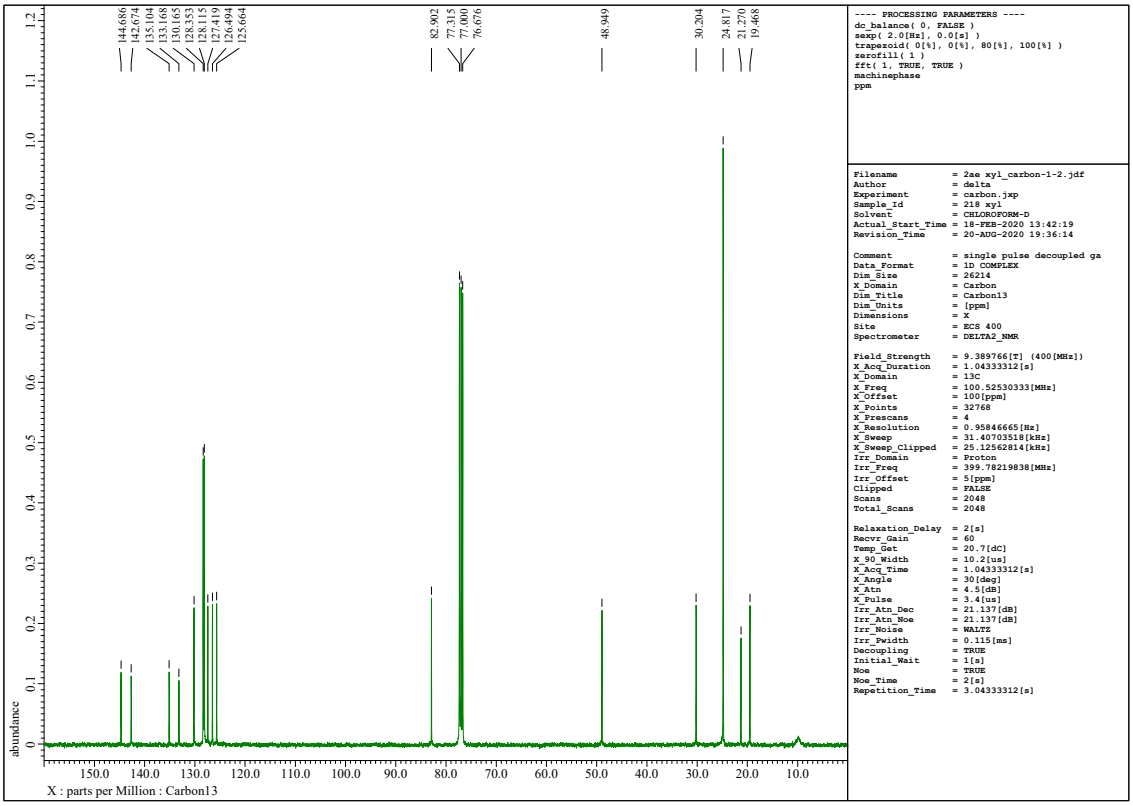
```
Filename          = ky4brtol_carbon0708-1-2.j
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = ky4brtol
Solvent           = CHLOROFORM-D
Actual_Start_Time =  8-JUL-2020 18:39:58
Revision_Time     =  8-JUL-2020 20:26:15

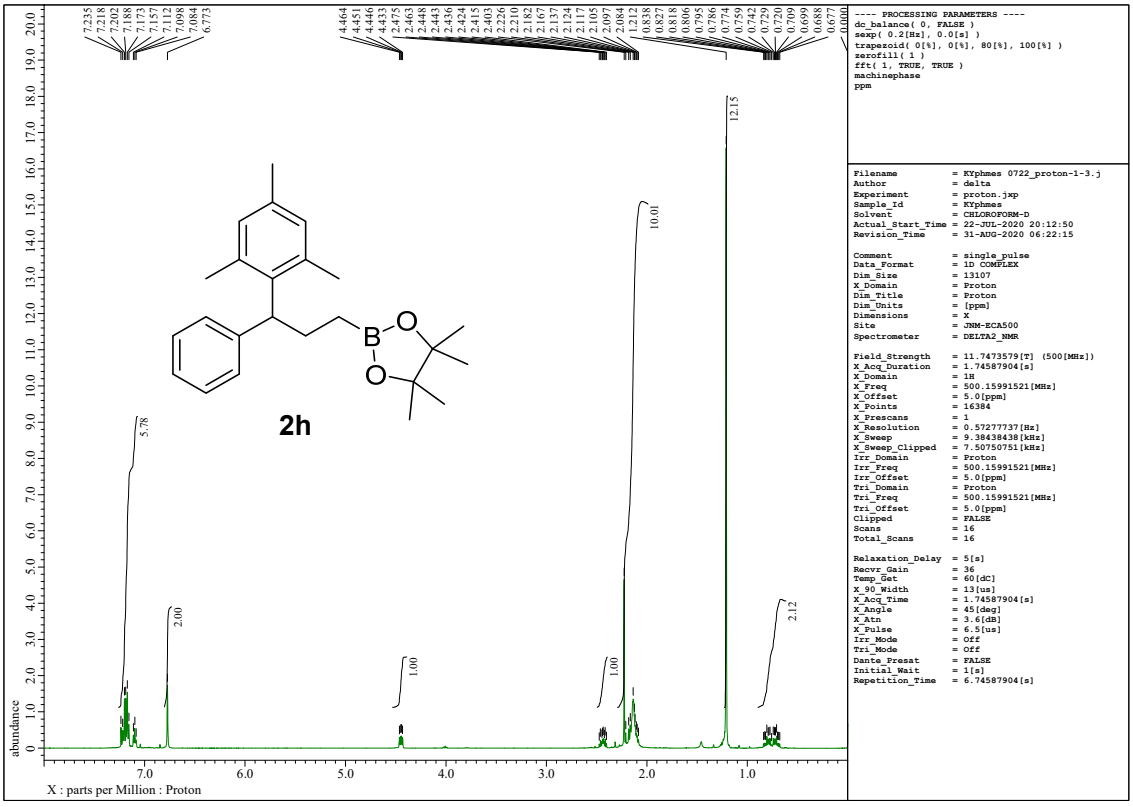
Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECS 400
Spectrometer      = DELTA2_NMR

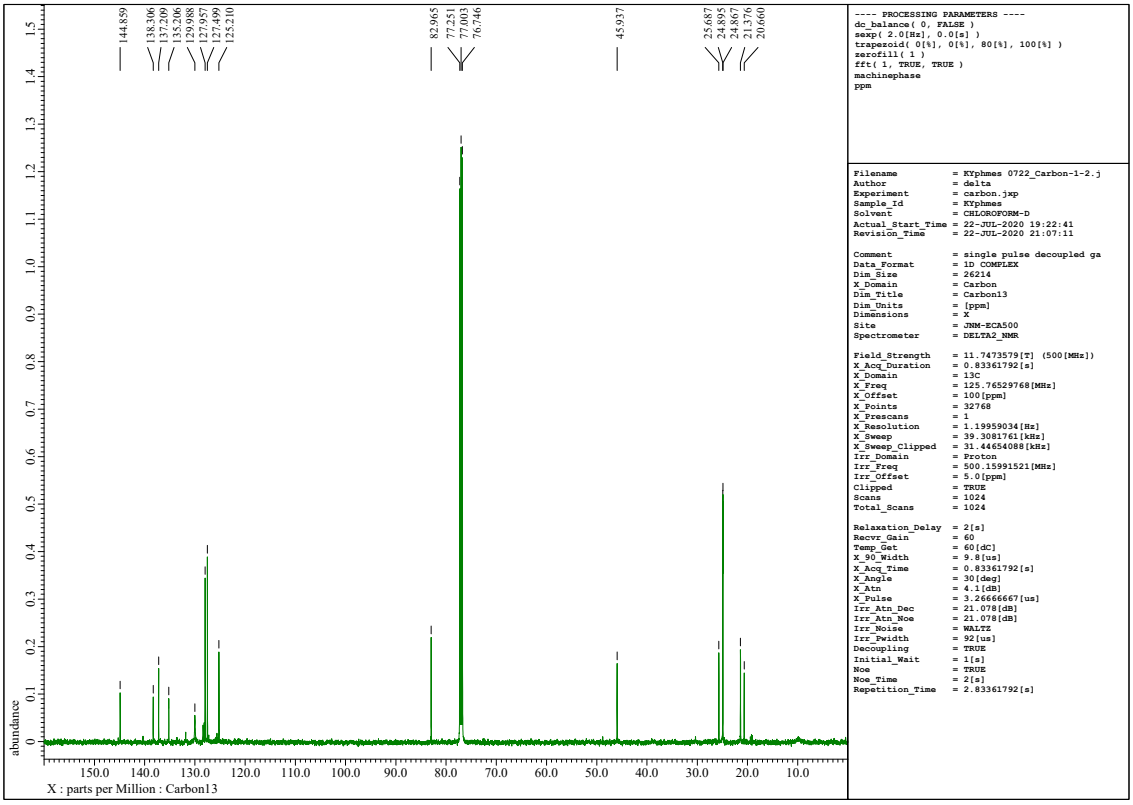
Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 1837
Total_Scans       = 1837

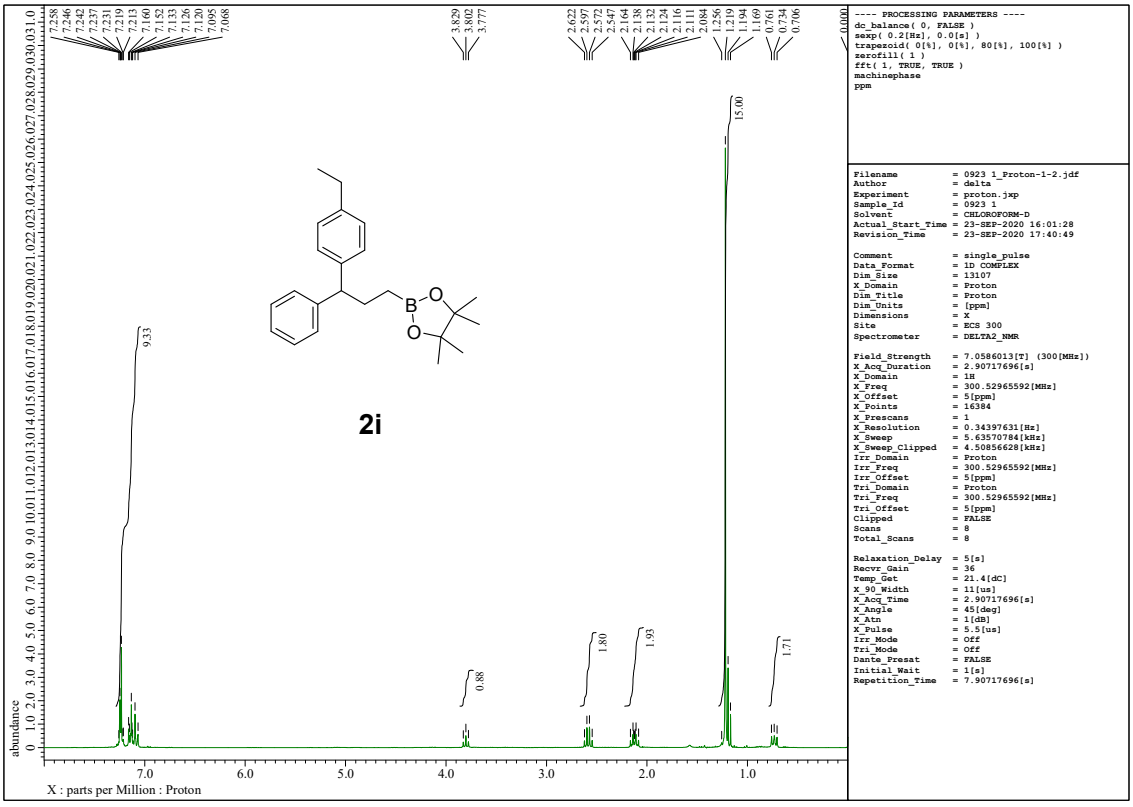
Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21[dC]
X_90_Width        = 8.6[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 4.7[dB]
X_Pulse           = 2.86666667[us]
Irr_Atn_Dec       = 22.07[dB]
Irr_Atn_Noe       = 22.07[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```

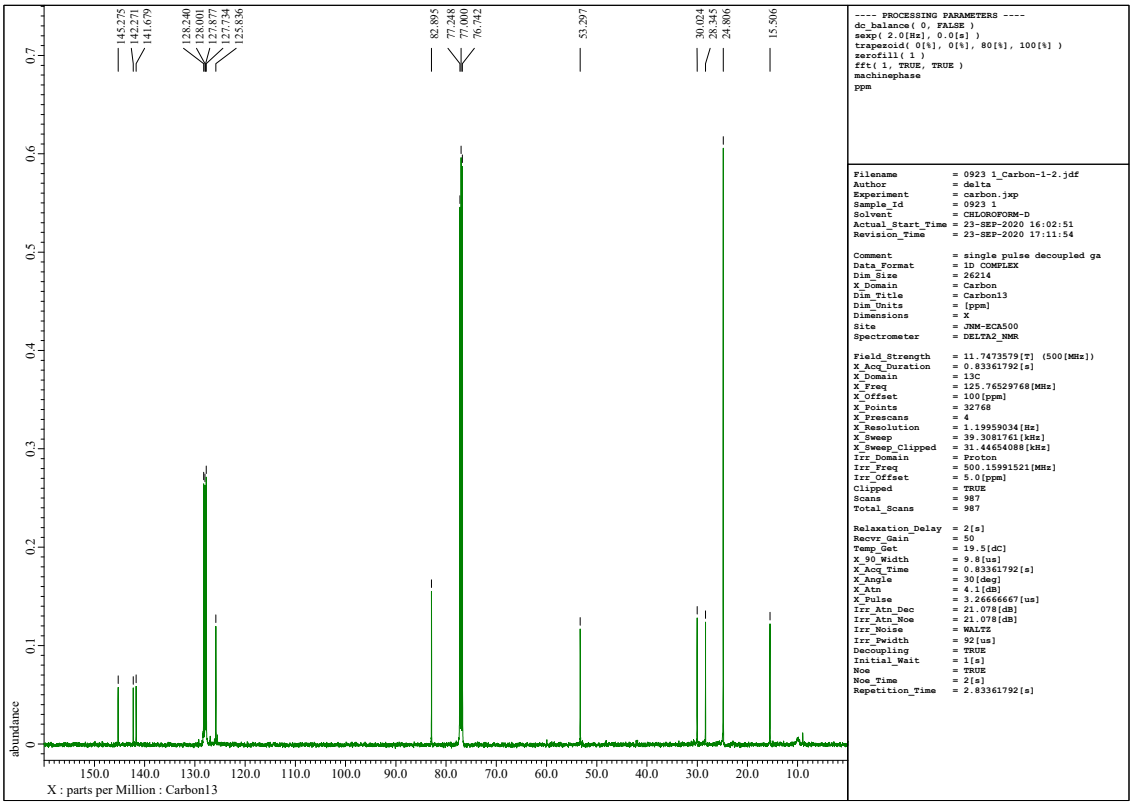

7.260
7.242
7.229
7.223
7.206
7.203
7.197
7.186
7.150
7.147
7.133
6.998
6.978
6.913
6.893
4.047
4.029
4.009
2.323
2.220
2.140
2.120
2.100
2.080
1.240
0.802
0.781
0.762
12.09
5.88
1.00
2.79
2.77
1.95
1.89
0.85
2g
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 2ae xyle_proton-1-3.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = xyle
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-FEB-2020 16:15:56
Revision_Time = 20-AUG-2020 19:31:49
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
X_Sweep_Clipped = 6.00240096[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 1[s]
Recvr_Gain = 34
Temp_Get = 20.4[dC]
X_90_Width = 13.3[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 6.65[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 3.18365952[s]

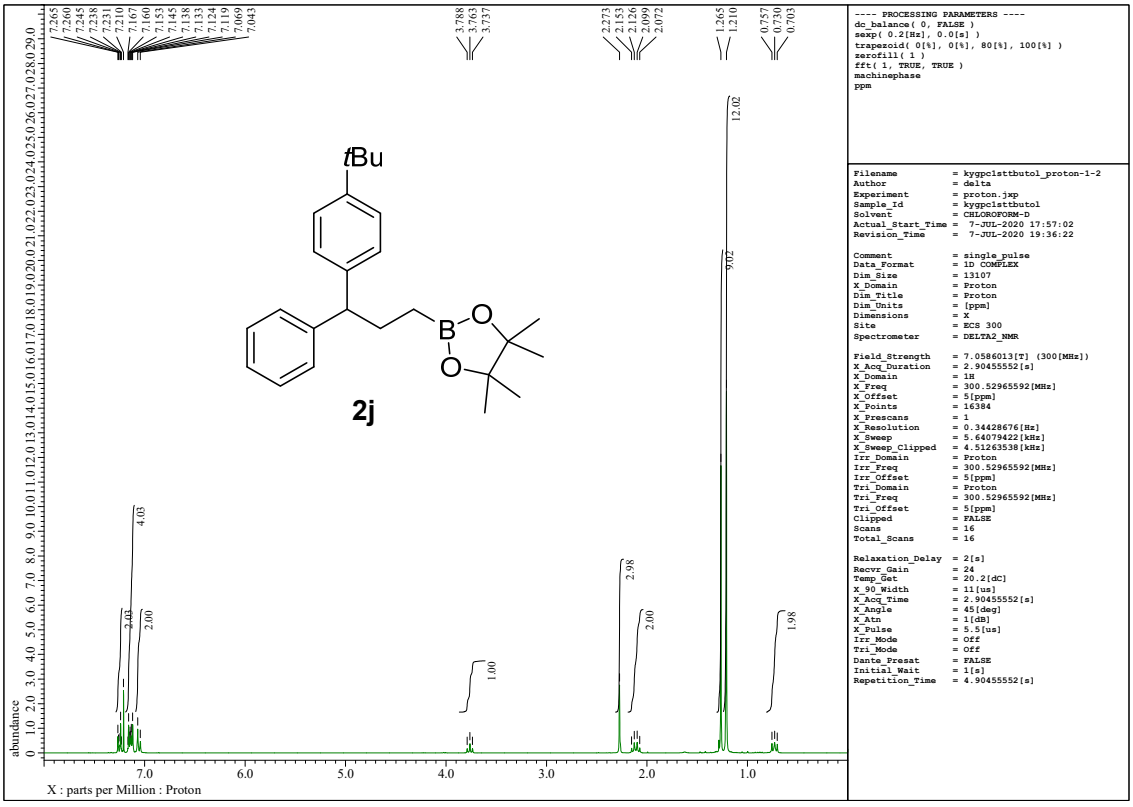

144.686
142.674
135.104
133.168
130.165
128.353
128.115
127.419
126.494
125.664
82.902
