Supplementary Information

A simple protocol for Cu-catalyzed protodecarboxylation of (hetero)aromatic carboxylic acids

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General considerations. The Reagents used for experiments were commercially available and were used as received unless otherwise noted. DMSO were distilled from CaH_2 under reduced pressure and stored under nitrogen. All Reactions were performed under nitrogen with the strict exclusion of moisture using Schlenk techniques. Column chromatography was performed on silica gel 300-400 mesh. The yields reported are the isolated yields and the average of two runs. Except for ^{13}C spectrum of product **2v**, ^{1}H, ^{13}C and ^{19}F NMR spectra of all protodecarboxylation products were recorded at 400, 100 and 377 MHz of Agilent 400MR DD2 with $CDCl_3$ as solvent respectively; ^{13}C spectrum of product **2v** was recorded at 100 MHz of Bruker Ascend400MR with $CDCl_3$ as solvent. All coupling constants (*J* values) were reported in Hertz (Hz). HRMS were performed by Shanghai Mass Spectrometry Centre, Shanghai Institute of Organic Chemistry, Chinese Academic of Sciences.

General procedure for Copper-Catalyzed Protodecarboxylation of (Hetero)Aromatic Carboxylic Acids. An oven-dried Schlenk tube equipped with a stir bar was charged with aryl carboxylic acid (0.2 mmol) and CuI (11.4 mg, 0.06 mmol, 0.3 equiv). The tube was fitted with a rubber septum, and then it was evacuated and refilled with nitrogen three times. Under nitrogen, the solution of Et_3N in DMSO (2 mL) was added via syringe. The rubber septum was replaced with a Teflon screwcap under nitrogen flow, and the Schlenk tube was pressurized to 1 atm. With stirring, the reaction mixtures were heated at 120 °C for the indicated amount of time (unless otherwise specified), and then cooled down to room temperature. The resultant mixture was filtered through a short plug of silica gel and then concentrated in vacuo. The residue was then purified by flash chromatography on silica gel to provide the corresponding product.

1-chloro-3-nitrobenzene (2a, Table 2). Procedure was followed using 4-chloro-2-nitrobenzoic acid (40.3 mg, 0.2 mmol), CuI (11.4 mg, 0.06 mmol, 0.3 equiv) and Et_3N (14 uL, 0.1 mmol, 0.5 equiv). The reaction mixtures were purified by flash column chromatography on silica gel (1% ether in hexane) to afford 24.9 mg (79%) of the product as a colourless liquid. Exhibited spectral data in accordance with

previous report.[1] ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.23 (t, J = 2.0 Hz, 1H), 8.14 (dd, J = 7.2, 0.8 Hz, 1H), 7.69 (ddd, J = 7.2, 1.8, 0.8 Hz, 1H), 7.51 (t, J = 8.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 135.4, 134.7, 130.4, 123.9, 121.7, 110.0.

1-chloro-4-nitrobenzene (2b, Table 2). Procedure was followed using 5-chloro-2-nitrobenzoic acid (40.3 mg, 0.2 mmol), CuI (11.4 mg, 0.06 mmol, 0.3 equiv) and Et_3N (14 uL, 0.1 mmol, 0.5 equiv). The reaction mixtures were purified by flash column chromatography on silica gel (1% ether in hexane) to afford 27.7 mg (88%) of the product as a colourless liquid. Exhibited spectral data in accordance with previous report.[2] ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.18 (d, J = 8.4 Hz, 2H), 7.51 (d, J = 8.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.4, 129.6, 124.9.

1-(methylsulfonyl)-3-nitrobenzene (2c, Table 2). Procedure was followed using 4-(methylsulfonyl)-2-nitrobenzoic acid (49.0 mg, 0.2 mmol), CuI (11.4 mg, 0.06 mmol, 0.3 equiv) and Et_3N (14 uL, 0.1 mmol, 0.5 equiv). The reaction mixtures were purified by flash column chromatography on silica gel (40% ether in hexane) to afford 35.0 mg (87%) of the product as a yellow solid. Exhibited spectral data in accordance with previous report.[3] ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.80 (s, 1H), 8.51-8.54 (m, 1H), 8.30 (d, J = 7.6 Hz, 1H), 7.84 (t, J = 8.0 Hz, 1H), 3.14 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 132.9, 130.9, 128.2, 122.9, 44.3.

1,3-dinitrobenzene (2d, Table 2). Procedure was followed using 2,4-dinitrobenzoic acid (42.4 mg, 0.2 mmol), CuI (11.4 mg, 0.06 mmol, 0.3 equiv) and Et_3N (14 uL, 0.1 mmol, 0.5 equiv). The reaction mixtures were purified by flash column chromatography on silica gel (10% ether in hexane) to afford 22.5 mg (67%) of the product as a white solid. Exhibited spectral data in accordance with previous report.[4] ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.08 (s, 1H), 8.59 (dd, J = 8.0, 1.2 Hz, 2H), 7.83 (t, J = 8.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 130.7, 128.9, 119.1.

3-nitrobenzoic acid (2e, Table 2). Procedure was followed using 2-nitroterephthalic acid (42.2 mg, 0.2 mmol), CuI (11.4 mg, 0.06 mmol, 0.3 equiv) and Et_3N (14 uL, 0.1 mmol, 0.5 equiv). The reaction mixtures were purified by flash column chromatography on silica gel (30% ether in hexane) to afford 13.7 mg (41%) of the product as a white solid. ^{1}H NMR (400 MHz, DMSO): δ 8.56 (s, 1H), 8.41 (dd, J = 8.0, 1.6 Hz, 1H), 8.29 (d, J = 8.0 Hz, 1H), 7.76 (t, J = 8.0 Hz, 1H). ^{13}C NMR (100 MHz, DMSO): δ 166.0, 148.3, 135.8, 132.9, 131.0, 127.8, 124.1. HRMS (MALDI-TOF) m/z: $[M]^+$ Calcd for $C_7H_5NO_4$ 167.0219; Found: 167.0215.

1-nitro-3-(trifluoromethyl)benzene (2f, Table 2). Procedure was followed using 2-nitro-4-(trifluoromethyl)benzoic acid (47.0 mg, 0.2 mmol), CuI (11.4 mg, 0.06 mmol, 0.3 equiv) and Et_3N (14 uL, 0.1 mmol, 0.5 equiv). The reaction mixtures were purified by flash column chromatography on silica gel (1% ether in hexane) to afford 20.6 mg (54%) of the product as a colourless liquid. Exhibited spectral data in accordance with previous report.[5] ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.52 (s, 1H), 8.45 (d, J = 8.4 Hz, 1H), 7.99 (d, J = 8.0 Hz, 1H), 7.75 (t, J = 8.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 131.2-131.1 (m), 130.3, 126.6, 124.2, 121.5, 120.9-120.8 (m). ^{19}F NMR (377 MHz, $CDCl_3$): δ -63.0 (s, 3F).

1-fluoro-3-nitrobenzene (2g, Table 2). Procedure was followed using 4-fluoro-2-nitrobenzoic acid (37.0 mg, 0.2 mmol), CuI (11.4 mg, 0.06 mmol, 0.3 equiv) and Et_3N (14 uL, 0.1 mmol, 0.5 equiv). The reaction mixtures were purified by flash column chromatography on silica gel (1% ether in hexane) to afford 14.7 mg (52%) of the product as a colourless liquid. Exhibited spectral data in accordance with previous report.[6] ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.06 (d, J = 7.6 Hz, 1H), 7.94 (d, J = 8.4 Hz, 1H), 7.56-7.52 (m, 1H), 7.45-7.41 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.6, 161.1, 130.7 (d, J = 8.2 Hz), 121.9 (d, J=22 Hz), 119.3 (d, J = 3.4 Hz), 111.4 (d, J=26 Hz). ^{19}F NMR (377 MHz, $CDCl_3$): δ -109.0 - -109.1 (m, 1F).

1-fluoro-4-nitrobenzene (2h, Table 2). Procedure was followed using 5-fluoro-2-nitrobenzoic acid (37.0 mg, 0.2 mmol), CuI (11.4 mg, 0.06 mmol, 0.3 equiv) and Et_3N (14 uL, 0.1 mmol, 0.5 equiv). The reaction mixtures were purified by flash column chromatography on silica gel (1% ether in hexane) to afford 15.2 mg (54%) of the product as a colourless liquid. Exhibited spectral data in accordance with previous report.[7] ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.29-8.26 (m, 2H), 7.26-7.19 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.5, 165.0, 126.4 (d, J = 10.0 Hz), 116.4 (d, J = 24.0 Hz). ^{19}F NMR (377 MHz, $CDCl_3$): δ -101.9 - -102.0 (m, 1F).

nitrobenzene (2i, Table 2). Procedure was followed using 2-nitrobenzoic acid (33.4 mg, 0.2 mmol), CuI (11.4 mg, 0.06 mmol, 0.3 equiv) and Et_3N (14 uL, 0.1 mmol, 0.5 equiv). The reaction mixtures were purified by flash column chromatography on silica gel (1% ether in hexane) to afford 15.5 mg (63%) of the product as a colourless liquid. Exhibited spectral data in accordance with previous report.[8] ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.24 (d, J = 7.6 Hz, 2H), 7.72-7.69 (m, 1H), 7.57-7.53 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 134.6, 129.3, 123.5.

1-methyl-2-nitrobenzene (2j, Table 2). Procedure was followed using 3-methyl-2-nitrobenzoic acid (36.2 mg, 0.2 mmol), CuI (11.4 mg, 0.06 mmol, 0.3 equiv) and Et_3N (14 uL, 0.1 mmol, 0.5 equiv). The reaction mixtures were purified by flash column chromatography on silica gel (1% ether in hexane) to afford 8.2 mg (30%) of the product as a colourless liquid. Exhibited spectral data in accordance with previous report.[9] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 (d, J = 8.4 Hz, 1H), 7.49 (d, J = 8.8 Hz, 1H), 7.35-7.34 (m, 2H), 2.61 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 133.5, 133.0, 132.7, 126.9, 124.6, 20.4.

1-methyl-3-nitrobenzene (2k, Table 2). Procedure was followed using 4-methyl-2-nitrobenzoic acid (36.2 mg, 0.2 mmol), CuI (11.4 mg, 0.06 mmol, 0.3 equiv) and Et_3N (14 uL, 0.1 mmol, 0.5 equiv). The reaction mixtures were purified by flash column chromatography on silica gel (1% ether in hexane) to afford 23.3 mg (85%) of the product as a colourless liquid. Exhibited spectral data in accordance with

previous report.[10] ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02 (d, J = 8.8 Hz, 2H), 7.50 (d, J = 7.6 Hz, 1H), 7.41 (t, J = 8.0 Hz, 1H), 2.46 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.8, 135.3, 129.0, 123.8, 120.6, 21.2.

1-methyl-4-nitrobenzene (2l, Table 2). Procedure was followed using 5-methyl-2-nitrobenzoic acid (36.2 mg, 0.2 mmol), CuI (11.4 mg, 0.06 mmol, 0.3 equiv) and Et_3N (14 uL, 0.1 mmol, 0.5 equiv). The reaction mixtures were purified by flash column chromatography on silica gel (1% ether in hexane) to afford 24.1 mg (88%) of the product as a colourless liquid. Exhibited spectral data in accordance with previous report.[11] ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.11 (d, J = 8.4 Hz, 2H), 7.31 (d, J = 8.0 Hz, 2H), 2.46 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.9, 129.8, 123.4, 21.7.

1-methoxy-3-nitrobenzene (2m, Table 2). Procedure was followed using 4-methoxy-2-nitrobenzoic acid (39.4 mg, 0.2 mmol), CuI (11.4 mg, 0.06 mmol, 0.3 equiv) and Et_3N (14 uL, 0.1 mmol, 0.5 equiv). The reaction mixtures were purified by flash column chromatography on silica gel (3% ether in hexane) to afford 27.3 mg (89%) of the product as a yellow liquid. Exhibited spectral data in accordance with previous report.[8] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.84-7.81 (m, 1H), 7.73 (s, 1H), 7.43 (t, J = 8.0 Hz, 1H), 7.23 (dd, J = 8.4, 1.2 Hz, 1H), 3.89 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.1, 129.9, 121.3, 115.7, 108.1, 55.8.

1-methoxy-4-nitrobenzene (2n, Table 2). Procedure was followed using 5-methoxy-2-nitrobenzoic acid (39.4 mg, 0.2 mmol), CuI (11.4 mg, 0.06 mmol, 0.3 equiv) and Et_3N (14 uL, 0.1 mmol, 0.5 equiv). The reaction mixtures were purified by flash column chromatography on silica gel (3% ether in hexane) to afford 26.0 mg (85%) of the product as a yellow solid. Exhibited spectral data in accordance with previous report.[12] ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17 (d, J = 8.0 Hz, 2H), 6.94 (d, J = 8.0 Hz, 2H), 3.90 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.6, 125.9, 114.0, 56.0.

1,2-dimethoxy-4-nitrobenzene (2o, Table 2). Procedure was followed using 4,5-dimethoxy-2-nitrobenzoic acid (45.4 mg, 0.2 mmol), and CuI (11.4 mg, 0.06 mmol, 0.3 equiv) and Et_3N (14 uL, 0.1 mmol, 0.5 equiv). The reaction mixtures were purified by flash column chromatography on silica gel (10% ether in hexane) to afford 34.1 mg (93%) of the product as a yellow solid. Exhibited spectral data in accordance with previous report.[13] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92-7.89 (m, 1H), 7.73 (d, J = 1.6 Hz, 1H), 6.90 (d, J = 8.8 Hz, 1H), 3.97 (s, 3H), 3.95 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.5, 148.8, 141.5, 117.8, 109.8, 106.4, 56.4, 56.3.

4-nitroaniline (2p, Table 2). Procedure was followed using 5-amino-2-nitrobenzoic acid (36.4 mg, 0.2 mmol), CuI (11.4 mg, 0.06 mmol, 0.3 equiv) and Et_3N (14 uL, 0.1 mmol, 0.5 equiv). The reaction mixtures were purified by flash column chromatography on silica gel (10% ether in hexane) to afford 24.3 mg (88%) of the product as a yellow solid. Exhibited spectral data in accordance with previous report.[14] ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.06 (d, J = 9.2 Hz, 2H), 6.62 (d, J = 9.2 Hz, 2H), 4.39 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.5, 126.4, 113.4.

N-(3-nitrophenyl)acetamide (2q, Table 2). Procedure was followed using 4-acetamido-2-nitrobenzoic acid (44.8 mg, 0.2 mmol), CuI (11.4 mg, 0.06 mmol, 0.3 equiv) and Et_3N (14 uL, 0.1 mmol, 0.5 equiv). The reaction mixtures were purified by flash column chromatography on silica gel (2% ether in hexane) to afford 23.1 mg (64%) of the product as a white solid. Exhibited spectral data in accordance with previous report.[15] ^{1}H NMR (400 MHz, DMSO): δ 10.53 (s, 1H), 8.14 (d, J = 8.8 Hz, 2H), 7.76 (d, J = 8.8 Hz, 2H), 2.06 (s, 3H). ^{13}C NMR (100 MHz, DMSO): δ 169.8, 145.9, 142.4, 125.4, 118.9, 24.7.

1-chloro-2,4-dimethoxy-5-nitrobenzene (2r, Table 2). Procedure was followed using 3-chloro-2,6-dimethoxy-5-nitrobenzoic acid (52.3 mg, 0.2 mmol), CuI (11.4 mg, 0.06 mmol, 0.3 equiv) and Et_3N (14 uL, 0.1 mmol, 0.5 equiv). The reaction mixtures were purified by flash column chromatography on

silica gel (10 % ether in hexane) to afford 38.7 mg (89%) of the product as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.05 (s, 1H), 6.54 (s, 1H), 3.99 (s, 3H), 3.98 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.0, 154.6, 127.9, 113.9, 97.0, 56.9, 56.7. HRMS (MALDI-TOF) m/z: $[M]^+$ Calcd for $C_8H_8NO_4Cl$ 217.0142; Found: 217.0140.

2*H*-chromen-2-one (2s, Table 2). Procedure was followed using 2-oxo-2H-chromene-3-carboxylic acid (38.0 mg, 0.2 mmol), CuI (11.4 mg, 0.06 mmol, 0.3 equiv) and Et_3N (14 uL, 0.1 mmol, 0.5 equiv). The reaction mixtures were purified by flash column chromatography on silica gel (5 % ether in hexane) to afford 16.7 mg (57%) of the product as a white solid.Exhibited spectral data in accordance with previous report.[16] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70 (d, J = 9.6 Hz, 1H), 7.54-7.47 (m, 2H), 7.33-7.25 (m, 2H), 6.42 (d, J = 9.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.7, 154.0, 143.3, 131.8, 127.8, 124.4, 118.8, 116.9, 116.7.

3-chlorobenzo[b]thiophene (2t, Table 2). Procedure was followed using 3-chlorobenzo[b]thiophene-2-carboxylic acid (42.5 mg, 0.2 mmol), CuI (11.4 mg, 0.06 mmol, 0.3 equiv) and Et_3N (14 uL, 0.1 mmol, 0.5 equiv). The reaction mixtures were purified by flash column chromatography on silica gel (1% ether in hexane) to afford 29.7 mg (88%) of the product as a colourless liquid. Exhibited spectral data in accordance with previous report.[17] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.86 (t, J = 8.8 Hz, 2H), 7.50-7.41(m, 2H), 7.32 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 138.4, 136.1, 125.4, 124.9, 122.9, 121.9, 121.2, 120.8.

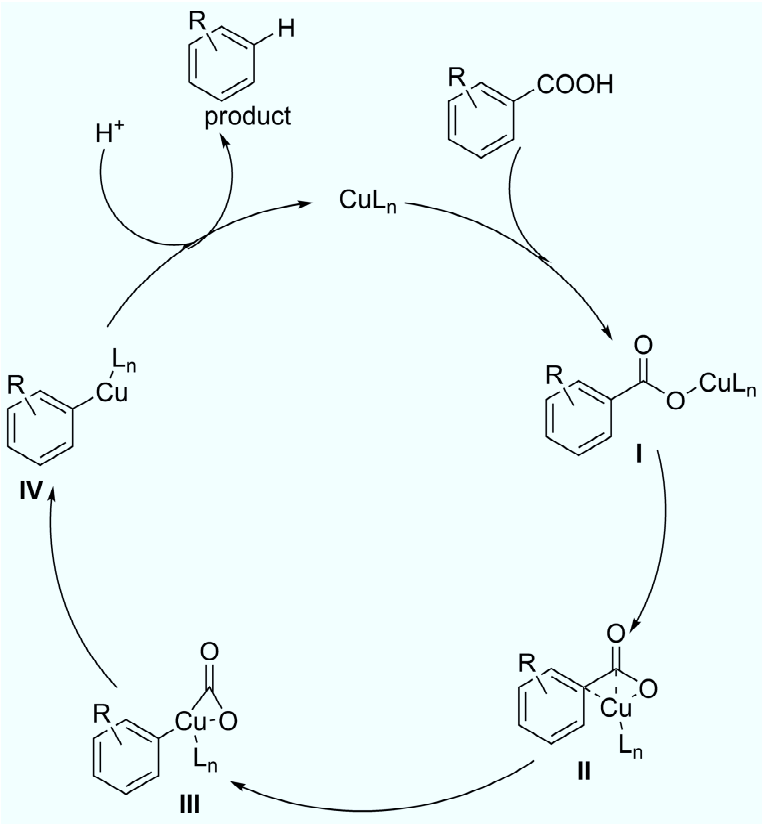
3-methylbenzo[b]thiophene (2u, Table 2). Procedure was followed using 3-methylbenzo[b]thiophene-2-carboxylic acid (38.4mg, 0.2 mmol), CuI (11.4 mg, 0.06 mmol, 0.3 equiv) and Et_3N (14 uL, 0.1 mmol, 0.5 equiv). The reaction mixtures were purified by flash column chromatography on silica gel (1% ether in hexane) to afford 26.4 mg (89%) of the product as a colourless liquid. Exhibited spectral data in accordance with previous report.[18] ^{1}H NMR (400 MHz,

$CDCl_3$): δ 7.89 (d, J = 7.6 Hz, 1H), 7.75 (d, J = 7.6 Hz, 1H), 7.45-7.36 (m, 2H), 7.10 (s, 1H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 140.3, 139.7, 132.2, 124.1, 123.9, 122.8, 121.8, 121.5, 14.0.

2,3,4-trichlorothiophene (2v, Table 2). Procedure was followed using 3,4,5-trichlorothiophene-2-carboxylic acid (46.3 mg, 0.2 mmol), CuI (11.4 mg, 0.06 mmol, 0.3 equiv) and Et_3N (14 uL, 0.1 mmol, 0.5 equiv). The reaction mixtures were purified by flash column chromatography on silica gel (1% ether in hexane) to afford 21.7 mg (58%) of the product as a yellow solid. ^1H NMR (400 MHz, $CDCl_3$): δ 7.06 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 125.2, 124.0, 123.6, 117.5. HRMS (MALDI-TOF) m/z: $[M]^+$ Calcd for C_4HSCl_3 185.8865; Found: 185.8863.

Mechanism discussion. some observations have been performed to gain insights into the reaction mechanism. Firstly, as shown in the entries of 14-15 of Table 1, the control experiments showed that both CuI and Et_3N were essential to this protodecarboxylation of (hetero)aromatic carboxylic acids. Secondly, when the model reaction was carried out under the standard conditions in the presence of radical inhibitor, such as 2,6-ditert-butyl-4-methylphenol (BHT), the reaction was obviously unaffected and gave the desired product in 92% yield. Thus, the result ruled out a radical pathway in our protocol. According to the above result and previous reports,[19,20] a tentative mechanism of our protocol (Fig S1) is proposed that copper catalyst was believed to initially react with aryl carboxylic acid substrate under heating to form copper carboxylate **I**, followed by coordination of copper atom to C-COO bond of the copper carboxylate **I** to provide intermediate **II**. Subsequently, copper inserted into C-C(O) bond of the intermediate **II** via oxidative addition immediately and then a reductive elimination generated aryl-copper intermediate **IV** from the intermediate **III**, which ultimately led to protodecarboxylation product and Cu(I) species. Therefore, it's understandable that the benefits of Et_3N in catalytic cycle is to assistant oxidative addition via its electron donating ability and accelerate reductive elimination through its steric hindrance.

