Supplementary Text 1

Materials and Methods

List of cell culture reagents.

Cell culture reagents were procured from Gibco Laboratories (Grand Island, NY, USA). ECL western blotting detection reagent was procured from GE Healthcare (Buckinghamshire, UK). Various primary antibodies used in the study were obtained from Cell Signaling Technology (MA, USA). Phorbol 12-myristate 13-acetate (PMA), monodansylcadaverine (MDC, a fluorescent dye that stains autophagic vacuoles), anti-rabbit HRP antibody, Bafilomycin A1 (Baf-A1, a vacuolar ATPase inhibitor), BCA kit, 100 × protease inhibitor cocktail and Fluoromount aqueous mounting medium were procured from Sigma (St. Louis, MO, USA). Middlebrook growth media 7H9 broth, 7H10 agar, 7H11 agar was ordered from BD (MD, USA). WST-1 cell viability assay kit and other general chemicals unless not mentioned were obtained from HiMedia Laboratory (Mumbai, India).

Chemical synthesis and characterization of various pyrazole derivatives

General procedure for the synthesis of compounds 3a-f.

For synthesis of the pyrazole derivatives, the commercially available acetylacetone (500 mg, 4.99 mmol) and compound 2a-f (4.99 mmol) were mixed in a round bottom flask containing 5 mL glycerol-water (1:1) mixture as a solvent and heated for 3-4 hrs at 90˚C with continuous stirring. The progress of the reaction was monitored by TLC and the reaction mixture was allowed to cool upon completion. The desired final product was extracted multiple times using ethyl acetate. The combined organic layer was washed with water, brine solution, dried by adding anhydrous Na_2SO_4 and the final product was purified by column chromatography.

1-(4-Methoxyphenyl)-3,5-dimethyl-1H-pyrazole (3a): Light yellow oil; Yield: 82%; IR (KBr, cm^{-1}): 2964, 1553, 1514, 1246, 745; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.23 (s, 3H), 2.28 (s, 3H), 3.83 (s, 3H), 5.95 (s, 1H), 6.94 (d, J = 8.70 Hz, 2H), 7.31 (d, J = 8.70 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 12.22, 13.58, 55.60, 106.32, 114.17, 126.46, 133.16, 139.56, 148.60, 158.84; ESI-HRMS (m/z) calculated for $C_{12}H_{14}N_2O$: 202.1106; observed: 203.2461 $(MH)^+$.

3,5-dimethyl-1-phenyl-1H-pyrazole (3b): Light yellow oil; Yield: 80%; IR (KBr, cm^{-1}): 2922, 1596, 1500, 1373, 1025, 753; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.30 (s, 6H), 5.99 (s, 1H), 7.32-7.35 (m, 1H), 7.41-7.46 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 12.46, 13.59, 106.99, 124.84, 127.33, 129.07, 139.48, 139.97, 149.04; ESI-HRMS (m/z) calculated for $C_{11}H_{12}N_2$: 172.1000; observed: 173.1453 $(MH)^+$.

3,5-dimethyl-1-(o-tolyl)-1H-pyrazole (3c): Brown liquid; Yield: 83%; IR (KBr, cm^{-1}): 2923, 1583, 1552, 1287, 1129, 1031, 775; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.05 (s, 6H), 2.29 (s, 3H), 5.96 (s, 1H), 7.22-7.33 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 11.35, 13.66, 17.30, 105.00, 126.50, 128.00, 129.00,

130.89, 136.39, 138.83, 140.29, 148.57; ESI-HRMS (m/z) calculated for $C_{12}H_{14}N_2$: 186.1157; observed: 187.1643 $(MH)^+$.

1-(2-Chlorophenyl)-3,5-dimethyl-1H-pyrazole (3d): Light yellow oil; Yield: 82%; IR (KBr, cm^{-1}): 2968, 1556, 1496, 1217, 1032, 745, 660; ^1H NMR (400 MHz, $CDCl_3$): δ 2.12 (s, 3H), 2.31 (s, 3H), 6.00 (s, 1H), 7.37-7.41 (m, 3H), 7.50-7.53 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 11.32, 13.69, 105.58, 127.61, 130.02, 130.24, 132.60, 137.56, 141.29, 149.36; ESI-HRMS (m/z) calculated for $C_{11}H_{11}ClN_2$: 206.0611; observed: 207.0686 $(MH)^+$, 209.0645 $(MH+2)^+$.

1-(3-Chlorophenyl)-3,5-dimethyl-1H-pyrazole (3e): Light yellow oil; Yield: 85%; IR (KBr, cm^{-1}): 2973, 1590, 1556, 1489, 1216, 744, 686; ^1H NMR (400 MHz, $CDCl_3$): δ 2.28 (s, 3H), 2.32 (s, 3H), 6.00 (s, 1H), 7.29-7.37 (m, 3H), 7.47-7.48 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 12.59, 13.57, 107.64, 122.56, 124.88, 127.29, 130.02, 134.74, 139.57, 141.03, 149.60; ESI-HRMS (m/z) calculated for $C_{11}H_{11}ClN_2$: 206.0611; observed: 207.0874 $(MH)^+$, 209.0732 $(MH+2)^+$.

1-(4-Chlorophenyl)-3,5-dimethyl-1H-pyrazole (3f): Light yellow oil; Yield: 75%; IR (KBr, cm^{-1}): 2973, 1554, 1498, 1216, 1037, 744, 665; ^1H NMR (400 MHz, $CDCl_3$): δ 2.28-2.29 (m, 6H), 5.99 (s, 1H), 7.35-7.42 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 12.48, 13.56, 107.42, 125.87, 129.22, 132.93, 138.41, 139.50, 149.43; ESI-HRMS (m/z) calculated for $C_{11}H_{11}ClN_2$: 206.0611; observed: 207.0848 $(MH)^+$, 209.0719 $(MH+2)^+$.

General procedure for the synthesis of compounds 5b-k.

Acetylacetone (500 mg, 4.99 mmol) was mixed in a round bottom flask containing diluted HCl (5 mL) and the mixture was cooled in ice bath to 37˚C followed by the addition of $NaNO_2$ (344.95 mg, 5 mmol, 5 mL H_2O) solution. The reaction mixture was subsequently left undisturbed for 20 mins. Simultaneously, substituted phenyl hydrazine hydrochloride (4.99 mmol) was dissolved in a mixture of polyethylene glycol-water (1:1) solvent system. The solution of substituted phenyl hydrazine hydrochloride was added dropwise to the above reaction mixture with continuous stirring and the temperature of the reaction mixture was slowly allowed to rise to 37˚C from room temperature. The obtained green precipitate was filtered, washed with 50% PEG solution, dried and purified by column chromatography using silica gel and ethyl acetate-hexane as a solvent system.

3,5-dimethyl-4-nitroso-1-phenyl-1H-pyrazole (5b): Greenish solid; Yield: 64%; mp 96-98 ºC; IR (KBr, cm^{-1}): 2923, 1543, 1511, 1383, 1088, 1016, 766; ^1H NMR (400 MHz, $CDCl_3$): δ 2.43 (s, 3H), 2.94 (s, 3H), 7.50-7.58 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 11.06, 12.98, 124.99, 129.14, 129.45, 137.61, 160.66; ESI-HRMS (m/z) calculated for $C_{11}H_{11}N_3O$: 201.0902 ; observed: 202.0976 $(MH)^+$.

3,5-dimethyl-4-nitroso-1-(o-tolyl)-1H-pyrazole (5c): Greenish solid; Yield: 66%; mp 68-70 ºC; IR (KBr, cm^{-1}): 2929, 1539, 1512, 1338, 1236, 1018, 771; ^1H NMR (400 MHz, $CDCl_3$): δ 2.14 (s, 3H), 2.45(brs, 3H), 2.66 (brs, 3H), 7.28-7.45 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 10.57, 13.16, 17.44, 127.16, 127.32, 130.42, 131.53, 135.69, 136.44, 160.27; ESI-HRMS (m/z) calculated for $C_{12}H_{13}N_3O$: 215.1059; observed: 216.1125 $(MH)^+$.

1-(2-Chlorophenyl)-3,5-dimethyl-4-nitroso-1H-pyrazole (5d): Greenish solid; Yield: 65%; mp 116-118 ºC; IR (KBr, cm^{-1}): 2920, 1546, 1513, 1349, 1225, 1098, 768, 718; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.44(brs, 3H), 2.76 (brs, 3H), 7.48-7.63 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 10.56, 13.20, 128.18, 129.39, 130.71, 131.67, 132.02, 135.31, 160.13; ESI-HRMS (m/z) calculated. for $C_{11}H_{10}ClN_3O$: 235.0512; observed: 236.0581 $(MH)^+$, 238.0557 $(MH+2)^+$.

1-(3-Chlorophenyl)-3,5-dimethyl-4-nitroso-1H-pyrazole (5e): Greenish solid; Yield: 69%; mp 87-89 ºC; IR (KBr, cm^{-1}): 2922, 1591, 1544, 1350,1222, 1078, 777, 682; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.41 (s, 3H), 2.97 (s, 3H), 7.42-7.43 (m, 1H), 7.49-7.50 (m, 2H), 7.57 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 11.27, 13.09, 123.12, 125.48, 129.46, 130.58, 135.43, 138.86, 160.65; ESI-HRMS (m/z) calculated for $C_{11}H_{10}ClN_3O$: 235.0512; observed: 236.0606 $(MH)^+$, 238.058 $(MH+2)^+$.

1-(2-Chlorophenyl)-3,5-dimethyl-4-nitroso-1H-pyrazole (5f) Greenish solid; Yield: 70%; mp 120-122 ºC; IR (KBr, cm^{-1}): 2927, 1543, 1508, 1344, 1235, 1085, 827, 769; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.40 (s, 3H), 2.95 (s, 3H), 7.47 (d, J = 8.70 Hz, 2H), 7.54 (d, J = 8.24 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 11.24, 13.10, 126.33, 129.84, 135.26, 136.32, 160.70; ESI-HRMS (m/z) calculated for $C_{11}H_{10}ClN_3O$: 235.0512; observed: 236.0597 $(MH)^+$, 238.0579 $(MH+2)^+$.

3,5-dimethyl-4-nitroso-1-(p-tolyl)-1H-pyrazole (5g): Greenish solid; Yield: 67%; mp 114-116 ºC; IR (KBr, cm^{-1}): 2926, 1541, 1517, 1342, 1232, 1080, 817; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.41-2.45 (m, 6H), 2.91 (brs, 3H), 7.33-7.39 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 9.02, 10.95, 19.12, 122.82, 127.98, 133.09, 137.38, 158.58; ESI-HRMS (m/z) calculated for $C_{12}H_{13}N_3O$: 215.1059; observed: 216.2504 $(MH)^+$.

1-(4-Bromophenyl)-3,5-dimethyl-4-nitroso-1H-pyrazole (5h): Greenish solid; Yield: 62%; mp 118-120 ºC; IR (KBr, cm^{-1}): 2925, 1543, 1508, 1348, 1228, 1072, 769, 705; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.40 (brs, 3H), 2.96 (brs, 3H), 7.41 (d, J = 8.24 Hz, 2H), 7.70 (d, J = 8.70 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 11.26, 13.11, 123.25, 126.57, 132.82, 136.83, 160.71; ESI-HRMS (m/z) calculated for $C_{11}H_{10}BrN_3O$: 279.0007; observed: 280.0074 $(MH)^+$, 282.0058 $(MH+2)^+$.

4-(3,5-dimethyl-4-nitroso-1H-pyrazol-1-yl)benzonitrile (5i): Greenish solid; Yield: 65%; mp 126-128 ºC; IR (KBr, cm^{-1}): 2932, 2227, 1544, 1510, 1336, 1230, 839, 771; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.39 (s, 3H), 3.06 (s, 3H), 7.73 (d, J = 8.24 Hz, 2H), 7.87 (d, J = 8.24,, Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 11.51, 13.14, 112.80, 117.78, 125.28, 133.59, 141.46, 160.62; ESI-HRMS (m/z) calculated for $C_{12}H_{10}N_4O$: 226.0855; observed: 227.0936 $(MH)^+$.

1-(3,4-dimethylphenyl)-3,5-dimethyl-4-nitroso-1H-pyrazole (5j): Greenish solid; Yield: 65%; mp 106-108 ºC; IR (KBr, cm^{-1}): 2922, 1541, 1514, 1323, 1172, 1043, 790; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.31-2.42 (m, 9H), 2.90 (brs, 3H), 7.19 (d, J = 7.79 Hz, 1H), 7.27-7.30 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 11.01, 12.93, 19.46, 19.75, 122.15, 125.93, 126.03, 130.31, 135.26, 138.02, 138.16, 160.66; ESI-HRMS (m/z) calculated for $C_{13}H_{15}N_3O$: 229.1215; observed: 230.1285 $(MH)^+$.

1-(2,5-dichlorophenyl)-3,5-dimethyl-4-nitroso-1H-pyrazole (5k): Greenish solid; Yield: 67%; mp 98-100 ºC; IR (KBr, cm^{-1}): 2926, 1541, 1465, 1344, 1255, 1095, 817, 777; ^{1}H NMR (400 MHz, $CDCl_3$):

δ 2.44 (s, 3H), 2.77 (s, 3H), 7.49-7.57 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 10.58, 13.13, 129.66, 130.42, 131.50, 131.80, 133.82, 136.16, 159.93; ESI-HRMS (m/z) calculated for $C_{11}H_9Cl_2N_3O$: 269.0123; observed: 270.0339 $(MH)^+$, 272.0264 $(MH+2)^+$, 274.0155$(MH+4)^+$.

Procedure for the synthesis of 3,5-dimethyl-1-phenyl-1H-pyrazol-4-amine (6).

Compound 3,5-dimethyl-4-nitroso-1-phenyl-1*H*-pyrazole (500 mg, 2.48 mmol) was dissolved in methanol (5 mL) and hydrogen gas was passed in the presence of Pd/C (50 mg) at 60 psi pressure followed by shaking for 3-4 hrs at room temperature. The completion of reaction was determined by TLC, palladium was removed by filtering through celite pad and followed by washing with methanol. The filtrate obtained was combined and dried using rotavapor at reduced pressure. Subsequently, 50 mL diluted HCL was added to the crude product with stirring. The impurities were removed by the addition of ethyl acetate, the-aqueous layer containing final product was neutralised with saturated K_2CO_3 solution and finally isolated by extraction with ethyl acetate.

3,5-dimethyl-1-phenyl-1H-pyrazol-4-amine (6): Yellow solid; Yield: 85%; mp 64-66 ºC 67 ºC; IR (KBr, cm^{-1}): 3323, 2921, 1598, 1438, 1368, 1215, 1074, 766; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.20 (s, 3H), 2.22 (s, 3H), 2.57 (brs, 2H), 7.24-7.42 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 10.41, 11.00, 124.20, 124.94, 126.81, 127.14, 129.08, 140.28, 140.98; ESI-HRMS (m/z) calculated for $C_{11}H_{13}N_3$: 187.1109; observed: 188.1328 $(MH)^+$.

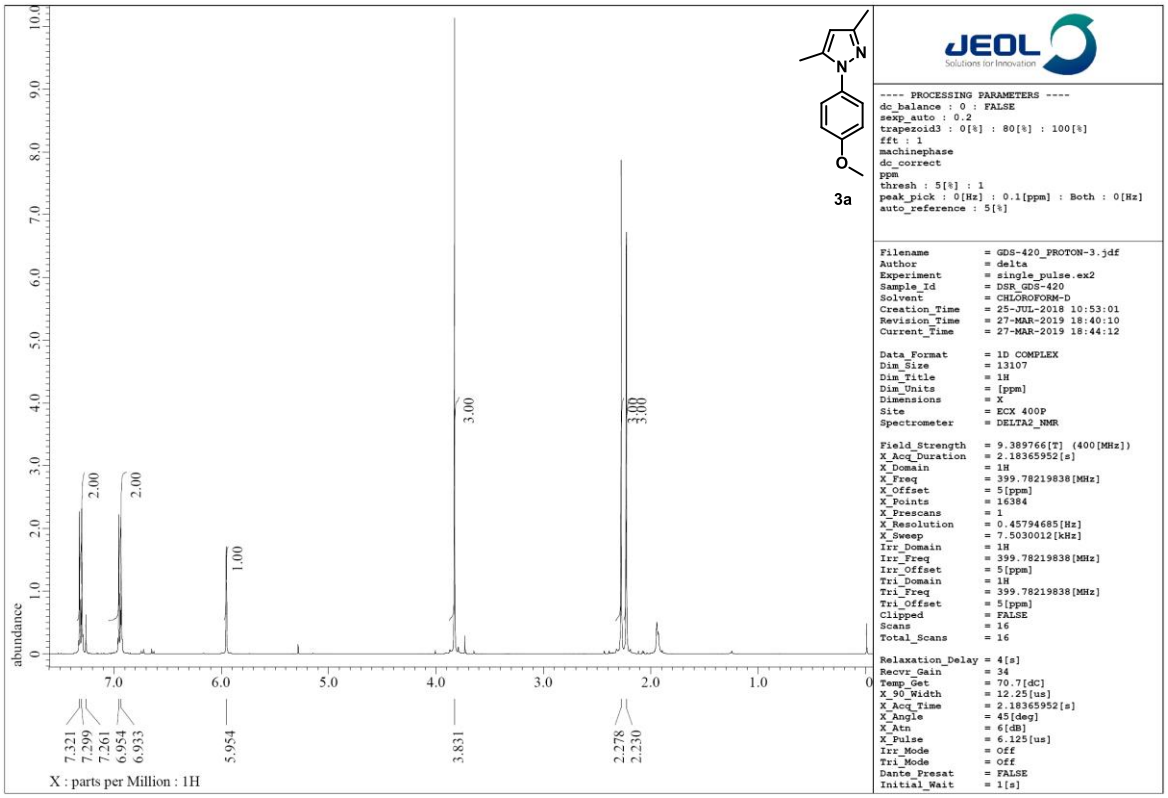
Procedure for the synthesis of 4-bromo/chloro-3,5-dimethyl-1-phenyl-1H-pyrazole (7a-b).