77.315
77.000
76.676
48.949
30.204
24.817
21.270
19.468
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 2ae xyl_carbon-1-2.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = 218 xyl
Solvent = CHLOROFORM-D
Actual_Start_Time = 18-FEB-2020 13:42:19
Revision_Time = 20-AUG-2020 19:36:14
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
X_Sweep_Clipped = 25.12562814[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 2048
Total_Scans = 2048
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 20.7[dC]
X_90_Width = 10.2[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 4.5[dB]
X_Pulse = 3.4[us]
Irr_Atn_Dec = 21.137[dB]
Irr_Atn_Noe = 21.137[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]


7.235
7.218
7.202
7.188
7.173
7.157
7.112
7.098
7.084
6.773
4.464
4.451
4.446
4.433
2.475
2.463
2.448
2.443
2.436
2.424
2.415
2.403
2.226
2.210
2.182
2.167
2.137
2.124
2.117
2.105
2.097
2.084
1.212
0.838
0.827
0.818
0.806
0.795
0.786
0.774
0.759
0.742
0.729
0.720
0.709
0.699
0.688
0.677
0.000
12.15
10.01
5.78
2.00
1.00
1.00
2.12
2h
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = KYphmes 0722_proton-1-3.j
Author = delta
Experiment = proton.jxp
Sample_Id = KYphmes
Solvent = CHLOROFORM-D
Actual_Start_Time = 22-JUL-2020 20:12:50
Revision_Time = 31-AUG-2020 06:22:15
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 36
Temp_Get = 60[dC]
X_90_Width = 13[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 3.6[dB]
X_Pulse = 6.5[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.74587904[s]


144.859
138.306
137.209
135.206
129.988
127.957
127.499
125.210
82.965
77.251
77.003
76.746
45.937
25.687
24.895
24.867
21.376
20.660
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = KYphmes 0722_Carbon-1-2.j
Author = delta
Experiment = carbon.jxp
Sample_Id = KYphmes
Solvent = CHLOROFORM-D
