Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Rh-Catalyzed Oxidation and Trifluoroethoxylation of *N*-Aryl-pyrrolidin-2-ones : A Domino Approach for the Synthesis of *N*-Aryl-5-(2,2,2-trifluoroethoxy)-1,5- dihydro-2*H*-pyrrol-2-ones

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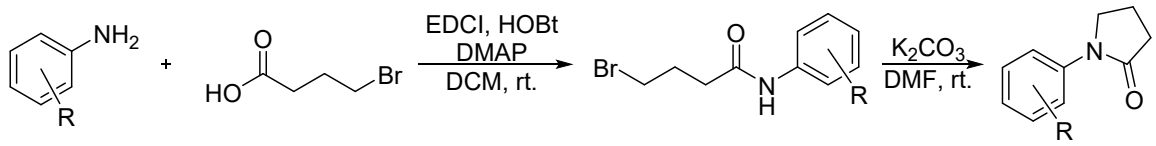
Tables of contents

1. General Information

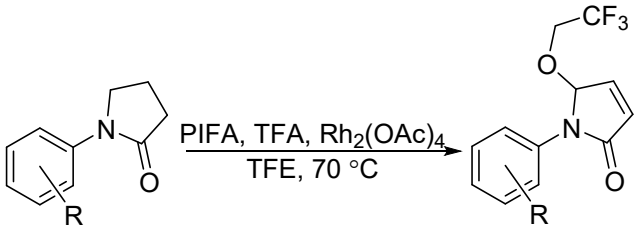
The Silica gel F254 plates were used for thin layer chromatography (TLC) in which the spots were examined under UV light at 254 nm. Flash chromatography was performed on silica gel (300-400 mesh). Anhydrous solvents were obtained according to standard procedures. Tetrahydrofuran (THF) was distilled from sodium-benzophenoneketyl. Methylene chloride (CH_2Cl_2) was distilled over P_2O_5. Methanol (MeOH) was distilled from magnesium. All other commercial reagents were purchased from commercial sources and used as received. NMR spectra were recorded on Varian Mercury spectrometer (400 MHz and 600 MHz). ^{1}H NMR spectra were recorded at ambient temperature at 400 MHz or 600 MHz. ^{13}C NMR spectra were recorded at ambient temperature at 100 MHz or 150 MHz. For ^{1}H NMR spectra acquired in $CDCl_3$, chemical shifts are reported as δ values in ppm and are calibrated according to internal $CHCl_3$ (7.26 ppm). For ^{13}C NMR spectra, chemical shifts are reported as δ values in ppm relative to $CHCl_3$. The NMR data are reported as follows: chemical shift in ppm on the δ scale, multiplicity (app = apparent, br = broad, s = singlet, d = doublet, t = triplet, q = quartet, quin = quintet, m = multiplet), coupling constants (Hz), and integration. LCMS/ HRMS were recorded on a Bruker Daltonics Data analysis 3.4 mass spectrometer.

2. Typical Procedure for the Synthesis of Substrates



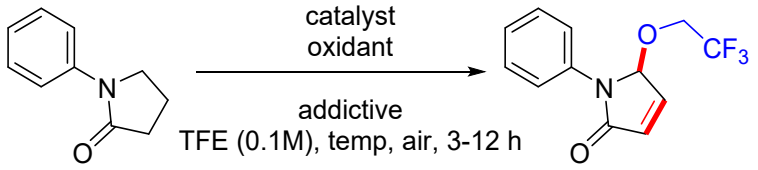
A flame-dried round-bottomed flask was charged with dry DCM (10 mL, 0.1 M), Aniline (1 mmol, 1 eq), 4-Bromobutyric acid (1.2 mmol, 1.2 eq), EDCI (1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride, 1.2 mmol, 1.2 eq.), HOBt (1-hydroxybenzotriazole, 1.2 mmol, 1.2 eq) and DMAP (0.2 mmol, 20 mol%). The reaction mixture was stirring for 30 minutes at room temperature, and then the substituted aniline (1 mmol, 1 eq.) was added. After consumption of the starting material (monitored by TLC) the reaction mixture was concentrated under reduced pressure. Then diluted with ethyl acetate (40 mL) and the mixture was washed with 1 M HCl (20 mL) three times. The organic layer was washed with brine and dried with anhydrous Na_2SO_4. The crude product was concentrated for next step without further purified. A solution of the above crude product in dry DMF (5 mL) was added K_2CO_3 (2.0 mmol) and the mixture was stirred overnight. After completion of the reaction monitored with TLC, the reaction mixture was diluted with ethyl acetate (40 mL) and washed with saturated NaCl solution (3×20 mL).The combined organic layers were dried over $MgSO_4$ and filtered. The solvent was removed in vacuo.The resulting product was purified by flash silica gel column chromatography using PE / EA (2:1) as eluent.

3. Typical Procedure for the Preparation of 1-substituted- 5-(2,2,2-trifluoroethoxy)-1,5-dihydro-2H-pyrrol-2-ones



To a solution of 1-substituted pyrrolidin-2-one (0.3 mmol) in TFE (3 mL) was added PIFA (1.05 mmol), $Rh_2(OAc)_4$ (2 mol%), TFA (0.3 mmol) at room temperature and the solution was stirred for 5 min. Then heat the mixture to 70 degrees. After consumption of the starting material (monitored by TLC) the reaction mixture was concentrated under reduced pressure. The resulting product was purified by flash silica gel column chromatography using PE / EA (2:1) as eluent.

4. Optimization of reaction conditions



1a **2a**

Table S1. Screening of catalyst[a]

Entry	Catalyst	Amount (mol%)	Yield (%)	Time (h)
1	$Cu(OAc)_2$	20	0	12
2	$Pd(OAc)_2$	20	0	12
3	$RhCl_3$	10	0	3
4	$Rh_2(OAc)_4$	10	59	3
5	$RhCl_3$	10	0	3
6	$Rh_2(OAc)_4$	5	59	3
7	$Rh_2(OAc)_4$	2	57	3
8	$Rh_2(OAc)_4$	1	29	9
9	$Rh_2(OAc)_4$	0	0	12
10[b]	$Rh_2(OAc)_4$	2	57	3
11[c]	$Rh_2(TFA)_4$	5	0	3
12	$Rh_2(TFA)_4$	5	62	3
13	$[Rh(C_8H_{15}O_2)_2]_2$	5	48	3

a. Reaction condition：substrate 1a (0.1 mmol), PIFA (0.35 mmol), $Rh_2(OAc)_4$ (x mol%), TFA (0.1

mmol), TFE (0.1M).

b.Reaction condition：air instead of N_2.

c. Reaction condition：substrate 1a (0.1 mmol), PIFA (0.35 mmol), TFE (0.1M).

Table S2. Screening of oxidant[a]

Entry	Oxidant	Amount(eq)	Yield(%)	Time
1	PIFA	3	53	6
2	PIDA	3.5	trace	12
3	$K_2S_2O_8$	3.5	5	12
4	$Na_2S_2O_8$	3.5	0	12
5	OXONE	3.5	0	12
6	selectfluor	3.5	46	12
7	PIFA	3.5	59	3
8	PIFA	4	57	3
9	PIFA	2	28	12
10	PIFA	0	0	12

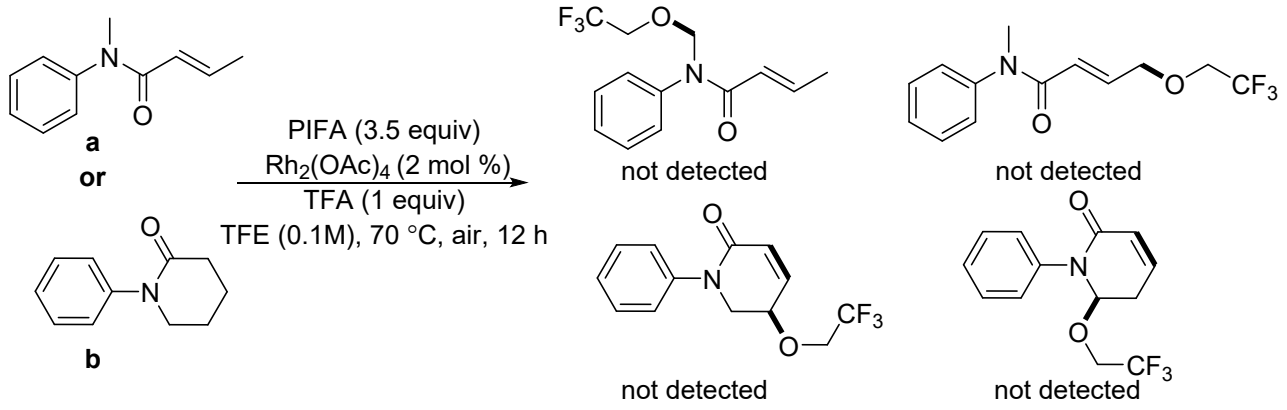
a. Reaction condition：substrate 1a (0.1 mmol), oxidant (x mmol), $Rh_2(OAc)_4$ (2 mol%), TFA (0.1 mmol), TFE (0.1M).

Table S3. Screening of additive[a]

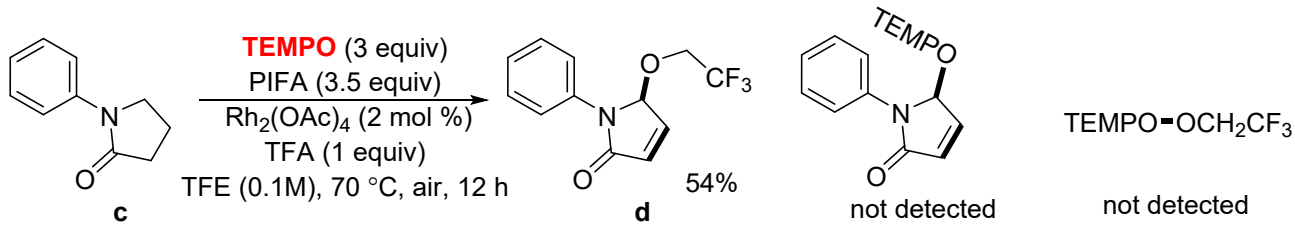
Entry	Additive	Amount (eq)	Yield (%)	Time (h)
1	TFA	10	59	3
2	TFA	5	56	3
3	TFA	1	57	3
4	TFA	0	trace	12

a. Reaction condition：substrate 1a (0.1 mmol), PIFA (0.35 mmol), $Rh_2(OAc)_4$ (2 mol%), TFA (x mmol), TFE (0.1M).

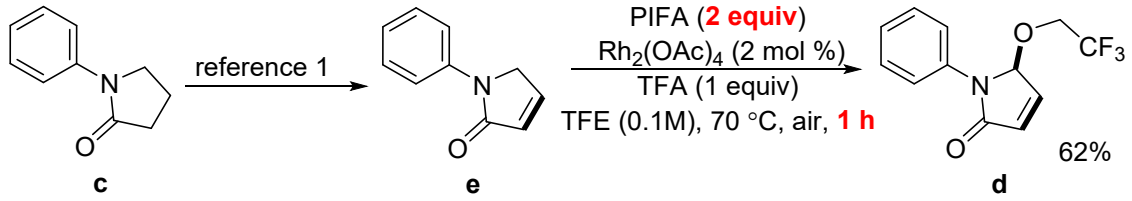
5. Mechanistic Experiments



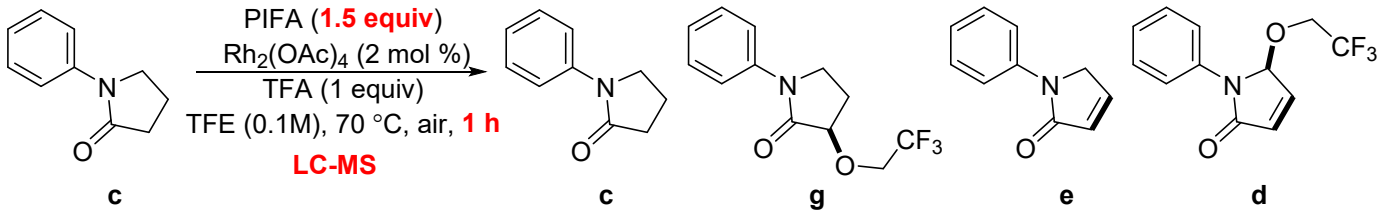
To a solution of **a** or **b** (0.3 mmol) in TFE (3 mL) was added PIFA (1.05 mmol), $Rh_2(OAc)_4$ (5 mol%), TFA (0.3 mmol) at room temperature and the solution was stirred for 5 min at that temperature before transfer to 70 ℃. Sampling after 12 h for LC-MS detection and analysis. The expected compound was not detected.



According to the typical procedure for the preparation of 1-substituted- 5-(2,2,2-trifluoroethoxy)-1,5-dihydro-2*H*-pyrrol-2-ones and added TEMPO (3 eq.). Sampling after 12 h for LC-MS detection and analysis. LC-MS results showed that no substrate or TFE captured by TEMPO was detected.



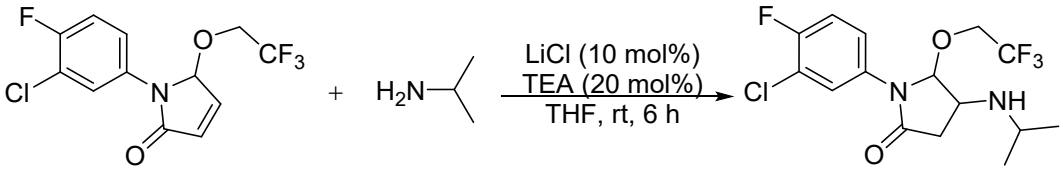
According to the reference 1 transfer **c** to **e**[1]. To a solution of **e** (0.3 mmol) in TFE (3 mL) was added PIFA (0.6 mmol), $Rh_2(OAc)_4$ (5 mol%), TFA (0.3 mmol) at room temperature and the solution was stirred for 5 min at that temperature before transfer to 70 ℃. After consumption of the starting material (monitored by TLC) the reaction mixture was concentrated under reduced pressure. The resulting product was purified by flash silica gel column chromatography using PE / EA (2:1) as eluent.



To a solution of **c** (0.3 mmol) in TFE (3 mL) was added PIFA (0.45 mmol), $Rh_2(OAc)_4$ (5 mol%), TFA (0.3 mmol) at room temperature and the solution was stirred for 5 min at that temperature before transfer to 70 ℃. Sampling after 1 h for LC-MS detection and analysis. The expected compound **c**, **g**, **e** and **d** was detected.

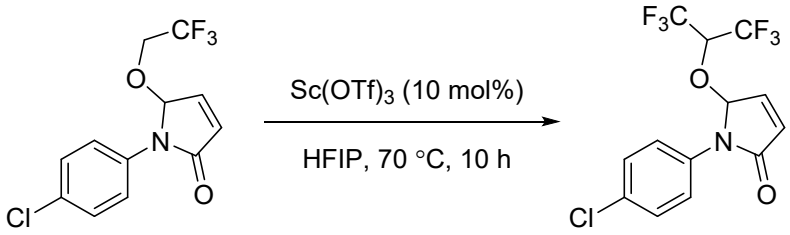
6. Further applications

6.1 Further reactions



2h **3h** 89%

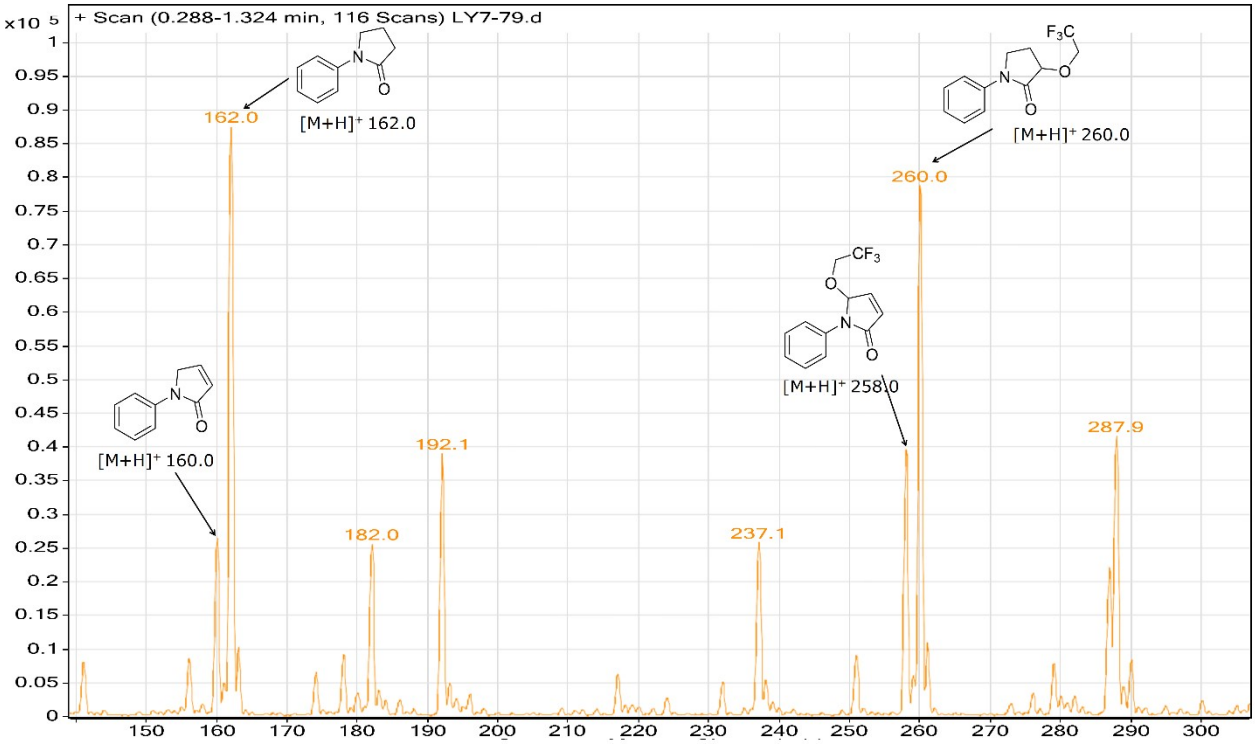
To a solution of **3h** (0.2 mmol) in THF (2 mL) was added isopropamide (0.4 mmol), LiCl (10 mol%), TEA (20 mol%) at room temperature and the solution was stirred for 6 h. Upon completion of reaction (monitored by TLC), the mixture was concentrated under reduced pressure and purified by flash column chromatography on silica gel using PE / EA (2:1) as eluent to afford the desired product.



2e **3e** 92%

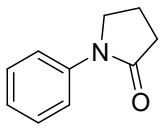
To a solution of **5h** (0.2 mmol) in HFIP (2 mL) was added $Sc(OTf)_3$ (10 mol%) and stirred for 10 h at 70 ℃. Upon completion of reaction (monitored by TLC), the mixture was concentrated under reduced pressure and purified by flash column chromatography on silica gel using PE / EA (2:1) as eluent to afford the desired product.

7. Mass spectrometry



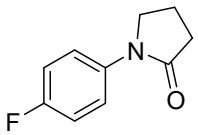
8. Analytic Date

phenylpyrrolidin-2-one（1a）[2]



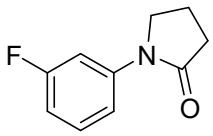
White solid, yield 80%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.61 (d, *J* = 7.7 Hz, 2H), 7.37 (t, *J* = 7.7 Hz, 2H), 7.14 (t, *J* = 7.4 Hz, 1H), 3.87 (t, *J* = 7.0 Hz, 2H), 2.62 (t, *J* = 8.1 Hz, 2H), 2.16 (p, *J* = 7.7 Hz, 2H).

(4-fluorophenyl)pyrrolidin-2-one（1b）[2]



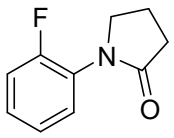
White solid, yield 73%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.59-7.54 (m, 2H), 7.06 (t, *J* = 8.7 Hz, 2H), 3.84 (t, *J* = 7.0 Hz, 2H), 2.61 (t, *J* = 8.1 Hz, 2H), 2.17 (p, *J* = 7.5 Hz, 2H).

(3-fluorophenyl)pyrrolidin-2-one（1c）[2]



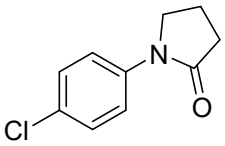
White solid, yield 67%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.52 (d, *J* = 11.5 Hz, 1H), 7.39 – 7.27 (m, 2H), 6.84 (t, *J* = 7.9 Hz, 1H), 3.85 (t, *J* = 7.0 Hz, 2H), 2.63 (t, *J* = 8.1 Hz, 2H), 2.18 (p, *J* = 7.5 Hz, 2H).

(2-fluorophenyl)pyrrolidin-2-one（1d）[2]



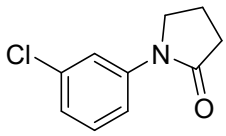
White solid, yield 63%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.46 – 7.37 (m, 1H), 7.26 – 7.21 (m, 1H), 7.20 – 7.09 (m, 2H), 3.83 (t, *J* = 7.0 Hz, 2H), 2.58 (t, *J* = 8.1 Hz, 2H), 2.21 (p, *J* = 7.5 Hz, 2H).

(4-chlorophenyl)pyrrolidin-2-one（1e）[2]



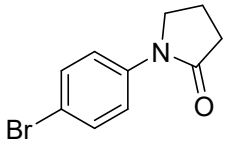
White solid, yield 72%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.58 (d, *J* = 9.0 Hz, 2H), 7.32 (d, *J* = 9.0 Hz, 2H), 3.84 (t, *J* = 7.0 Hz, 2H), 2.62 (t, *J* = 8.1 Hz, 2H), 2.17 (p, *J* = 7.5 Hz, 2H).

1-(3-chlorophenyl)pyrrolidin-2-one（1f）[2]



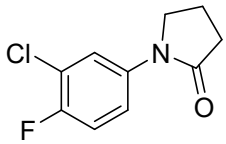
White solid, yield 65%. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.67 (t, J = 2.0 Hz, 1H), 7.60 – 7.48 (m, 1H), 7.28 (s, 1H), 7.19 – 7.03 (m, 1H), 3.84 (t, J = 7.0 Hz, 2H), 2.62 (t, J = 8.1 Hz, 2H), 2.17 (p, J = 7.6 Hz, 2H).

(4-bromophenyl)pyrrolidin-2-one（1g）[3]



White solid, yield 20%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.53 (d, *J* = 8.8 Hz, 2H), 7.47 (d, *J* = 8.8 Hz, 2H), 3.84 (t, *J* = 7.0 Hz, 2H), 2.61 (t, *J* = 8.0 Hz, 2H), 2.17 (p, *J* = 7.4 Hz, 2H).

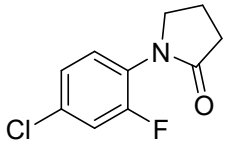
1-(3-chloro-4-fluorophenyl)pyrrolidin-2-one（1h）



White solid, yield 64%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.73 (dd, *J* = 6.5, 2.6 Hz, 1H), 7.52-7.48 (m, 1H), 7.12 (t, *J* = 8.8 Hz, 1H), 3.82 (t, *J* = 7.0 Hz, 2H), 2.61 (t, *J* = 8.1 Hz, 2H), 2.18 (p, *J* = 7.6 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.2, 154.8 (d, *J* = 246.6 Hz), 136.1 (d, J = 3.3 Hz), 121.9,

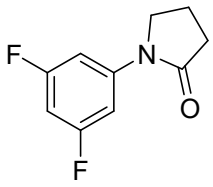
120.9 (d, J = 18.5 Hz), 119.4 (d, J = 6.9 Hz), 116.4 (d, J = 21.9 Hz), 48.8, 32.5, 17.8. HRMS(ESI) *m/z*: calculated for $C_{10}H_{10}ClFNO$ $[M+H]^+$ 214.0430, found 214.0429.

1-(4-chloro-2-fluorophenyl)pyrrolidin-2-one（1i）



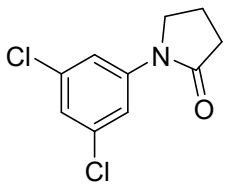
White solid, yield 58%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.42 – 7.33 (m, 1H), 7.21 – 7.12 (m, 2H), 3.81 (t, *J* = 6.6 Hz, 2H), 2.56 (t, *J* = 8.1 Hz, 2H), 2.21 (p, *J* = 7.5 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.8, 156.8 (d, *J* = 253.7 Hz), 132.9 (d, *J* = 9.9 Hz), 128.5 (d, *J* = 2.9 Hz), 125.2 (d, *J* = 11.8 Hz), 124.9 (d, *J* = 3.6 Hz), 117.4 (d, *J* = 23.6 Hz), 49.8, 30.9, 19.0. HRMS(ESI) *m/z*: calculated for $C_{10}H_{10}ClFNO$ $[M+H]^+$ 214.0430, found 214.0430.

1-(3,5-difluorophenyl)pyrrolidin-2-one（1j）



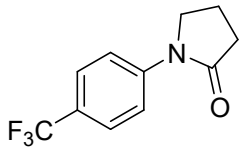
White solid, yield 61%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.27 (d, *J* = 7.8 Hz, 2H), 6.58 (t, *J* = 8.8 Hz, 1H), 3.82 (t, *J* = 7.0 Hz, 2H), 2.63 (t, *J* = 8.1 Hz, 2H), 2.18 (p, *J* = 7.6 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.5, 164.3 (d, *J* = 14.8 Hz), 161.9 (d, *J* = 14.7 Hz), 141.5 (t, *J* = 13.1 Hz), 102.4 (dd, J = 60.6, 9.0 Hz), 99.4 (t, *J* = 25.7 Hz), 48.5, 32.9, 17.7. HRMS(ESI) *m/z*: calculated for $C_{10}H_{10}F_2NO$ $[M+H]^+$ 198.0725, found 198.0729.

1-(3,5-dichlorophenyl)pyrrolidin-2-one（1k）[4]



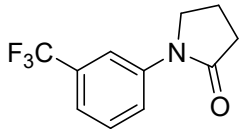
White solid, yield 63%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.61 (s, 2H), 7.13 (s, 1H), 3.82 (t, *J* = 7.0 Hz, 2H), 2.63 (t, *J* = 8.1 Hz, 2H), 2.18 (p, *J* = 7.5 Hz, 2H).

1-(4-(trifluoromethyl)phenyl)pyrrolidin-2-one（1l）[2]



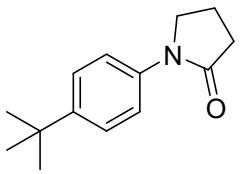
White solid, yield 20%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.77 (d, *J* = 8.6 Hz, 2H), 7.62 (d, *J* = 8.6 Hz, 2H), 3.90 (t, *J* = 7.0 Hz, 2H), 2.65 (t, *J* = 8.1 Hz, 2H), 2.20 (p, *J* = 7.6 Hz, 2H).

1-(3-(trifluoromethyl)phenyl)pyrrolidin-2-one（1m）[2]



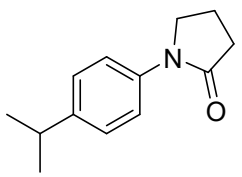
White solid, yield 59%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 (d, *J* = 8.1 Hz, 1H), 7.84 (s, 1H), 7.49 (t, *J* = 8.0 Hz, 1H), 7.40 (d, *J* = 8.0 Hz, 1H), 3.90 (t, *J* = 7.0 Hz, 2H), 2.65 (t, *J* = 8.1 Hz, 2H), 2.20 (p, *J* = 7.4 Hz, 2H).

1-(4-(tert-butyl)phenyl)pyrrolidin-2-one（1n）[2]



White solid, yield 79%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.51 (d, *J* = 8.7 Hz, 2H), 7.38 (d, *J* = 8.7 Hz, 2H), 3.85 (t, *J* = 7.0 Hz, 2H), 2.60 (t, *J* = 8.1 Hz, 2H), 2.15 (p, *J* = 7.5 Hz, 2H), 1.31 (s, 9H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.1, 147.5, 136.8, 125.7, 119.8, 48.9, 34.4, 32.7, 31.4.

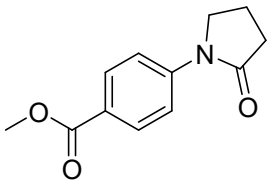
1-(4-isopropylphenyl)pyrrolidin-2-one（1o）[2]



White solid, yield 77%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.50 (d, *J* = 8.4 Hz, 2H), 7.23 (d, *J* = 8.4 Hz, 2H), 3.85 (t, *J* = 7.0 Hz, 2H), 2.89 (hept, *J* = 6.8

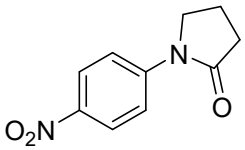
Hz, 1H), 2.60 (t, *J* = 8.1 Hz, 2H), 2.15 (p, *J* = 7.5 Hz, 2H), 1.24 (d, *J* = 6.9 Hz, 6H).

methyl 4-(2-oxopyrrolidin-1-yl)benzoate（1p）[5]



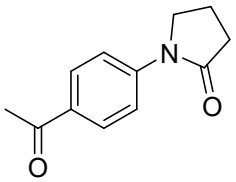
White solid, yield 44%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.04 (d, J = 8.8 Hz, 2H), 7.73 (d, J = 8.8 Hz, 2H), 4.00 – 3.83 (m, 5H), 2.65 (t, J = 8.1 Hz, 2H), 2.19 (p, J = 7.6 Hz, 2H).

1-(4-nitrophenyl)pyrrolidin-2-one（1q）[6]



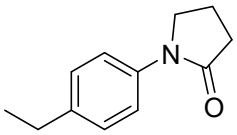
White solid, yield 23%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.24 (d, *J* = 9.3 Hz, 2H), 7.85 (d, *J* = 9.3 Hz, 2H), 3.94 (t, *J* = 7.1 Hz, 2H), 2.68 (t, *J* = 8.1 Hz, 2H), 2.24 (p, *J* = 7.6 Hz, 2H).

1-(4-acetylphenyl)pyrrolidin-2-one（1r）[7]



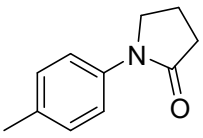
White solid, yield 34%. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.98 (d, J = 8.8 Hz, 2H), 7.76 (d, J = 8.9 Hz, 2H), 3.91 (t, J = 7.0 Hz, 2H), 2.66 (t, J = 8.1 Hz, 2H), 2.59 (s, 3H), 2.20 (p, J = 7.6 Hz, 2H).

1-(4-ethylphenyl)pyrrolidin-2-one（1s）[2]



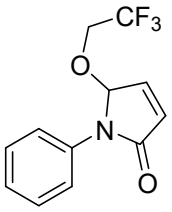
White solid, yield 75%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.50 (d, *J* = 8.4 Hz, 2H), 7.19 (d, *J* = 8.4 Hz, 2H), 3.85 (t, *J* = 7.0 Hz, 2H), 2.70 – 2.49 (m, 4H), 2.15 (p, *J* = 7.5 Hz, 2H), 1.22 (t, *J* = 7.6 Hz, 3H).

1-(p-tolyl)pyrrolidin-2-one（1t）[2]



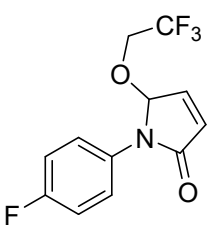
White solid, yield 78%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.48 (d, *J* = 8.4 Hz, 2H), 7.17 (d, *J* = 8.4 Hz, 2H), 3.84 (t, *J* = 7.0 Hz, 2H), 2.60 (t, *J* = 8.1 Hz, 2H), 2.33 (s, 3H), 2.15 (p, *J* = 7.6 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.1, 136.9, 134.2, 129.4, 120.1, 48.9, 32.7, 20.9, 18.1.

1-phenyl-5-(2,2,2-trifluoroethoxy)-1,5-dihydro-2*H*-pyrrol-2-one (2a)



Slight yellow viscous liquid, yield 59%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.74 – 7.61 (m, 2H), 7.42 (t, *J* = 8.0 Hz, 2H), 7.26 – 7.18 (m, 1H), 7.01 (dd, *J* = 6.1, 1.8 Hz, 1H), 6.45 (d, *J* = 6.1 Hz, 1H), 6.18 (s, 1H), 3.68 – 3.53 (m, 2H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 168.1, 141.9, 136.3, 131.8, 129.3, 125.5, 123.4 (q, *J* = 277.6 Hz), 120.6, 88.1, 60.3 (q, *J* = 35.5 Hz). 19F NMR (376 MHz, $CDCl_3$) δ -73.96. HRMS(ESI) *m/z*: calculated for $C_{12}H_{11}F_3NO_2$ $[M+H]^+$ 258.0736, found 258.0734.

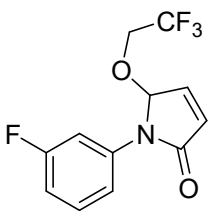
1-(4-fluorophenyl)-5-(2,2,2-trifluoroethoxy)-1,5-dihydro-2*H*-pyrrol-2-one(2b)



Slight yellow viscous liquid, yield 89%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.72 – 7.52 (m, 2H), 7.11 (t, *J* = 8.7 Hz, 2H), 7.05 – 6.95 (m, 1H), 6.45 (d, *J* = 6.1 Hz, 1H), 6.11 (s, 1H), 3.70 – 3.51 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ

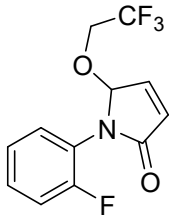
168.1, 160.2 (d, *J* = 245.6 Hz), 141.9, 132.4 (d, *J* = 3.0 Hz), 131.7, 123.3 (q, *J* = 277.6 Hz), 122.6 (d, *J* = 8.1 Hz), 116.1 (d, *J* = 22.6 Hz), 88.3, 60.4 (q, *J* = 35.6 Hz). HRMS(ESI) *m/z*: calculated for $C_{12}H_{10}F_4NO_2$ $[M+H]^+$ 276.0642, found 276.0639.

1-(3-fluorophenyl)-5-(2,2,2-trifluoroethoxy)-1,5-dihydro-2*H*-pyrrol-2-one(2c)



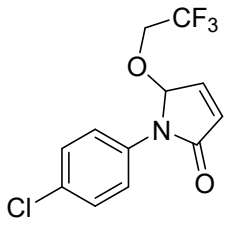
Slight yellow viscous liquid, yield 76%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.67 – 7.56 (m, 1H), 7.50 – 7.42 (m, 1H), 7.42 – 7.31 (m, 1H), 7.02 (dd, *J* = 6.0, 1.8 Hz, 1H), 6.96 – 6.87 (m, 1H), 6.51 – 6.39 (m, 1H), 6.15 (s, 1H), 3.69 – 3.50 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 168.0, 163.1 (d, *J* = 245.4 Hz), 142.1, 137.9 (d, *J* = 10.6 Hz), 131.8, 130.4 (d, *J* = 9.3 Hz), 123.3 (q, *J* = 277.6 Hz), 115.1 (d, *J* = 3.1 Hz), 112.1 (d, *J* = 21.2 Hz), 107.5 (d, *J* = 26.5 Hz), 87.9, 60.1 (q, *J* = 35.7 Hz). HRMS(ESI) *m/z*: calculated for $C_{12}H_{10}F_4NO_2$ $[M+H]^+$ 276.0642, found 276.0630.