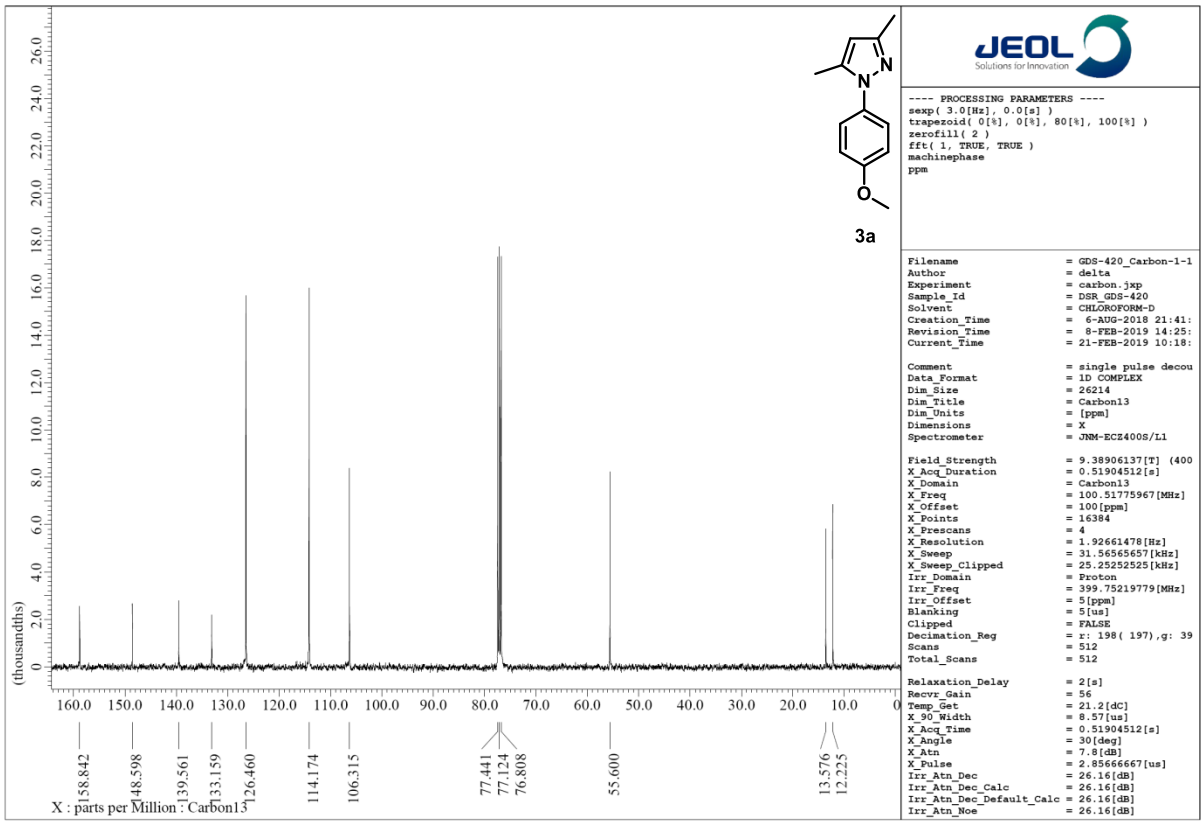
The synthesized compound 3,5-dimethyl-1-phenyl-1*H*-pyrazole (300 mg, 1.74 mmol) and N-halo-succinimide (1.74 mmol) were taken in a round bottom flask containing 5 mL of water. The reaction mixture containing N-bromosuccinimide or N-chlorosuccinimide was stirred at room temperature or at 37 ˚C, respectively for 2 hrs. The completion of reaction was confirmed by TLC and the product was extracted with ethyl acetate multiple times. The combined organic layer was washed with water and brine, dried by the addition of Na_2SO_4 and ethyl acetate to purify the desired products.

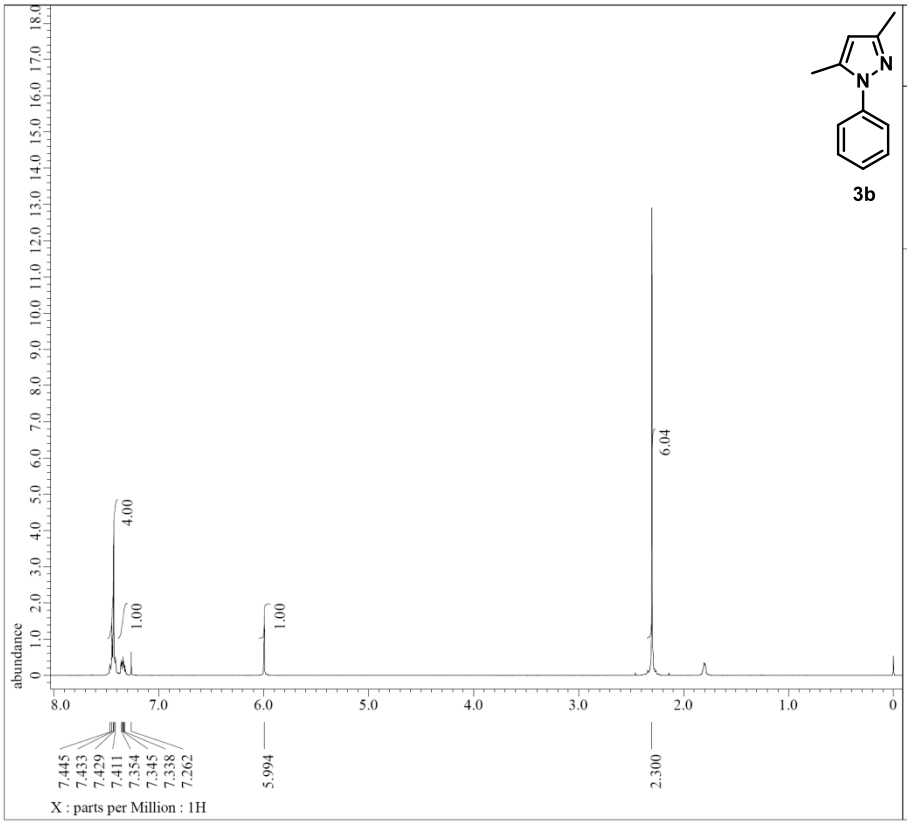
4-Bromo-3,5-dimethyl-1-phenyl-1H-pyrazole (7a): Yellow oil; Yield: 75%; IR (KBr, cm^{-1}): 2982, 1597, 1502, 1373, 1216, 1080, 744, 691; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.30 (s, 6H), 7.38-7.41 (m, 3H), 7.45-7.47 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 11.69, 12.29, 96.07, 124.60, 127.75, 129.10, 137.44, 139.70, 147.50; ESI-HRMS (m/z) calculated for $C_{11}H_{11}BrN_2$: 250.0106; observed: 251.0179 $(MH)^+$, 253.0159 $(MH+2)^+$.

4-Chloro-3,5-dimethyl-1-phenyl-1H-pyrazole (7b): Yellow oil; Yield: 75%; IR (KBr, cm^{-1}): 2923, 1596, 1501, 1374, 1272, 1099, 760, 692; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.30 (s, 6H), 7.37-7.46 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 10.91, 11.49, 109.89, 124.62, 127.81, 129.26, 135.79, 139.82, 146.14; ESI-HRMS (m/z) calculated for $C_{11}H_{11}ClN_2$: 206.0611; observed: 207.0930 $(MH)^+$, 209.0757 $(MH+2)^+$.

Characterization details of various scaffolds prepared in the present study.





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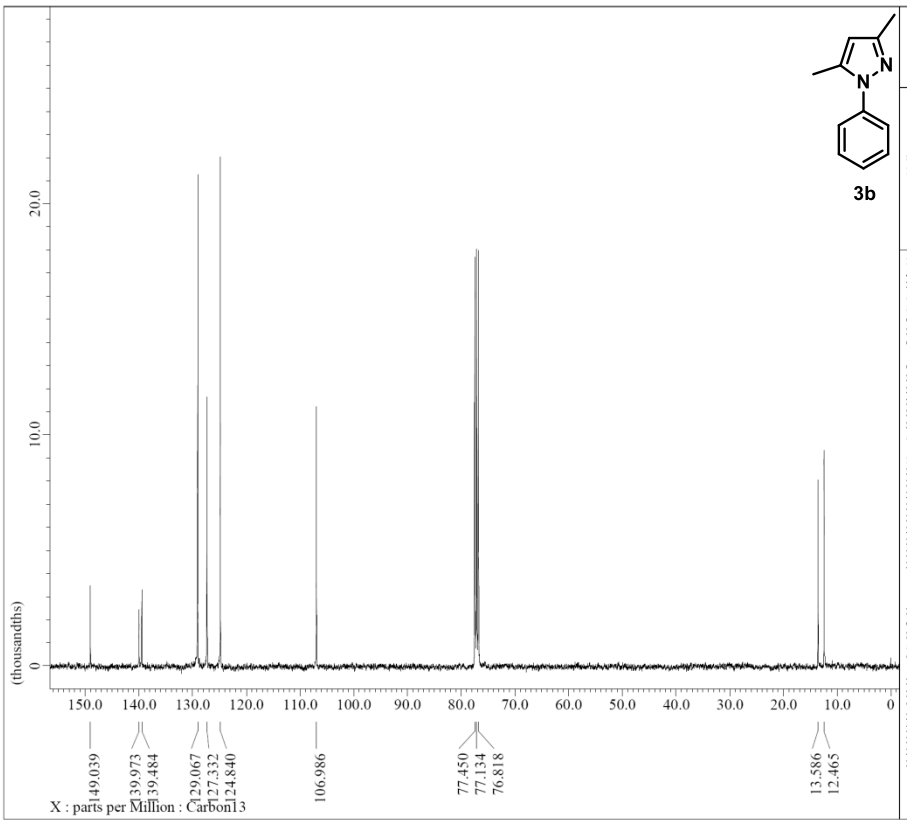


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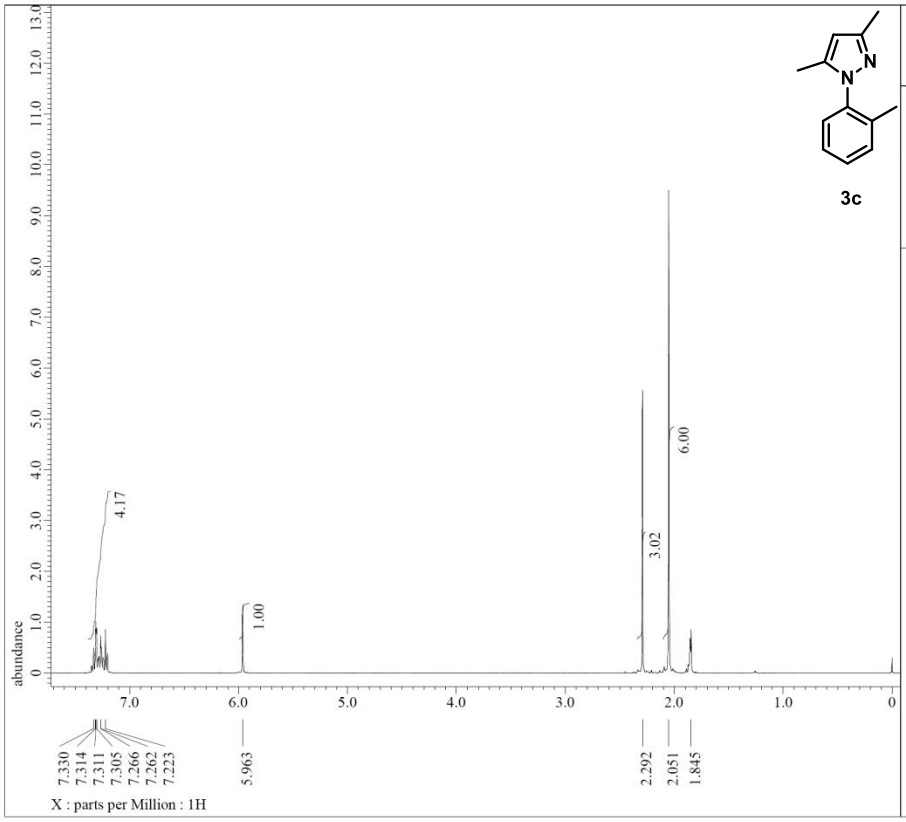


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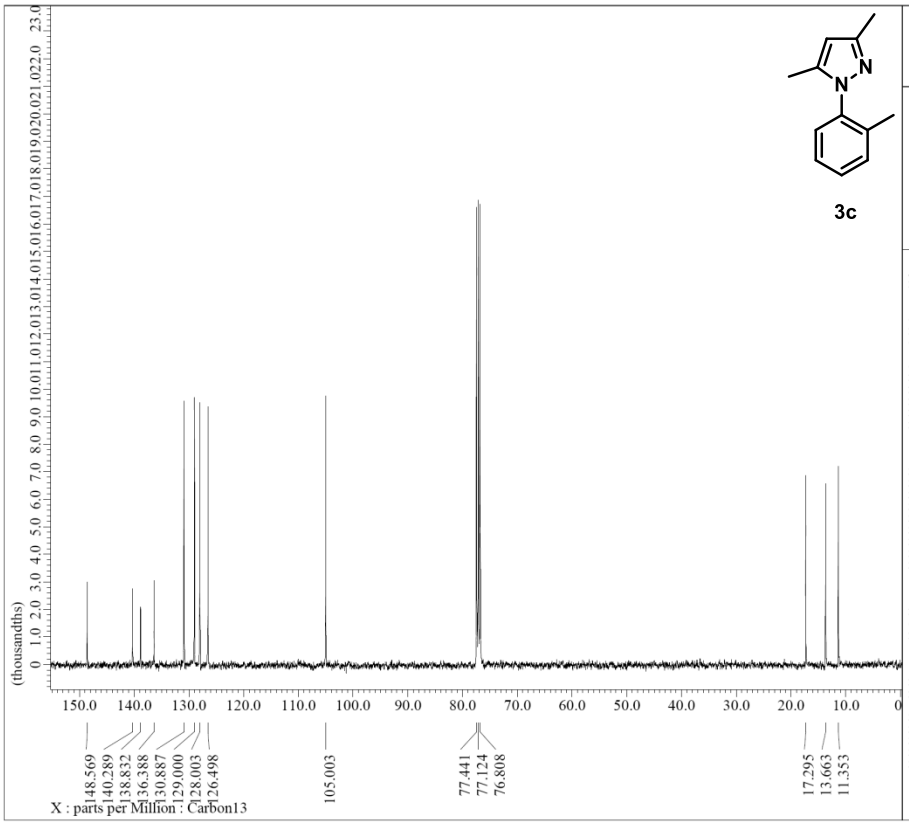
X_Angle             = 45[deg]
X_Atn               = 6[dB]
X_Pulse             = 6.125[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
```



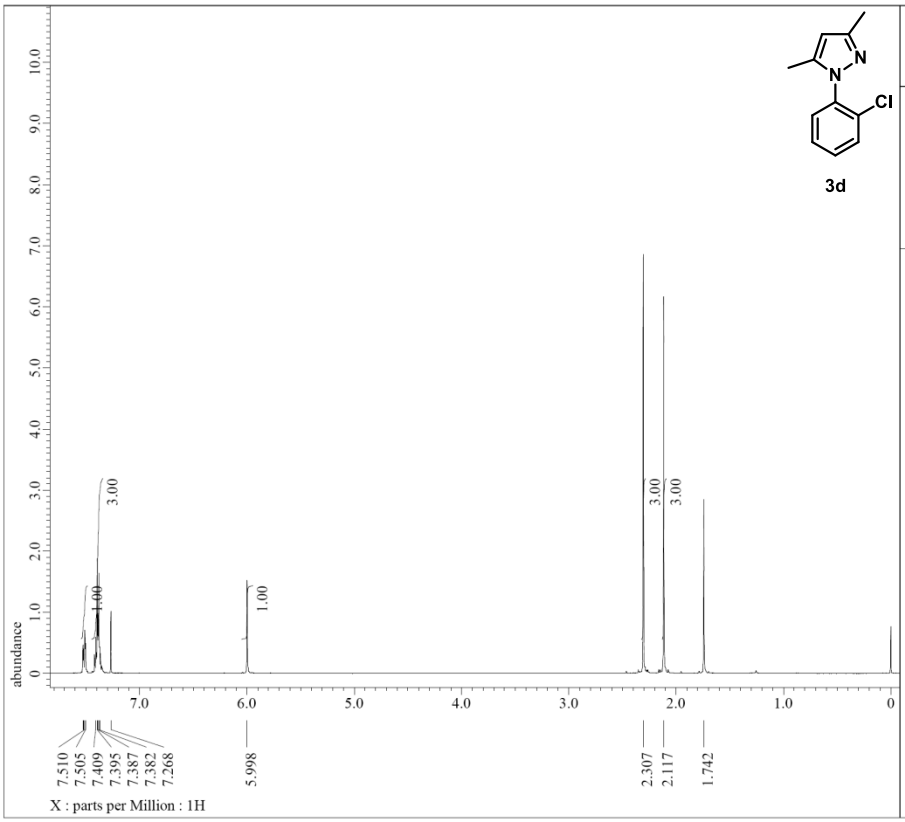

```
---- PROCESSING PARAMETERS ----
sexp( 3.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 2 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                = GDS-423_Carbon-1-1
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = DSR_GDS-423
Solvent                 = CHLOROFORM-D
Creation_Time           =  6-AUG-2018 21:15:
Revision_Time           =  8-FEB-2019 14:51:
Current_Time            = 21-FEB-2019 12:02:

Comment                 = single pulse decou
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.38906137[T] (400
X_Acq_Duration          = 0.51904512[s]
X_Domain                = Carbon13
X_Freq                  = 100.51775967[MHz]
X_Offset                = 100[ppm]
X_Points                = 16384
X_Prescans              = 4
X_Resolution            = 1.92661478[Hz]
X_Sweep                 = 31.56565657[kHz]
X_Sweep_Clipped         = 25.25252525[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.75219779[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 5[us]
Clipped                 = FALSE
Decimation_Reg          = x: 198( 197),g: 39
Scans                   = 512
Total_Scans             = 512

