Supporting Information

Regioselective Hydrochlorination of Unactivated Alkenes through Combined Acid System

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1. General

^{1}H and ^{13}C NMR spectra were recorded at 400 MHz and 101 MHz using $CDCl_3$ as a solvent. The chemical shifts are reported in δ (ppm) values (^{1}H and ^{13}C NMR relative to $CHCl_3$, δ 7.26 ppm for ^{1}H NMR and δ 77.0 ppm for ^{13}C NMR and $CFCl_3$ (δ 0 ppm for ^{19}F NMR), multiplicities are indicated by s (singlet), d (doublet), t (triplet), q (quartet), p (pentet), h (hextet), m (multiplet) and br (broad). Coupling constants (*J*), are reported in Hertz (Hz). All reagents and solvents were employed without further purification. The products were purified using a commercial flash chromatography system. TLC was developed on silica gel 60 F254 aluminum sheets. All reagents were purchased from Sigma-Aldrich or Alfa Aesar and used as received without any further purification. HCl/DMPU (43% w/w) was prepared following our reported work.[1]

2. General procedures

2.1 General procedure for hydrochlorination of alkenes with combined acid system

HCl/DMPU (43% w/w, 8 equiv) was added to a solution of alkene **1** (0.2 mmol) in AcOH (0.5 ml), the mixture was stirred at room temperature for designated time. Then the reaction mixture was diluted with Et_2O (1 ml), sequentially washed with water (1 ml), $NaHCO_3$ aqueous solution (2 × 1 ml) and brine (1 ml). The organic layer was dried over Na_2SO_4 and concentrated to dryness. The residue was purified by flash chromatography on silica gel (hexanes/ethyl acetate) to obtain pure product **2**.

2.2 Additive-based screening for heterocycles

HCl/DMPU (43% w/w, 8 equiv) and heterocycle additives (0.2 mmol, 1 equiv) were added to a solution of styrene **1a** (0.2 mmol) in AcOH (0.5 ml), the mixture was stirred at room temperature for 6 h. Then internal standard CH_2Br_2 (0.2 mmol, 1 equiv) was added into the reaction mixture. Both reaction yield and additive remaining were determined through analysis of crude ^{1}H NMR.

2.3 Comparison of efficiency with different HCl sources

HCl sources (8 equiv) was added to a solution of styrene **1a** (0.4 mmol) in AcOH (1 ml), the mixture was stirred at room temperature for 5 h. The reaction yield was monitored at 20 min, 40 min, 1 h, 1.5 h, 2 h, 3 h and 5 h through analysis of crude ^{1}H NMR.

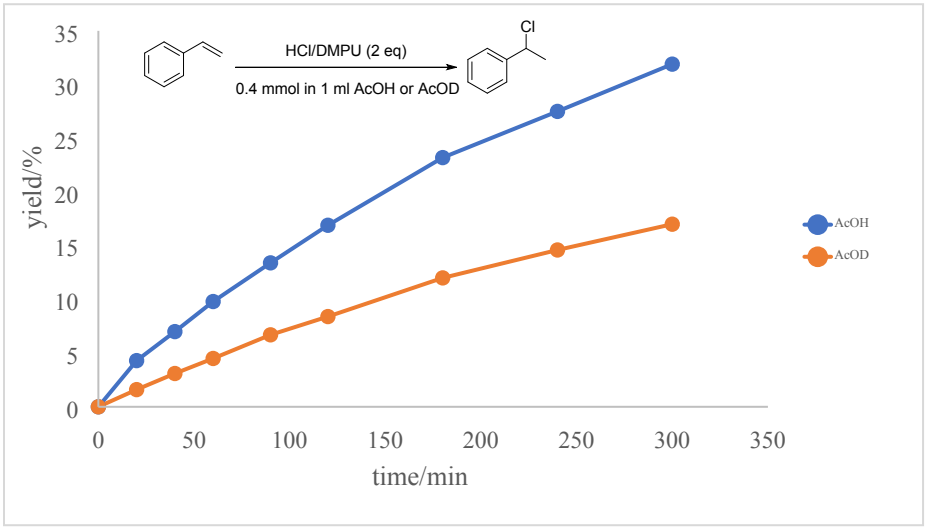
2.4 Study of the effect of chloride concentration

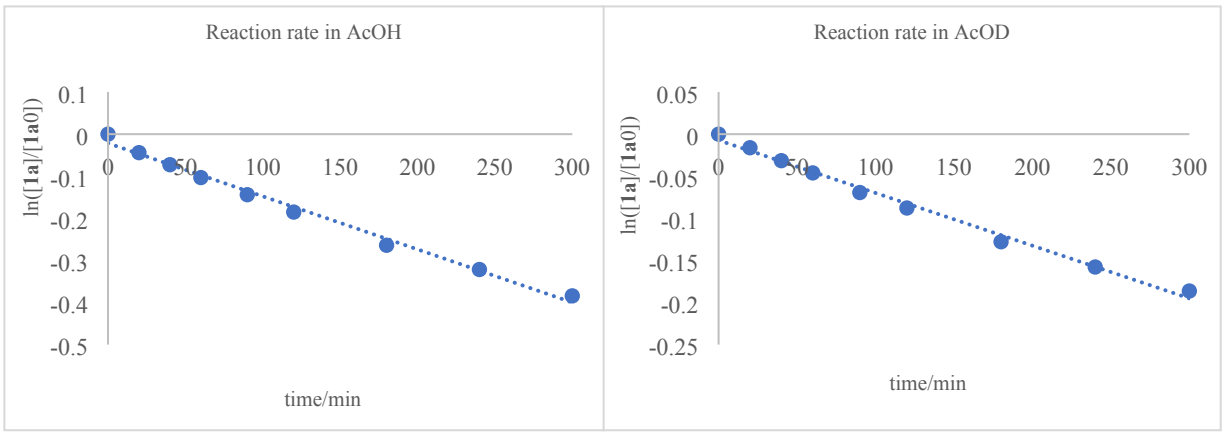
Four parallel reactions with styrene **1a** (0.4 mmol), HCl/DMPU (43% w/w, 2 equiv) in AcOH (1 ml) were set up, then 0, 1, 2 and 4 equivalents of LiCl was added respectively, the reaction mixtures were stirred at room temperature for 5 h. The reaction yields were monitored at 20 min, 40 min, 1 h, 1.5 h, 2 h, 3 h and 5 h through analysis of crude ^{1}H NMR.

2.5 Mechanism study of hydrochlorination of styrene

A) KIE study for hydrochlorination of styrene

Two parallel reactions with styrene **1a** (0.4 mmol), HCl/DMPU (43% w/w, 2 equiv) in AcOH (1 ml) and AcOD (1 ml) were set up, then the reaction mixtures were stirred at room temperature for 5 h. The reaction yields were monitored at 20 min, 40 min, 1 h, 1.5 h, 2 h, 3 h and 5 h through analysis of crude ^{1}H NMR. The reaction rates were showed in Scheme S1.

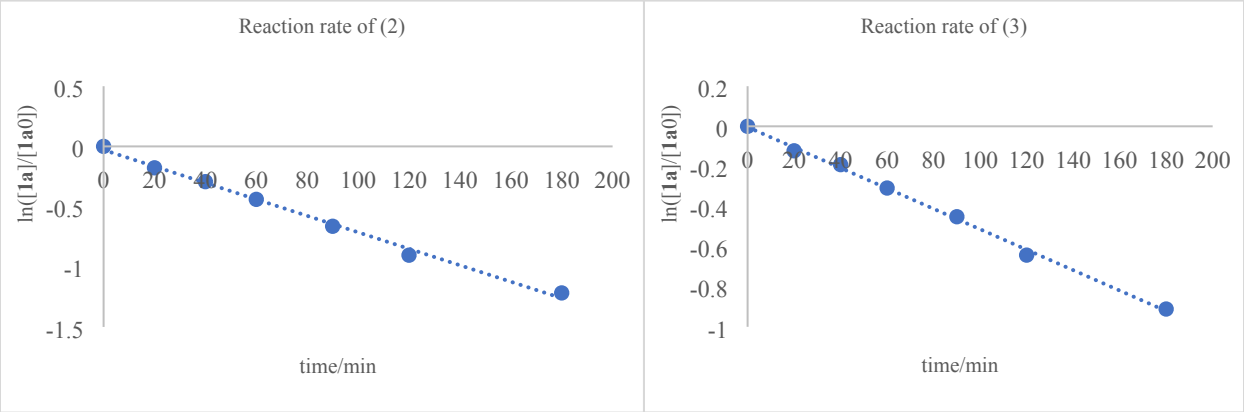




Scheme S1. Reaction rates in AcOH and AcOD.

B) Mechanism study for step 1: acetylation of styrene

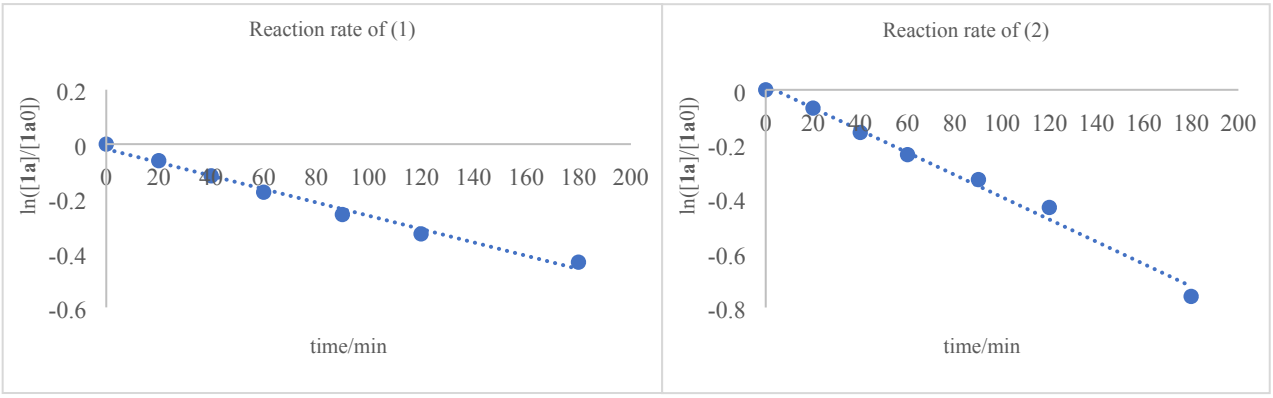
Four parallel reactions were set up: (1) styrene **1a** (0.4 mmol), TfOH (2 equiv) in AcOH (1 ml); (2) styrene **1a** (0.4 mmol), $Ga(OTf)_3$ (2 equiv) in AcOH (1 ml); (3) styrene **1a** (0.4 mmol), $Ga(OTf)_3$ (2 equiv) in AcOD (1 ml); (4) styrene **1a** (0.4 mmol) in AcOH (1 ml). Then the reaction mixtures were stirred at room temperature for 5 h. The reaction yields were monitored at 20 min, 40 min, 1 h, 1.5 h, 2 h, 3 h and 5 h through analysis of crude ^{1}H NMR. The reaction rates of reaction (2) and (3) were showed in Scheme S2.



Scheme S2. Reaction rates of reaction (2) and (3).

C) Mechanism study for step 2: chlorination

Five parallel reactions with 1-phenylethyl acetate (0.4 mmol), HCl/DMPU (2 equiv) in solvents: (1) AcOH (1 ml); (2) AcOD (1 ml); (3) DCM (1 ml); (4) Tol (1 ml); (5) DMF were set up. Then the reaction mixtures were stirred at room temperature for 5 h. The reaction yields were monitored at 20 min, 40 min, 1 h, 1.5 h, 2 h, 3 h and 5 h through analysis of crude ^{1}H NMR. The reaction rates of reaction (1) and (2) were showed in Scheme S3.



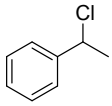
Scheme S3. Reaction rates of reaction (1) and (2).

2.6 Gram-scale synthesis of 2a

HCl/DMPU (43% w/w, 8 equiv) was added to a solution of styrene **1a** (1.04g, 10 mmol) in AcOH (25 ml), the mixture was stirred at room temperature for 6 h. Then the reaction mixture was diluted with Et_2O (25 ml), sequentially washed with water (25 ml), $NaHCO_3$ aqueous solution (2 × 25 ml) and brine (25 ml). The organic layer was dried over Na_2SO_4 and concentrated to dryness. The residue was purified by flash chromatography on silica gel to obtain pure product **2a** with 90% yield.

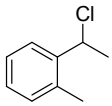
3. Characterization of product 2

(1-chloroethyl)benzene (**2a**)[2]



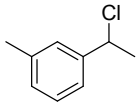
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.25 (m, 5H), 5.09 (q, *J* = 6.8 Hz, 1H), 1.85 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.78, 141.69, 128.60, 128.22, 126.47, 58.76, 26.50. Colorless oil (24.4 mg).

1-(1-chloroethyl)-2-methylbenzene (**2b**)[3]



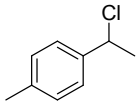
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.5 Hz, 1H), 7.25 – 7.15 (m, 3H), 5.35 (q, *J* = 6.7 Hz, 1H), 2.42 (s, 3H), 1.87 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.42, 135.22, 130.55, 128.14, 156.50, 125.69, 55.00, 25.16, 18.99. Colorless oil (28.0 mg).

1-(1-chloroethyl)-3-methylbenzene (**2c**)[3]



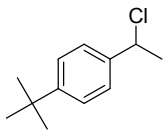
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 – 7.21 (m, 3H), 7.12 (d, *J* = 7.1 Hz, 1H), 5.07 (q, *J* = 6.8 Hz, 1H), 2.37 (s, 3H), 1.84 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.71, 138.33, 129.02, 128.52, 127.19, 123.51, 58.91, 26.48, 21.41. Colorless oil (29.5 mg).

1-(1-chloroethyl)-4-methylbenzene (**2d**)[4]



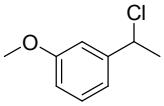
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (d, *J* = 7.8 Hz, 2H), 7.16 (d, *J* = 7.8 Hz, 2H), 5.08 (q, *J* = 6.9 Hz, 1H), 2.34 (s, 3H), 1.84 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.87, 138.10, 129.27, 126.39, 58.81, 26.43, 21.13. Colorless oil (27.7 mg).

1-(tert-butyl)-4-(1-chloroethyl)benzene (**2e**)[5]



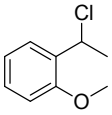
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.30 (m, 4H), 5.10 (q, *J* = 6.8 Hz, 1H), 1.85 (d, *J* = 6.8 Hz, 3H), 1.31 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.27, 139.74, 126.18, 125.54, 58.74, 34.58, 31.28, 26.36. Colorless oil (33.8 mg).

1-(1-chloroethyl)-3-methoxybenzene (**2f**)[6]



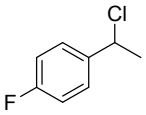
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 (d, *J* = 8.2 Hz, 1H), 7.02 – 6.95 (m, 2H), 6.84 (d, *J* = 8.2 Hz, 1H), 5.06 (q, *J* = 6.8 Hz, 1H), 3.82 (s, 3H), 1.84 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.70, 144.32, 129.64, 118.75, 113.62, 112.23, 58.64, 55.26, 26.50. Colorless oil (32.4 mg).

1-(1-chloroethyl)-2-methoxybenzene (**2g**)[7]



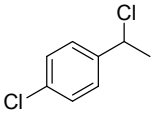
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (d, J = 7.5 Hz, 1H), 7.24 (t, J = 7.8 Hz, 1H), 6.96 (t, J = 7.4 Hz, 1H), 6.87 (d, J = 8.2 Hz, 1H), 5.09 (d, J = 6.3 Hz, 1H), 3.85 (s, 2H), 1.50 (d, J = 6.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.51, 133.35, 128.28, 126.07, 120.76, 110.38, 66.53, 55.23, 22.81. Colorless oil (30.7 mg).

1-(1-chloroethyl)-4-fluorobenzene (**2h**)[3]



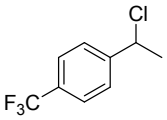
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.37 (m, 2H), 7.05 – 7.01 (m, 2H), 5.08 (q, *J* = 6.8 Hz, 1H), 1.83 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.36 (d, J = 246.0 Hz), 138.69, 128.25 (d, J = 9.0 Hz), 115.47 (d, J = 21.0 Hz), 57.92, 26.56. Colorless oil (29.5 mg).

1-chloro-4-(1-chloroethyl)benzene (**2i**)[4]



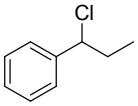
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.26 (m, 4H), 5.05 (q, J = 6.8 Hz, 1H), 1.82 (d, J = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.29, 133.95, 128.77, 127.89. Colorless oil (32.9 mg).

1-(1-chloroethyl)-4-(trifluoromethyl)benzene (**2j**)[8]



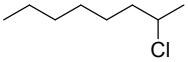
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, J = 8.2 Hz, 2H), 7.53 (d, J = 8.1 Hz, 2H), 5.10 (q, J = 6.9 Hz, 1H), 1.84 (d, J = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.56, 130.18 (m), 126.89, 125.65 (d, J = 3.0 Hz), 57.47, 26.45. Colorless oil (32.5 mg).

(1-chloropropyl)benzene (**2k**)[9]



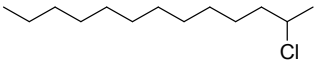
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.28 (m, 5H), 4.79 (t, *J* = 8.0 Hz, 1H), 2.22 – 1.99 (m, 2H), 1.00 (t, *J* = 8.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.75, 128.54, 128.14, 126.95, 65.46, 33.20, 11.69. Colorless oil (22.6 mg).

2-chlorooctane (**2m**)[10]



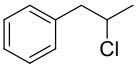
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.02 (q, *J* = 6.6 Hz, 1H), 1.73 – 1.66 (m, 2H), 1.56 – 1.28 (m, 11H), 0.89 – 0.86 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 58.88, 40.36, 31.67, 28.76, 26.59, 25.31, 22.54, 14.00. Colorless oil (19.33 mg).

2-chlorotridecane (**2n**)[11]



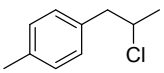
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.02 (q, *J* = 6.7 Hz, 1H), 1.70 (td, *J* = 5.7, 3.0 Hz, 2H), 1.55 – 1.17 (m, 21H), 0.93 – 0.78 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 58.95, 40.37, 31.89, 29.61, 29.55, 29.48, 29.32, 29.11, 26.65, 26.51, 25.33, 22.67, 14.09. Colorless oil (31.1 mg).

(2-chloropropyl)benzene (**2o**)[12]



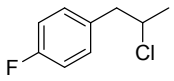
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.15 (m, 5H), 4.24 – 4.19 (m, 1H), 3.02 (ddd, *J* = 50.8, 13.8, 6.8 Hz, 2H), 1.50 (d, *J* = 6.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.94, 129.31, 128.38, 126.76, 58.50, 46.66, 24.64. Colorless oil (24.4 mg).

1-(2-chloropropyl)-4-methylbenzene (**2p**)[13]



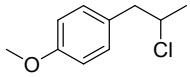
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.11 (m, 4H), 4.24 – 4.16 (m, 1H), 2.99 (ddd, *J* = 50.7, 13.8, 6.9 Hz, 2H), 2.33 (s, 3H), 1.50 (d, *J* = 6.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.33, 134.90, 129.19, 129.08, 58.70, 46.26, 24.62, 21.06. Colorless oil (27.3 mg).

1-(2-chloropropyl)-4-fluorobenzene (**2q**)[13]



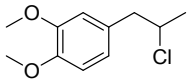
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 – 6.97 (m, 4H), 4.21 – 4.13 (m, 1H), 3.12 – 2.83 (m, 2H), 1.50 (d, *J* = 6.5 Hz, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 161.8 (d, *J* = 244.0 Hz), 133.60, 130.79 (d, *J* = 7.0 Hz), 115.19 (d, *J* = 21.0 Hz), 58.44, 45.69, 24.61. Colorless oil (24.9 mg).

1-(2-chloropropyl)-4-methoxybenzene (**2r**)[14]



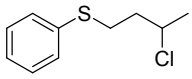
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.11 (d, *J* = 8.1 Hz, 2H), 6.84 (d, *J* = 7.8 Hz, 2H), 4.20 – 4.12 (m, 1H), 3.78 (s, 3H), 2.95 (ddd, *J* = 49.0, 13.9, 6.8 Hz, 2H), 1.48 (d, *J* = 6.5 Hz, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ = 158.42, 130.30, 130.04, 113.76, 58.84, 55.21, 45.77, 24.52. Colorless oil (28.1 mg).

4-(2-chloropropyl)-1,2-dimethoxybenzene (**2s**)



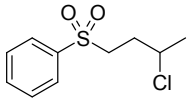
^{1}H NMR (400 MHz, $CDCl_3$) δ 6.82 – 6.70 (m, 3H), 4.24 – 4.11 (m, 1H), 3.87 (s, 3H), 3.86 (s, 3H), 3.07 – 2.79 (m, 2H), 1.50 (d, *J* = 8.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.79, 147.91, 130.55, 121.39, 112.59, 111.14, 58.70, 55.86, 46.27, 24.60, 24.55. HRMS(CI) calcd. for [$C_{11}H_{16}ClO_2$] ([M+H]) 215.0839; found 215.0828. Colorless oil (32.6 mg).

(3-chlorobutyl)(phenyl)sulfane (**2t**)



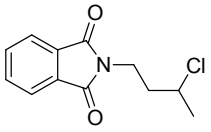
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.19 (m, 5H), 4.23 – 4.17 (m, 1H), 3.19 – 2.98 (m, 2H), 2.03 – 1.97 (m, 2H), 1.52 (d, *J* = 8.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.85, 129.32, 128.95, 126.13, 57.05, 39.48, 30.72, 25.24. Colorless oil (30.1 mg). HRMS(CI) calcd. for [$C_{10}H_{12}ClS$] ([M-H]) 199.0348; found 199.0338. Colorless oil (110.6 mg).

((3-chlorobutyl)sulfonyl)benzene (**2u**)[15]



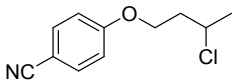
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 – 7.90 (m, 2H), 7.69 – 7.65 (m, 1H), 7.60 – 7.56 (m, 2H), 4.13 – 4.05 (m, 1H), 3.38 – 3.18 (m, 2H), 2.27 – 1.98 (m, 2H), 1.51 (d, *J* = 8.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.99, 133.87, 129.39, 127.95, 56.18, 53.66, 32.88, 25.18. Colorless oil (39.6 mg).

2-(3-chlorobutyl)isoindoline-1,3-dione (**2v**)[16]



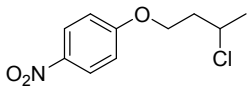
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 – 7.68 (m, 4H), 7.69 – 7.65 (m, 1H), 7.60 – 7.56 (m, 2H), 4.06 – 4.01 (m, 1H), 3.91 – 3.77 (m, 2H), 2.13 – 2.01 (m, 2H), 1.54 (d, *J* = 8.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.17, 133.96, 132.03, 123.24, 55.54, 38.63, 35.64, 25.27. Colorless oil (39.5 mg).

4-(3-chlorobutoxy)benzonitrile (**2x**)



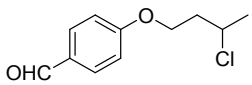
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.0 Hz, 2H), 6.94 (d, *J* = 8.0 Hz, 2H), 4.31 – 4.12 (m, 3H), 2.28 – 2.06 (m, 2H), 1.60 (d, *J* = 8.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.96, 133.99, 119.09, 115.17, 65.24, 54.72, 39.38, 25.50. HRMS(CI) calcd. for [$C_{11}H_{13}ClNO$] ([M+H]) 210.0686; found 210.0679. White solid (26.0 mg).

1-(3-chlorobutoxy)-4-nitrobenzene (**2y**)



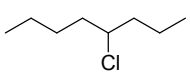
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, *J* = 8.0 Hz, 2H), 6.95 (d, *J* = 8.0 Hz, 2H), 4.33 – 4.17 (m, 3H), 2.31 – 2.08 (m, 2H), 1.61 (d, *J* = 8.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.71, 141.60, 125.90, 114.42, 65.70, 54.70, 39.35, 25.51. HRMS(CI) calcd. for [$C_{10}H_{13}ClNO_3$] ([M+H]) 230.0584; found 230.0576. Colorless oil (41.3 mg).

4-(3-chlorobutoxy)benzaldehyde (**2z**)



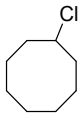
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.88 (s, 1H), 7.83 (d, *J* = 8.0 Hz, 2H), 7.00 (d, *J* = 8.0 Hz, 2H), 4.32 – 4.17 (m, 3H), 2.29 – 2.08 (m, 2H), 1.61 (d, *J* = 8.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.69, 163.72, 131.96, 130.09, 114.75, 65.23, 54.81, 39.48, 25.50. HRMS(CI) calcd. for [$C_{11}H_{14}ClO_2$] ([M+H]) 213.0682; found 213.0673. Colorless oil (29.8 mg).

