Supporting Information

Two-step Conversion of Carboxylic Esters into Distally Fluorinated Ketones via Ring Cleavage of Cyclopropanol Intermediates: Application of Sulfinate Salts as Fluoroalkylating Reagents

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I. Preparation of cyclopropanols

General procedure for cyclopropanation of carboxylic esters. Preparation of cyclopropanols 1a-c, 1g, 1i.[1] To a stirred solution of ester (25 mmol) and titanium(IV) isopropoxide (0.74 mL, 2.5 mmol, 10 mol%) in diethyl ether (50 mL) was added slowly over 2–3 h at room temperature a solution of EtMgBr (60 mmol) in diethyl ether (60 mL). The reaction mixture was stirred for additional 30 min and then cooled with an ice bath. The reaction mixture was hydrolyzed by slow addition of cold 10% H_2SO_4 solution (50 mL) and then extracted with ether (3 × 40 mL). The combined organic layers were washed with saturated $NaHCO_3$ solution, brine and dried ($MgSO_4$). After evaporation of solvent under reduced pressure the cyclopropanol products can be purified using distillation or column chromatography on silica gel. However, in most cases they are pure enough to be used directly in the next step. The following cyclopropanol product were synthesized using the procedure described above:

1-Benzylcyclopropanol (1a), starting from isopropyl phenylacetate.[2] Yield 88%. Purified using short-column silica gel chromatography. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.37−7.22 (m, 5H), 2.89 (s, 2H), 1.93 (s, 1H), 0.82 (m, 2H), 0.64 (m, 2H). ^{13}C NMR (100.6 MHz, $CDCl_3$): δ = 138.73, 129.57, 128.68, 126.79, 56.30, 44.26, 13.41.

1-Amylcyclopropanol (1b), starting from methyl hexanoate.[1] Yield 95%. Used as obtained without any purification. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.82 (br s, 1H), 1.57−1.46 (m, 4H), 1.36−1.27 (m, 4H), 0.90 (m, 3H), 0.72 (m. 2H), 0.43 (m, 2H). ^{13}C NMR (100.6 MHz, $CDCl_3$): δ = 56.02, 38.41, 32.02, 25.74, 22.86, 14.20, 13.64.

1-(3-Chloropropyl)cyclopropanol (1c), starting from ethyl 4-chlorobutanoate.[3] Yield 86%. Purified using short-column silica gel chromatography. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.64 (t, J = 6.5 Hz, 2H), 2.04 (m, 2H), 1.80 (br s, 1H), 1.70 (m, 2H), 0.77 (m, 2H), 0.49 (m, 2H). ^{13}C NMR (100.6 MHz, $CDCl_3$): δ = 55.25, 45.22, 35.63, 29.34, 13.82.

1-(2-Phenylethyl)cyclopropanol (1g), starting from ethyl 2-phenylpropanoate.[4] Yield 97%. Purified using short-column silica gel chromatography. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.32−7.16 (m, 5H), 2.86 (m, 2H), 1.88 (m, 2H), 1.80 (s, 1H), 0.76 (m, 2H), 0.46 (m, 2H). ^{13}C NMR (100.6 MHz, $CDCl_3$): δ = 142.33, 128.57, 128.55, 125.99, 55.96, 40.57, 32.65, 13.85.

1-(9-Decenyl)cyclopropanol (1j), starting from methyl 10-undecenoate. Yield 84%. Purified using short-column silica gel chromatography. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 5.81 (ddt, *J* = 17.0, 10.2, 6.7 Hz, 1H), 4.99 (ddt, *J* = 17.0, 2.2, 1.7 Hz, 1H), 4.93 (ddt, *J* = 10.2, 2.2, 1.2 Hz, 1H), 2.04 (m, 2H), 1.75 (s, 1H), 1.58−1.44 (m, 4H), 1.43–1.23 (m, 10H), 0.73 (m, 2H), 0.44 (m, 2H). ^{13}C NMR (100.6 MHz, $CDCl_3$): δ = 139.38, 114.26, 56.05, 38.44, 33.96, 29.81, 29.78, 29.59, 29.28, 29.08, 26.06, 13.67.

Preparation of cyclopropanols 1h, 1d, 1f, 1e. To a stirred solution of ester (10 mmol) and titanium(IV) isopropoxide (0.75 mL, 2.5 mmol, 25 mol%) in THF (60 mL) was added slowly over 3–4 h at room temperature a solution of EtMgBr (25 mmol) in THF (25 mL). The reaction mixture was stirred overnight and then hydrolyzed with water (1–2 mL) and filtered to afford compound **1h** after evaporation of the solvent. For compounds **1d-e**, solvent (THF) was evaporated under reduced pressure prior the hydrolysis. The reaction mixture was diluted with CH_2Cl_2 (50 mL), cooled with ice bath, hydrolyzed with water (1–2 mL) and filtered through layer of silica. The filter cake was thoroughly washed with CH_2Cl_2 or ethyl acetate (5 × 40 mL). After evaporation of solvent under reduced pressure the cyclopropanol products were purified by column chromatography on silica gel, recrystallization or used directly in the next step without any purification.

1-(*tert*-Butyldiphenylsiloxymethyl)cyclopropanol (1h), starting from ethyl *tert*-butyldiphenylsiloxyacetate.[5] Yield 97%. Used as obtained without any purification. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.73–7.65 (m, 4H), 7.48–7.36 (m, 6H), 3.69 (s, 2H), 2.69 (s, 1H), 1.08 (s, 9H), 0.79 (m, 2H), 0.44 (m, 2H). ^{13}C NMR (100.6 MHz, $CDCl_3$): δ = 135.74, 133.53, 129.92, 127.89, 69.49, 56.62, 27.04, 19.47, 11.53.

1-(Tetrahydro-2H-pyran-4-yl)cyclopropanol (1d), starting from the corresponding ethyl ester. Yield 83%. Purified using short-column silica gel chromatography. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 4.02 (dt, *J* = 11.0, 3.2 Hz, 2H), 3.45–3.27 (m, 2H), 2.12 (s, 1H), 1.67– 1.52 (m, 4H), 1.33–1.21 (m, 1H), 0.71 (m, 2H), 0.47 (m, 2H). ^{13}C NMR (100.6 MHz, $CDCl_3$): δ = 68.16, 58.66, 42.22, 28.84, 12.35.

***tert*-Butyl 4-(1-hydroxycyclopropyl)piperidine-1-carboxylate (1f)**, starting from the corresponding ethyl ester. Yield 68%. Purified by recrystallization from cyclohexane (mp 118 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 4.19 (br s, 2H), 2.63 (br t, *J* = 12.9 Hz, 2H), 1.81 (br s,

1H), 1.71–1.63 (m, 2H), 1.55–1.35 (m, 2H), 1.46 (s, 9H), 1.12 (tt, J = 12.1, 3.5 Hz, 1H), 0.73 (m, 2H), 0.48 (m, 2H). ^{13}C NMR (100.6 MHz, $CDCl_3$): δ = 154.97, 79.50, 58.74, 44.00, 43.50, 28.62, 28.09, 12.77.

1-(2,2-Diethoxyethyl)cyclopropanol (1e).[6] Yield 90%. Used as obtained without any purification. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 4.80 (t, J = 5.8 Hz, 1H), 3.79–3.67 (m, 2H), 3.62–3.52 (m, 3H), 1.89 (d, J = 5.8 Hz, 2H), 1.23 (t, J = 7.1 Hz, 6H), 0.76 (m, 2H), 0.45 (m, 2H).

Preparation of 1-(3-methoxyphenyl)cyclopropanol (1i).[7] A 1.5 M solution of MeMgBr in diethyl ether (20 mL, 30 mmol) was added within 5 min to a solution of titanium isopropoxide (5.68 g, 20 mmol) in Et_2O. The resulting yellow solution was cooled to 0 °C and methyl 3-methoxybenzoate (20 mmol, 3.32 g, in 10 mL of Et_2O) was then added. EtMgBr (30 mL of a 1 M solution in Et_2O, 30 mmol) was added over 30–40 min. The resulting reaction mixture was allowed to warm to room temperature, then stirred for an additional hour, quenched at 0 °C by careful addition of cold 10% H_2SO_4 solution (80 mL), and was extracted with Et_2O (3 × 20 mL). The combined organic layers were washed with saturated $NaHCO_3$ solution, brine and dried ($MgSO_4$). After evaporation of solvent under reduced pressure the cyclopropanol product was isolated by column chromatography on silica gel (petroleum ether/EtOAc). Yield 45% (1.5 g). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.24 (t, J = 8.0 Hz, 1H), 6.91 (dd, J = 2.6, 1.8 Hz, 1H), 6.83 (ddd, J = 8.0, 1.8, 0.9 Hz, 1H), 6.76 (ddd, J = 8.0, 2.6, 0.9 Hz, 1H), 3.81 (s, 3H), 2.39 (br s, 1H), 1.26 (m, 2H), 1.04 (m, 2H). ^{13}C NMR (100.6 MHz, $CDCl_3$): δ = 159.85, 146.27, 129.52, 116.64, 111.82, 110.62, 56.71, 55.37, 18.19.

References:

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2. M. Limbach, S. Dalai, A. de Meijere. *Adv. Synth. Catal*. **2004**, *346*, 760.
3. O. Kulinkovich, N. Masalov, V. Tyvorskii, N. De Kimpe, M. Keppens. *Tetrahedron Lett*. **1996**, *37*, 1095.
4. D. Rosa, A. Orellana, *Chem. Comm*. **2013**, *49*, 5420.
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6. M. V. Raiman, A. V. Pukin, V. I. Tyvorski, N. De Kimpe, O. G. Kulinkovich, *Tetrahedron*, **2003**, *59*, 5265.
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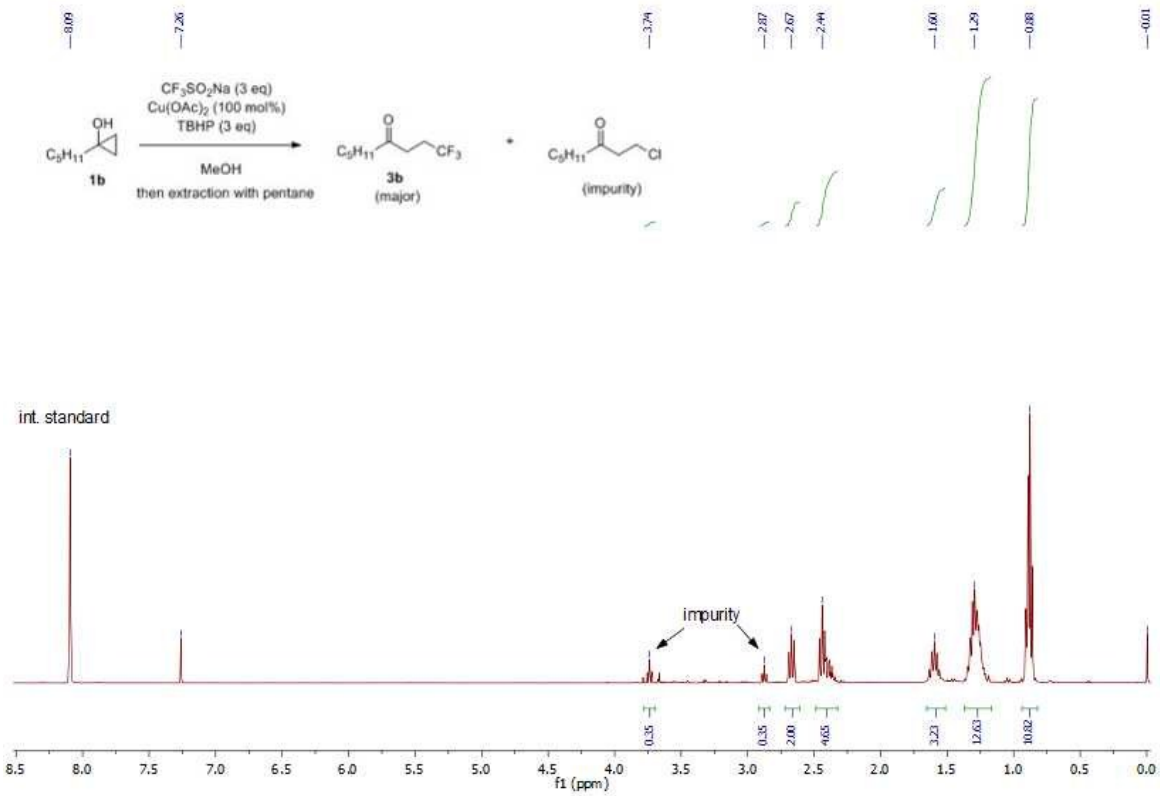
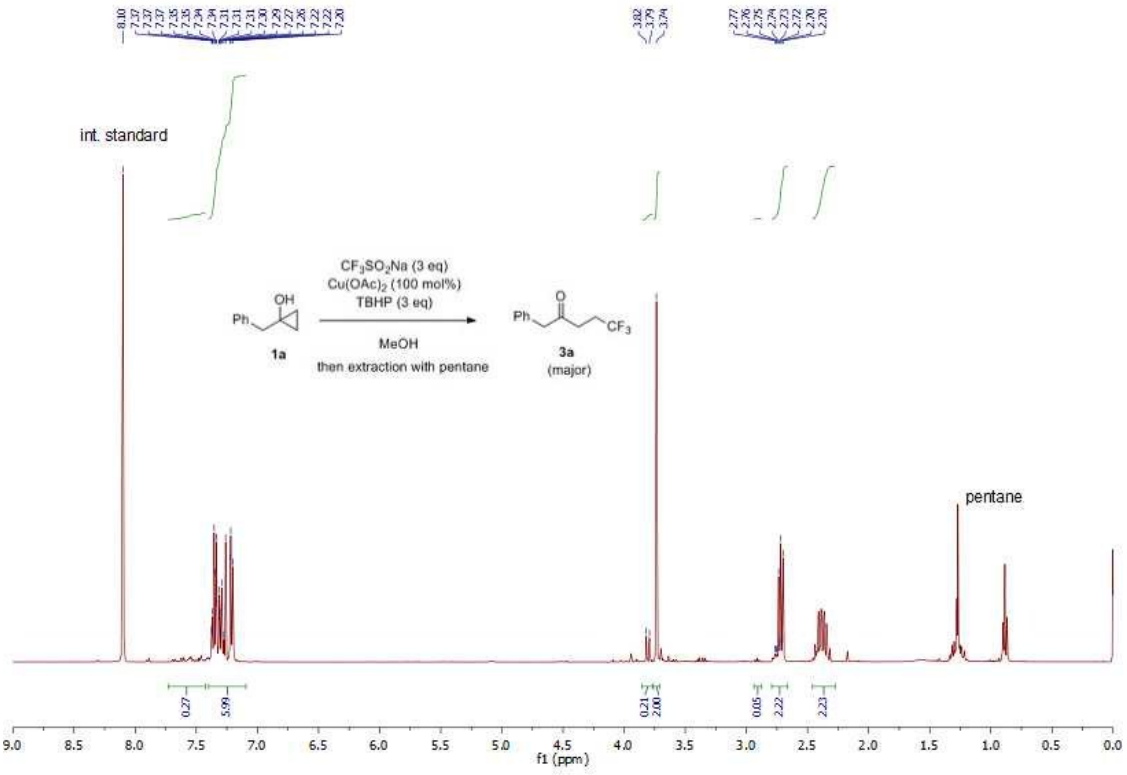
II. Selected NMR spectra of the reaction mixtures

Produced from 1-amylcyclopropanol (**1b**) after extraction with pentane:

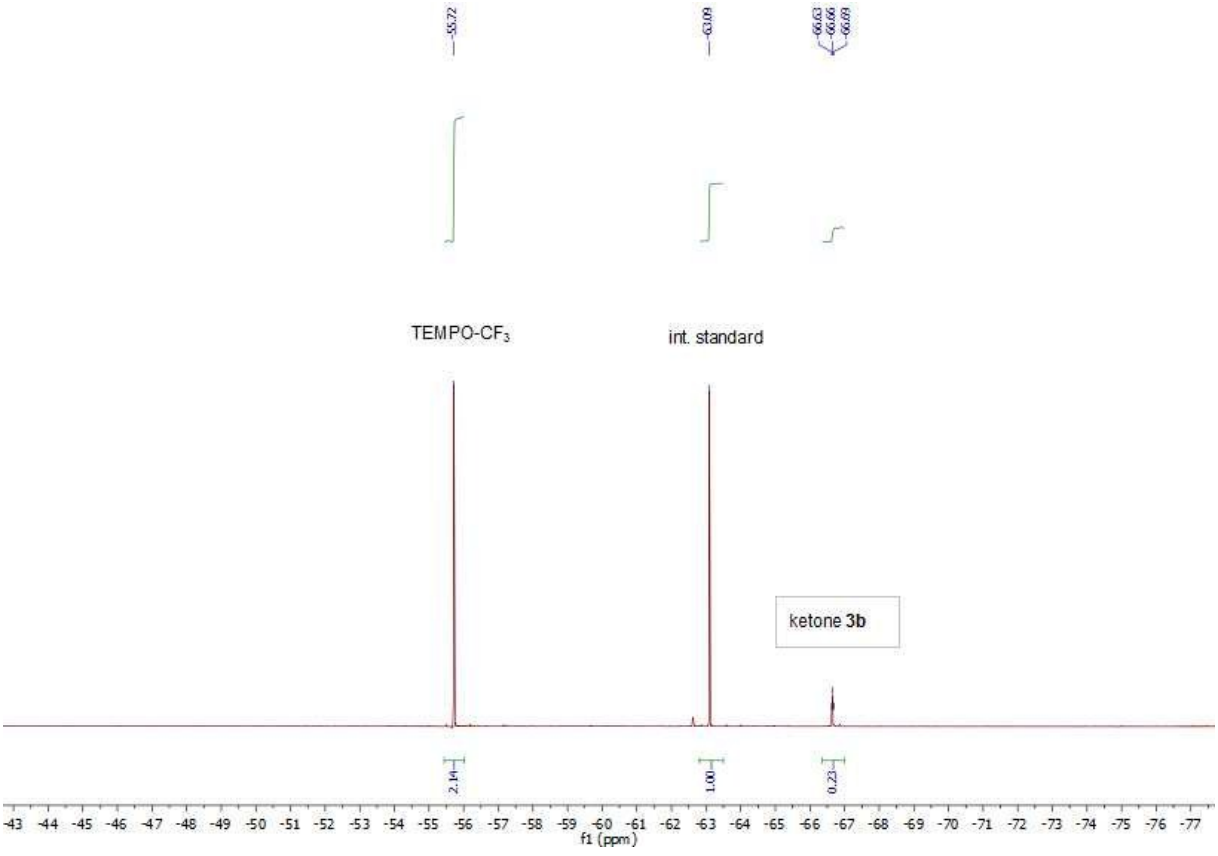


Produced from 1-benzylcyclopropanol (**1a**) after extraction with pentane:

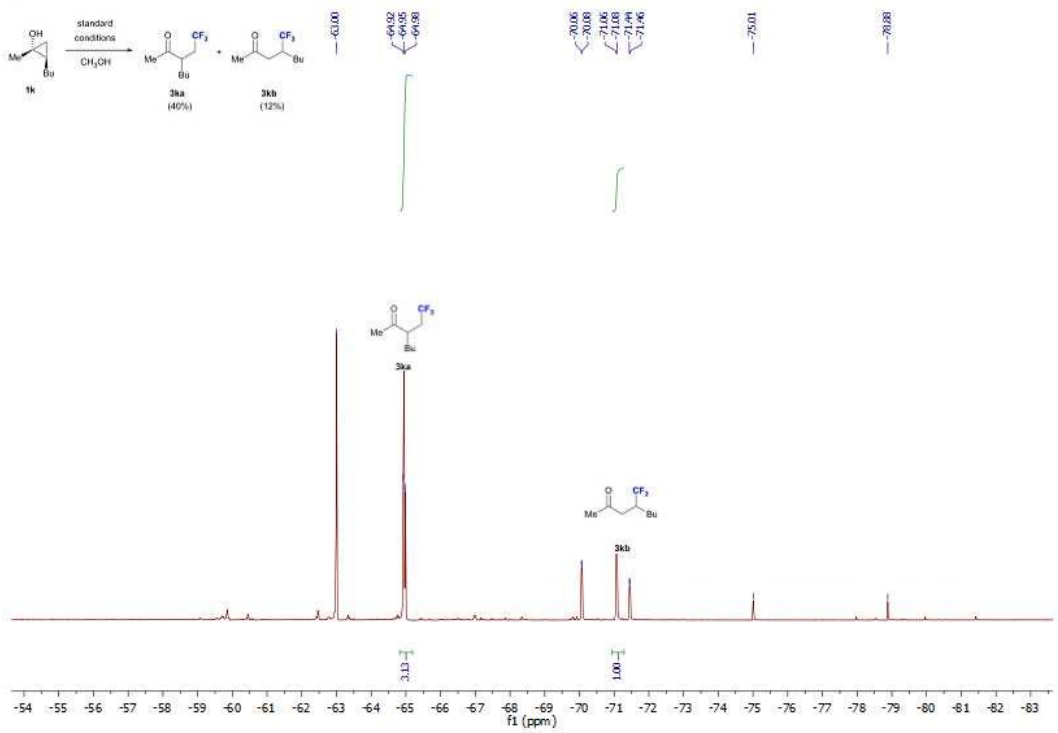


III. Mechanism proving experiments

TEMPO inhibition experiment. A 5 mL vial was charged with $Cu(OAc)_2 \cdot H_2O$ (40 mg, 0.2 mmol, 100 mol%), TEMPO (94 mg, 0.6 mmol) and CF_3SO_2Na (94 mg, 0.6 mmol). Then a solution of cyclopropanol **1b** (0.2 mmol) and internal standard (1,3-bis(trifluoromethyl)-5-bromobenzene) in CD_3OD (1 mL) was added. After that, *tert*-butyl hydroperoxide solution (70% in water, 0.08 mL, 0.6 mmol) was added dropwise via syringe (without a metal needle). The reaction mixture was then filtered through a thin layer of $MgSO_4$ atop of short layer of SiO_2 into a NMR tube and examined by ^{19}F NMR. The internal standard was employed to calculate yields of TEMPO-CF_3 adduct and β-trifluoromethyl ketone **3b**. After 24h, the solution was diluted with 1 mL of D_2O, extracted with $CDCl_3$ and passed through a thin layer of $MgSO_4$ again to remove traces of paramagnetic Cu^{II} species. ^{19}F NMR spectrum was measured again to refine the initial data.

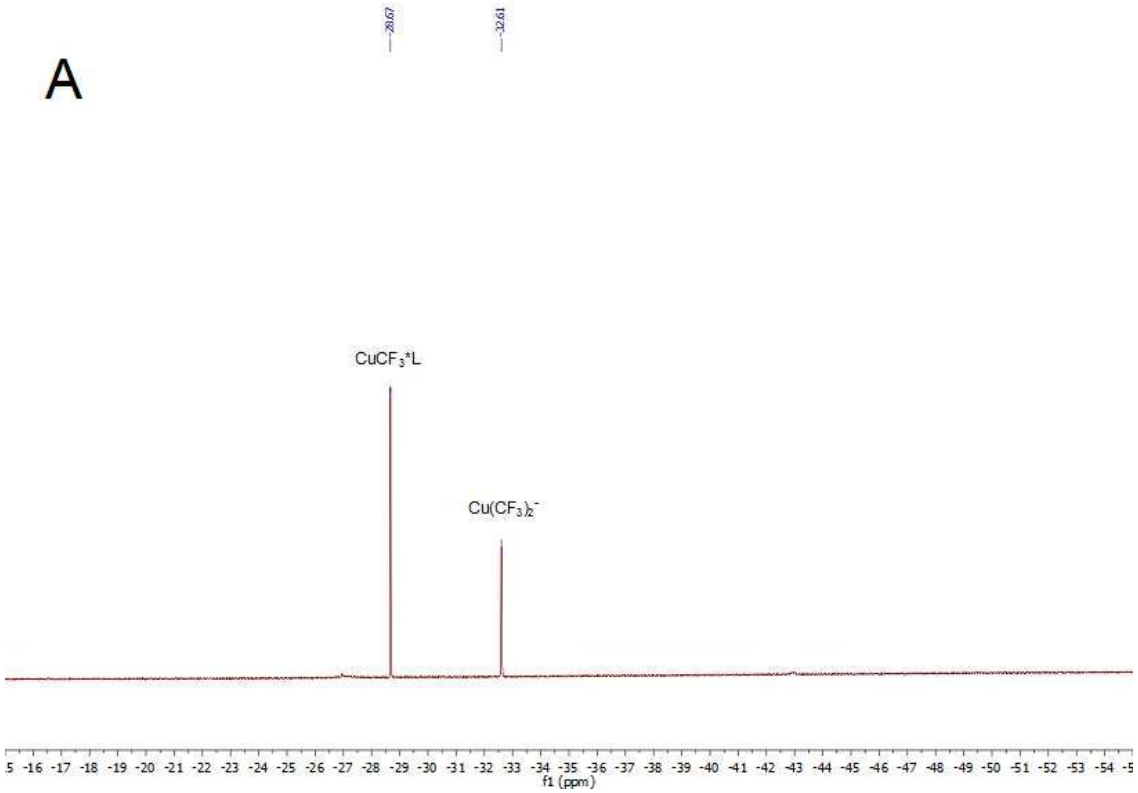


^{19}F NMR spectrum of reaction mixture produced from 2-butyl-1-methylcyclopropanol:

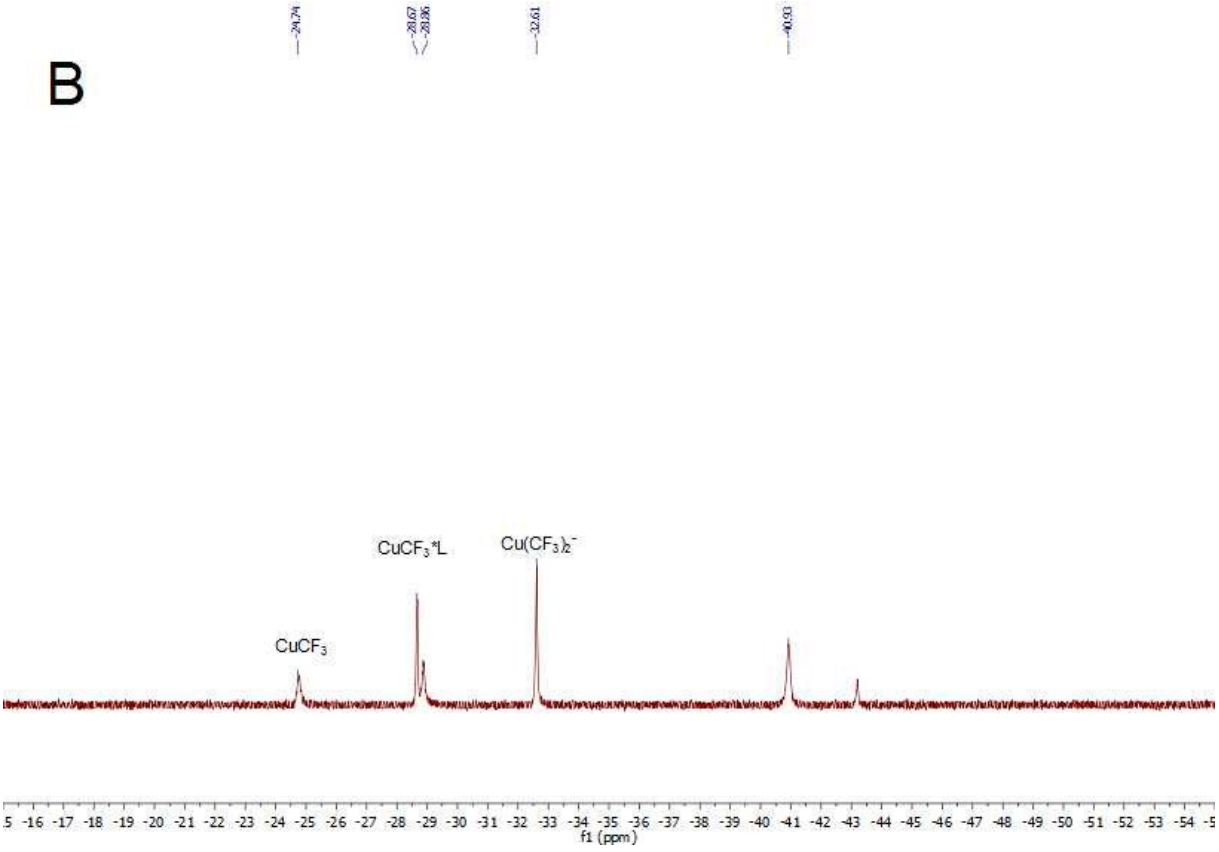


Direct monitoring of reaction in NMR tube. Detection of $CuCF_3$ species.

^{19}F NMR spectra were acquired in DMF-d_7 after addition of 1 equiv. of TBHP (spectrum A), 3 equiv. of TBHP (spectrum B), and after 48 h (spectrum C).



B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-40.93
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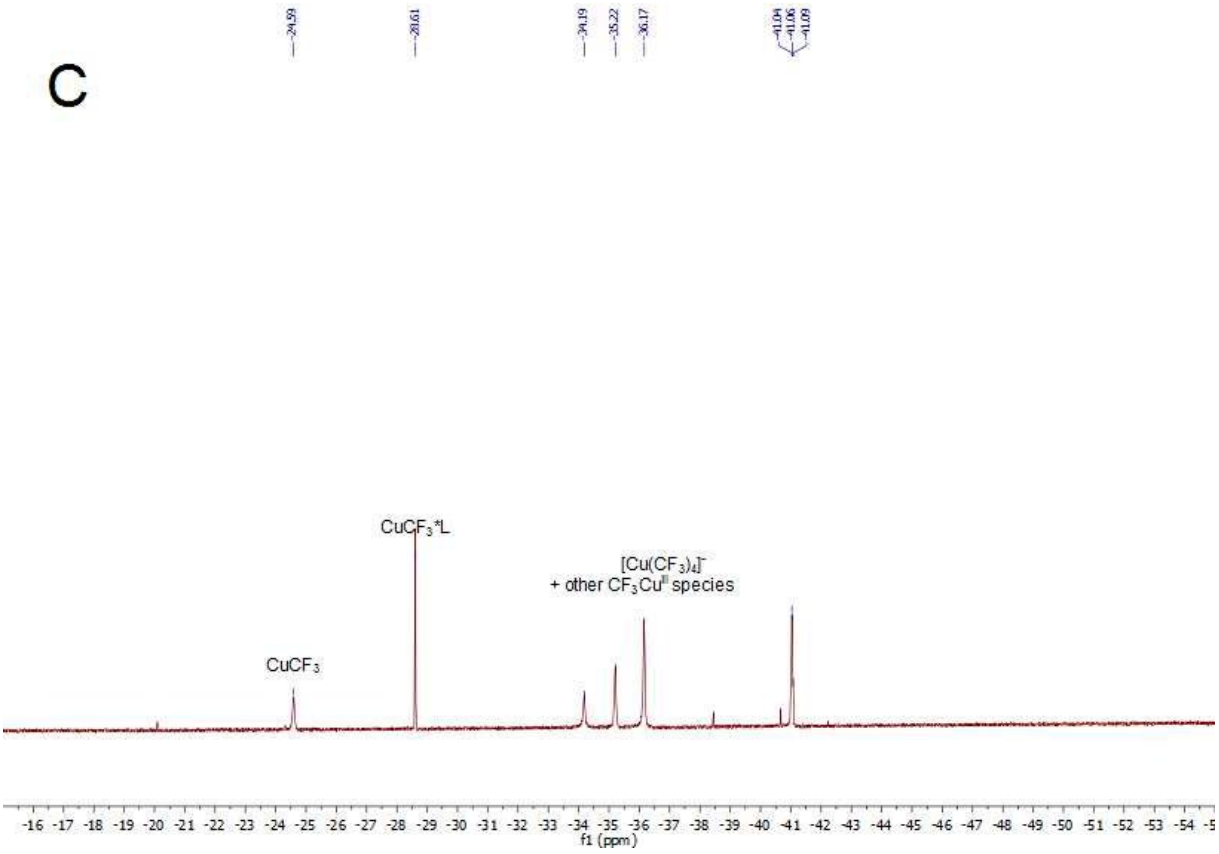
Cu(CF3)2-
CuCF3
f1 (ppm)

C


-24.59
-28.61
-29.19
-35.22
-36.17
-41.04
-41.06
-41.09
CuCF3*L
[Cu(CF3)4]-
+ other CF3CuIII species
CuCF3
f1 (ppm)

IV. X-Ray data for compound 6

Single crystal X-ray diffraction analysis

Crystal data for **6:**

$C_{18}H_{17}BrF_2O$, M_r =367.22g/mol, orthorhombic, *Pnma* (no. 62), a = 34.5876(4) Å, b = 9.19962(10) Å, c = 4.92247(5) Å, V = 1566.29(3) Å^3, Z = 4, T = 123.0 K, μ(Cu-$K\alpha$) = 3.762 mm^{-1}, ρ_{calc} = 1.557 g/cm^3, 13397 reflections measured (5.11° ≤ 2Θ ≤ 134.43°) of which 1462 unique (R_{int} = 0.0195, R_{sigma} = 0.0074), final R_1 [F^2>2σ(F^2)] = 0.0235, wR_2 = 0.0627. The crystallographic data is deposited with the Cambridge Crystallographic Data Centre (CCDC 1536256) and can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif.