Relaxation_Delay        = 2[s]
Recvr_Gain              = 56
Temp_Get                = 21.1[dC]
X_90_Width              = 8.57[us]
X_Acq_Time              = 0.51904512[s]
X_Angle                 = 30[deg]
X_Atn                   = 7.8[dB]
X_Pulse                 = 2.85666667[us]
Irr_Atn_Dec             = 26.16[dB]
Irr_Atn_Dec_Calc        = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe             = 26.16[dB]
```



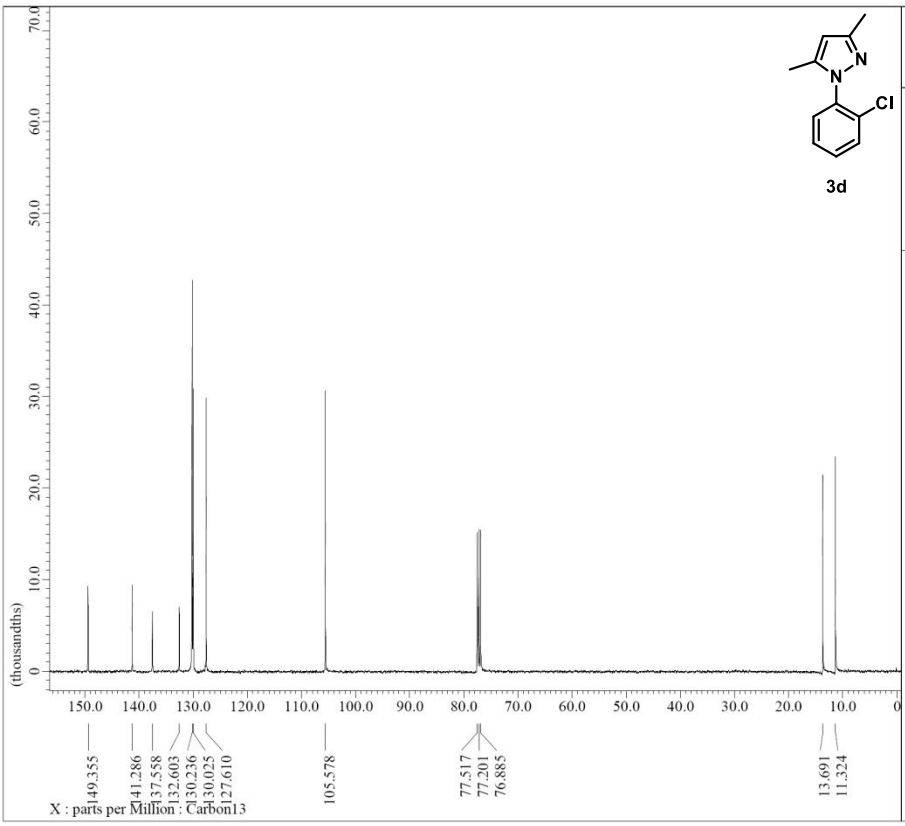

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
```

```
Filename          = GDS-421_PROTON-2.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = DSM_GDS-421
Solvent           = CHLOROFORM-D
Creation_Time     = 26-JUL-2018 09:34:21
Revision_Time     = 21-FEB-2019 12:10:18
Current_Time      = 21-FEB-2019 12:10:39

Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
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]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 16
Total_Scans       = 16

Relaxation_Delay  = 4[s]
Recvr_Gain        = 38
Temp_Get          = 71.7[dC]
X_90_Width        = 12.25[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 6[dB]
X_Pulse           = 6.125[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
```



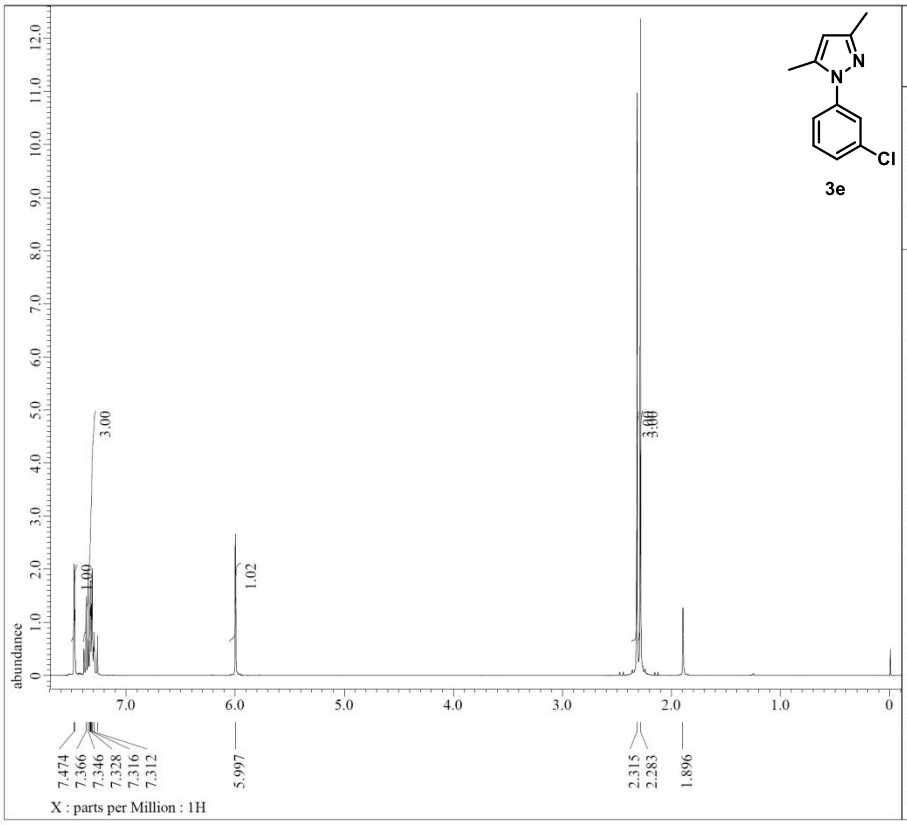

```
---- PROCESSING PARAMETERS ----
sexp( 3.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 2 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                = GDS-421_Carbon-1-1
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = DB_GDS-421
Solvent                 = CHLOROFORM-D
Creation_Time           =  7-AUG-2018 23:09:
Revision_Time           =  8-FEB-2019 14:37:
Current_Time            = 21-FEB-2019 12:15:

Comment                 = single pulse decou
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.38906137[T] (400
X_Acq_Duration          = 0.51904512[s]
X_Domain                = Carbon13
X_Freq                  = 100.51775967[MHz]
X_Offset                = 100[ppm]
X_Points                = 16384
X_Prescans              = 4
X_Resolution            = 1.92661478[Hz]
X_Sweep                 = 31.56565657[kHz]
X_Sweep_Clipped         = 25.25252525[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.75219779[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 5[us]
Clipped                 = FALSE
Decimation_Reg          = r: 198( 197),g: 39
Scans                   = 512
Total_Scans             = 512

Relaxation_Delay        = 2[s]
Recvr_Gain              = 56
Temp_Get                = 20.7[dC]
X_90_Width              = 8.57[us]
X_Acq_Time              = 0.51904512[s]
X_Angle                 = 30[deg]
X_Atn                   = 7.8[dB]
X_Pulse                 = 2.85666667[us]
Irr_Atn_Dec             = 26.16[dB]
Irr_Atn_Dec_Calc        = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe             = 26.16[dB]
```



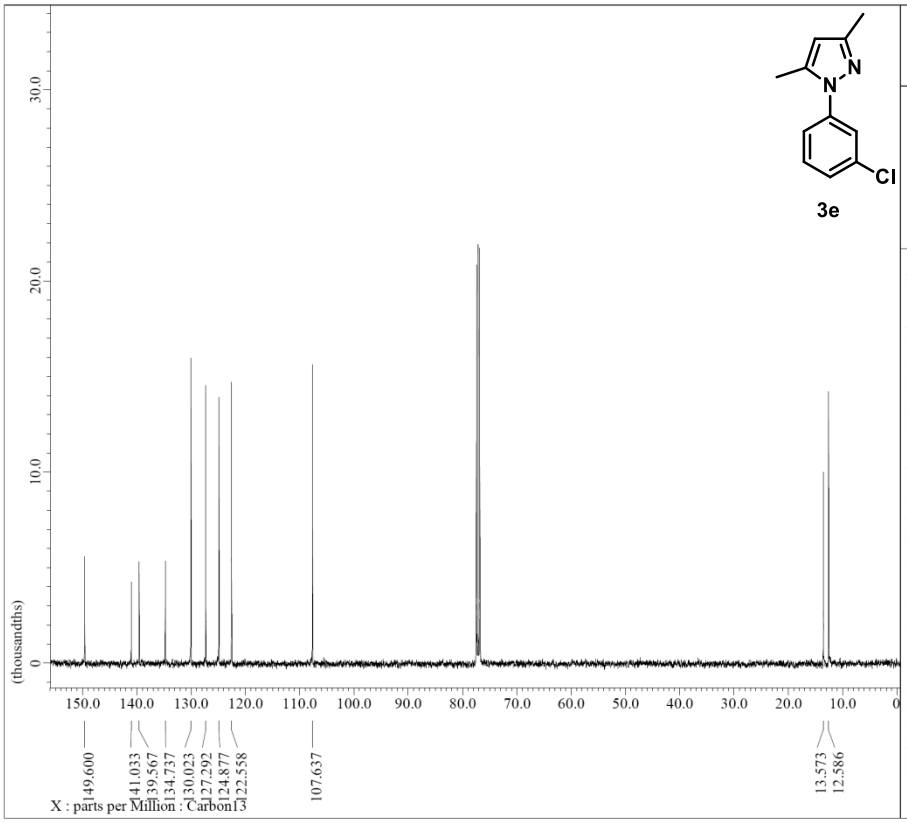

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
```

```
Filename          = GDS-419-P_PROTON-2.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = DSR_GDS-419-P
Solvent           = CHLOROFORM-D
Creation_Time     = 24-JUL-2018 08:31:41
Revision_Time     = 21-FEB-2019 12:26:02
Current_Time      = 21-FEB-2019 12:26:24

Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
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]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 16
Total_Scans       = 16

Relaxation_Delay  = 4[s]
Recvr_Gain        = 34
Temp_Get          = 73.4[dC]
X_90_Width        = 12.25[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 6[dB]
X_Pulse           = 6.125[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
```



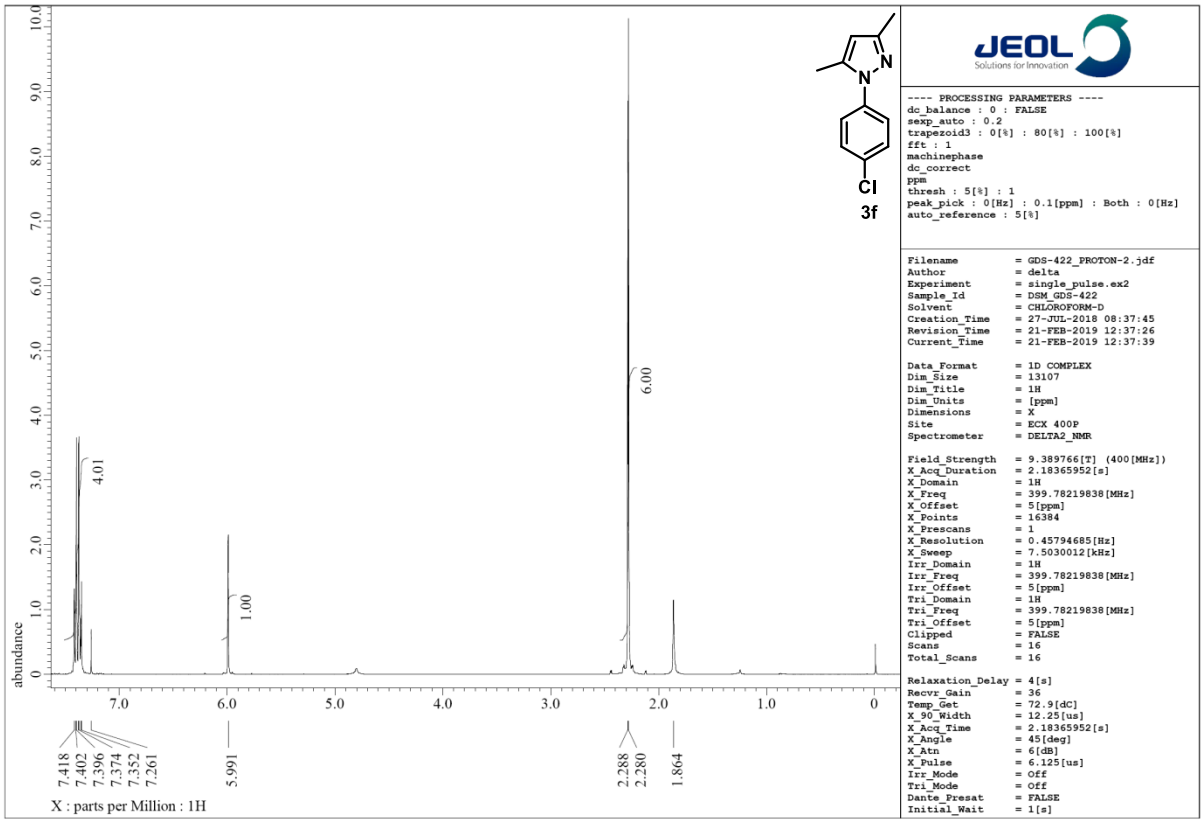

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                = GDS-419P_Carbon_co
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = DSR_GDS-419P
Solvent                 = CHLOROFORM-D
Creation_Time           = 26-JUL-2018 15:43:
Revision_Time           =  8-FEB-2019 13:02:
Current_Time            = 21-FEB-2019 12:33:

Comment                 = single pulse decou
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (400[M
X_Acq_Duration          = 0[s]
X_Domain                = Carbon13
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz]
X_Sweep_Clipped         = 25.25252525[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 5[us]
Clipped                 = FALSE
Decimation_Reg          = r: 198( 197),g: 39
Incomplete_Copy         = TRUE
Scans                   = 372
Total_Scans             = 372

Relaxation_Delay        = 2[s]
Recvr_Gain              = 56
Temp_Get                = 20[dC]
X_90_Width              = 8.57[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 7.8[dB]
X_Pulse                 = 2.85666667[us]
Irr_Atn_Dec             = 26.16[dB]
Irr_Atn_Dec_Calc        = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
```



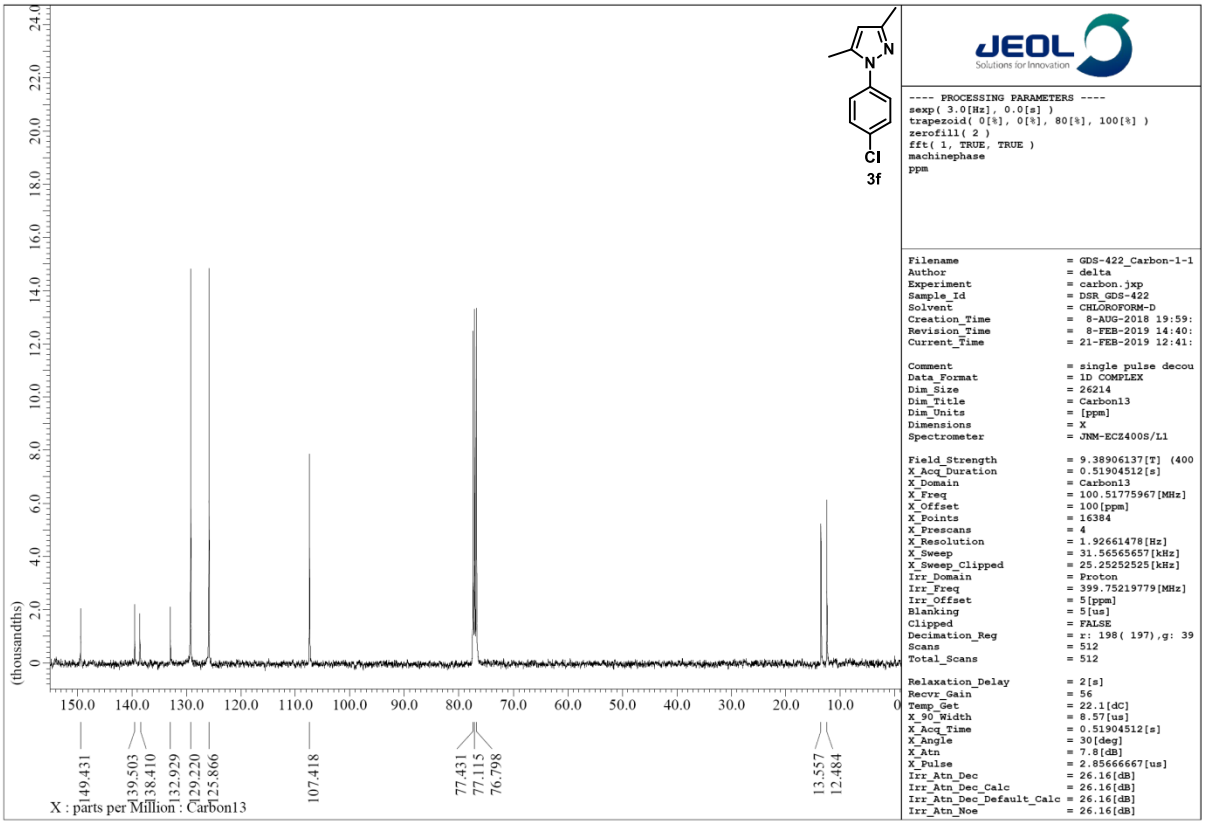

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
```

```
Filename          = GDS-422_PROTON-2.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = DSM_GDS-422
Solvent           = CHLOROFORM-D
Creation_Time     = 27-JUL-2018 08:37:45
Revision_Time     = 21-FEB-2019 12:37:26
Current_Time      = 21-FEB-2019 12:37:39

Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
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]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 16
Total_Scans       = 16

Relaxation_Delay  = 4[s]
Recvr_Gain        = 36
Temp_Get          = 72.9[dC]
X_90_Width        = 12.25[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 6[dB]
X_Pulse           = 6.125[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
```



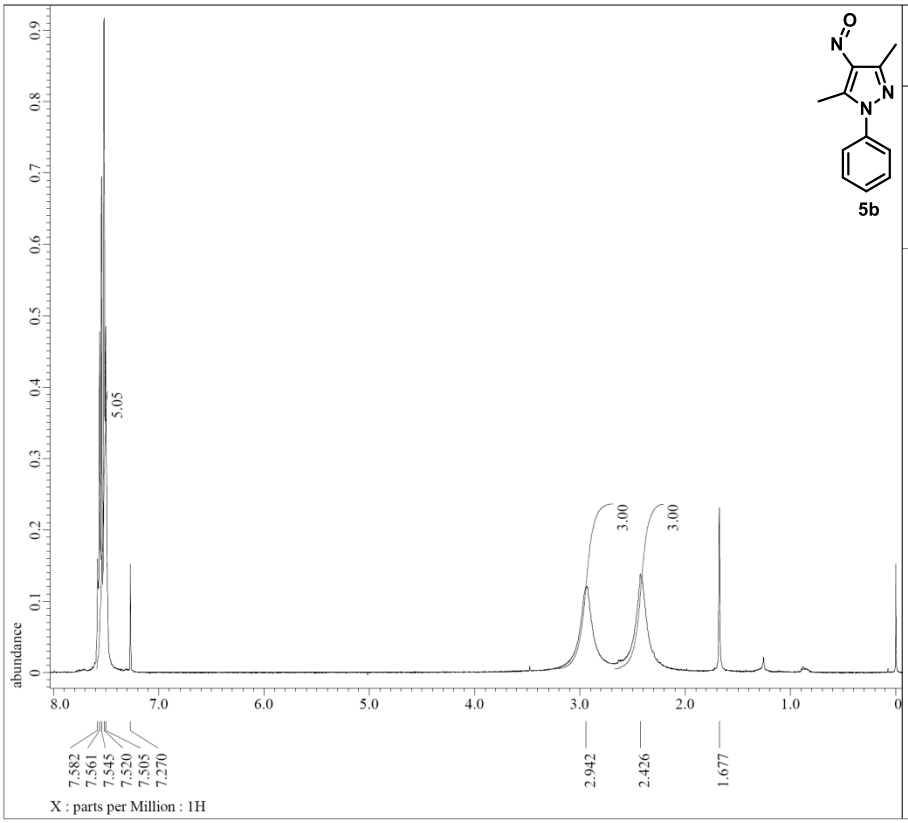