1-(2-fluorophenyl)-5-(2,2,2-trifluoroethoxy)-1,5-dihydro-2*H*-pyrrol-2-one(2d)



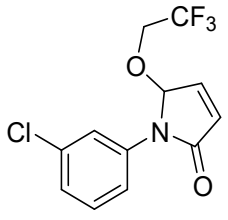
Slight yellow viscous liquid, yield 82%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.45 – 7.29 (m, 2H), 7.26 – 7.16 (m, 2H), 7.08 (d, *J* = 6.0 Hz, 1H), 6.48 (d, *J* = 6.0 Hz, 1H), 6.11 (s, 1H), 3.71 (q, *J* = 8.4 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 168.2, 157.6 (d, *J* = 249.9 Hz), 143.5, 130.9, 129.4 (d, *J* = 8.1 Hz), 128.7 (d, *J* = 1.1 Hz), 124.9 (d, *J* = 3.7 Hz), 123.3 (q, *J* = 277.9 Hz), 122.7 (d, *J* = 11.9 Hz), 116.8 (d, *J* = 20.2 Hz), 89.4 (d, *J* = 4.7 Hz), 61.7 (q, *J* = 35.4 Hz). HRMS(ESI) *m/z*: calculated for $C_{12}H_{10}F_4NO_2$ $[M+H]^+$ 276.0642, found 276.0641.

1-(4-chlorophenyl)-5-(2,2,2-trifluoroethoxy)-1,5-dihydro-2*H*-pyrrol-2-one(2e)



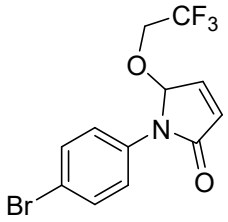
Slight yellow viscous liquid, yield 86%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.67 (d, *J* = 8.9 Hz, 2H), 7.38 (d, *J* = 8.9 Hz, 2H), 7.07 – 6.94 (m, 1H), 6.45 (d, *J* = 6.1 Hz, 1H), 6.14 (s, 1H), 3.67 – 3.49 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 167.9, 141.9, 135.0, 131.8, 130.7, 129.4, 123.3 (q, *J* = 277.6 Hz), 121.4, 87.9, 60.2 (q, *J* = 35.7 Hz). HRMS(ESI) *m/z*: calculated for $C_{12}H_{10}ClF_3NO_2$ $[M+H]^+$ 292.0347, found 292.0344.

1-(3-chlorophenyl)-5-(2,2,2-trifluoroethoxy)-1,5-dihydro-2*H*-pyrrol-2-one(2f)



Slight yellow viscous liquid, yield 79%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.82 (s, 1H), 7.58 (d, *J* = 8.1 Hz, 1H), 7.34 (t, *J* = 8.1 Hz, 1H), 7.19 (d, *J* = 8.0 Hz, 1H), 7.03 (d, *J* = 6.0 Hz, 1H), 6.45 (d, *J* = 6.0 Hz, 1H), 6.15 (s, 1H), 3.68 – 3.52 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 167.9, 142.1, 137.6, 135.0, 131.8, 130.3, 125.4, 123.3 (q, *J* = 277.6 Hz), 120.2, 117.9, 87.8, 60.2 (q, *J* = 35.7 Hz). HRMS(ESI) *m/z*: calculated for $C_{12}H_{10}ClF_3NO_2$ $[M+H]^+$ 292.0347, found 292.0343.

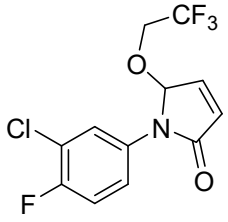
1-(4-bromophenyl)-5-(2,2,2-trifluoroethoxy)-1,5-dihydro-2*H*-pyrrol-2-one(2g)



Slight yellow viscous liquid, yield 71%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.62 (d, *J* = 8.9 Hz, 2H), 7.52 (d, *J* = 8.9 Hz, 2H), 7.02 (d, *J* = 5.9 Hz, 1H), 6.44 (d, *J* = 6.0 Hz, 1H), 6.14 (s, 1H), 3.69 – 3.46 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 167.9, 141.9, 135.6, 132.3, 131.9, 123.3 (q, *J* = 277.6 Hz), 121.6,

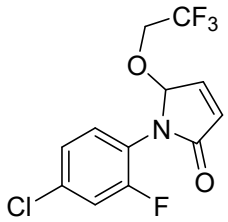
118.4, 87.8, 60.2 (q, J = 35.7 Hz).HRMS(ESI) *m/z*: calculated for $C_{12}H_{10}F_3BrNO_2$ $[M+H]^+$ 335.9842, found 335.9840.

1-(3-chloro-4-fluorophenyl)-5-(2,2,2-trifluoroethoxy)-1,5-dihydro-2*H*-pyrrol-2-one(2h)



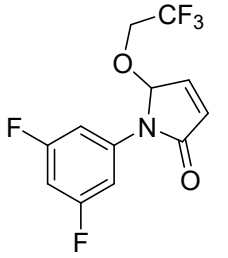
Slight yellow viscous liquid, yield 81%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.87 (dd, J = 6.4, 2.6 Hz, 1H), 7.62 – 7.51 (m, 1H), 7.18 (t, J = 8.8 Hz, 1H), 7.03 (d, J = 6.0 Hz, 1H), 6.45 (d, J = 6.0 Hz, 1H), 6.10 (s, 1H), 3.69 – 3.52 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 167.9, 155.5 (d, J = 247.9 Hz), 142.1, 133.1 (d, J = 3.4 Hz), 131.7, 123.2 (q, J = 277.6 Hz), 122.6, 121.6 (d, J = 18.6 Hz), 119.9 (d, J = 7.0 Hz), 116.9 (d, J = 22.1 Hz), 88.1, 60.3 (q, J = 35.7 Hz). HRMS(ESI) *m/z*: calculated for $C_{12}H_8ClF_4NO_2Na$ $[M+Na]^+$ 332.0072, found 332.0088.

1-(4-chloro-2-fluorophenyl)-5-(2,2,2-trifluoroethoxy)-1,5-dihydro-2*H*-pyrrol-2-one(2i)



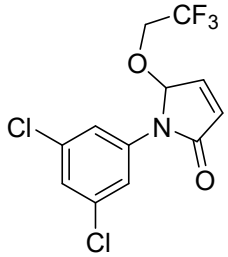
Slight yellow viscous liquid, yield 70%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.34 (t, J = 8.4 Hz, 1H), 7.26 – 7.19 (m, 2H), 7.12 – 7.06 (m, 1H), 6.47 (d, J = 6.0 Hz, 1H), 6.08 (s, 1H), 3.70 (q, J = 8.3 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 167.9, 157.2 (d, J = 253.4 Hz), 143.6, 134.3 (d, J = 10.0 Hz), 130.9, 129.3 (d, J = 2.1 Hz), 125.4 (d, J = 3.7 Hz), 123.2 (q, J = 277.9 Hz), 121.5 (d, J = 12.0 Hz), 117.7 (d, J = 23.6 Hz), 89.2, 61.8 (q, J = 35.5 Hz). HRMS(ESI) *m/z*: calculated for $C_{12}H_8ClF_4NO_2Na$ $[M+Na]^+$ 332.0072, found 332.0084.

1-(3,5-difluorophenyl)-5-(2,2,2-trifluoroethoxy)-1,5-dihydro-2*H*-pyrrol-2-one(2j)



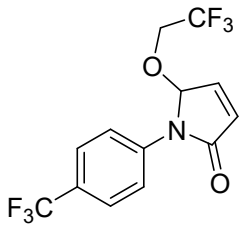
Slight yellow viscous liquid, yield 73%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.42 (d, J = 7.4 Hz, 2H), 7.04 (d, J = 6.0 Hz, 1H), 6.65 (t, J = 8.7 Hz, 1H), 6.45 (d, J = 6.1 Hz, 1H), 6.12 (s, 1H), 3.70 – 3.49 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 167.9, 163.3 (dd, J = 246.7, 14.6 Hz), 142.2, 138.7 (t, J = 13.2 Hz), 131.8, 123.2 (q, J = 277.6 Hz), 102.5 (d, J = 30.3 Hz), 100.3 (t, J = 25.5 Hz), 87.7, 59.9 (q, J = 35.9 Hz). HRMS(ESI) *m/z*: calculated for $C_{12}H_9F_5NO_2$ $[M+H]^+$ 294.0548, found 294.0547.

1-(3,5-dichlorophenyl)-5-(2,2,2-trifluoroethoxy)-1,5-dihydro-2*H*-pyrrol-2-one(2k)



Slight yellow viscous liquid, yield 69%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.73 (d, J = 1.4 Hz, 2H), 7.20 (s, 1H), 7.04 (d, J = 6.0 Hz, 1H), 6.45 (d, J = 6.0 Hz, 1H), 6.13 (s, 1H), 3.70 – 3.49 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 167.8, 142.3, 138.3, 135.6, 131.7, 125.2, 123.2 (q, J = 277.7 Hz), 117.9, 87.7, 60.1 (q, J = 35.8 Hz). HRMS(ESI) *m/z*: calculated for $C_{12}H_8Cl_2F_3NO_2Na$ $[M+Na]^+$ 347.9776, found 347.9778.

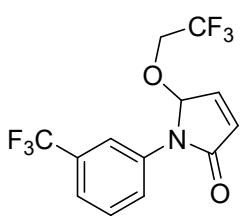
5-(2,2,2-trifluoroethoxy)-1-(4-(trifluoromethyl)phenyl)-1,5-dihydro-2*H*-pyrrol-2-one(2l)



Slight yellow viscous liquid, yield 72%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.90 (d, J = 8.6 Hz, 2H), 7.67 (d, J = 8.6 Hz, 2H), 7.06 (d, J = 6.0 Hz, 1H), 6.47

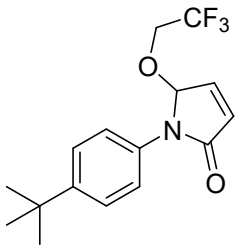
(d, *J* = 6.1 Hz, 1H), 6.22 (s, 1H), 3.69 – 3.49 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 168.1, 142.2, 139.5, 131.9, 126.4 (q, *J* = 3.8 Hz), 126.9 (q, *J* = 32.9 Hz), 123.9 (q, *J* = 271.8 Hz), 123.2 (q, *J* = 277.6 Hz), 119.3, 87.6, 60.1 (q, *J* = 35.8 Hz). HRMS(ESI) *m/z*: calculated for $C_{13}H_9F_6NO_2Na$ $[M+Na]^+$ 348.0430, found 348.0434.

5-(2,2,2-trifluoroethoxy)-1-(3-(trifluoromethyl)phenyl)-1,5-dihydro-2*H*-pyrrol-2-one(2m)



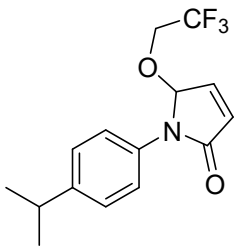
Slight yellow viscous liquid, yield 69%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.06 (s, 1H), 7.93 (d, *J* = 8.1 Hz, 1H), 7.54 (t, *J* = 8.0 Hz, 1H), 7.46 (d, *J* = 7.7 Hz, 1H), 7.10 – 7.02 (m, 1H), 6.47 (d, *J* = 6.1 Hz, 1H), 6.21 (s, 1H), 3.71 – 3.51 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 168.0, 142.2, 137.1, 131.8, 131.7 (q, *J* = 32.7 Hz), 129.8, 123.8 (q, *J* = 272.5 Hz), 123.2 (q, *J* = 277.6 Hz), 122.9, 121.8 (q, *J* = 3.8 Hz), 116.7 (q, *J* = 4.0 Hz), 87.8, 60.2 (q, *J* = 35.8 Hz). HRMS(ESI) *m/z*: calculated for $C_{13}H_9F_6NO_2Na$ $[M+Na]^+$ 348.0430, found 348.0428.

1-(4-(tert-butyl)phenyl)-5-(2,2,2-trifluoroethoxy)-1,5-dihydro-2*H*-pyrrol-2-one(2n)



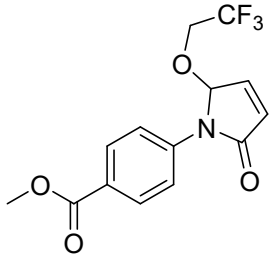
Slight yellow viscous liquid, yield 42%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.55 (d, *J* = 8.9 Hz, 2H), 7.43 (d, *J* = 8.9 Hz, 2H), 6.98 (dd, *J* = 6.1, 1.7 Hz, 1H), 6.43 (dd, *J* = 6.1, 0.8 Hz, 1H), 6.12 (s, 1H), 3.62 (q, *J* = 8.4 Hz, 2H), 1.32 (s, 9H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 168.2, 148.6, 141.9, 133.7, 131.8, 126.2, 123.5 (q, *J* = 277.6 Hz), 120.7, 88.4, 60.3 (q, *J* = 35.4 Hz), 34.5, 31.3. HRMS(ESI) *m/z*: calculated for $C_{16}H_{19}F_3NO_2$ $[M+H]^+$ 314.1362, found 314.1363.

1-(4-isopropylphenyl)-5-(2,2,2-trifluoroethoxy)-1,5-dihydro-2*H*-pyrrol-2-one（2o）



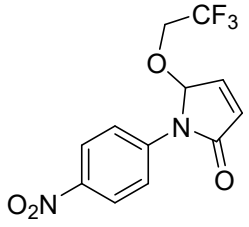
Slight yellow viscous liquid, yield 19%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.54 (d, *J* = 8.5 Hz, 2H), 7.27 (d, *J* = 8.5 Hz, 2H), 6.99 (d, *J* = 6.0 Hz, 1H), 6.43 (d, *J* = 5.9 Hz, 1H), 6.12 (s, 1H), 3.62 (q, *J* = 8.4 Hz, 2H), 2.91 (hept, *J* = 6.7 Hz, 1H), 1.25 (d, *J* = 6.9 Hz, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 168.2, 146.4, 141.9, 133.9, 131.8, 127.3, 123.4 (q, *J* = 277.7 Hz), 121.1, 88.4, 60.4 (q, *J* = 35.5 Hz), 33.7, 23.9. HRMS(ESI) *m/z*: calculated for $C_{15}H_{17}F_3NO_2$ $[M+H]^+$ 300.1206, found 300.1204.

methyl 4-(2-oxo-5-(2,2,2-trifluoroethoxy)-2,5-dihydro-1*H*-pyrrol- 1-yl)benzoate(2p)



Slight yellow viscous liquid, yield 73%. ^{1}H NMR (400 MHz, Chloroform-d) δ 8.08 (d, J = 8.7 Hz, 2H), 7.86 (d, *J* = 8.7 Hz, 2H), 7.06 (d, *J* = 6.0 Hz, 1H), 6.47 (d, *J* = 6.1 Hz, 1H), 6.24 (s, 1H), 3.92 (s, 3H), 3.69 – 3.50 (m, 2H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 168.0, 166.4, 142.2, 140.5, 131.9, 130.8, 126.4, 123.2 (q, *J* = 277.6 Hz), 118.8, 87.5, 60.0 (q, *J* = 35.8 Hz), 52.1. HRMS(ESI) *m/z*: calculated for $C_{14}H_{13}F_3NO_4$ $[M+H]^+$ 316.0791, found 316.0792.

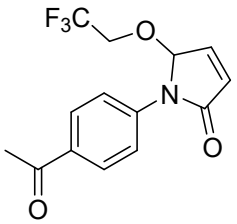
1-(4-nitrophenyl)-5-(2,2,2-trifluoroethoxy)-1,5-dihydro-2*H*-pyrrol-2-one (2q)



Slight yellow solid, yield 66%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.29 (d, *J* = 9.3 Hz, 2H), 8.01 (d, *J* = 9.3 Hz, 2H), 7.12 (dd, *J* = 6.1, 1.9 Hz, 1H), 6.51

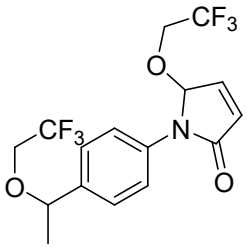
(d, *J* = 6.1 Hz, 1H), 6.28 (s, 1H), 3.72 – 3.49 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 168.0, 143.9, 142.6, 142.2, 131.9, 125.0, 123.1 (q, *J* = 277.6 Hz), 118.7, 87.4, 60.1 (q, *J* = 35.9 Hz). HRMS(ESI) *m/z*: calculated for $C_{12}H_8F_3N_2O_4$ $[M-H]^-$ 301.0442, found 301.0440.

1-(4-acetylphenyl)-5-(2,2,2-trifluoroethoxy)-1,5-dihydro-2H-pyrrol-2-one (2r)



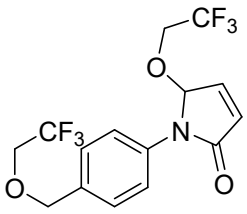
Slight yellow solid, yield 85%. ^{1}H NMR (400 MHz, DMSO-d6) δ 8.01 (d, J = 8.7 Hz, 2H), 7.83 (d, J = 8.7 Hz, 2H), 7.43 (d, J = 6.0 Hz, 1H), 6.59 (s, 1H), 6.54 (d, J = 6.2 Hz, 1H), 4.11 – 3.86 (m, 2H), 2.57 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d6) δ 197.3, 168.6, 141.1, 133.1, 130.7, 129.7, 129.20 – 120.11 (m), 120.05, 87.6, 61.15 (q, J = 34.0 Hz), 27.0.

5-(2,2,2-trifluoroethoxy)-1-(4-(1-(2,2,2-trifluoroethoxy)ethyl)phenyl)-1,5-dihydro-2*H*-pyrrol-2-one(2s)



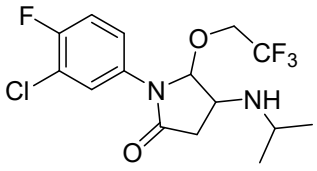
Slight yellow viscous liquid, yield 13%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.68 (dd, *J* = 8.7, 2.2 Hz, 2H), 7.37 (d, *J* = 8.6 Hz, 2H), 7.02 (dd, *J* = 6.1, 1.7 Hz, 1H), 6.46 (dd, *J* = 6.1, 0.8 Hz, 1H), 6.17 (s, 1H), 4.58 (qd, *J* = 6.4, 2.2 Hz, 1H), 3.80 – 3.51 (m, 4H), 1.50 (dd, *J* = 6.5, 1.3 Hz, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 168.1, 142.9, 138.9 (d, *J* = 4.0 Hz), 136.1 (d, *J* = 6.4 Hz), 131.8, 130.2, 127.2 (d, *J* = 4.2 Hz), 124.0 (q, *J* = 278.9 Hz), 123.3 (q, *J* = 277.6 Hz), 120.8, 120.8, 88.0 (d, *J* = 2.4 Hz), 79.0 (d, *J* = 2.6 Hz), 65.8 (q, *J* = 34.0 Hz), 60.2 (q, *J* = 35.3 Hz), 23.7. HRMS(ESI) *m/z*: calculated for $C_{16}H_{16}F_6NO_3$ $[M+H]^+$ 384.1029, found 384.1029.

5-(2,2,2-trifluoroethoxy)-1-(4-((2,2,2-trifluoroethoxy)methyl)phenyl)-1,5-dihydro-2*H*-pyrrol-2-one(2t)



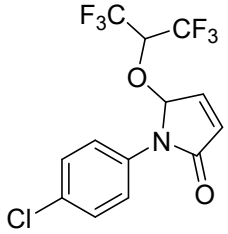
Slight yellow viscous liquid, yield 11%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.70 (d, *J* = 8.4 Hz, 2H), 7.40 (d, *J* = 8.4 Hz, 2H), 7.02 (d, *J* = 6.0 Hz, 1H), 6.45 (d, *J* = 6.0 Hz, 1H), 6.18 (s, 1H), 4.67 (s, 2H), 3.83 (q, *J* = 8.7 Hz, 2H), 3.71 – 3.48 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 168.1, 141.9, 136.4, 133.5, 131.8, 128.9, 124.0 (q, *J* = 279.3 Hz), 123.3 (q, *J* = 277.6 Hz), 120.5, 87.9, 73.5, 67.2 (q, *J* = 34.1 Hz), 60.2 (q, *J* = 35.6 Hz). HRMS(ESI) *m/z*: calculated for $C_{15}H_{14}F_6NO_3$ $[M+H]^+$ 370.0872, found 370.0879.

1-(3-chloro-4-fluorophenyl)-4-(isopropylamino)-5-(2,2,2-trifluoroethoxy)pyrrolidin-2-one (3h)



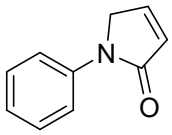
Slight yellow viscous liquid, yield 89%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.56 (dd, *J* = 6.6, 2.6 Hz, 1H), 7.33 (ddd, *J* = 8.9, 4.1, 2.6 Hz, 1H), 7.18 (t, *J* = 8.7 Hz, 1H), 5.10 (s, 1H), 3.95 – 3.75 (m, 2H), 3.53 – 3.46 (m, 1H), 3.06 – 2.88 (m, 2H), 2.35 – 2.25 (m, 1H), 1.12 (t, *J* = 6.5 Hz, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.1, 156.7 (d, *J* = 249.5 Hz), 133.8 (d, *J* = 3.7 Hz), 126.7, 124.1 (d, *J* = 7.3 Hz), 123.3 (q, *J* = 278.8 Hz), 121.6 (d, *J* = 18.7 Hz), 117.0 (d, *J* = 22.1 Hz), 97.7, 65.5 (q, *J* = 35.1 Hz), 53.9, 46.6, 37.4, 23.1. HRMS(ESI) *m/z*: calculated for $C_{15}H_{18}ClF_4N_2O_2$ $[M+H]^+$ 369.0987, found 369.0992.

1-(4-chlorophenyl)-5-((1,1,1,3,3,3-hexafluoropropan-2-yl)oxy)-1,5-dihydro-2*H*-pyrrol-2-one (3e)



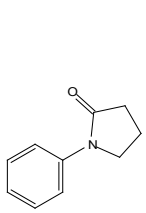
White solid, yield 92%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.58 (d, *J* = 8.9 Hz, 2H), 7.38 (d, *J* = 8.9 Hz, 2H), 7.06 (d, *J* = 5.9 Hz, 1H), 6.49 (d, *J* = 6.1 Hz, 1H), 6.31 (s, 1H), 4.13 (hept, *J* = 5.6 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-d) δ 167.9, 140.9, 134.9, 132.1, 130.9, 129.2, 121.9, 120.9 (q, J = 285.8), 120.8 (q, J = 284.8), 88.9, 70.0 (hept, J = 67.0). HRMS(ESI) m/z: calculated for C13H7ClF6NO2 [M-H]- 358.0075, found 358.0076.

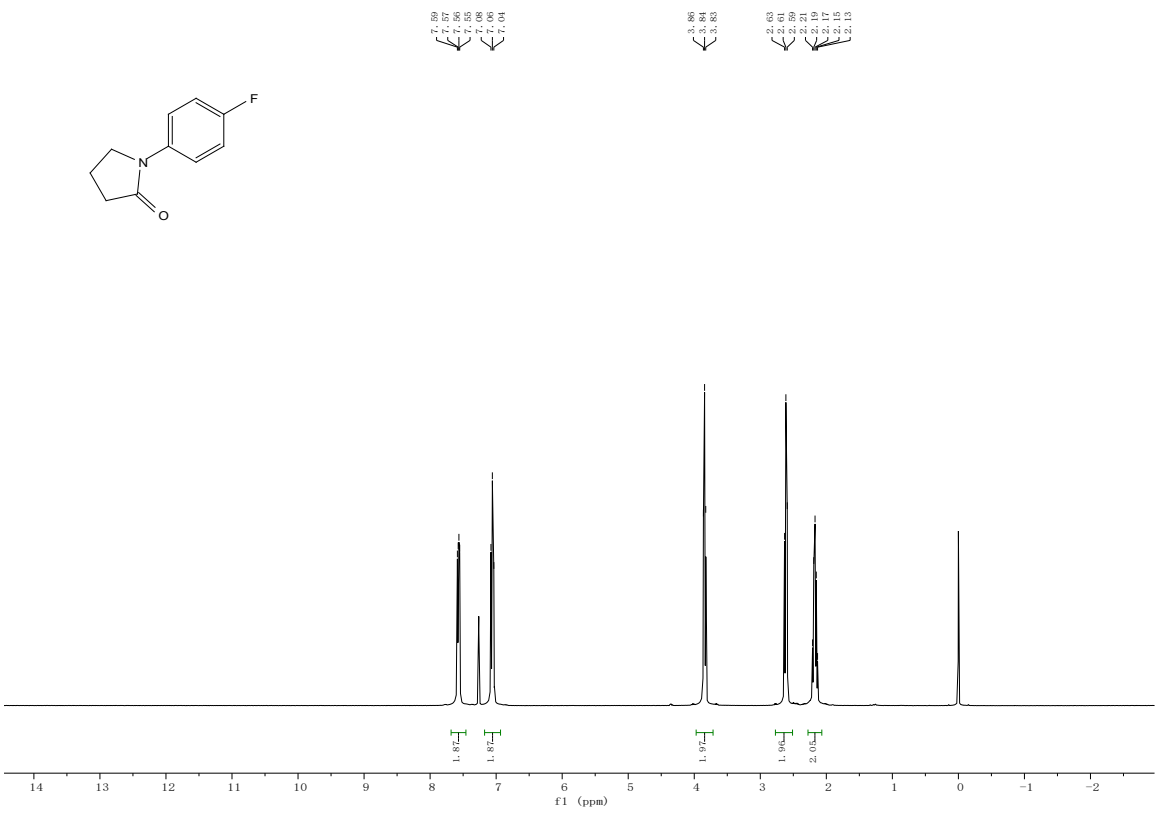
1-phenyl-1,5-dihydro-2*H*-pyrrol-2-one (compound e)[1]



Brown solid, Yield 95%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.71 (d, J = 8.0 Hz, 2H), 7.38 (t, J = 8.0 Hz, 2H), 7.18 (dt, J = 6.1, 1.9 Hz, 1H), 7.14 (t, J = 6.1 Hz, 1H), 6.28 (dt, J = 6.0, 1.9 Hz, 1H), 4.45 (t, J = 1.9 Hz, 2H).