4-chlorooctane (**2a'**)[17]



^{1}H NMR (400 MHz, $CDCl_3$) δ 3.93 – 3.87 (m, 1H), 1.73 – 1.20 (m, 10H), 0.94 – 0.83 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 63.94, 40.57, 38.22, 28.62, 22.25, 19.67, 13.92, 13.55. Colorless oil (21.4 mg).

chlorocyclooctane (**2b'**)[18]

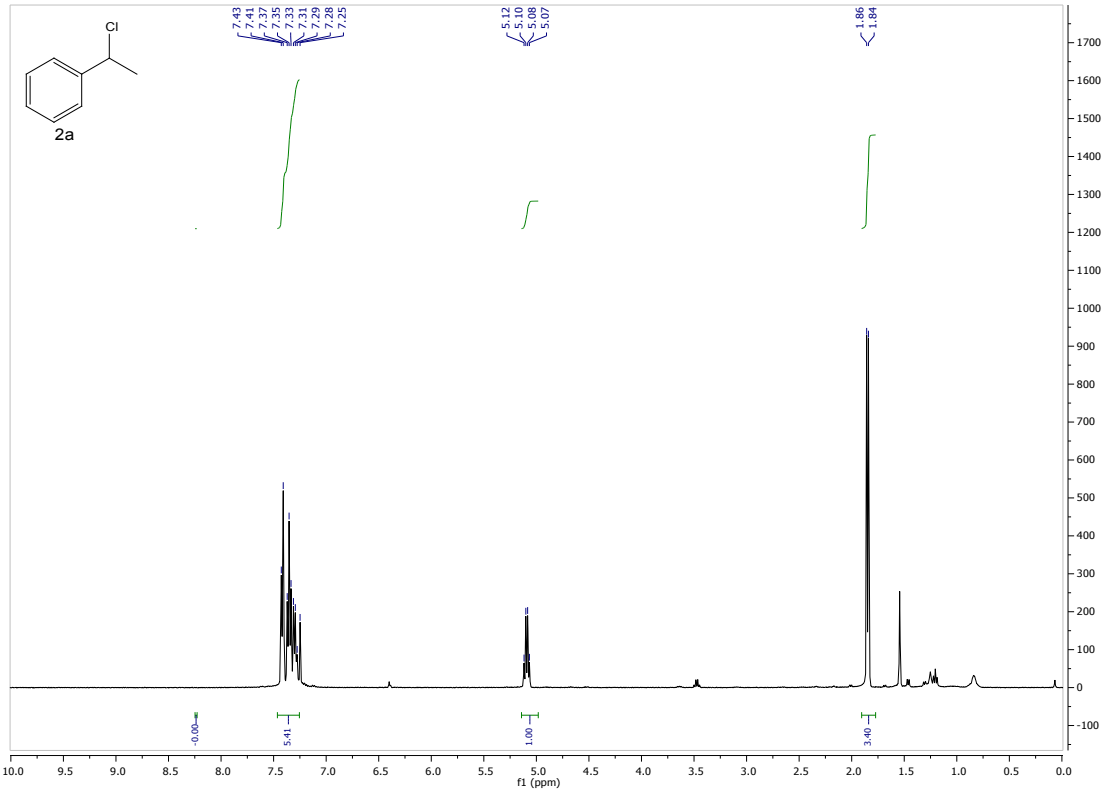


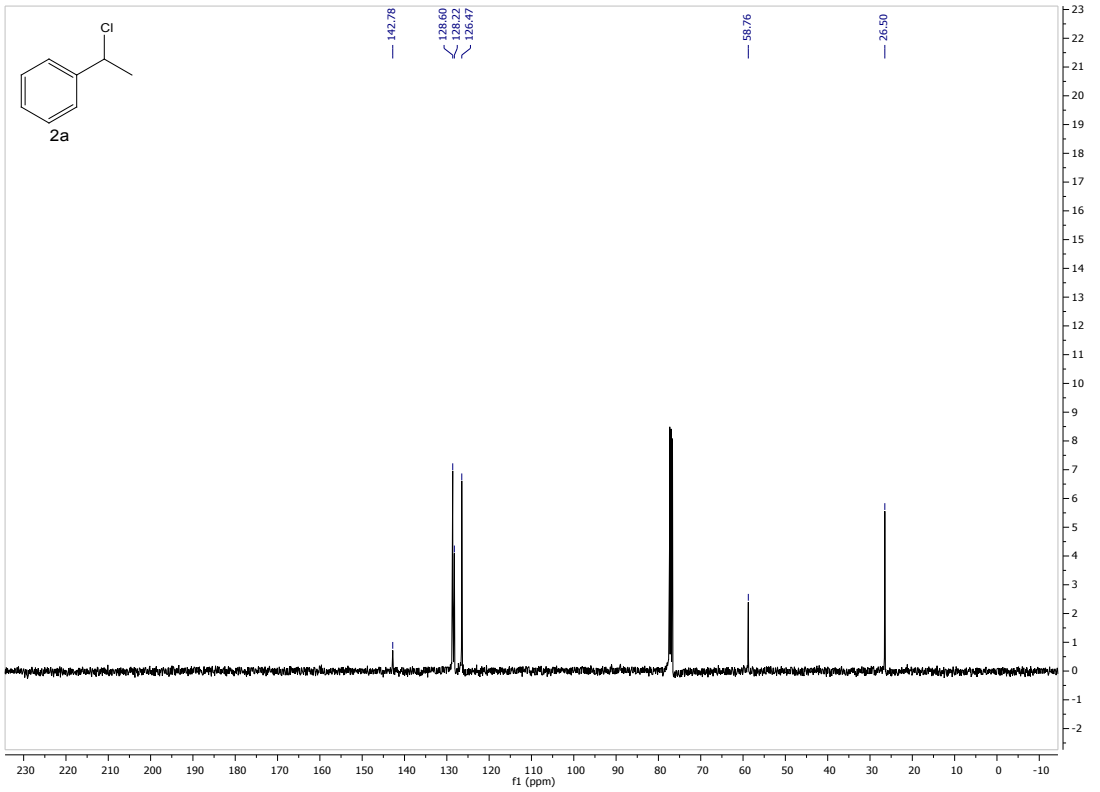
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.25 – 4.18 (m, 1H), 2.13 – 1.93 (m, 4H), 1.77 – 1.72 (m, 2H), 1.58 – 1.50 (m, 8H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 63.54, 35.13, 27.37, 24.89, 23.54. Colorless oil (24.4 mg).

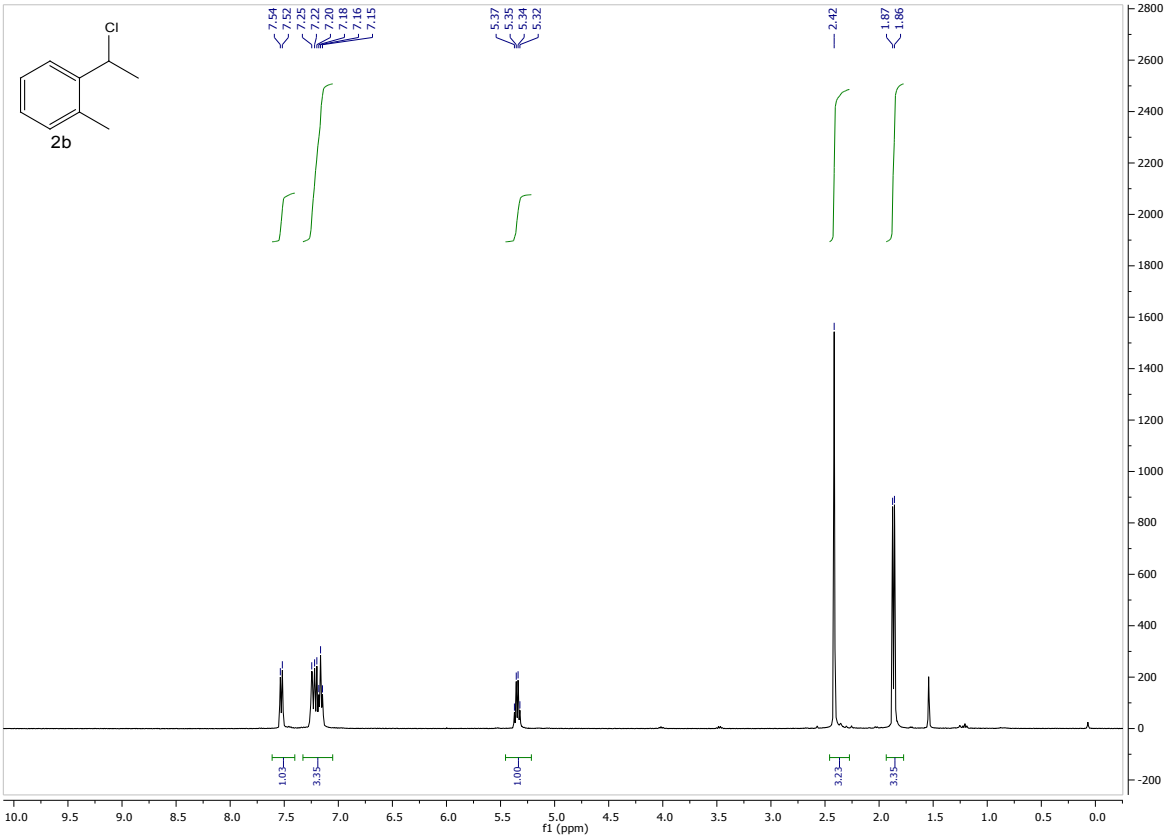
1-chloro-1-methylcyclohexane (**2c'**)[19]

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.94 – 1.85 (m, 2H), 1.76 – 1.50 (m, 10H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 72.43, 41.55, 33.46, 25.18, 22.62. Colorless oil (23.1 mg).

4. Copies of NMR spectra of product 2






Cl
2b
7.54
7.52
7.25
7.22
7.20
7.18
7.16
7.15
5.37
5.35
5.34
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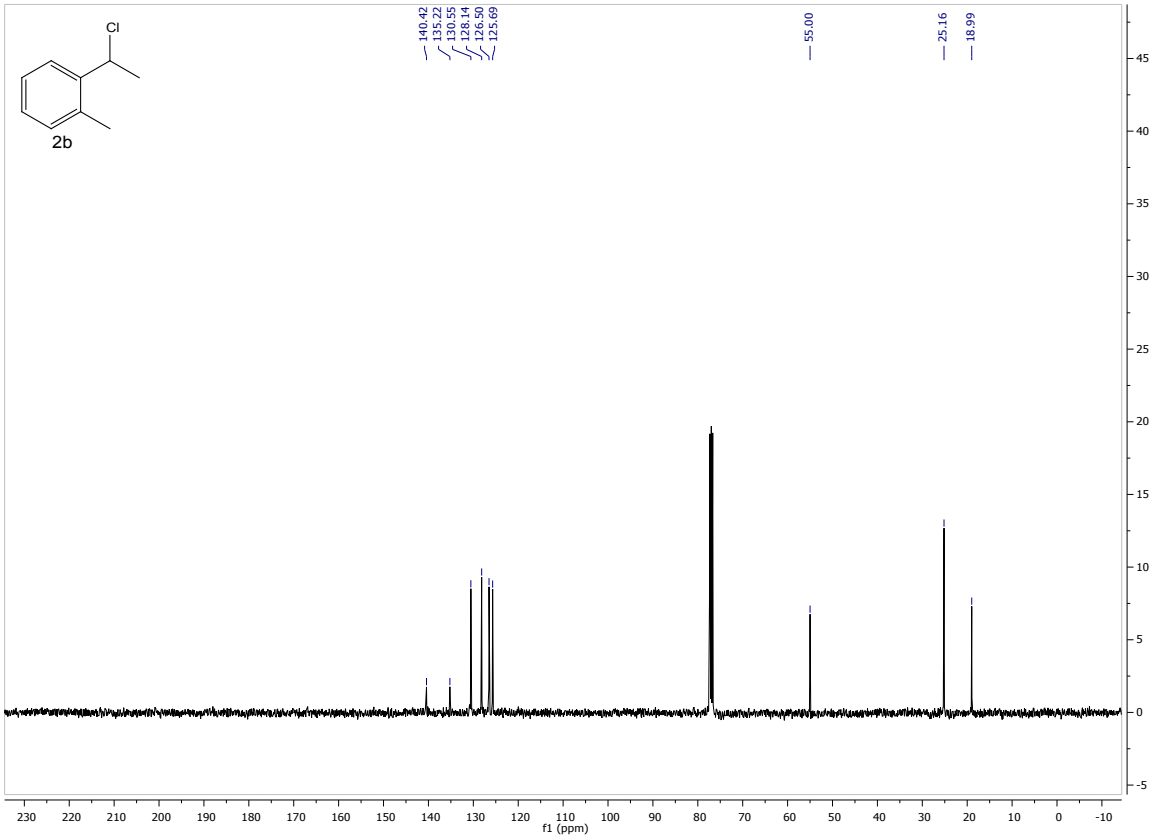
1.87
1.86
1.03
3.35
1.00
3.23
3.35
f1 (ppm)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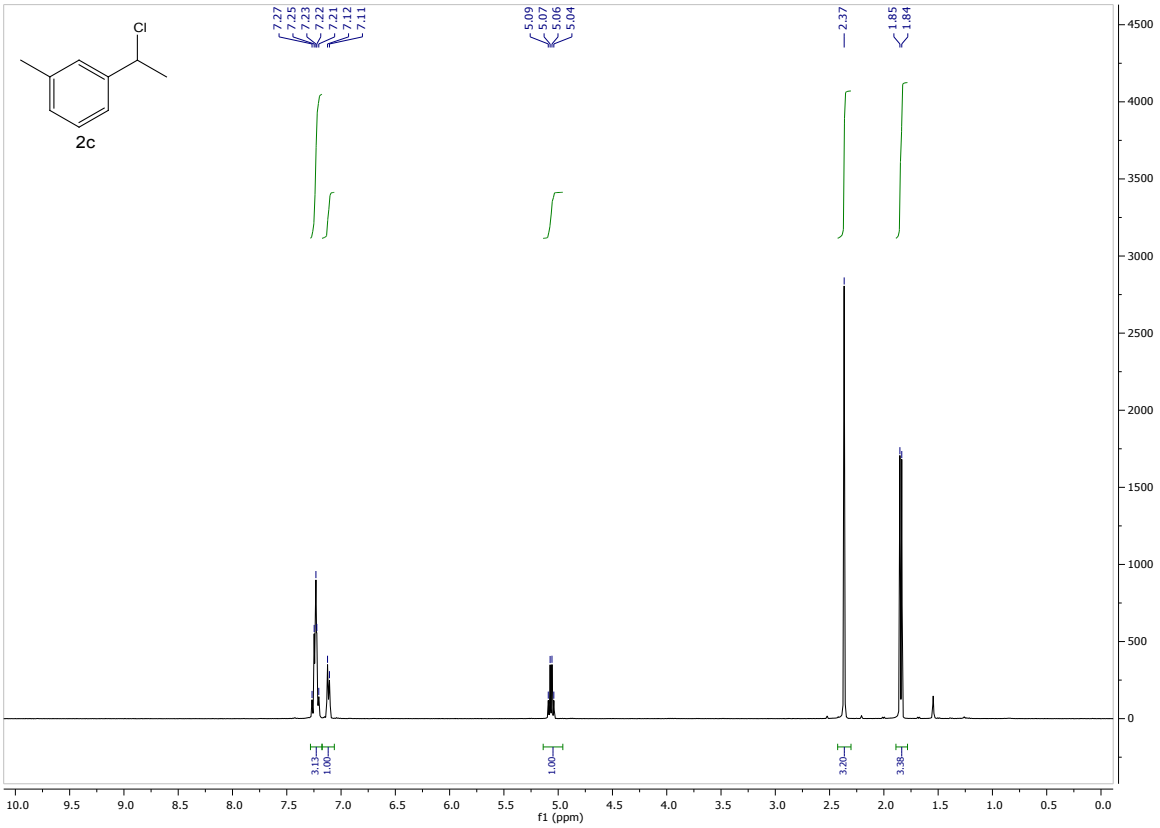
55.00
25.16
18.99
f1 (ppm)


Cl
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7.21
7.12
7.11
5.09
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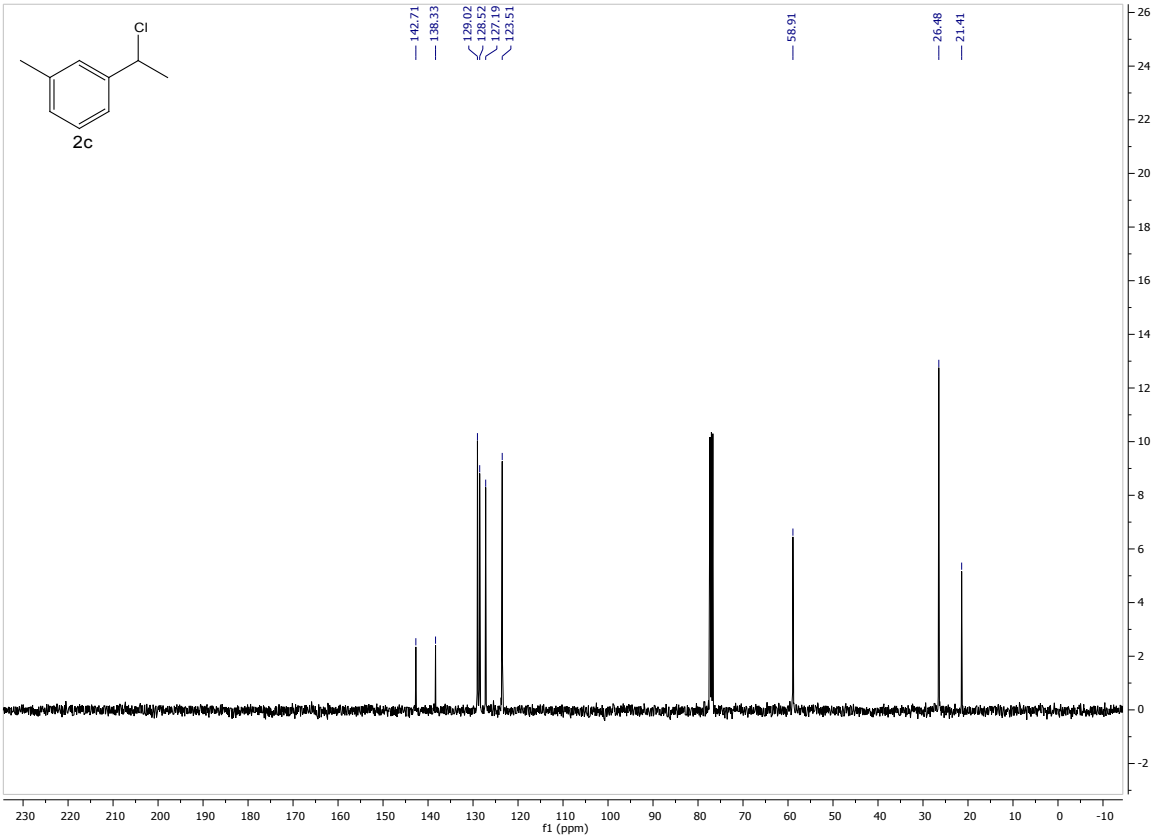
1.00
1.00
3.20
3.38
f1 (ppm)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127.19
123.51
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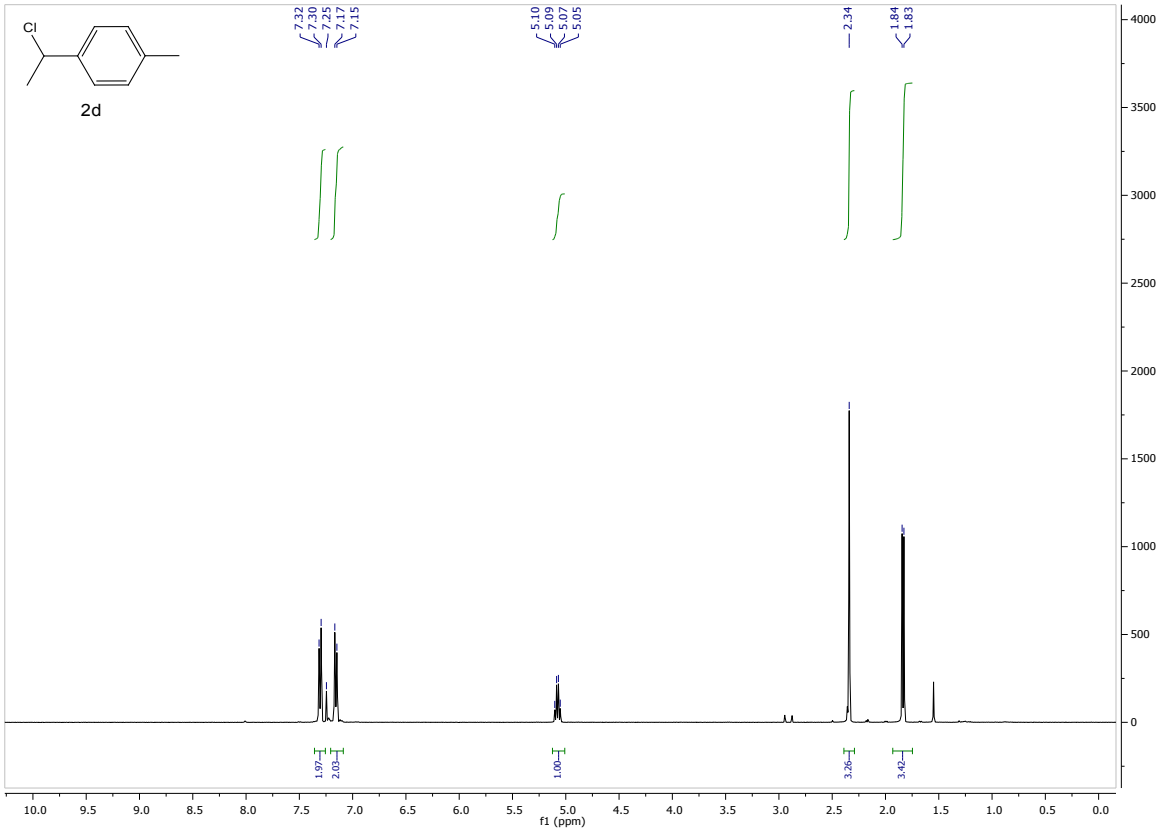
21.41
f1 (ppm)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5.10
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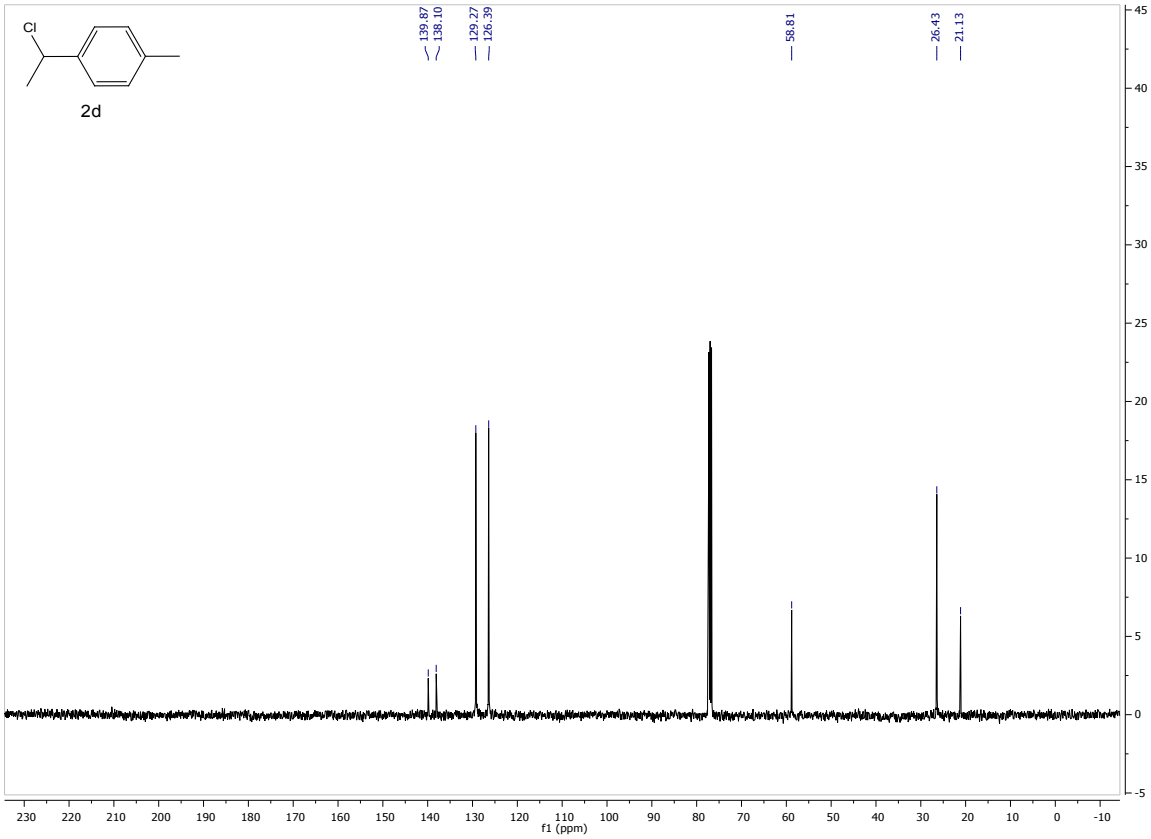
2.03
1.00
3.26
3.42
f1 (ppm)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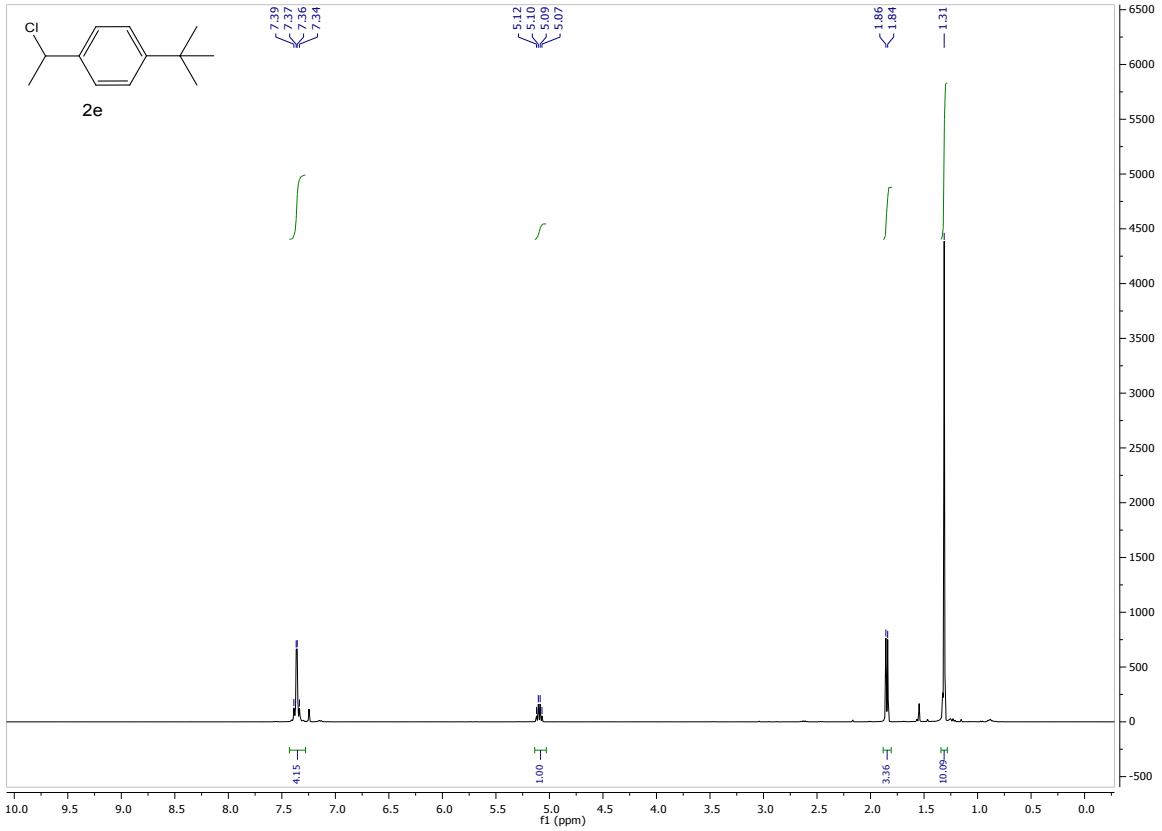
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7.34
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5.09
5.07
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1.84
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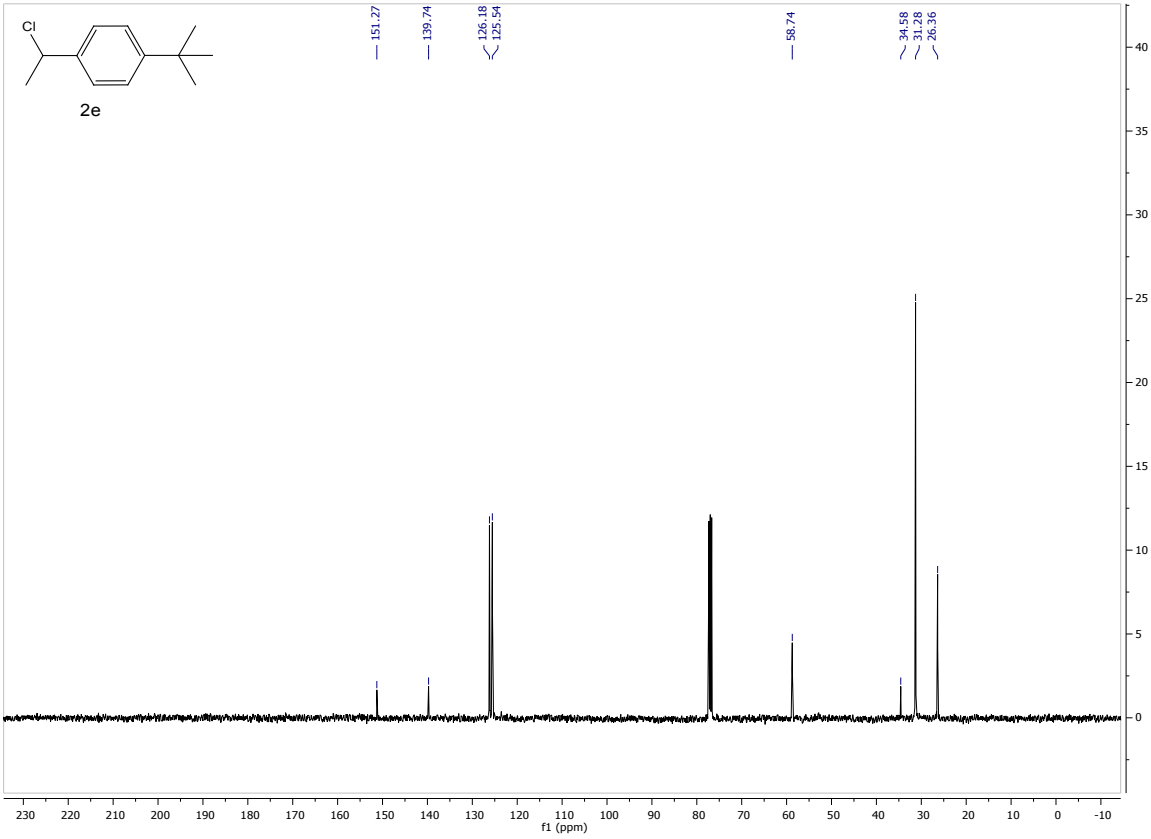
4.15
1.00
3.36
10.09
f1 (ppm)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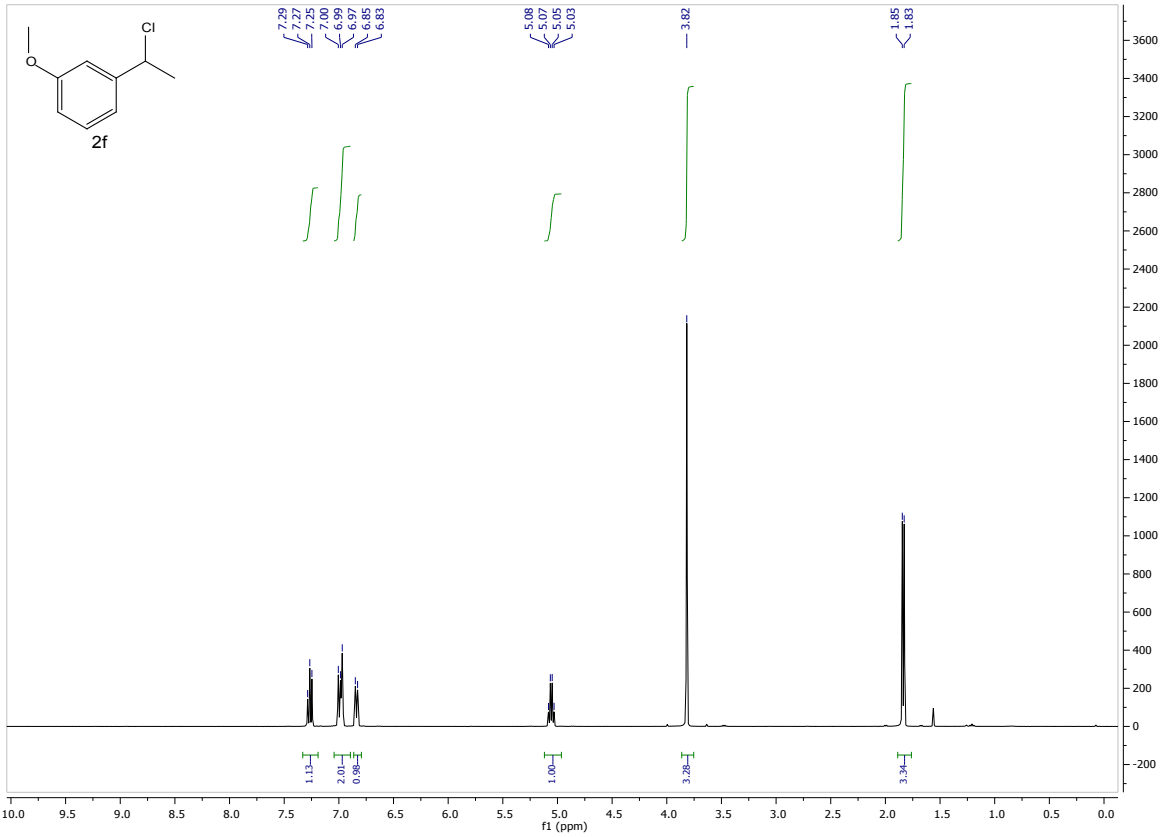
31.28
26.36
f1 (ppm)