```
---- PROCESSING PARAMETERS ----
sexp( 3.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 2 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                = GDS-422_Carbon-1-1
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = DSR_GDS-422
Solvent                 = CHLOROFORM-D
Creation_Time           =  8-AUG-2018 19:59:
Revision_Time           =  8-FEB-2019 14:40:
Current_Time            = 21-FEB-2019 12:41:

Comment                 = single pulse decou
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.38906137[T] (400
X_Acq_Duration          = 0.51904512[s]
X_Domain                = Carbon13
X_Freq                  = 100.51775967[MHz]
X_Offset                = 100[ppm]
X_Points                = 16384
X_Prescans              = 4
X_Resolution            = 1.92661478[Hz]
X_Sweep                 = 31.56565657[kHz]
X_Sweep_Clipped         = 25.25252525[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.75219779[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 5[us]
Clipped                 = FALSE
Decimation_Reg          = r: 198( 197),g: 39
Scans                   = 512
Total_Scans             = 512

Relaxation_Delay        = 2[s]
Recvr_Gain              = 56
Temp_Get                = 22.1[dC]
X_90_Width              = 8.57[us]
X_Acq_Time              = 0.51904512[s]
X_Angle                 = 30[deg]
X_Atn                   = 7.8[dB]
X_Pulse                 = 2.85666667[us]
Irr_Atn_Dec             = 26.16[dB]
Irr_Atn_Dec_Calc        = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe             = 26.16[dB]
```



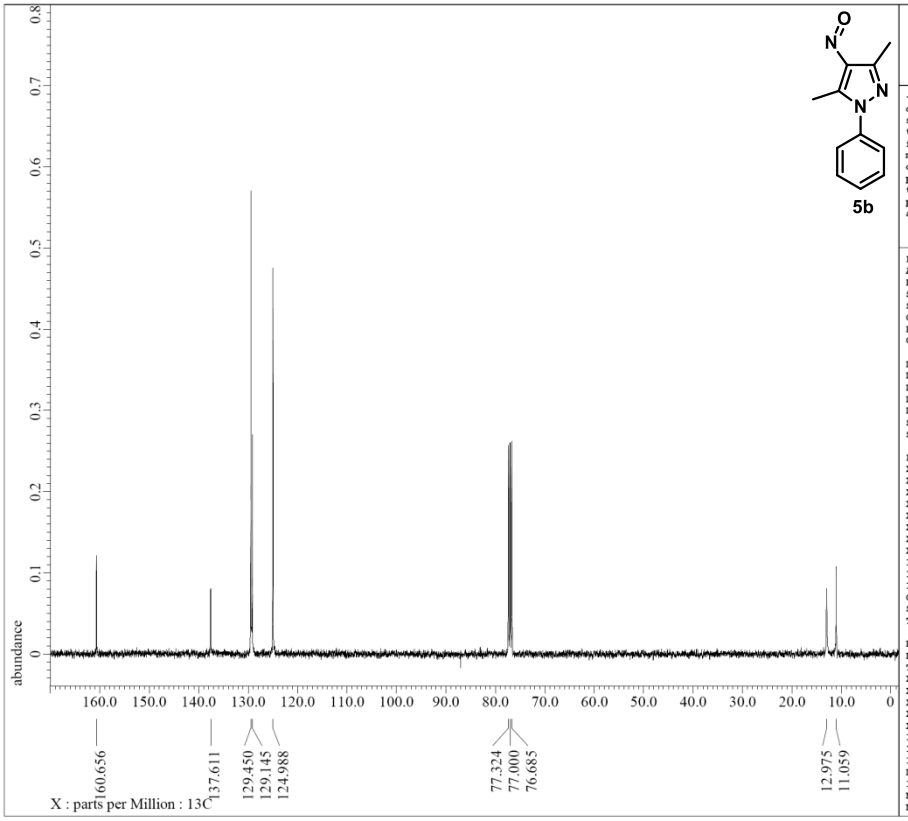

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
```

```
Filename          = GDS-401_PROTON-2.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = DSR_GDS-401
Solvent           = CHLOROFORM-D
Creation_Time     = 20-MAR-2018 12:32:45
Revision_Time     = 21-FEB-2019 14:24:01
Current_Time      = 21-FEB-2019 14:24:12

Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
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]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 16
Total_Scans       = 16

Relaxation_Delay  = 4[s]
Recvr_Gain        = 36
Temp_Get          = 404.2[dC]
X_90_Width        = 12.25[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 6[dB]
X_Pulse           = 6.125[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
```



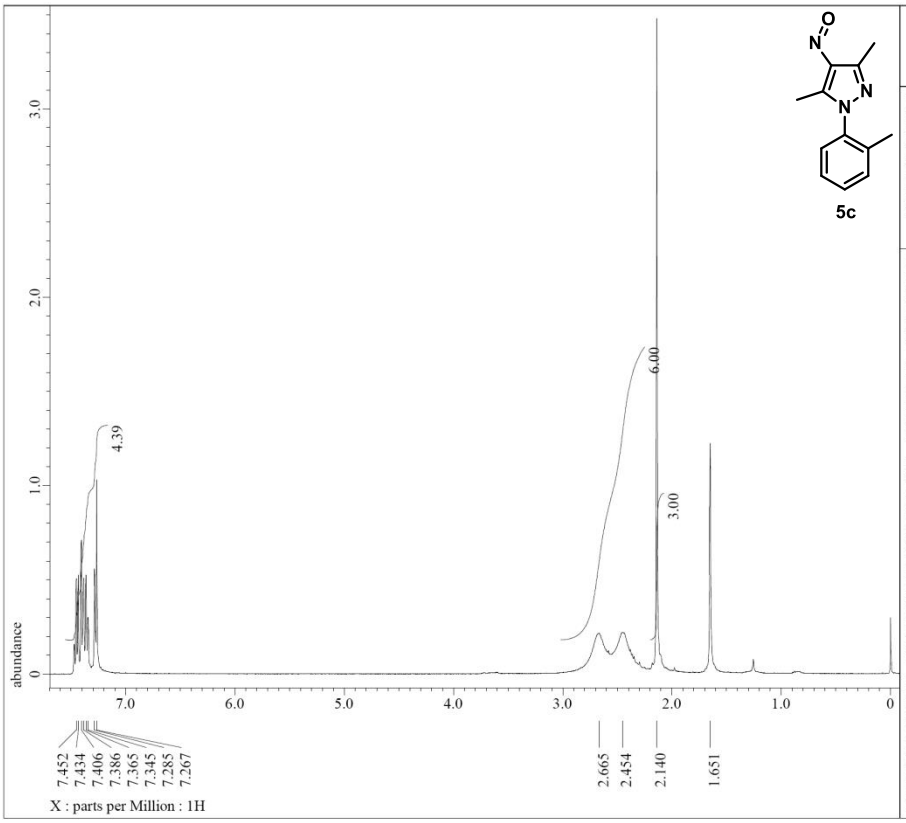

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
```

```
Filename          = GDS-401_CARBON-1.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = DB_GDS-401
Solvent           = CHLOROFORM-D
Creation_Time     = 14-MAR-2018 17:21:10
Revision_Time     =  8-FEB-2019 11:00:44
Current_Time      = 21-FEB-2019 14:53:16

Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
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]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 224
Total_Scans       = 224

Relaxation_Delay  = 2[s]
Recvr_Gain        = 54
Temp_Get          = 404.6[dC]
X_90_Width        = 9.25[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 9[dB]
X_Pulse           = 3.08333333[us]
Irr_Atn_Dec       = 25.45[dB]
Irr_Atn_Noe       = 25.45[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
```



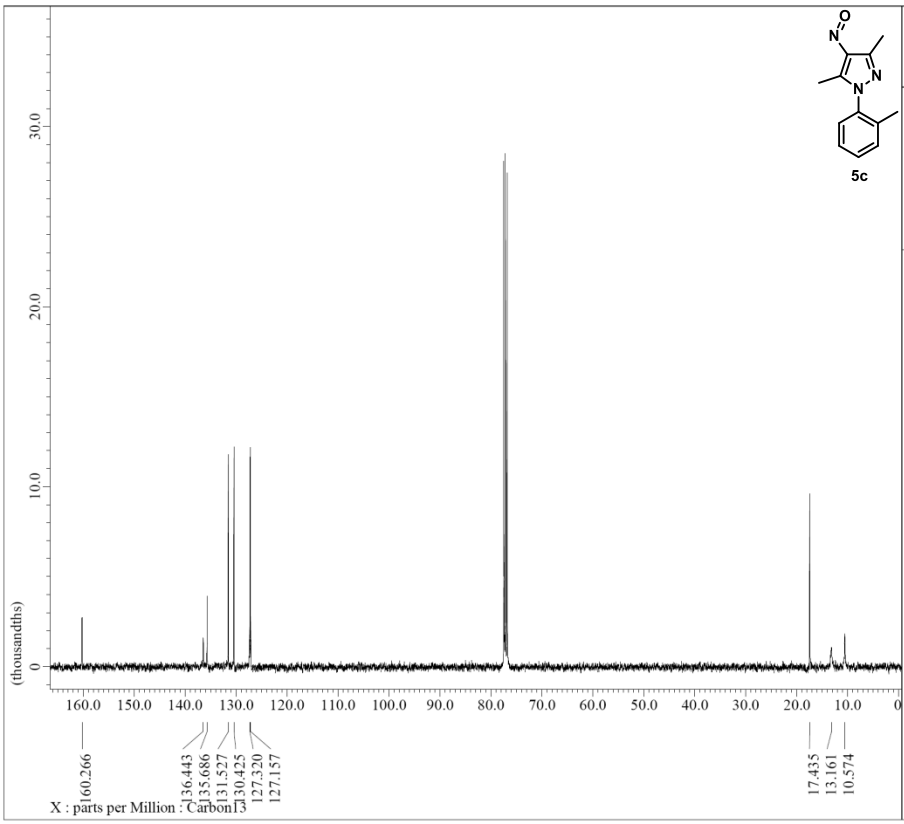

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
```

```
Filename          = GDS-410_PROTON-2.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = DSR_GDS-410
Solvent           = CHLOROFORM-D
Creation_Time     = 12-JUL-2018 12:44:44
Revision_Time     = 10-MAR-2019 12:12:36
Current_Time      = 10-MAR-2019 12:13:27

Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.09051904[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 1[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.91699454[Hz]
X_Sweep           = 15.02403846[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 10
Total_Scans       = 10

Relaxation_Delay  = 4[s]
Recvr_Gain        = 34
Temp_Get          = 64.9[dC]
X_90_Width        = 12.25[us]
X_Acq_Time        = 1.09051904[s]
X_Angle           = 45[deg]
X_Atn             = 6[dB]
X_Pulse           = 6.125[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
```



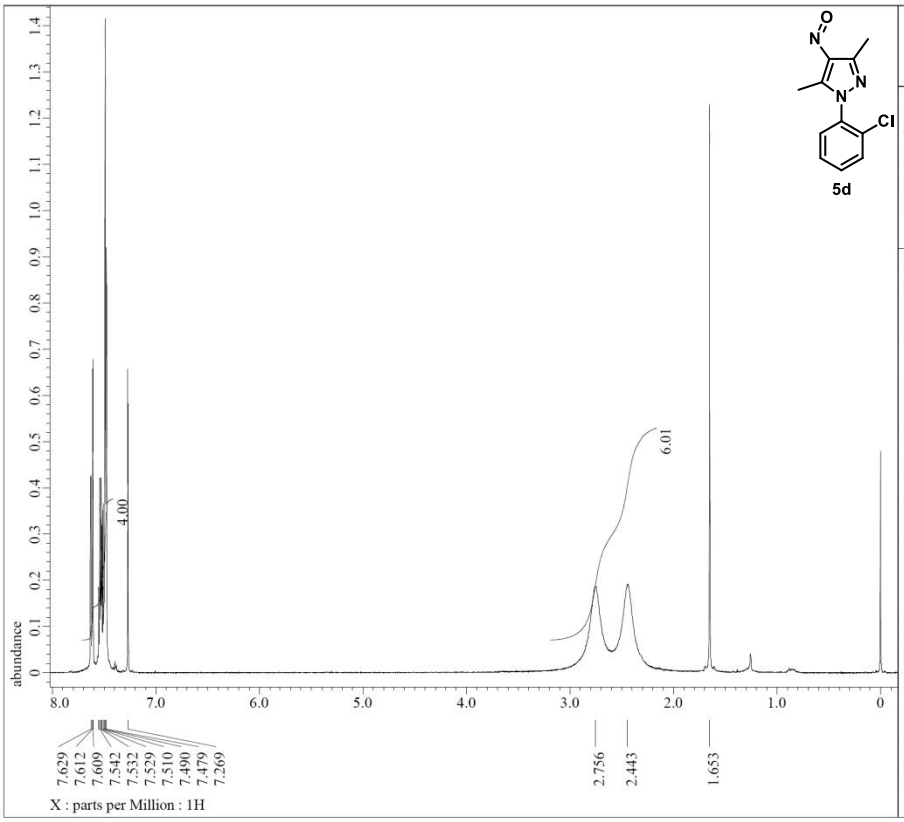

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                = GDS-410_Carbon-1-1
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = DSM_GDS-410
Solvent                 = CHLOROFORM-D
Creation_Time           = 18-JUL-2018 07:54:
Revision_Time           =  8-FEB-2019 12:39:
Current_Time            = 21-FEB-2019 15:12:

Comment                 = single pulse decou
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (400[M
X_Acq_Duration          = 1.03809024[s]
X_Domain                = Carbon13
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz]
X_Sweep_Clipped         = 25.25252525[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 5[us]
Clipped                 = FALSE
Decimation_Reg          = r: 198( 197),g: 39
Scans                   = 300
Total_Scans             = 300

Relaxation_Delay        = 2[s]
Recvr_Gain              = 56
Temp_Get                = 17.5[dC]
X_90_Width              = 8.57[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 7.8[dB]
X_Pulse                 = 2.85666667[us]
Irr_Atn_Dec             = 26.16[dB]
Irr_Atn_Dec_Calc        = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe             = 26.16[dB]
```



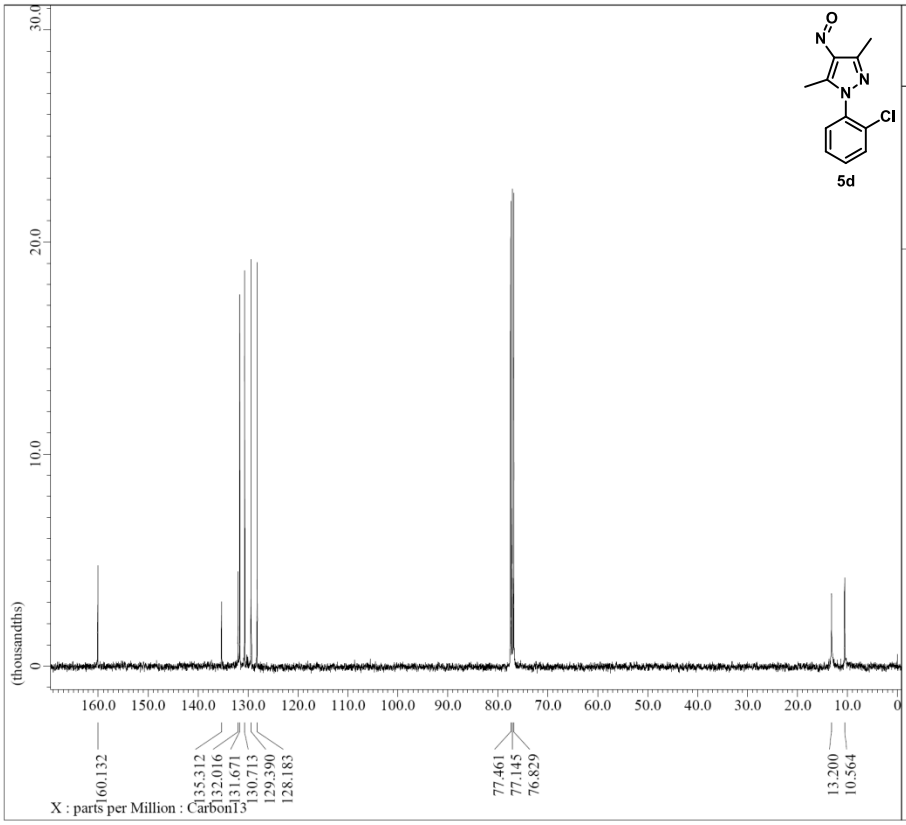

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
```

```
Filename          = GDS-414-P_PROTON-2.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = DSM_GDS-414-P
Solvent           = CHLOROFORM-D
Creation_Time     = 17-JUL-2018 12:27:26
Revision_Time     = 21-FEB-2019 15:26:49
Current_Time      = 21-FEB-2019 15:27:58

Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
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]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 4[s]
Recvr_Gain        = 36
Temp_Get          = 68.3[dC]
X_90_Width        = 12.25[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 6[dB]
X_Pulse           = 6.125[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
```