Single crystals of **6** were obtained as large colourless blocks, by slow evaporation of a solution of **6** in Et_2O and pentane. Single crystal X-ray diffraction data was collected at 123.0K on a Rigaku Compact HomeLab diffractometer, equipped with a Saturn 944 HG CCD detector and Oxford Cryostream cooling system using monochromatic Cu-$K\alpha$ radiation (1.54178Å) from a MicroMax™-003 sealed tube microfocus X-ray source. The strategy for data collection was calculated using *Rigaku CollectionStrategy* [1]. Data was collected using ω-scans. *CrysAlisPro* [2] was used for data reduction and empirical absorption correction using spherical harmonics implemented in *SCALE3 ABSPACK* scaling algorithm [3]. The structure was solved using *SHELXT* [4] and refined by full-matrix least-squares method against F^2 with *SHELXL-2014* [4] through *OLEX2* [5] program package. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. Hydrogen atoms were treated as riding on parent atoms, using isotropic displacement parameters U_{iso}(H) = 1.2U_{iso}(C) for CH and CH_2. The asymmetric unit contains only half of the molecule, which is situated on a mirror plane (perpendicular to [0, 1, 0]). A part of the molecule was found to be disordered around the mirror plane and was modelled in one position with 50% occupancy, with the other disorder component generated by the symmetry element (Figure S1). Restraints were applied to the geometry of the disordered phenyl ring (FLAT, SADI) and to the sp^2 carbon C9 with the atoms bound to it (FLAT). Anisotropic atomic displacement parameters were also restrained (RIGU). The figure was drawn using the program Mercury CSD 3.9 [6] and POV-Ray 3.7 [7].

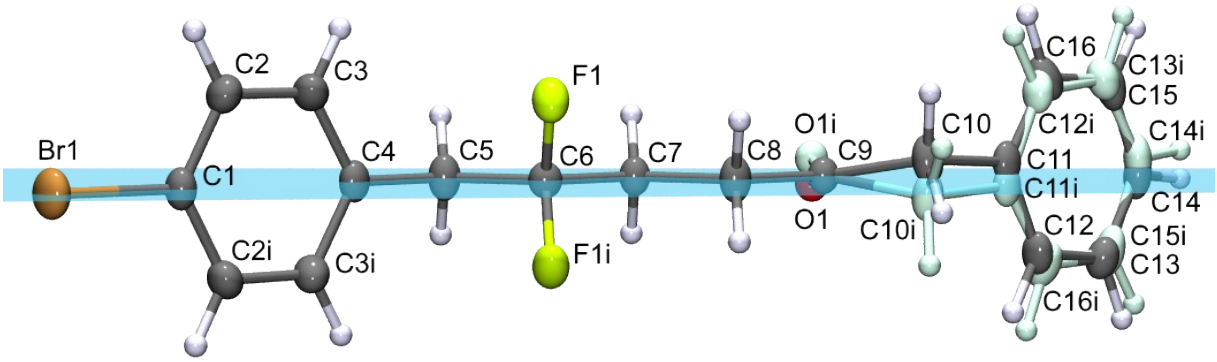


Figure S1. The molecule of **6** in the crystal structure, showing the mirror plane (perpendicular to [0, 1, 0]) in light blue. The symmetry-generated disorder component is drawn in light aquamarine, symmetry code: i) x, ½ − y, z. The atomic displacement ellipsoids are drawn at 50% probability level.

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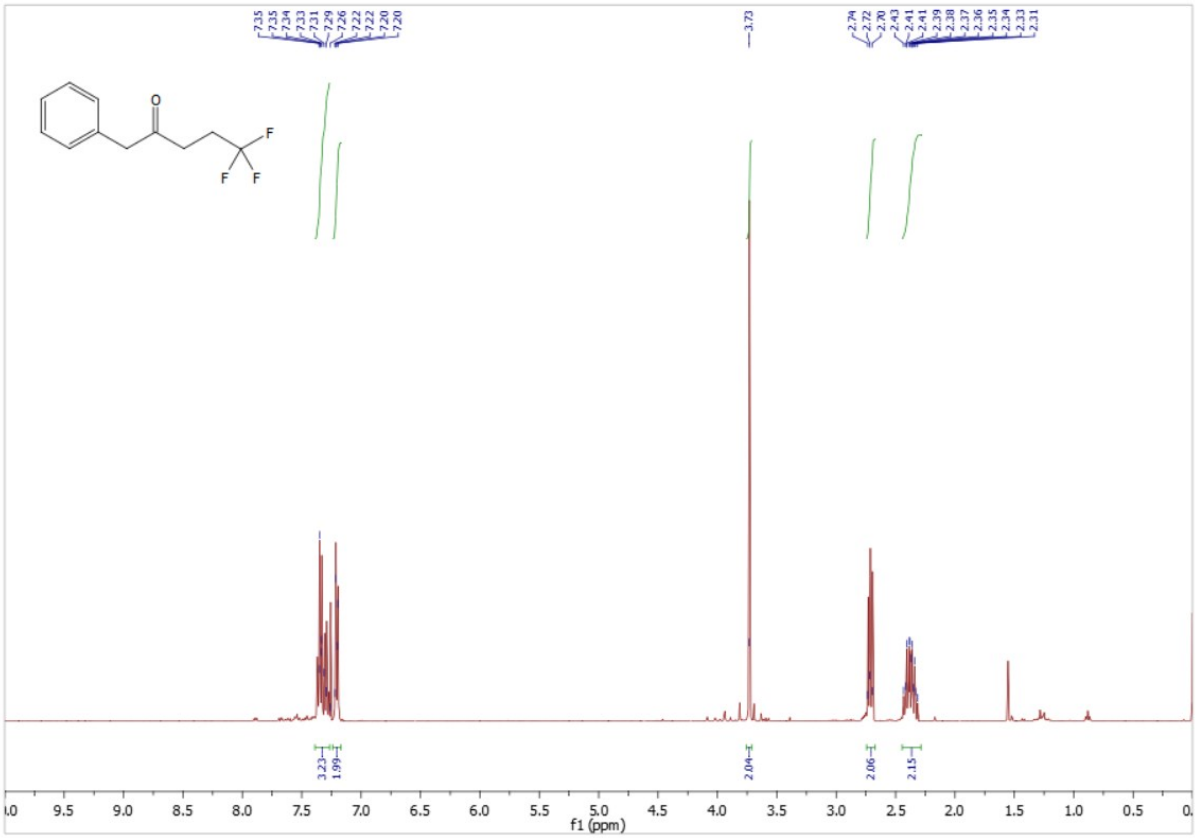
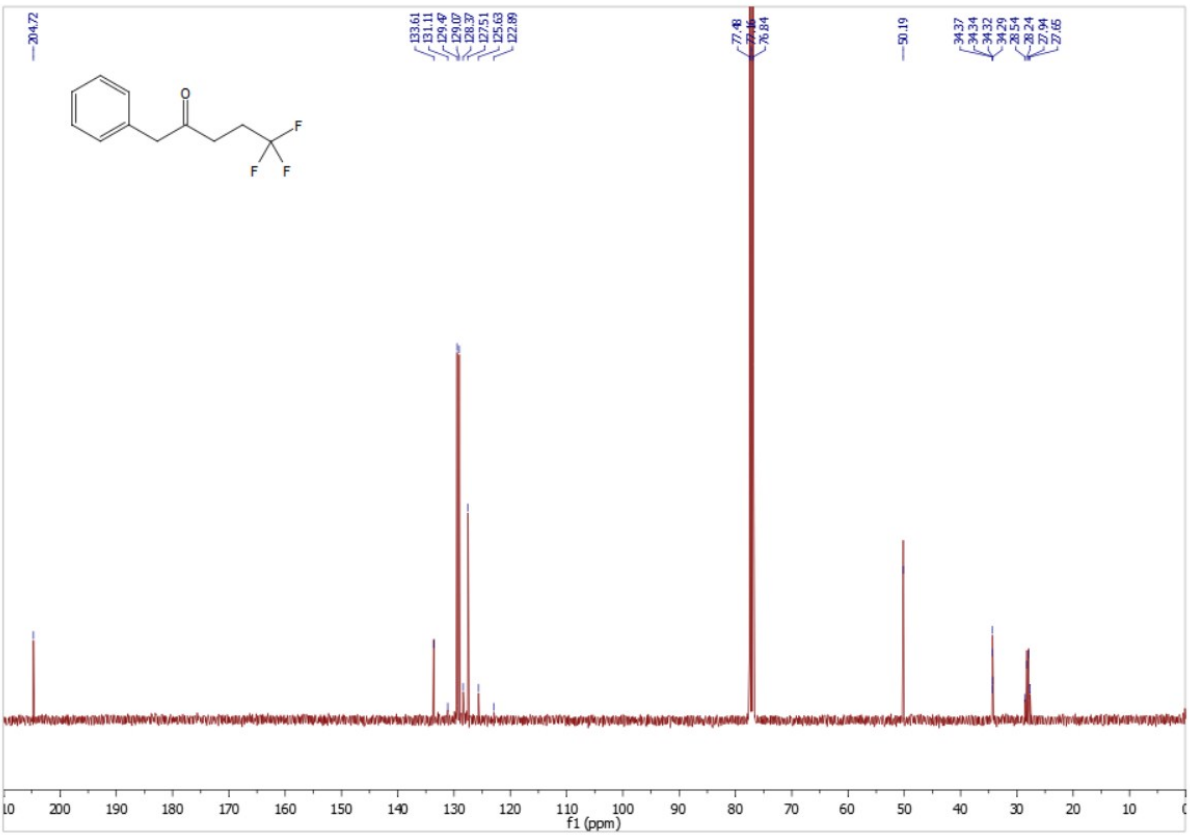
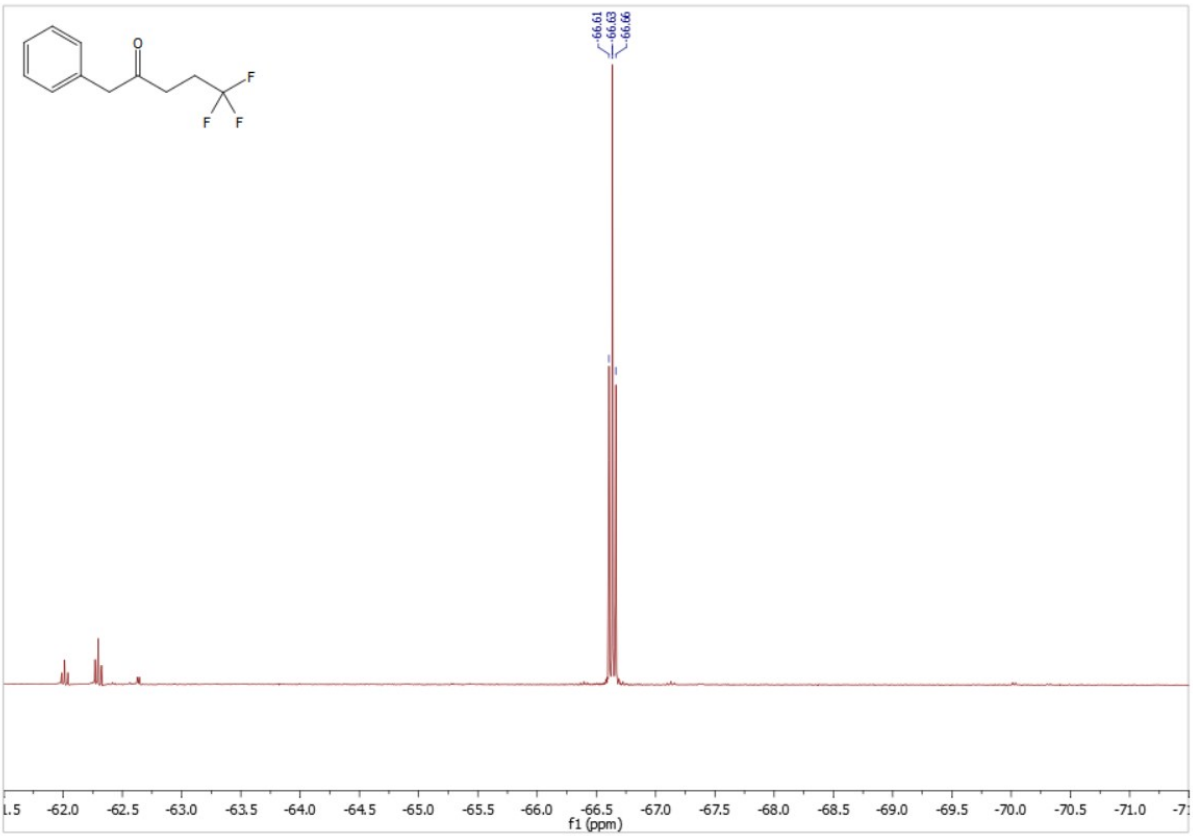
V. Copies of ^{1}H, ^{13}C and ^{19}F NMR spectra of fluorinated ketones



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F
F
F
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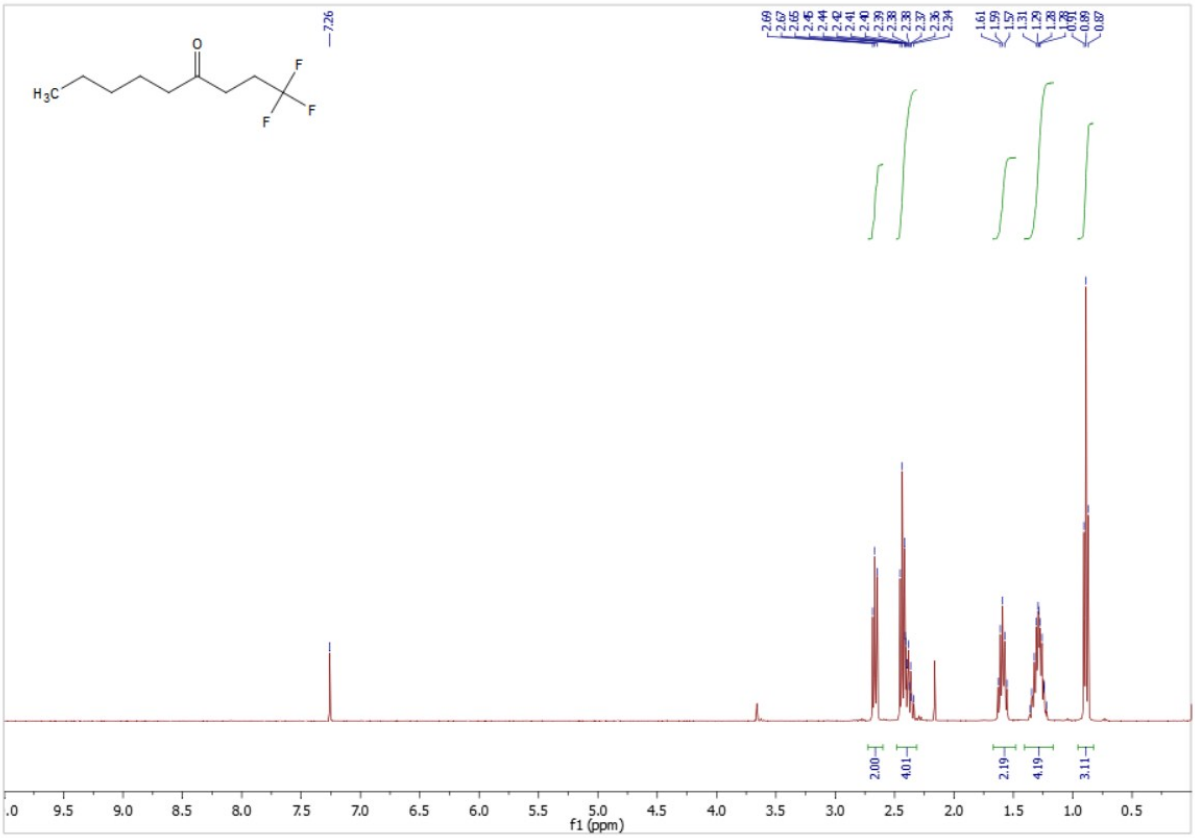
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F
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2.38
2.38
2.37
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2.34
1.61
1.59
1.57
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1.29
1.28
0.89
0.87
2.00
4.01
2.19
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3.11
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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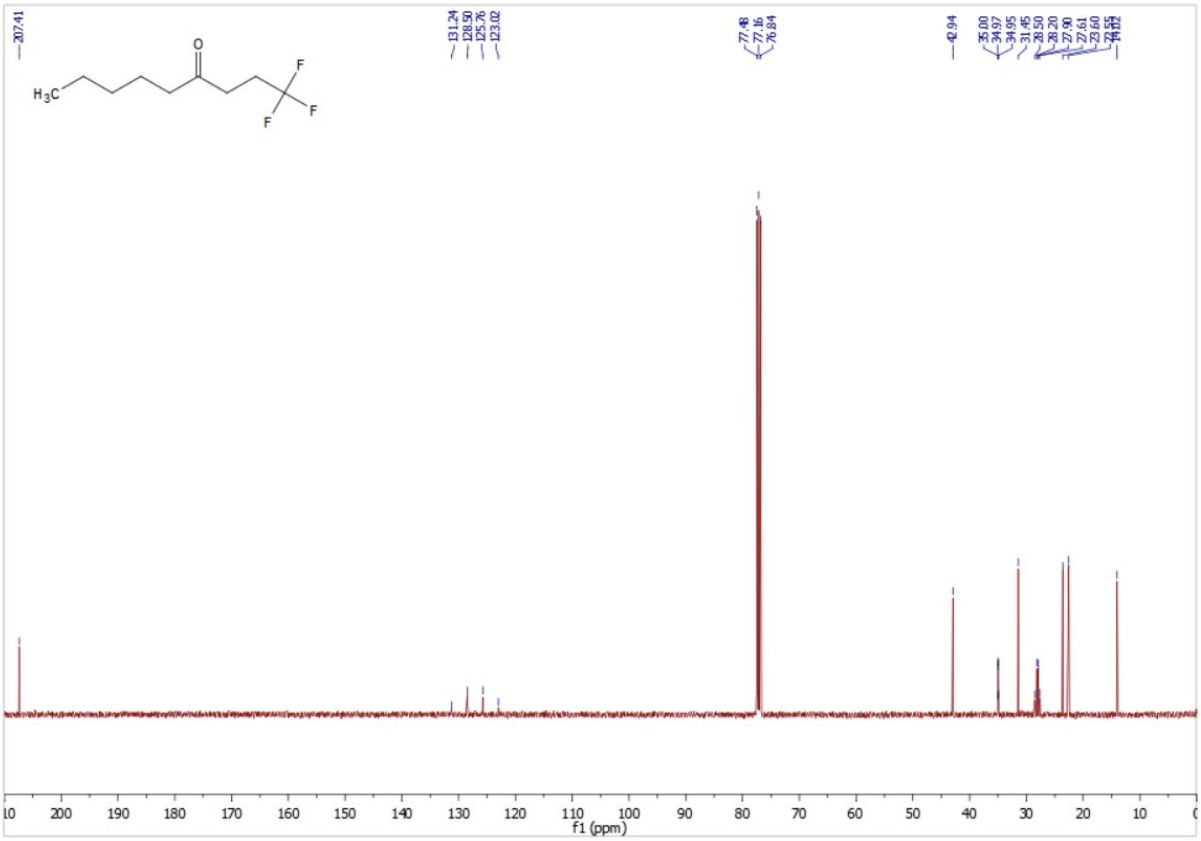
1.0
0.5
f1 (ppm)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F
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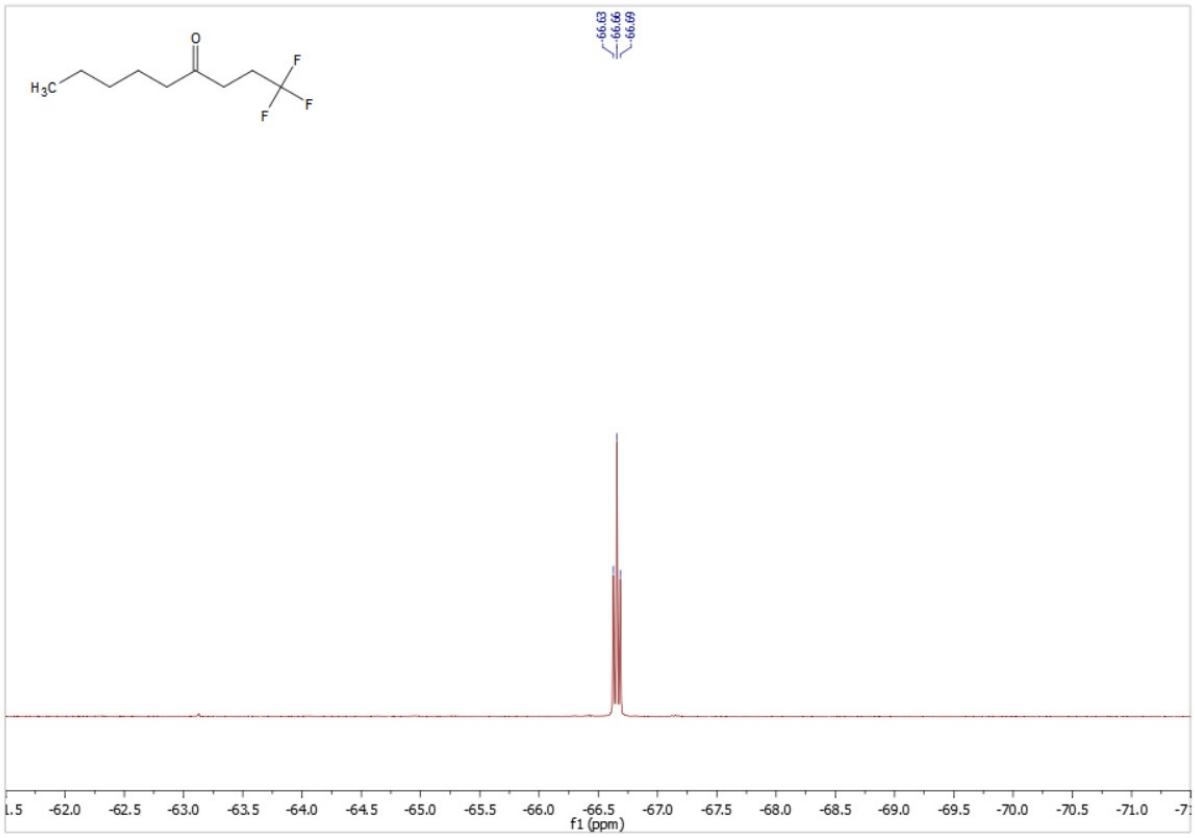
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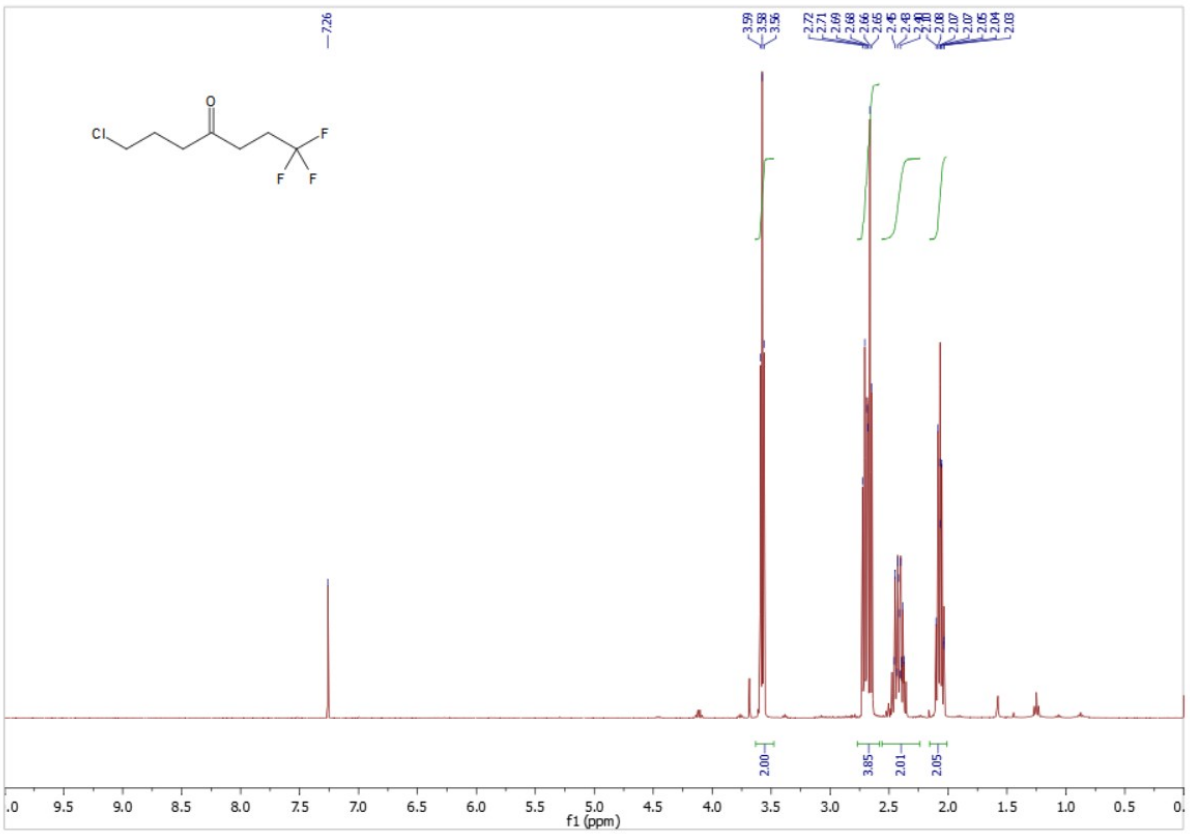
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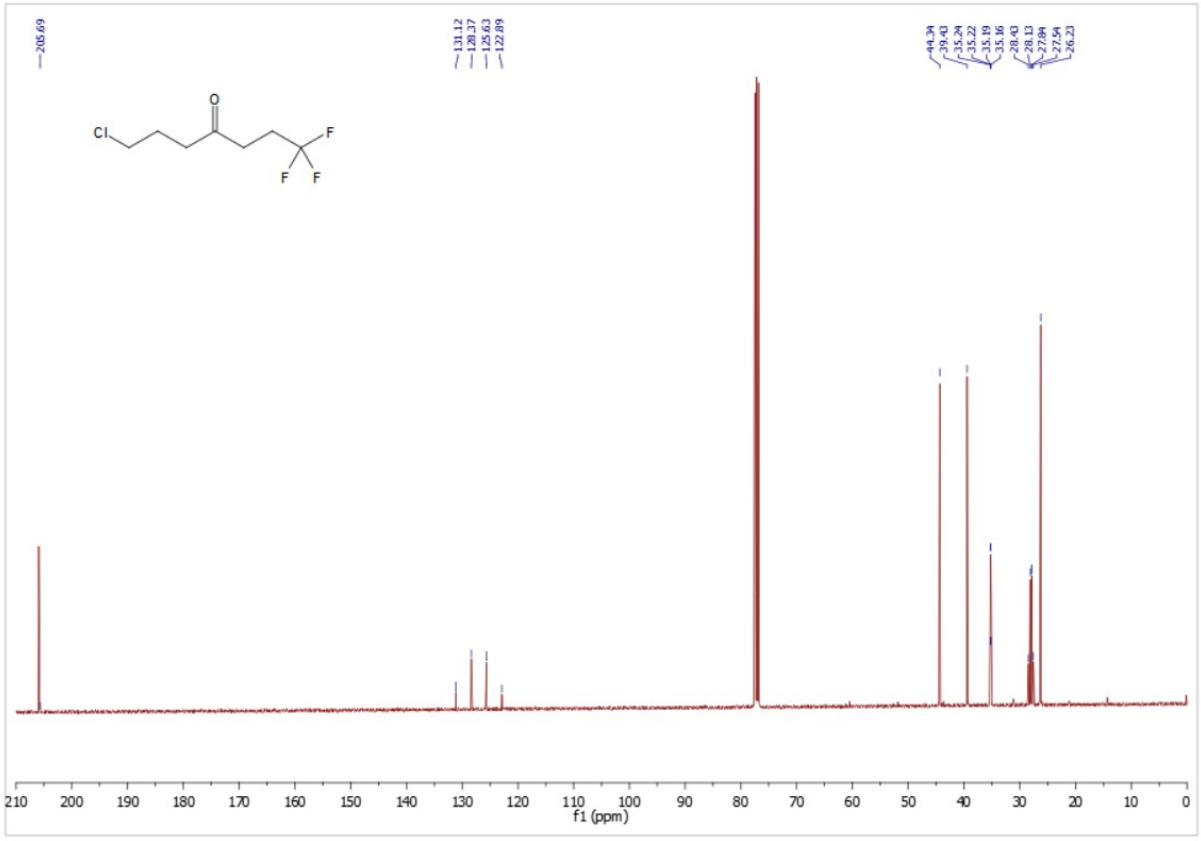
2.01
2.05
f1 (ppm)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O
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F
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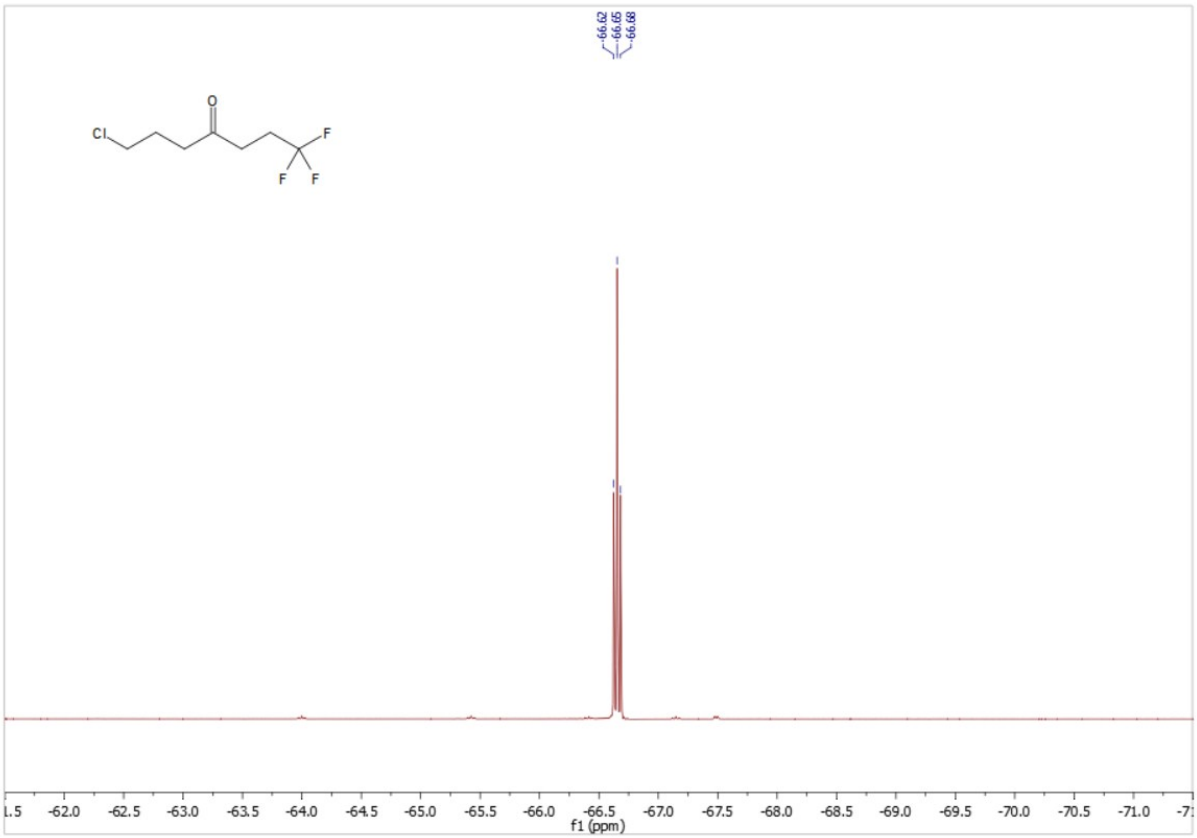
f1 (ppm)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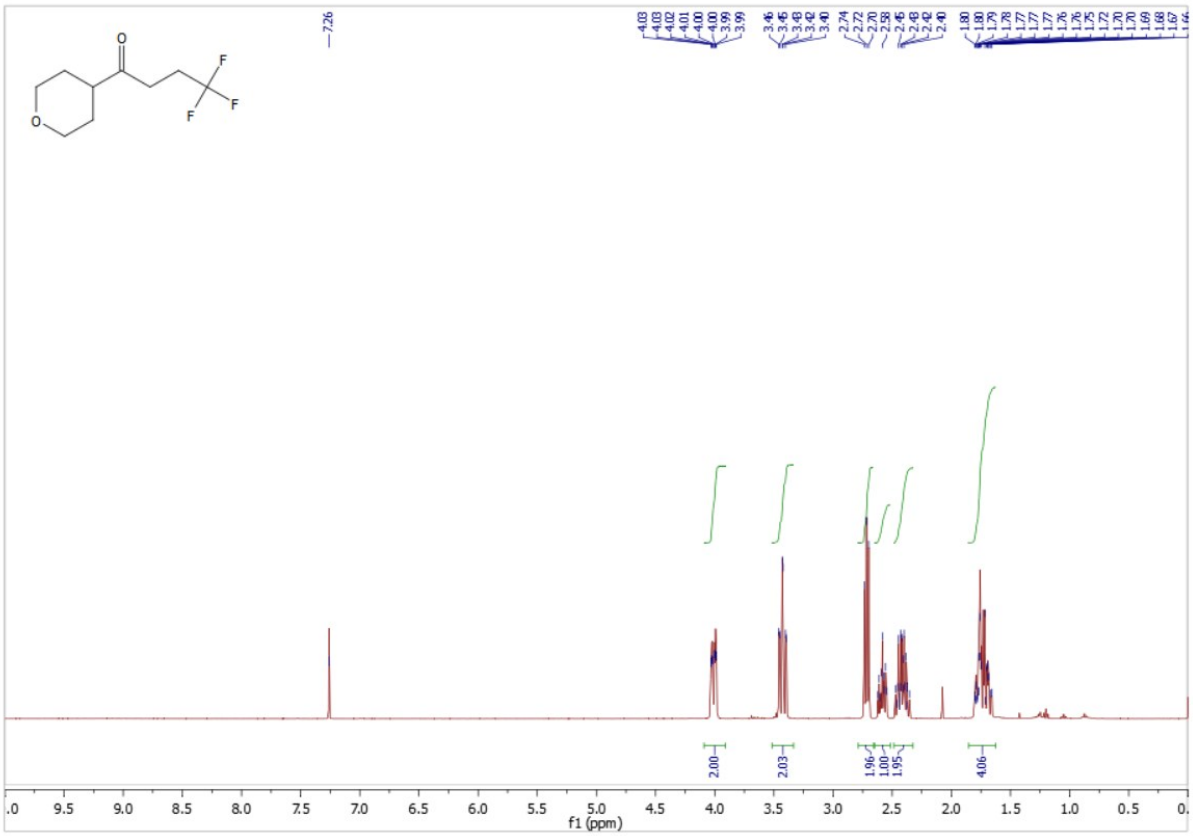
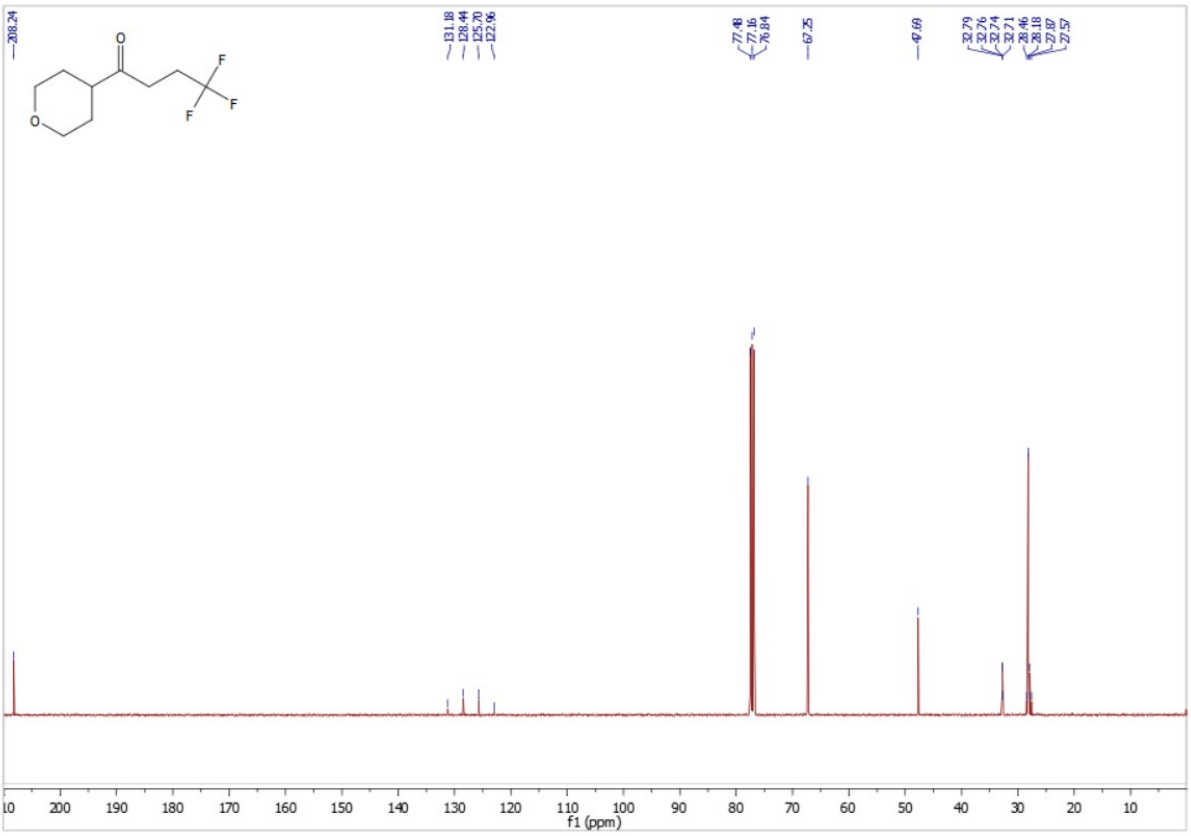
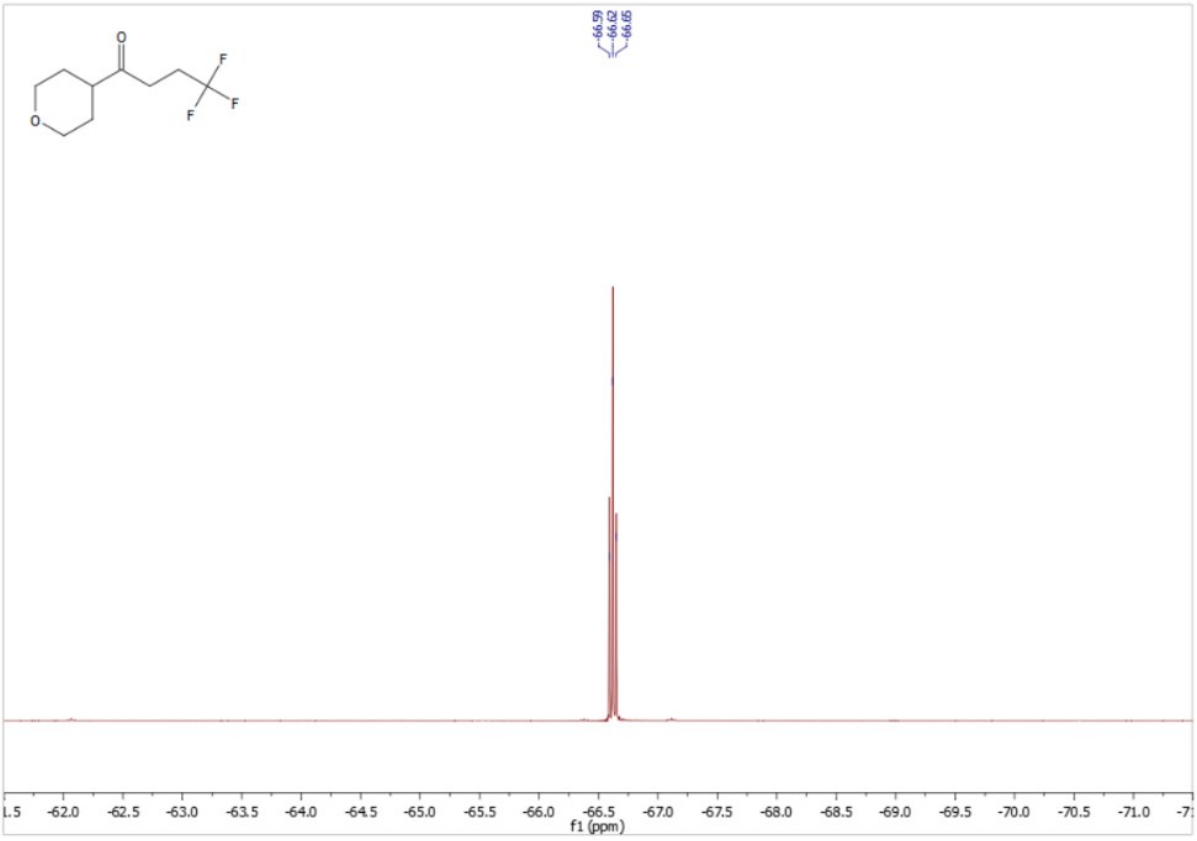
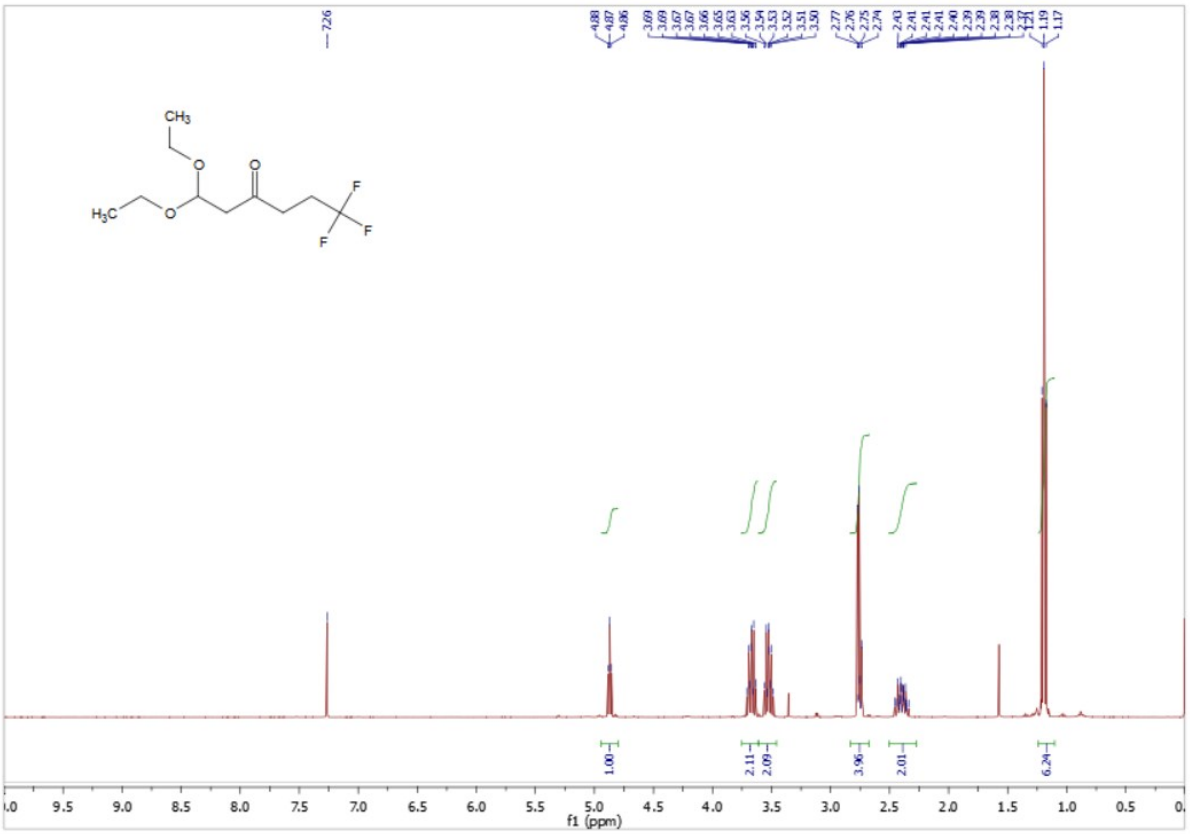
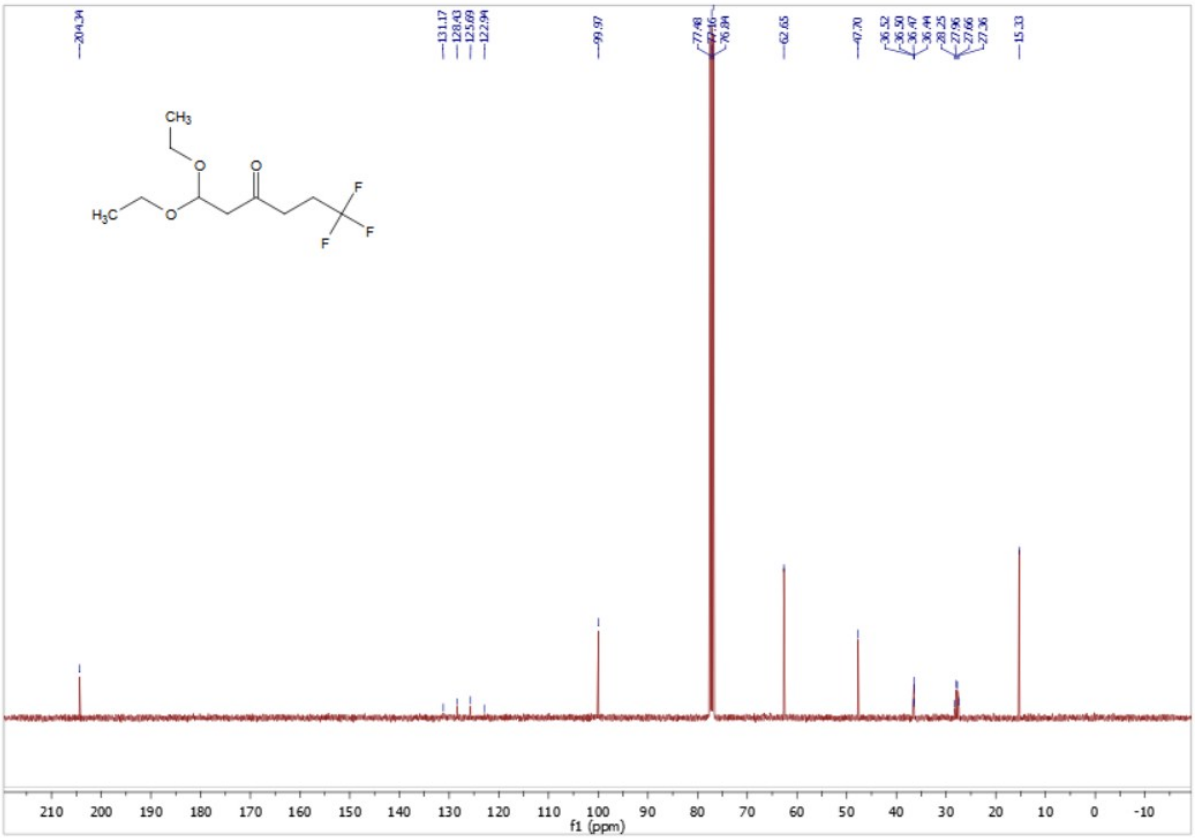
f1 (ppm)