Cl
O
2f
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7.27
7.25
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6.97
6.85
6.83
5.08
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1.85
1.83
1.13
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0.98
1.00
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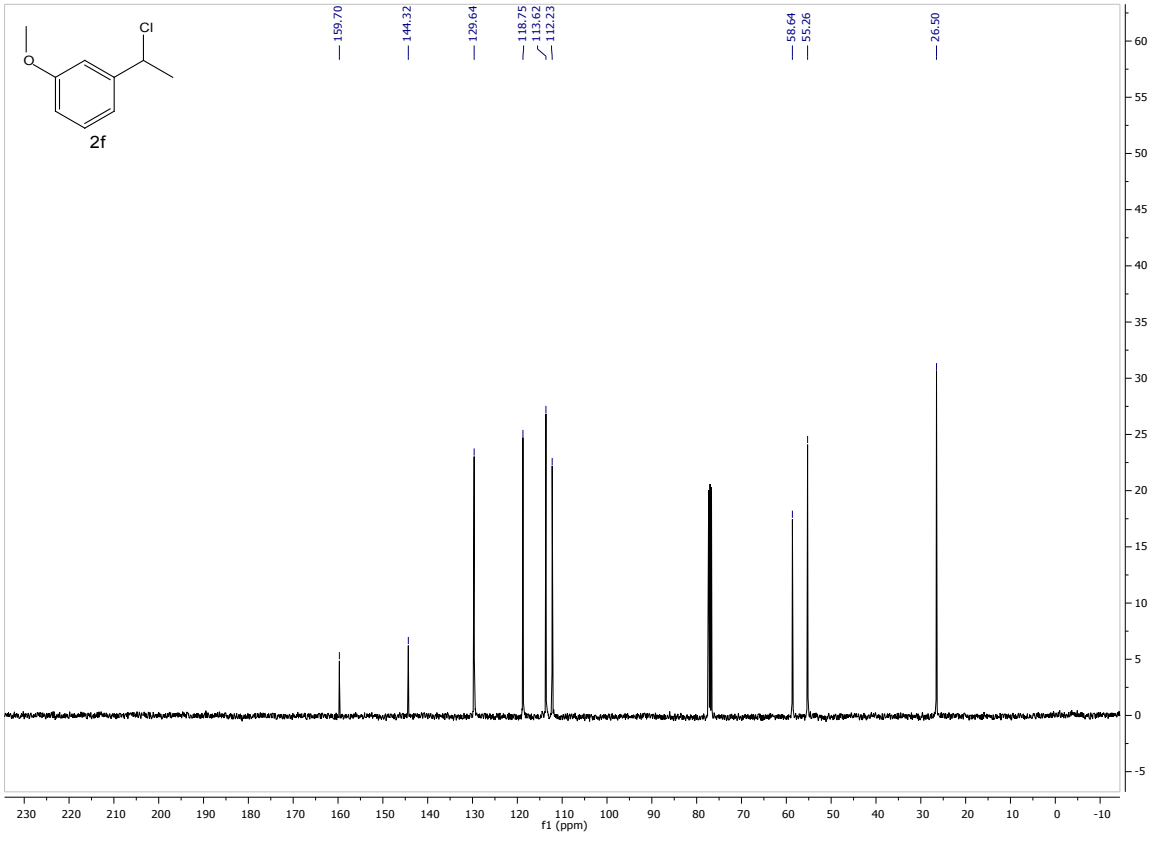
3.34
f1 (ppm)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112.23
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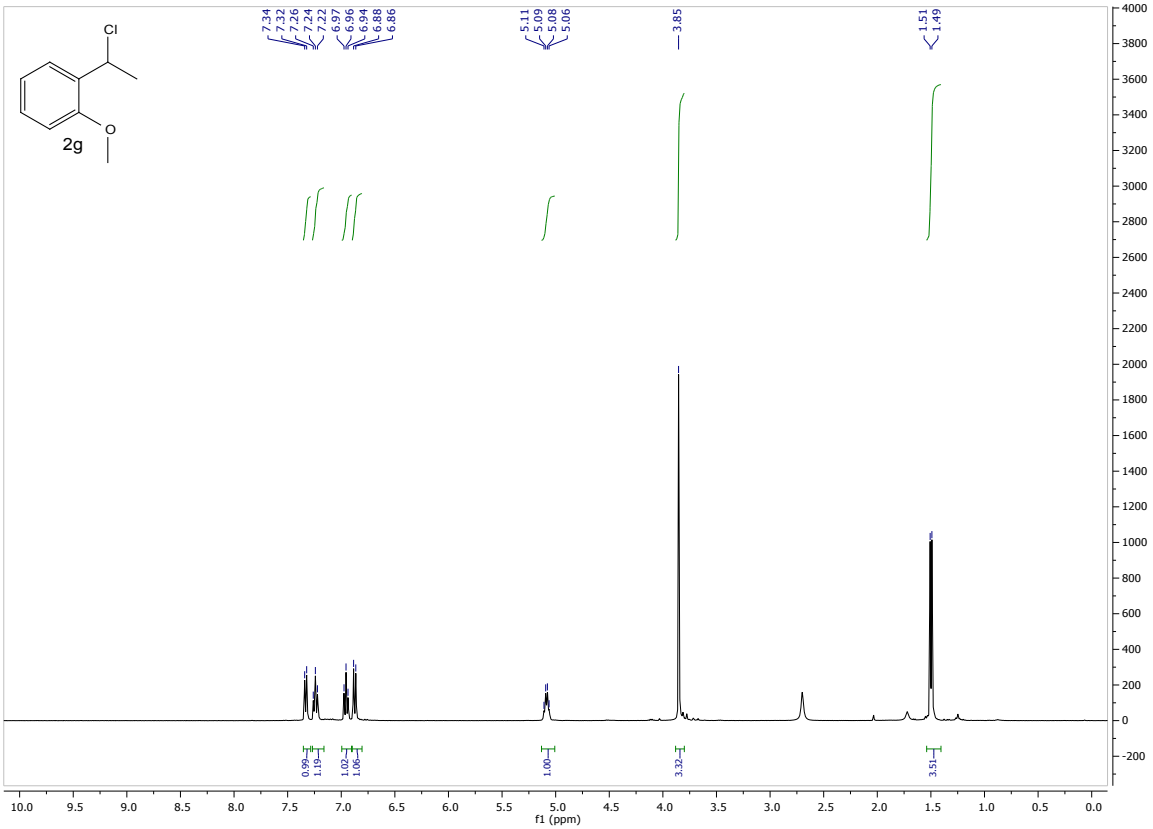
55.26
26.50
f1 (ppm)


Cl
O
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7.24
7.22
6.97
6.96
6.94
6.88
6.86
5.11
5.09
5.08
5.06
3.85
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1.49
0.99
1.19
1.02
1.06
1.00
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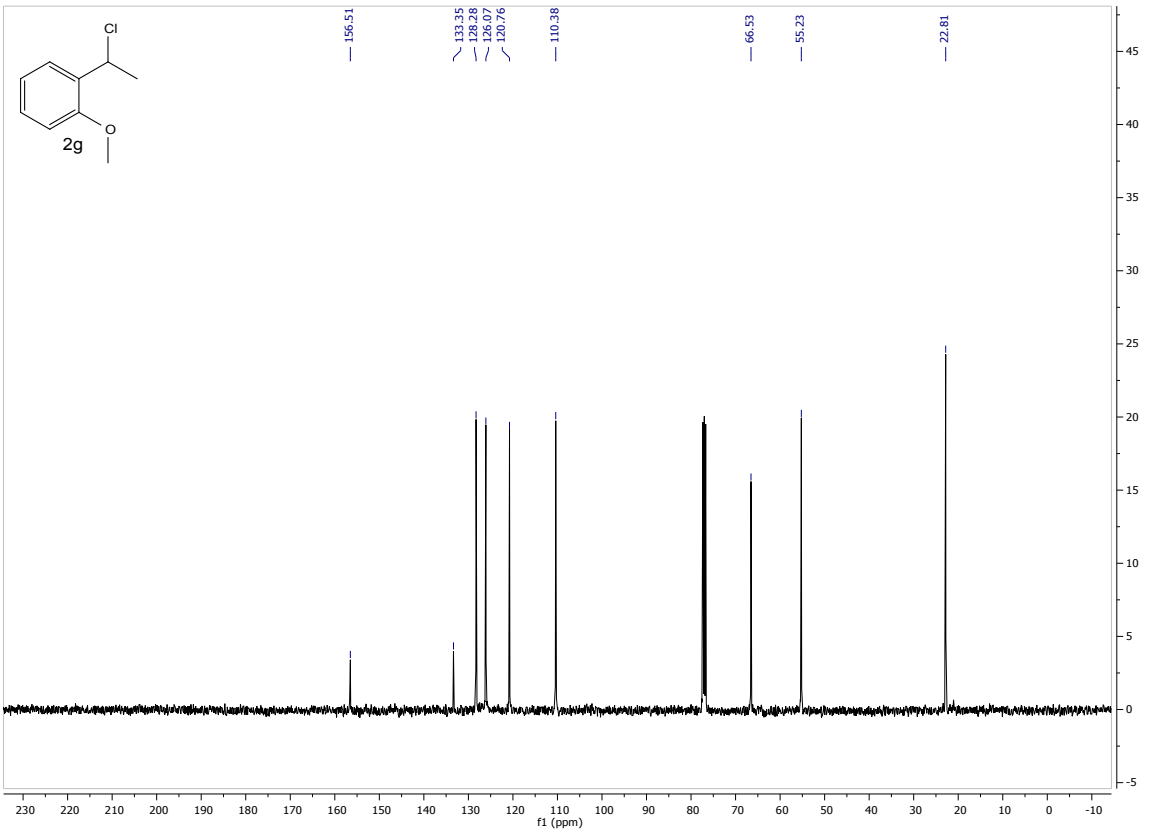
3.51
f1 (ppm)


Cl
O
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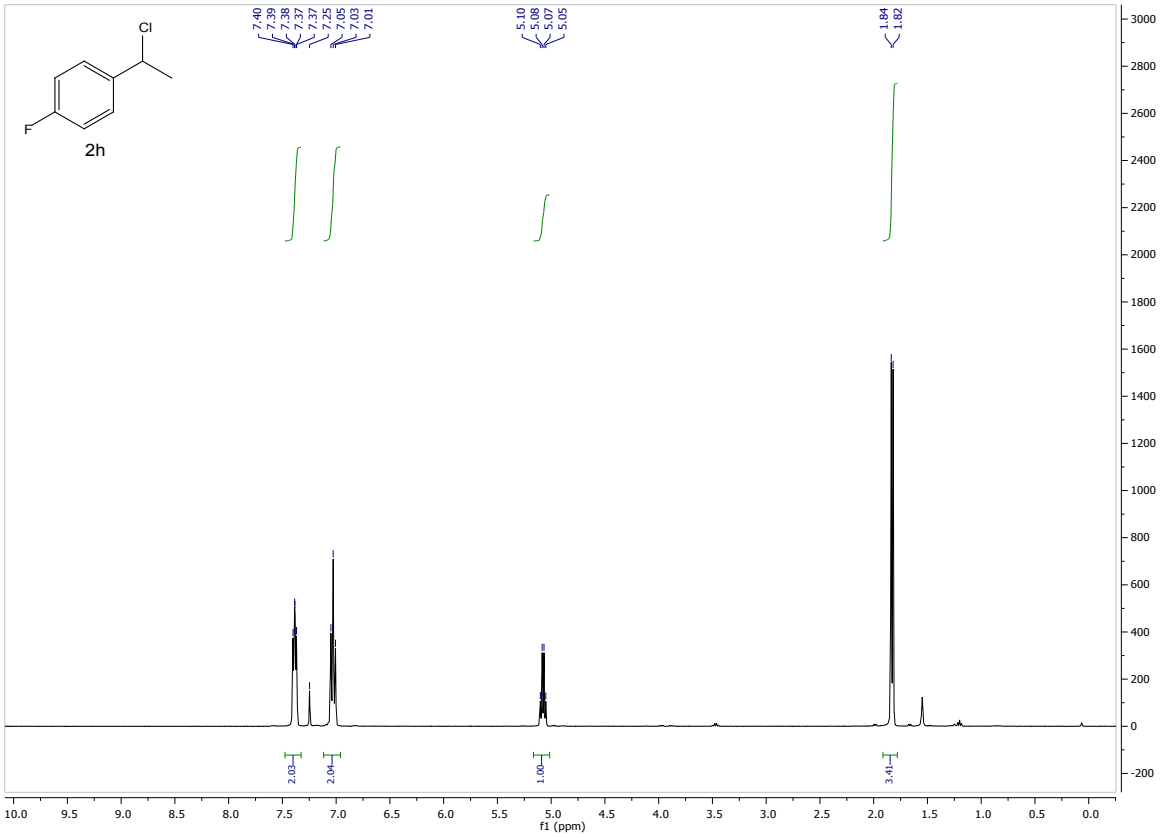
22.81
f1 (ppm)


Cl
F
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7.03
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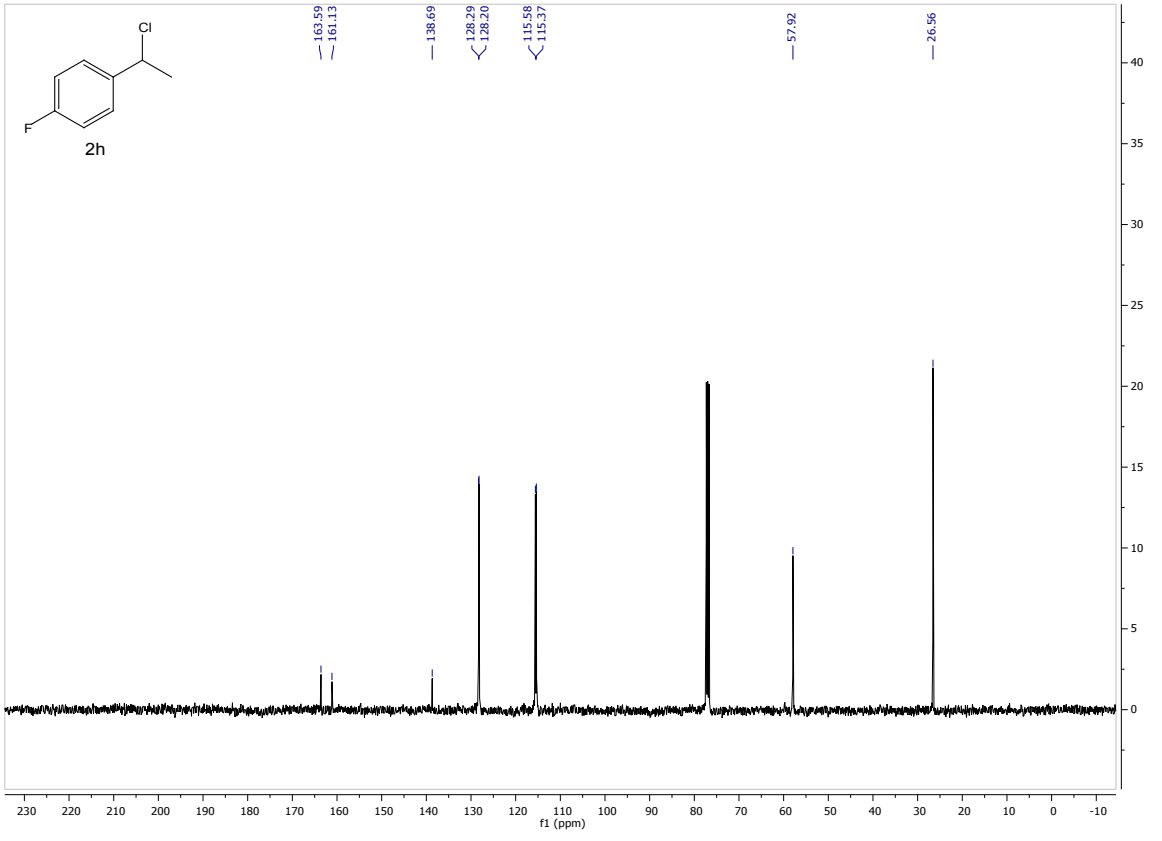
5.07
5.05
1.84
1.82
2.03
2.04
1.00
3.41
f1 (ppm)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F
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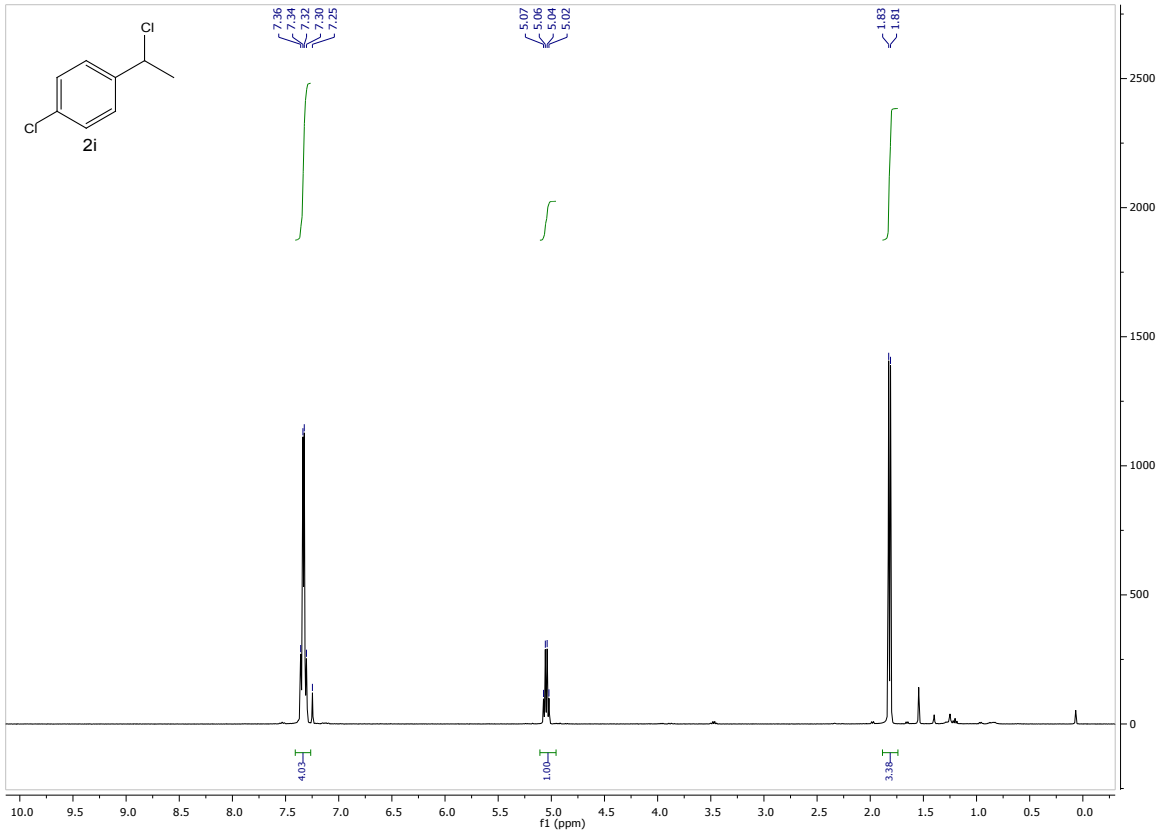
128.20
115.58
115.37
57.92
26.56
f1 (ppm)