***Fig S1**. A tentative mechanism of this protocol*



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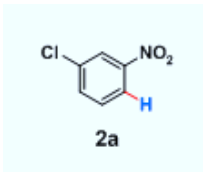
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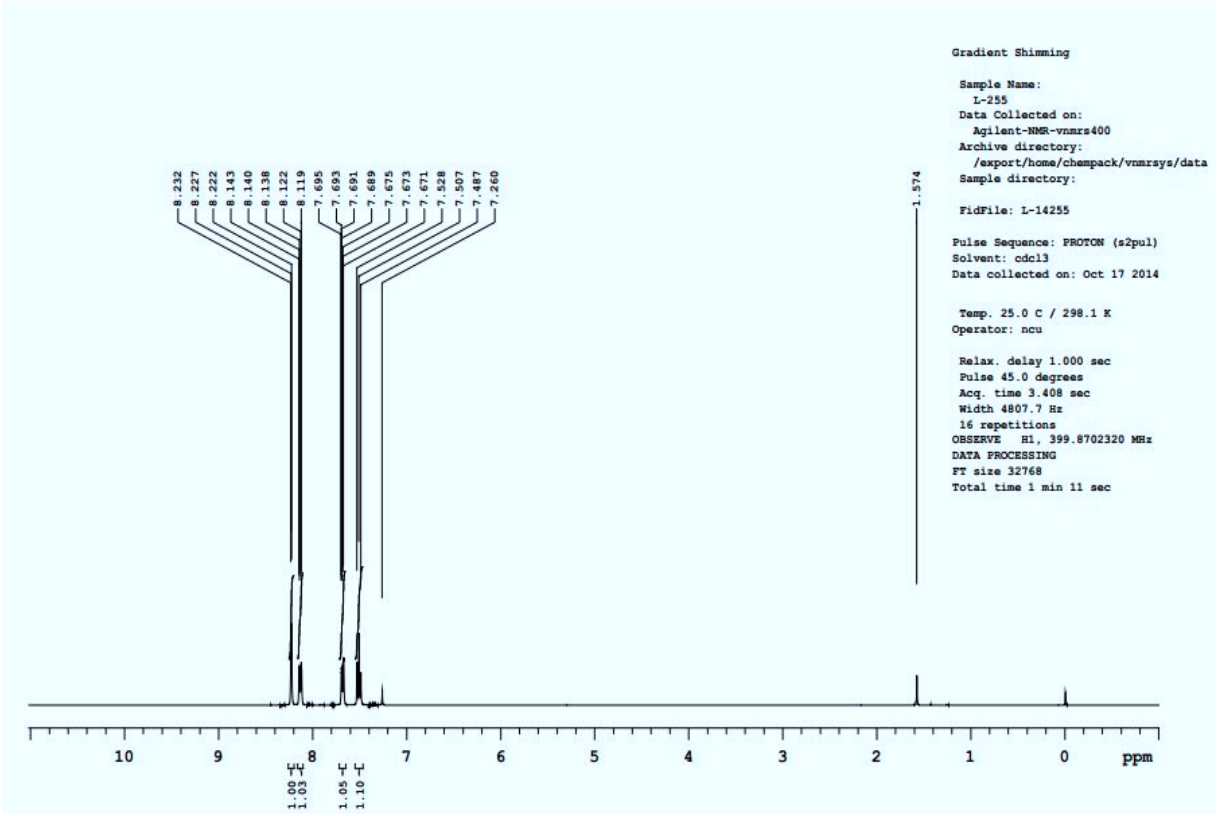
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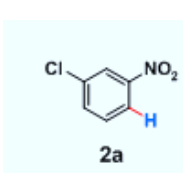
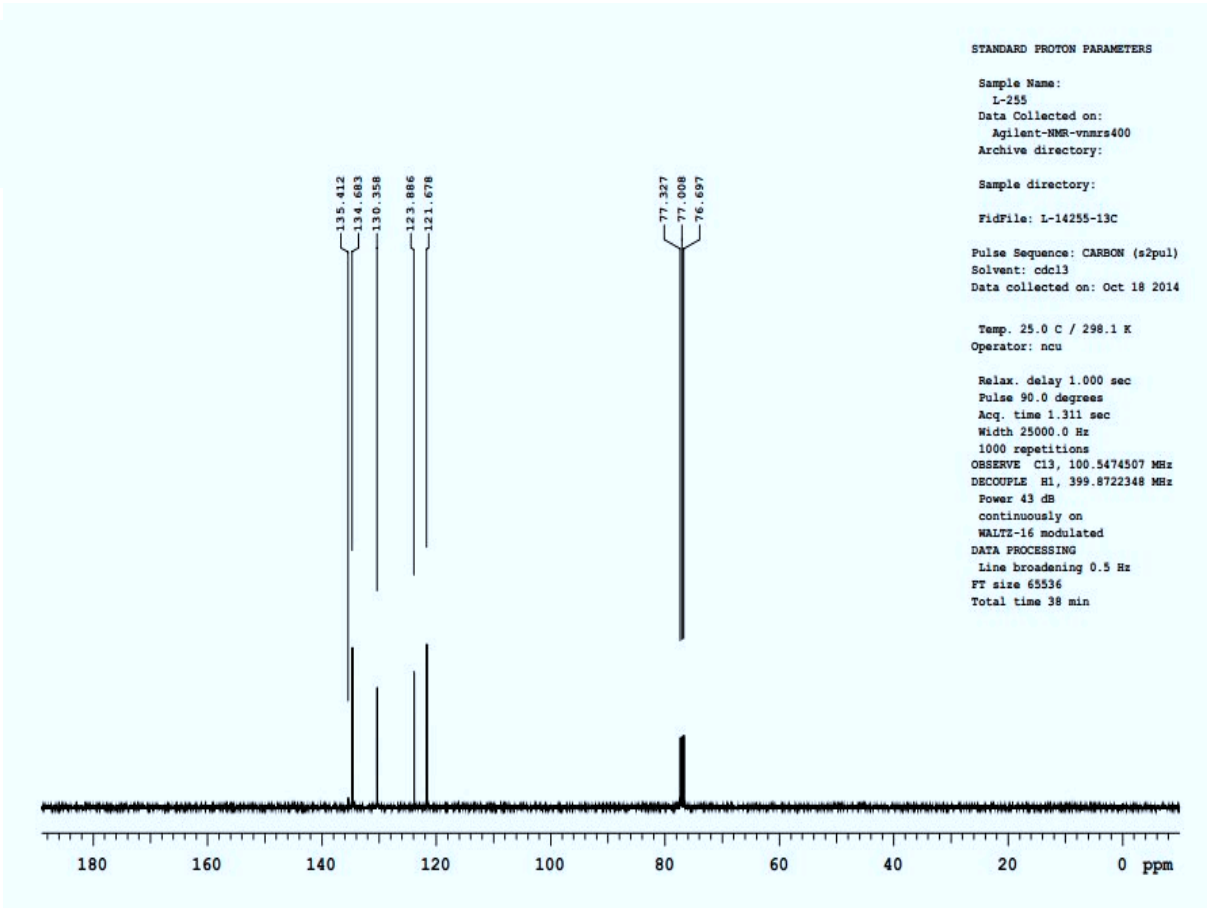
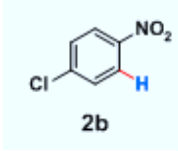
FT size 32768
Total time 1 min 11 sec

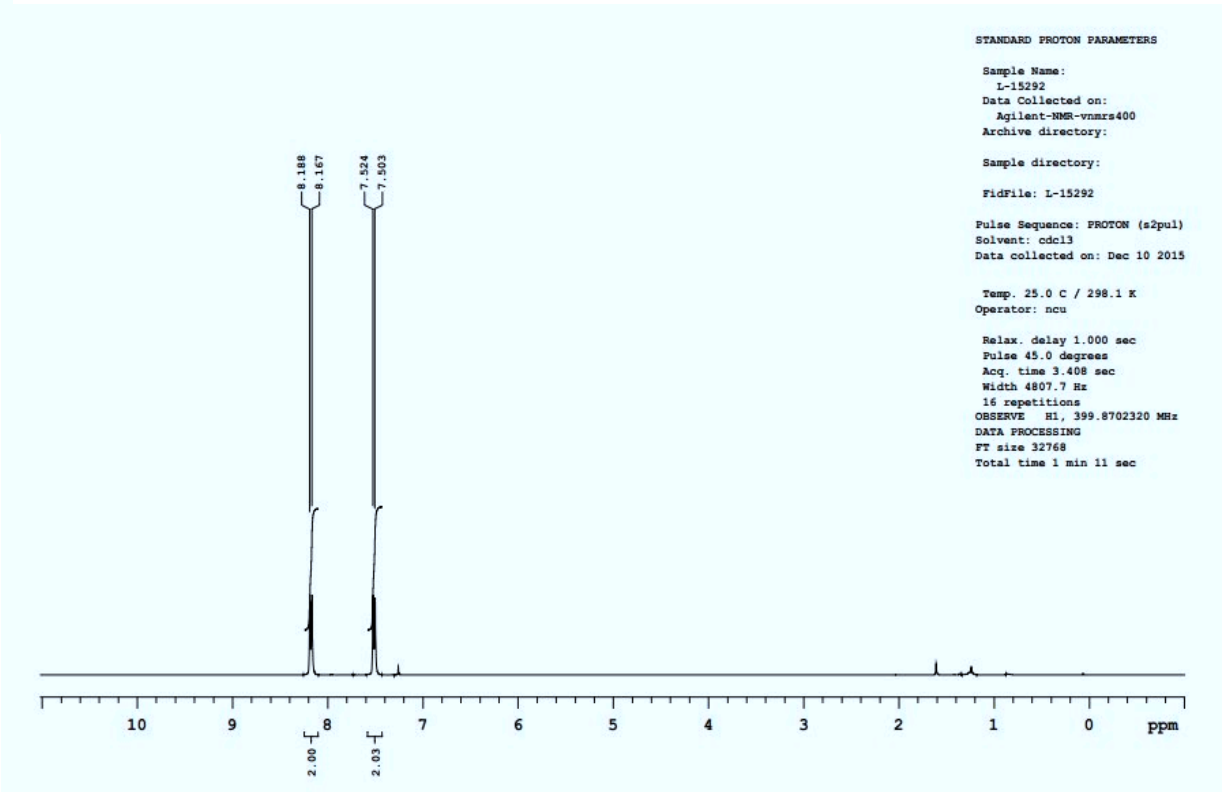

Cl
NO2
H

2a


135.412
134.683
130.358
123.886
121.678
77.327
77.008
76.697
180
160
140
120
100
80
60
40
20
0
ppm
STANDARD PROTON PARAMETERS
Sample Name:
L-255
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: L-14255-13C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 18 2014
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1000 repetitions
OBSERVE C13, 100.5474507 MHz
DECOUPLE H1, 399.8722348 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 38 min

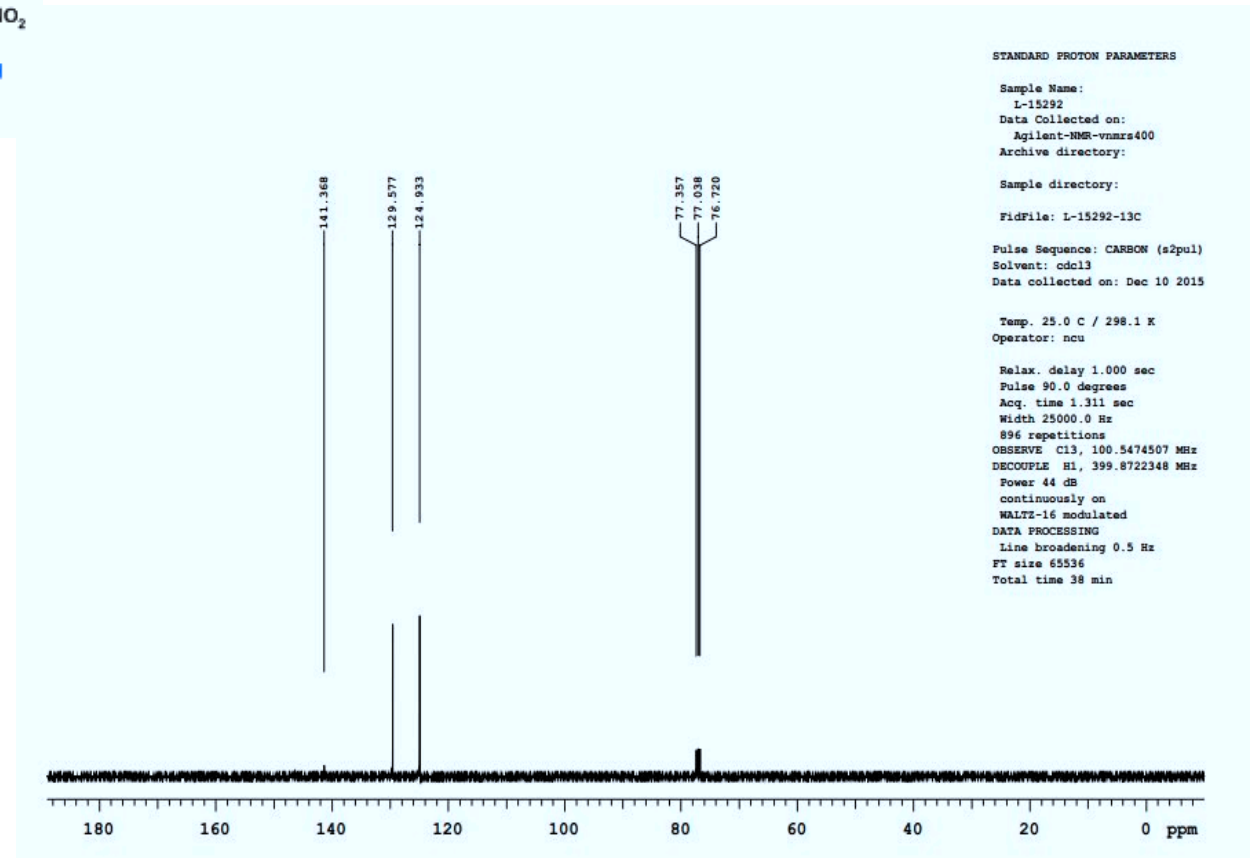

NO2
Cl
H

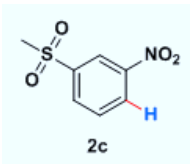
2b


8.188
8.167
7.524
7.503
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.03
STANDARD PROTON PARAMETERS
Sample Name:
L-15292
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: L-15292
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Dec 10 2015
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.408 sec
Width 4807.7 Hz
16 repetitions
OBSERVE H1, 399.8702320 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 11 sec

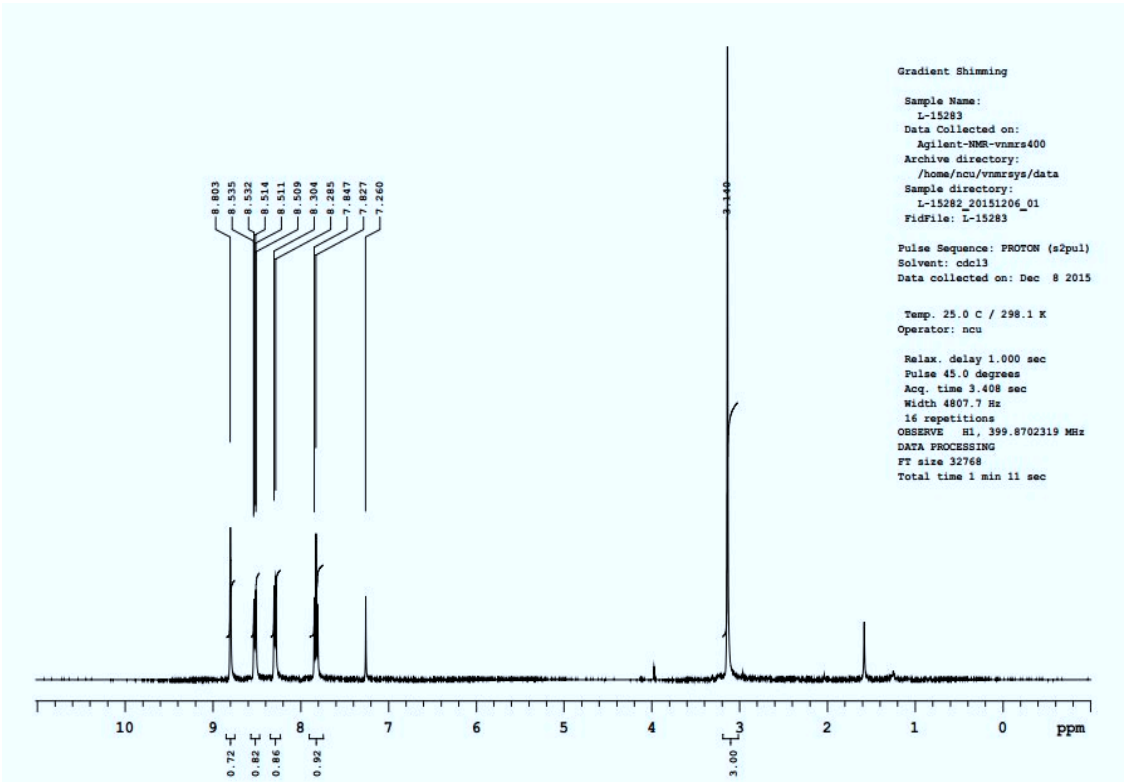

NO2
Cl
H

2b


141.368
129.577
124.933
77.357
77.038
76.720
180
160
140
120
100
80
60
40
20
0
ppm
STANDARD PROTON PARAMETERS
Sample Name:
L-15292
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: L-15292-13C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Dec 10 2015
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
896 repetitions
OBSERVE C13, 100.5474507 MHz
DECOUPLE H1, 399.8722348 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 38 min

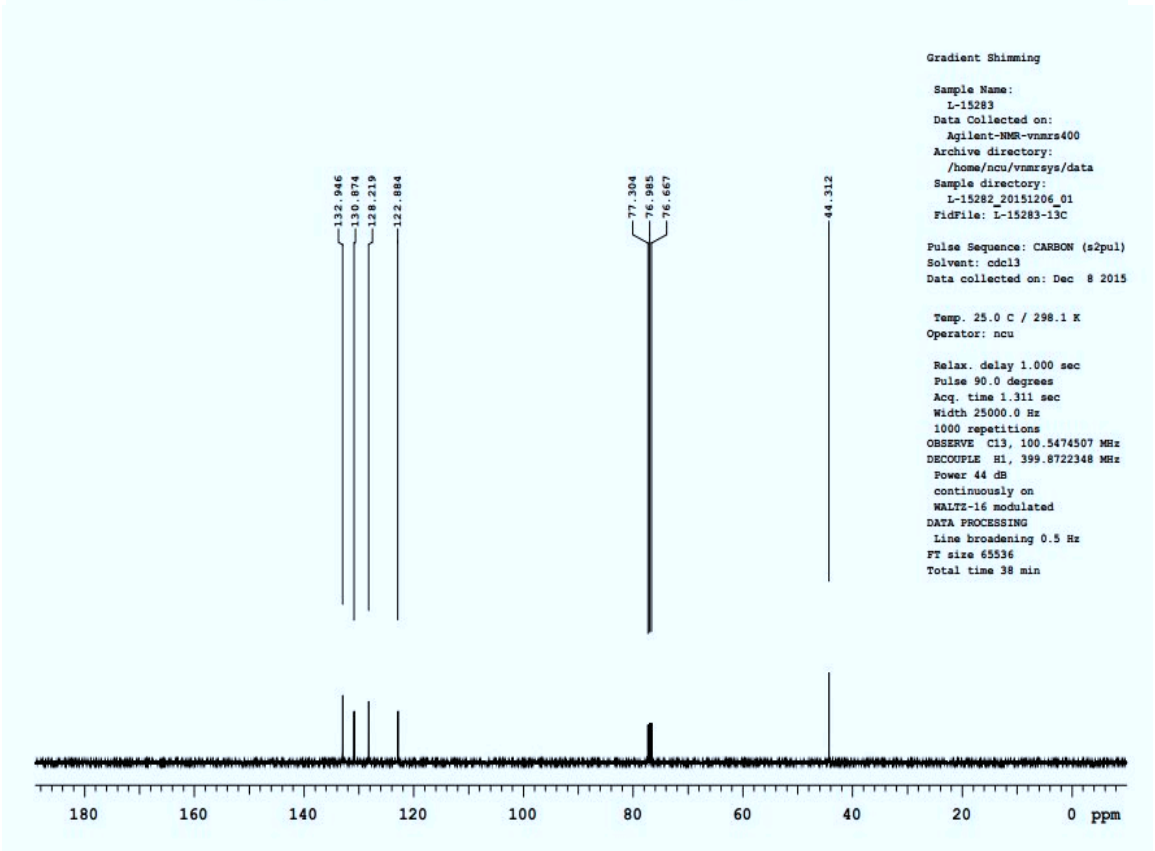

O
S
O
NO2
H

2c


8.803
8.535
8.532
8.514
8.511
8.509
8.304
8.285
7.847
7.827
7.260
3.140
10
9
8
7
6
5
4
3
2
1
0
ppm
0.72
0.82
0.86
0.92
3.00
Gradient Shimming
Sample Name:
L-15283
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
/home/ncu/vnmrsys/data
Sample directory:
L-15282_20151206_01
FidFile: L-15283
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Dec 8 2015
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.408 sec
Width 4807.7 Hz
16 repetitions
OBSERVE H1, 399.8702319 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 11 sec