9. NMR Spectra

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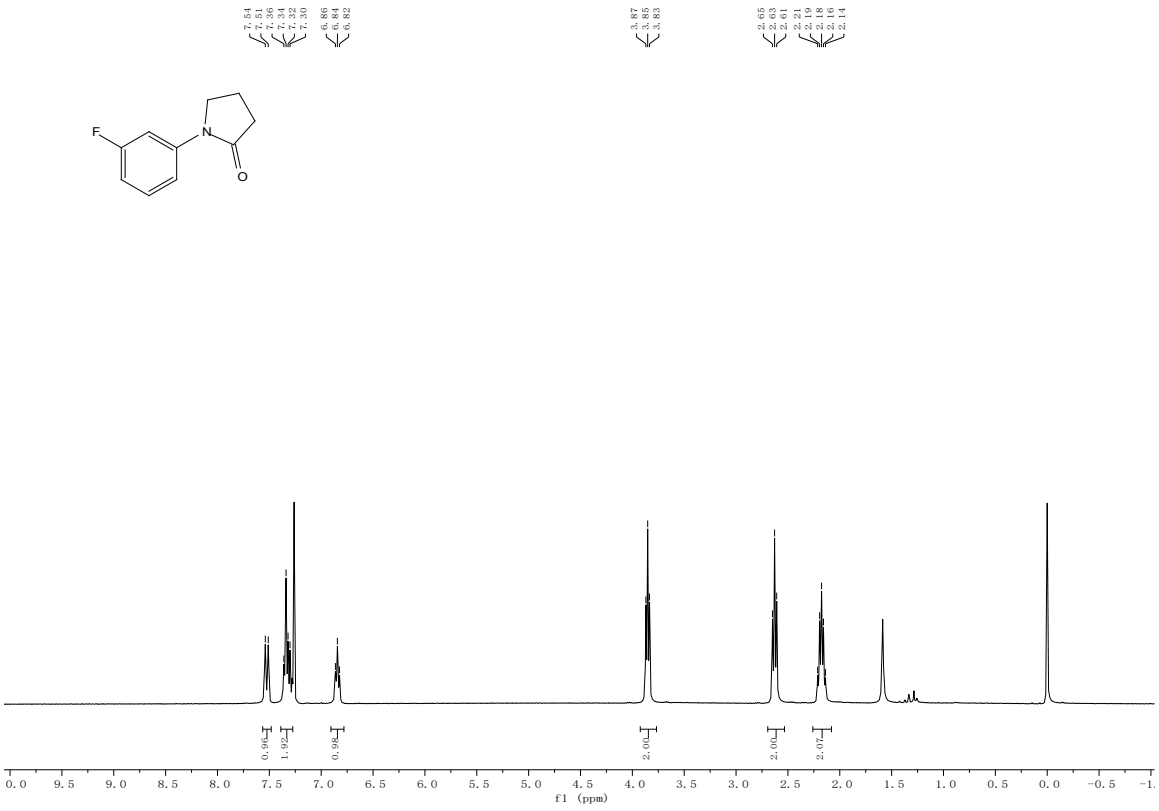
7.57
7.56
7.55
7.08
7.06
7.04
3.88
3.84
3.83
2.63
2.61
2.59
2.21
2.19
2.17
2.15
2.13
F
N
O
1.87
1.87
1.97
1.94
2.05
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2
f1 (ppm)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7.34
7.32
7.30
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6.84
6.82
3.87
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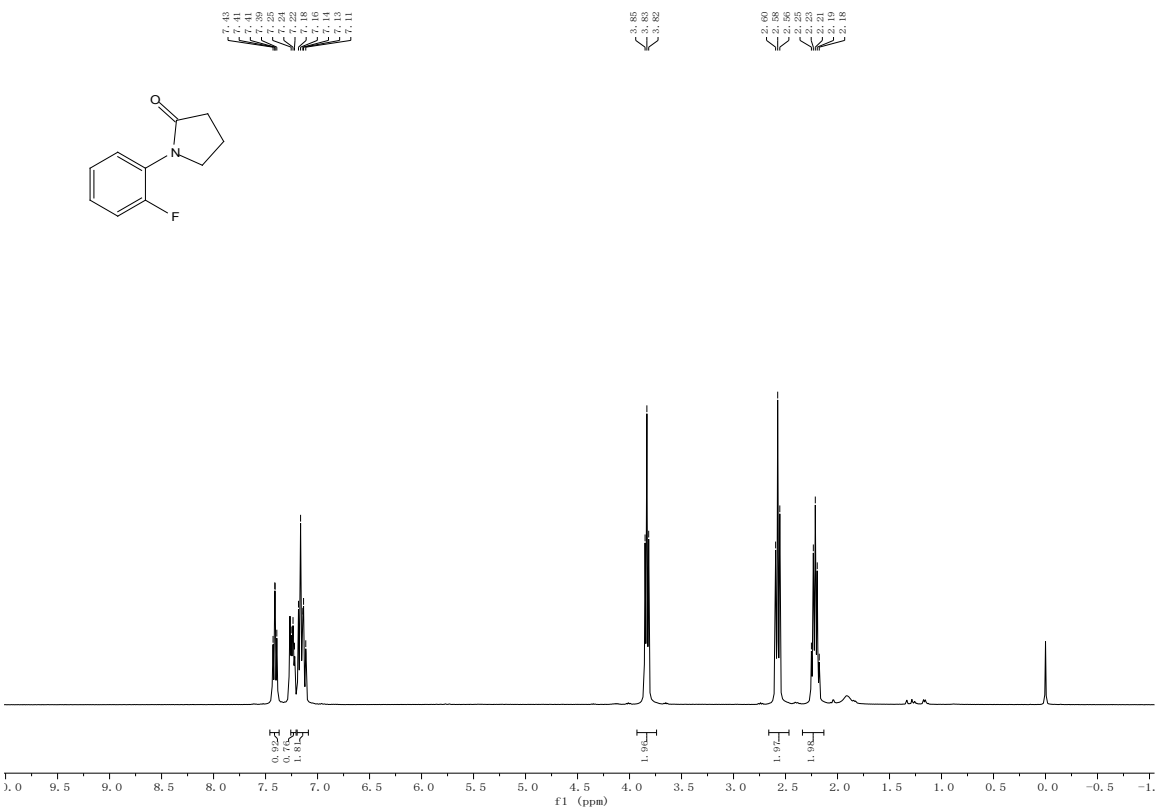
2.65
2.63
2.61
2.21
2.19
2.18
2.16
2.14
F
N
O
0.96
1.92
0.98
2.00
2.00
2.07
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.
f1 (ppm)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7.24
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7.18
7.16
7.14
7.13
7.11
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3.83
3.82
2.60
2.58
2.56
2.25
2.23
2.21
2.19
2.18
O
N
F
0.92
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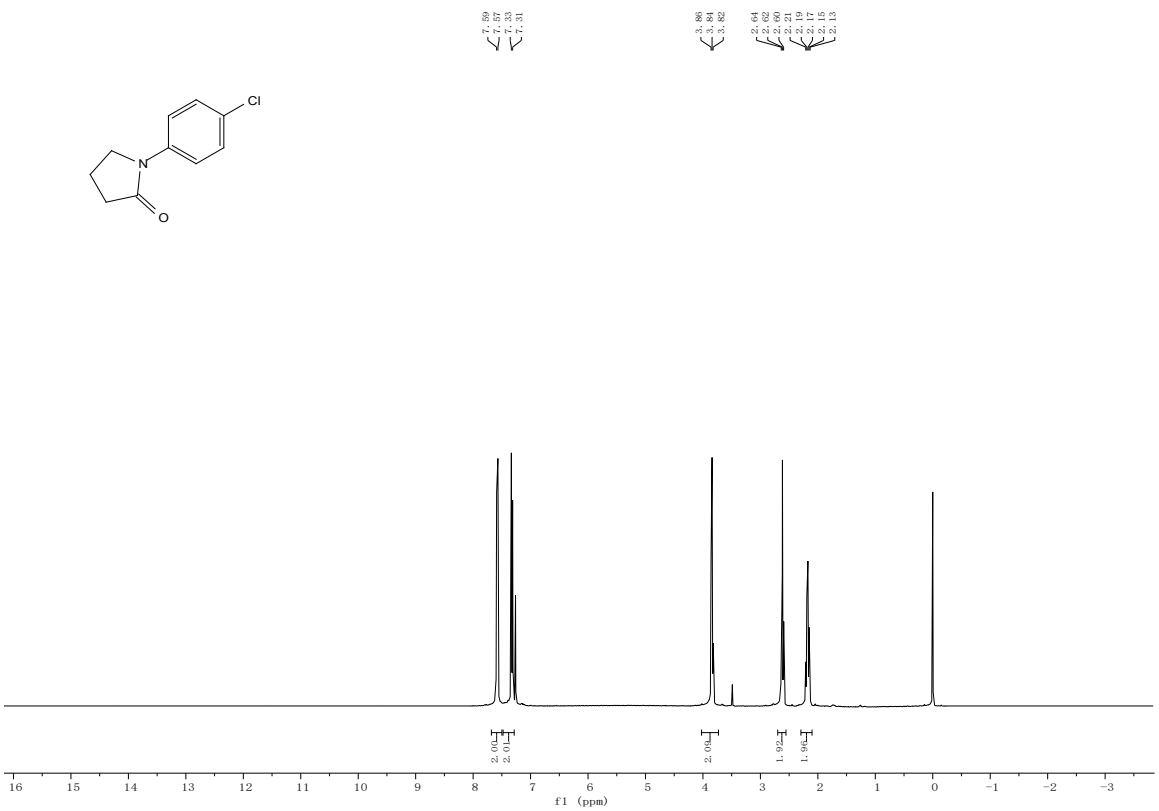
1.84
1.96
1.97
1.98
f1 (ppm)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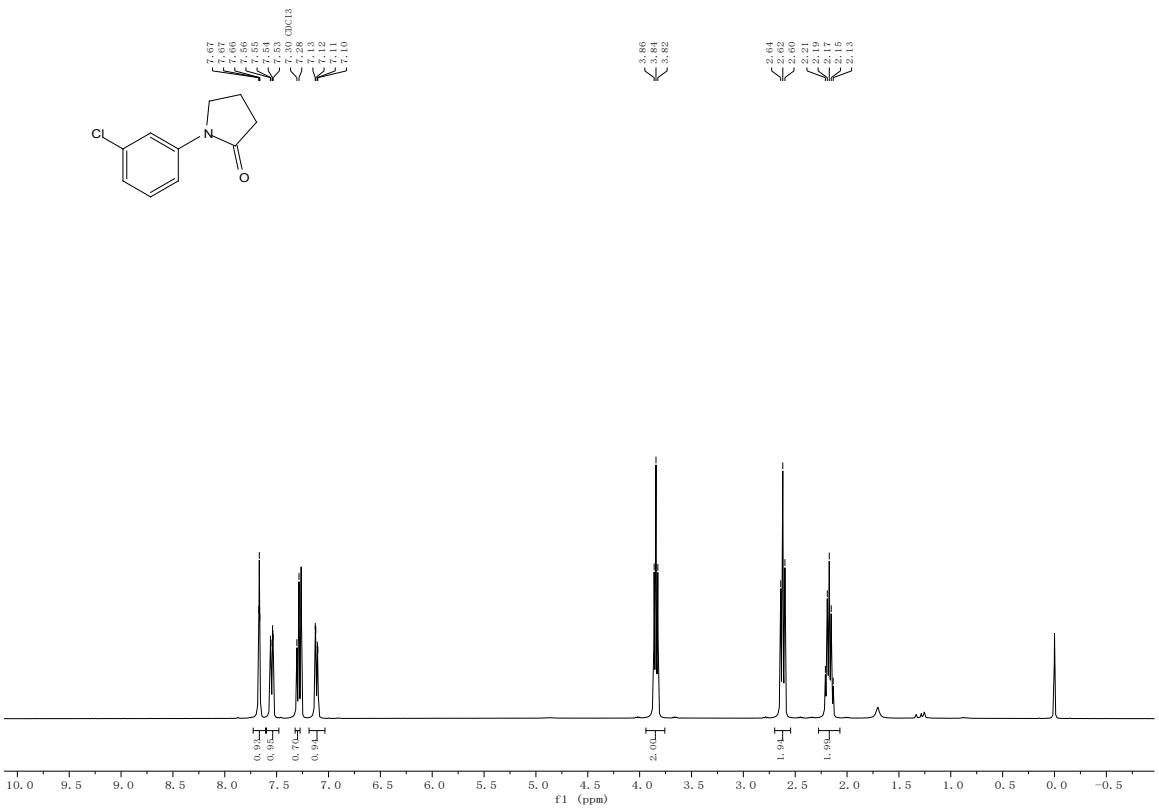
2.64
2.62
2.60
2.21
2.19
2.17
2.15
2.13
Cl
N
O
2.07
2.07
2.00
1.92
1.96
f1 (ppm)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7.54
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7.30
CDCl3
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7.13
7.12
7.11
7.10
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2.62
2.60
2.21
2.19
2.17
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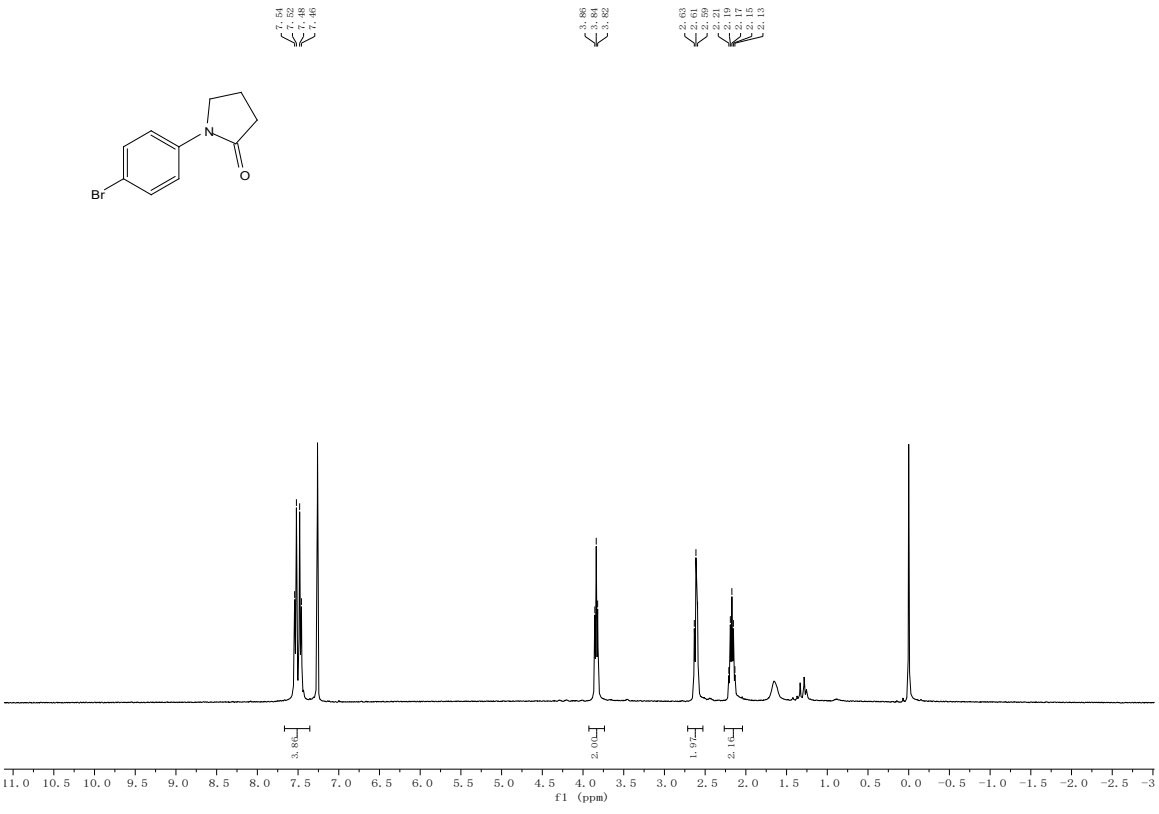
1.99
f1 (ppm)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7.52
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2.15
2.13
N
O
Br
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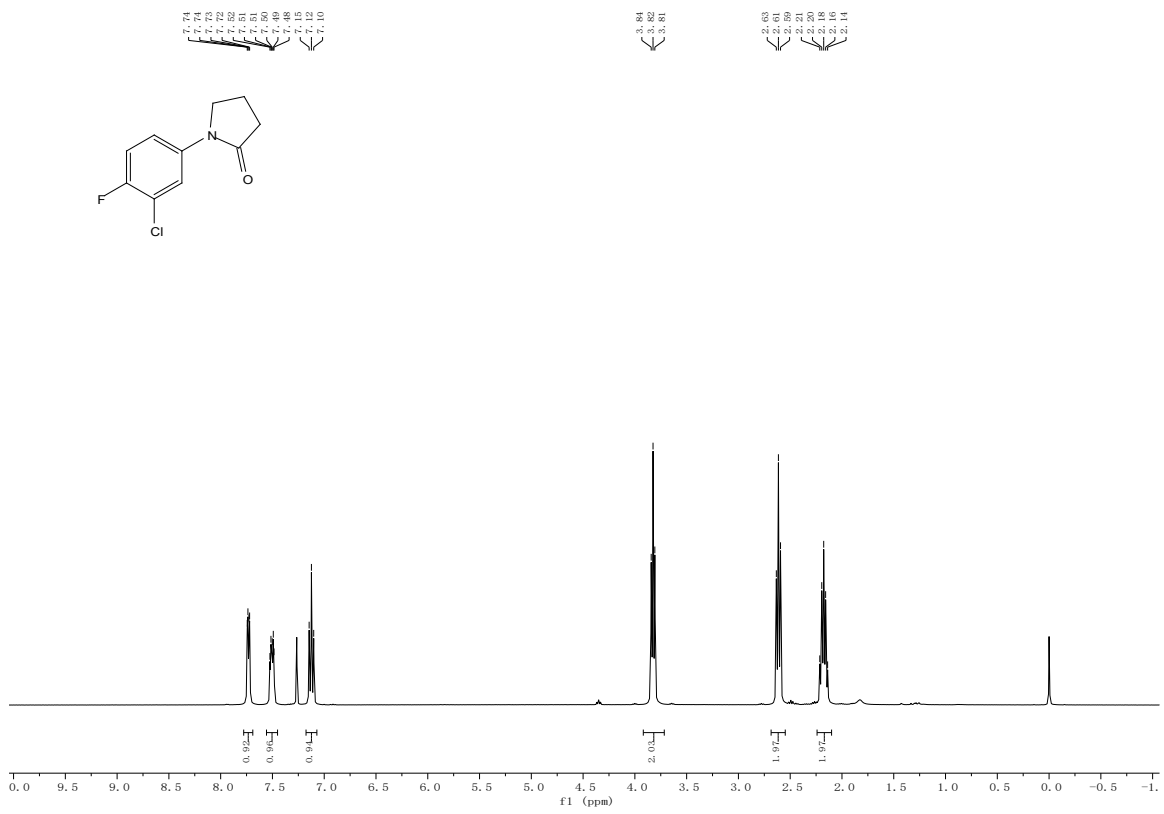
2.00
1.97
2.16
f1 (ppm)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7.74
7.73
7.72
7.52
7.51
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7.49
7.48
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7.12
7.10
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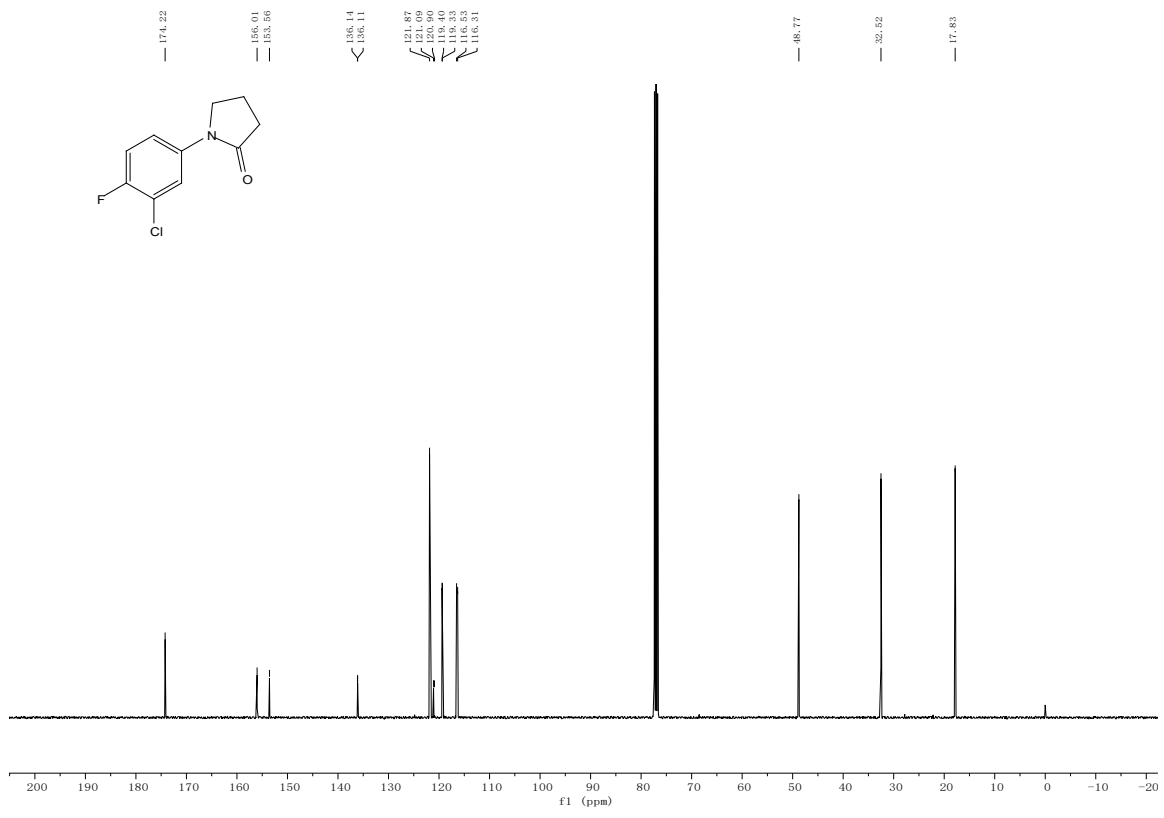
3.82
3.81
2.63
2.61
2.59
2.21
2.20
2.18
2.16
2.14
N
O
F
Cl
0.92
0.96
0.94
2.03
1.97
1.97
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.
f1 (ppm)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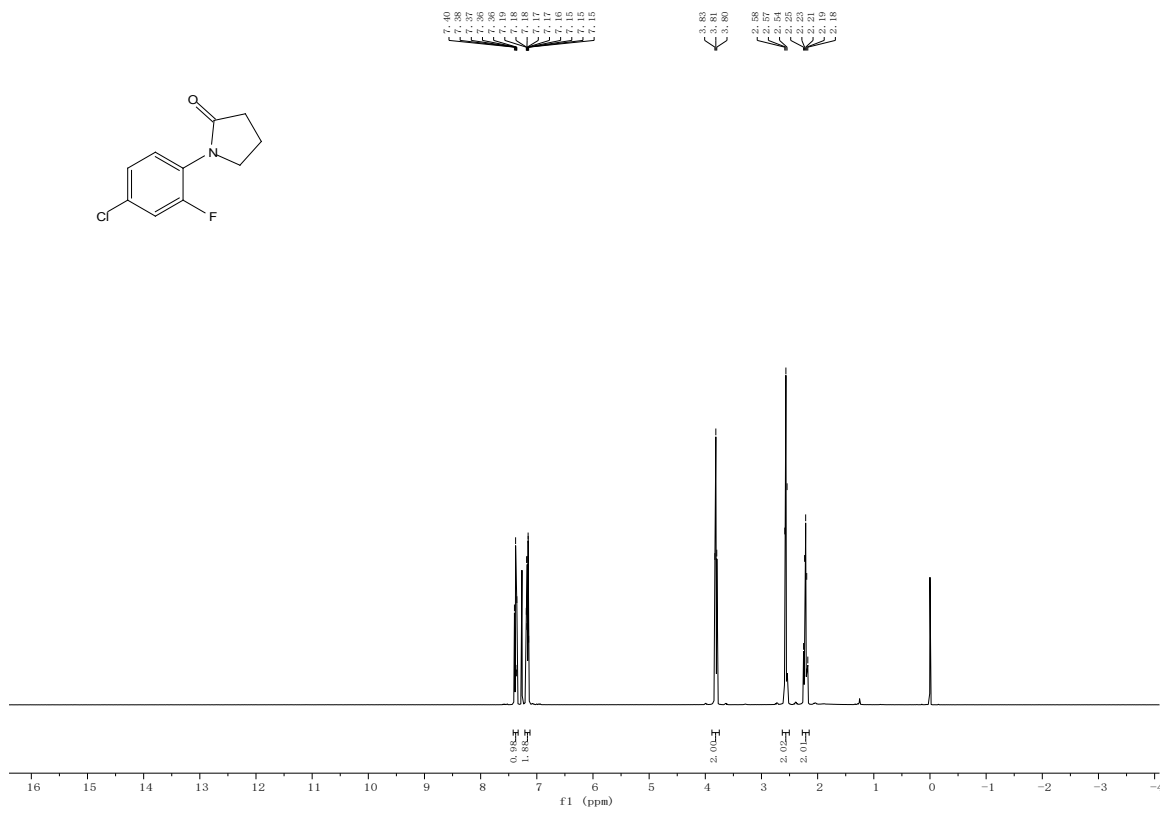
136.11
121.87
121.09
120.90
119.40
119.33
116.53
116.31
48.77
32.52
17.83
N
O
F
Cl
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20
f1 (ppm)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7.16
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7.15
3.83
3.81
3.80
2.58
2.57
2.54
2.25
2.23
2.21
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2.18
O
N
Cl
F
0.98
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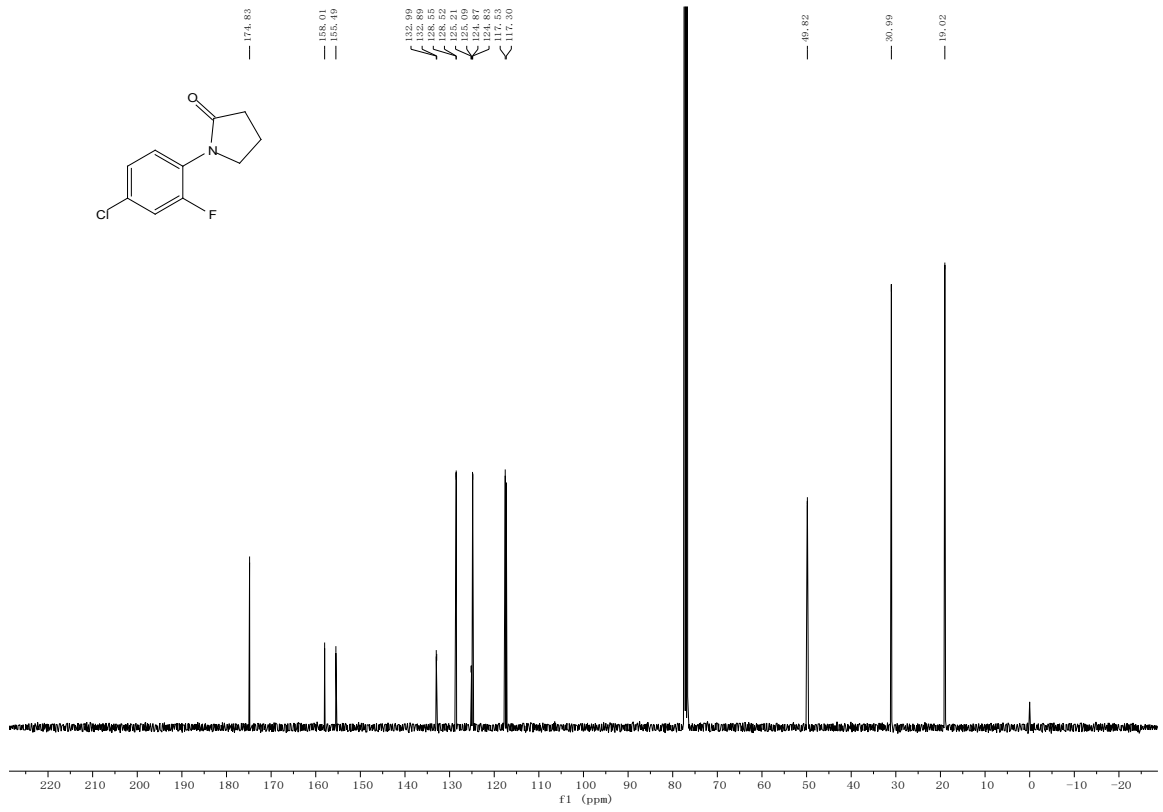
2.01
2.02
2.01
f1 (ppm)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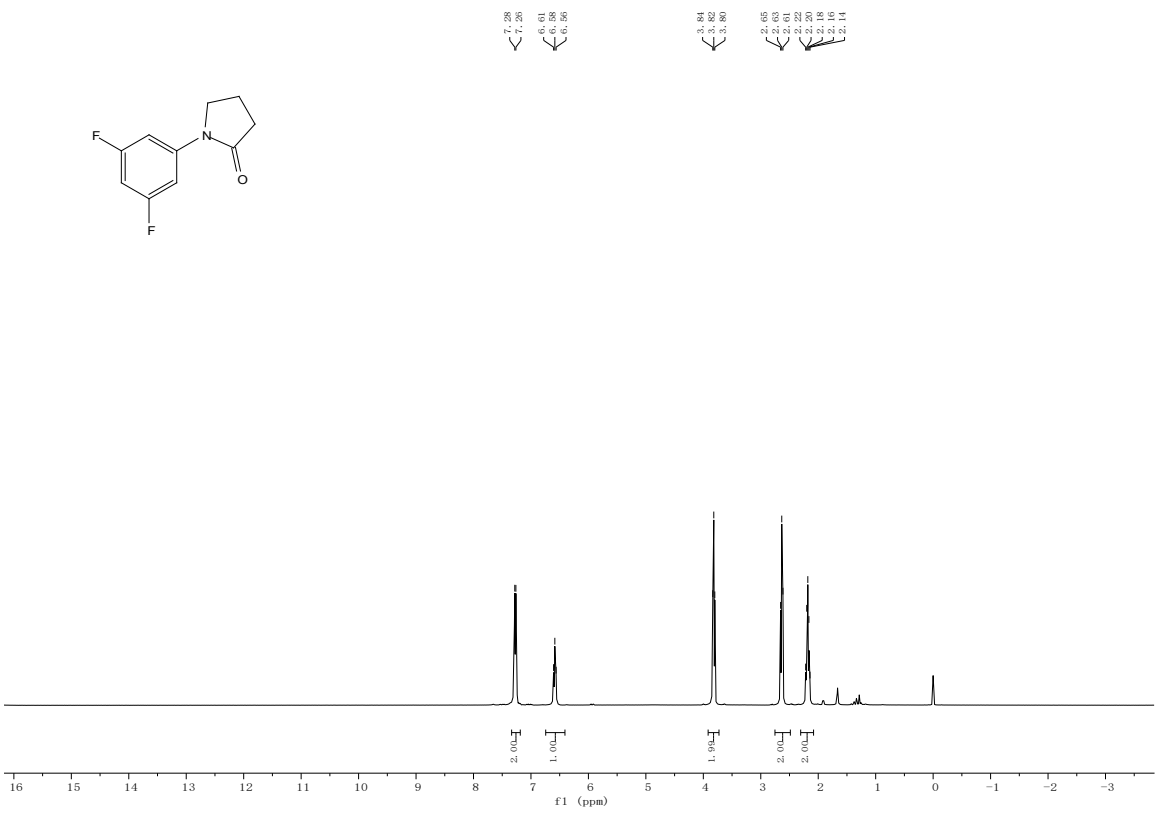
30.99
19.02
O
N
Cl
F
f1 (ppm)