Cl
Cl
2i
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7.34
7.32
7.30
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5.06
5.04
5.02
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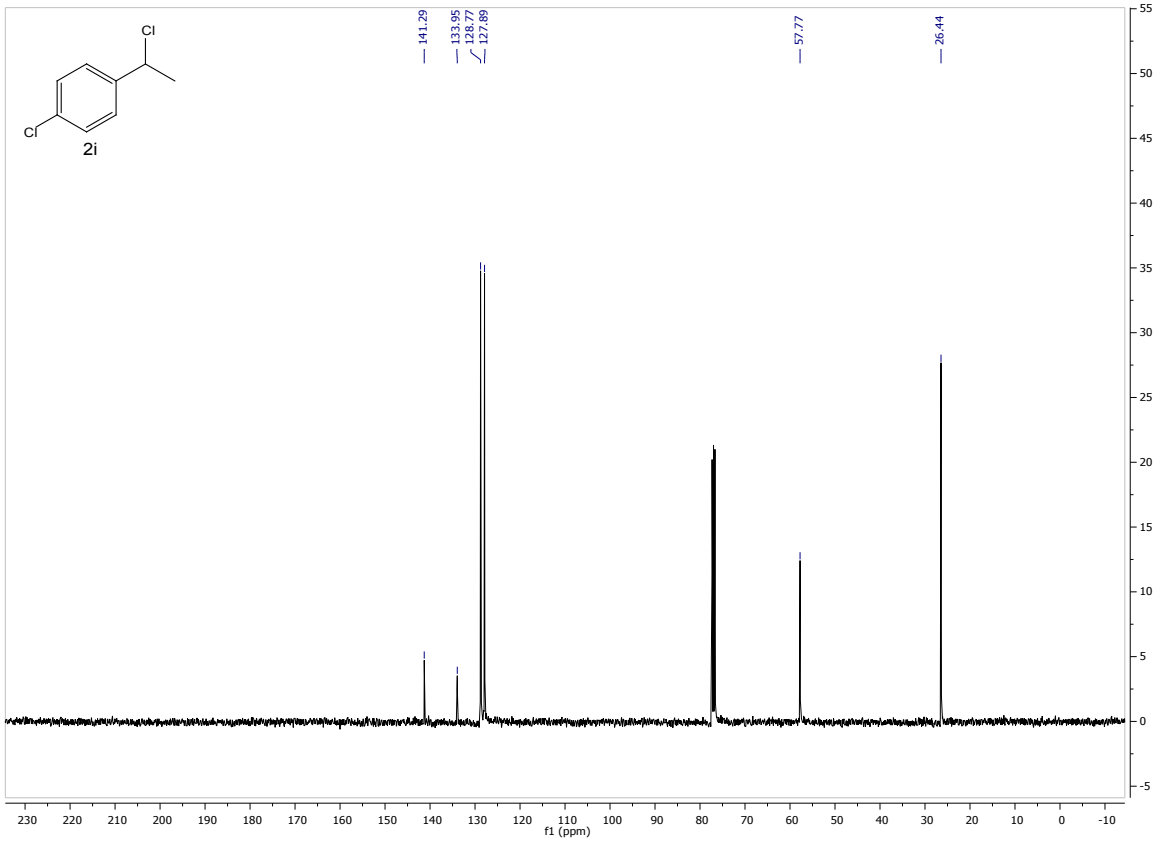
1.81
4.03
1.00
3.38
f1 (ppm)


Cl
Cl
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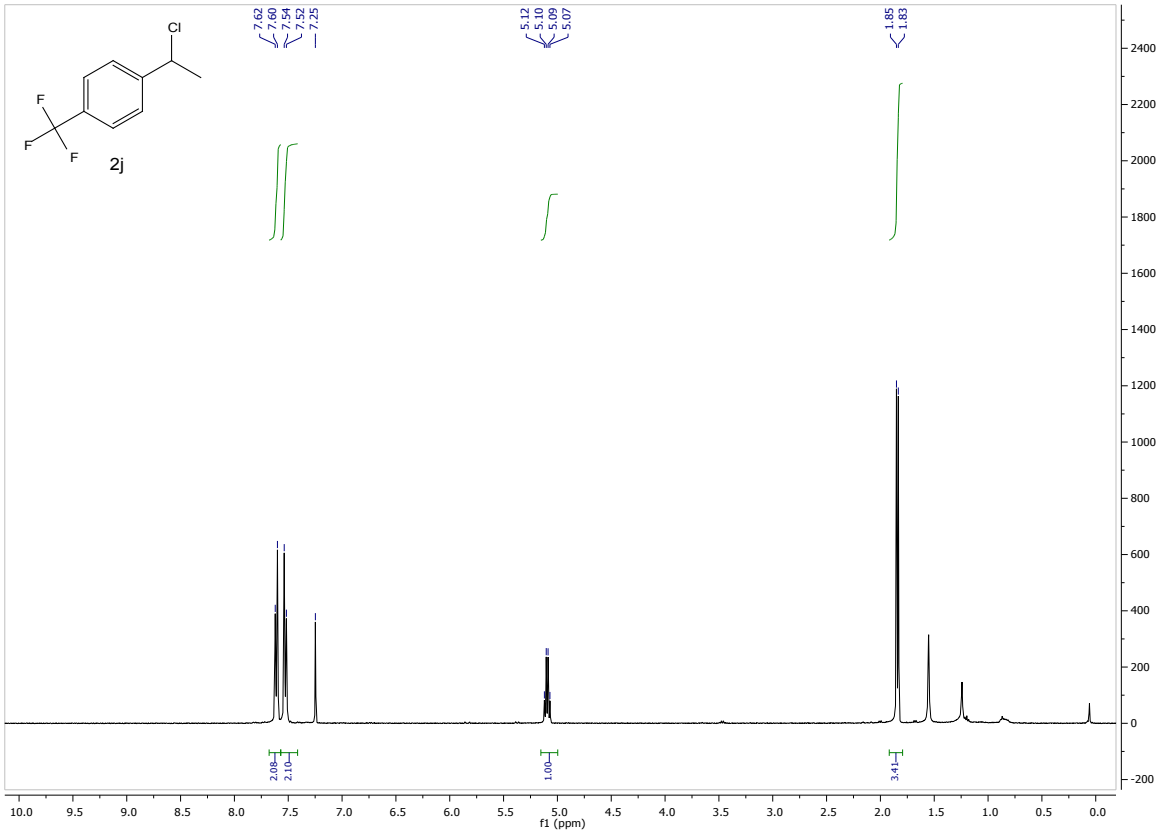
Cl
F
F
F
2j
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7.54
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7.25
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5.09
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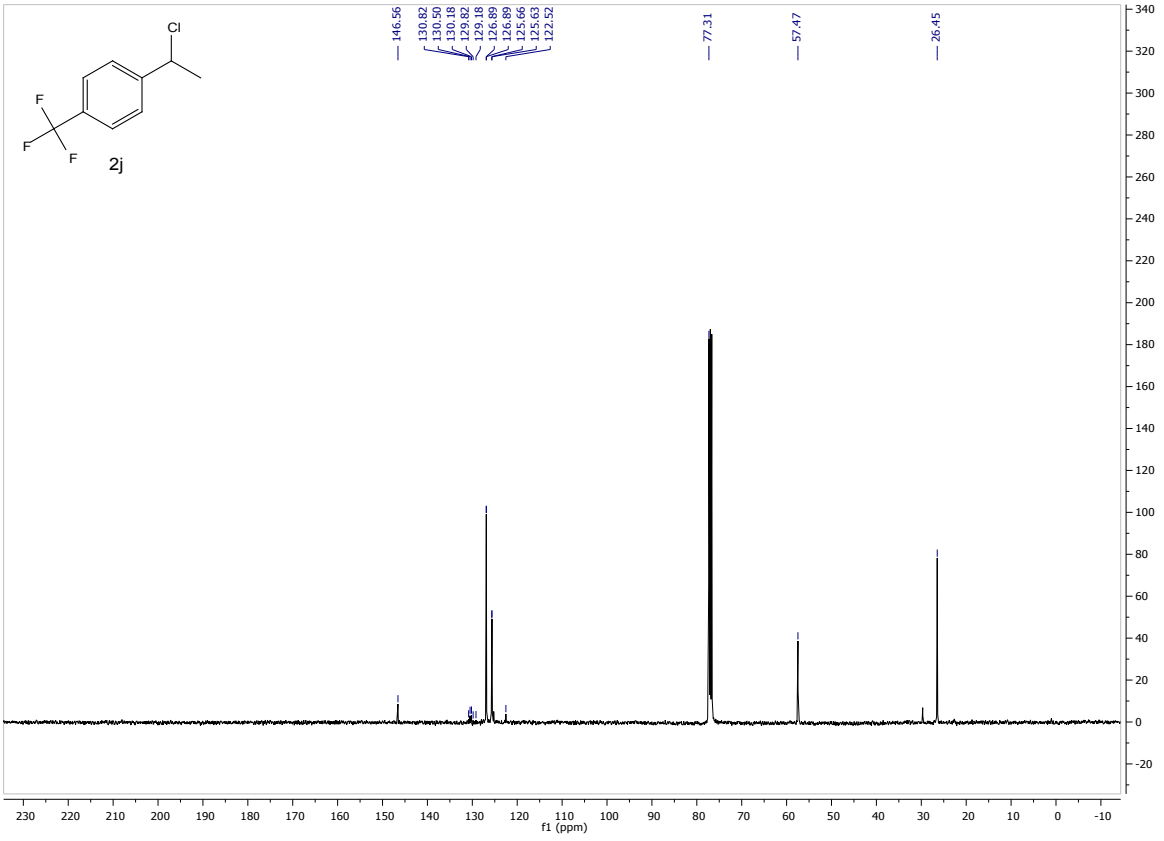
2.08
2.10
1.00
3.41
f1 (ppm)


Cl
F
F
F
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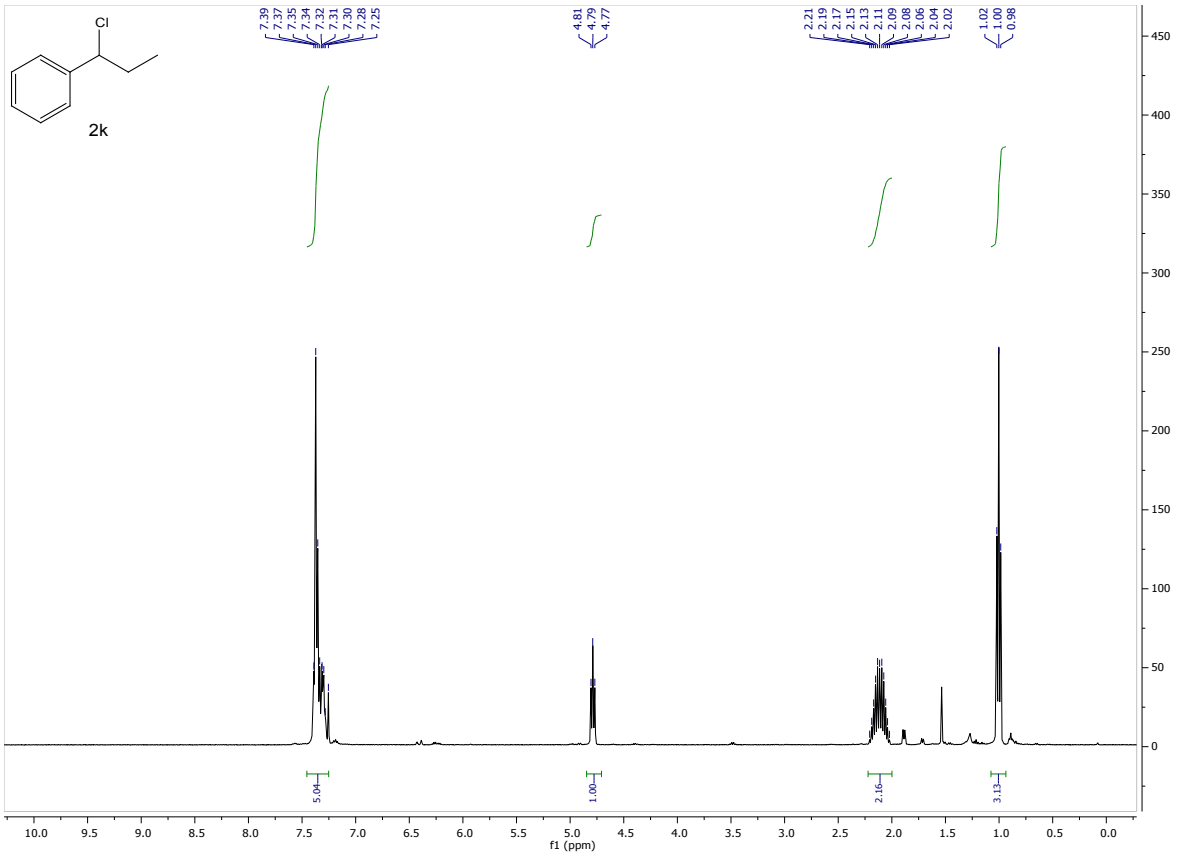
122.52
77.31
57.47
26.45
f1 (ppm)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7.25
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2.19
2.17
2.15
2.13
2.11
2.09
2.08
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2.04
2.02
1.02
1.00
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5.04
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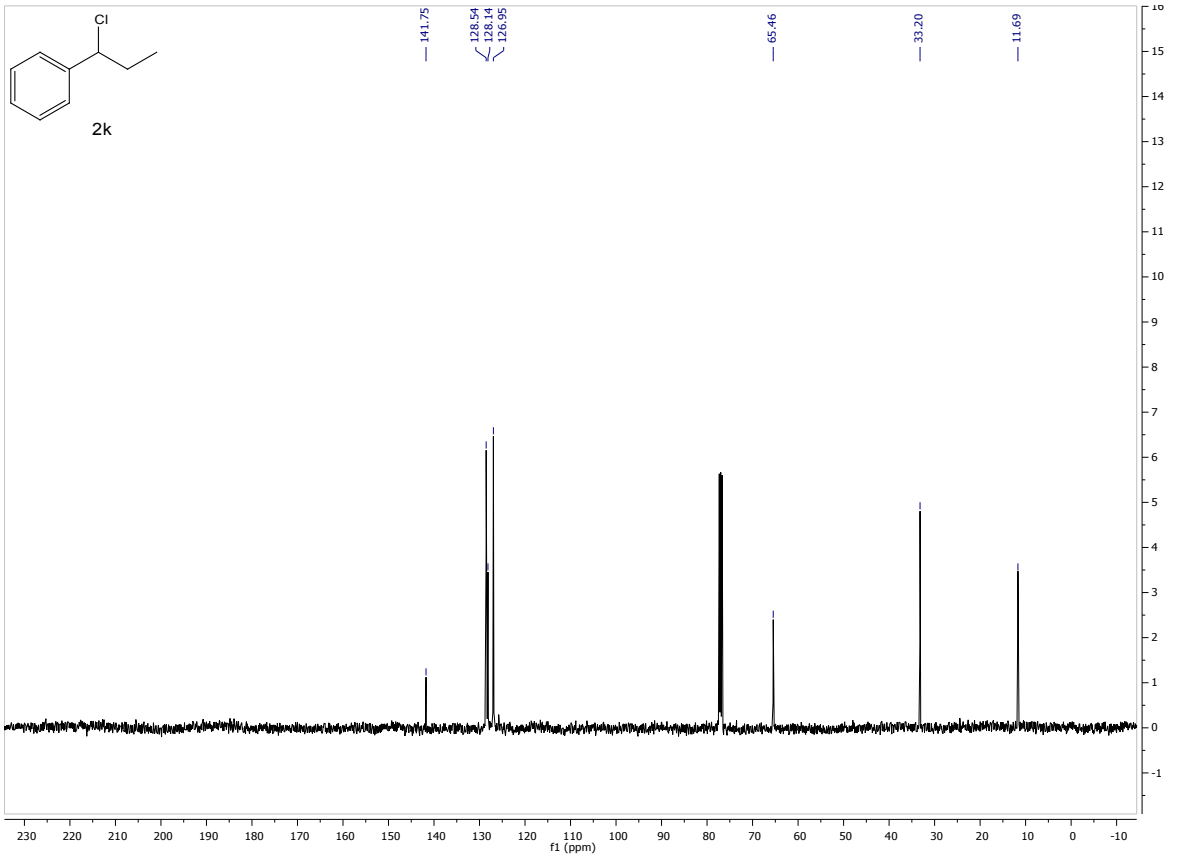
f1 (ppm)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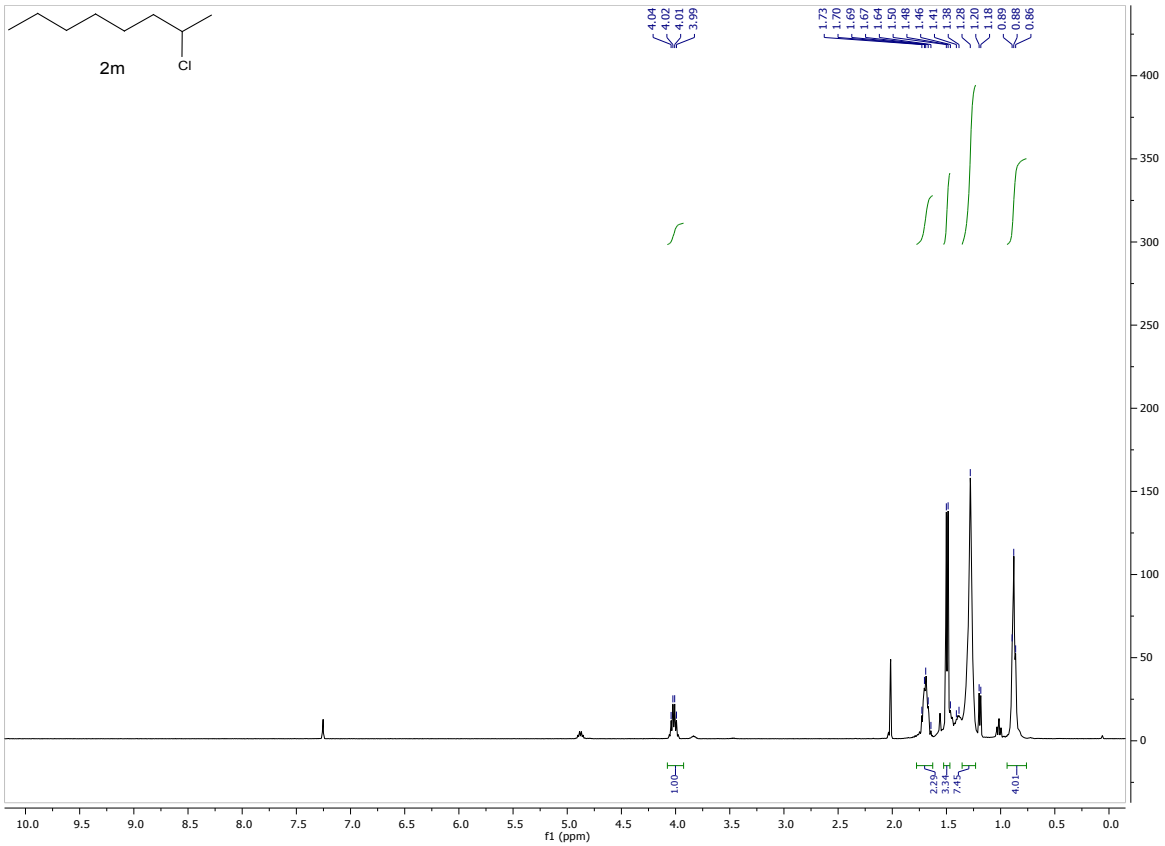
2m
Cl
4.04
4.02
4.01
3.99
1.73
1.70
1.69
1.67
1.64
1.50
1.48
1.46
1.41
1.38
1.28
1.20
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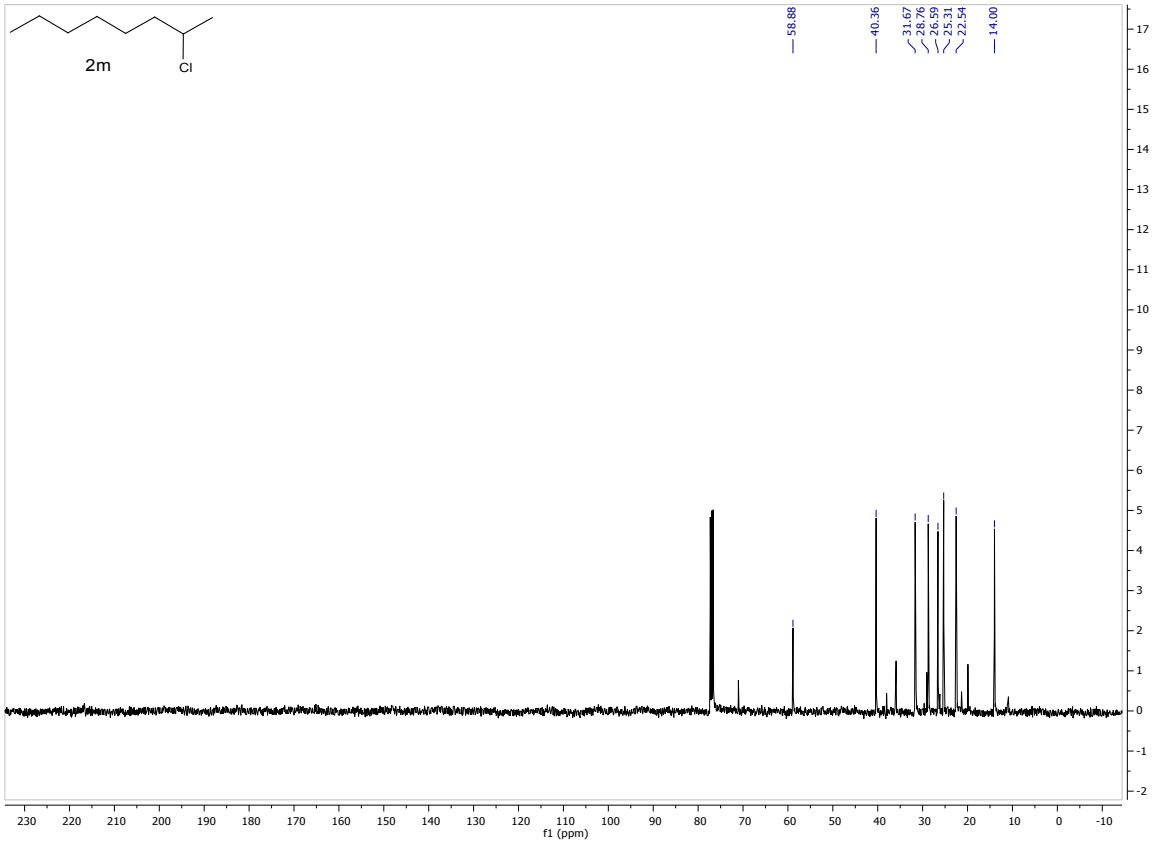
0.88
0.86
1.00
2.29
3.34
7.45
4.01
f1 (ppm)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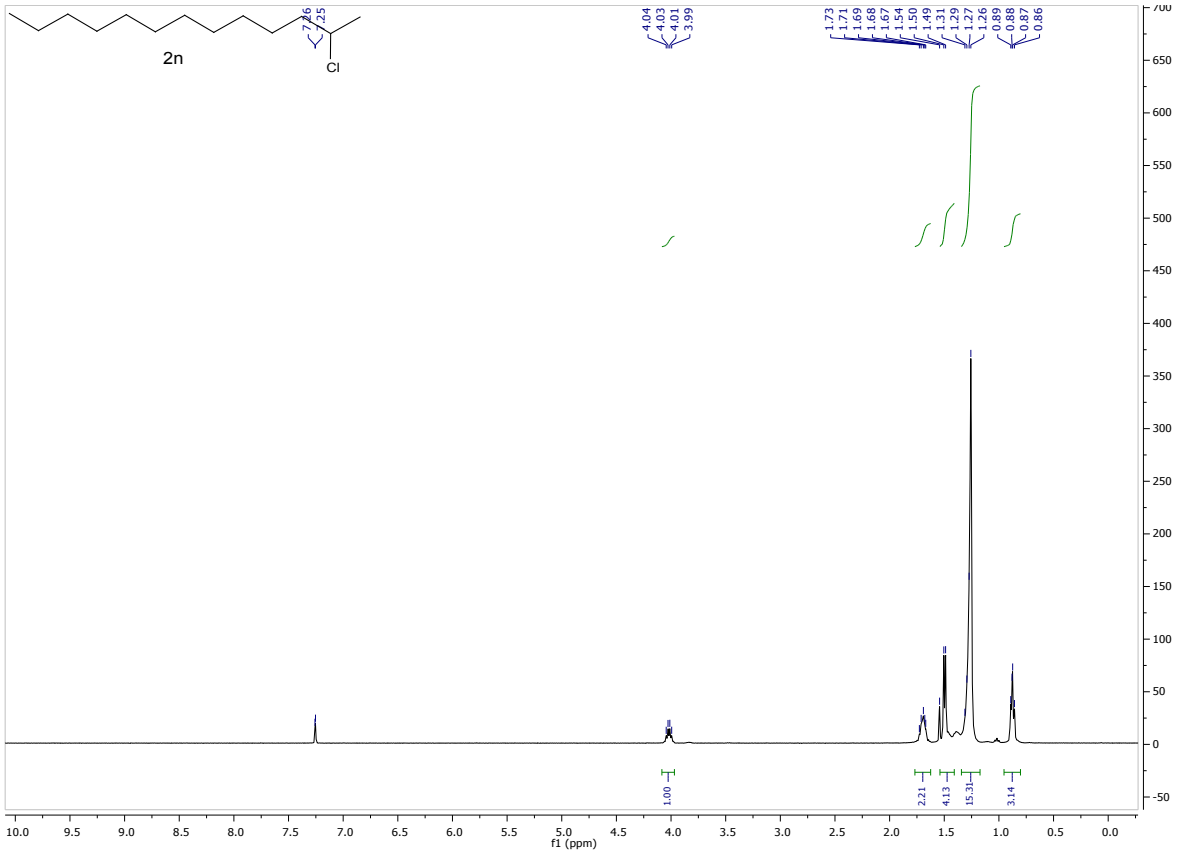
25.31
22.54
14.00
f1 (ppm)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1.69
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1.67
1.54
1.50
1.49
1.31
1.29
1.27
1.26
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0.88
0.87
0.86
1.00
2.21
4.13
15.31
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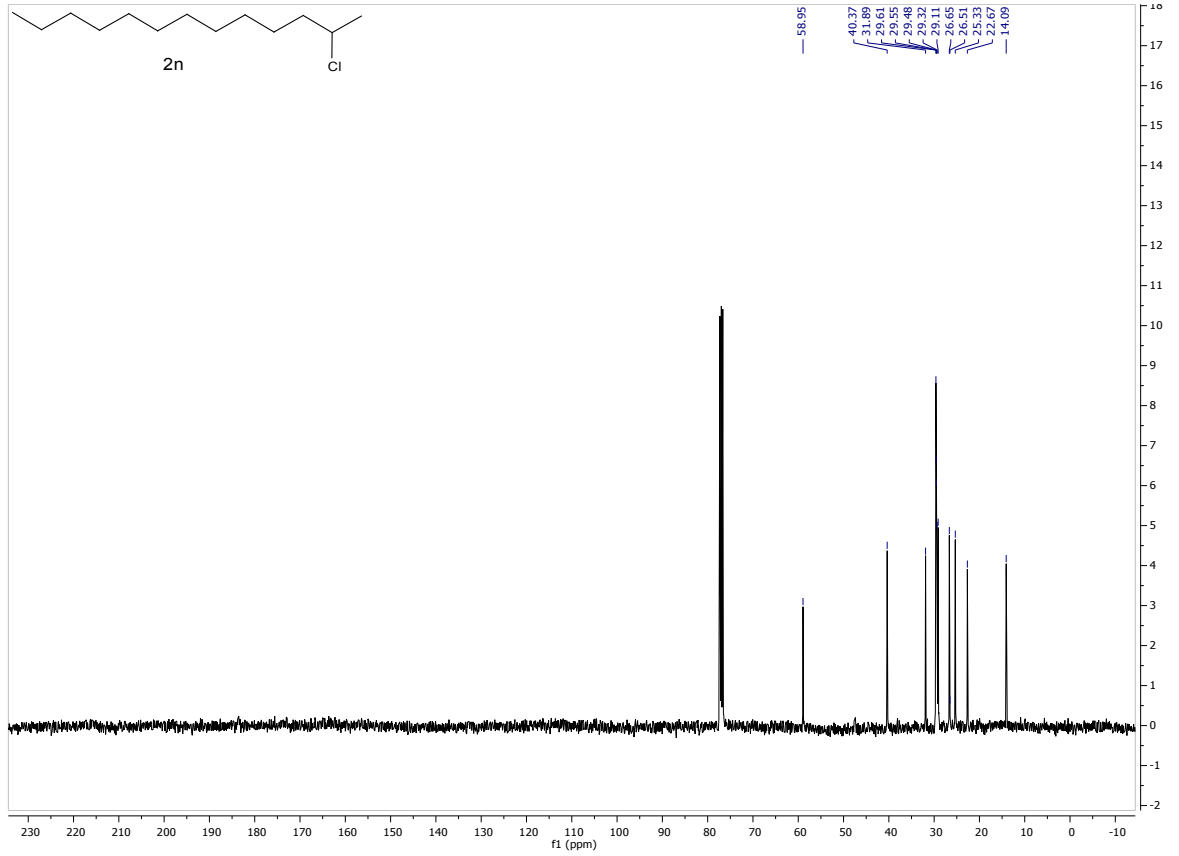
f1 (ppm)


