Copper(II)-catalyzed C-O coupling of aryl bromides with aliphatic diols: synthesis of ethers, phenols, and benzo-fused cyclic ethers

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Supporting Information

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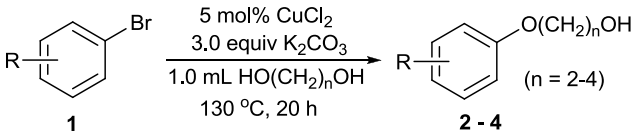
1. General considerations

Reagents: All the copper catalysts have purity greater than 97% and aliphatic diols were reagent grade. All reagents and solvent were obtained from commercial suppliers and used without further purification. Dichloromethane was dried by CaH_2. All manipulations were carried out under Ar.

Analytical methods: ^1H and ^{13}C NMR spectra were recorded on a 500 MHz spectrometer (125 MHz for ^{13}C). Multiplicities are indicated as s (singlet), d (doublet), t (triplet), q (quadruplet), quintet, m (multiplet), and coupling constants (*J*) are reported in hertz units. Spectrometer with chemical shifts reported in ppm relative to residual solvent peaks or to TMS as the internal standard. GC-MS analysis conducted on a GC-MSD system and products described in GC yield were accorded to the authentic sample/*n*-dodecane calibration standard from GC-MSD. LC-MS and HRMS spectra were recorded using ESI mode. IR spectra were recorded in neat. Column chromatography was performed on silica gel60 (230-400 mesh) and TLC was performed on silica gel 60 F_{254} glass plate.

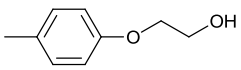
2. Copper(II)-catalyzed coupling of aryl bromides with aliphatic diols (Table 2 and Table3)



2.1. General experimental procedure (I)

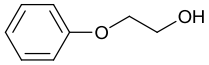
To a Schlenk test tube charged with a mixture of aryl bromide (**1**) (1.0 mmol) and potassium carbonate (415 mg, 3.0 mmol) was added copper chloride (6.7 mg, 0.05 mmol) and aliphatic diols (1.0 mL) under Ar. The resulting mixture was stirred for 20 h at 130 ℃. The reaction mixture was then acidified to pH=3 with 1N HCl solution. The aqueous phase was extracted twice with EtOAc and the combined organic layers was washed with H_2O and brine, dried over $MgSO_4$, and concentrated in vacuo. Purification of the crude product by column chromatography afforded the desired product (**2, 3, 4**).

2.2. Synthesis and characterization of the products

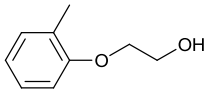


2-(*p*-tolyloxy)ethanol (**2a**)[1] [CAS: 15149-10-7] As the general procedure I, 1-bromo-4-methylbenzene (171 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 130 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as white solid (146 mg, 96%). ^1H NMR (500 MHz, $CDCl_3$) δ 7.08 (d, *J* = 8.5 Hz, 2H), 6.82 (d, *J* = 8.5 Hz, 2H), 4.05 (t, *J* = 5.0 Hz, 2H), 3.96-3.93 (m, 2H), 2.29 (s, 3H), 2.12 (t, *J* = 5.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.5, 130.4, 130.0, 114.4, 69.2, 61.6, 20.5; MS (EI) *m/z* = 152, 108 (100), 91, 77, 65.

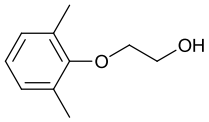
[1]Capparelli, M. P.; Deschepper, R. E.; Swenton, J. S. *J. Org. Chem*., **1987**, *52*, 4953-4966.



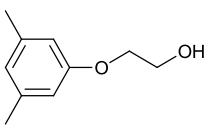
2-phenoxyethanol (**2b**) [CAS: 122-99-6] As the general procedure I, bromobenzene (157 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 130 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as colorless liquid (136 mg, 99%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31-7.28 (m, 2H), 6.97-6.91 (m, 3H), 4.08 (t, *J* = 4.0 Hz, 2H), 3.98-3.94 (m, 2H), 2.20 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.8, 129.8, 121.4, 114.8, 69.2, 61.7; Elemental analysis (%) : Calcd. for C 69.54, H 7.30; Found C 69.56, H 7.21; MS (EI) *m/z* = 138, 94(100), 77, 66, 51.



2-(*o*-tolyloxy)ethanol (**2c**) [CAS:6161-86-0] As the general procedure I, 1-bromo-2-methylbenzene (171 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 130 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as colorless liquid (150 mg, 99%). ^{1}H NMR (500 MHz, $CDCl_3$) δ7.14-7.12 (m, 2H), 6.88-6.85 (t, *J* = 7.0 Hz, 1H), 6.81-6.79 (d, *J* = 9.0 Hz, 1H), 4.05-4.04 (m, 2H), 2.23 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.9, 121.1, 127.12, 127.07, 121.1, 111.6, 69.5, 61.8, 16.5; Elemental analysis (%) : Calcd. for C 71.03, H 7.95; Found C 71.04, H 8.01; FT-IR 3465, 2936, 1737, 1593, 1496, 1375, 1242, 1123, 1043, 917, 812, 743; MS (EI) m/z = 152, 108(100), 91, 77, 65.

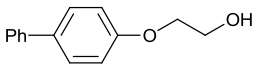


2-(2,6-dimethylphenoxy)ethanol (**2d**) [CAS: 16737-71-6] As the general procedure I, 2-bromo-1,3-dimethylbenzene (185 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 140 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as white solid (156 mg, 94%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.02 (d, *J* = 7.5 Hz, 2H), 6.96-6.91 (m, 1H), 3.98-3.93 (m, 2H), 3.91-3.75 (m, 2H), 2.30 (s, 6H), 2.21 (t, *J* = 6.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.6, 131.0, 129.2, 124.3, 73.1, 62.7, 16.5; HRMS (FAB) *m/z* calcd for $C_6H_{14}O_2$ $[M]^+$: 116.0994, found: 116.0991. IR (neat): 3294, 2948, 2912, 2871, 1466, 1223, 1202, 1076, 1045, 1031, 824, 771, 752, 673 cm^{-1}.

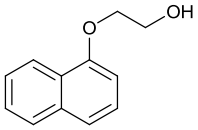


2-(3,5-dimethylphenoxy)ethanol (**2e**) [CAS: 5960-05-4] As the general procedure I, 1-bromo-3,5-dimethylbenzene(185 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 130 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the

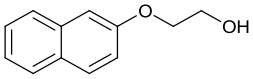
desired product as white-yellow solid (164 mg, 99%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.03-7.01 (m, 2H), 6.95-6.92 (m, 1H), 3.96 (t, *J* = 4.5 Hz, 2H), 3.90 (t, *J* = 5.0 Hz, 2H), 2.30 (s, 6H), 2.23 (t, *J* = 5.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.3, 130.8, 128.9, 72.9, 62.4, 16.3; Elemental analysis (%) : Calcd. for C 72.26, H 8.49; Found C 72.27, H 8.50; MS (EI) *m/z* = 166, 122 (100), 107, 77.



2-(biphenyl-4-yloxy)ethanol[2] (**2f**) [CAS: 19070-95-2] As the general procedure I, 4-bromobiphenyl (233 mg, 1.0 mmol) in a Schlenk flask was stirred for 20 h at 130 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as white solid (203 mg, 95%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56-7.53 (m, 4H), 7.42 (t, *J* = 7.5 Hz, 2H), 7.33-7.30 (m, 1H), 7.00 (d, *J* = 7.0 Hz, 2H), 4.13 (t, *J* = 3.0 Hz, 2H), 4.00 (t, *J* = 3.0 Hz, 2H), 2.04 (t, *J* = 6.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.2, 140.7, 134.2, 128.7, 128.2, 126.7, 114.8, 69.3, 61.5; MS (EI) *m/z* = 214, 170 (100), 141, 115.



2-(naphthalen-1-yloxy)ethanol[3] (**2g**) [CAS: 711-82-0] As the general procedure I, 1-bromonaphthalene (207 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 130 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as red solid (180 mg, 96%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.27 (d, *J* = 9.0 Hz, 1H), 7.81 (d, *J* = 7.5 Hz, 1H), 7.50-7.45 (m, 3H), 7.38 (t, *J* = 8.0 Hz, 1H), 6.84 (d, *J* = 7.5 Hz, 1H), 4.10 (t, *J* = 4.5 Hz, 2H), 3.98 (t, *J* = 4.5 Hz, 2H), 2.81 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 154.3, 134.5, 127.6, 126.5, 125.8, 125.5, 125.3, 121.7, 120.8, 104.9, 69.5, 61.6; MS (ESI) *m/z* = 189.1 (M^+).



2-(naphthalen-2-yloxy)ethanol (2h)[4] [CAS: 93-20-9] As the general procedure I, 2-bromonaphthalene (207 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 130 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as white solid (174 mg, 94%). ^{1}H NMR (500 MHz, $CDCl_3$)δ 7.81-7.70 (m, 3H), 7.49-7.41 (m, 1H), 7.40-7.33 (m, 1H), 7.21-7.13 (m, 2H), 4.22 (t, *J* = 6.5 Hz, 2H), 4.04 (t, *J* = 6.5 Hz, 2H), 2.06 (t, *J* = 6.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.8, 134.7, 129.8, 129.4, 127.9, 127.0, 126.7, 124.1, 119.0, 107.1, 69.4, 61.8.

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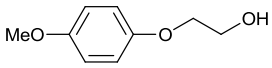
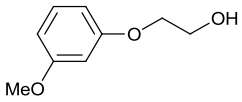
[2]Zhang, T.; Park, S.-Y.; Farmer, B. L.; Interrante, L. V. *J. Polym. Sci., Part A: Polym. Chem.***2003**, *41*, 984-997.

[3]Bolchi, C.; Catalano, P.; Fumagalli, L.; Gobbi, M.; Pallavicini, M.; Pedretti, A.; Villa, L.; Vistolia, D.; Valotia, E. *Bioorg. Med. Chem*., **2004**, *12*, 4937-4951.

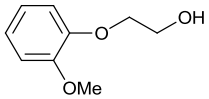
[4]Kessler, S. N.; Wegner, H. A., *Org. Lett.**2010,*** 12, 4062-4065.



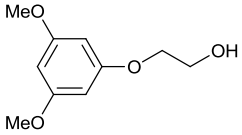
2-(4-methoxyphenoxy)ethanol [5] (**2i**) [CAS: 5394-57-0] As the general procedure I, 1-bromo-4-methoxybenzene (187 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 130 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as white solid (156 mg, 93%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.88-6.83 (m, 4H), 4.04 (t, *J* = 5.0 Hz, 2H), 3.94 (t, *J* = 5.0 Hz, 2H), 3.77 (s, 3H), 2.08-2.04 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 154.3, 152.9, 115.8, 114.9, 70.1, 61.8, 55.9; MS (EI) *m/z* = 168, 124 (100), 109, 81.



2-(3-methoxyphenoxy)ethanol (**2j**) As the general procedure I, 1-bromo-3-methoxybenzene (187mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 130 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as white solid (154 mg, 92%).^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.20-7.17 (t, *J* = 8.5 Hz, 1H), 6.54-6.48 (m, 3H), 4.08-4.06 (m, 2H), 3.96-3.95 (m, 2H), 3.79 (s, 3H); ^{13}C-NMR (125 MHz, $CDCl_3$) δ 160.8, 159.8, 129.9, 106.68, 106.65, 101.1, 69.2, 61.5, 55.3; MS (EI) *m/z* = 168, 124 (100), 94, 77. Elemental analysis (%): Calcd for C 64.27, H 7.19; Found C 64.23, H 7.20; FT-IR 3354, 2939, 2875, 1729, 1588, 1492, 1453, 1335, 1264, 1199, 1038, 994, 834, 761, 686.



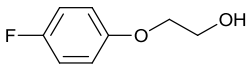
2-(2-methoxyphenoxy)ethanol [6] (**2k**) [CAS: 118181-71-0] As the general procedure I, 1-bromo-2-methoxybenzene (187 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 130 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as colorless liquid (154 mg, 92%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.98-6.89 (m, 4H), 4.13 (t, *J* = 4.0 Hz, 2H), 3.92 (t, *J* = 4.0 Hz, 2H), 3.87 (s, 3H), 2.91(m, 1H) ; ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.9, 148.3, 122.1, 121.3, 114.8, 112.1, 71.4, 61.3, 55.8; MS (ESI) *m/z* = 169.1 (M^+).



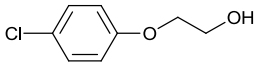
2-(3,5-dimethoxyphenoxy)ethanol (**2l**) [CAS: 27318-86-1] As the general procedure I, 1-bromo-3,5-dimethoxybenzene (217 mg, 1.0 mmol) in a Schlenk flask was stirred for 20 h at 130 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as white solid (196 mg, 99%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.10 (s, 3H), 4.05-4.03 (m, 2H),

[5]Brand,J. P.;Charpentier, J.;Waser, J. *Angew. Chem. Int. Ed*. **2009**, *48*, 9346-9349.
[6]Ochoa-Teran, A.; Rivero, I. A. *ARKIVOC*, **2008**, *2*, 235-242.

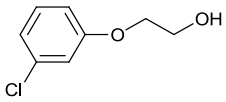
3.94-3.93 (m, 2H), 3.76 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.7, 160.7, 93.7, 69.4, 61.6, 55.6; Elemental analysis (%) : Calcd. for C 60.59, H 7.12; Found C 60.60, H 7.11; MS (ESI) *m/z* = 199.1 (M^+).



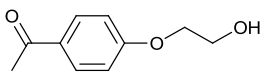
2-(4-fluorophenoxy)ethanol (**2m**) [CAS: 49650-88-6] As the general procedure I, 1-bromo-4-fluorobenzene (175 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 130 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as colorless liquid (149 mg, 96%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.97 (t, *J* = 8.0 Hz, 2H), 6.86-6.84 (m, 2H), 4.04 (m, 2H), 3.96-3.94 (m, 2H), 2.38 (t, *J* = 4.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.7 (d, *J* = 237.25 Hz, C-F), 155.0 (d, *J* = 2.13 Hz, C-F), 116.1(d, *J* = 22.87 Hz, C-F), 115.8 (d, *J* = 8.0 Hz, C-F), 70.1, 61.6; Elemental analysis (%) : Calcd. for C 61.53, H 5.81; Found C 61.52, H 5.85; MS (EI) *m/z* = 156.



2-(4-chlorophenoxy)ethanol (**2n**) [CAS: 2924-66-5] As the general procedure I, 1-bromo-4-chlorobenzene (191 mg, 1.0 mmol) in a Schlenk flask was stirred for 20 h at 130 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as colorless solid (165 mg, 96%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.23 (t, *J* = 9.0 Hz, 2H), 6.84 (t, *J* = 7.0 Hz, 2H), 4.05 (t, *J* = 5.0 Hz, 2H), 3.97-3.94 (m, 2H), 2.10-2.06 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.2, 129.4, 126.0, 115.8, 69.5, 61.4; Elemental analysis (%) : Calcd. for C 55.67, H 5.26; Found C 55.62, H 5.19; MS (ESI) *m/z* = 170.9 (M^-).



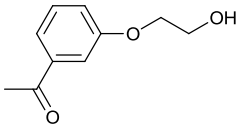
2-(3-chlorophenoxy)ethanol (2o) [CAS: 6161-83-7] As the general procedure I, 1-bromo-4-chlorobenzene (191 mg, 1.0 mmol) in a Schlenk flask was stirred for 20 h at 130 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as colorless solid (163 mg, 95%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.20 (t, *J* = 7.5 Hz, 1H), 7.01-6.88 (m, 2H), 6.81 (d, *J* = 7.5 Hz, 1H), 4.10-4.04 (m, 2H), 3.98-3.92 (m, 2H), 2.09 (br-s, 1H).^{13}C NMR (125 MHz, $CDCl_3$) δ 159.3, 134.9, 130.3, 121.3, 115.0, 113.0, 69.4, 61.3.



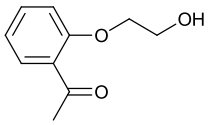
1-(4-(2-hydroxyethoxy)phenyl)ethanone [7] (**2p**) [CAS: 31769-45-6] As the general procedure I, 4'-Bromoacetophenone (200 mg, 1.0 mmol) in a Schlenk flask was stirred for 36 h at 110 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as orange solid (158 mg, 88%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.94 (dd, *J* = 6.5, 2.0 Hz, 2H),

[7]Mello, R.; Martinez-Ferrer, J.; Asensio, G.; Gonzalez-Nunez, M. E. *J. Org. Chem.*,**2007**, *72*, 9376-9378.

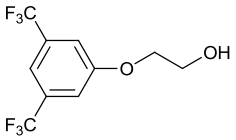
6.96 (dd, *J* = 6.5, 2.0 Hz, 2H), 4.16 (t, *J* = 4.0 Hz, 2H), 4.00 (t, *J* = 4.0 Hz, 2H), 2.56 (s, 3H), 2.13 (t, *J* = 4.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 196.8, 162.5, 130.65, 130.64, 114.2, 69.4, 61.3, 26.4; MS (ESI) *m/z* = 181.0 (M^+).



1-(3-(2-hydroxyethoxy)phenyl)ethanone [8] (**2q**) [CAS: 1892-43-9] As the general procedure I, 1-(3-bromophenyl)ethanone(200 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 110 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as white solid (162 mg, 90%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57-7.55 (m, 1H), 7.53-7.50 (m, 1H), 7.42-7.35 (m, 1H), 7.15-7.13 (m, 1H), 4.14 (t, *J* = 5.0 Hz, 2H), 4.01-3.96 (m, 2H), 2.60 (s, 3H), 2.18 (t, *J* = 5.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 198.2, 159.1, 138.7, 129.9, 121.8, 120.3, 113.3, 69.6, 61.6, 27.0; MS (ESI) *m/z* = 180, 165, 121(100), 93, 65.



1-(2-(2-hydroxyethoxy)phenyl)ethanone [9] (**2r**) [CAS: 126572-94-9] As the general procedure I, 2'-bromoacetophenone (200 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 110 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as white solid (150 mg, 83%). ^{1}H NMR (500 MHz, CD_3Cl_3) δ 7.72 (d, *J* = 2.0 Hz, 1H), 7.48-7.44 (m, 1H), 7.05-7.01 (m, 1H), 6.98 (d, *J* = 2.0 Hz, 1H), 4.21 (t, *J* = 5.0 Hz, 2H), 4.00 (t, *J* = 5.0 Hz, 2H), 2.89 (s, 1H), 2.63 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 199.9, 157.9, 133.7, 130.5, 128.6, 121.1, 113.6, 70.6, 61.2, 31.3; MS (ESI) *m/z* = 180, 165, 121(100), 93, 65.

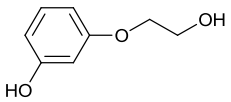


2-(3,5-bis(trifluoromethyl)phenoxy)ethanol (**2s**) [CAS: 887268-12-4] As the general procedure I, 1-bromo-3,5-bis (trifluoromethyl)benzene (293 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 130 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as white solid (249 mg, 91%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49 (s, 1H), 7.34 (s, 2H), 4.18 (t, *J* = 4.0 Hz, 2H), 4.04 (t, *J* = 4.0 Hz, 2H), 2.03 (t, *J* = 6.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.20, 133.9 (q, *J* = 33.38 Hz, C-F), 123.1 (q, *J* = 271.13 Hz, C-F), 114.9 (m, *J* = 4.0 Hz, C-F), 114.7

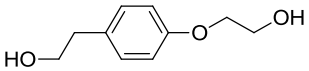
[8]Riggio, G.; Raeber, A. J.; Hopff, W. H. *Helv.Chim.Acta*.,**1989**, *72*, 1216-1224.

[9]Fumagalli,L.;Bolchi, C.; Colleoni, S.; Gobbi, M.; Moroni, B.; Pallavicini, M.; Pedretti, A.; Villa, L.; Vistolia, G.; Valoti, E. *Bioorg. Med. Chem*., **2005**, *13*, 2547-2559.

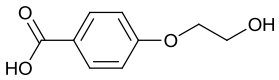
(q, *J* = 3.75 Hz, C-F), 70.0, 61.1; Elemental analysis (%) : Calcd. for C 43.81, H 2.93; Found C 43.87, H 2.93; MS (EI) *m/z* = 274.



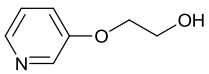
3-(2-hydroxyethoxy)phenol[10] (**2t**) [CAS: 850895-55-5] As the general procedure I, 3-bromophenol (173 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 130 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as white solid (145 mg, 94%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.15-7.12 (m, 1H), 6.52-6.49 (m, 1H), 6.46-6.43 (m, 2H), 5.00 (s, 1H), 4.08-4.02 (m, 2H), 3.99-3.88 (m, 2H), 2.10-2.07 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.0, 156.7, 130.2, 108.2, 107.0, 102.2, 69.1, 61.5; MS (EI) *m/z* = 154, 110(100), 93, 82, 65.



2-(4-(2-hydroxyethoxy)phenyl)ethanol (**2u**) [CAS: 4960-67-2] As the general procedure I, 2-(4-bromophenyl)ethanol (201mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 130 ℃. Following aqueous workup, purification of the crude product by column chromatography (10% methanol in CH_2Cl_2) afforded the desired product as white solid (145 mg, 94%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.16 (d, *J* = 7.1 Hz, 2H), 6.88 (d, *J* = 7.1 Hz, 2H), 4.10-4.02 (m, 2H), 4.02-3.90 (m, 2H), 3.83 (q, *J* = 6.0 Hz, 2H), 2.82 (t, *J* = 6.5 Hz, 2H), 2.03 (t, *J* = 6.0 Hz, 1H), 1.38 (t, *J* = 6.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.3, 130.9, 130.1, 114.7, 69.2, 63.8, 61.5, 38.3; MS (EI) *m/z* = 182, 151, 107(100), 77.



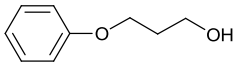
4-(2-hydroxyethoxy)benzoic acid (**2v**) [CAS: 1711-24-6] As the general procedure I, 4-bromobenzoic acid (201 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 hat 130 ℃. Following aqueous workup, purification of the crude product by column chromatography (10% methanol in CH_2Cl_2) afforded the desired product as white solid (173 mg, 95%). ^{1}H NMR (500 MHz, CD_3OD) δ 7.88 (d, *J* = 8.0 Hz, 2H), 7.00 (d, *J* = 8.0 Hz, 2H), 4.11 (t, *J* = 3.0 Hz, 2H), 3.73 (t, *J* = 3.0 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.4, 162.8, 131.8, 123.3,114.7, 70.2, 59.9; Elemental analysis (%) : Calcd. for C 59.34, H 5.53; Found C 59.38, H 5.41; MS (ESI) *m/z* = 181.1 (M^-).



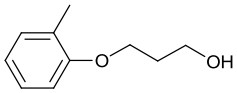
2-(pyridin-3-yloxy)ethanol[11] (**2w**) [CAS: 119967-49-6] As the general procedure I, 3-bromopyridine (158 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 hat 130 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as white solid

[10]Singh, A.; Yip, W. –T.; Halterman, R. L. *Org. Lett*., **2012**, *14*, 4046-4049.
[11]Kocak, A.; Kurbanli, S.; Malkondu, S. *Synth.Commun*.,**2007**, *37*, 3697-3708.

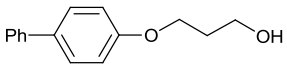
(125 mg, 90%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.33(t, *J* = 5.0 Hz, 1H), 8.23(t, *J* = 5.0 Hz, 1H), 7.28-7.23 (m, 2H), 4.15-4.13 (m, 2H), 4.02-3.99 (m, 2H), 3.85 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.0, 142.2, 138.0, 124.0, 121.2, 69.7, 61.1; MS (EI) *m/z* = 139, 95(100), 78, 67, 51.



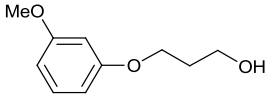
3-phenoxypropan-1-ol[12] (**3b**) [CAS: 6180-61-6] As the general procedure I, bromobenzene(157mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 130 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as white solid (137 mg, 90%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30-7.27 (m, 2H), 6.96-6.90 (m, 3H), 4.12 (t, *J* = 6.0 Hz,2H), 3.87-3.84 (m, 2H), 2.06-2.03 (m, 2H), 1.96 (t, J = 5.0 Hz,1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.7, 129.5, 120.9, 114.5, 65.6, 60.5, 32.0; MS (EI) *m/z* = 166, 108(100), 91, 77.



3-(o-tolyloxy)propan-1-ol[12] (**3c**) [CAS: 52448-99-4] As the general procedure I, 1-bromo-2-methylbenzene (171 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 130 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as white solid (128 mg, 77%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.19-7.10 (m, 2H), 6.88-6.83 (m, 2H), 4.13 (t, *J* = 5.0 Hz,2H), 3.90-3.88 (m, *2*H), 2.22 (s, 3H), 2.10-2.04 (m, 2H), 1.96-1.92 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.8, 130.7, 126.8, 126.5, 120.5, 110.8, 65.9, 60.9, 32.1, 16.3; MS (EI) *m/z* = 180, 122(100), 107, 91, 77.

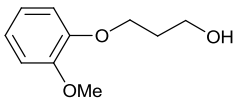


3-([1,1'-biphenyl]-4-yloxy)propan-1-ol[2] (**3f**) [CAS: 173025-78-0] As the general procedure I, 4-bromo-1,1'-biphenyl (233 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 130 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as white solid (187 mg, 82%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56-7.43 (m, 4H), 7.41-7.35 (m, 2H), 7.30-7.27 (m, 1H), 6.98 (d, *J* = 8.0 Hz, 2H), 4.18 (t, *J* = 6.0 Hz, 2H), 3.88 (t, *J* = 6.0 Hz,2H),2.10- 2.05 (m, 2H), 1.70 (m, 1H);^{13}C NMR (125 MHz, CDCl3) δ 158.3, 140.8, 134.0, 128.7, 126.8, 126.72, 126.68, 114.8, 65.9, 60.6, 32.0; MS (EI) *m/z* = 228.

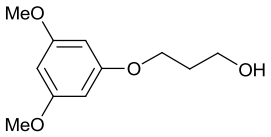


[12]Sugimura, T.; Hagiya, K.; Sato, Y.;Tei, T.; Tai, A.Okuyama, T. *Org. Lett*., **2001**, *3*, 37-40.

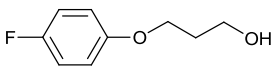
3-(3-methoxyphenoxy)propan-1-ol [13] (**3j**) [CAS:136167-42-5] As the general procedure I, 1-bromo-3-methoxybenzene (187 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 130 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as white solid (169 mg, 93%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.18 (t, *J* = 8.0 Hz, 1H), 6.53-6.50 (m, 2H), 6.47 (t, *J* = 2.5 Hz, 1H), 4.11 (t, *J* = 6.0 Hz, 2H), 3.88-3.84 (m, 2H), 3.79 (s, 3H), 2.04 (quintet, *J* = 6.0 Hz, 2H), 1.80-1.78 (m, 1H);^{13}C NMR (125 MHz, $CDCl_3$) δ 160.8, 160.0, 129.9, 106.6, 106.5, 100.9, 65.8, 60.6, 55.3, 32.0; MS (EI) *m/z* = 182, 124(100), 94.



3-(2-methoxyphenoxy)propan-1-ol [14] (**3k**) [CAS: 136167-44-7] As the general procedure I, 1-bromo-2-methoxybenzene (187 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 130 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as white solid (149 mg, 82%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.94-6.80 (m, 4H), 4.20 (t, *J* = 6.0 Hz, 2H), 3.89-3.85 (m, 5H), 2.74 (t, *J* = 5.0 Hz, 1H), 2.10-2.06 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.4, 148.1, 121.5, 120.8, 113.3, 111.5, 68.5, 61.6, 55.8, 31.8; MS (EI) *m/z* = 182.



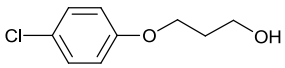
3-(3,5-dimethoxyphenoxy)propan-1-ol(**3l**) [CAS: 1082823-86-6] As the general procedure I, 1-bromo-3,5-dimethoxybenzene (217 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 130 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as white solid (182 mg, 86%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.09 (s, 3H), 4.09 (t, *J* = 6.0 Hz, 2H), 3.89-3.85 (m, 2H), 3.74 (s, 6H), 2.03 (quintet, *J* = 6.0Hz, 2H), 1.73 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.5, 160.6, 93.4, 65.8, 60.6, 55.4, 32.0; HRMS (FAB) *m/z* calcd for $C_{11}H_{16}O_4$ $[M+H]^+$: 213.1127, found: 212.1126. IR (neat): 3387, 2941, 1592, 1470, 1193, 1146, 1060, 818, 752, 681 cm^{-1}.



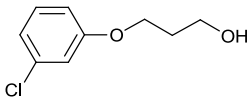
3-(4-fluorophenoxy)propan-1-ol [15] **(3m**) [CAS: 104413-57-2] As the general procedure I, 1-bromo-4-fluorobenzene (175 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 130 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as white solid (138 mg, 81%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.99-6.94 (m, 2H), 6.85-6.82 (m, 2H), 4.08 (t, *J* = 5.0 Hz,2H), 3.89-3.85 (m, 2H), 2.03 (p, *J* = 6.0 Hz, 2H), 1.79 (t, *J* = 5.0 Hz,1H);^{13}C NMR (125

[13]Zettl, H.;Steri, R.;Lammerhofer,M.; Schubert-Zsilavecz, M. *Bioorg. Med. Chem. Lett*., **2009**, *19*, 4421-4426.
[14]Panchgalle, S. P.;Kunte, S. S.;Chavan, S. P.; Kalkote, U. R.*Synth.Commun*.,**2011**, *41*, 1938-1944.
[15]Peprah, K.; Zhu, X. Y.; Eyunni, S. V.K.; Etukala, J. R.;Setola, V.; Roth, B. L.; Ablordeppey, S. Y.*Bioorg. Med. Chem*., **2012**, *20*, 1671-1678.

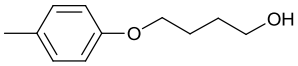
MHz, $CDCl_3$) δ 157.3 (d, *J* = 236.75 Hz, C-F),154.9 (d, *J* = 2.13 Hz, C-F), 115.8 (d, *J* = 228.75 Hz, C-F), 115.4 (d, *J* = 7.87 Hz, C-F), 66.3, 60.4, 32.0; MS (EI)*m/z* = 170, 112(100), 83, 57.



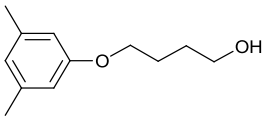
3-(4-chlorophenoxy)propan-1-ol [16] (**3n**) [CAS: 18673-04-6] As the general procedure I, 1-bromo-4-chlorobenzene (191 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 130 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as white solid (147 mg, 79%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.24-7.22 (m, 2H), 6.85-6.82 (m, 2H), 4.09 (t, *J* = 6.0Hz, 2H), 3.86 (t, *J* = 6.0 Hz, 2H), 2.04 (p, *J* = 6.0Hz, 2H), 1.69 (s, 1H);^{13}C NMR (125 MHz, $CDCl_3$) δ 157.4, 129.3, 125.7, 115.7, 104.7, 85.9, 60.3, 31.9; MS (EI) *m/z* = 186.



3-(3-chlorophenoxy)propan-1-ol[16] (**3o**) [CAS: 57264-55-8] As the general procedure I, 1-bromo-3-chlorobenzene (191 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 130 ℃. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as white solid (153 mg, 82%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.19 (t, *J* = 8.0 Hz, 1H), 6.95-6.90 (m, 2H), 6.79 (dd, *J* = 8.5, 2.5 Hz, 1H), 4.10 (t, *J* = 5.0 Hz, 2H), 3.87-3.84 (m, 2H), 2.06-2.01 (m, 2H), 1.77 (t, J = 5.0 Hz, 1H);^{13}C NMR (125 MHz, $CDCl_3$) δ 159.5, 134.9, 130.2, 121.0, 114.9, 113.0, 65.7, 60.1, 31.9; MS (EI) *m/z* = 186.



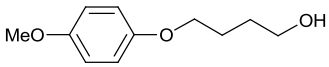
4-(*p*-tolyloxy)butan-1-ol[17] (**4a**) [CAS: 60222-64-2] As the general procedure I, 1-bromo-4-methylbenzene (171 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 130 ℃ using Cs_2CO_3 as base instead of K_2CO_3. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as white solid (144 mg, 80%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.07 (d, *J* = 8.5 Hz, 2H), 6.80 (d, *J* = 8.5 Hz, 2H), 3.98 (t, *J* = 6.0 Hz, 2H), 3.71 (t, *J* = 6.0 Hz, 2H), 2.28 (s, 3H), 1.91-1.83 (m, 2H), 1.81-1.71 (m, 2H), 1.68 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.7, 129.93, 129.88, 114.3, 67.8, 62.0, 29.6, 25.9, 20.5; MS (EI) *m/z* = 180, 108(100), 77.



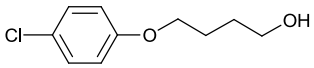
4-(3,5-dimethylphenoxy)butan-1-ol (**4e**) [CAS: 40324-48-9] As the general procedure I, 1-bromo-3,5-dimethylbenzene (185 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 130 ℃using Cs_2CO_3 as base

[16]Goosen, A.; Marais, C. F.; McCleland, C. W.; Rinaldi, F. C. *J. Chem. Soc. Perkin Trans. 2*, **1995**, 1227-1236.
[17]Sword, R.; Baldwin, L. A.; Murphy, J. A. *Org. Biomol. Chem.*, **2011**, *9*, 3560-3570.

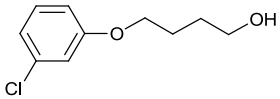
instead of K_2CO_3. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as white solid (120 mg, 62%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.60 (d, *J* = 4.5 Hz, 1H), 6.53 (d, *J* = 5.0 Hz, 2H), 3.99-3.96 (m, 2H), 3.73-3.69 (m, 2H), 2.27 (s, 6H), 1.88-1.85(m, 2H), 1.76-1.73 (m, 2H);^{13}C NMR (125 MHz, $CDCl_3$) δ 159.1, 139.4, 122.8, 112.5, 67.8, 62.8, 29.8, 26.2, 21.7; HRMS (FAB) *m/z* calcd for $C_{12}H_{18}O_2$ $[M+H]^+$: 195.1385, found: 195.1388. IR (neat): 3338, 2918, 2870,1593, 1467, 1322, 1294, 1167, 1154, 1057, 826, 687 cm^{-1}.



4-(4-methoxyphenoxy)butan-1-ol (**4i**) [CAS: 123731-28-2] As the general procedure I, 1-bromo-4-methoxybenzene (187 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 130 ℃using Cs_2CO_3 as base instead of K_2CO_3. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as white solid (153 mg, 78%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.86-6.81 (m, 4H), 3.96-3.94 (m, 2H), 3.77 (s, 3H), 3.73-3.70 (m, 2H), 1.89-1.85 (m, 3H), 1.77-1.75 (2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 153.6, 153.1, 115.7, 115.0, 68.2, 60.9, 55.8, 29.5, 26.0; HRMS (FAB) *m/z* calcd for $C_{11}H_{16}O_3$ $[M]^+$: calcd for 196.1099, found: 196.1100. IR (neat): 3294, 2949, 2911, 2877, 1508, 1223, 1114, 1032, 824, 737 cm^{-1}.

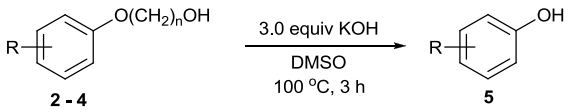


4-(4-chlorophenoxy)butan-1-ol (**4n**) [CAS: 55129-23-2] As the general procedure I, 1-bromo-4-chlorobenzene (191 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 130 ℃using Cs_2CO_3 as base instead of K_2CO_3. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as white solid (124 mg, 62%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.22 (d, *J* = 9.0 Hz, 2H), 6.82 (d, *J* = 9.0 Hz, 2H), 3.97 (t, *J* = 6.0 Hz, 2H), 3.72 (t, *J* = 6.5 Hz, 2H), 1.94-1.82 (m, 2H), 1.81-1.70 (m, 2H), 1.58 (s, 1H);^{13}C NMR (125 MHz, $CDCl_3$) δ 157.5, 132.2, 129.3, 125.5, 116.3, 115.7, 68.0, 62.5,48.2, 29.4, 25.7;HRMS (FAB) *m/z* calcd for $C_{10}H_{13}ClO_2$ $[M+H]^+$: calcd for 201.0682, found: 201.0682. IR (neat): 3351, 2943, 2873, 1491, 1240, 1046, 822, 664,507 cm^{-1}.



4-(3-chlorophenoxy)butan-1-ol (**4o**) [CAS: 1153244-52-0] As the general procedure I, 1-bromo-3-chlorobenzene (191 mg, 1.0 mmol) in a Schlenk test tube was stirred for 20 h at 130 ℃using Cs_2CO_3 as base instead of K_2CO_3. Following aqueous workup, purification of the crude product by column chromatography (25% EtOAc in *n*-hexane) afforded the desired product as white solid (144 mg, 72%). ^{1}H NMR (500 MHz, $CDCl_3$)δ 7.21-7.18 (m, 1H), 6.94-6.89 (m, 2H), 6.83-6.73 (m, 1H), 4.08-3.92 (m, 2H), 3.75-3.71 (m, 2H), 1.90-1.87 (m, 2H), 1.81-1.69 (m, 2H), 1.59 (s, 1H);^{13}C NMR (125 MHz, $CDCl_3$) δ 159.9, 135.1, 130.4, 121.1, 115.1, 113.3, 68.2, 62.7, 29.6, 25.9; HRMS (FAB) *m/z* calcd for $C_{10}H_{13}ClO_2$ $[M+H]^+$: calcd for 201.0682, found: 201.0681. IR (neat): 3335, 2943, 2874, 1593, 1468, 1283, 1245, 1230, 1046, 765, 629,444 cm^{-1}.

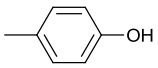
3. Synthesis of phenols using arylalkyl ethers (Scheme 1)



3.1. General experimental procedure (II)

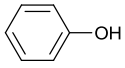
To a solution of aryloxy-aliphatic alcohol (**2, 3, 4**) (1.0 mmol) in a Schlenk flask was added potassium hydroxide (168 mg, 3.0 mmol) and DMSO (3.0 mL). The resulting mixture was stirred at 100 ℃ for 3 h (120 ℃and5 h for **3**).The reaction mixture was then acidified to pH=3 with 1N HCl solution. The aqueous phase was extracted twice with EtOAc and the combined organic layers were washed with H_2O and brine, and dried over $MgSO_4$ and concentrated in vacuo. Purification of the crude product by column chromatography afforded the desired phenolic product (**5**).

3.2. Synthesis and characterization of the products



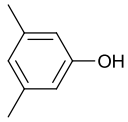
***p*-cresol**[18] (**5a**) [CAS: 106-44-5] from **2a**: As the general procedure II, 2-(*p*-tolyloxy)ethanol(152 mg, 1.0 mmol) in a Schlenk flask was stirred for 3 h at 100 ℃. Following aqueous workup, purification of the crude product by column chromatography (20% EtOAc in *n*-hexane) afforded the desired product as colorless liquid (107 mg, 99%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.03 (t, *J* = 8.0 Hz, 2H), 6.75-6.71 (m, 2H), 4.98 (s, 1H), 2.27 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 153.2, 130.1, 130.0, 115.1, 20.5; MS (EI) *m/z* = 108(100), 77, 51.

***p*-cresol**[18] (**5a**) [CAS: 106-44-5] from **4a**: As the general procedure II, 4-(*p*-tolyloxy)butan-1-ol(180 mg, 1.0 mmol) in a Schlenk flask was stirred for 3 h at 100 ℃. Following aqueous workup, purification of the crude product by column chromatography (20% EtOAc in *n*-hexane) afforded the desired product as colorless liquid (105 mg, 98%).

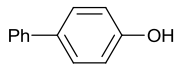


Phenol[19] (**5b**) [CAS: 108-95-2] As the general procedure II, 2-phenoxyethanol (138 mg, 1.0 mmol) in a Schlenk flask was stirred for 3 h at 100 ℃. Following aqueous workup, purification of the crude product by column chromatography (20% EtOAc in *n*-hexane) afforded the desired product as colorless solid (93 mg, 99%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.23-7.20 (m, 2H), 6.93-6.90 (m, 1H), 6.83-6.82 (m, 2H), 5.84 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.1, 129.7, 121.0, 115.4; MS (EI) *m/z* =94.

[18]Yang,K.; Li, Z.; Wang, Z.; Yao, Z.; Jiang, S.*Org. Lett.***2011**, *13*, 4340-4343.

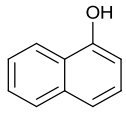


3,5-dimethylphenol[18] (**5e**) [CAS: 108-68-9] As the general procedure II, 2-(3,5-dimetyl phenoxy)ethanol (166 mg, 1.0 mmol) in a Schlenk flask was stirred for 3 h at 100 ℃. Following aqueous workup, purification of the crude product by column chromatography (20% EtOAc in *n*-hexane) afforded the desired product as yellow solid (120 mg, 99%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.58 (s, 1H), 6.46 (s, 2H), 4.76 (s, 1H), 2.26 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.6, 157.3, 94.2, 93.2, 55.4; MS (EI) *m/z* = 122.

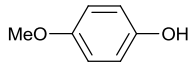


4-biphenol[19] (**5f**) [CAS: 92-69-3] from **2e**: As the general procedure II, 2-(biphenyl-4- yloxy)ethanol (214 mg, 1.0 mmol) in a Schlenk flask was stirred for 3 h at 100 ℃. Following aqueous workup, purification of the crude product by column chromatography (20% EtOAc in *n*-hexane) afforded the desired product as white liquid (168 mg, 99%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55-7.53 (m, 2H), 7.50-7.47 (m, 2H), 7.43-7.40 (m, 2H), 7.32-7.29 (m, 1H), 6.92-6.90 (m, 2H), 4.77 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.0, 140.7, 134.0, 128.7, 128.4, 126.71, 126.70, 115.6; MS (ESI) *m/z* = 170 (100), 141, 115.

4-biphenol[19] (**5f**) [CAS: 92-69-3] from **3e**: As the general procedure II, 3-(biphenyl-4-yloxy)propan-1-ol (228 mg, 1.0 mmol) in a Schlenk flask was stirred for 5 h at 120 ℃. Following aqueous workup, purification of the crude product by column chromatography (20% EtOAc in *n*-hexane) afforded the desired product as white liquid (158 mg, 93%).



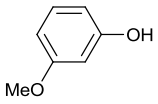
Naphthalen-1-ol[20] (**5g**) [CAS: 90-15-3] As the general procedure II, 2-(naphthalen-1-yloxy)ethanol (188 mg, 1.0 mmol) in a Schlenk flask was stirred for 3 h at 100 ℃. Following aqueous workup, purification of the crude product by column chromatography (20% EtOAc in *n*-hexane) afforded the desired product as white solid (115 mg, 80%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.76 (t, *J* = 8.0 Hz, 2H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.43 (t, *J* = 7.0 Hz, 1H), 7.33 (t, *J* = 7.0 Hz, 1H), 7.15 (s, 1H), 7.10 (dd, *J* = 8.5, 2.5 Hz, 1H), 4.98 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 153.3, 134.6, 129.8, 128.9, 127.8, 126.5, 126.4, 123.6, 117.7, 109.5; MS (EI) *m/z* = 144 (100), 115, 89.



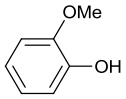
4-methoxyphenol[18] (**5i**) [CAS: 150-76-5] from **2g**: As the general procedure II, 2-(4-methoxylphenoxy) ethanol (168 mg, 1.0 mmol) in a Schlenk flask was stirred for 3 h at 100 ℃. Following aqueous workup, purification of the crude product by column chromatography (20% EtOAc in *n*-hexane) afforded the desired product as

[19]Mann, G.;Incarvito, C.; Rheingold, A. L.;Hartwig, J. F. *J. Am. Chem. Soc.***1999**, *121*, 3224-3225.
[20]Chae, J. H. *Arch. Pharm. Res.* **2008**, *31*, 305-309.

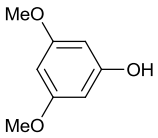
colorless liquid (123 mg, 99%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.80-6.75 (m,4H), 5.53 (s, 1H), 3.76 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.8, 156.8, 130.2, 107.9, 106.4, 101.6, 55.3; MS (EI) *m/z* = 124, 109 (100), 81, 53. 4-methoxyphenol[18] (**5g**) from **4g**: As the general procedure II, 4-(4-methoxyphenoxy)butan-1-ol (196mg, 1.0 mmol) in a Schlenk flask was stirred for 3 h at 100 ℃. Following aqueous workup, purification of the crude product by column chromatography (20% EtOAc in *n*-hexane) afforded the desired product as colorless liquid (121 mg, 98%).



3-methoxyphenol (**5j**)[21] As the general procedure II,2-(3-methoxyphenoxy)ethanol (168mg, 1.0 mmol) in a Schlenk flask was stirred for 3 h at 100 ℃. Following aqueous workup, purification of the crude product by column chromatography (20% EtOAc in *n*-hexane) afforded the desired product as colorless liquid (114 mg, 92%). ^{1}H NMR (500 MHz, $CDCl_3$) δ7.14-7.11 (m, 1H), 6.50-6.48 (m, 1H), 6.45-6.42 (m, 2H), 3.77 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ160.8, 156.7, 130.2, 107.9, 106.4, 101.6, 55.3; MS (EI) *m/z* = 124 (100), 94, 81, 66, 53.



2-methoxyphenol[22] (**5k**) [CAS: 90-05-1] As the general procedure II, 2-(2-methylphenoxy) ethanol (168mg, 1.0 mmol) in a Schlenk flask was stirred for 3 h at 100 ℃. Following aqueous workup, purification of the crude product by column chromatography (20% EtOAc in *n*-hexane) afforded the desired product as yellow solid (109 mg, 88%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.92 (m, 1H), 6.87-6.85 (m, 3H), 5.62 (s, 1H), 3.89 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 146.5, 145.6, 121.4, 120.1, 114.5, 110.6, 55.8; MS (EI) *m/z* = 124.

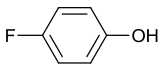


3,5-dimethoxyphenol[22] (**5l**) [CAS: 500-99-2] from **2j**: As the general procedure II, 2-(3,5-dimethoxyphenoxy)ethanol(198 mg, 1.0 mmol) in a Schlenk flask was stirred for 5 hat 120 ℃. Following aqueous workup, purification of the crude product by column chromatography (20% EtOAc in *n*-hexane) afforded the desired product as orange liquid (140 mg, 90%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.08 (s, 1H), 6.03 (t, *J* = 2.0 Hz, 2H), 5.29 (s, 1H), 3.75 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.6, 157.3, 94.3, 93.2, 55.3; MS (ESI) *m/z* = 153.1 (M^-).

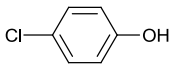
3,5-dimethoxyphenol[22] (**5l**) [CAS: 500-99-2] from **3j**: As the general procedure II, 3-(3,5-dimethoxyphenoxy)propan-1-ol (212 mg, 1.0 mmol) in a Schlenk flask was stirred for 5 hat 120 ℃. Following

[21]Thakur, K. G.; Sekar, G. *Chem. Commun.*, **2011**, *47*, 6692-6694.
[22]Jing, L.; Wei, J.; Zhou, L.; Huang, Z.; Li, Z.; Zhou, X.*Chem.Commun.***2010**, *46*, 4767-4769.

aqueous workup, purification of the crude product by column chromatography (20% EtOAc in *n*-hexane) afforded the desired product as orange liquid (141 mg, 91%).

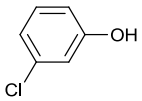


4-fluorophenol[18] (**5m**) [CAS: 371-41-5] As the general procedure II, 2-(4-fluorophenoxy) ethanol (156 mg, 1.0 mmol) in a Schlenk flask was stirred for 3 h at 100 ℃. Following aqueous workup, purification of the crude product by column chromatography (20% EtOAc in *n*-hexane) afforded the desired product as brown liquid (109 mg, 98%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.94-6.91 (m, 2H), 6.78-6.76 (m, 2H), 4.85 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.2 (d, *J* = 236.25 Hz, C-F), 151.5 (d, *J* = 2.25 Hz, C-F), 116.1 (d, *J* = 7.88 Hz, C-F), 116.0 (d, *J* = 23.25 Hz, C-F); MS (EI) *m/z* = 112.

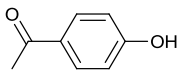


4-chlorophenol[18] (**5n**) [CAS: 106-48-9] As the general procedure II, 2-(4-chlorophenoxy) ethanol (172 mg, 1.0 mmol,) in a Schlenk flask was stirred for 3 h at 100 ℃. Following aqueous workup, purification of the crude product by column chromatography (20% EtOAc in *n*-hexane) afforded the desired product as colorless liquid (127 mg, 99%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.18 (d, *J* = 8.5 Hz, 2H), 6.76 (d, *J* = 8.5 Hz, 2H), 5.37 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 154.1, 129.8, 126.1, 117.0; MS (ESI) *m/z* = 130, 128 (100), 65.

4-chlorophenol[18] (**5n**) [CAS: 106-48-9] As the general procedure II, 3-(4-chlorophenoxy) propan-1-ol (186mg, 1.0 mmol,) in a Schlenk flask was stirred for 5 h at 120 ℃. Following aqueous workup, purification of the crude product by column chromatography (20% EtOAc in *n*-hexane) afforded the desired product as colorless liquid (122 mg, 95%).

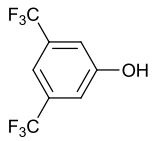


3-chlorophenol[18] (**5o**) [CAS: 108-43-0] As the general procedure II, 4-(3-chlorophenoxy)butan-1-ol (200 mg, 1.0 mmol) in a Schlenk flask was stirred for 3 h at 100 ℃. Following aqueous workup, purification of the crude product by column chromatography (20% EtOAc in *n*-hexane) afforded the desired product as colorless liquid (127 mg, 99%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.18-7.14 (m, 1H), 6.94-6.91 (m, 1H),6.87-6.85 (m, 1H),6.73-6.71 (m, 1H),5.05 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.2, 134.9, 130.5, 121.1, 115.9, 113.7; MS (ESI) *m/z* = 130 (M^+), 128 (M^+, 100), 100, 65.

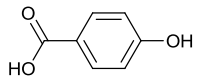


1-(4-hydroxyphenyl)ethanone[19] (**5p**) [CAS: 99-93-4] As the general procedure II, 1-(4-(2-hydroxyethoxy) phenyl)ethanone (0.18 mg, 1.0 mmol) in a Schlenk flask was stirred for 3 h at 100 ℃. Following aqueous workup, purification of the crude product by column chromatography (20% EtOAc in *n*-hexane) afforded the desired product as white solid (134 mg, 99%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.93-7.91 (m,2H), 6.93-6.91 (m,

2H), 6.45 (s, 1H), 2.58 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 198.2, 161.0, 131.2, 129.8, 115.5, 26.4.; MS (EI) *m/z* = 136, 121 (100), 93, 65.

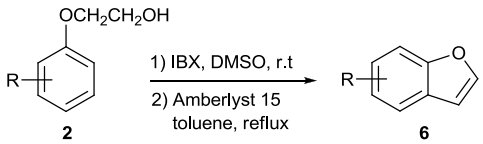


3,5-bis(trifluoromethyl)phenol [23] (**5s**) [CAS: 349-58-6] As the general procedure II, 2-(3,5-bis (trifluoromethyl)phenoxy)ethanol (274 mg, 1.0 mmol) in a Schlenk flask was stirred for 3 h at 100 ℃. Following aqueous workup, purification of the crude product by column chromatography (20% EtOAc in *n*-hexane) afforded the desired product as brown liquid (218 mg, 95%). ^{1}H NMR (500 MHz, DMSO) δ 10.93 (s, 1H), 7.45 (s, 1H), 7.36 (m, 2H); ^{13}C NMR (125 MHz, DMSO) δ 156.4, 133.0 (q, *J* = 8.38 Hz, C-F), 123.6 (d, *J* = 3.0 Hz, C-F), 122.6 (q, *J* = 271.38 Hz, C-F), 121.4 (quintet, *J* = 3.5 Hz, C-F); MS (EI) *m/z* = 230.



4-hydroxybenzoic acid[18] (**5v**) [CAS: 99-96-7] As the general procedure II, 4-(2-hydroxyethoxy)benzoic acid (182 mg, 1.0 mmol) in a Schlenk flask was stirred for 3 h at 100 ℃. Following aqueous workup, purification of the crude product by column chromatography (10% methanol in CH_2Cl_2) afforded the desired product as white solid (124 mg, 90%). ^{1}H NMR (500 MHz, DMSO) δ 12.42 (s, 1H), 10.22 (s, 1H), 7.78 (t, *J* = 5.0 Hz, 2H), 6.82 (d, *J* = 5.0 Hz, 2H); ^{13}C NMR (125 MHz, DMSO) δ 167.8, 162.3, 132.2, 122.1, 115.8.

4. Synthesis of benzofurans using arylalkyl ethers (Scheme 2)

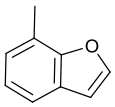


4.1 General experimental procedure (III)

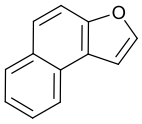
To a solution of aryloxyethanol (**2**) (2 mmol) in DMSO, was added IBX (846 mg, 3 mmol). Then the mixture was stirred at room temperature for 12 h. 20 mL of water was added and filtered. The filtrate was extracted with ethyl acetate and the organic layer was washed with brine, dried with anhydrous Na_2SO_4 and then condensed. The crude product was directly used for the next step. It was dissolved in toluene (10 mL) and Amberlyst (0.4g) was added. Then the mixture was stirred at 50 ^{o}C for 2 h. After filtration, toluene was removed in vacuum and the resulting crude product was purified by column chromatography (10% EtOAc in *n*-hexane) to afford the desired product (**6**).

4.2. Synthesis and characterization of the products

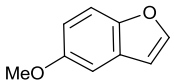
[23]Zhao, D.; Wu,N.; Zhang,S.; Xi, P.; Su, X.; Lan, J.; You, J.*Angew. Chem. Int. Ed.***2009**, *48*, 8729-8732.



7-methylbenzofuran[24] (6c) [CAS: 17059-52-8] As the general procedure (III), 2-(*o*-tolyloxy)ethanol (304 mg, 2 mmol) was used as substrate. After reaction, purification by column chromatography (10% EtOAc in *n*-hexane) afforded colorless liquid (161 mg, 68%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 (d, *J* = 2.0 Hz, 1H), 7.49-7.35 (m, 1H), 7.17-7.05 (m, 2H), 6.79-6.66 (m, 1H), 2.53 (s, 3H); ^{13}C NMR (125 MHz,$CDCl_3$) δ 154.0, 144.6, 126.8, 125.0, 122.7, 121.6, 118.6, 106.8, 15.1.

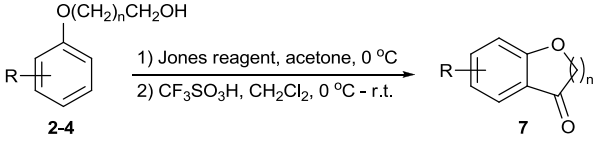


naphtho[2,1-b]furan[25] (6h) [CAS: 232-95-1] As the general procedure (III), 2-(naphthalen-2-yloxy)ethanol (376 mg, 2 mmol) was used as substrate. After reaction, purification by column chromatography (10% EtOAc in *n*-hexane) afforded white solid (211 mg, 63%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.0 Hz, 1H), 7.94 (d, *J* = 8.0 Hz, 1H), 7.75 (d, *J* = 2.0 Hz, 1H), 7.73-6.66 (m, 2H), 7.60-7.56 (m, 1H), 7.50-7.46 (m, 1H), 7.26-7.23 (m,1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.8, 144.4, 130.6, 129.0, 128.1, 126.5, 125.4, 124.7, 123.7, 122.9, 112.8, 105.8.



5-methoxybenzofuran[26] (6i) [CAS: 13391-28-1] As the general procedure (III), 2-(4-methoxyphenoxy)ethanol (336 mg, 2 mmol) was used as substrate. After reaction, purification by column chromatography (10% EtOAc in *n*-hexane) afforded yellow liquid (223 mg, 75%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 (s, 1H), 7.39 (d, *J* = 8.5 Hz, 1H), 7.05 (s, 1H), 6.98-6.84 (m, 1H), 6.71 (s, 1H), 3.85 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.9, 149.9, 145.7, 127.9, 113.1, 111.8, 106.7, 103.5, 55.9.

5. Synthesis of benzo-fused cyclic ethers using arylalkyl ethers (Scheme 3)



5.1. General experimental procedure (IV)

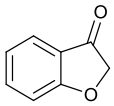
To a solution of aryloxy-aliphatic alcohol (**2, 3, 4**) (2.0 mmol) in a flask, was added Jones reagent (2 mL, 8.0 mmol) and acetone (10.0 mL) under ice bath. After stirring for 1 h at the same temperature, the reaction was quenched with water, and then extracted twice with EtOAc and the combined organic layer was washed with

[24]Barker, P.; Finke, P.; Thompson, K. *Synth.Commun.* **1989,***19*, 257-265.

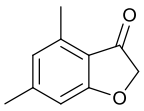
[25]Antelo, B.; Castedo, L.; Delamano, J.; Gómez, A.; López, C.; Tojo, G. *J. Org. Chem.* **1996,***61*, 1188-1189.
[26]Hu, Y.; Kamitanaka, T.; Mishima, Y.; Dohi, T.; Kita, Y. *J. Org. Chem.***2013,***78*, 5530-5543.

H_2O and brine, dried over anhydrous $MgSO_4$ and concentrated in vacuo. Purification of the crude product by recrystallization afforded the intermediate compounds.The intermediate compound was further dissolved in the dry CH_2Cl_2 (3 mL), and triflic acid (1.0 mL) was added by injection in small portions under ice bath. Then the reaction mixture was stirred at room temperature overnight. The reaction was quenched with ice water, then extracted twice with CH_2Cl_2 and the combined organic layer was washed with H_2O and saturated Na_2CO_3 solution, dried over anhydrous $MgSO_4$ and concentrated in vacuo. Purification of the crude product by column chromatography afforded the desired benzo-fused cyclic ethers (**7**).

5.2. Synthesis and characterization of the products

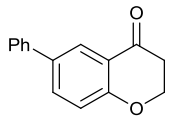


benzofuran-3(2H)-one[27] (**7b**) [CAS: 7169-34-8] As the general procedure IV, 2-phenoxyethanol (276 mg, 2.0 mmol) in a flask was stirred for 1 h under ice bath. Following aqueous workup, purification of the crude product by recrystallization afforded the intermediate product (2-phenoxyacetic acid[CAS: 122-59-8]: ^{1}H NMR (500 MHz, DMSO) δ 7.33-7.27 (m, 2H), 6.97-6.89 (m, 3H), 4.66 (s, 2H); ^{13}C NMR (125 MHz, DMSO) δ 171.0, 158.4, 130.2, 121.7, 115.1, 65.1) as white solid (228 mg, 75%). Then 2-phenoxyacetic acid (152 mg, 1.0 mmol) in a Schlenk test tube was stirred overnight at room temperature after adding triflic acid (1.0 mL) under ice bath. Following aqueous workup, purification of the crude product by column chromatography (10% EtOAc in *n*-hexane) afforded the desired product (**7c**) as light yellow liquid (111 mg, 83%). ^{1}HNMR (500 MHz,$CDCl_3$)δ 7.69-7.67 (m, 1H), 7.62 (t, *J* =10.0 Hz,1H),7.15 (d, *J* =10.0 Hz,1H), 7.11 (d, *J* =10.0 Hz,1H),4.63 (s,2H); ^{13}CNMR (125MHz,$CDCl_3$) δ 198.9, 173.0, 136.9, 123.0, 121.0, 120.1, 112.6, 73.7.

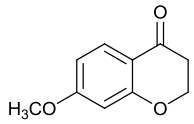


4,6-dimethylbenzofuran-3(2H)-one[28] (**7d**) [CAS: 20895-44-7] As the general procedure IV, 2-(3,5-dimetyl phenoxy)ethanol (332 mg, 2.0 mmol) in a flask was stirred for 1 h under ice bath. Following aqueous workup, purification of the crude product by recrystallization afforded the intermediate product (2-(3,5-dimethylphenoxy)acetic acid[CAS: 5406-14-4]: ^{1}H NMR (500 MHz, DMSO) δ 6.67 (s, 1H), 6.55 (s, 2H), 4.65 (s, 2H), 2.29 (s, 6H).^{13}C NMR (125 MHz, DMSO) δ 171.0, 155.9, 131.0, 129.4, 124.7, 69.4, 16.6;) as white solid (317 mg, 88%). Then the intermediate product(180 mg, 1.0 mmol) in a Schlenk test tube was stirred overnight at room temperature after adding triflic acid (1.0 mL) under ice bath. Following aqueous workup, purification of the crude product by column chromatography (10% EtOAc in *n*-hexane) afforded the desired product (**7d**) as white solid (130 mg, 91%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.73 (s, 1H), 6.65 (s, 1H), 4.57 (s, 2H), 2.55 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 200.0, 175.0, 149.3, 139.0, 124.8, 117.0, 110.8, 74.9, 22.4, 17.7. MS (EI) *m/z* = 162 (100), 133, 105, 77.

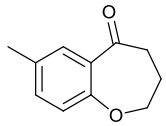
[27]Lockner, J. W.; Dixon, D. D.;Risgaard, R.;Baran, P. S. *Org. Lett.*,**2011**, *13*, 5628-5631.
[28]Sebej, P.; Lim, B. H.; Park, B. S.; Givens, R. S.; Klan, P. *Org. Lett.*, **2011**, *13*, 644-647.



6-phenylchroman-4-one (**7f**) [CAS: 73316-17-3] As the general procedure IV, 3-([1,1'-biphenyl]-4-yloxy)propan-1-ol (556 mg, 2.0 mmol) in a flask was stirred for 1 h under ice bath. Following aqueous workup, purification of the crude product by recrystallization afforded the intermediate compound (3-([1,1'-biphenyl]-4-yloxy)propanoic acid[CAS: 63472-21-9]: ^{1}H NMR (500 MHz, DMSO) δ 12.40 (s, 1H), 7.60 (dd, *J* = 11.0 Hz, 5.0 Hz, 4H), 7.45-7.42 (m, 2H), 7.32 (dd, *J* = 11.0, 4.0 Hz, 1H), 7.05-7.02 (m, 2H), 4.29-4.11 (m, 2H), 2.71-2.67 (m, 2H); ^{13}C NMR (125 MHz, DMSO) δ 172.9, 158.7, 140.5, 133.4, 129.6, 128.5, 127.4, 126.9, 115.6, 64.4, 34.8) as white solid (440 mg, 91%). Then the intermediate compounds(242 mg, 1.0 mmol) in a Schlenk test tube was stirred overnight at room temperature after adding triflic acid (1.0 mL) under ice bath. Following aqueous workup, purification of the crude product by column chromatography (10% EtOAc in *n*-hexane) afforded the desired product (**7f**) as white solid (210 mg, 94%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (d, *J* = 2.5 Hz, 1H), 7.74 (dd, *J* = 8.5, 2.5 Hz, 1H), 7.58 (d, *J* = 7.5 Hz, 2H), 7.46- 7.42 (m, 2H), 7.35-7.33 (m, 1H), 7.06 (d, *J* = 8.5 Hz, 1H), 4.58 (t, *J* = 8.5 Hz, 2H), 2.86 (t, *J* = 8.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.0, 161.5, 139.8, 134.9, 134.8, 129.1, 127.6, 127.0, 125.4, 121.6, 118.6, 67.3, 38.1.HRMS (FAB) *m/z* calcd for $C_{15}H_{12}O_2$ $[M+H]^+$: calcd for 225.0916, found: 225.0916; IR (neat): 2876, 1683, 1611, 1476, 1454, 1402, 1295, 1247, 1219, 1172, 1030, 832, 762, 691, 557, 528 cm^{-1}.