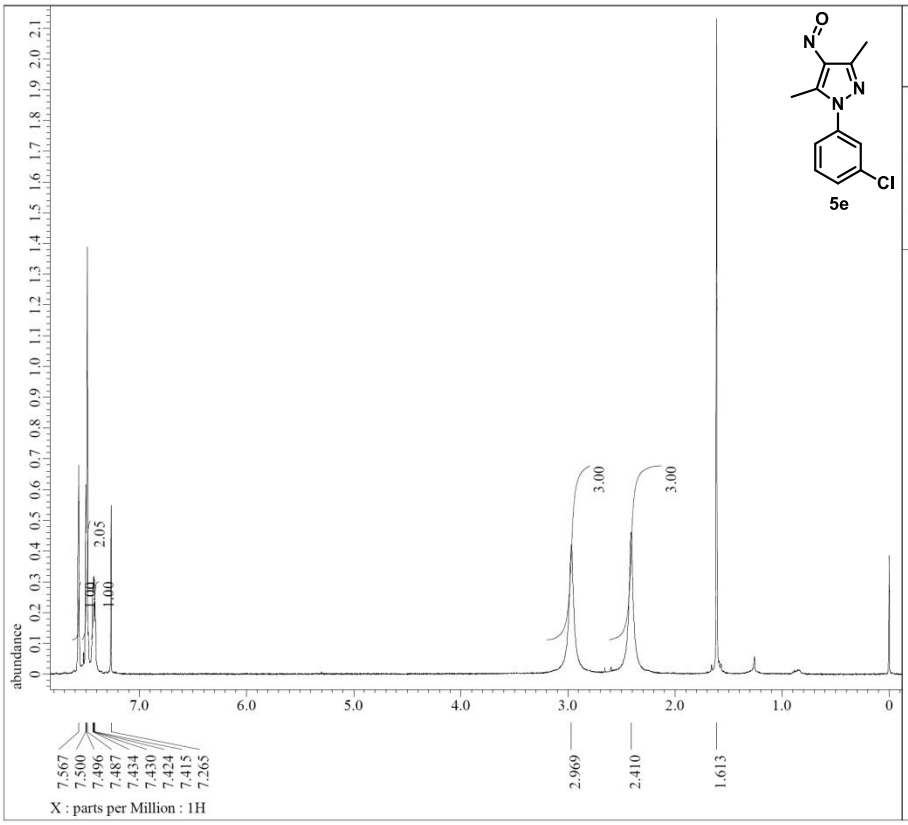

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                = GDS-414_Carbon-1-1
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = DSR_GDS-414
Solvent                 = CHLOROFORM-D
Creation_Time           = 18-JUL-2018 01:17:
Revision_Time           =  8-FEB-2019 12:48:
Current_Time            = 21-FEB-2019 22:14:

Comment                 = single pulse decou
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (400[M
X_Acq_Duration          = 1.03809024[s]
X_Domain                = Carbon13
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz]
X_Sweep_Clipped         = 25.25252525[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 5[us]
Clipped                 = FALSE
Decimation_Reg          = r: 198( 197),g: 39
Scans                   = 500
Total_Scans             = 500

Relaxation_Delay        = 2[s]
Recvr_Gain              = 56
Temp_Get                = 18.1[dC]
X_90_Width              = 8.57[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 7.8[dB]
X_Pulse                 = 2.85666667[us]
Irr_Atn_Dec             = 26.16[dB]
Irr_Atn_Dec_Calc        = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe             = 26.16[dB]
```



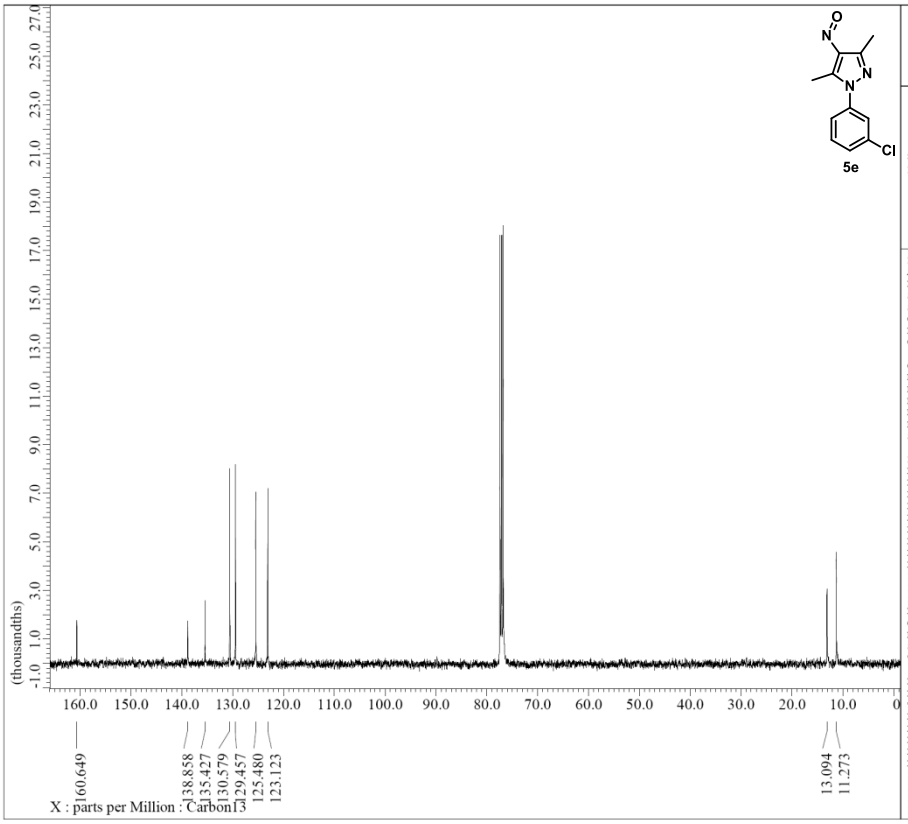

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
```

```
Filename            = GDS-413_PROTON-2.jdf
Author              = delta
Experiment          = single_pulse.ex2
Sample_Id           = DSR_GDS-413
Solvent             = CHLOROFORM-D
Creation_Time       = 11-JUL-2018 15:28:27
Revision_Time       = 21-FEB-2019 22:23:55
Current_Time        = 21-FEB-2019 22:32:16

Data_Format         = 1D COMPLEX
Dim_Size            = 13107
Dim_Title           = 1H
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400P
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]
Irr_Domain          = 1H
Irr_Freq            = 399.78219838[MHz]
Irr_Offset          = 5[ppm]
Tri_Domain          = 1H
Tri_Freq            = 399.78219838[MHz]
Tri_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 9
Total_Scans         = 9

Relaxation_Delay    = 4[s]
Recvr_Gain          = 40
Temp_Get            = 64.3[dC]
X_90_Width          = 12.25[us]
X_Acq_Time          = 2.18365952[s]
X_Angle             = 45[deg]
X_Atn               = 6[dB]
X_Pulse             = 6.125[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
```



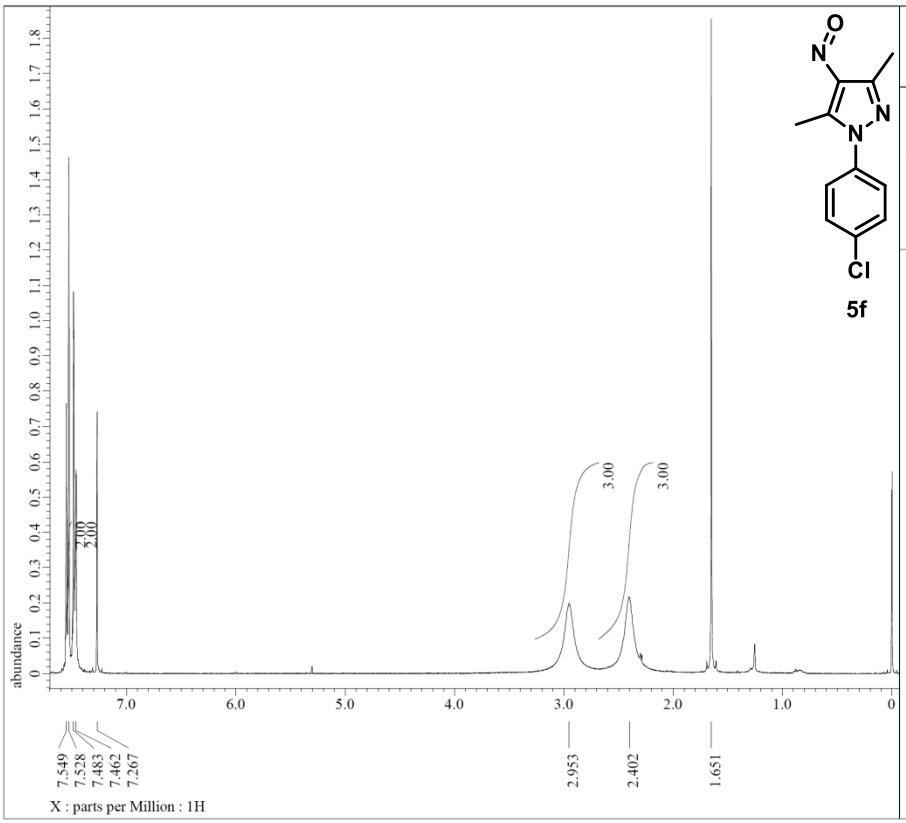

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                = GDS-413_Carbon-1-1
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = DSR_GDS-413
Solvent                 = CHLOROFORM-D
Creation_Time           = 13-JUL-2018 00:25:
Revision_Time           =  8-FEB-2019 12:42:
Current_Time            = 21-FEB-2019 22:35:

Comment                 = single pulse decou
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (400[M
X_Acq_Duration          = 1.03809024[s]
X_Domain                = Carbon13
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz]
X_Sweep_Clipped         = 25.25252525[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 5[us]
Clipped                 = FALSE
Decimation_Reg          = r: 198( 197),g: 39
Scans                   = 500
Total_Scans             = 500

Relaxation_Delay        = 2[s]
Recvr_Gain              = 56
Temp_Get                = 22.6[dC]
X_90_Width              = 8.57[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 7.8[dB]
X_Pulse                 = 2.85666667[us]
Irr_Atn_Dec             = 26.16[dB]
Irr_Atn_Dec_Calc        = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe             = 26.16[dB]
```



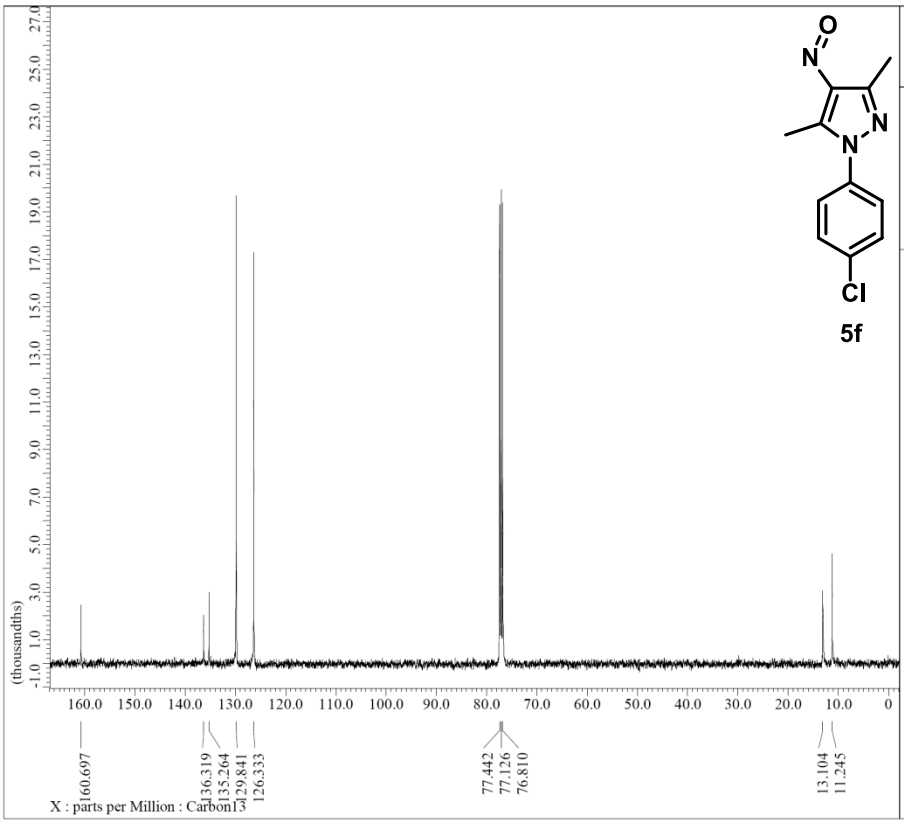

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]

Filename            = GDS-415_PROTON-2.jdf
Author              = delta
Experiment          = single_pulse.ex2
Sample_Id           = DSR_GDS-415
Solvent             = CHLOROFORM-D
Creation_Time       = 19-JUL-2018 10:57:46
Revision_Time       = 21-FEB-2019 22:41:36
Current_Time        = 21-FEB-2019 22:42:00

Data_Format         = 1D COMPLEX
Dim_Size            = 13107
Dim_Title           = 1H
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400P
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]
Irr_Domain          = 1H
Irr_Freq            = 399.78219838[MHz]
Irr_Offset          = 5[ppm]
Tri_Domain          = 1H
Tri_Freq            = 399.78219838[MHz]
Tri_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 16
Total_Scans         = 16

Relaxation_Delay    = 4[s]
Recvr_Gain          = 38
Temp_Get            = 68.9[dC]
X_90_Width          = 12.25[us]
X_Acq_Time          = 2.18365952[s]
X_Angle             = 45[deg]
X_Atn               = 6[dB]
X_Pulse             = 6.125[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
```



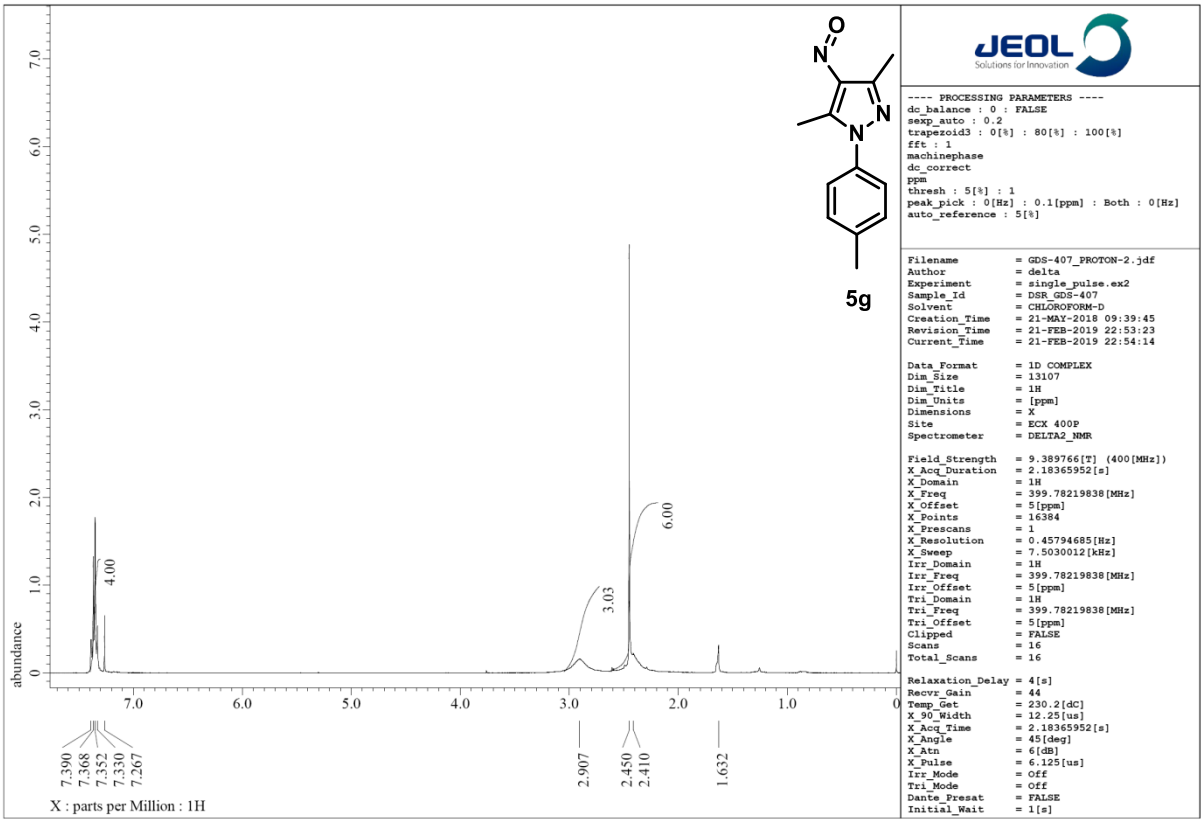

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename                = GDS-415_Carbon-1-1
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = DSR_GDS-415
Solvent                 = CHLOROFORM-D
Creation_Time           = 20-JUL-2018 07:15:
Revision_Time           =  8-FEB-2019 12:51:
Current_Time            = 21-FEB-2019 22:48:

Comment                 = single pulse decou
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (400[M
X_Acq_Duration          = 1.03809024[s]
X_Domain                = Carbon13
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz]
X_Sweep_Clipped         = 25.25252525[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 5[us]
Clipped                 = FALSE
Decimation_Reg          = r: 198( 197),g: 39
Scans                   = 500
Total_Scans             = 500