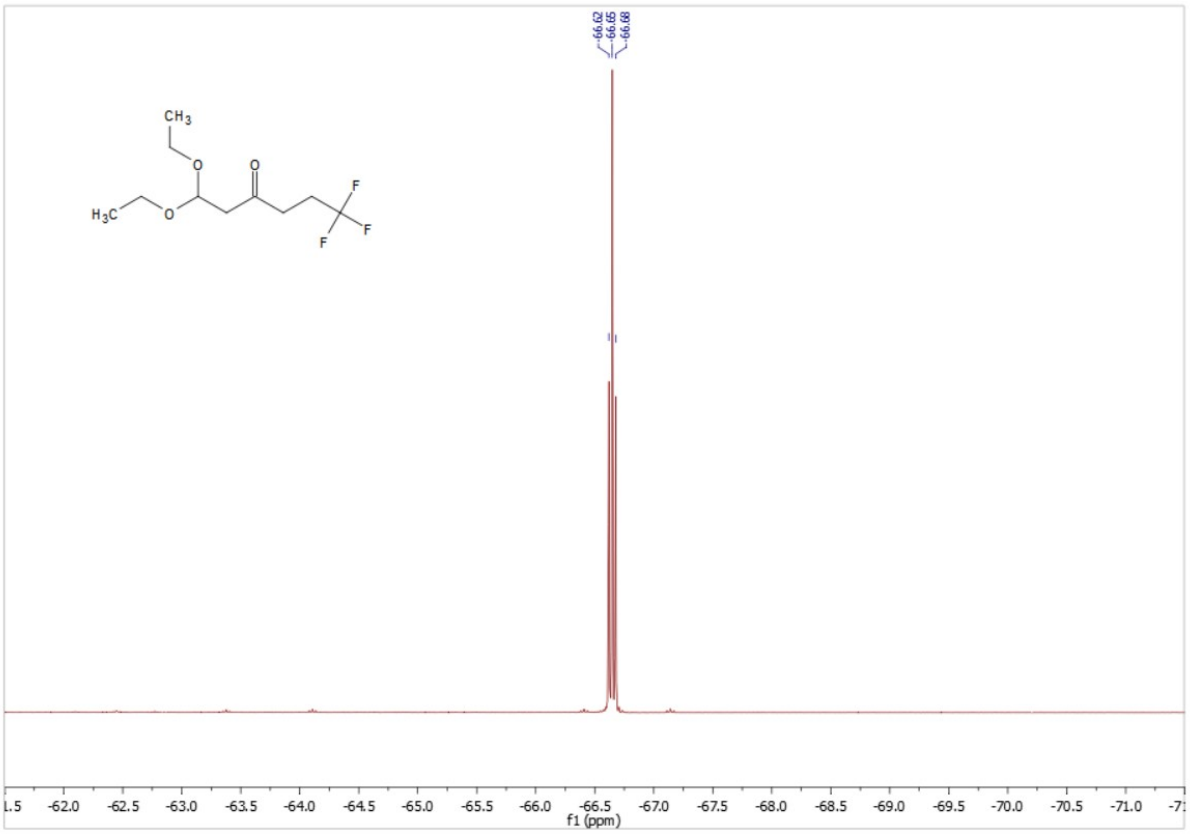

7.26
O
O
F
F
F
2.00
2.03
1.96
1.00
1.95
4.06
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

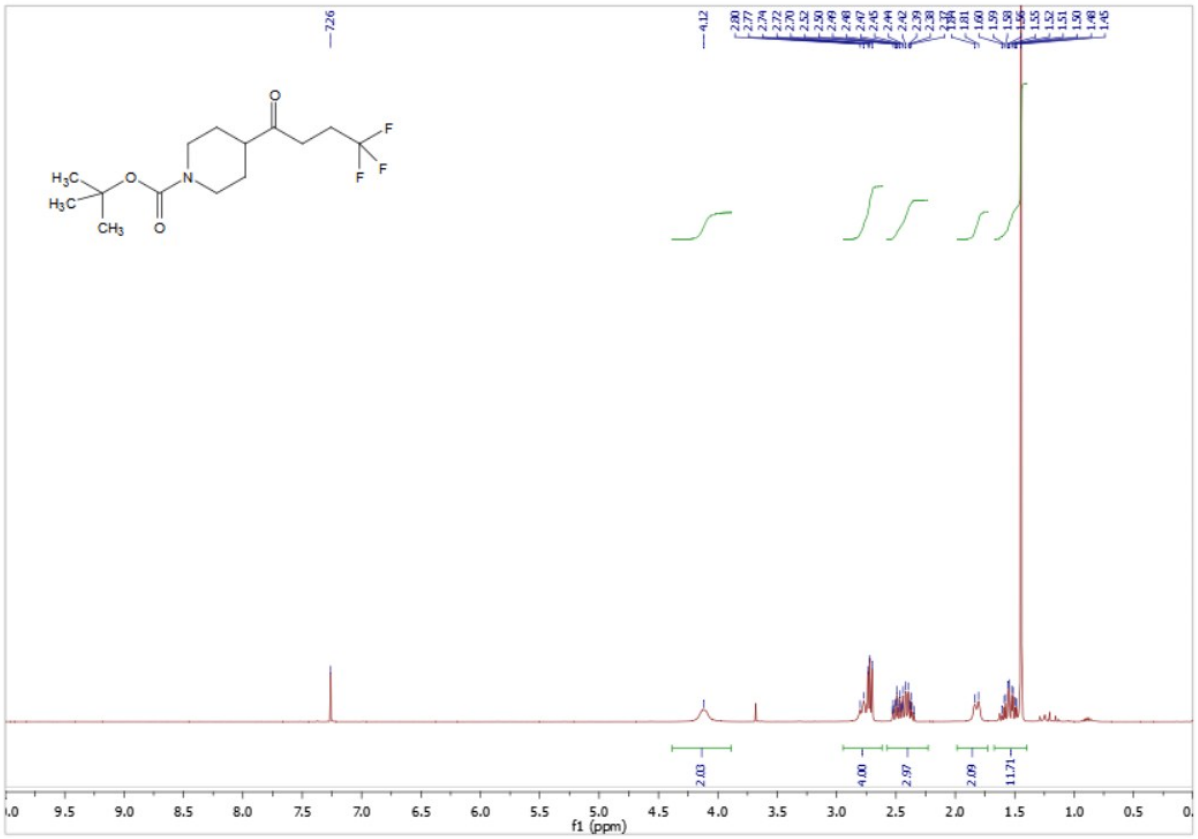

208.24
131.88
128.44
125.70
122.96
77.48
77.16
76.84
67.25
49.69
32.79
32.76
32.74
32.71
28.46
28.18
27.87
27.57
O
F
F
F
O
f1 (ppm)

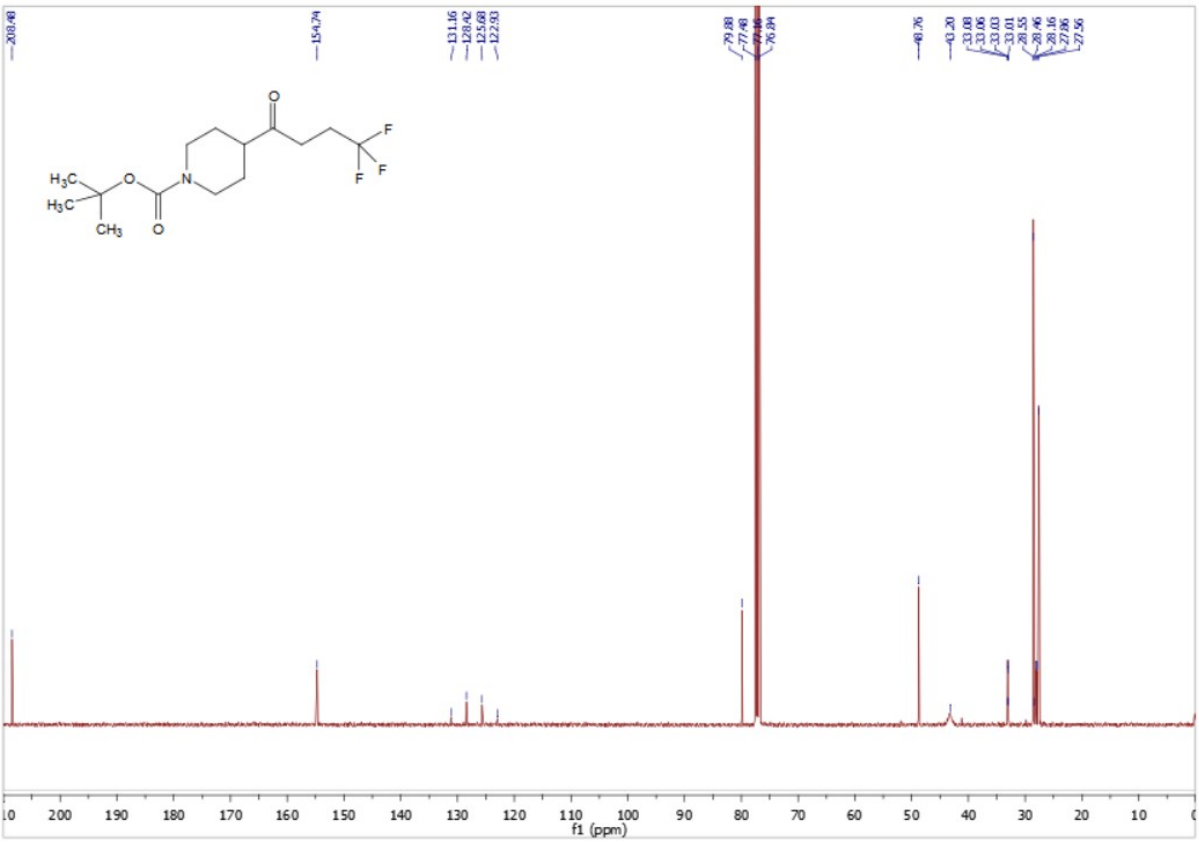

66.59
66.62
66.65
O
F
F
F
O
f1 (ppm)


7.26
4.88
4.87
4.86
3.69
3.67
3.66
3.65
3.63
3.56
3.54
3.53
3.52
3.51
3.50
2.77
2.76
2.75
2.74
2.43
2.41
2.40
2.39
2.38
1.19
1.17
CH3
O
O
H3C
O
F
F
F
1.00
2.11
2.09
3.96
2.01
6.24
f1 (ppm)

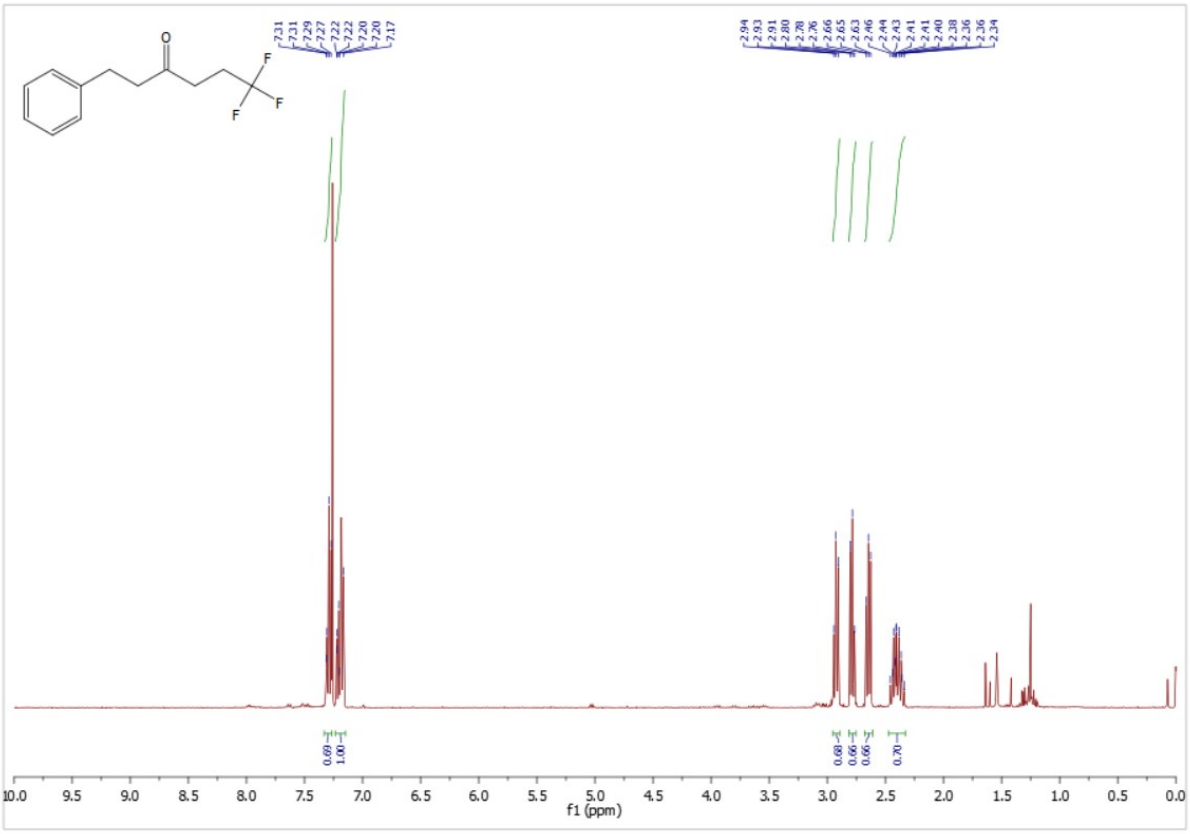

204.34
131.17
128.43
125.69
122.94
99.97
77.48
77.16
76.84
62.65
47.70
36.52
36.50
36.47
36.44
28.25
27.95
27.66
27.36
15.33
CH3
O
O
H3C
O
F
F
F
f1 (ppm)

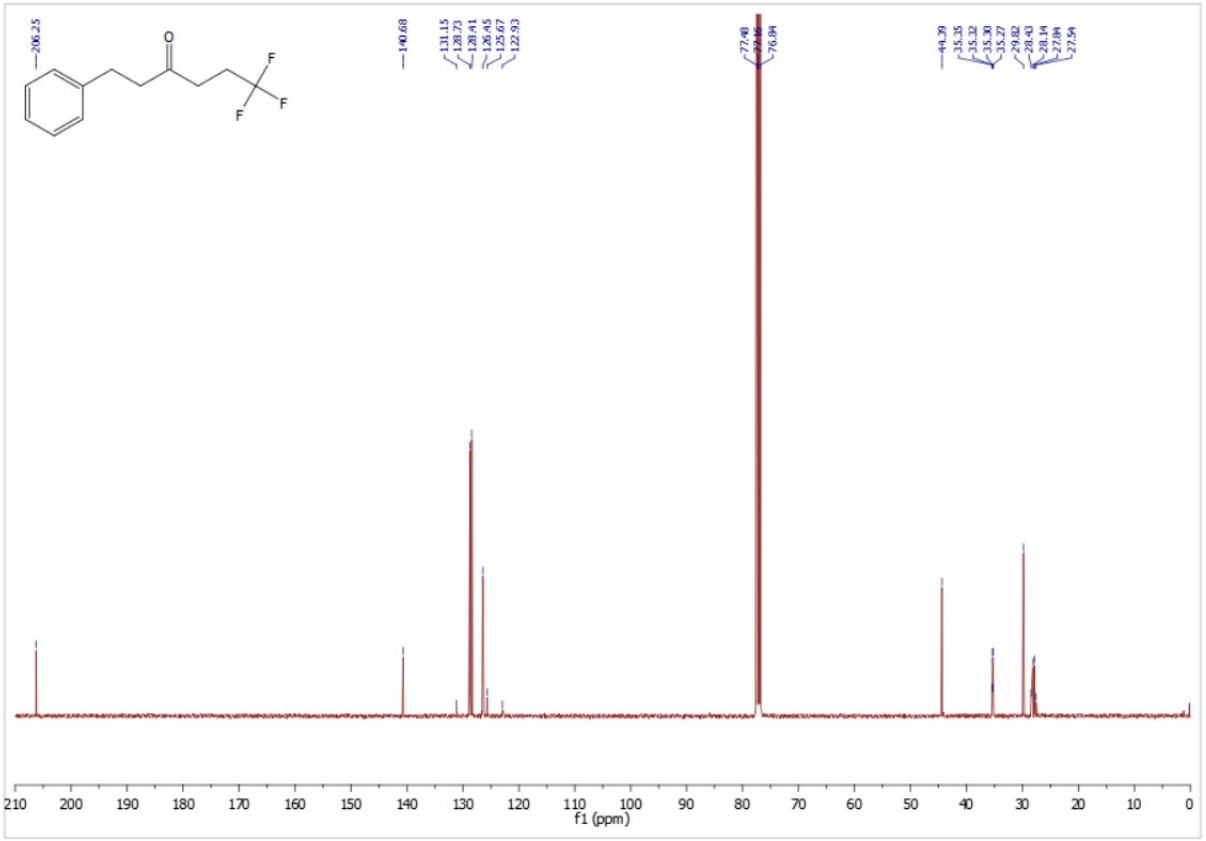

-66.62
-66.65
-66.68
CH3
O
O
O
H3C
F
F
F
-62.0
-62.5
-63.0
-63.5
-64.0
-64.5
-65.0
-65.5
-66.0
-66.5
-67.0
-67.5
-68.0
-68.5
-69.0
-69.5
-70.0
-70.5
-71.0
f1 (ppm)

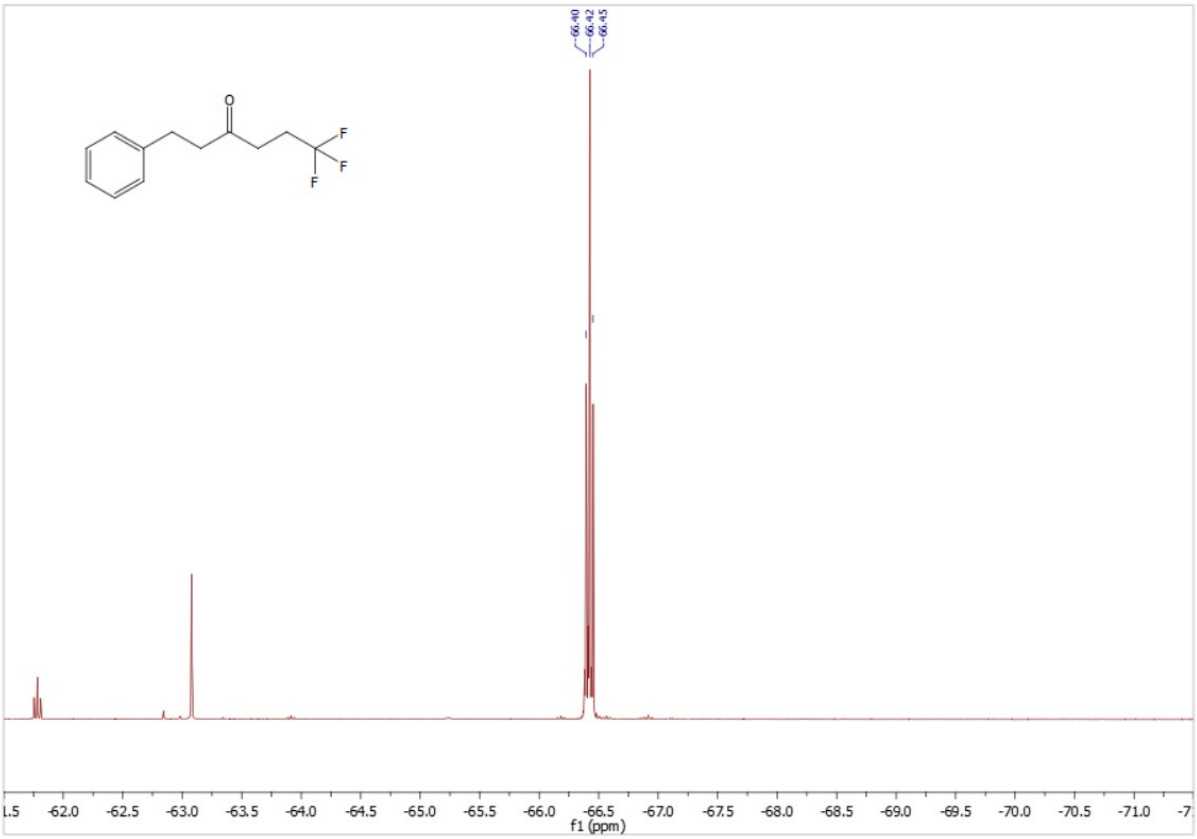

7.26
4.12
2.80
2.77
2.74
2.72
2.70
2.52
2.50
2.49
2.48
2.47
2.45
2.44
2.42
2.39
2.38
1.81
1.60
1.59
1.58
1.55
1.52
1.51
1.50
1.48
1.45
O
F
F
F
H3C
H3C
CH3
O
O
N
2.03
4.00
2.97
2.09
11.71
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