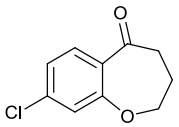


7-methoxychroman-4-one [29] (**7j**) [CAS: 863309-86-8] As the general procedure IV, 3-(2-methoxyphenoxy)propan-1-ol (364 mg, 2.0 mmol) in a flask was stirred for 1 h under ice bath. Following aqueous workup, purification of the crude product by recrystallization afforded the intermediate compound (3-(3-methoxyphenoxy)propanoic acid[CAS: 49855-03-0]: ^{1}H NMR (500 MHz, DMSO) δ 12.40 (s, 1H), 7.17 (t, J = 8.0 Hz, 1H), 6.52-6.46 (m, 3H), 4.13 (t, *J* = 8.0 Hz, 2H), 3.72 (s, 3H), 2.67 (t, *J* = 8.0 Hz, 2H); ^{13}C NMR (125 MHz, DMSO) δ 173.0, 161.2, 160.3, 130.7, 107.2, 107.1, 101.3, 64.2, 55.8, 34.8) as brown solid (314 mg, 80%). Then the intermediate compound (196mg, 1.0 mmol) in a Schlenk test tube was stirred overnight at room temperature after addingtriflic acid (1.0 mL) under ice bath. Following aqueous workup, purification of the crude product by column chromatography (10% EtOAc in *n*-hexane) afforded the desired product (**7j**) as white solid (160 mg, 90%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (d, *J* = 8.0 Hz, 1H), 6.58 (d, *J* = 8.0 Hz, 1H), 6.41 (s, 1H), 4.52 (t, *J* = 5.0 Hz, 2H), 3.84 (s, 3H), 2.76 (t, *J* = 5.0 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 190.5, 166.0, 163.8, 128.9, 115.3, 109.9, 100.7, 67.4, 55.6, 37.4.



[29]Siddaiah,V.; Rao,C. V.;Venkateswarlu,S.; Krishnaraju, A. V.;Subbaraju, G. V.*Bioorg. Med. Chem*. **2006**, *14*, 2545-2551.

7-methyl-3,4-dihydrobenzo[b]oxepin-5(2H)-one[30] (**7a**) [CAS: 41177-66-6] As the general procedure IV, 4-(p-tolyloxy)butan-1-ol (360 mg, 2.0 mmol) in a flask was stirred for 1 h under ice bath. Following aqueous workup, purification of the crude product by recrystallization afforded the intermediate compound (4-(p-tolyloxy)butanoic acid[CAS: 22180-02-5]: ^{1}H NMR (500 MHz, DMSO) δ 12.17 (s, 1H), 7.07 (d, *J* = 8.0 Hz, 2H), 6.80 (d, *J* = 8.0 Hz, 1H), 3.92 (t, *J* = 6.5 Hz, 2H), 2.39-2.35 (m, 2H), 2.22 (s, 3H), 1.95-1.85 (m, 2H); ^{13}C NMR (125 MHz, DMSO) δ 174.8, 157.1, 130.5, 129.8, 114.9, 67.1, 30.8, 25.0, 20.8) white solid (369 mg, 95%). Then the intermediate compound (194 mg, 1.0 mmol) in a Schlenk test tube was stirred overnight at room temperature after adding triflic acid (1.0 mL) under ice bath. Following aqueous workup, purification of the crude product by column chromatography (10% EtOAc in *n*-hexane) afforded the desired product (**7a**) as white solid (162 mg, 92%). ^{1}H NMR (500 MHz, DMSO) δ 7.44-7.43 (m, 1H), 7.33-7.31 (m, 1H), 7.01 (dd, *J* = 8.0, 2.0 Hz, 1H), 4.17-4.14 (m, 2H), 2.78-2.75 (m, 2H), 2.28 (s, 3H), 2.10-2.08 (m, 2H); ^{13}C NMR (125 MHz, DMSO) δ 200.9, 159.8, 135.3, 132.5, 129.5, 129.4, 121.5, 73.0, 41.0, 26.0, 20.7.



8-chloro-3,4-dihydrobenzo[b]oxepin-5(2H)-one (**7o**) [CAS: 37483-57-1] As the general procedure IV, 4-(3-chlorophenoxy)butan-1-ol (400 mg, 2.0 mmol) in a flask was stirred for 1 h under ice bath. Following aqueous workup, purification of the crude product by recrystallization afforded the intermediate compound (4-(3-chlorophenoxy)butanoic acid [CAS: 5057-51-2]: ^{1}H NMR (500 MHz, DMSO) δ 12.16 (s, 1H), 7.32-7.28 (m, 1H), 7.02-6.97 (m, 2H), 6.92-6.90 (m, 1H), 4.01-4.00 (m, 2H), 2.38 (t, *J* = 6.0 Hz, 2H), 1.94-1.93 (m, 2H).^{13}C NMR (125 MHz, DMSO) δ 174.7, 160.2, 134.4, 131.6, 121.2, 115.2, 114.2, 67.7, 30.7, 24.8) as white solid (360 mg, 84%). Then the intermediate compound (214mg, 1.0 mmol) in a Schlenk test tube was stirred overnight at room temperature after adding triflic acid (1.0 mL) under ice bath. Following aqueous workup, purification of the crude product by column chromatography (10% EtOAc in *n*-hexane) afforded the desired product (**7o**) as white solid (182mg, 93%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.0 Hz, 1H), 7.10-7.05 (m, 2H), 4.27-4.24 (m, 2H), 2.90-2.88 (m, 2H), 2.24-2.21 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 199.7, 162.8, 139.6, 130.9, 127.8, 123.5, 121.3, 73.5, 40.8, 26.4. HRMS (FAB) *m/z* calcd for $C_{10}H_9ClO_2$ $[M+H]^+$: calcd for 197.0369, found: 197.0369; IR (neat): 2969, 1680, 1590, 1558, 1414, 1372, 1268, 1198, 1086, 1050, 985, 819, 767, 592, 515 cm^{-1}.

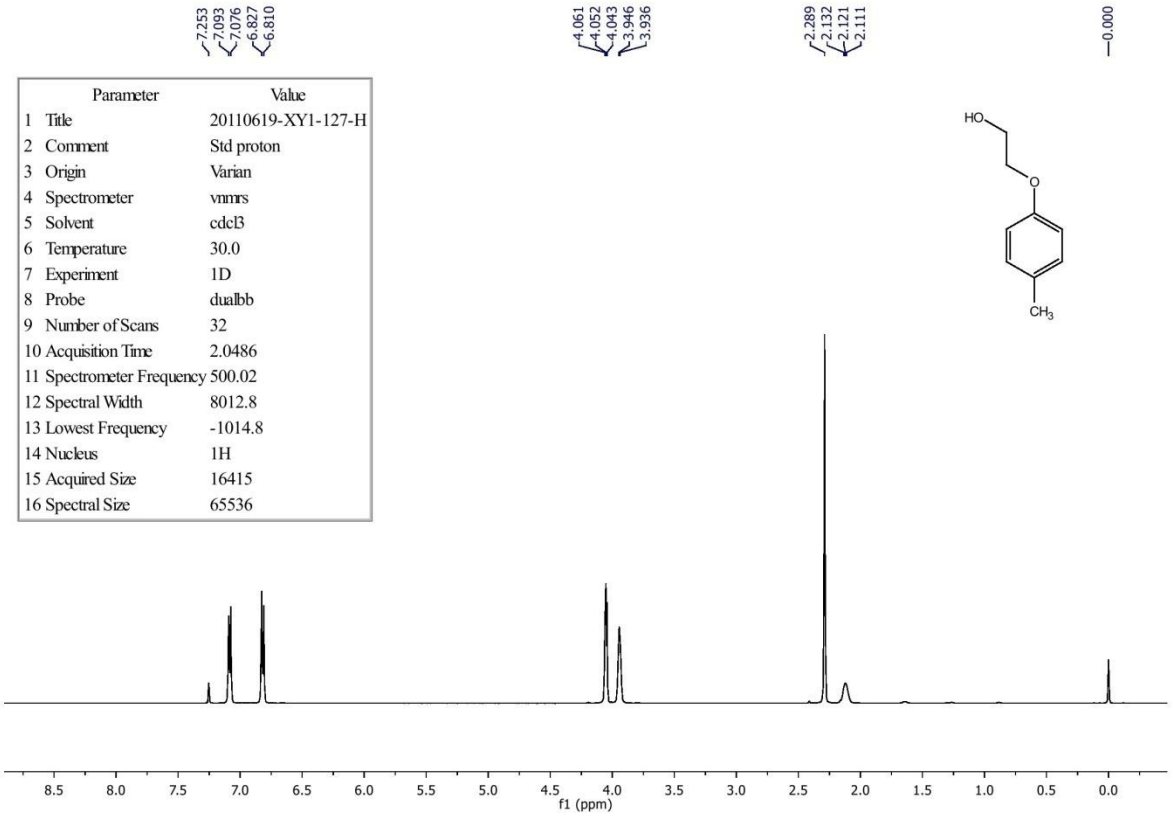
6. Synthesis of phenol in 0.1 mol scale

Bromodobenzene (**1b**, 15.7 g, 0.1 mol), $CuCl_2$ (0.67 g, 5 mmol) and K_2CO_3 (41 g, 0.3 mol) were stirred in 56 mL of ethylene glycol (1.0 mol, ~2 M) under Ar atmosphere at 130 ^oC for 20 h. The reaction mixture was diluted with 100 mL of water after cooling to room temperature, acidified with concentrated HCl to pH=3 under ice bath, and then extracted with ethyl acetate (200 mL x 2). The combined organic layer was washed with water for twice and brine, dried over anhydrous magnesium sulphate and concentrated in vacuum to give a pale yellow liquid **2b** (13.7 g, 0. 099 mol, crude yield 99%). The concentrated crude coupled product was directly used for

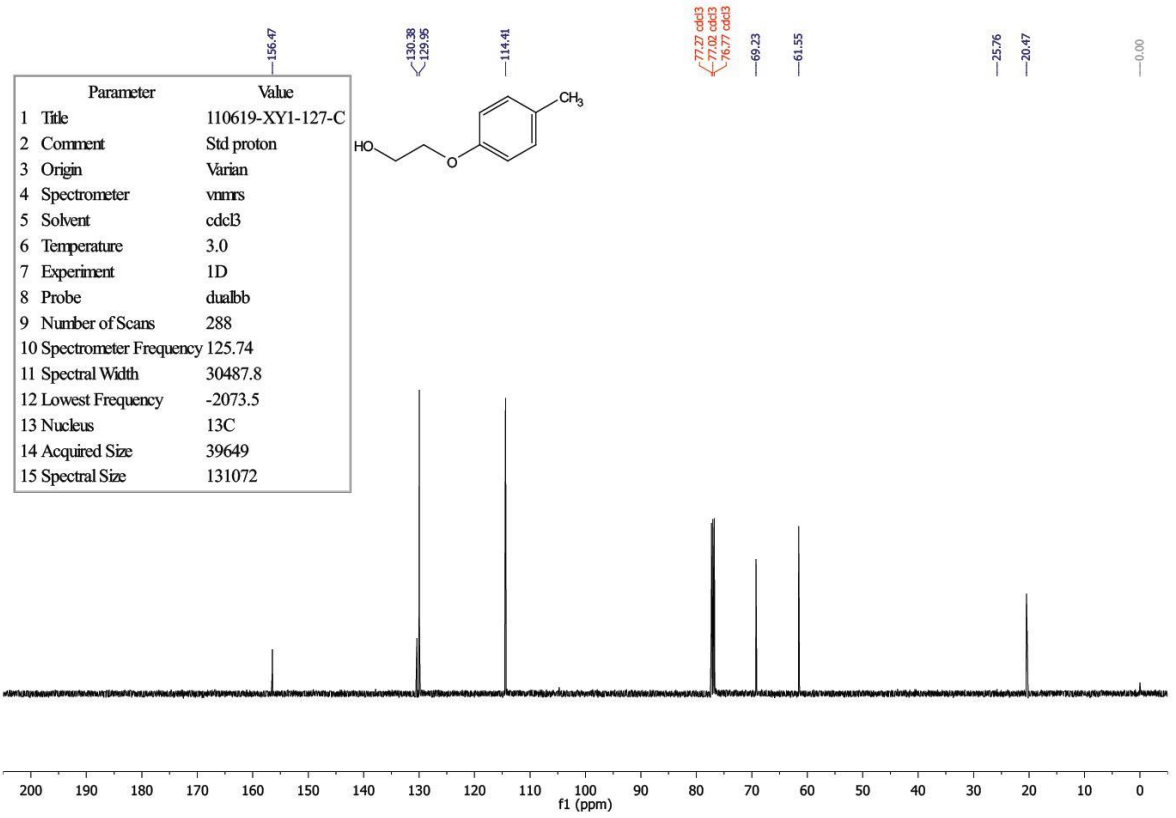
[30]Nikitin, K. V.; Andryukhova, N. P. *Can. J. Chem.*, **2004**, *82*, 571-578.

the next reaction and well cleaved at 100 ^{o}C after 5 h in the presence of KOH (16.8 g, 0.3 mol) in 200 mL of DMSO under N_2 atmosphere. The reaction mixture was cooled to room temperature, diluted with 200 mL of water, acidified with concentrated HCl under ice bath to pH=3, and then extracted with ether (200 mL x 4). The combined organic layer was washed with water for twice and brine, dried over anhydrous magnesium sulphate and concentrated in vacuum to afford the crude phenol, which was further purified by distillation under reduced pressure to give phenol **5b** (8.75 g, 0.093 mol, yield 93% over 2 steps) as colorless liquid.

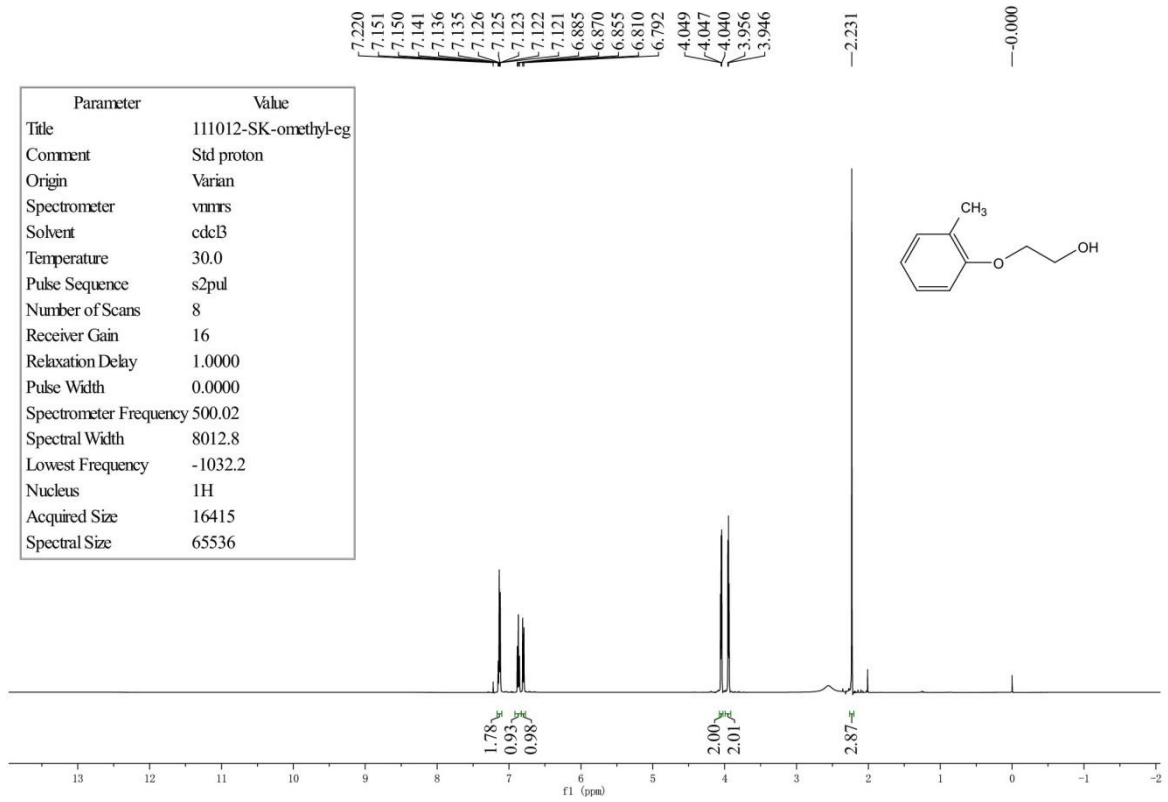
7. Copies of ^{1}H and ^{13}C NMR spectra



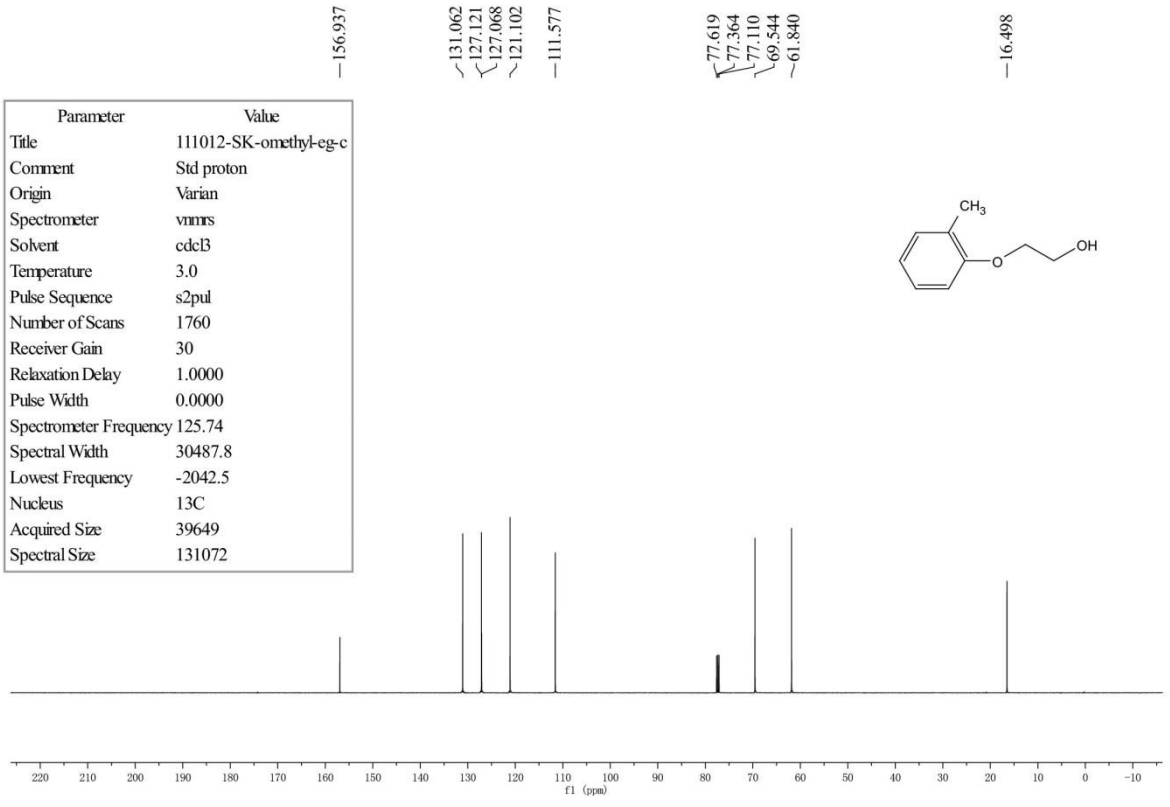
Parameter	Value
1 Title	20110619-XY1-127-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	32
10 Acquisition Time	2.0486
11 Spectrometer Frequency	500.02
12 Spectral Width	8012.8
13 Lowest Frequency	-1014.8
14 Nucleus	1H
15 Acquired Size	16415
16 Spectral Size	65536



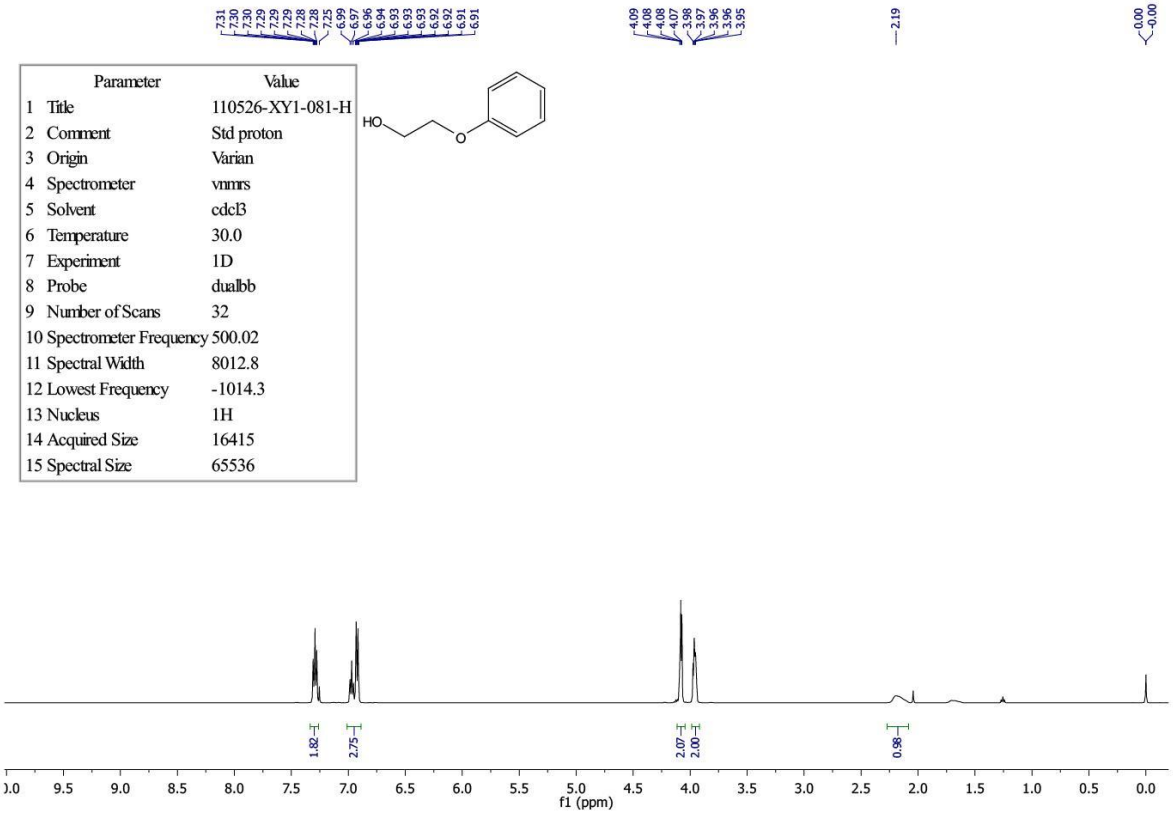
Parameter	Value
1 Title	110619-XY1-127-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	288
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2073.5
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072



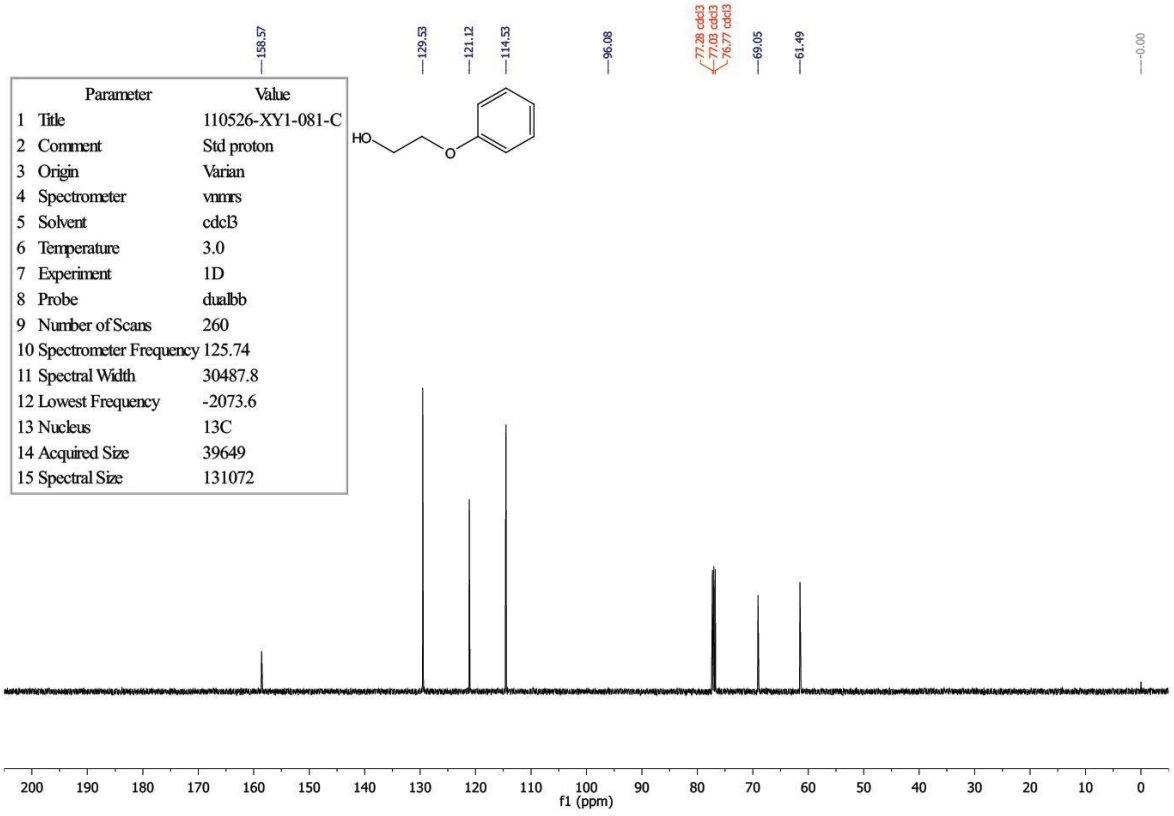
Parameter	Value
Title	111012-SK-omethyl-eg
Comment	Std proton
Origin	Varian
Spectrometer	vnmrs
Solvent	cdcl3
Temperature	30.0
Pulse Sequence	s2pul
Number of Scans	8
Receiver Gain	16
Relaxation Delay	1.0000
Pulse Width	0.0000
Spectrometer Frequency	500.02
Spectral Width	8012.8
Lowest Frequency	-1032.2
Nucleus	1H
Acquired Size	16415
Spectral Size	65536



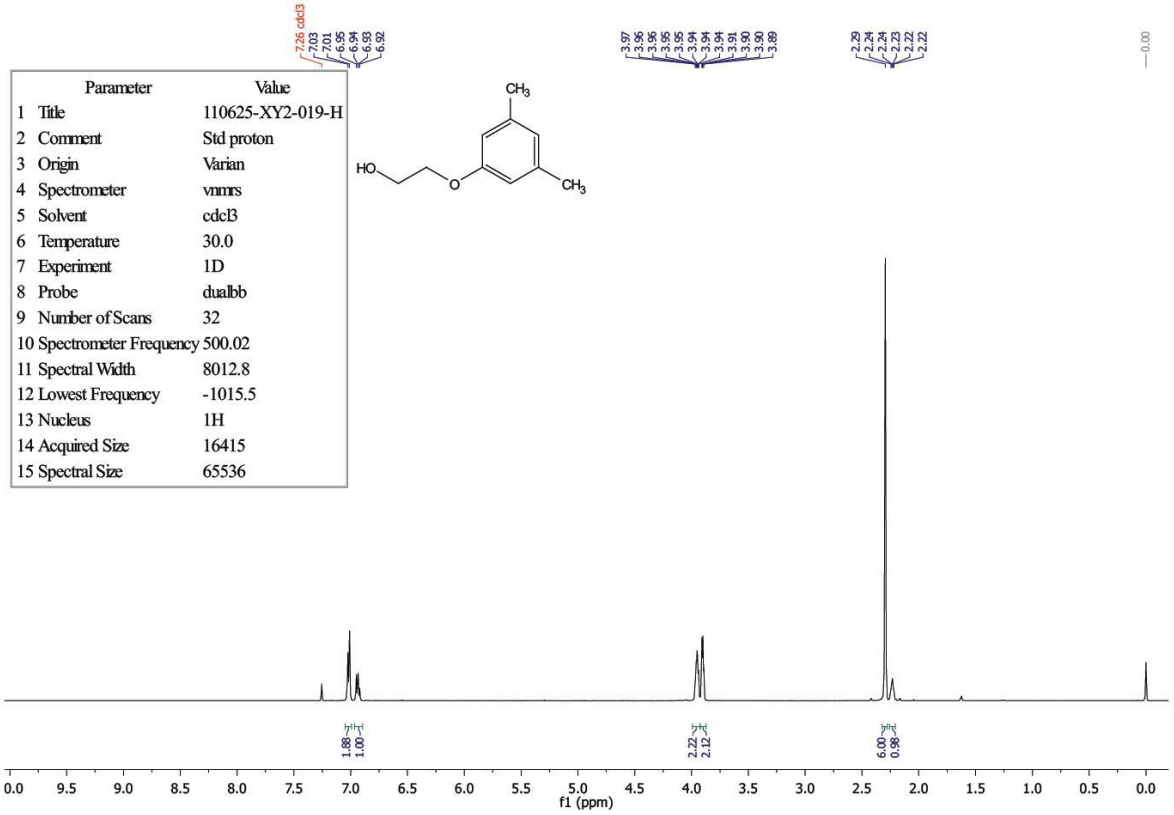
Parameter	Value
Title	111012-SK-omethyl-eg-c
Comment	Std proton
Origin	Varian
Spectrometer	vnmrs
Solvent	cdcl3
Temperature	3.0
Pulse Sequence	s2pul
Number of Scans	1760
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	0.0000
Spectrometer Frequency	125.74
Spectral Width	30487.8
Lowest Frequency	-2042.5
Nucleus	13C
Acquired Size	39649
Spectral Size	131072



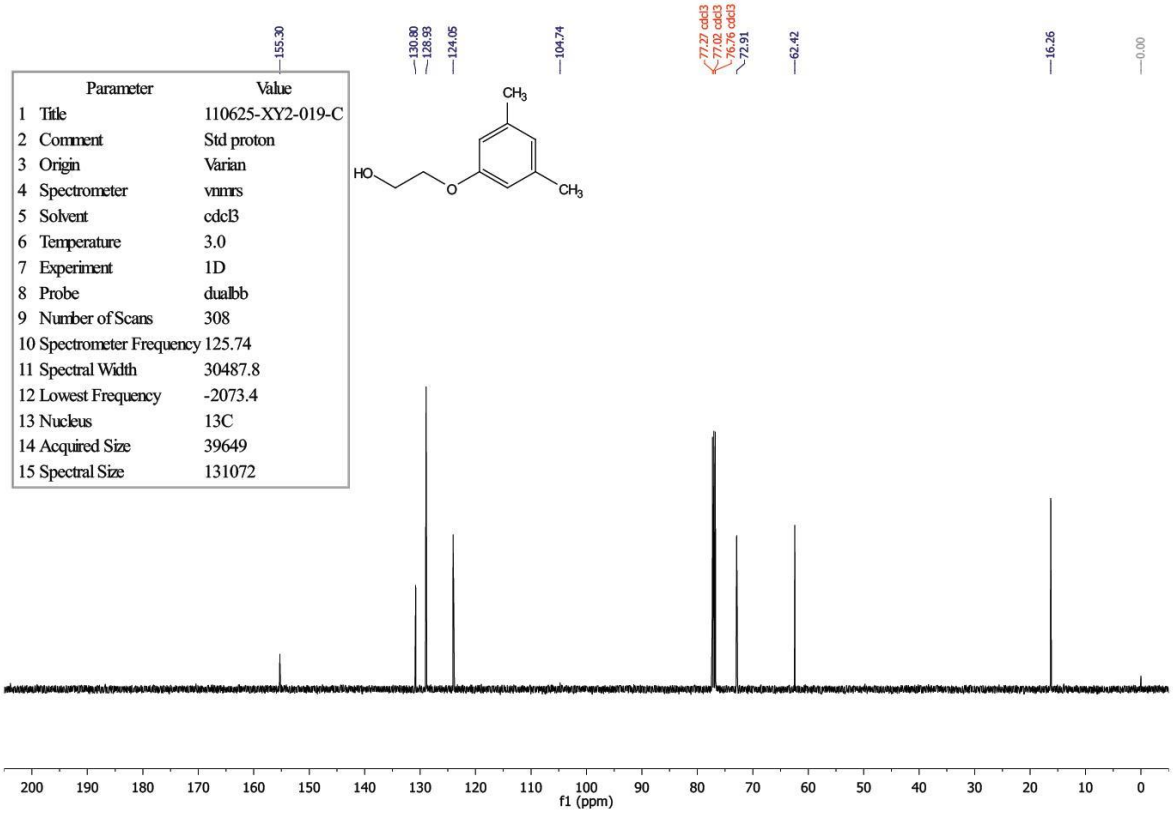
Parameter	Value
1 Title	110526-XY1-081-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	32
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1014.3
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



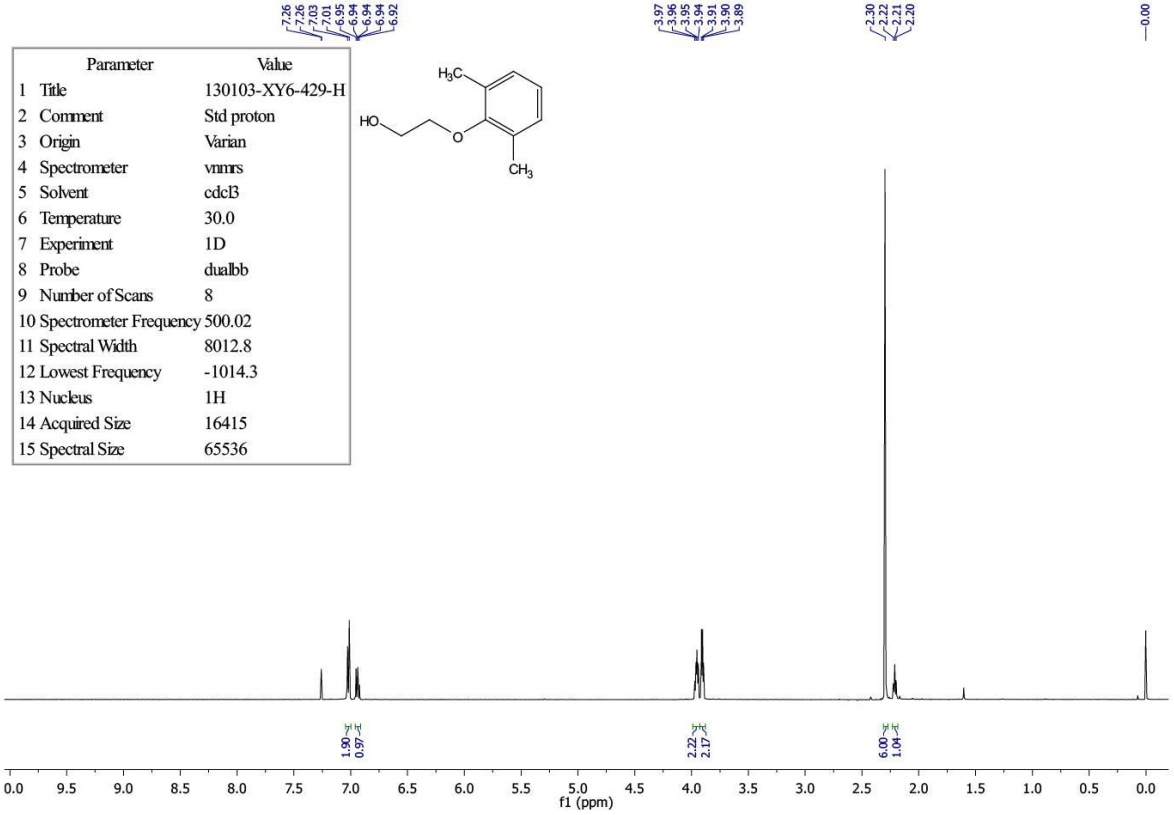
Parameter	Value
1 Title	110526-XY1-081-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	260
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2073.6
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072



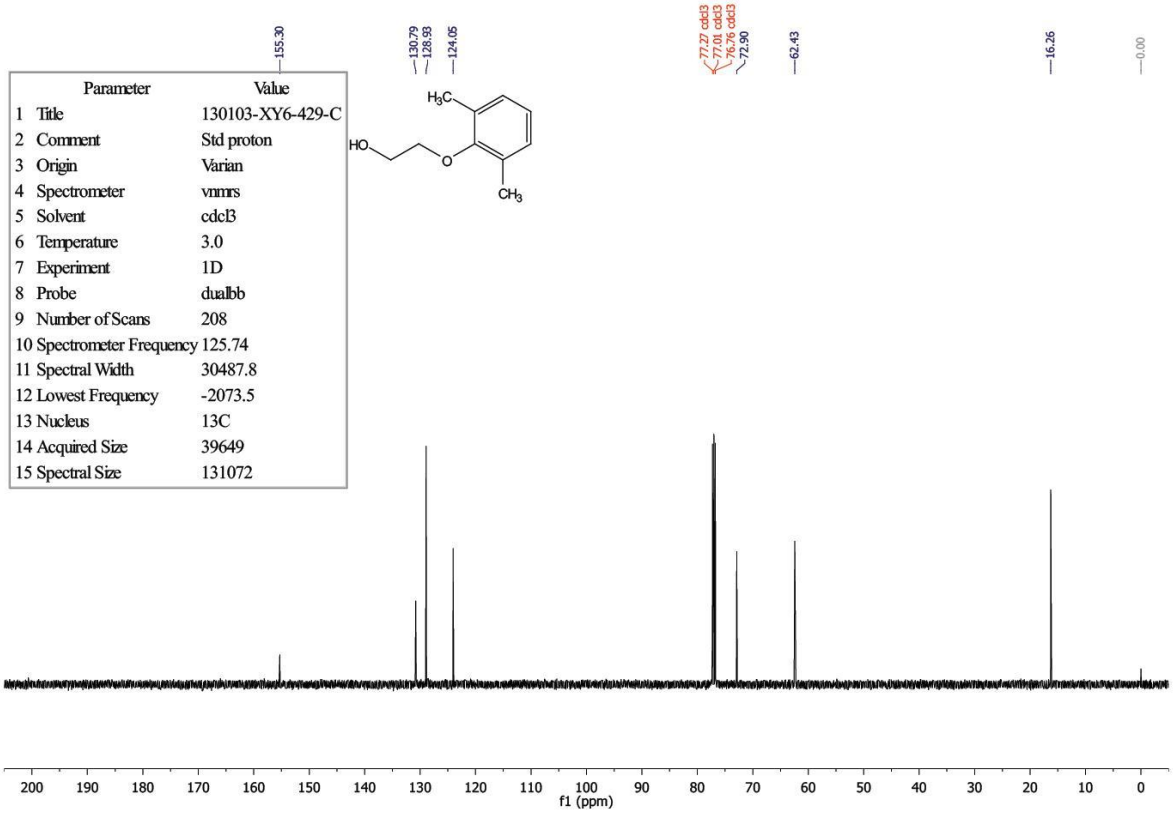
Parameter	Value
1 Title	110625-XY2-019-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	32
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1015.5
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



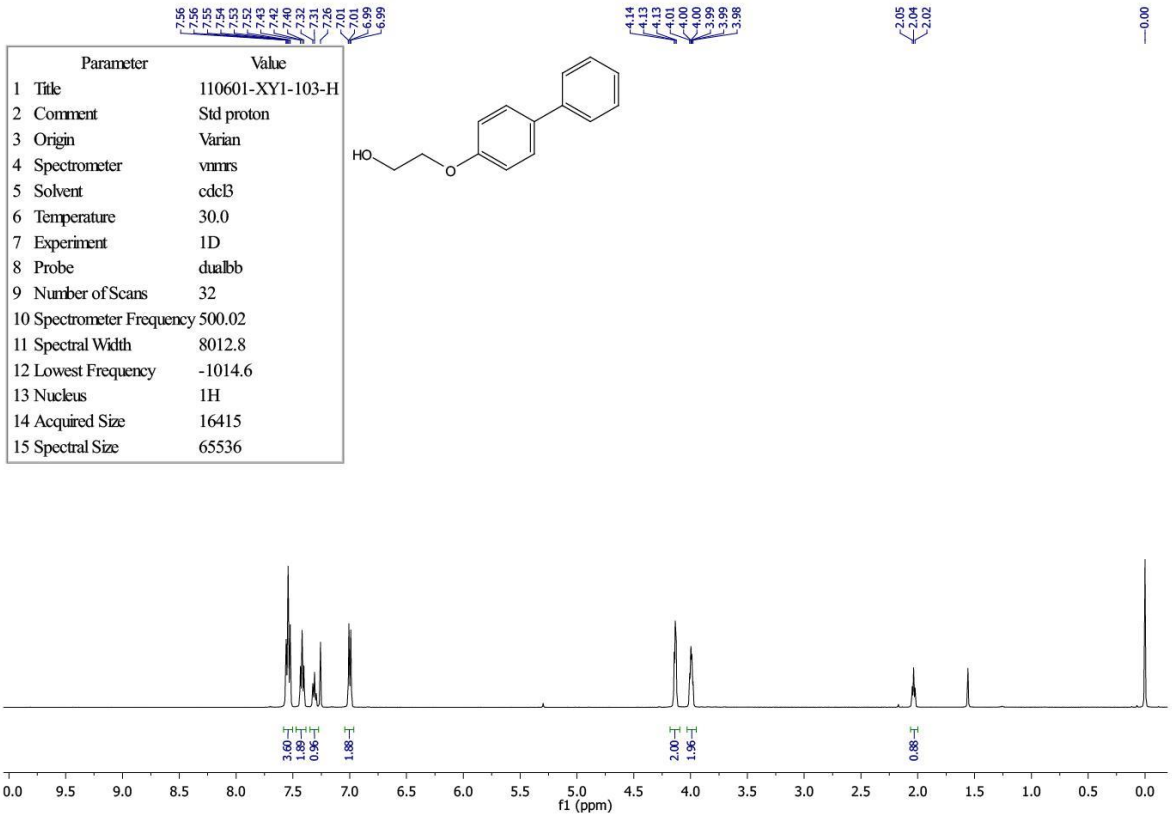
Parameter	Value
1 Title	110625-XY2-019-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	308
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2073.4
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072



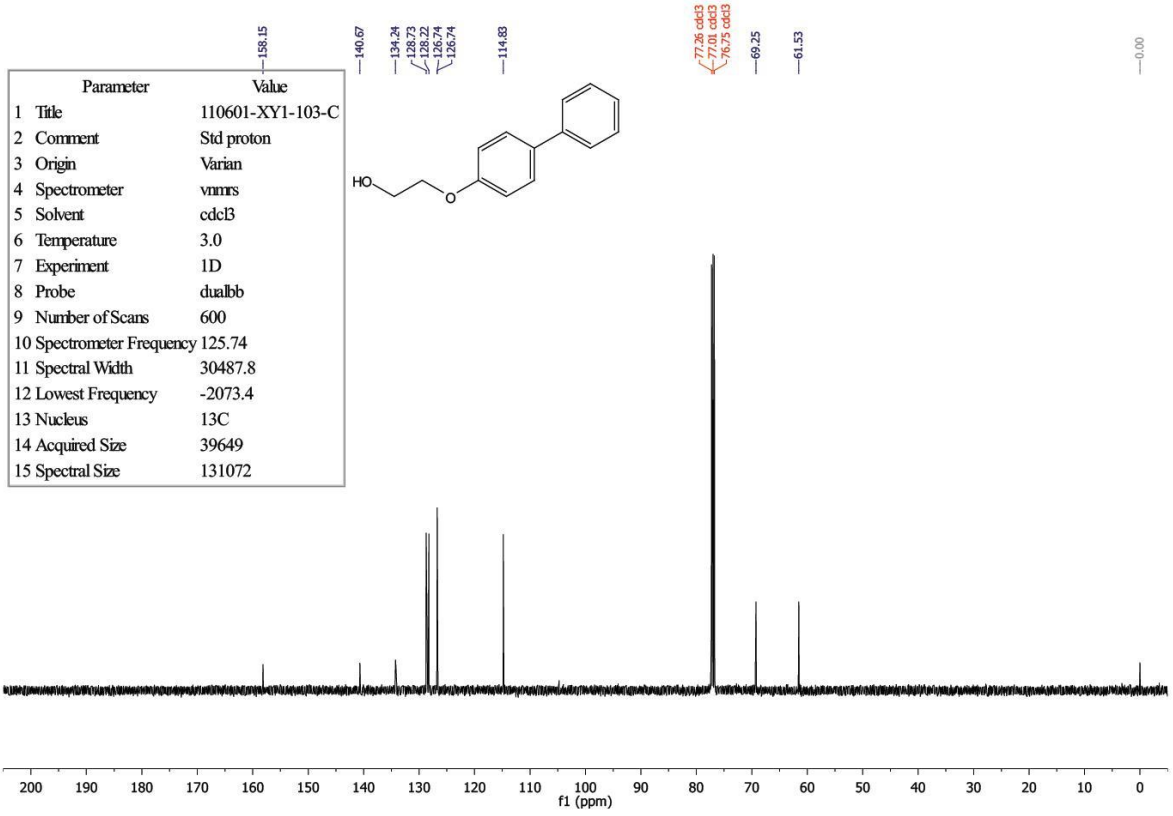
Parameter	Value
1 Title	130103-XY6-429-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	8
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1014.3
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



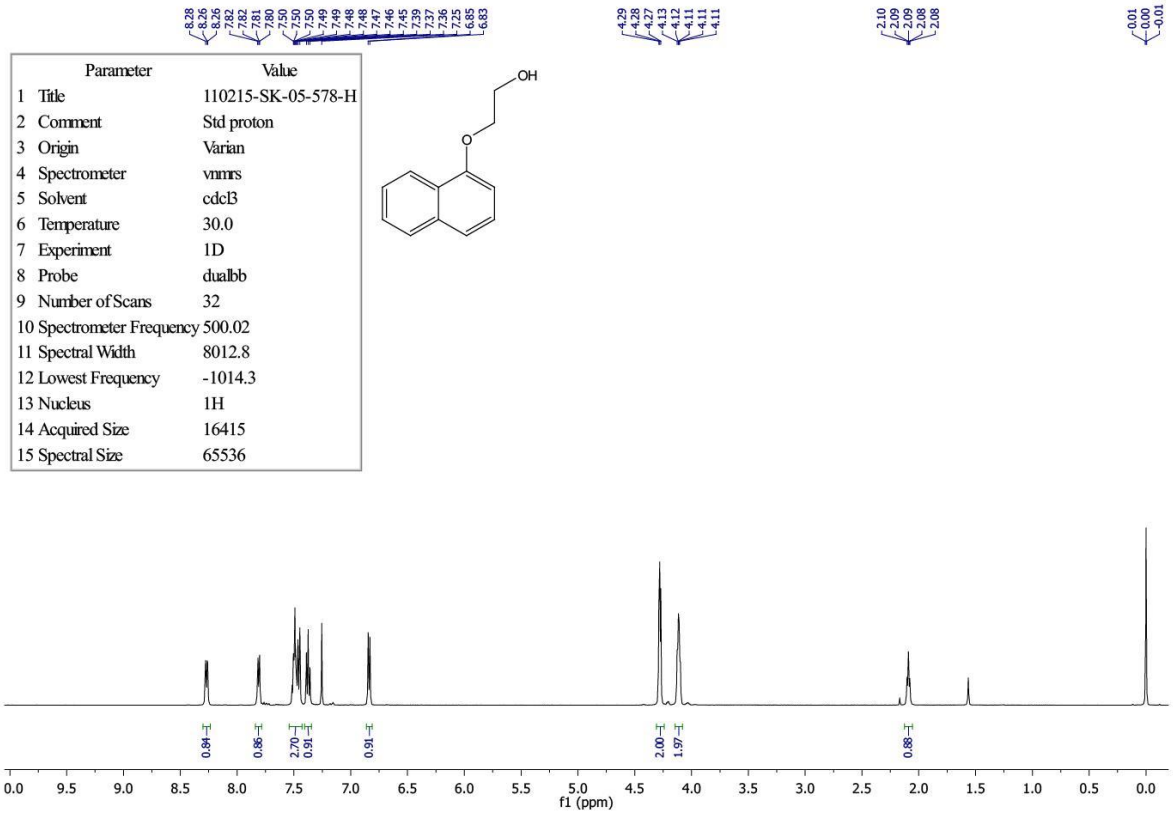
Parameter	Value
1 Title	130103-XY6-429-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	208
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2073.5
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072



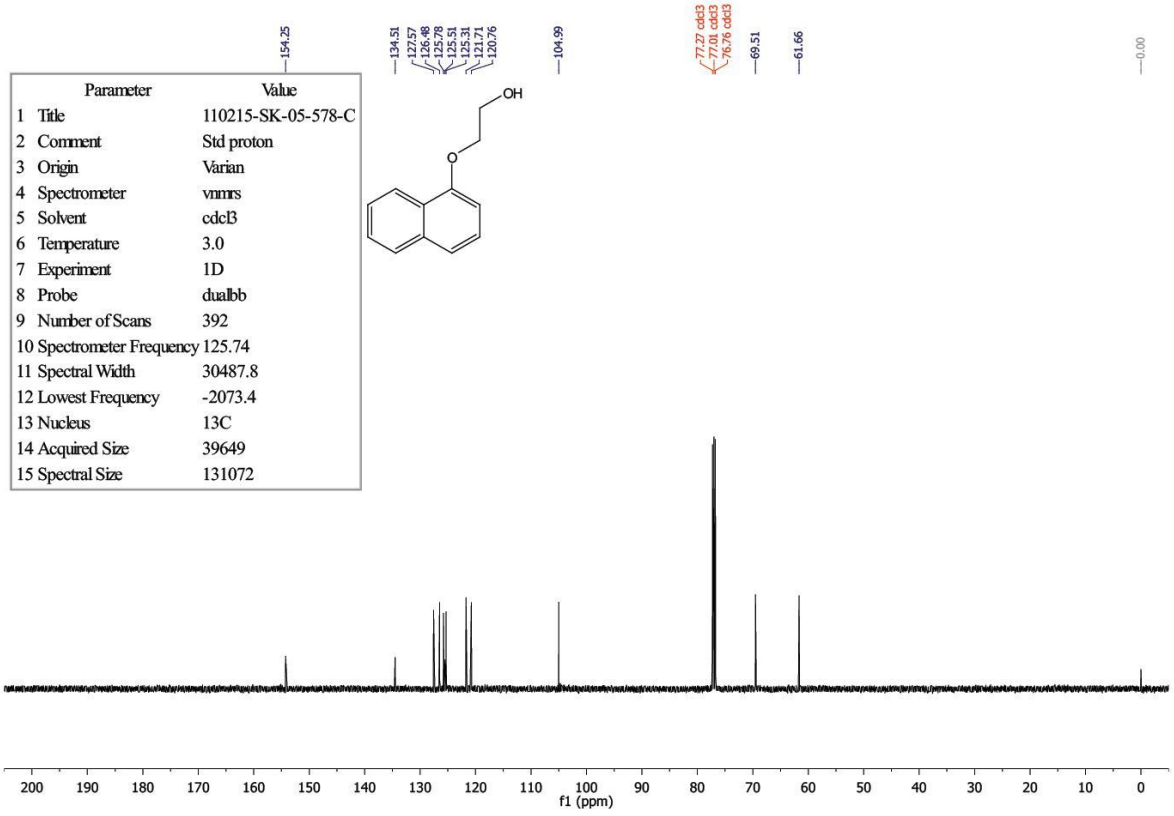
Parameter	Value
1 Title	110601-XY1-103-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	32
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1014.6
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



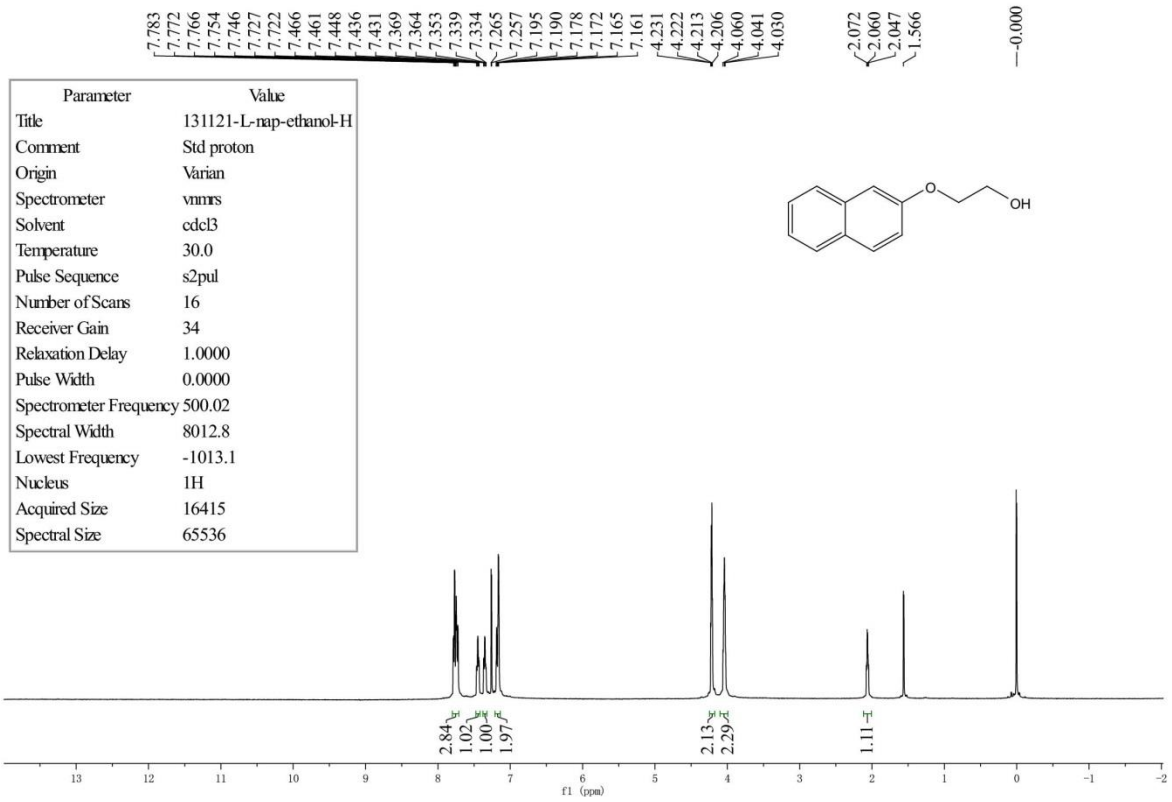
Parameter	Value
1 Title	110601-XY1-103-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	600
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2073.4
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072



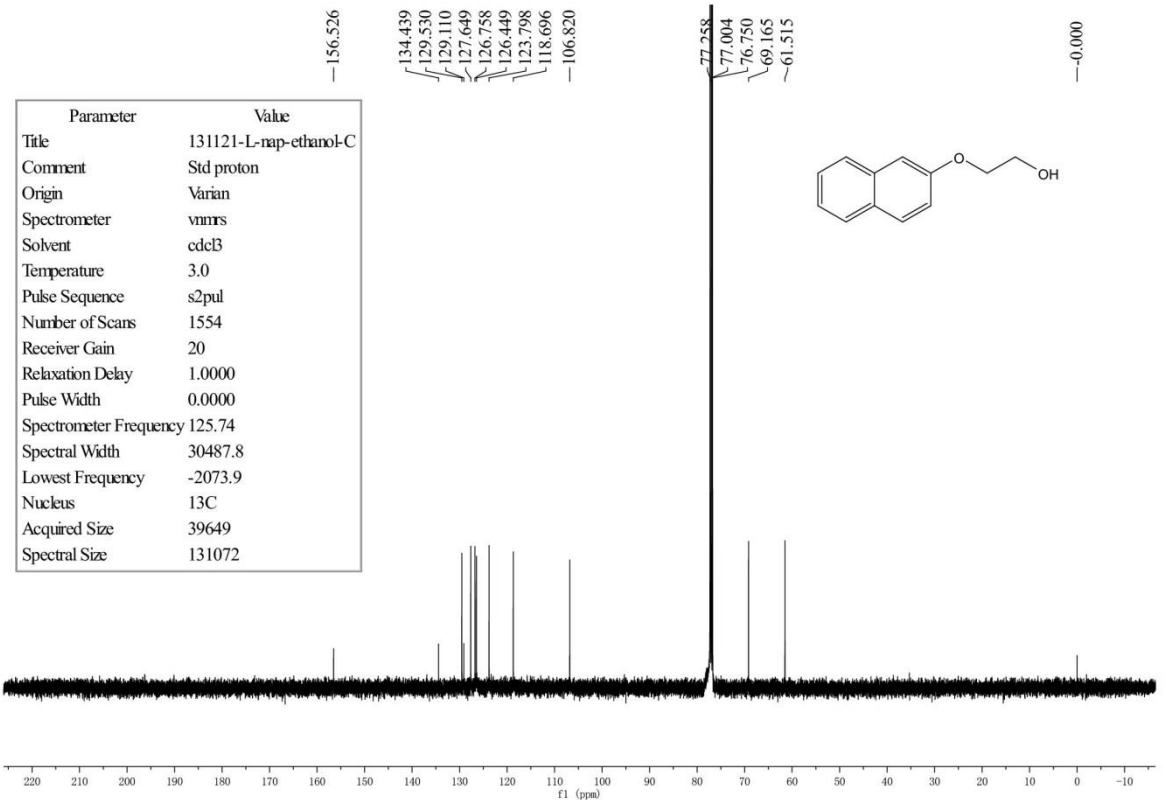
Parameter	Value
1 Title	110215-SK-05-578-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	32
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1014.3
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



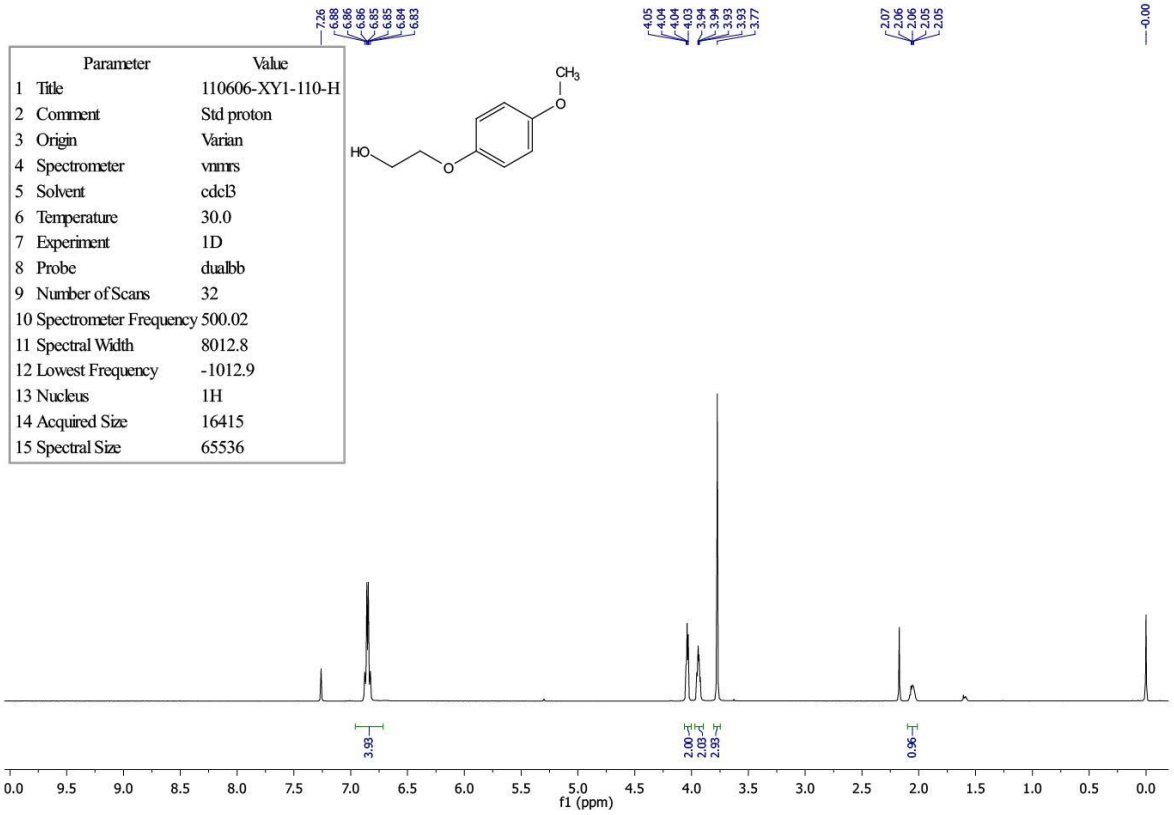
Parameter	Value
1 Title	110215-SK-05-578-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	392
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2073.4
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072



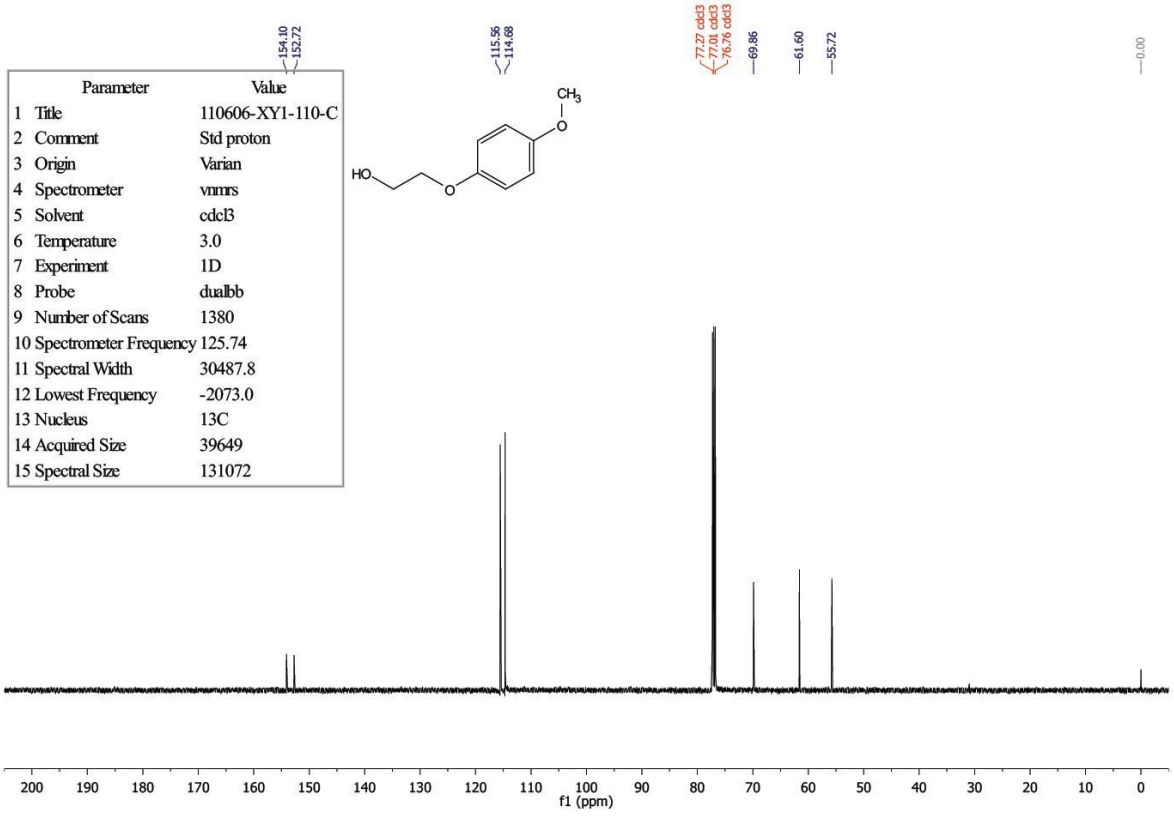
Parameter	Value
Title	131121-L-nap-ethanol-H
Comment	Std proton
Origin	Varian
Spectrometer	vnmrs
Solvent	cdcl3
Temperature	30.0
Pulse Sequence	s2pul
Number of Scans	16
Receiver Gain	34
Relaxation Delay	1.0000
Pulse Width	0.0000
Spectrometer Frequency	500.02
Spectral Width	8012.8
Lowest Frequency	-1013.1
Nucleus	1H
Acquired Size	16415
Spectral Size	65536