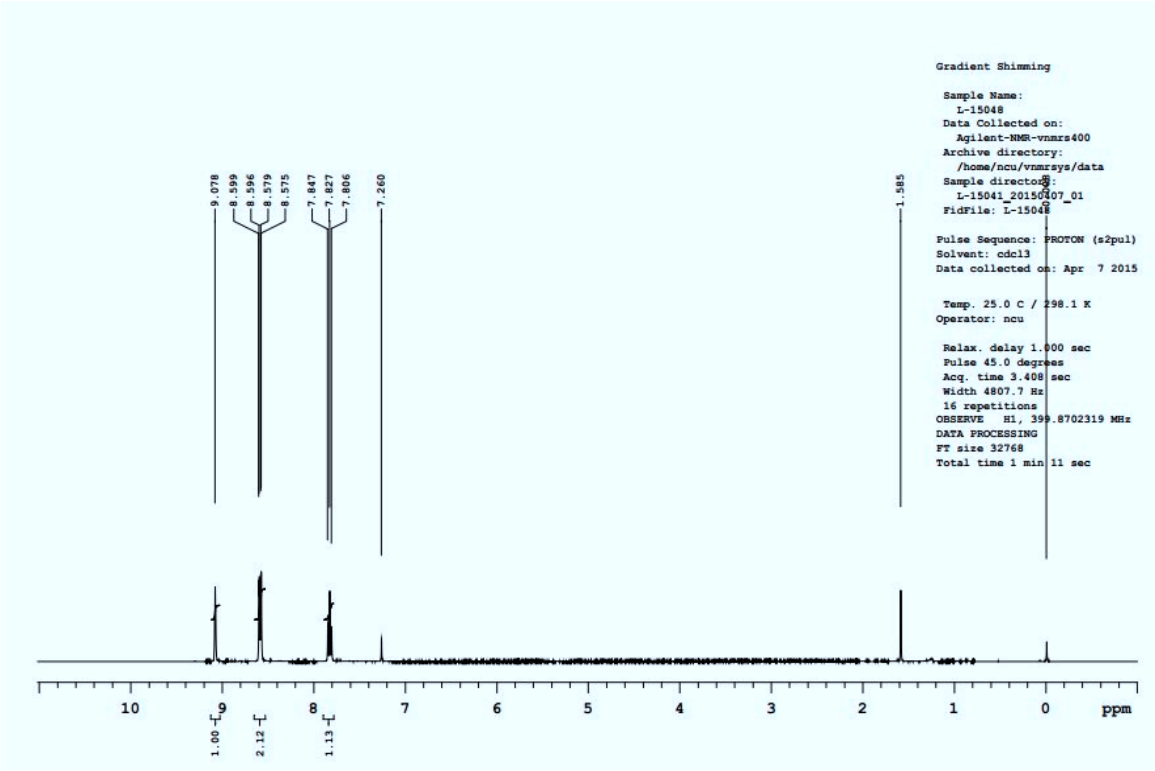

O
S
O
NO2
H

2c


132.946
130.874
128.219
122.884
77.304
76.985
76.667
44.312
180
160
140
120
100
80
60
40
20
0
ppm
Gradient Shimming
Sample Name:
L-15283
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
/home/ncu/vnmrsys/data
Sample directory:
L-15282_20151206_01
FidFile: L-15283-13C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Dec 8 2015
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1000 repetitions
OBSERVE C13, 100.5474507 MHz
DECOUPLE H1, 399.8722348 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 38 min

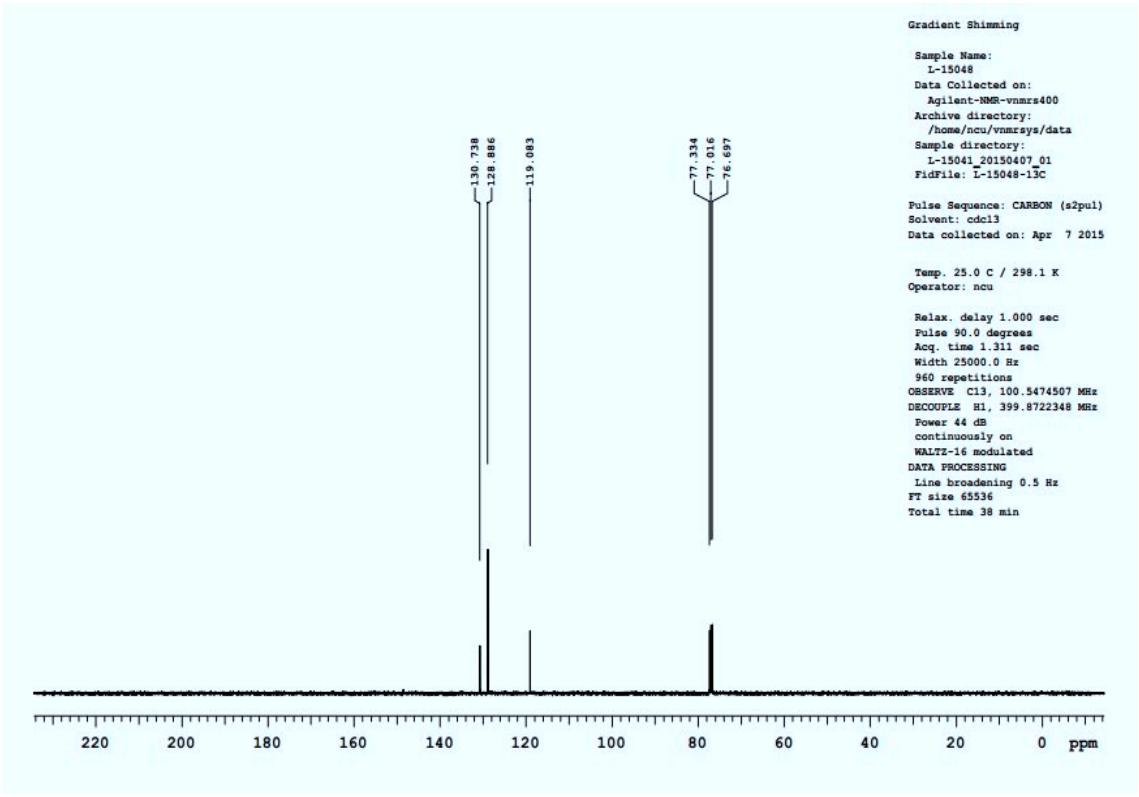

O_2N
NO_2
H

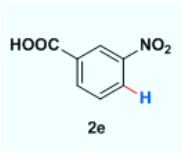
2d


Gradient Shimming
Sample Name:
L-15048
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
/home/ncu/vnmrsys/data
Sample directory:
L-15041_20150407_01
FidFile: L-15048
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 7 2015
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.408 sec
Width 4807.7 Hz
16 repetitions
OBSERVE H1, 399.8702319 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 11 sec
9.078
8.599
8.596
8.579
8.575
7.847
7.827
7.806
7.260
1.585
1.00
2.12
1.13
10
9
8
7
6
5
4
3
2
1
0
ppm

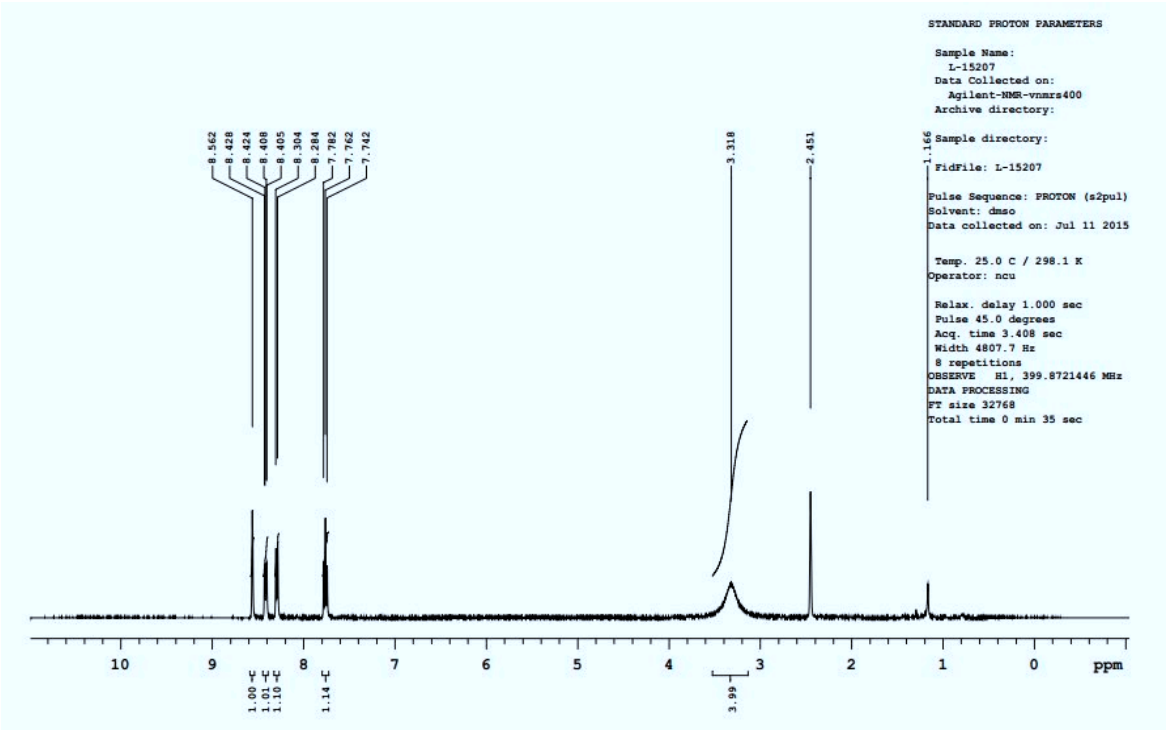

O_2N
NO_2
H

2d


Gradient Shimming
Sample Name:
L-15048
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
/home/ncu/vnmrsys/data
Sample directory:
L-15041_20150407_01
FidFile: L-15048-13C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 7 2015
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
960 repetitions
OBSERVE C13, 100.5474507 MHz
DECOUPLE H1, 399.8722348 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 38 min
130.738
128.886
119.083
77.334
77.016
76.697
220
200
180
160
140
120
100
80
60
40
20
0
ppm

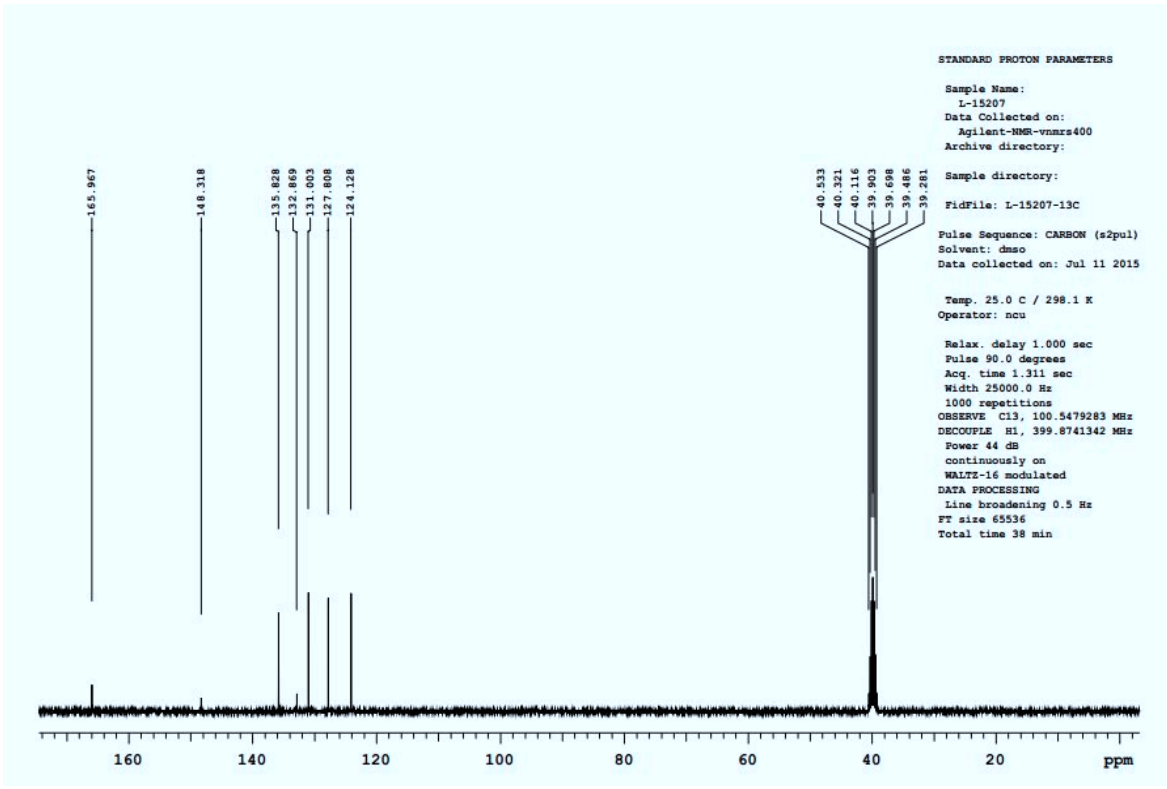

HOOC
NO2
H

2e


STANDARD PROTON PARAMETERS
Sample Name:
L-15207
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: L-15207
Pulse Sequence: PROTON (s2pul)
Solvent: dmso
Data collected on: Jul 11 2015
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.408 sec
Width 4807.7 Hz
8 repetitions
OBSERVE H1, 399.8721446 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 35 sec
8.562
8.428
8.424
8.408
8.405
8.304
8.284
7.782
7.762
7.742
3.318
2.451
1.166
1.00
1.01
1.10
1.14
3.99
ppm

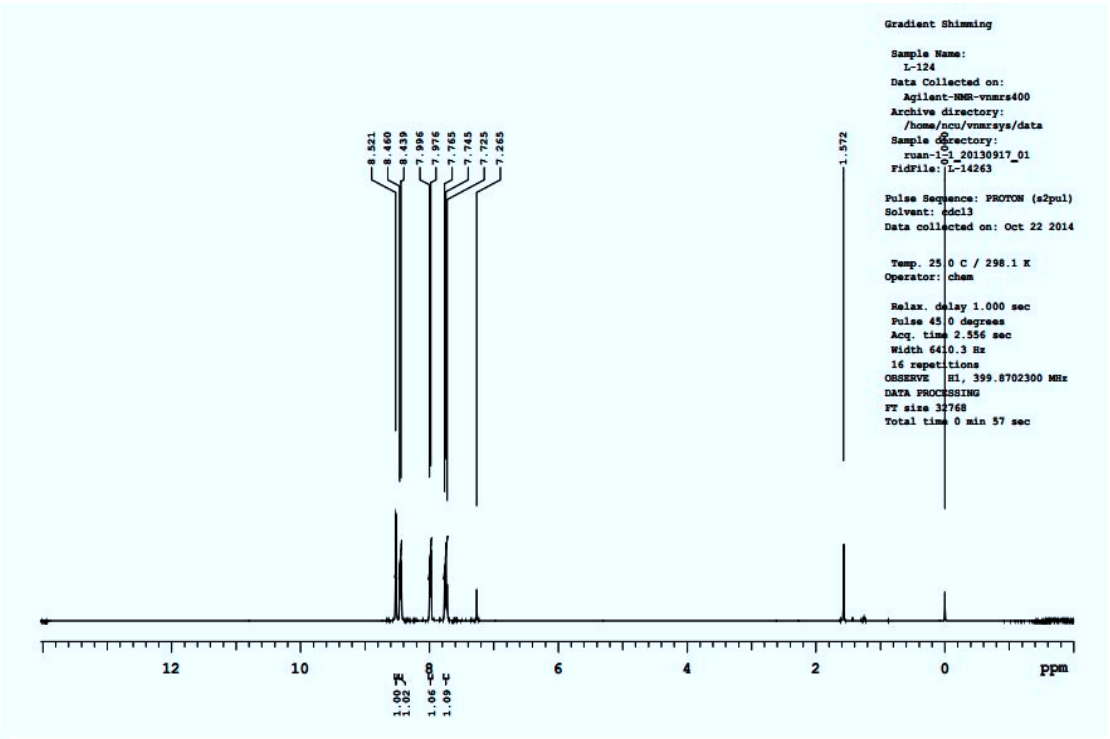

HOOC
NO2
H

2e


STANDARD PROTON PARAMETERS
Sample Name:
L-15207
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: L-15207-13C
Pulse Sequence: CARBON (s2pul)
Solvent: dmso
Data collected on: Jul 11 2015
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1000 repetitions
OBSERVE C13, 100.5479283 MHz
DECOUPLE H1, 399.8741342 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 38 min
165.967
148.318
135.828
132.869
131.003
127.808
124.128
40.533
40.321
40.116
39.903
39.698
39.486
39.281
ppm

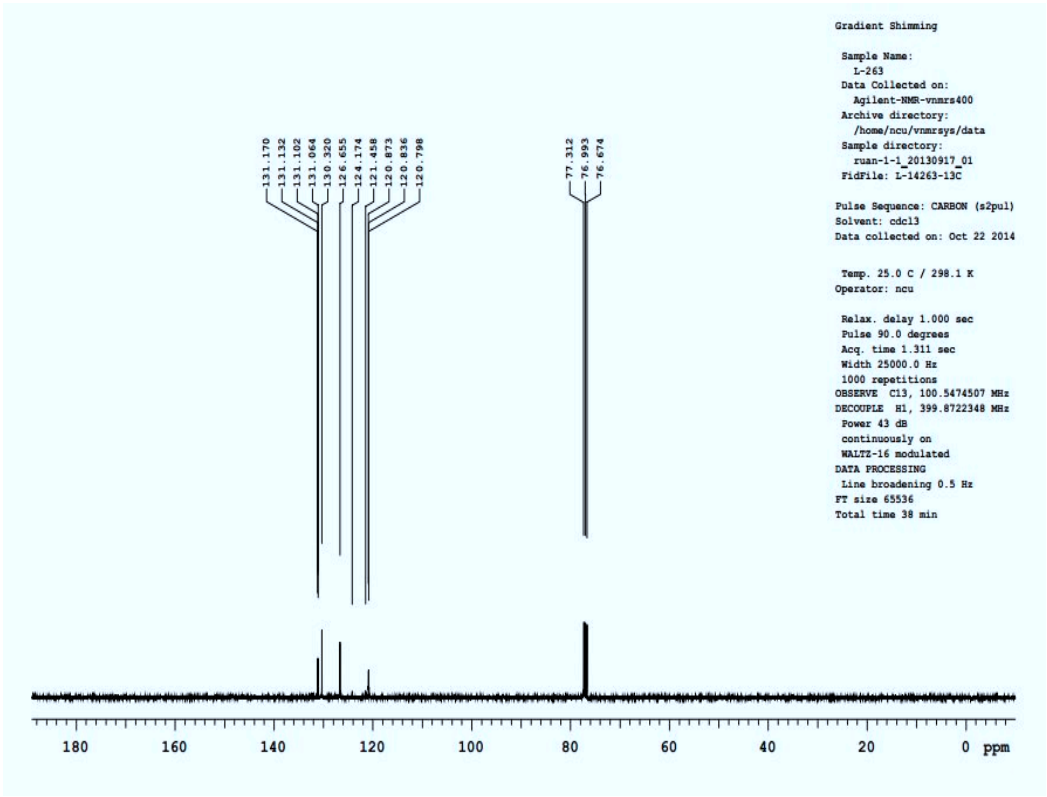

F3C
NO2
H

2f


8.521
8.460
8.439
7.996
7.976
7.765
7.745
7.725
7.265
1.572
1.00
1.02
1.06
1.09
12
10
8
6
4
2
0
ppm
Gradient Shimming
Sample Name:
L-124
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
/home/ncu/vnmrsys/data
Sample directory:
ruan-1-1_20130917_01
FidFile: L-14263
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 22 2014
Temp. 25.0 C / 298.1 K
Operator: chem
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 399.8702300 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 57 sec

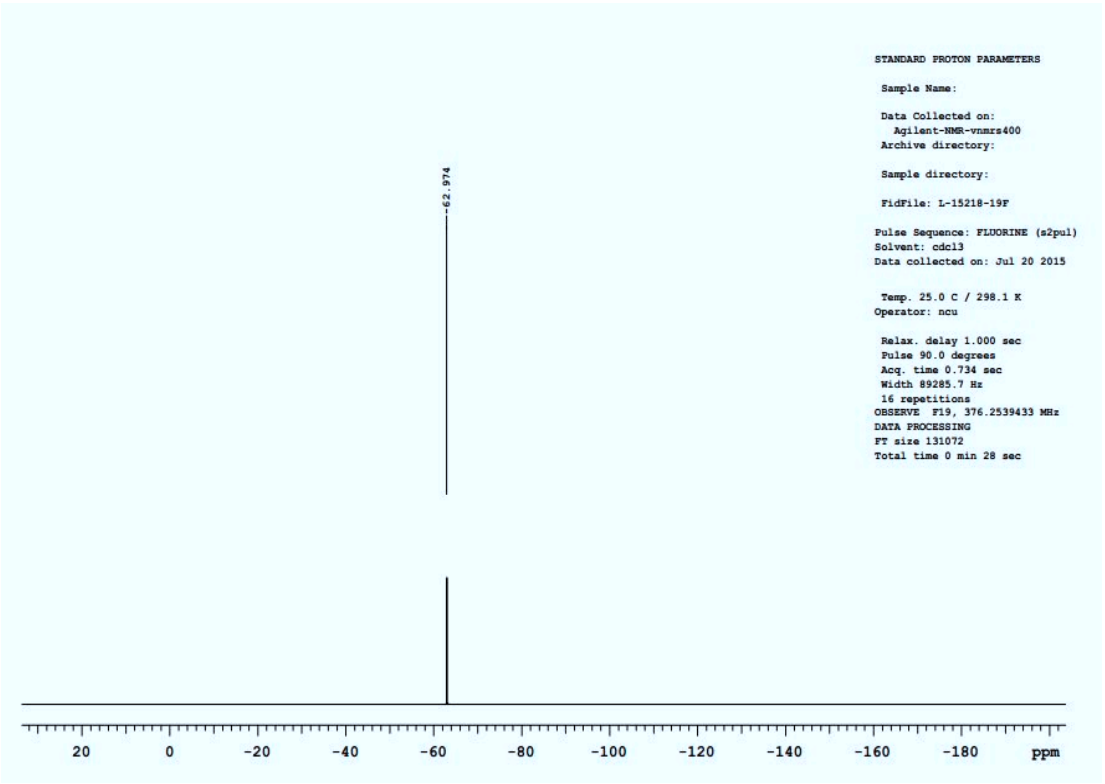

F3C
NO2
H

2f


131.170
131.132
131.102
131.064
130.320
126.655
124.174
121.458
120.873
120.836
120.798
77.312
76.993
76.674
180
160
140
120
100
80
60
40
20
0
ppm
Gradient Shimming
Sample Name:
L-263
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
/home/ncu/vnmrsys/data
Sample directory:
ruan-1-1_20130917_01
FidFile: L-14263-13C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 22 2014
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1000 repetitions
OBSERVE C13, 100.5474507 MHz
DECOUPLE H1, 399.8722348 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 38 min