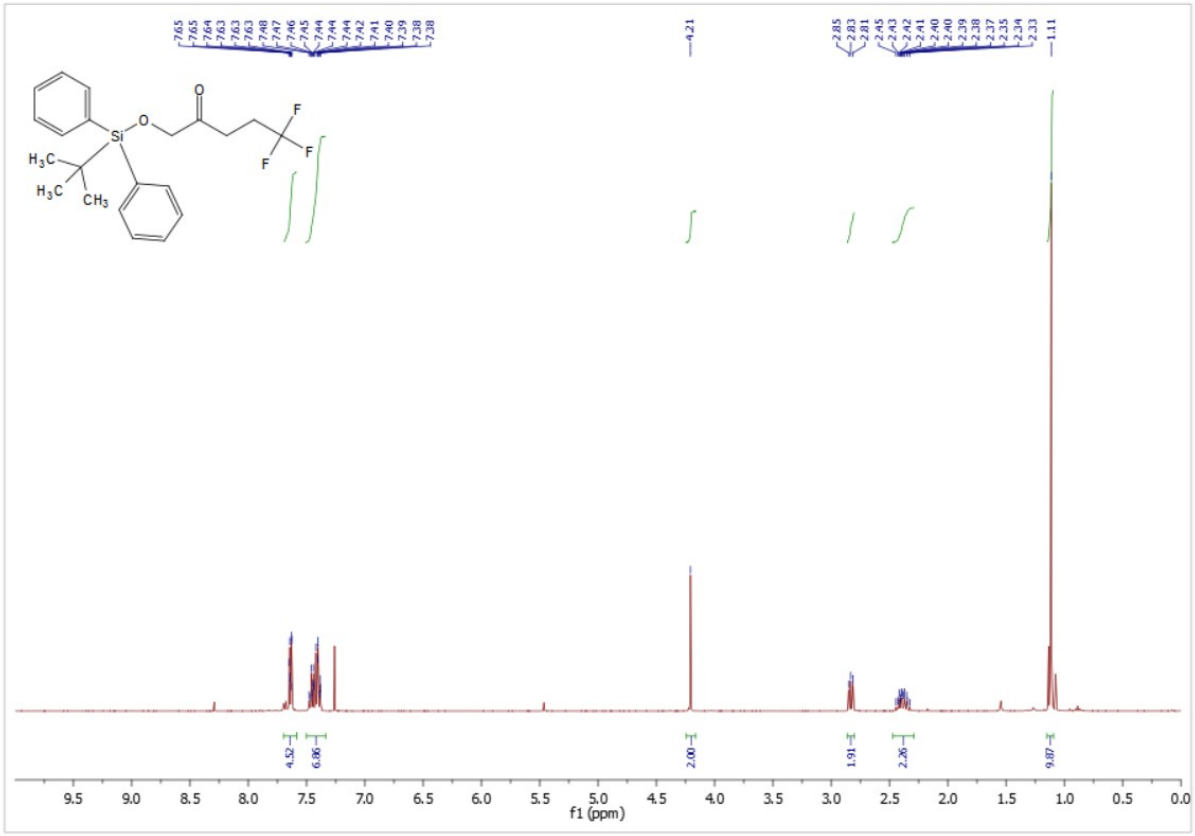

208.48
154.74
131.16
128.42
125.68
122.93
79.88
77.48
77.16
76.84
48.76
43.20
33.08
33.06
33.03
33.01
28.55
28.46
28.16
27.96
27.56
O
F
F
F
H3C
H3C
CH3
O
O
N
f1 (ppm)

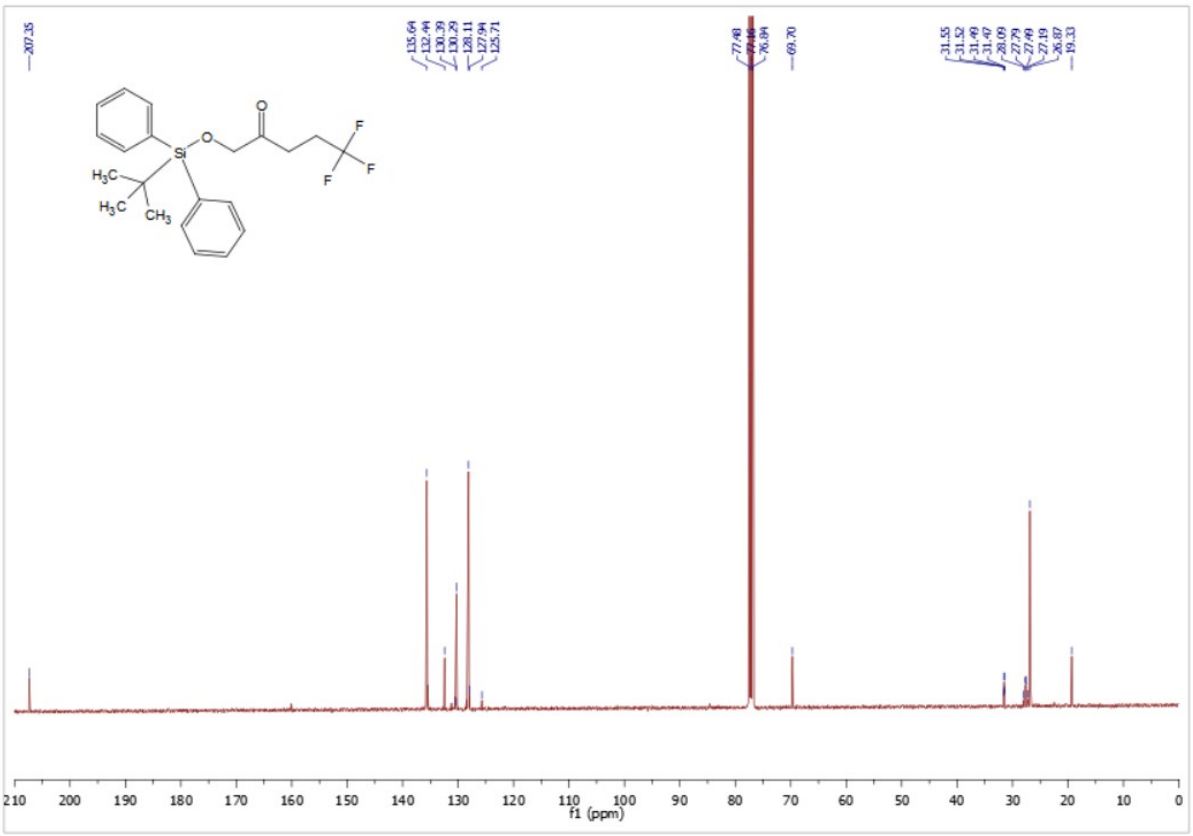

66.58
66.61
66.64
O
F
F
F
H3C
H3C
CH3
O
O
N
f1 (ppm)

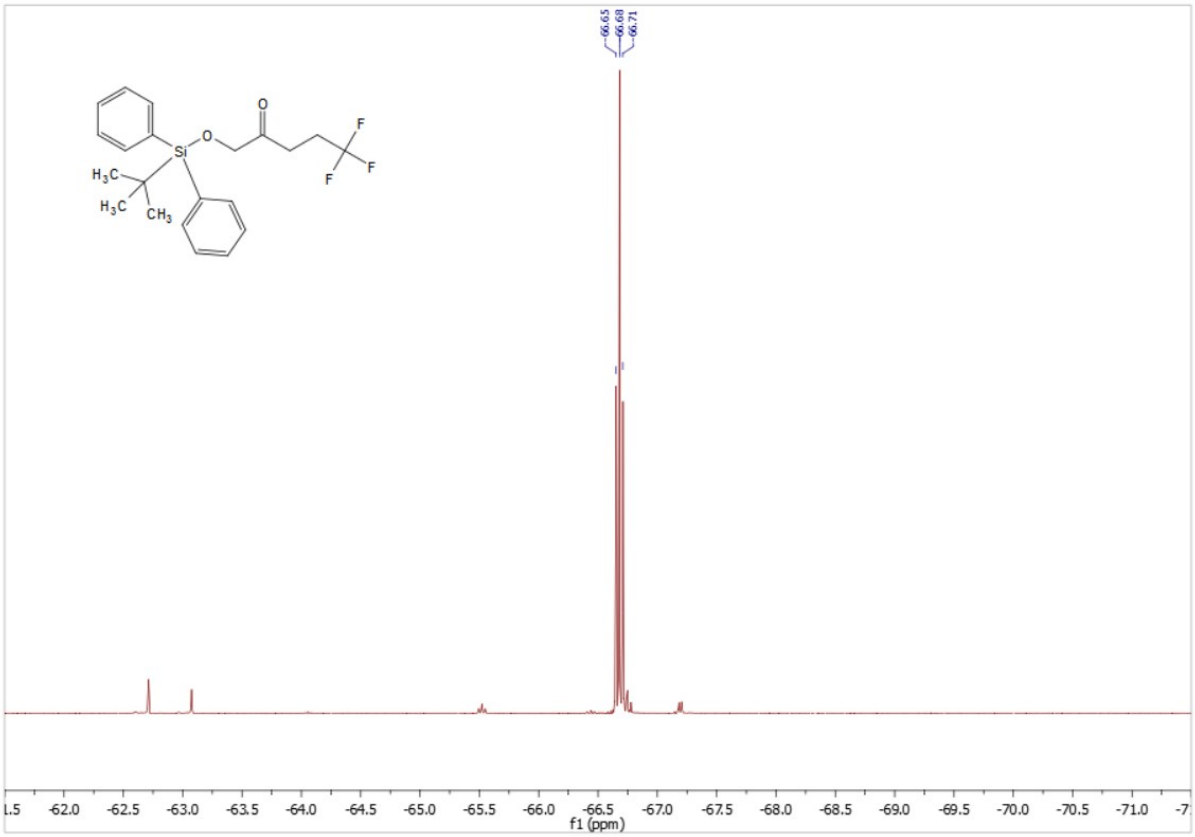

O
F
F
F
7.31
7.31
7.29
7.27
7.22
7.22
7.20
7.20
7.17
2.94
2.93
2.91
2.80
2.78
2.76
2.66
2.65
2.63
2.46
2.44
2.43
2.41
2.41
2.40
2.38
2.36
2.36
2.34
0.69
1.00
0.68
0.66
0.66
0.70
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

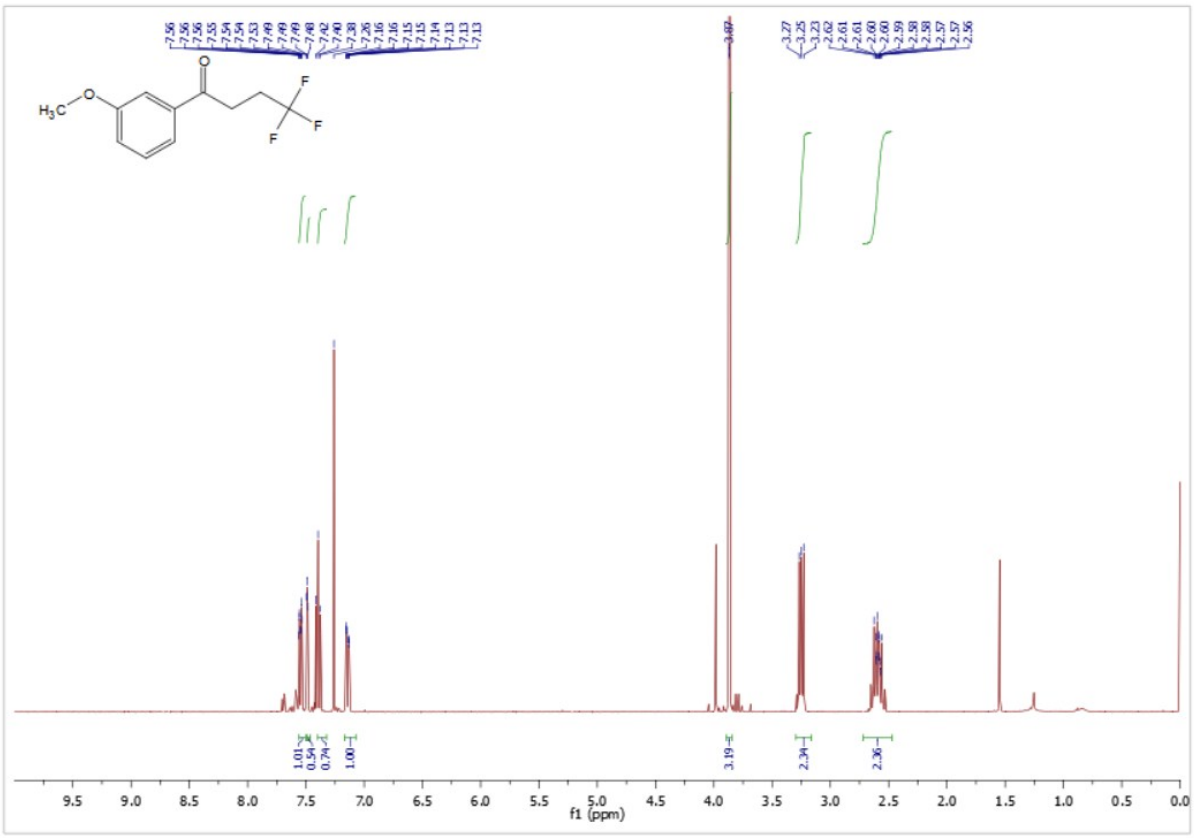

O
F
F
F
206.25
140.68
131.15
128.73
128.41
126.45
125.67
122.93
77.48
77.16
76.84
44.39
35.35
35.32
35.30
35.27
29.82
28.43
28.14
27.84
27.54
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

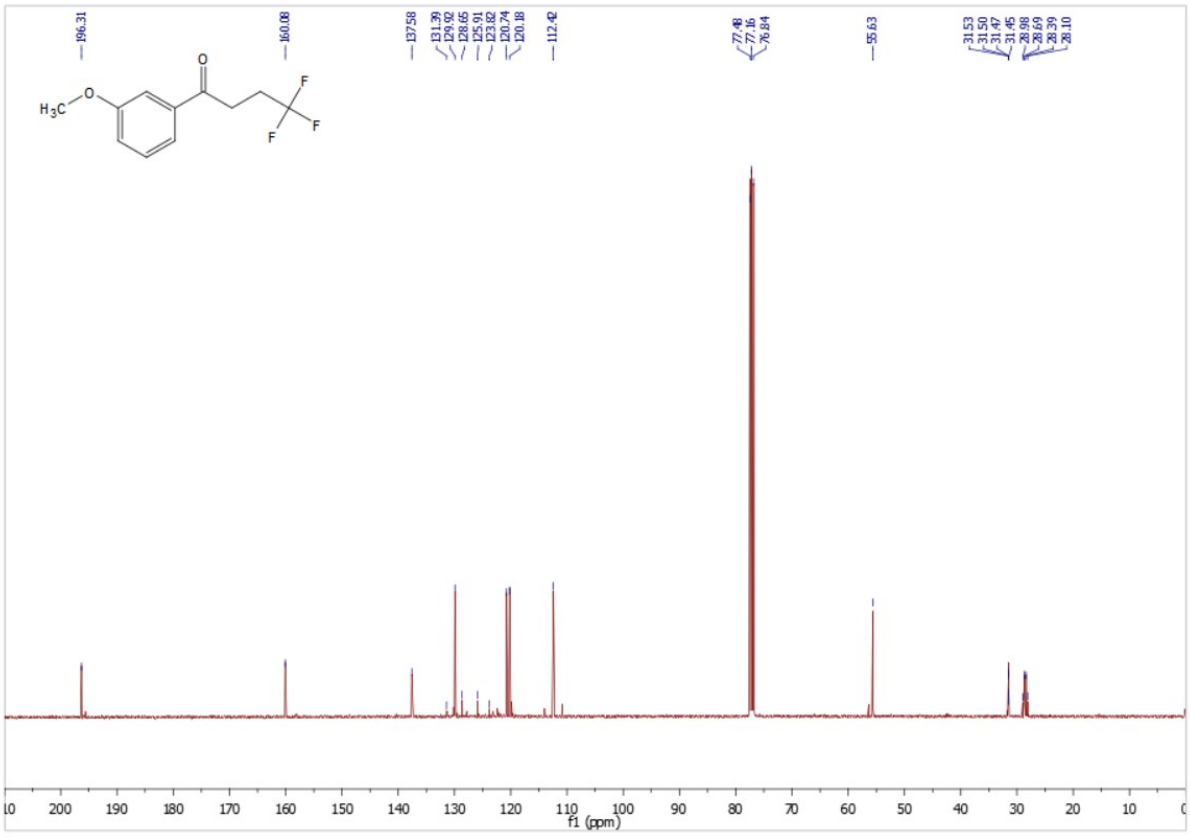

O
F
F
F
-66.40
-66.42
-66.45
-62.0
-62.5
-63.0
-63.5
-64.0
-64.5
-65.0
-65.5
-66.0
-66.5
-67.0
-67.5
-68.0
-68.5
-69.0
-69.5
-70.0
-70.5
-71.0
f1 (ppm)

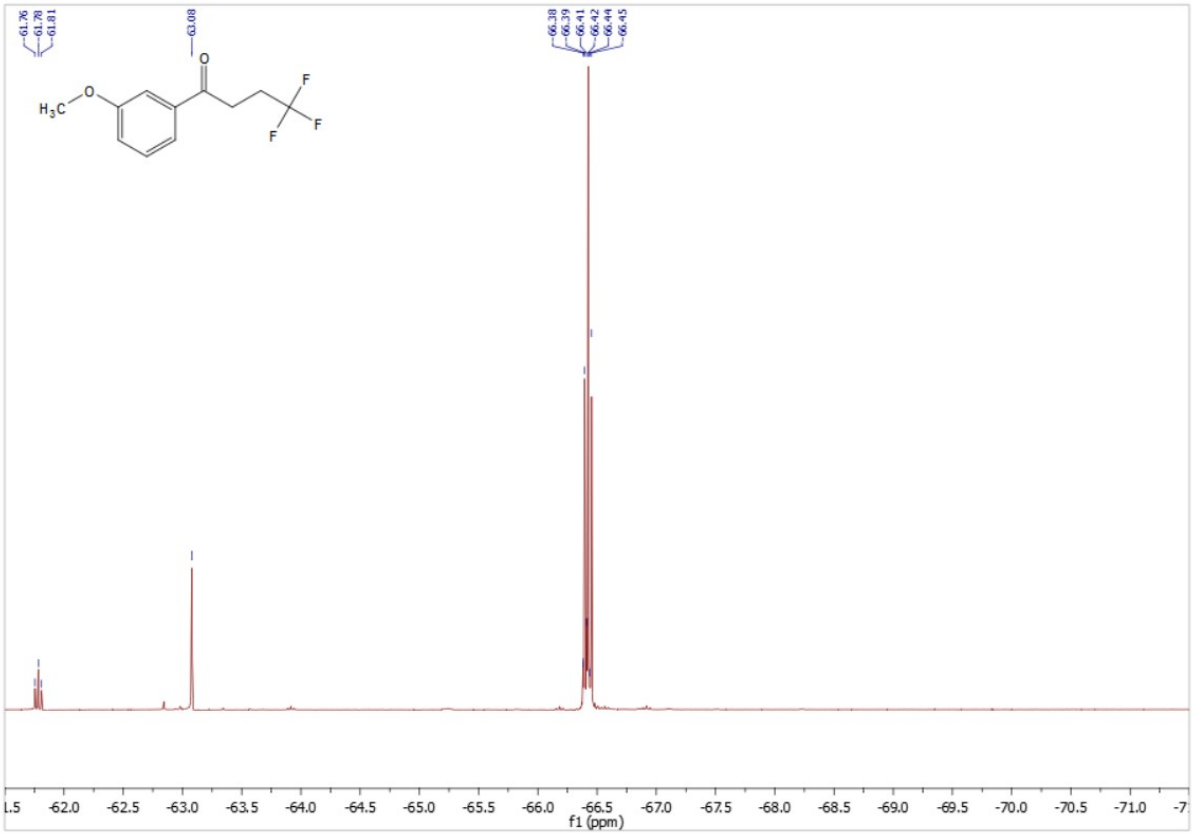

Si
O
O
F
F
F
H3C
H3C
CH3
4.21
1.11
4.52
6.86
2.00
1.91
2.26
9.87
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

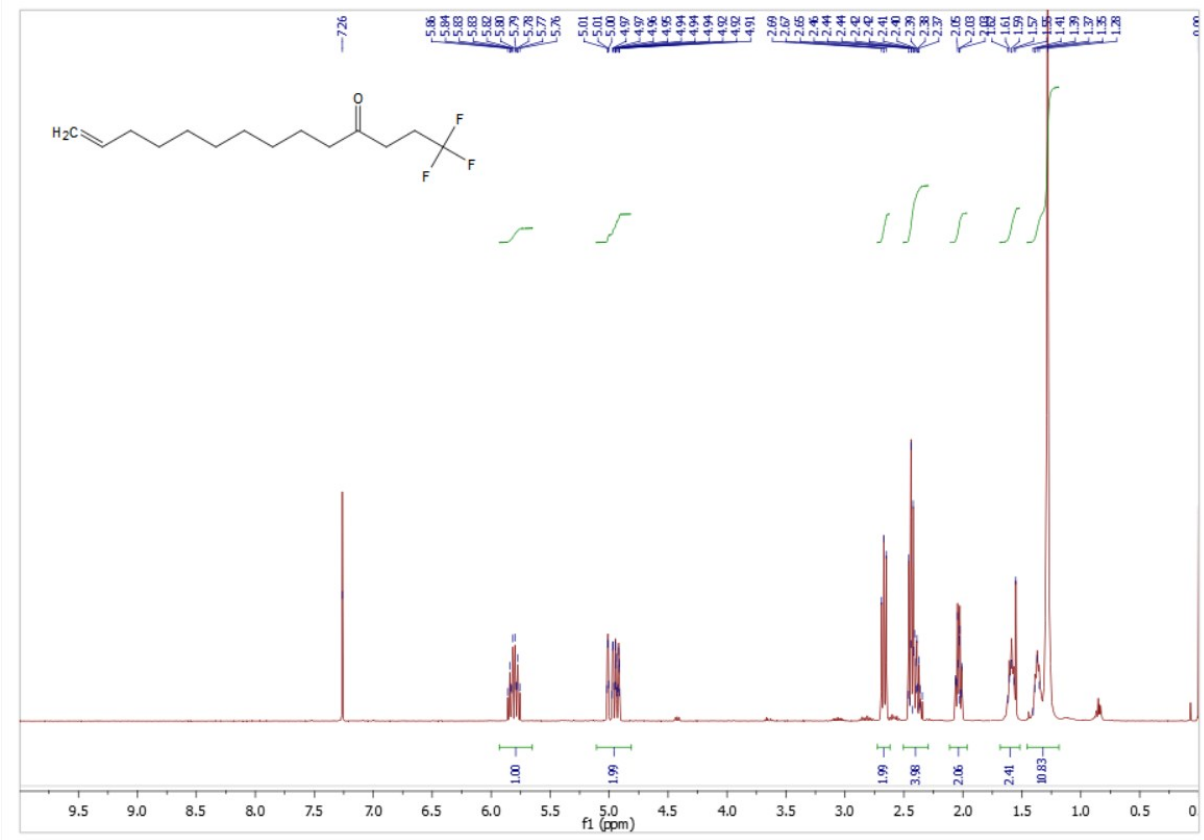

207.35
135.64
132.44
130.39
130.29
128.11
127.94
125.71
77.48
77.16
76.84
69.70
31.55
31.52
31.49
31.47
28.09
27.79
27.49
27.19
26.87
19.33
O
Si
O
F
F
F
H3C
H3C
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

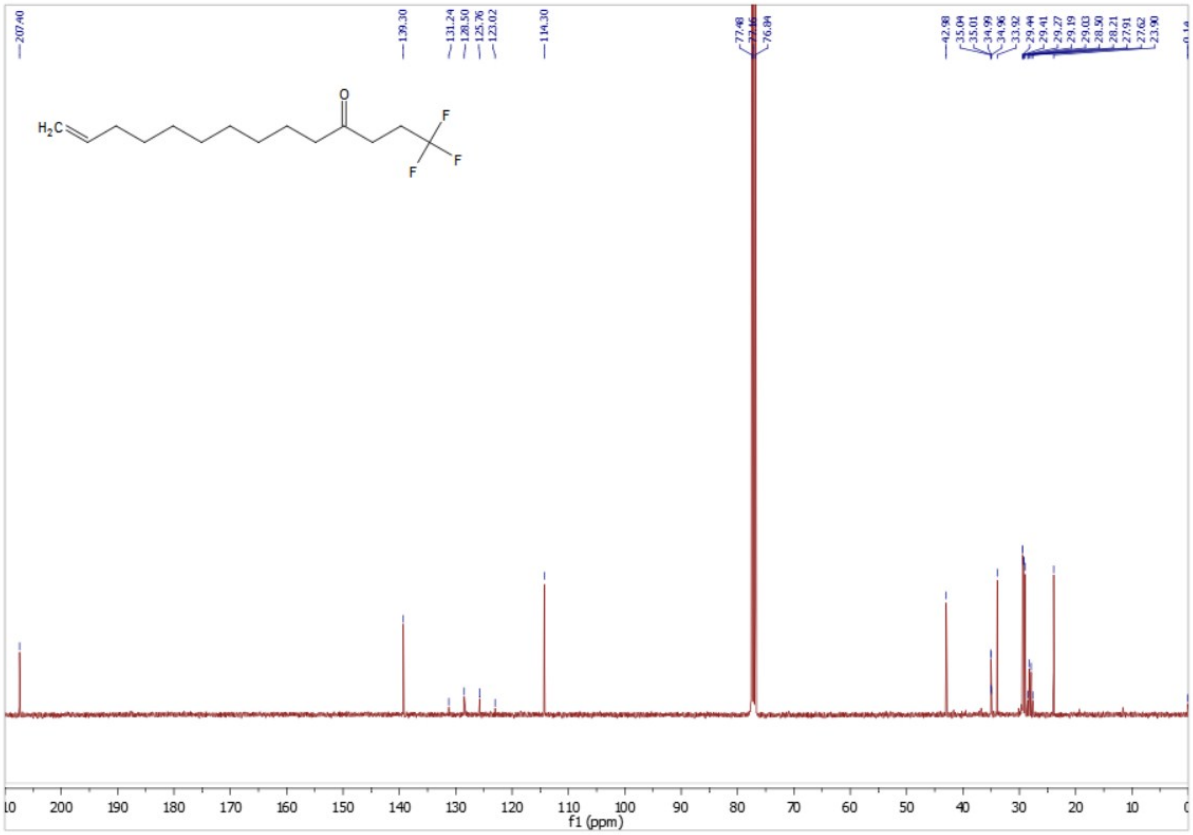

66.65
66.68
66.71
O
Si
O
F
F
F
H3C
H3C
CH3
-62.0 -62.5 -63.0 -63.5 -64.0 -64.5 -65.0 -65.5 -66.0 -66.5 -67.0 -67.5 -68.0 -68.5 -69.0 -69.5 -70.0 -70.5 -71.0
f1 (ppm)

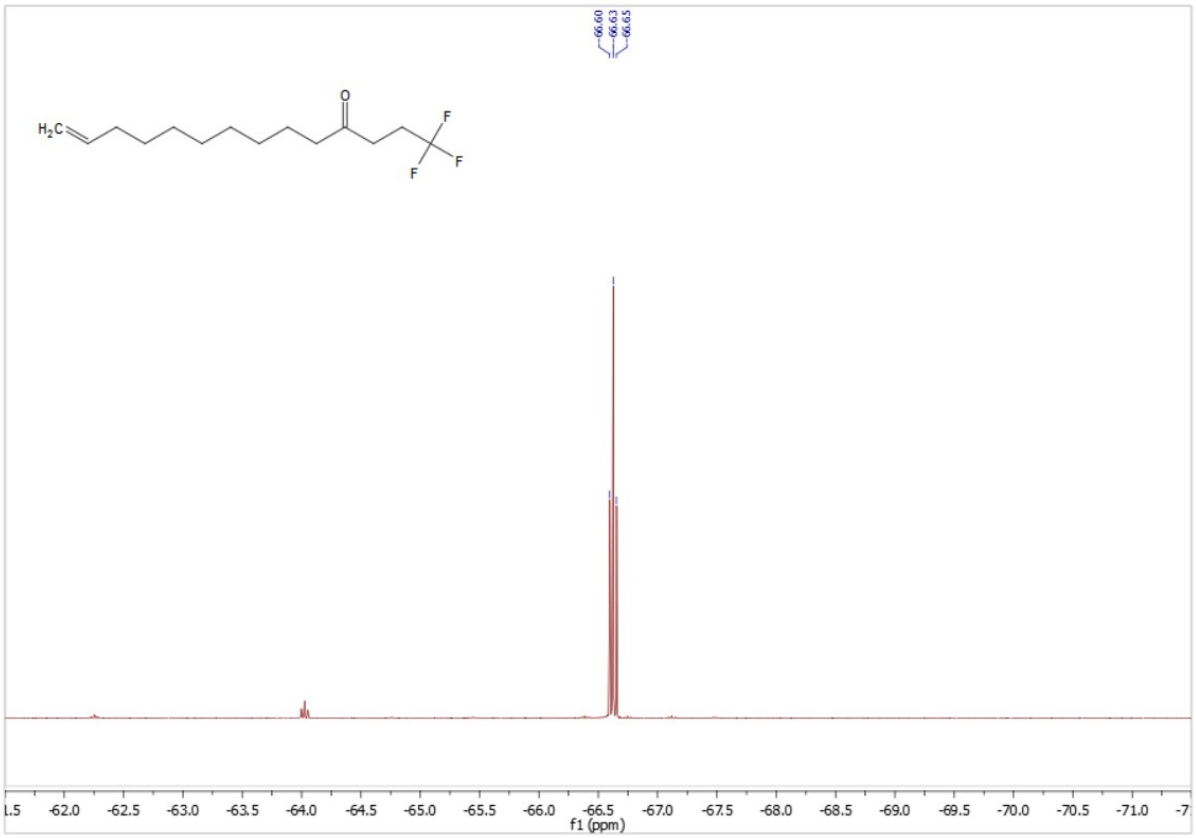

7.56
7.56
7.56
7.55
7.54
7.54
7.53
7.49
7.49
7.49
7.48
7.42
7.40
7.38
7.26
7.16
7.15
7.15
7.14
7.13
7.13
7.13
3.87
3.27
3.25
3.23
2.62
2.61
2.61
2.60
2.60
2.59
2.58
2.58
2.57
2.57
2.56
O
H3C
O
F
F
F
1.01
0.54
0.74
1.00
3.19
2.34
2.36
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