2n
Cl
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29.32
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26.51
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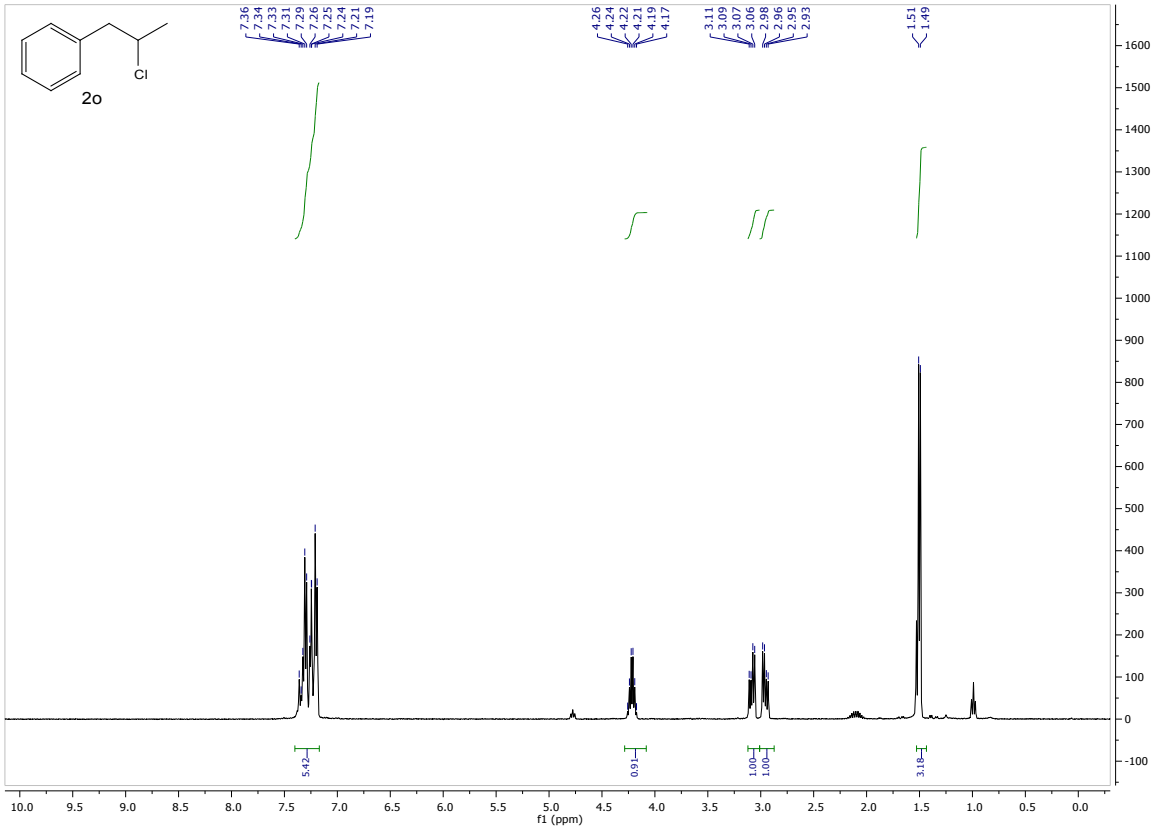
22.67
14.09
f1 (ppm)


Cl
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7.26
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7.21
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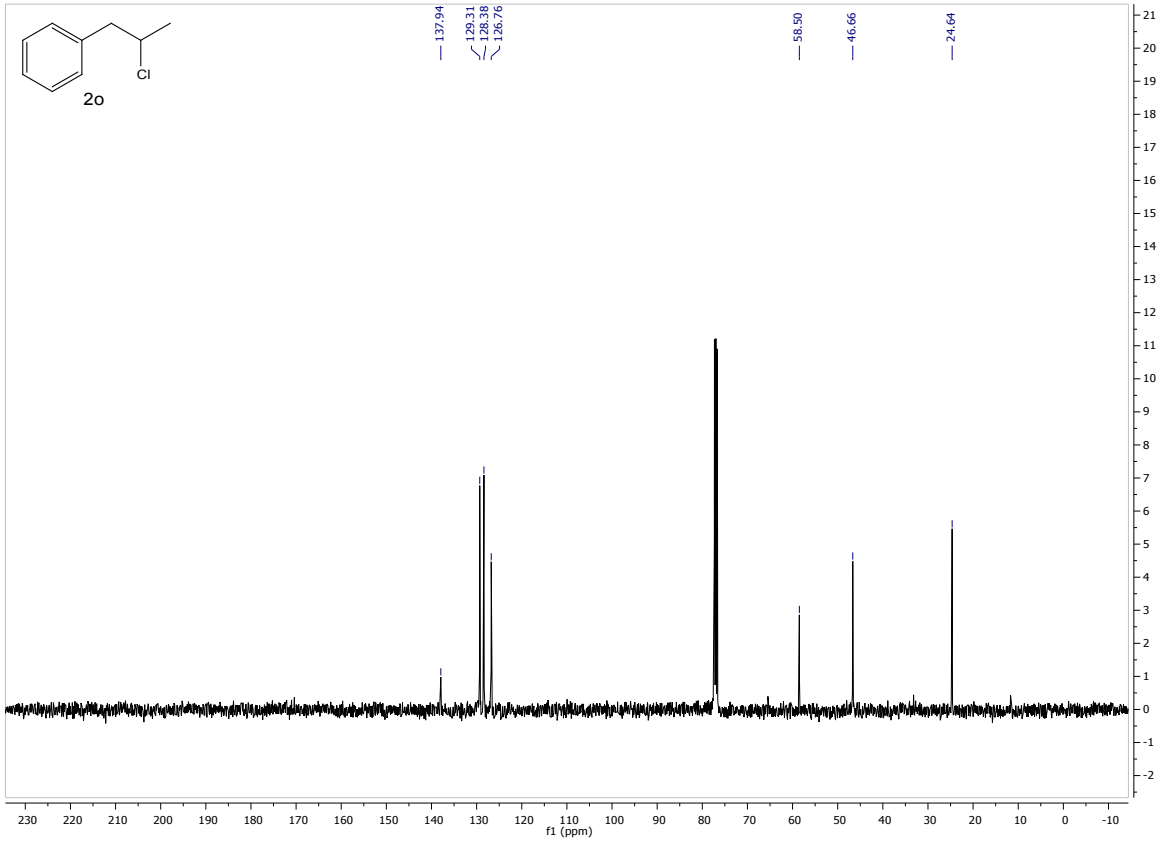
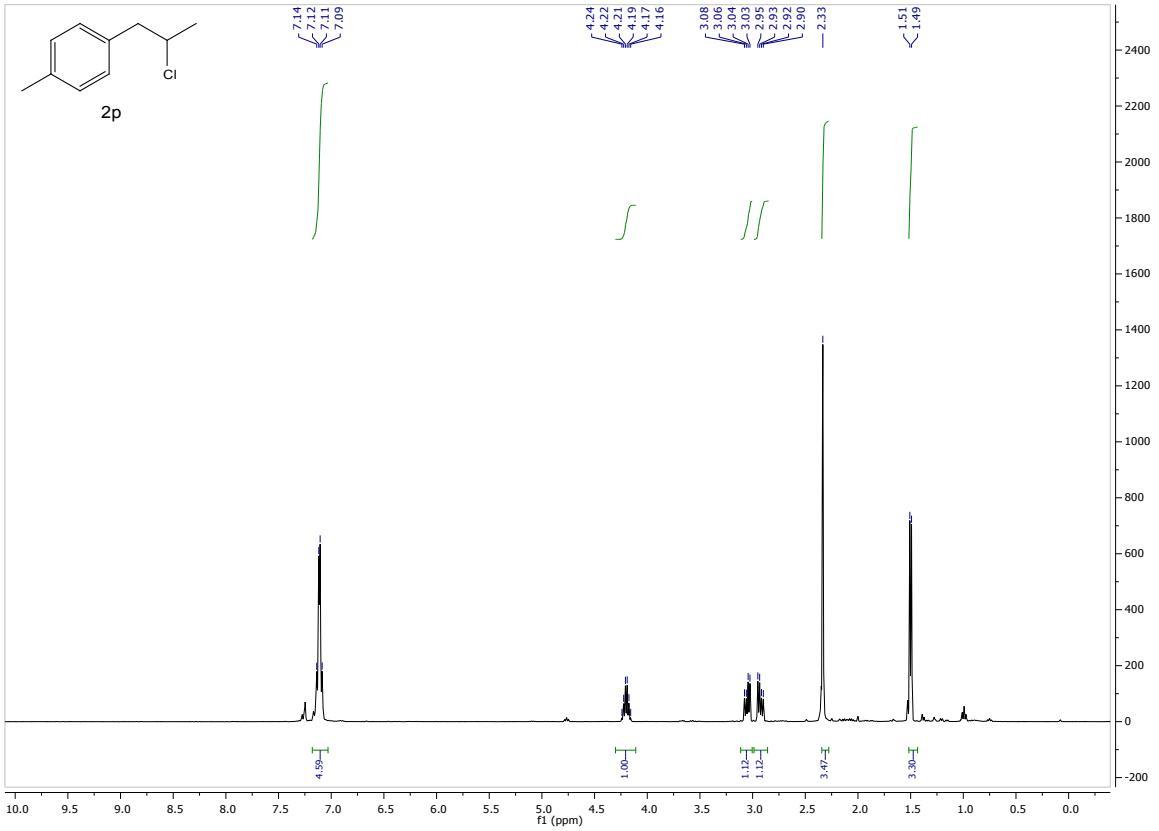
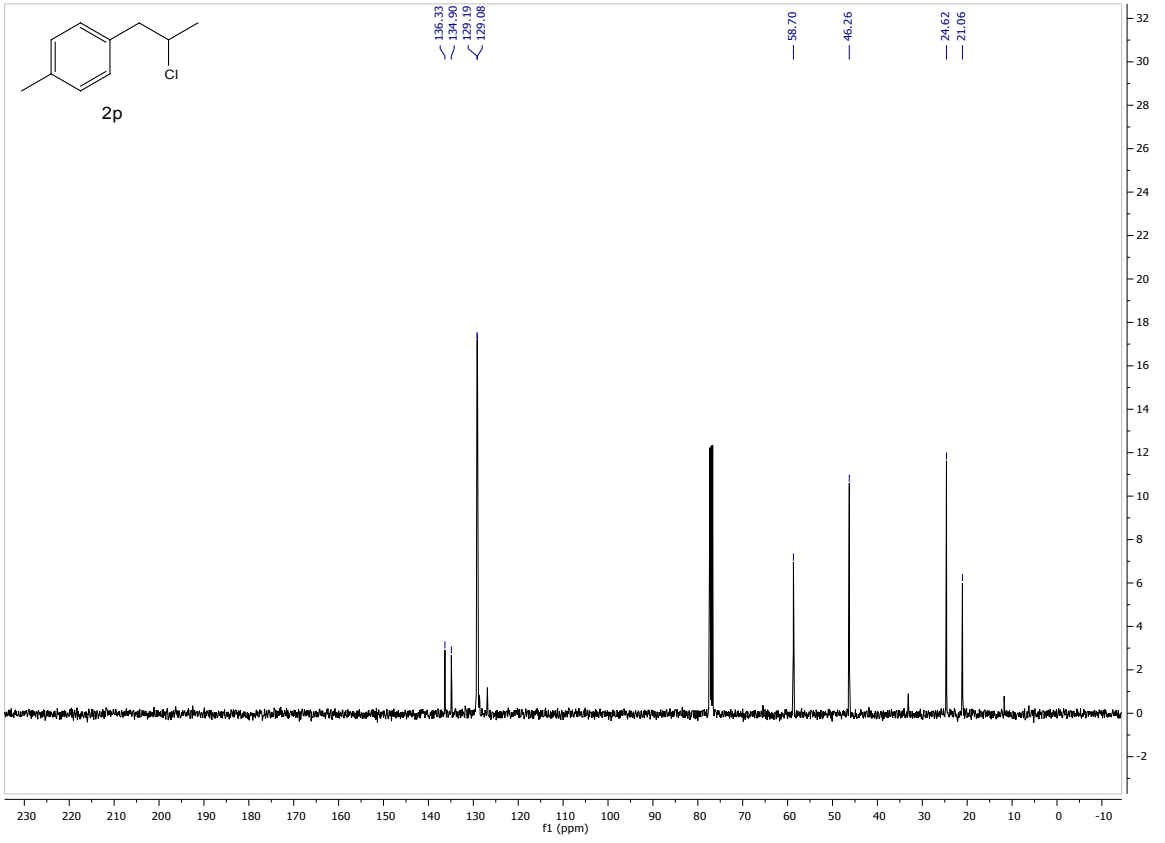
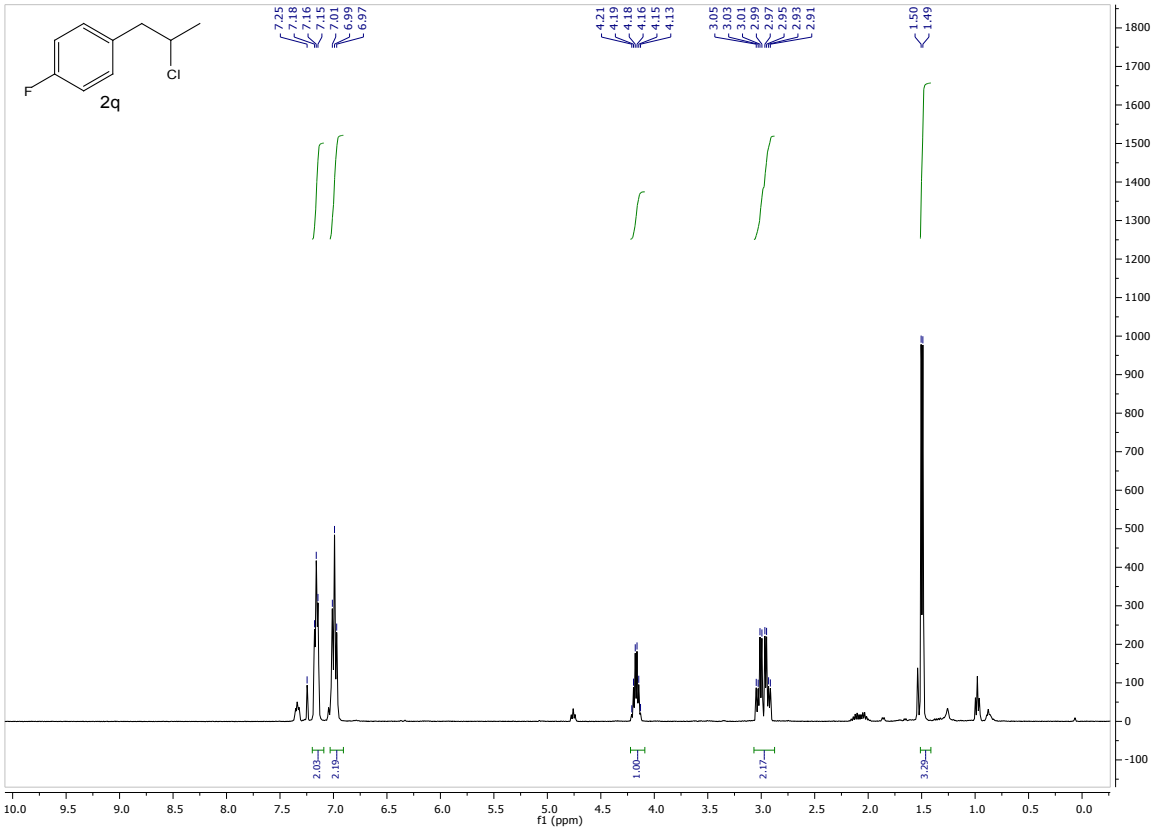
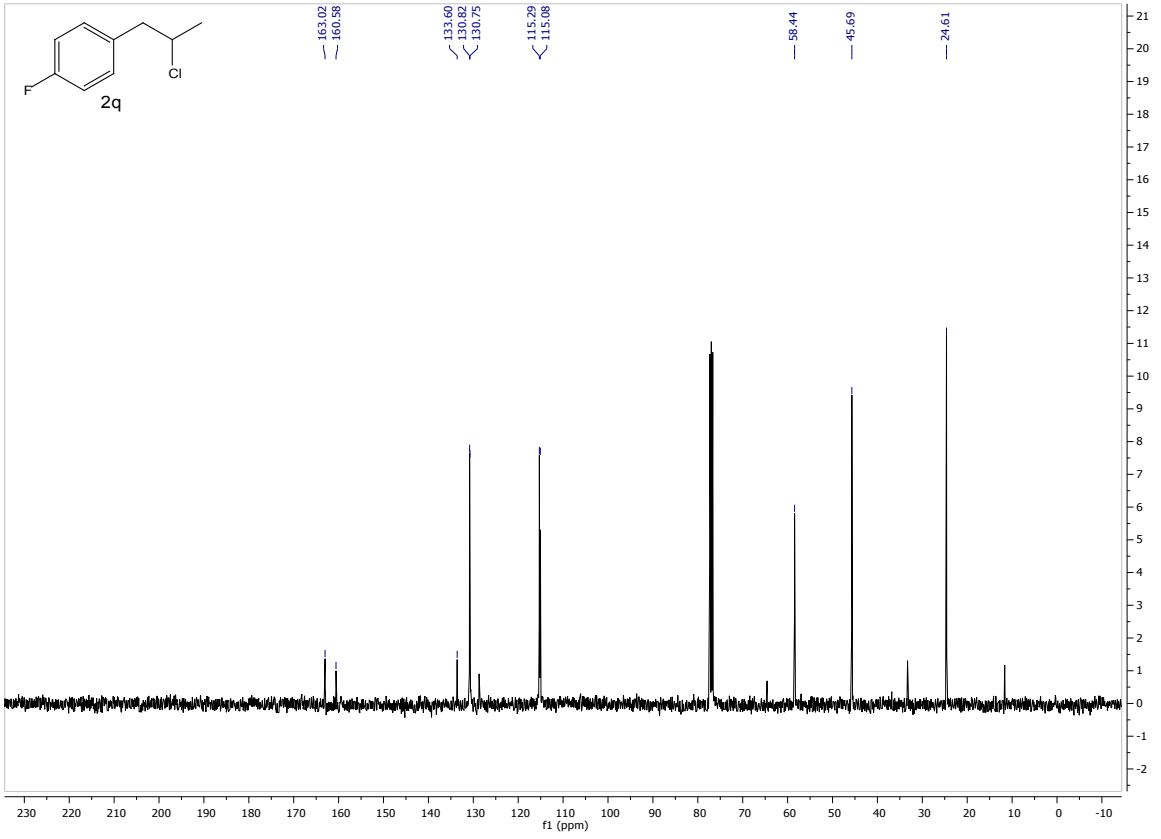
4.19
4.17
3.11
3.09
3.07
3.06
2.98
2.96
2.95
2.93
1.51
1.49
5.42
0.91
1.00
1.00
3.18
f1 (ppm)