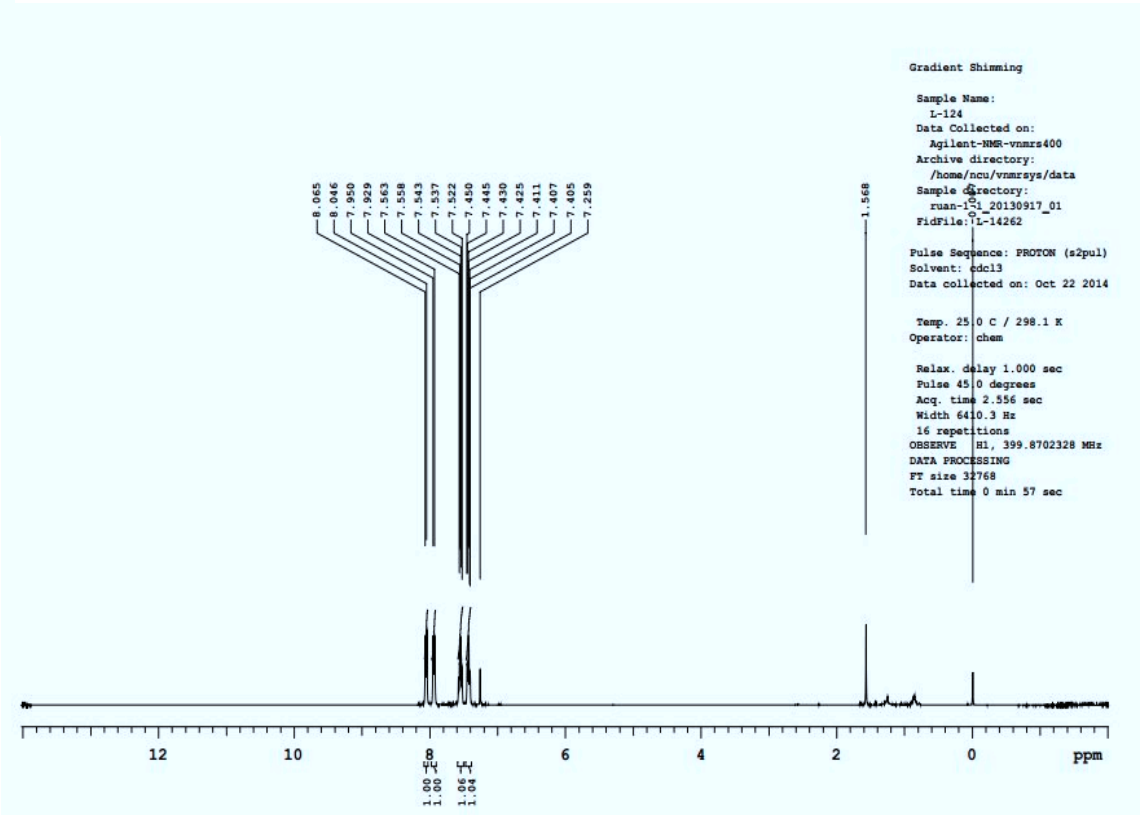

F3C
NO2
H

2f


-62.974
STANDARD PROTON PARAMETERS
Sample Name:
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: L-15218-19F
Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: Jul 20 2015
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 0.734 sec
Width 89285.7 Hz
16 repetitions
OBSERVE F19, 376.2539433 MHz
DATA PROCESSING
FT size 131072
Total time 0 min 28 sec
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

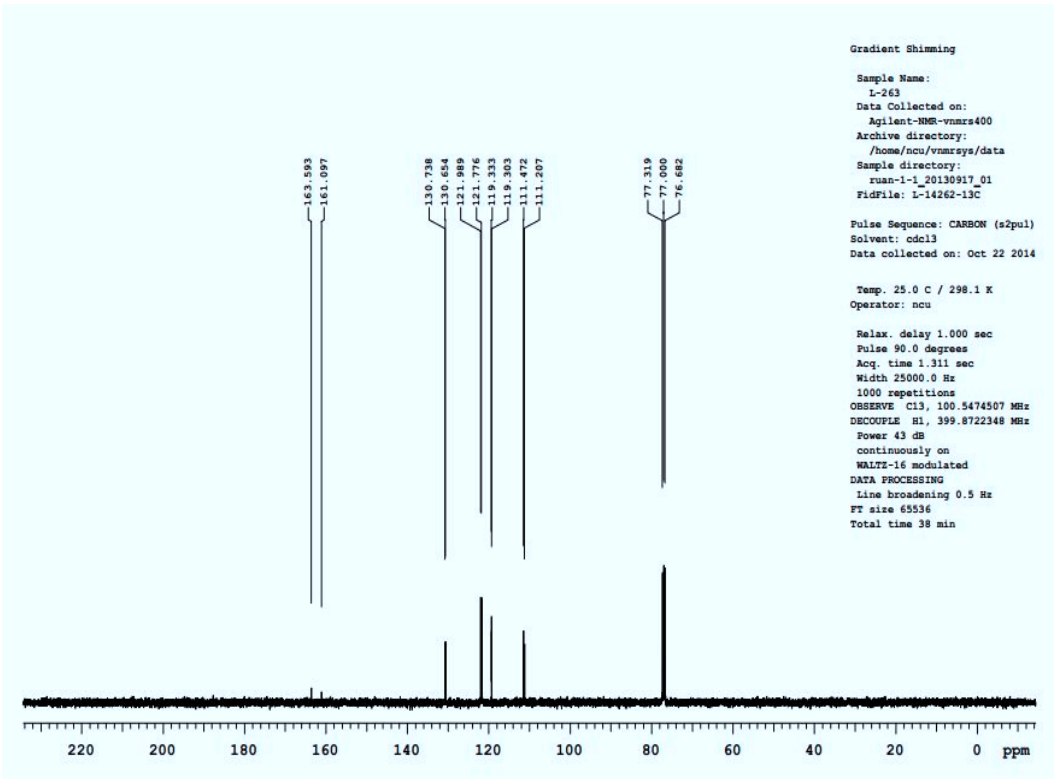

F
NO2
H

2g


8.065
8.046
7.950
7.929
7.563
7.558
7.543
7.537
7.522
7.450
7.445
7.430
7.425
7.411
7.407
7.405
7.259
1.568
Gradient Shimming
Sample Name:
L-124
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
/home/ncu/vnmrsys/data
Sample directory:
ruan-1-1_20130917_01
FidFile: L-14262
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 22 2014
Temp. 25.0 C / 298.1 K
Operator: chem
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 399.8702328 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 57 sec
12
10
8
6
4
2
0
ppm
1.00
1.00
1.06
1.04

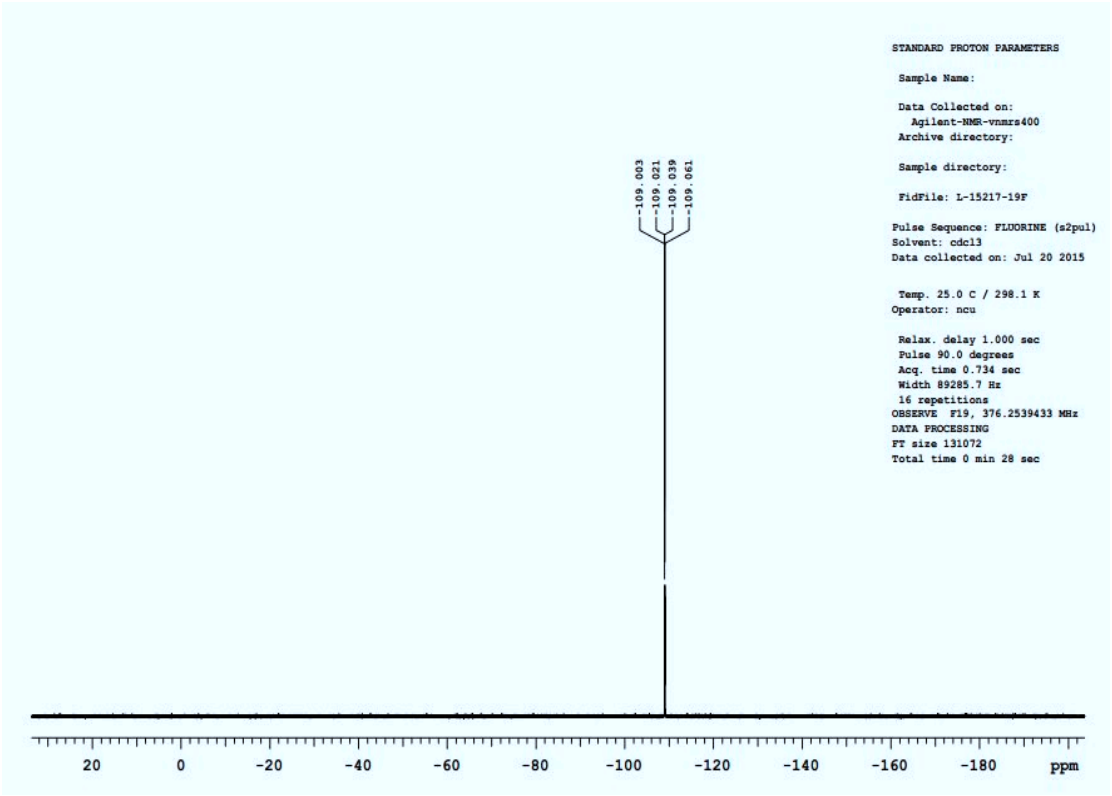

F
NO2
H

2g


163.593
161.097
130.738
130.654
121.989
121.776
119.333
119.303
111.472
111.207
77.319
77.000
76.682
Gradient Shimming
Sample Name:
L-263
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
/home/ncu/vnmrsys/data
Sample directory:
ruan-1-1_20130917_01
FidFile: L-14262-13C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 22 2014
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1000 repetitions
OBSERVE C13, 100.5474507 MHz
DECOUPLE H1, 399.8722348 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 38 min
220
200
180
160
140
120
100
80
60
40
20
0
ppm

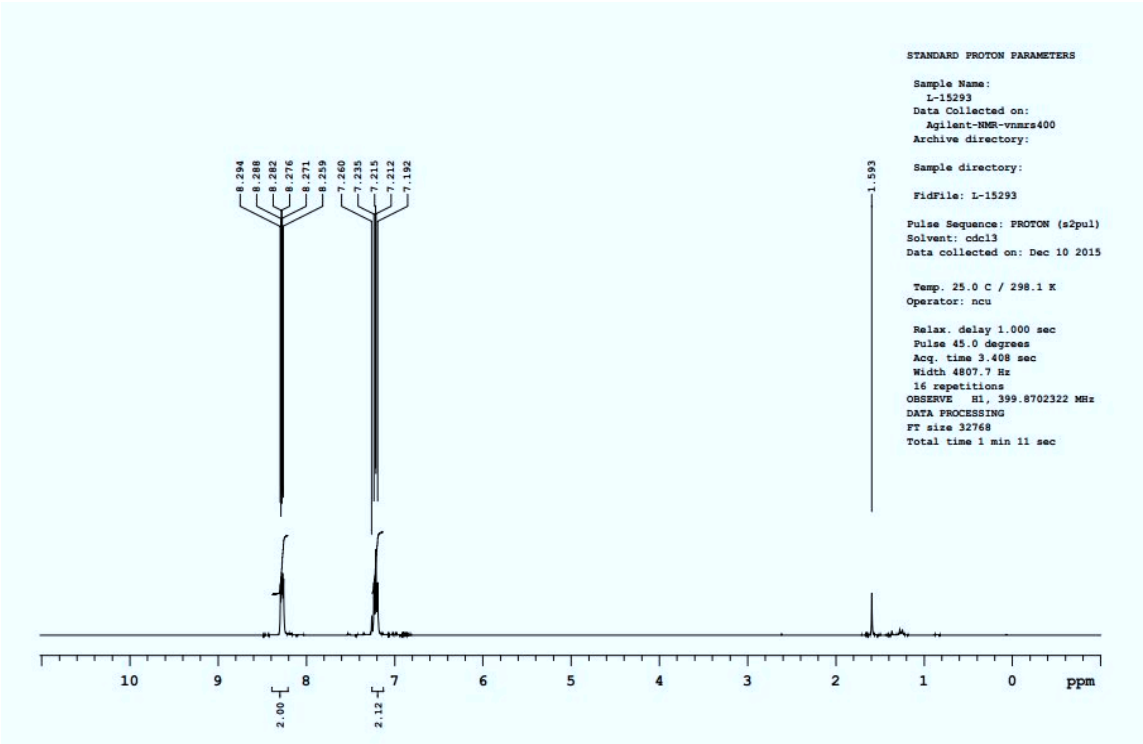

F
NO2
H

2g


-109.003
-109.021
-109.039
-109.061
STANDARD PROTON PARAMETERS
Sample Name:
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: L-15217-19F
Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: Jul 20 2015
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 0.734 sec
Width 89285.7 Hz
16 repetitions
OBSERVE F19, 376.2539433 MHz
DATA PROCESSING
FT size 131072
Total time 0 min 28 sec
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

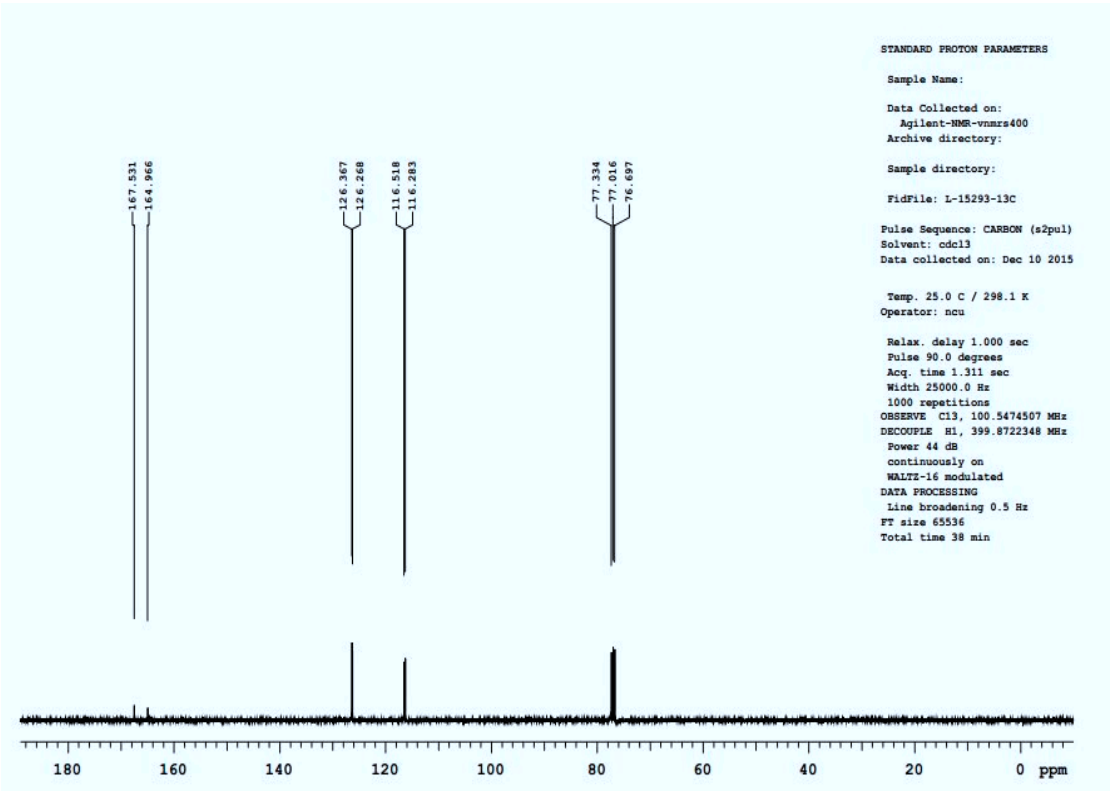

NO2
F
H

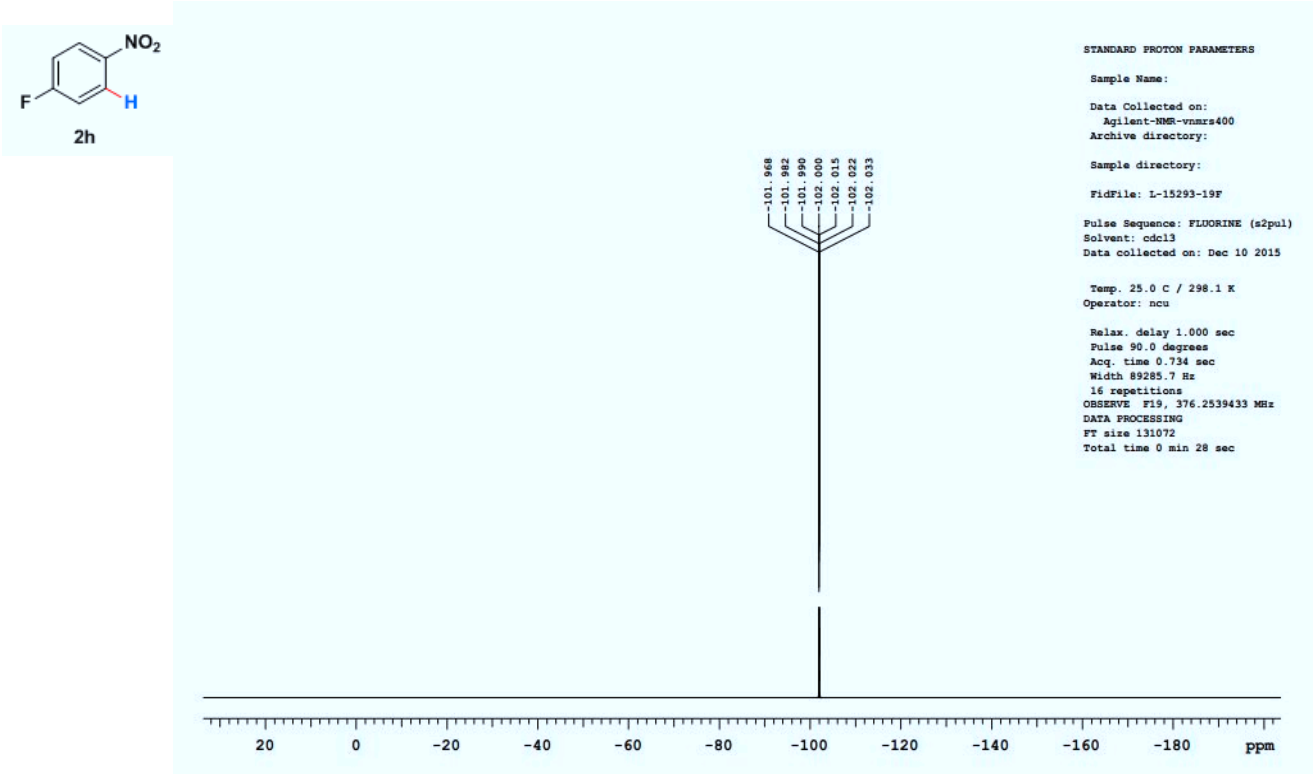
2h

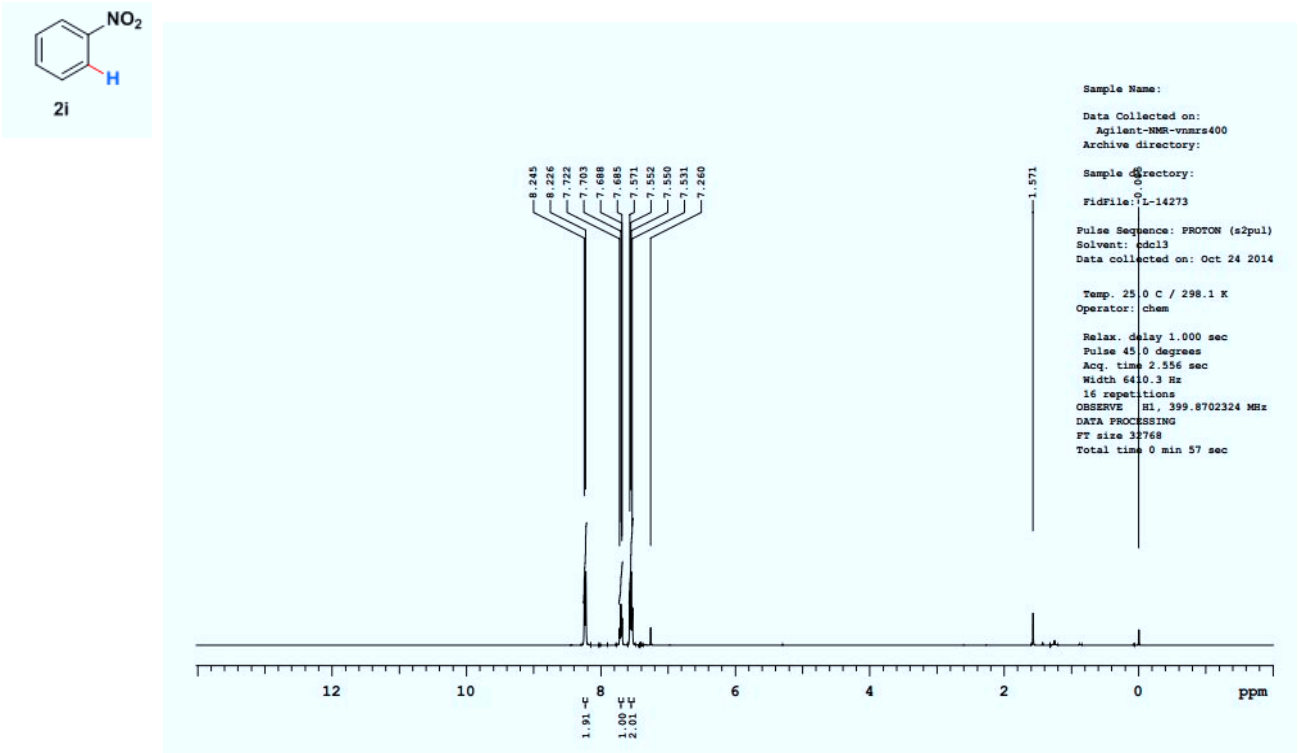

8.294
8.288
8.282
8.276
8.271
8.259
7.260
7.235
7.215
7.212
7.192
1.593
STANDARD PROTON PARAMETERS
Sample Name:
L-15293
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: L-15293
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Dec 10 2015
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.408 sec
Width 4807.7 Hz
16 repetitions
OBSERVE H1, 399.8702322 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 11 sec
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.12