Actual_Start_Time = 22-JUL-2020 19:22:41
Revision_Time = 22-JUL-2020 21:07:11
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 0.83361792[s]
X_Domain = 13C
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 1.19959034[Hz]
X_Sweep = 39.3081761[kHz]
X_Sweep_Clipped = 31.44654088[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Clipped = TRUE
Scans = 1024
Total_Scans = 1024
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 60[dC]
X_90_Width = 9.8[us]
X_Acq_Time = 0.83361792[s]
X_Angle = 30[deg]
X_Atn = 4.1[dB]
X_Pulse = 3.26666667[us]
Irr_Atn_Dec = 21.078[dB]
Irr_Atn_Noe = 21.078[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 92[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.83361792[s]


7.258
7.246
7.242
7.237
7.231
7.219
7.213
7.160
7.152
7.133
7.126
7.120
7.095
7.068
3.829
3.802
3.777
2.622
2.597
2.572
2.547
2.164
2.138
2.132
2.124
2.116
2.111
2.084
1.256
1.219
1.194
1.169
0.761
0.734
0.706
0.000
15.00
9.33
1.80
1.93
1.71
0.88
B
O
O
2i
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 0923 1_Proton-1-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = 0923 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 23-SEP-2020 16:01:28
Revision_Time = 23-SEP-2020 17:40:49
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = ECS 300
Spectrometer = DELTA2_NMR
Field_Strength = 7.0586013[T] (300[MHz])
X_Acq_Duration = 2.90717696[s]
X_Domain = 1H
X_Freq = 300.52965592[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.34397631[Hz]
X_Sweep = 5.63570784[kHz]
X_Sweep_Clipped = 4.50856628[kHz]
Irr_Domain = Proton
Irr_Freq = 300.52965592[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 300.52965592[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 36
Temp_Get = 21.4[dC]
X_90_Width = 11[us]
X_Acq_Time = 2.90717696[s]
X_Angle = 45[deg]
X_Atn = 1[dB]