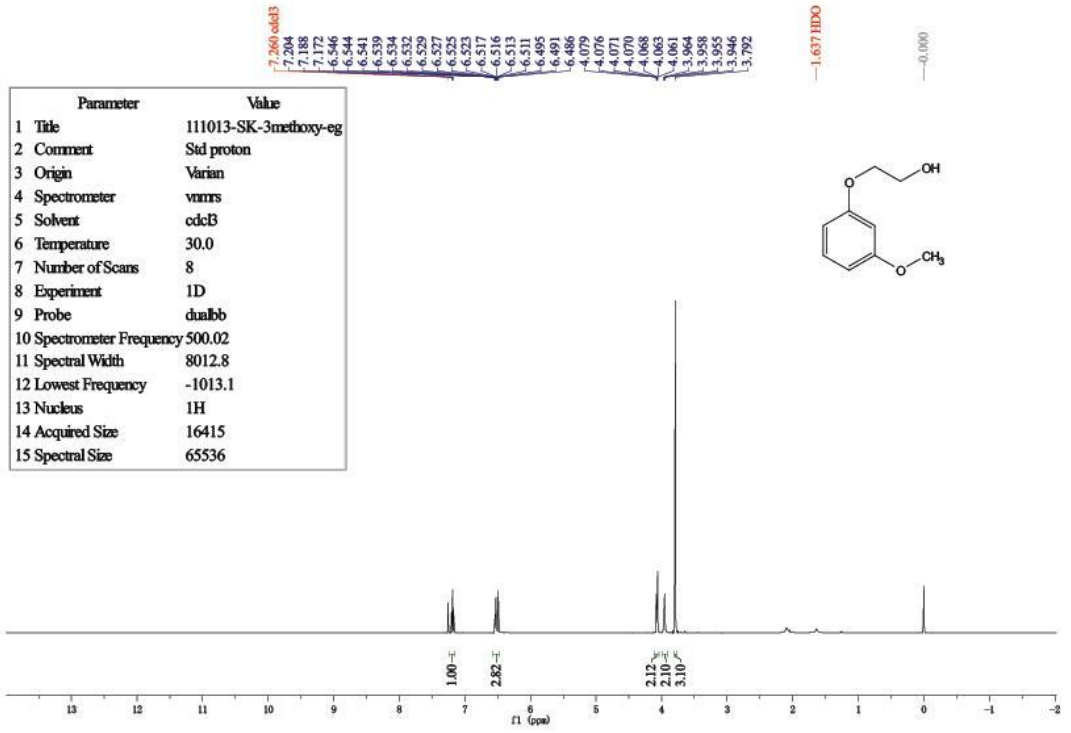
Parameter	Value
Title	131121-L-nap-ethanol-C
Comment	Std proton
Origin	Varian
Spectrometer	vnmrs
Solvent	cdcl3
Temperature	3.0
Pulse Sequence	s2pul
Number of Scans	1554
Receiver Gain	20
Relaxation Delay	1.0000
Pulse Width	0.0000
Spectrometer Frequency	125.74
Spectral Width	30487.8
Lowest Frequency	-2073.9
Nucleus	13C
Acquired Size	39649
Spectral Size	131072



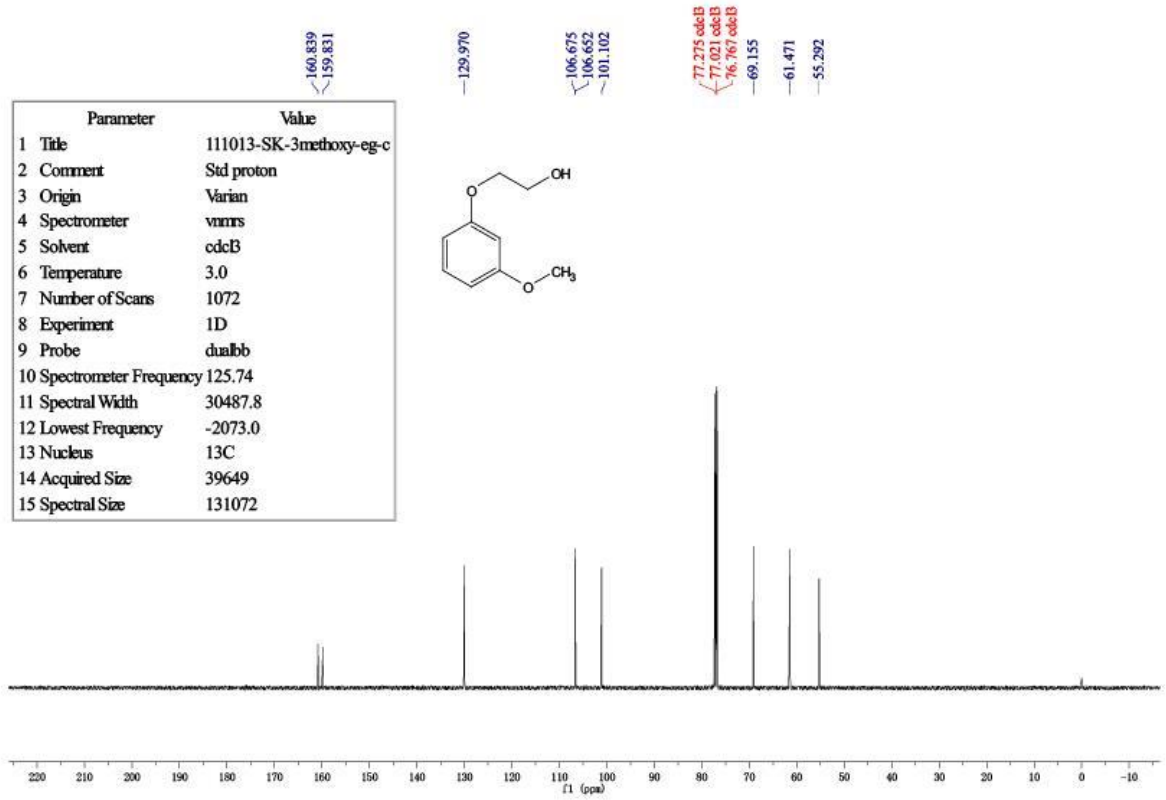
Parameter	Value
1 Title	110606-XY1-110-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	32
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1012.9
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



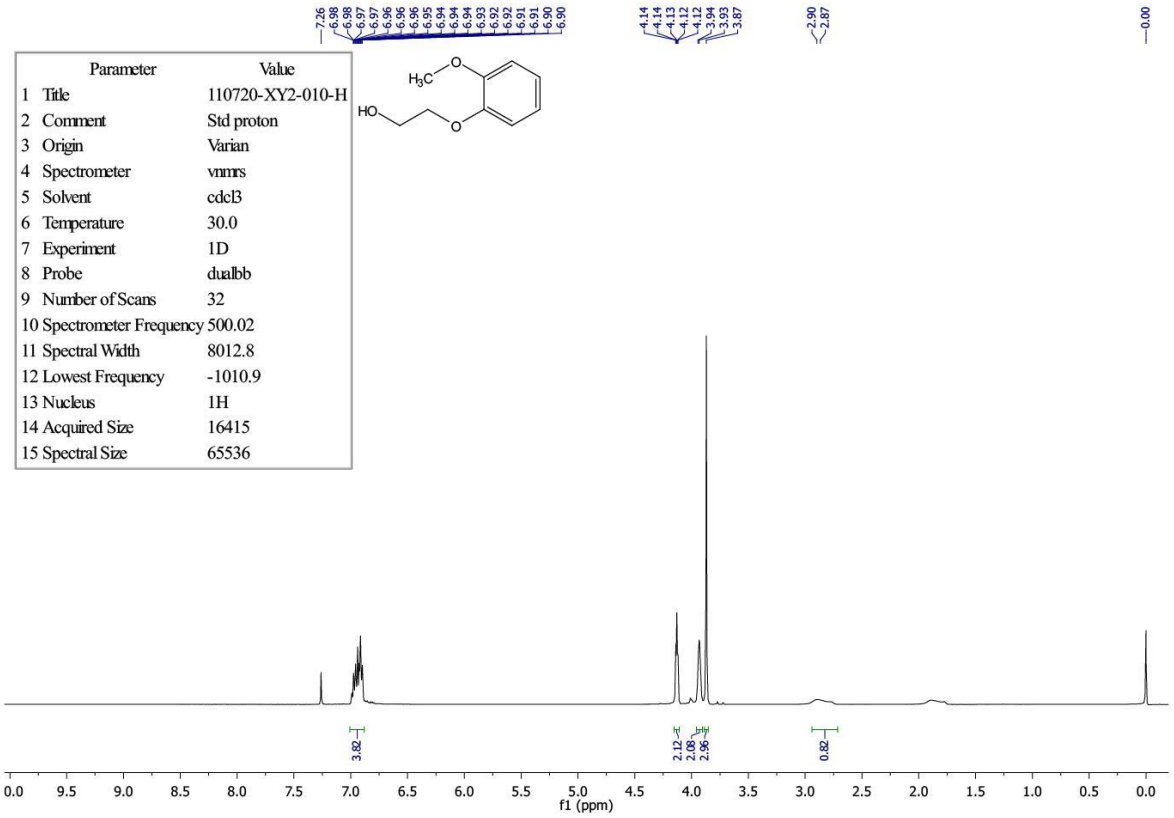
Parameter	Value
1 Title	110606-XY1-110-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	1380
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2073.0
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072



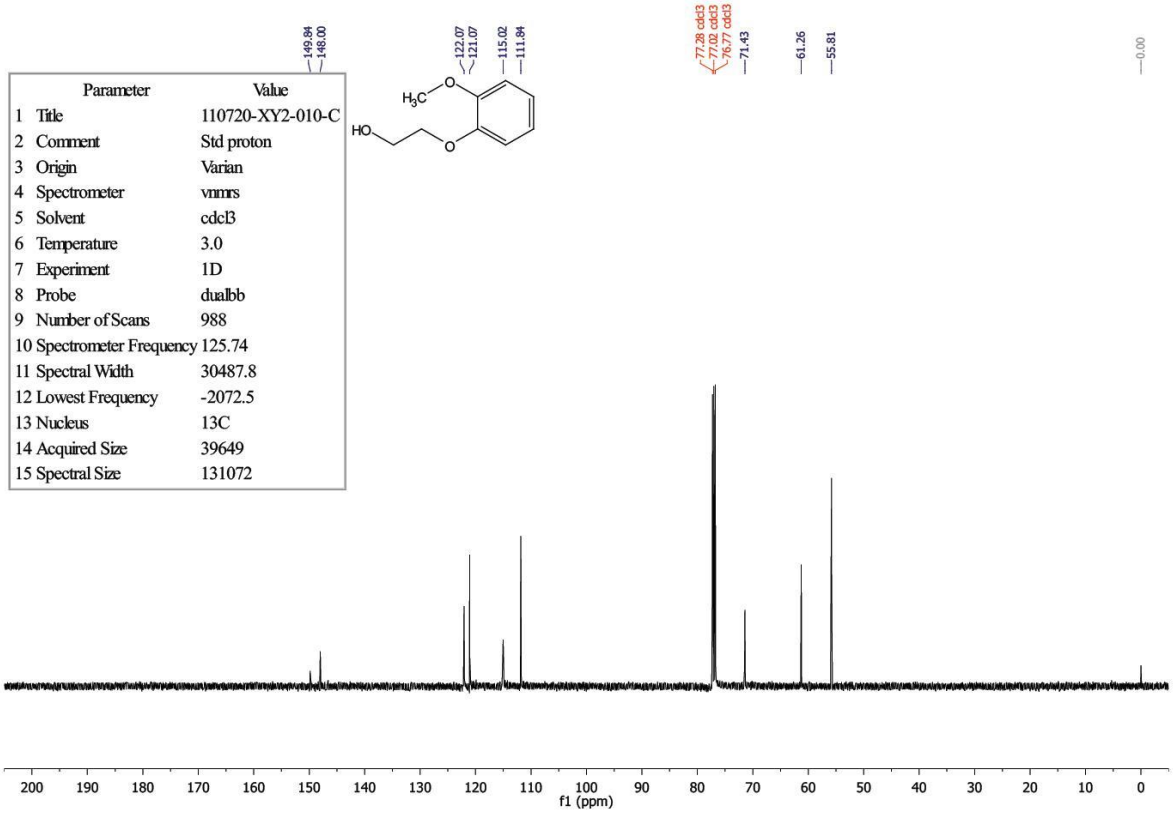
Parameter	Value
1 Title	111013-SK-3methoxy-eg
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Number of Scans	8
8 Experiment	1D
9 Probe	dualbb
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1013.1
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



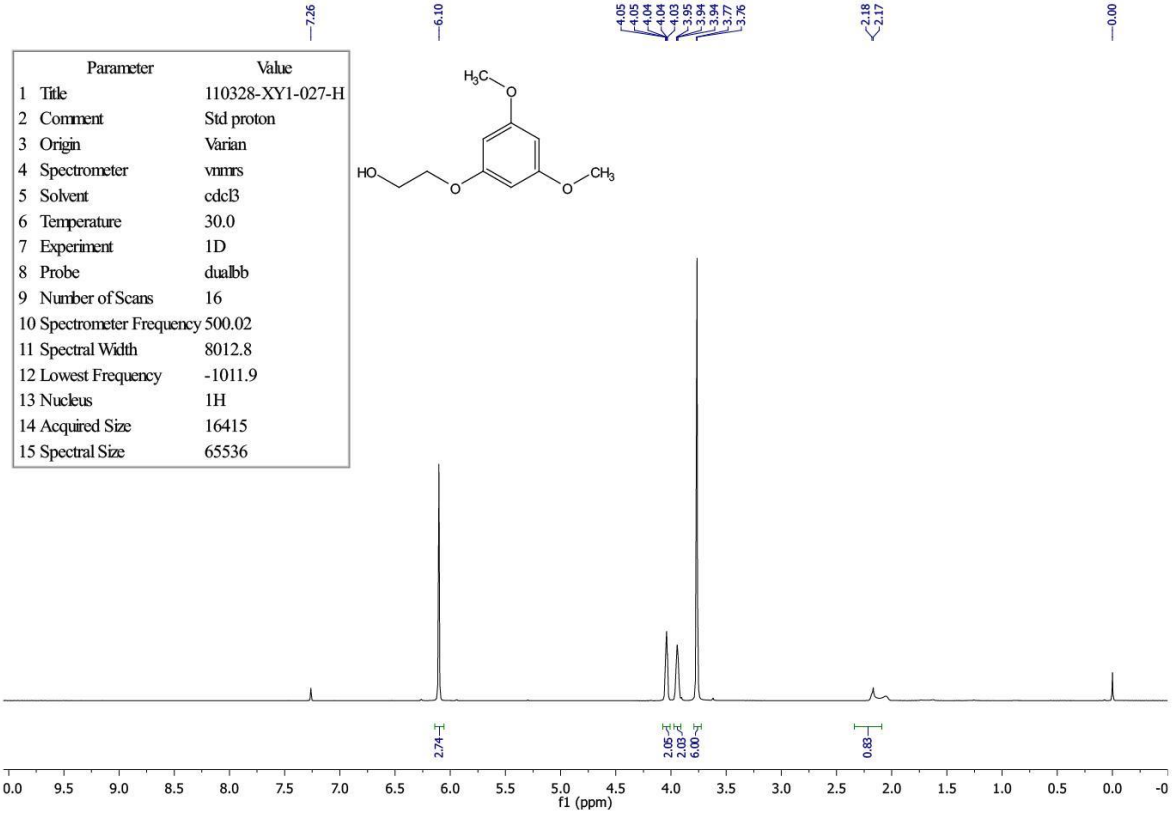
Parameter	Value
1 Title	111013-SK-3methoxy-eg-c
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Number of Scans	1072
8 Experiment	1D
9 Probe	dualbb
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2073.0
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072

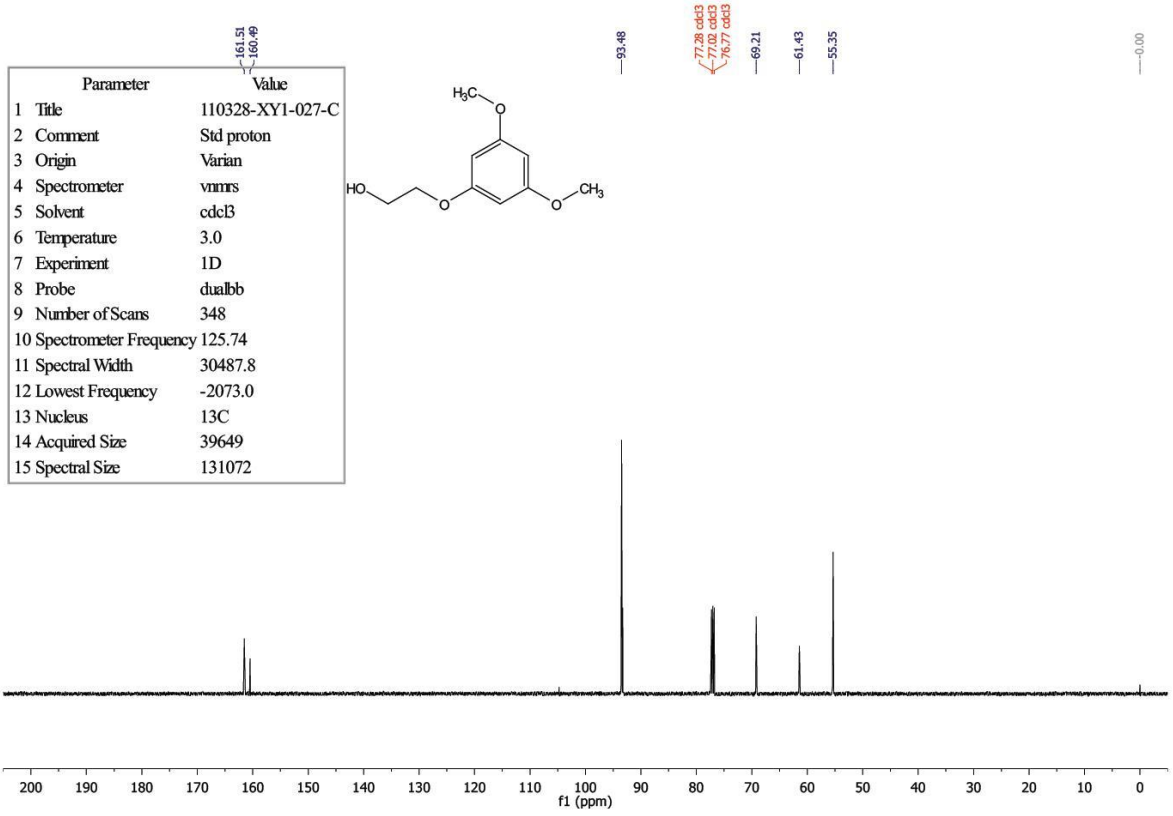


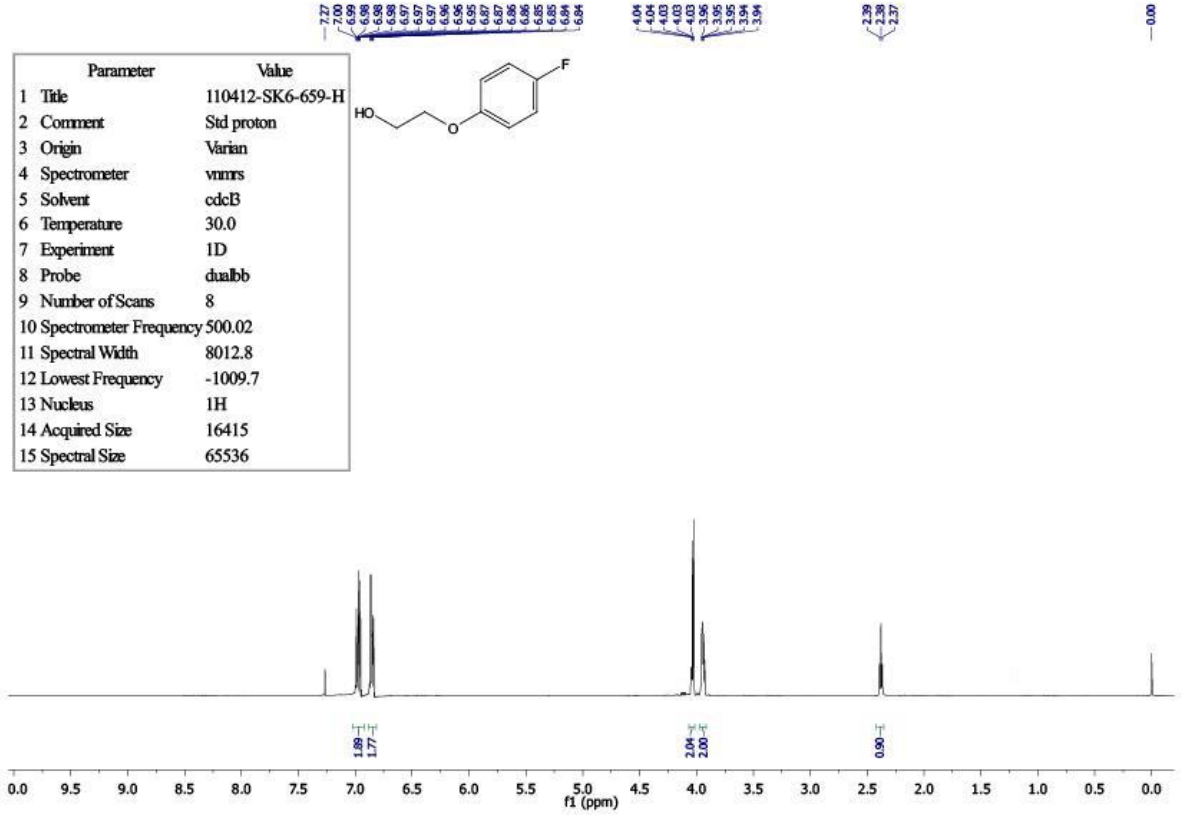
Parameter	Value
1 Title	110720-XY2-010-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	32
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1010.9
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



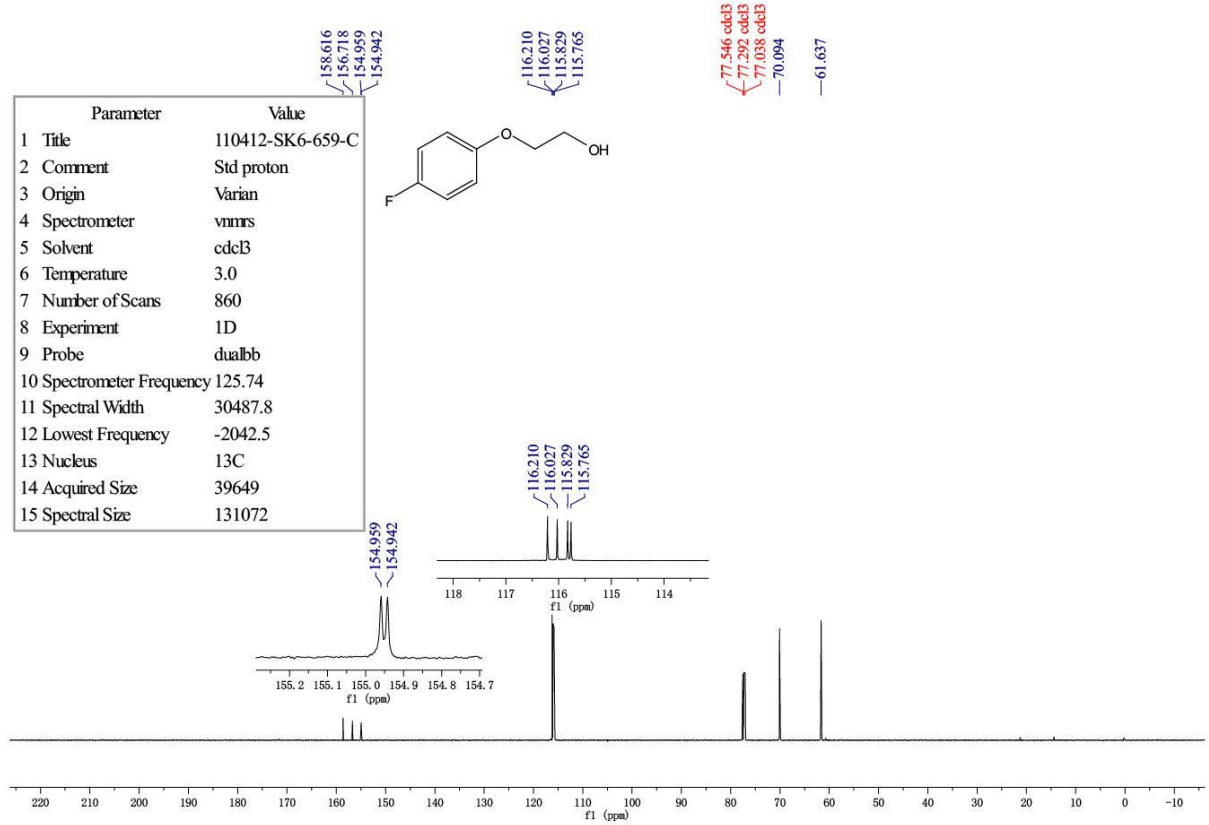
Parameter	Value
1 Title	110720-XY2-010-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	988
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2072.5
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072


7.26
6.10
4.05
4.05
4.04
4.04
4.03
3.95
3.94
3.94
3.77
3.76
2.18
2.17
0.00
Parameter Value
1 Title 110328-XY1-027-H
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent cdcl3
6 Temperature 30.0
7 Experiment 1D
8 Probe dualbb
9 Number of Scans 16
10 Spectrometer Frequency 500.02
11 Spectral Width 8012.8
12 Lowest Frequency -1011.9
13 Nucleus 1H
14 Acquired Size 16415
15 Spectral Size 65536
H3C
O
HO
O
O
CH3
2.74
2.05
2.03
6.00
0.83
f1 (ppm)

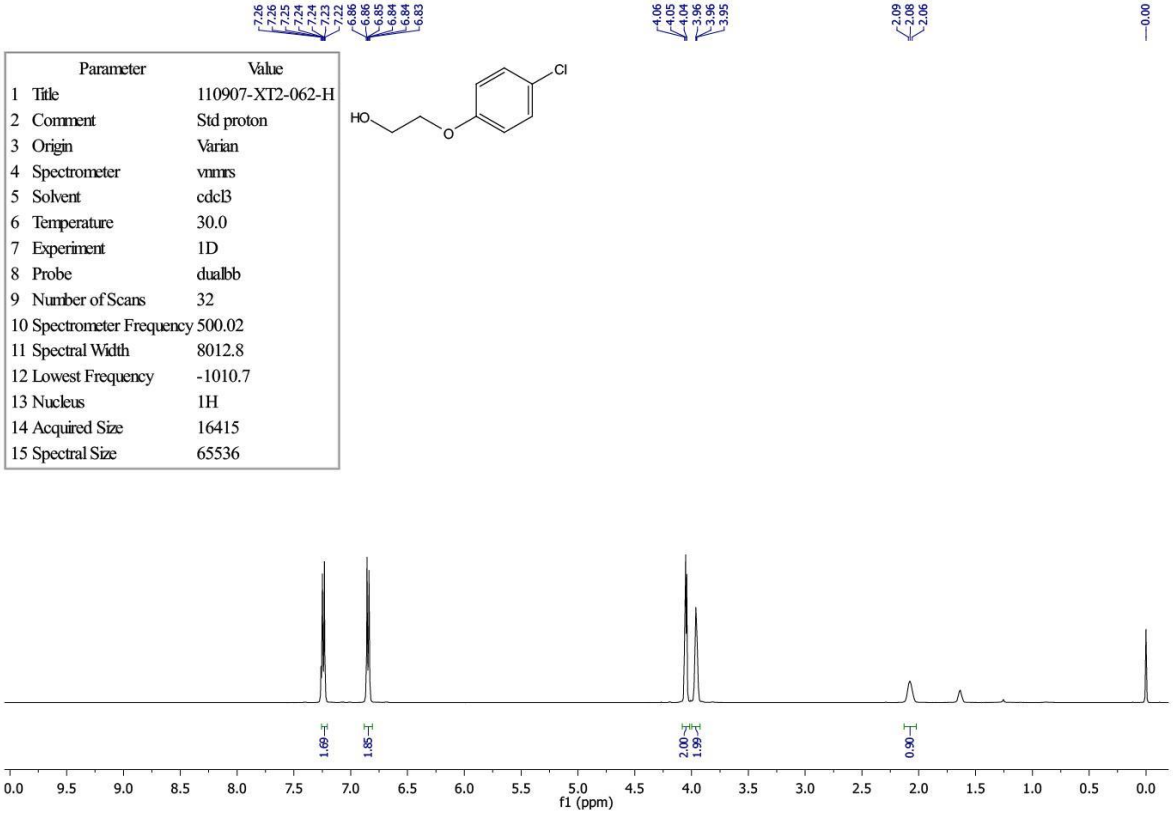

161.51
160.49
93.48
77.28 cdcl3
77.02 cdcl3
76.77 cdcl3
69.21
61.43
55.35
0.00
Parameter Value
1 Title 110328-XY1-027-C
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent cdcl3
6 Temperature 3.0
7 Experiment 1D
8 Probe dualbb
9 Number of Scans 348
10 Spectrometer Frequency 125.74
11 Spectral Width 30487.8
12 Lowest Frequency -2073.0
13 Nucleus 13C
14 Acquired Size 39649
15 Spectral Size 131072
H3C
O
HO
O
O
CH3
f1 (ppm)



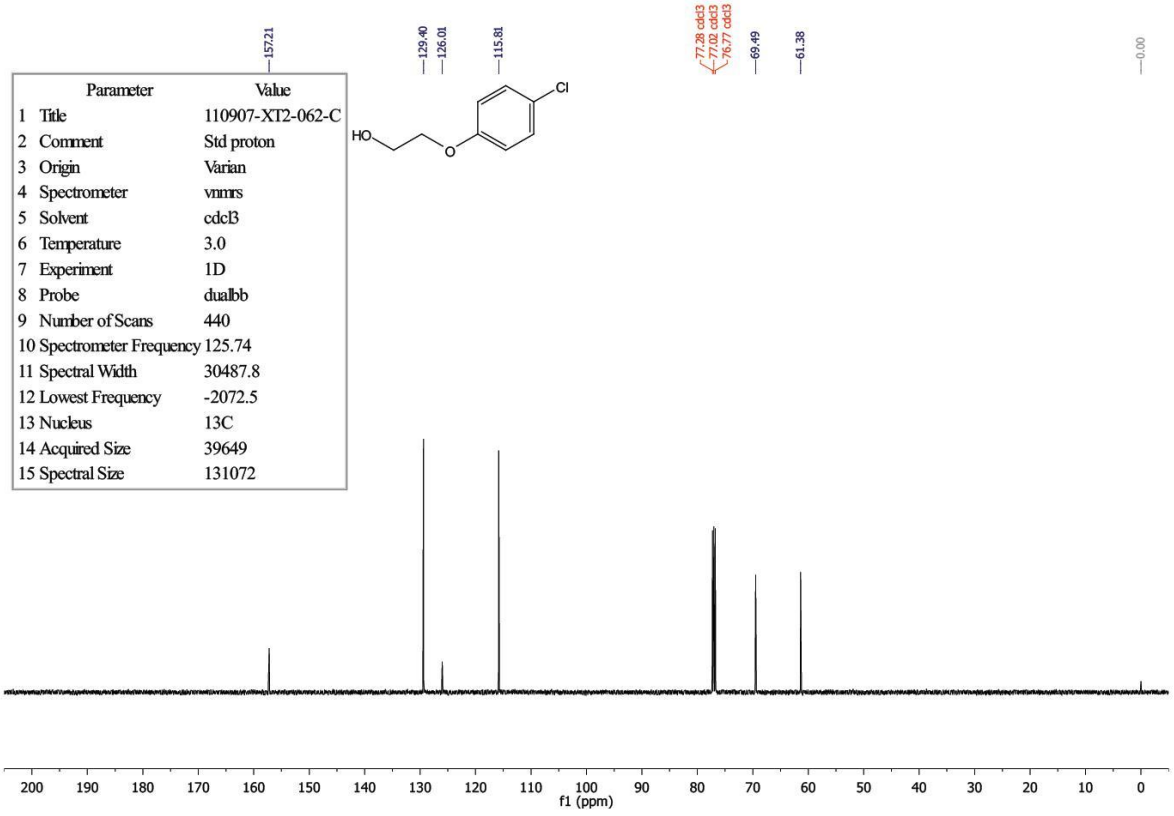
Parameter	Value
1 Title	110412-SK6-659-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	8
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1009.7
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



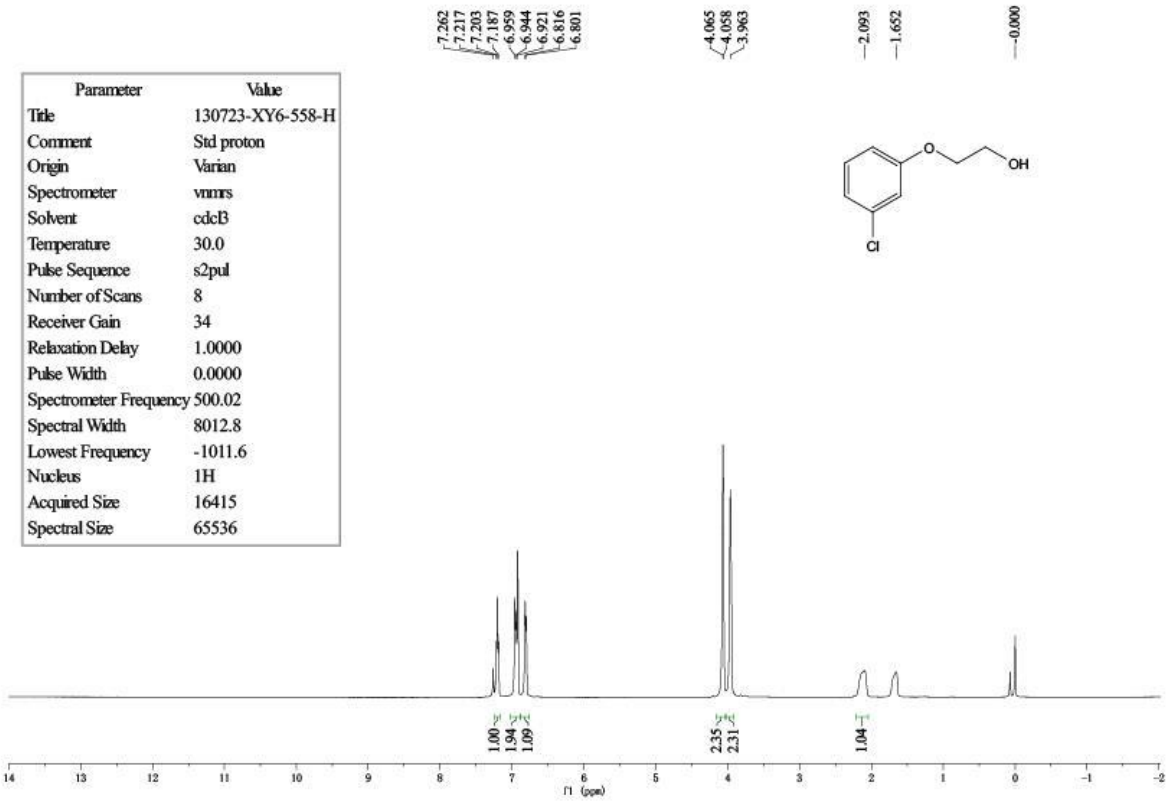
Parameter	Value
1 Title	110412-SK6-659-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Number of Scans	860
8 Experiment	1D
9 Probe	dualbb
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2042.5
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072

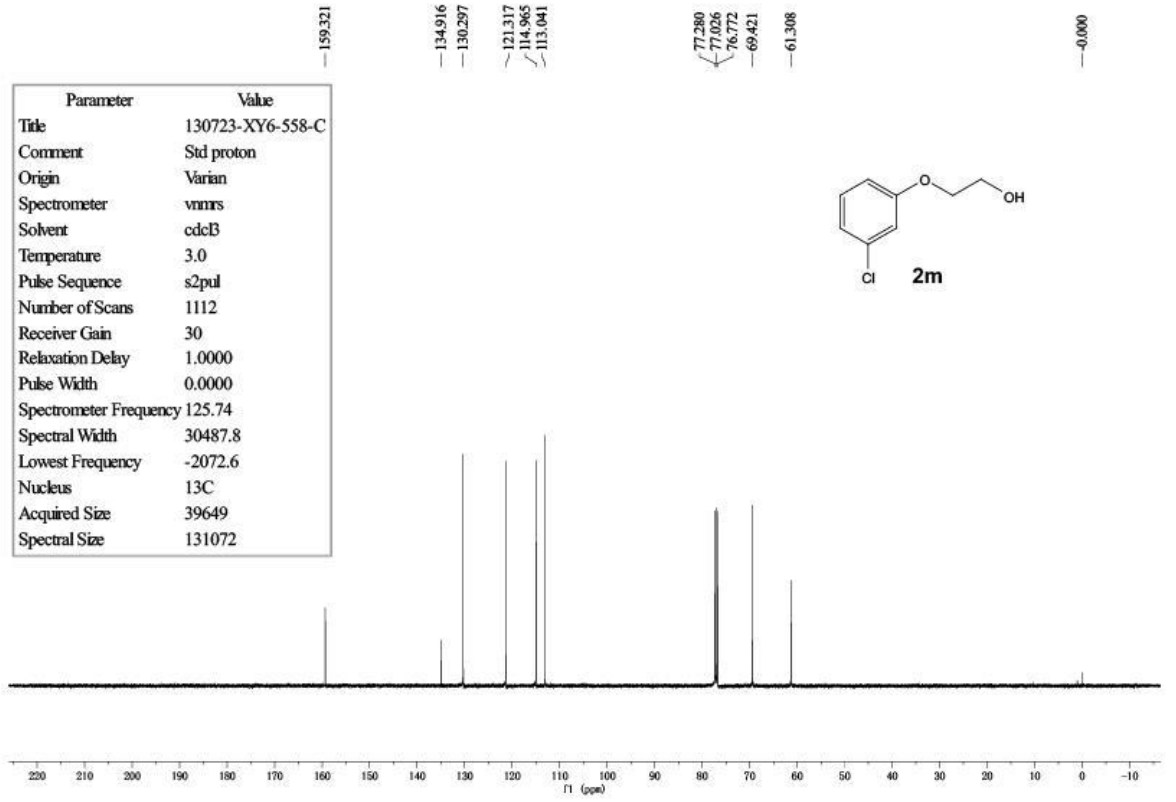


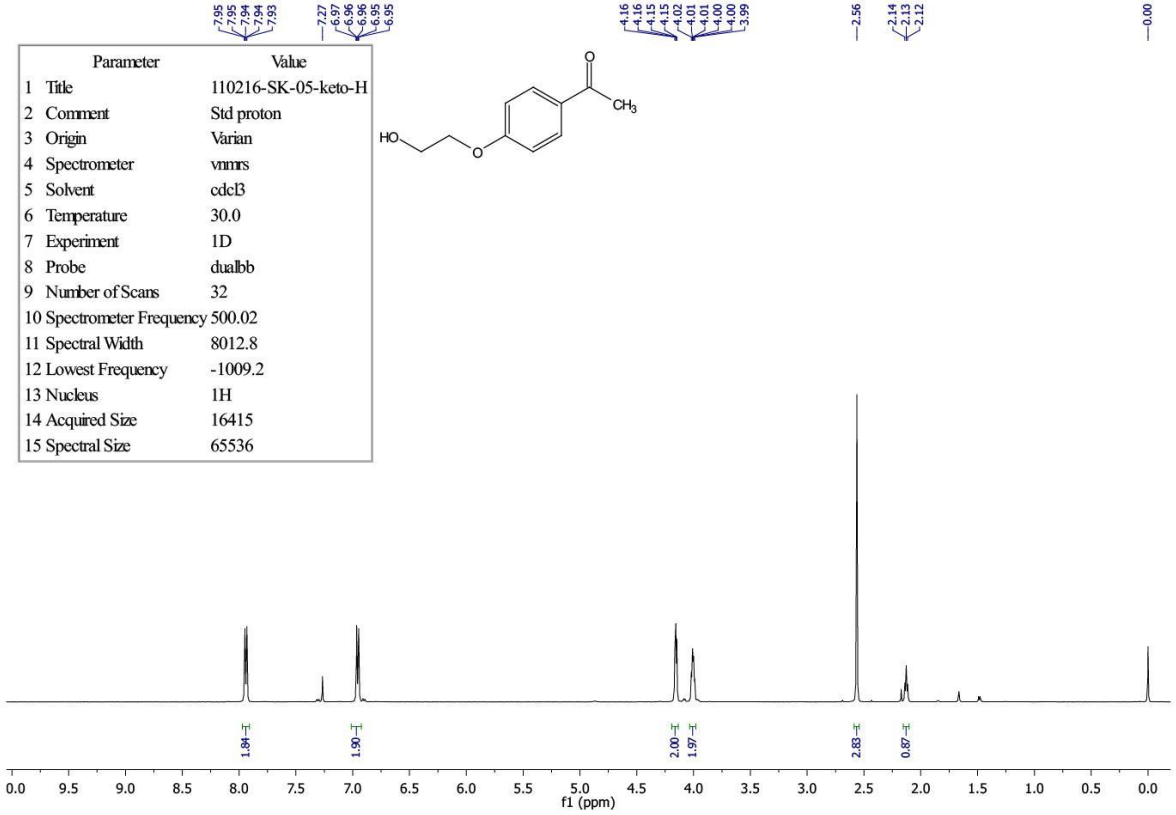
Parameter	Value
1 Title	110907-XT2-062-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	32
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1010.7
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536

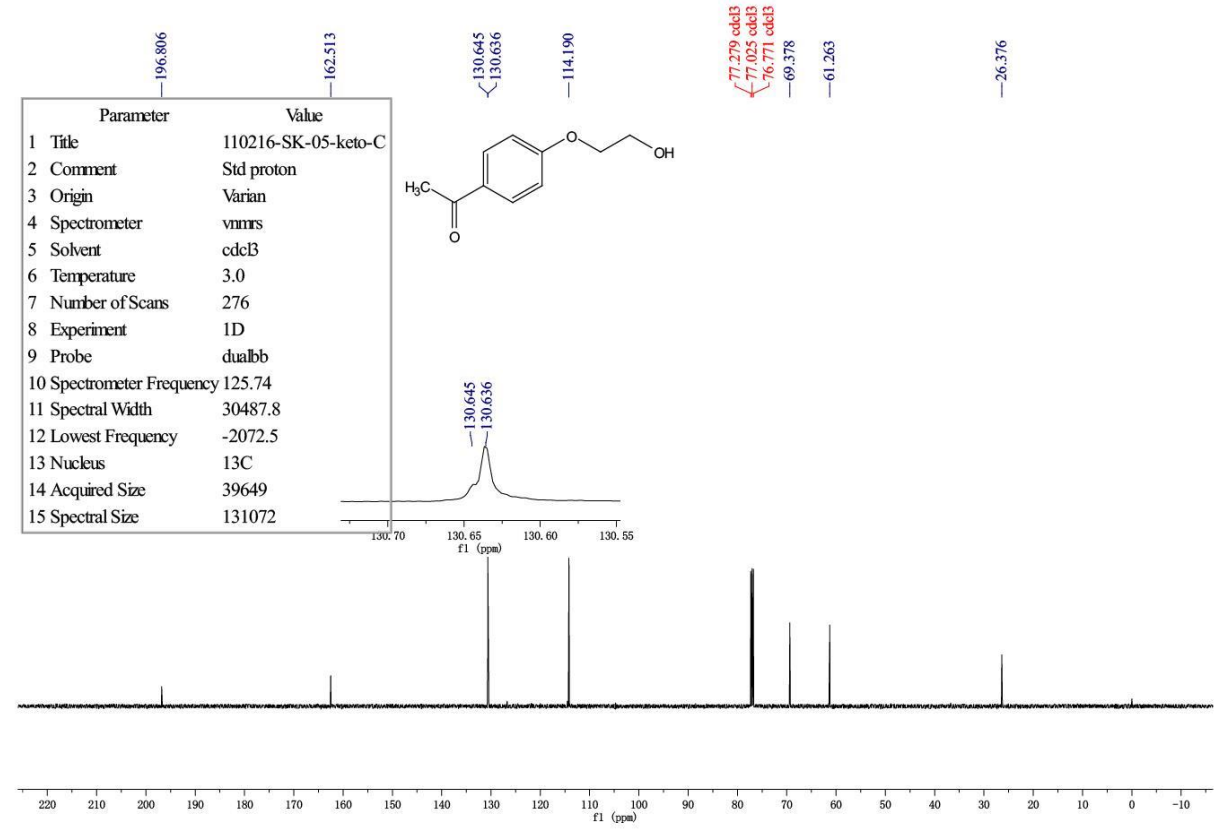


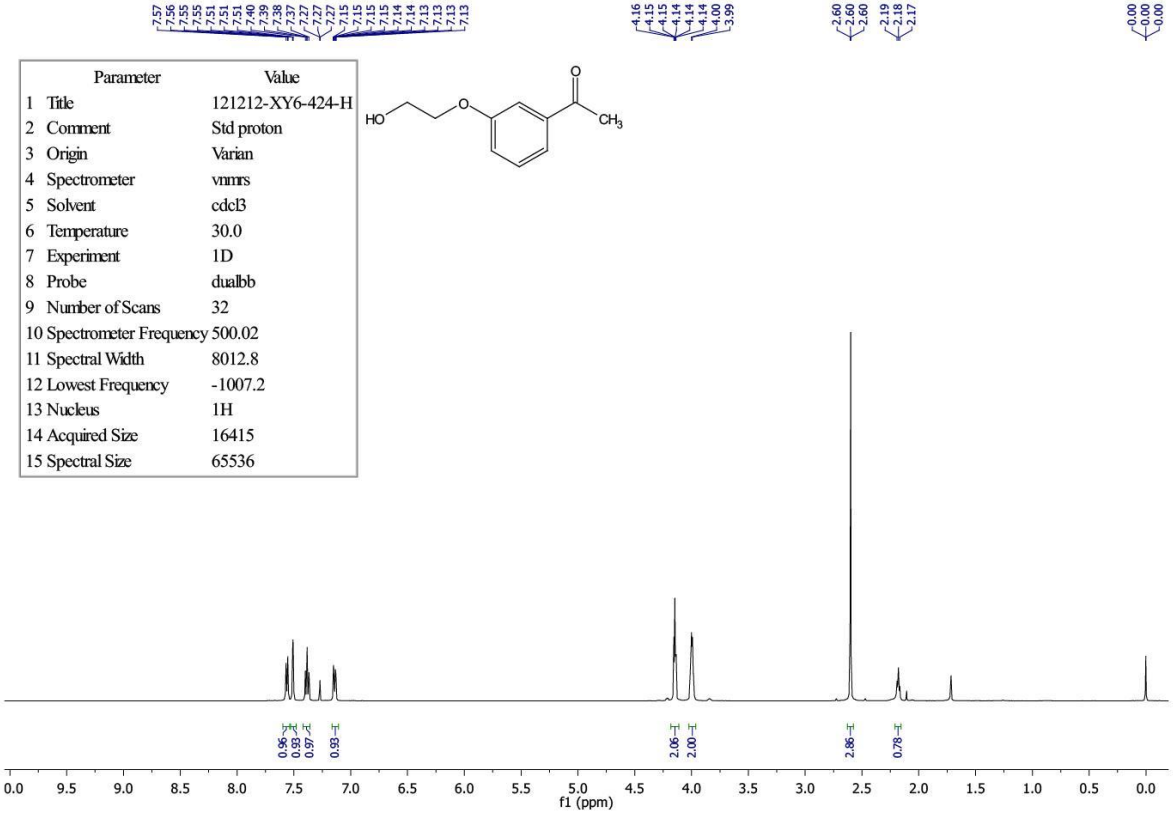
Parameter	Value
1 Title	110907-XT2-062-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	440
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2072.5
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072

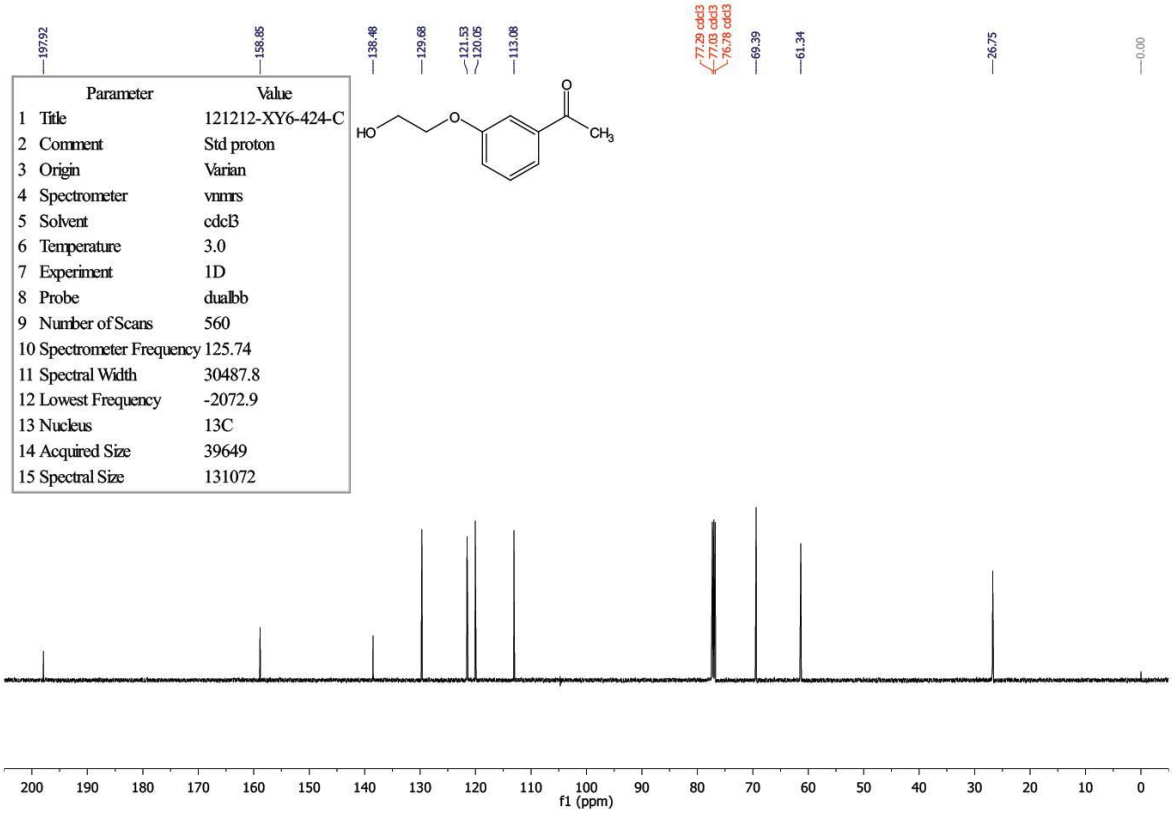

7.262
7.217
7.203
7.187
6.959
6.944
6.921
6.816
6.801
4.065
4.058
3.963
2.093
1.652
0.000
Parameter Value
Title 130723-XY6-558-H
Comment Std proton
Origin Varian
Spectrometer vnmrs
Solvent cdcl3
Temperature 30.0
Pulse Sequence s2pul
Number of Scans 8
Receiver Gain 34
Relaxation Delay 1.0000
Pulse Width 0.0000
Spectrometer Frequency 500.02
Spectral Width 8012.8
Lowest Frequency -1011.6
Nucleus 1H
Acquired Size 16415
Spectral Size 65536
O
OH
Cl
1.00
1.94
1.09
2.35
2.31
1.04
f1 (ppm)

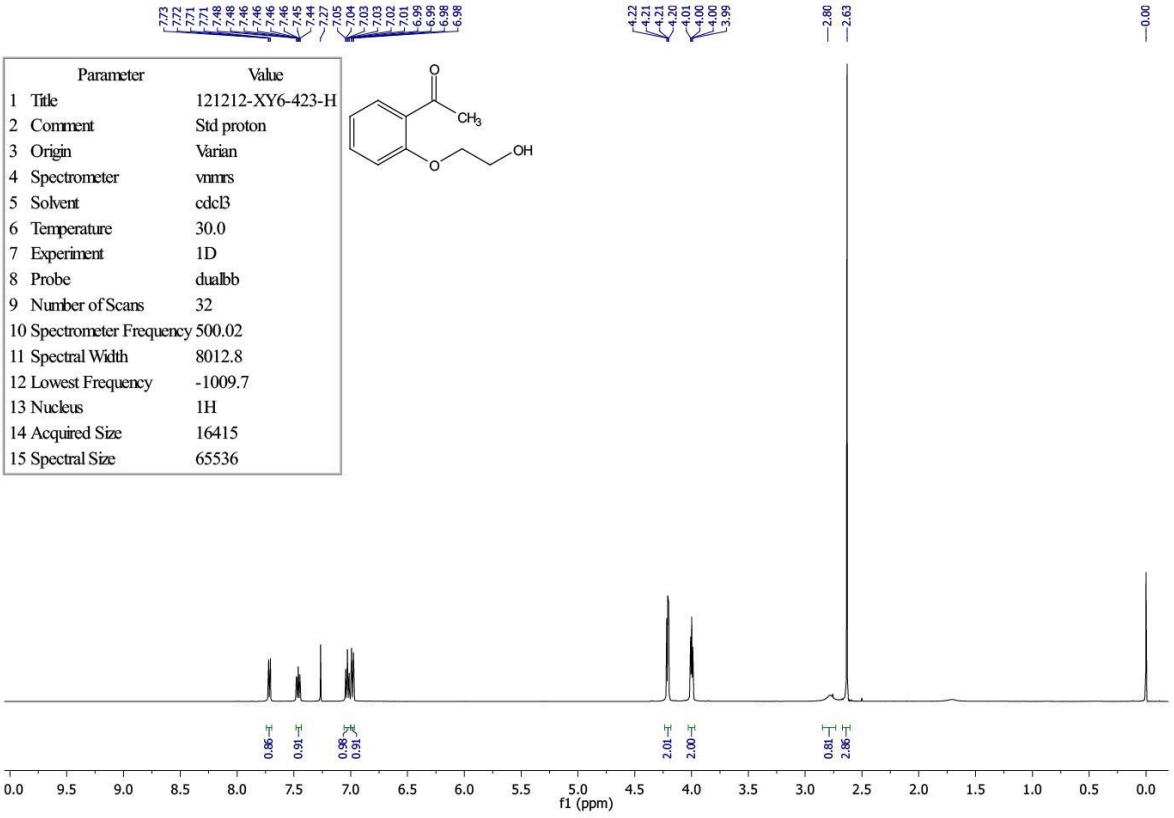

159.321
134.916
130.297
121.317
114.965
113.041
77.280
77.026
76.772
69.421
61.308
0.000
Parameter Value
Title 130723-XY6-558-C
Comment Std proton
Origin Varian
Spectrometer vnmrs
Solvent cdcl3
Temperature 3.0
Pulse Sequence s2pul
Number of Scans 1112
Receiver Gain 30
Relaxation Delay 1.0000
Pulse Width 0.0000
Spectrometer Frequency 125.74
Spectral Width 30487.8
Lowest Frequency -2072.6
Nucleus 13C
Acquired Size 39649
Spectral Size 131072
O
OH
Cl
2m
f1 (ppm)

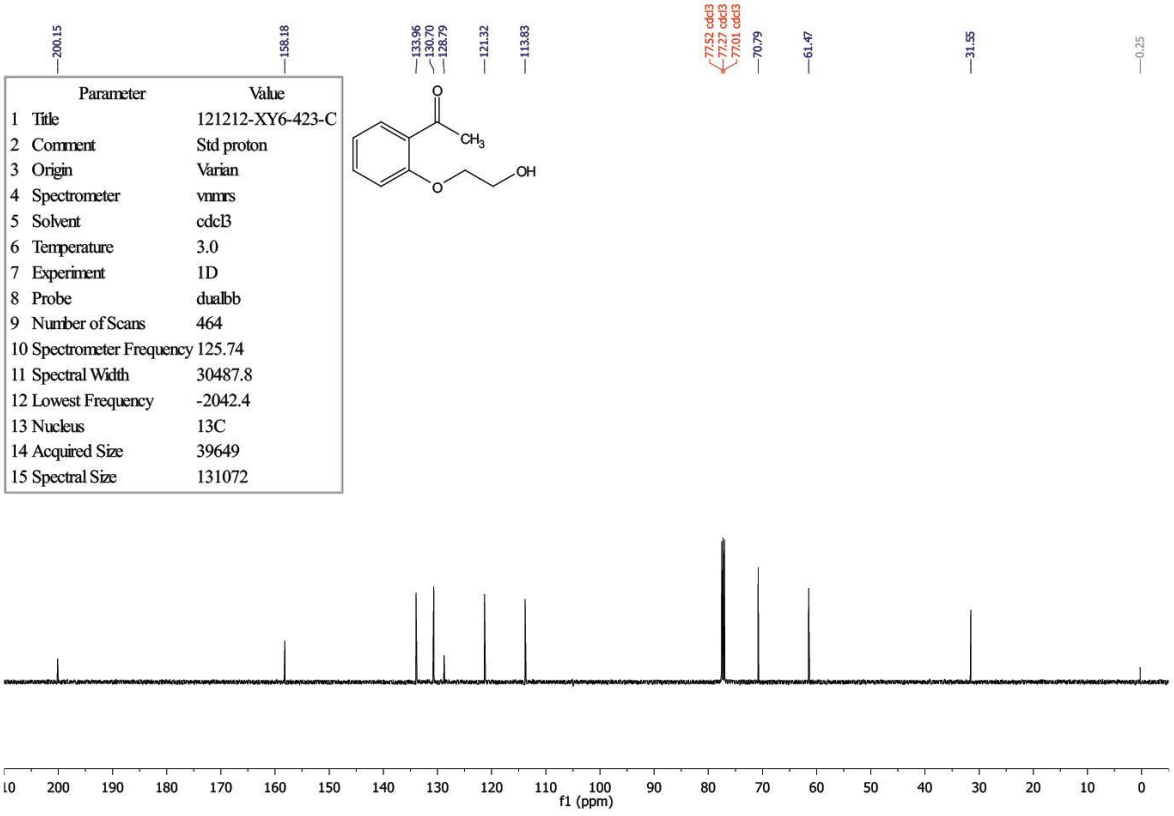

7.95
7.95
7.94
7.94
7.93
7.27
6.97
6.96
6.96
6.95
6.95
4.16
4.16
4.15
4.15
4.02
4.01
4.01
4.00
4.00
3.99
2.56
2.14
2.13
2.12
0.00
Parameter Value
1 Title 110216-SK-05-keto-H
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent cdcl3
6 Temperature 30.0
7 Experiment 1D
8 Probe dualbb
9 Number of Scans 32
10 Spectrometer Frequency 500.02
11 Spectral Width 8012.8
12 Lowest Frequency -1009.2
13 Nucleus 1H
14 Acquired Size 16415
15 Spectral Size 65536
HO
O
O
CH3
1.84
1.90
2.00
1.97
2.83
0.87
f1 (ppm)

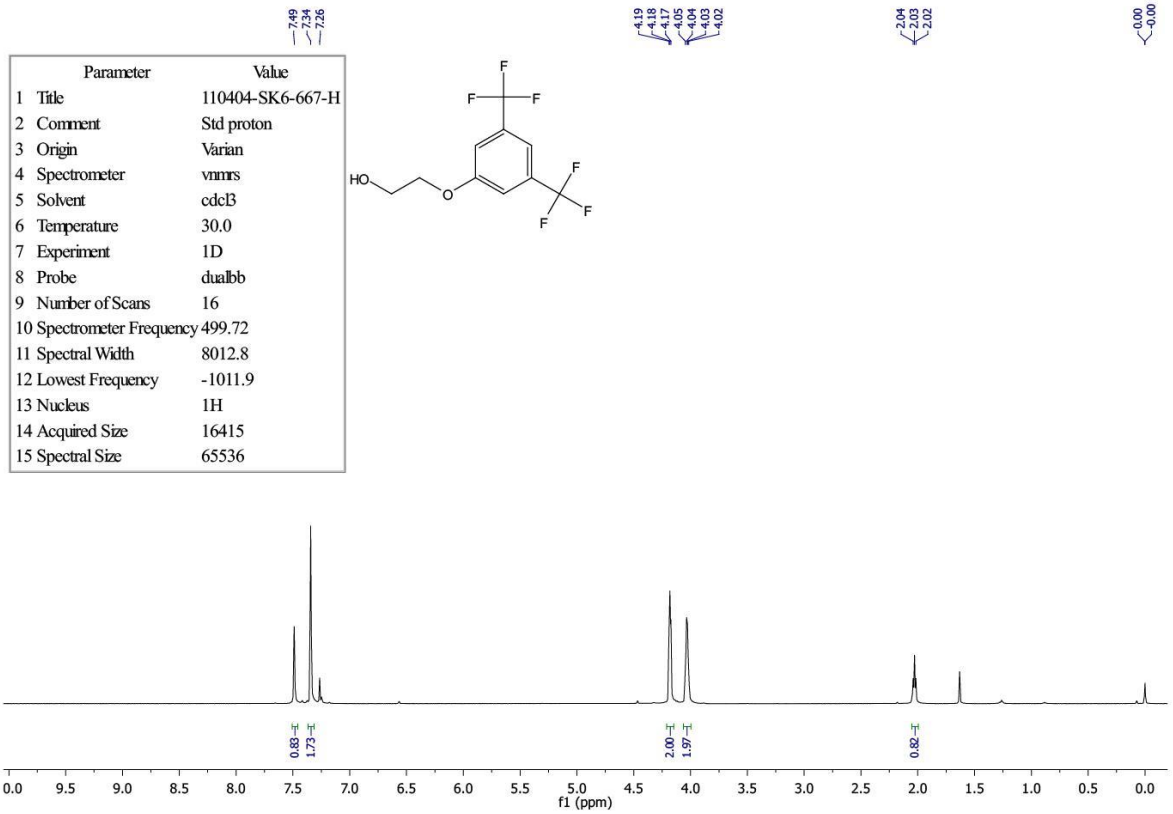

196.806
162.513
130.645
130.636
114.190
77.279 cdcl3
77.025 cdcl3
76.771 cdcl3
69.378
61.263
26.376
Parameter Value
1 Title 110216-SK-05-keto-C
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent cdcl3
6 Temperature 3.0
7 Number of Scans 276
8 Experiment 1D
9 Probe dualbb
10 Spectrometer Frequency 125.74
11 Spectral Width 30487.8
12 Lowest Frequency -2072.5
13 Nucleus 13C
14 Acquired Size 39649
15 Spectral Size 131072
H3C
O
O
OH
130.645
130.636
f1 (ppm)
f1 (ppm)