7.28
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2.63
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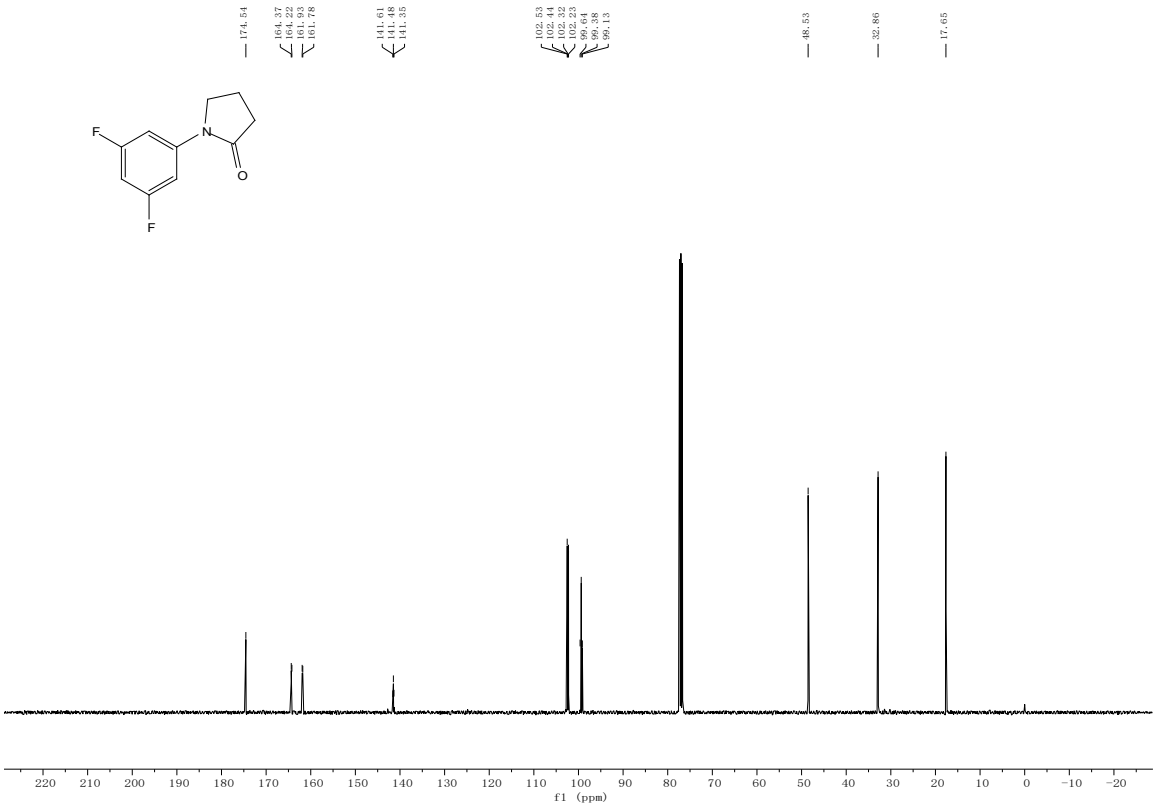
2.18
2.16
2.14
F
N
O
F
2.00
1.00
1.99
2.00
2.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)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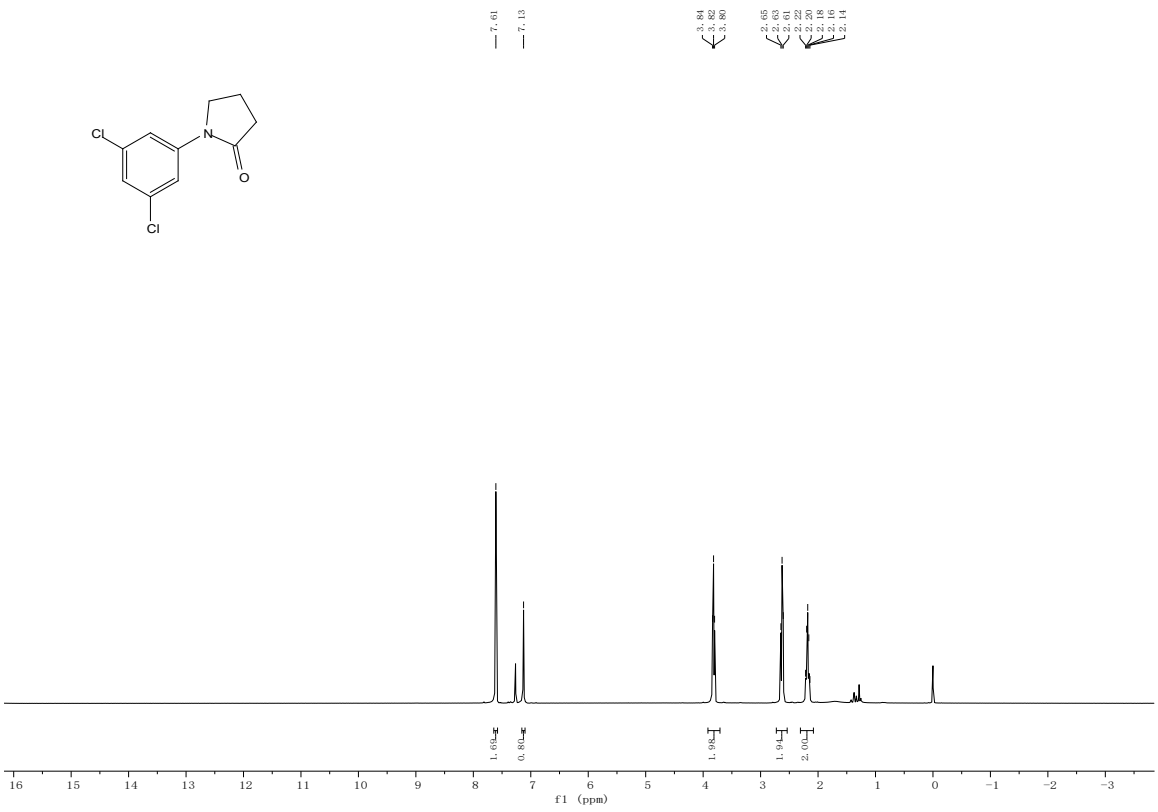
164.22
161.93
161.78
141.61
141.48
141.35
102.53
102.44
102.32
102.25
99.64
99.38
99.13
48.53
32.86
17.65
F
N
O
F
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20
f1 (ppm)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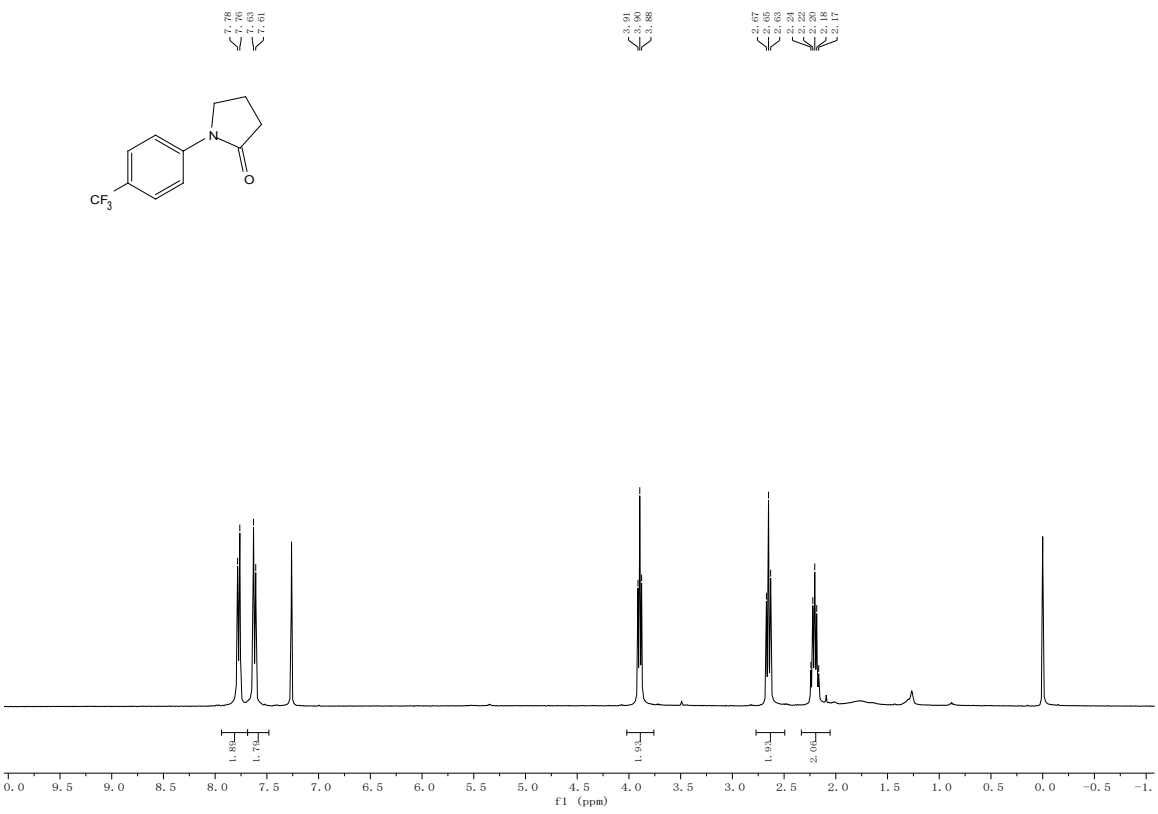
7.13
3.84
3.82
3.80
2.65
2.63
2.61
2.22
2.20
2.18
2.16
2.14
Cl
N
O
Cl
1.69
0.80
1.98
1.94
2.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)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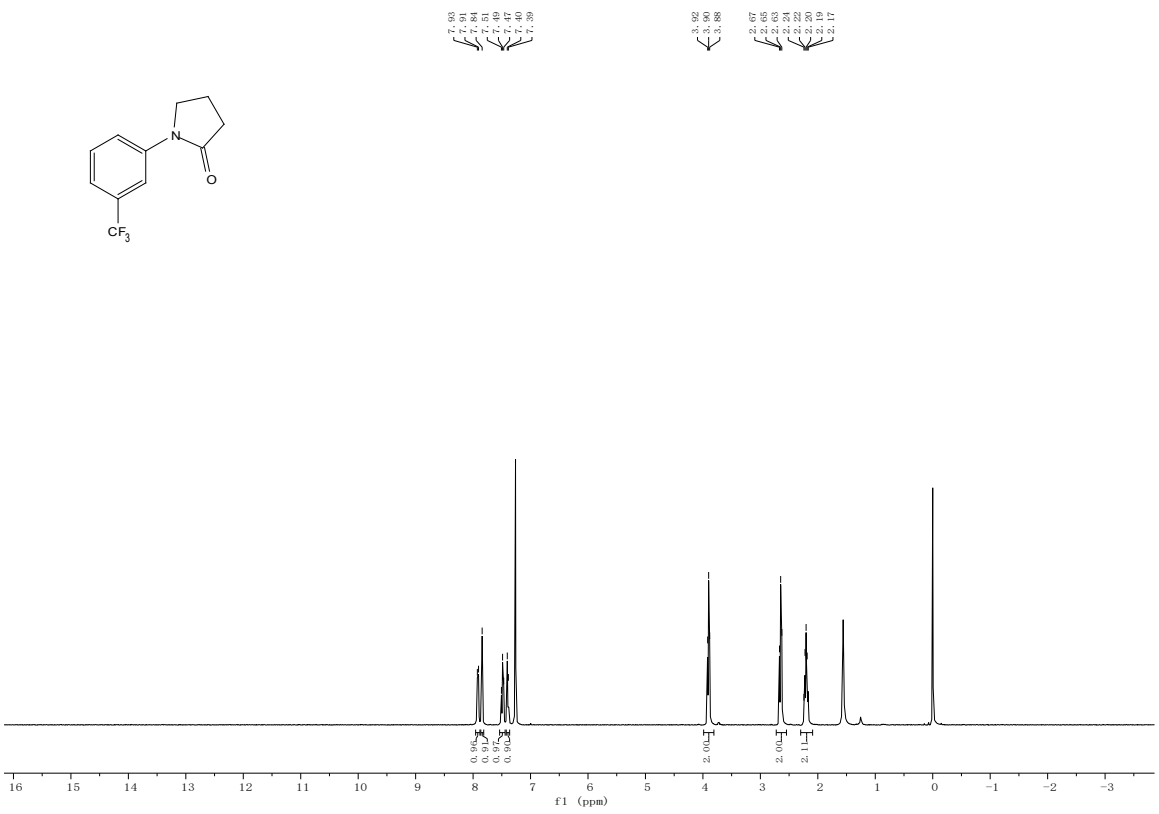
7.61
3.91
3.90
3.88
2.67
2.65
2.63
2.24
2.22
2.20
2.18
2.17
N
O
CF3
1.89
1.79
1.93
1.93
2.06
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.
f1 (ppm)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7.91
7.84
7.51
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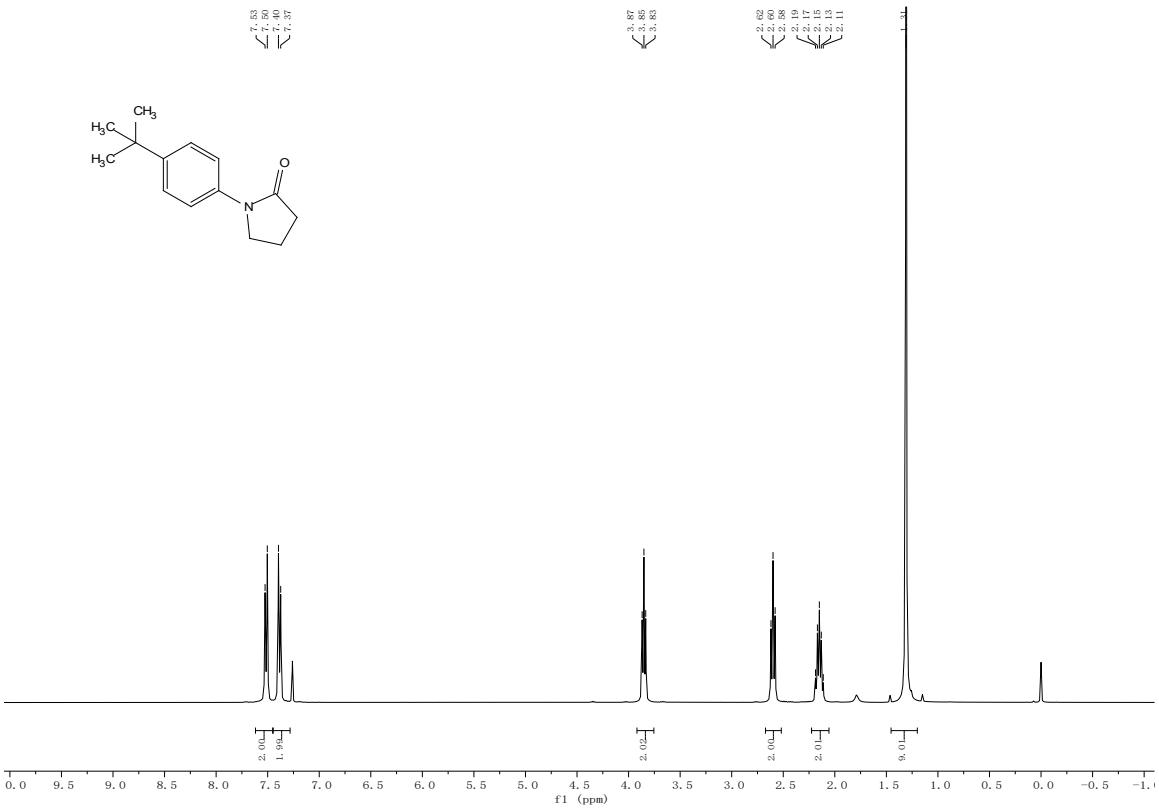
7.47
7.40
7.39
3.92
3.90
3.88
2.67
2.65
2.63
2.24
2.22
2.20
2.19
2.17
N
O
CF3
0.94
0.91
0.97
0.96
2.00
2.00
2.11
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)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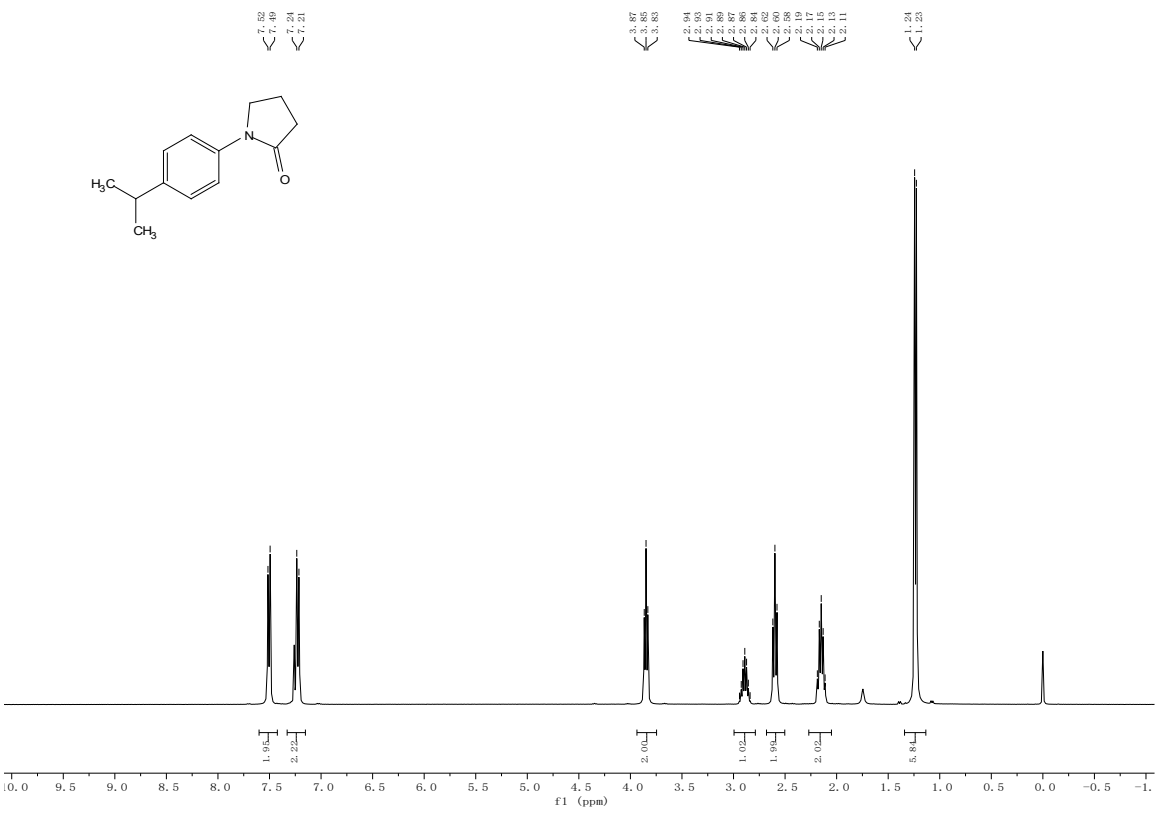
3.85
3.83
2.62
2.60
2.58
2.19
2.17
2.15
2.13
2.11
1.30
CH3
H3C
H3C
O
N
2.00
1.94
2.02
2.00
2.01
9.01
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.
f1 (ppm)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2.91
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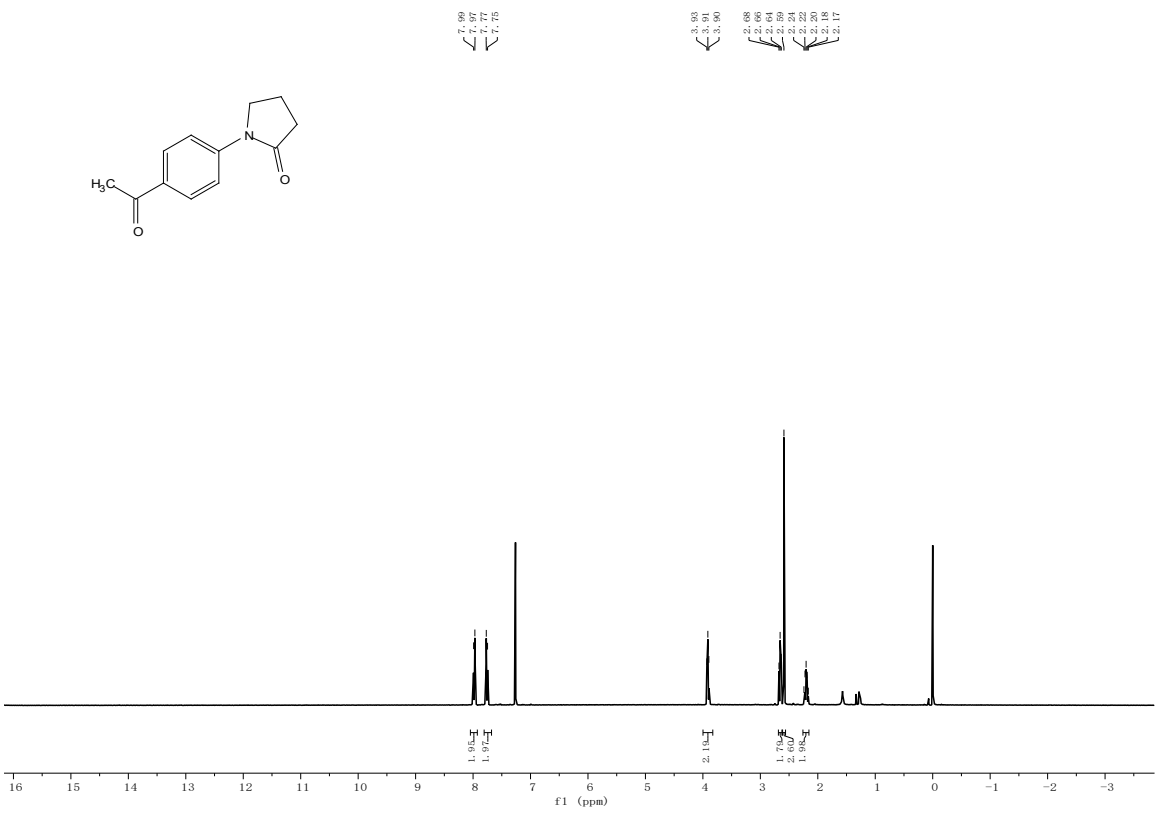
2.87
2.86
2.84
2.62
2.60
2.58
2.19
2.17
2.15
2.13
2.11
1.24
1.23
H3C
CH3
N
O
1.95
2.22
2.00
1.02
1.94
2.02
5.84
f1 (ppm)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3.91
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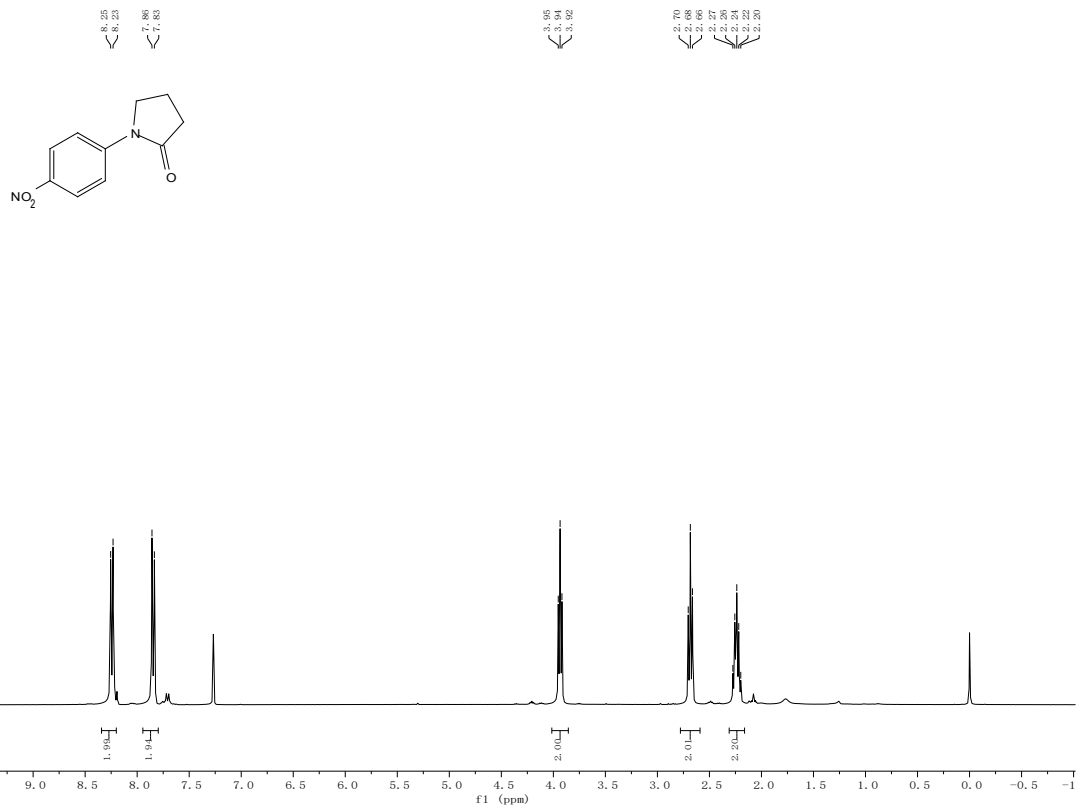
2.64
2.59
2.24
2.22
2.20
2.18
2.17
H3C
O
N
O
1.95
1.97
2.18
1.76
2.60
1.98
f1 (ppm)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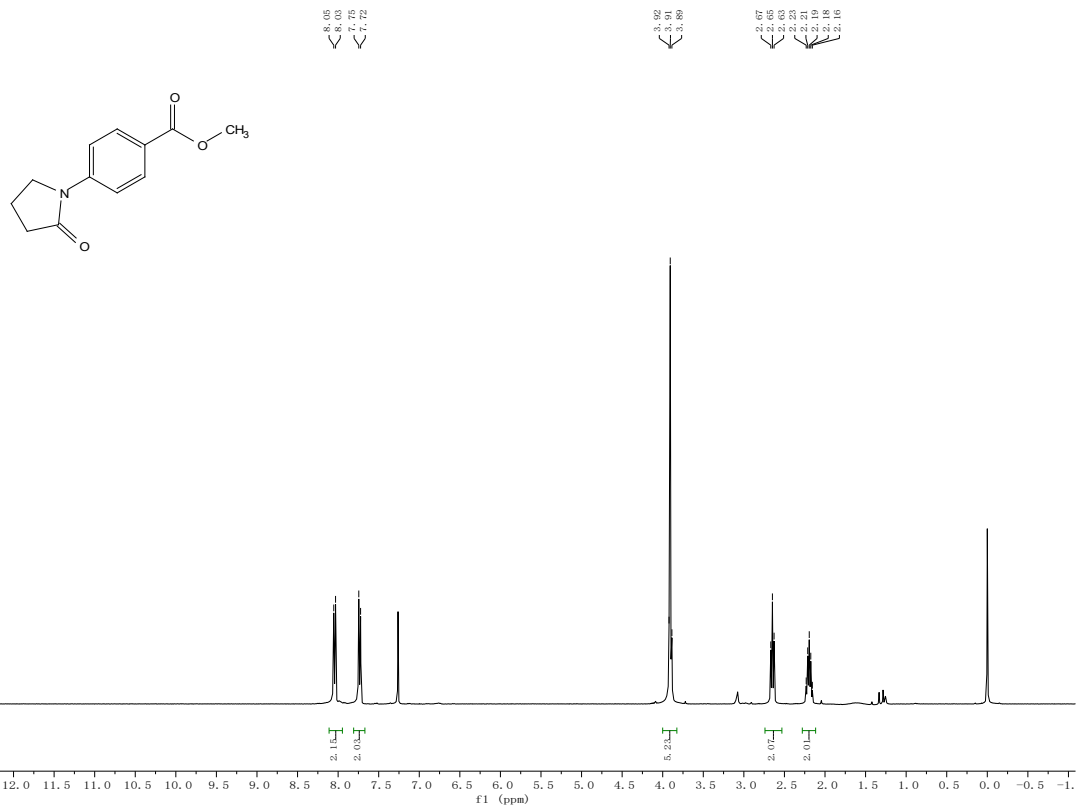
8.23
7.86
7.83
3.95
3.94
3.92
2.70
2.68
2.66
2.27
2.26
2.24
2.22
2.20
N
O
NO2
1.94
1.94
2.00
2.01
2.20
f1 (ppm)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8.03
7.75
7.72
3.92
3.91
3.89
2.67
2.65
2.63
2.23
2.21
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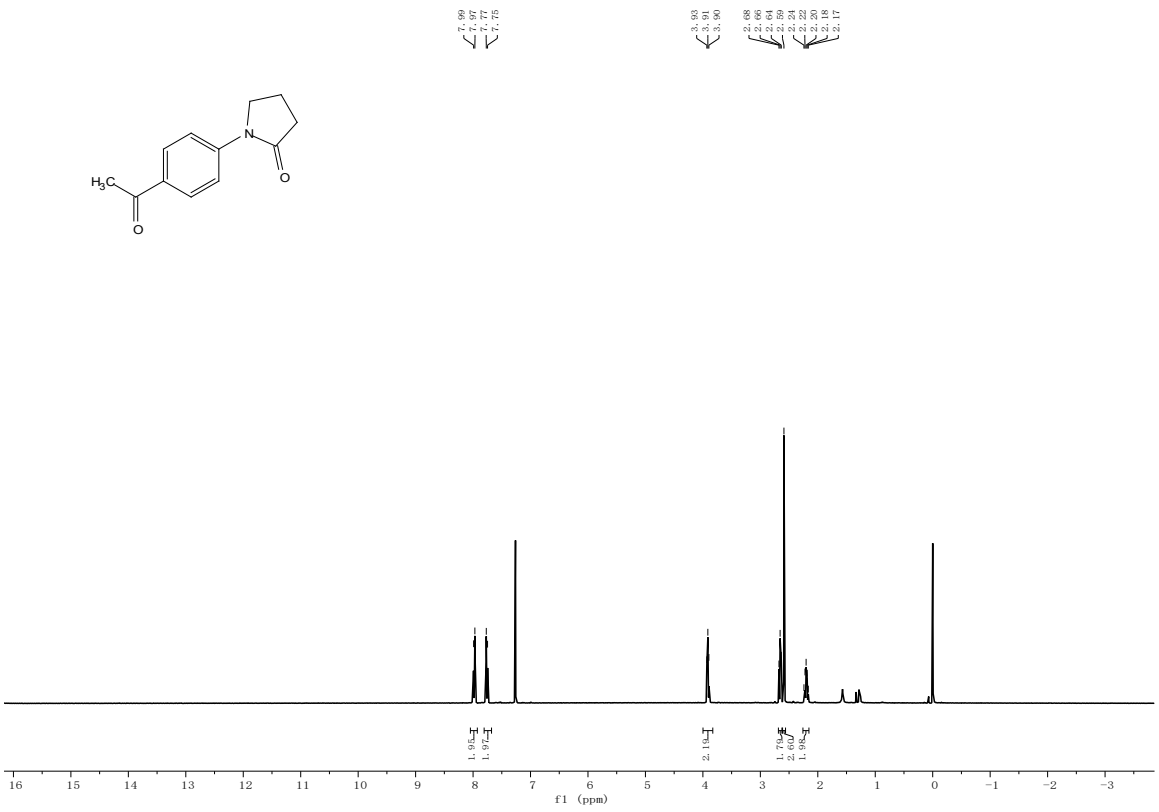
2.03
5.23
2.07
2.01
f1 (ppm)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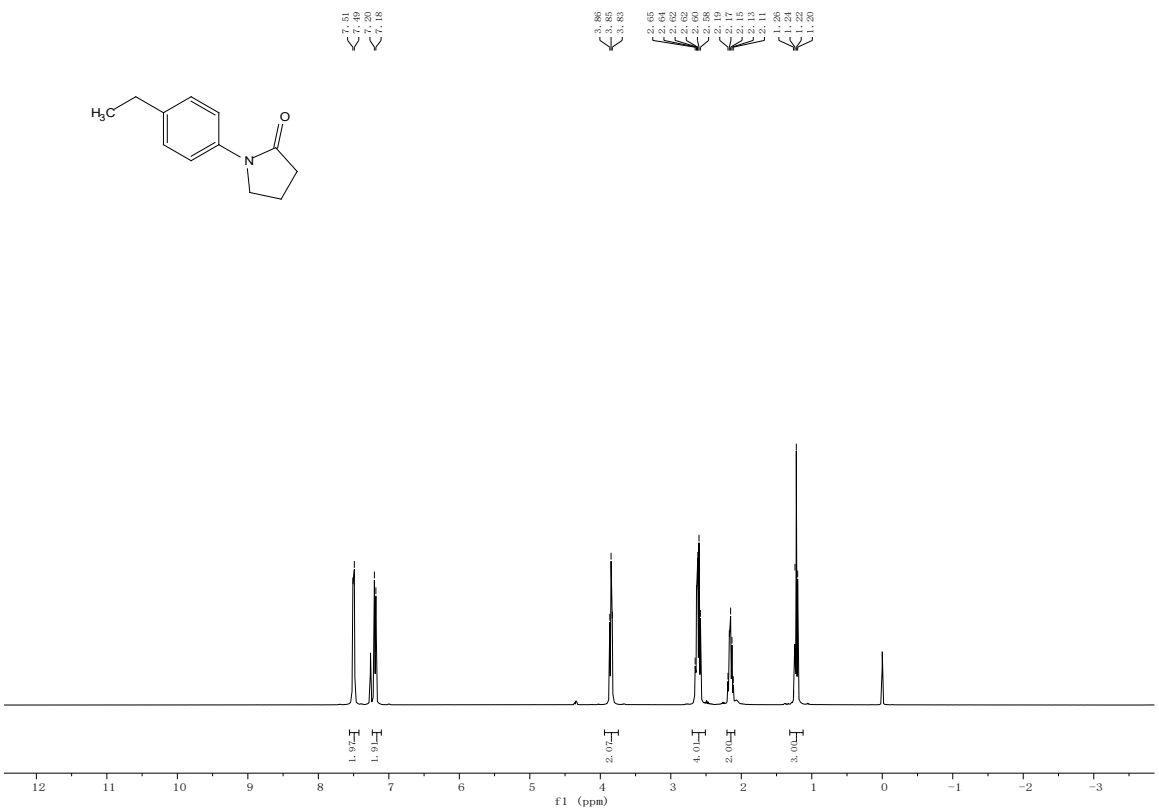
7.97
7.77
7.75
3.93
3.91
3.90
2.68
2.66
2.64
2.59
2.24
2.22
2.20
2.18
2.17
H3C
O
N
O
1.95
1.97
2.19
1.74
2.60
1.96
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)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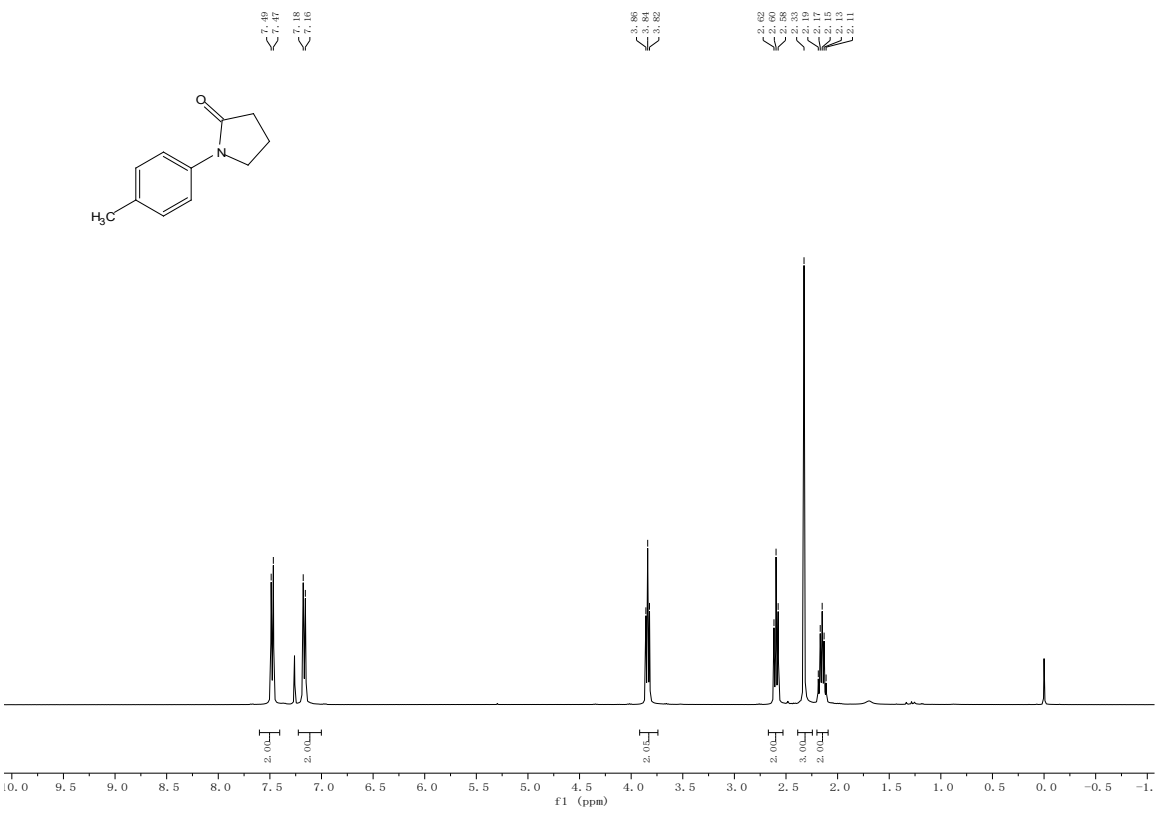
7.49
7.20
7.18
3.86
3.85
3.83
2.65
2.64
2.62
2.62
2.60
2.58
2.19
2.17
2.15
2.13
2.11
1.26
1.24
1.22
1.20
H3C
O
N
1.91
1.91
2.07
4.01
2.07
3.01
12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)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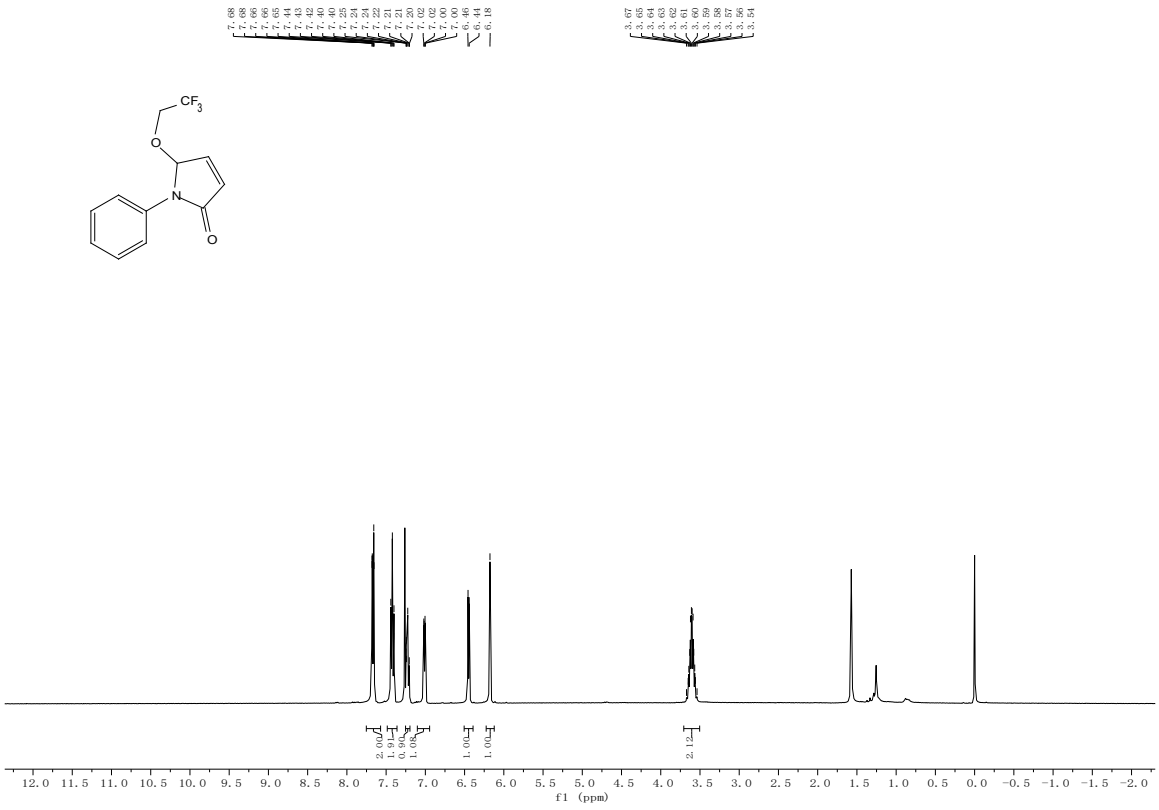
3.84
3.82
2.62
2.60
2.58
2.33
2.19
2.17
2.15
2.13
2.11
O
N
H3C
2.01
2.01
2.05
2.01
3.01
2.01
f1 (ppm)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7.42
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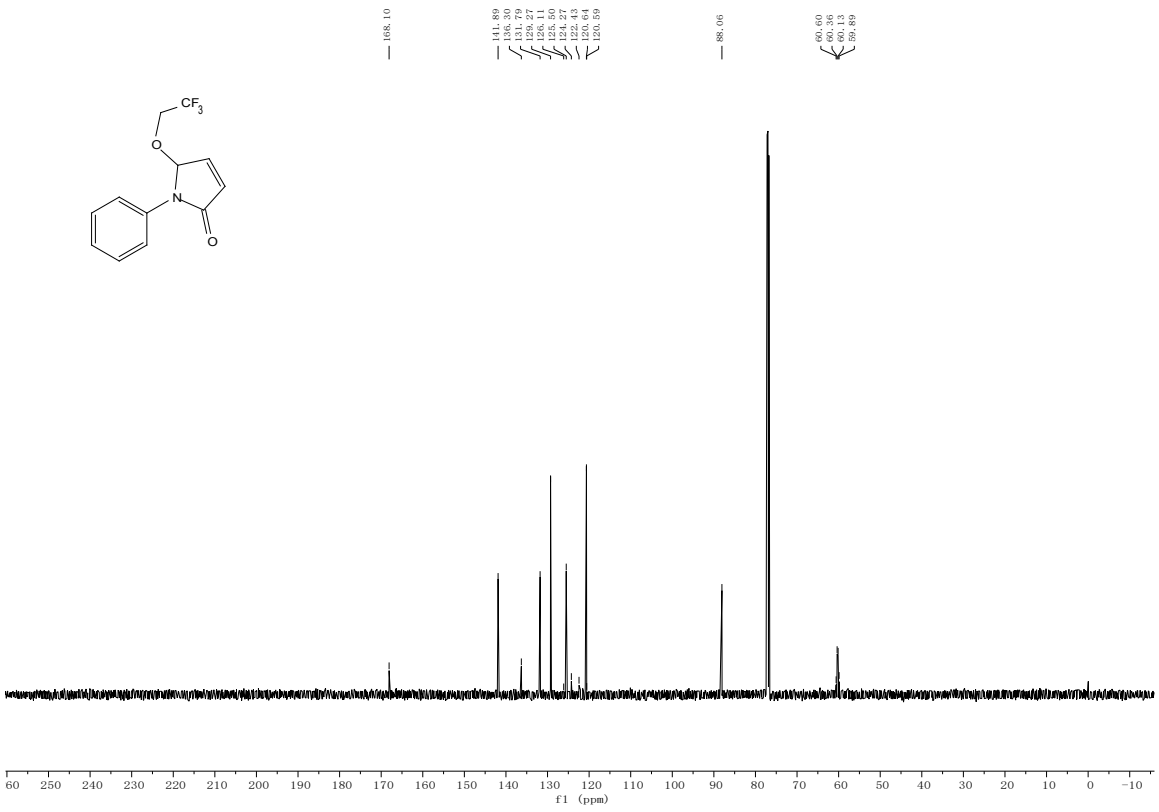
7.40
7.25
7.24
7.24
7.22
7.21
7.21
7.20
7.02
7.02
7.00
7.00
6.46
6.44
6.18
3.67
3.65
3.64
3.63
3.62
3.61
3.60
3.59
3.58
3.57
3.56
3.54
CF3
O
N
O
2.07
1.97
0.90
1.00
1.00
1.00
2.12
f1 (ppm)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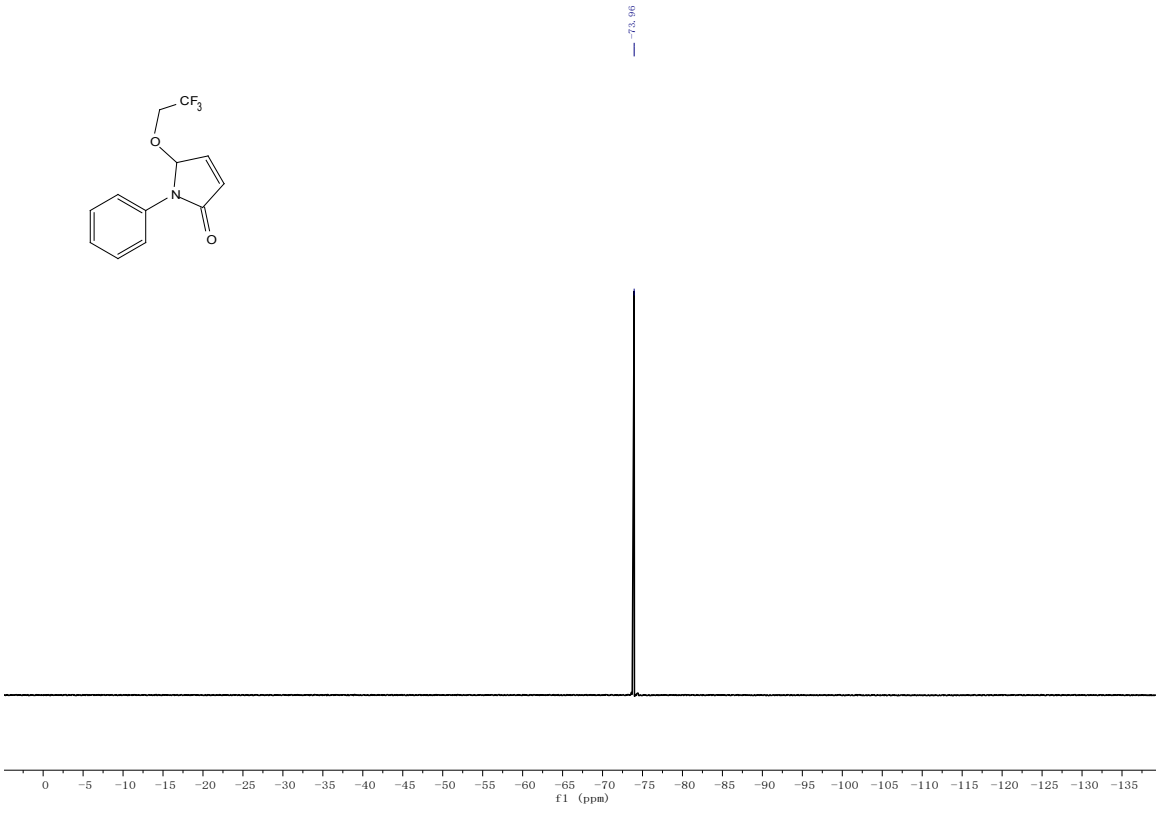
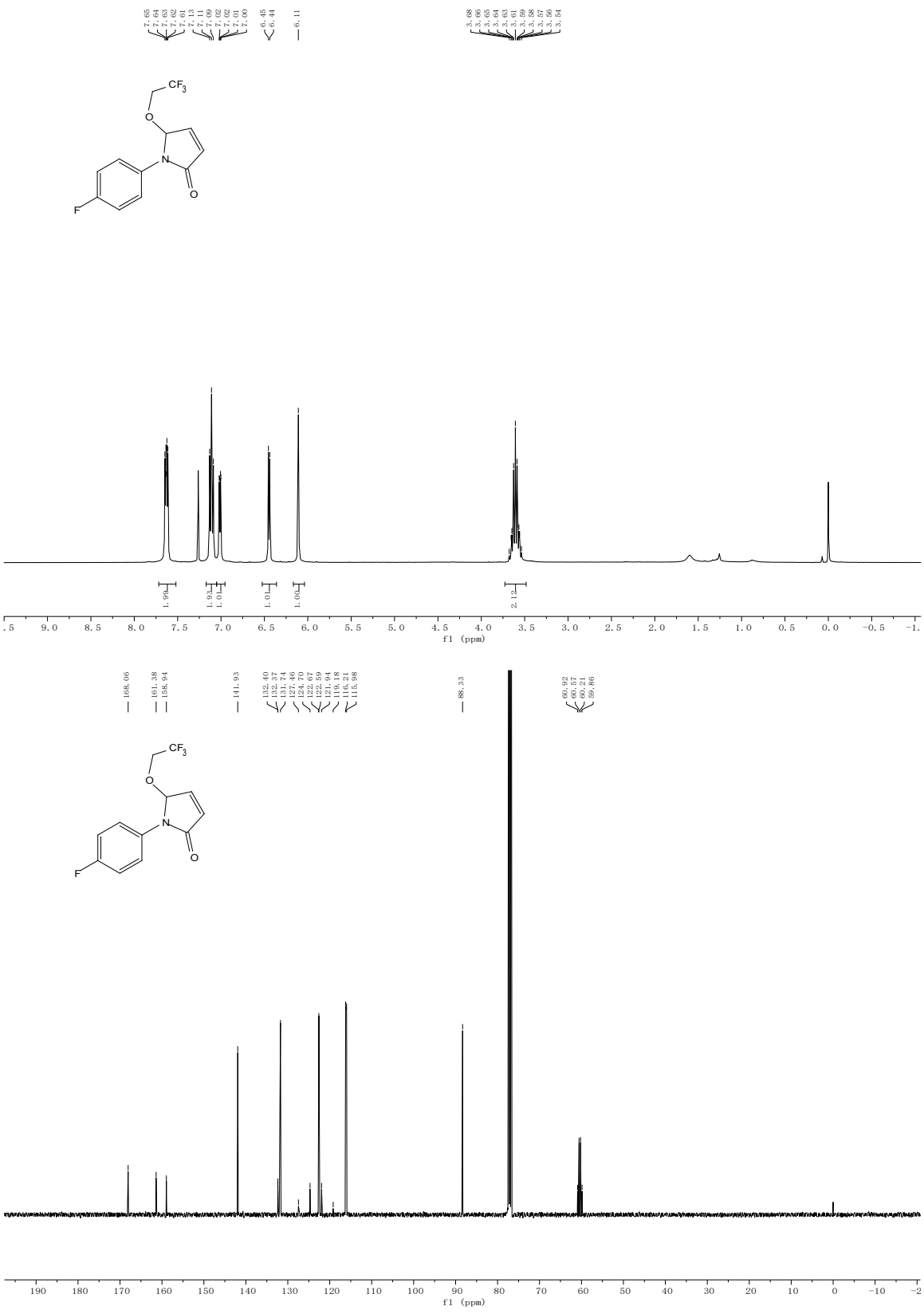
129.27
126.11
125.50
124.27
122.43
120.64
120.59
88.06
60.60
60.36
60.13
59.89
CF3
O
N
O
60 250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