X_Pulse = 5.5[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.90717696[s]


145.275
142.271
141.679
128.240
128.001
127.877
127.734
125.836
82.895
77.248
77.000
76.742
53.297
30.024
28.345
24.806
15.806
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 0923 1_Carbon-1-2.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = 0923 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 23-SEP-2020 16:02:51
Revision_Time = 23-SEP-2020 17:11:54
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 0.83361792[s]
X_Domain = 13C
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.19959034[Hz]
X_Sweep = 39.3081761[kHz]
X_Sweep_Clipped = 31.44654088[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Clipped = TRUE
Scans = 987
Total_Scans = 987
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 19.5[dC]
X_90_Width = 9.8[us]
X_Acq_Time = 0.83361792[s]
X_Angle = 30[deg]
X_Atn = 4.1[dB]
X_Pulse = 3.26666667[us]
Irr_Atn_Dec = 21.078[dB]
Irr_Atn_Noe = 21.078[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 92[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.83361792[s]



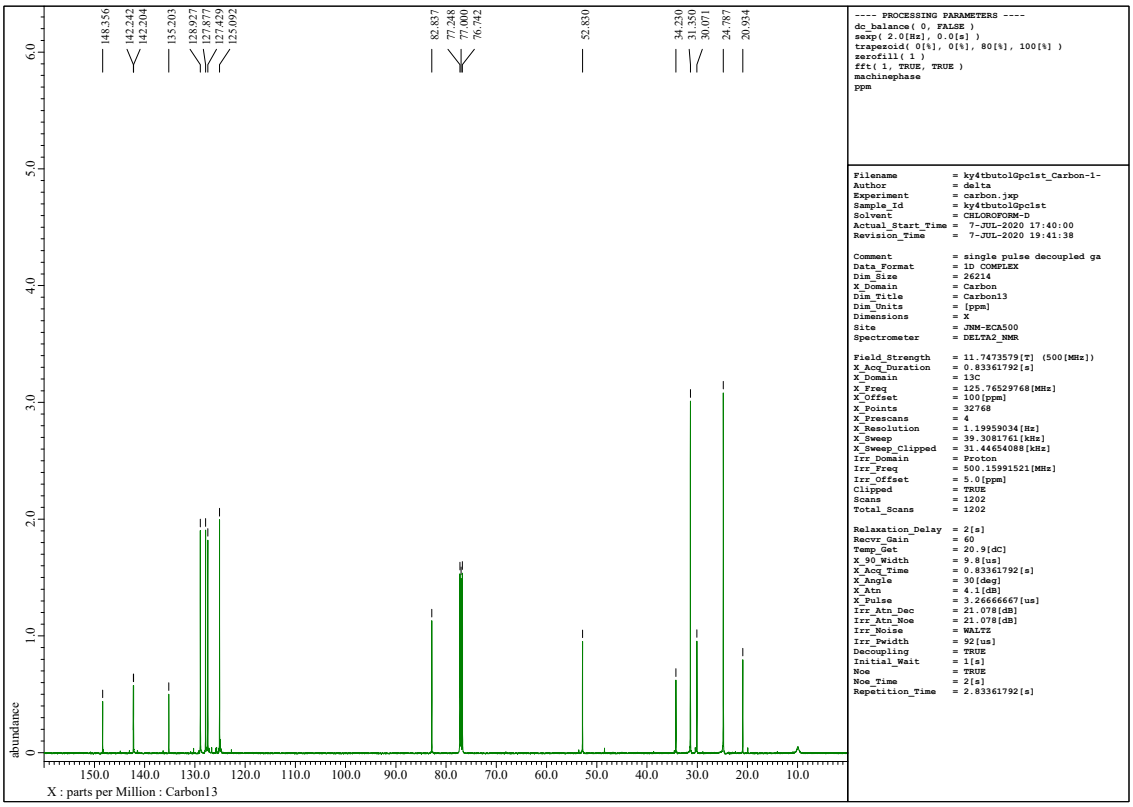

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = kygpc1sttbutol_proton-1-2
Author            = delta
Experiment        = proton.jxp
Sample_Id         = kygpc1sttbutol
Solvent           = CHLOROFORM-D
Actual_Start_Time =  7-JUL-2020 17:57:02
Revision_Time     =  7-JUL-2020 19:36:22

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECS 300
Spectrometer      = DELTA2_NMR

Field_Strength    = 7.0586013[T] (300[MHz])
X_Acq_Duration    = 2.90455552[s]
X_Domain          = 1H
X_Freq            = 300.52965592[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.34428676[Hz]
X_Sweep           = 5.64079422[kHz]
X_Sweep_Clipped   = 4.51263538[kHz]
Irr_Domain        = Proton