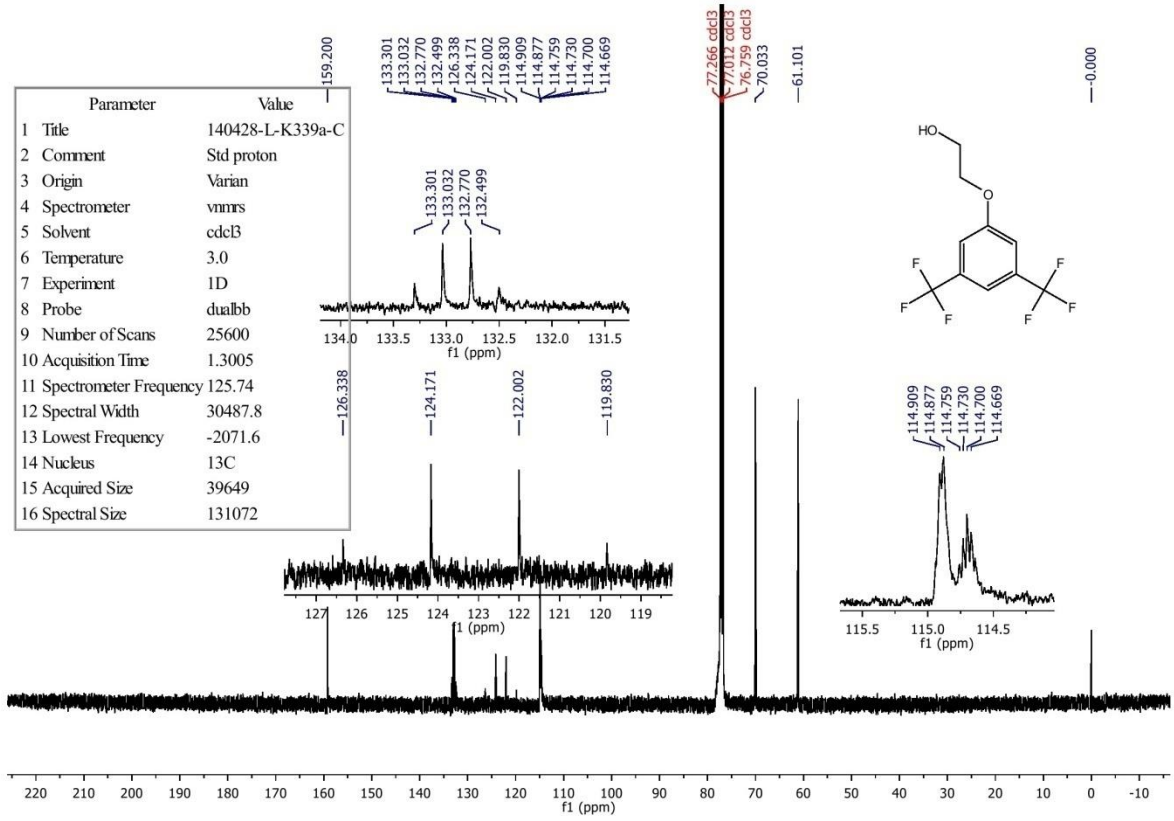

7.57 7.56 7.55 7.55 7.51 7.51 7.51 7.40 7.39 7.38 7.37 7.27 7.27 7.27 7.15 7.15 7.15 7.15 7.14 7.14 7.13 7.13 7.13 7.13
4.16 4.15 4.15 4.14 4.14 4.14 4.00 3.99
2.60 2.60 2.60
2.19 2.18 2.17
0.00 0.00 0.00
Parameter Value
1 Title 121212-XY6-424-H
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent cdcl3
6 Temperature 30.0
7 Experiment 1D
8 Probe dualbb
9 Number of Scans 32
10 Spectrometer Frequency 500.02
11 Spectral Width 8012.8
12 Lowest Frequency -1007.2
13 Nucleus 1H
14 Acquired Size 16415
15 Spectral Size 65536
HO
O
O
CH3
0.96 0.93 0.97 0.93
2.06 2.00
2.86
0.78
f1 (ppm)

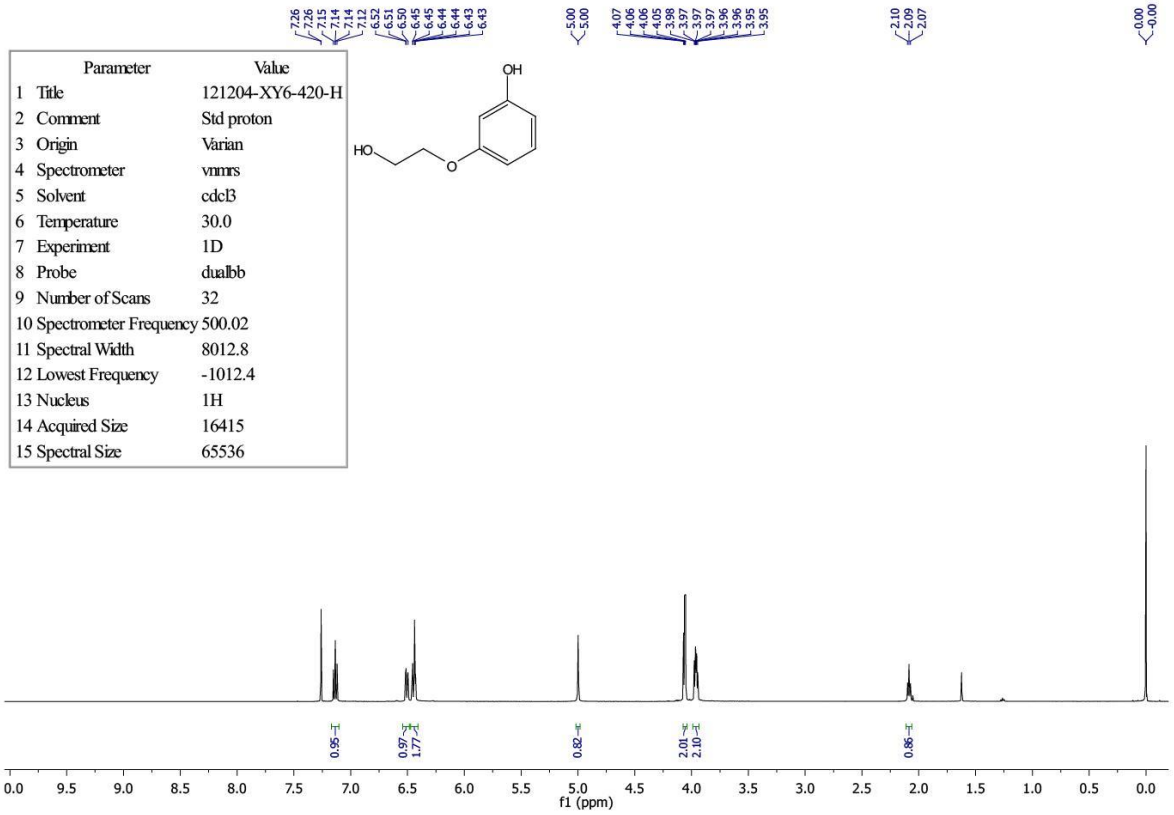

197.92
158.85
138.48
129.68
121.53 120.05
113.08
77.29 cdcl3 77.03 cdcl3 76.78 cdcl3
69.39
61.34
26.75
0.00
Parameter Value
1 Title 121212-XY6-424-C
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent cdcl3
6 Temperature 3.0
7 Experiment 1D
8 Probe dualbb
9 Number of Scans 560
10 Spectrometer Frequency 125.74
11 Spectral Width 30487.8
12 Lowest Frequency -2072.9
13 Nucleus 13C
14 Acquired Size 39649
15 Spectral Size 131072
HO
O
O
CH3
f1 (ppm)


7.73 7.72 7.71 7.71 7.48 7.48 7.46 7.46 7.46 7.46 7.45 7.44 7.07 7.05 7.04 7.03 7.03 7.02 7.01 6.99 6.99 6.98 6.98
4.22 4.21 4.21 4.20 4.01 4.00 4.00 3.99
2.80 2.63
0.00
Parameter Value
1 Title 121212-XY6-423-H
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent cdcl3
6 Temperature 30.0
7 Experiment 1D
8 Probe dualbb
9 Number of Scans 32
10 Spectrometer Frequency 500.02
11 Spectral Width 8012.8
12 Lowest Frequency -1009.7
13 Nucleus 1H
14 Acquired Size 16415
15 Spectral Size 65536
O
CH3
OH
O
0.86 0.91 0.98 0.91 2.01 2.00 0.81 2.86
f1 (ppm)

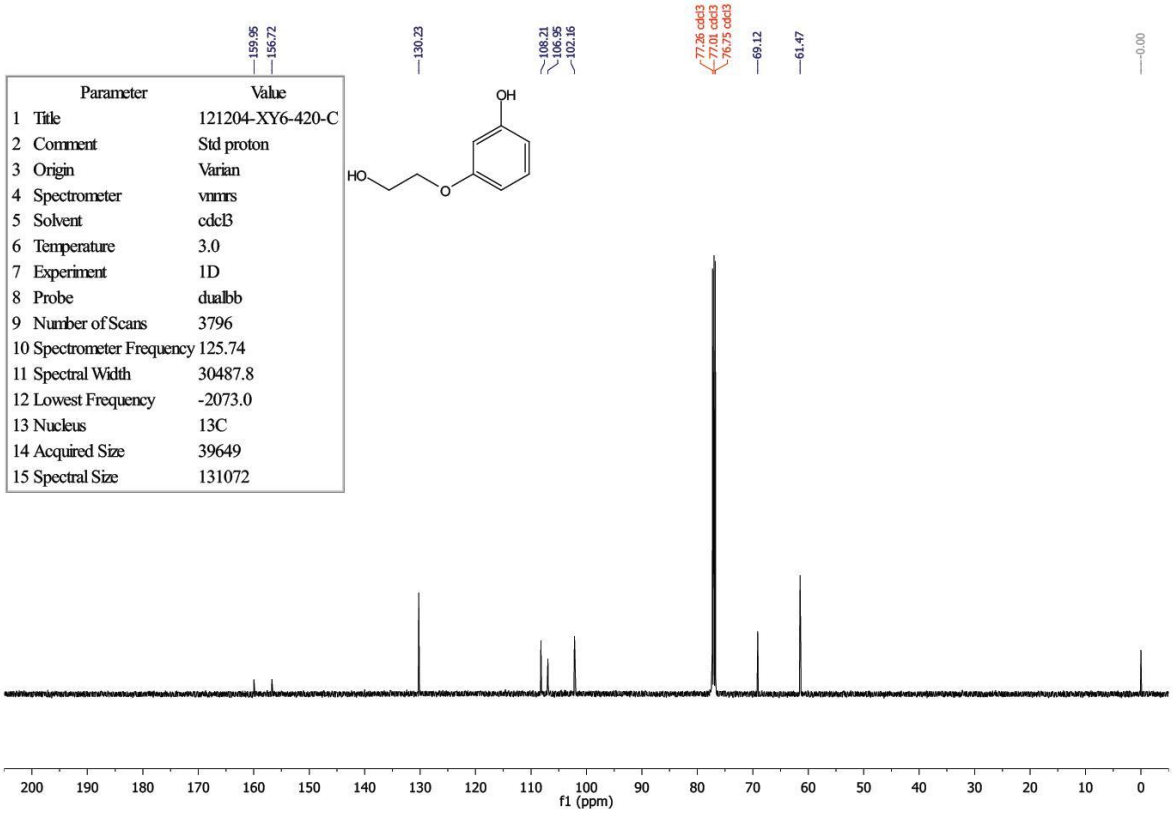

200.15 158.18 133.96 130.70 128.79 121.32 113.83 77.52 cdcl3 77.27 cdcl3 77.01 cdcl3 70.79 61.47 31.55 0.25
Parameter Value
1 Title 121212-XY6-423-C
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent cdcl3
6 Temperature 3.0
7 Experiment 1D
8 Probe dualbb
9 Number of Scans 464
10 Spectrometer Frequency 125.74
11 Spectral Width 30487.8
12 Lowest Frequency -2042.4
13 Nucleus 13C
14 Acquired Size 39649
15 Spectral Size 131072
O
CH3
OH
f1 (ppm)


7.49
7.34
7.26
4.19
4.18
4.17
4.05
4.04
4.03
4.02
2.04
2.03
2.02
0.00
-0.00
Parameter Value
1 Title 110404-SK6-667-H
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent cdcl3
6 Temperature 30.0
7 Experiment 1D
8 Probe dualbb
9 Number of Scans 16
10 Spectrometer Frequency 499.72
11 Spectral Width 8012.8
12 Lowest Frequency -1011.9
13 Nucleus 1H
14 Acquired Size 16415
15 Spectral Size 65536
HO
O
F
0.83
1.73
2.00
1.97
0.82
f1 (ppm)

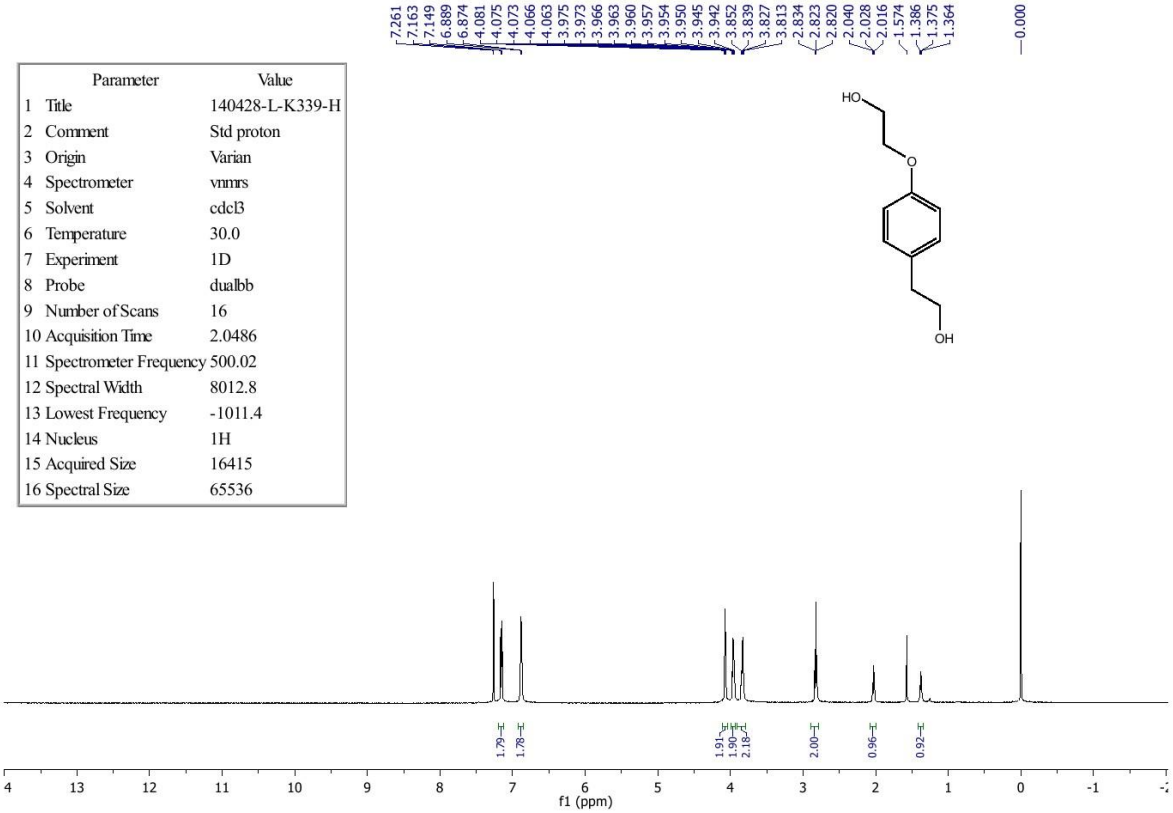

159.200
133.301
133.032
132.770
132.499
126.338
124.171
122.002
119.830
114.909
114.877
114.759
114.730
114.700
114.669
77.266 cdcl3
77.012 cdcl3
76.759 cdcl3
70.033
61.101
-0.000
Parameter Value
1 Title 140428-L-K339a-C
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent cdcl3
6 Temperature 3.0
7 Experiment 1D
8 Probe dualbb
9 Number of Scans 25600
10 Acquisition Time 1.3005
11 Spectrometer Frequency 125.74
12 Spectral Width 30487.8
13 Lowest Frequency -2071.6
14 Nucleus 13C
15 Acquired Size 39649
16 Spectral Size 131072
HO
O
F
f1 (ppm)



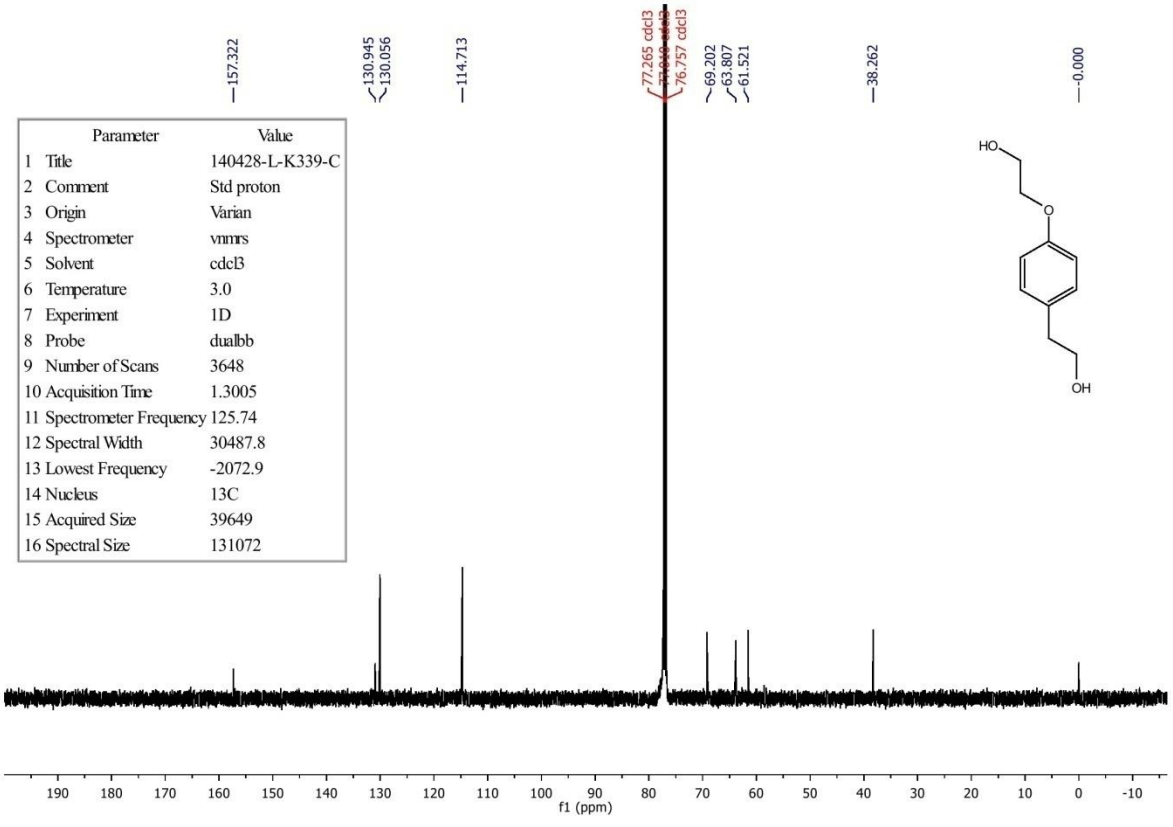
Parameter	Value
1 Title	121204-XY6-420-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	32
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1012.4
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



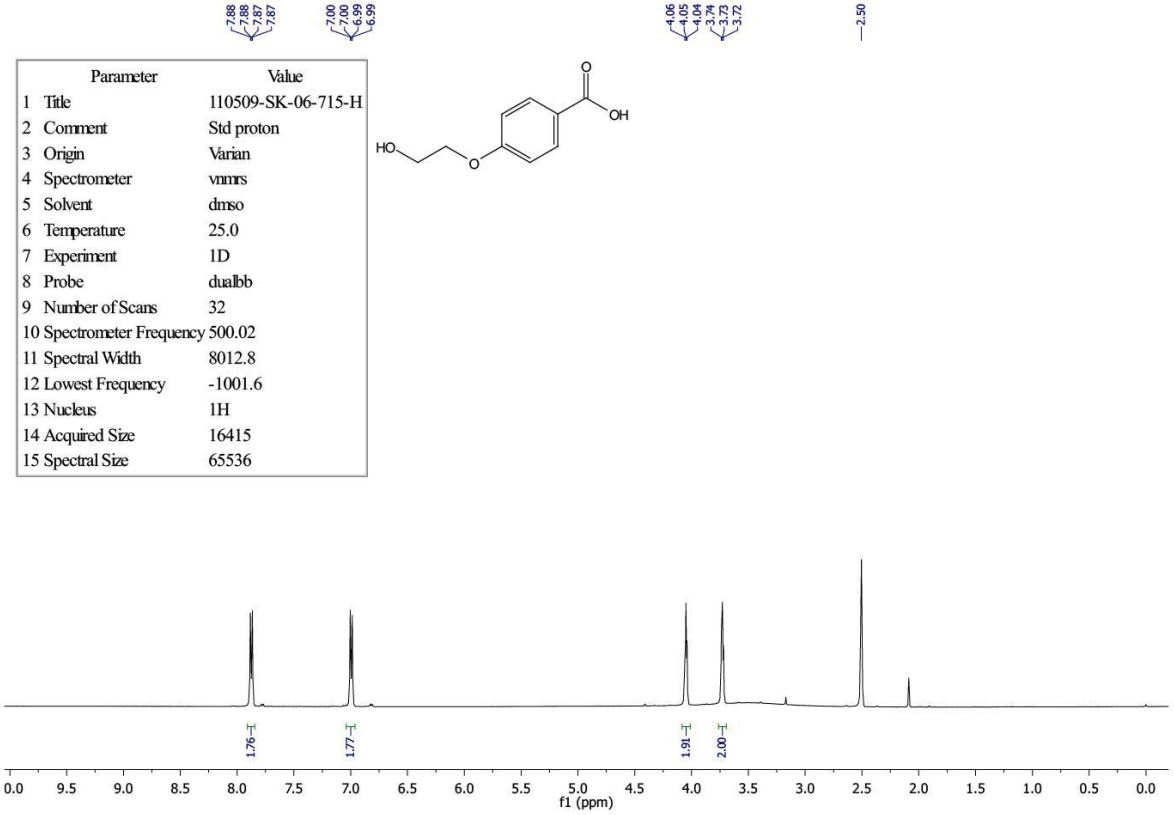
Parameter	Value
1 Title	121204-XY6-420-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	3796
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2073.0
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072

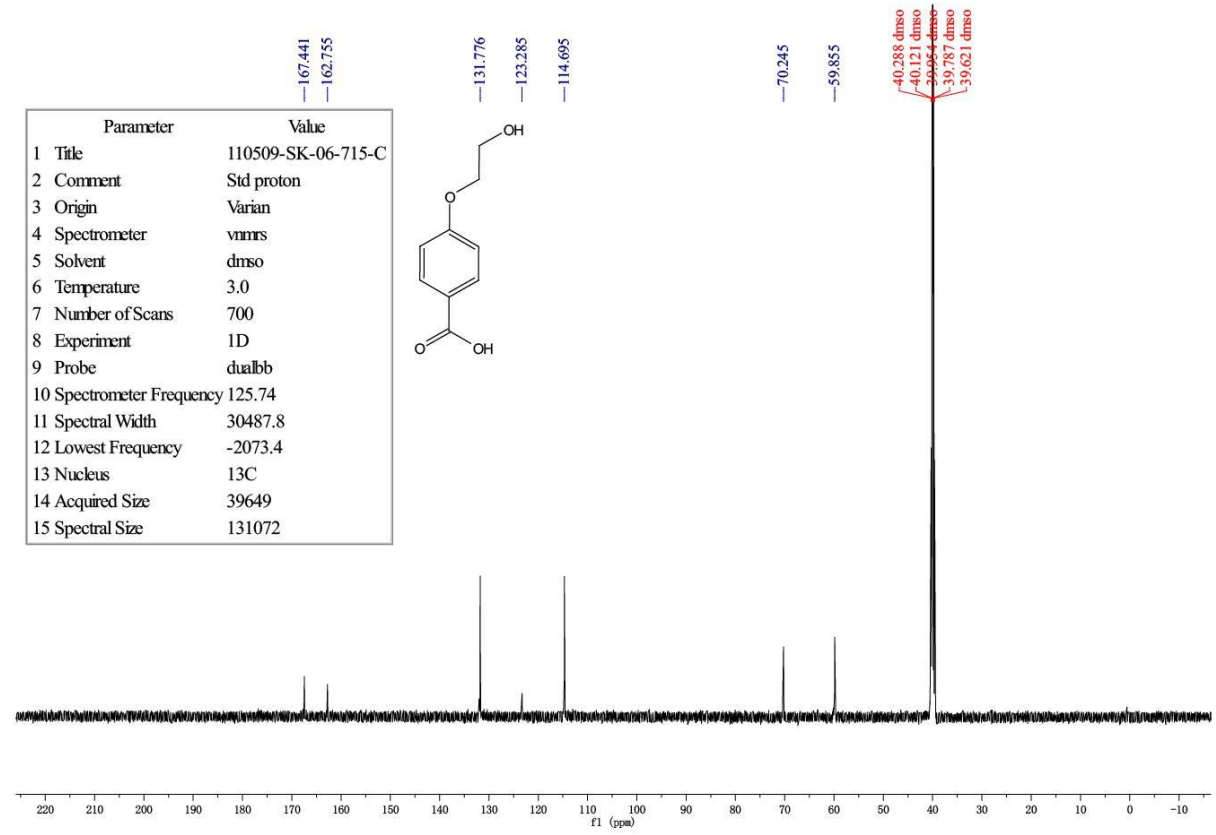


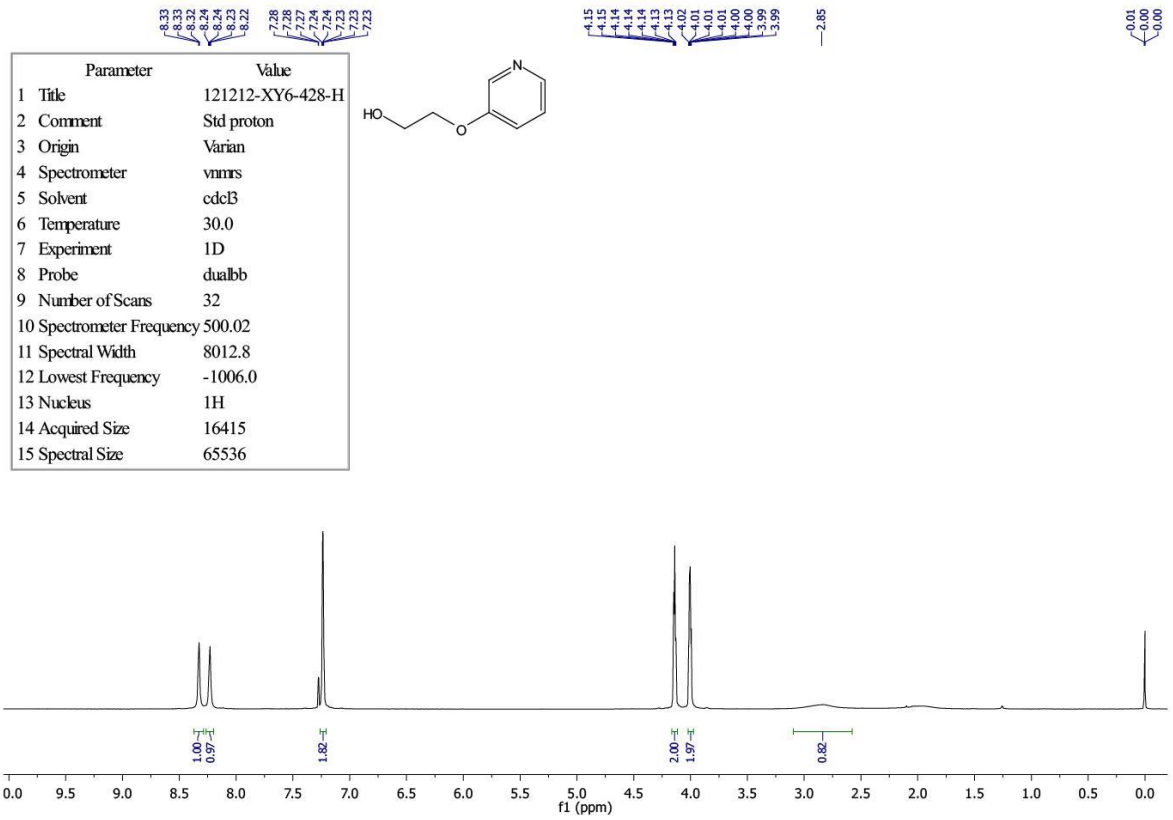
Parameter	Value
1 Title	140428-L-K339-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	16
10 Acquisition Time	2.0486
11 Spectrometer Frequency	500.02
12 Spectral Width	8012.8
13 Lowest Frequency	-1011.4
14 Nucleus	1H
15 Acquired Size	16415
16 Spectral Size	65536



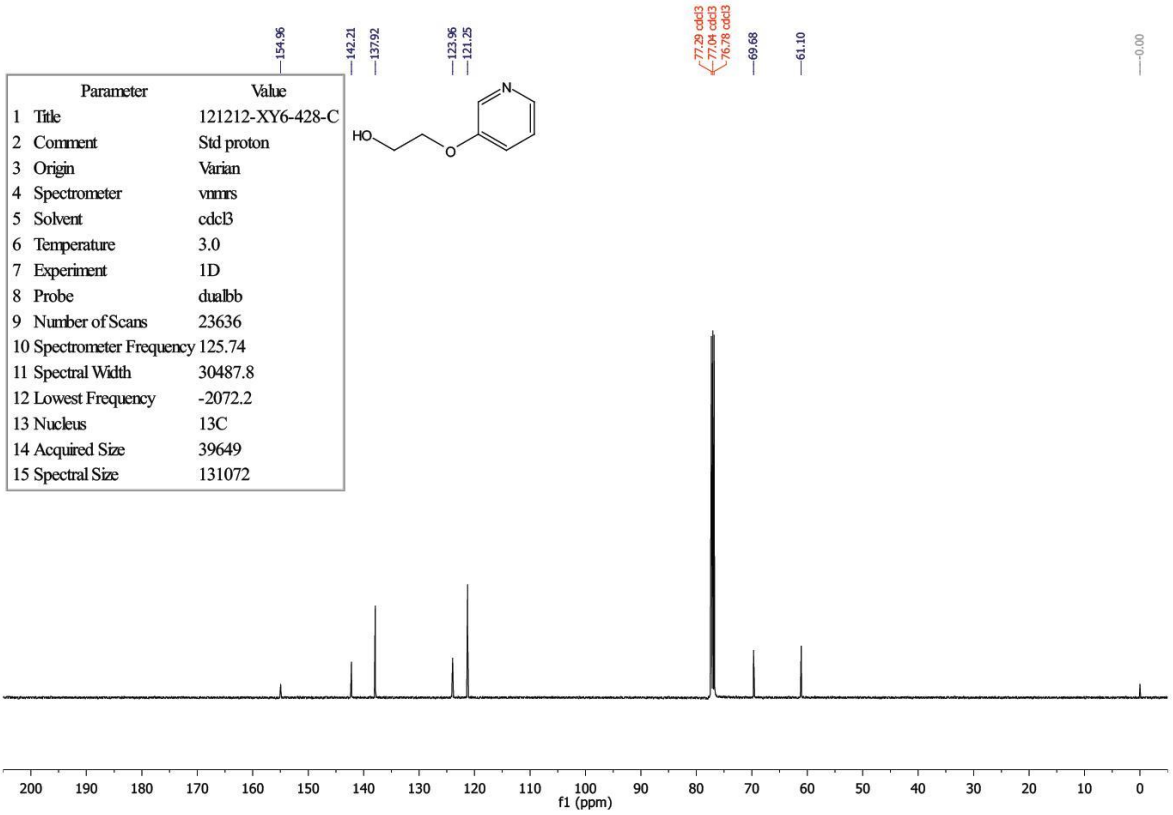
Parameter	Value
1 Title	140428-L-K339-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	3648
10 Acquisition Time	1.3005
11 Spectrometer Frequency	125.74
12 Spectral Width	30487.8
13 Lowest Frequency	-2072.9
14 Nucleus	13C
15 Acquired Size	39649
16 Spectral Size	131072


7.88
7.88
7.87
7.87
7.00
7.00
6.99
6.99
4.06
4.05
4.04
3.74
3.73
3.72
2.50
Parameter Value
1 Title 110509-SK-06-715-H
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent dmso
6 Temperature 25.0
7 Experiment 1D
8 Probe dualbb
9 Number of Scans 32
10 Spectrometer Frequency 500.02
11 Spectral Width 8012.8
12 Lowest Frequency -1001.6
13 Nucleus 1H
14 Acquired Size 16415
15 Spectral Size 65536
HO
O
O
OH
1.76
1.77
1.91
2.00
f1 (ppm)

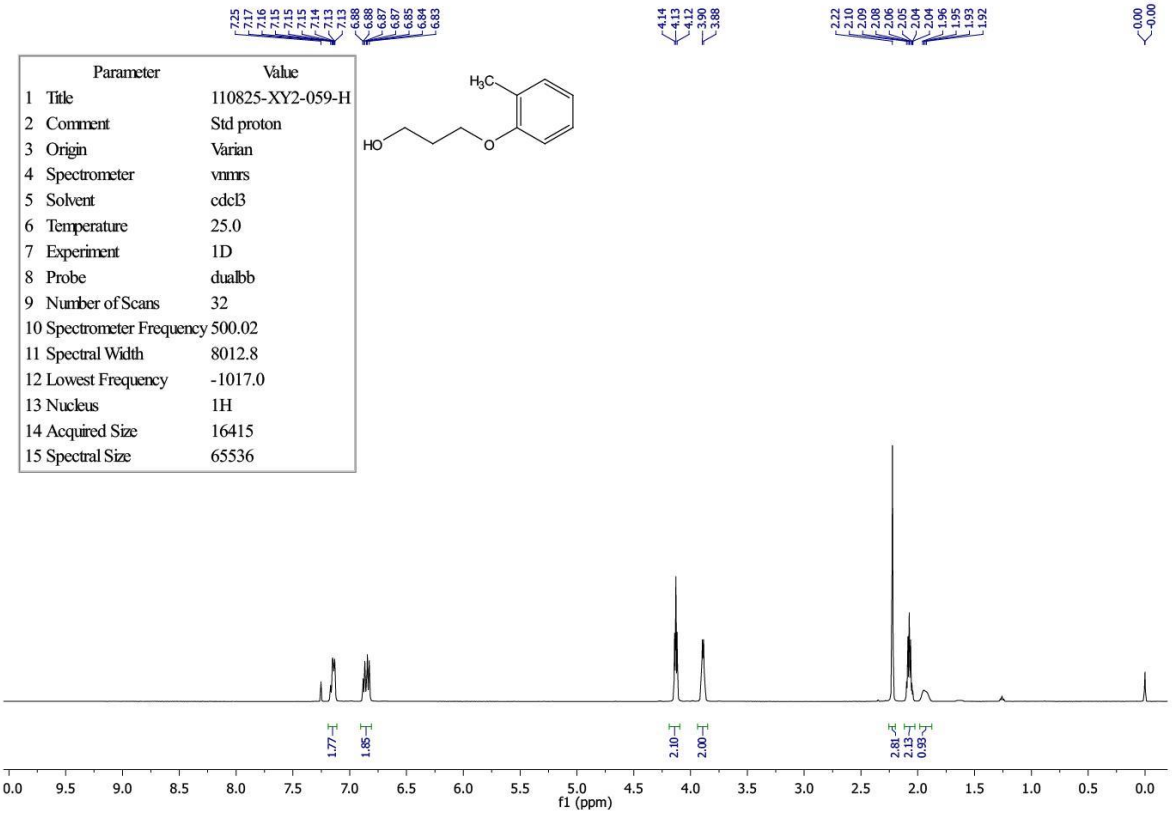

167.441
162.755
131.776
123.285
114.695
70.245
59.855
40.288 dmso
40.121 dmso
39.954 dmso
39.787 dmso
39.621 dmso
Parameter Value
1 Title 110509-SK-06-715-C
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent dmso
6 Temperature 3.0
7 Number of Scans 700
8 Experiment 1D
9 Probe dualbb
10 Spectrometer Frequency 125.74
11 Spectral Width 30487.8
12 Lowest Frequency -2073.4
13 Nucleus 13C
14 Acquired Size 39649
15 Spectral Size 131072
OH
O
O
OH
f1 (ppm)

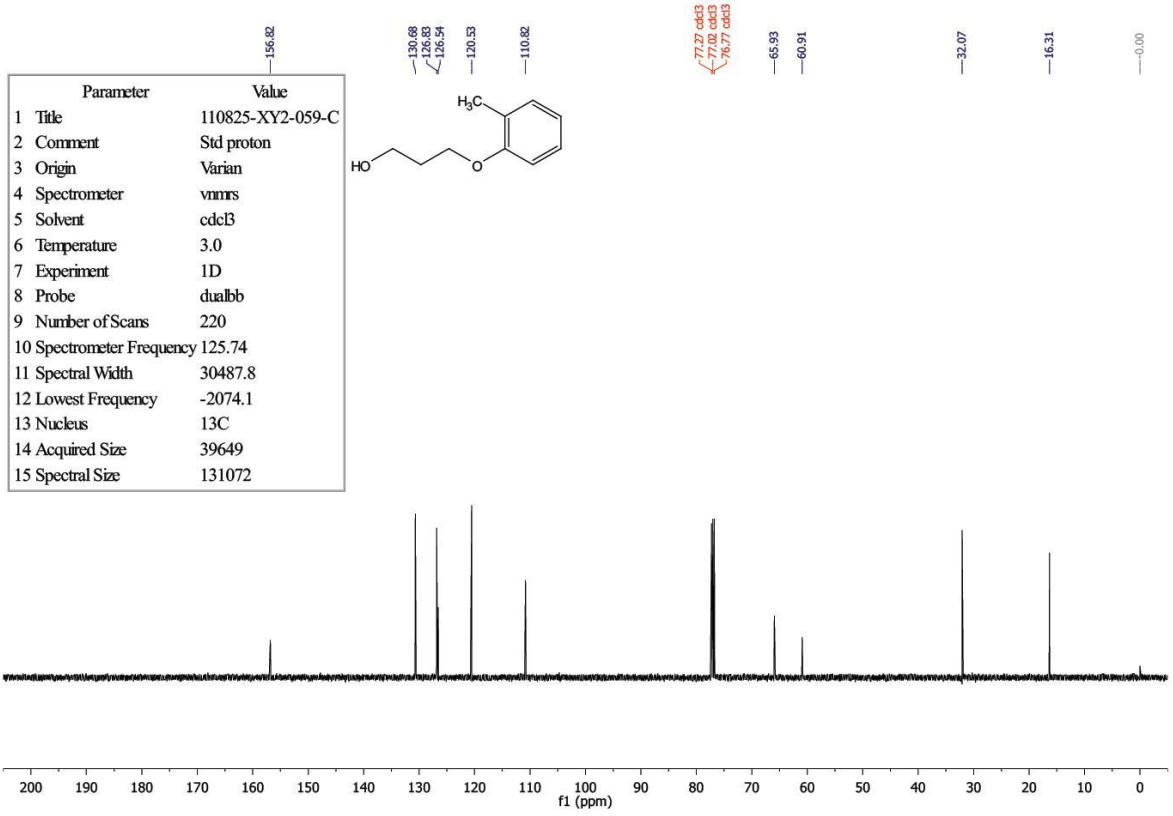


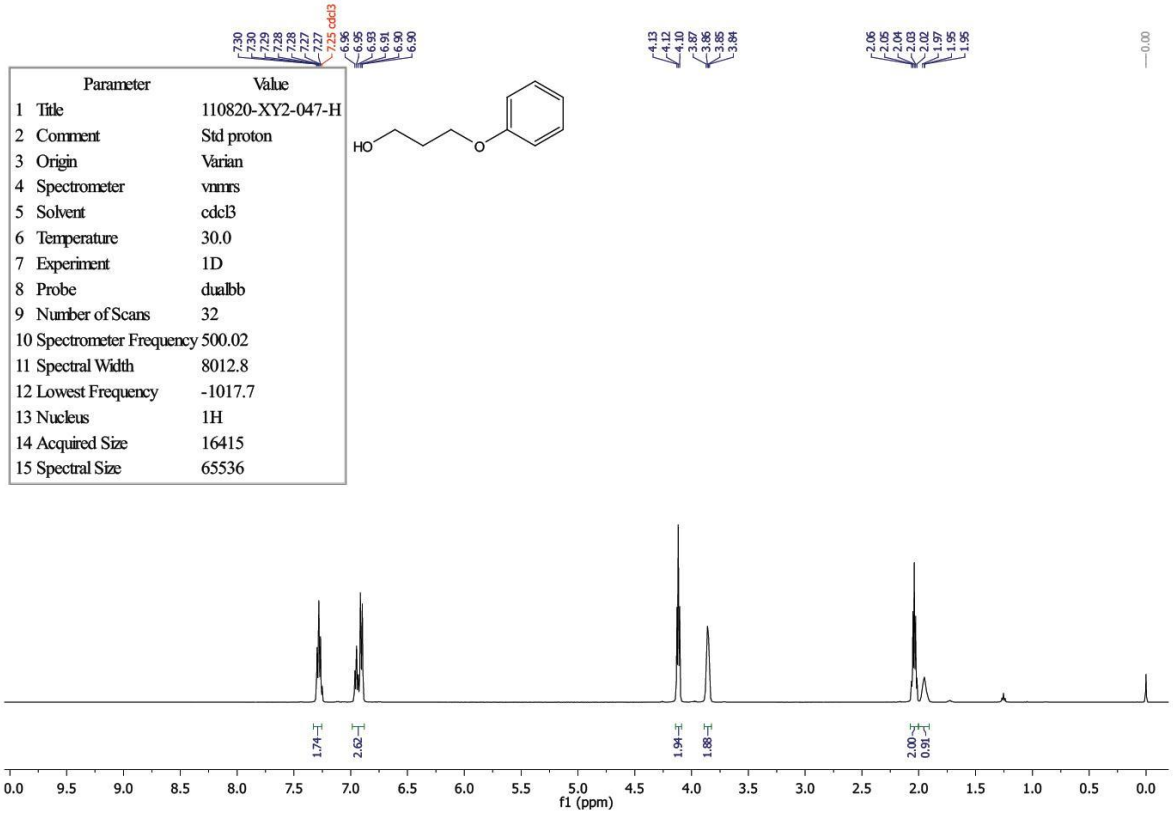
Parameter	Value
1 Title	121212-XY6-428-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	32
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1006.0
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



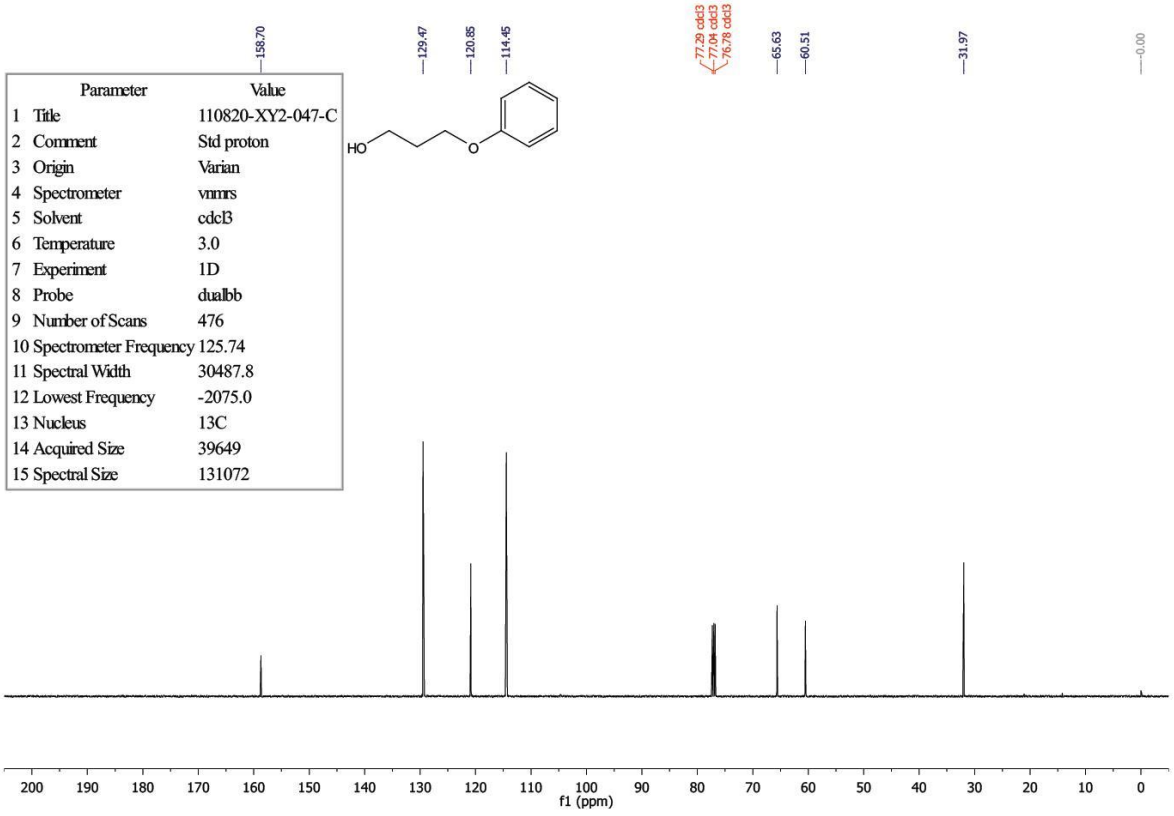
Parameter	Value
1 Title	121212-XY6-428-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	23636
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2072.2
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072


7.25 7.17 7.16 7.15 7.15 7.15 7.14 7.13 7.13 6.88 6.88 6.87 6.87 6.85 6.84 6.83
4.14 4.13 4.12 3.90 3.88
2.22 2.10 2.09 2.08 2.06 2.05 2.04 2.04 1.96 1.95 1.93 1.92
0.00 -0.00
Parameter Value
1 Title 110825-XY2-059-H
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent cdcl3
6 Temperature 25.0
7 Experiment 1D
8 Probe dualbb
9 Number of Scans 32
10 Spectrometer Frequency 500.02
11 Spectral Width 8012.8
12 Lowest Frequency -1017.0
13 Nucleus 1H
14 Acquired Size 16415
15 Spectral Size 65536
H3C
HO
O
1.77 1.85 2.10 2.00 2.81 2.13 0.93
f1 (ppm)

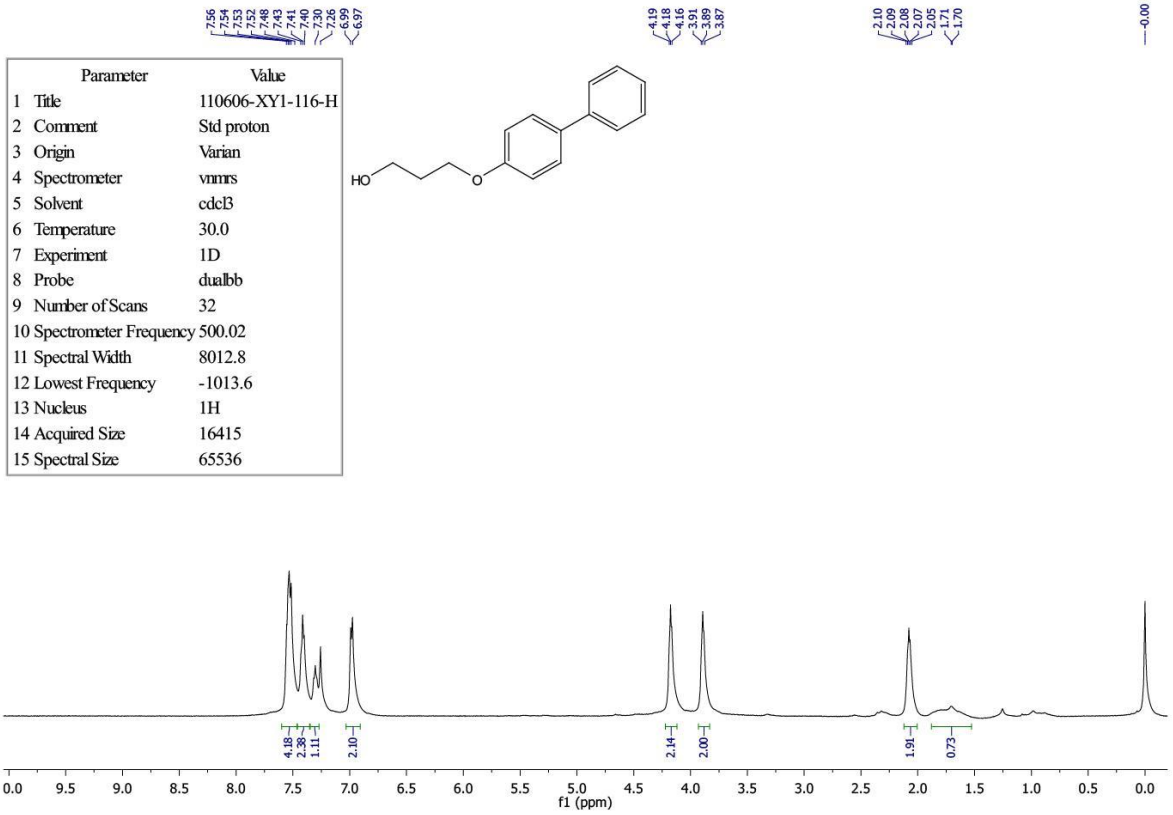

156.82
130.68 126.83 126.54 120.53 110.82
77.27 cdcl3 77.02 cdcl3 76.77 cdcl3
65.93 60.91 32.07 16.31 -0.00
Parameter Value
1 Title 110825-XY2-059-C
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent cdcl3
6 Temperature 3.0
7 Experiment 1D
8 Probe dualbb
9 Number of Scans 220
10 Spectrometer Frequency 125.74
11 Spectral Width 30487.8
12 Lowest Frequency -2074.1
13 Nucleus 13C
14 Acquired Size 39649
15 Spectral Size 131072
H3C
HO
O
f1 (ppm)



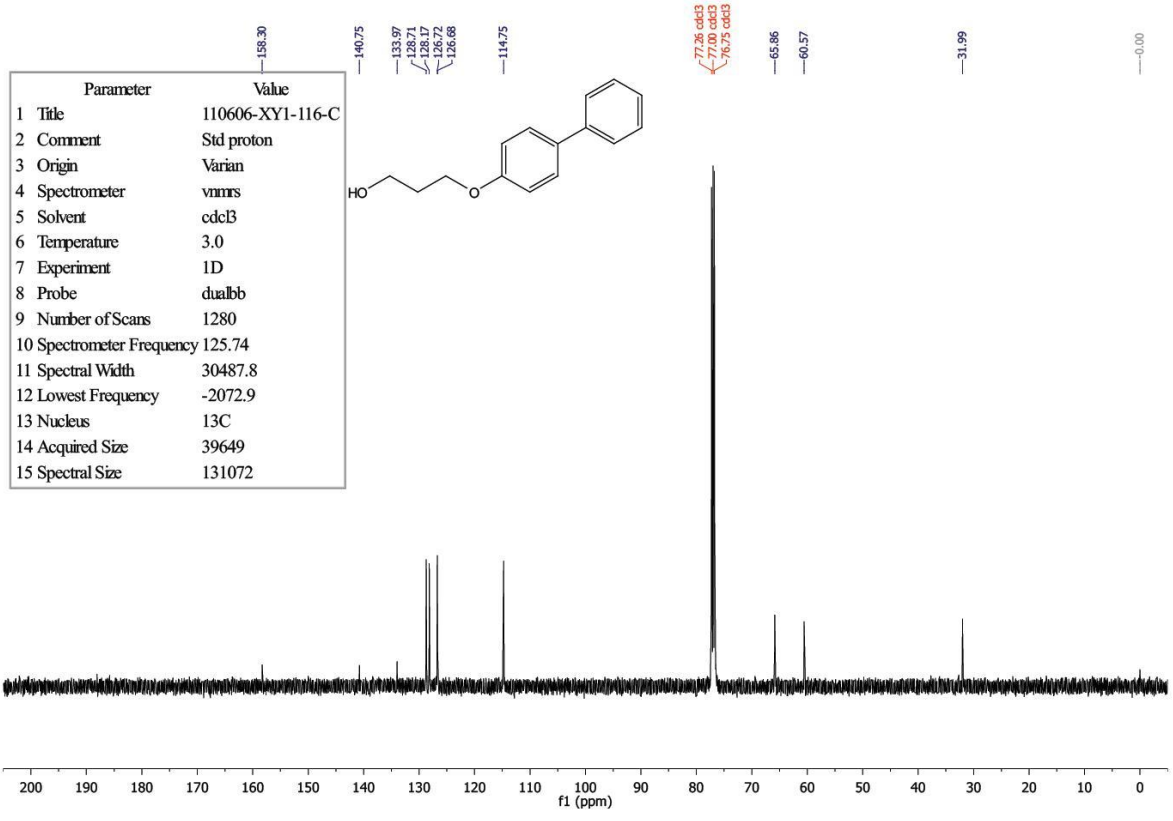
Parameter	Value
1 Title	110820-XY2-047-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	32
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1017.7
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



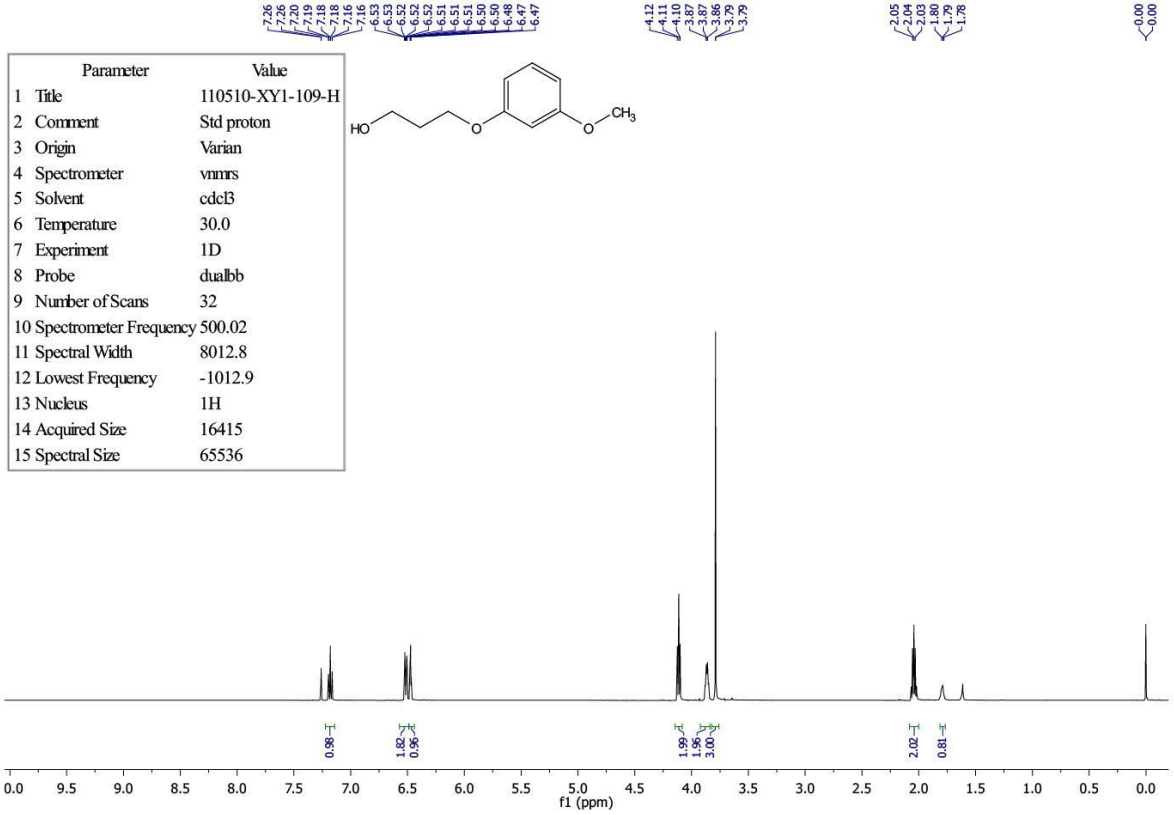
Parameter	Value
1 Title	110820-XY2-047-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	476
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2075.0
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072

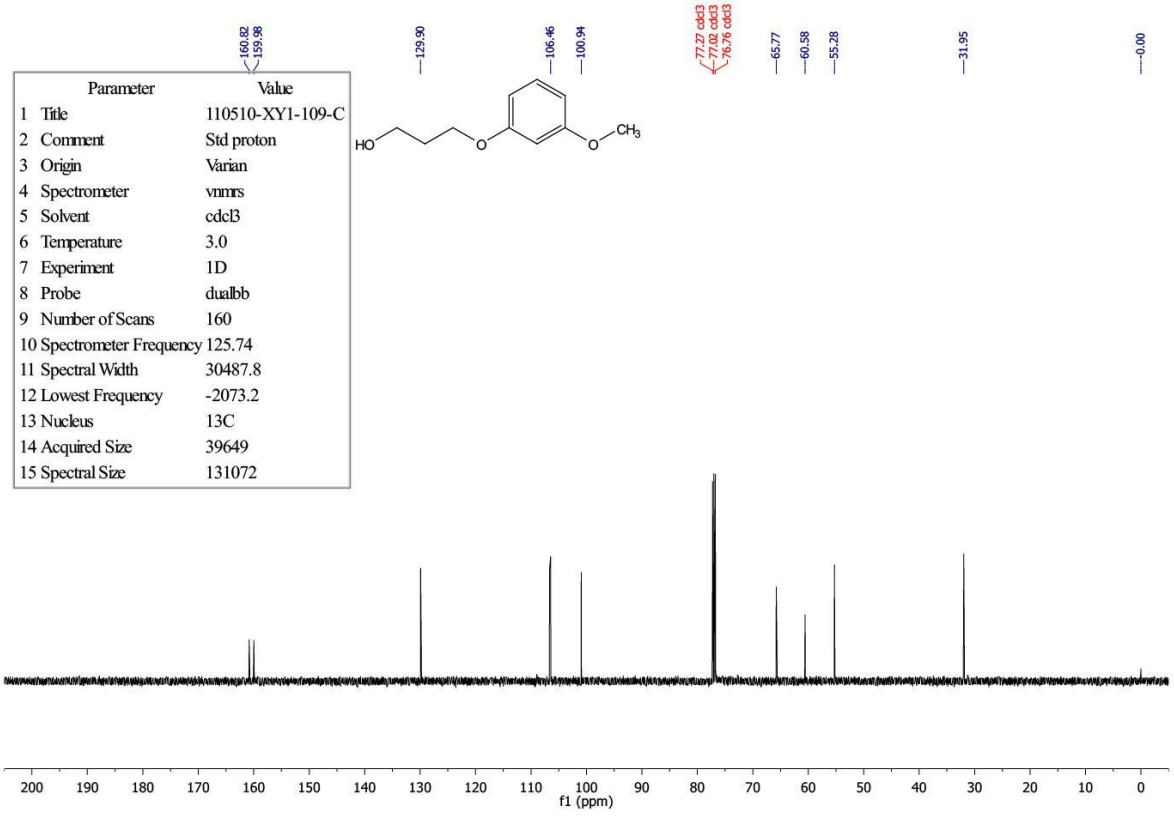


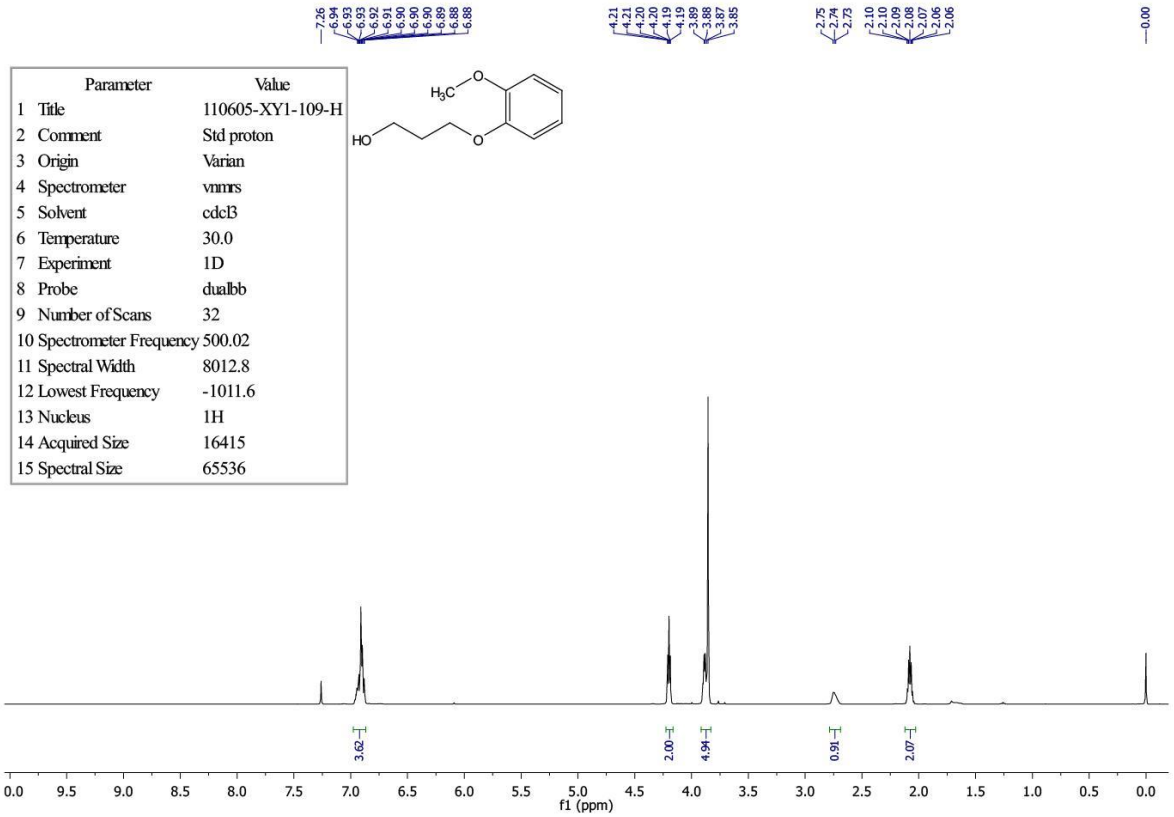
Parameter	Value
1 Title	110606-XY1-116-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	32
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1013.6
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



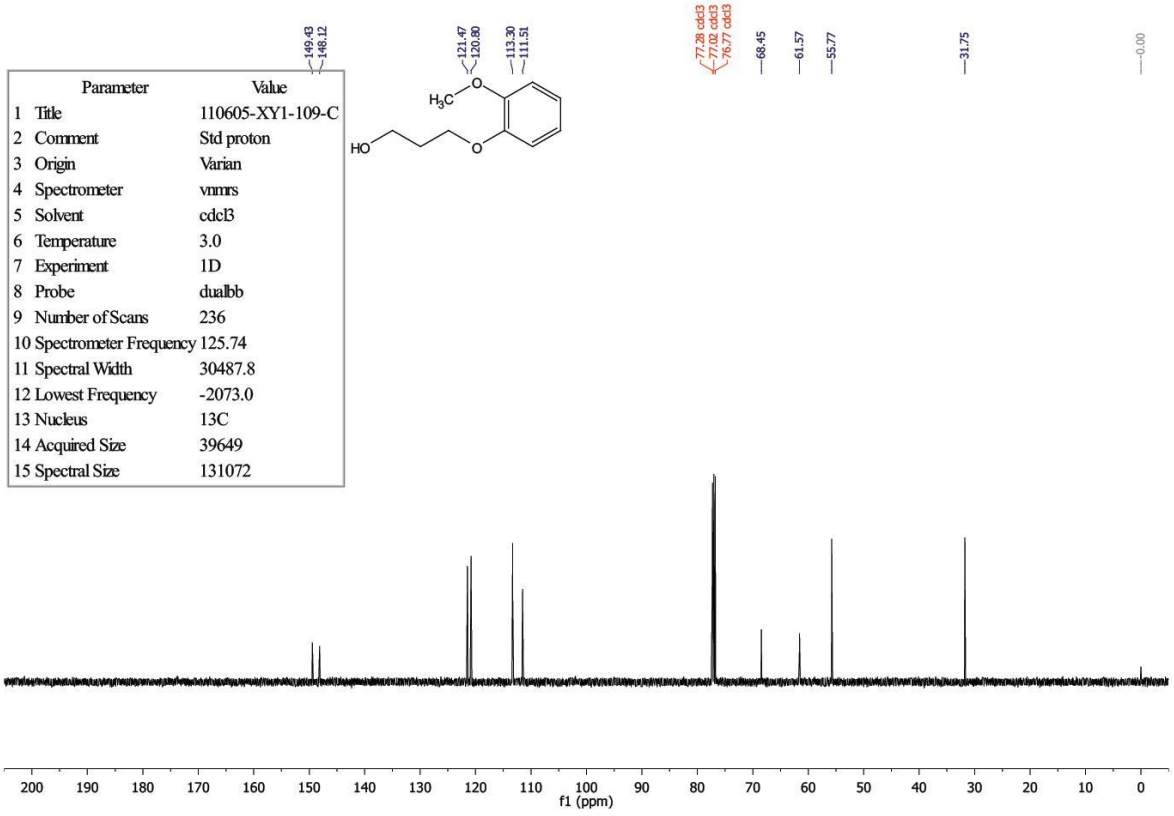
Parameter	Value
1 Title	110606-XY1-116-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	1280
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2072.9
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072