−73.96
CF3
O
N
O
0 −5 −10 −15 −20 −25 −30 −35 −40 −45 −50 −55 −60 −65 −70 −75 −80 −85 −90 −95 −100 −105 −110 −115 −120 −125 −130 −135
f1 (ppm)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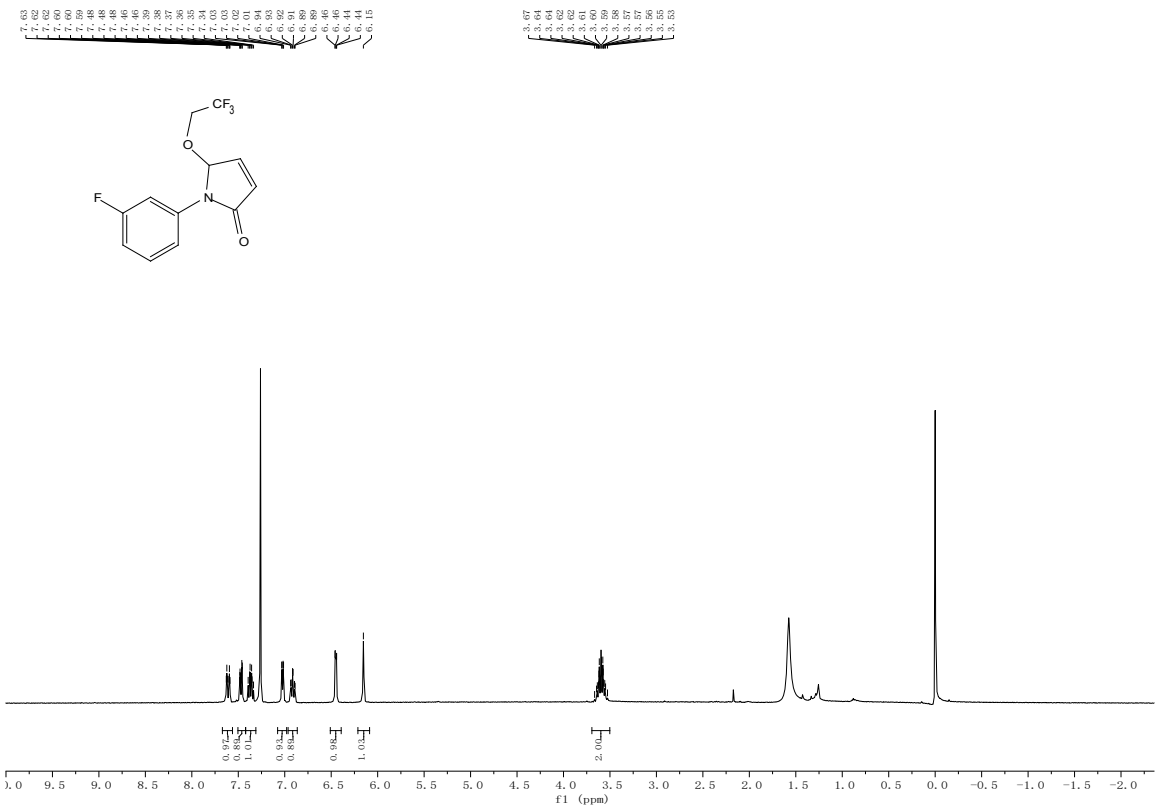
7.61
7.13
7.11
7.09
7.02
7.02
7.01
7.00
6.45
6.44
6.11
3.68
3.66
3.65
3.64
3.63
3.61
3.59
3.58
3.57
3.56
3.54
CF3
O
N
O
F
1.94
1.93
1.01
1.01
1.00
2.12
f1 (ppm)
168.06
161.38
158.94
141.93
132.40
132.37
131.74
127.46
124.70
122.67
122.59
121.94
119.18
116.21
115.98
88.33
60.92
60.57
60.21
59.86
f1 (ppm)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7.46
7.46
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7.38
7.37
7.37
7.36
7.35
7.34
7.03
7.03
7.02
7.01
6.94
6.93
6.92
6.91
6.89
6.89
6.46
6.46
6.44
6.44
6.15
3.67
3.64
3.64
3.62
3.62
3.61
3.60
3.59
3.58
3.57
3.57
3.56
3.55
3.53
CF3
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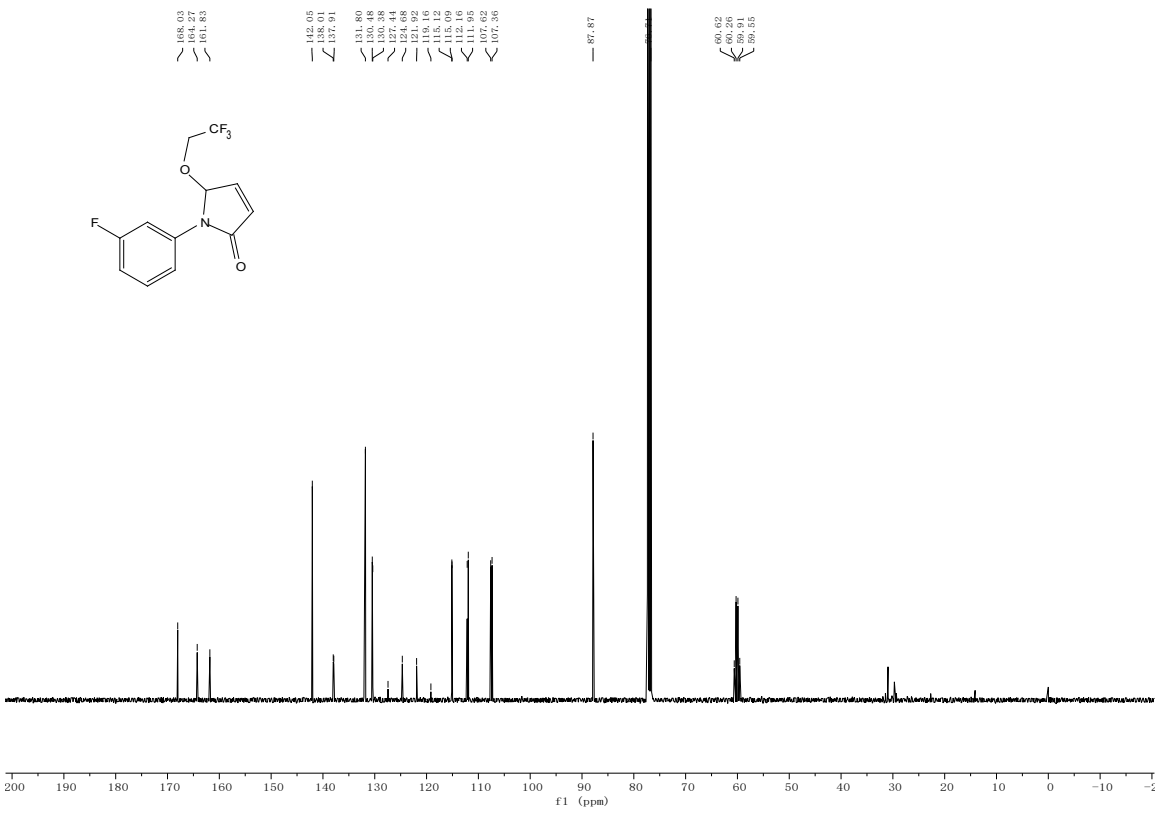
F
N
O
0.97
0.88
1.01
0.93
0.88
0.98
1.03
2.04
f1 (ppm)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161.83
142.05
138.01
137.91
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130.48
130.38
127.44
124.68
121.92
119.16
115.12
115.09
112.16
111.95
107.62
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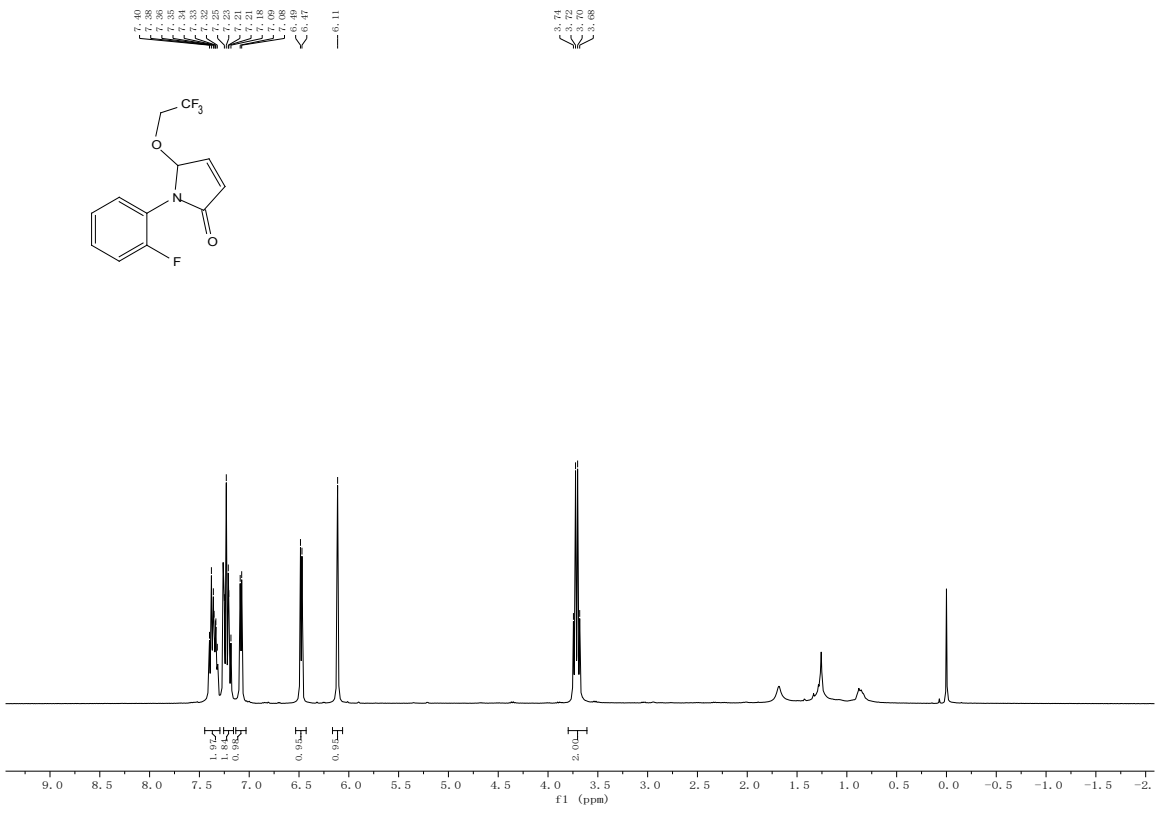
87.87
60.62
60.26
59.91
59.55
CF3
O
F
N
O
f1 (ppm)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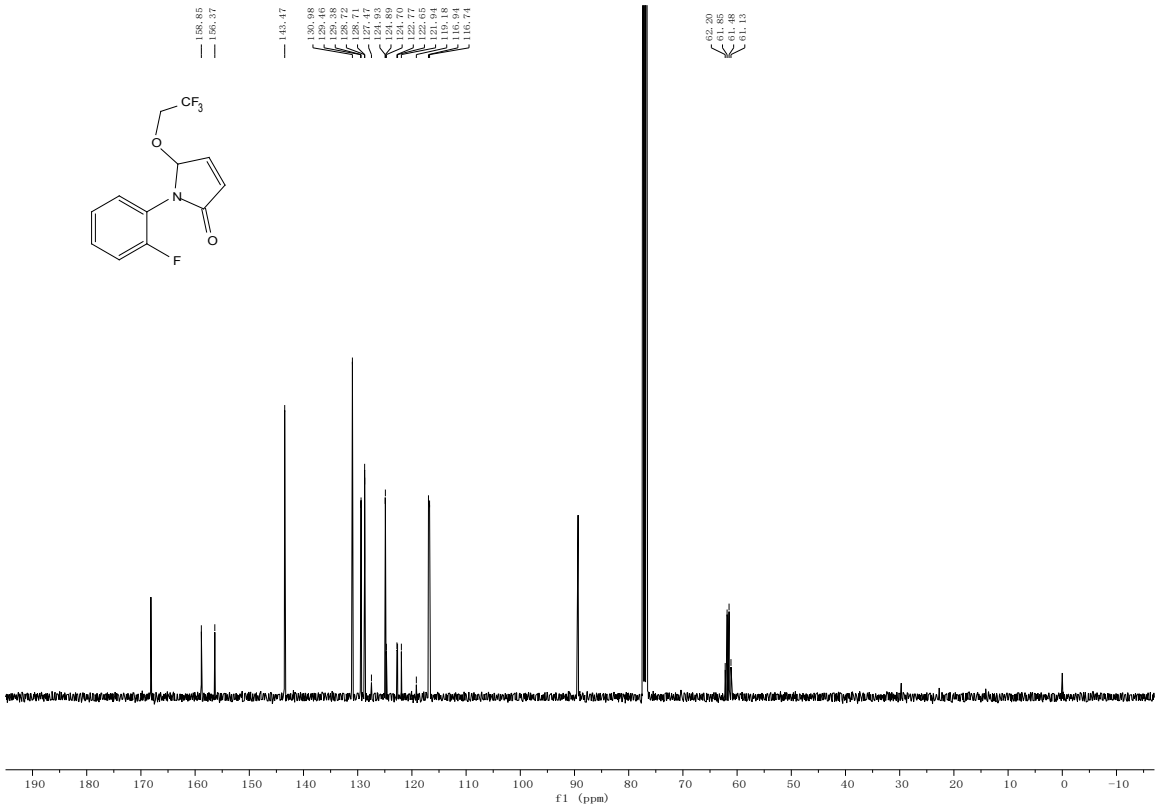
7.33
7.32
7.25
7.23
7.21
7.18
7.09
7.08
6.49
6.47
6.11
3.74
3.72
3.70
3.68
CF3
O
N
O
F
1.67
1.84
0.98
0.95
0.95
2.00
f1 (ppm)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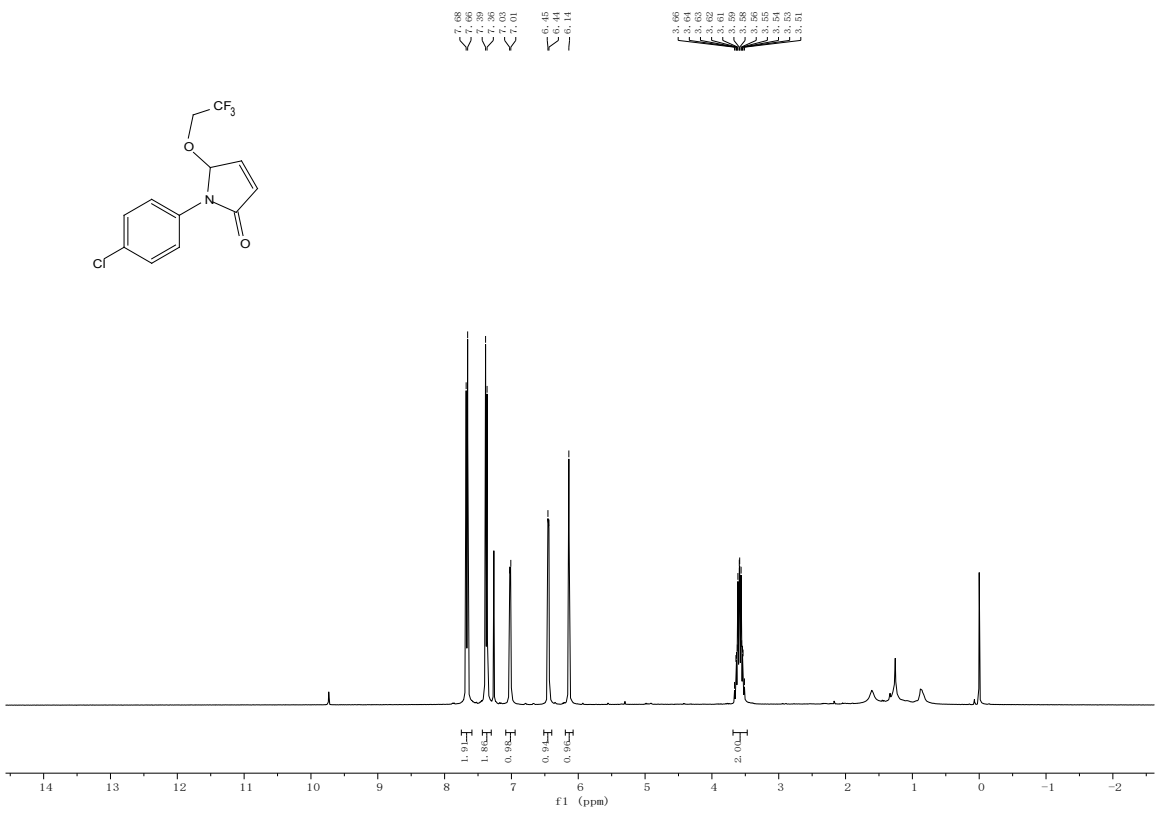
125.35
124.89
124.70
122.77
122.65
121.94
119.18
116.94
116.74
62.20
61.85
61.48
61.13
CF3
O
N
O
F
f1 (ppm)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7.36
7.03
7.01
6.45
6.44
6.14
3.66
3.64
3.63
3.62
3.61
3.59
3.58
3.56
3.55
3.54
3.53
3.51
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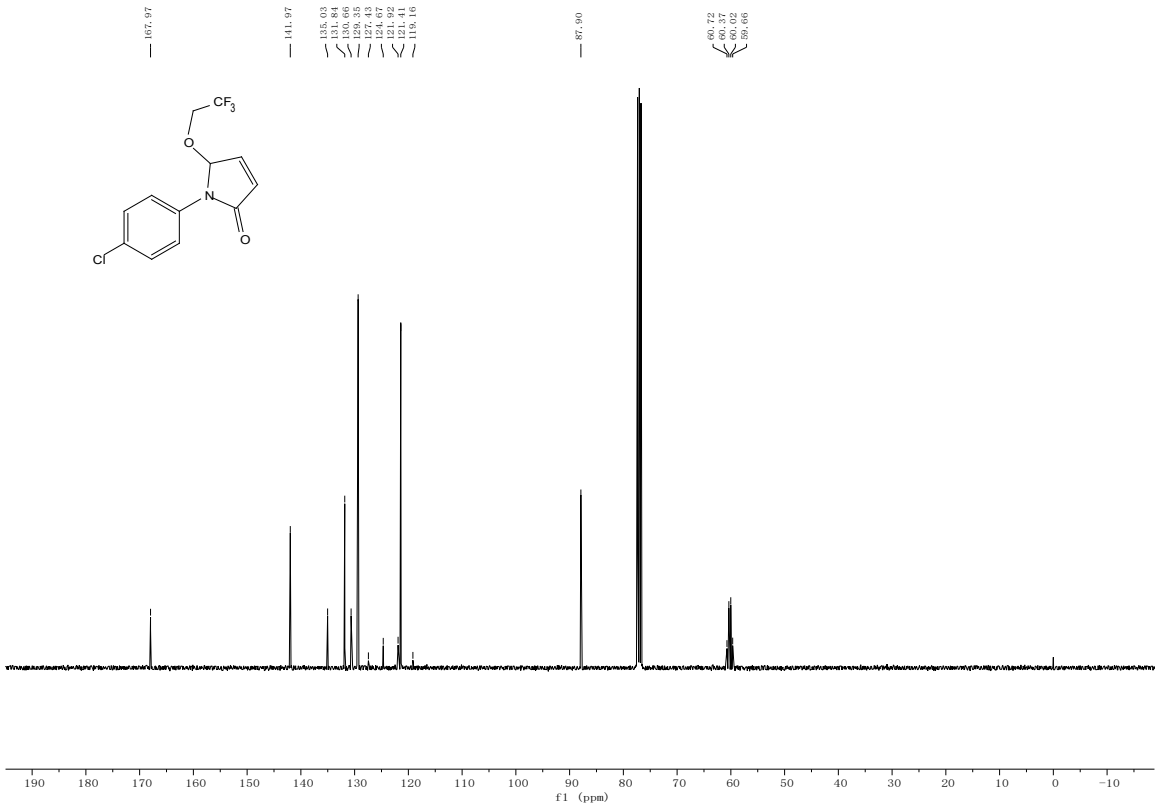
O
N
O
Cl
1.91
1.88
0.98
0.94
0.96
2.04
f1 (ppm)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124.67
121.92
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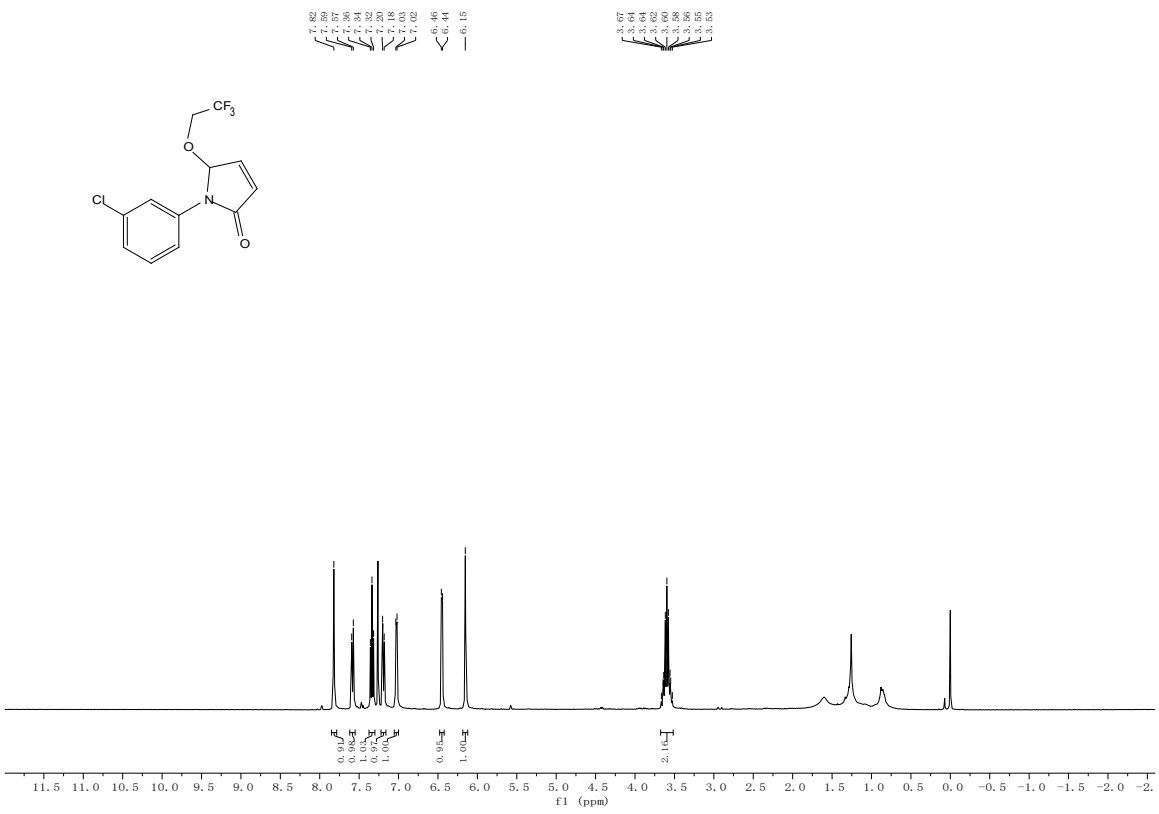
87.90
60.72
60.37
60.02
59.66
CF3
O
N
O
Cl
f1 (ppm)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7.32
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7.18
7.03
7.02
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6.44
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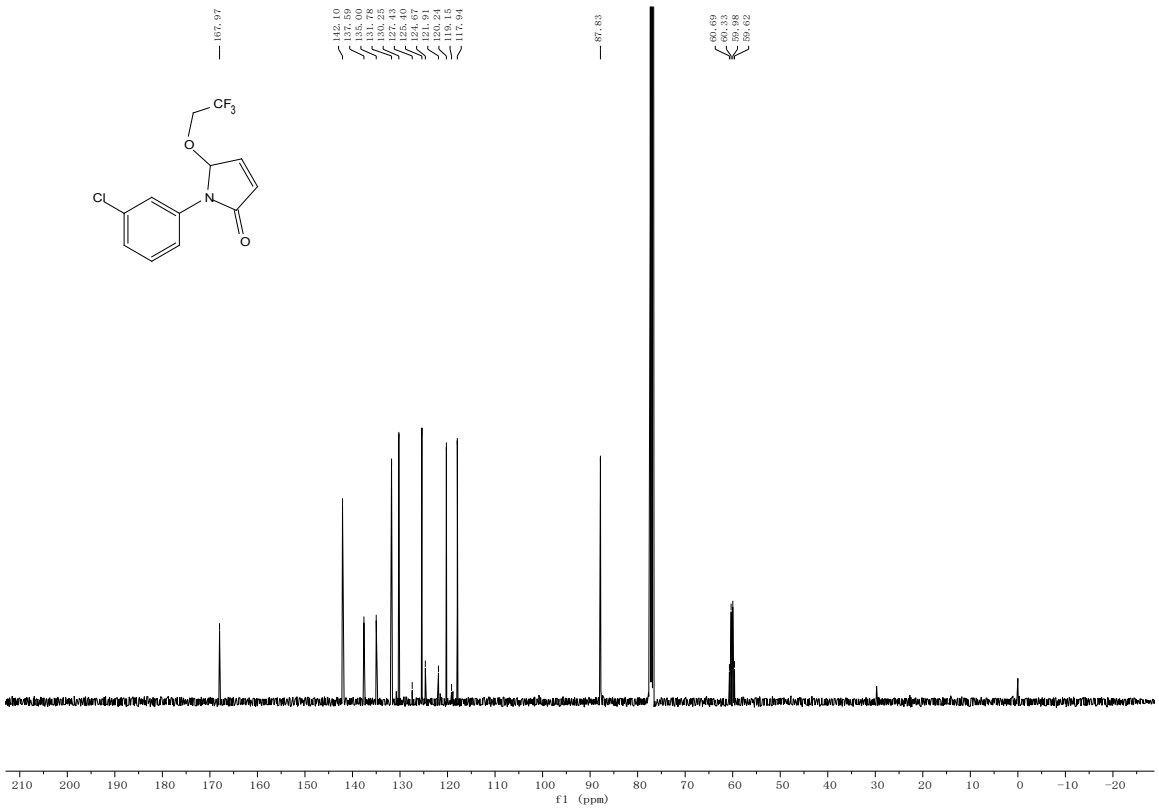
3.67
3.64
3.64
3.62
3.60
3.58
3.56
3.55
3.53
CF3
O
N
Cl
O
0.91
0.94
1.03
0.97
1.00
0.95
1.00
2.16
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0 -2.
f1 (ppm)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125.40
124.67
121.91
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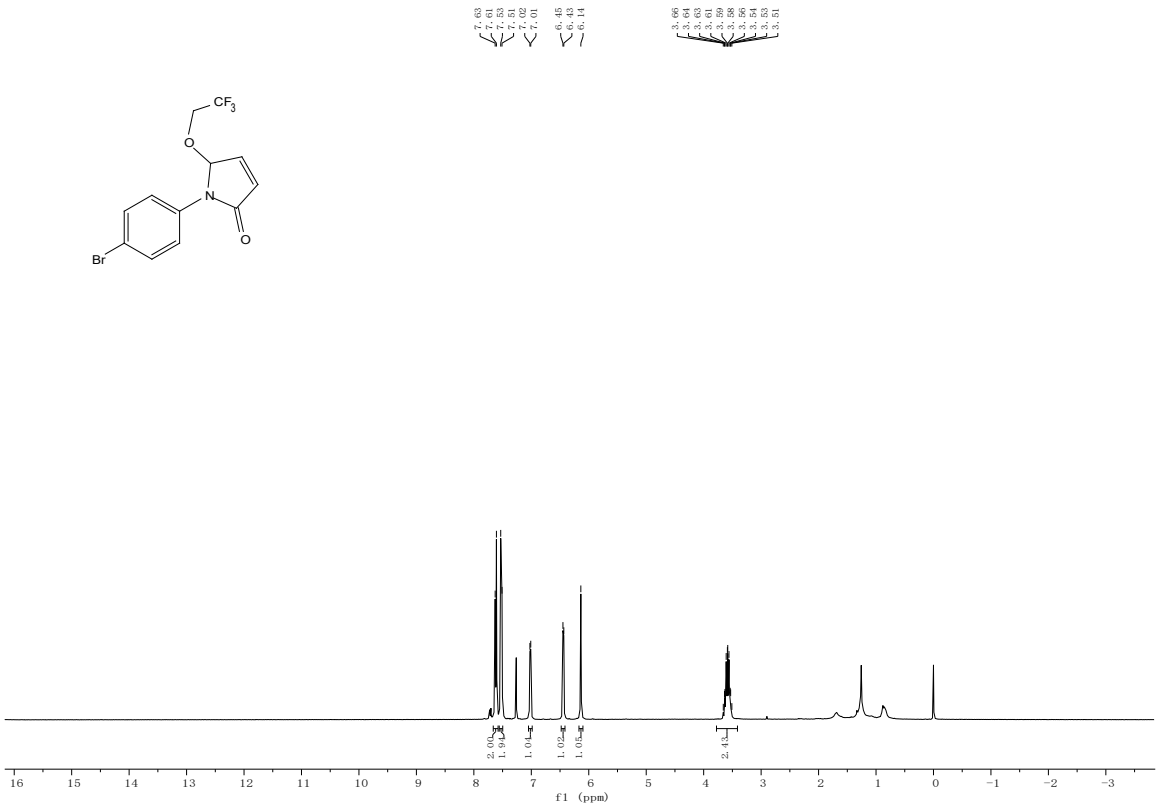
117.94
87.83
60.69
60.33
59.98
59.62
CF3
O
N
Cl
O
f1 (ppm)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7.01
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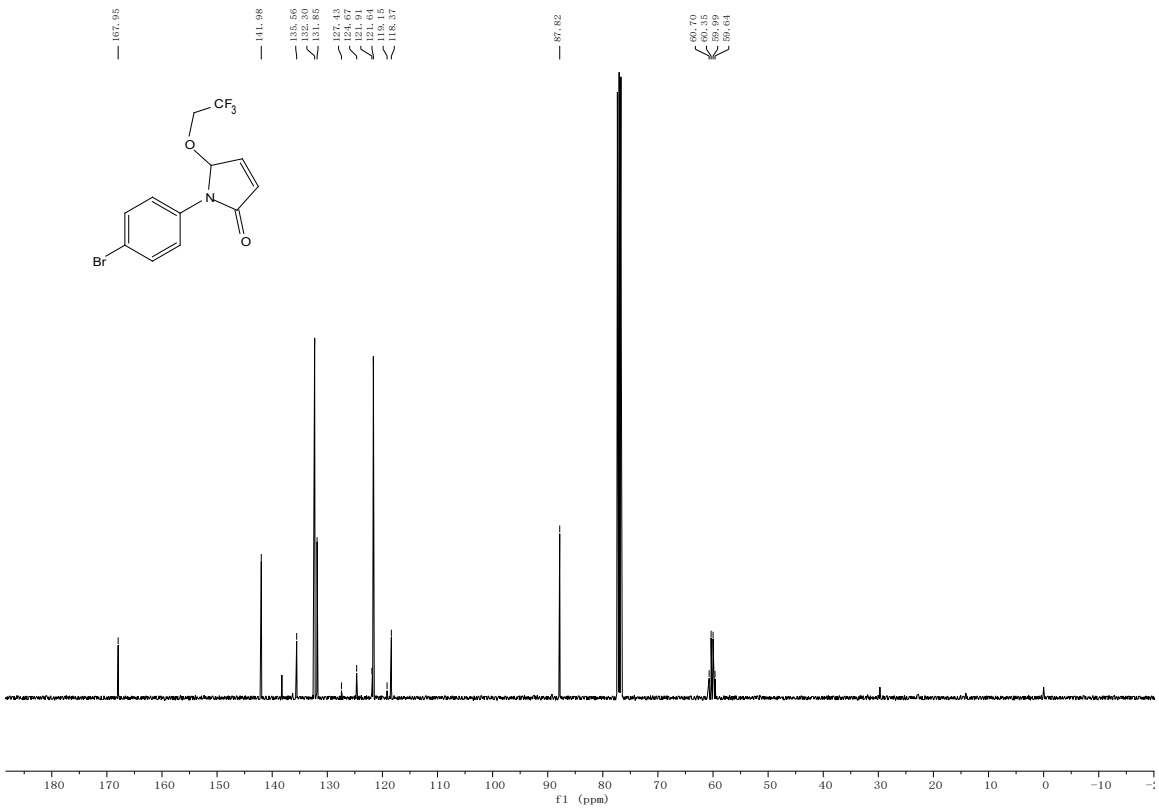
6.14
3.66
3.64
3.63
3.61
3.59
3.58
3.56
3.54
3.53
3.51
CF3
O
N
Br
O
2.00
1.93
1.01
1.02
1.05
2.43
f1 (ppm)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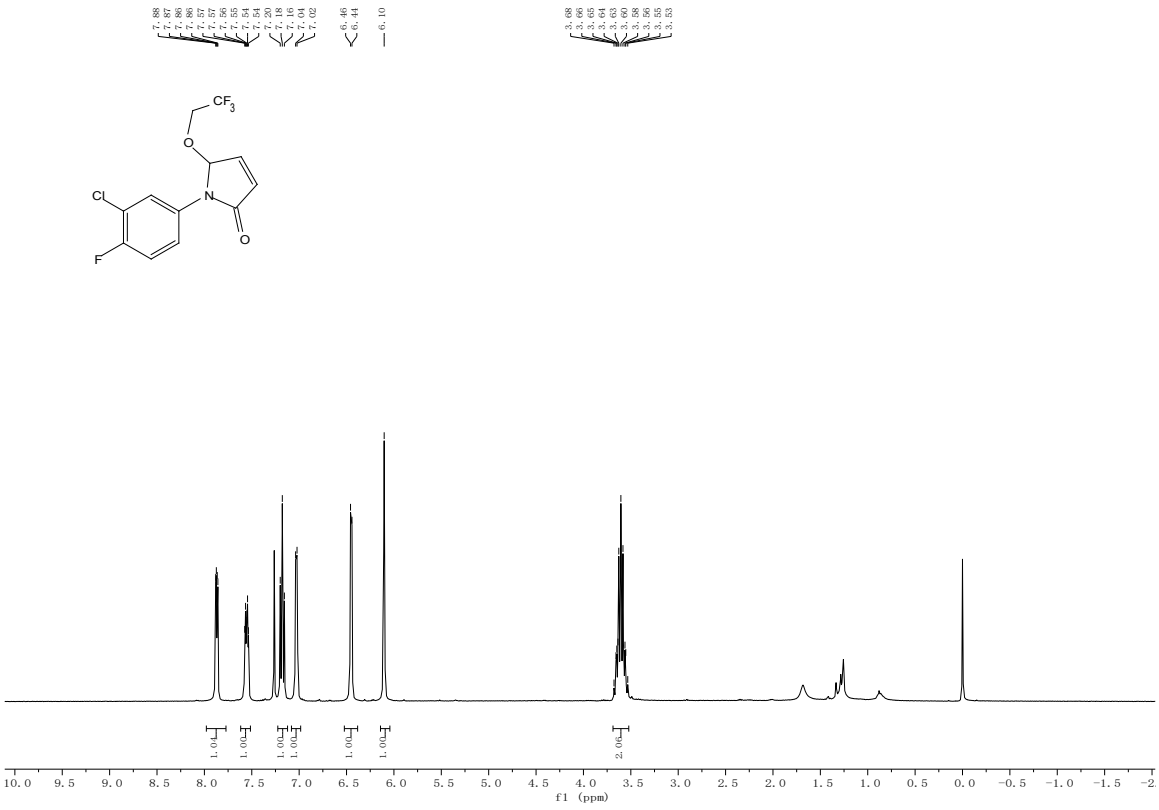
132.30
131.85
127.43
124.67
121.91
121.64
119.15
118.37
87.82
60.70
60.35
59.99
59.64
CF3
O
N
O
Br