Irr_Freq          = 300.52965592[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 300.52965592[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 16
Total_Scans       = 16

Relaxation_Delay  = 2[s]
Recvr_Gain        = 24
Temp_Get          = 20.2[dC]
X_90_Width        = 11[us]
X_Acq_Time        = 2.90455552[s]
X_Angle           = 45[deg]
X_Atn             = 1[dB]
X_Pulse           = 5.5[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 4.90455552[s]
```



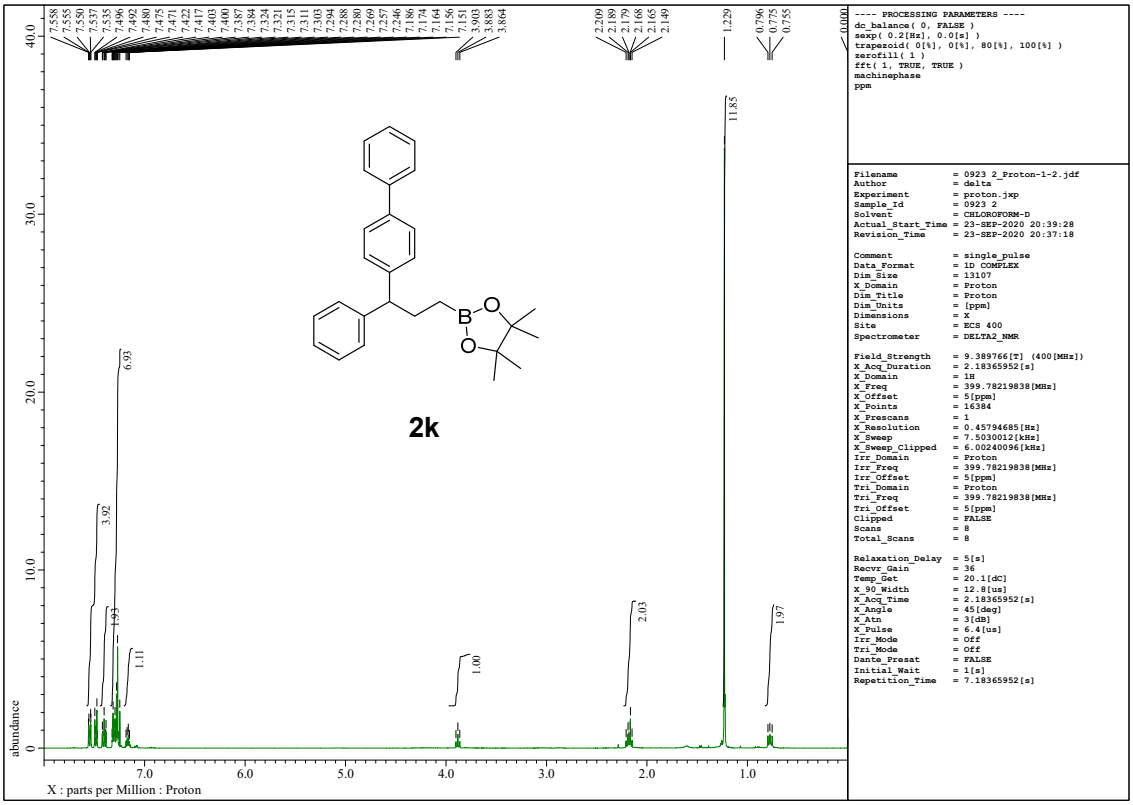

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = ky4tbutolGpc1st_Carbon-1-
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = ky4tbutolGpc1st
Solvent           = CHLOROFORM-D
Actual_Start_Time =  7-JUL-2020 17:40:00
Revision_Time     =  7-JUL-2020 19:41:38

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = TRUE
Scans             = 1202
Total_Scans       = 1202

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 20.9[dC]
X_90_Width        = 9.8[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 4.1[dB]
X_Pulse           = 3.26666667[us]
Irr_Atn_Dec       = 21.078[dB]
Irr_Atn_Noe       = 21.078[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```



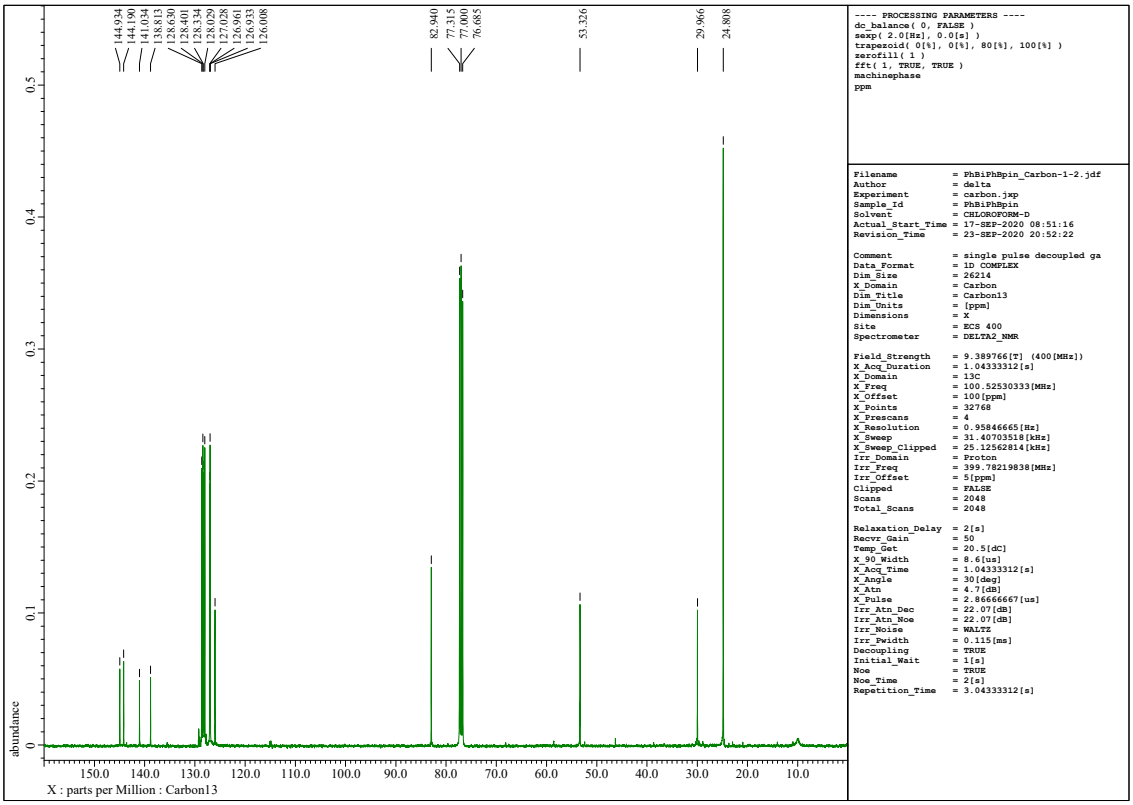

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = 0923 2_Proton-1-2.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 0923 2
Solvent           = CHLOROFORM-D
Actual_Start_Time = 23-SEP-2020 20:39:28
Revision_Time     = 23-SEP-2020 20:37:18

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECS 400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 36
Temp_Get          = 20.1[dC]
X_90_Width        = 12.8[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 3[dB]
X_Pulse           = 6.4[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.18365952[s]
```