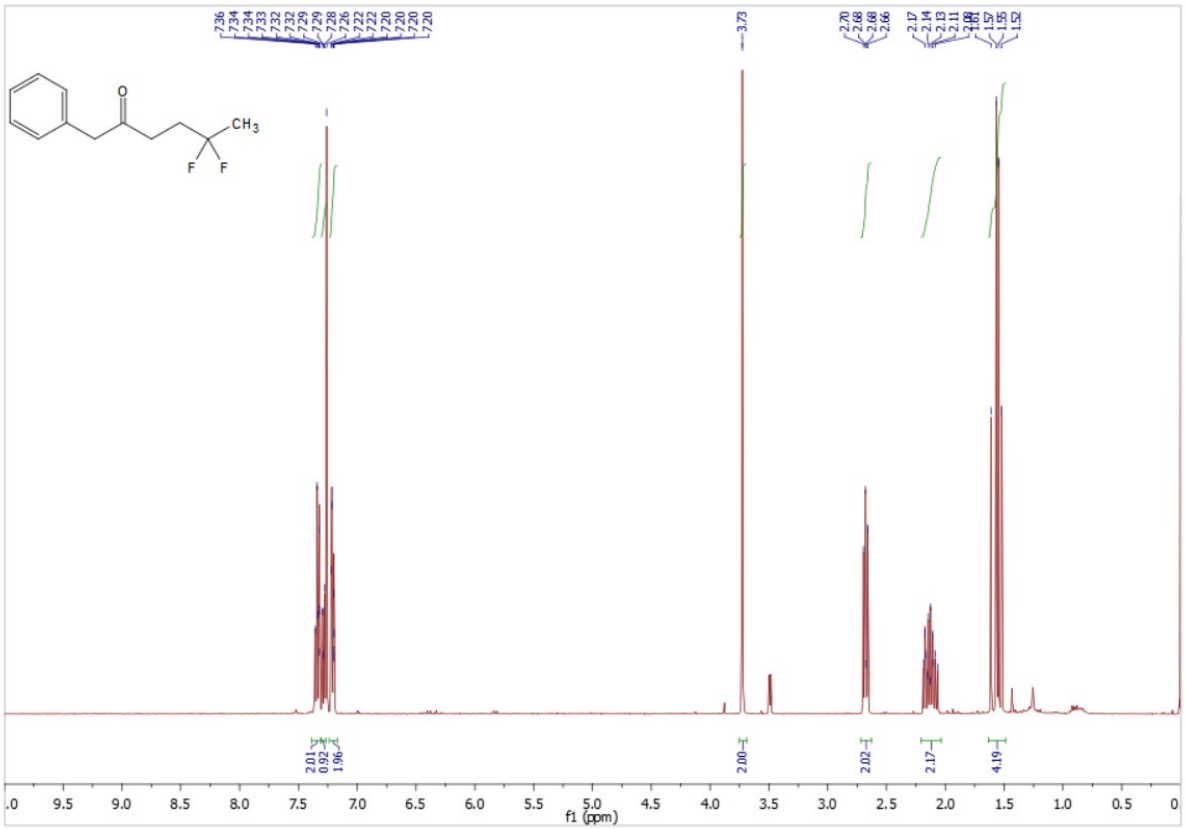

196.31
160.08
137.58
131.39
129.92
128.65
125.91
123.82
120.74
120.18
112.42
77.48
77.16
76.84
55.63
31.53
31.50
31.47
31.45
28.98
28.69
28.39
28.10
O
H3C
O
F
F
F
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

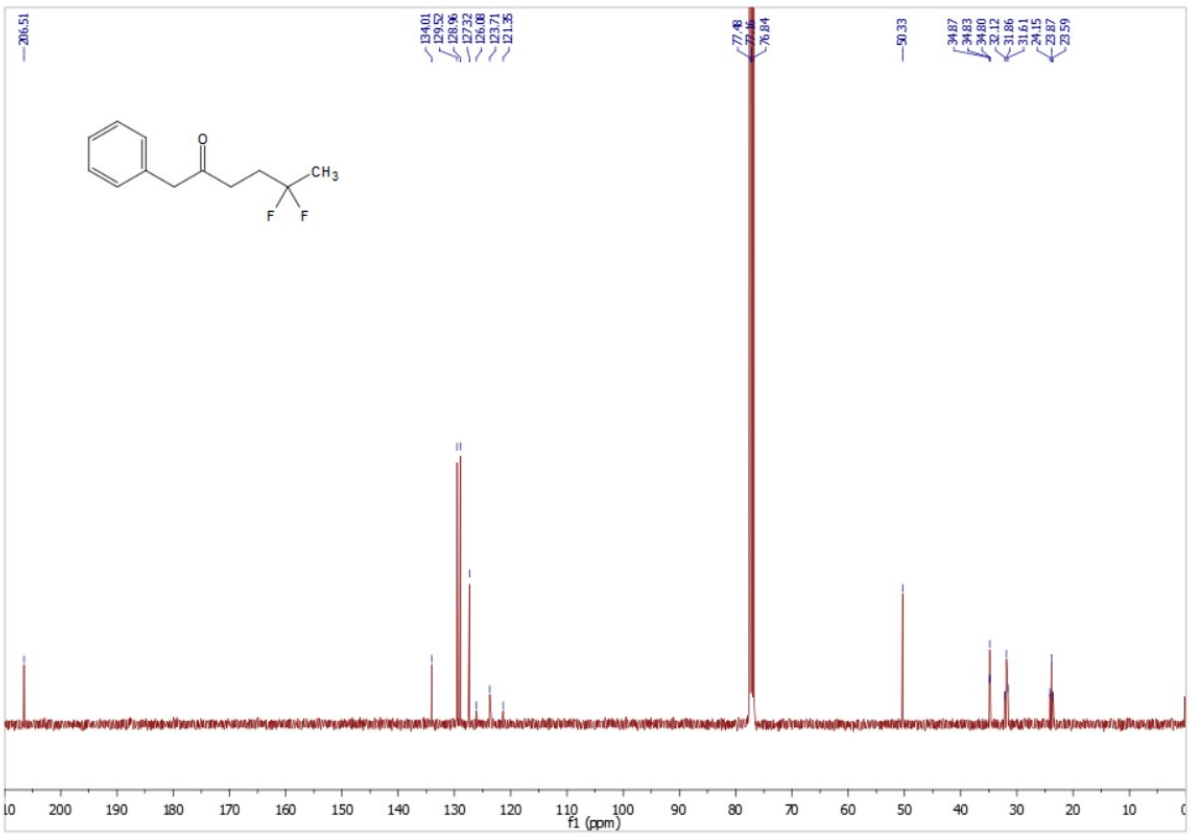

-61.76
-61.78
-61.81
-63.08
-66.38
-66.39
-66.41
-66.42
-66.44
-66.45
O
H3C
O
F
F
F
f1 (ppm)

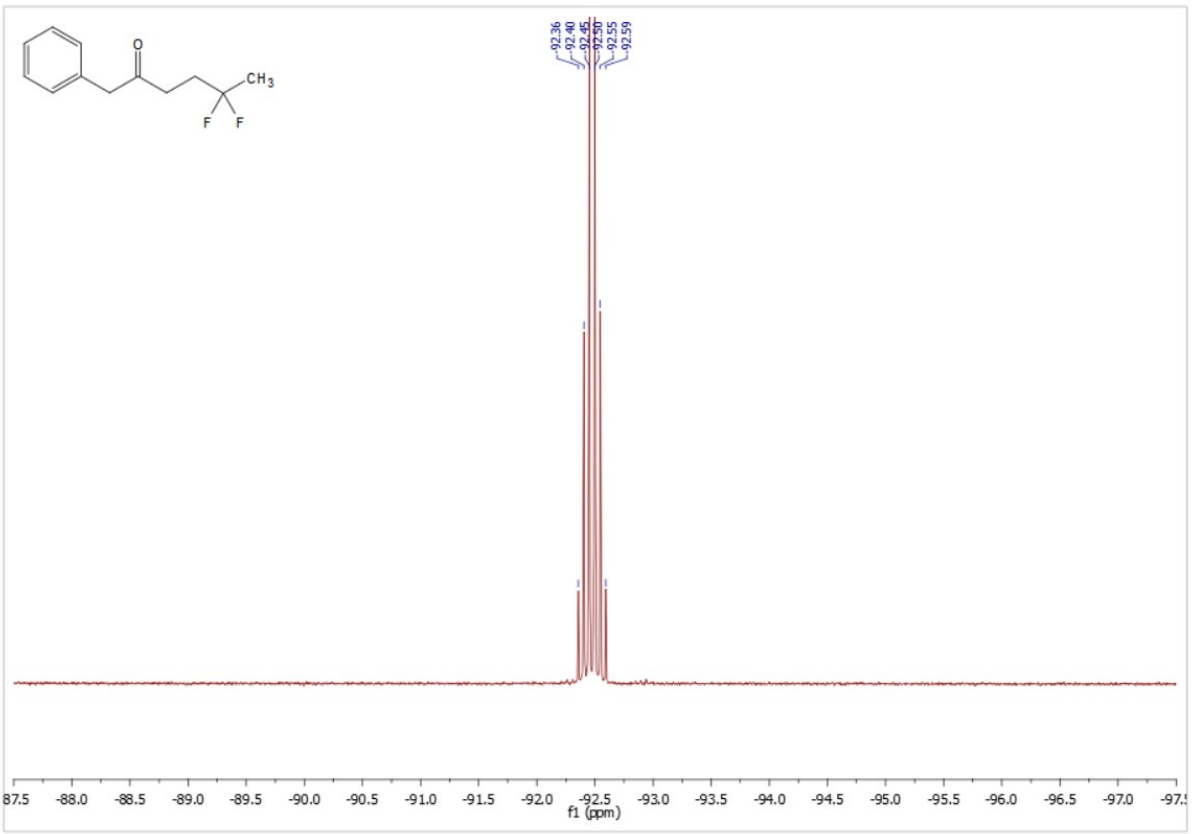

7.26
O
H2C
F
F
F
1.00
1.99
1.99
3.98
2.06
2.41
10.83
f1 (ppm)

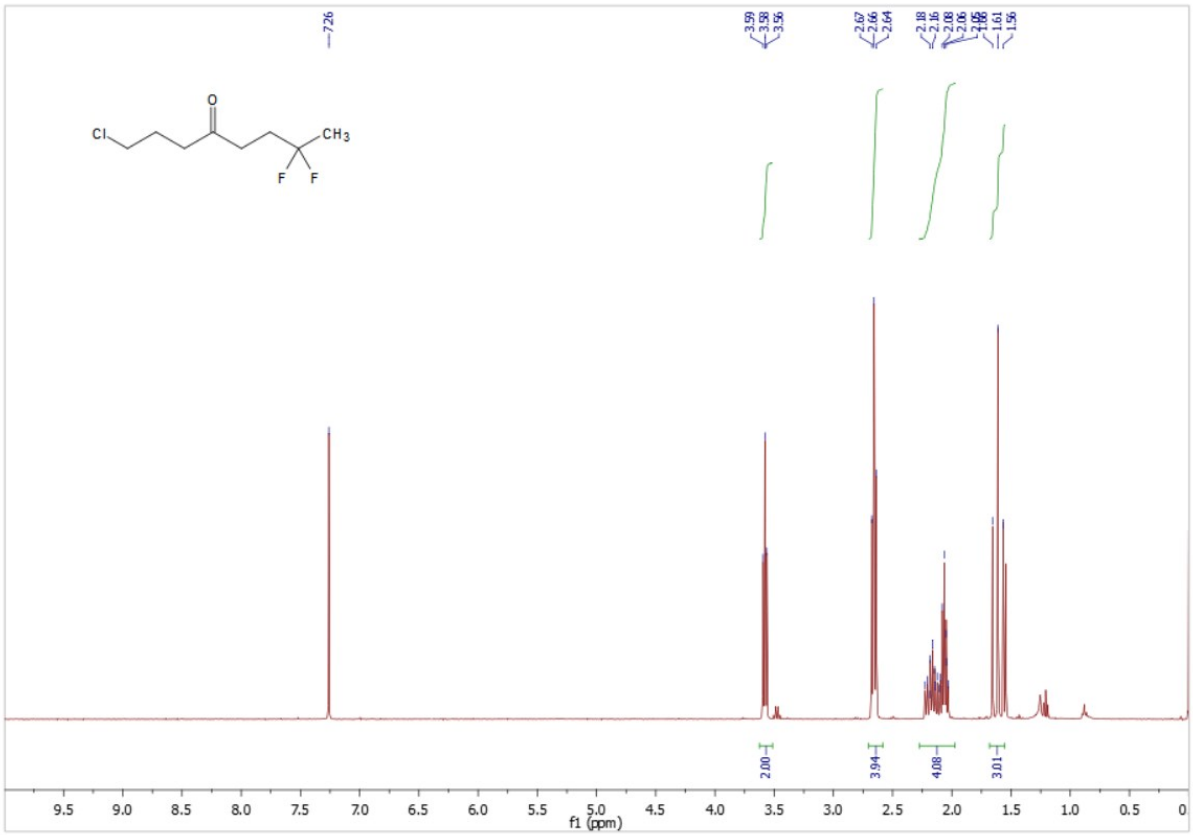

207.40
139.30
131.24
128.50
125.76
123.02
114.30
77.48
76.84
42.98
35.09
35.01
34.99
34.96
33.92
29.44
29.41
29.27
29.19
29.03
28.90
28.21
27.91
27.62
23.90
O
H2C
F
F
F
f1 (ppm)

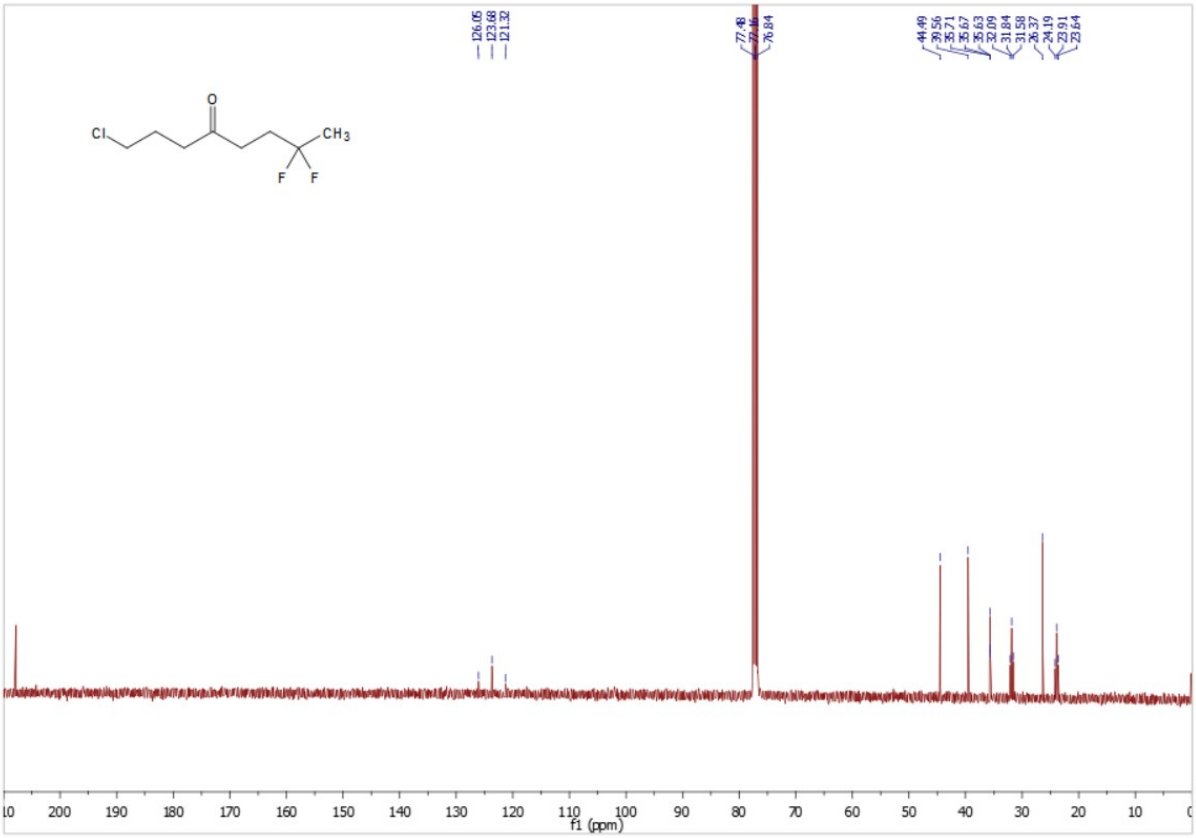

66.60
66.63
66.65
O
H2C
F
F
F
f1 (ppm)

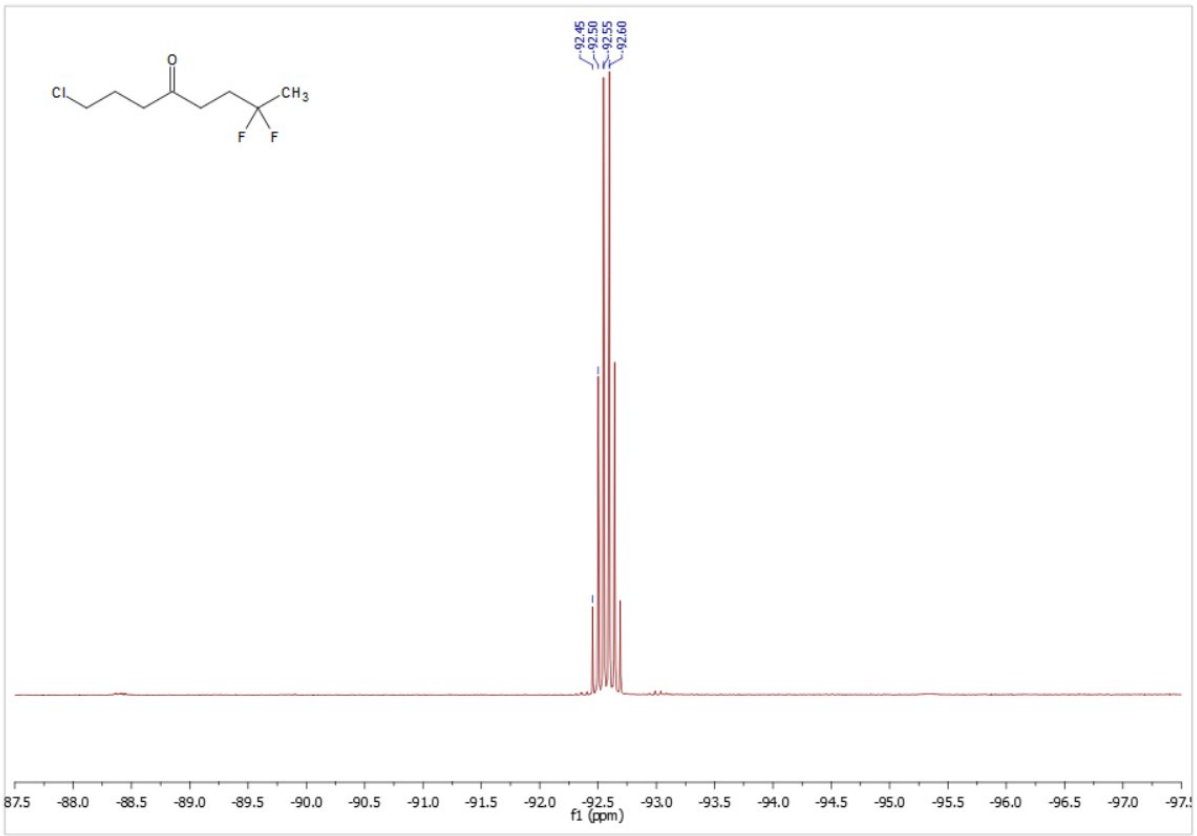

O
CH3
F
F
f1 (ppm)

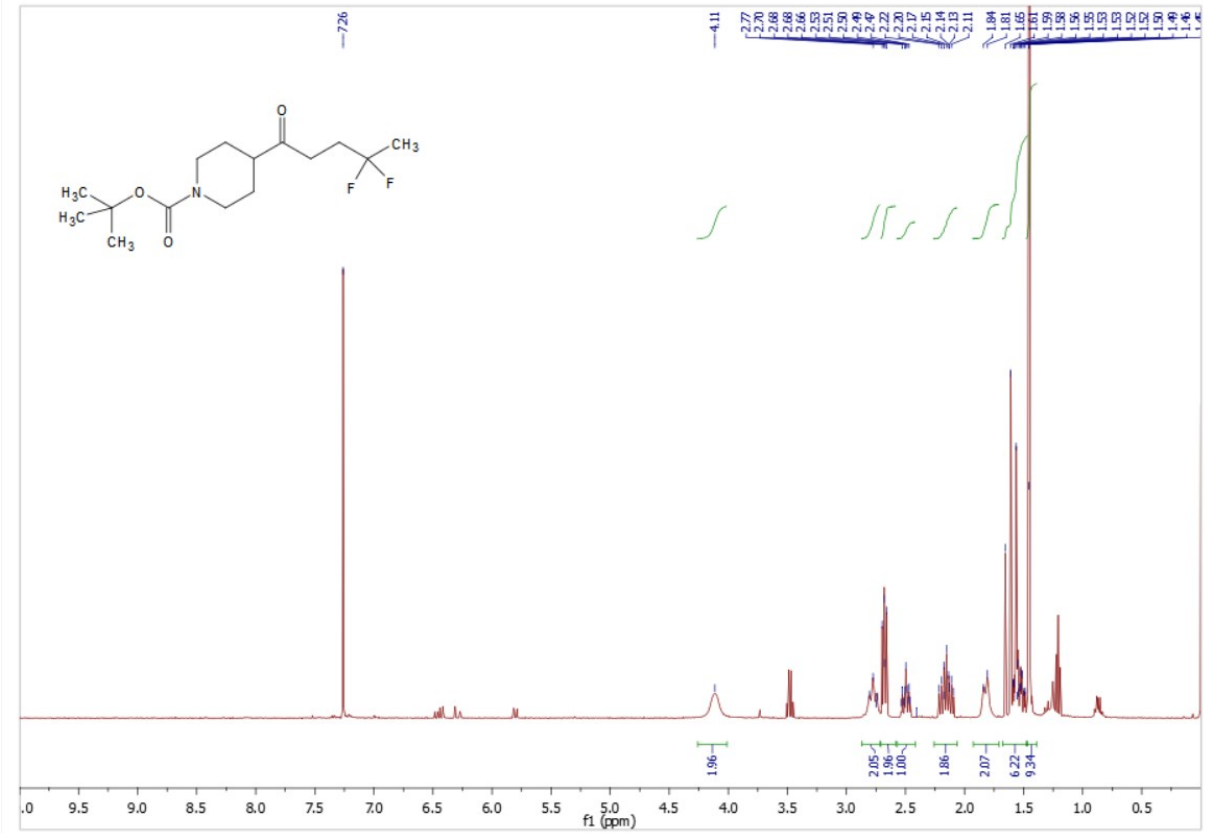

O
CH3
F
F
f1 (ppm)

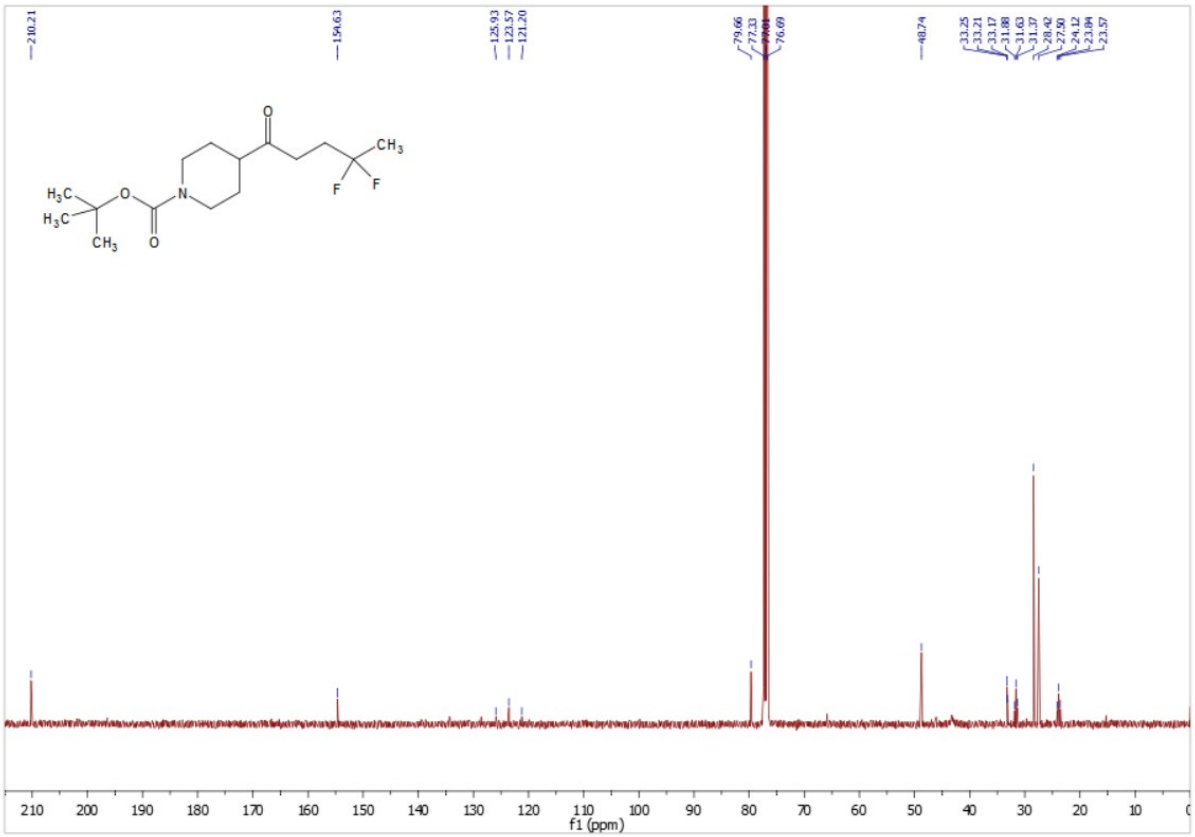

O
CH3
F F
-92.36
-92.40
-92.45
-92.50
-92.55
-92.59
f1 (ppm)

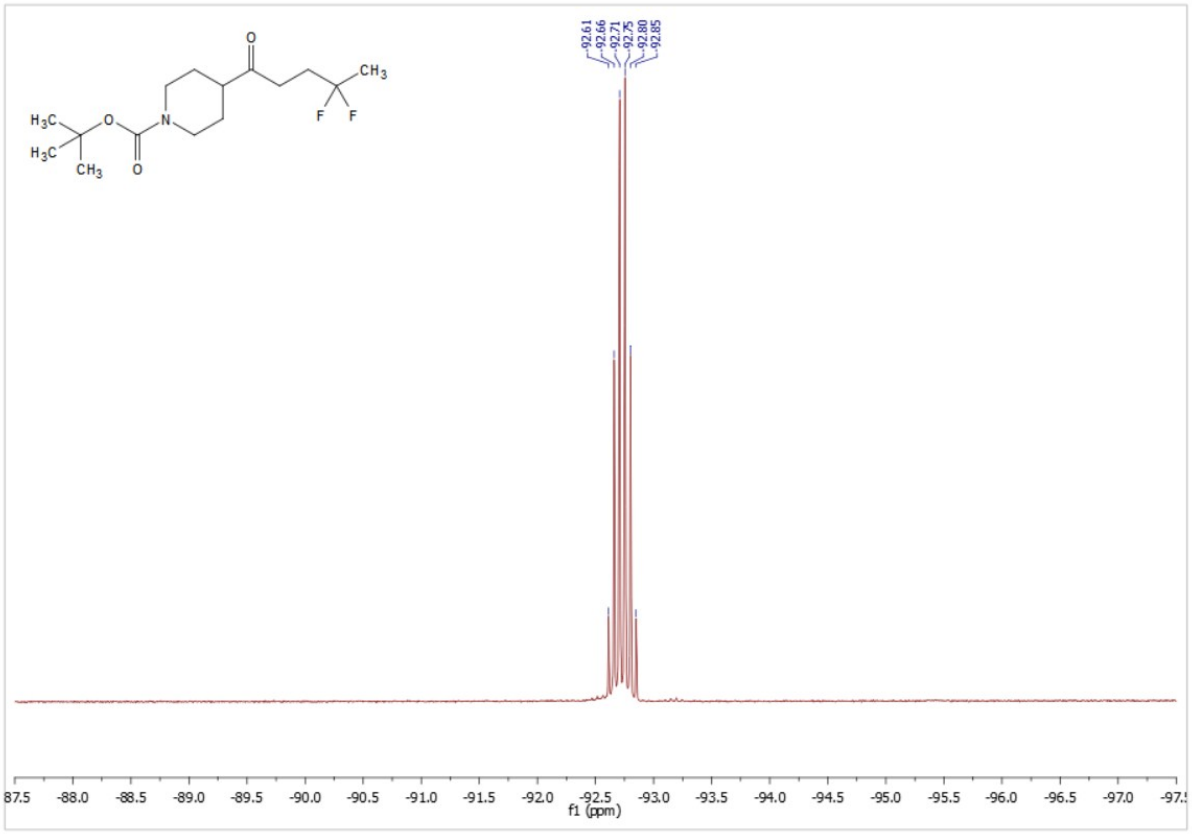

7.26
3.59
3.58
3.56
2.67
2.66
2.64
2.18
2.16
2.08
2.06
1.61
1.56
O
Cl
CH3
F F
2.00
3.94
4.08
3.01
f1 (ppm)

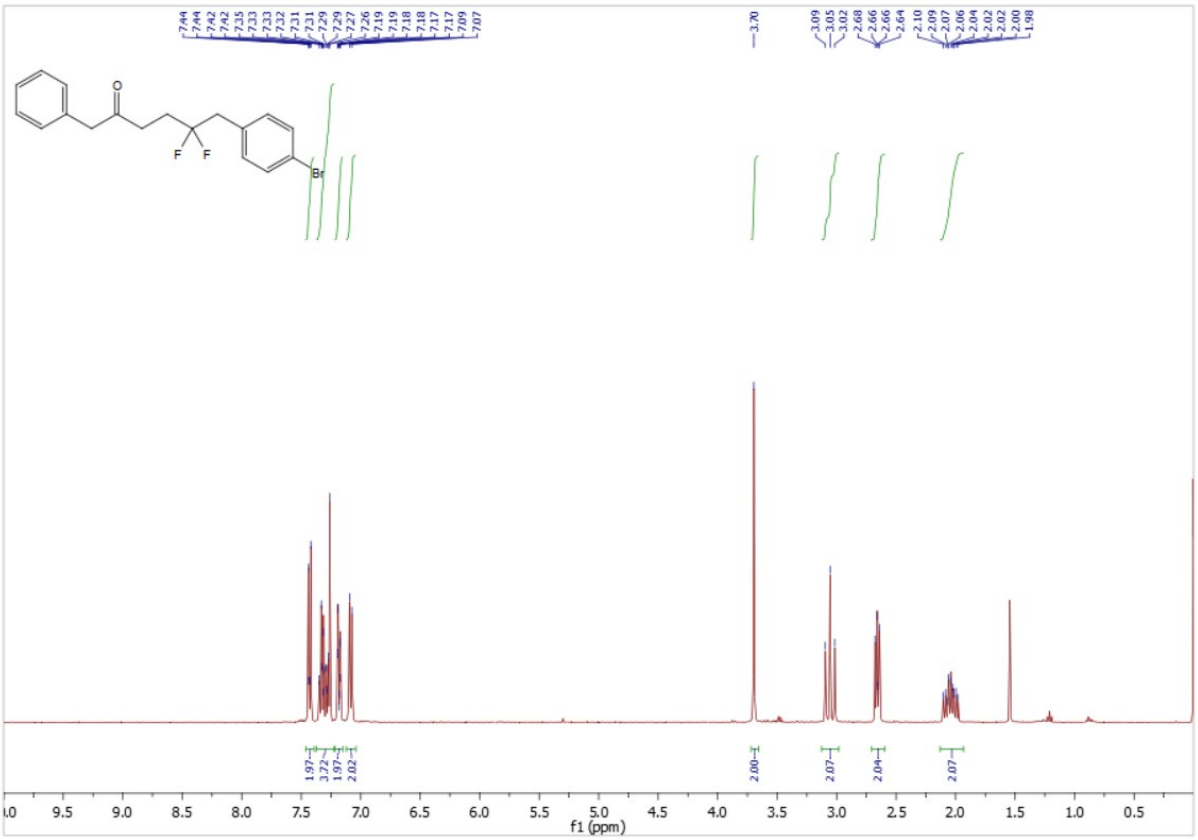

126.05
123.68
121.32
77.48
77.16
76.84
44.49
39.56
35.71
35.67
35.63
32.09
31.84
31.58
26.37
24.19
23.91
23.64
O
Cl
CH3
F
F
f1 (ppm)

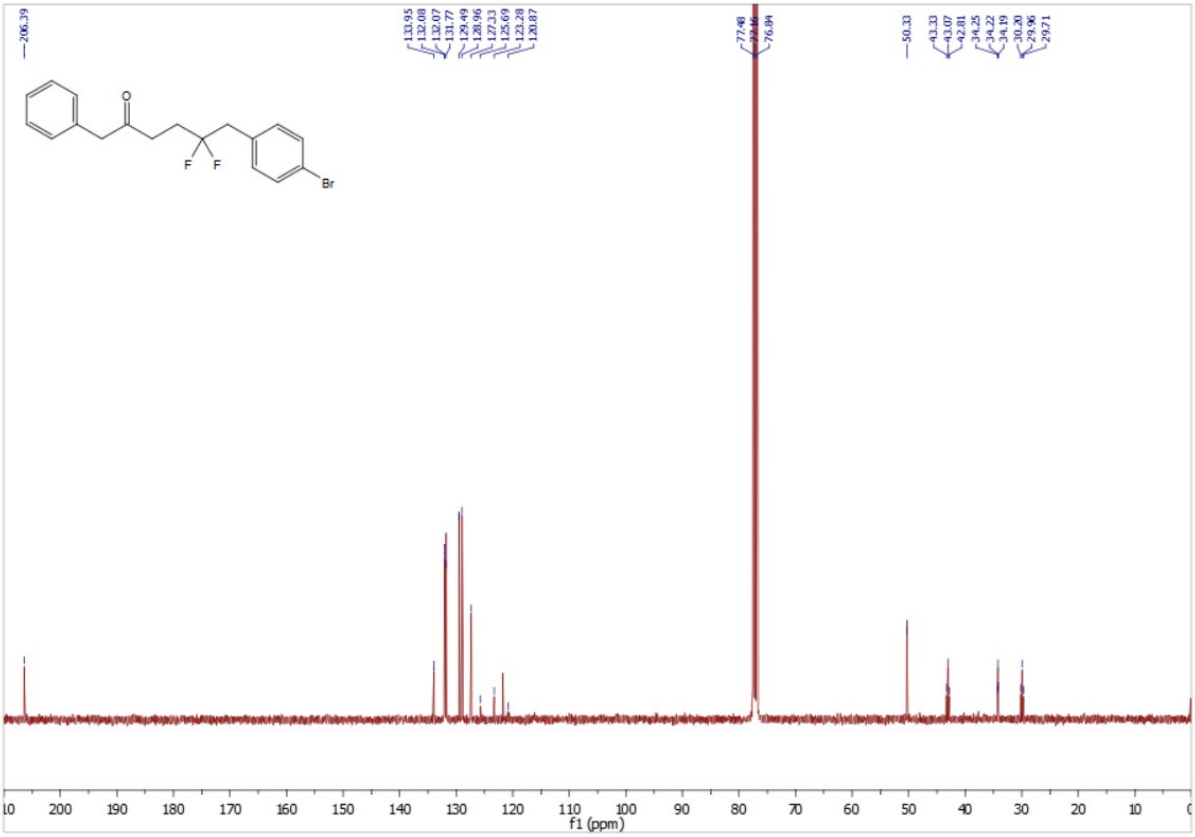

-92.45
-92.50
-92.55
-92.60
O
Cl
CH3
F
F
f1 (ppm)