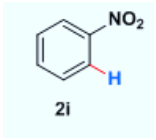

NO2
F
H

2h

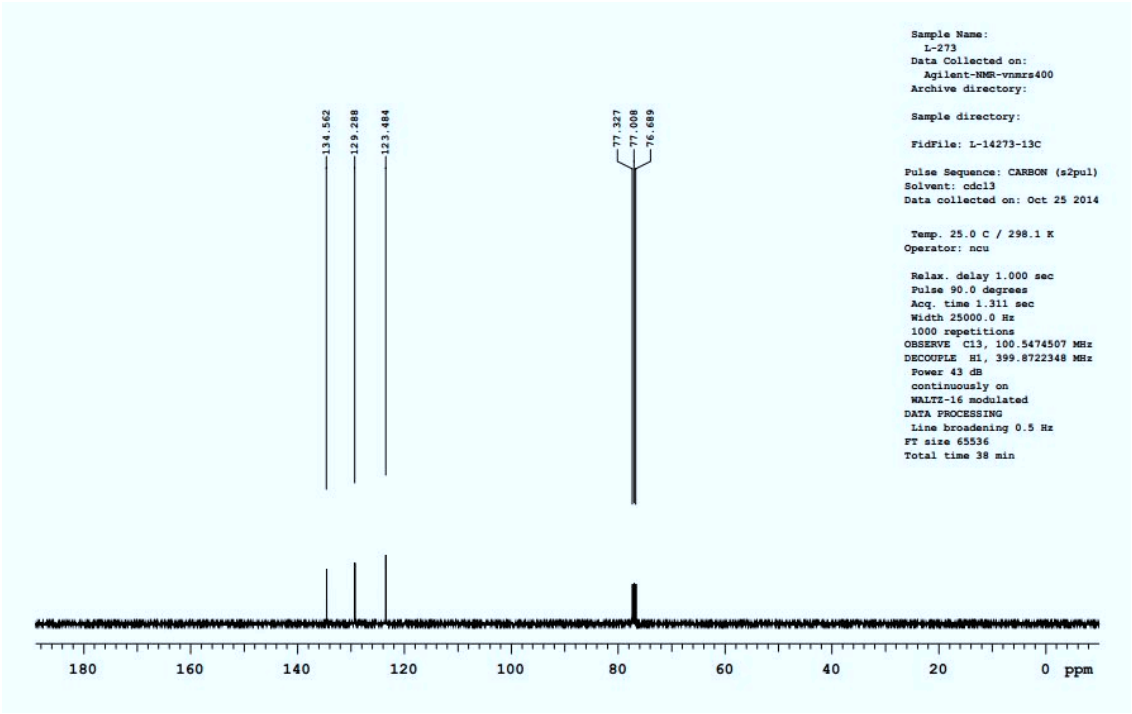

167.531
164.966
126.367
126.268
116.518
116.283
77.334
77.016
76.697
STANDARD PROTON PARAMETERS
Sample Name:
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: L-15293-13C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Dec 10 2015
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1000 repetitions
OBSERVE C13, 100.5474507 MHz
DECOUPLE H1, 399.8722348 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 38 min
180
160
140
120
100
80
60
40
20
0
ppm

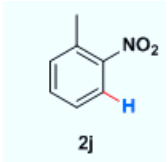

NO2
F
H
2h
STANDARD PROTON PARAMETERS
Sample Name:
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: L-15293-19F
Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: Dec 10 2015
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 0.734 sec
Width 89285.7 Hz
16 repetitions
OBSERVE F19, 376.2539433 MHz
DATA PROCESSING
FT size 131072
Total time 0 min 28 sec
-101.968
-101.982
-101.990
-102.000
-102.015
-102.022
-102.033
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm


NO2
H
2i
Sample Name:
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: L-14273
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 24 2014
Temp. 25.0 C / 298.1 K
Operator: chem
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 399.8702324 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 57 sec
8.245
8.226
7.722
7.703
7.688
7.685
7.571
7.552
7.550
7.531
7.260
1.571
0.000
12
10
8
6
4
2
0
ppm
1.91
1.00
2.01

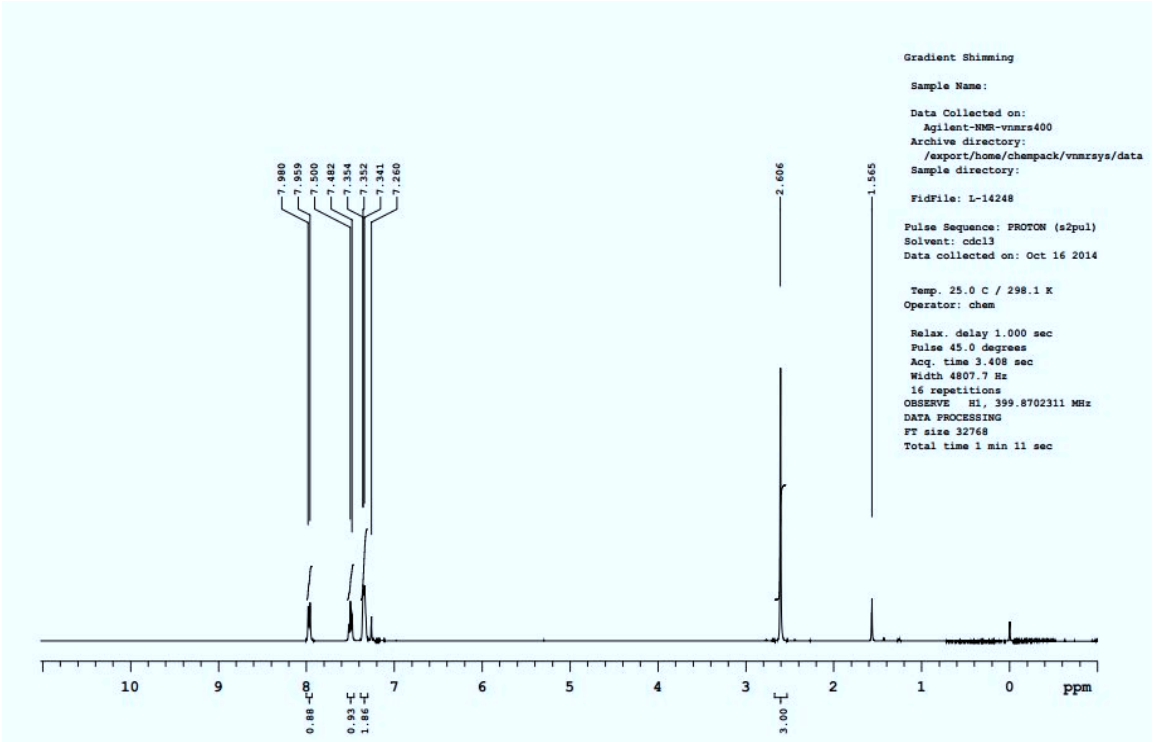

NO2
H

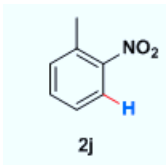
2i


134.562
129.288
123.484
77.327
77.008
76.689
Sample Name:
L-273
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: L-14273-13C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 25 2014
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1000 repetitions
OBSERVE C13, 100.5474507 MHz
DECOUPLE H1, 399.8722348 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 38 min
180
160
140
120
100
80
60
40
20
0 ppm

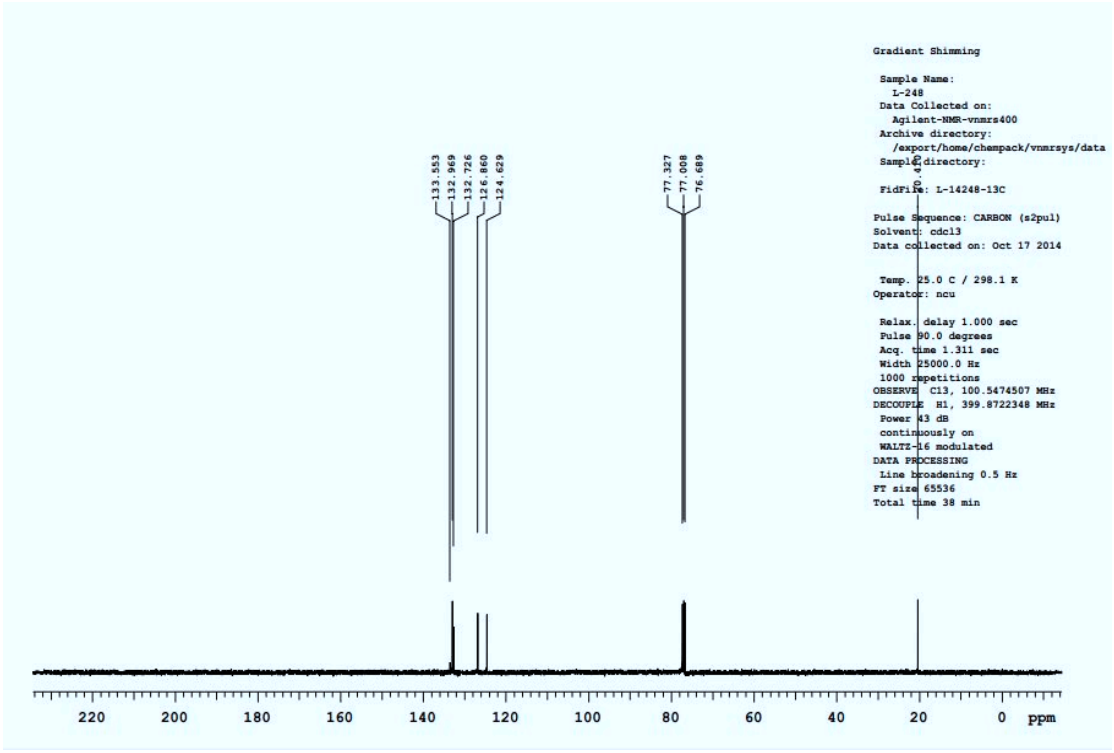

NO2
H

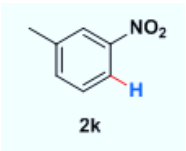
2j


7.980
7.959
7.500
7.482
7.354
7.352
7.341
7.260
2.606
1.565
Gradient Shimming
Sample Name:
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
/export/home/chempack/vnmrsys/data
Sample directory:
FidFile: L-14248
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 16 2014
Temp. 25.0 C / 298.1 K
Operator: chem
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.408 sec
Width 4807.7 Hz
16 repetitions
OBSERVE H1, 399.8702311 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 11 sec
10
9
8
7
6
5
4
3
2
1
0
ppm
0.88
0.93
1.86
3.00

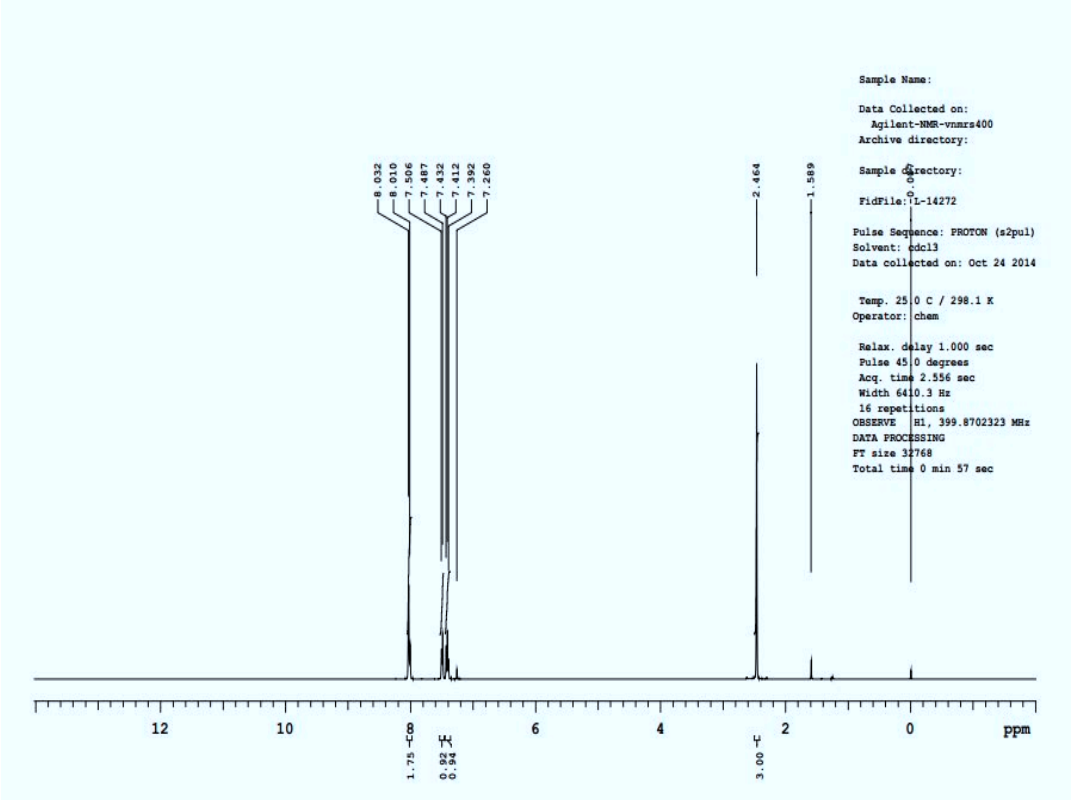

NO2
H

2j


133.553
132.969
132.726
126.860
124.629
77.327
77.008
76.689
Gradient Shimming
Sample Name:
L-248
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
/export/home/chempack/vnmrsys/data
Sample directory:
FidFile: L-14248-13C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 17 2014
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1000 repetitions
OBSERVE C13, 100.5474507 MHz
DECOUPLE H1, 399.8722348 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 38 min
220
200
180
160
140
120
100
80
60
40
20
0
ppm

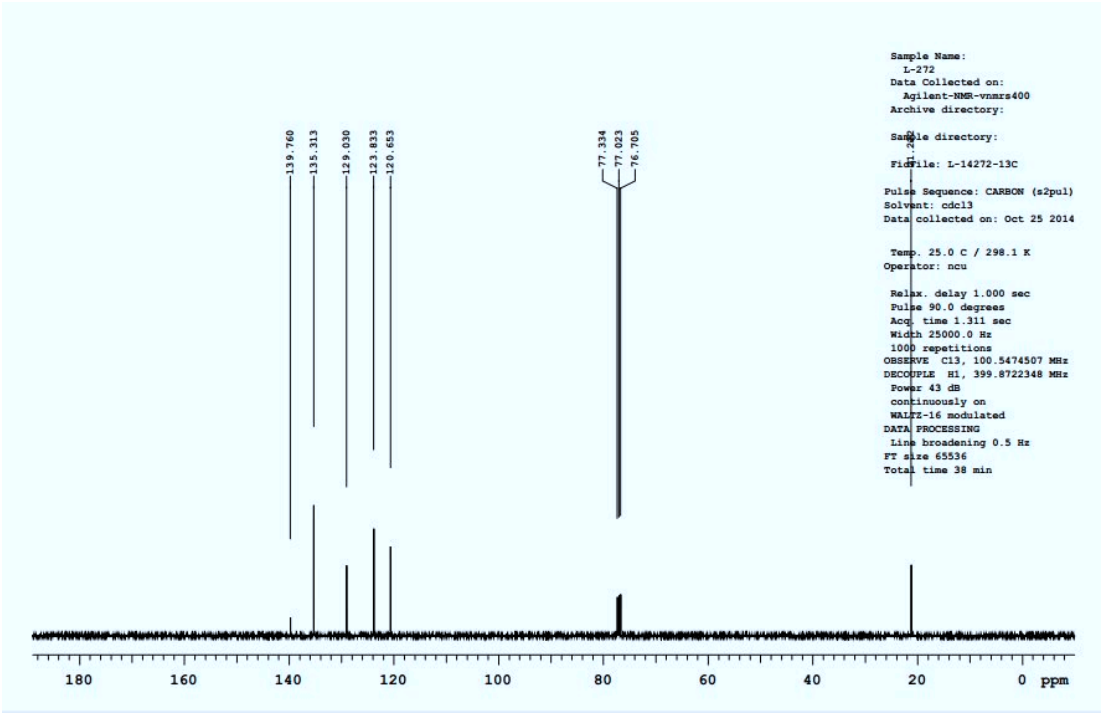

NO2
H

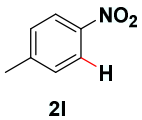
2k


8.032
8.010
7.506
7.487
7.432
7.412
7.392
7.260
2.464
1.589
Sample Name:
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: L-14272
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 24 2014
Temp. 25.0 C / 298.1 K
Operator: chem
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 399.8702323 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 57 sec
12
10
8
6
4
2
0
ppm
1.75
0.92
0.94
3.00

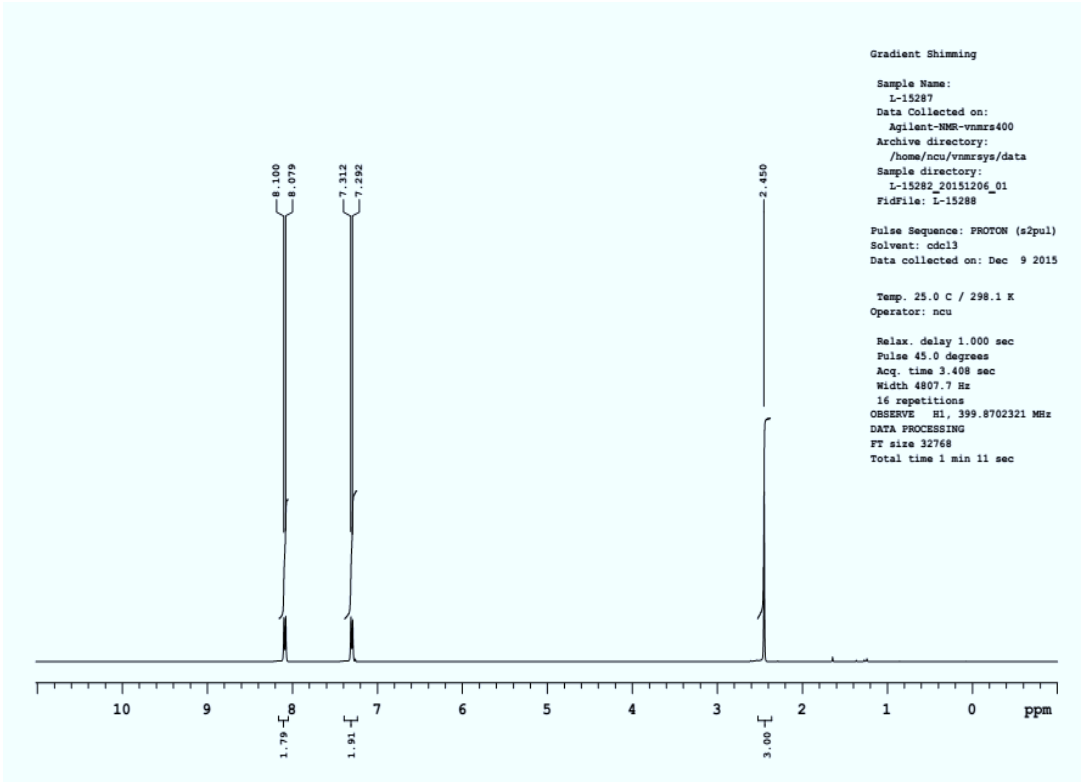

NO2
H

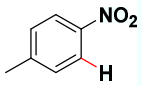
2k


139.760
135.313
129.030
123.833
120.653
77.334
77.023
76.705
20.811
Sample Name:
L-272
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: L-14272-13C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 25 2014
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1000 repetitions
OBSERVE C13, 100.5474507 MHz
DECOUPLE H1, 399.8722348 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 38 min
180
160
140
120
100
80
60
40
20
0
ppm