7.26 7.26 7.20 7.19 7.18 7.18 7.16 7.16 6.53 6.53 6.52 6.52 6.52 6.51 6.51 6.50 6.50 6.48 6.47 6.47
4.12 4.11 4.10 3.87 3.87 3.86 3.79 3.79
2.05 2.04 2.03 1.80 1.79 1.78
0.00 0.00
Parameter Value
1 Title 110510-XY1-109-H
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent cdcl3
6 Temperature 30.0
7 Experiment 1D
8 Probe dualbb
9 Number of Scans 32
10 Spectrometer Frequency 500.02
11 Spectral Width 8012.8
12 Lowest Frequency -1012.9
13 Nucleus 1H
14 Acquired Size 16415
15 Spectral Size 65536
HO
O
O
CH3
0.98 1.82 0.96 1.99 1.96 3.00 2.02 0.81
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

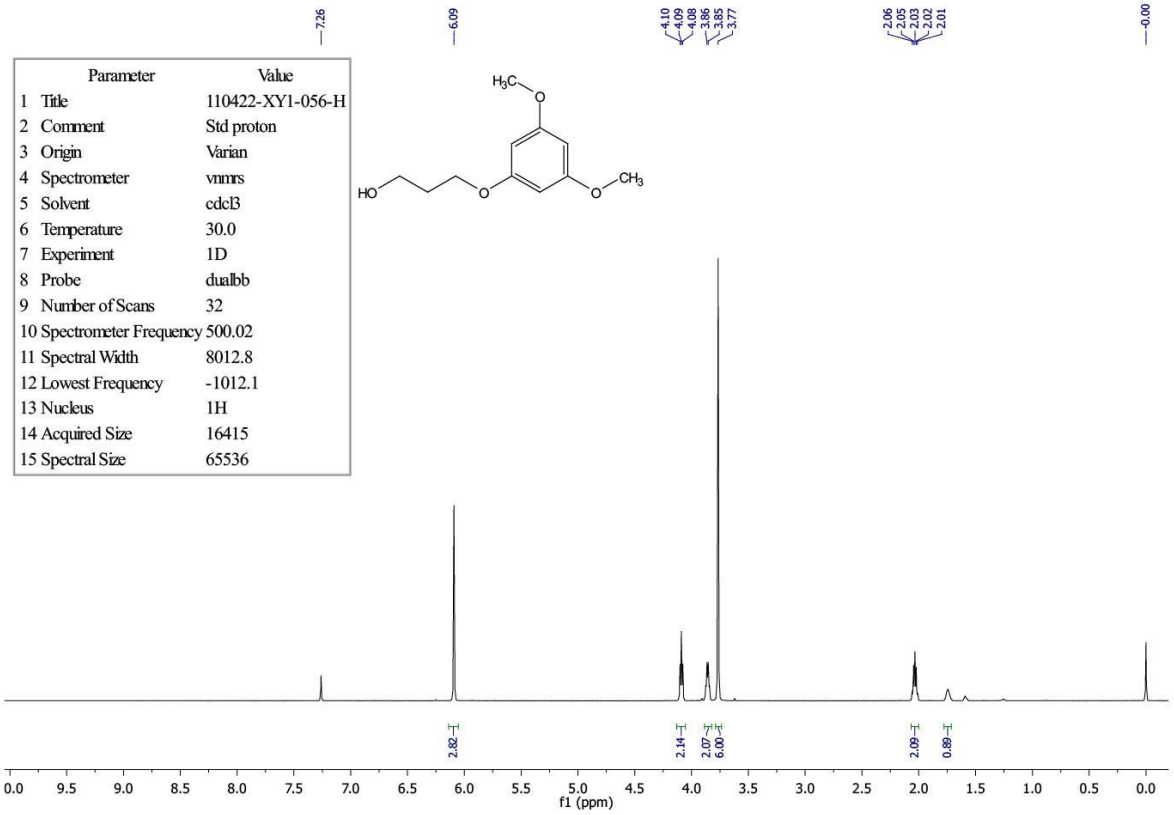

160.82 159.98
129.90
106.46 100.94
77.27 cdcl3 77.02 cdcl3 76.76 cdcl3
65.77 60.58 55.28
31.95
0.00
Parameter Value
1 Title 110510-XY1-109-C
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent cdcl3
6 Temperature 3.0
7 Experiment 1D
8 Probe dualbb
9 Number of Scans 160
10 Spectrometer Frequency 125.74
11 Spectral Width 30487.8
12 Lowest Frequency -2073.2
13 Nucleus 13C
14 Acquired Size 39649
15 Spectral Size 131072
HO
O
O
CH3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

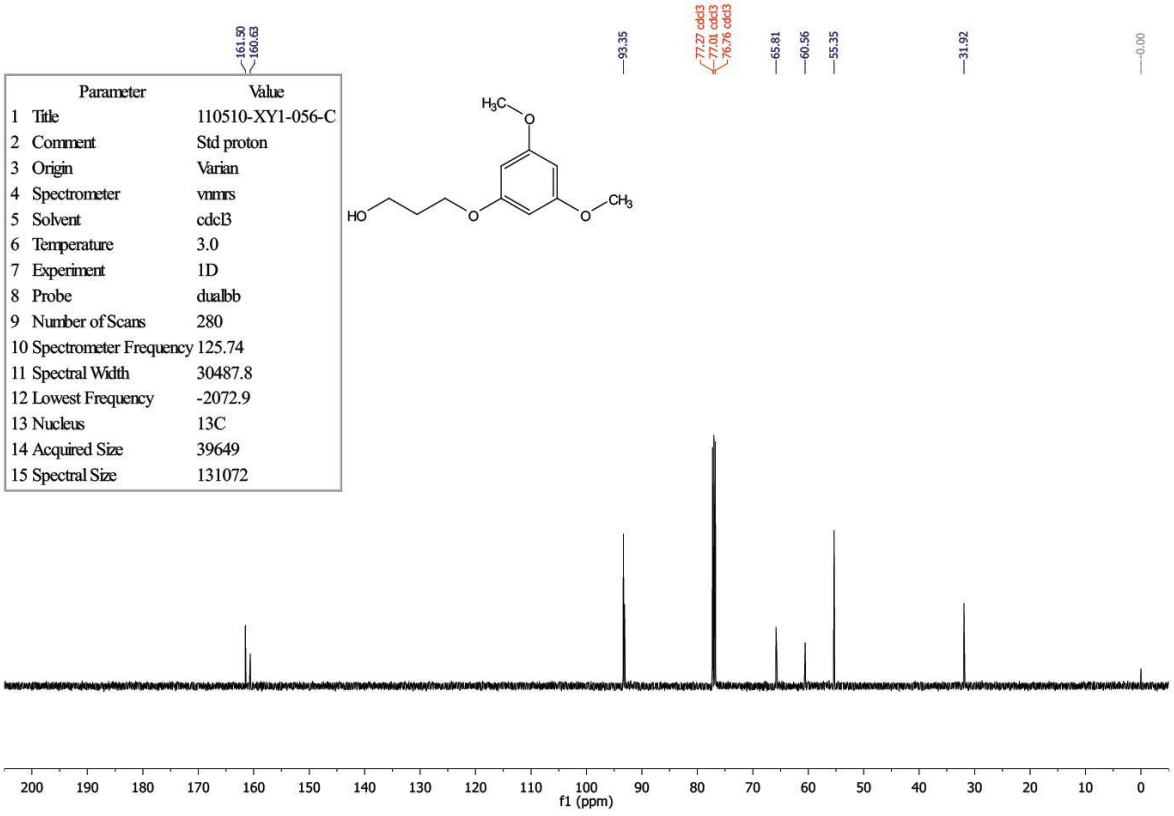


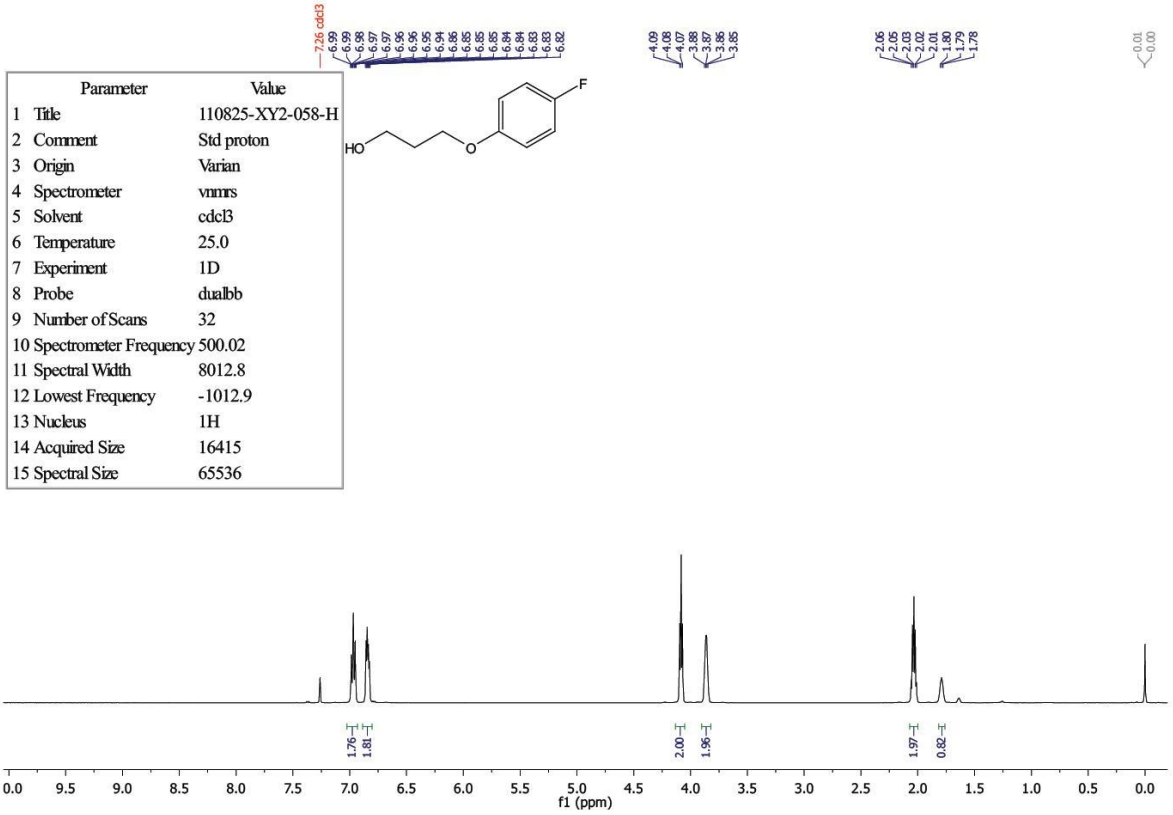
Parameter	Value
1 Title	110605-XY1-109-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	32
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1011.6
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



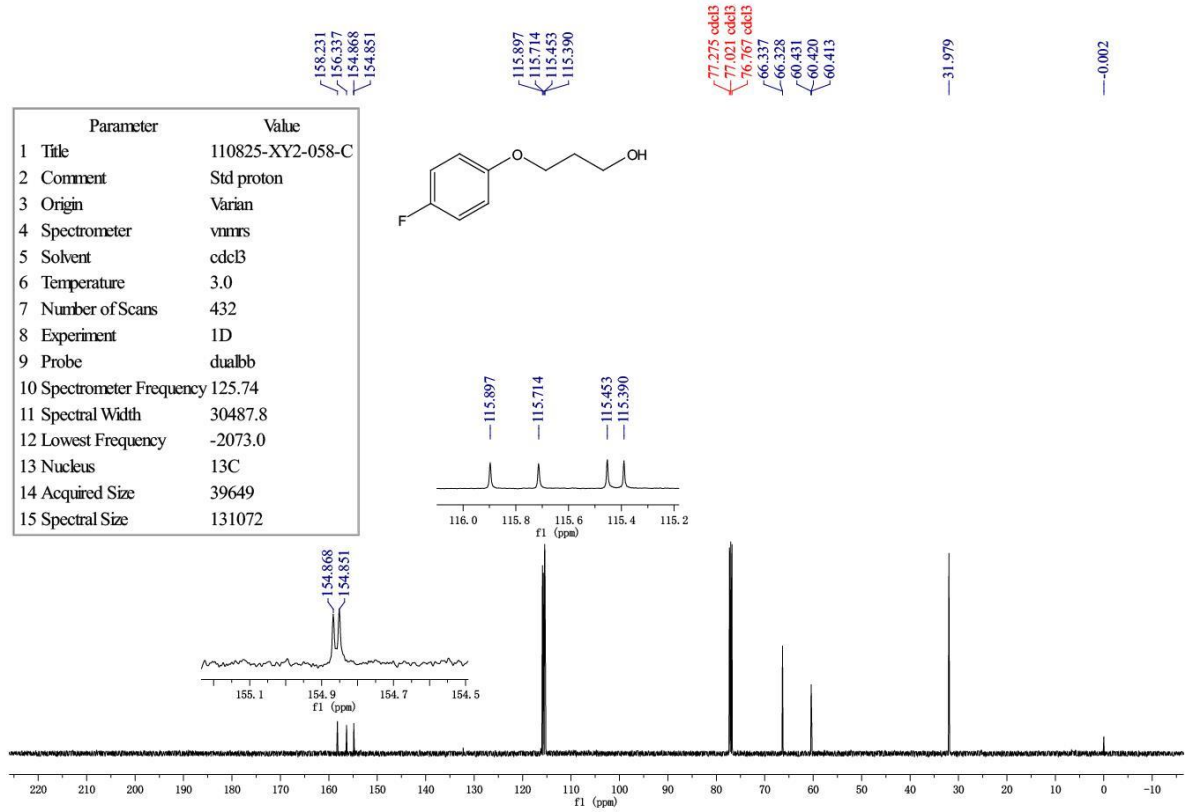
Parameter	Value
1 Title	110605-XY1-109-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	236
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2073.0
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072


7.26
6.09
4.10
4.09
4.08
3.86
3.85
3.77
2.06
2.05
2.03
2.02
2.01
0.00
Parameter Value
1 Title 110422-XY1-056-H
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent cdcl3
6 Temperature 30.0
7 Experiment 1D
8 Probe dualbb
9 Number of Scans 32
10 Spectrometer Frequency 500.02
11 Spectral Width 8012.8
12 Lowest Frequency -1012.1
13 Nucleus 1H
14 Acquired Size 16415
15 Spectral Size 65536
H3C
O
HO
O
O
CH3
2.62
2.14
2.07
6.00
2.09
0.89
f1 (ppm)

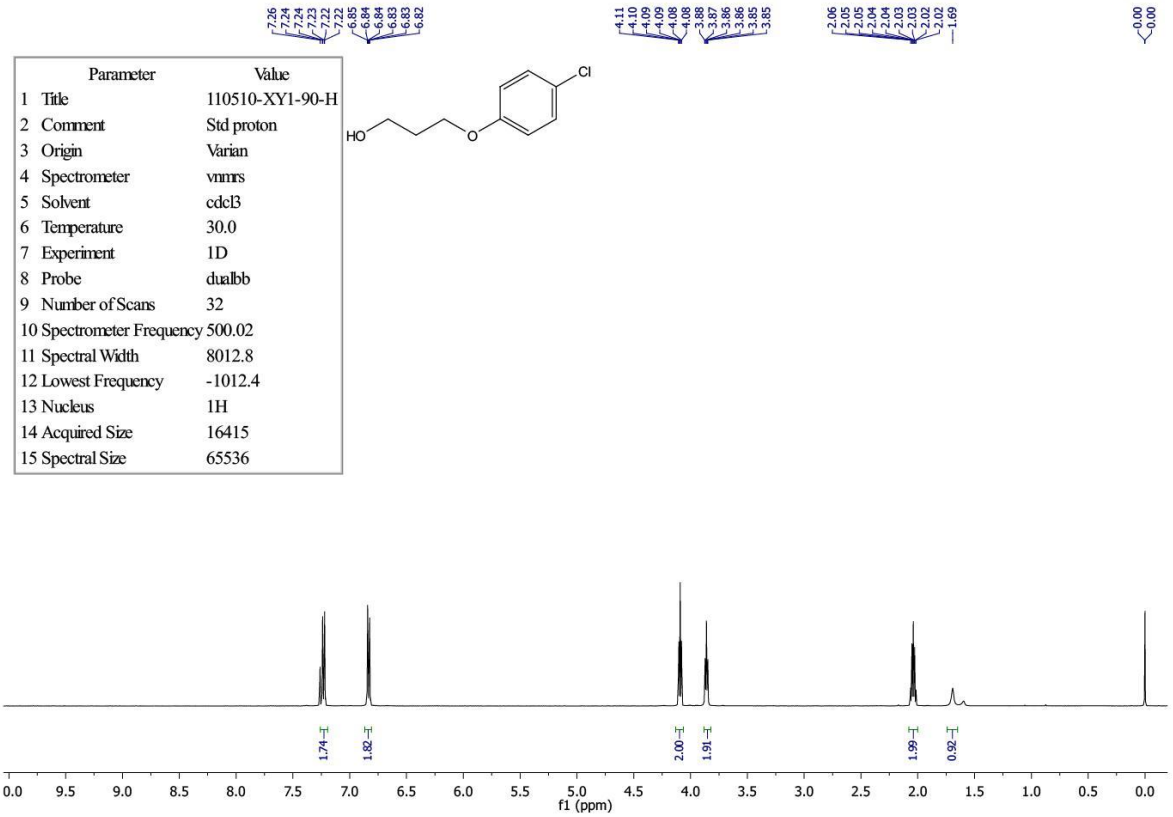

161.50
160.63
93.35
77.27 cdcl3
77.01 cdcl3
76.76 cdcl3
65.81
60.56
55.35
31.92
0.00
Parameter Value
1 Title 110510-XY1-056-C
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent cdcl3
6 Temperature 3.0
7 Experiment 1D
8 Probe dualbb
9 Number of Scans 280
10 Spectrometer Frequency 125.74
11 Spectral Width 30487.8
12 Lowest Frequency -2072.9
13 Nucleus 13C
14 Acquired Size 39649
15 Spectral Size 131072
H3C
O
HO
O
O
CH3
f1 (ppm)



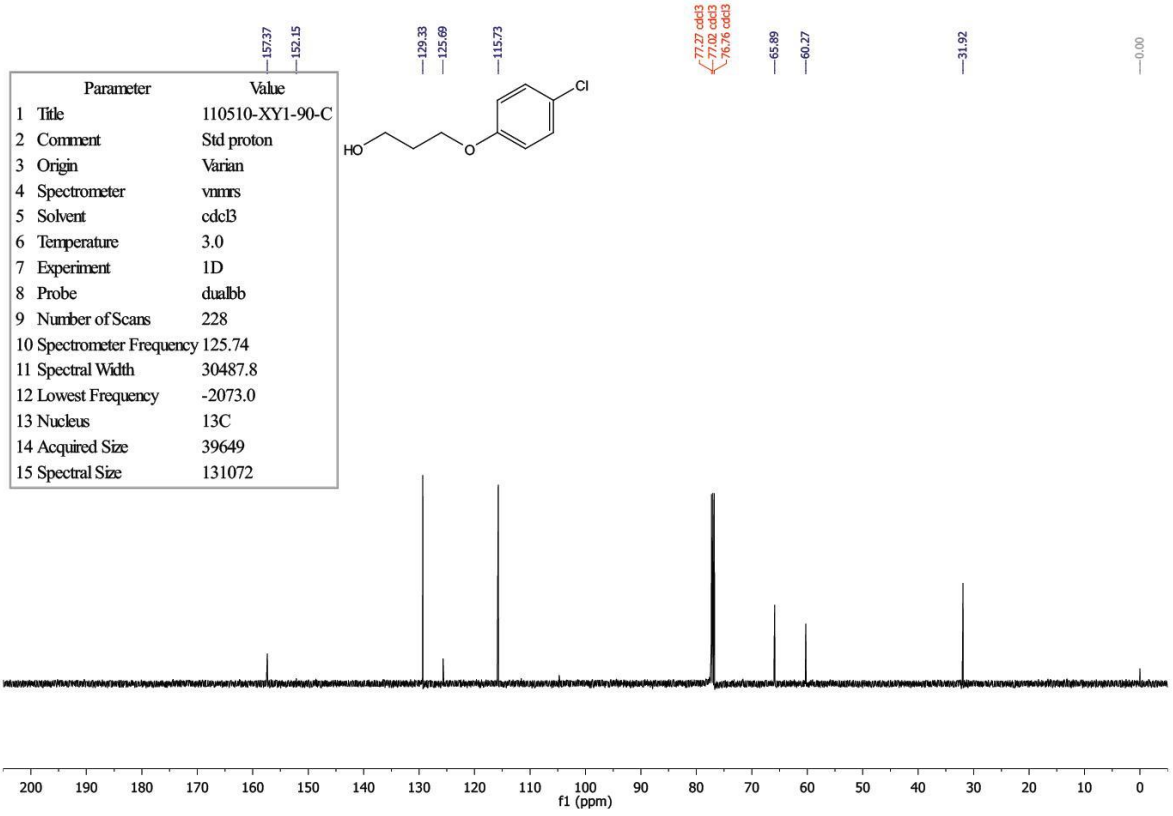
Parameter	Value
1 Title	110825-XY2-058-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	25.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	32
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1012.9
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



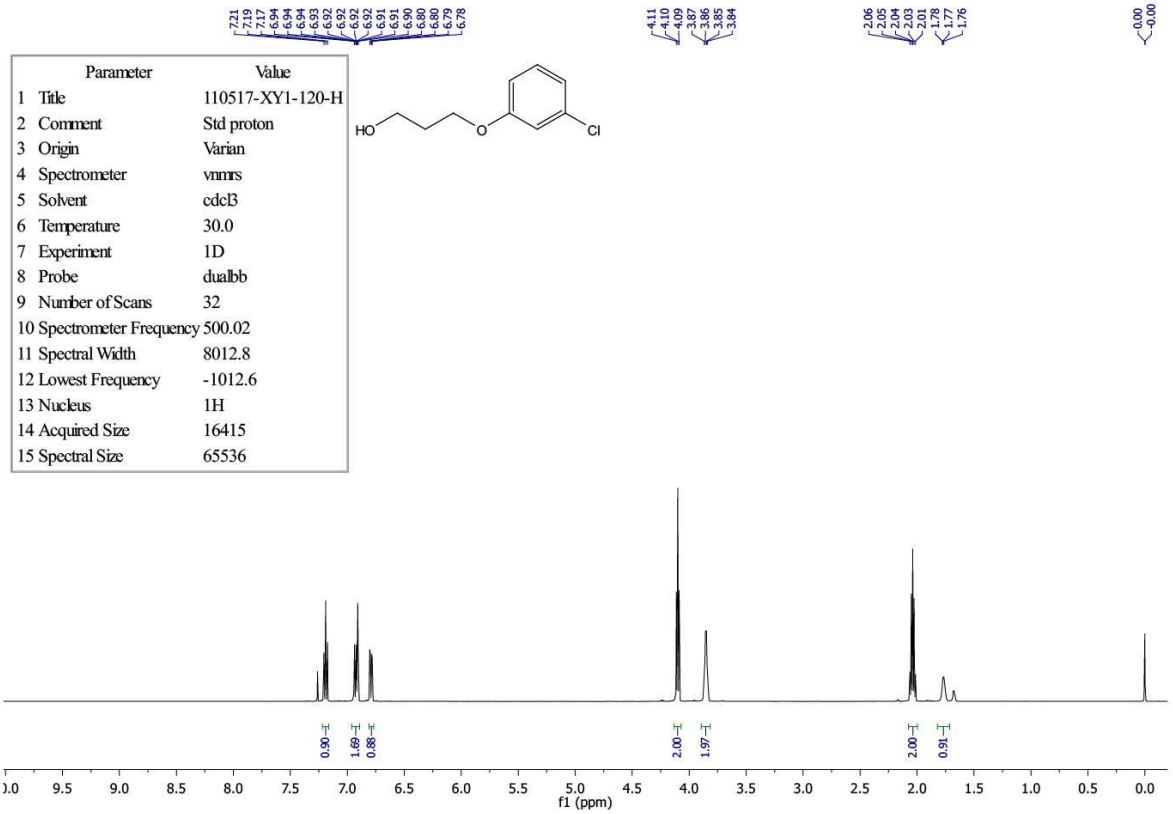
Parameter	Value
1 Title	110825-XY2-058-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Number of Scans	432
8 Experiment	1D
9 Probe	dualbb
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2073.0
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072



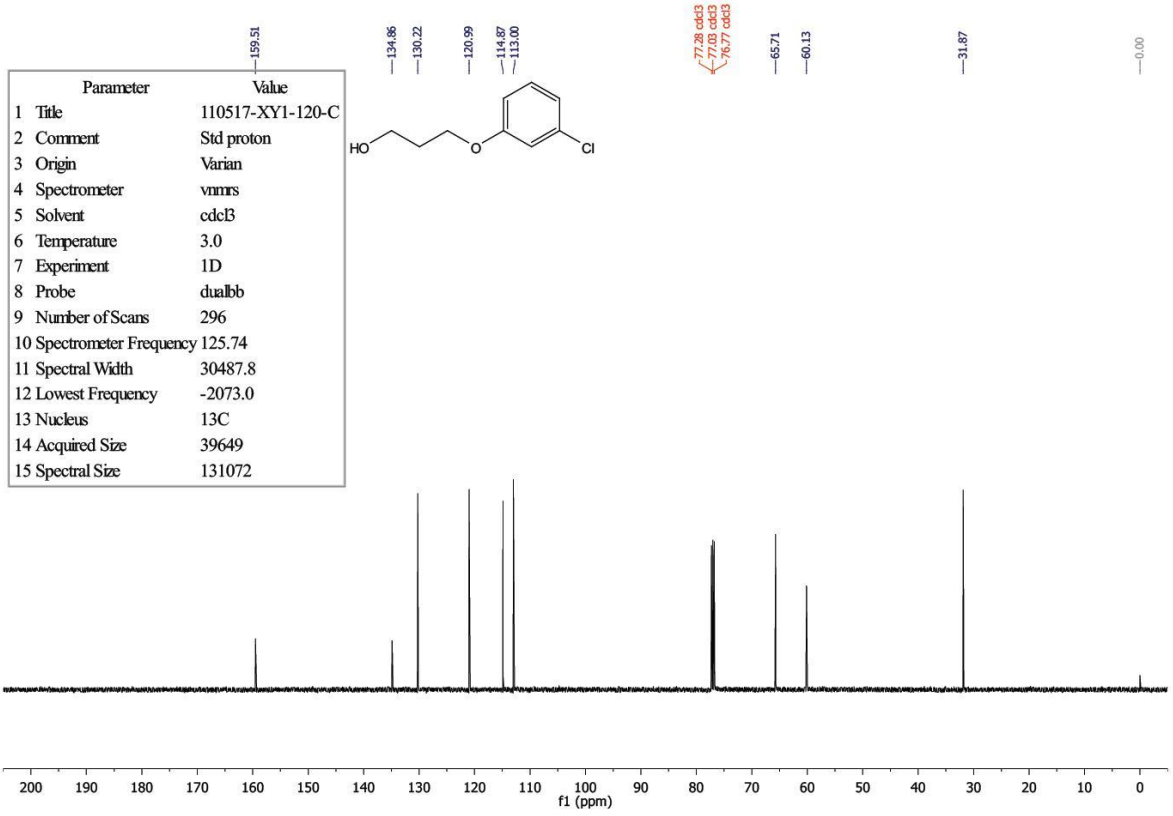
Parameter	Value
1 Title	110510-XY1-90-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	32
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1012.4
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



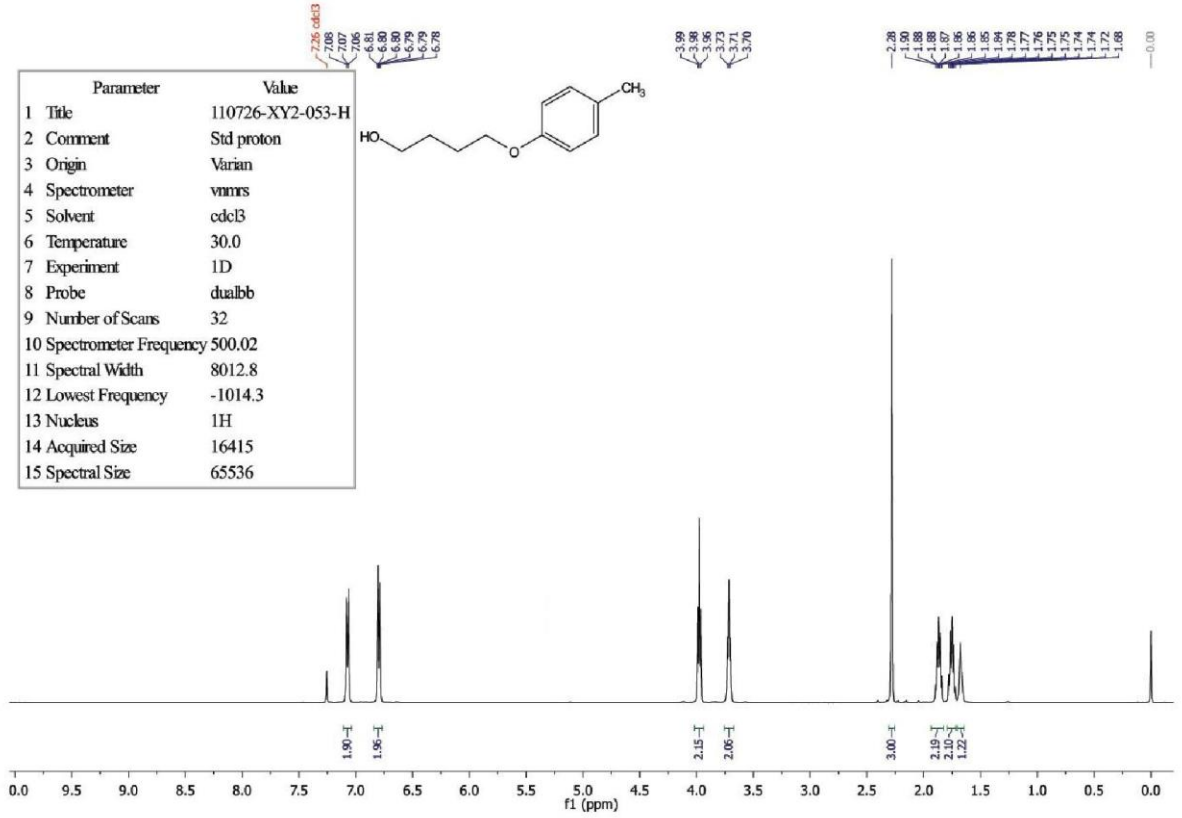
Parameter	Value
1 Title	110510-XY1-90-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	228
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2073.0
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072



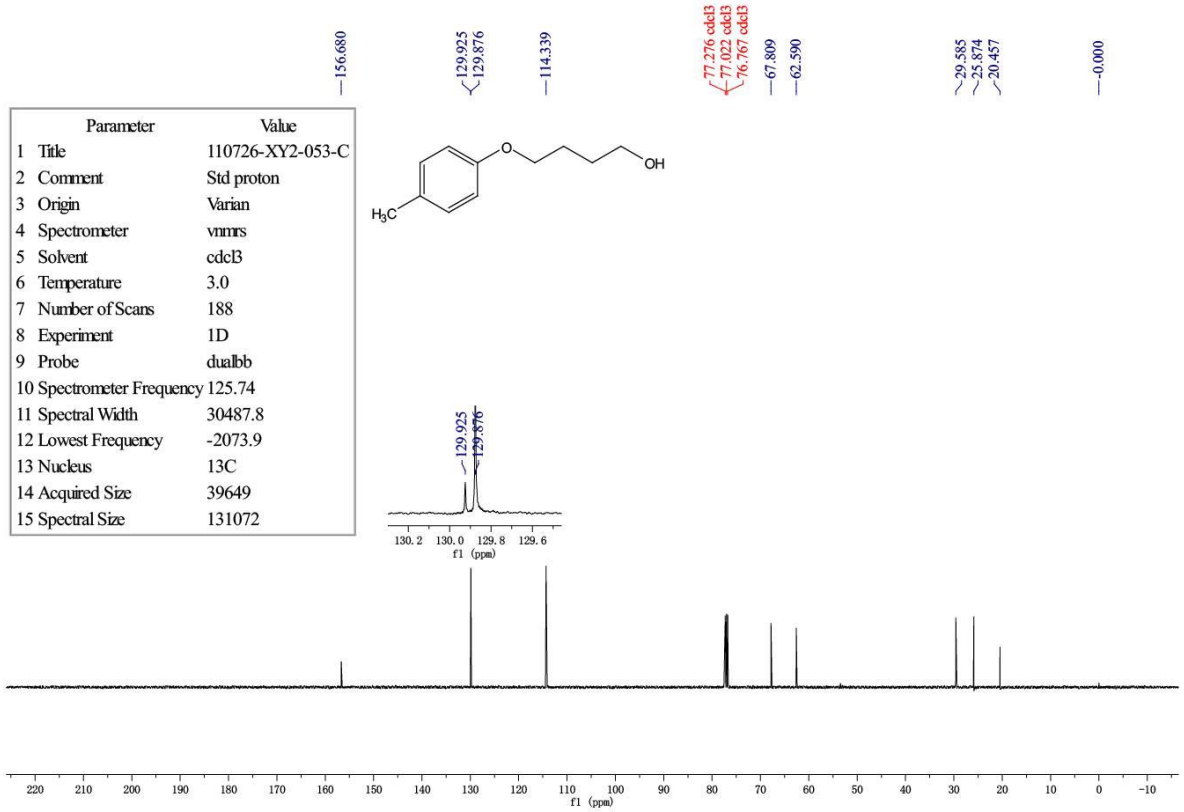
Parameter	Value
1 Title	110517-XY1-120-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	32
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1012.6
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



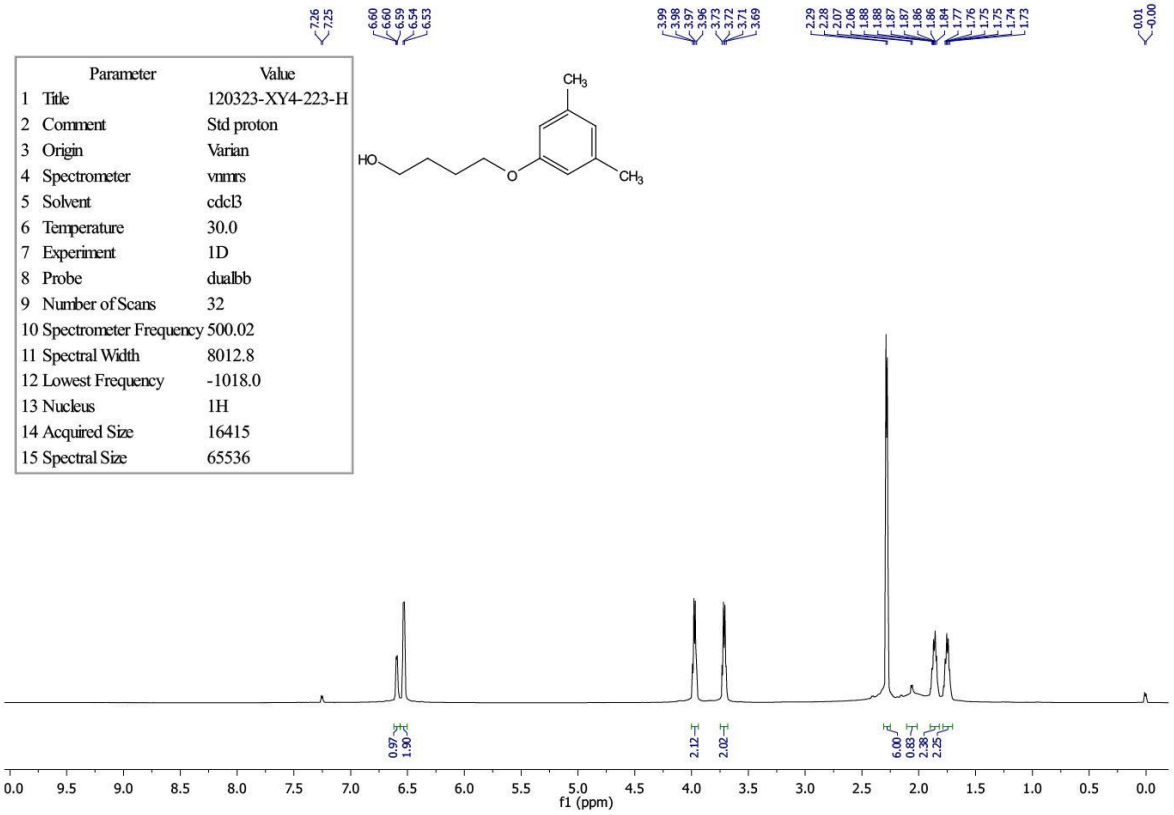
Parameter	Value
1 Title	110517-XY1-120-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	296
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2073.0
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072



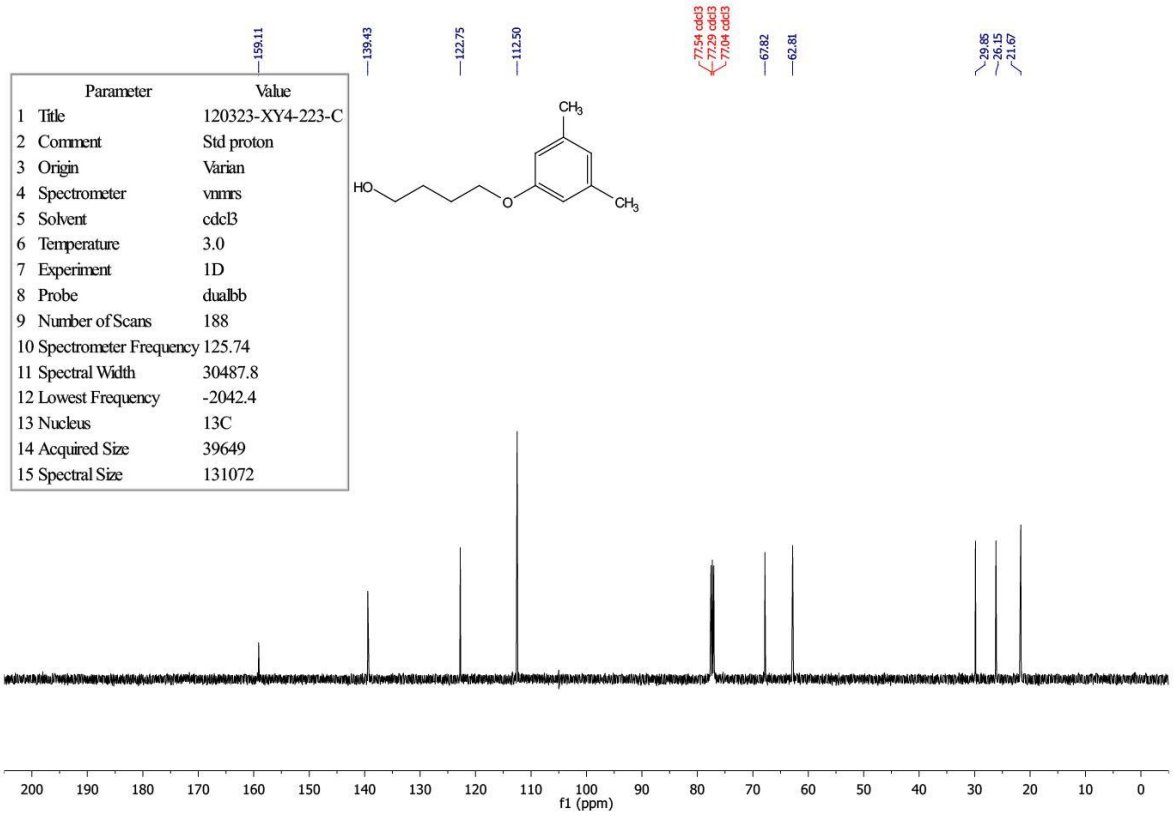
Parameter	Value
1 Title	110726-XY2-053-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	32
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1014.3
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



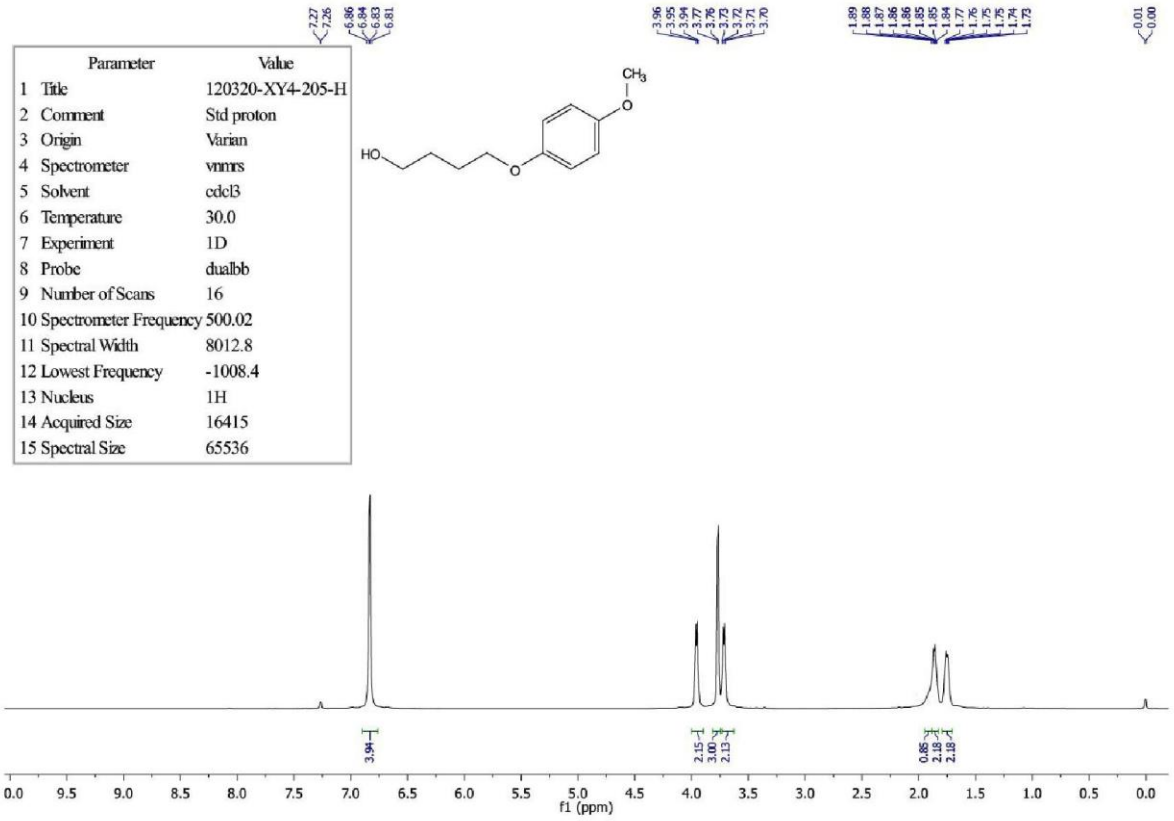
Parameter	Value
1 Title	110726-XY2-053-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Number of Scans	188
8 Experiment	1D
9 Probe	dualbb
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2073.9
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072



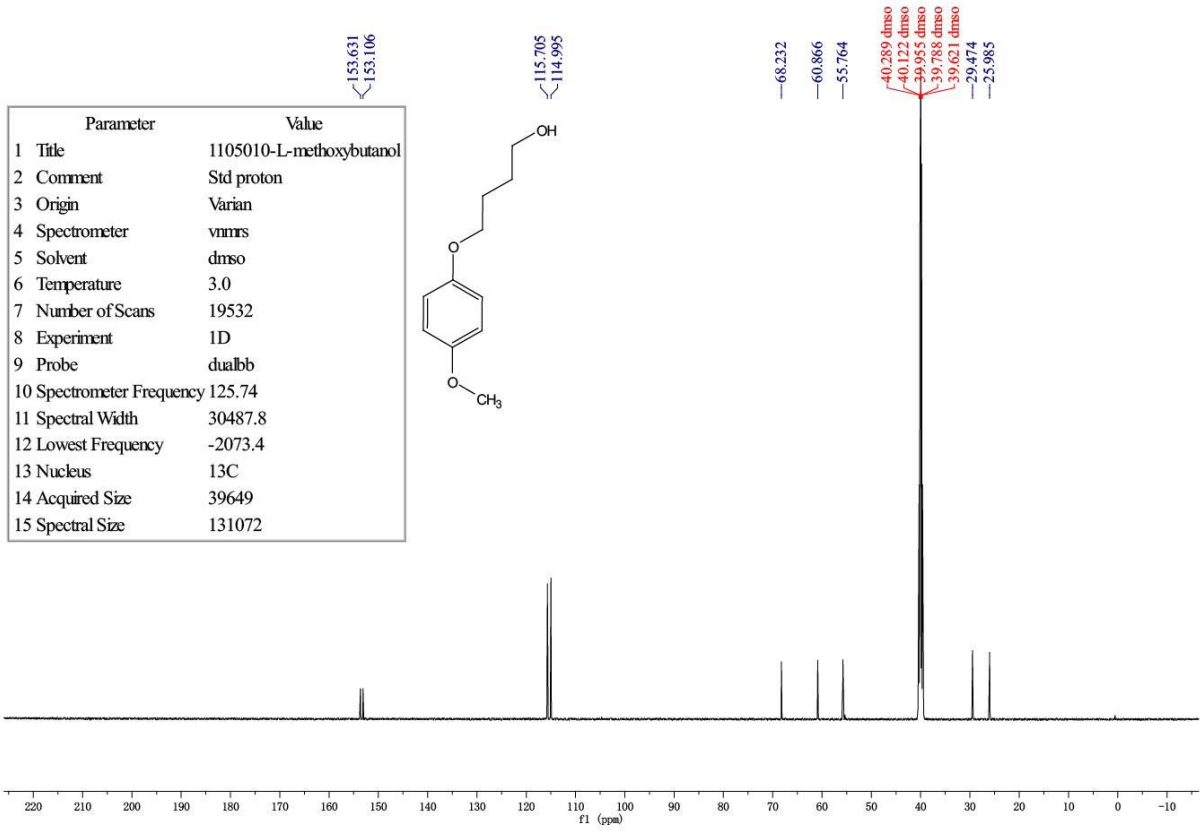
Parameter	Value
1 Title	120323-XY4-223-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	32
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1018.0
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



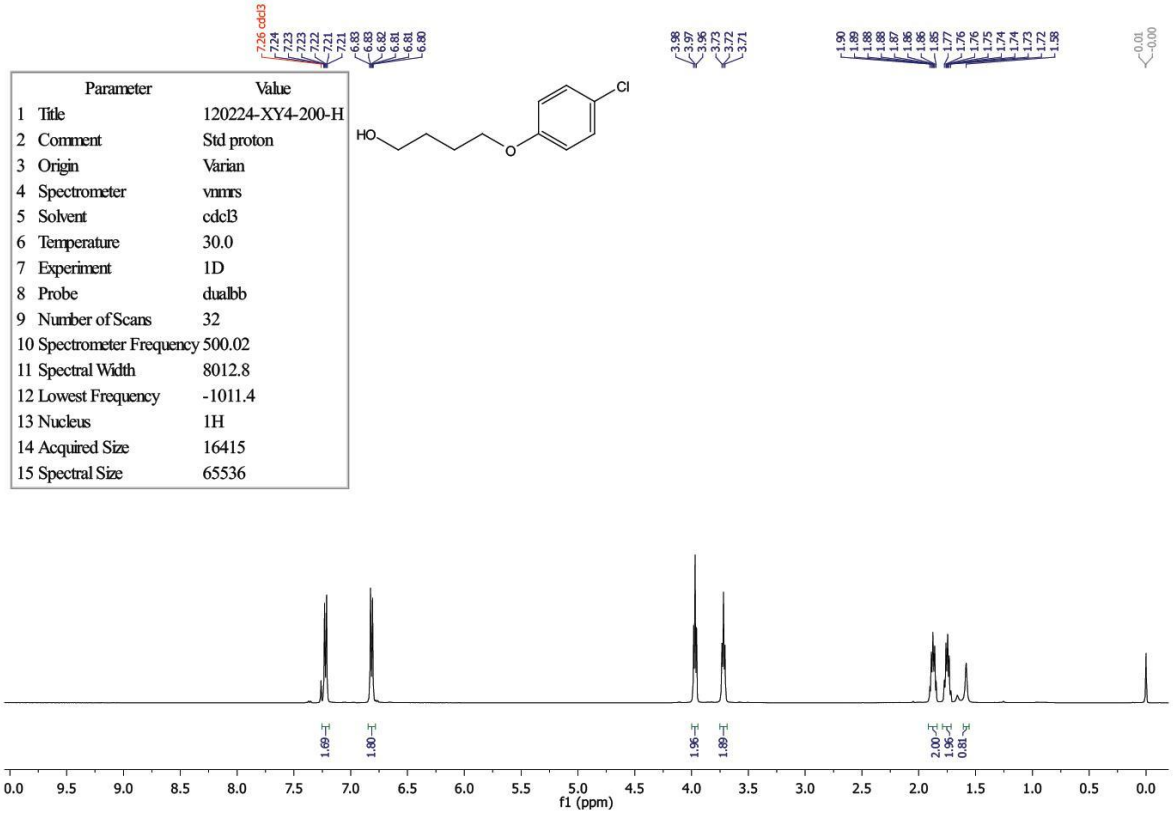
Parameter	Value
1 Title	120323-XY4-223-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	188
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2042.4
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072



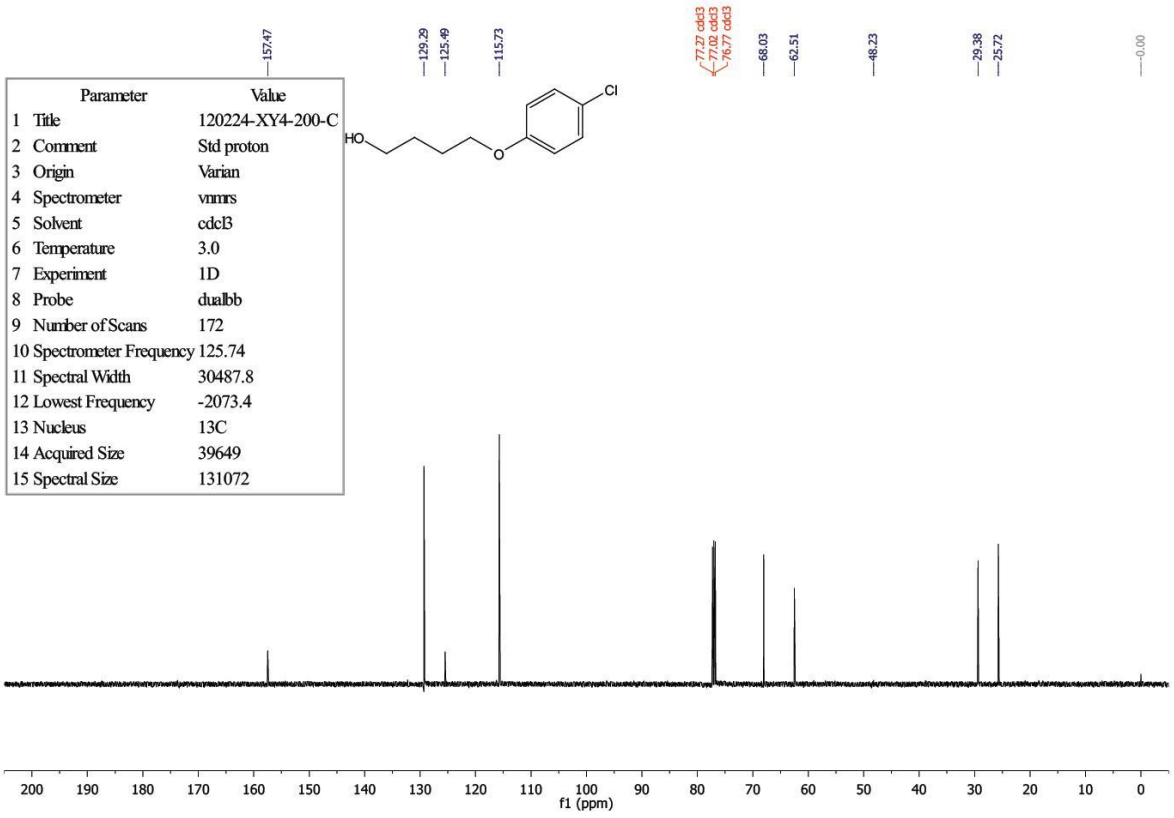
Parameter	Value
1 Title	120320-XY4-205-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	16
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1008.4
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



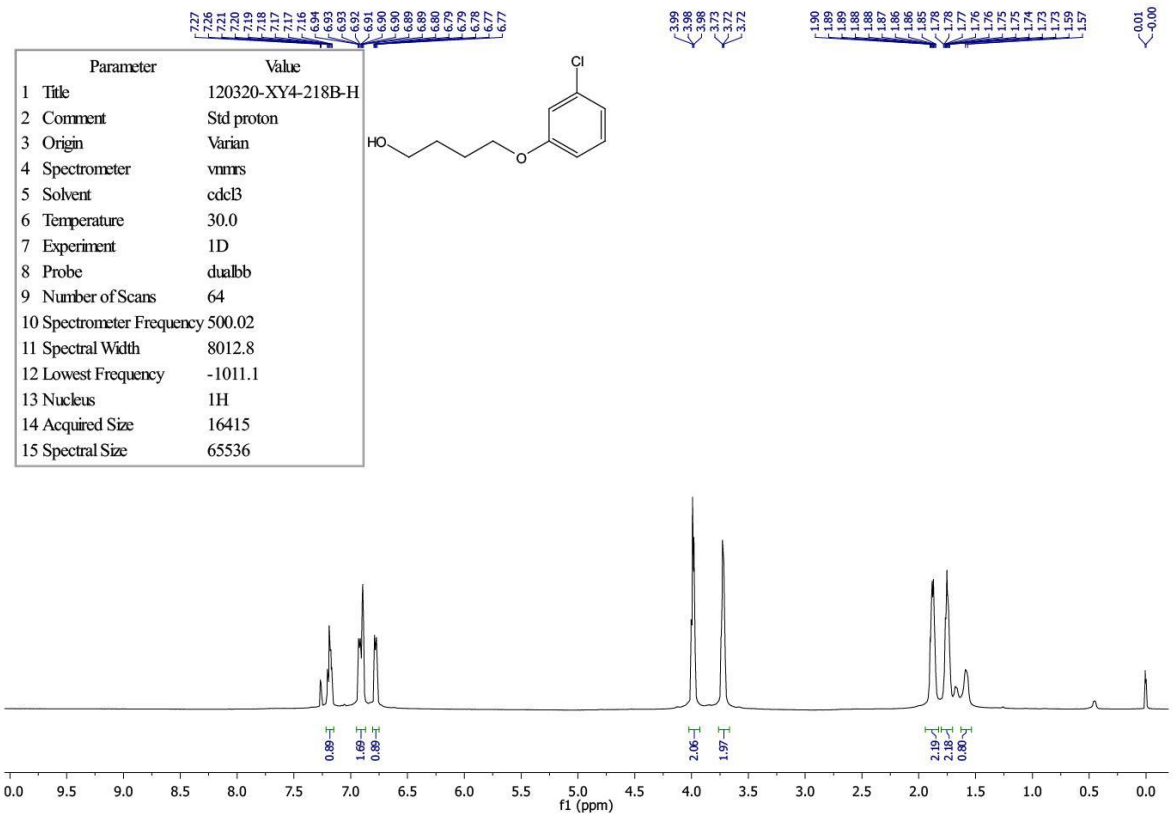
Parameter	Value
1 Title	1105010-L-methoxybutanol
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	dmso
6 Temperature	3.0
7 Number of Scans	19532
8 Experiment	1D
9 Probe	dualbb
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2073.4
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072



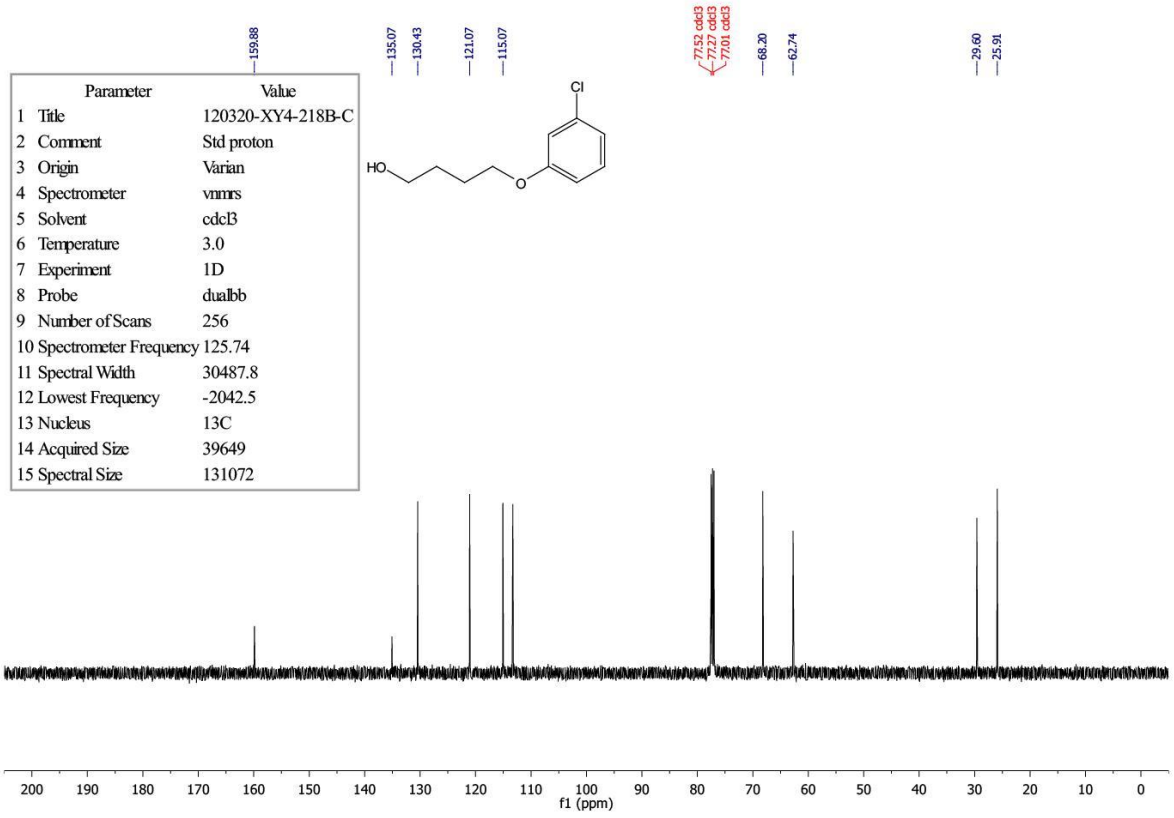
Parameter	Value
1 Title	120224-XY4-200-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	32
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1011.4
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



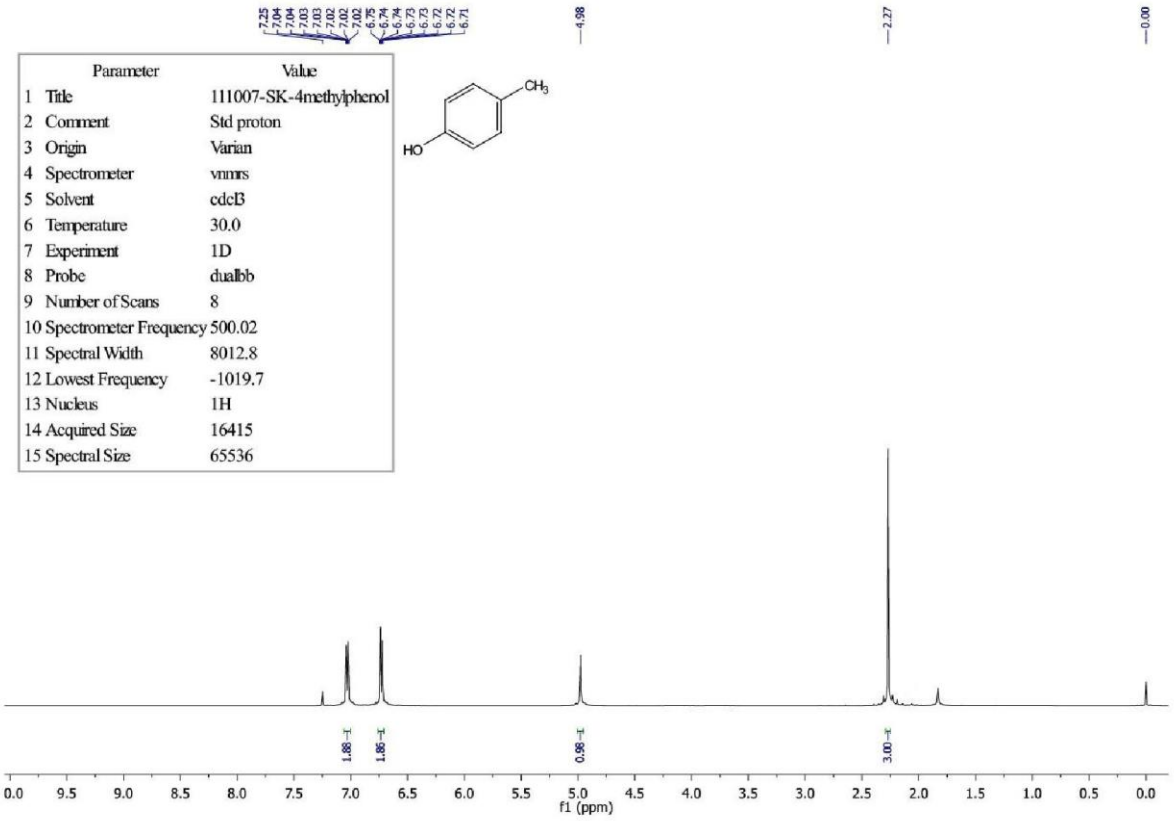
Parameter	Value
1 Title	120224-XY4-200-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	172
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2073.4
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072