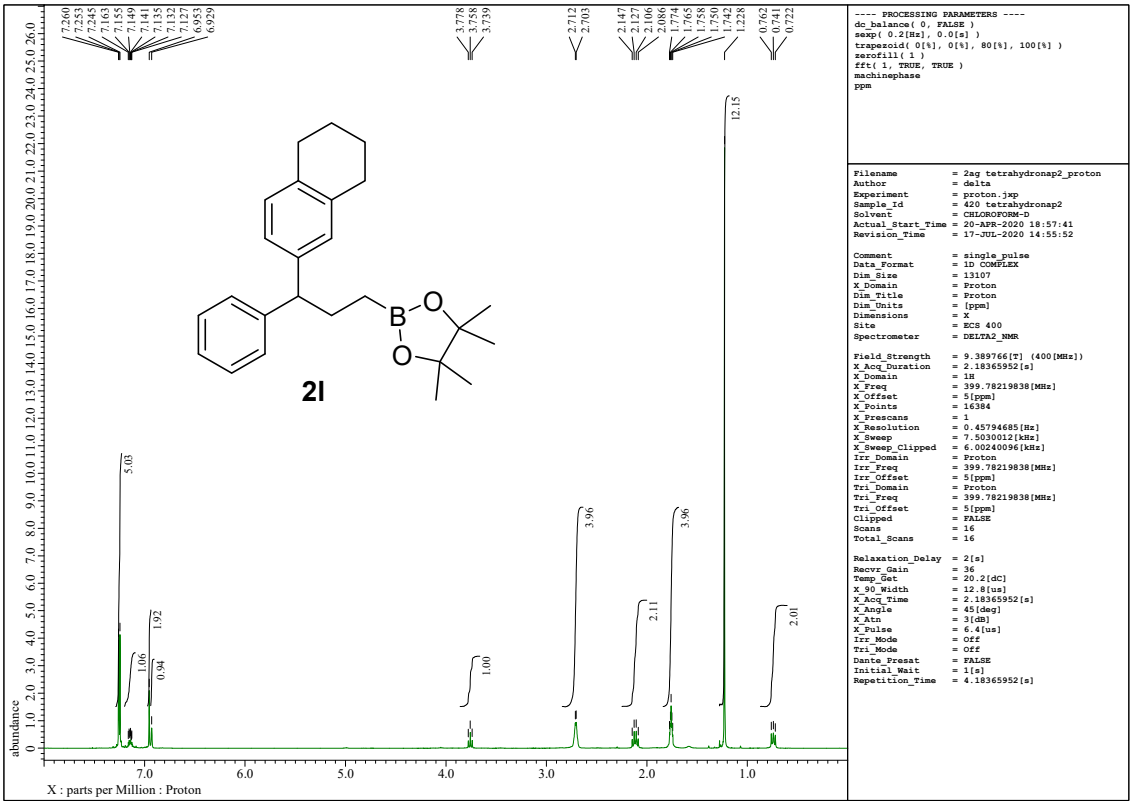

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = PhBiPhBpin_Carbon-1-2.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = PhBiPhBpin
Solvent           = CHLOROFORM-D
Actual_Start_Time = 17-SEP-2020 08:51:16
Revision_Time     = 23-SEP-2020 20:52:22

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECS 400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 2048
Total_Scans       = 2048

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 20.5[dC]
X_90_Width        = 8.6[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 4.7[dB]
X_Pulse           = 2.86666667[us]
Irr_Atn_Dec       = 22.07[dB]
Irr_Atn_Noe       = 22.07[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```



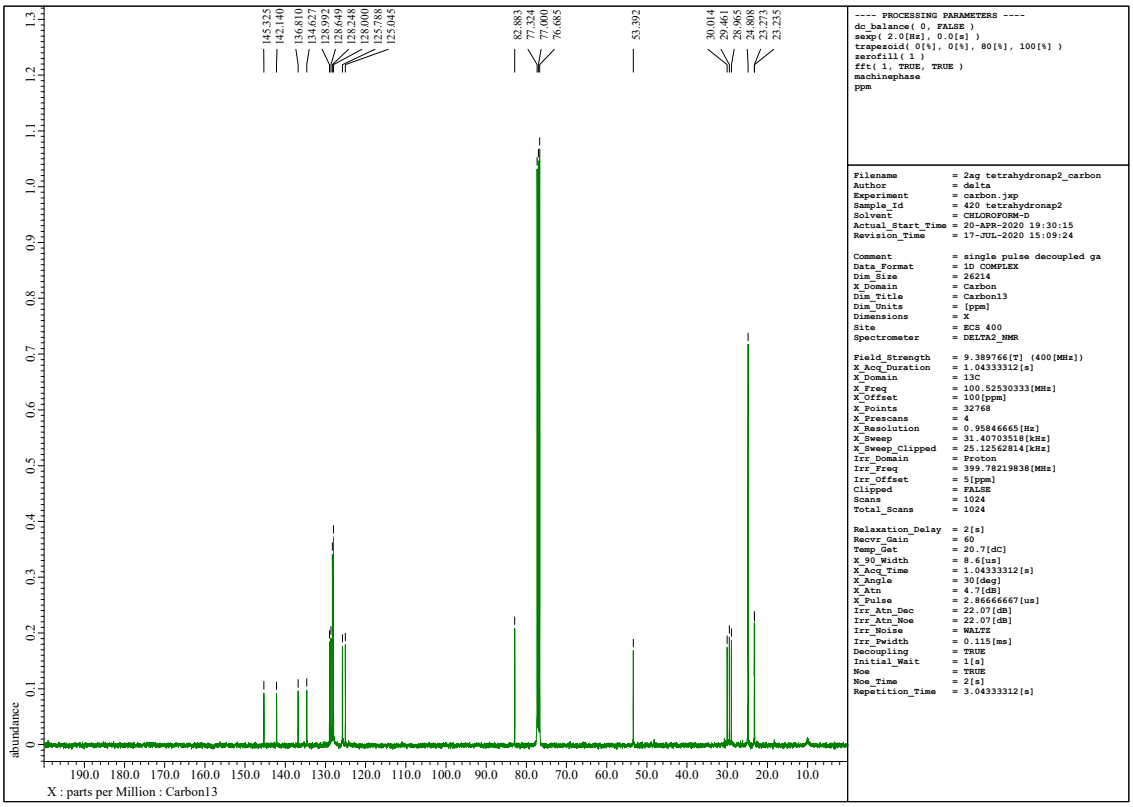

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = 2ag tetrahydronap2_proton
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 420 tetrahydronap2
Solvent           = CHLOROFORM-D
Actual_Start_Time = 20-APR-2020 18:57:41
Revision_Time     = 17-JUL-2020 14:55:52

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECS 400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 16
Total_Scans       = 16

Relaxation_Delay  = 2[s]
Recvr_Gain        = 36
Temp_Get          = 20.2[dC]
X_90_Width        = 12.8[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 3[dB]
X_Pulse           = 6.4[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 4.18365952[s]
```



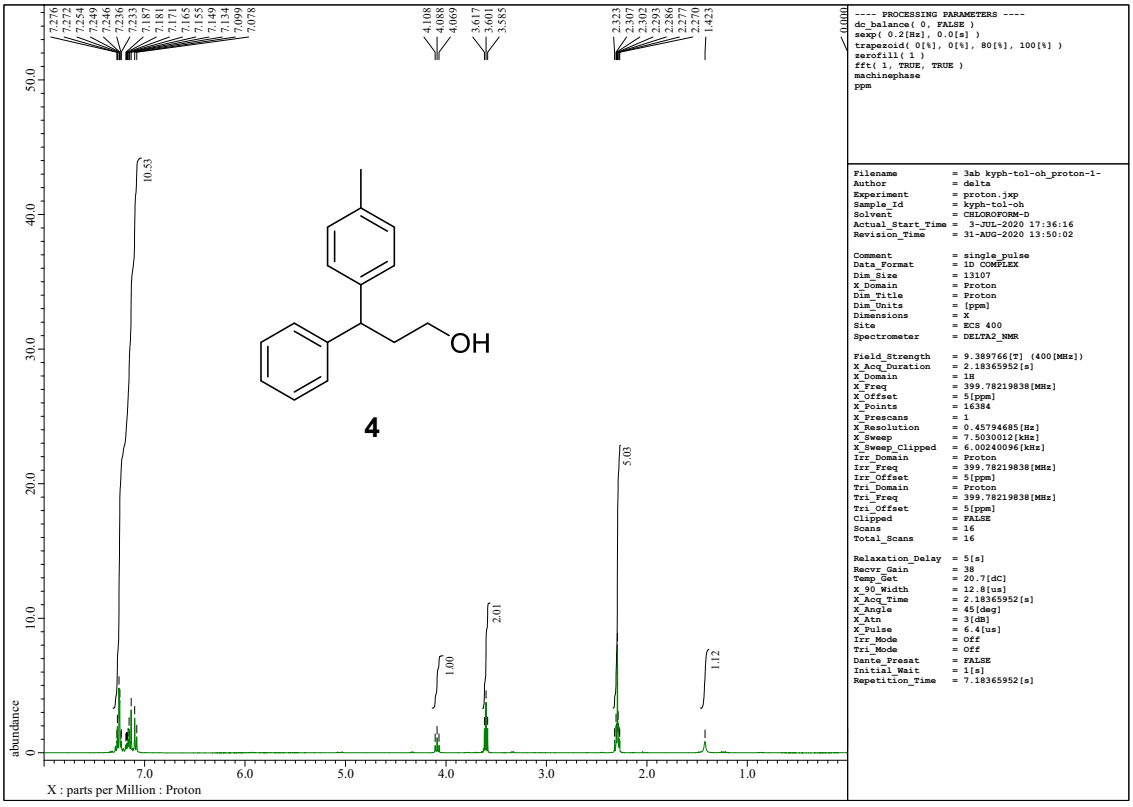

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

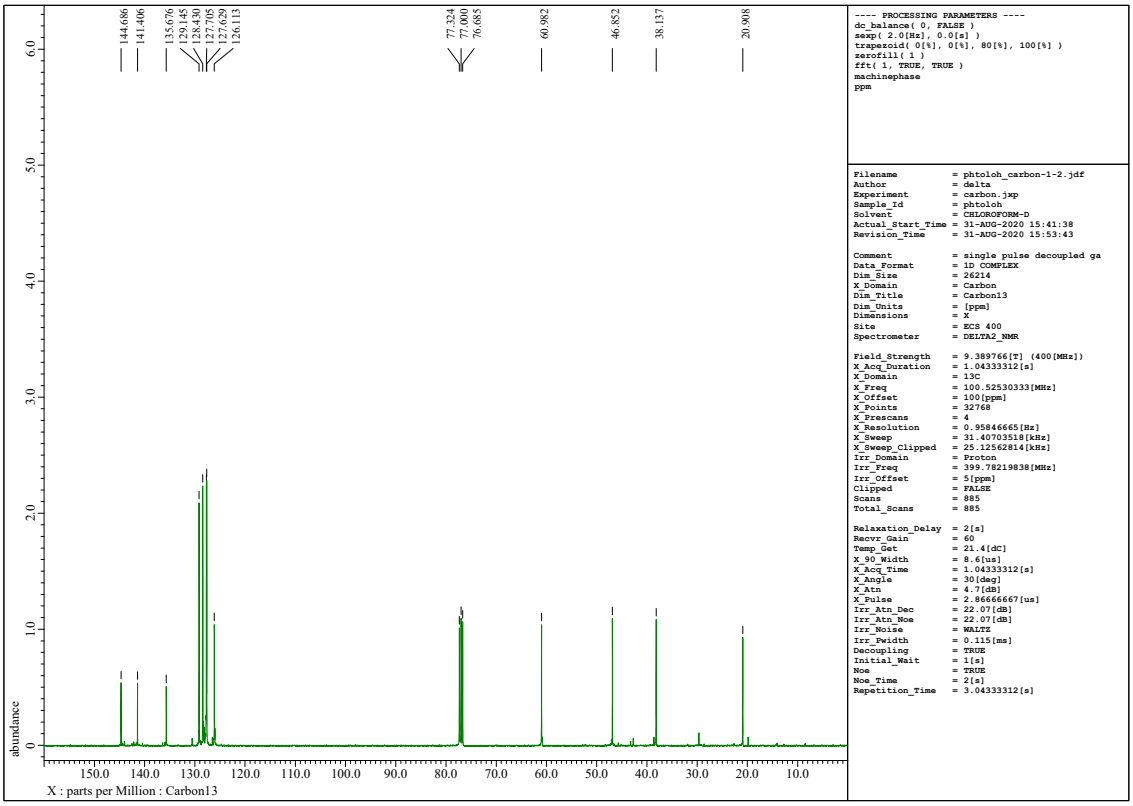
```
Filename          = 2ag tetrahydronap2_carbon
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 420 tetrahydronap2
Solvent           = CHLOROFORM-D
Actual_Start_Time = 20-APR-2020 19:30:15
Revision_Time     = 17-JUL-2020 15:09:24