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)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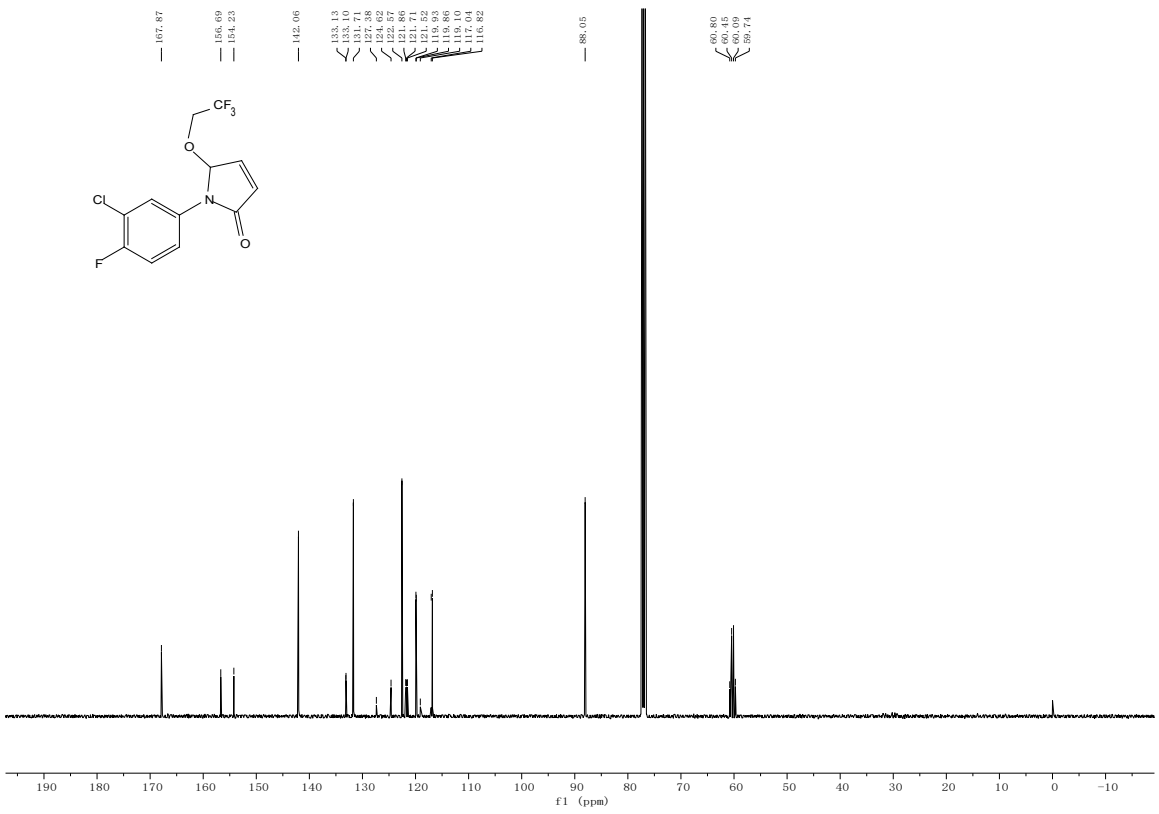
7.02
6.46
6.44
6.10
3.68
3.66
3.65
3.64
3.63
3.60
3.58
3.56
3.55
3.53
CF3
O
N
O
Cl
F
1.01
1.00
1.00
1.00
1.00
1.00
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.0 −1.5 −2
f1 (ppm)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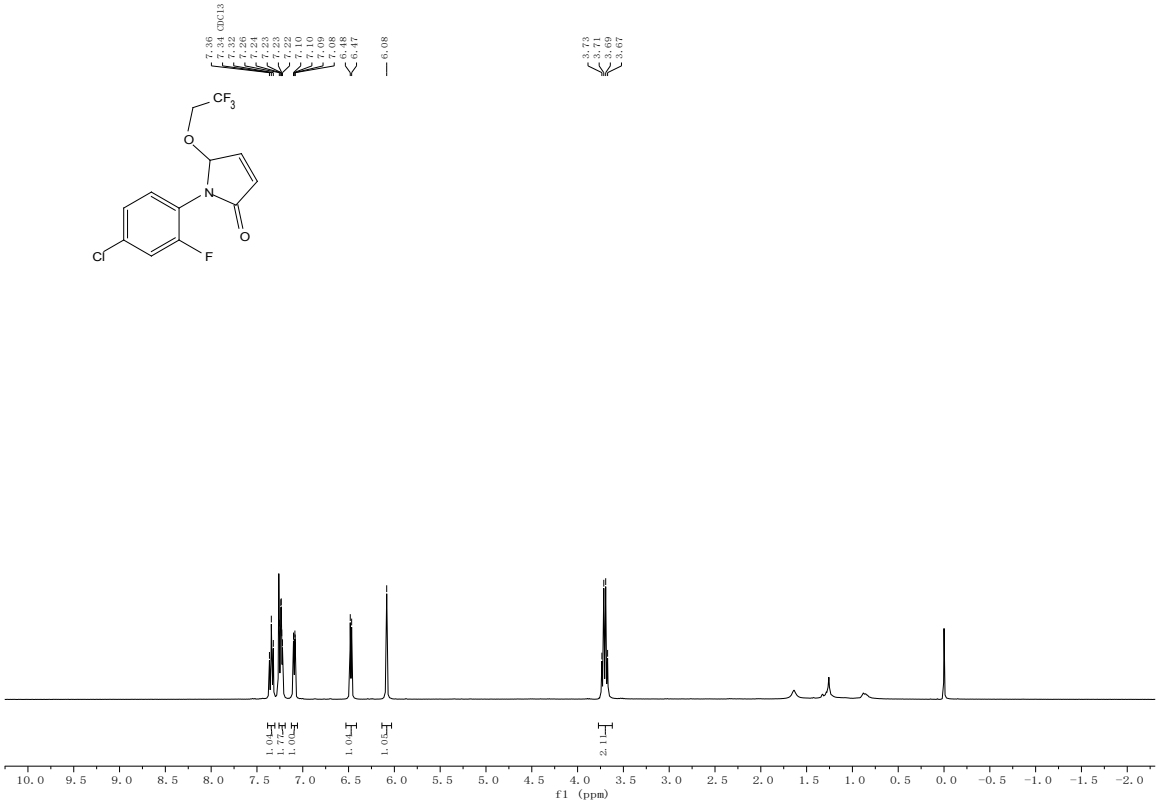
156.69
154.23
142.06
133.13
133.10
131.71
127.38
124.62
122.57
121.86
121.71
121.52
119.93
119.86
119.10
117.04
116.82
88.05
60.80
60.45
60.09
59.74
CF3
O
N
O
Cl
F
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)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7.34 CDCl3
7.32
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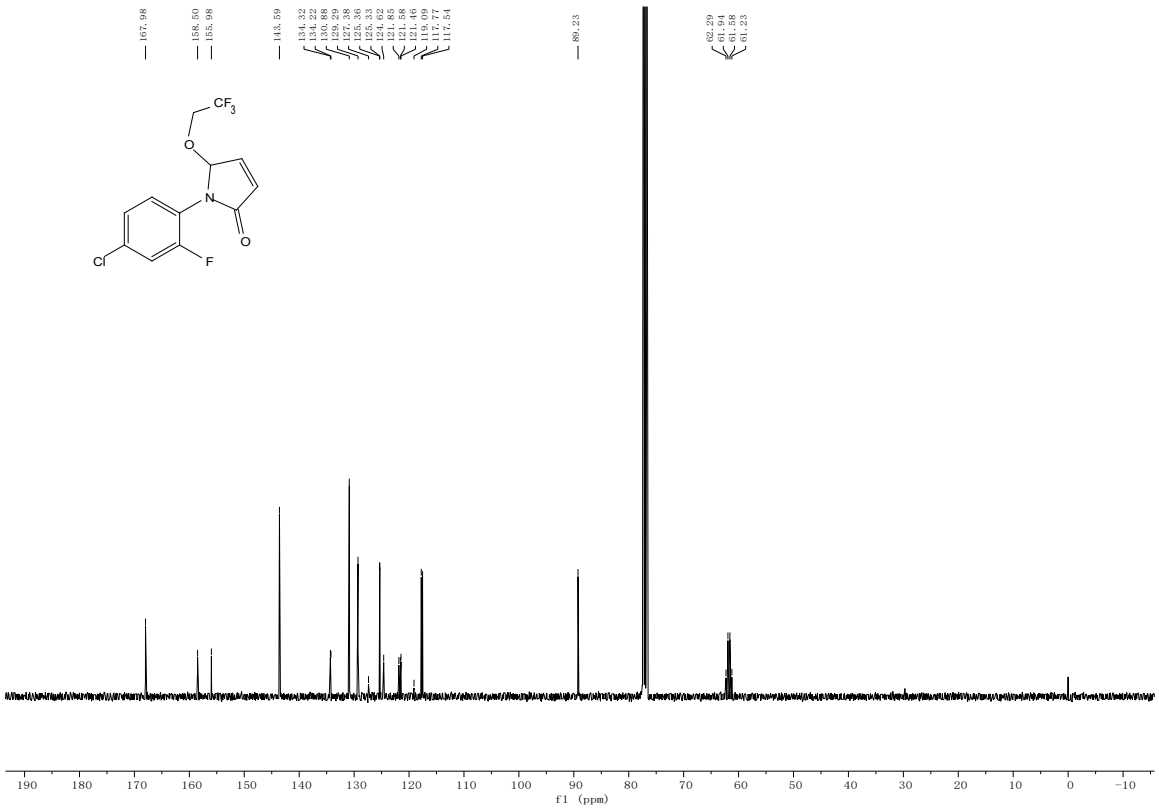
7.24
7.23
7.22
7.10
7.10
7.09
7.08
6.48
6.47
6.08
3.73
3.71
3.69
3.67
CF3
O
N
O
Cl
F
1.04
1.72
1.00
1.04
1.05
2.11
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.0 −1.5 −2.0
f1 (ppm)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134.22
130.88
129.29
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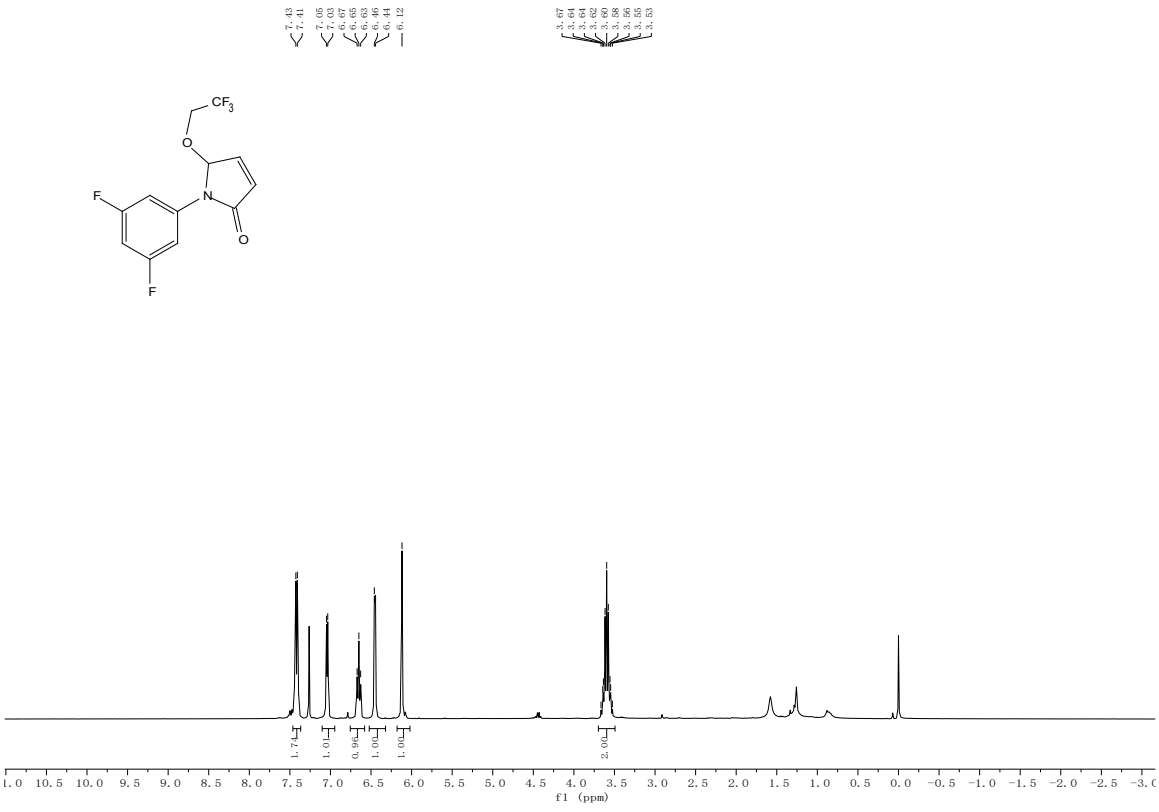
125.36
125.33
124.62
121.85
121.58
121.46
119.09
117.77
117.54
89.23
62.29
61.94
61.58
61.23
CF3
O
N
O
Cl
F
f1 (ppm)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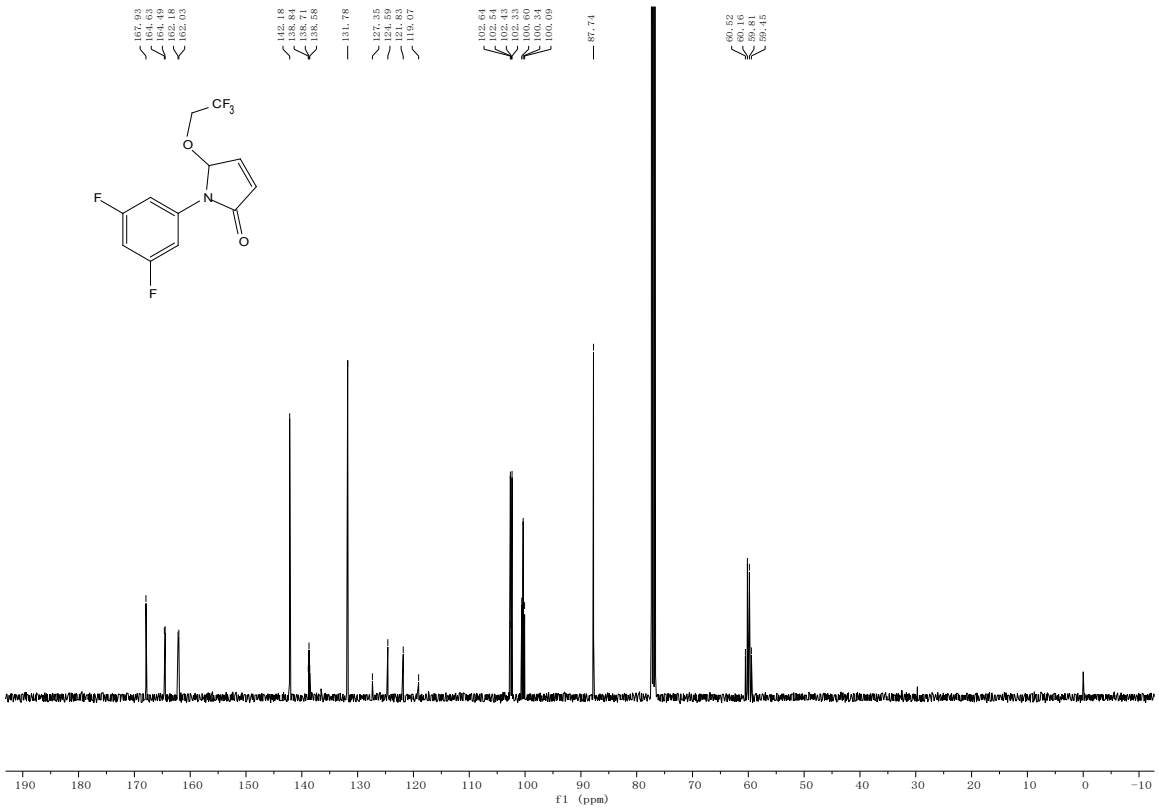
7.41
7.05
7.03
6.67
6.65
6.63
6.46
6.44
6.12
3.67
3.64
3.62
3.60
3.58
3.56
3.55
3.53
CF3
O
N
O
F
F
1.74
1.01
0.99
1.00
1.00
2.00
f1 (ppm)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164.49
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138.71
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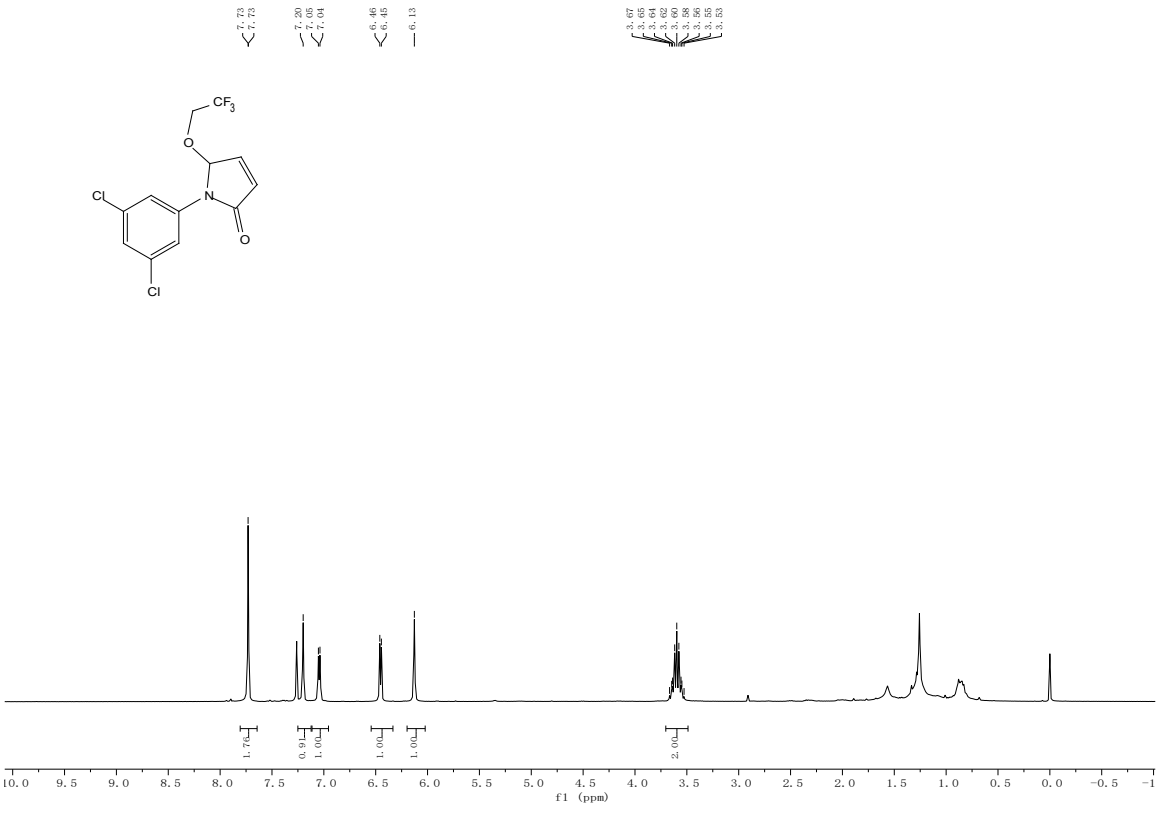
127.35
124.59
121.83
119.07
102.64
102.54
102.43
102.33
100.60
100.34
100.09
87.74
60.52
60.16
59.81
59.45
CF3
O
N
O
F
F
f1 (ppm)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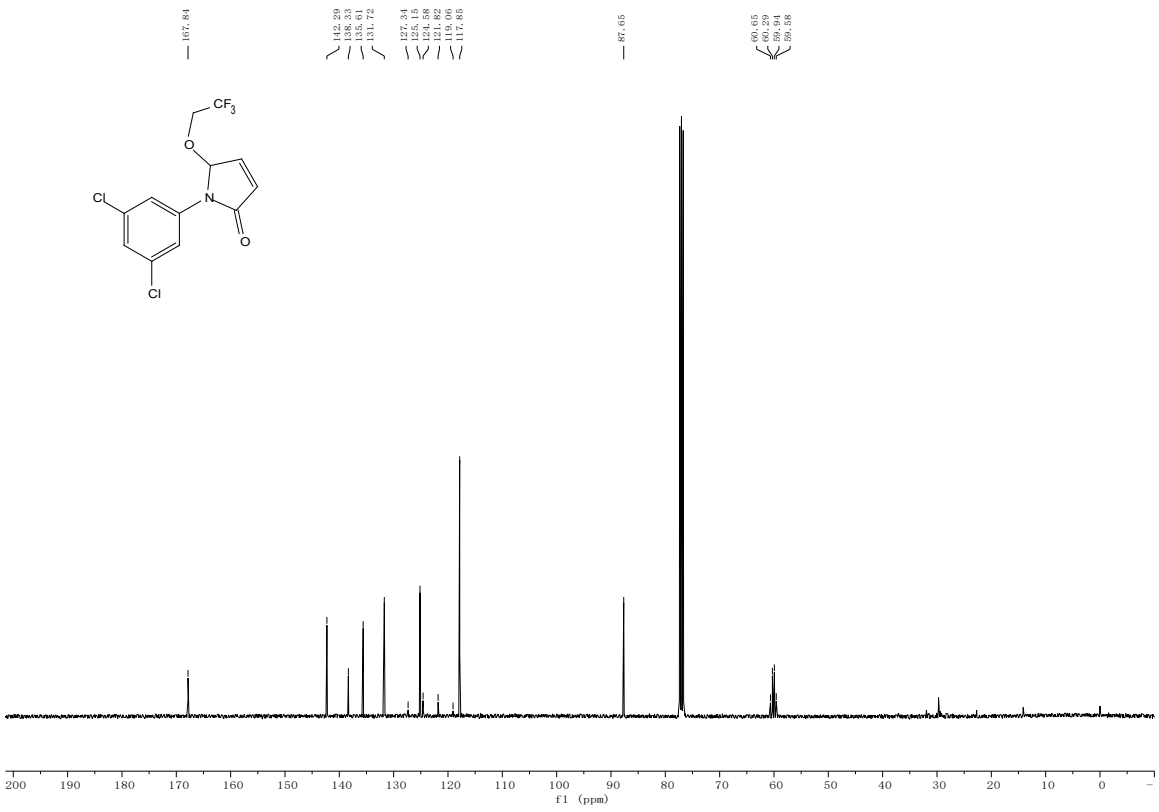
7.72
7.20
7.05
7.04
6.46
6.45
6.13
3.67
3.65
3.64
3.62
3.60
3.58
3.56
3.55
3.53
CF3
O
N
O
Cl
Cl
1.76
0.91
1.00
1.00
1.00
2.00
f1 (ppm)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142.29
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135.61
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127.34
125.15
124.58
121.82
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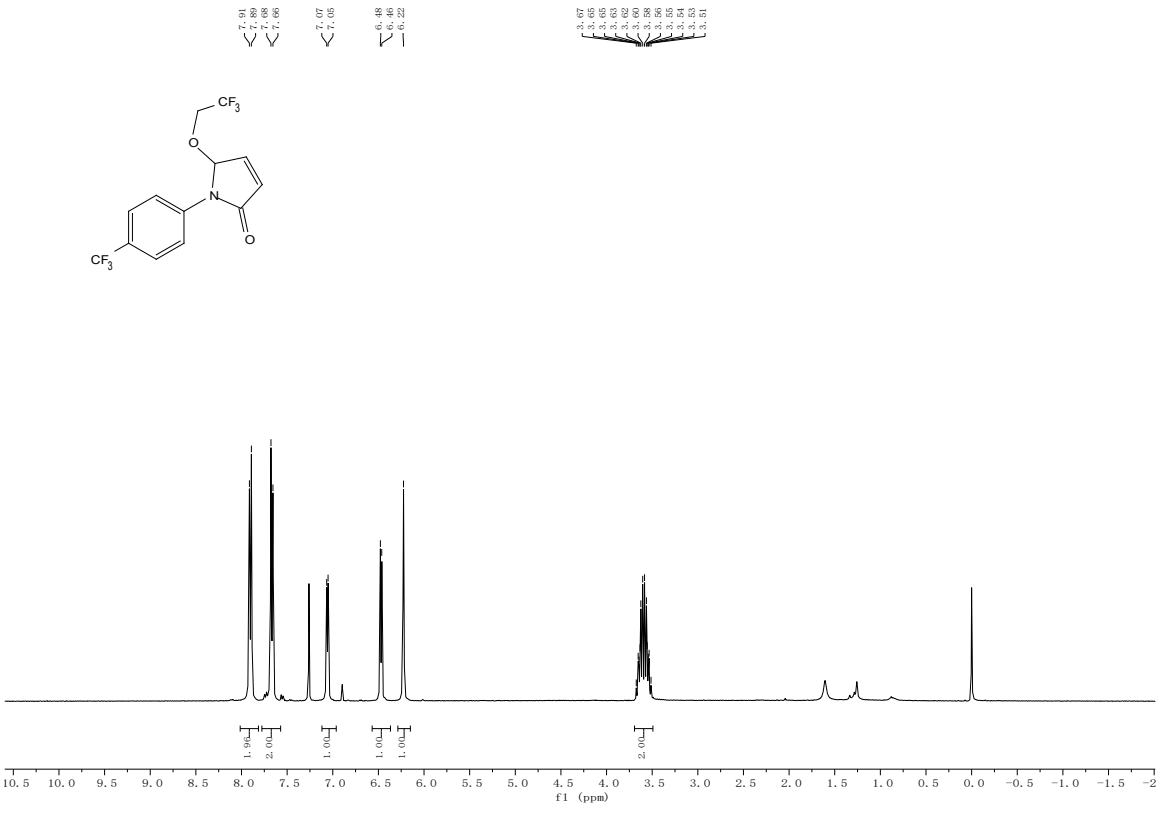
60.65
60.29
59.94
59.58
CF3
O
N
O
Cl
Cl
f1 (ppm)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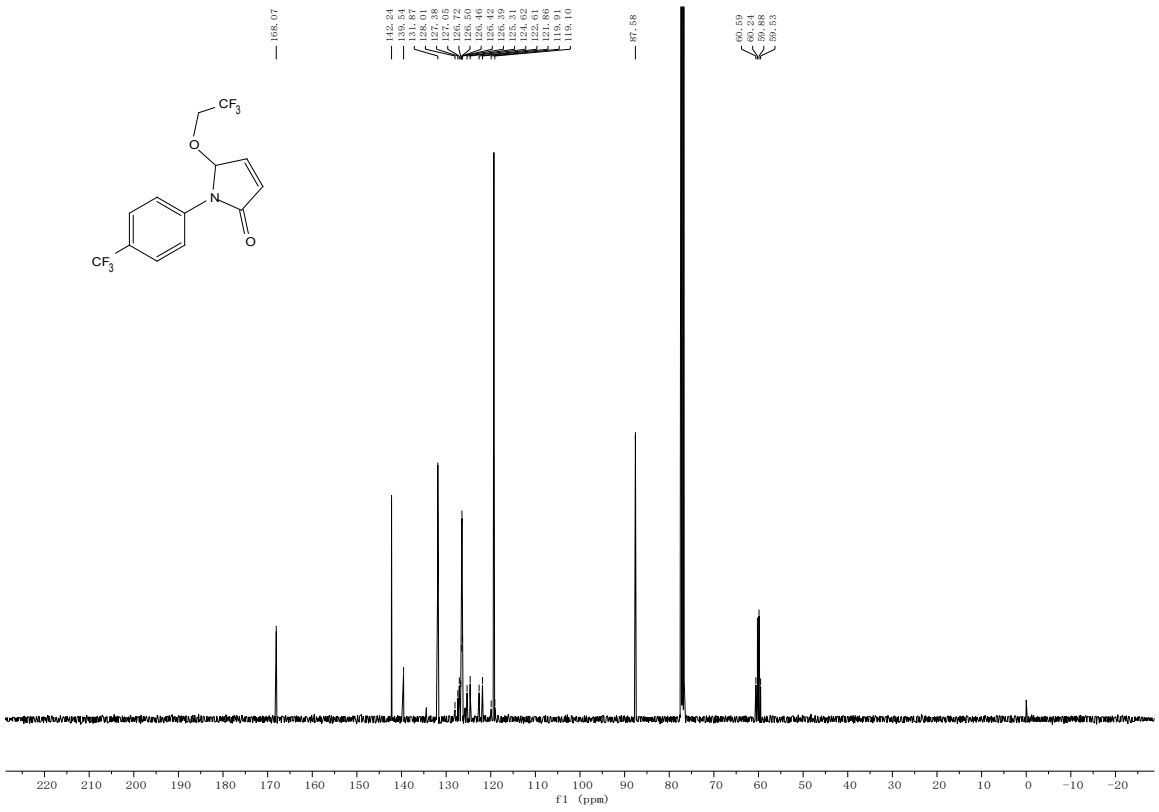
7.88
7.68
7.66
7.07
7.05
6.48
6.46
6.22
3.67
3.65
3.65
3.63
3.62
3.60
3.58
3.56
3.55
3.54
3.53
3.51
CF3
O
N
O
CF3
1.96
2.00
1.00
1.00
1.00
2.00
f1 (ppm)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142.24
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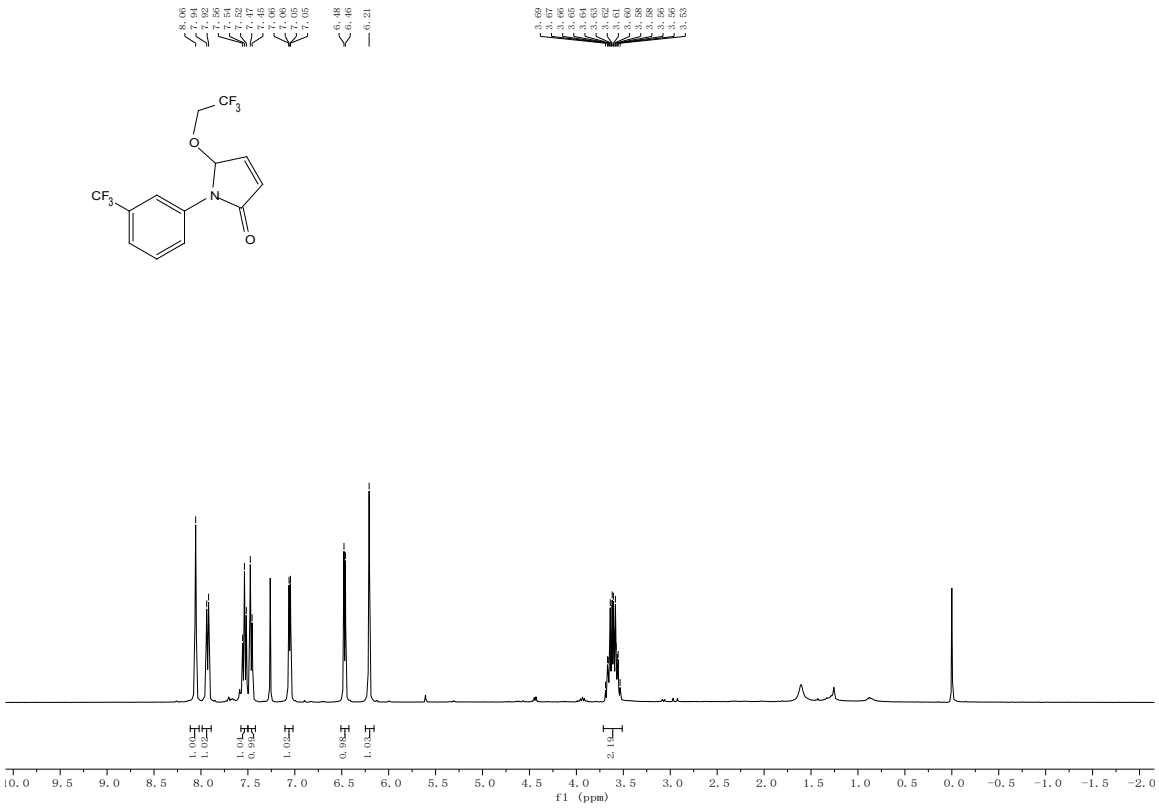
131.87
128.91
128.30
127.38
127.05
126.72
126.50
126.46
126.42
126.39
125.31
124.62
122.61
121.86
119.91
119.10
87.58
60.59
60.24
59.88
59.53
CF3
O
N
O
CF3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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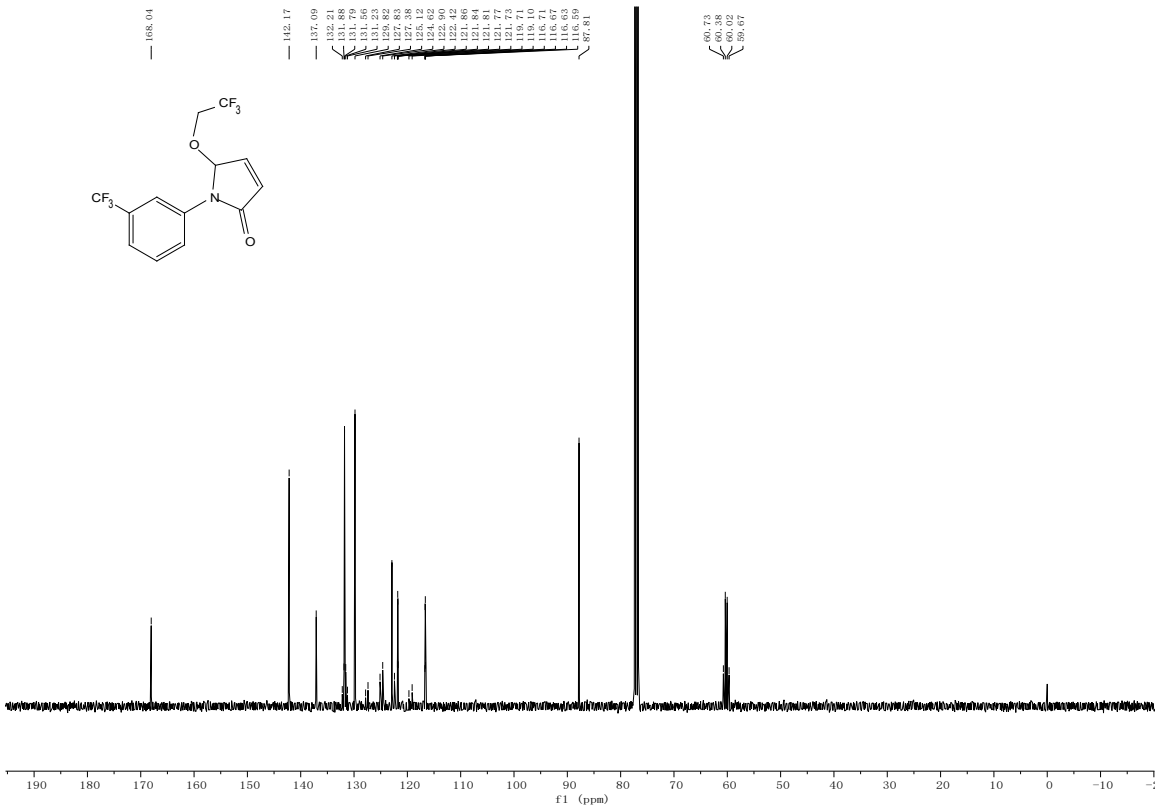
7.94
7.92
7.56
7.54
7.52
7.47
7.45
7.06
7.06
7.05
7.05
6.48
6.46
6.21
3.69
3.67
3.66
3.65
3.64
3.63
3.62
3.61
3.60
3.58
3.56
3.56
3.53
CF3
O
N
O
CF3
1.00
1.02
1.04
0.96
1.02
0.98
1.03
2.19
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)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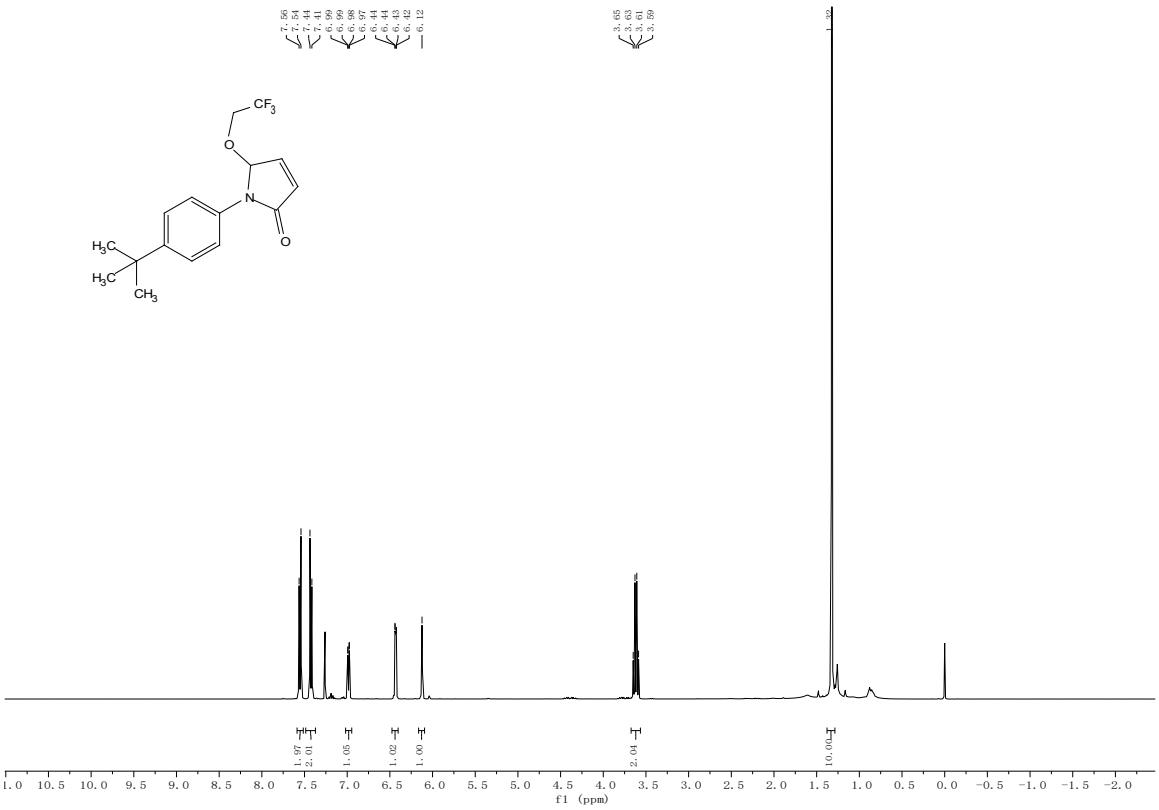