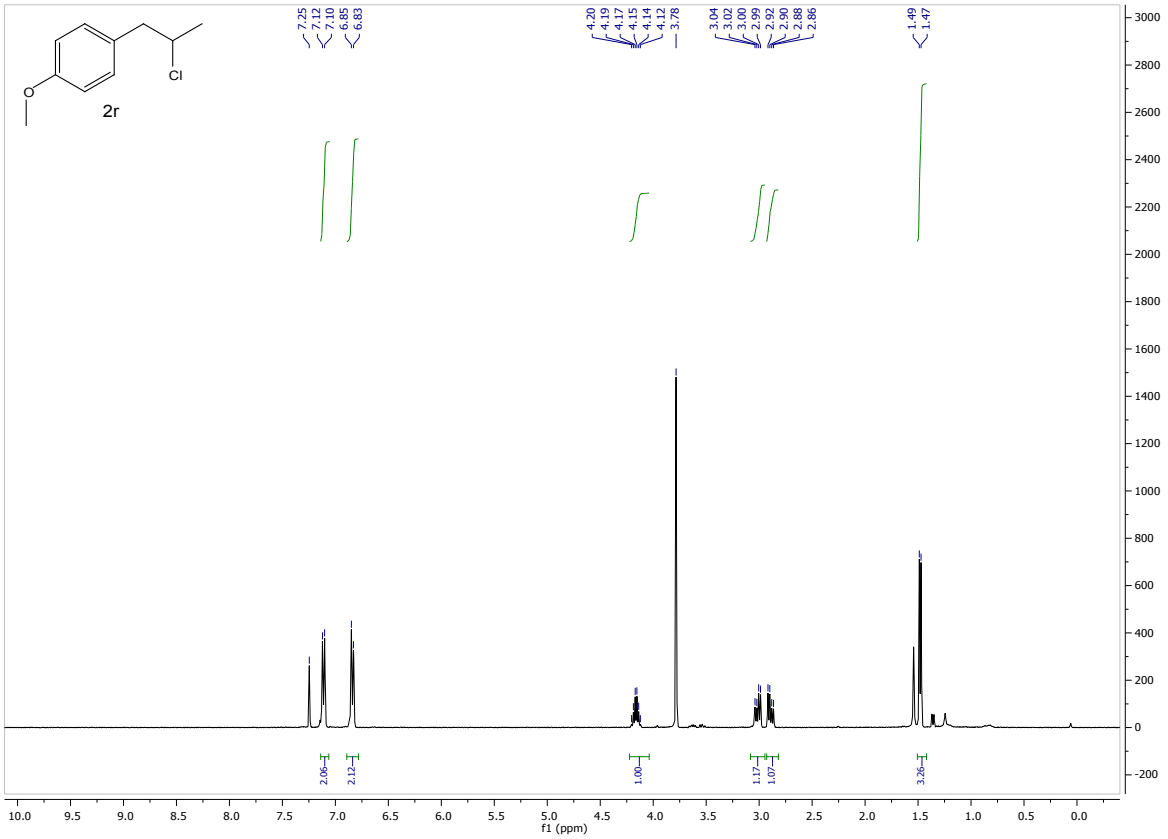

Cl
2o
137.94
129.31
128.38
126.76
58.50
46.66
24.64
f1 (ppm)


Cl
2p
7.14
7.12
7.11
7.09
4.24
4.22
4.21
4.19
4.17
4.16
3.08
3.06
3.04
3.03
2.95
2.93
2.92
2.90
2.33
1.51
1.49
4.59
1.00
1.12
1.12
3.47
3.30
f1 (ppm)


Cl
2p
136.33
134.90
129.19
129.08
58.70
46.26
24.62
21.06
f1 (ppm)


F
Cl
2q
7.25
7.18
7.16
7.15
7.01
6.99
6.97
4.21
4.19
4.18
4.16
4.15
4.13
3.05
3.03
3.01
2.99
2.97
2.95
2.93
2.91
1.50
1.49
2.03
2.19
1.00
2.17
3.29
f1 (ppm)


F
Cl
2q
163.02
160.58
133.60
130.82
130.75
115.29
115.08
58.44
45.69
24.61
f1 (ppm)


2r
Cl
O
7.25
7.12
7.10
6.85
6.83
4.20
4.19
4.17
4.15
4.14
4.12
3.78
3.04
3.02
3.00
2.99
2.92
2.90
2.88
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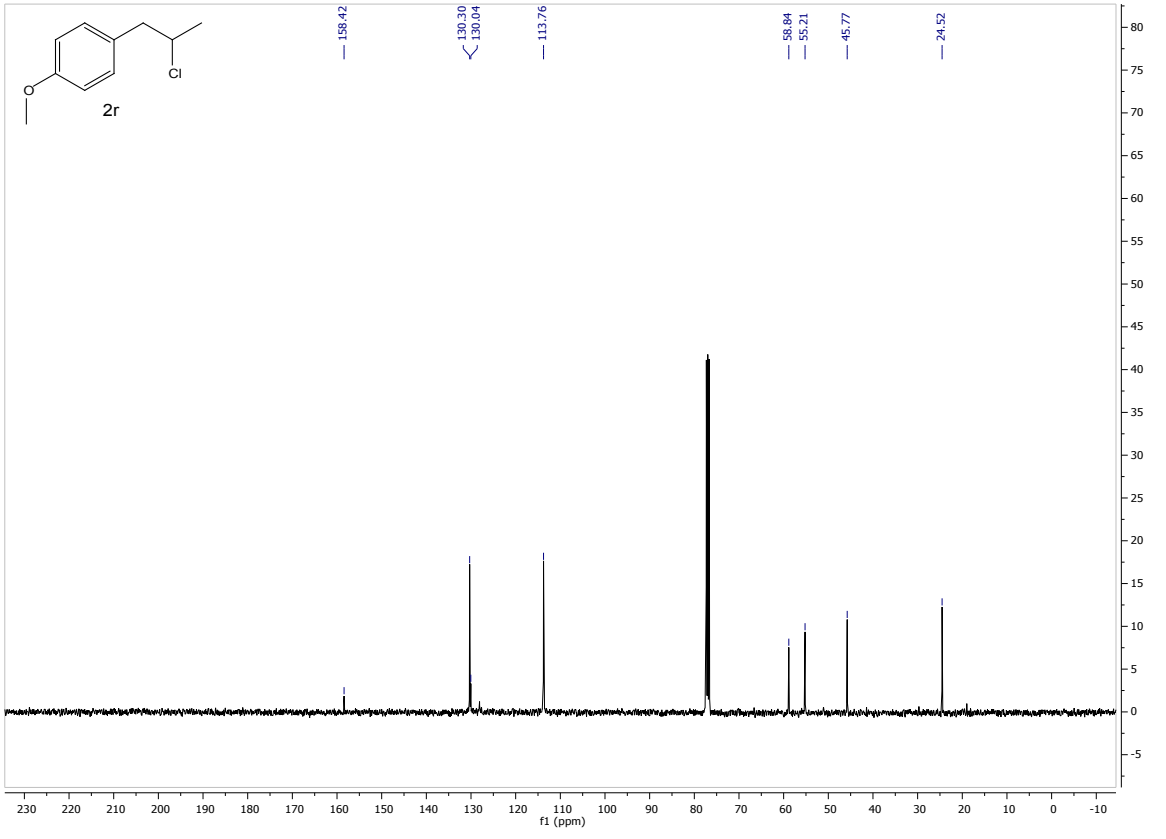
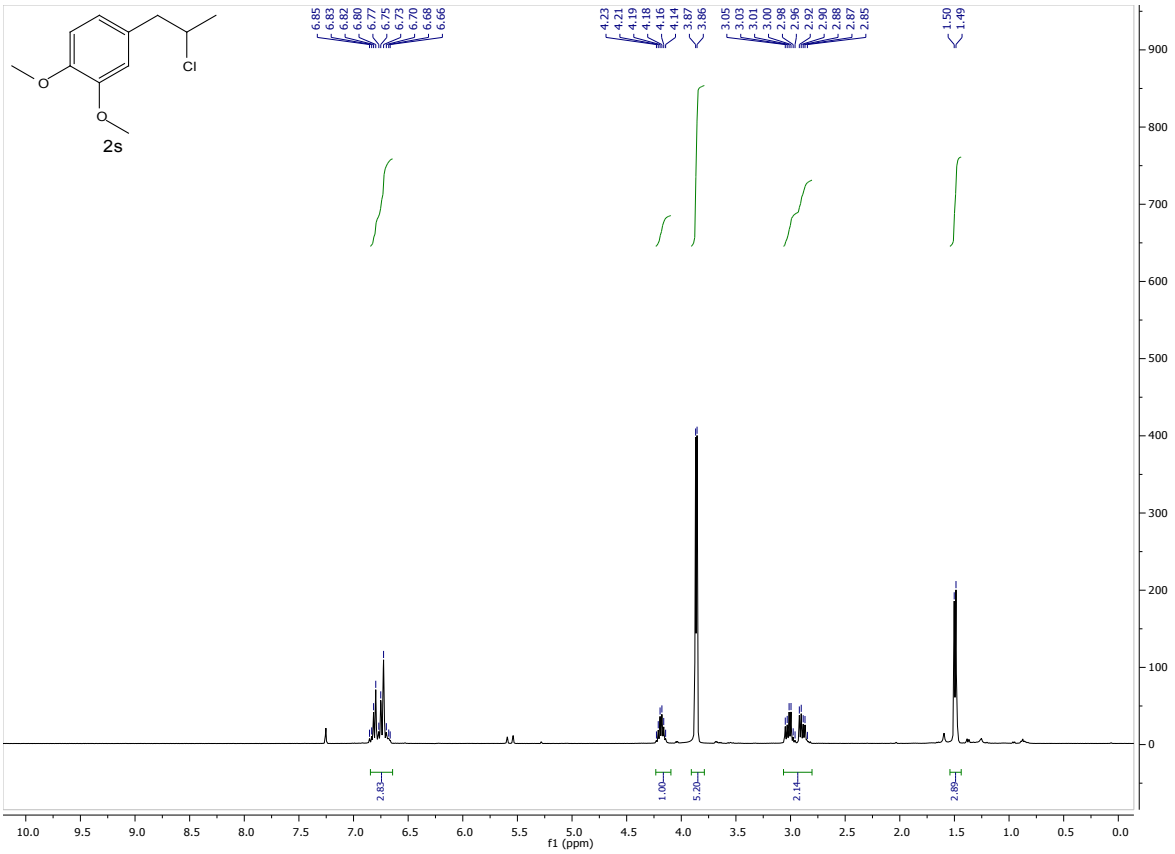
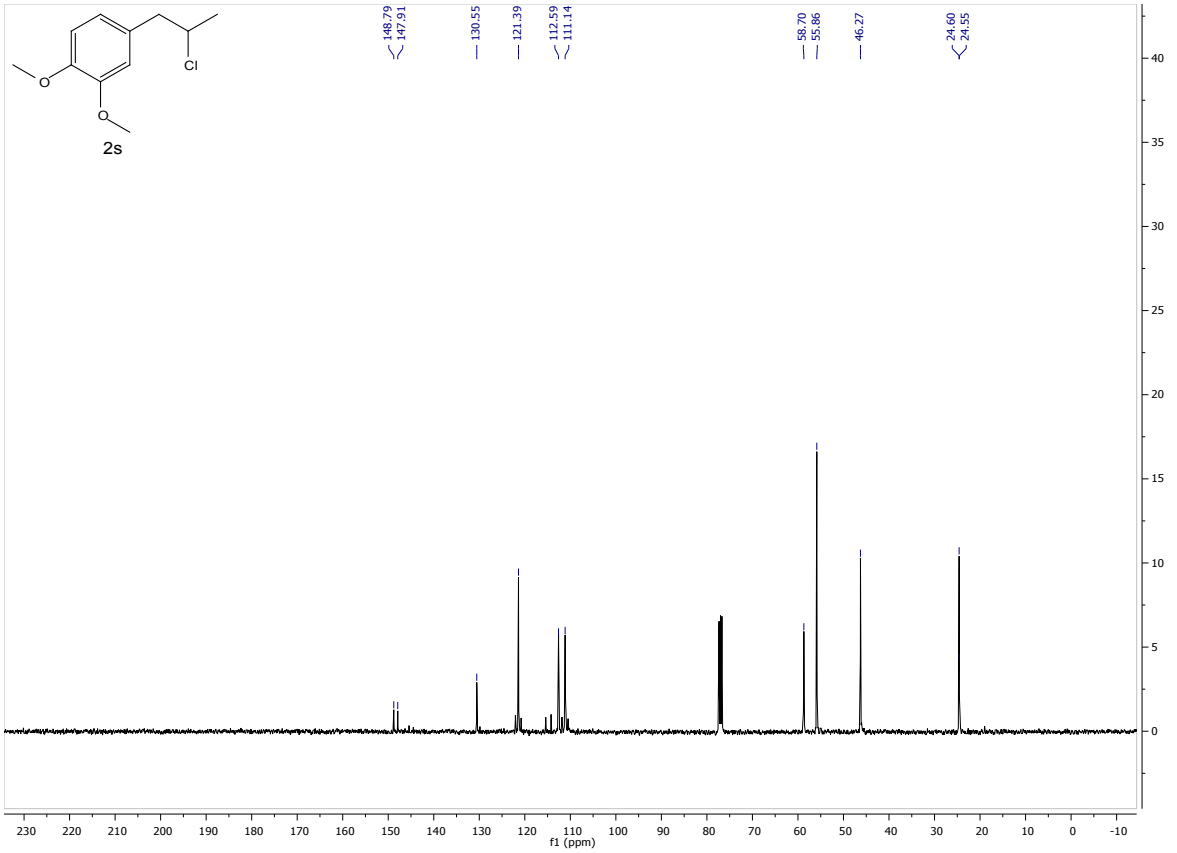
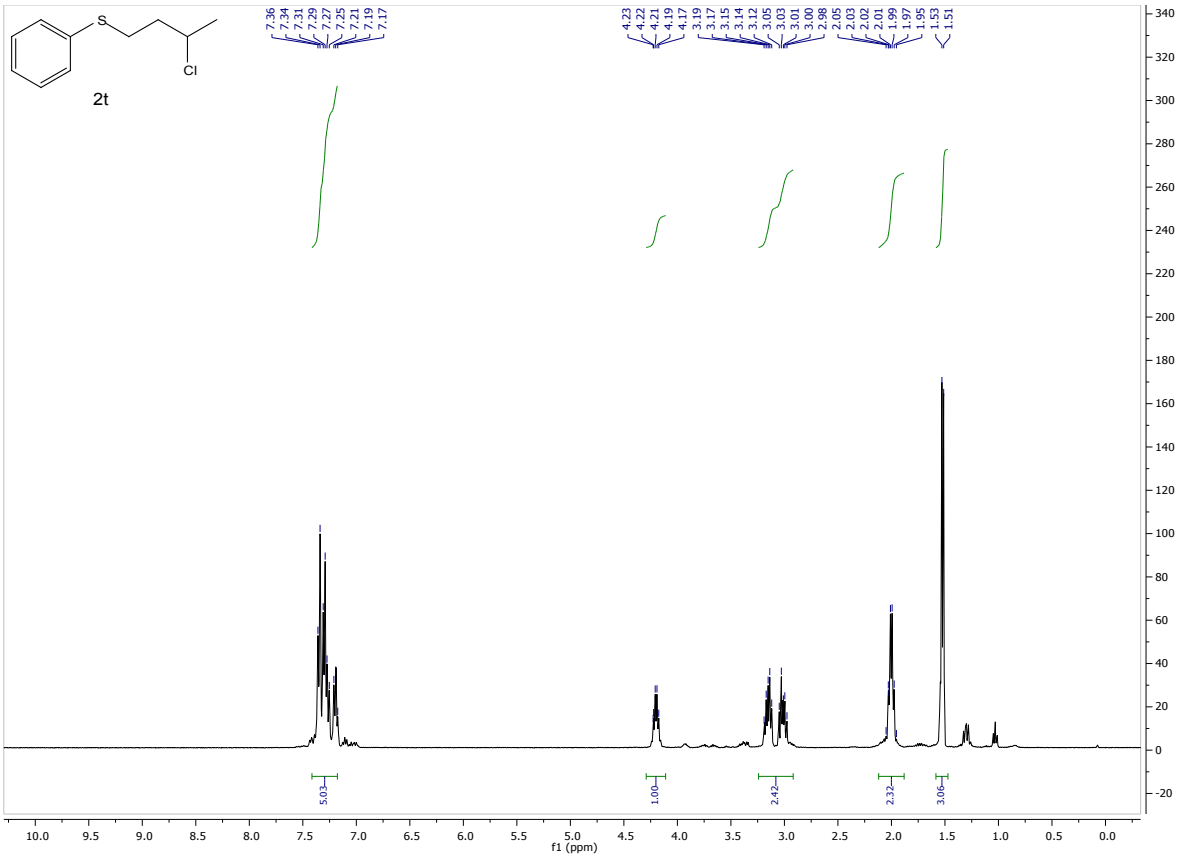
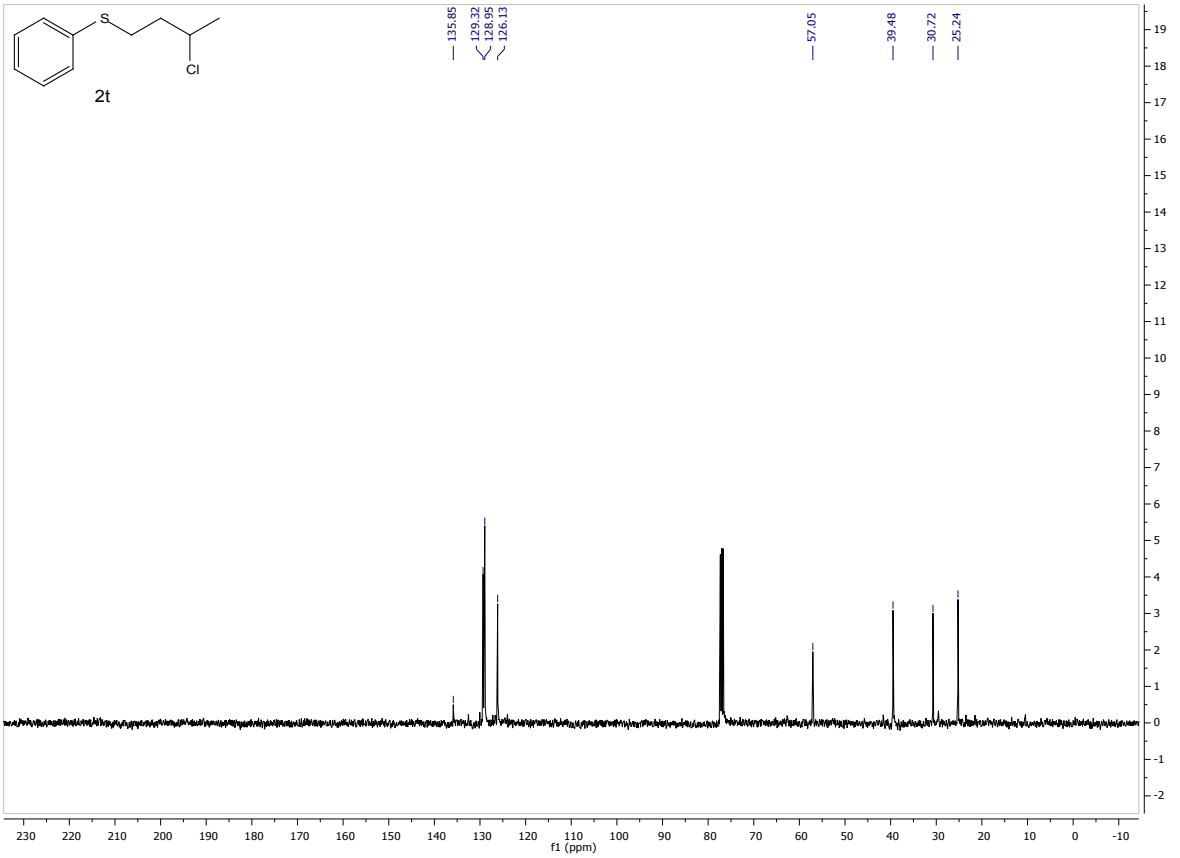
1.49
1.47
2.06
2.12
1.00
1.17
1.07
3.26
f1 (ppm)

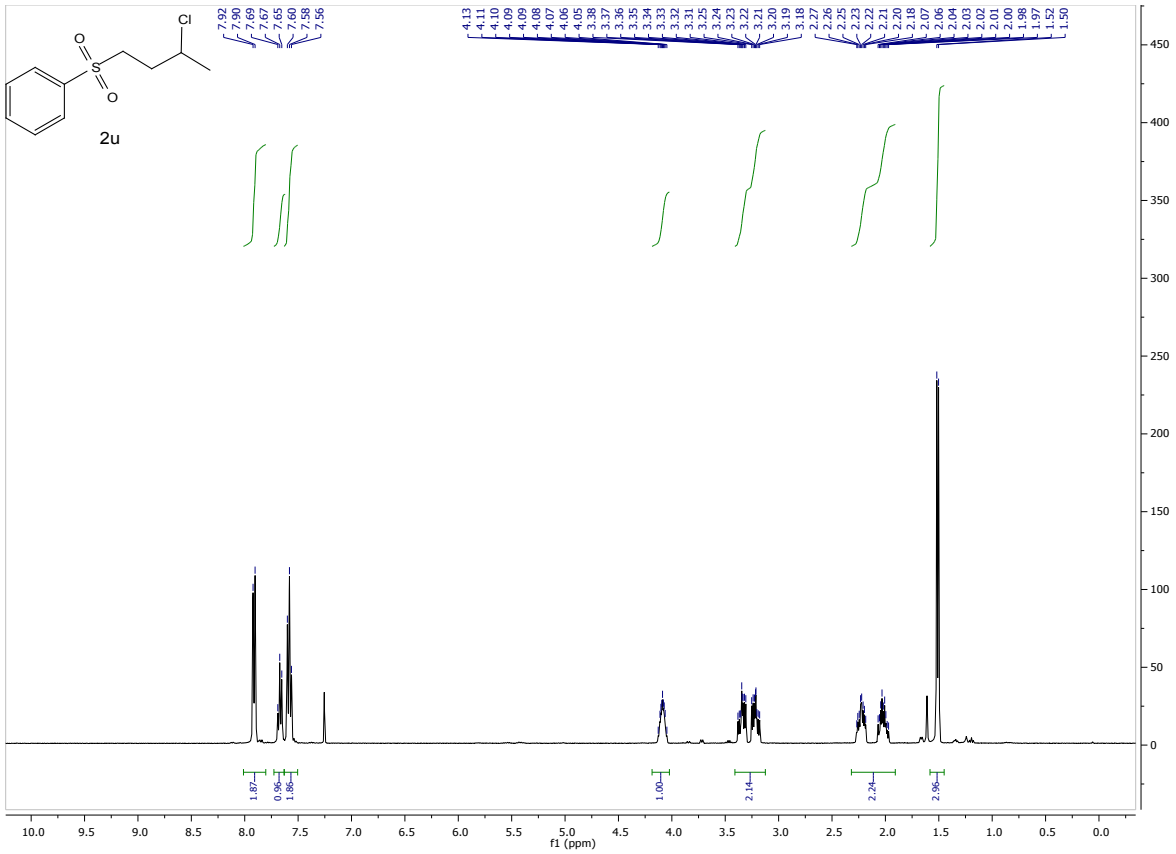

2r
Cl
O
158.42
130.30
130.04
113.76
58.84
55.21
45.77
24.52
f1 (ppm)

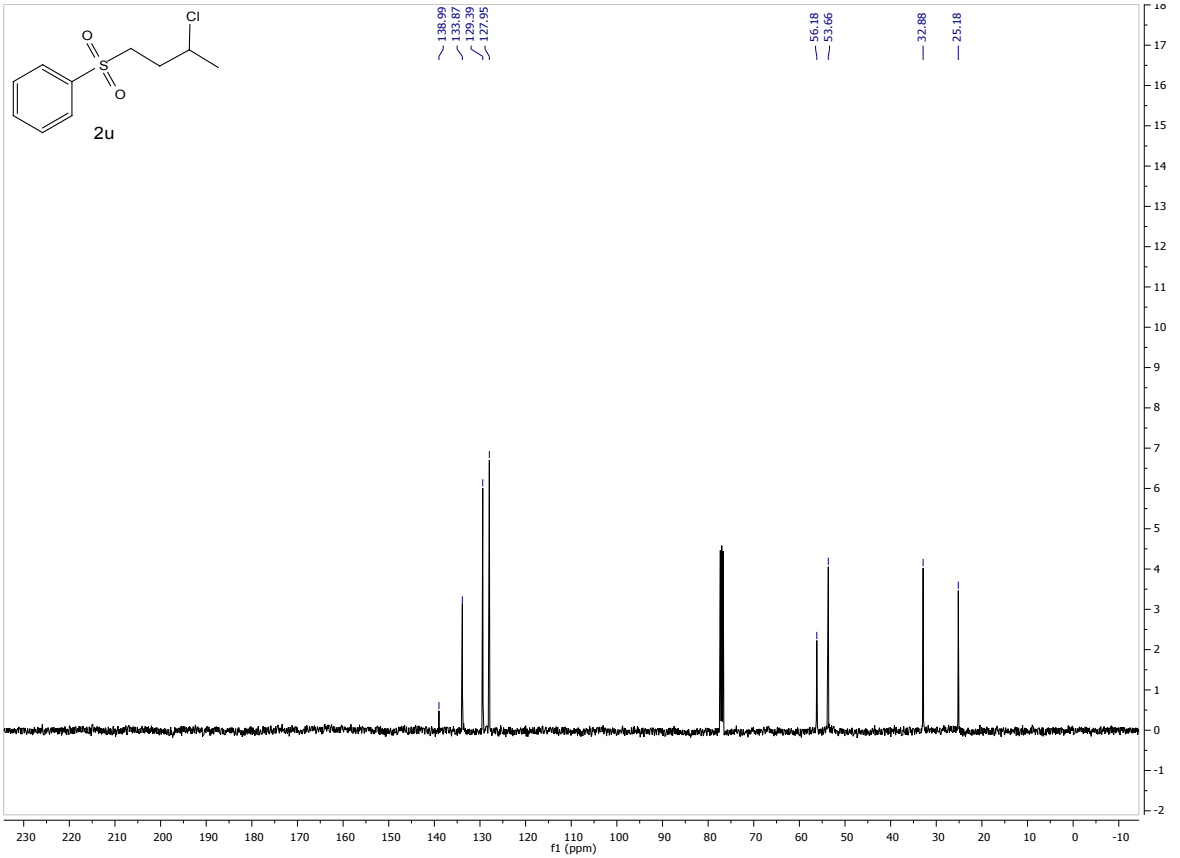

2s
6.85
6.83
6.82
6.80
6.77
6.75
6.73
6.70
6.68
6.66
4.23
4.21
4.19
4.18
4.16
4.14
3.87
3.86
3.05
3.03
3.01
3.00
2.98
2.96
2.92
2.90
2.88
2.87
2.85
1.50
1.49
2.63
1.00
5.20
2.14
2.89
f1 (ppm)