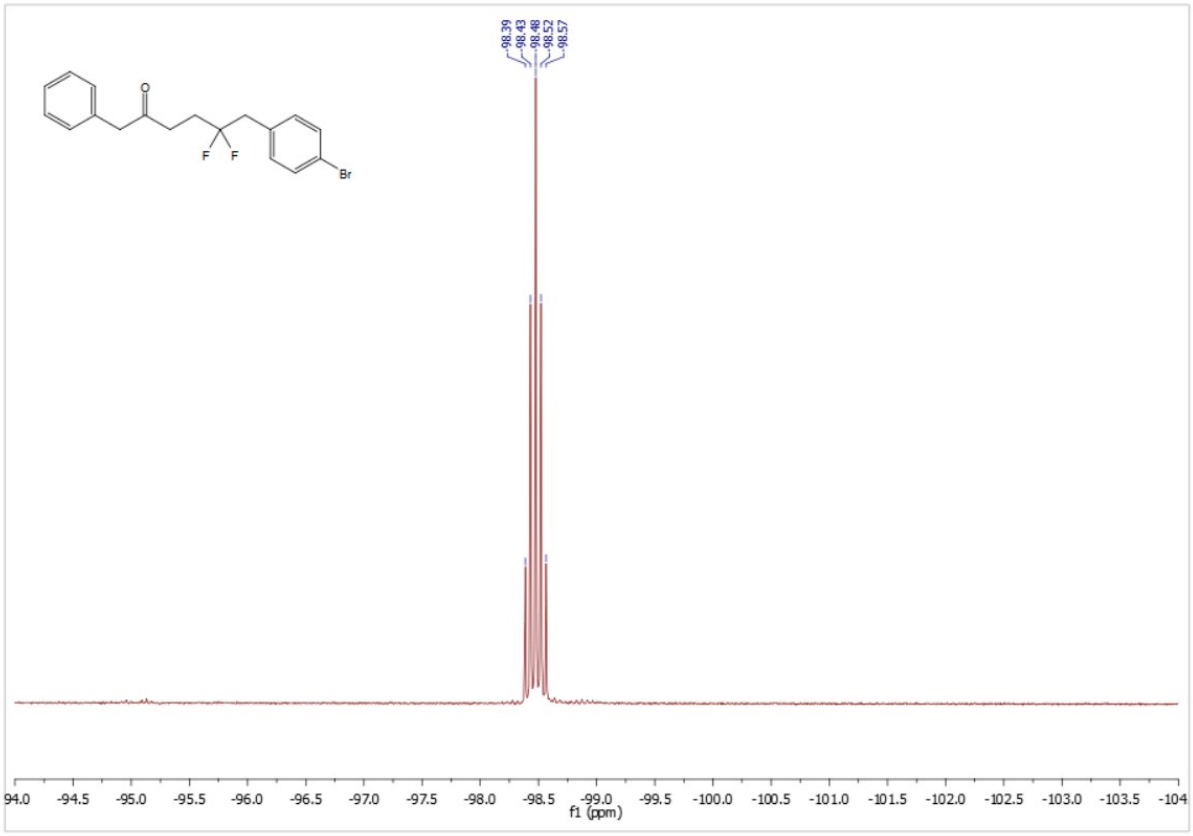

7.26
4.11
1.96
2.05
1.96
1.00
1.86
2.07
6.22
9.34
f1 (ppm)

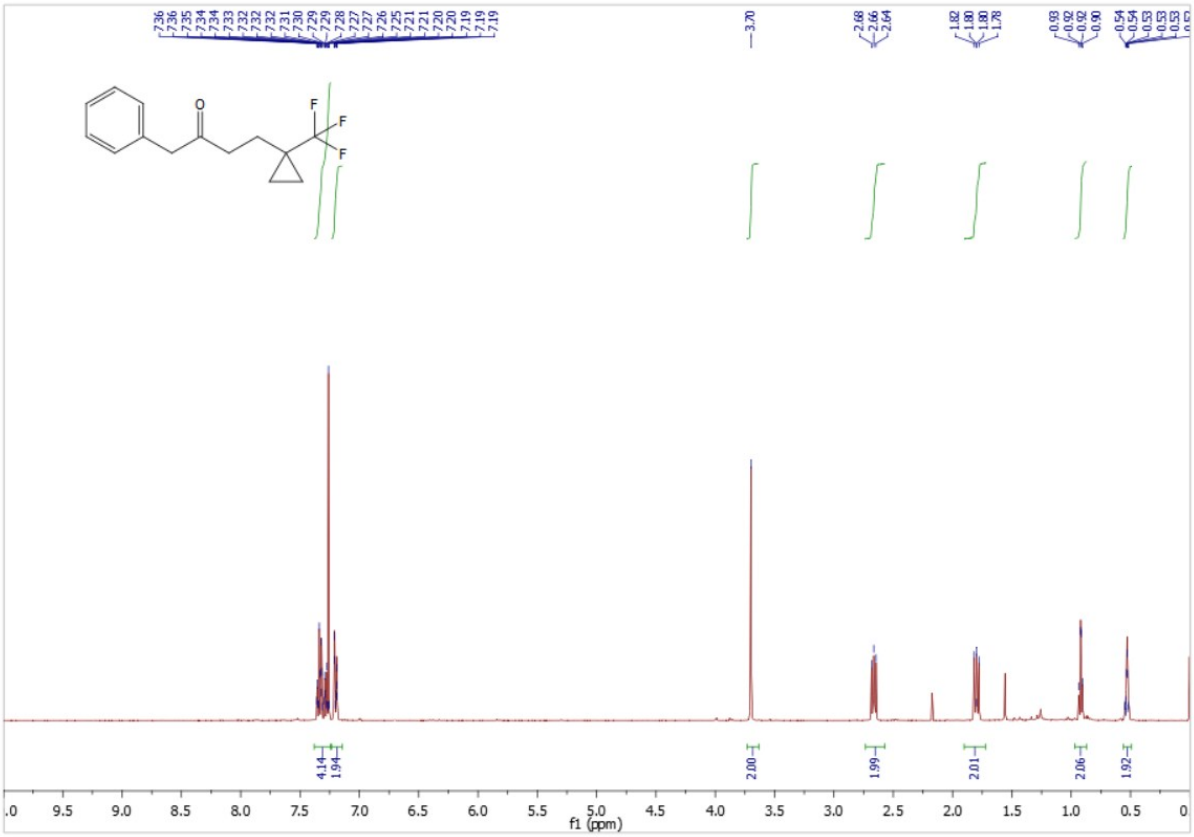

210.21
154.63
125.93
123.57
121.20
79.66
77.33
77.01
76.69
48.74
33.25
33.21
33.17
31.88
31.63
31.37
28.42
27.50
24.12
23.04
23.57
f1 (ppm)

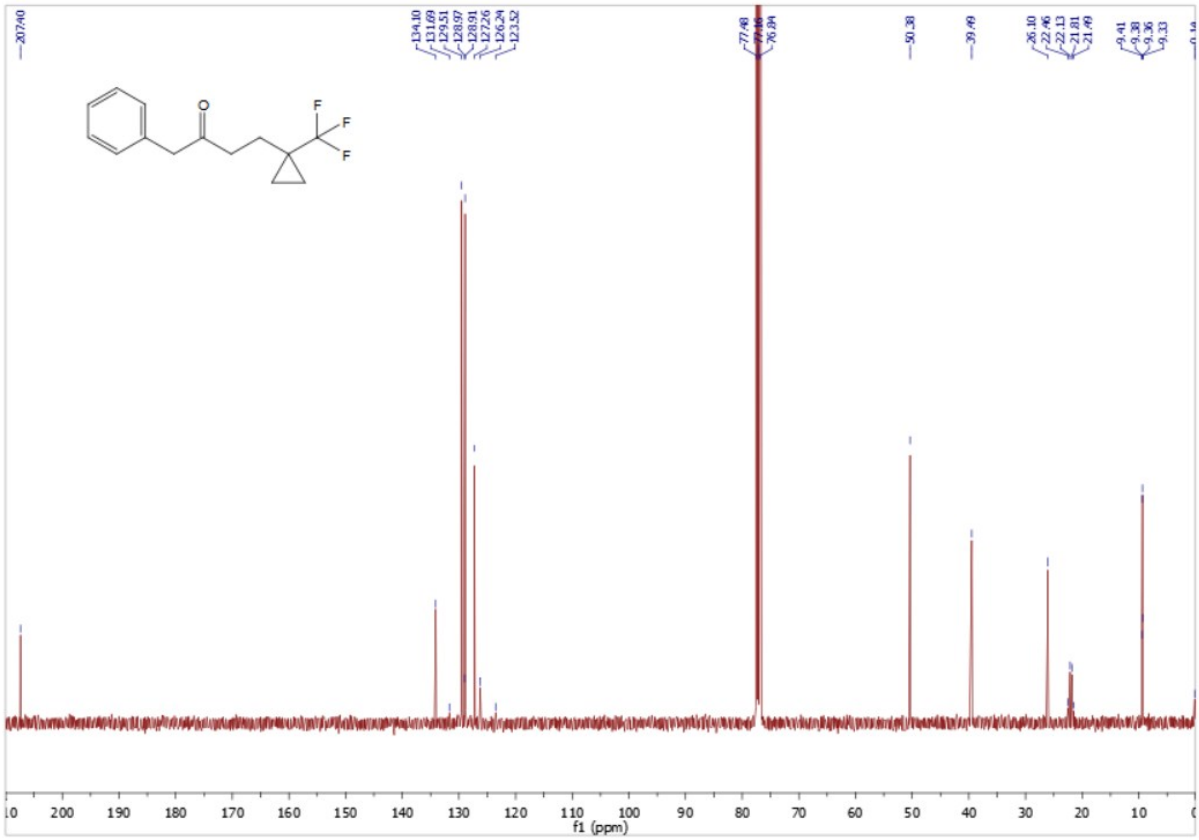

-92.61
-92.66
-92.71
-92.75
-92.80
-92.85
f1 (ppm)

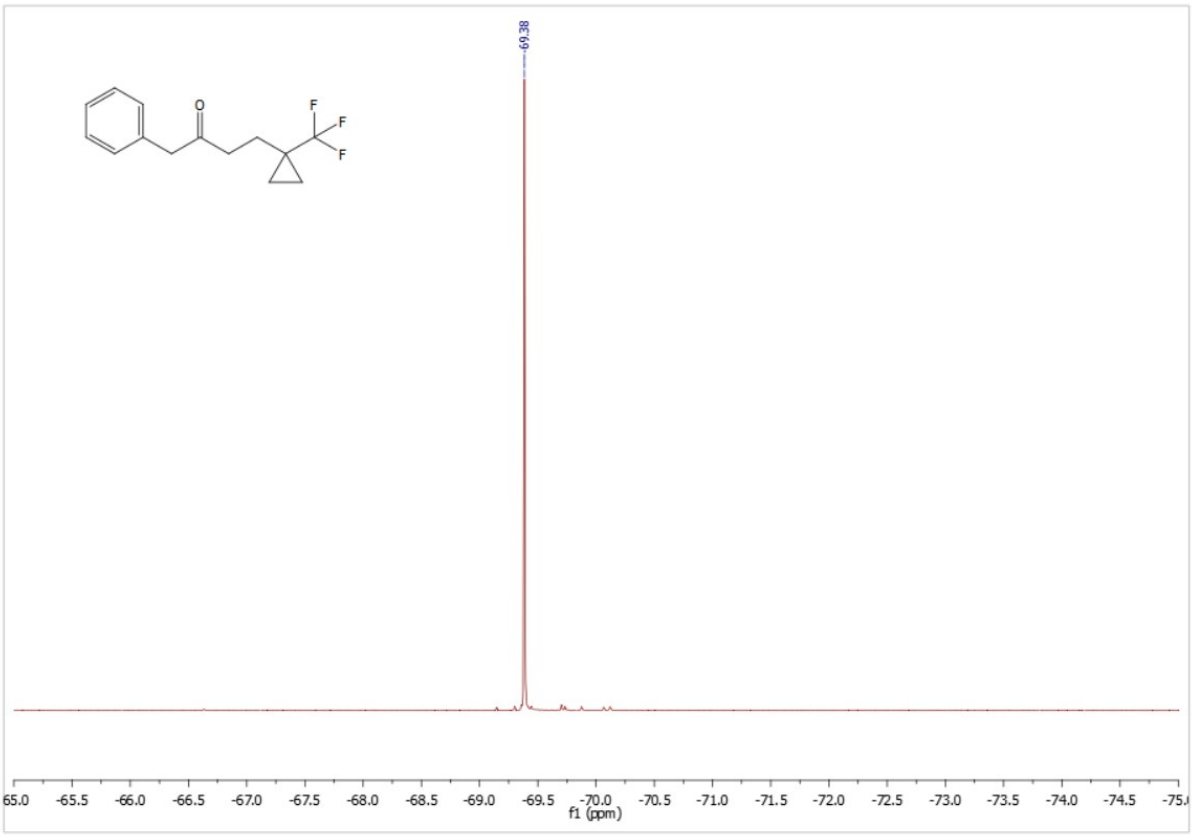

7.44
7.44
7.42
7.42
7.35
7.33
7.33
7.32
7.31
7.31
7.29
7.29
7.27
7.26
7.19
7.19
7.18
7.18
7.17
7.17
7.09
7.07
3.70
3.09
3.05
3.02
2.68
2.66
2.66
2.64
2.10
2.09
2.07
2.06
2.04
2.02
2.02
2.00
1.98
1.97
3.72
1.97
2.02
2.00
2.07
2.04
2.07
f1 (ppm)

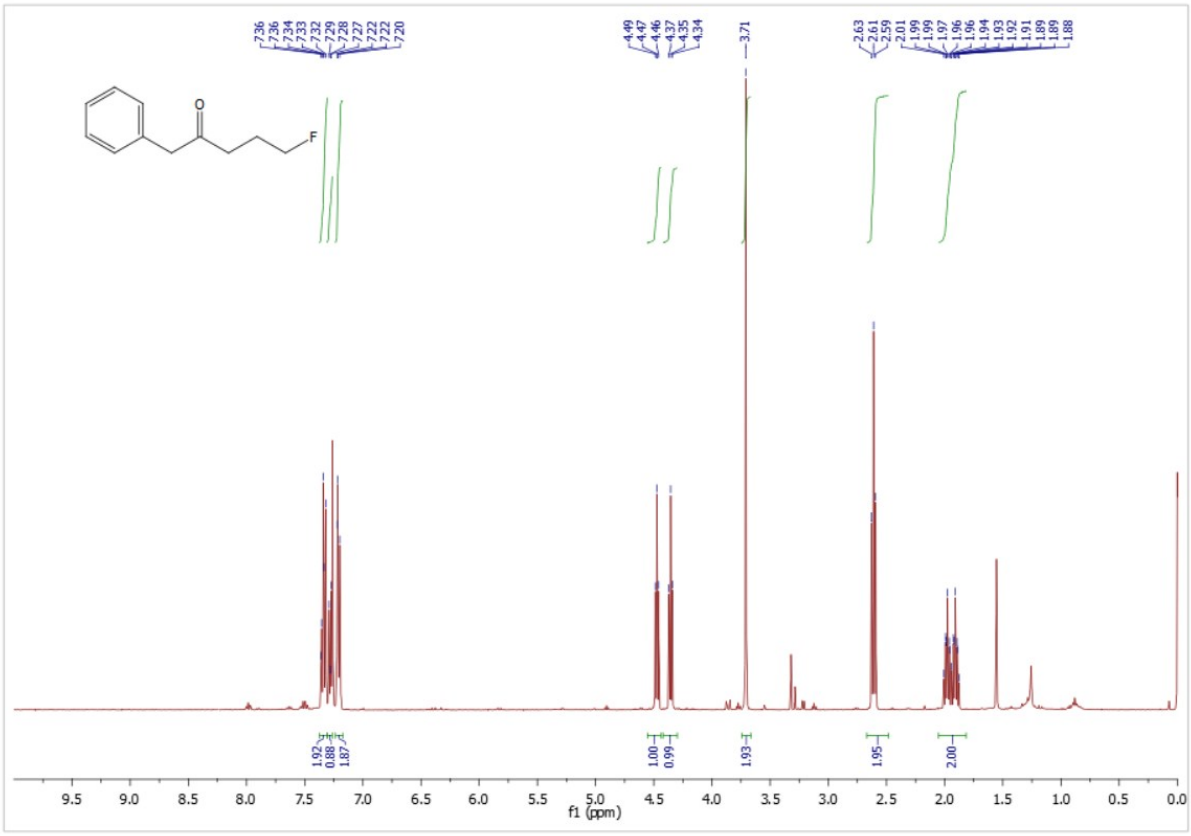

206.39
133.95
132.08
132.07
131.77
129.49
128.96
127.33
125.69
123.28
120.87
77.48
77.16
76.84
50.33
43.33
43.07
42.81
34.25
34.22
34.19
30.30
29.96
29.71
O
F
F
Br
f1 (ppm)

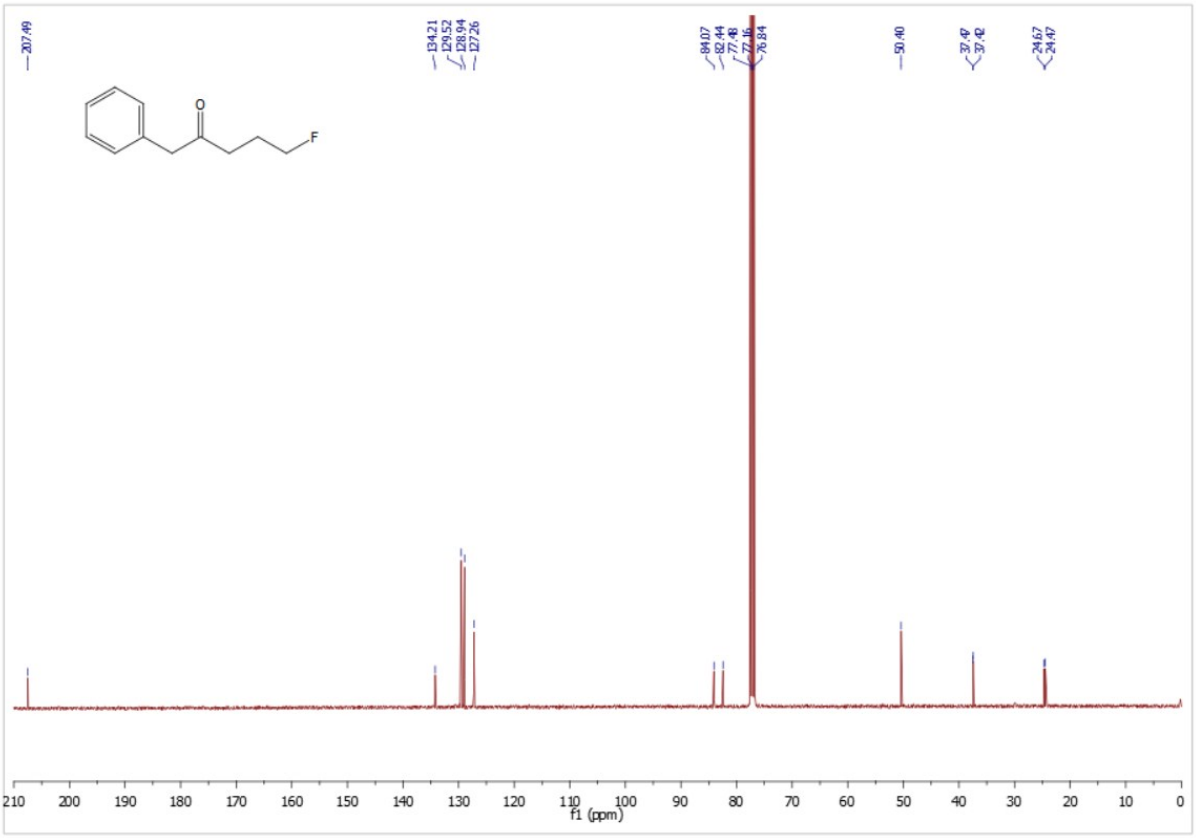

98.39
98.43
98.48
98.52
98.57
O
F
F
Br
f1 (ppm)

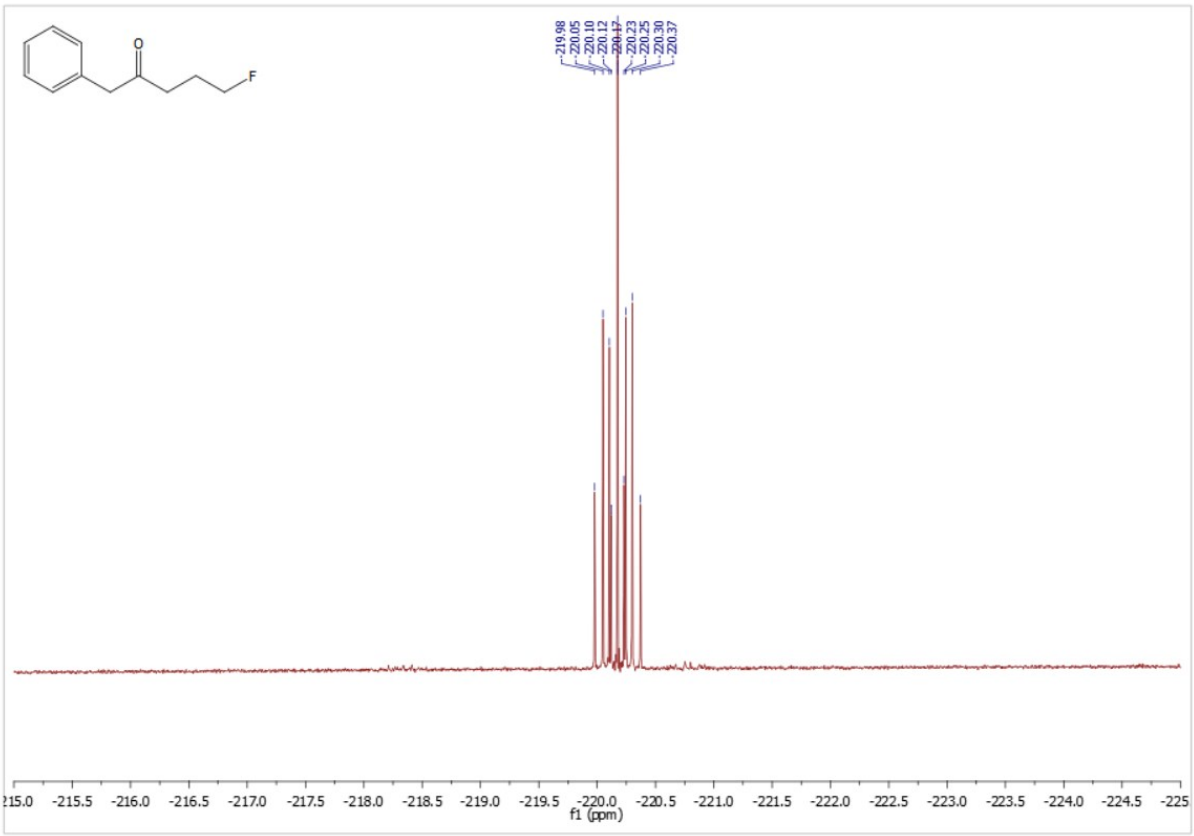

O
F
F
F
f1 (ppm)

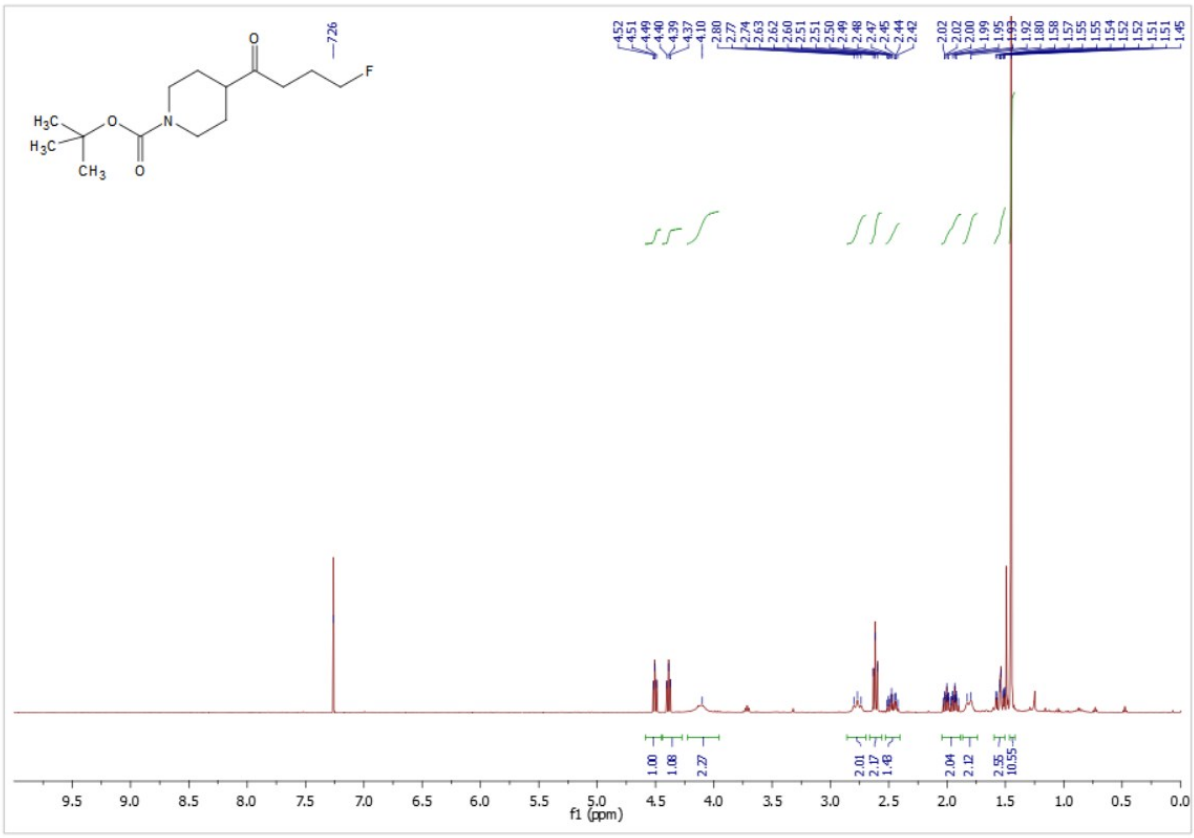

O
F
F
F
f1 (ppm)

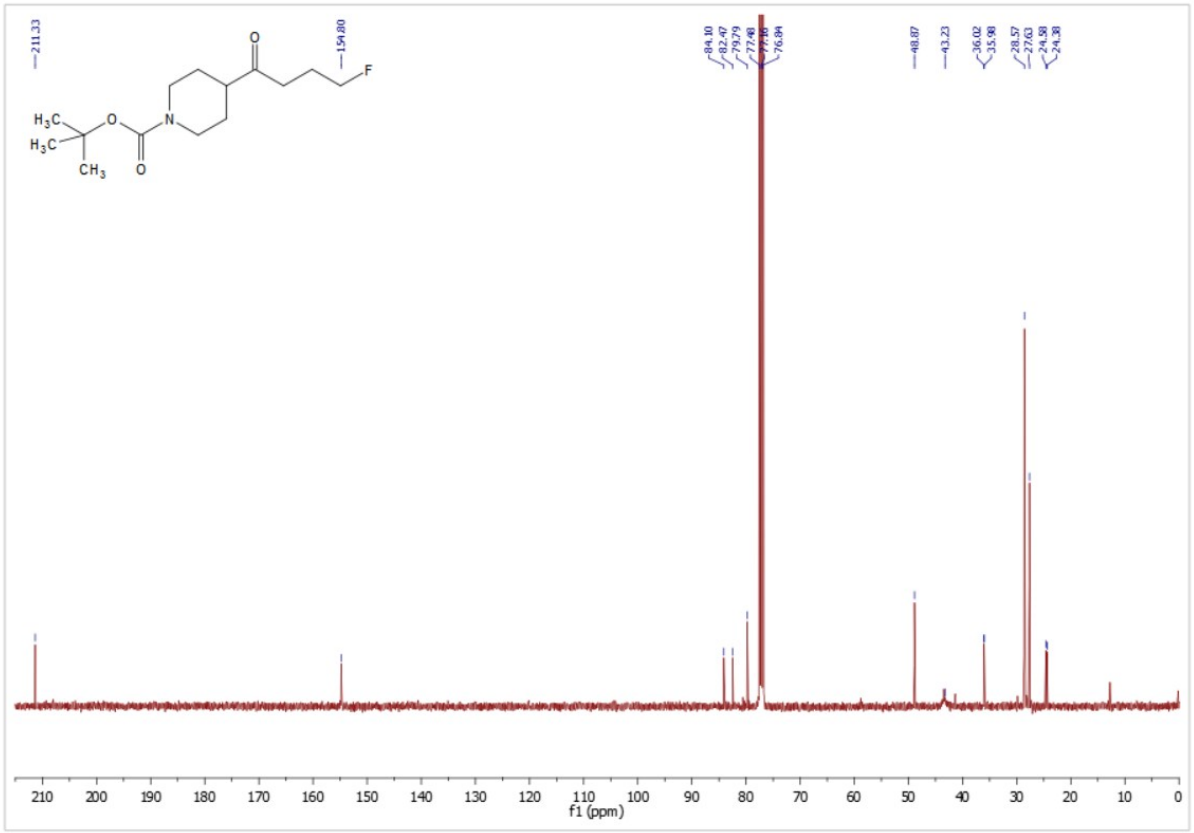

O
F
F
F
-69.38
65.0
-65.5
-66.0
-66.5
-67.0
-67.5
-68.0
-68.5
-69.0
-69.5
-70.0
-70.5
-71.0
-71.5
-72.0
-72.5
-73.0
-73.5
-74.0
-74.5
f1 (ppm)

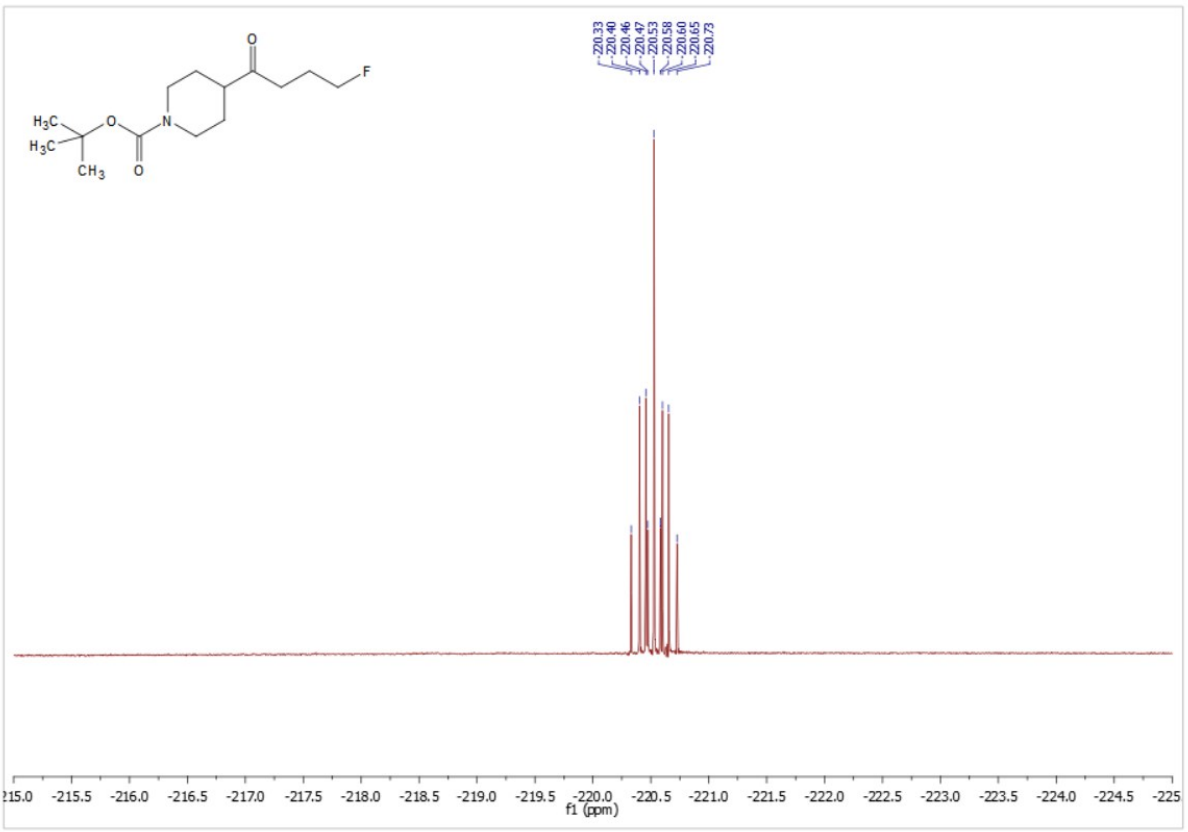

7.36
7.36
7.34
7.33
7.32
7.29
7.28
7.27
7.22
7.22
7.20
4.49
4.47
4.46
4.37
4.35
4.34
3.71
2.63
2.61
2.59
2.01
1.99
1.99
1.97
1.96
1.96
1.94
1.93
1.92
1.91
1.89
1.89
1.88
O
F
1.92
0.88
1.87
1.00
0.99
1.93
1.95
2.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