142.17
137.09
132.21
131.88
131.79
131.56
131.23
129.82
127.83
127.38
125.12
124.62
122.90
122.42
121.86
121.84
121.81
121.77
121.73
119.71
119.10
116.71
116.67
116.63
116.59
87.81
60.73
60.38
60.02
59.67
CF3
O
N
CF3
O
f1 (ppm)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7.54
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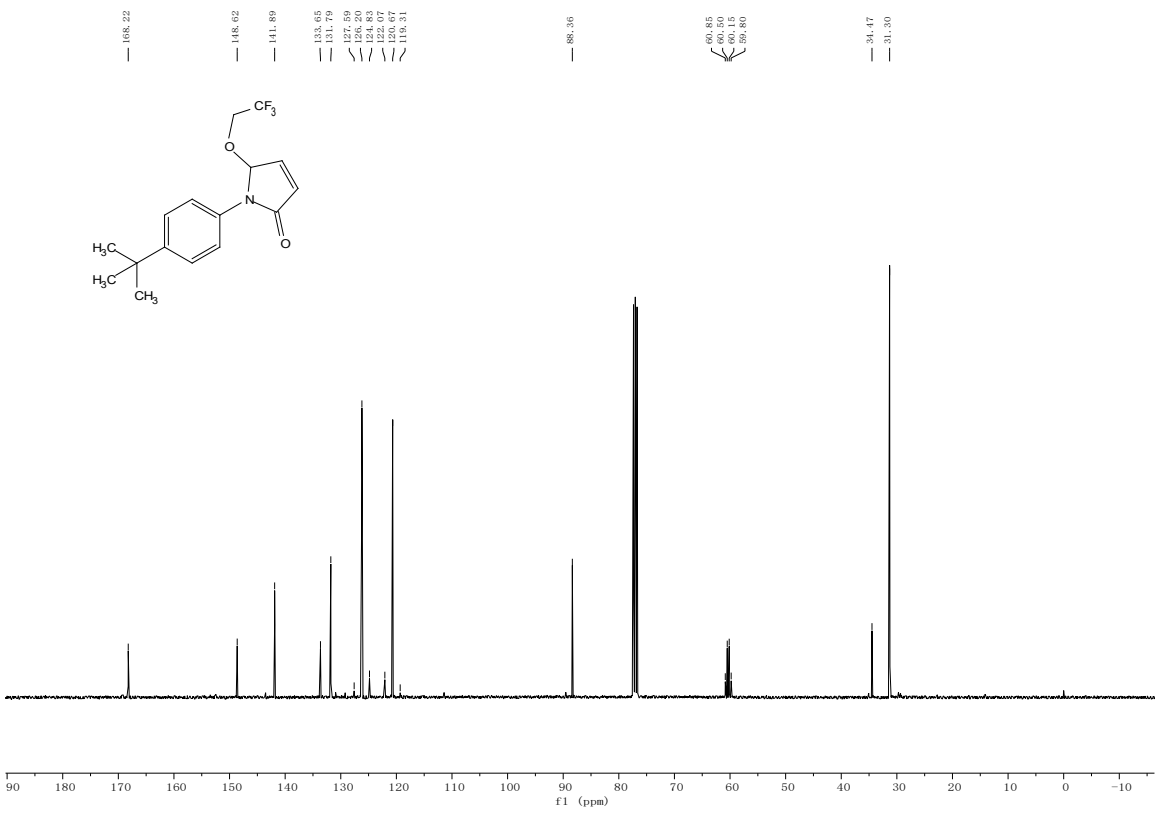
7.41
6.99
6.98
6.97
6.44
6.43
6.42
6.12
3.65
3.63
3.61
3.59
1.33
CF3
O
N
O
H3C
H3C
CH3
1.97
2.01
1.05
1.02
1.00
2.04
10.00
f1 (ppm)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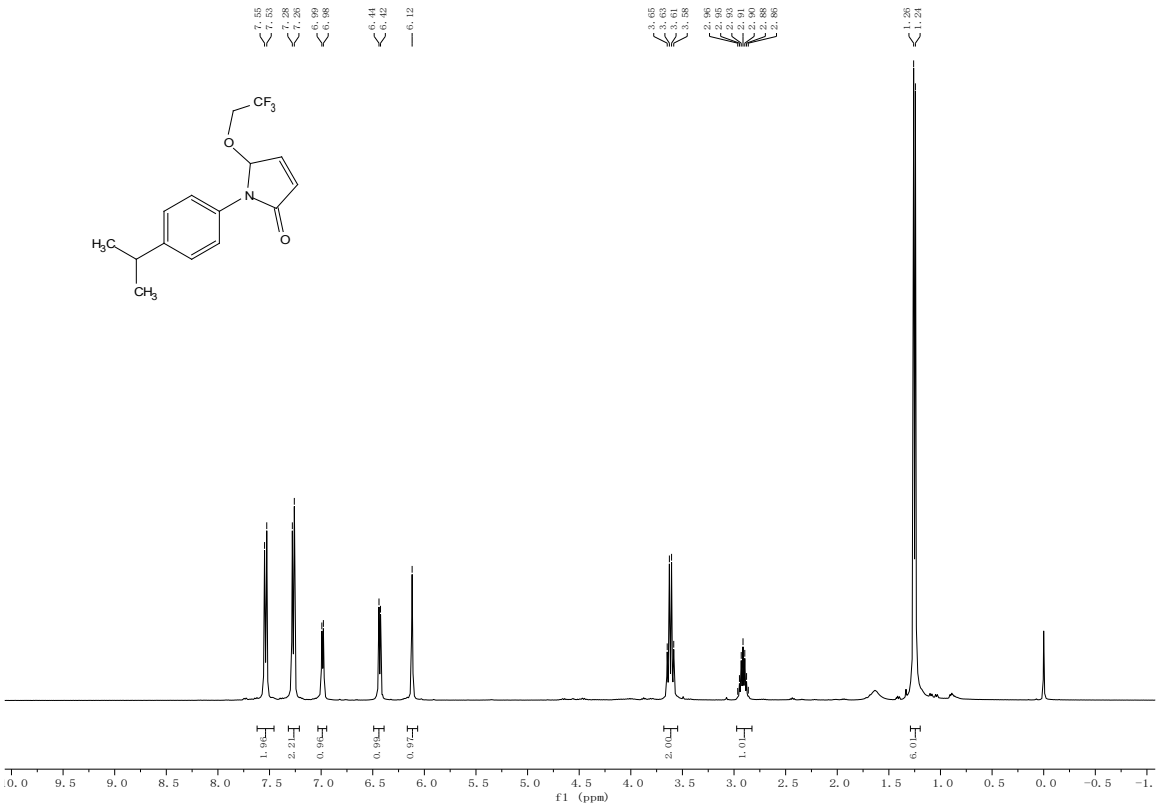
148.62
141.89
133.65
131.79
127.59
126.20
124.83
122.07
120.67
119.31
88.36
60.85
60.50
60.15
59.80
34.47
31.30
CF3
O
N
O
H3C
H3C
CH3
f1 (ppm)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7.53
7.28
7.26
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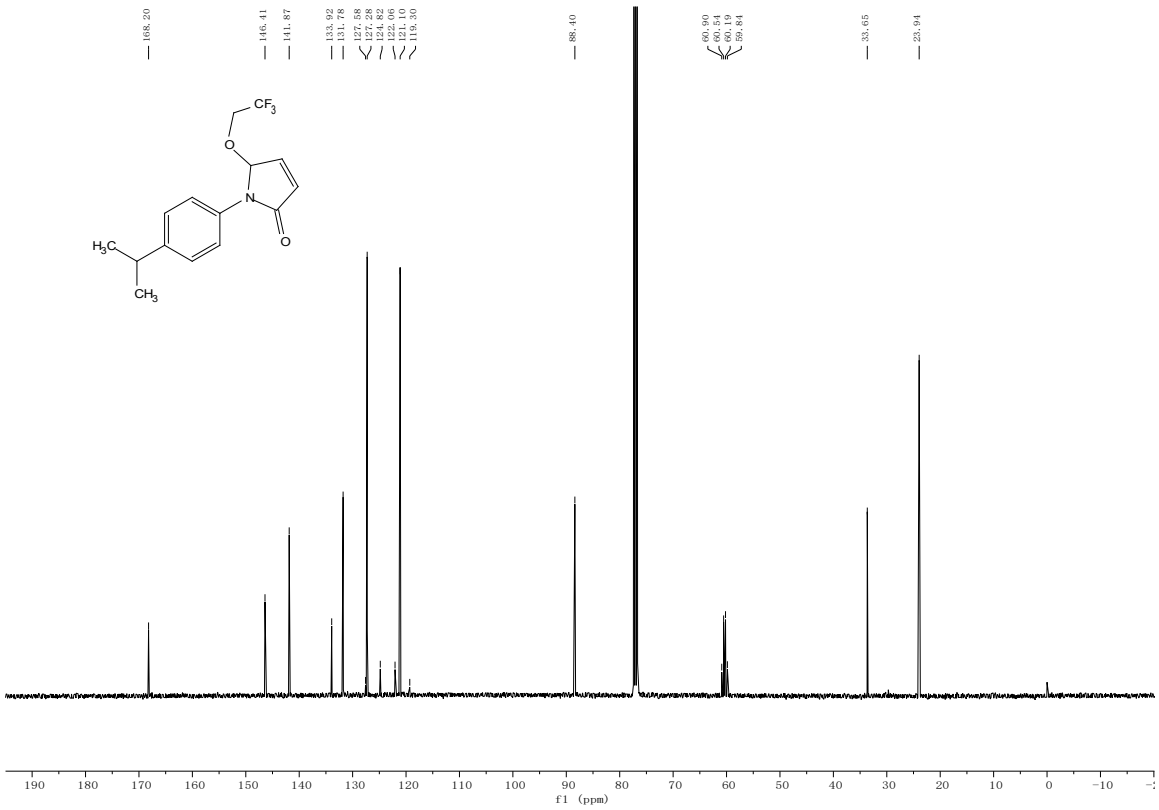
6.98
6.44
6.42
6.12
3.65
3.63
3.61
3.58
2.96
2.95
2.93
2.91
2.90
2.88
2.86
1.26
1.24
1.96
2.21
0.96
0.98
0.97
2.00
1.01
6.01
CF3
O
N
O
H3C
CH3
f1 (ppm)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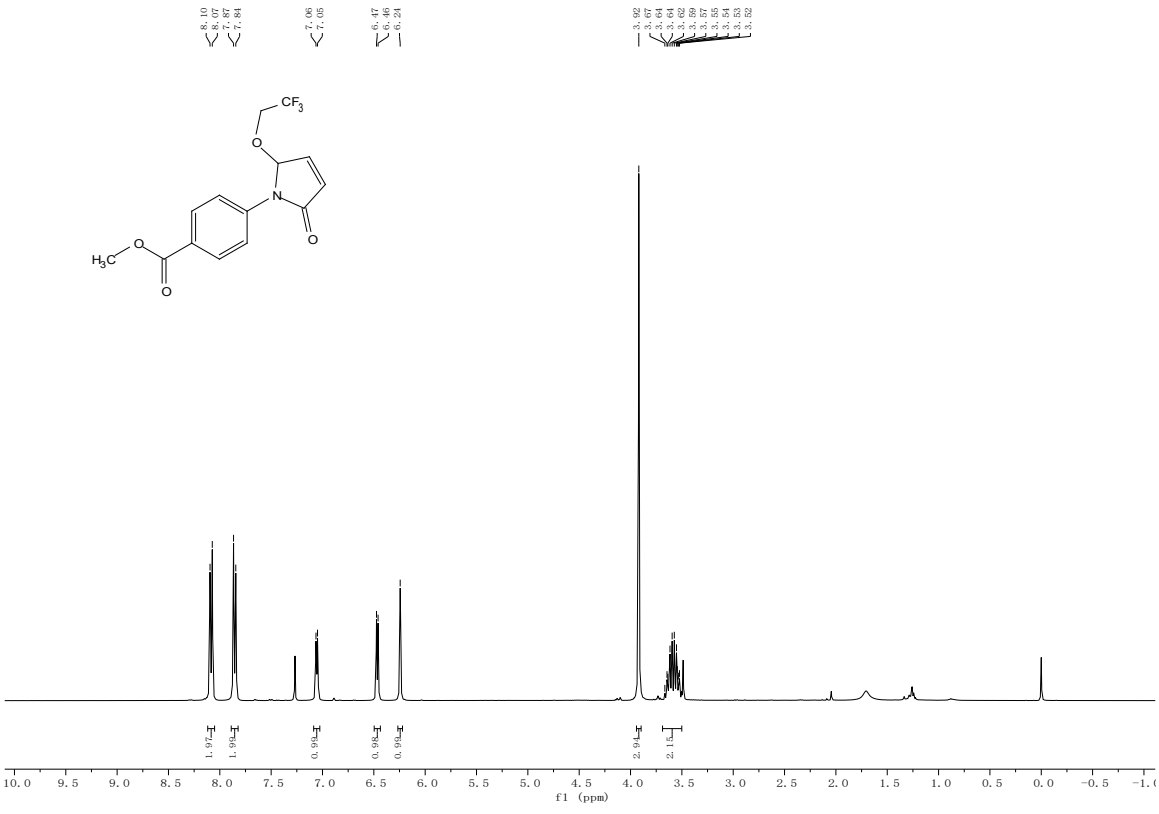
127.68
127.28
124.82
122.06
121.10
119.30
88.40
60.90
60.54
60.19
59.84
33.65
23.94
CF3
O
N
O
H3C
CH3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)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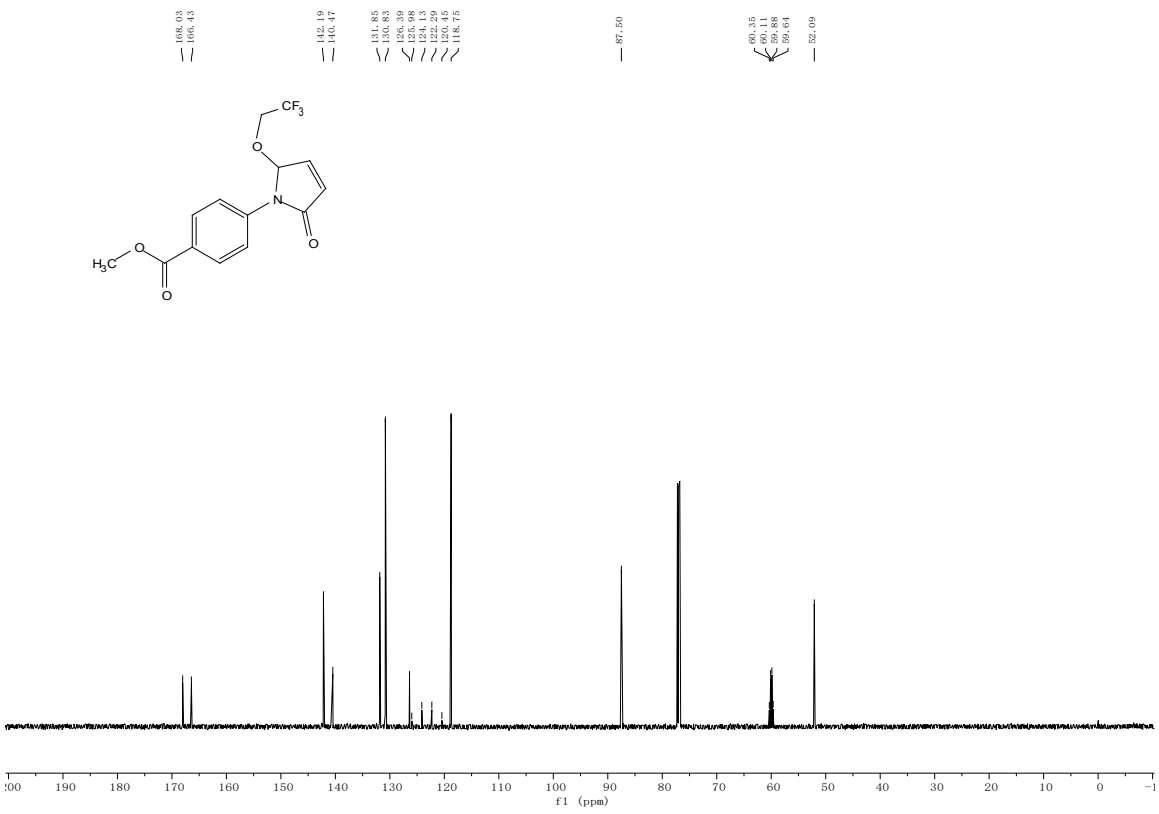
8.07
7.87
7.84
7.06
7.05
6.47
6.46
6.24
3.92
3.67
3.64
3.62
3.59
3.57
3.55
3.54
3.53
3.52
CF3
O
N
O
H3C
O
O
1.97
1.99
0.99
0.98
0.99
2.94
2.15
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5
f1 (ppm)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166.43
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130.83
126.39
125.98
124.13
122.59
120.45
118.75
87.50
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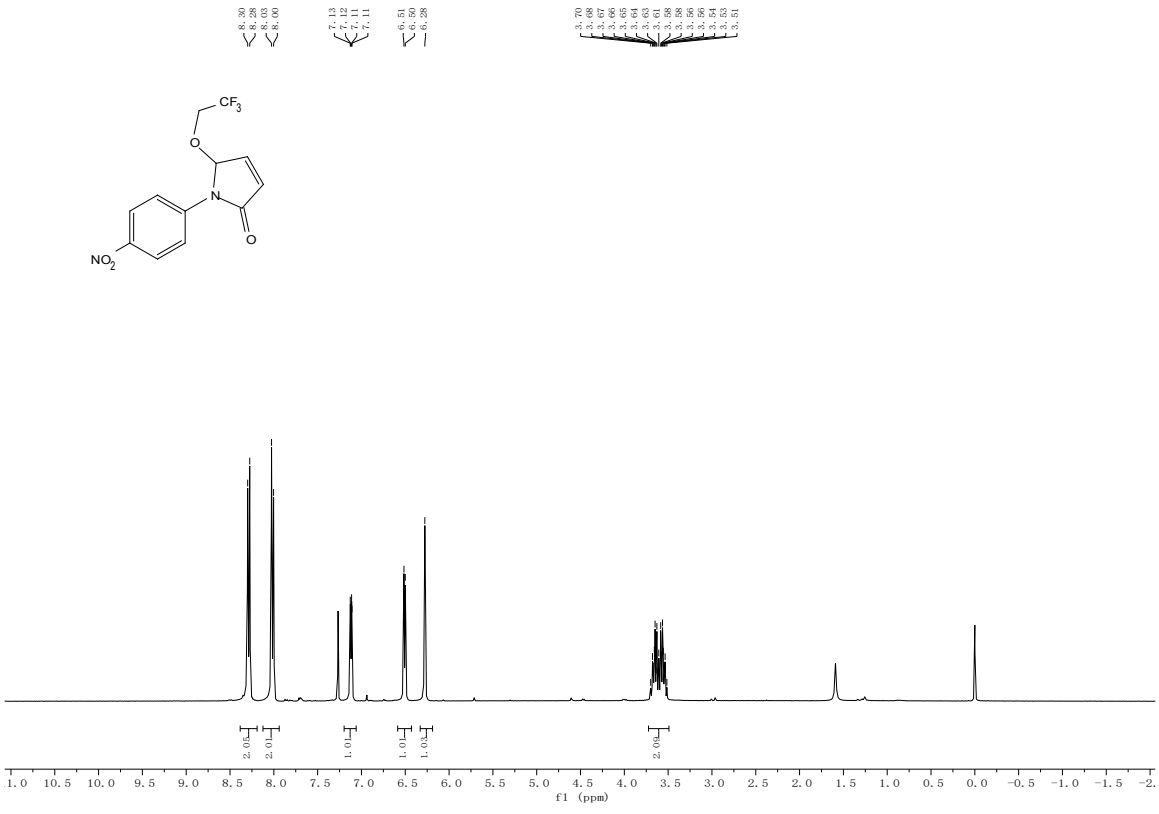
60.11
59.88
59.64
52.09
CF3
O
N
O
H3C
O
O
f1 (ppm)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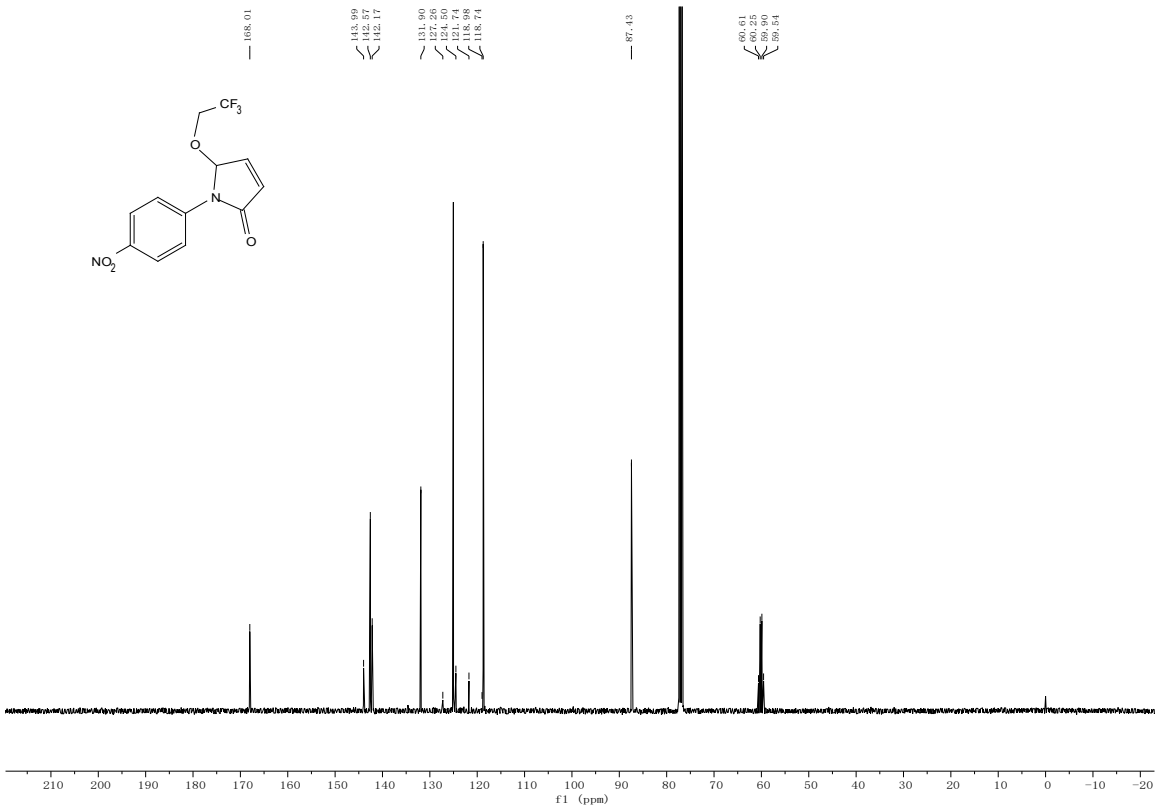
8.03
8.00
7.13
7.12
7.11
7.11
6.51
6.50
6.28
3.70
3.68
3.67
3.65
3.64
3.63
3.61
3.58
3.56
3.55
3.54
3.53
3.51
CF3
O
N
O
NO2
2.05
2.01
1.00
1.01
1.03
2.09
f1 (ppm)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127.26
124.50
121.74
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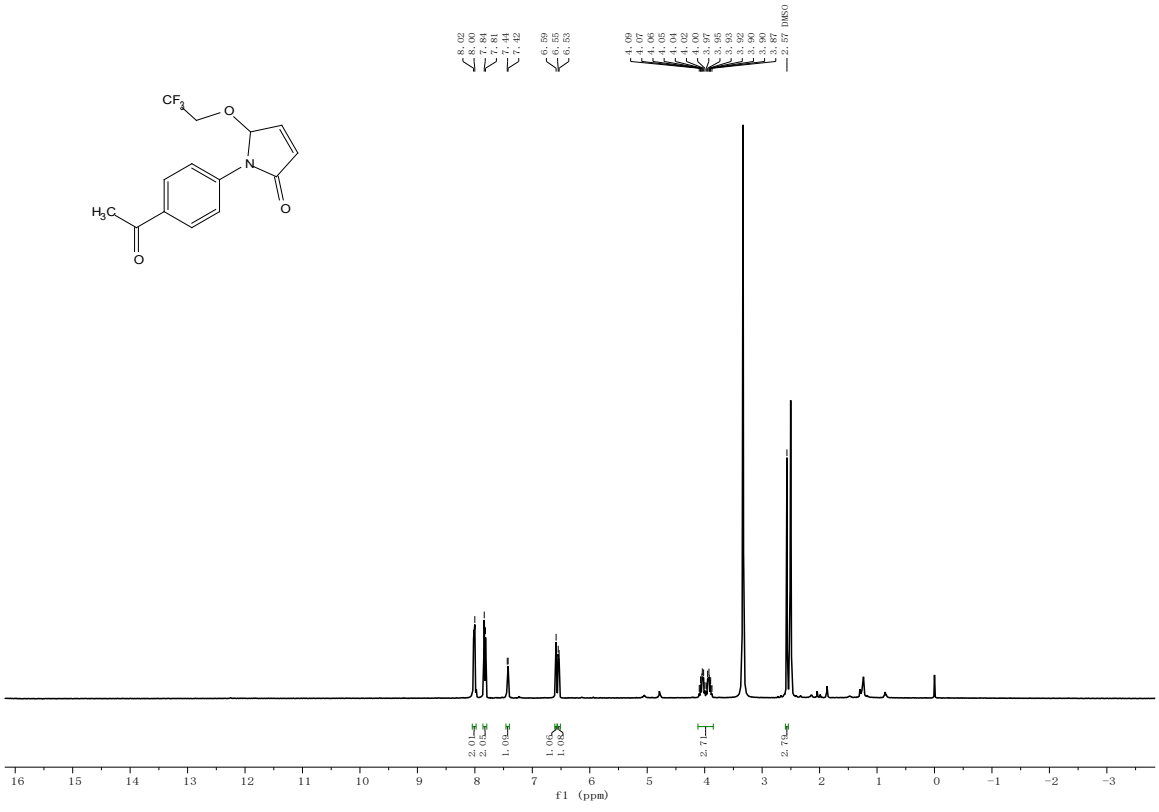
60.61
60.25
59.90
59.54
CF3
O
N
O
NO2
f1 (ppm)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7.42
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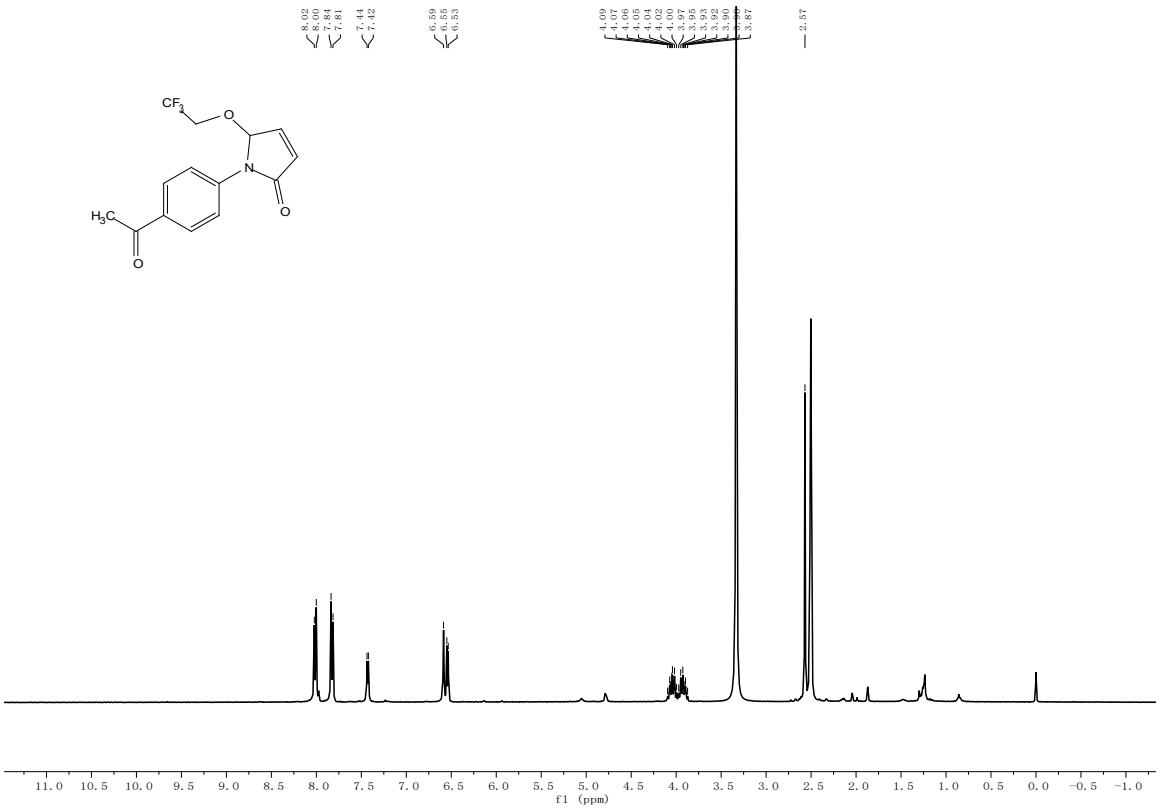
6.55
6.53
4.09
4.07
4.06
4.05
4.04
4.02
4.00
3.97
3.95
3.93
3.92
3.90
3.87
2.97
DMSO
CF3
O
N
O
H3C
O
2.01
2.05
1.09
1.06
1.00
2.71
2.79
f1 (ppm)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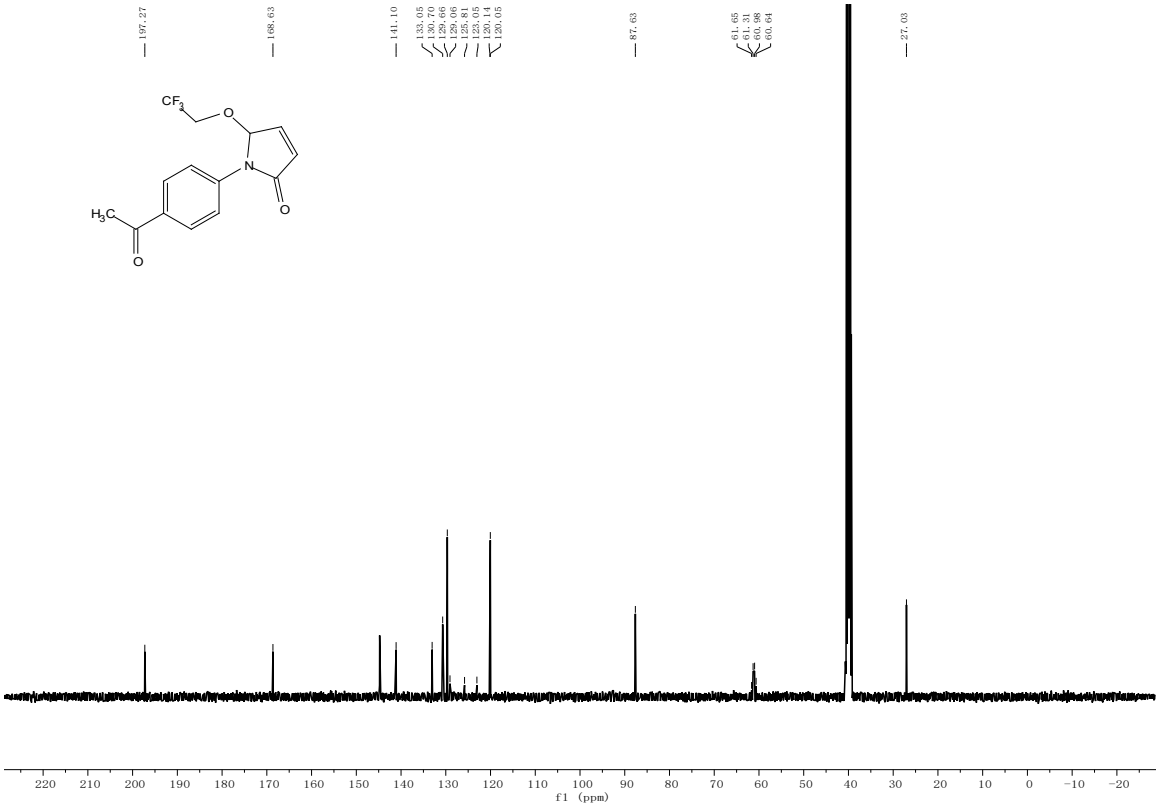
8.00
7.84
7.81
7.44
7.42
6.59
6.55
6.53
4.09
4.07
4.06
4.05
4.04
4.02
4.00
3.97
3.95
3.93
3.92
3.90
3.88
3.87
2.57
CF3
O
N
O
H3C
O
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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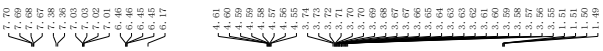
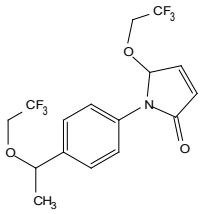
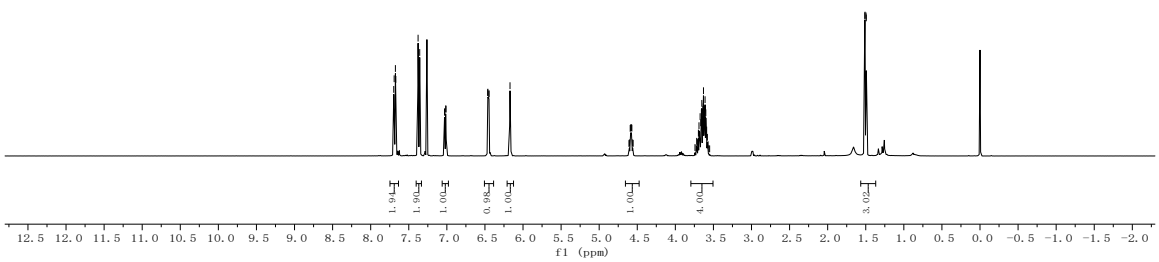
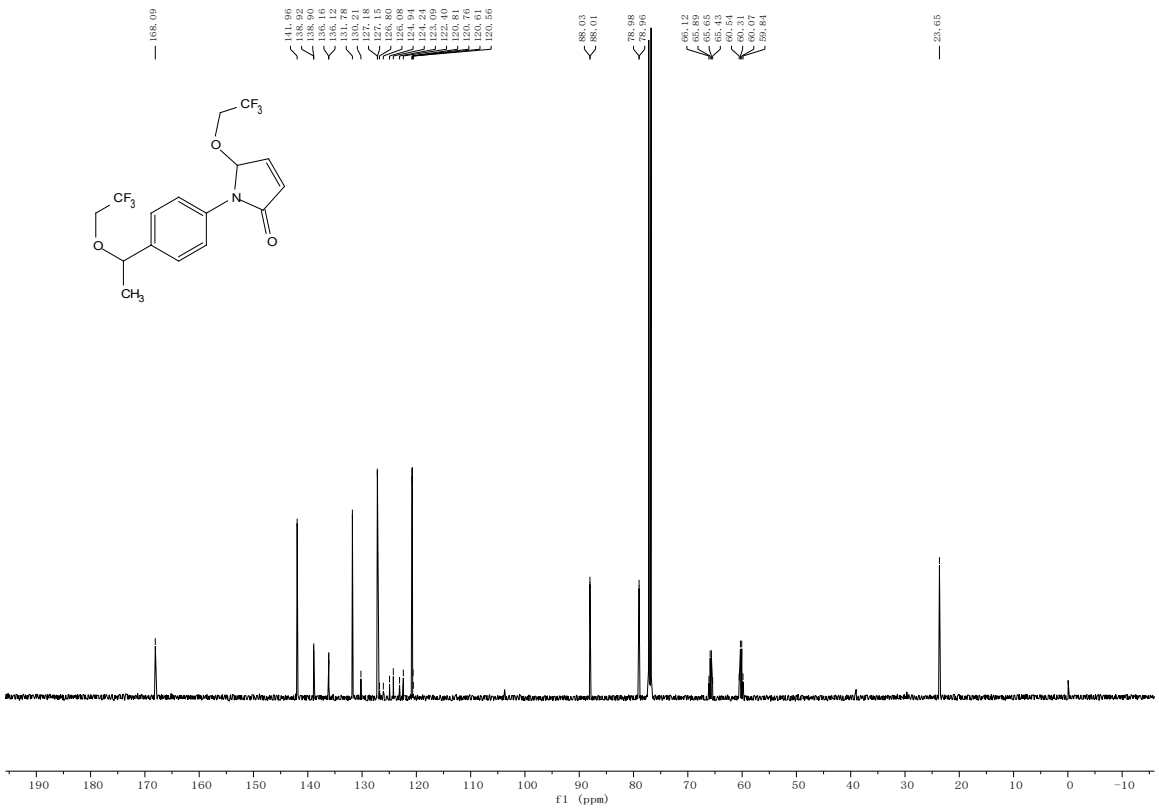
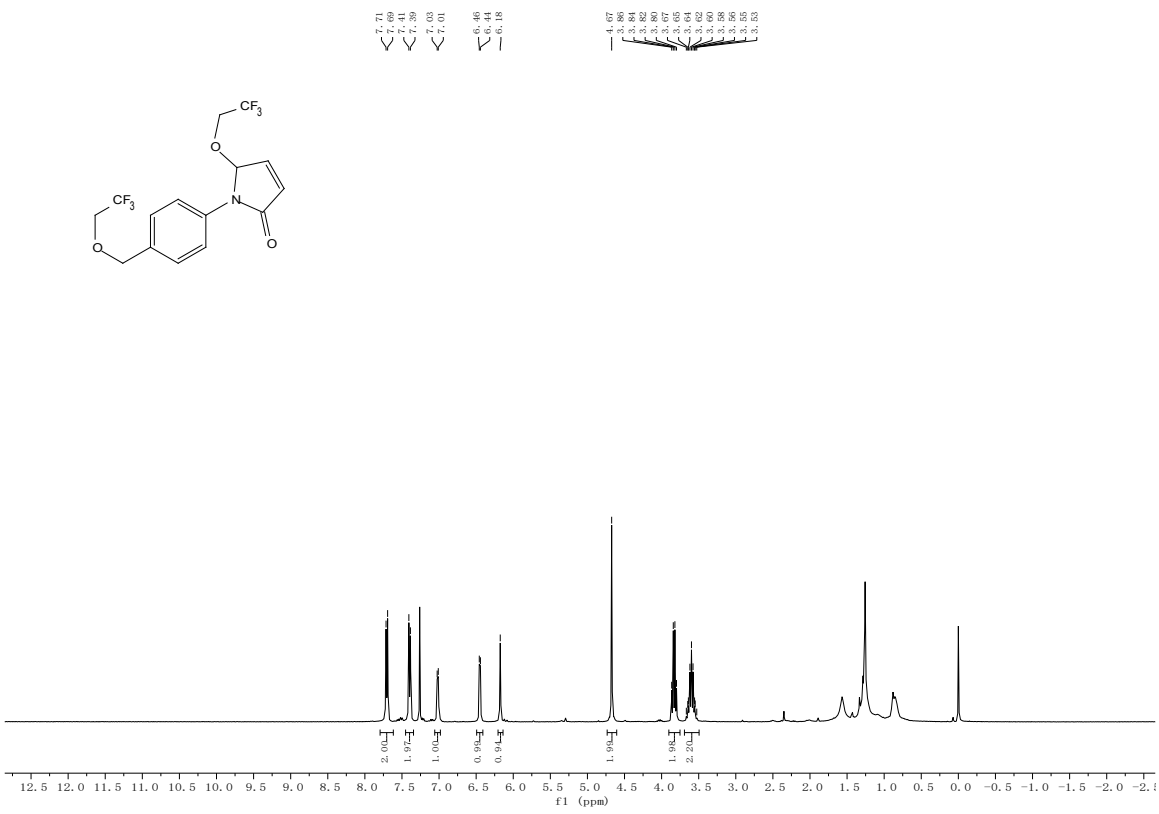
129.66
129.06
125.61
125.05
120.14
120.05
87.63
61.65
61.31
60.98
60.64
27.03
CF3
O
N
O
H3C
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)