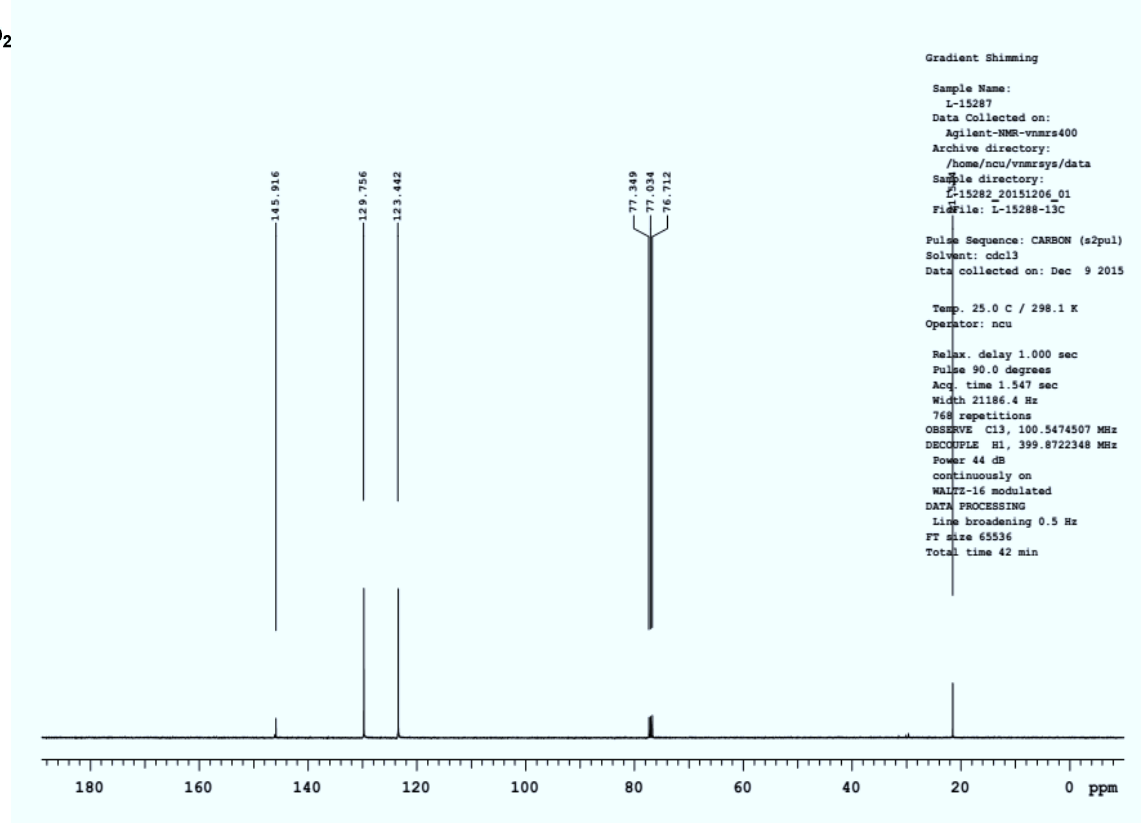

NO2
H

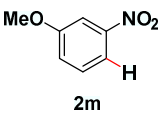
2l


8.100
8.079
7.312
7.292
2.450
Gradient Shimming
Sample Name:
L-15287
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
/home/ncu/vnmrsys/data
Sample directory:
L-15282_20151206_01
FidFile: L-15288
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Dec 9 2015
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.408 sec
Width 4807.7 Hz
16 repetitions
OBSERVE H1, 399.8702321 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 11 sec
10
9
8
7
6
5
4
3
2
1
0
ppm
1.79
1.91
3.00

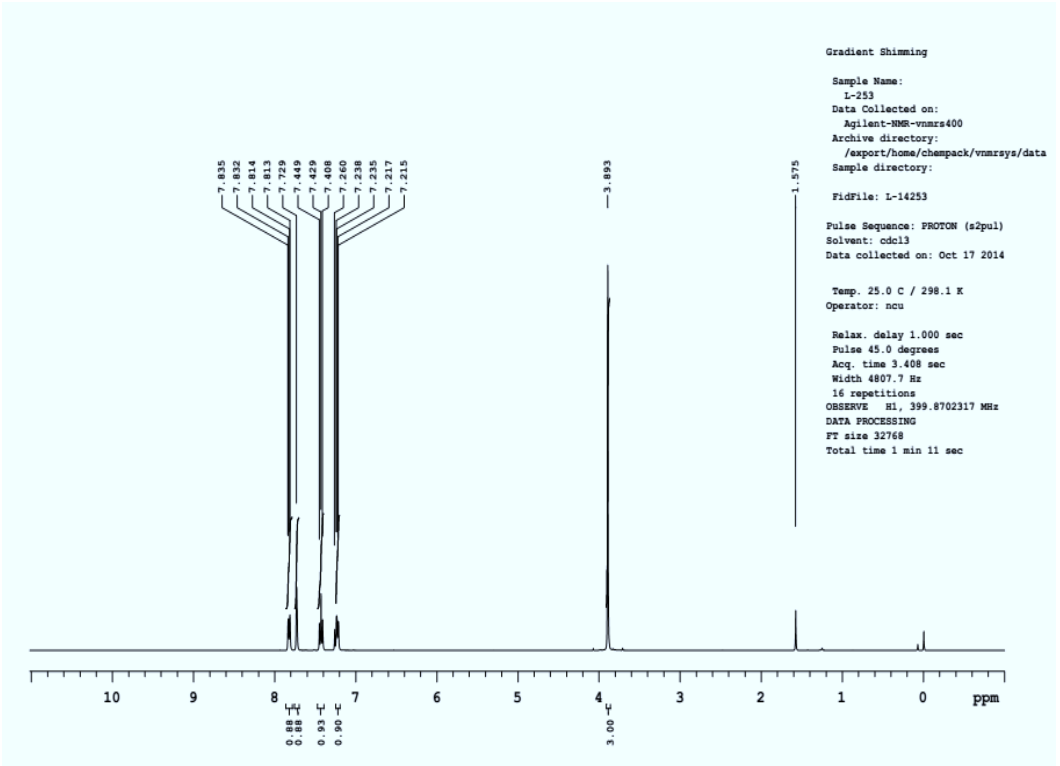

NO2
H

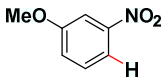
2l


145.916
129.756
123.442
77.349
77.034
76.712
Gradient Shimming
Sample Name:
L-15287
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
/home/ncu/vnmrsys/data
Sample directory:
L-15282_20151206_01
FidFile: L-15288-13C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Dec 9 2015
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.547 sec
Width 21186.4 Hz
768 repetitions
OBSERVE C13, 100.5474507 MHz
DECOUPLE H1, 399.8722348 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 42 min
180
160
140
120
100
80
60
40
20
0 ppm

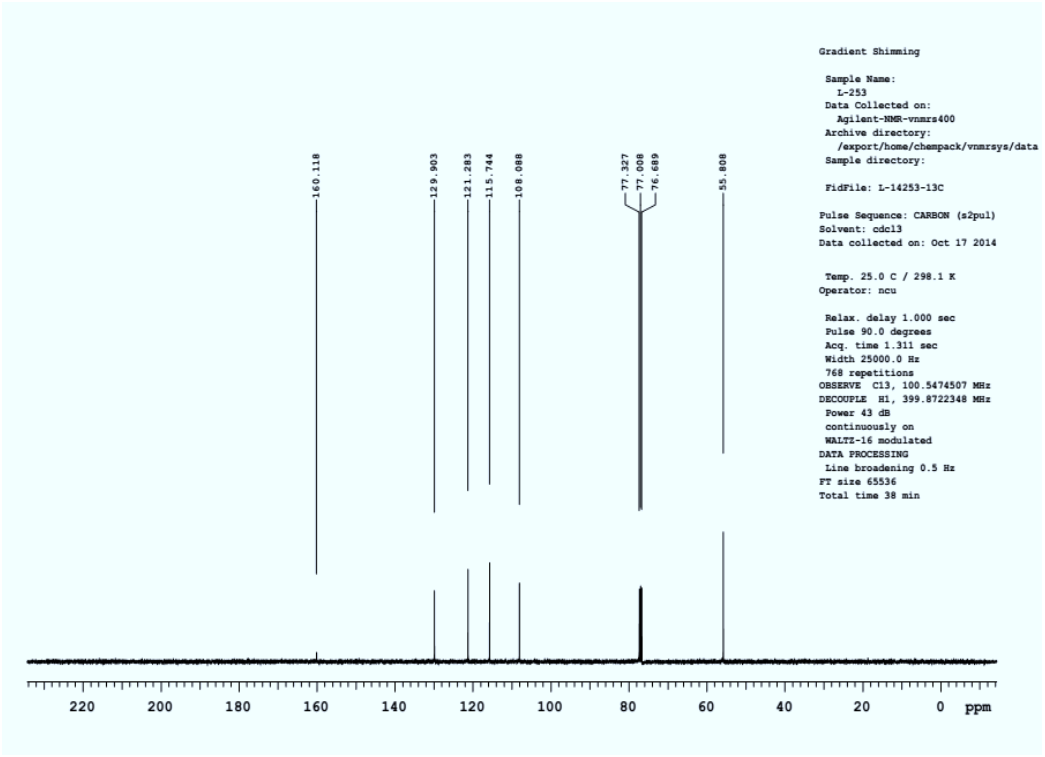

MeO
NO2
H

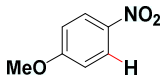
2m


7.835
7.832
7.814
7.813
7.729
7.449
7.429
7.408
7.260
7.238
7.235
7.217
7.215
3.893
1.575
Gradient Shimming
Sample Name:
L-253
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
/export/home/chempack/vnmrsys/data
Sample directory:
FidFile: L-14253
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 17 2014
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.408 sec
Width 4807.7 Hz
16 repetitions
OBSERVE H1, 399.8702317 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 11 sec
10
9
8
7
6
5
4
3
2
1
0
ppm
0.88
0.88
0.93
0.90
3.00

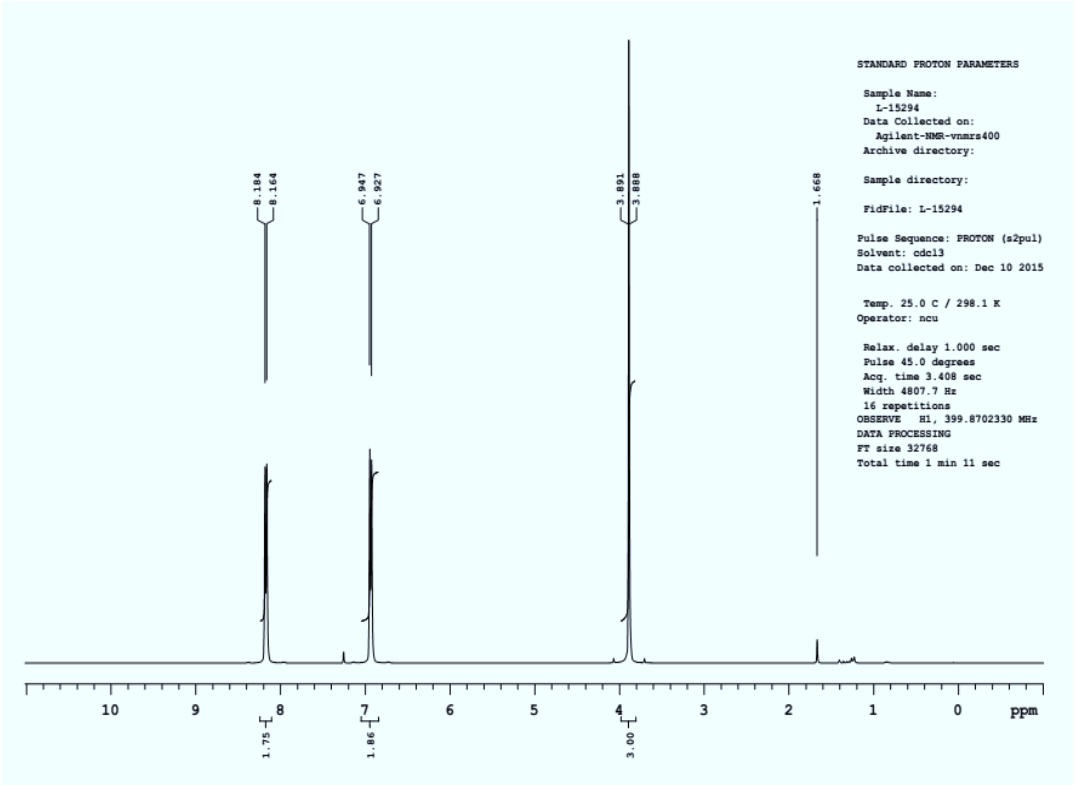

MeO
NO2
H

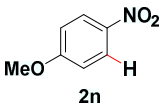
2m


Gradient Shimming
Sample Name:
L-253
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
/export/home/chempack/vnmrsys/data
Sample directory:
FidFile: L-14253-13C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 17 2014
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
768 repetitions
OBSERVE C13, 100.5474507 MHz
DECOUPLE H1, 399.8722348 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 38 min
160.118
129.903
121.283
115.744
108.088
77.327
77.008
76.689
55.808
220
200
180
160
140
120
100
80
60
40
20
0
ppm

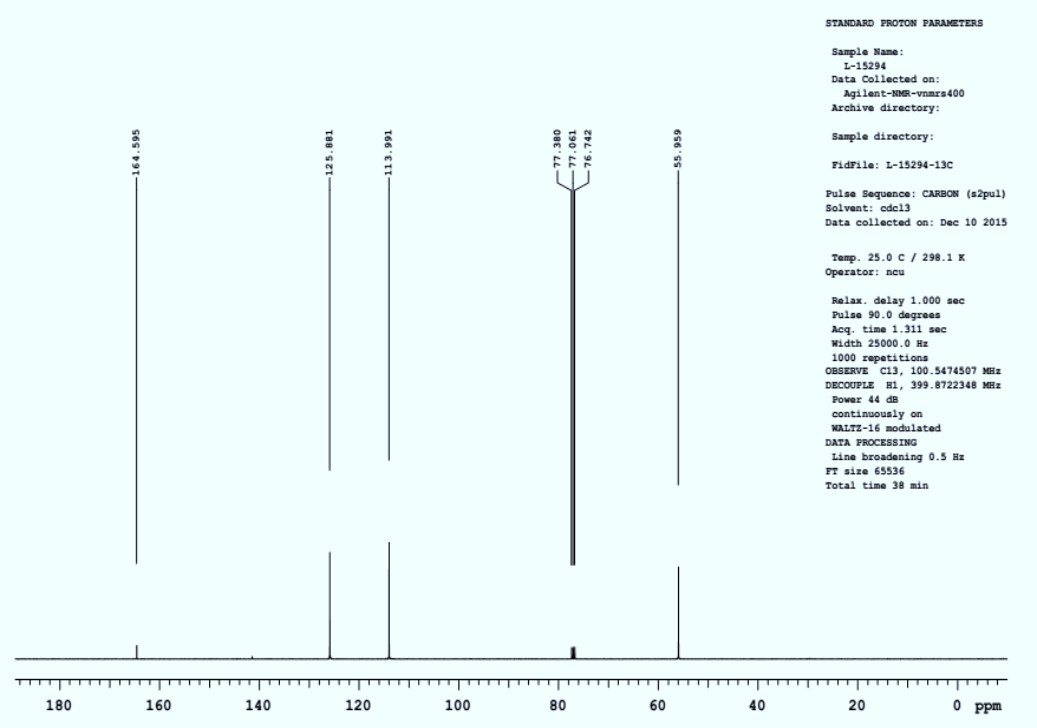

NO2
MeO
H

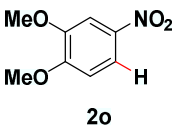
2n


STANDARD PROTON PARAMETERS
Sample Name:
L-15294
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: L-15294
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Dec 10 2015
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.408 sec
Width 4807.7 Hz
16 repetitions
OBSERVE H1, 399.8702330 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 11 sec
8.184
8.164
6.947
6.927
3.891
3.888
1.668
10
9
8
7
6
5
4
3
2
1
0
ppm
1.75
1.86
3.00

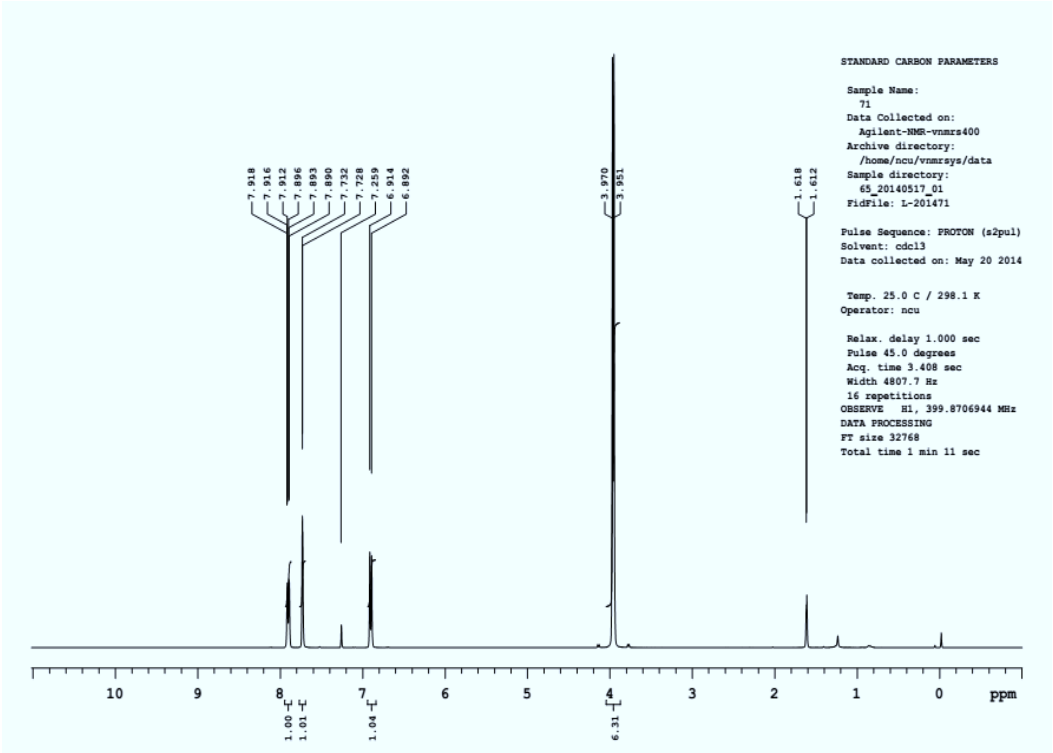

NO2
MeO
H

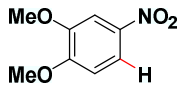
2n


164.595
125.881
113.991
77.380
77.061
76.742
55.959
180
160
140
120
100
80
60
40
20
0 ppm
STANDARD PROTON PARAMETERS
Sample Name:
L-15294
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: L-15294-13C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Dec 10 2015
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1000 repetitions
OBSERVE C13, 100.5474507 MHz
DECOUPLE H1, 399.8722348 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 38 min

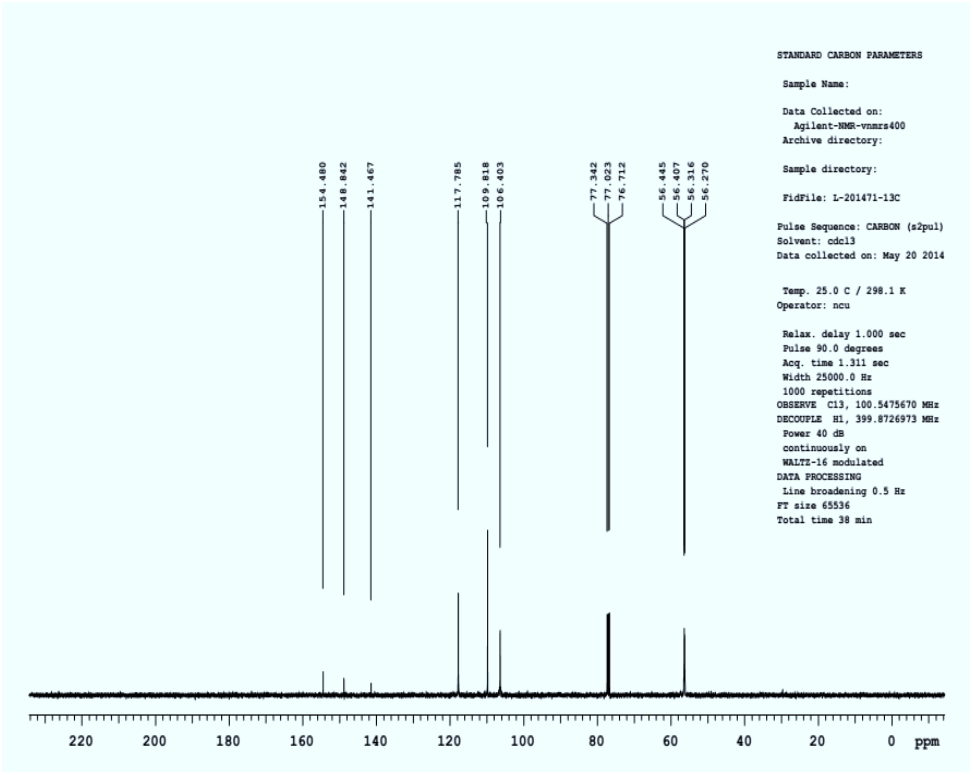

MeO
NO2
MeO
H

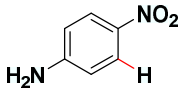
2o


7.918
7.916
7.912
7.896
7.893
7.890
7.732
7.728
7.259
6.914
6.892
3.970
3.951
1.618
1.612
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.01
1.04
6.31
STANDARD CARBON PARAMETERS
Sample Name:
71
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
/home/ncu/vnmrsys/data
Sample directory:
65_20140517_01
FidFile: L-201471
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: May 20 2014
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.408 sec
Width 4807.7 Hz
16 repetitions
OBSERVE H1, 399.8706944 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 11 sec