Relaxation_Delay        = 2[s]
Recvr_Gain              = 56
Temp_Get                = 19.9[dC]
X_90_Width              = 8.57[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 7.8[dB]
X_Pulse                 = 2.85666667[us]
Irr_Atn_Dec             = 26.16[dB]
Irr_Atn_Dec_Calc        = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe             = 26.16[dB]
```



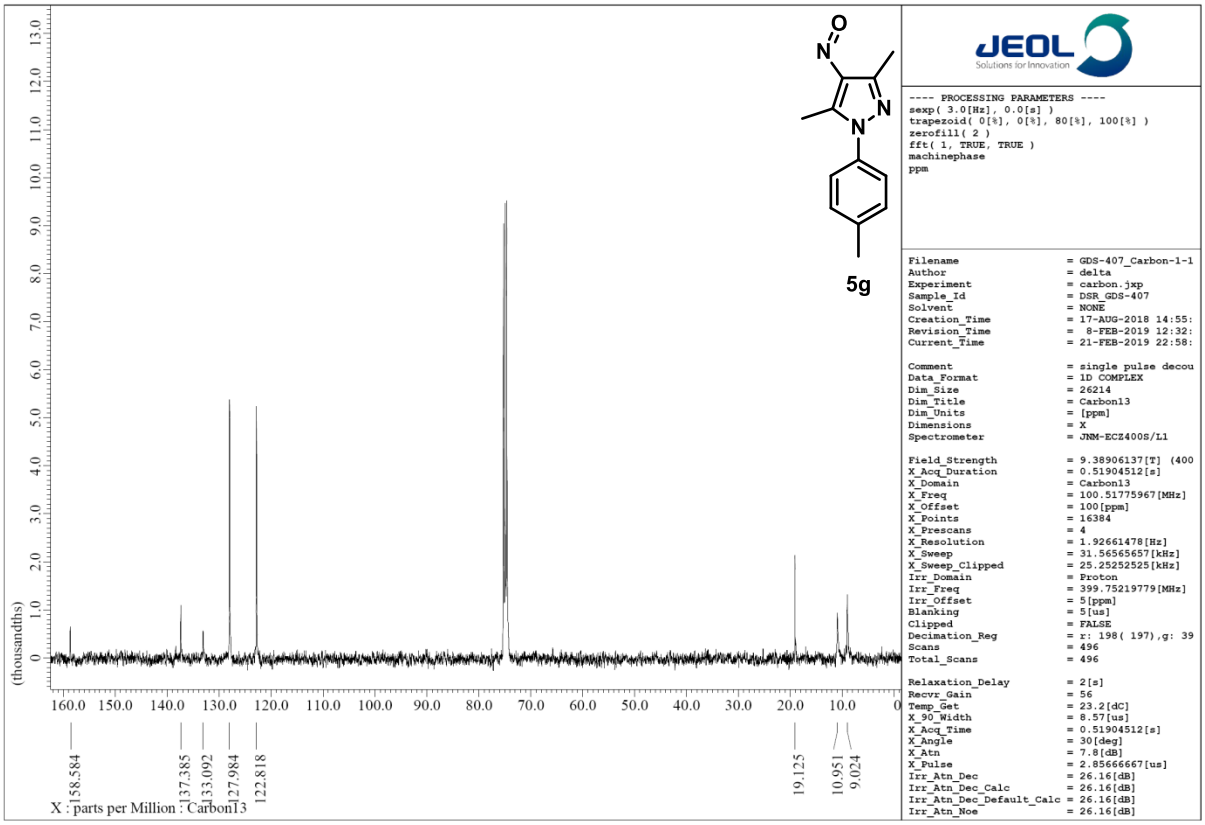

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
```

```
Filename          = GDS-407_PROTON-2.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = DSR_GDS-407
Solvent           = CHLOROFORM-D
Creation_Time     = 21-MAY-2018 09:39:45
Revision_Time     = 21-FEB-2019 22:53:23
Current_Time      = 21-FEB-2019 22:54:14

Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
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]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 16
Total_Scans       = 16

Relaxation_Delay = 4[s]
Recvr_Gain        = 44
Temp_Get          = 230.2[dC]
X_90_Width        = 12.25[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 6[dB]
X_Pulse           = 6.125[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
```



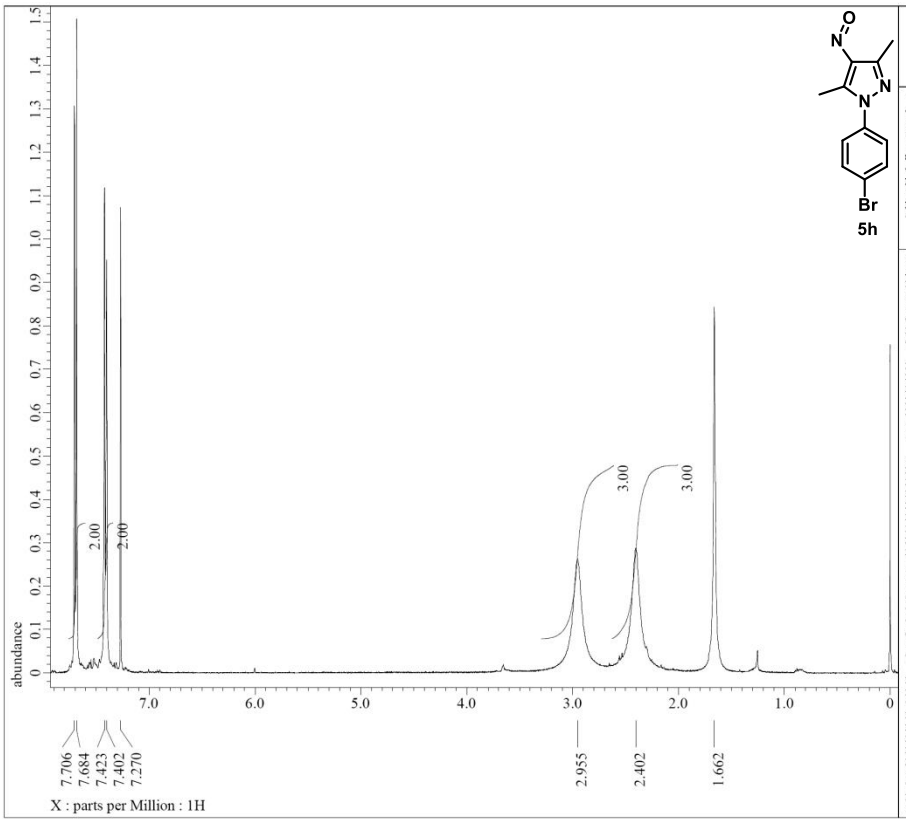

```
---- PROCESSING PARAMETERS ----
sexp( 3.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 2 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                = GDS-407_Carbon-1-1
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = DSR_GDS-407
Solvent                 = NONE
Creation_Time           = 17-AUG-2018 14:55:
Revision_Time           =  8-FEB-2019 12:32:
Current_Time            = 21-FEB-2019 22:58:

Comment                 = single pulse decou
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.38906137[T] (400
X_Acq_Duration          = 0.51904512[s]
X_Domain                = Carbon13
X_Freq                  = 100.51775967[MHz]
X_Offset                = 100[ppm]
X_Points                = 16384
X_Prescans              = 4
X_Resolution            = 1.92661478[Hz]
X_Sweep                 = 31.56565657[kHz]
X_Sweep_Clipped         = 25.25252525[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.75219779[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 5[us]
Clipped                 = FALSE
Decimation_Reg          = r: 198( 197),g: 39
Scans                   = 496
Total_Scans             = 496

Relaxation_Delay        = 2[s]
Recvr_Gain              = 56
Temp_Get                = 23.2[dC]
X_90_Width              = 8.57[us]
X_Acq_Time              = 0.51904512[s]
X_Angle                 = 30[deg]
X_Atn                   = 7.8[dB]
X_Pulse                 = 2.85666667[us]
Irr_Atn_Dec             = 26.16[dB]
Irr_Atn_Dec_Calc        = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe             = 26.16[dB]
```



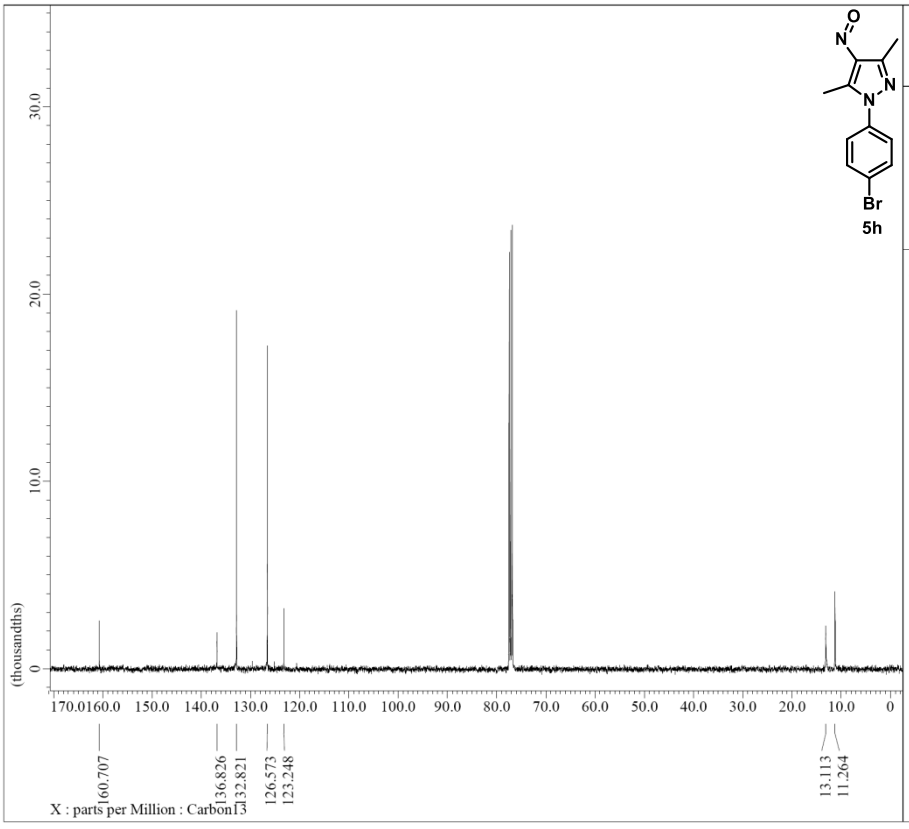

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
```

```
Filename          = gds-408_PROTON-2.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = DSR_KKY-408
Solvent           = CHLOROFORM-D
Creation_Time     = 24-JUL-2018 10:02:34
Revision_Time     = 21-FEB-2019 23:02:43
Current_Time      = 21-FEB-2019 23:02:56

Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
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]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 16
Total_Scans       = 16

Relaxation_Delay  = 4[s]
Recvr_Gain        = 40
Temp_Get          = 71.8[dC]
X_90_Width        = 12.25[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 6[dB]
X_Pulse           = 6.125[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
```



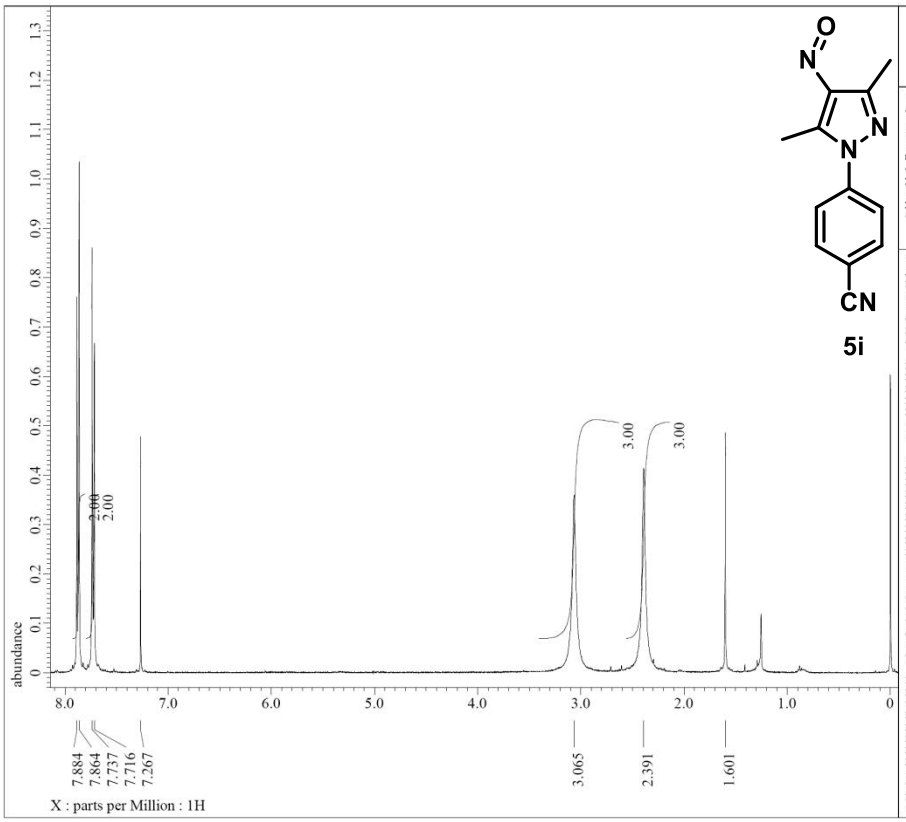

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                = GDS-408_Carbon-1-1
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = DSR_GDS-408
Solvent                 = CHLOROFORM-D
Creation_Time           = 26-JUL-2018 16:06:
Revision_Time           =  8-FEB-2019 12:35:
Current_Time            = 21-FEB-2019 23:08:

Comment                 = single pulse decou
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (400[M
X_Acq_Duration          = 1.03809024[s]
X_Domain                = Carbon13
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz]
X_Sweep_Clipped         = 25.25252525[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 5[us]
Clipped                 = FALSE
Decimation_Reg          = z: 198( 197),g: 39
Scans                   = 500
Total_Scans             = 500

Relaxation_Delay        = 2[s]
Recvr_Gain              = 56
Temp_Get                = 20[dC]
X_90_Width              = 8.57[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 7.8[dB]
X_Pulse                 = 2.85666667[us]
Irr_Atn_Dec             = 26.16[dB]
Irr_Atn_Dec_Calc        = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe             = 26.16[dB]
```



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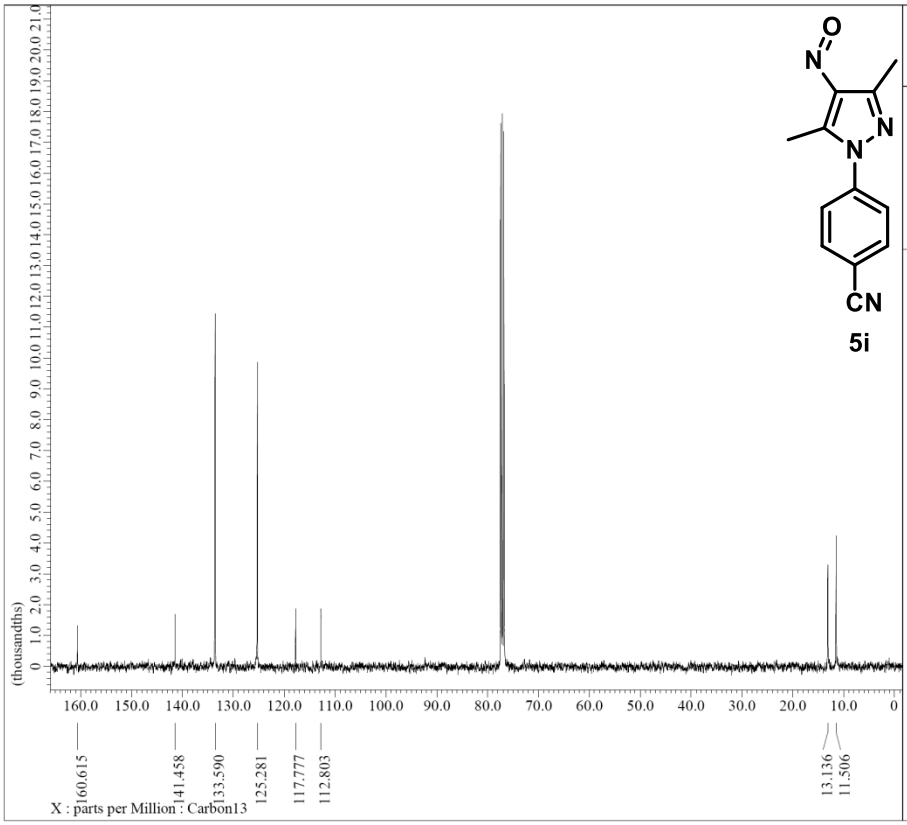
```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
```

```
Filename            = GDS-424_PROTON-2.jdf
Author              = delta
Experiment          = single_pulse.ex2
Sample_Id           = DSR_GDS-424
Solvent             = CHLOROFORM-D
Creation_Time       =  1-AUG-2018 13:55:35
Revision_Time       = 21-FEB-2019 23:14:14
Current_Time        = 21-FEB-2019 23:14:39

Data_Format         = 1D COMPLEX
Dim_Size            = 13107
Dim_Title           = 1H
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400P
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]
Irr_Domain          = 1H
Irr_Freq            = 399.78219838[MHz]
Irr_Offset          = 5[ppm]
Tri_Domain          = 1H
Tri_Freq            = 399.78219838[MHz]
Tri_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 12
Total_Scans         = 12

Relaxation_Delay    = 4[s]
Recvr_Gain          = 38
Temp_Get            = 71.8[dC]
X_90_Width          = 12.25[us]
X_Acq_Time          = 2.18365952[s]
X_Angle             = 45[deg]
X_Atn               = 6[dB]
X_Pulse             = 6.125[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
```



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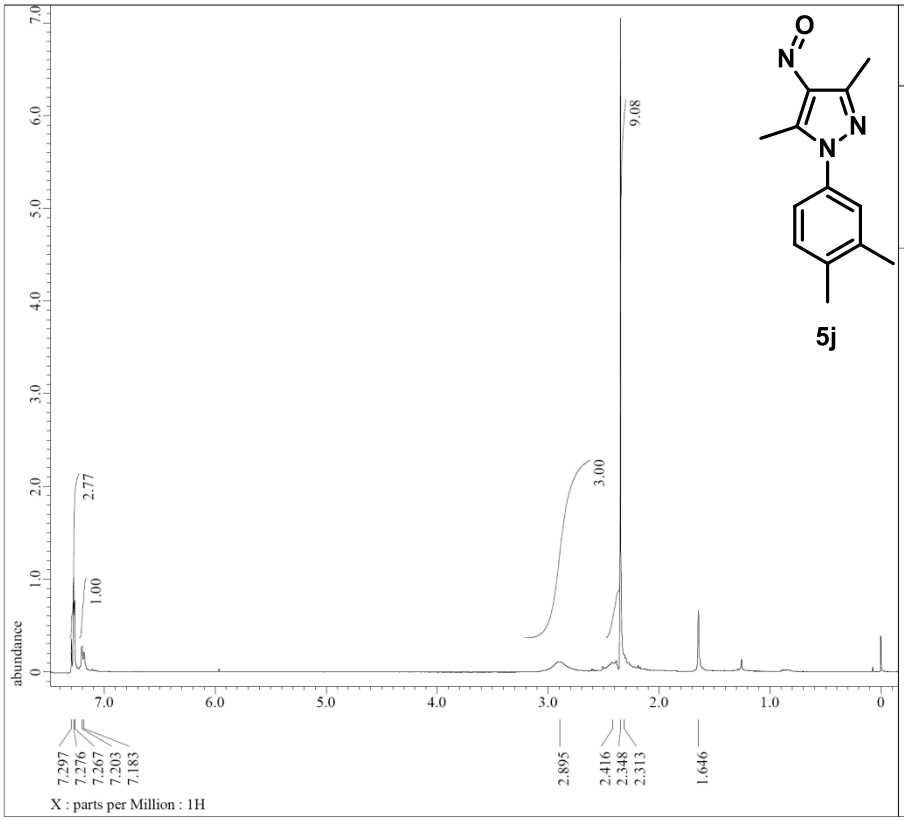
```
---- PROCESSING PARAMETERS ----
sexp( 3.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 2 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                = GDS-424_Carbon-1-1
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = DSR_GDS-424
Solvent                 = CHLOROFORM-D
Creation_Time           =  4-AUG-2018 16:44:
Revision_Time           = 12-FEB-2019 10:54:
Current_Time            = 21-FEB-2019 23:19:

Comment                 = single pulse decou
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.38906137[T] (400
X_Acq_Duration          = 0.51904512[s]
X_Domain                = Carbon13
X_Freq                  = 100.51775967[MHz]
X_Offset                = 100[ppm]
X_Points                = 16384
X_Prescans              = 4
X_Resolution            = 1.92661478[Hz]
X_Sweep                 = 31.56565657[kHz]
X_Sweep_Clipped         = 25.25252525[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.75219779[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 5[us]
Clipped                 = FALSE
Decimation_Reg          = r: 198( 197),g: 39
Scans                   = 365
Total_Scans             = 365

Relaxation_Delay        = 2[s]
Recvr_Gain              = 56
Temp_Get                = 20.9[dC]
X_90_Width              = 8.57[us]
X_Acq_Time              = 0.51904512[s]
X_Angle                 = 30[deg]
X_Atn                   = 7.8[dB]
X_Pulse                 = 2.85666667[us]
Irr_Atn_Dec             = 26.16[dB]
Irr_Atn_Dec_Calc        = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe             = 26.16[dB]
```