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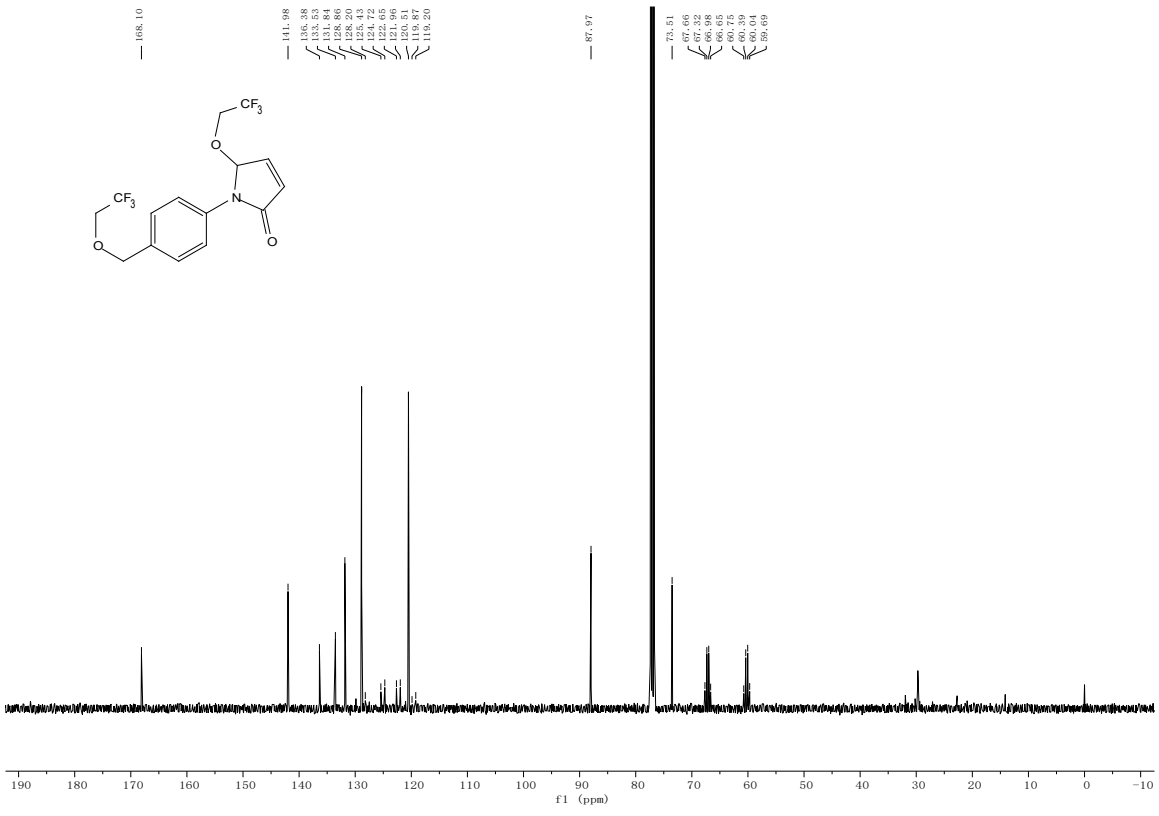
3.84
3.82
3.80
3.67
3.65
3.64
3.62
3.60
3.58
3.56
3.55
3.53
CF3
O
N
O
CF3
O
O
2.00
1.97
1.00
0.99
0.94
1.99
1.98
2.20
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.0 −1.5 −2.0
f1 (ppm)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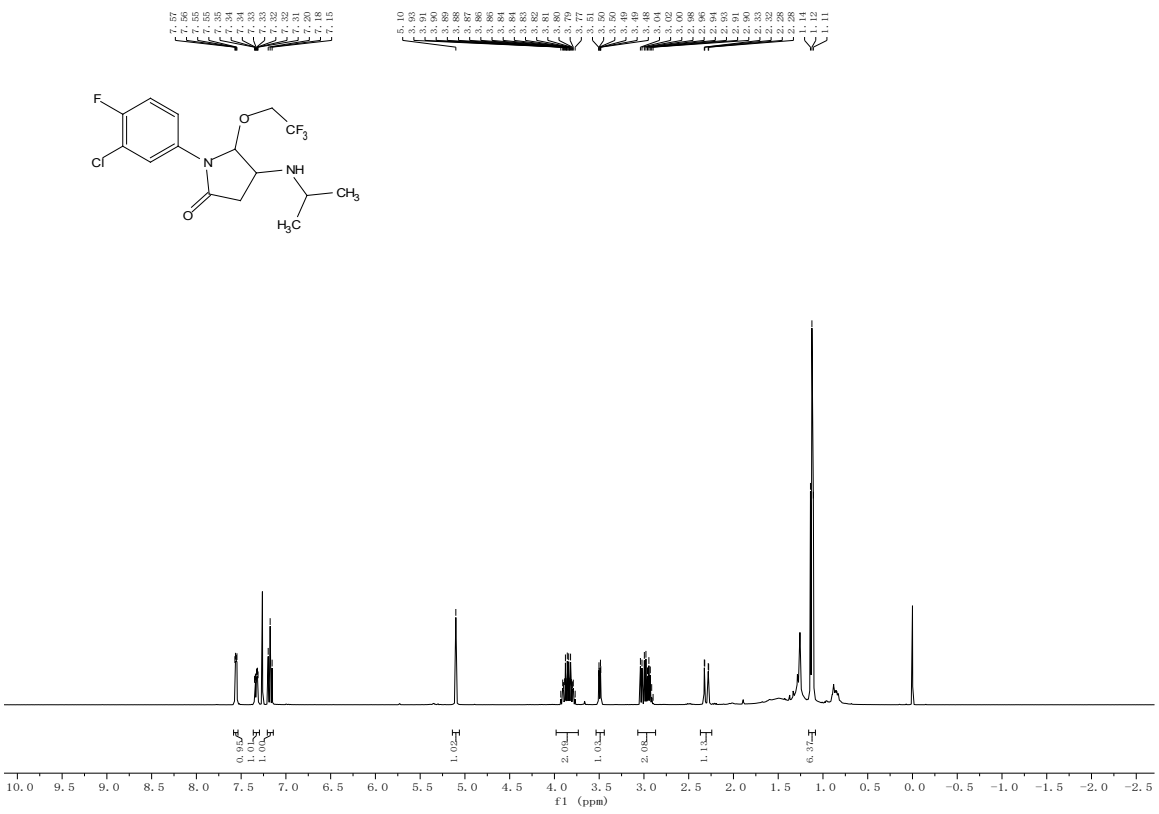
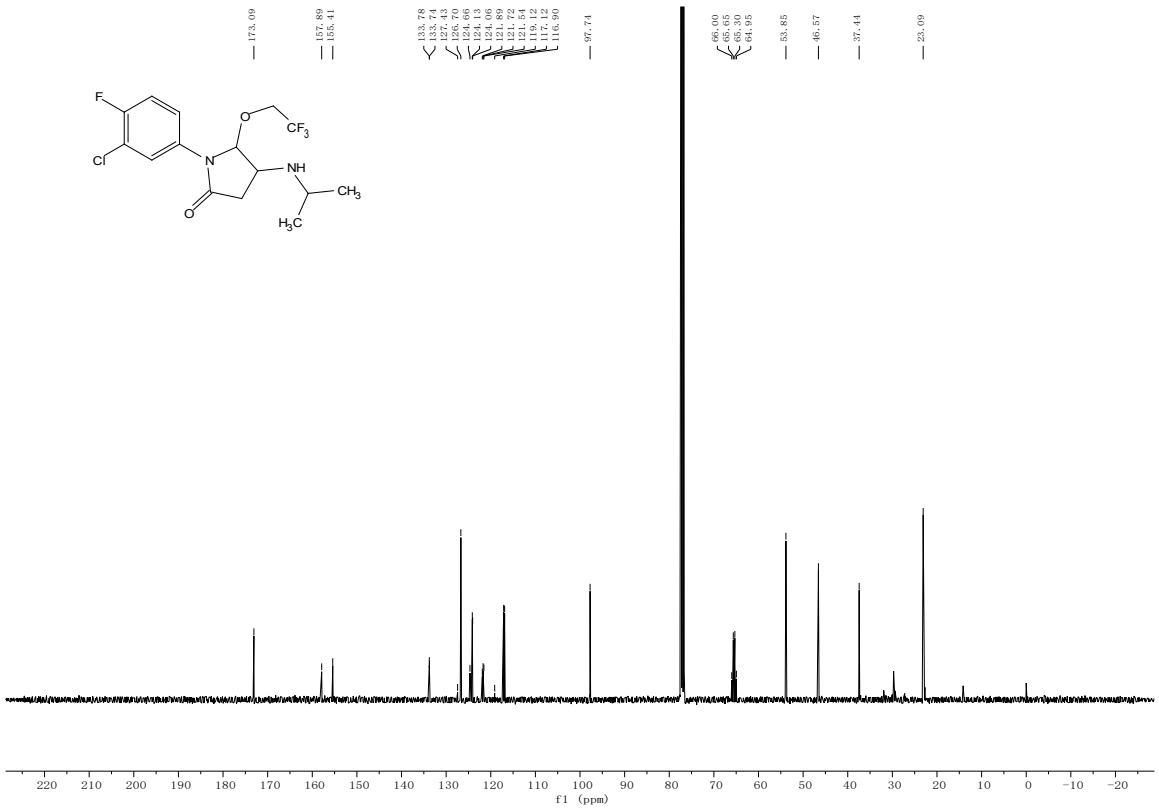
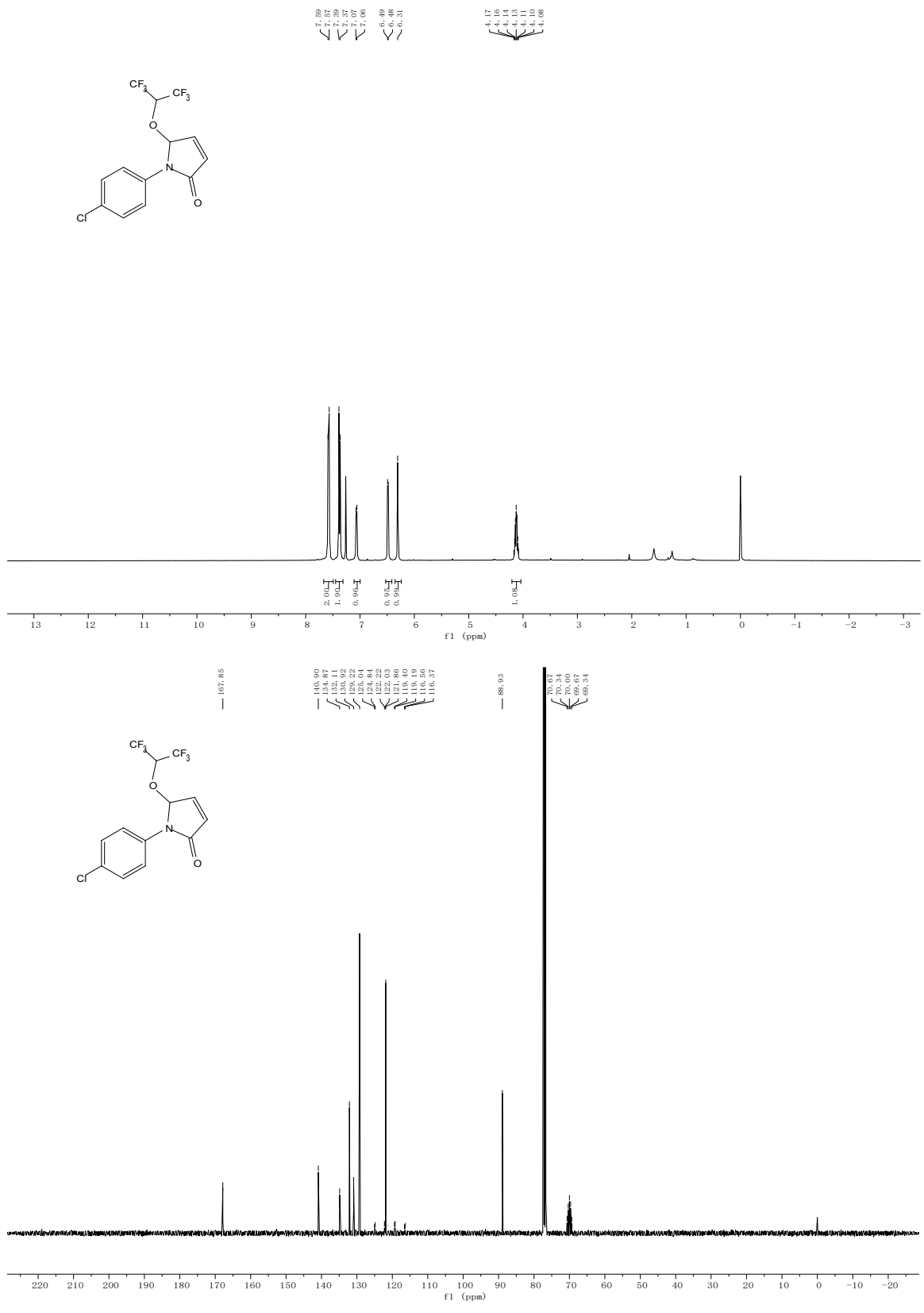
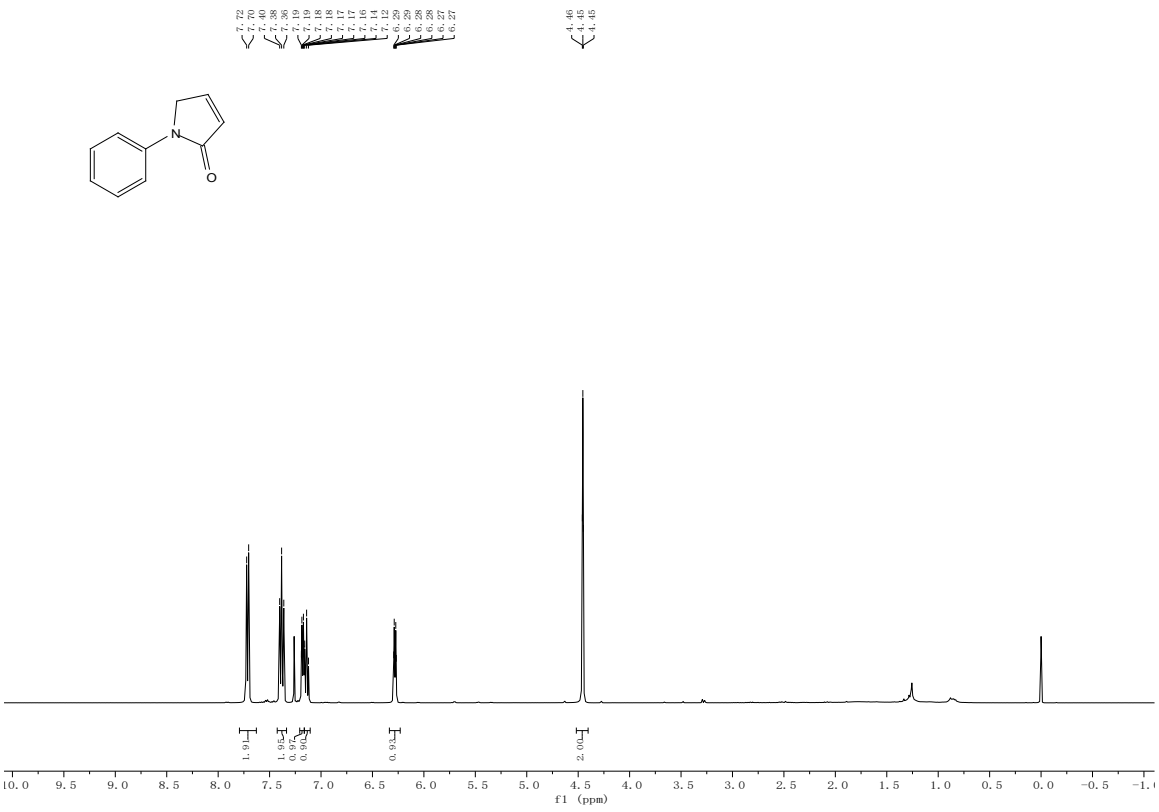
128.86
128.20
125.43
124.72
122.65
121.96
120.51
119.87
119.20
87.97
73.51
67.66
67.32
66.98
66.65
66.75
66.39
60.04
59.69
CF3
O
N
O
CF3
O
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


F
Cl
O
CF3
N
NH
CH3
O
H3C
f1 (ppm)


F
Cl
O
CF3
N
NH
CH3
O
H3C
f1 (ppm)


7.59
7.57
7.39
7.37
7.07
7.06
6.49
6.48
6.31
4.17
4.16
4.14
4.13
4.11
4.10
4.08
CF3
CF3
O
N
O
Cl
2.00
1.90
0.96
0.95
0.95
1.08
f1 (ppm)
167.85
140.90
134.87
132.11
130.92
129.22
125.04
123.84
122.22
122.03
121.86
119.40
119.19
116.56
116.37
88.93
70.67
70.34
70.00
69.67
69.34
f1 (ppm)



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