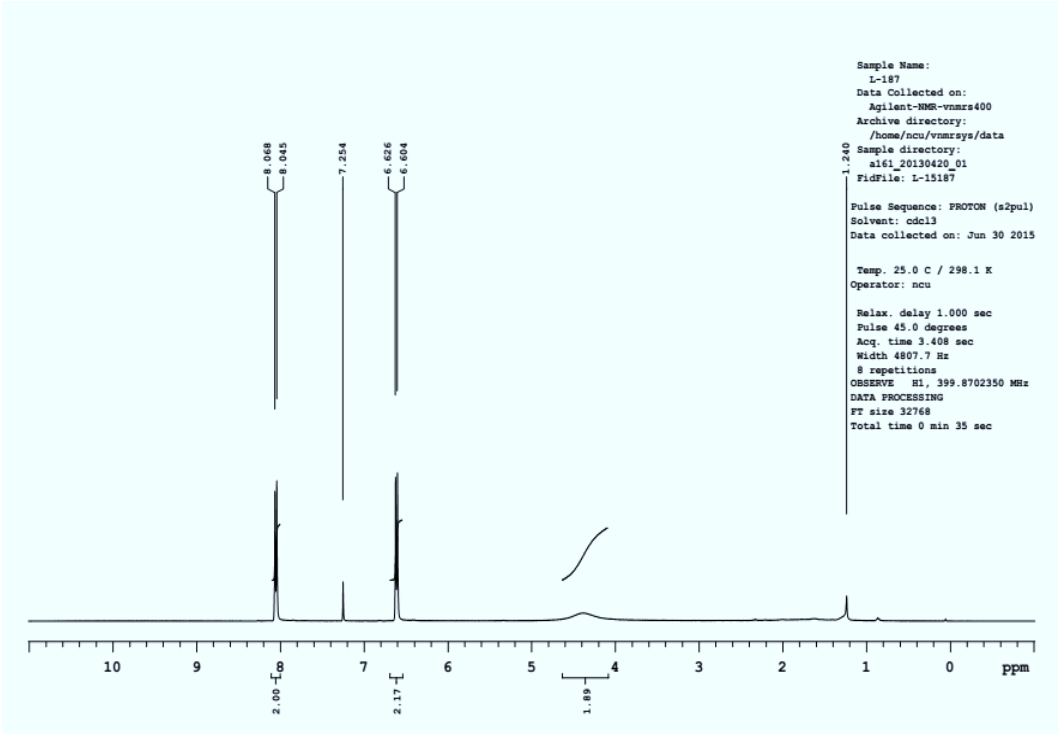

MeO
NO2
MeO
H

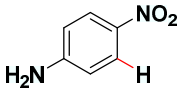
2o


STANDARD CARBON PARAMETERS
Sample Name:
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: L-201471-13C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 20 2014
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1000 repetitions
OBSERVE C13, 100.5475670 MHz
DECOUPLE H1, 399.8726973 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 38 min
154.480
148.842
141.467
117.785
109.818
106.403
77.342
77.023
76.712
56.445
56.407
56.316
56.270
220
200
180
160
140
120
100
80
60
40
20
0
ppm

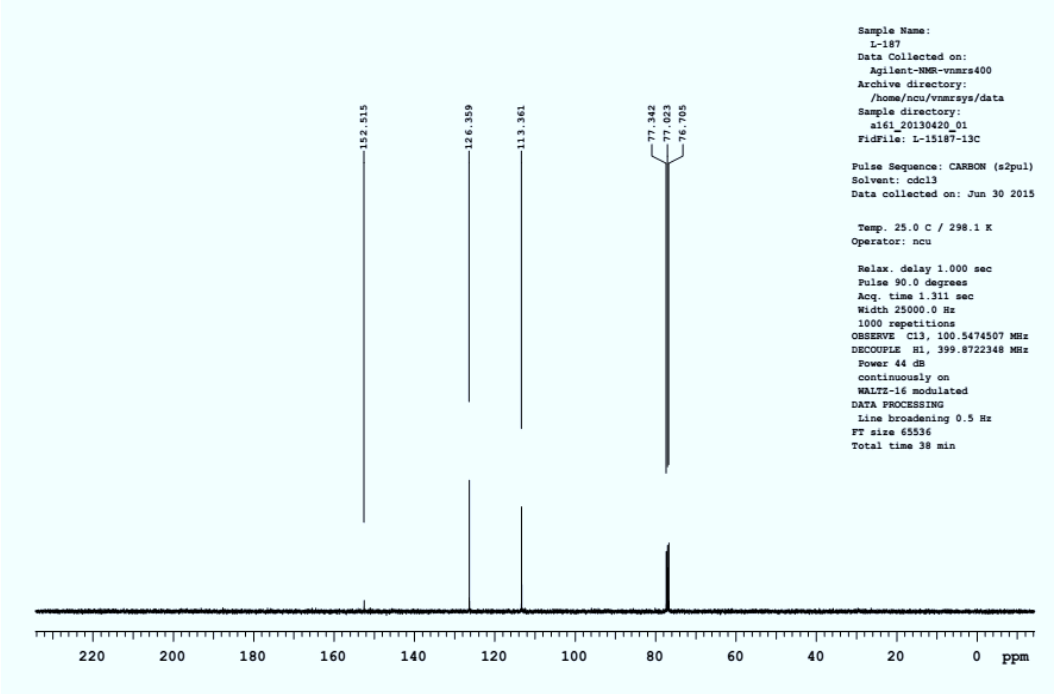

NO2
H2N
H

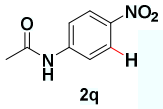
2p


Sample Name:
L-187
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
/home/ncu/vnmrsys/data
Sample directory:
a161_20130420_01
FidFile: L-15187
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 30 2015
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.408 sec
Width 4807.7 Hz
8 repetitions
OBSERVE H1, 399.8702350 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 35 sec
8.068
8.045
7.254
6.626
6.604
1.240
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.17
1.89

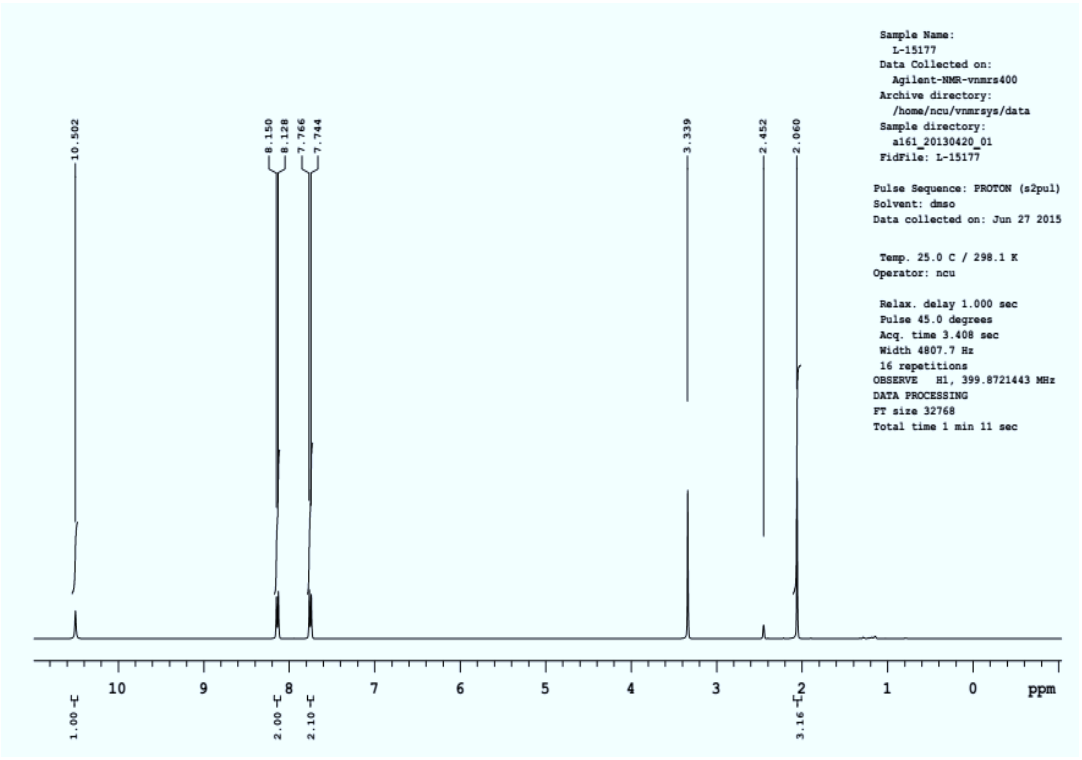

NO2
H2N
H

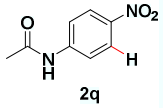
2p


152.515
126.359
113.361
77.342
77.023
76.705
Sample Name:
L-187
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
/home/ncu/vnmrsys/data
Sample directory:
a161_20130420_01
FidFile: L-15187-13C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 30 2015
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1000 repetitions
OBSERVE C13, 100.5474507 MHz
DECOUPLE H1, 399.8722348 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 38 min
220
200
180
160
140
120
100
80
60
40
20
0
ppm

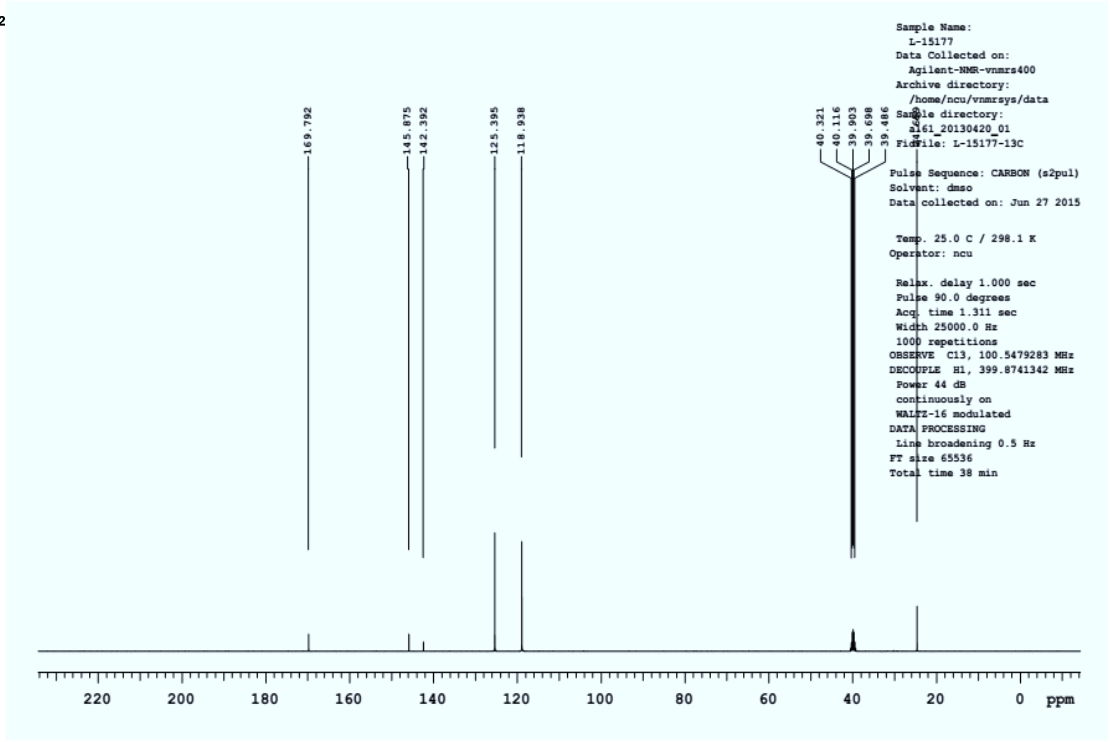

O
N
H
NO2
H

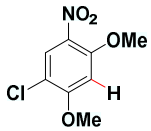
2q


10.502
8.150
8.128
7.766
7.744
3.339
2.452
2.060
Sample Name:
L-15177
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
/home/ncu/vnmrsys/data
Sample directory:
a161_20130420_01
FidFile: L-15177
Pulse Sequence: PROTON (s2pul)
Solvent: dmso
Data collected on: Jun 27 2015
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.408 sec
Width 4807.7 Hz
16 repetitions
OBSERVE H1, 399.8721443 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 11 sec
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
2.00
2.10
3.16

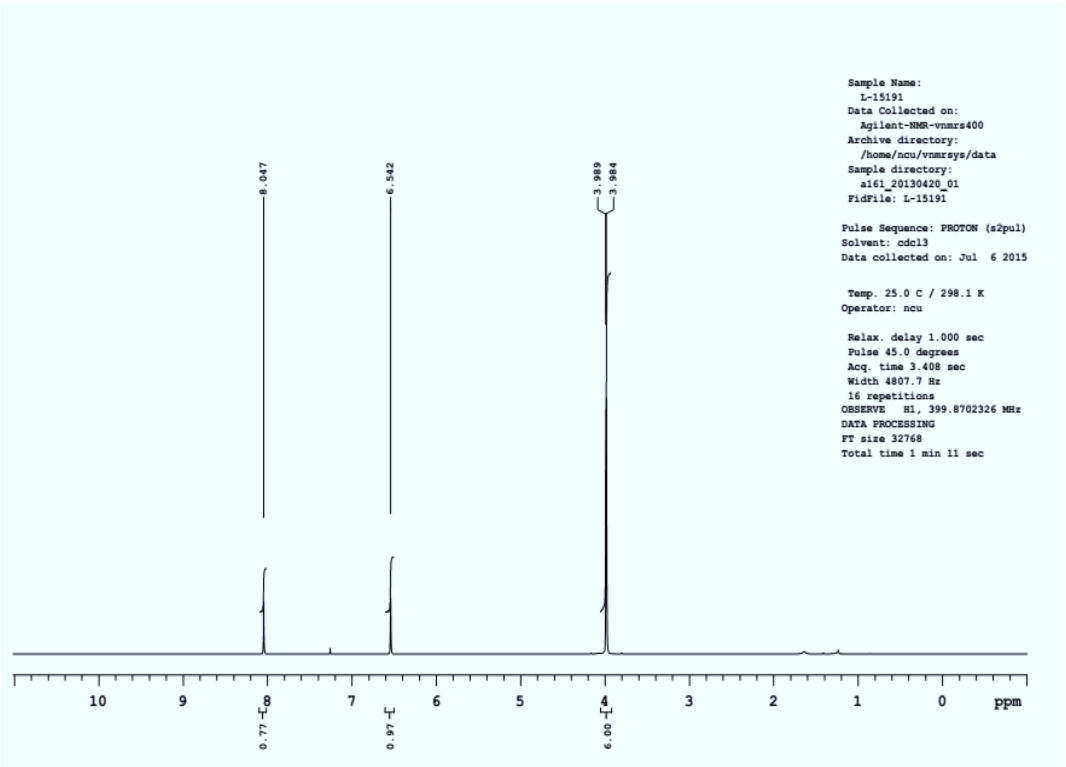

O
N
H
NO2
H

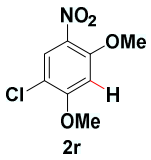
2q


169.792
145.875
142.392
125.395
118.938
40.321
40.116
39.903
39.698
39.486
Sample Name:
L-15177
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
/home/ncu/vnmrsys/data
Sample directory:
a161_20130420_01
FidFile: L-15177-13C
Pulse Sequence: CARBON (s2pul)
Solvent: dmso
Data collected on: Jun 27 2015
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1000 repetitions
OBSERVE C13, 100.5479283 MHz
DECOUPLE H1, 399.8741342 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 38 min
220
200
180
160
140
120
100
80
60
40
20
0
ppm

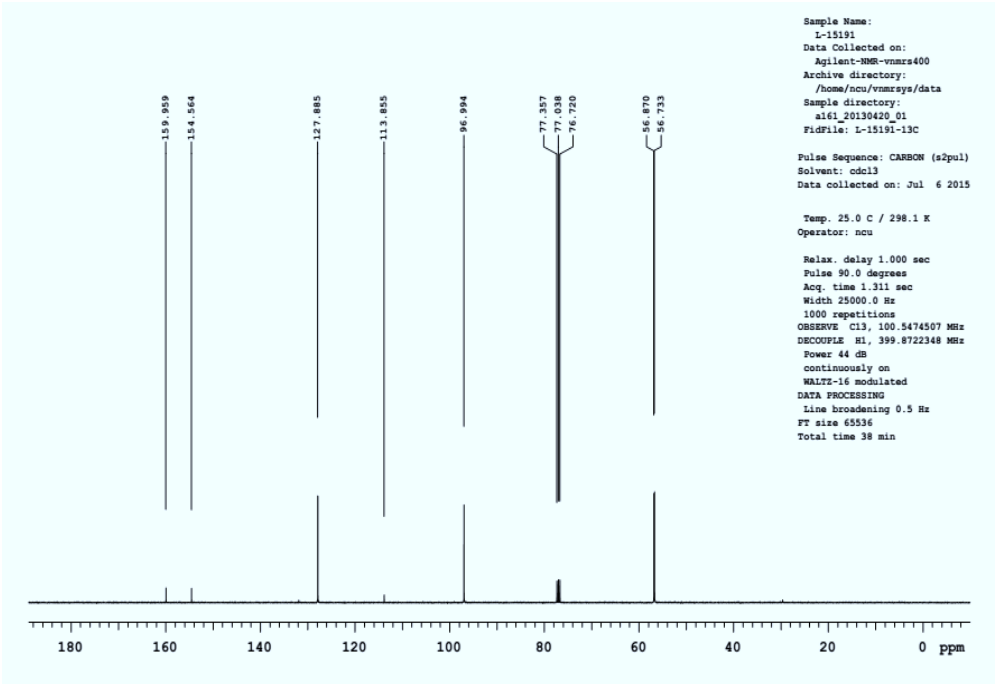

NO2
OMe
Cl
H
OMe

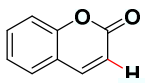
2r


8.047
6.542
3.989
3.984
Sample Name:
L-15191
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
/home/ncu/vnmrsys/data
Sample directory:
a161_20130420_01
FidFile: L-15191
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 6 2015
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.408 sec
Width 4807.7 Hz
16 repetitions
OBSERVE H1, 399.8702326 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 11 sec
10
9
8
7
6
5
4
3
2
1
0
ppm
0.77
0.97
6.00

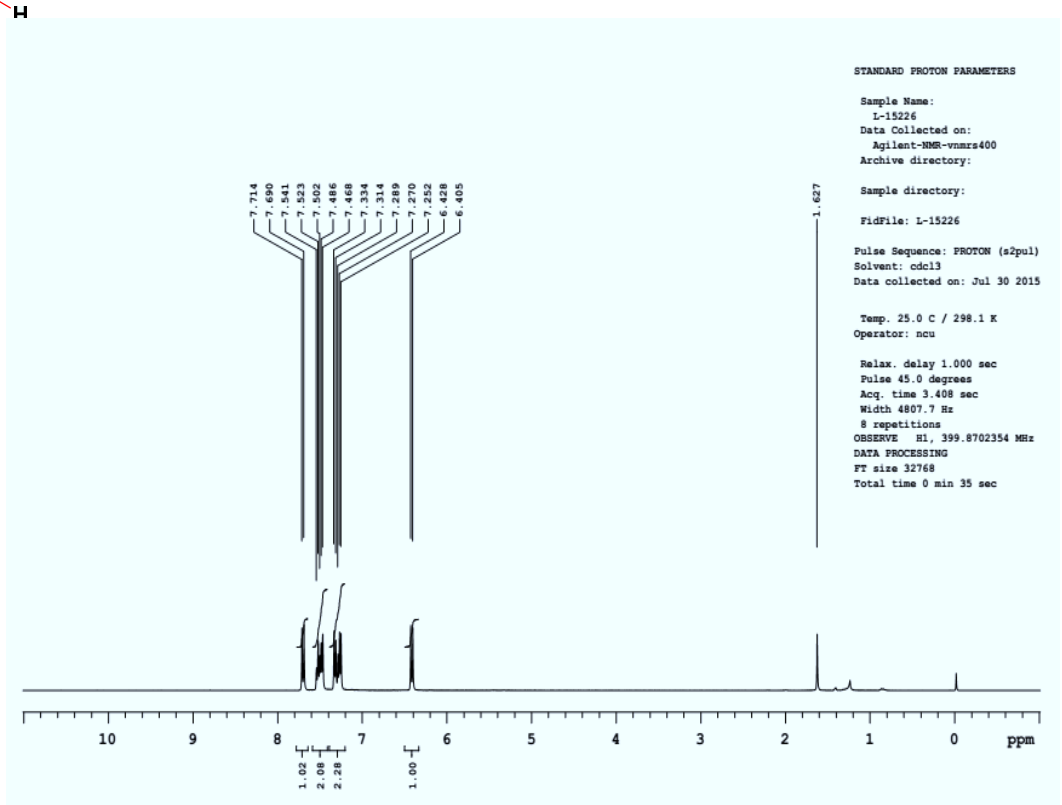

NO2
OMe
Cl
H
OMe

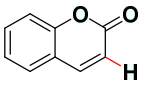
2r


159.959
154.564
127.885
113.855
96.994
77.357
77.038
76.720
56.870
56.733
180
160
140
120
100
80
60
40
20
0 ppm
Sample Name:
L-15191
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
/home/ncu/vnmrsys/data
Sample directory:
a161_20130420_01
FidFile: L-15191-13C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 6 2015
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1000 repetitions
OBSERVE C13, 100.5474507 MHz
DECOUPLE H1, 399.8722348 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 38 min