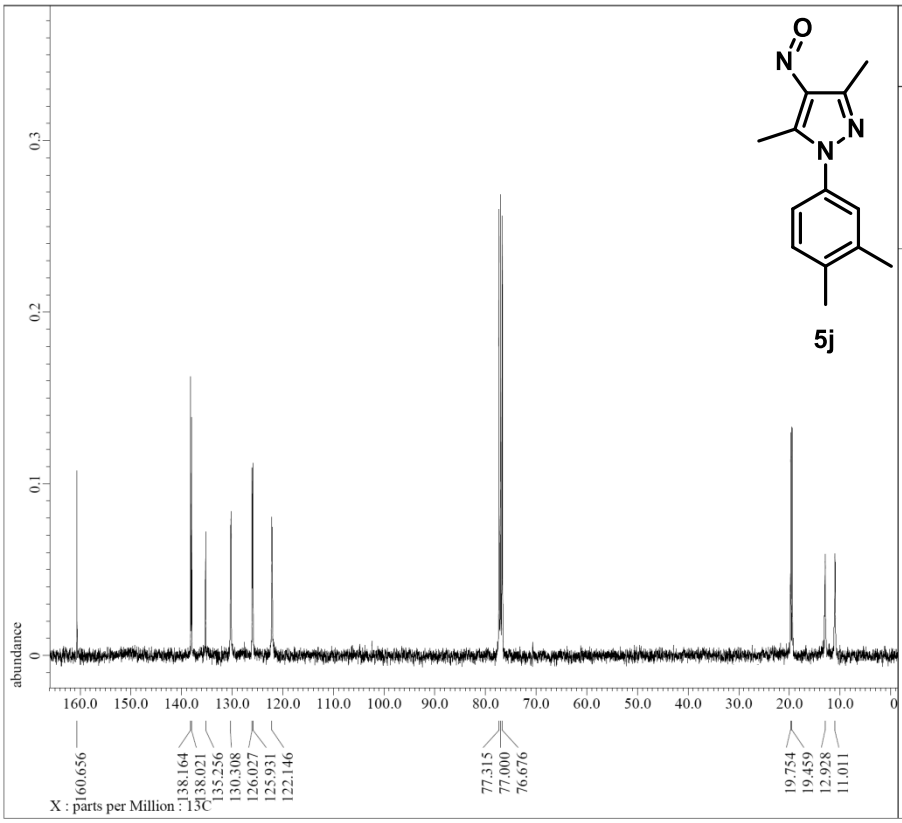

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
```

```
Filename          = GDS-405_PROTON-1.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = DSR_GDS-405
Solvent           = CHLOROFORM-D
Creation_Time     =  3-MAY-2018 10:10:46
Revision_Time     = 26-JAN-2019 10:04:19
Current_Time      = 21-FEB-2019 23:27:04

Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
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]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 16
Total_Scans       = 16

Relaxation_Delay = 4[s]
Recvr_Gain        = 36
Temp_Get          = 82.9[dC]
X_90_Width        = 12.25[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 6[dB]
X_Pulse           = 6.125[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
```



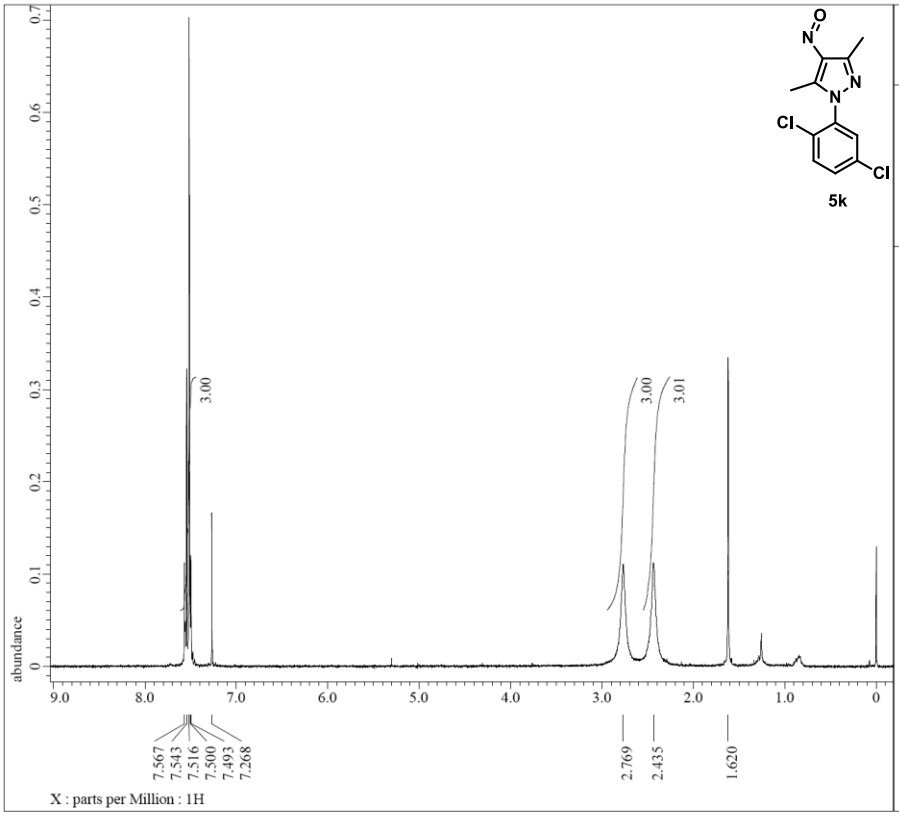

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Peaks : 0[Hz]
auto_reference : 5[%]
```

```
Filename          = GDS-405_CARBON-1.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = DSR_GDS-405
Solvent           = CHLOROFORM-D
Creation_Time     =  5-MAY-2018 11:12:04
Revision_Time     =  8-FEB-2019 12:26:24
Current_Time      = 21-FEB-2019 23:33:23

Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
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]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 286
Total_Scans       = 286

Relaxation_Delay = 2[s]
Recvr_Gain        = 54
Temp_Get          = 73.6[dC]
X_90_Width        = 9.25[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 9[dB]
X_Pulse           = 3.08333333[us]
Irr_Atn_Dec       = 25.45[dB]
Irr_Atn_Noe       = 25.45[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
```



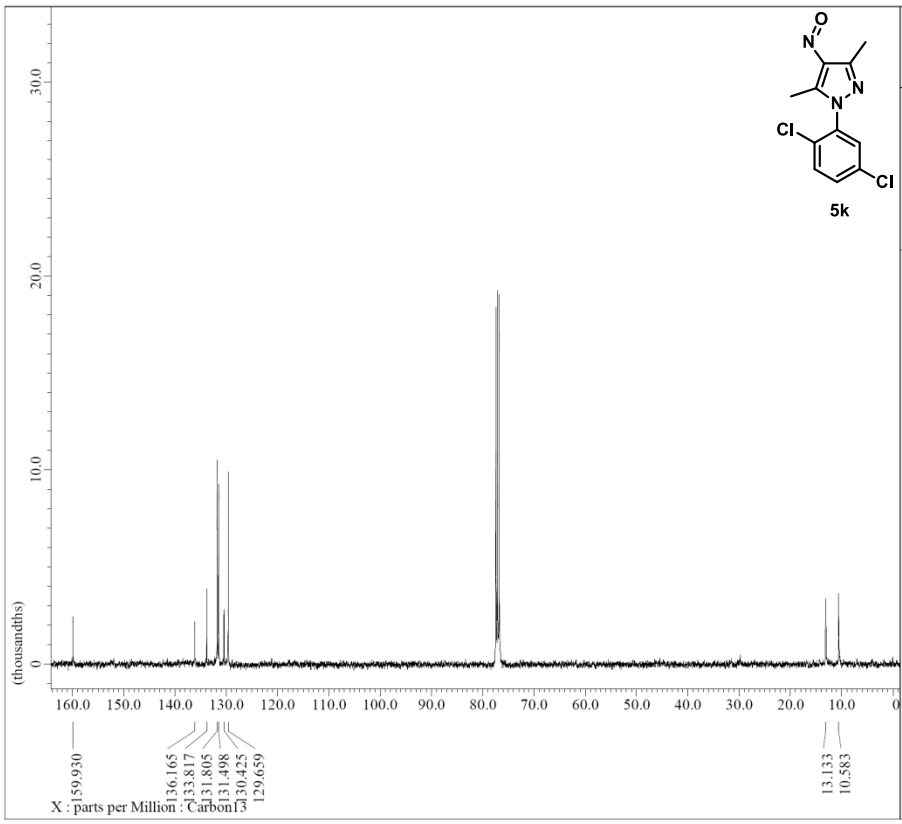

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
```

```
Filename            = GDS-406_PROTON-2.jdf
Author              = delta
Experiment          = single_pulse.ex2
Sample_Id           = DSR_GDS-406
Solvent             = CHLOROFORM-D
Creation_Time       =  9-MAY-2018 11:42:10
Revision_Time       =  1-JUL-2019 19:41:04
Current_Time        =  1-JUL-2019 19:41:19

Data_Format         = 1D COMPLEX
Dim_Size            = 13107
Dim_Title           = 1H
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400P
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]
Irr_Domain          = 1H
Irr_Freq            = 399.78219838[MHz]
Irr_Offset          = 5[ppm]
Tri_Domain          = 1H
Tri_Freq            = 399.78219838[MHz]
Tri_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 5
Total_Scans         = 5

Relaxation_Delay    = 4[s]
Recvr_Gain          = 38
Temp_Get            = 72.9[dC]
X_90_Width          = 12.25[us]
X_Acq_Time          = 2.18365952[s]
X_Angle             = 45[deg]
X_Atn               = 6[dB]
X_Pulse             = 6.125[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
```



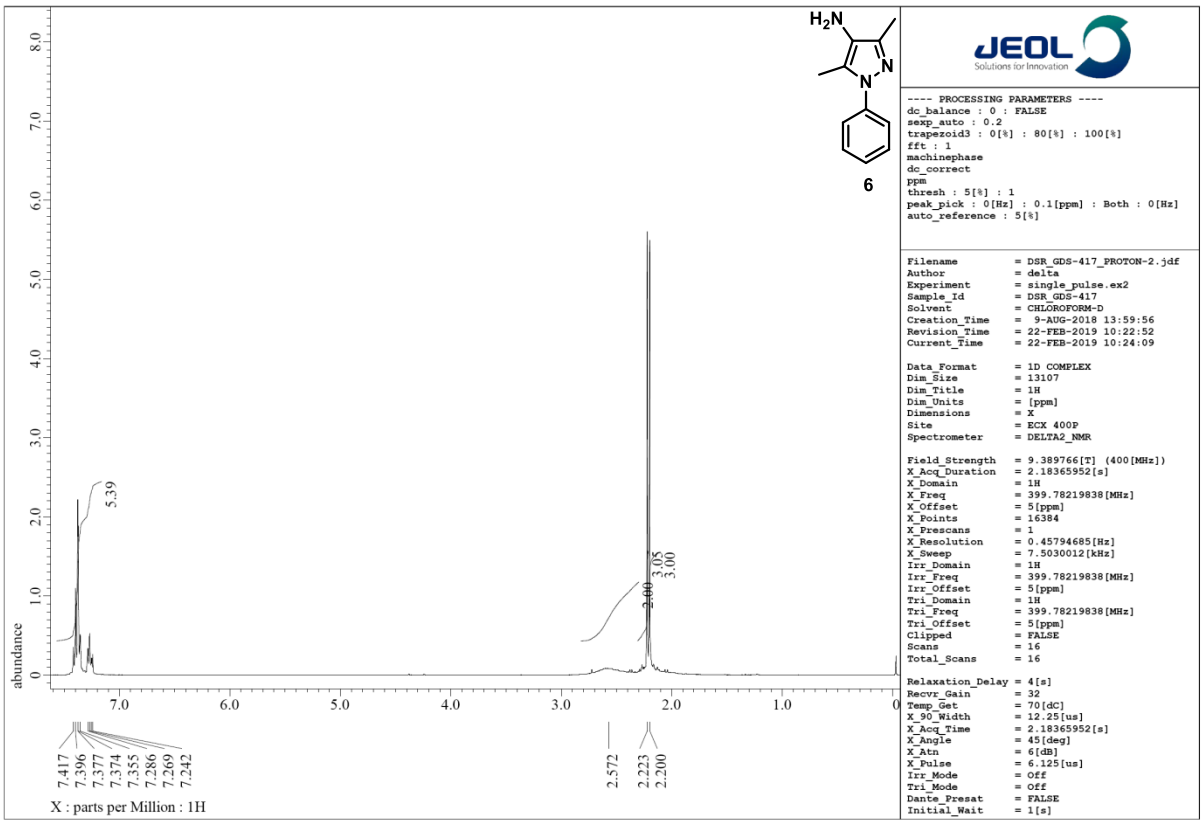

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                = GDS-406_Carbon-1-1
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = DSR_GDS-406
Solvent                 = CHLOROFORM-D
Creation_Time           = 20-JUL-2018 06:45:
Revision_Time           =  8-FEB-2019 12:29:
Current_Time            = 21-FEB-2019 23:52:

Comment                 = single pulse decou
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (400[M
X_Acq_Duration          = 1.03809024[s]
X_Domain                = Carbon13
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz]
X_Sweep_Clipped         = 25.25252525[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 5[us]
Clipped                 = FALSE
Decimation_Reg          = r: 198( 197),g: 39
Scans                   = 500
Total_Scans             = 500

Relaxation_Delay        = 2[s]
Recvr_Gain              = 56
Temp_Get                = 19.8[dC]
X_90_Width              = 8.57[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 7.8[dB]
X_Pulse                 = 2.85666667[us]
Irr_Atn_Dec             = 26.16[dB]
Irr_Atn_Dec_Calc        = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe             = 26.16[dB]
```



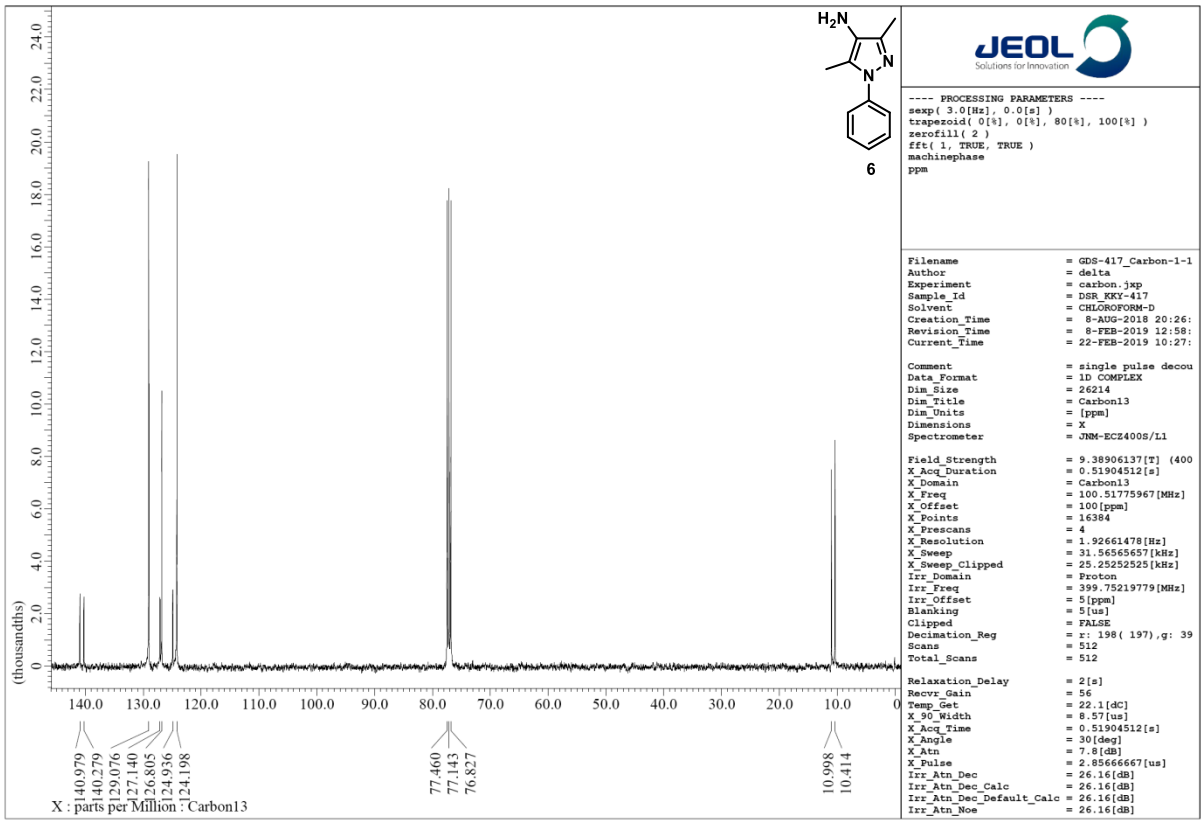

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
```

```
Filename            = DSR_GDS-417_PROTON-2.jdf
Author              = delta
Experiment          = single_pulse.ex2
Sample_Id           = DSR_GDS-417
Solvent             = CHLOROFORM-D
Creation_Time       =  9-AUG-2018 13:59:56
Revision_Time       = 22-FEB-2019 10:22:52
Current_Time        = 22-FEB-2019 10:24:09

Data_Format         = 1D COMPLEX
Dim_Size            = 13107
Dim_Title           = 1H
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400P
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]
Irr_Domain          = 1H
Irr_Freq            = 399.78219838[MHz]
Irr_Offset          = 5[ppm]
Tri_Domain          = 1H
Tri_Freq            = 399.78219838[MHz]
Tri_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 16
Total_Scans         = 16