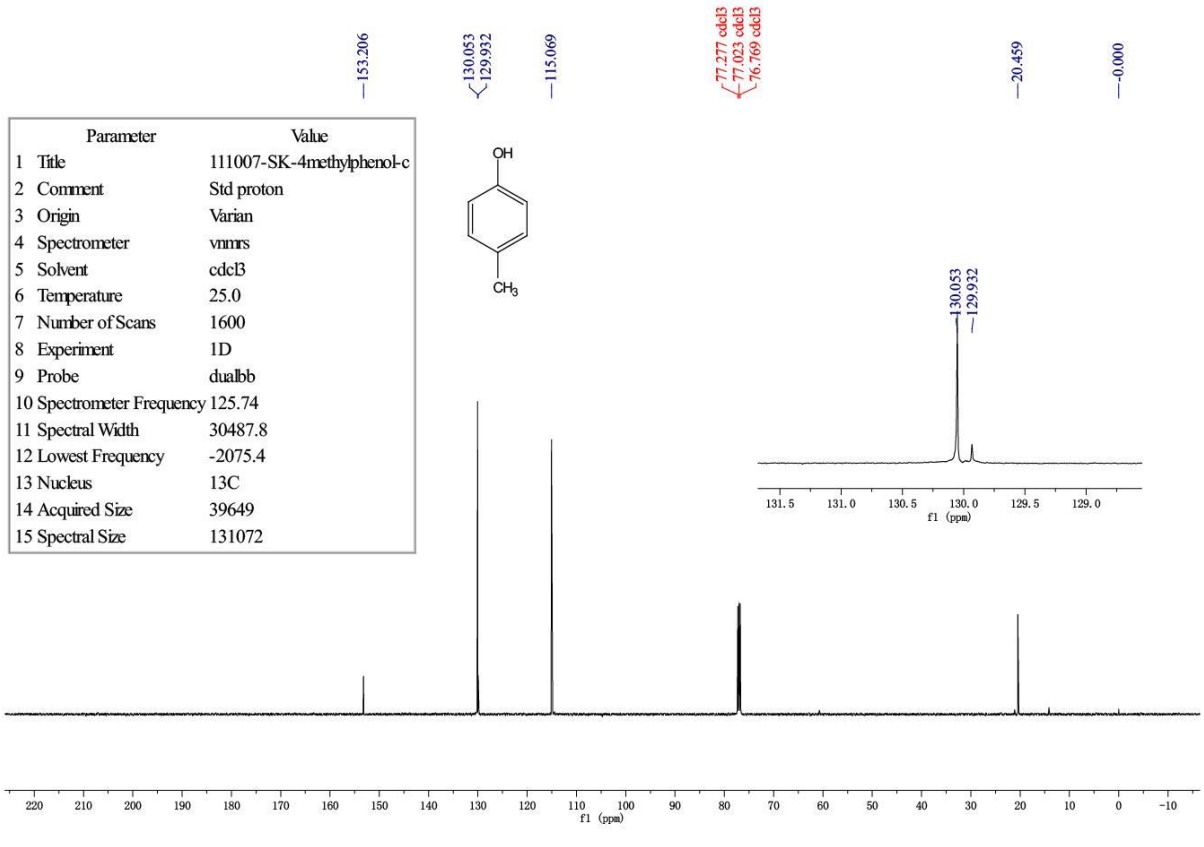
Parameter	Value
1 Title	120320-XY4-218B-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	64
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1011.1
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



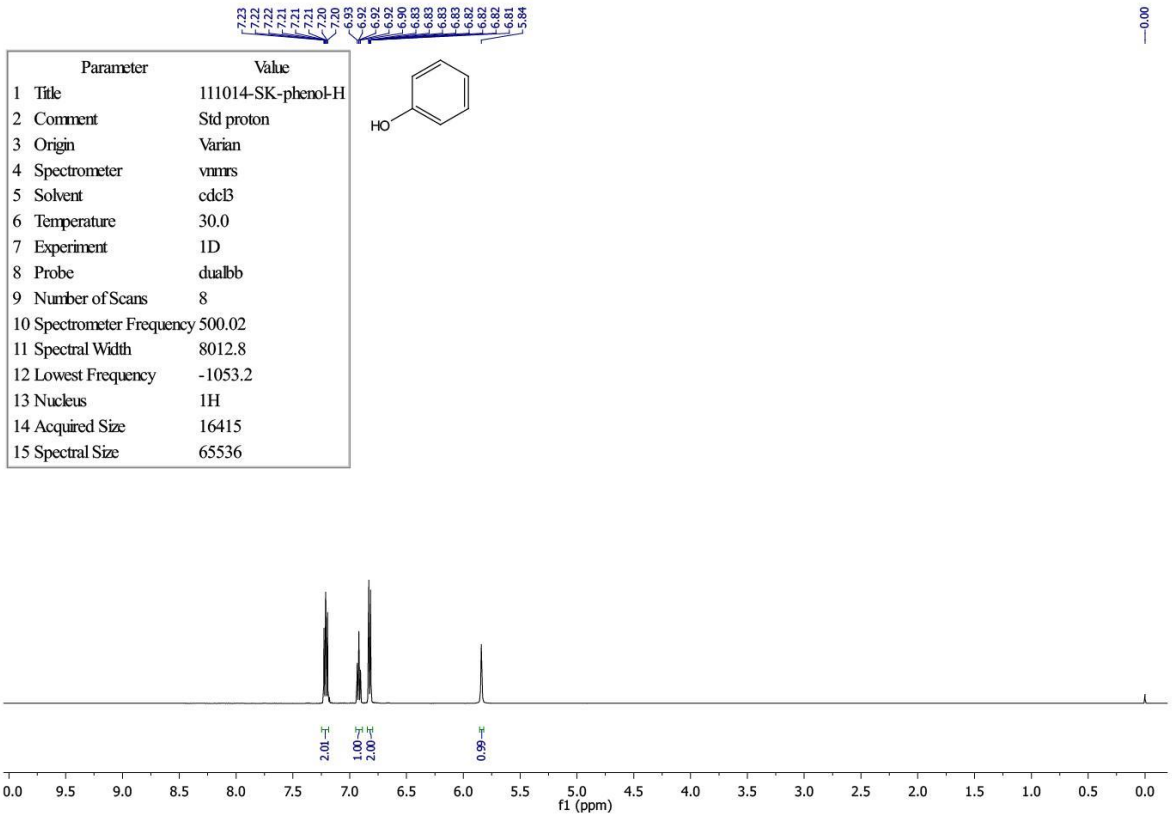
Parameter	Value
1 Title	120320-XY4-218B-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	256
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2042.5
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072



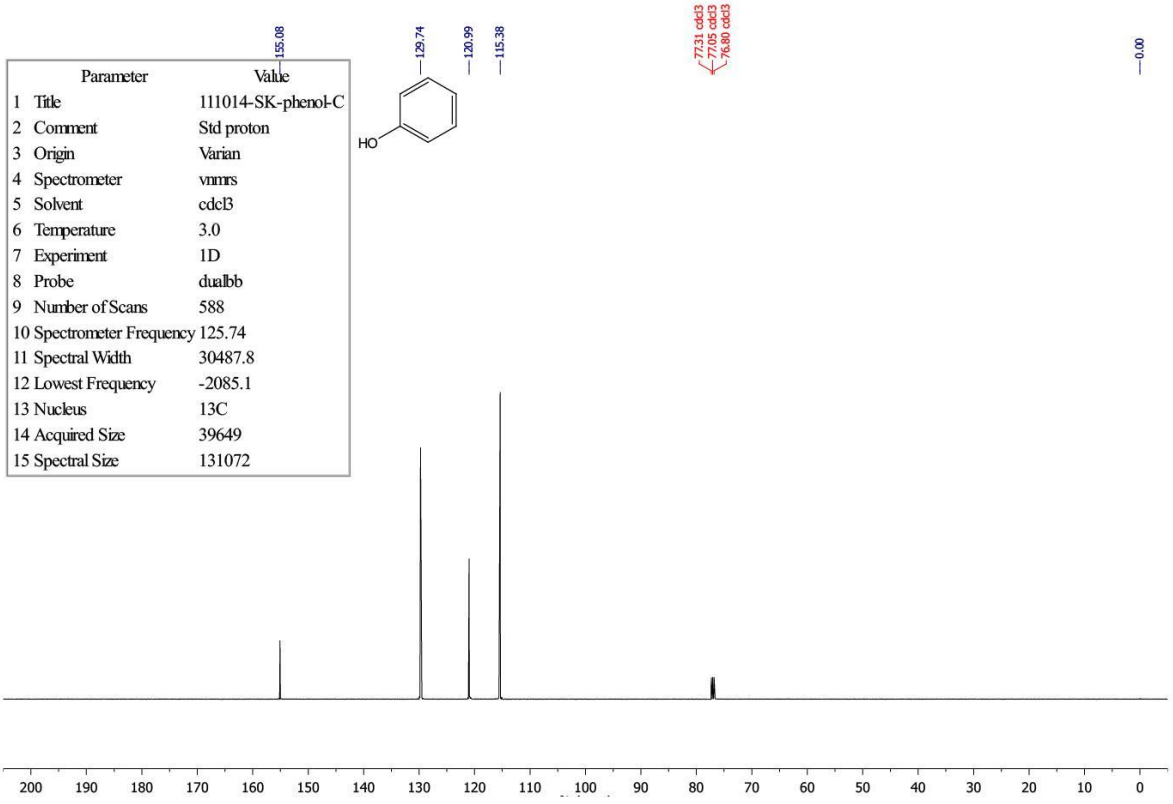
Parameter	Value
1 Title	111007-SK-4methylphenol
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	8
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1019.7
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



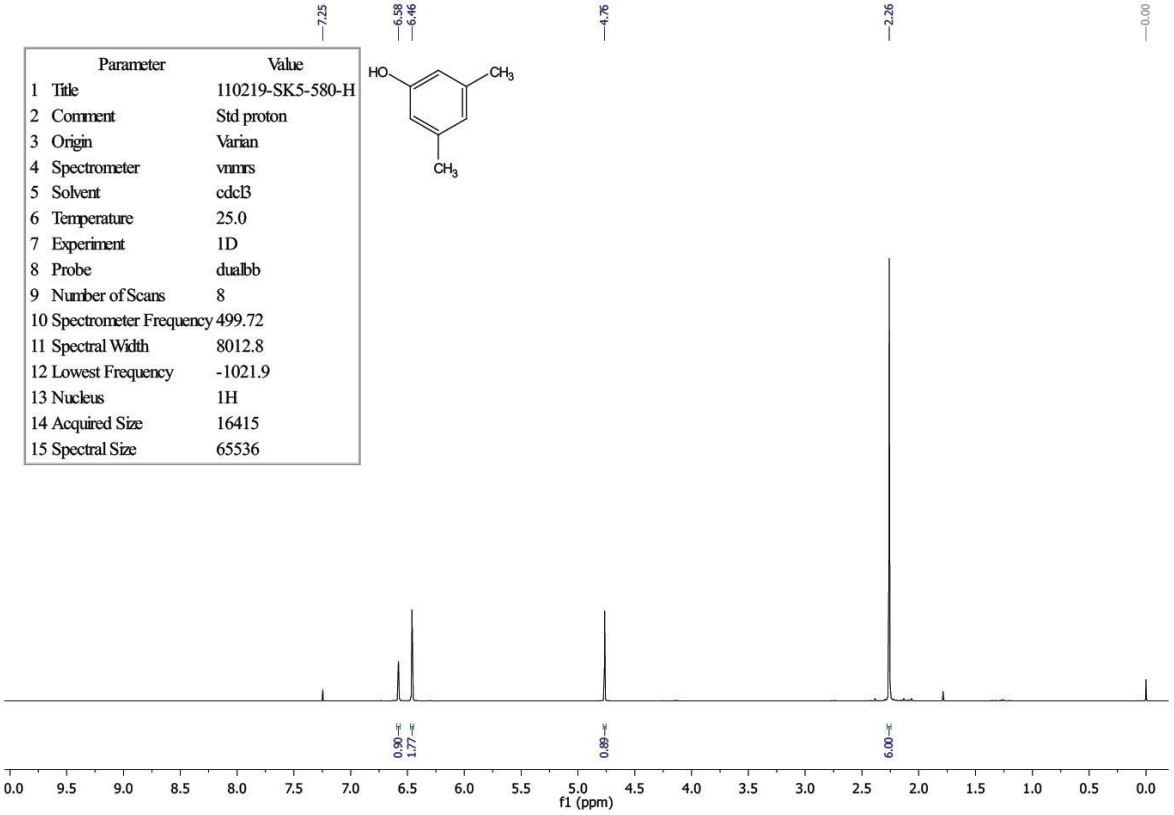
Parameter	Value
1 Title	111007-SK-4methylphenol-c
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	25.0
7 Number of Scans	1600
8 Experiment	1D
9 Probe	dualbb
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2075.4
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072



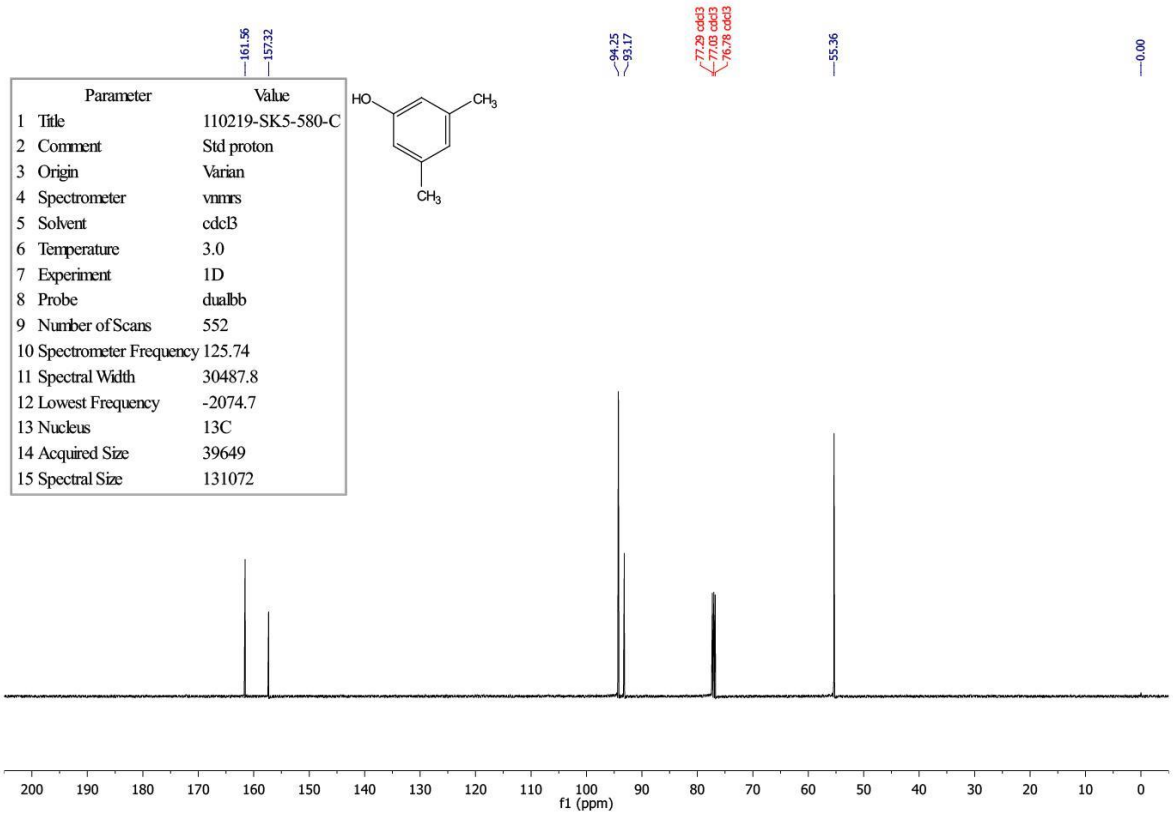
Parameter	Value
1 Title	111014-SK-phenol-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	8
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1053.2
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



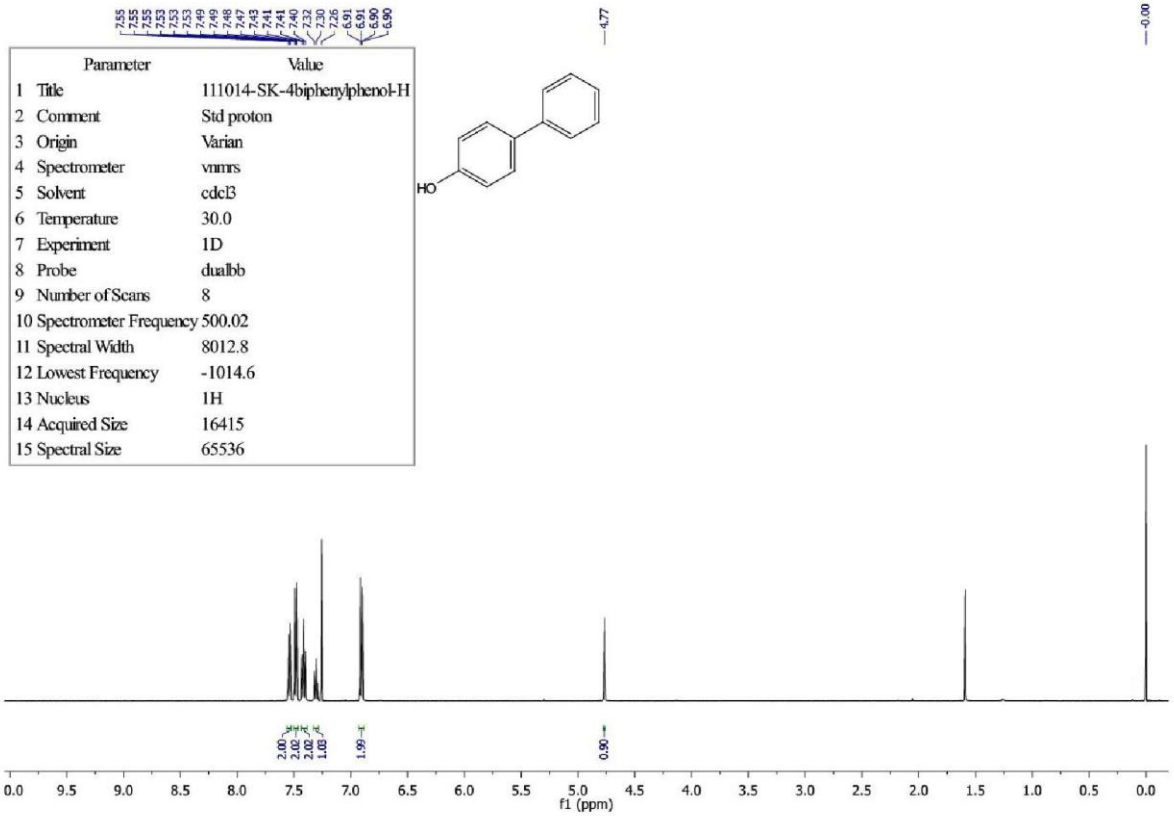
Parameter	Value
1 Title	111014-SK-phenol-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	588
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2085.1
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072



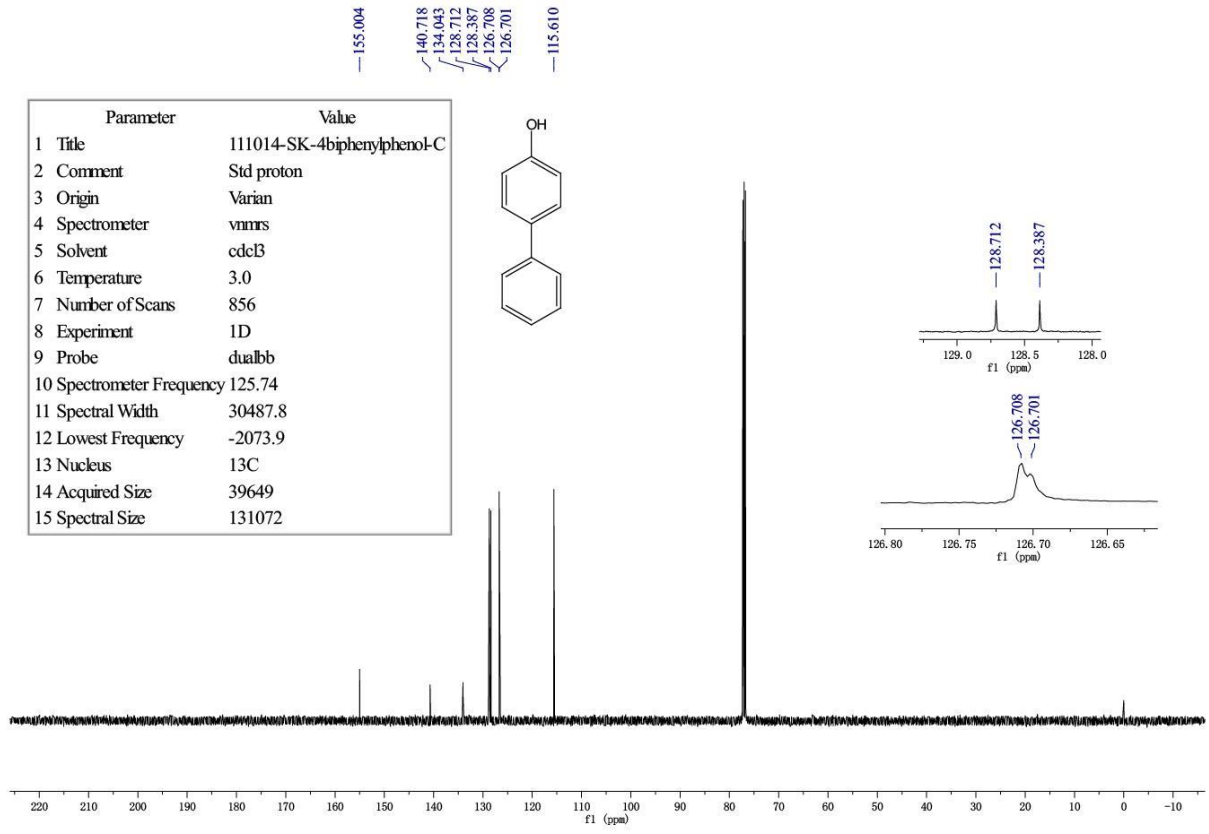
Parameter	Value
1 Title	110219-SK5-580-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	25.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	8
10 Spectrometer Frequency	499.72
11 Spectral Width	8012.8
12 Lowest Frequency	-1021.9
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



Parameter	Value
1 Title	110219-SK5-580-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	552
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2074.7
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072

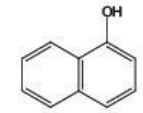


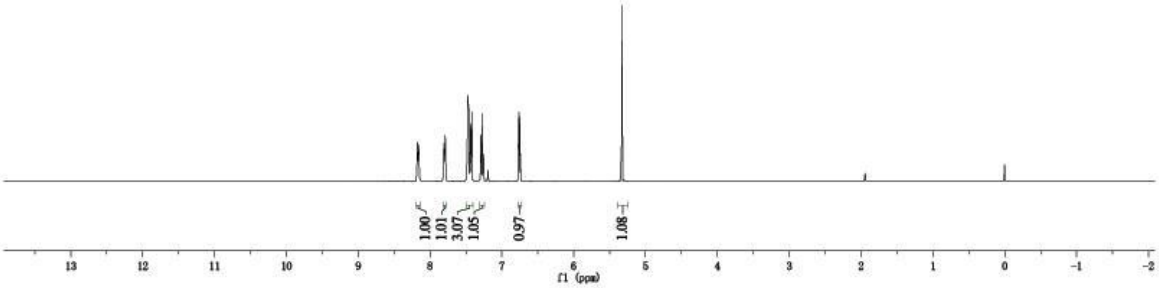
Parameter	Value
1 Title	111014-SK-4biphenylphenol-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	8
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1014.6
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



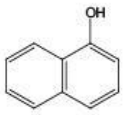
Parameter	Value
1 Title	111014-SK-4biphenylphenol-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Number of Scans	856
8 Experiment	1D
9 Probe	dualbb
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2073.9
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072

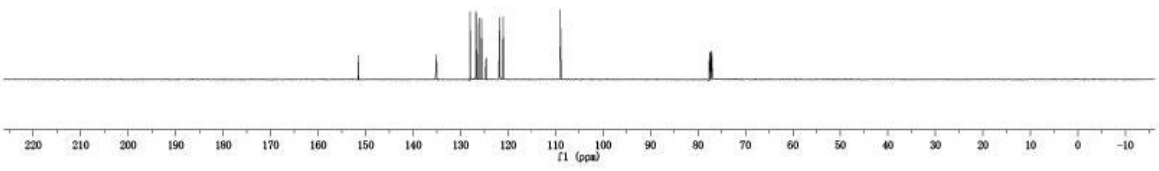
Parameter	Value
1 Title	121103-XY3-nap-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Number of Scans	8
8 Experiment	1D
9 Probe	dualbb
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1045.4
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536

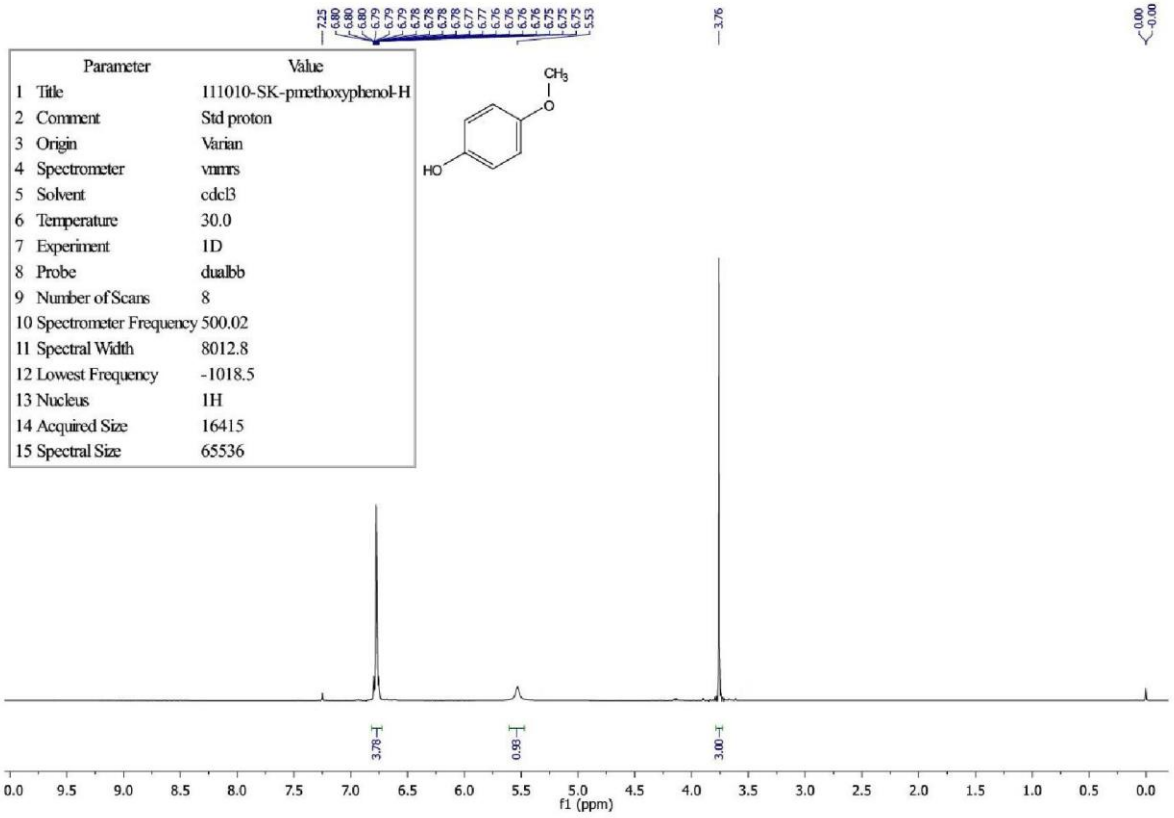




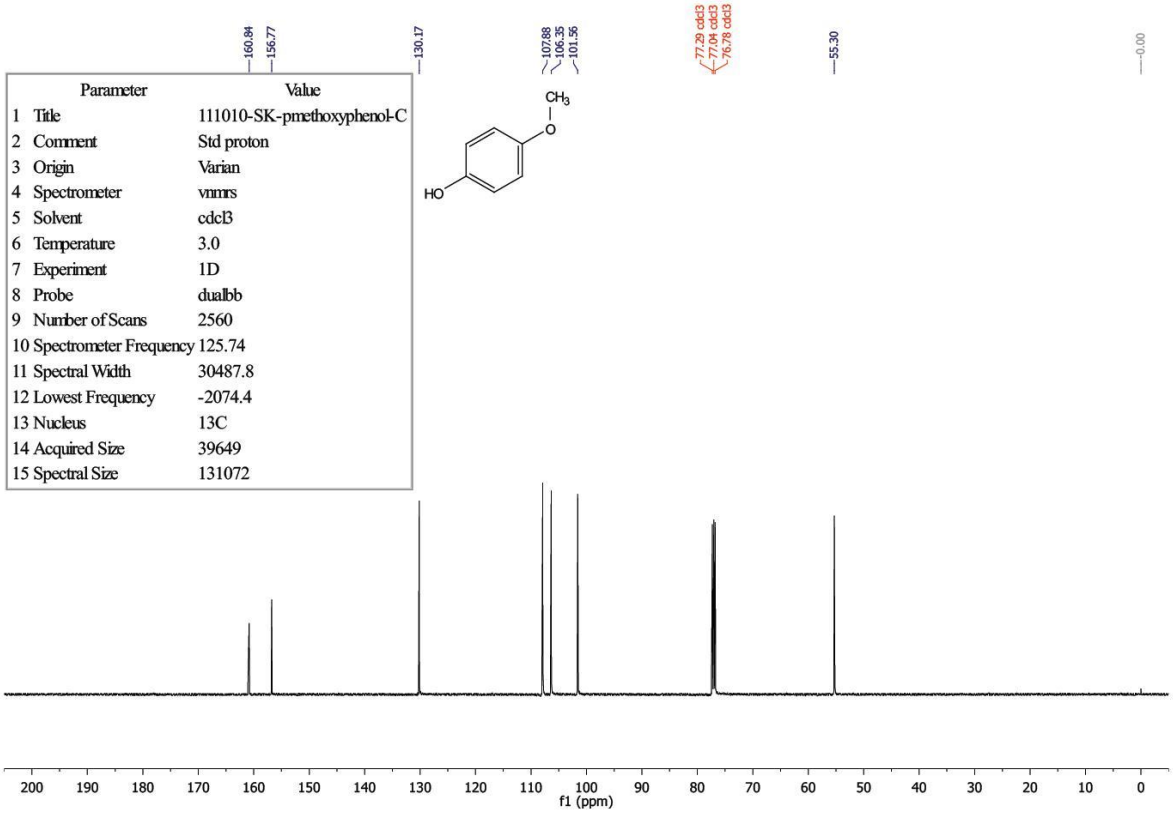
Parameter	Value
1 Title	121103-XY3-nap-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Number of Scans	564
8 Experiment	1D
9 Probe	dualbb
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2042.5
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072



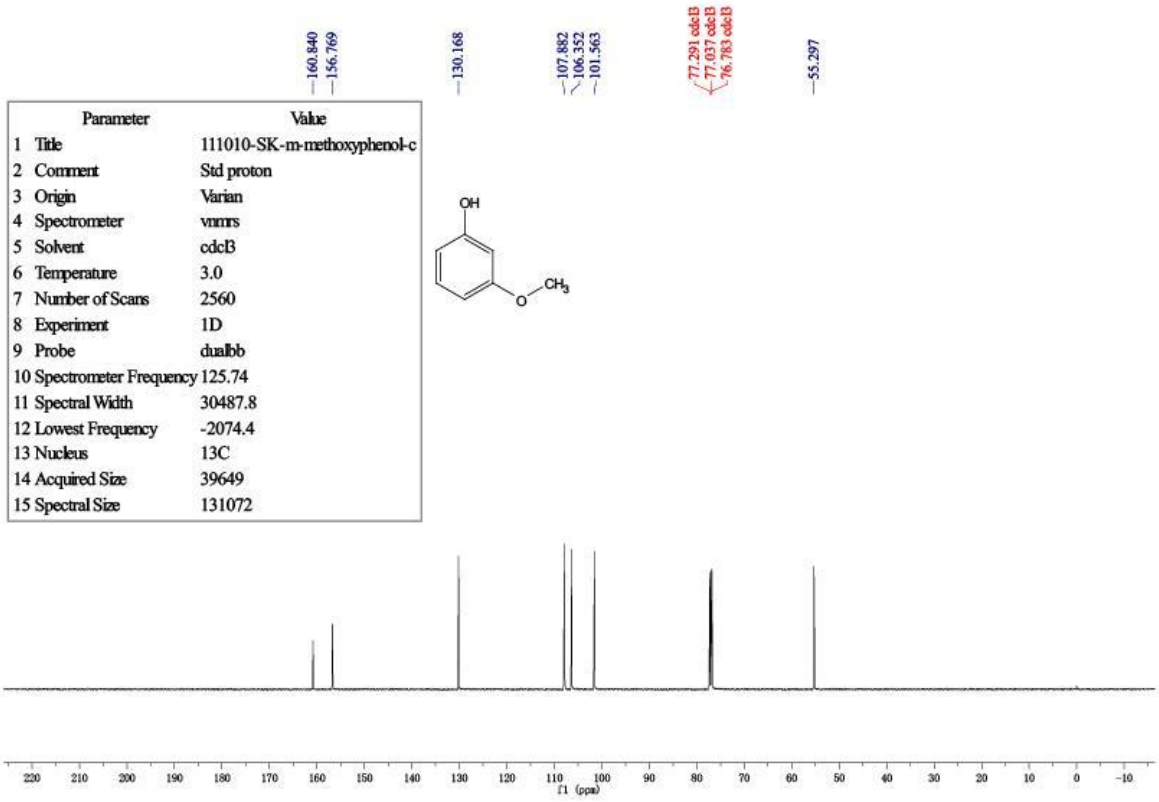




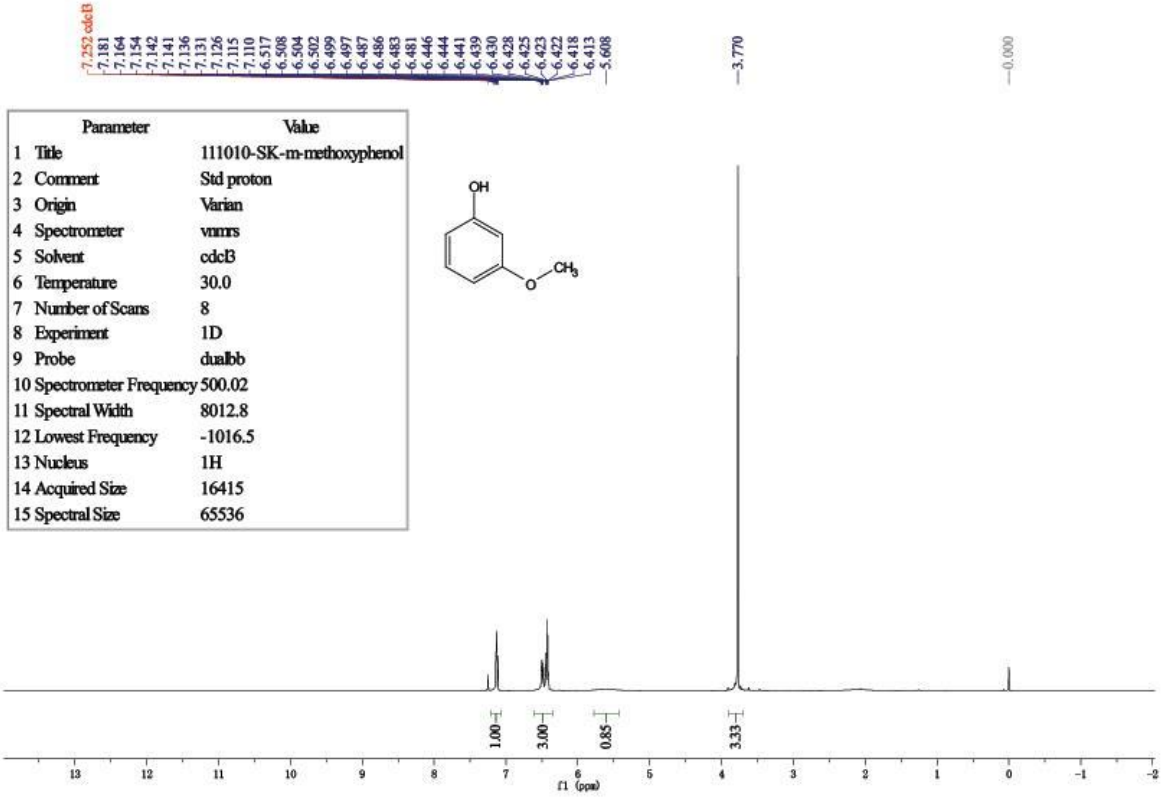
Parameter	Value
1 Title	111010-SK-pmethoxyphenol-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	8
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1018.5
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



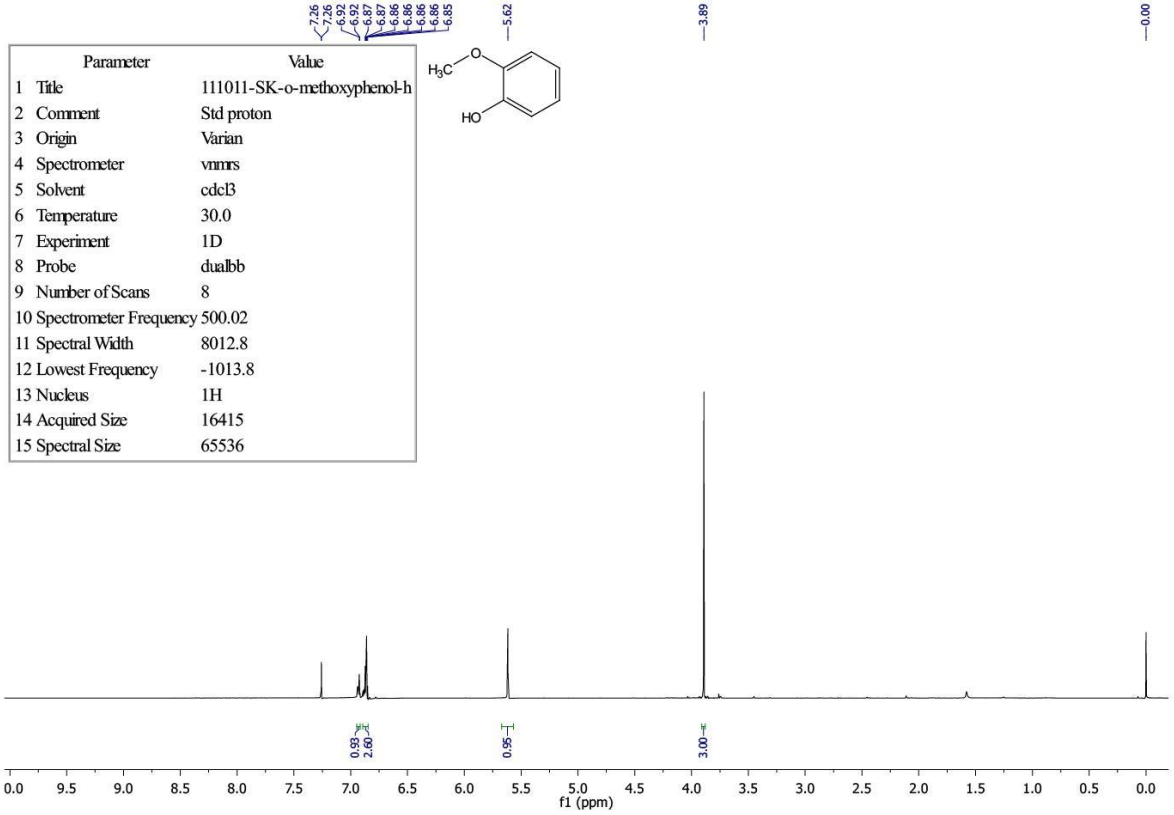
Parameter	Value
1 Title	111010-SK-pmethoxyphenol-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	2560
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2074.4
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072



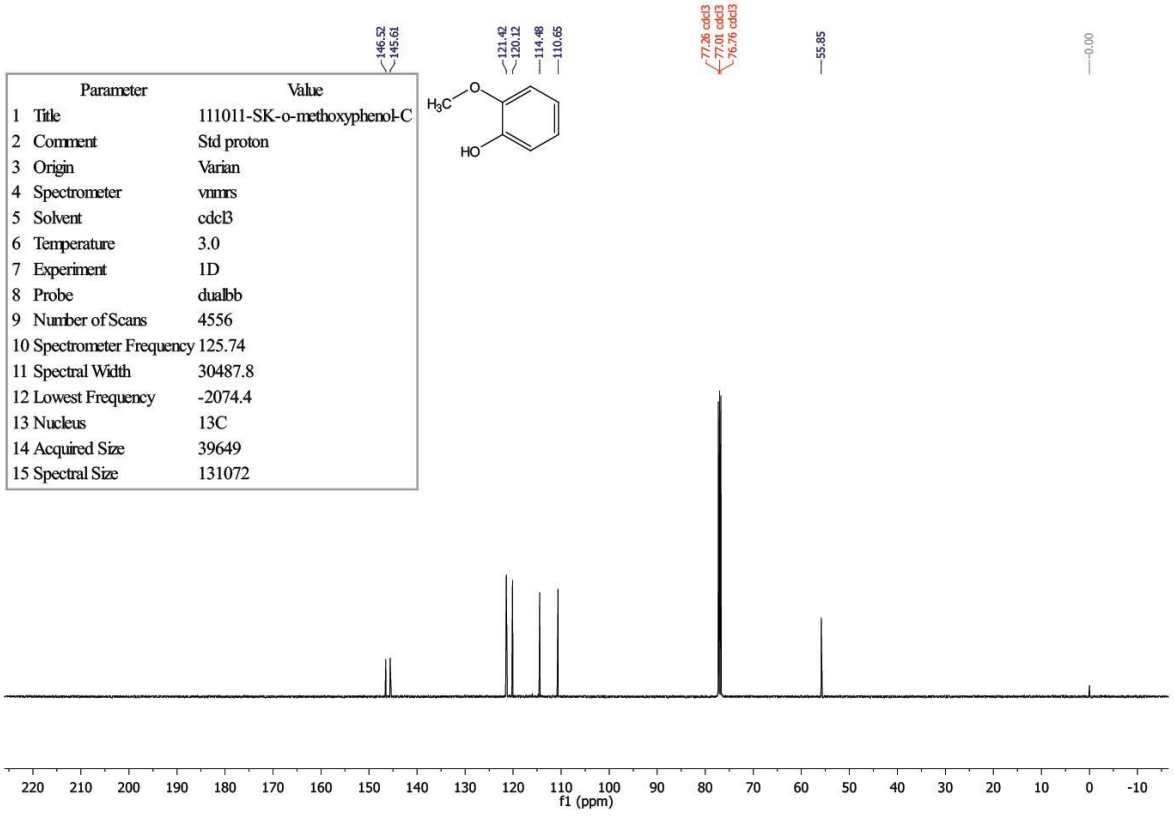
Parameter	Value
1 Title	111010-SK-m-methoxyphenol-c
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Number of Scans	2560
8 Experiment	1D
9 Probe	dualbb
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2074.4
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072



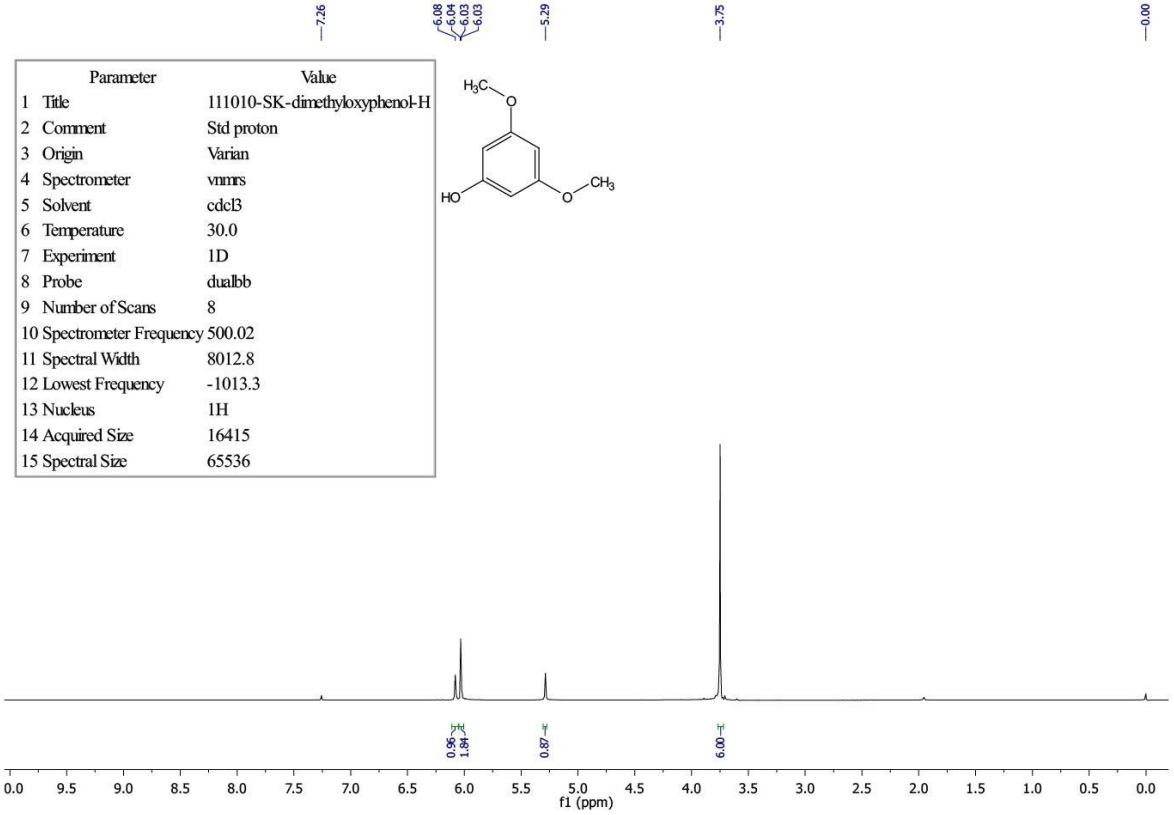
Parameter	Value
1 Title	111010-SK-m-methoxyphenol
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Number of Scans	8
8 Experiment	1D
9 Probe	dualbb
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1016.5
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



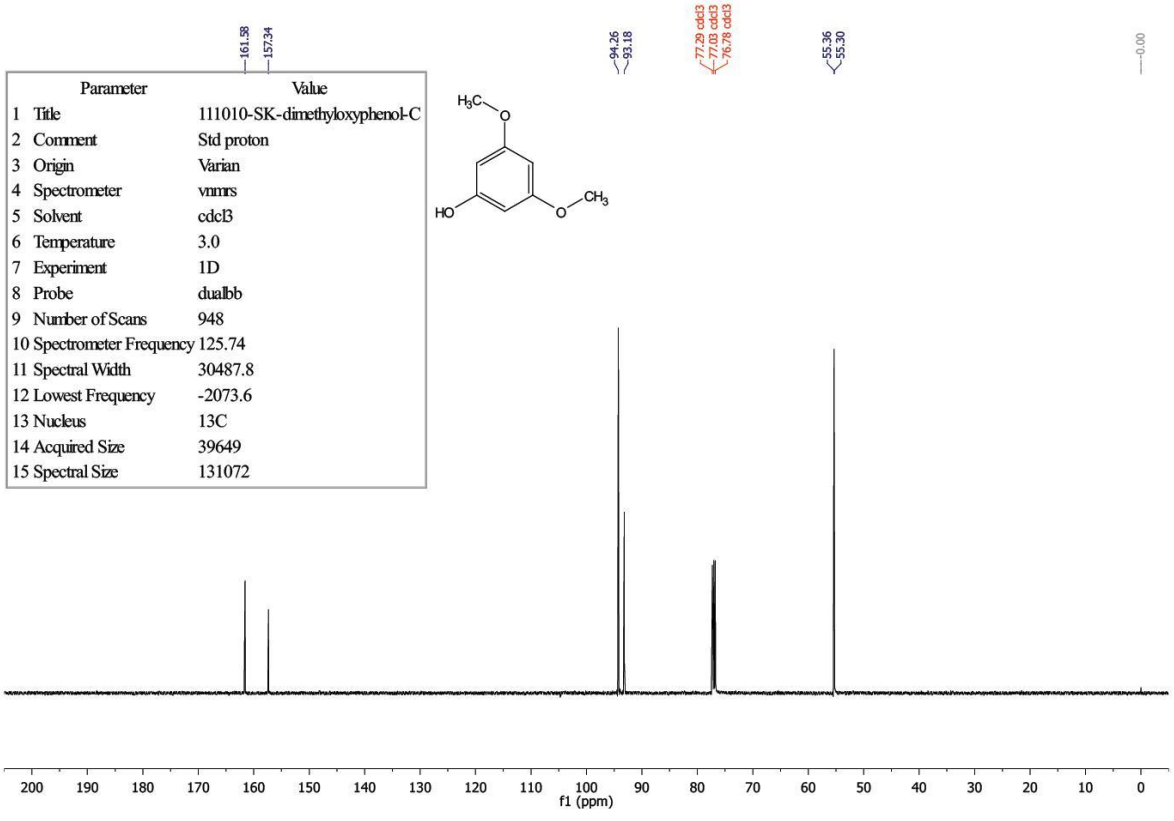
Parameter	Value
1 Title	111011-SK-o-methoxyphenol-h
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	8
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1013.8
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



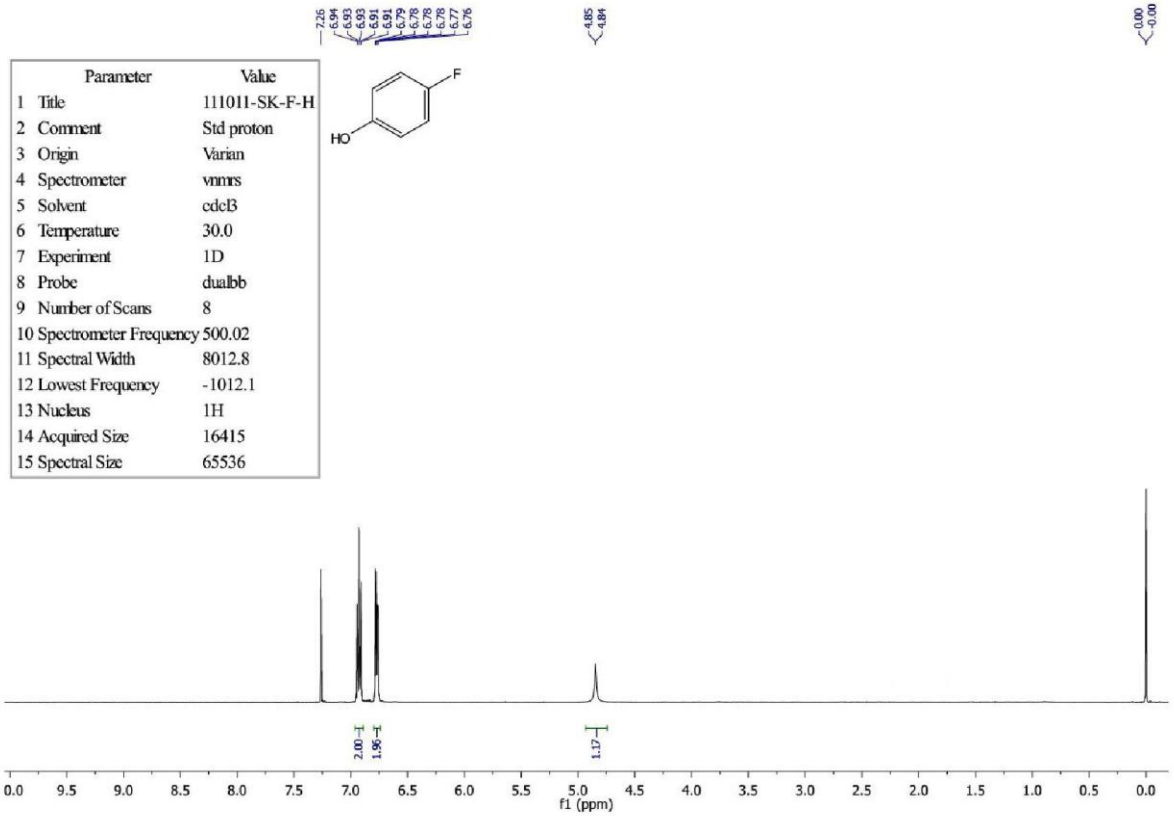
Parameter	Value
1 Title	111011-SK-o-methoxyphenol-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	4556
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2074.4
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072



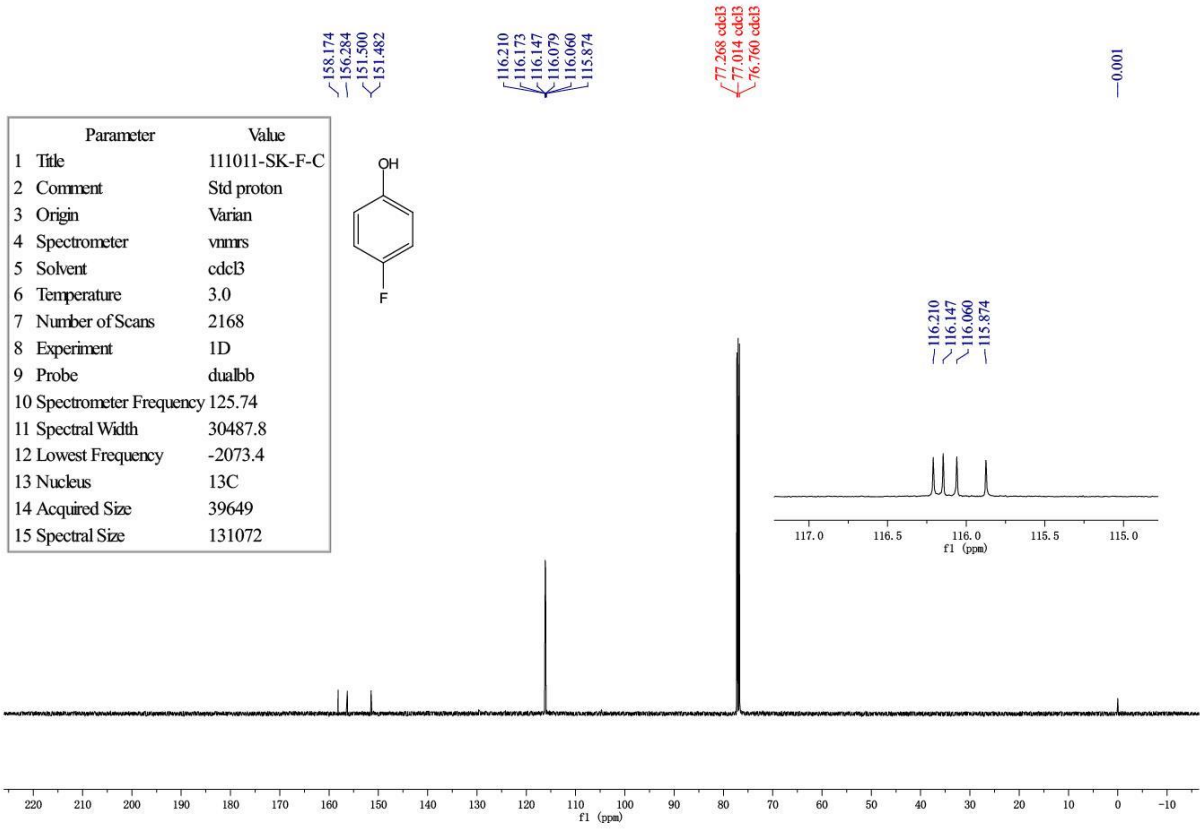
Parameter	Value
1 Title	111010-SK-dimethyloxyphenol-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	8
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1013.3
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



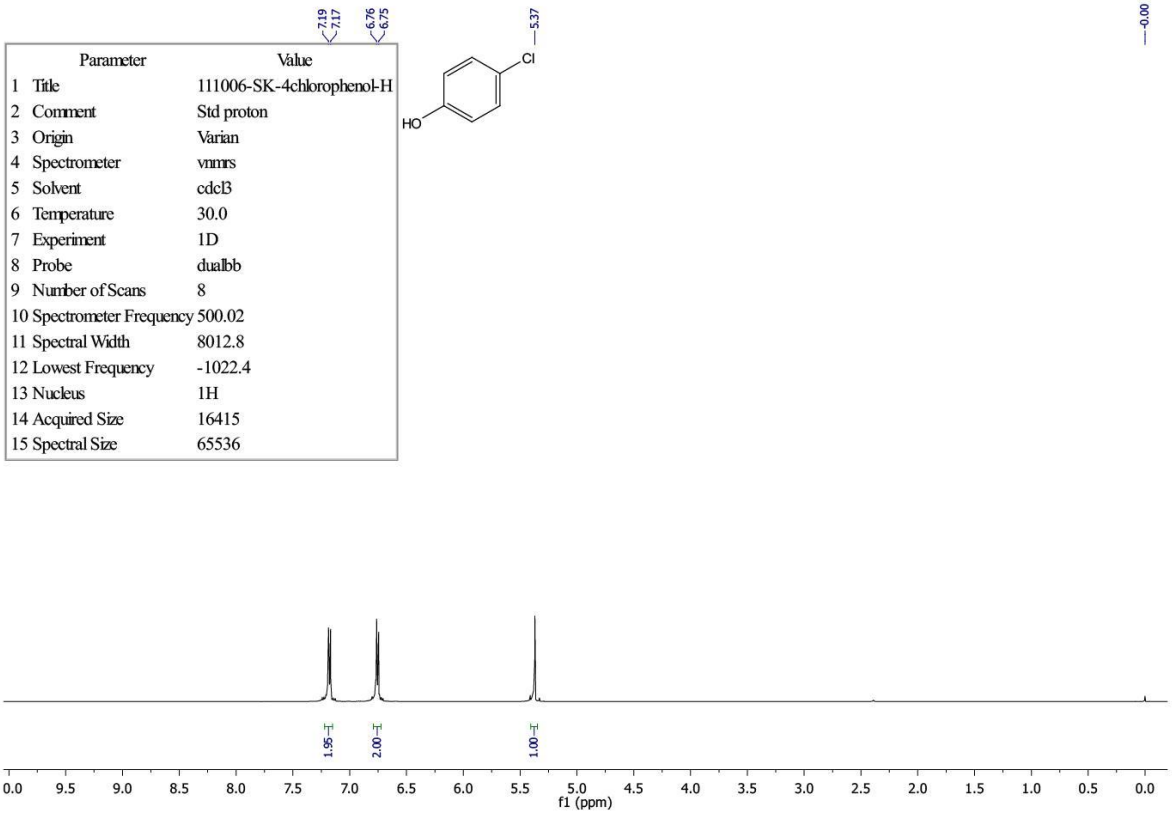
Parameter	Value
1 Title	111010-SK-dimethyloxyphenol-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	948
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2073.6
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072



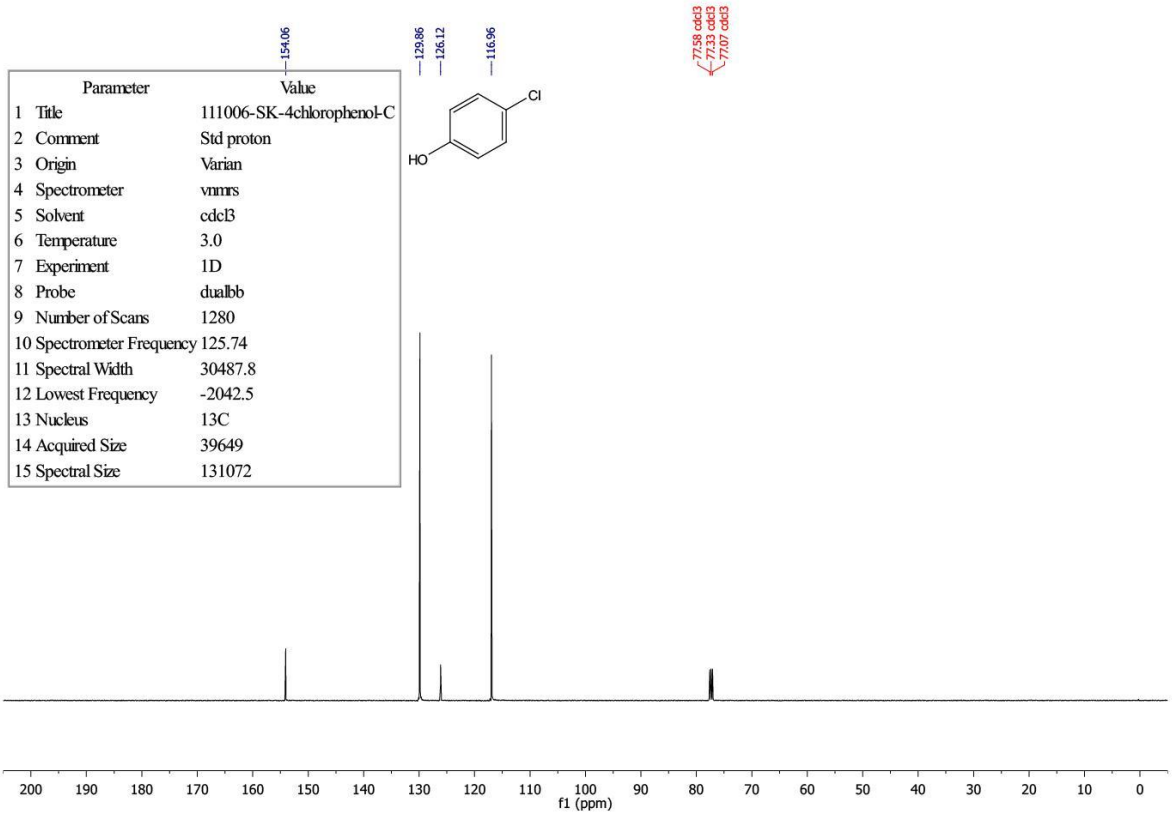
Parameter	Value
1 Title	111011-SK-F-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	8
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1012.1
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



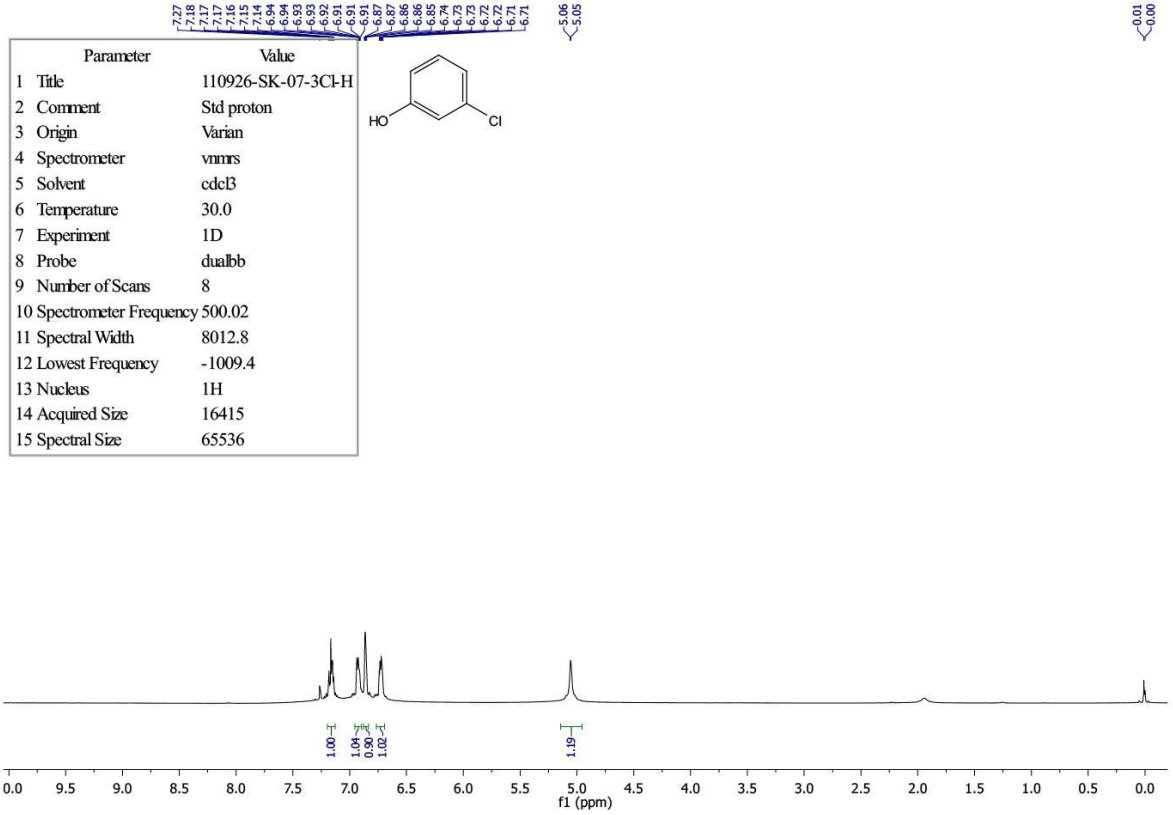
Parameter	Value
1 Title	111011-SK-F-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Number of Scans	2168
8 Experiment	1D
9 Probe	dualbb
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2073.4
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072