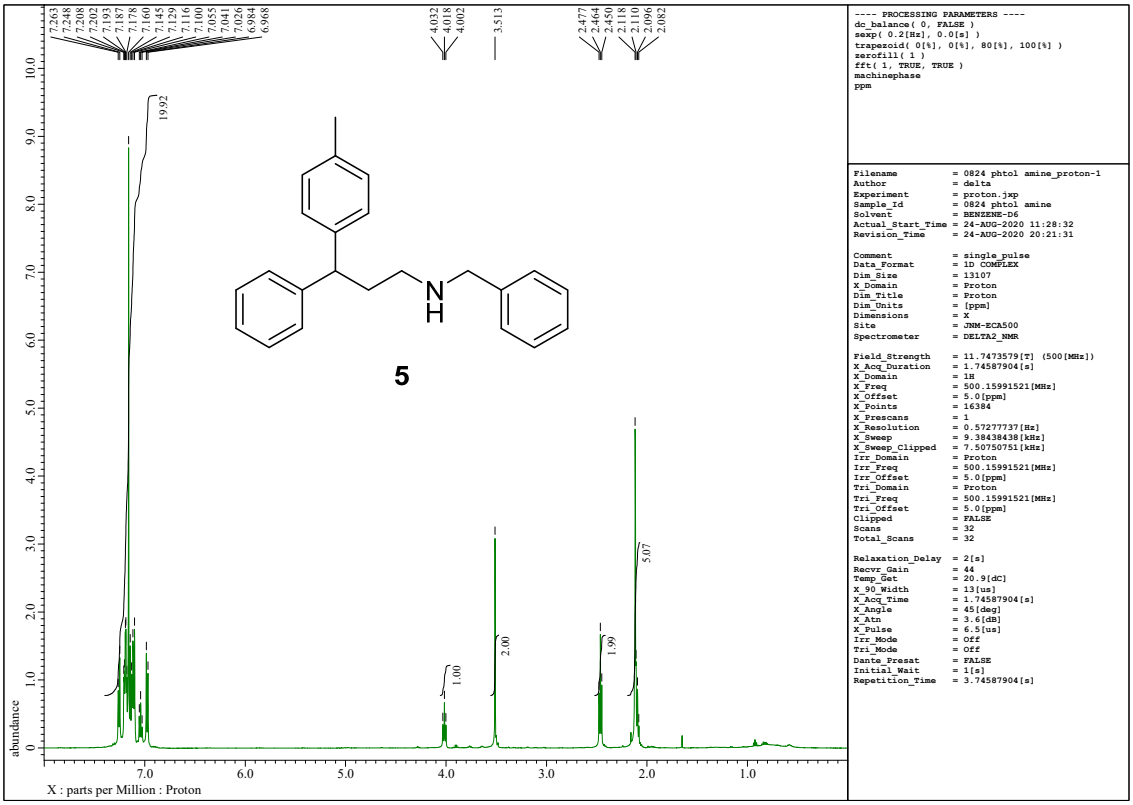
Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECS 400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 20.7[dC]
X_90_Width        = 8.6[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 4.7[dB]
X_Pulse           = 2.86666667[us]
Irr_Atn_Dec       = 22.07[dB]
Irr_Atn_Noe       = 22.07[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```

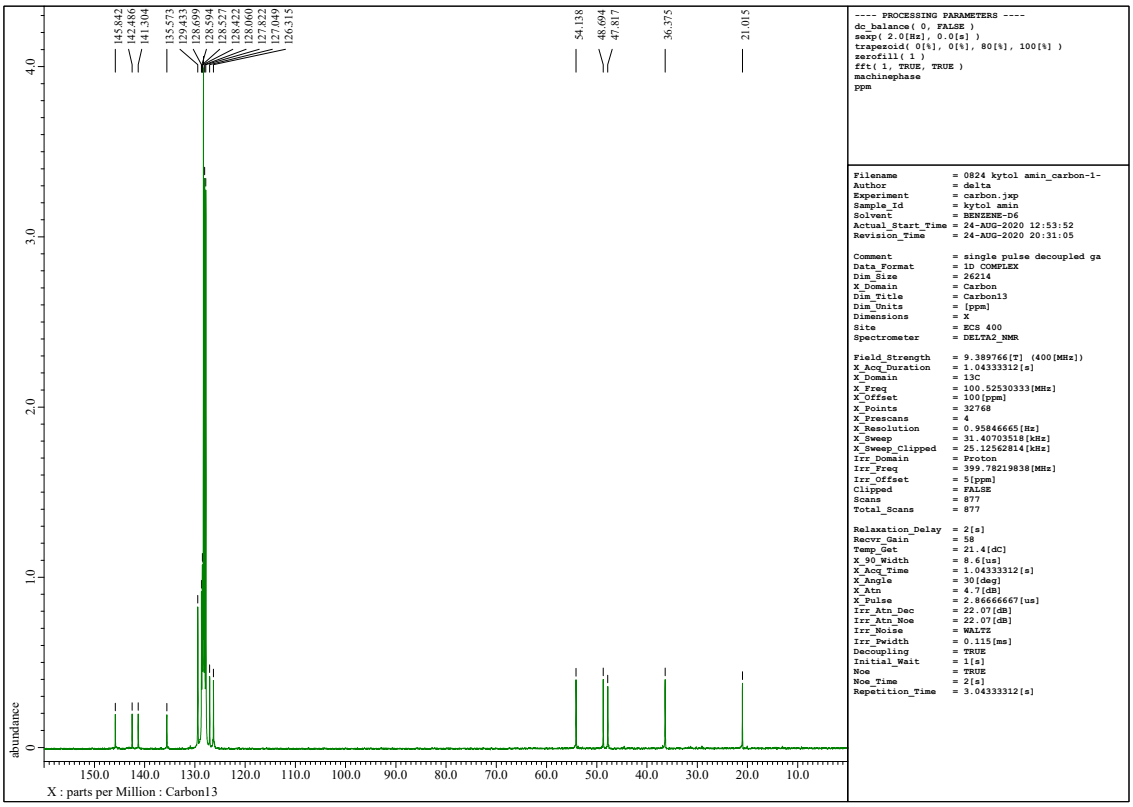

7.276
7.272
7.254
7.249
7.246
7.236
7.233
7.187
7.181
7.171
7.165
7.155
7.149
7.134
7.099
7.078
4.108
4.088
4.069
3.617
3.601
3.585
2.323
2.307
2.302
2.293
2.286
2.277
2.270
1.423
0.000
10.53
5.03
2.01
1.00
1.12
OH
4
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 3ab kyph-tol-oh_proton-1-
Author = delta
Experiment = proton.jxp
Sample_Id = kyph-tol-oh
Solvent = CHLOROFORM-D
Actual_Start_Time = 3-JUL-2020 17:36:16
Revision_Time = 31-AUG-2020 13:50:02
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
X_Sweep_Clipped = 6.00240096[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 38
Temp_Get = 20.7[dC]
X_90_Width = 12.8[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 3[dB]
X_Pulse = 6.4[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.18365952[s]


144.686
141.406
135.676
129.145
128.430
127.705
127.409
126.113
77.324
77.000
76.685
60.982
46.852
38.137
20.908
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = phtoloh_carbon-1-2.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = phtoloh
Solvent = CHLOROFORM-D
Actual_Start_Time = 31-AUG-2020 15:41:38
Revision_Time = 31-AUG-2020 15:53:43
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95846665[Hz]
X_Sweep = 31.40703518[kHz]
X_Sweep_Clipped = 25.12562814[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 885
Total_Scans = 885
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 21.4[dC]