Relaxation_Delay    = 4[s]
Recvr_Gain          = 32
Temp_Get            = 70[dC]
X_90_Width          = 12.25[us]
X_Acq_Time          = 2.18365952[s]
X_Angle             = 45[deg]
X_Atn               = 6[dB]
X_Pulse             = 6.125[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
```



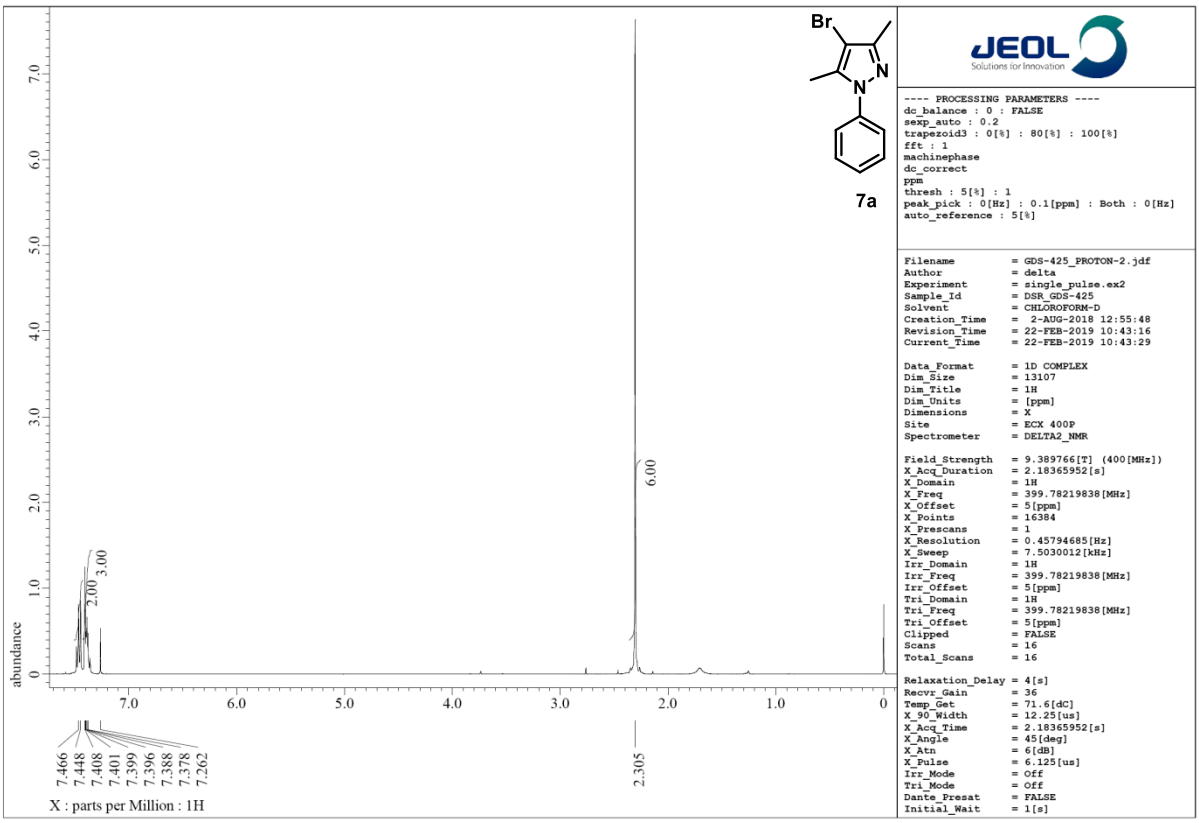

```
---- PROCESSING PARAMETERS ----
sexp( 3.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 2 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                = GDS-417_Carbon-1-1
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = DSR_KKY-417
Solvent                 = CHLOROFORM-D
Creation_Time           =  8-AUG-2018 20:26:
Revision_Time           =  8-FEB-2019 12:58:
Current_Time            = 22-FEB-2019 10:27:

Comment                 = single pulse decou
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.38906137[T] (400
X_Acq_Duration          = 0.51904512[s]
X_Domain                = Carbon13
X_Freq                  = 100.51775967[MHz]
X_Offset                = 100[ppm]
X_Points                = 16384
X_Prescans              = 4
X_Resolution            = 1.92661478[Hz]
X_Sweep                 = 31.56565657[kHz]
X_Sweep_Clipped         = 25.25252525[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.75219779[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 5[us]
Clipped                 = FALSE
Decimation_Reg          = r: 198( 197),g: 39
Scans                   = 512
Total_Scans             = 512

Relaxation_Delay        = 2[s]
Recvr_Gain              = 56
Temp_Get                = 22.1[dC]
X_90_Width              = 8.57[us]
X_Acq_Time              = 0.51904512[s]
X_Angle                 = 30[deg]
X_Atn                   = 7.8[dB]
X_Pulse                 = 2.85666667[us]
Irr_Atn_Dec             = 26.16[dB]
Irr_Atn_Dec_Calc        = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe             = 26.16[dB]
```



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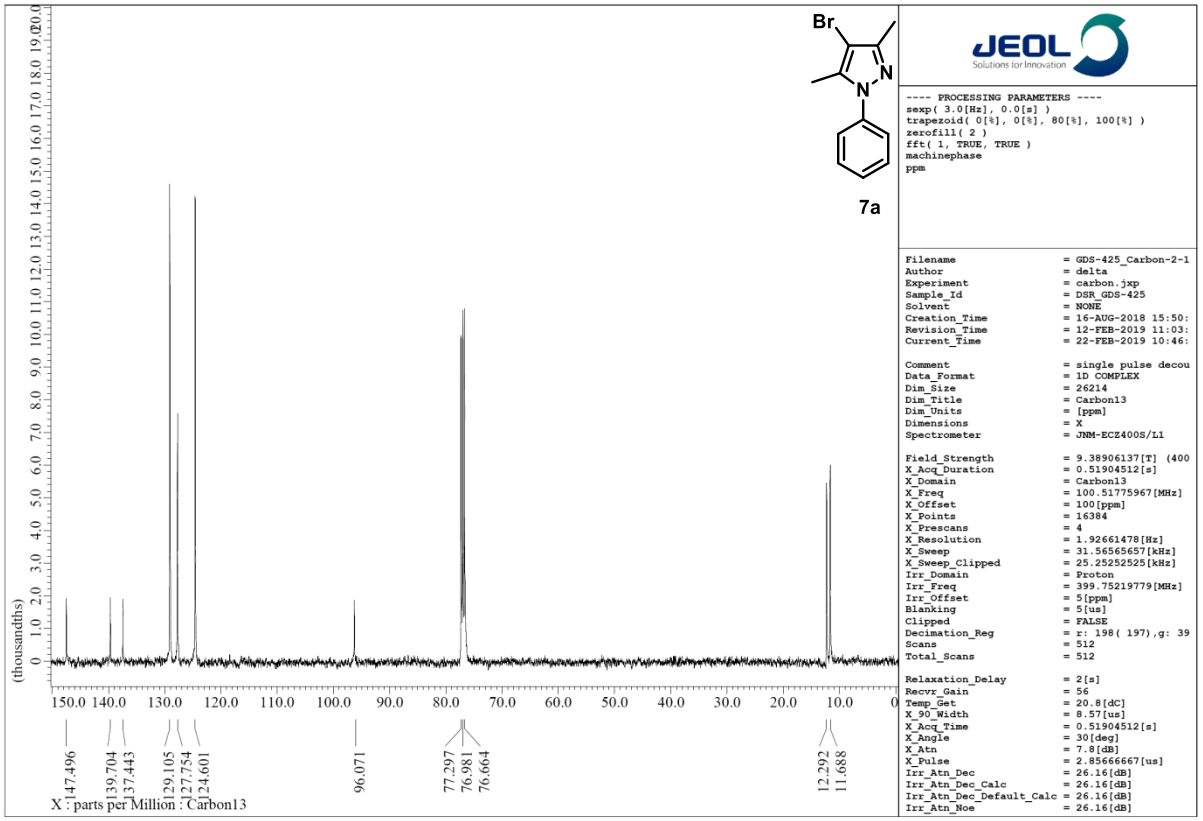
```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
```

```
Filename          = GDS-425_PROTON-2.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = DSR_GDS-425
Solvent           = CHLOROFORM-D
Creation_Time     =  2-AUG-2018 12:55:48
Revision_Time     = 22-FEB-2019 10:43:16
Current_Time      = 22-FEB-2019 10:43:29

Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
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]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 16
Total_Scans       = 16

Relaxation_Delay  = 4[s]
Recvr_Gain        = 36
Temp_Get          = 71.6[dC]
X_90_Width        = 12.25[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 6[dB]
X_Pulse           = 6.125[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
```



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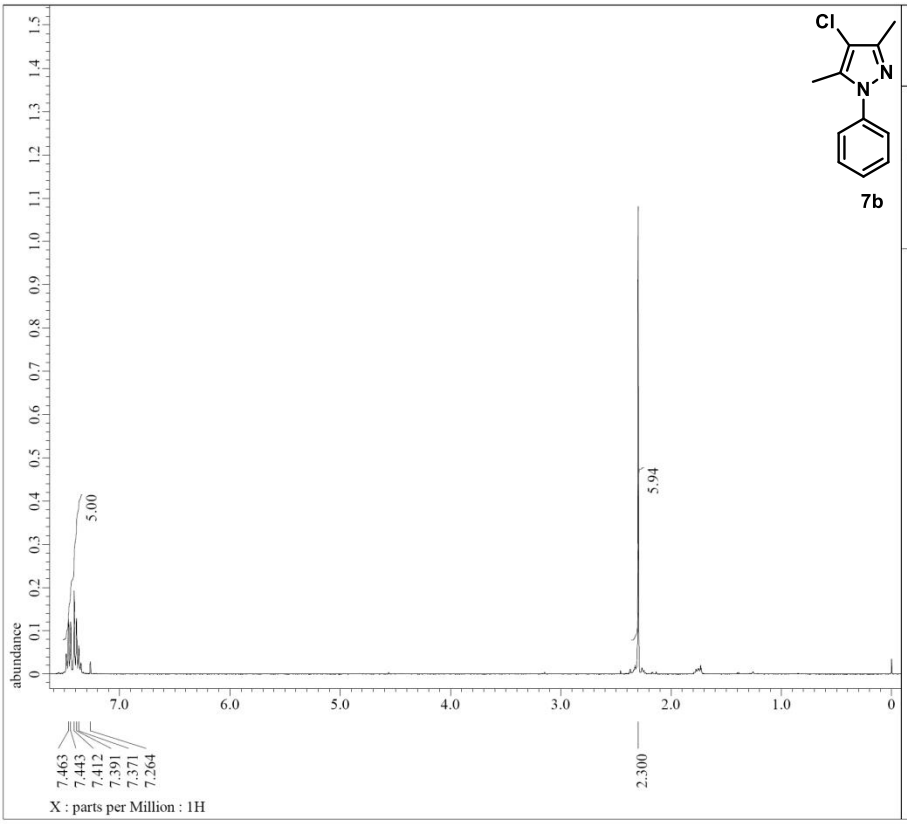
```
---- PROCESSING PARAMETERS ----
sexp( 3.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 2 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                = GDS-425_Carbon-2-1
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = DSR_GDS-425
Solvent                 = NONE
Creation_Time           = 16-AUG-2018 15:50:
Revision_Time           = 12-FEB-2019 11:03:
Current_Time            = 22-FEB-2019 10:46:

Comment                 = single pulse decou
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.38906137[T] (400
X_Acq_Duration          = 0.51904512[s]
X_Domain                = Carbon13
X_Freq                  = 100.51775967[MHz]
X_Offset                = 100[ppm]
X_Points                = 16384
X_Prescans              = 4
X_Resolution            = 1.92661478[Hz]
X_Sweep                 = 31.56565657[kHz]
X_Sweep_Clipped         = 25.25252525[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.75219779[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 5[us]
Clipped                 = FALSE
Decimation_Reg          = r: 198( 197),g: 39
Scans                   = 512
Total_Scans             = 512

Relaxation_Delay        = 2[s]
Recvr_Gain              = 56
Temp_Get                = 20.8[dC]
X_90_Width              = 8.57[us]
X_Acq_Time              = 0.51904512[s]
X_Angle                 = 30[deg]
X_Atn                   = 7.0[dB]
X_Pulse                 = 2.85666667[us]
Irr_Atn_Dec             = 26.16[dB]
Irr_Atn_Dec_Calc        = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe             = 26.16[dB]
```



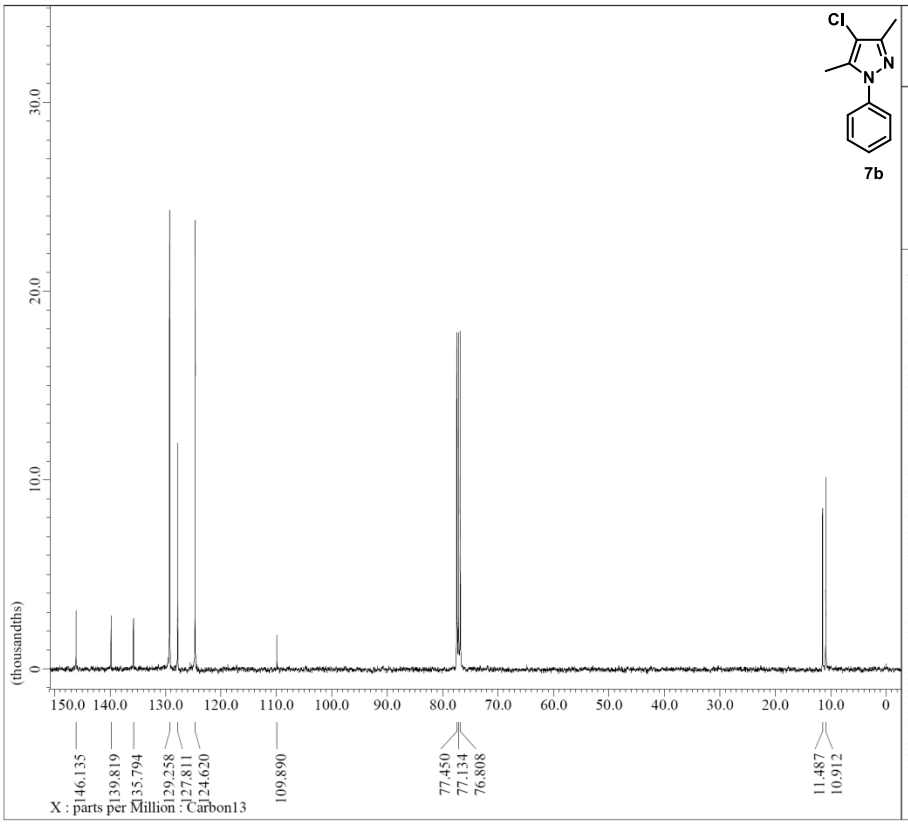

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp_auto : 0.2
trapezoid3 : 0[%] : 80[%] : 100[%]
fft : 1
machinephase
dc_correct
ppm
thresh : 5[%] : 1
peak_pick : 0[Hz] : 0.1[ppm] : Both : 0[Hz]
auto_reference : 5[%]
```

```
Filename            = GDS-426_PROTON-2.jdf
Author              = delta
Experiment          = single_pulse.ex2
Sample_Id           = DSM_GDS-426
Solvent             = CHLOROFORM-D
Creation_Time       =  6-AUG-2018 10:31:18
Revision_Time       = 22-FEB-2019 10:54:40
Current_Time        = 22-FEB-2019 10:54:56

Data_Format         = 1D COMPLEX
Dim_Size            = 13107
Dim_Title           = 1H
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400P
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]
Irr_Domain          = 1H
Irr_Freq            = 399.78219838[MHz]
Irr_Offset          = 5[ppm]
Tri_Domain          = 1H
Tri_Freq            = 399.78219838[MHz]
Tri_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 16
Total_Scans         = 16

Relaxation_Delay    = 4[s]
Recvr_Gain          = 34
Temp_Get            = 71.2[dC]
X_90_Width          = 12.25[us]
X_Acq_Time          = 2.18365952[s]
X_Angle             = 45[deg]
X_Atn               = 6[dB]
X_Pulse             = 6.125[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 3.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 2 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                = GDS-426_Carbon-1-1
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = DB_GDS-426
Solvent                 = CHLOROFORM-D
Creation_Time           =  7-AUG-2018 22:43:
Revision_Time           = 12-FEB-2019 11:11:
Current_Time            = 22-FEB-2019 10:56:

Comment                 = single pulse decou
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.38906137[T] (400
X_Acq_Duration          = 0.51904512[s]
X_Domain                = Carbon13
X_Freq                  = 100.51775967[MHz]
X_Offset                = 100[ppm]
X_Points                = 16384
X_Prescans              = 4
X_Resolution            = 1.92661478[Hz]
X_Sweep                 = 31.56565657[kHz]
X_Sweep_Clipped         = 25.25252525[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.75219779[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 5[us]
Clipped                 = FALSE
Decimation_Reg          = r: 198( 197),g: 39
Scans                   = 512
Total_Scans             = 512

Relaxation_Delay        = 2[s]
Recvr_Gain              = 56
Temp_Get                = 20.7[dC]
X_90_Width              = 8.57[us]
X_Acq_Time              = 0.51904512[s]
X_Angle                 = 30[deg]
X_Atn                   = 7.8[dB]
X_Pulse                 = 2.85666667[us]
Irr_Atn_Dec             = 26.16[dB]
Irr_Atn_Dec_Calc        = 26.16[dB]
Irr_Atn_Dec_Default_Calc = 26.16[dB]
Irr_Atn_Noe             = 26.16[dB]
```

LEGENDS FOR SUPPLEMENTARY FIGURES

Supplementary Figure 1: This figure shows the chemical structures of shortlisted compounds obtained from phenotypic screens performed in *M. bovis* BCG.

Supplementary Figure 2: Two drug checkerboard assay to study the interaction of NSC 18725 with INH, RIF, EMB, BDQ, BTZ043 or PA-824. Fractional inhibitory concentrations (FICs) and fractional inhibitory concentration index (∑FIC) for various drug combinations were calculated using the following formula: FIC=MIC in combination/MIC alone. ∑FIC = FIC of drug A + FIC of drug B. ∑FIC value ≤ 0.5 indicate synergistic activity, ∑FIC of ≥ 4.0 indicate antagonistic activity, and values in between (≤ 4.0 and > .5) indicate an additive interaction. Wells showing + sign denote growth, - sign denote no growth, and (-) sign denote activity due to a combination. The data shown in this panel is representative of three independent experiments.