207.49
134.21
129.52
128.94
127.26
84.07
82.44
77.48
77.16
76.84
50.40
37.49
37.42
24.67
24.47
O
F
f1 (ppm)

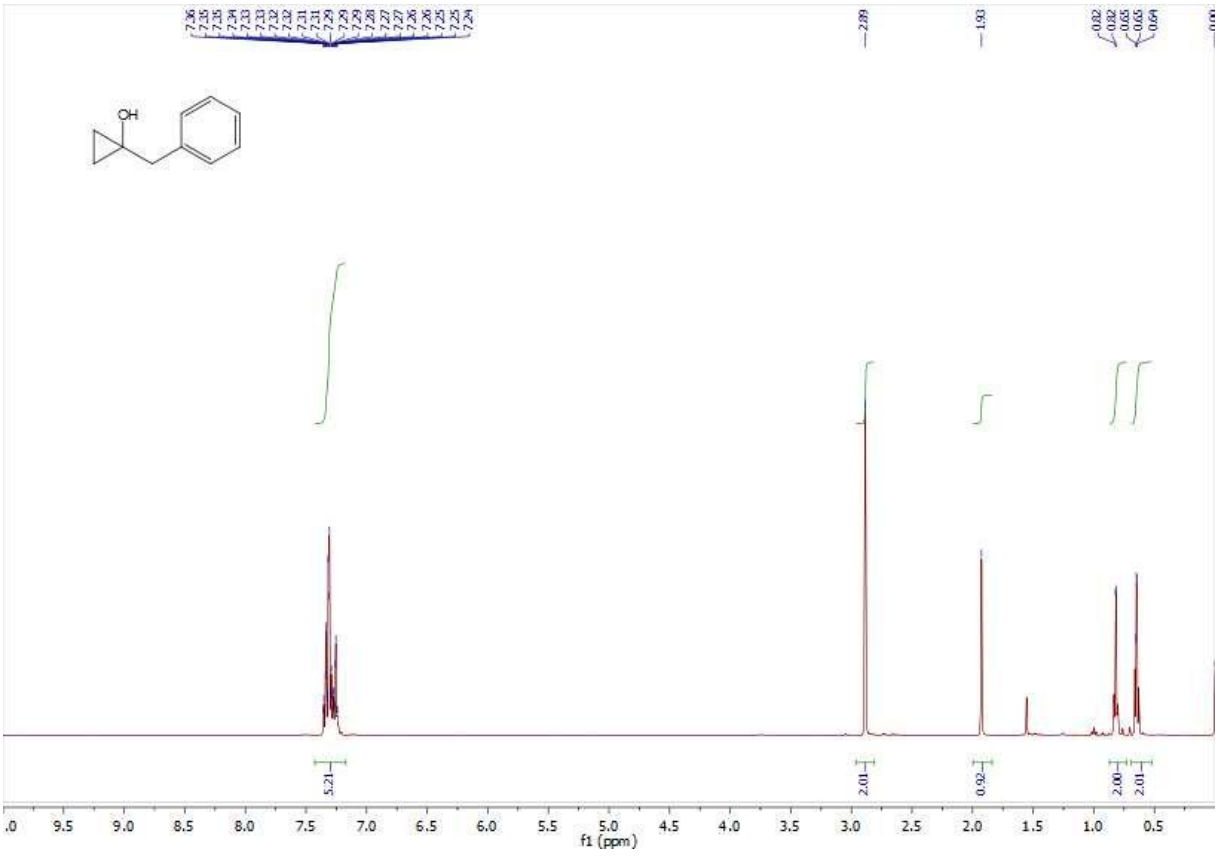

219.98
220.05
220.10
220.12
220.17
220.23
220.25
220.30
220.37
O
F
f1 (ppm)

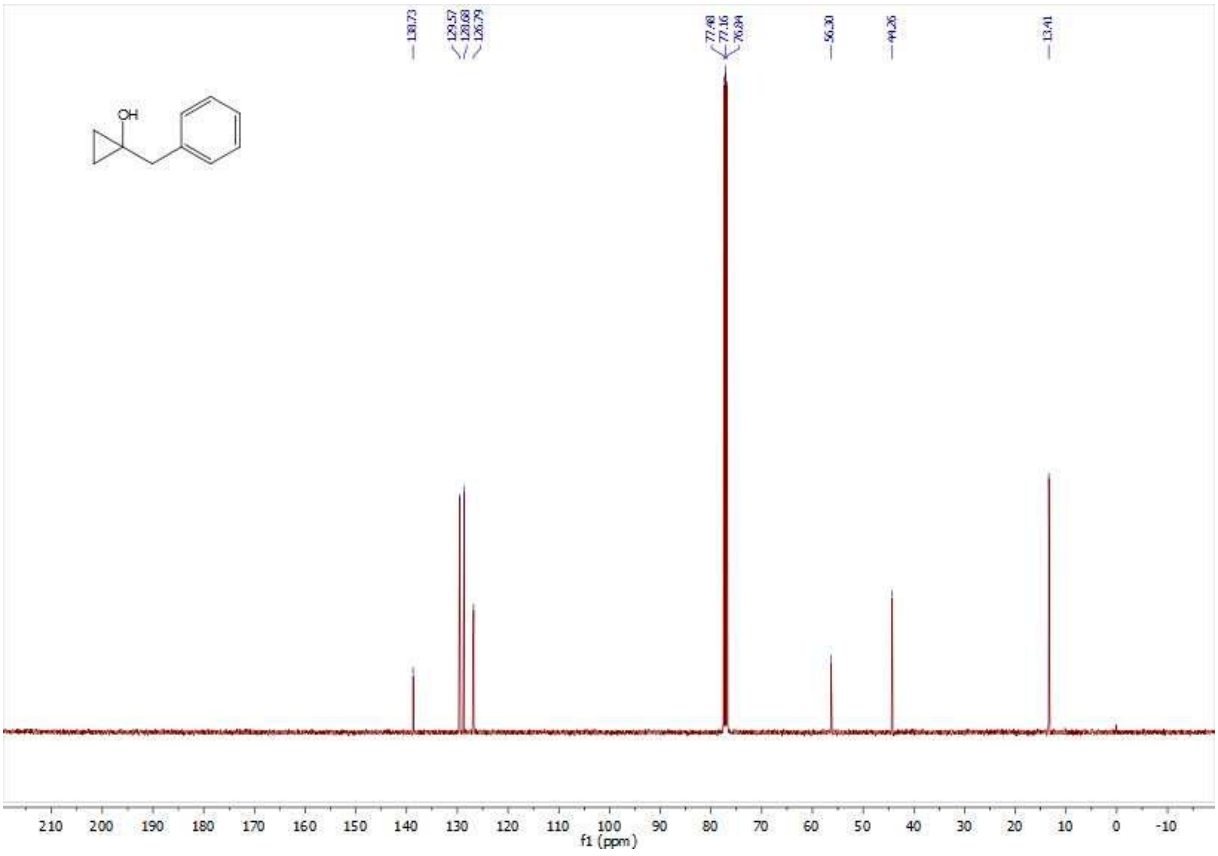

7.26
4.52
4.51
4.49
4.40
4.39
4.37
4.10
2.80
2.77
2.74
2.63
2.62
2.60
2.51
2.51
2.50
2.49
2.48
2.47
2.45
2.44
2.42
2.02
2.02
2.00
1.99
1.95
1.93
1.92
1.80
1.58
1.57
1.55
1.55
1.54
1.52
1.52
1.51
1.51
1.45
1.00
1.08
2.27
2.01
2.17
1.48
2.04
2.12
2.55
10.55
f1 (ppm)

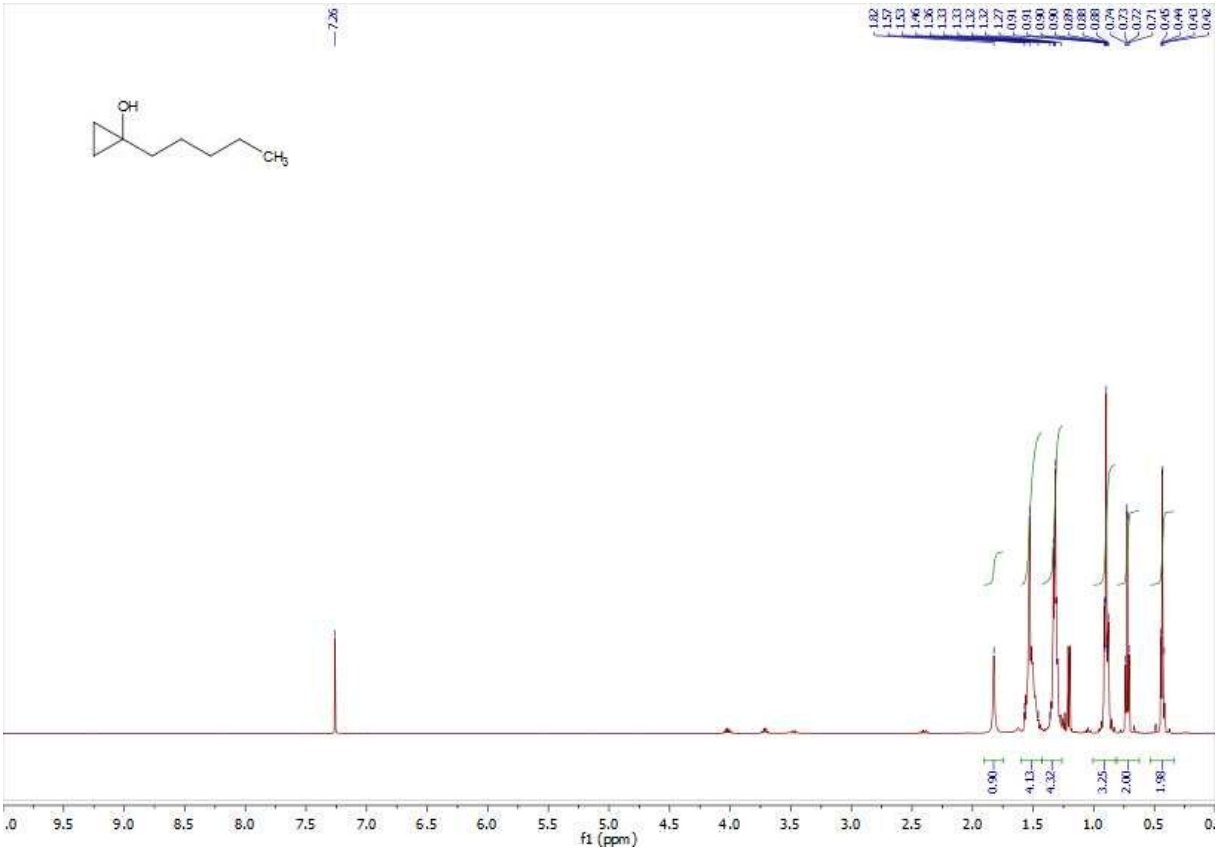

211.33
159.80
84.10
82.47
79.79
77.48
77.16
76.84
48.87
43.23
36.02
35.98
28.57
27.63
24.58
24.38
f1 (ppm)

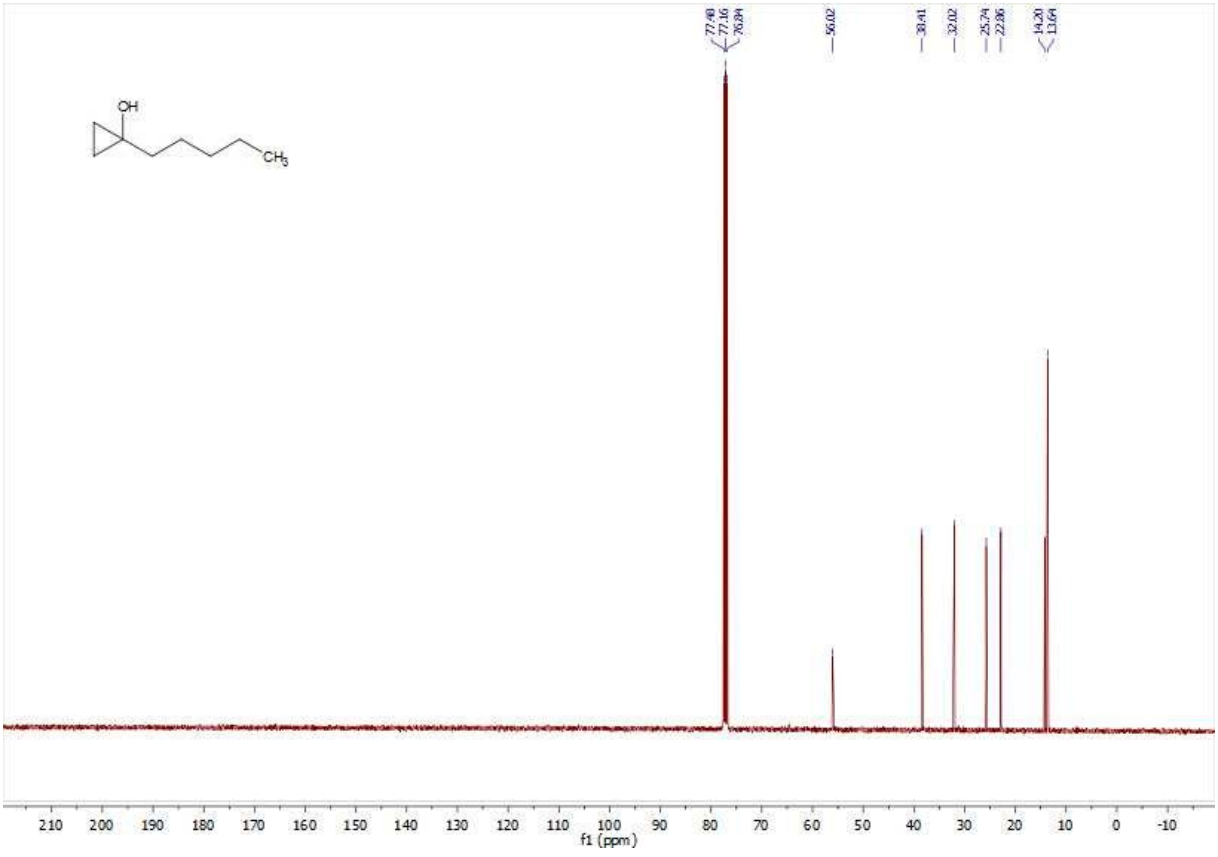

220.33
220.40
220.46
220.47
220.53
220.58
220.60
220.65
220.73
O
F
H3C
O
N
H3C
CH3
O
-215.0
-215.5
-216.0
-216.5
-217.0
-217.5
-218.0
-218.5
-219.0
-219.5
-220.0
-220.5
-221.0
-221.5
-222.0
-222.5
-223.0
-223.5
-224.0
-224.5
-225
f1 (ppm)

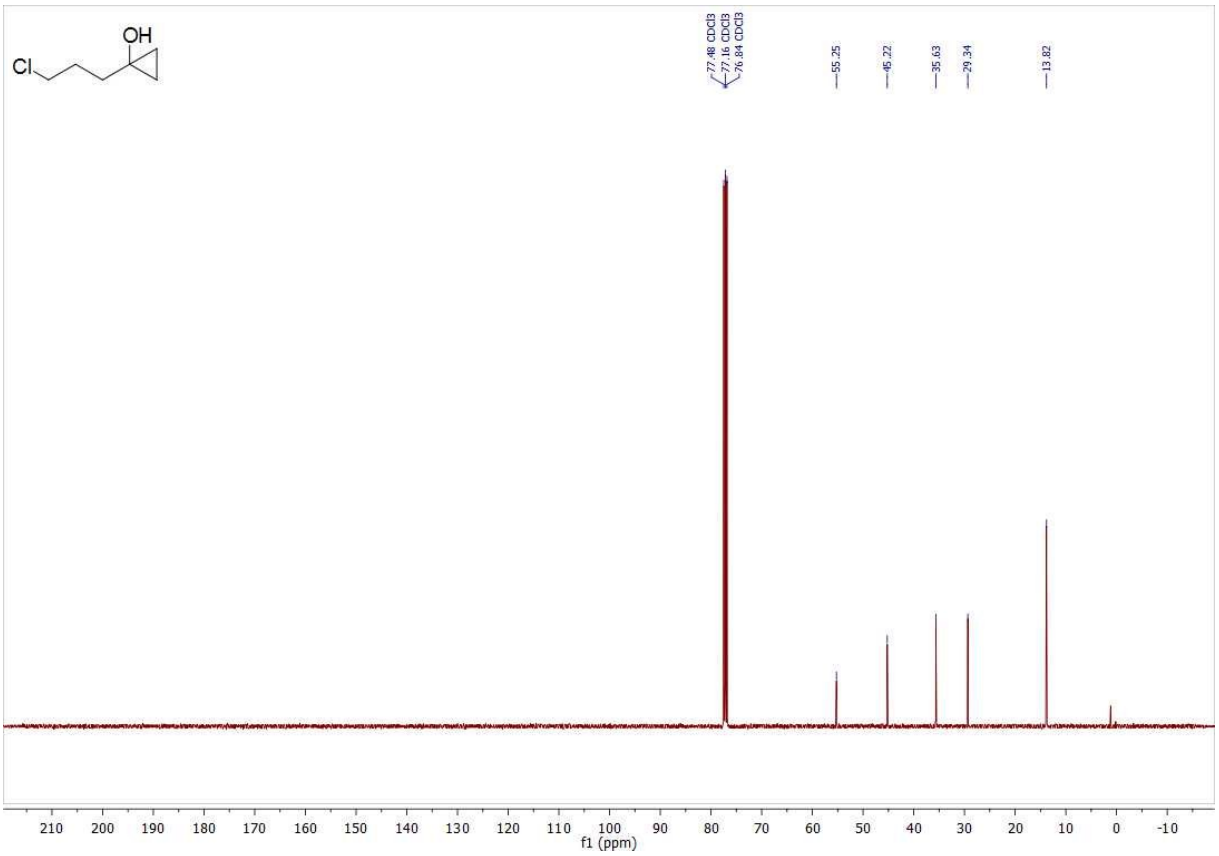
VI. Copies of ^{1}H, ^{13}C NMR for cyclopropanols

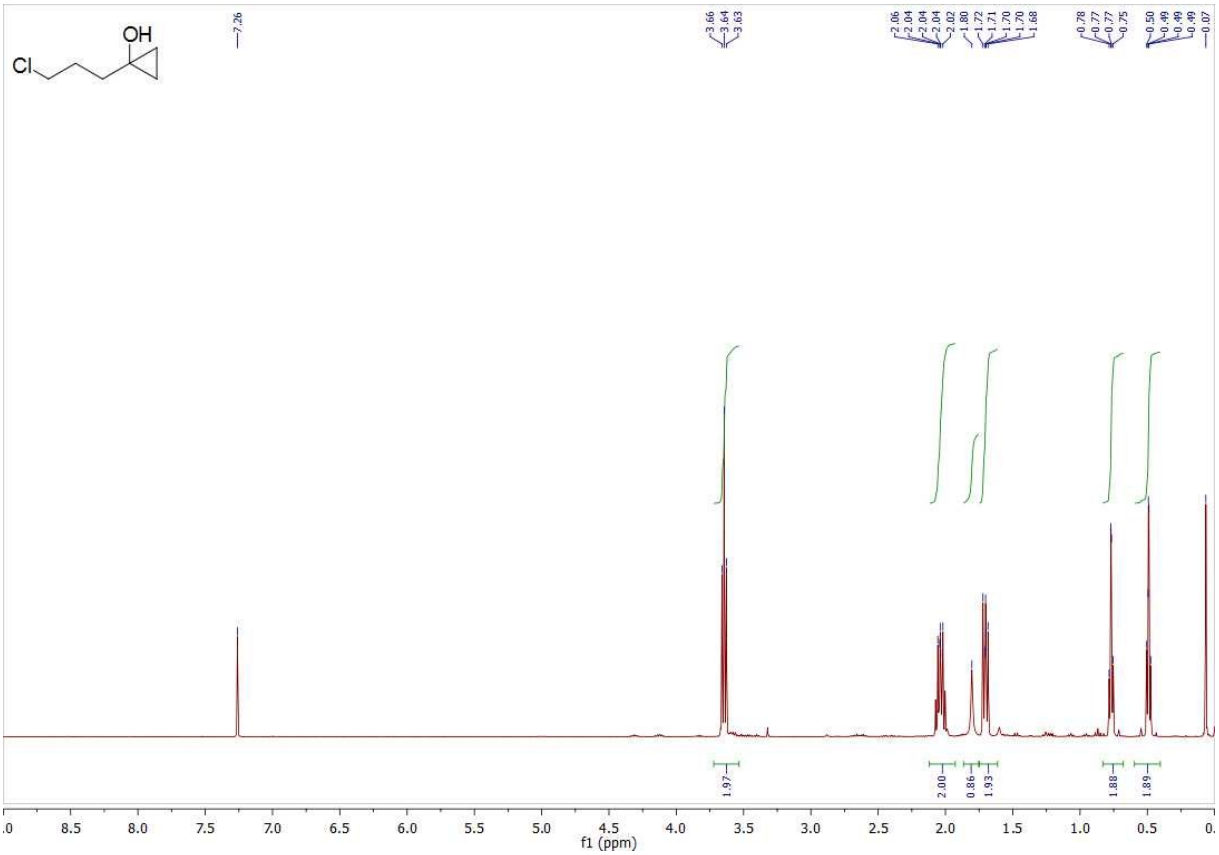


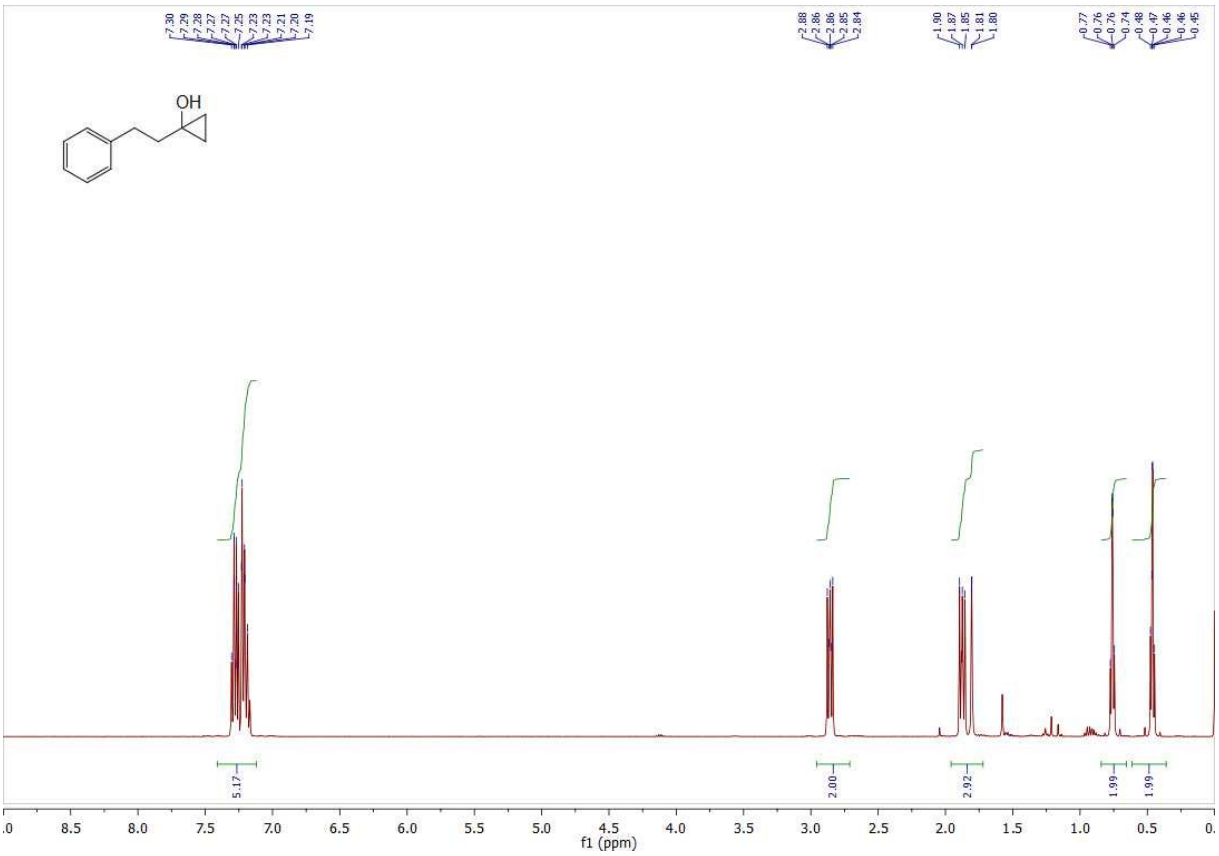


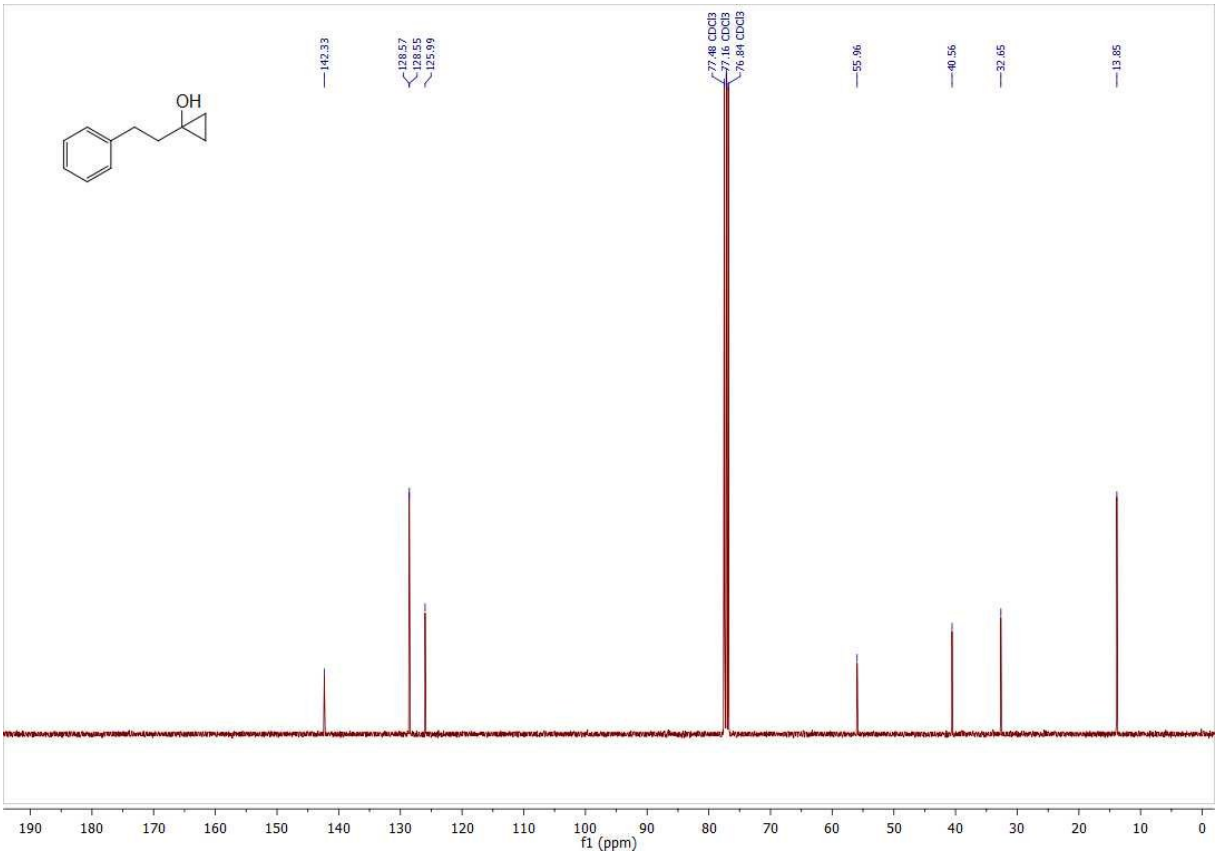

OH
CH3
f1 (ppm)

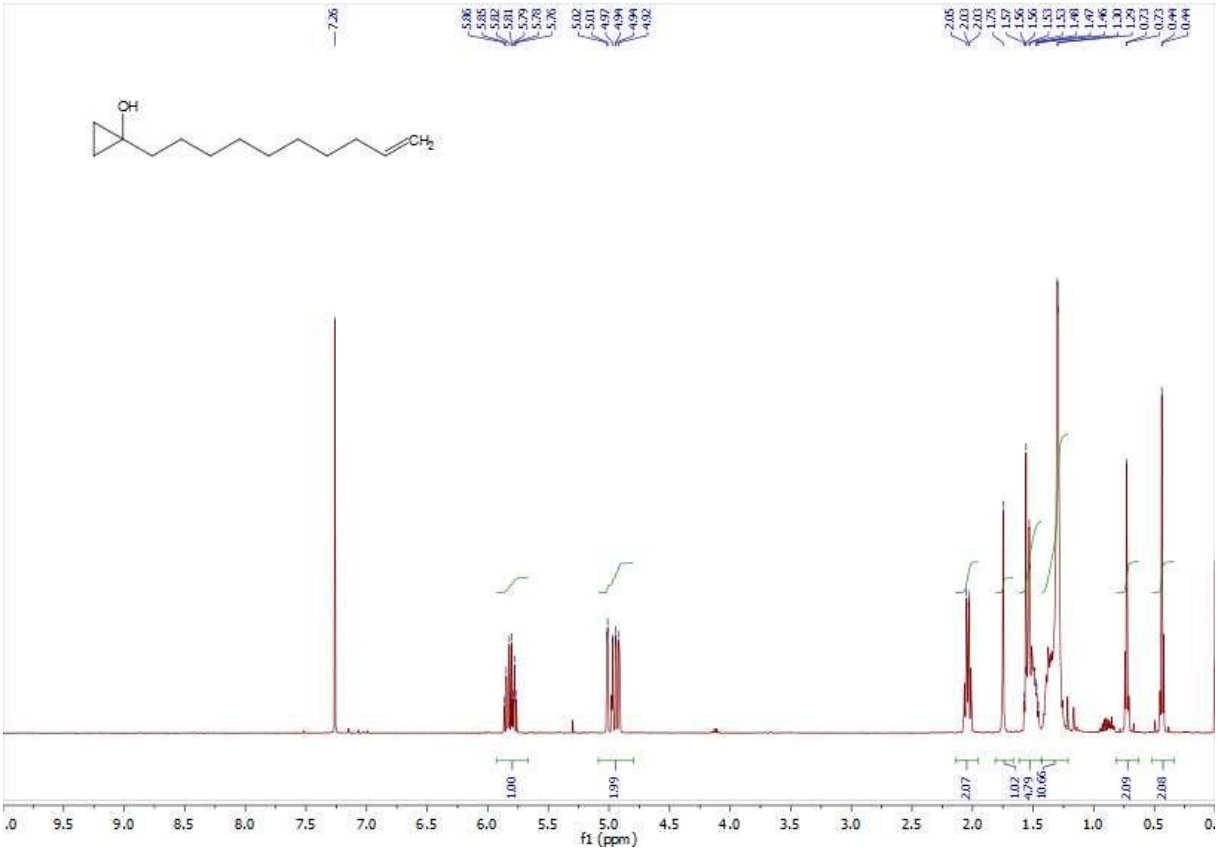

OH
CH3
f1 (ppm)