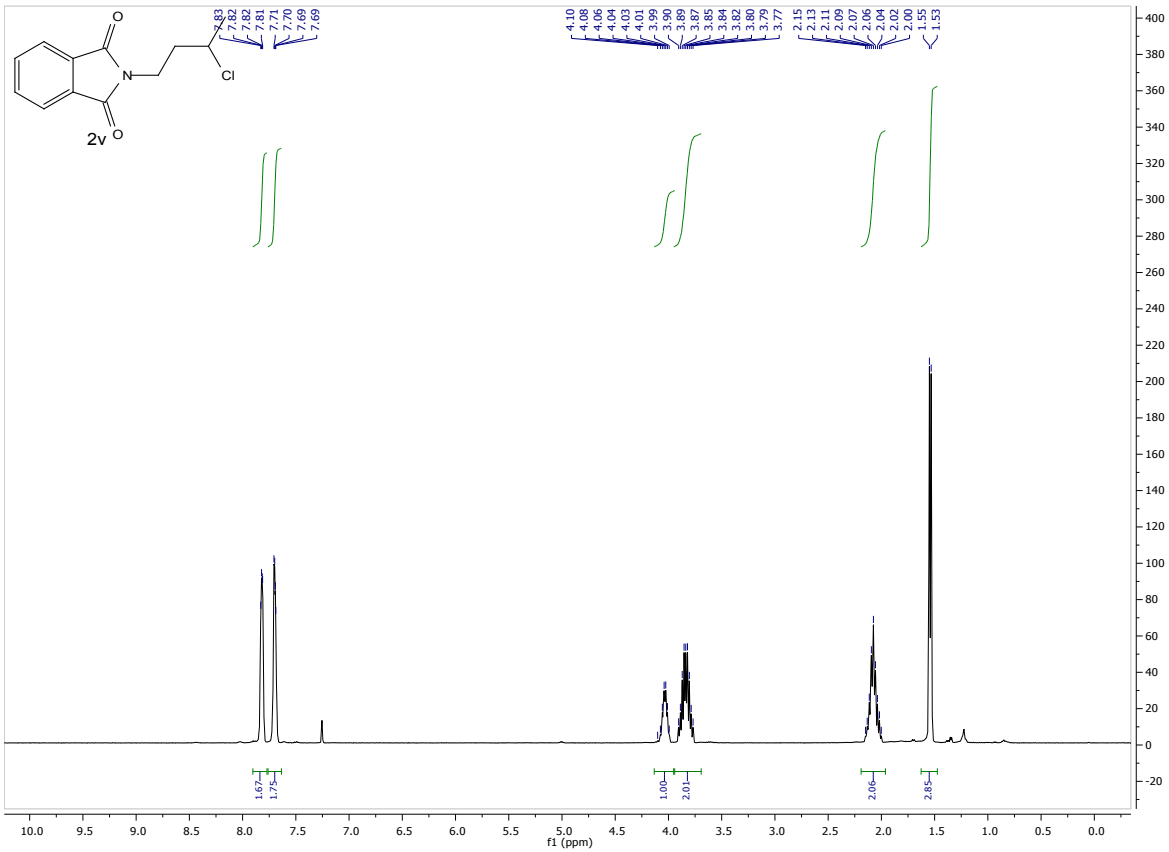

2s
148.79
147.91
130.55
121.39
112.59
111.14
58.70
55.86
46.27
24.60
24.55
f1 (ppm)

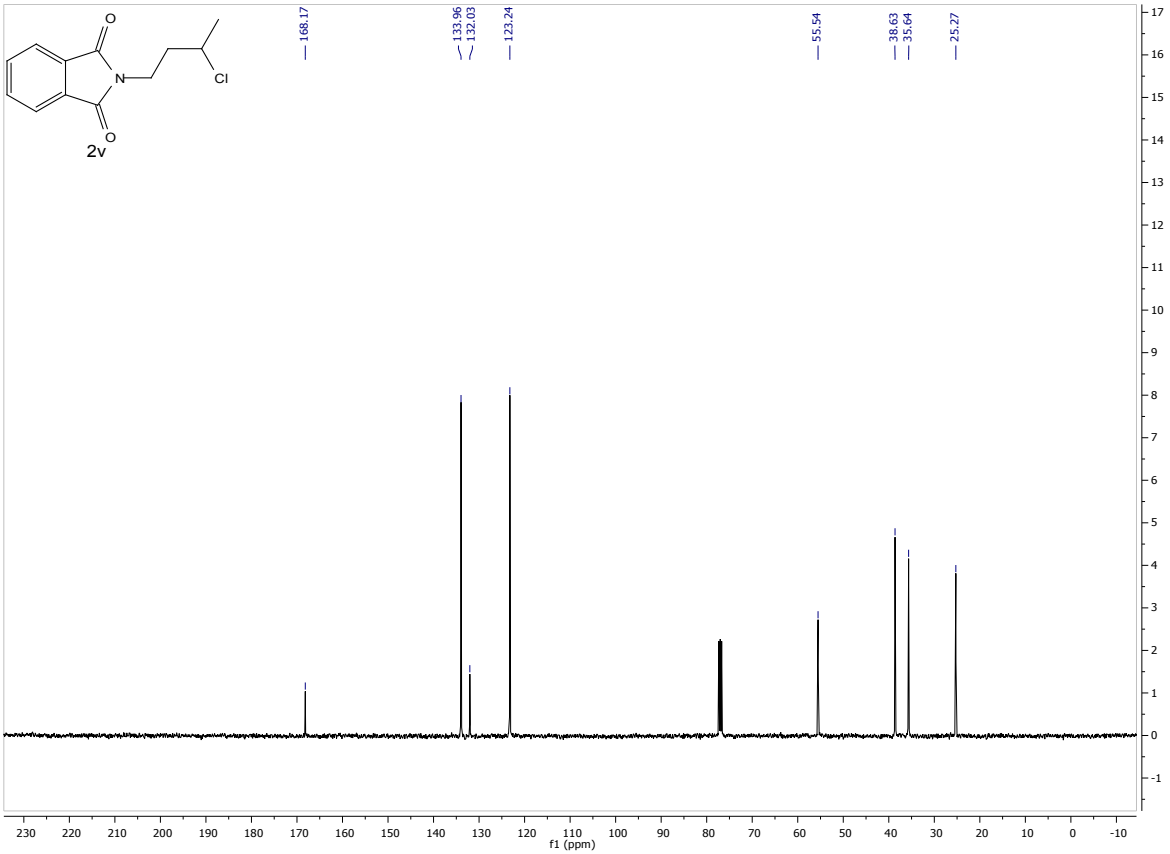

S
Cl
2t
7.36
7.34
7.31
7.29
7.27
7.25
7.21
7.19
7.17
4.23
4.22
4.21
4.19
4.17
3.19
3.17
3.15
3.14
3.12
3.05
3.03
3.01
3.00
2.98
2.05
2.03
2.02
2.01
1.99
1.97
1.95
1.53
1.51
5.03
1.00
2.42
2.32
3.06
f1 (ppm)

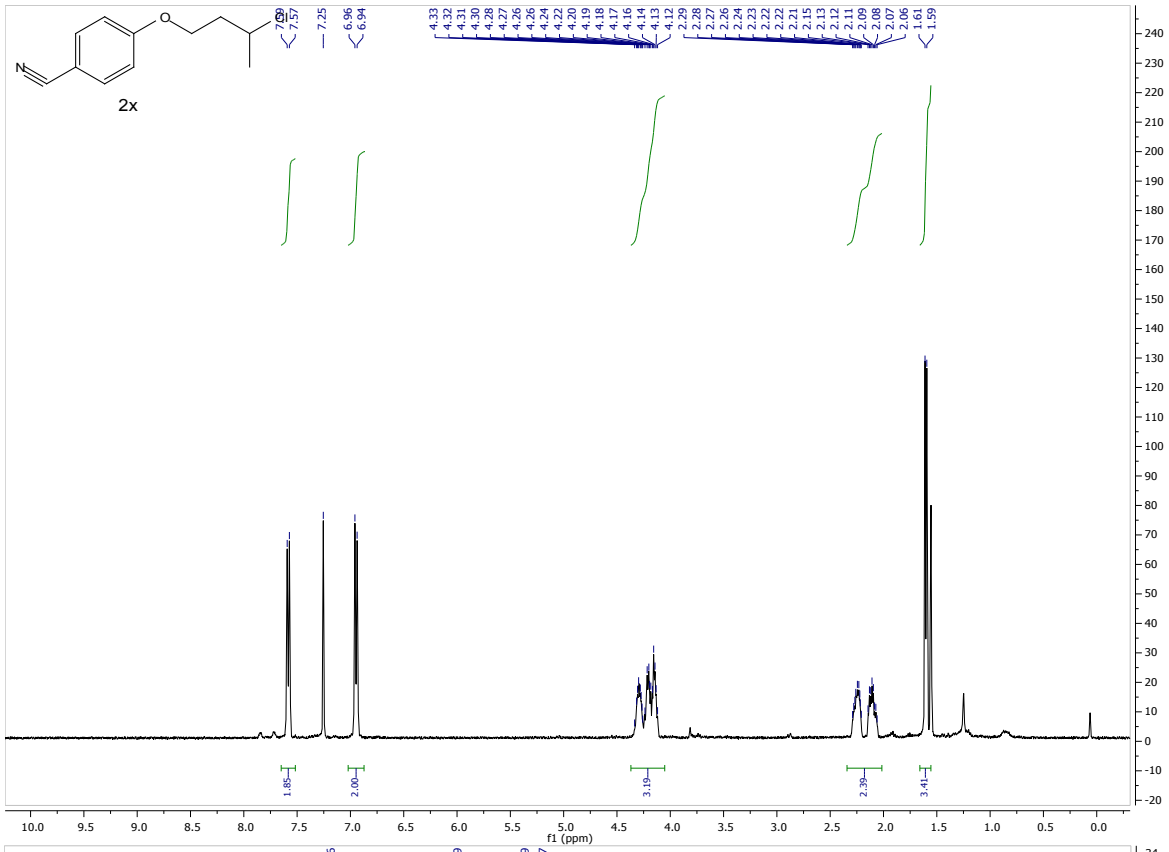

S
Cl
2t
135.85
129.32
128.95
126.13
57.05
39.48
30.72
25.24
f1 (ppm)

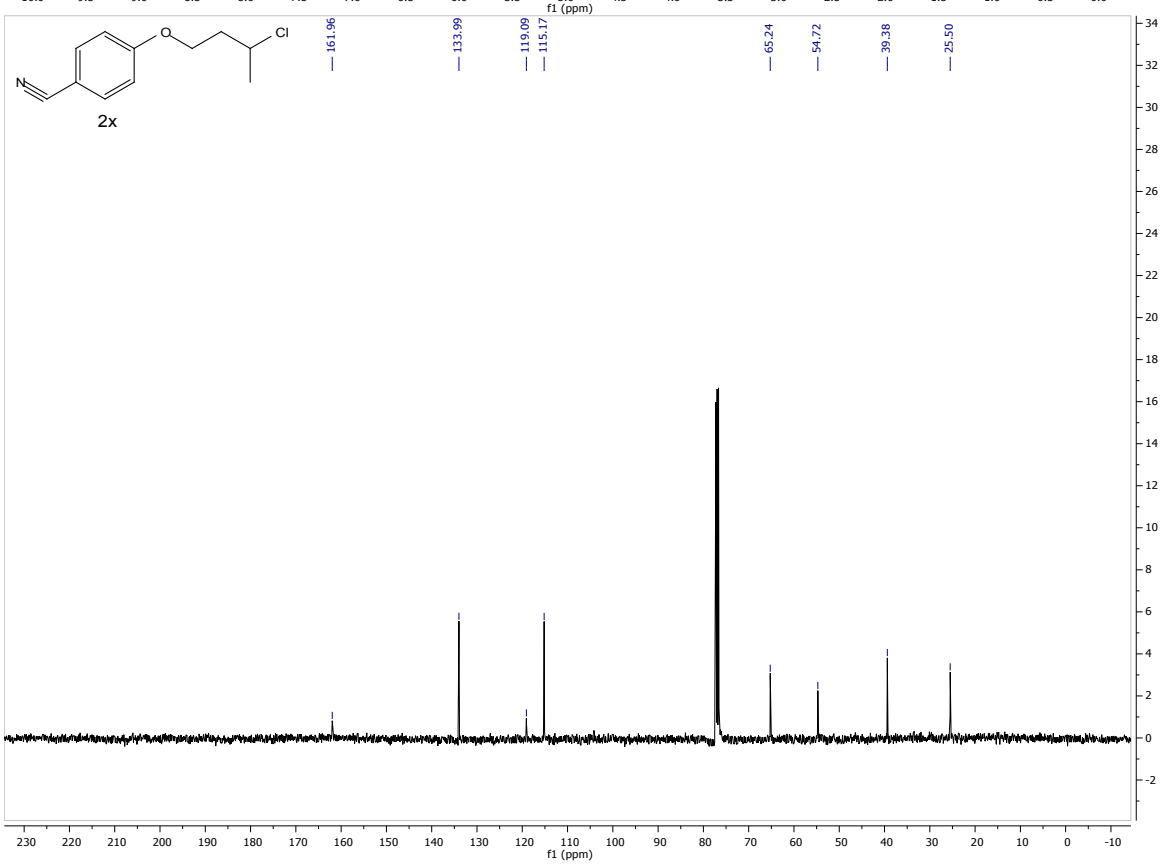

Cl
O
S
O
2u
7.92
7.90
7.69
7.67
7.65
7.60
7.58
7.56
4.13
4.11
4.10
4.09
4.09
4.08
4.07
4.06
4.05
3.38
3.37
3.36
3.35
3.34
3.33
3.32
3.31
3.25
3.24
3.23
3.22
3.21
3.20
3.19
3.18
3.17
2.27
2.26
2.25
2.23
2.22
2.21
2.20
2.18
2.07
2.06
2.04
2.03
2.02
2.01
2.00
1.98
1.97
1.52
1.50
1.87
0.96
1.86
1.00
2.14
2.24
2.96
f1 (ppm)

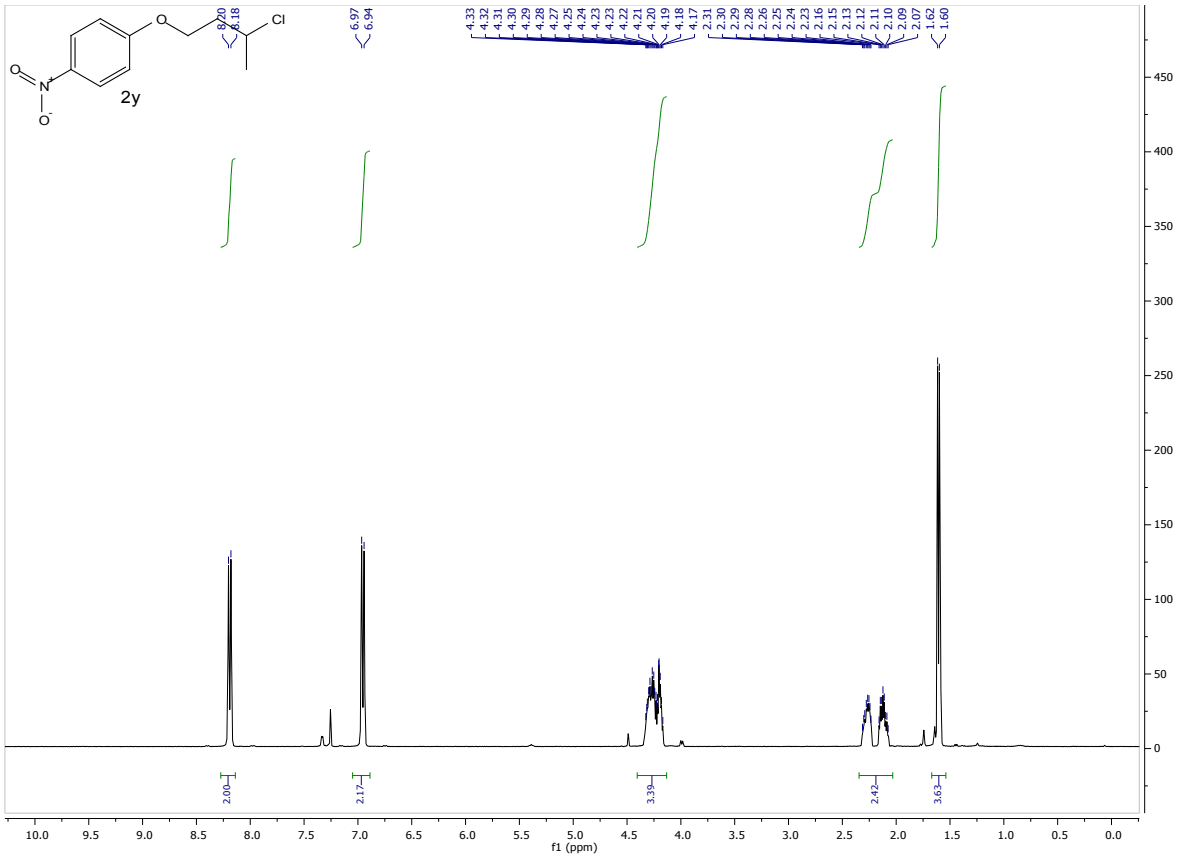

Cl
O
S
O
2u
138.99
133.87
129.39
127.95
56.18
53.66
32.88
25.18
f1 (ppm)

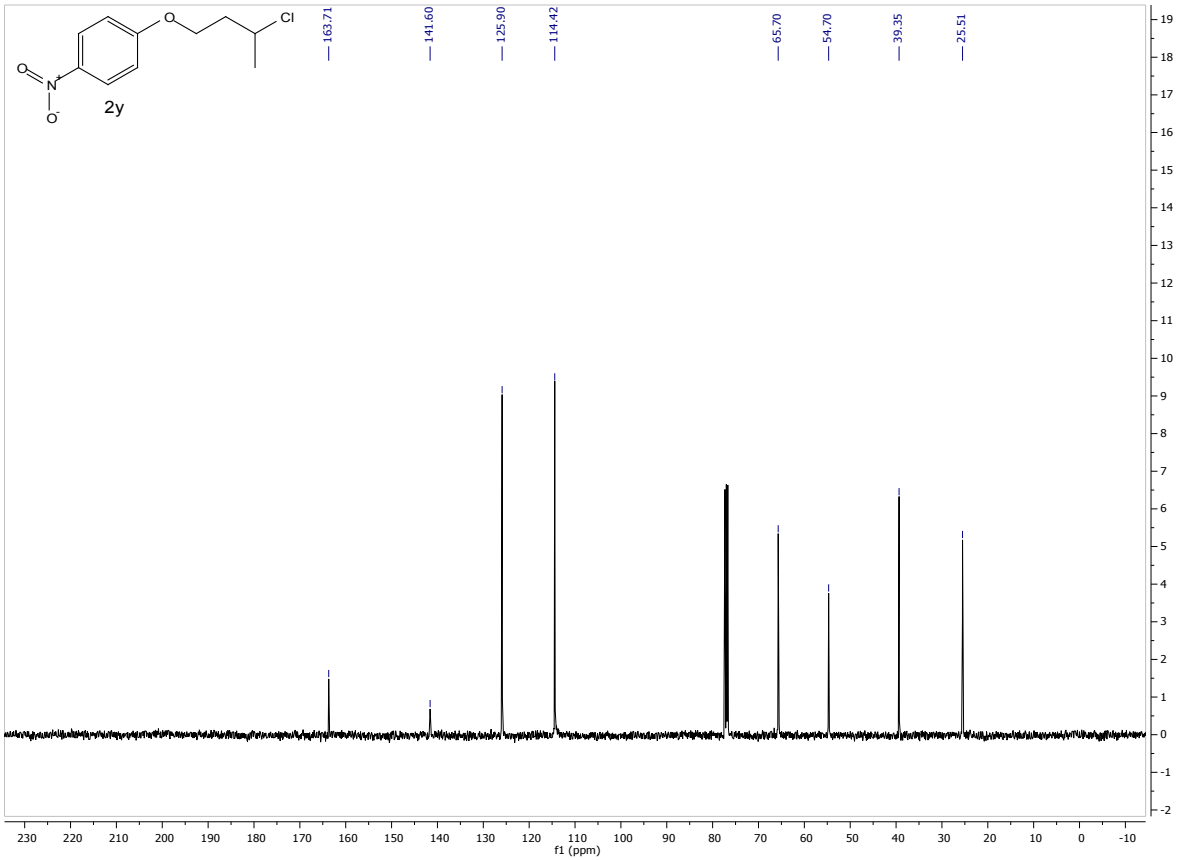

2v
7.83
7.82
7.82
7.81
7.71
7.70
7.69
7.69
4.10
4.08
4.06
4.04
4.03
4.01
3.99
3.90
3.89
3.87
3.85
3.84
3.82
3.80
3.79
3.77
2.15
2.13
2.11
2.09
2.07
2.06
2.04
2.02
2.00
1.55
1.53
1.67
1.75
1.00
2.01
2.06
2.85
f1 (ppm)

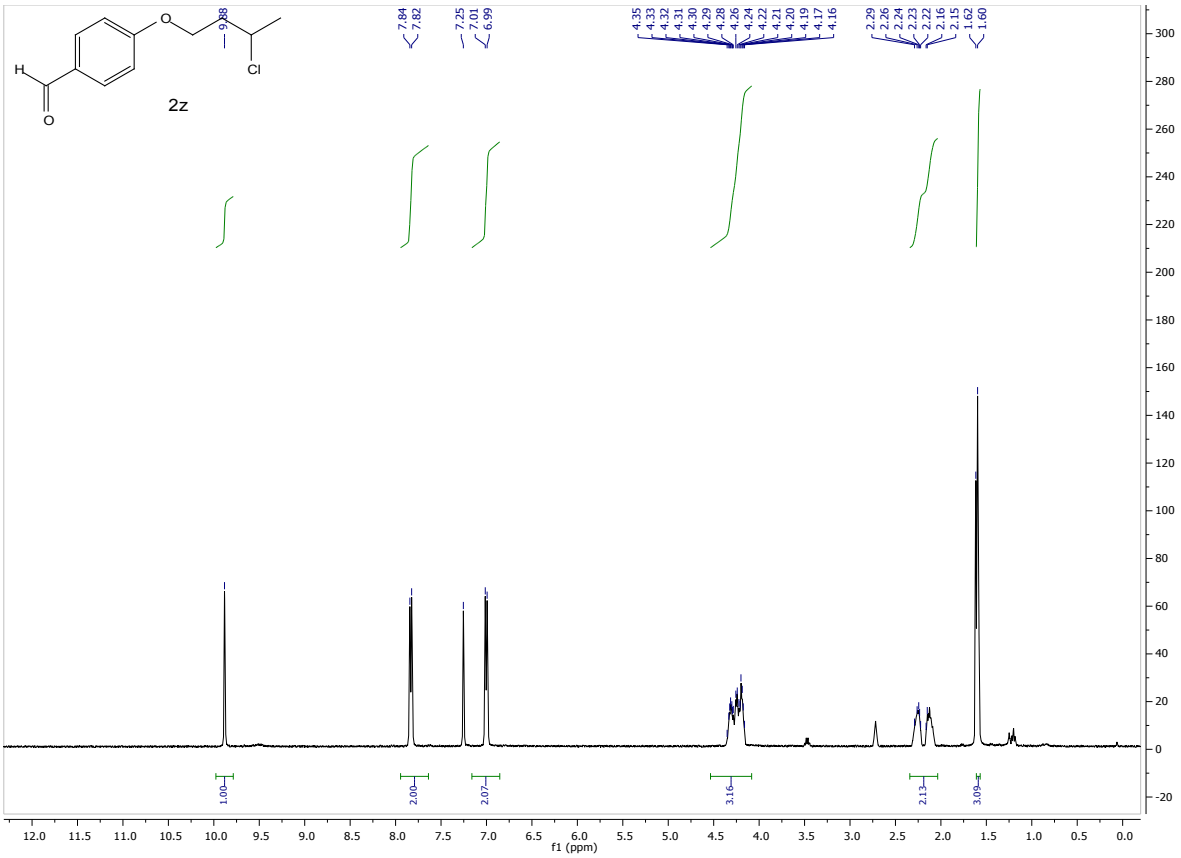

2v
168.17
133.96
132.03
123.24
55.54
38.63
35.64
25.27
f1 (ppm)