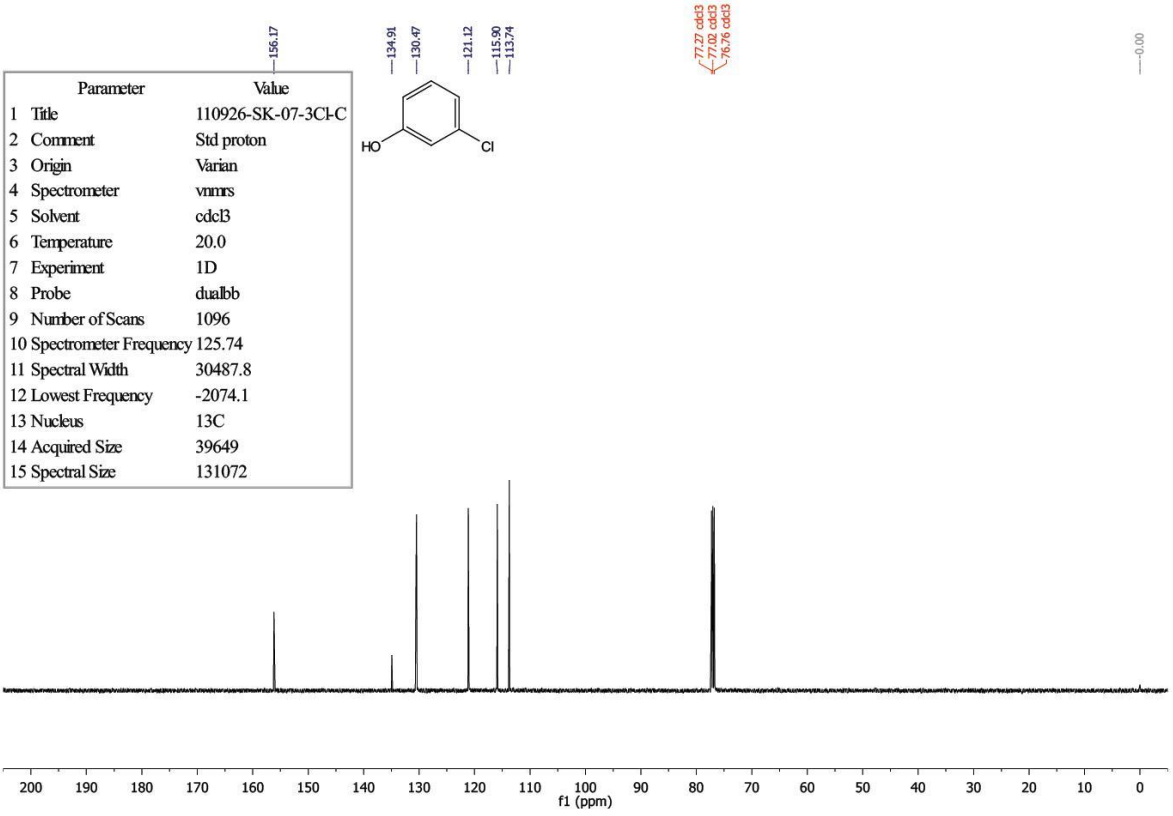
Parameter	Value
1 Title	111006-SK-4chlorophenol-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	8
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1022.4
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



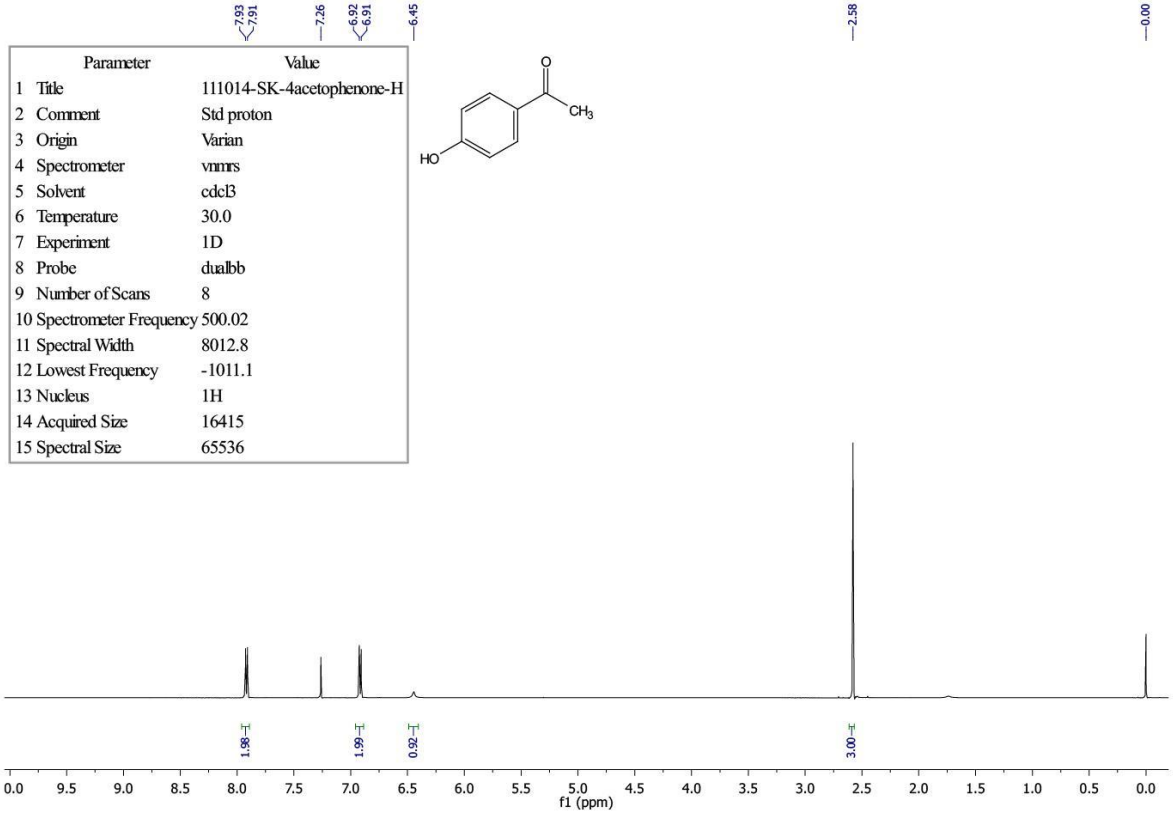
Parameter	Value
1 Title	111006-SK-4chlorophenol-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	1280
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2042.5
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072



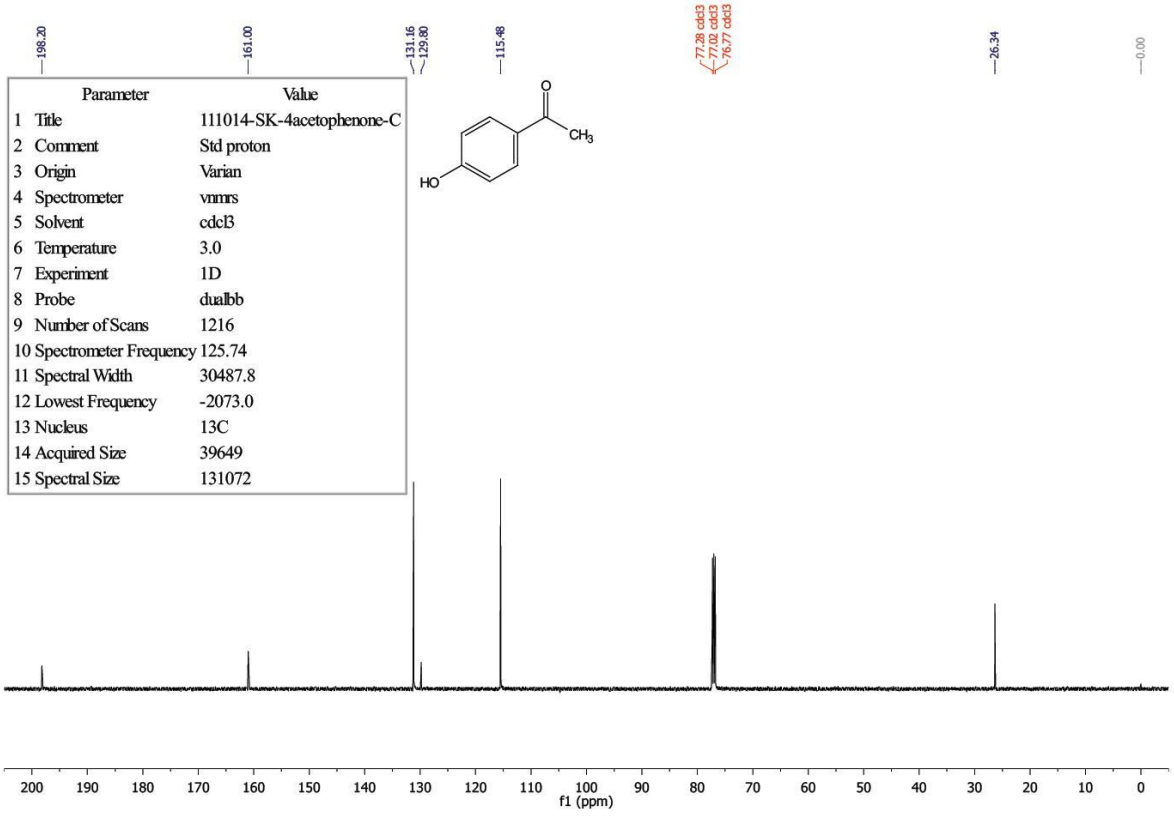
Parameter	Value
1 Title	110926-SK-07-3Cl-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	8
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1009.4
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



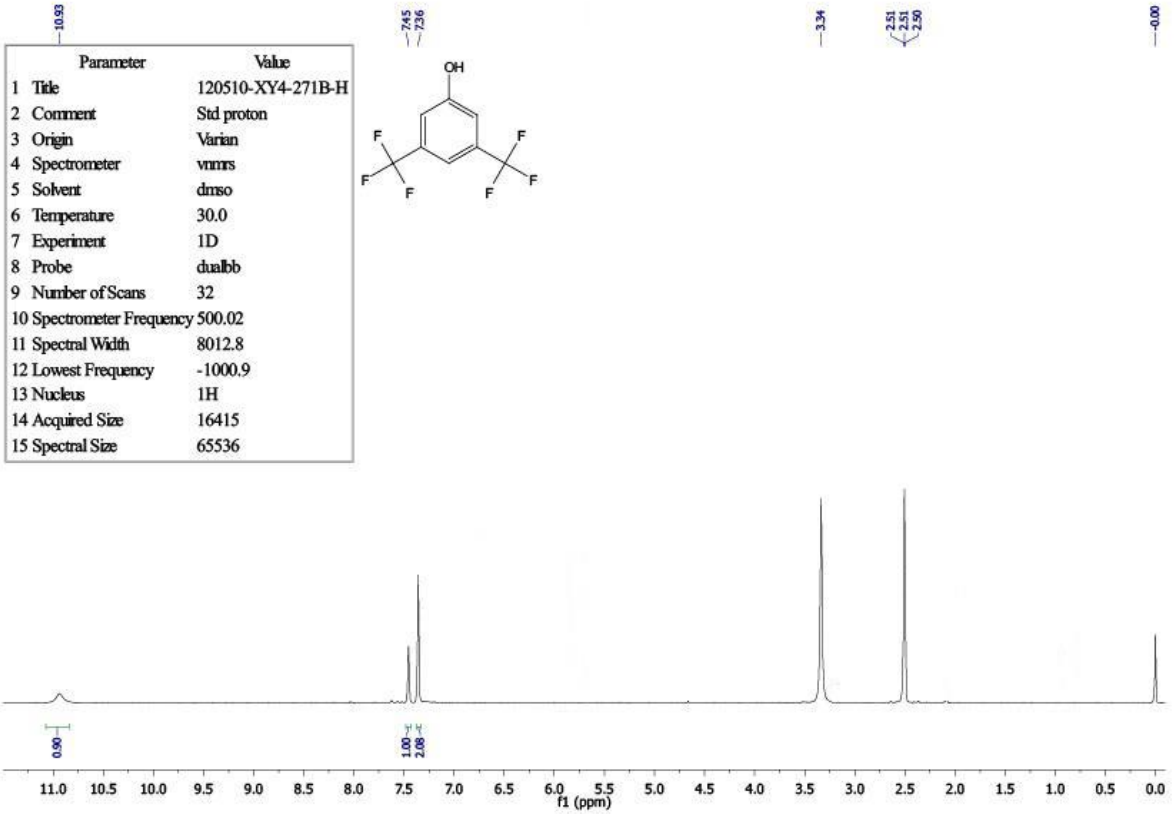
Parameter	Value
1 Title	110926-SK-07-3Cl-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	20.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	1096
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2074.1
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072



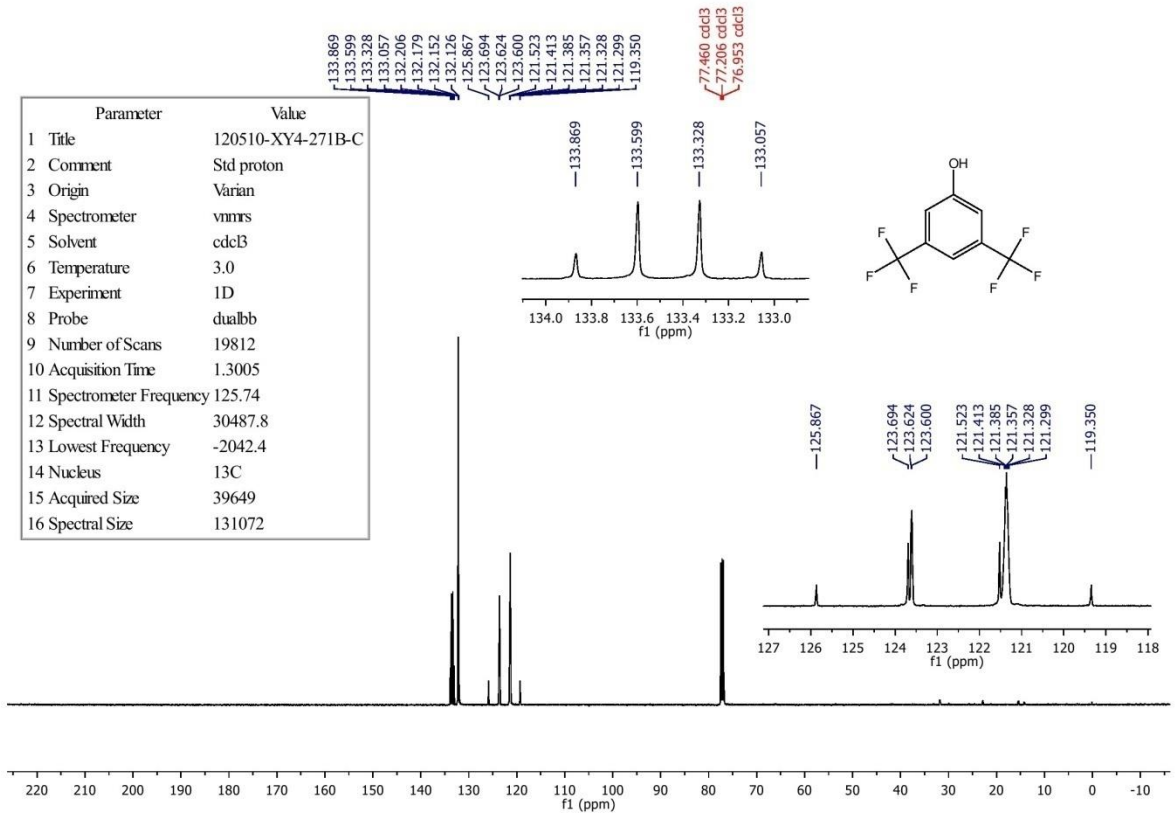
Parameter	Value
1 Title	111014-SK-4acetophenone-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	8
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1011.1
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



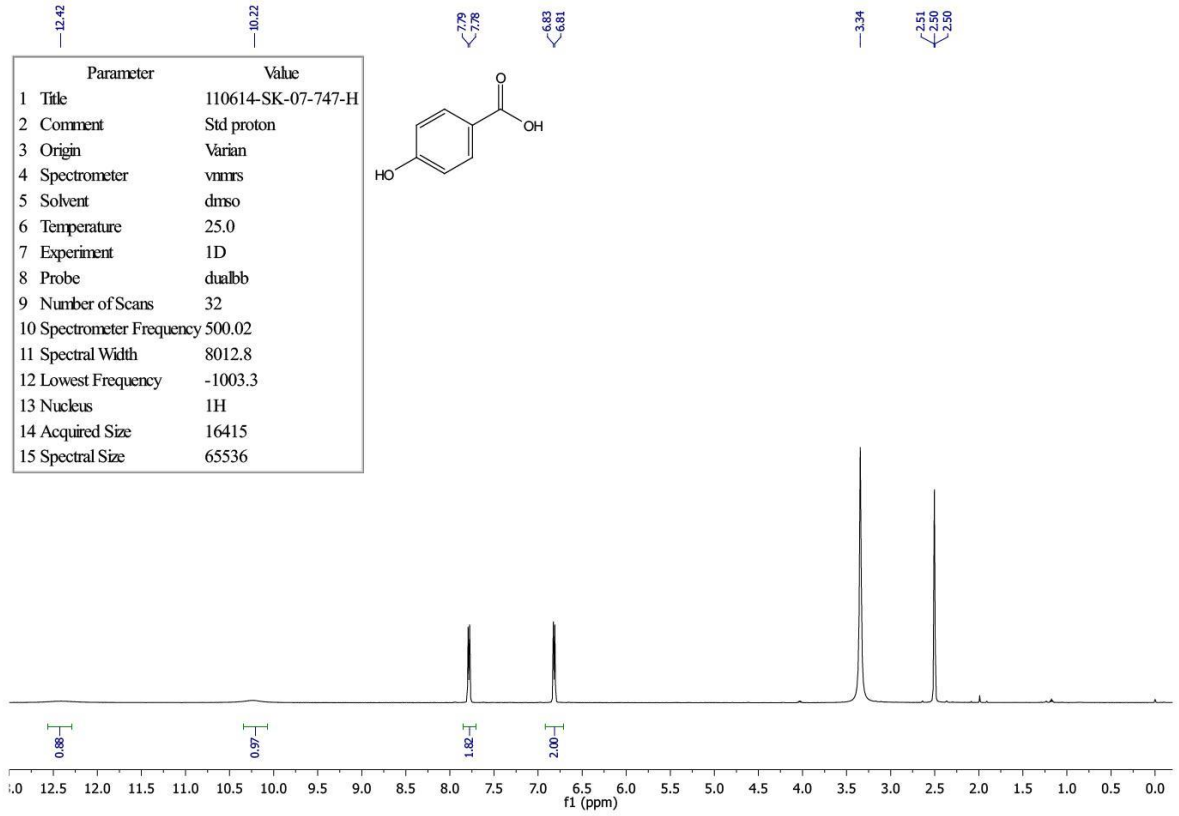
Parameter	Value
1 Title	111014-SK-4acetophenone-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	1216
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2073.0
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072



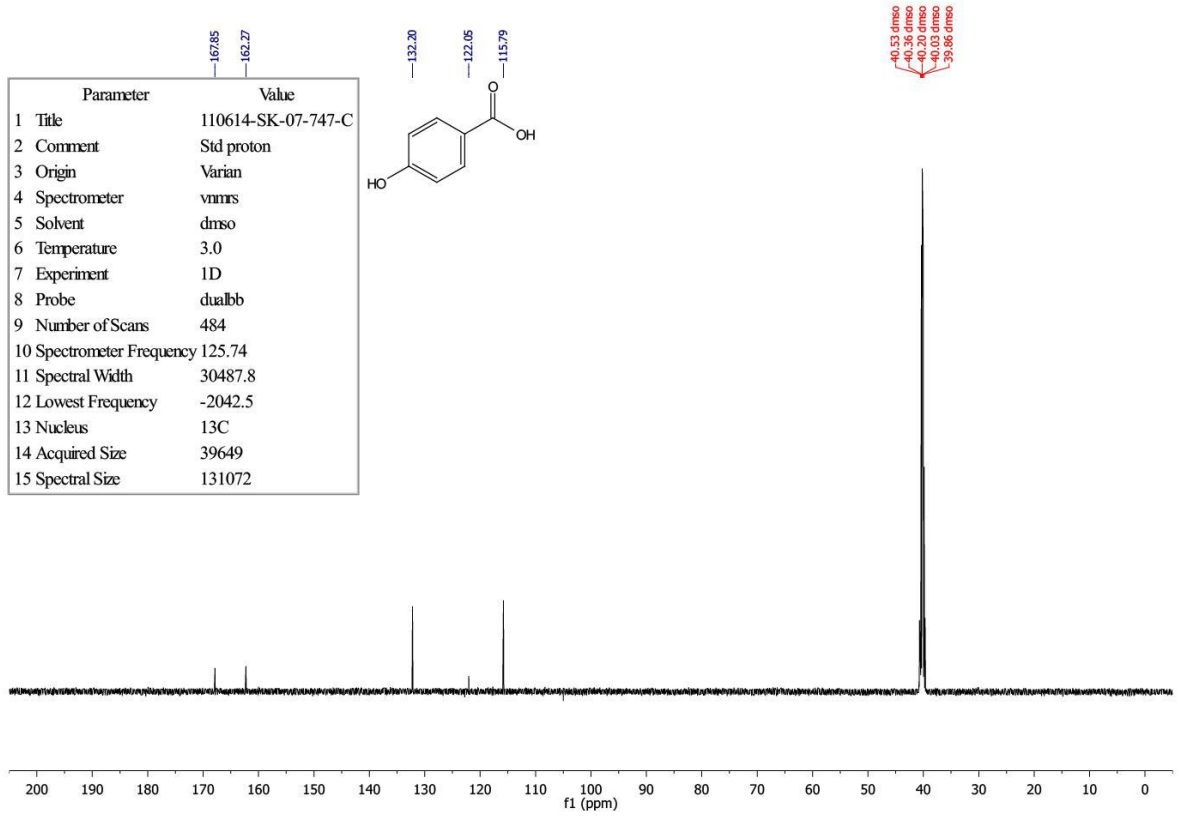
Parameter	Value
1 Title	120510-XY4-271B-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	dmso
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	32
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1000.9
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



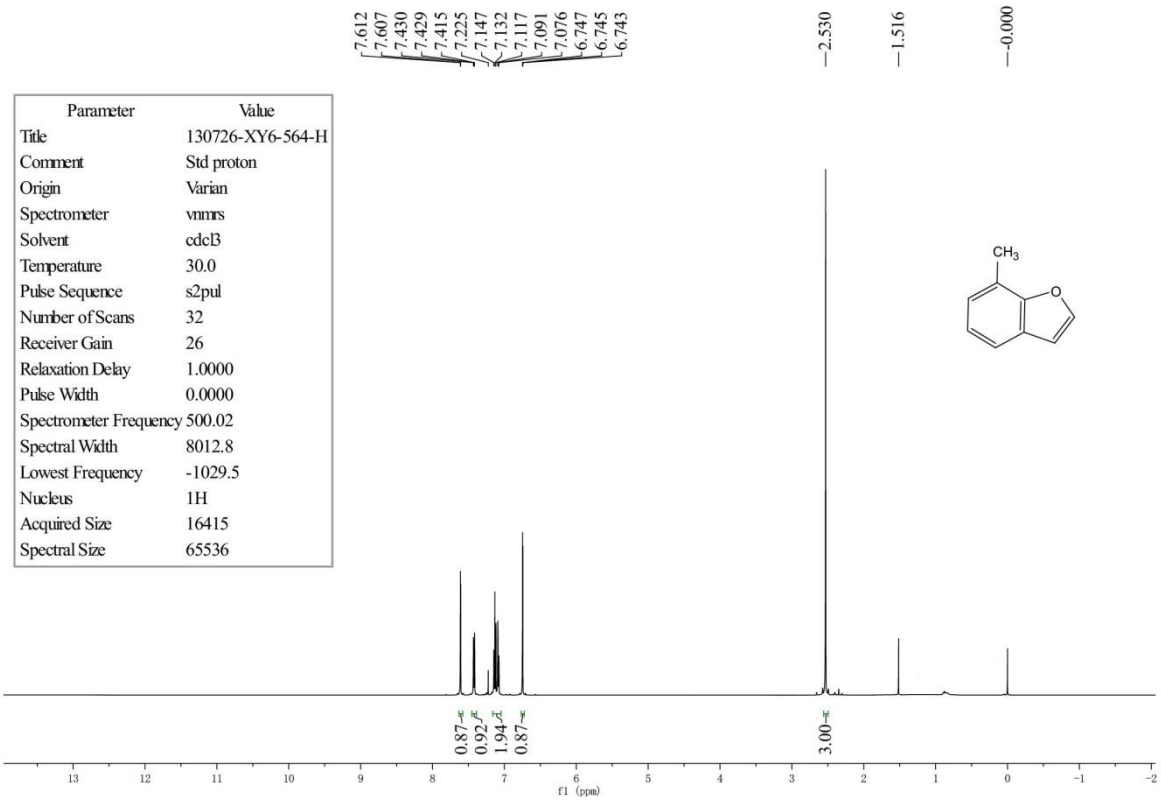
Parameter	Value
1 Title	120510-XY4-271B-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	19812
10 Acquisition Time	1.3005
11 Spectrometer Frequency	125.74
12 Spectral Width	30487.8
13 Lowest Frequency	-2042.4
14 Nucleus	13C
15 Acquired Size	39649
16 Spectral Size	131072



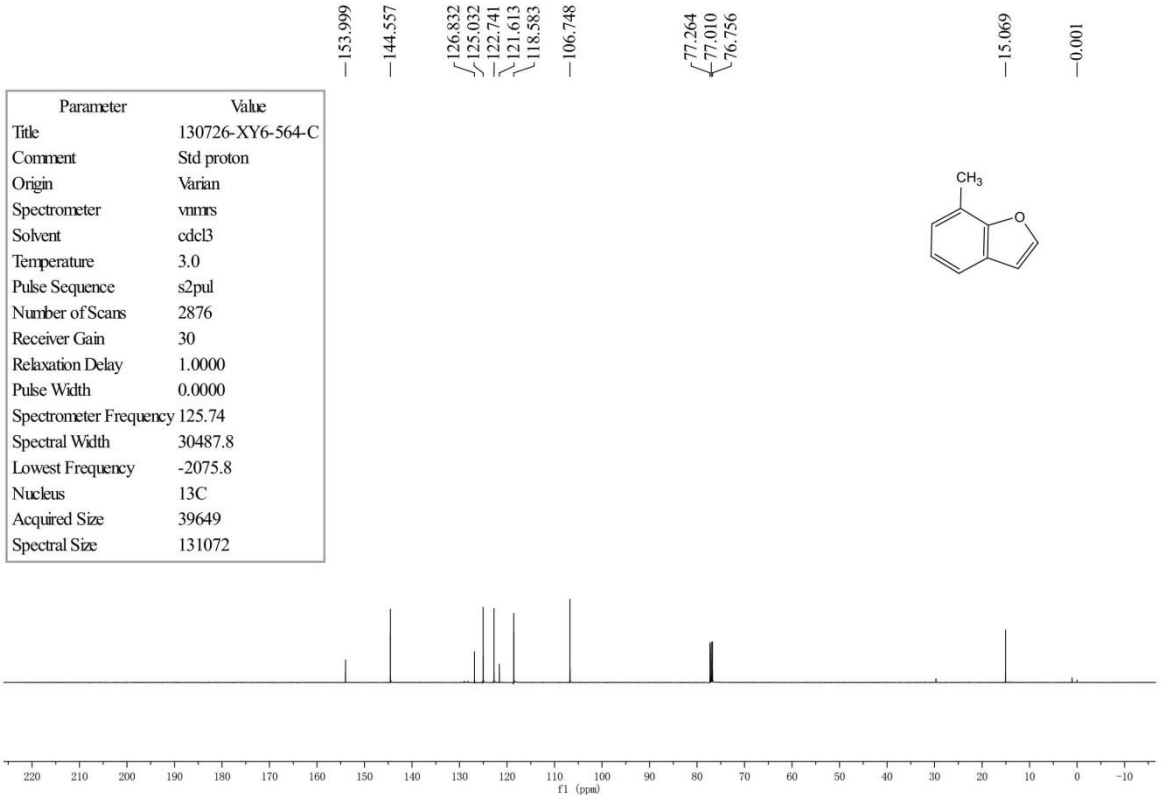
	Parameter	Value
1	Title	110614-SK-07-747-H
2	Comment	Std proton
3	Origin	Varian
4	Spectrometer	vnmrs
5	Solvent	dmso
6	Temperature	25.0
7	Experiment	1D
8	Probe	dualbb
9	Number of Scans	32
10	Spectrometer Frequency	500.02
11	Spectral Width	8012.8
12	Lowest Frequency	-1003.3
13	Nucleus	1H
14	Acquired Size	16415
15	Spectral Size	65536



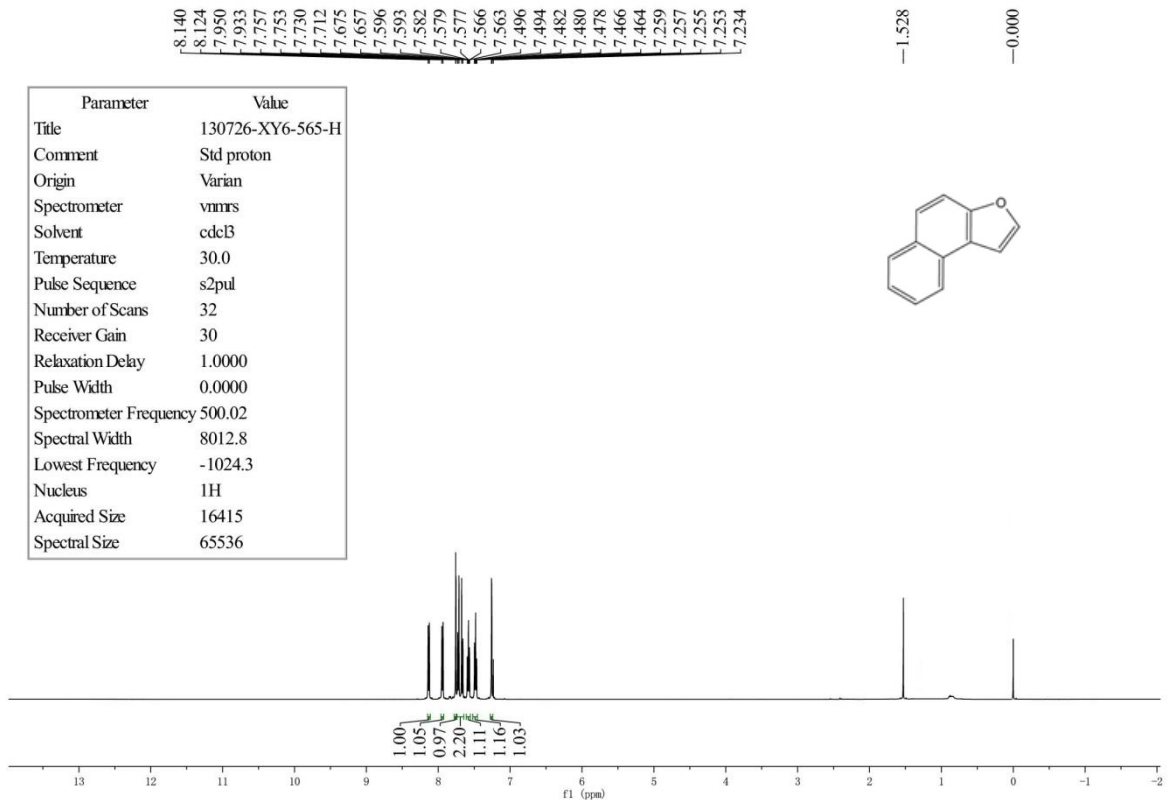
	Parameter	Value
1	Title	110614-SK-07-747-C
2	Comment	Std proton
3	Origin	Varian
4	Spectrometer	vnmrs
5	Solvent	dmso
6	Temperature	3.0
7	Experiment	1D
8	Probe	dualbb
9	Number of Scans	484
10	Spectrometer Frequency	125.74
11	Spectral Width	30487.8
12	Lowest Frequency	-2042.5
13	Nucleus	13C
14	Acquired Size	39649
15	Spectral Size	131072



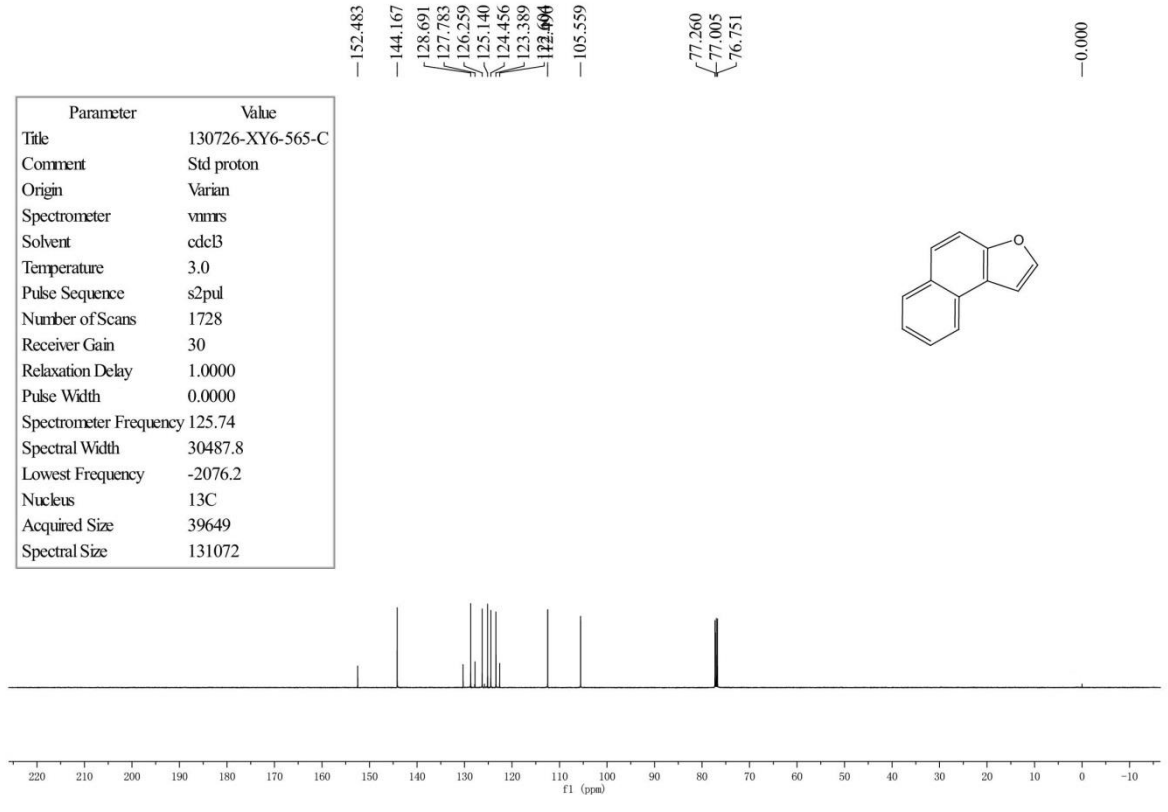
Parameter	Value
Title	130726-XY6-564-H
Comment	Std proton
Origin	Varian
Spectrometer	vnmrs
Solvent	cdcl3
Temperature	30.0
Pulse Sequence	s2pul
Number of Scans	32
Receiver Gain	26
Relaxation Delay	1.0000
Pulse Width	0.0000
Spectrometer Frequency	500.02
Spectral Width	8012.8
Lowest Frequency	-1029.5
Nucleus	1H
Acquired Size	16415
Spectral Size	65536



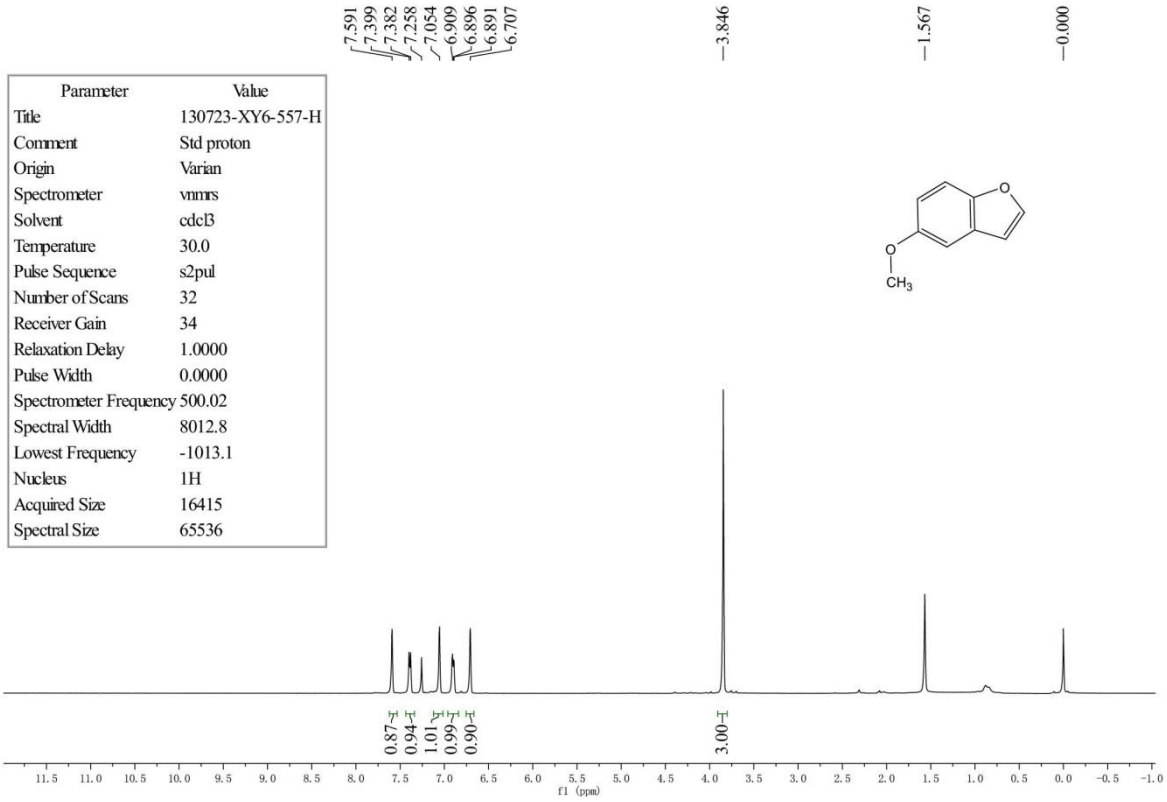
Parameter	Value
Title	130726-XY6-564-C
Comment	Std proton
Origin	Varian
Spectrometer	vnmrs
Solvent	cdcl3
Temperature	3.0
Pulse Sequence	s2pul
Number of Scans	2876
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	0.0000
Spectrometer Frequency	125.74
Spectral Width	30487.8
Lowest Frequency	-2075.8
Nucleus	13C
Acquired Size	39649
Spectral Size	131072



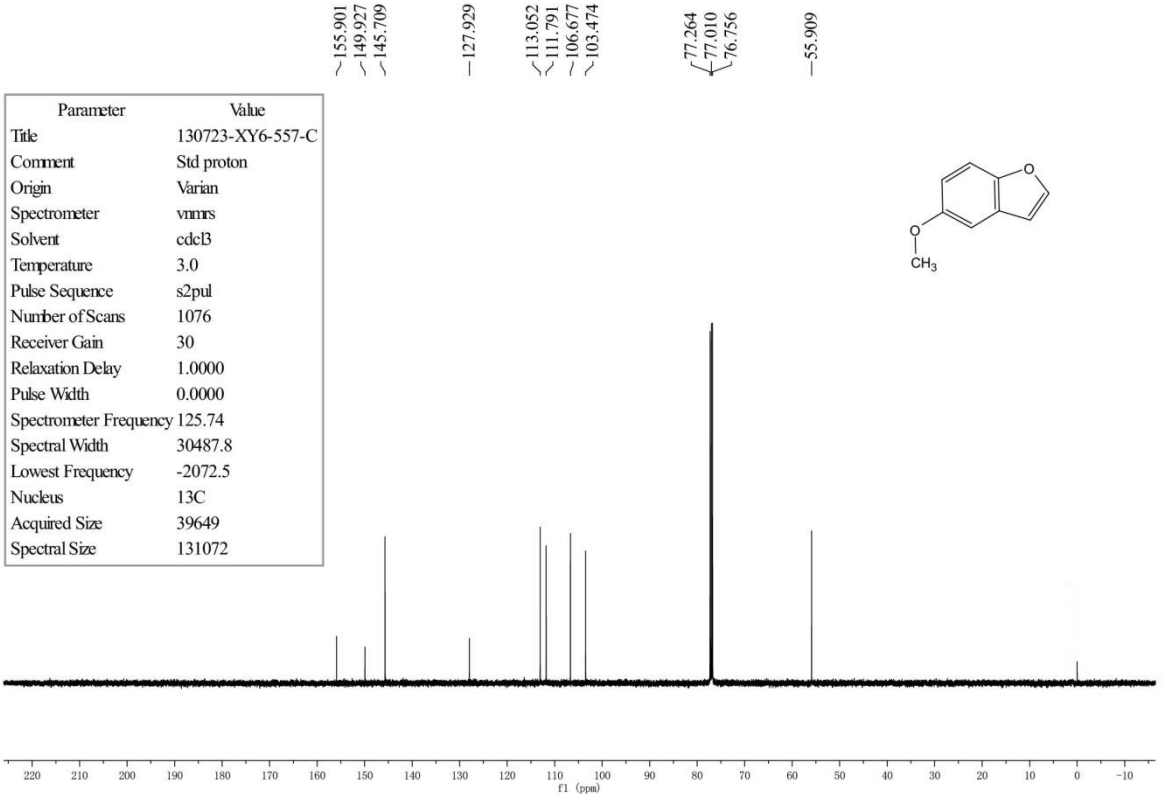
Parameter	Value
Title	130726-XY6-565-H
Comment	Std proton
Origin	Varian
Spectrometer	vnmrs
Solvent	cdcl3
Temperature	30.0
Pulse Sequence	s2pul
Number of Scans	32
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	0.0000
Spectrometer Frequency	500.02
Spectral Width	8012.8
Lowest Frequency	-1024.3
Nucleus	1H
Acquired Size	16415
Spectral Size	65536



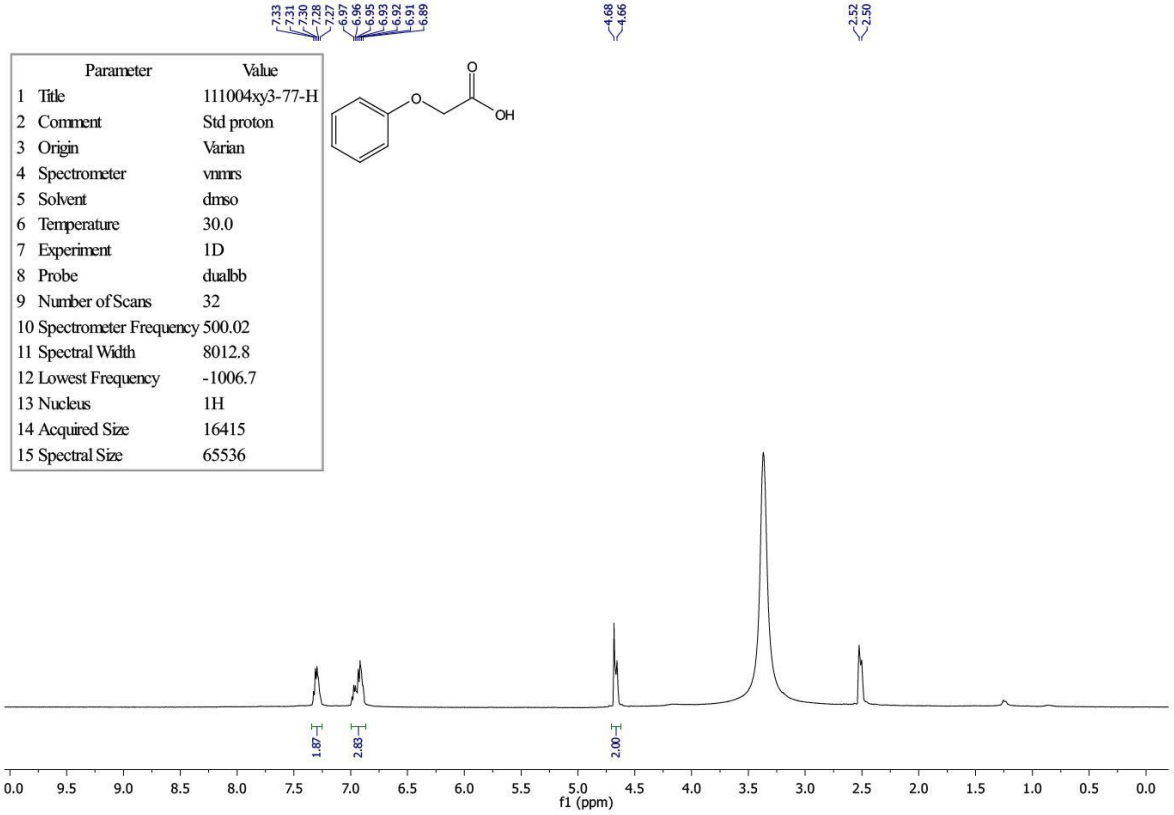
Parameter	Value
Title	130726-XY6-565-C
Comment	Std proton
Origin	Varian
Spectrometer	vnmrs
Solvent	cdcl3
Temperature	3.0
Pulse Sequence	s2pul
Number of Scans	1728
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	0.0000
Spectrometer Frequency	125.74
Spectral Width	30487.8
Lowest Frequency	-2076.2
Nucleus	13C
Acquired Size	39649
Spectral Size	131072



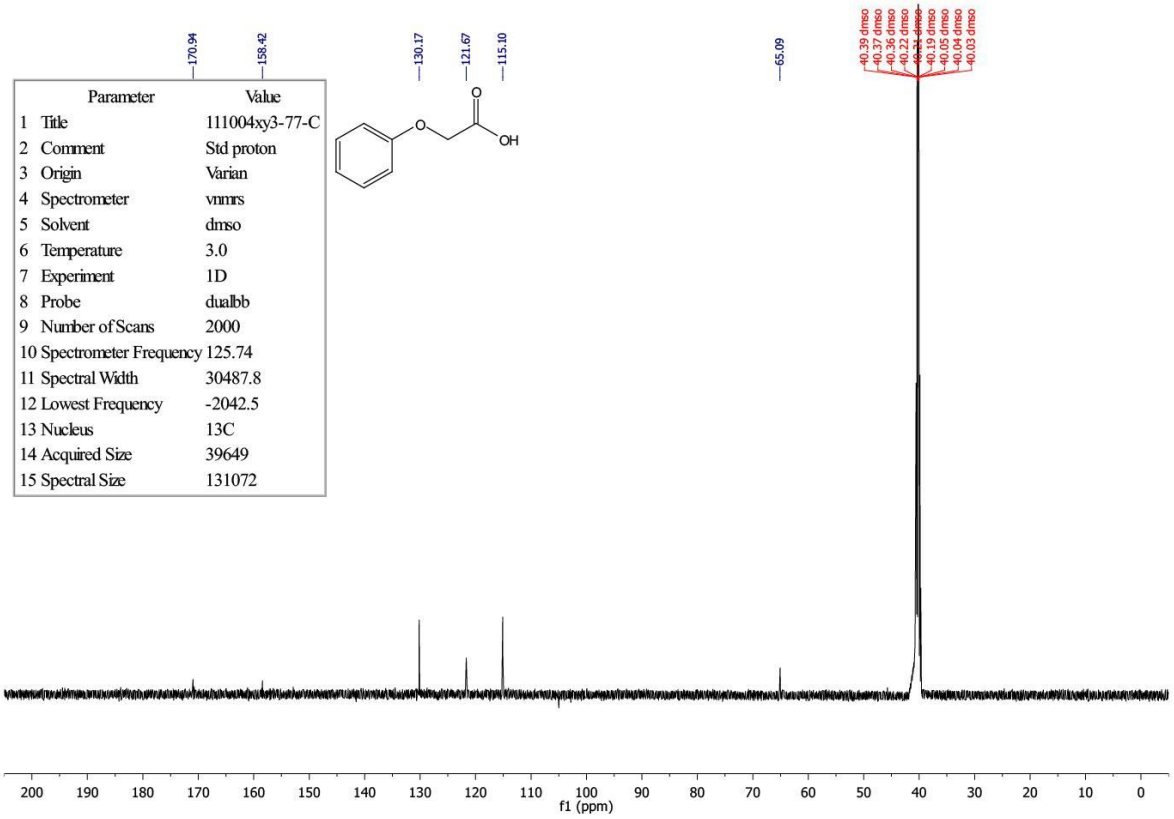
Parameter	Value
Title	130723-XY6-557-H
Comment	Std proton
Origin	Varian
Spectrometer	vnmrs
Solvent	cdcl3
Temperature	30.0
Pulse Sequence	s2pul
Number of Scans	32
Receiver Gain	34
Relaxation Delay	1.0000
Pulse Width	0.0000
Spectrometer Frequency	500.02
Spectral Width	8012.8
Lowest Frequency	-1013.1
Nucleus	1H
Acquired Size	16415
Spectral Size	65536



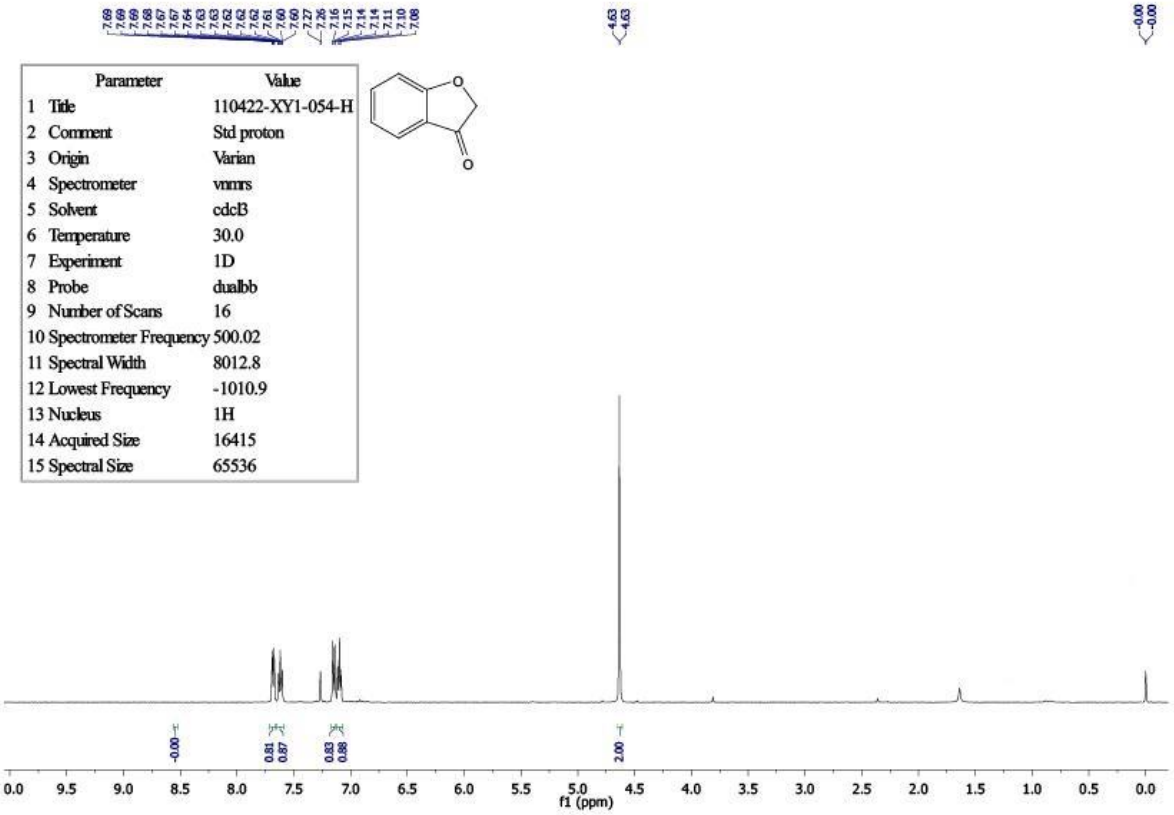
Parameter	Value
Title	130723-XY6-557-C
Comment	Std proton
Origin	Varian
Spectrometer	vnmrs
Solvent	cdcl3
Temperature	3.0
Pulse Sequence	s2pul
Number of Scans	1076
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	0.0000
Spectrometer Frequency	125.74
Spectral Width	30487.8
Lowest Frequency	-2072.5
Nucleus	13C
Acquired Size	39649
Spectral Size	131072

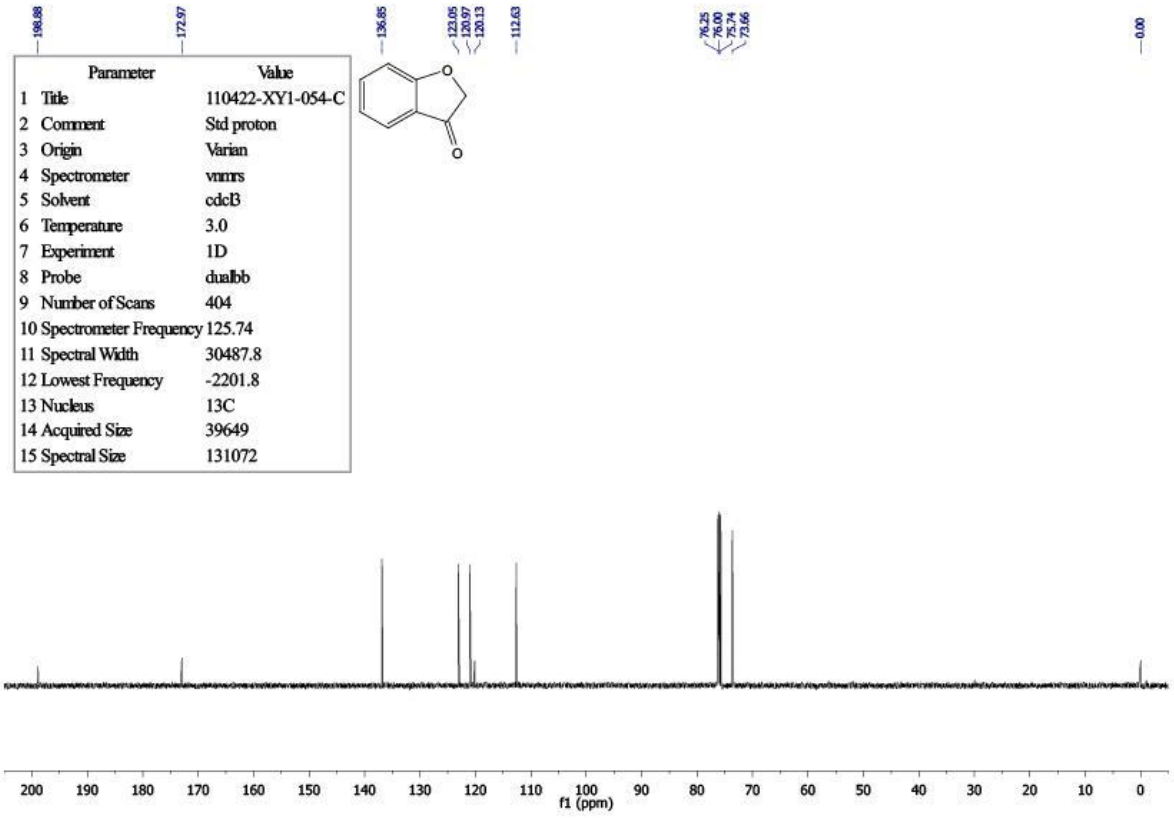


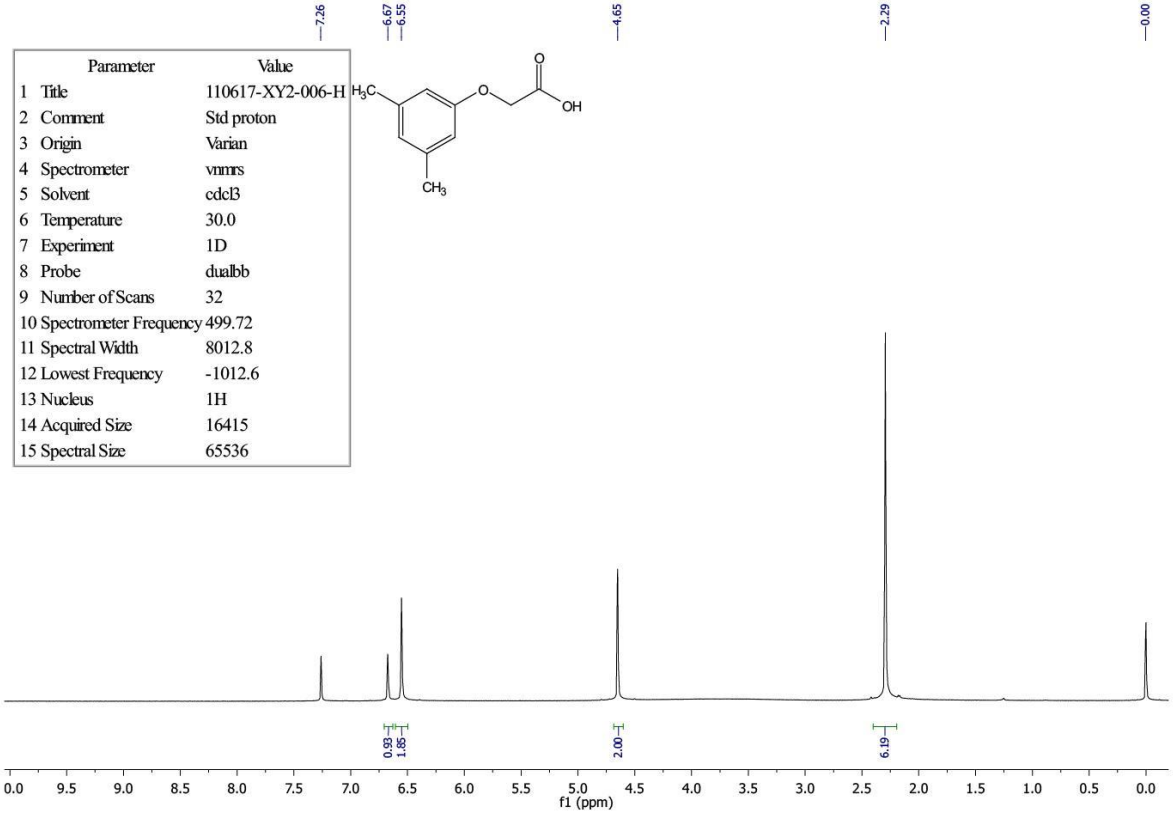
Parameter	Value
1 Title	111004xy3-77-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	dmso
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	32
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1006.7
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



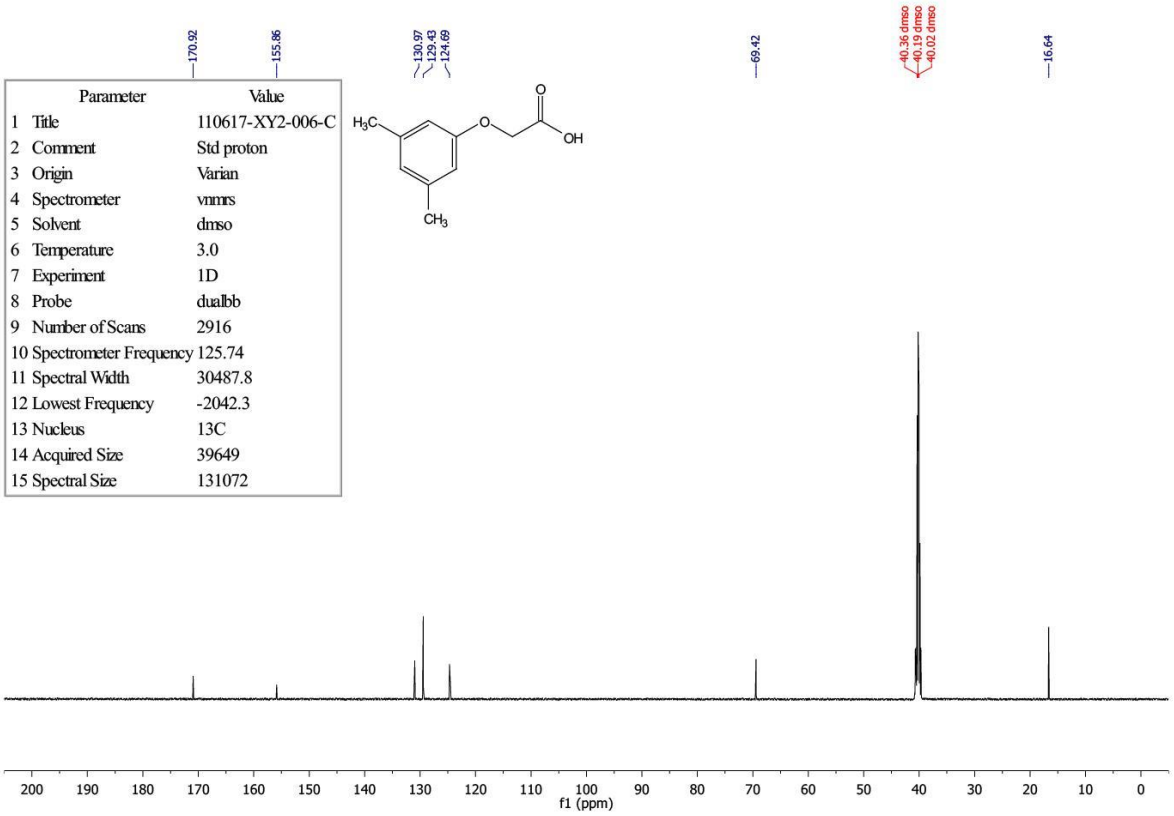
Parameter	Value
1 Title	111004xy3-77-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	dmso
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	2000
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2042.5
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072


7.69 7.69 7.69 7.68 7.67 7.67 7.64 7.63 7.63 7.62 7.62 7.62 7.61 7.60 7.60 7.27 7.26 7.16 7.15 7.14 7.14 7.11 7.10 7.08
4.63 4.63
0.00 0.00
Parameter Value
1 Title 110422-XY1-054-H
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent cdcl3
6 Temperature 30.0
7 Experiment 1D
8 Probe dualbb
9 Number of Scans 16
10 Spectrometer Frequency 500.02
11 Spectral Width 8012.8
12 Lowest Frequency -1010.9
13 Nucleus 1H
14 Acquired Size 16415
15 Spectral Size 65536
O
O
0.00 0.81 0.87 0.83 0.88 2.00
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