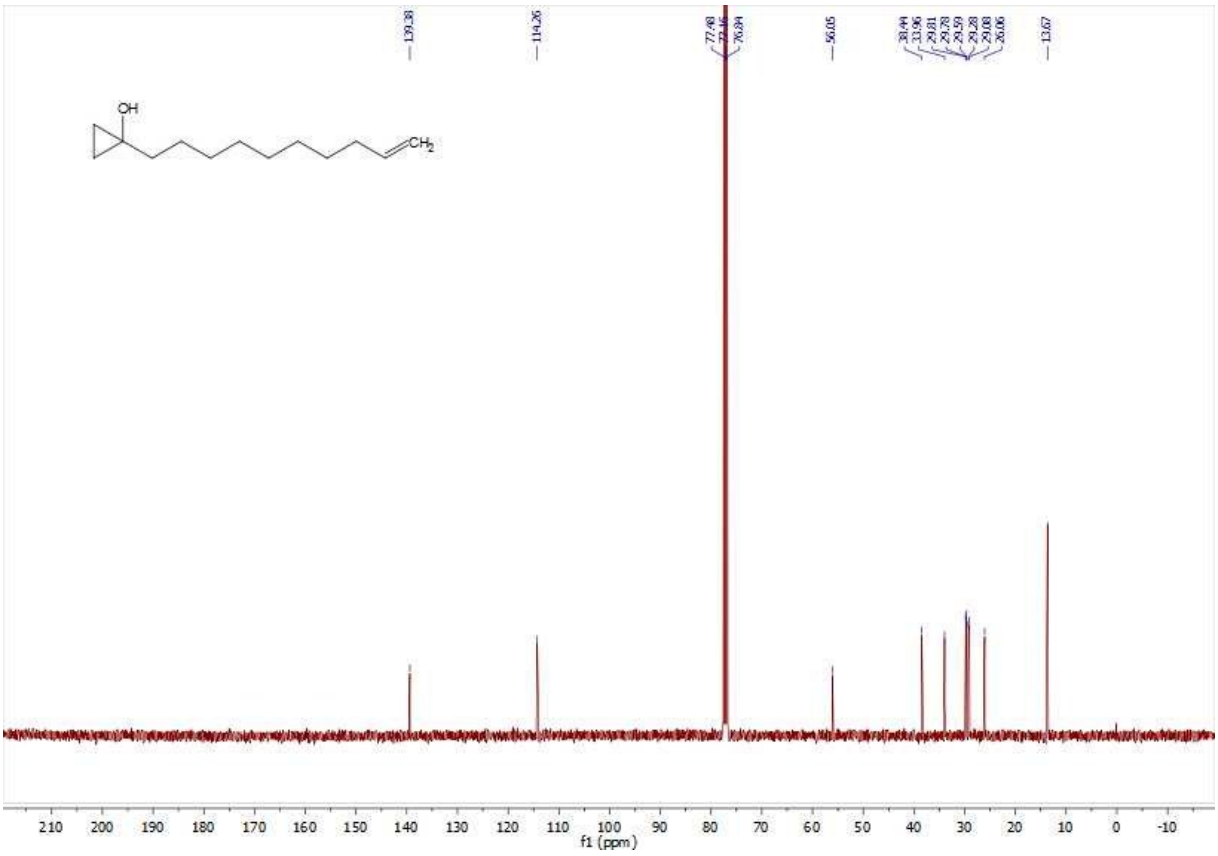

OH
Cl
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
55.25
45.22
35.63
29.34
13.82
f1 (ppm)

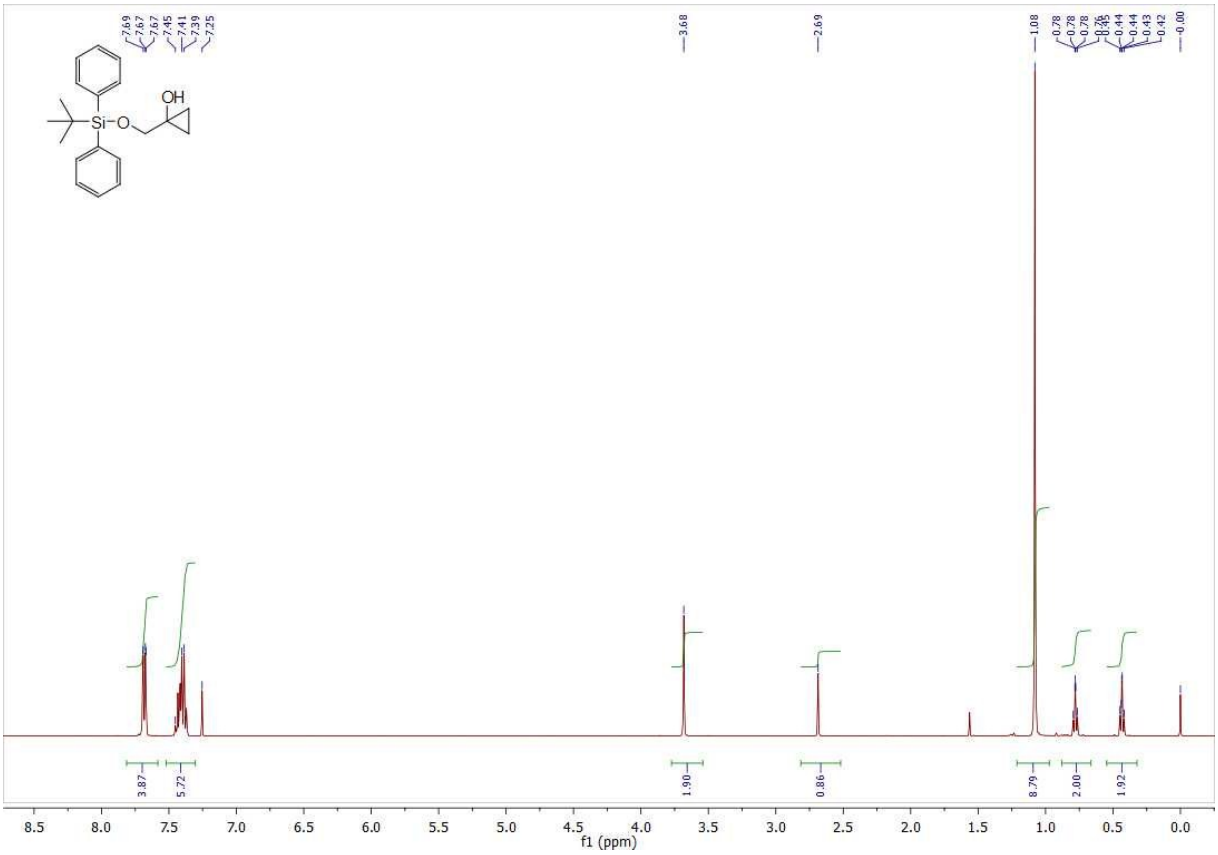

OH
Cl
7.26
3.66
3.64
3.63
2.06
2.04
2.04
2.04
2.02
1.80
1.72
1.71
1.70
1.70
1.68
0.78
0.77
0.77
0.75
0.50
0.49
0.49
0.49
0.07
1.97
2.00
0.86
1.93
1.88
1.89
f1 (ppm)

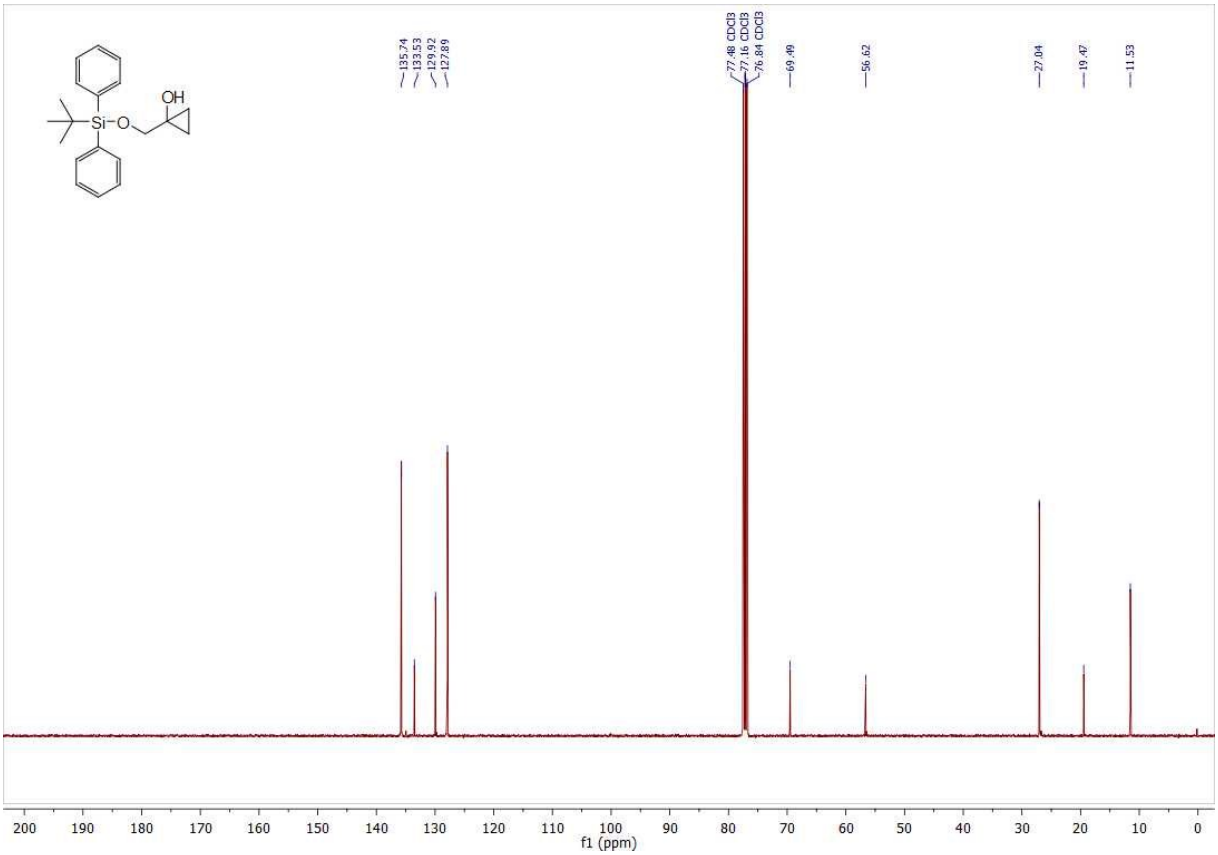

OH
7.30
7.29
7.28
7.27
7.27
7.27
7.25
7.23
7.23
7.21
7.20
7.19
2.88
2.86
2.86
2.85
2.84
1.90
1.87
1.85
1.81
1.80
0.77
0.76
0.76
0.74
0.48
0.47
0.46
0.46
0.45
5.17
2.00
2.92
1.99
1.99
f1 (ppm)

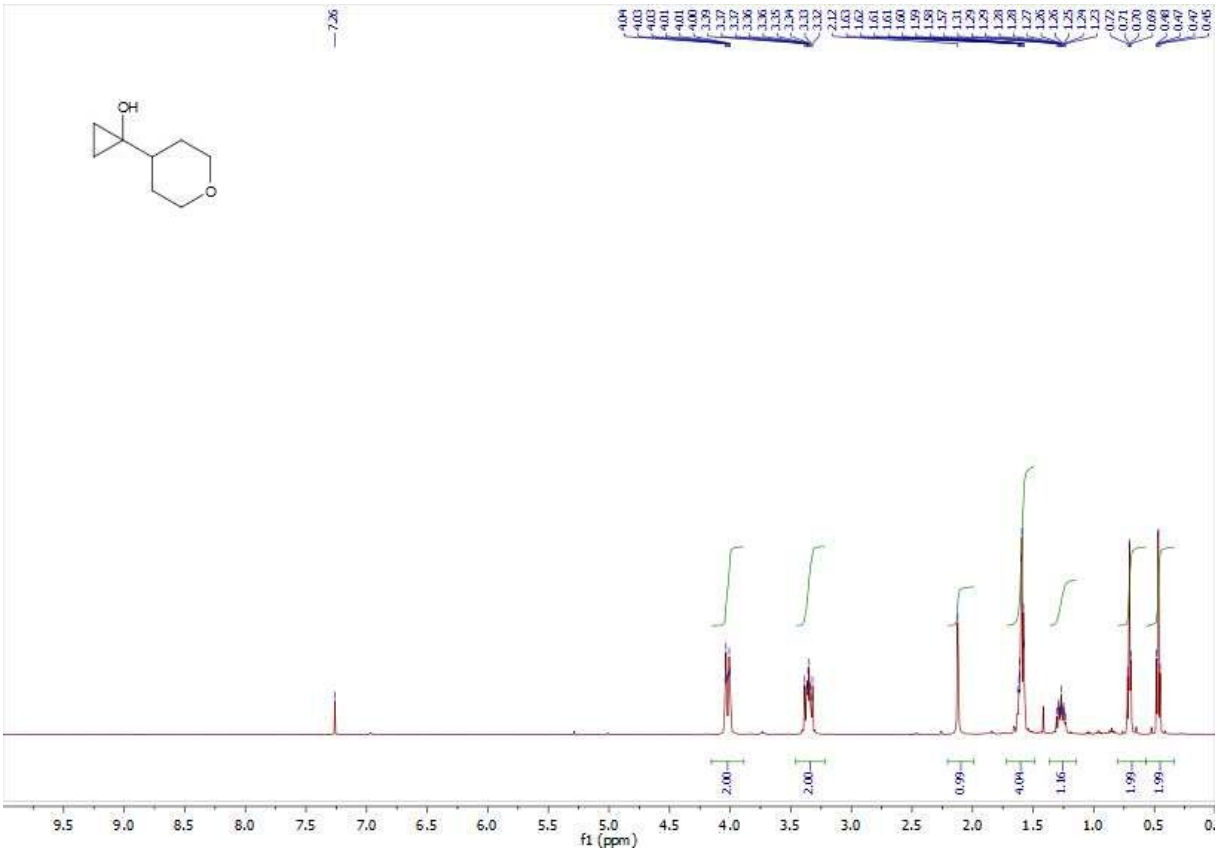

OH
142.33
128.57
128.55
125.99
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
55.96
40.56
32.65
13.85
f1 (ppm)

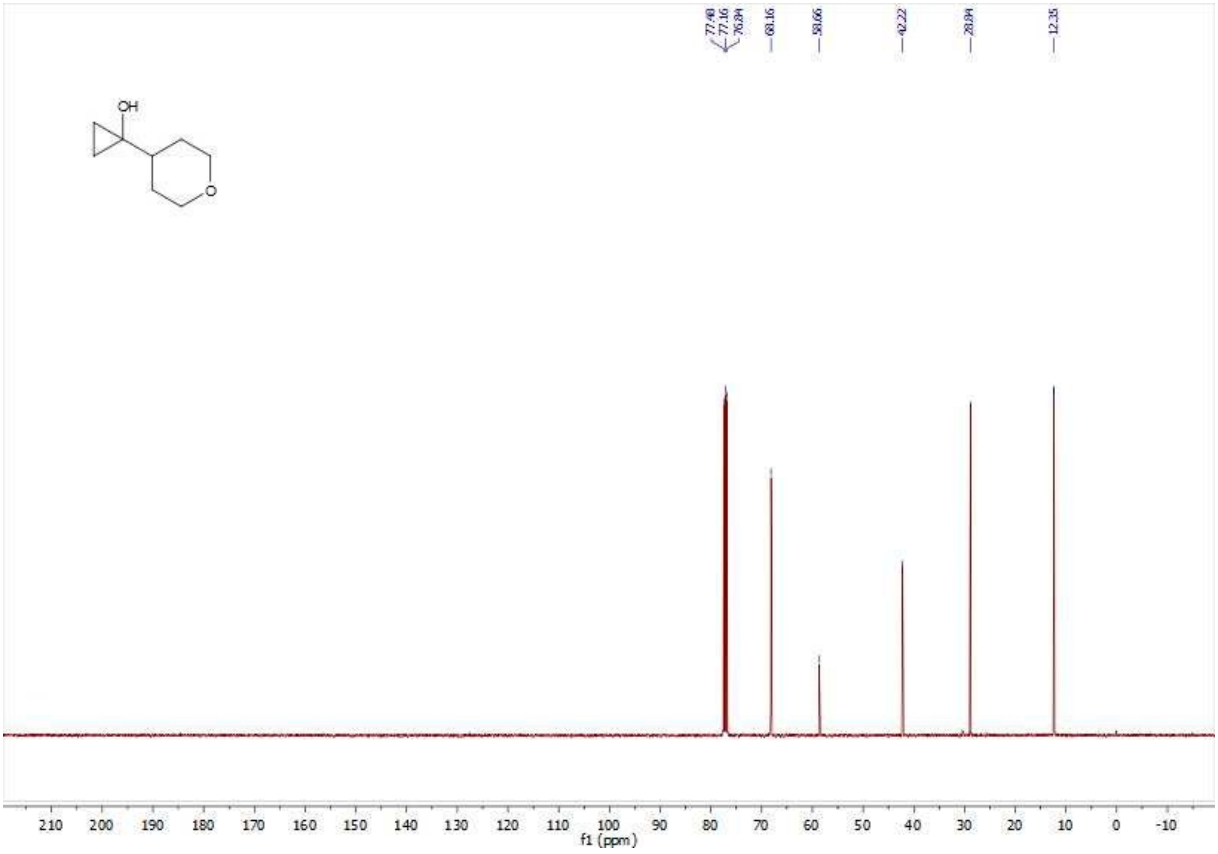

OH
CH2
f1 (ppm)

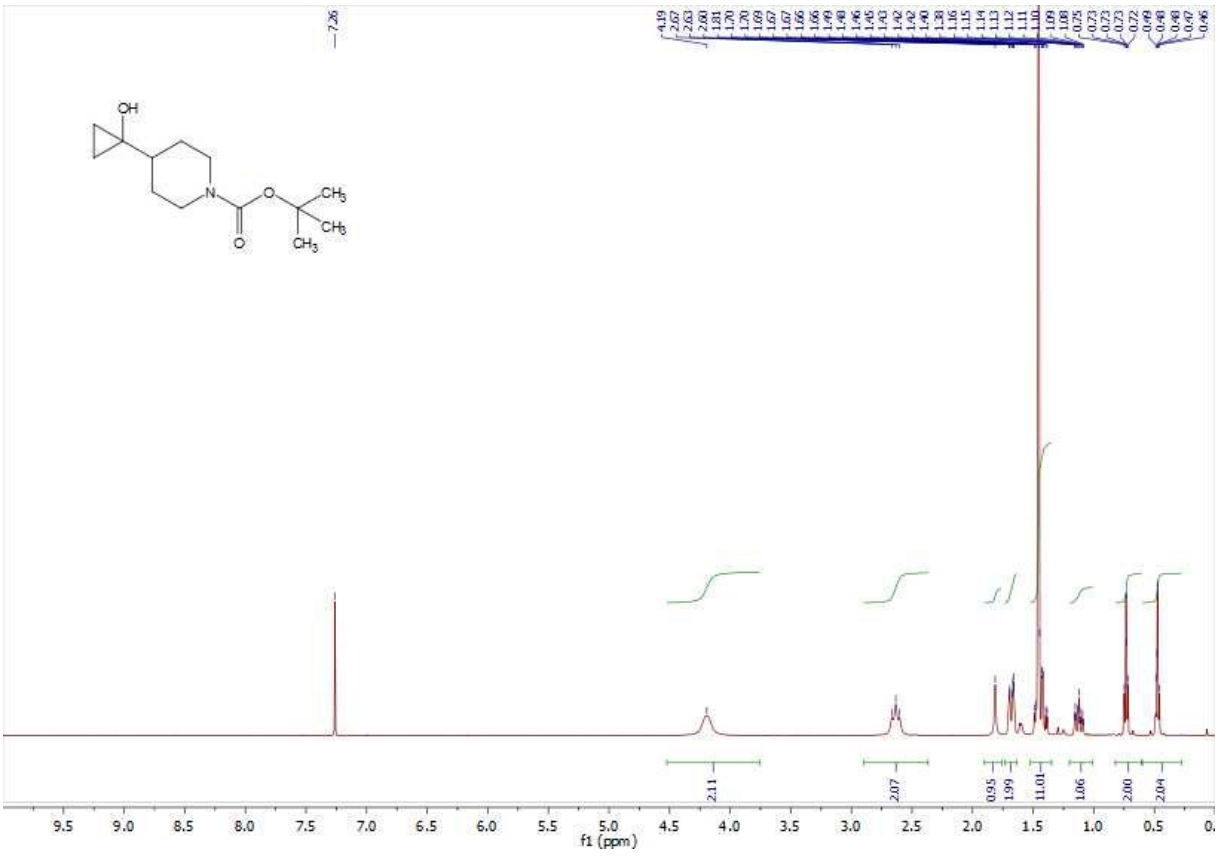

OH
CH2
f1 (ppm)

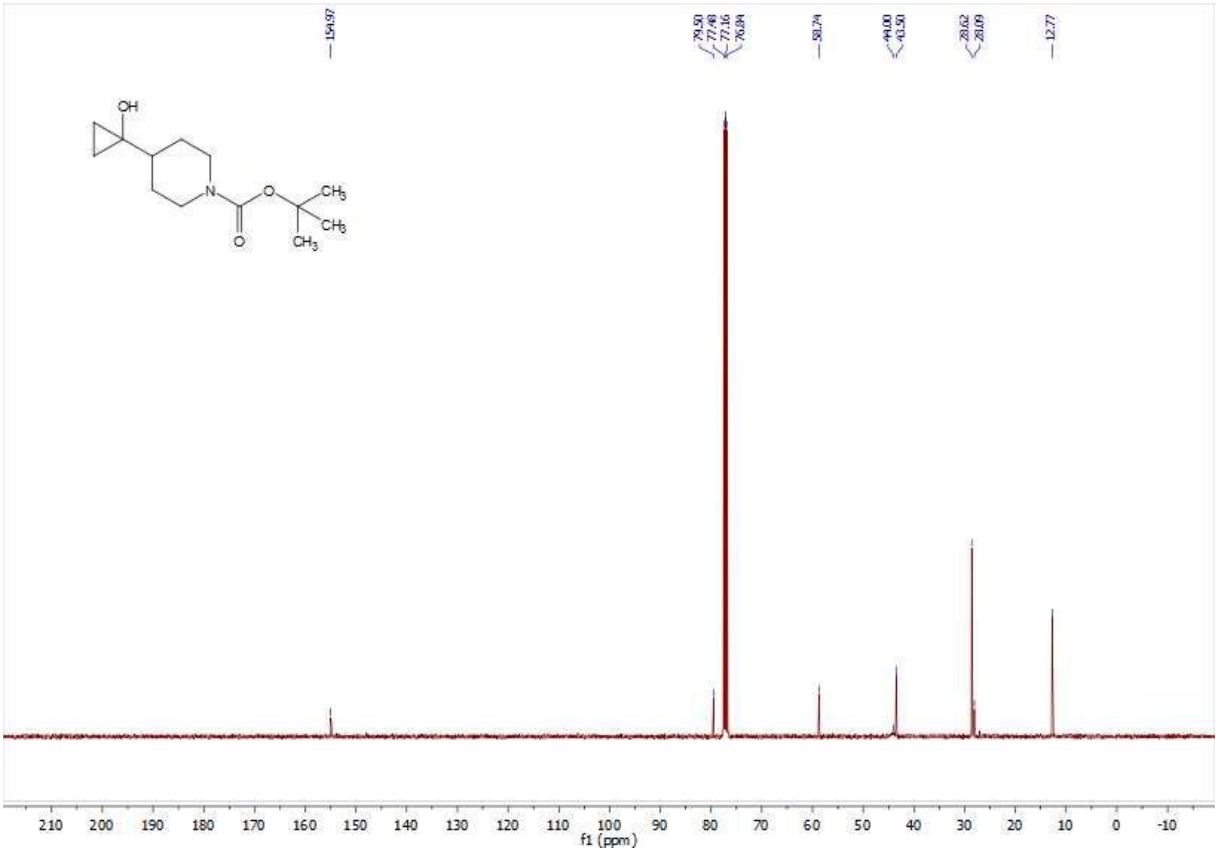

OH
Si
O
f1 (ppm)

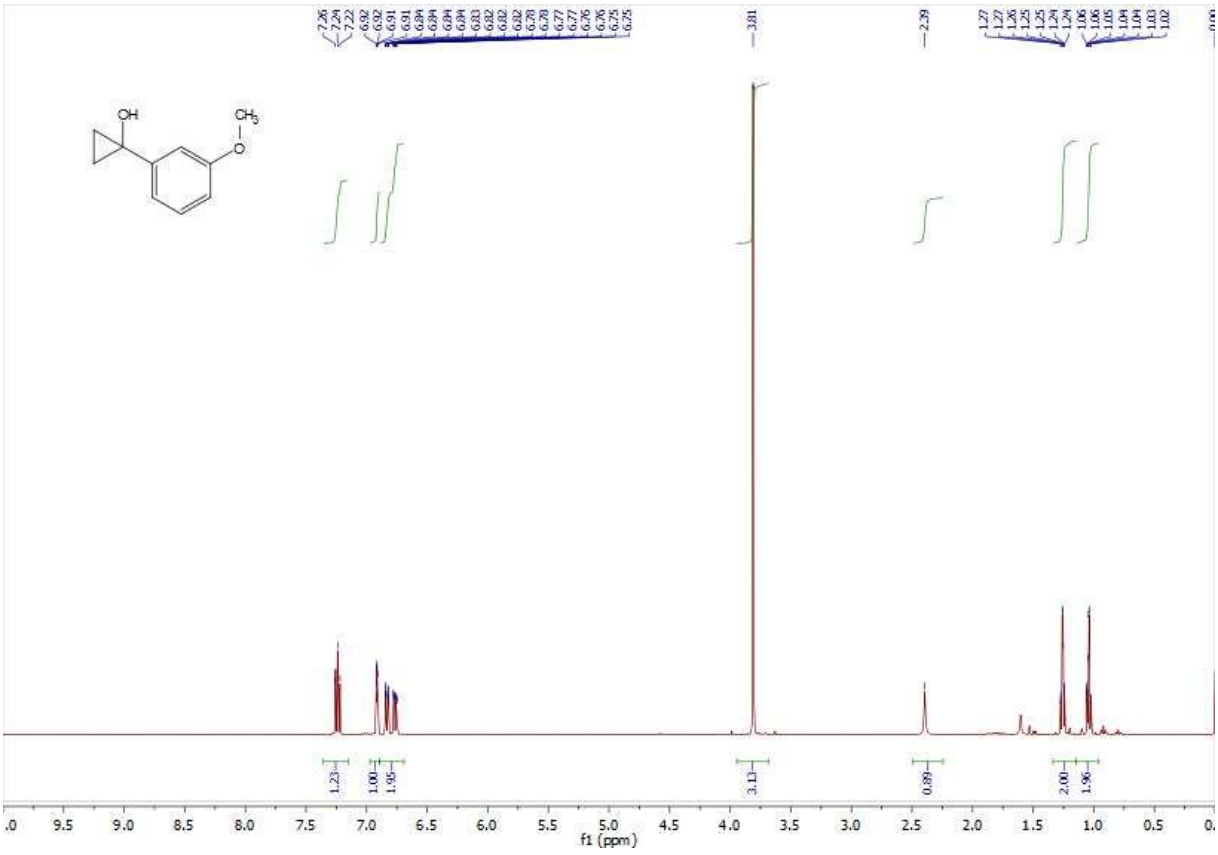

OH
Si
O
f1 (ppm)

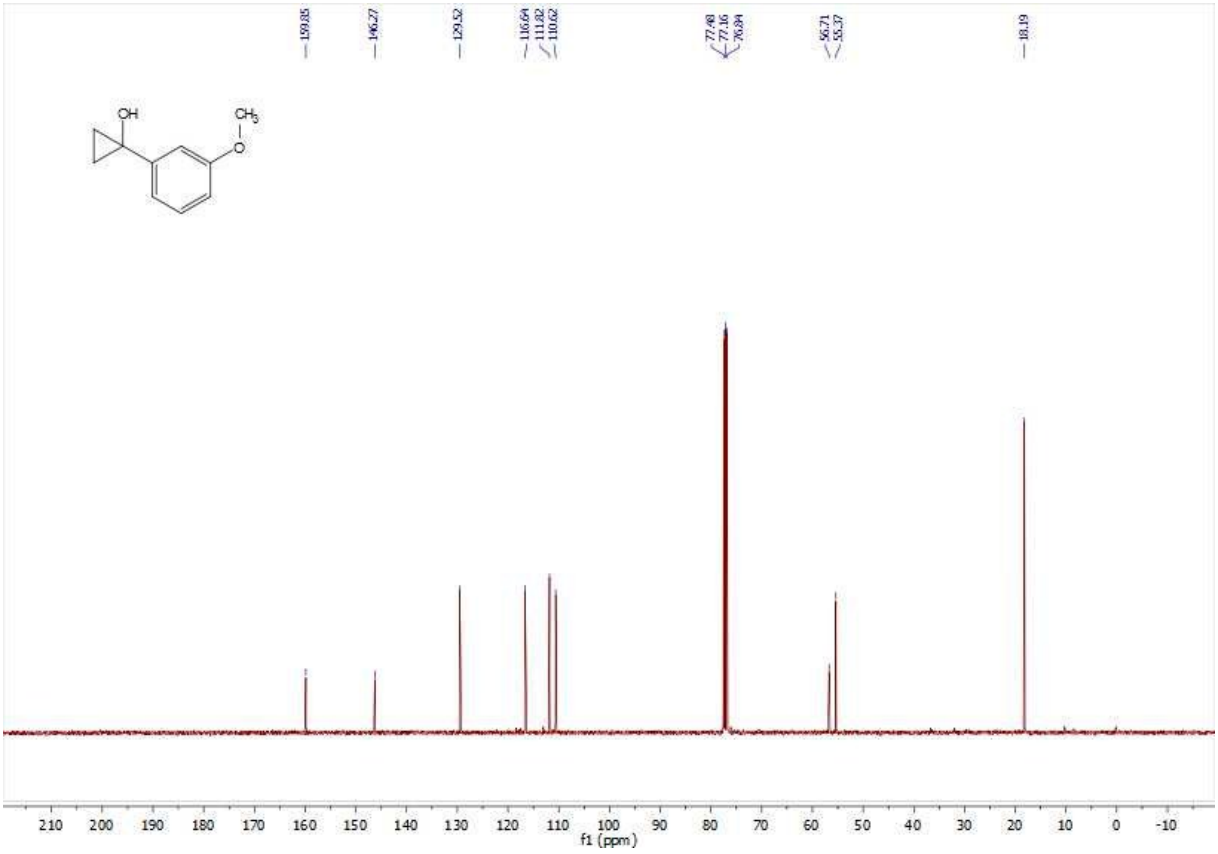

OH
O
f1 (ppm)

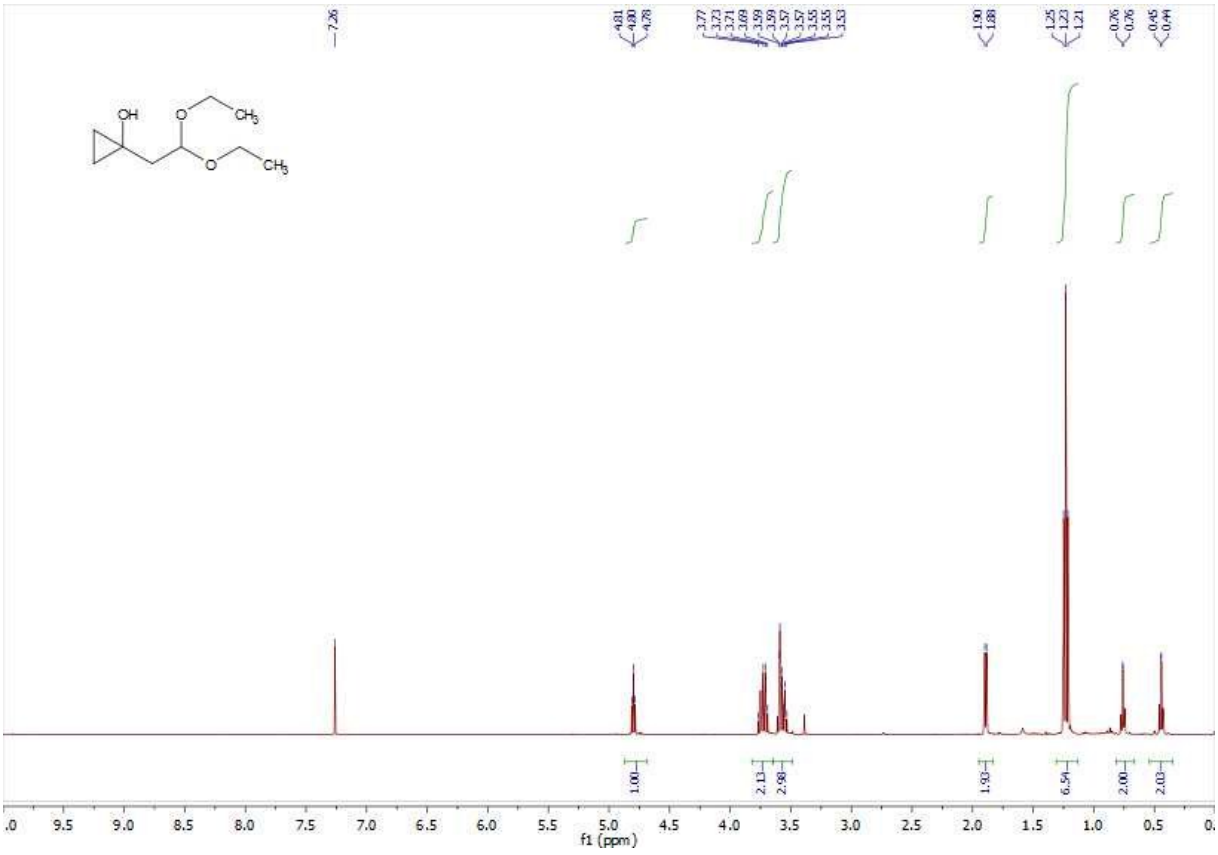

OH
O
f1 (ppm)


OH
N
O
O
CH3
CH3
CH3
f1 (ppm)


OH
N
O
O
CH3
CH3
CH3
f1 (ppm)


OH
CH3
O
f1 (ppm)


OH
CH3
O
f1 (ppm)


OH
O
CH3
O
CH3
7.26
4.81
4.80
4.78
3.77
3.73
3.71
3.69
3.59
3.59
3.57
3.57
3.55
3.55
3.53
1.90
1.88
1.25
1.23
1.21
0.76
0.76
0.45
0.44
1.00
2.13
2.98
1.93
6.54
2.00
2.03
f1 (ppm)