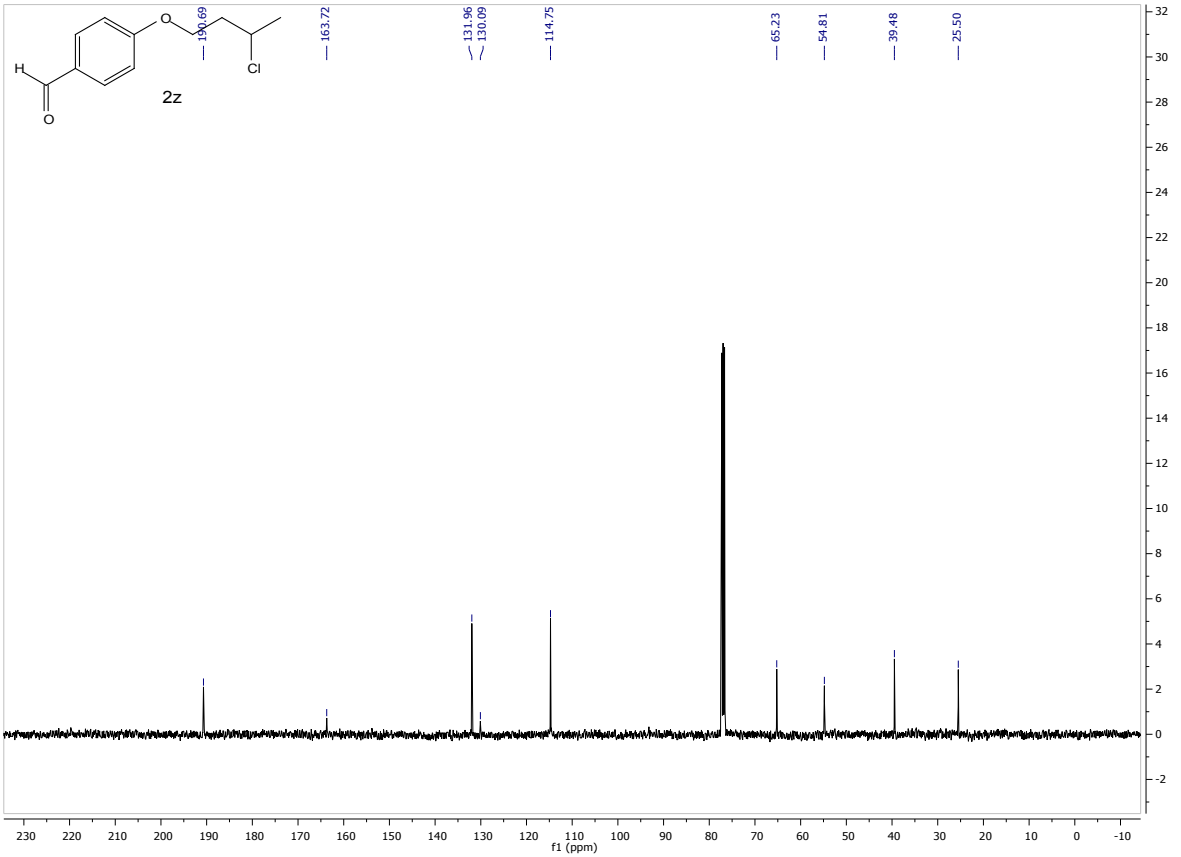

2x
7.59
7.57
7.25
6.96
6.94
4.33
4.32
4.31
4.30
4.28
4.27
4.26
4.26
4.24
4.22
4.20
4.19
4.18
4.17
4.16
4.14
4.13
4.12
2.29
2.28
2.27
2.26
2.24
2.23
2.22
2.22
2.21
2.15
2.13
2.12
2.11
2.09
2.08
2.07
2.06
1.61
1.59
1.85
2.00
3.19
2.39
3.41
f1 (ppm)

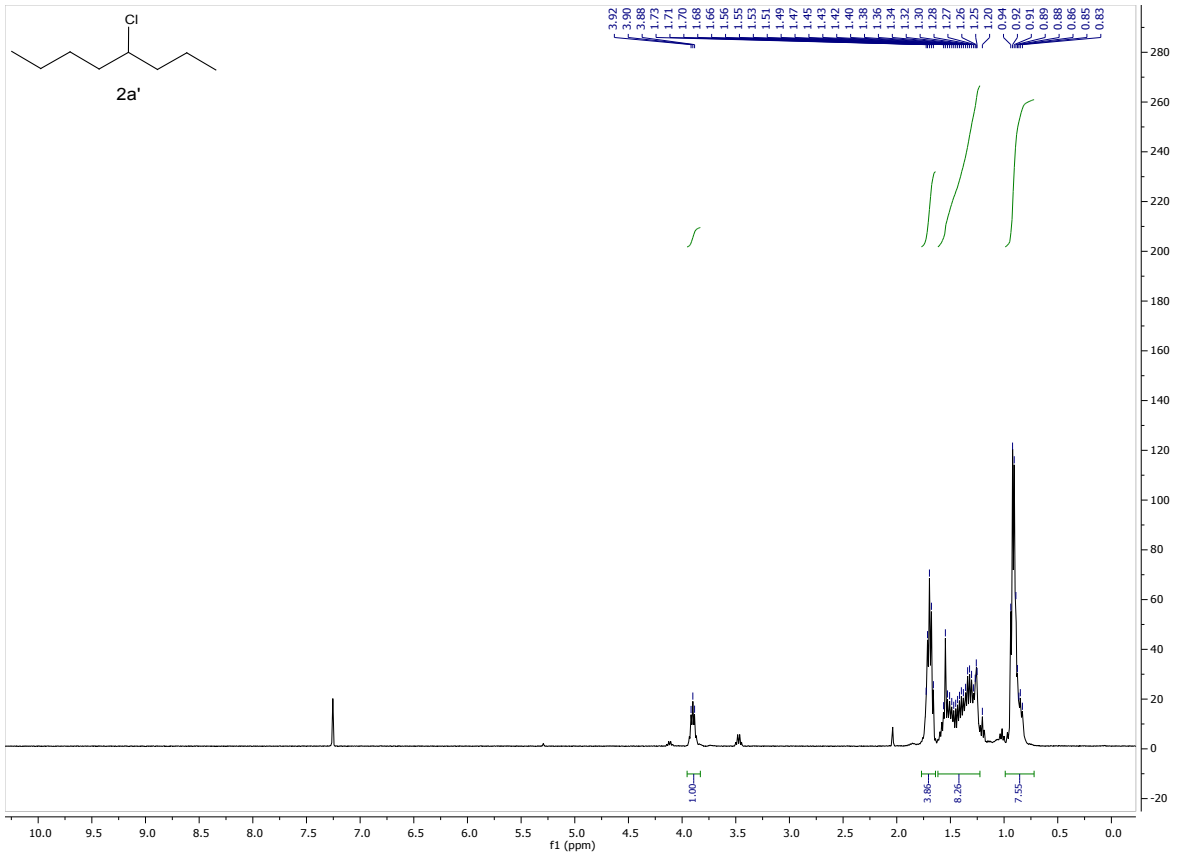

2x
161.96
133.99
119.09
115.17
65.24
54.72
39.38
25.50
f1 (ppm)

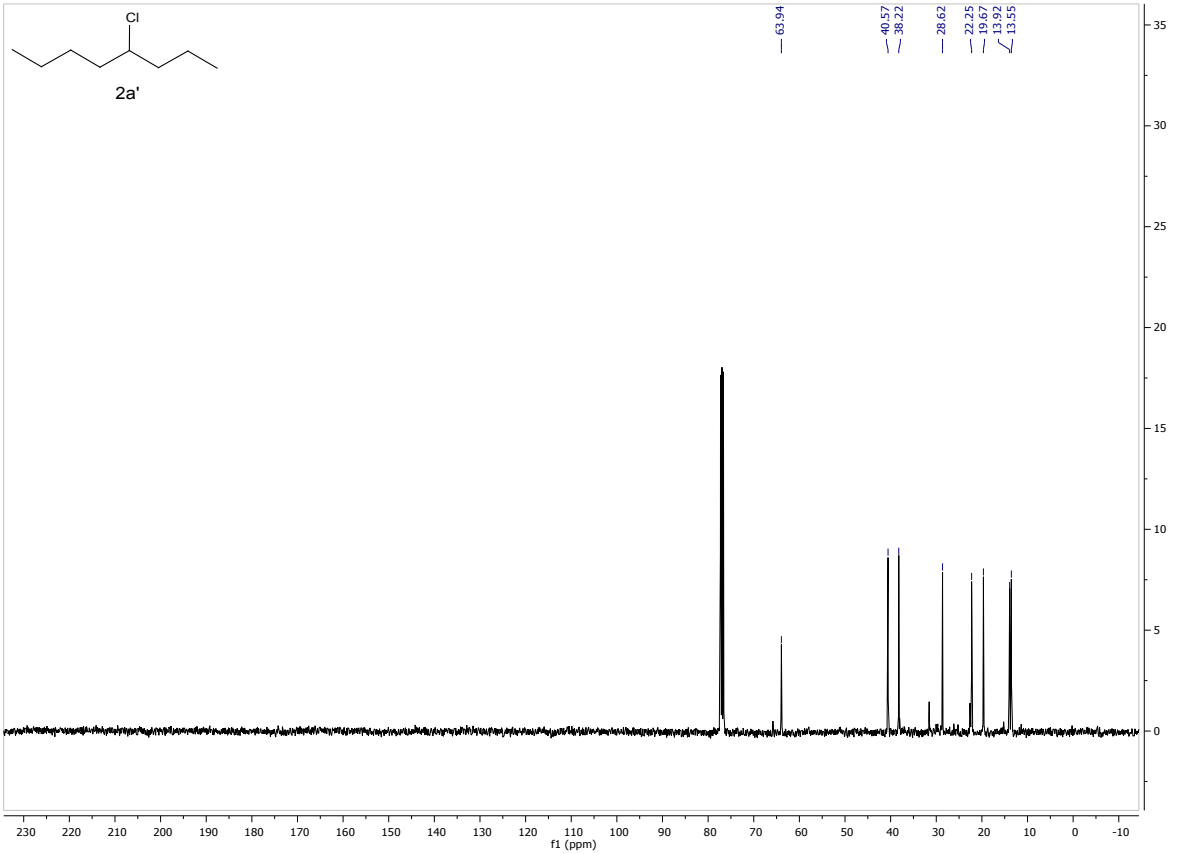

2y
8.20
8.18
6.97
6.94
4.33
4.32
4.31
4.30
4.29
4.28
4.27
4.25
4.24
4.23
4.23
4.22
4.21
4.20
4.19
4.18
4.17
2.31
2.30
2.29
2.28
2.26
2.25
2.24
2.23
2.16
2.15
2.13
2.12
2.11
2.10
2.09
2.07
1.62
1.60
2.00
2.17
3.39
2.42
3.63
f1 (ppm)

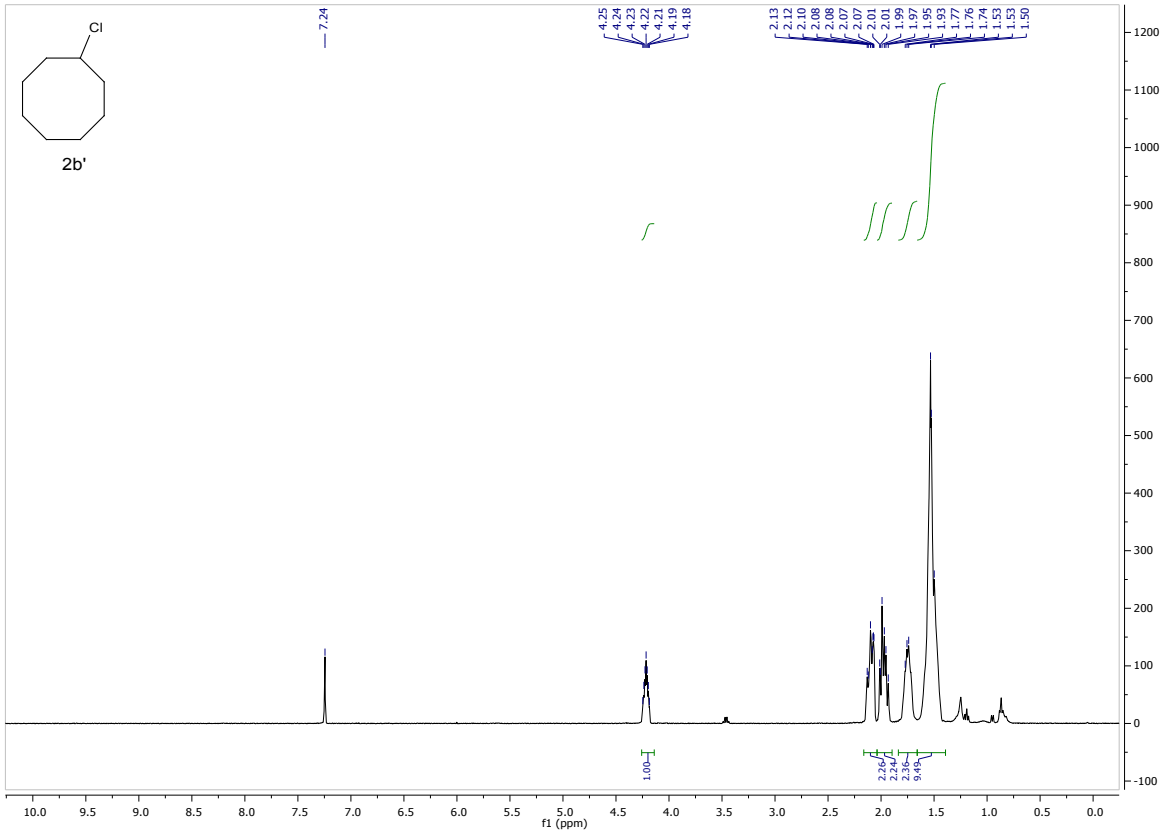

2y
163.71
141.60
125.90
114.42
65.70
54.70
39.35
25.51
f1 (ppm)

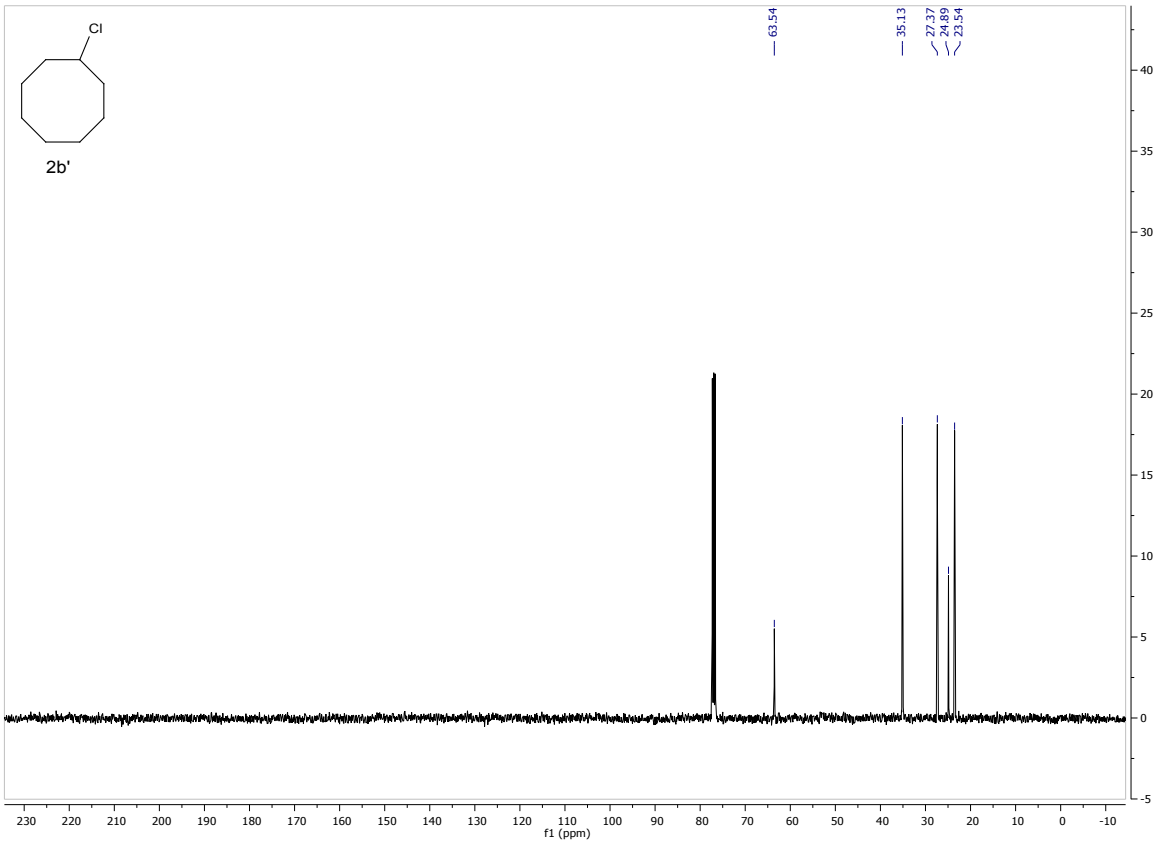

2z
9.88
7.84
7.82
7.25
7.01
6.99
4.35
4.33
4.32
4.31
4.30
4.29
4.28
4.26
4.24
4.22
4.21
4.20
4.19
4.17
4.16
2.29
2.26
2.24
2.23
2.22
2.16
2.15
1.62
1.60
1.00
2.00
2.07
3.16
2.13
3.09
f1 (ppm)

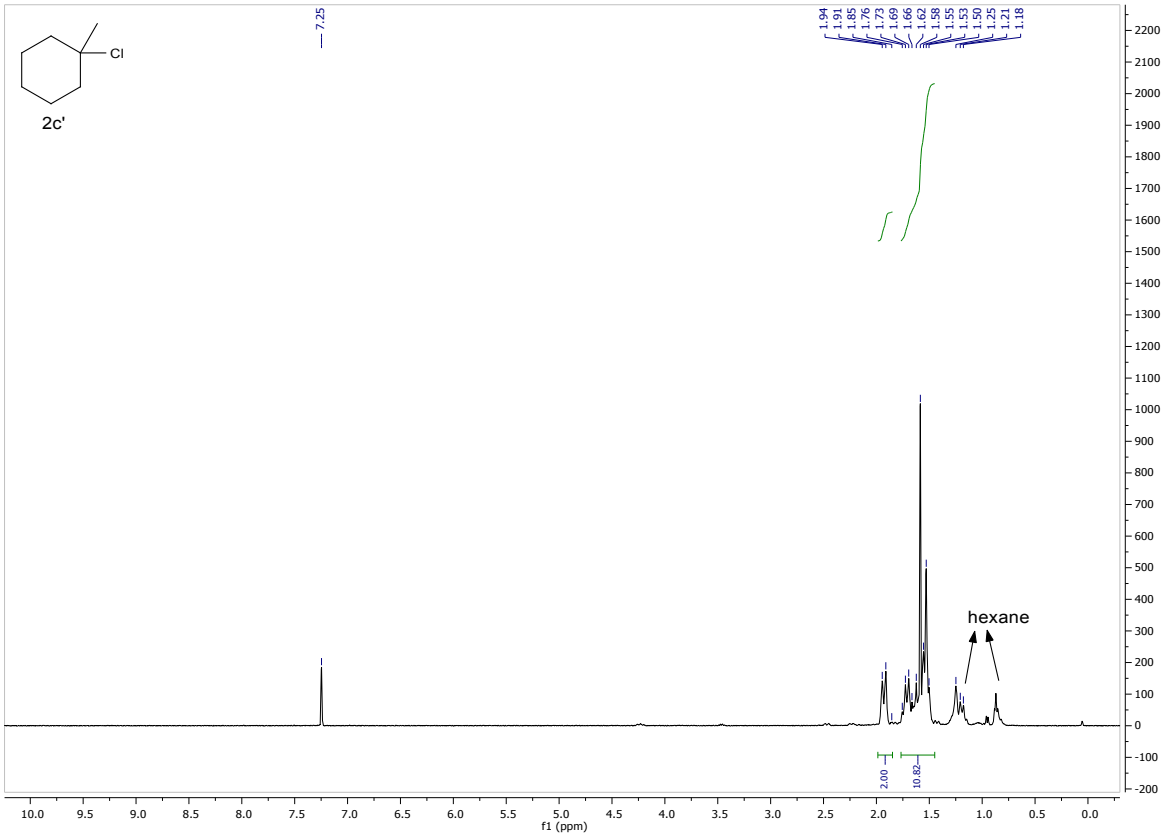

2z
190.69
163.72
131.96
130.09
114.75
65.23
54.81
39.48
25.50
f1 (ppm)

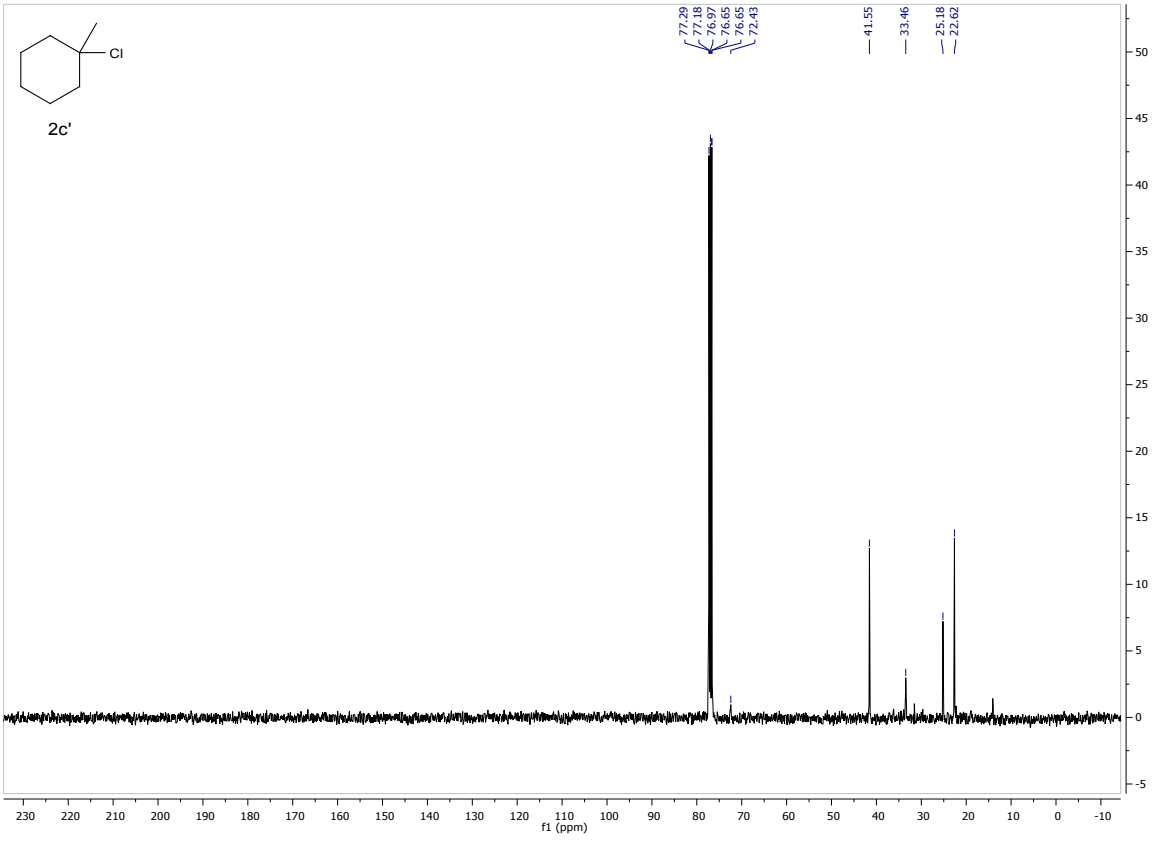

Cl
2a'
3.92
3.90
3.88
3.73
1.71
1.70
1.68
1.66
1.56
1.55
1.53
1.51
1.49
1.47
1.45
1.43
1.42
1.40
1.38
1.36
1.34
1.32
1.30
1.28
1.27
1.26
1.25
1.20
0.94
0.92
0.91
0.89
0.88
0.86
0.85
0.83
1.00
3.86
8.26
7.55
f1 (ppm)


Cl
2a'
63.94
40.57
38.22
28.62
22.25
19.67
13.92
13.55
f1 (ppm)


Cl
2b'
7.24
4.25
4.24
4.23
4.22
4.21
4.19
4.18
2.13
2.12
2.10
2.08
2.08
2.07
2.07
2.01
2.01
1.99
1.97
1.95
1.93
1.77
1.76
1.74
1.53
1.53
1.50
1.00
2.26
2.24
2.16
9.48
f1 (ppm)


Cl
2b'
63.54
35.13
27.37
24.89
23.54
f1 (ppm)


Cl
2c'
7.25
1.94
1.91
1.85
1.76
1.73
1.69
1.66
1.62
1.58
1.55
1.53
1.50
1.25
1.21
1.18
hexane
2.00
10.82
f1 (ppm)


Cl
2c'
77.29
77.18
76.97
76.65
76.65
72.43
41.55
33.46
25.18
22.62
f1 (ppm)

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