X_90_Width = 8.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 4.7[dB]
X_Pulse = 2.86666667[us]
Irr_Atn_Dec = 22.07[dB]
Irr_Atn_Noe = 22.07[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 0824 phtol amine_proton-1
Author	= delta
Experiment	= proton.jxp
Sample_Id	= 0824 phtol amine
Solvent	= BENZENE-D6
Actual_Start_Time	= 24-AUG-2020 11:28:32
Revision_Time	= 24-AUG-2020 20:21:31
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECA500
Spectrometer	= DELTA2_NMR
Field_Strength	= 11.7473579[T] (500[MHz])
X_Acq_Duration	= 1.74587904[s]
X_Domain	= 1H
X_Freq	= 500.15991521[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.57277737[Hz]
X_Sweep	= 9.38438438[kHz]
X_Sweep_Clipped	= 7.50750751[kHz]
Irr_Domain	= Proton
Irr_Freq	= 500.15991521[MHz]
Irr_Offset	= 5.0[ppm]
Tri_Domain	= Proton
Tri_Freq	= 500.15991521[MHz]
Tri_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 32
Total_Scans	= 32
Relaxation_Delay	= 2[s]
Recvr_Gain	= 44
Temp_Get	= 20.9[dC]
X_90_Width	= 13[us]
X_Acq_Time	= 1.74587904[s]
X_Angle	= 45[deg]
X_Atn	= 3.6[dB]
X_Pulse	= 6.5[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 3.74587904[s]




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 0824 kytol amin_carbon-1-
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= kytol amin
Solvent	= BENZENE-D6
Actual_Start_Time	= 24-AUG-2020 12:53:52
Revision_Time	= 24-AUG-2020 20:31:05
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.52530333[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 877
Total_Scans	= 877
Relaxation_Delay	= 2[s]
Recvr_Gain	= 58
Temp_Get	= 21.4[dC]
X_90_Width	= 8.6[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 4.7[dB]
X_Pulse	= 2.86666667[us]
Irr_Atn_Dec	= 22.07[dB]
Irr_Atn_Noe	= 22.07[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.04333312[s]