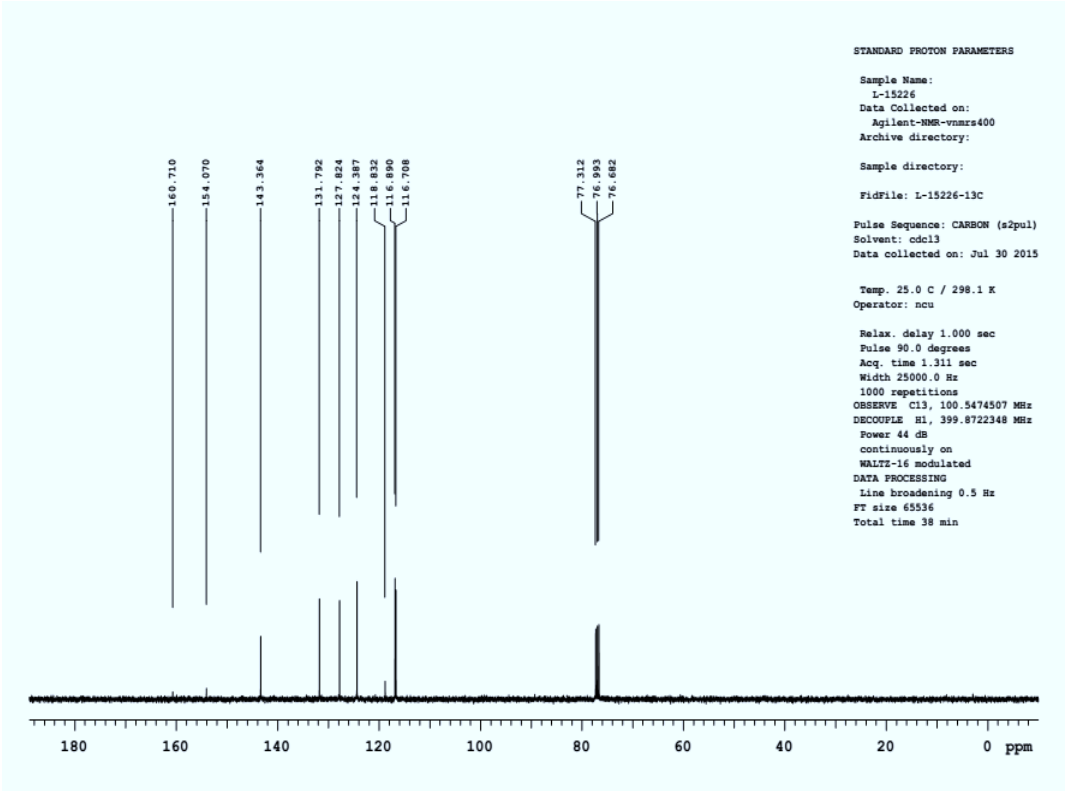

O
O
H

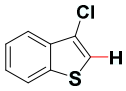
2s


7.714
7.690
7.541
7.523
7.502
7.486
7.468
7.334
7.314
7.289
7.270
7.252
6.428
6.405
1.627
10
9
8
7
6
5
4
3
2
1
0
ppm
1.02
2.08
2.28
1.00
STANDARD PROTON PARAMETERS
Sample Name:
L-15226
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: L-15226
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 30 2015
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.408 sec
Width 4807.7 Hz
8 repetitions
OBSERVE H1, 399.8702354 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 35 sec

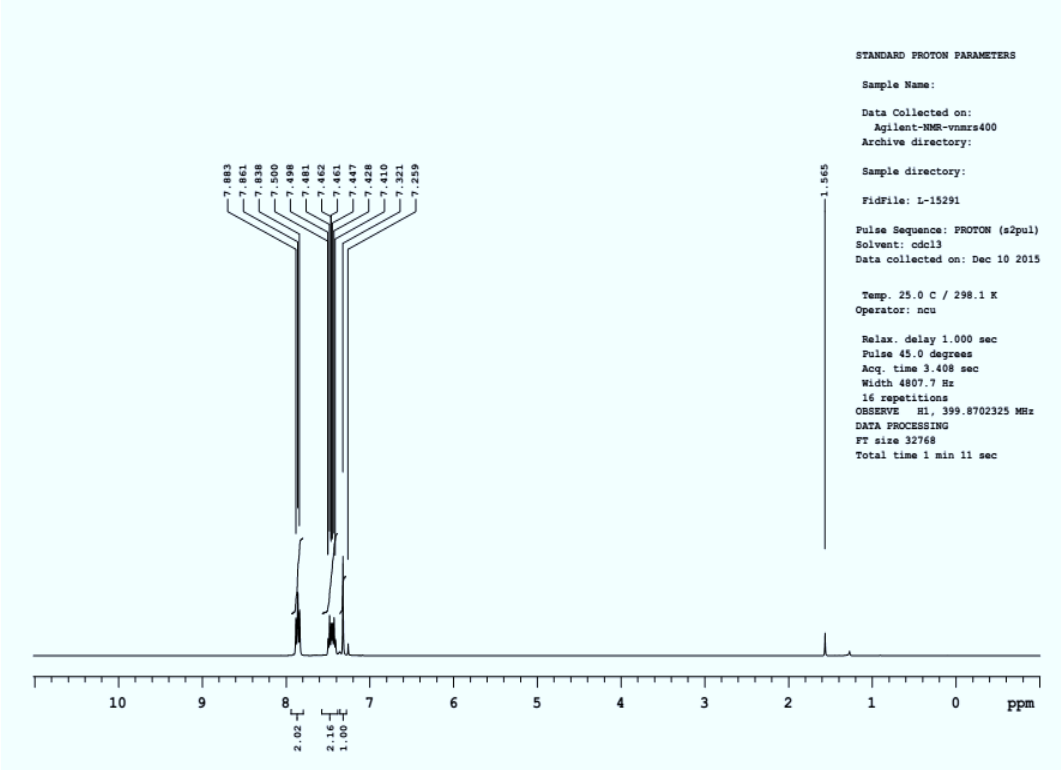

O
O
H

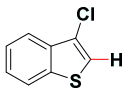
2s


160.710
154.070
143.364
131.792
127.824
124.387
118.832
116.890
116.708
77.312
76.993
76.682
STANDARD PROTON PARAMETERS
Sample Name:
L-15226
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: L-15226-13C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 30 2015
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1000 repetitions
OBSERVE C13, 100.5474507 MHz
DECOUPLE H1, 399.8722348 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 38 min
180
160
140
120
100
80
60
40
20
0
ppm

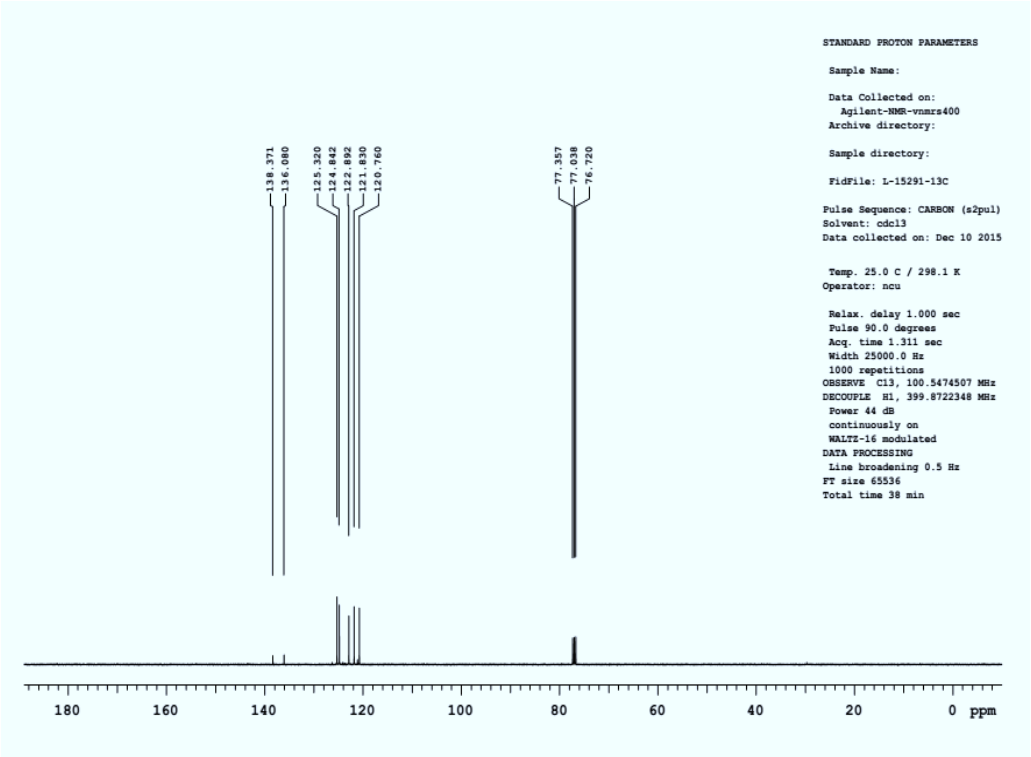

Cl
H
S

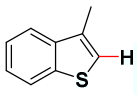
2t


7.883
7.861
7.838
7.500
7.498
7.481
7.462
7.461
7.447
7.428
7.410
7.321
7.259
1.565
STANDARD PROTON PARAMETERS
Sample Name:
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: L-15291
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Dec 10 2015
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.408 sec
Width 4807.7 Hz
16 repetitions
OBSERVE H1, 399.8702325 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 11 sec
10
9
8
7
6
5
4
3
2
1
0
ppm
2.02
2.16
1.00

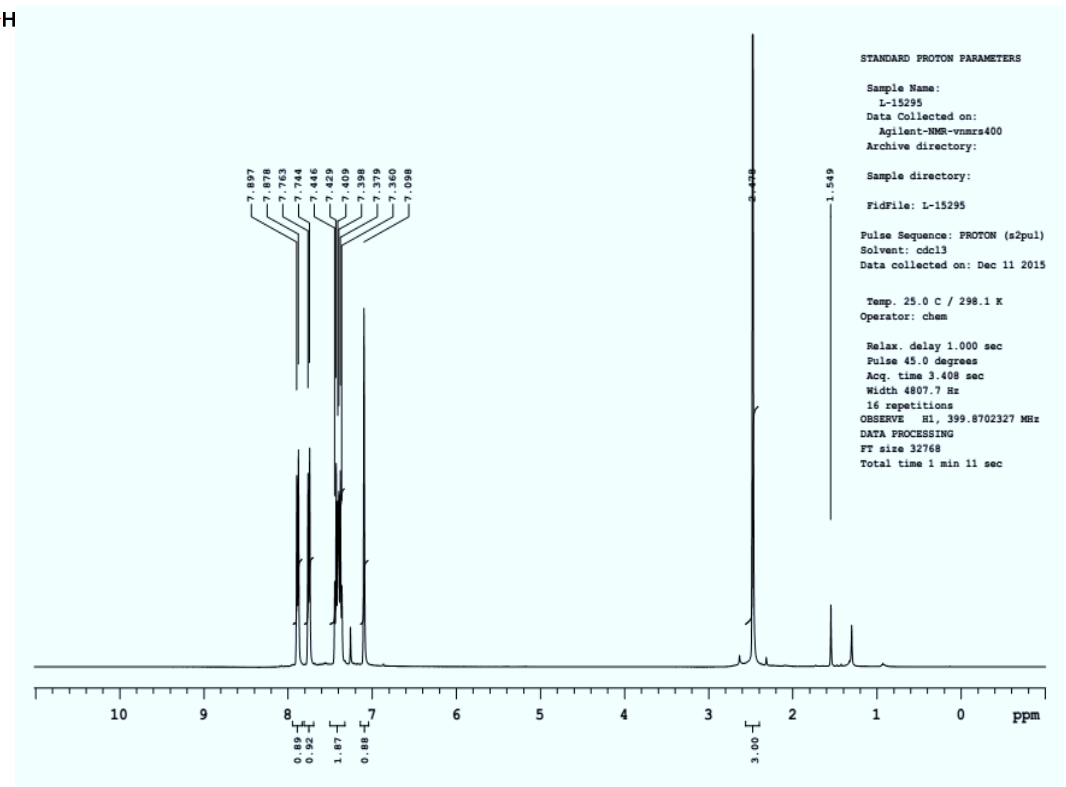

Cl
H
S

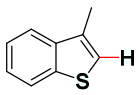
2t


138.371
136.080
125.320
124.842
122.892
121.830
120.760
77.357
77.038
76.720
STANDARD PROTON PARAMETERS
Sample Name:
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: L-15291-13C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Dec 10 2015
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1000 repetitions
OBSERVE C13, 100.5474507 MHz
DECOUPLE H1, 399.8722348 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 38 min
180
160
140
120
100
80
60
40
20
0 ppm

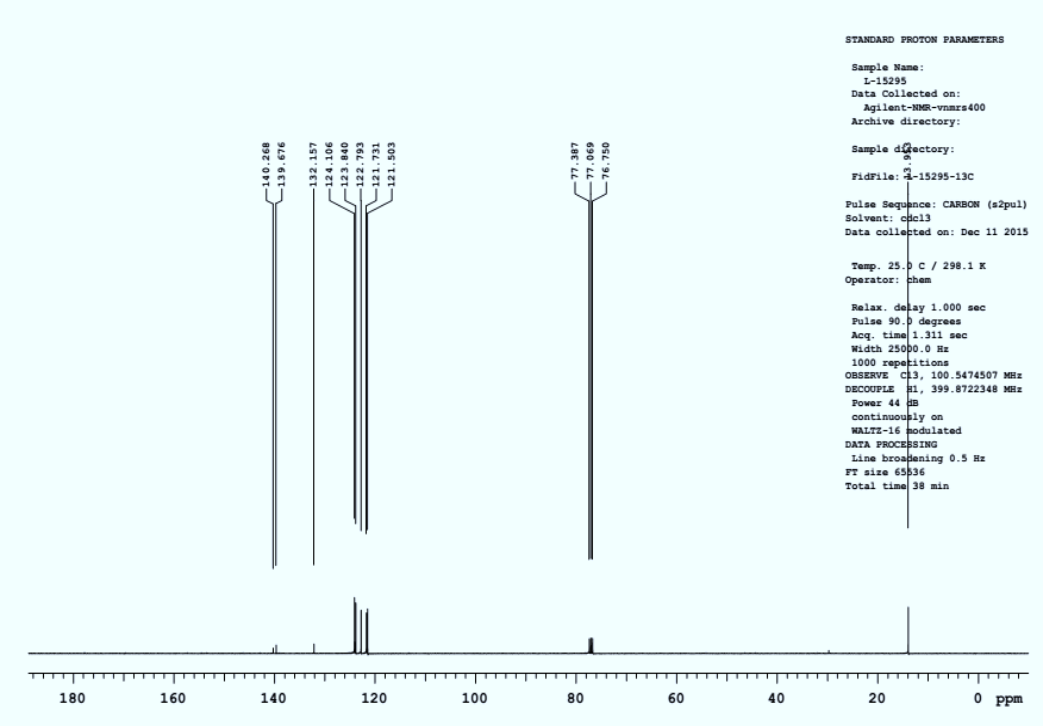

H
S

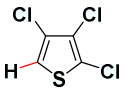
2u


7.897
7.878
7.763
7.744
7.446
7.429
7.409
7.398
7.379
7.360
7.098
2.478
1.549
STANDARD PROTON PARAMETERS
Sample Name:
L-15295
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: L-15295
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Dec 11 2015
Temp. 25.0 C / 298.1 K
Operator: chem
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.408 sec
Width 4807.7 Hz
16 repetitions
OBSERVE H1, 399.8702327 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 11 sec
10
9
8
7
6
5
4
3
2
1
0
ppm
0.89
0.92
1.87
0.88
3.00

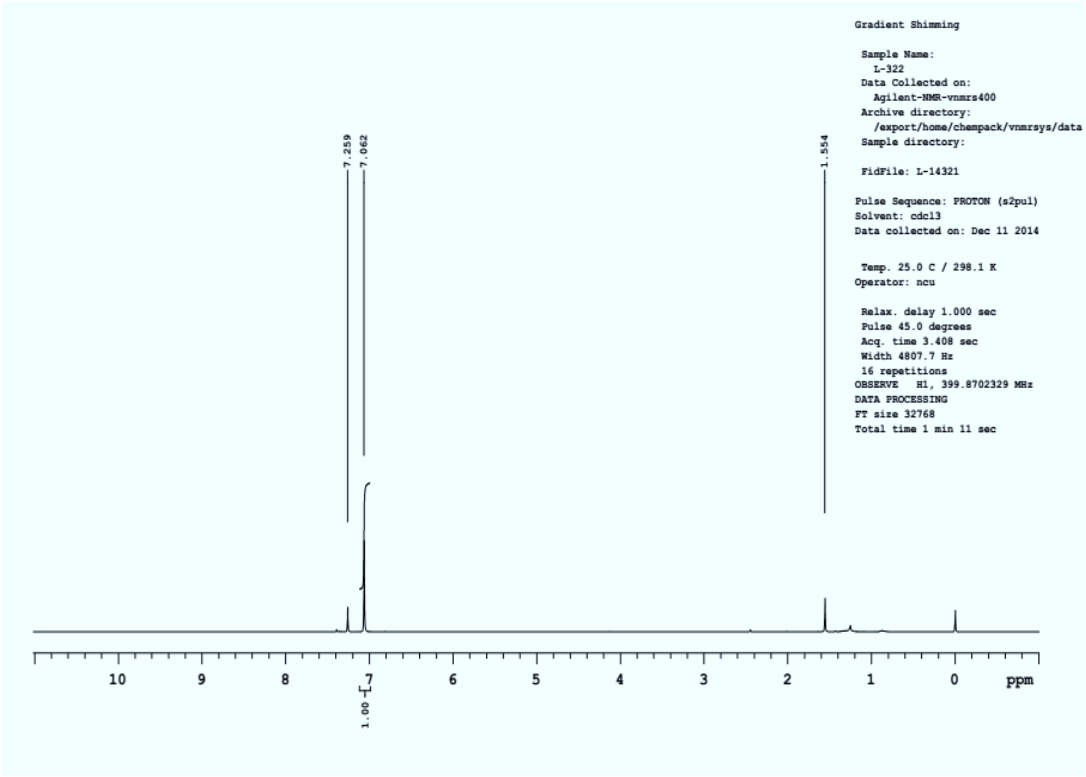


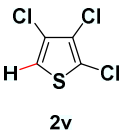
2u


STANDARD PROTON PARAMETERS
Sample Name:
L-15295
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: L-15295-13C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Dec 11 2015
Temp. 25.0 C / 298.1 K
Operator: chem
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1000 repetitions
OBSERVE C13, 100.5474507 MHz
DECOUPLE H1, 399.8722348 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 38 min
140.268
139.676
132.157
124.106
123.840
122.793
121.731
121.503
77.387
77.069
76.750
180
160
140
120
100
80
60
40
20
0 ppm

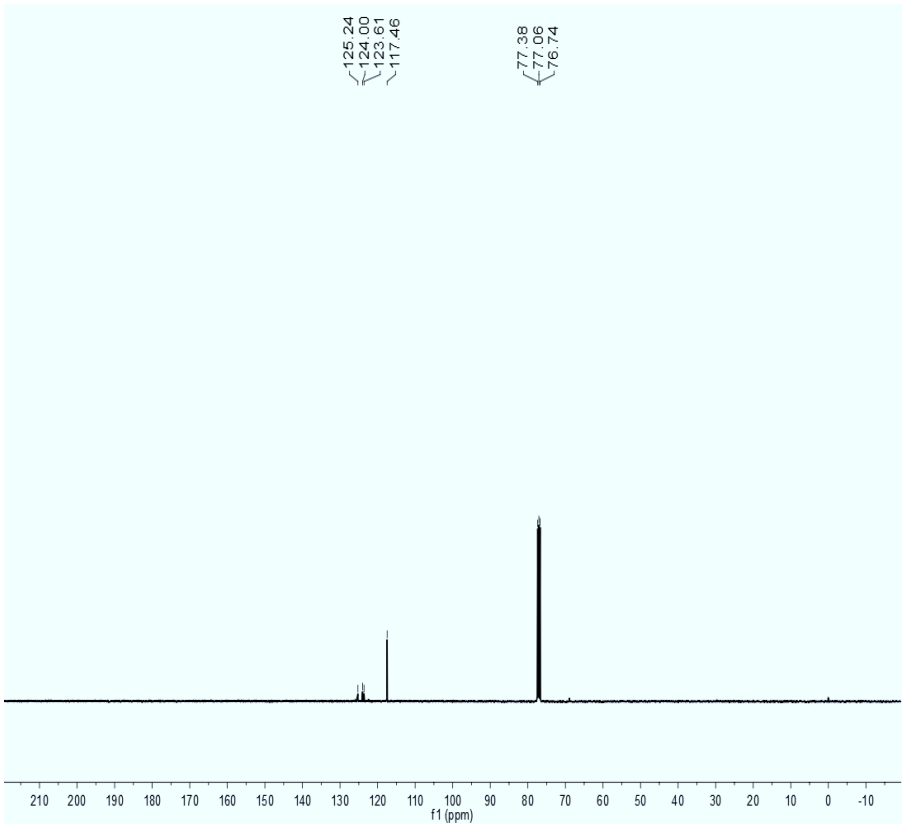


2v


Gradient Shimming
Sample Name:
L-322
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
/export/home/chempack/vnmrsys/data
Sample directory:
FidFile: L-14321
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Dec 11 2014
Temp. 25.0 C / 298.1 K
Operator: ncu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.408 sec
Width 4807.7 Hz
16 repetitions
OBSERVE H1, 399.8702329 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 11 sec
7.259
7.062
1.554
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00



2v



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2	Title	L-14321
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	290.2
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	1024
14	Receiver Gain	196
15	Relaxation Delay	2.0000
16	Pulse Width	10.0000
17	Acquisition Time	1.3631
18	Acquisition Date	2015-01-28T 23:16:00
19	Modification Date	2015-01-28T 23:16:48
20	Spectrometer Frequency	100.61
21	Spectral Width	24038.5
22	Lowest Frequency	-1958.4
23	Nucleus	13C
24	Acquired Size	32768
25	Spectral Size	65536