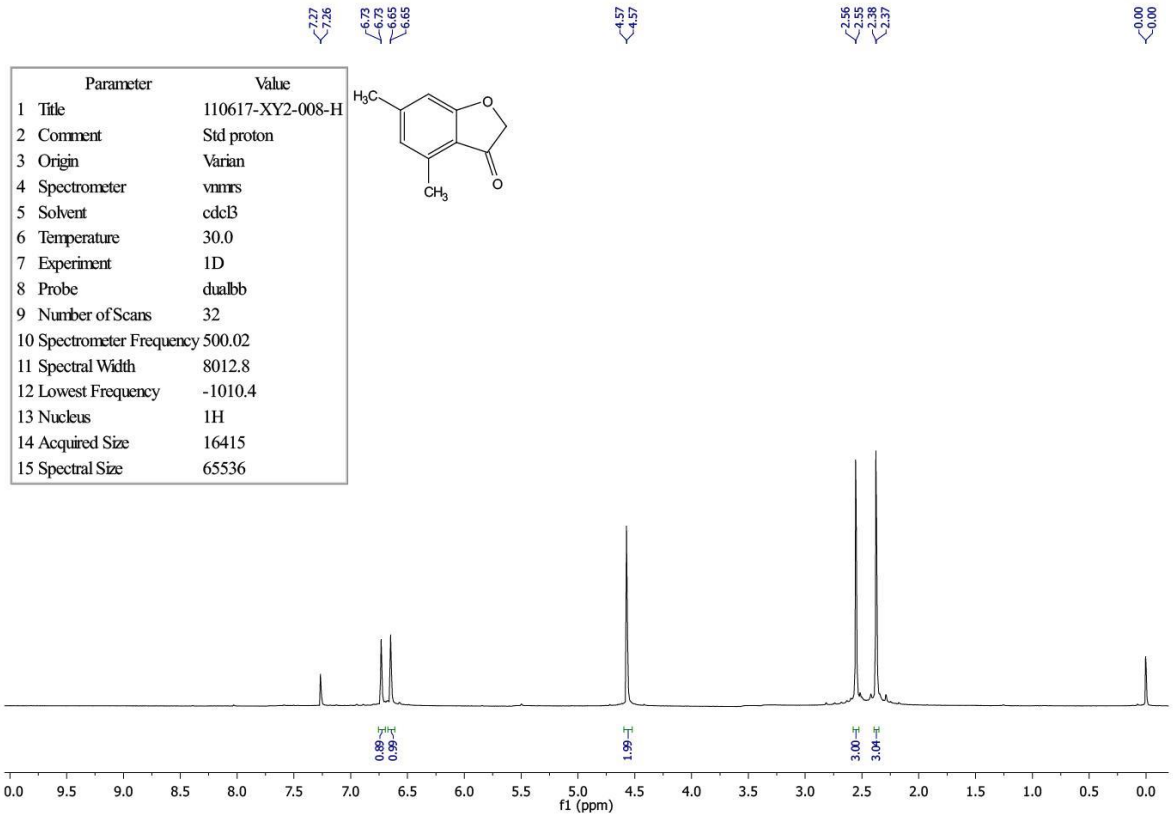

198.88 172.97 136.85 123.06 120.97 120.13 112.63 76.25 76.00 75.74 73.66 0.00
Parameter Value
1 Title 110422-XY1-054-C
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent cdcl3
6 Temperature 3.0
7 Experiment 1D
8 Probe dualbb
9 Number of Scans 404
10 Spectrometer Frequency 125.74
11 Spectral Width 30487.8
12 Lowest Frequency -2201.8
13 Nucleus 13C
14 Acquired Size 39649
15 Spectral Size 131072
O
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

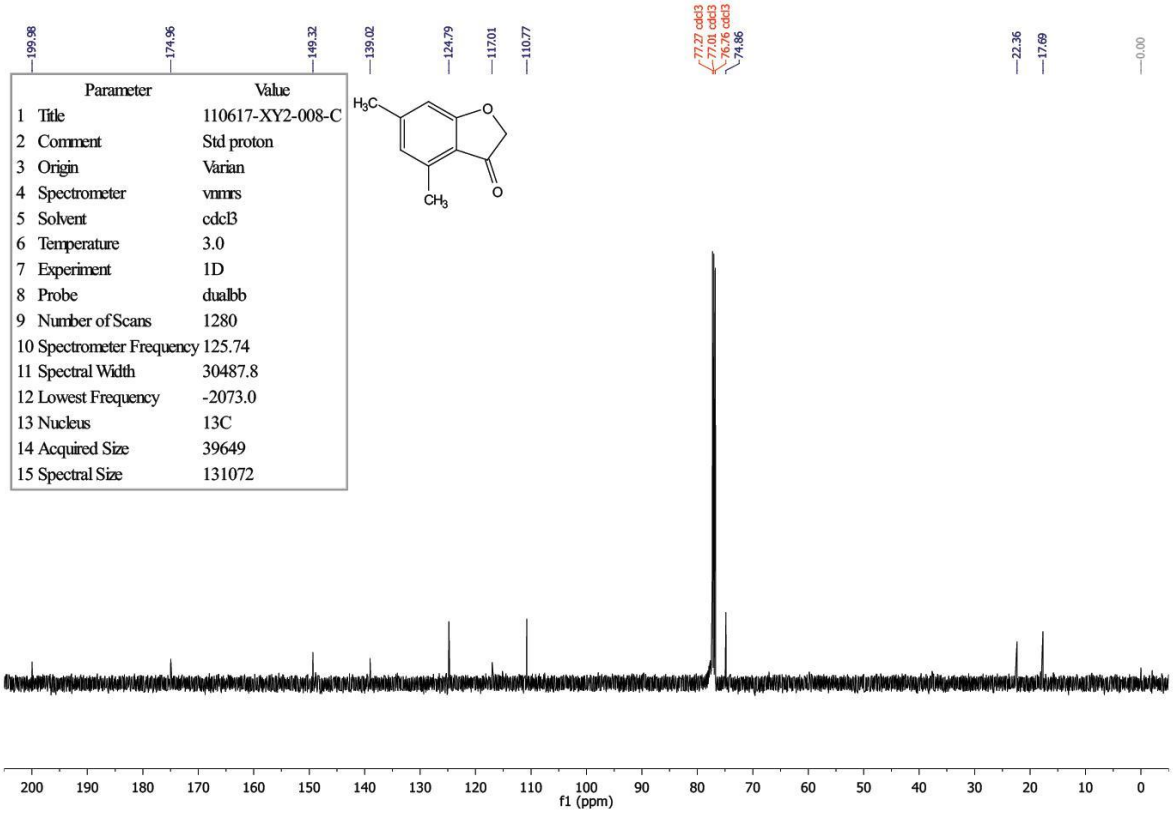


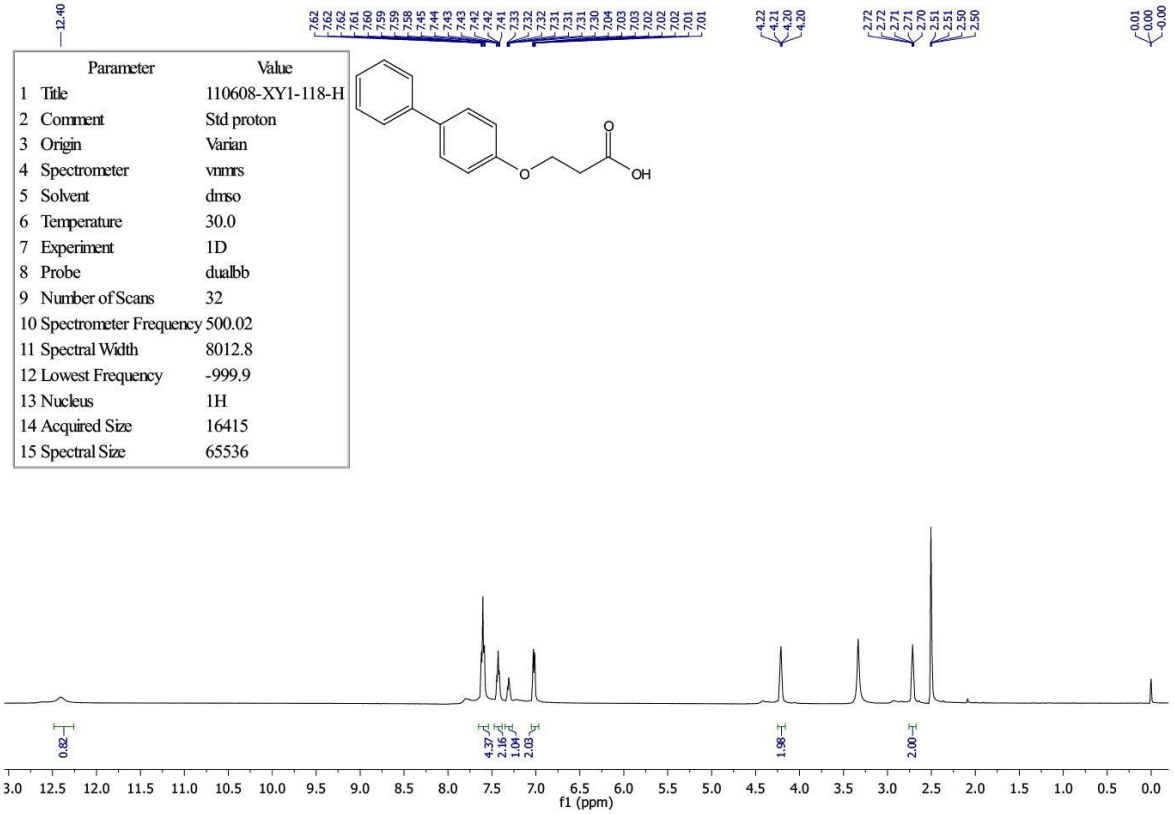
Parameter	Value
1 Title	110617-XY2-006-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	32
10 Spectrometer Frequency	499.72
11 Spectral Width	8012.8
12 Lowest Frequency	-1012.6
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536

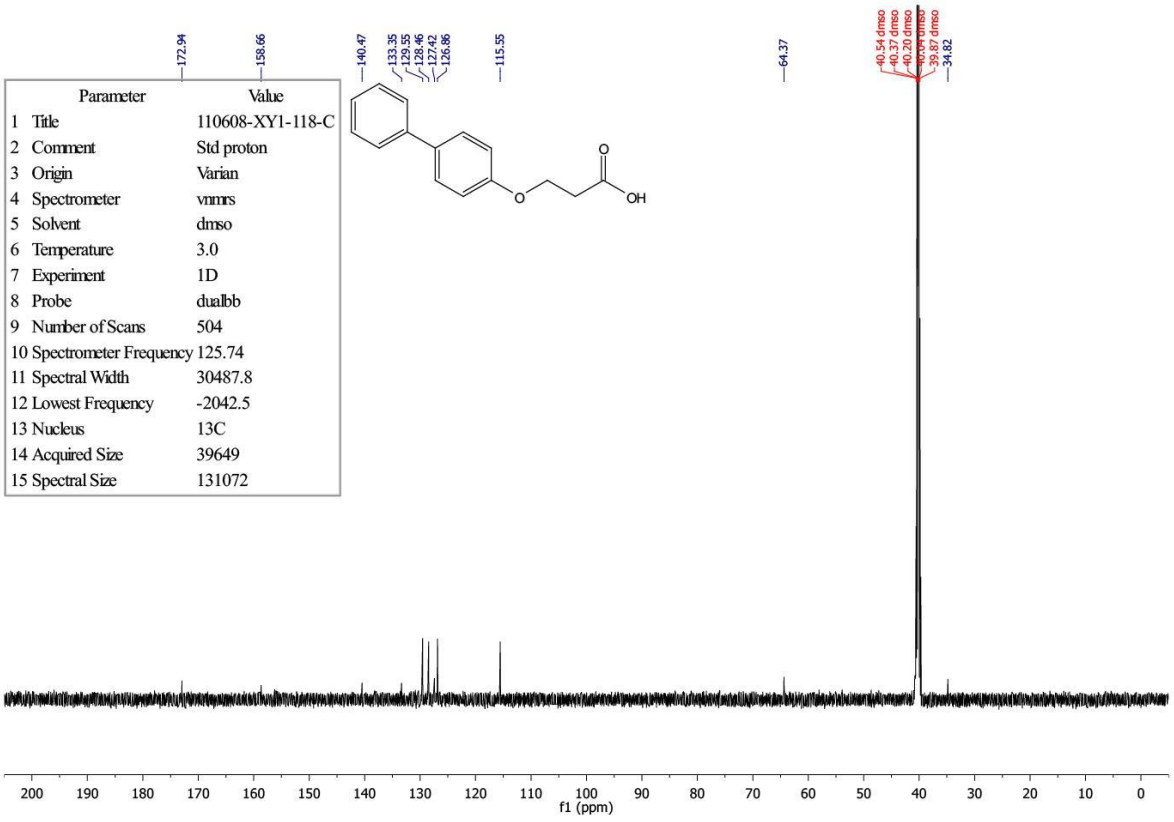


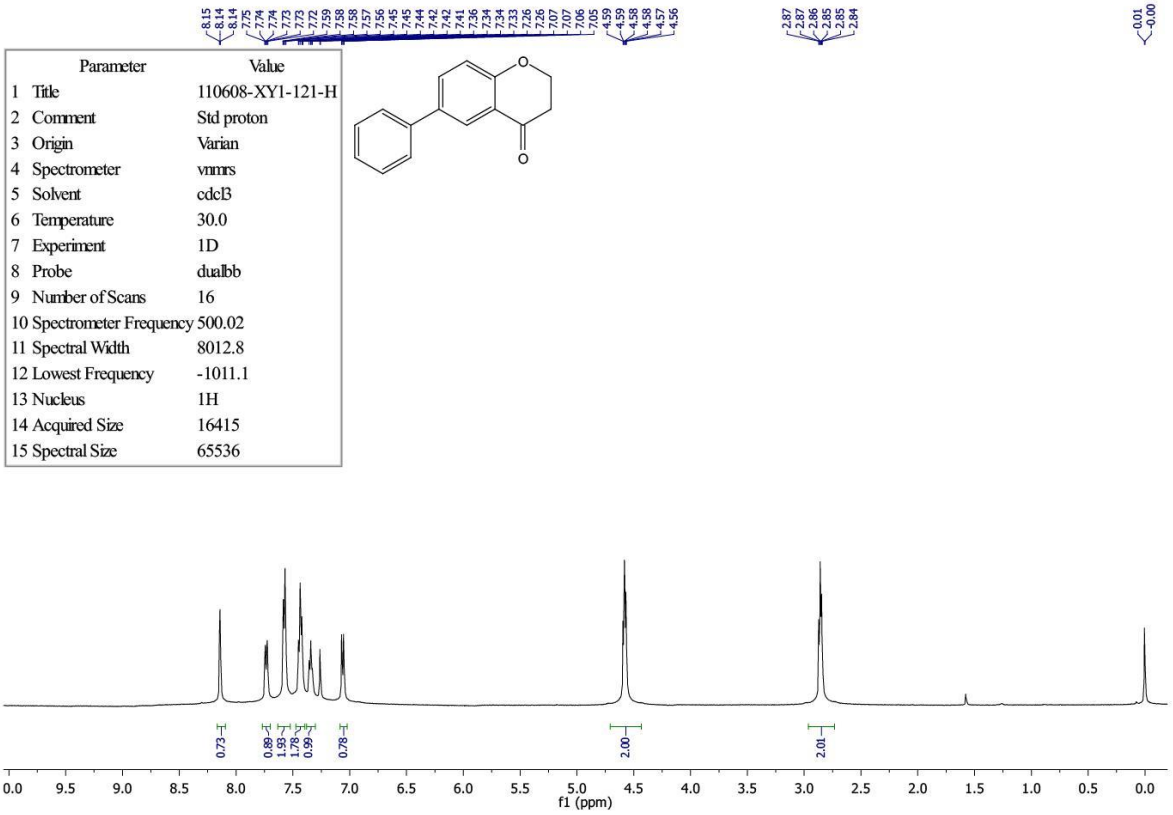
Parameter	Value
1 Title	110617-XY2-006-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	dmso
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	2916
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2042.3
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072

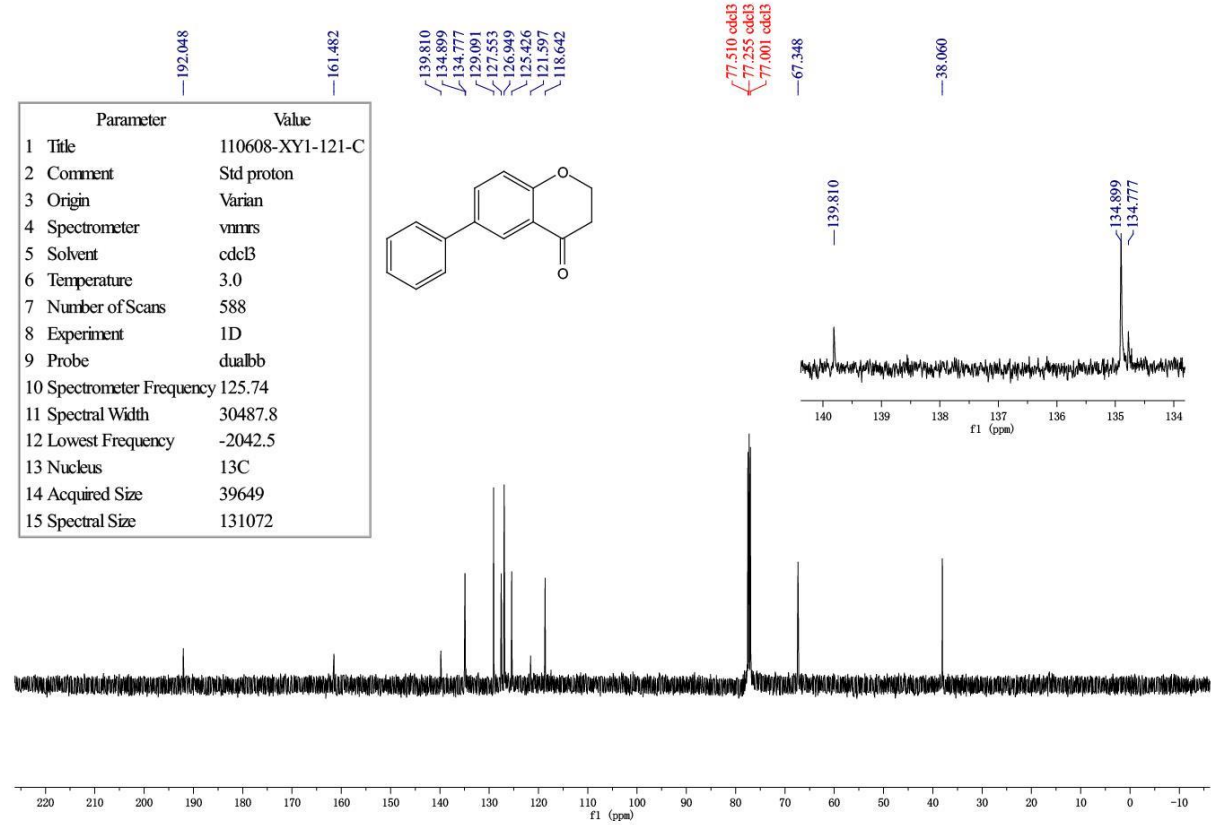

7.27
7.26
6.73
6.73
6.65
6.65
4.57
4.57
2.56
2.55
2.38
2.37
0.00
0.00
Parameter Value
1 Title 110617-XY2-008-H
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent cdcl3
6 Temperature 30.0
7 Experiment 1D
8 Probe dualbb
9 Number of Scans 32
10 Spectrometer Frequency 500.02
11 Spectral Width 8012.8
12 Lowest Frequency -1010.4
13 Nucleus 1H
14 Acquired Size 16415
15 Spectral Size 65536
H3C
O
O
CH3
0.99
0.99
1.99
3.00
3.04
f1 (ppm)

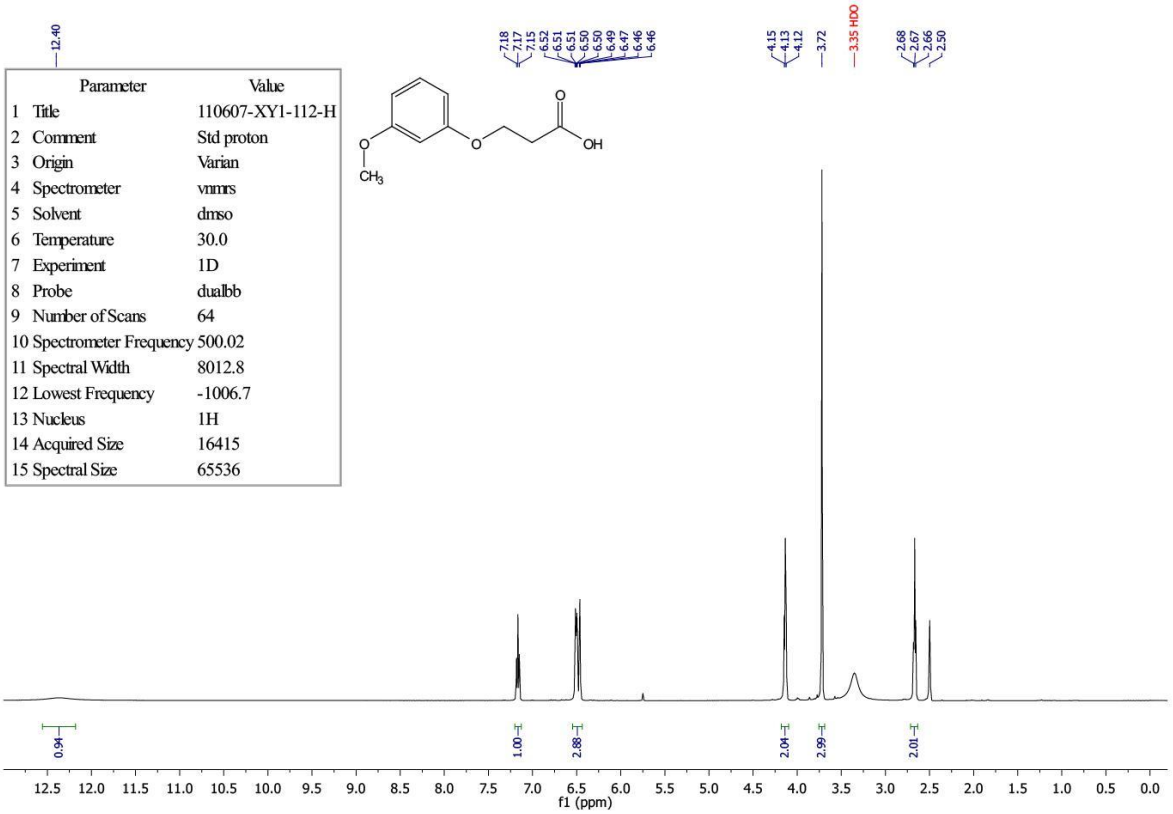

199.98
174.96
149.32
139.02
124.79
117.01
110.77
77.27 cdcl3
77.01 cdcl3
76.76 cdcl3
74.86
22.36
17.69
0.00
Parameter Value
1 Title 110617-XY2-008-C
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent cdcl3
6 Temperature 3.0
7 Experiment 1D
8 Probe dualbb
9 Number of Scans 1280
10 Spectrometer Frequency 125.74
11 Spectral Width 30487.8
12 Lowest Frequency -2073.0
13 Nucleus 13C
14 Acquired Size 39649
15 Spectral Size 131072
H3C
O
O
CH3
f1 (ppm)


12.40
7.62 7.62 7.62 7.61 7.60 7.59 7.59 7.58 7.45 7.44 7.43 7.43 7.42 7.42 7.41 7.33 7.32 7.32 7.31 7.31 7.31 7.30 7.04 7.03 7.03 7.02 7.02 7.02 7.01 7.01
4.22 4.21 4.20 4.20
2.72 2.72 2.71 2.71 2.70 2.51 2.51 2.50 2.50
0.01 0.00 -0.00
Parameter Value
1 Title 110608-XY1-118-H
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent dmso
6 Temperature 30.0
7 Experiment 1D
8 Probe dualbb
9 Number of Scans 32
10 Spectrometer Frequency 500.02
11 Spectral Width 8012.8
12 Lowest Frequency -999.9
13 Nucleus 1H
14 Acquired Size 16415
15 Spectral Size 65536
O
OH
O
0.82
4.37
2.16
1.04
2.03
1.98
2.00
f1 (ppm)

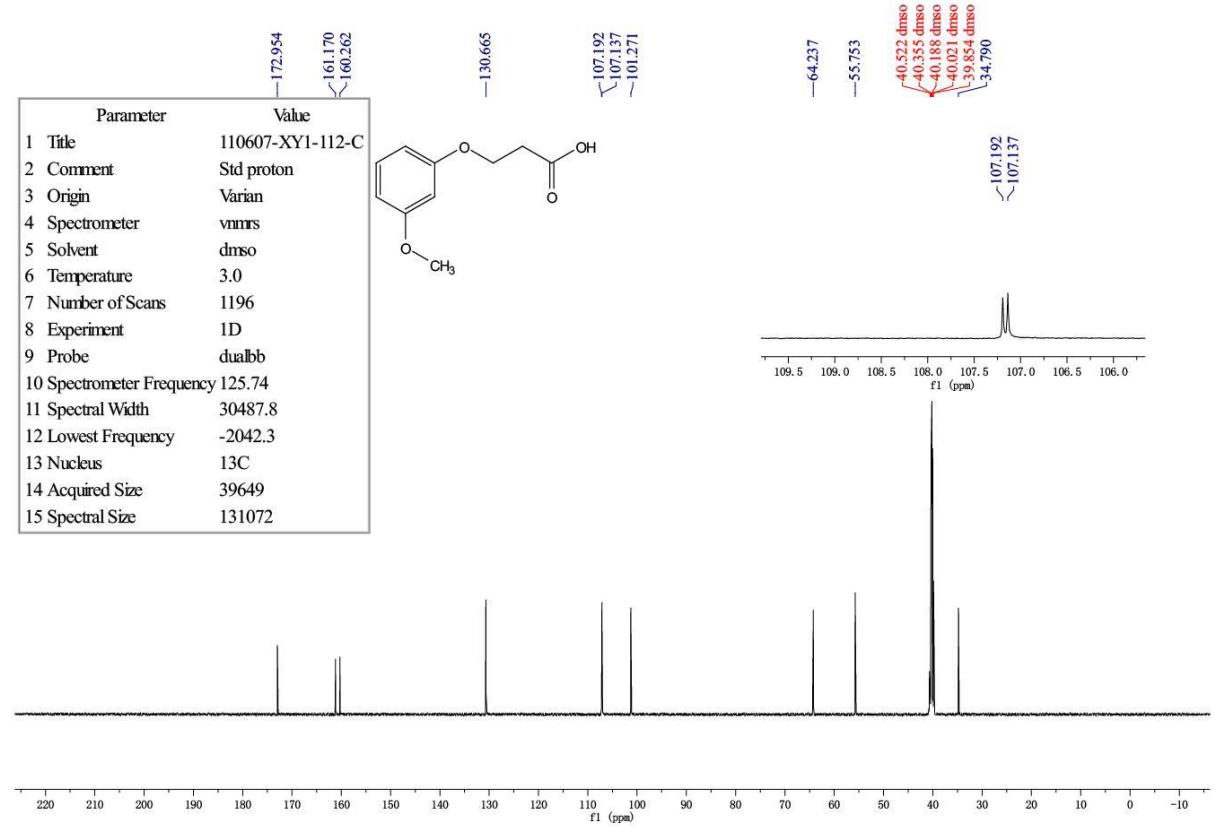

172.94
158.66
140.47
133.35
129.55
128.46
127.42
126.86
115.55
64.37
40.54 dmso
40.37 dmso
40.20 dmso
40.04 dmso
39.87 dmso
34.82
Parameter Value
1 Title 110608-XY1-118-C
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent dmso
6 Temperature 3.0
7 Experiment 1D
8 Probe dualbb
9 Number of Scans 504
10 Spectrometer Frequency 125.74
11 Spectral Width 30487.8
12 Lowest Frequency -2042.5
13 Nucleus 13C
14 Acquired Size 39649
15 Spectral Size 131072
O
OH
O
f1 (ppm)


8.15 8.14 8.14 7.75 7.74 7.74 7.73 7.73 7.72 7.59 7.58 7.58 7.57 7.56 7.45 7.44 7.44 7.42 7.41 7.36 7.34 7.34 7.33 7.26 7.07 7.07 7.06 7.05 4.59 4.59 4.58 4.58 4.57 4.56
2.87 2.87 2.86 2.85 2.85 2.84
0.01 -0.00
Parameter Value
1 Title 110608-XY1-121-H
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent cdcl3
6 Temperature 30.0
7 Experiment 1D
8 Probe dualbb
9 Number of Scans 16
10 Spectrometer Frequency 500.02
11 Spectral Width 8012.8
12 Lowest Frequency -1011.1
13 Nucleus 1H
14 Acquired Size 16415
15 Spectral Size 65536
O
O
0.73 0.89 1.53 1.78 0.99 0.78 2.00 2.01
f1 (ppm)

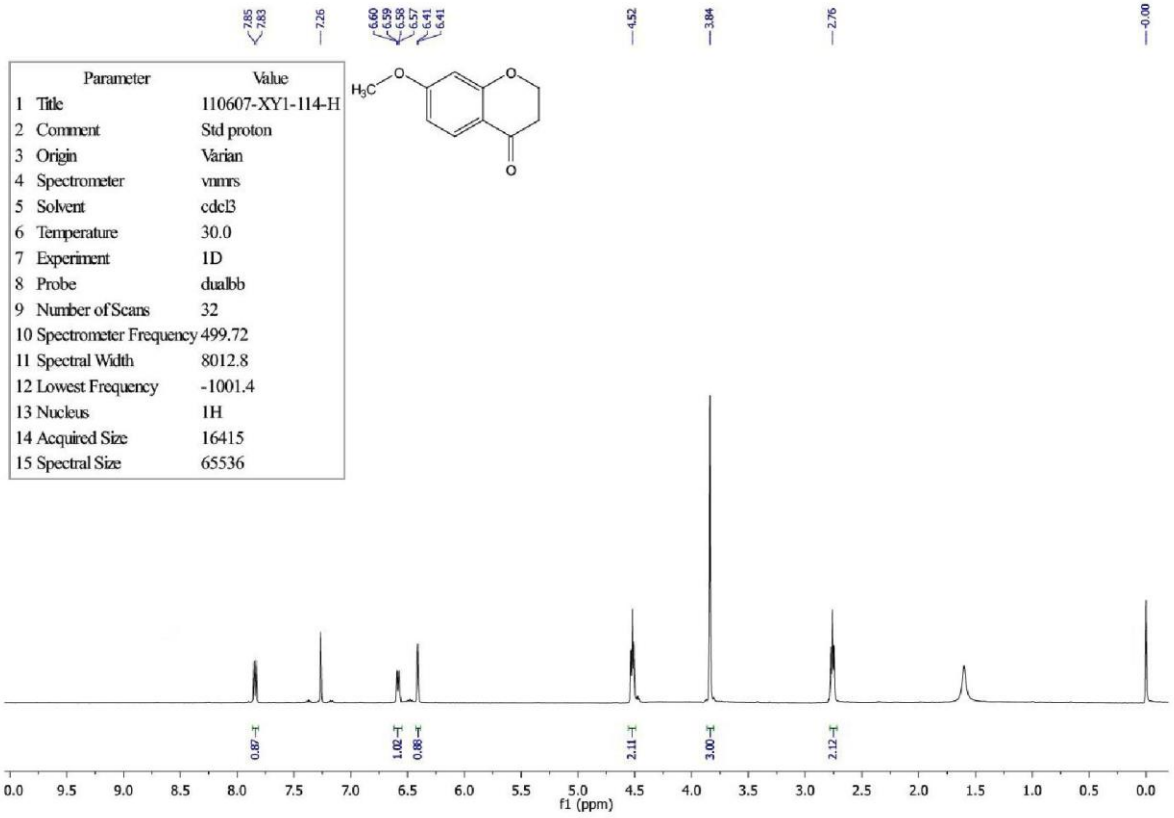

192.048 161.482 139.810 134.899 134.777 129.091 127.553 126.949 125.426 121.597 118.642
77.510 cdcl3 77.255 cdcl3 77.001 cdcl3 67.348 38.060
Parameter Value
1 Title 110608-XY1-121-C
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent cdcl3
6 Temperature 3.0
7 Number of Scans 588
8 Experiment 1D
9 Probe dualbb
10 Spectrometer Frequency 125.74
11 Spectral Width 30487.8
12 Lowest Frequency -2042.5
13 Nucleus 13C
14 Acquired Size 39649
15 Spectral Size 131072
O
O
139.810 134.899 134.777
f1 (ppm)
f1 (ppm)

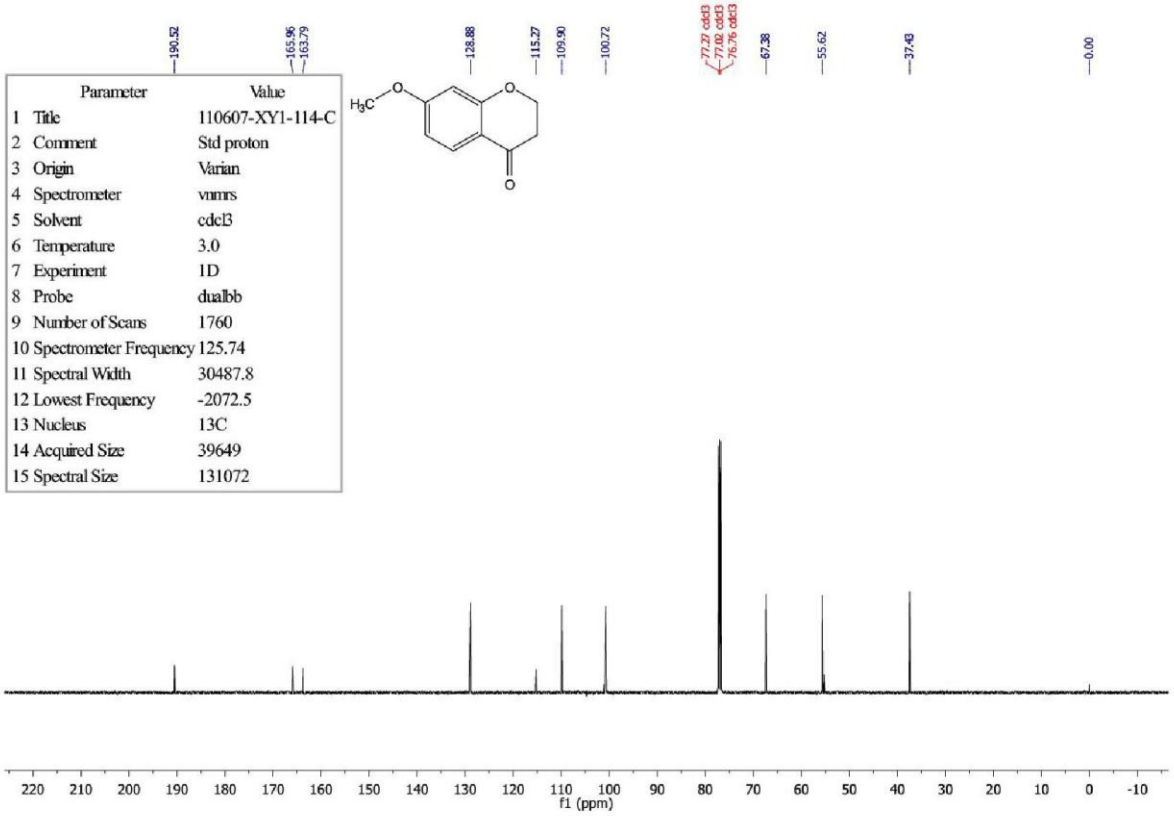


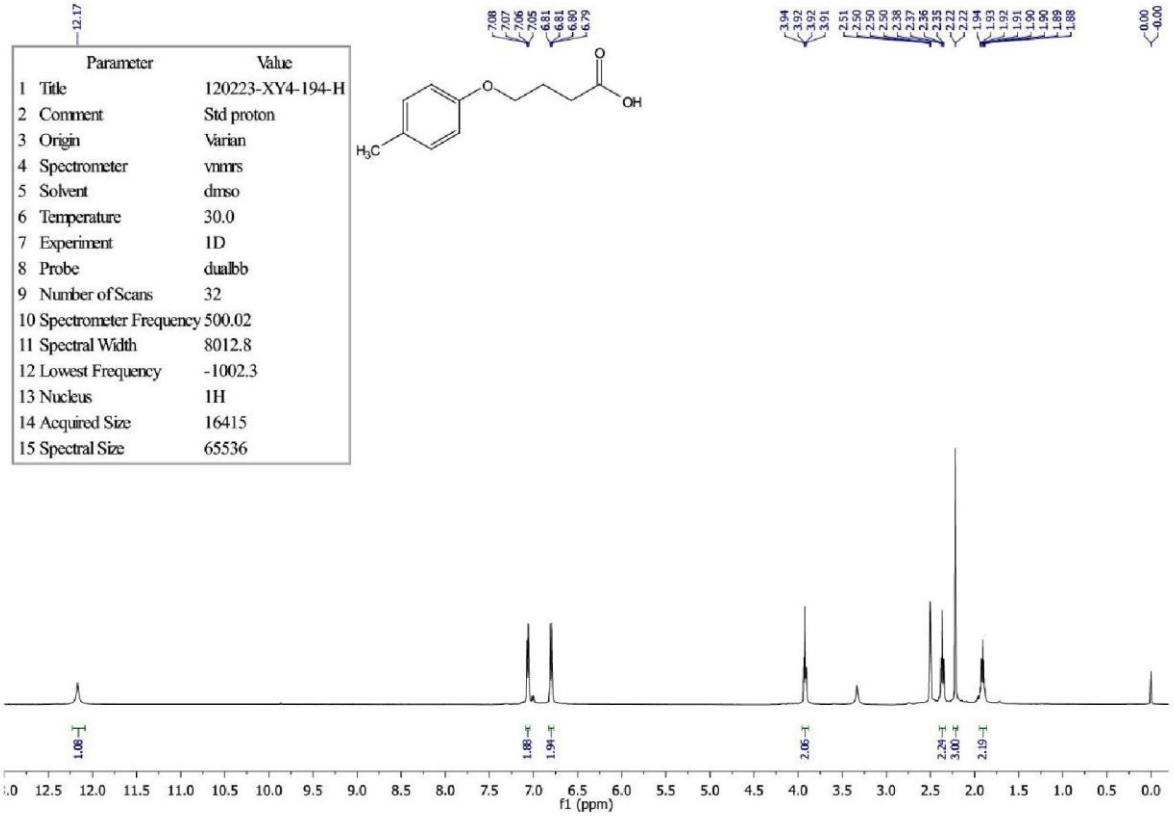
Parameter	Value
1 Title	110607-XY1-112-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	dmso
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	64
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1006.7
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



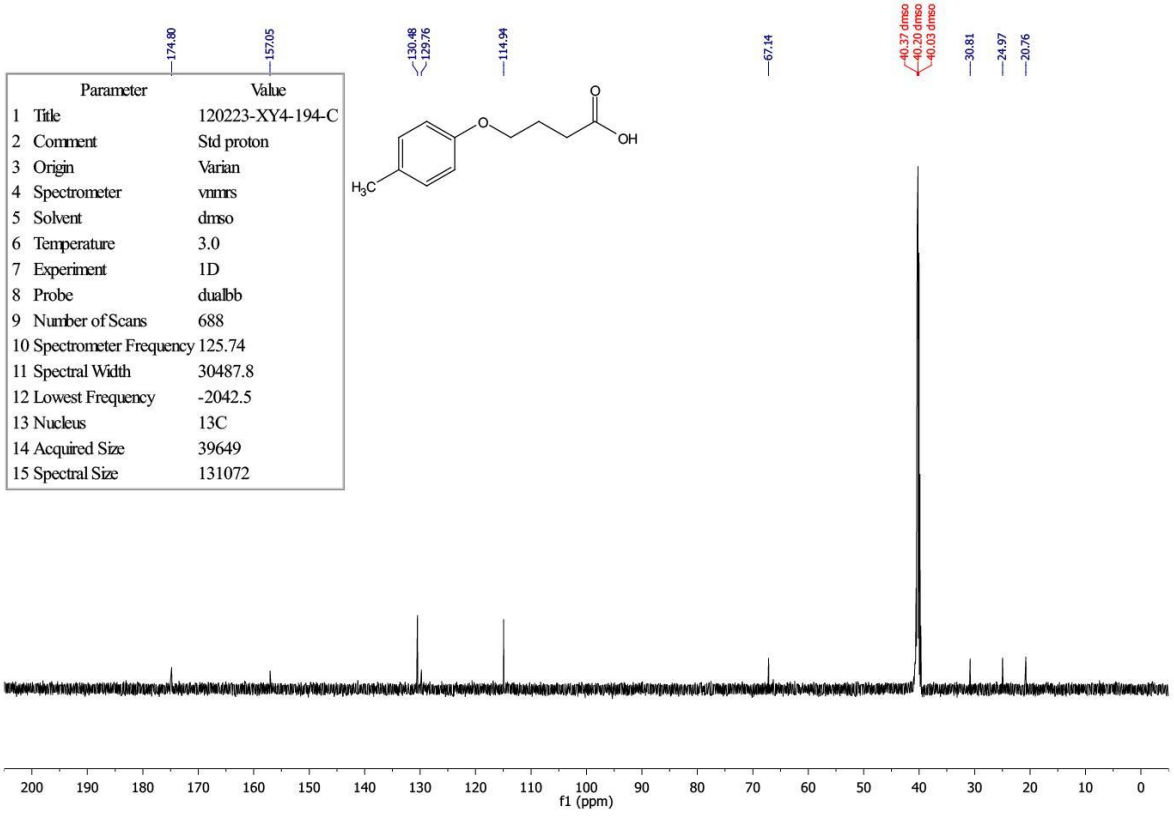
Parameter	Value
1 Title	110607-XY1-112-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	dmso
6 Temperature	3.0
7 Number of Scans	1196
8 Experiment	1D
9 Probe	dualbb
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2042.3
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072


7.85
7.83
7.26
6.60
6.59
6.58
6.57
6.41
6.41
4.52
3.84
2.76
0.00
Parameter Value
1 Title 110607-XY1-114-H
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent cdcl3
6 Temperature 30.0
7 Experiment 1D
8 Probe dualbb
9 Number of Scans 32
10 Spectrometer Frequency 499.72
11 Spectral Width 8012.8
12 Lowest Frequency -1001.4
13 Nucleus 1H
14 Acquired Size 16415
15 Spectral Size 65536
H3C
O
O
O
0.87
1.02
0.88
2.11
3.00
2.12
f1 (ppm)

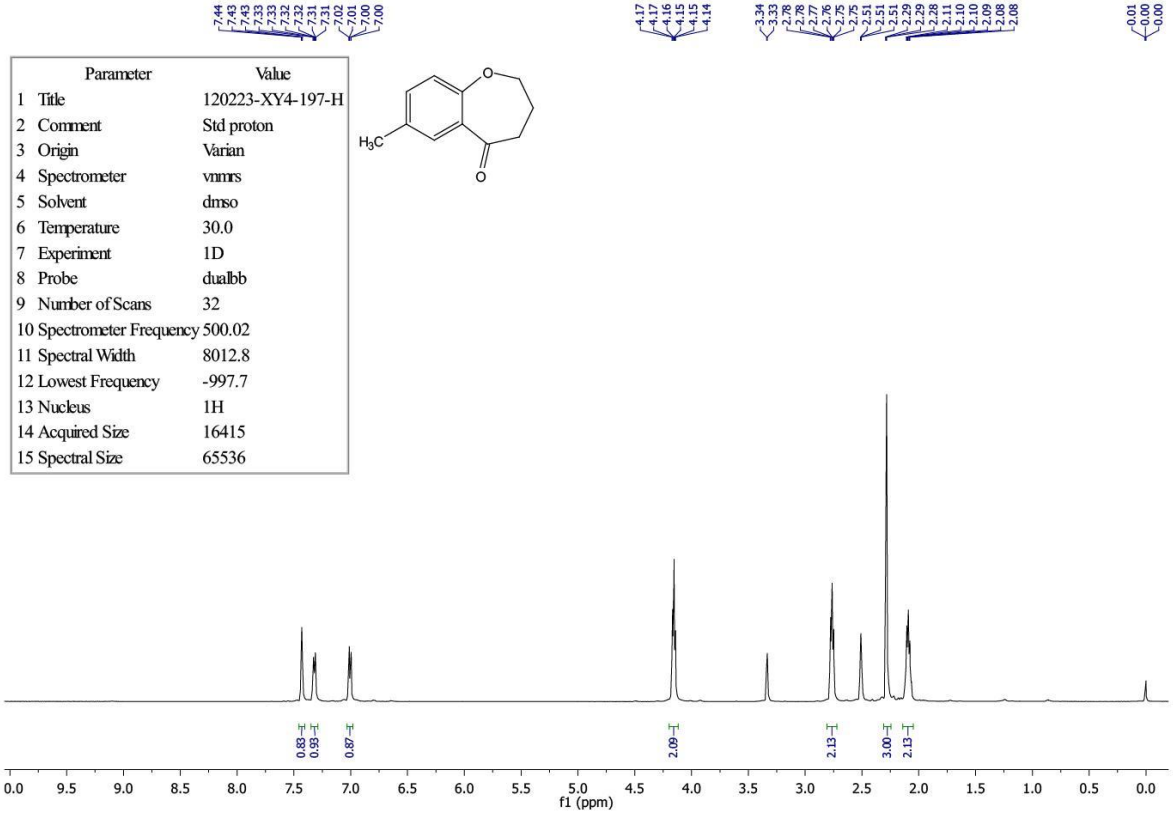

190.52
165.96
163.79
128.88
115.27
109.90
100.72
77.27 cdcl3
77.02 cdcl3
76.76 cdcl3
67.38
55.62
37.43
0.00
Parameter Value
1 Title 110607-XY1-114-C
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent cdcl3
6 Temperature 3.0
7 Experiment 1D
8 Probe dualbb
9 Number of Scans 1760
10 Spectrometer Frequency 125.74
11 Spectral Width 30487.8
12 Lowest Frequency -2072.5
13 Nucleus 13C
14 Acquired Size 39649
15 Spectral Size 131072
H3C
O
O
O
f1 (ppm)

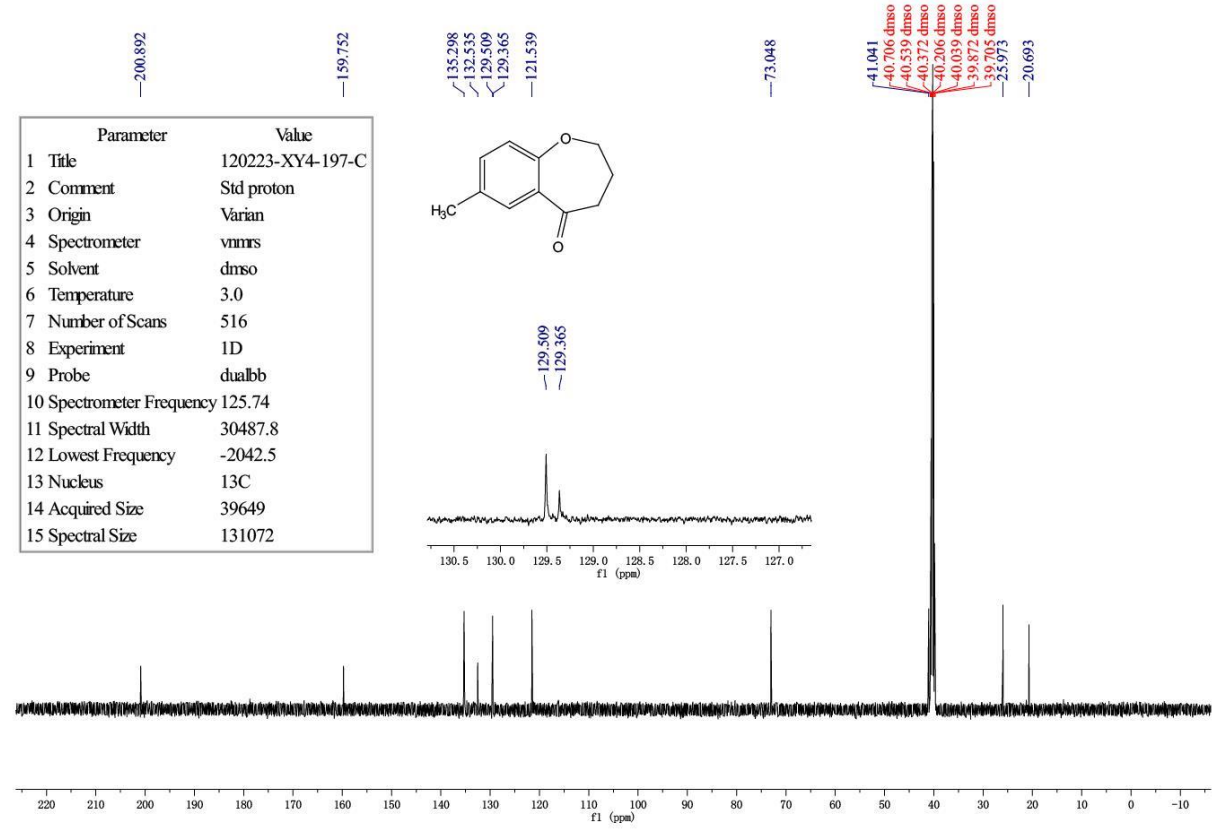


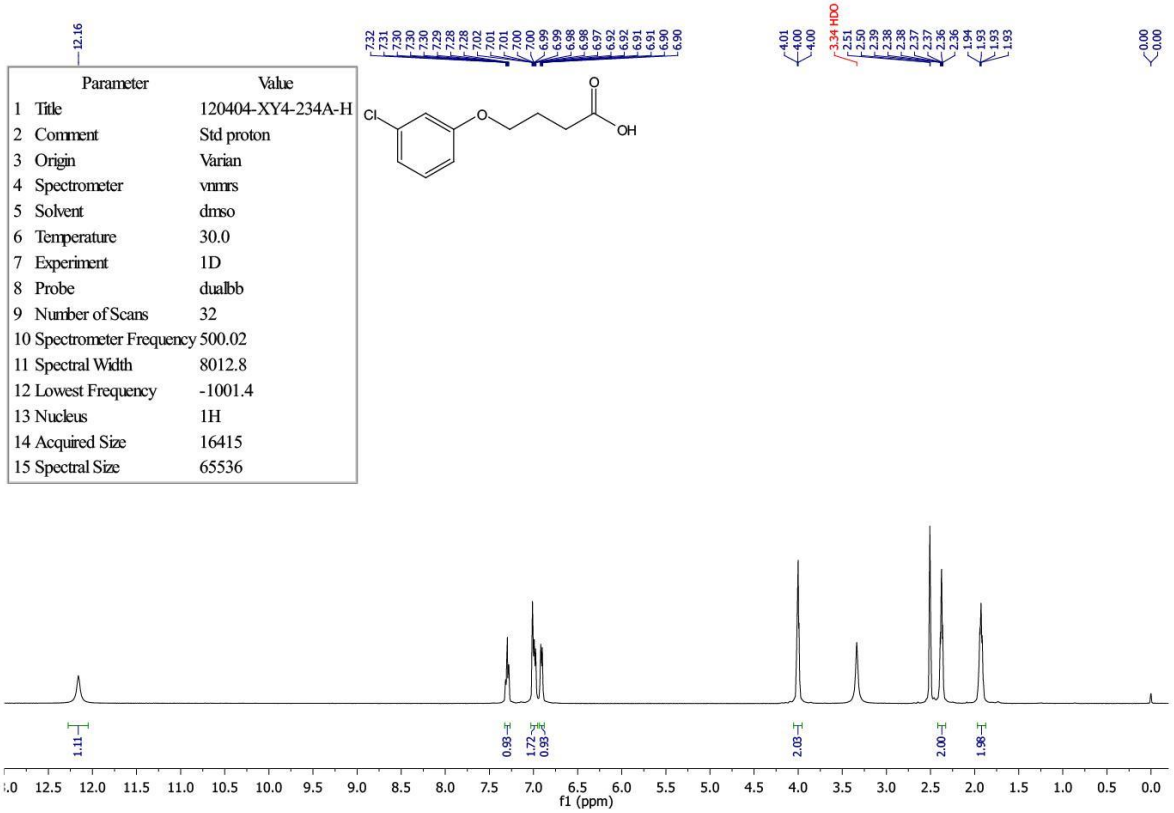
Parameter	Value
1 Title	120223-XY4-194-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	dmso
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	32
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1002.3
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



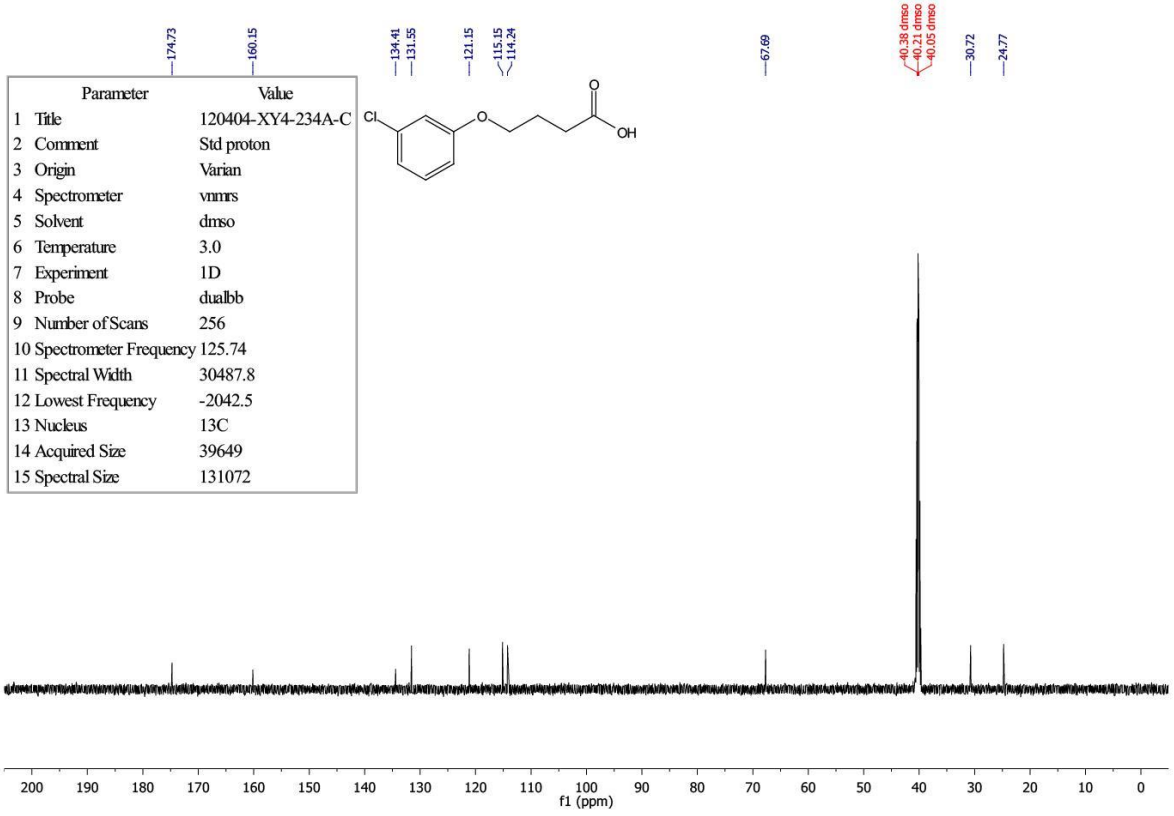
Parameter	Value
1 Title	120223-XY4-194-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	dmso
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	688
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2042.5
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072


7.44 7.43 7.43 7.33 7.33 7.32 7.32 7.31 7.31 7.02 7.01 7.00 7.00
4.17 4.17 4.16 4.15 4.15 4.14
3.34 3.33 2.78 2.78 2.77 2.76 2.75 2.75 2.51 2.51 2.51 2.29 2.29 2.28 2.11 2.10 2.09 2.08 2.08
0.01 0.00 0.00
Parameter Value
1 Title 120223-XY4-197-H
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent dmso
6 Temperature 30.0
7 Experiment 1D
8 Probe dualbb
9 Number of Scans 32
10 Spectrometer Frequency 500.02
11 Spectral Width 8012.8
12 Lowest Frequency -997.7
13 Nucleus 1H
14 Acquired Size 16415
15 Spectral Size 65536
H3C
O
O
0.83 0.93 0.87 2.09 2.13 3.00 2.13
f1 (ppm)

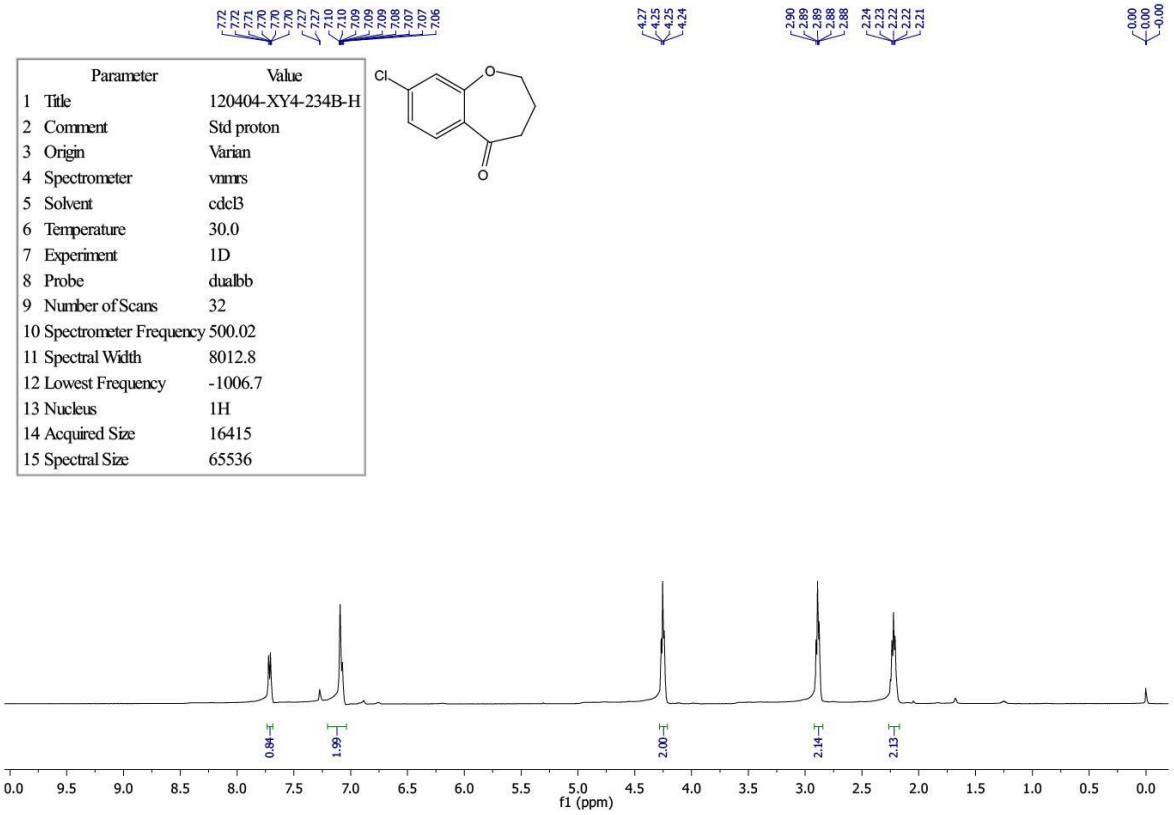

200.892 159.752 135.298 132.535 129.509 129.365 121.539 73.048
41.041 40.706 dmso 40.539 dmso 40.372 dmso 40.206 dmso 40.039 dmso 39.872 dmso 39.705 dmso 25.973 20.693
Parameter Value
1 Title 120223-XY4-197-C
2 Comment Std proton
3 Origin Varian
4 Spectrometer vnmrs
5 Solvent dmso
6 Temperature 3.0
7 Number of Scans 516
8 Experiment 1D
9 Probe dualbb
10 Spectrometer Frequency 125.74
11 Spectral Width 30487.8
12 Lowest Frequency -2042.5
13 Nucleus 13C
14 Acquired Size 39649
15 Spectral Size 131072
H3C
O
O
129.509 129.365
f1 (ppm)
f1 (ppm)



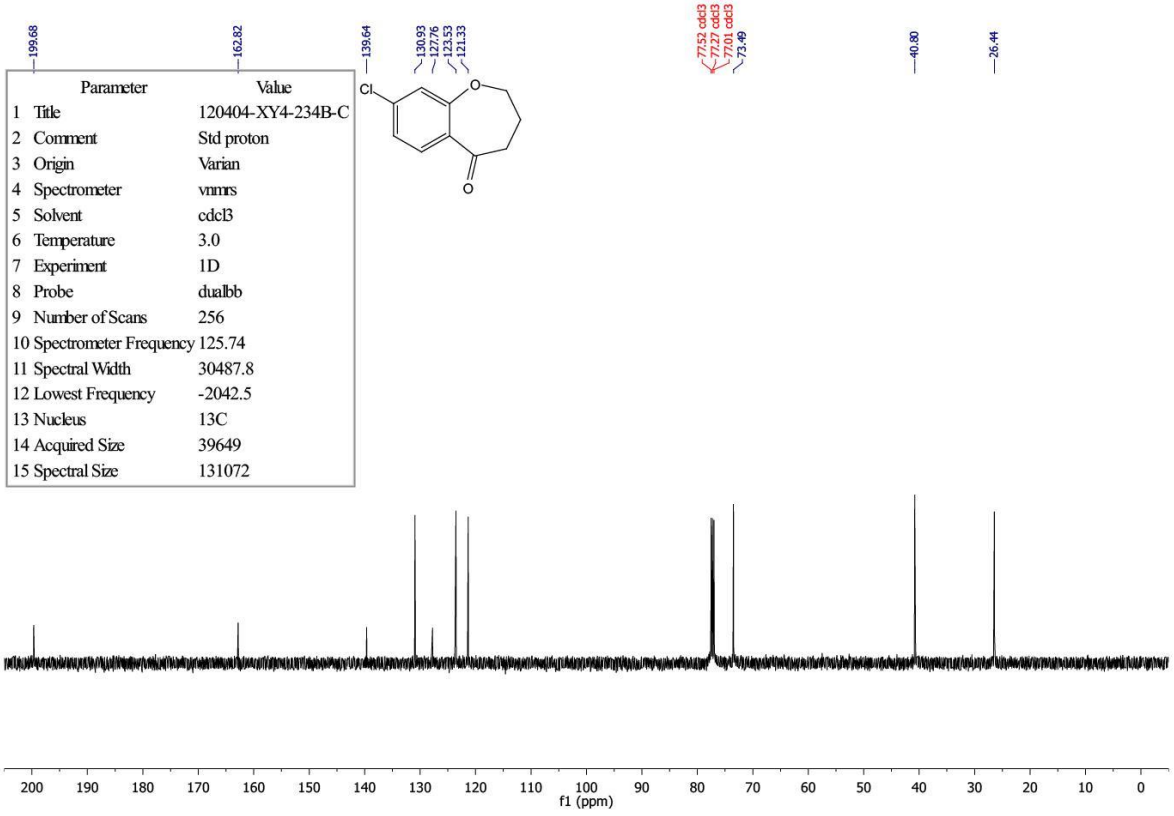
Parameter	Value
1 Title	120404-XY4-234A-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	dmso
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	32
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1001.4
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



Parameter	Value
1 Title	120404-XY4-234A-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	dmso
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	256
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2042.5
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072



Parameter	Value
1 Title	120404-XY4-234B-H
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	30.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	32
10 Spectrometer Frequency	500.02
11 Spectral Width	8012.8
12 Lowest Frequency	-1006.7
13 Nucleus	1H
14 Acquired Size	16415
15 Spectral Size	65536



Parameter	Value
1 Title	120404-XY4-234B-C
2 Comment	Std proton
3 Origin	Varian
4 Spectrometer	vnmrs
5 Solvent	cdcl3
6 Temperature	3.0
7 Experiment	1D
8 Probe	dualbb
9 Number of Scans	256
10 Spectrometer Frequency	125.74
11 Spectral Width	30487.8
12 Lowest Frequency	-2042.5
13 Nucleus	13C
14 Acquired Size	39649
15 Spectral Size	131072