Supporting Information

The Cyclization/Rearrangement of α-Hydroxy Ketones with Trifluoromethyl N-acylhydrazones to Synthesize Multi-substituted Trifluoromethyloxazolines

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Contents:

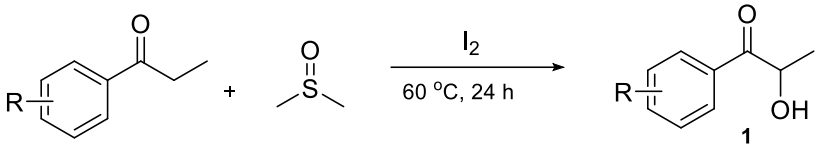
1. General Information 2
2. General Procedures 3
2.1. General procedure for the synthesis of α-hydroxy ketones 1 3
2.2. General procedure for the synthesis of trifluoromethyl N-acylhydrazones 2 3
2.3. General procedure for the synthesis of compounds 3 and 4: 4
2.4. Partial condition optimization 4
2.5. Characterization data of compounds 3 and 4 6
3. References and notes 24
4. Single Crystal X-Ray Structure Determinations of Compounds 3a 25
5. Copies of NMR Spectra 33
6. Control experiments 106
7. Theoretical caculation 108
8. HRMS(ESI) copy of active intermediates 113
9. References and notes 117
10. Cartesian coordinates 118

1. General Information

All reactions were performed in dried glassware with magnetic stirring bar and sealed with a rubber septum. The solvents were distilled by standard methods. Reagents were obtained from commercial suppliers and used without further purification unless otherwise noted. Silica gel column chromatography was carried out using silica Gel 60 (230–400 mesh). Analytical thin layer chromatography (TLC) was done using silica Gel (silica gel 60 F254). TLC plates were analyzed by an exposure to ultraviolet (UV) light and/or submersion in phosphomolybdic acid solution or submersion in $KMnO_4$ solution or in Iodine vapor. NMR experiments were carried out in $CDCl_3$ or acetone-d_6. ^{1}H NMR, ^{13}C{^{1}H} NMR and ^{19}F NMR spectra were recorded at 400 MHz or 600 MHz, 100 MHz or 150 MHz and 376 MHz spectrometers, respectively. Chemical shifts are reported as δ values relative to internal TMS (δ 0.00 ppm for ^{1}H NMR), chloroform (δ 7.26 ppm for ^{1}H NMR), chloroform (δ 77.00 ppm for ^{13}C NMR) and $CFCl_3$ (δ 0.00 ppm for ^{19}F NMR) in parts per million (ppm). The following abbreviations are used for the multiplicities: s: singlet, d: doublet, dd: doublet of doublet, t: triplet, q: quartet, m: multiplet; Coupling constants (J) are reported in Hertz (Hz). Melting points were uncorrected. High resolution mass spectra (HRMS) were recorded on Micro TOF-QII mass instrument (ESI). The relative configuration of **3a** was determined by NMR Data, molecular weight and x-ray single crystal diffraction. Substrates **1** were synthesized according to the published procedures.[1] Substrates **2** were prepared according to the literature method.[2]

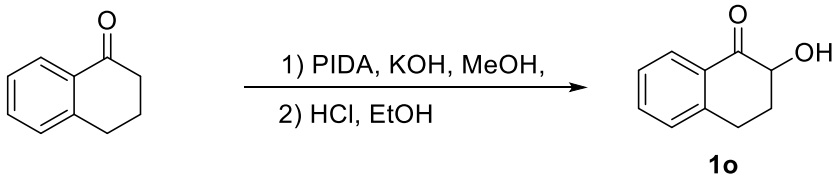
2. General Procedures

2.1. General procedure for the synthesis of α-hydroxy ketones 1



Scheme S1 Preparation of the *α*-hydroxy ketone 1a-1m

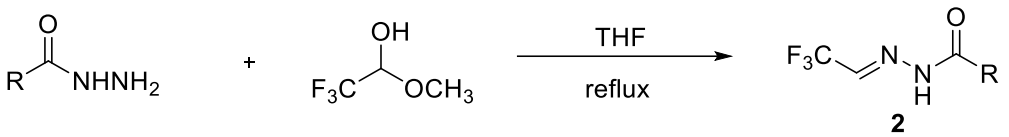
Ketone (10 mmol), I_2 (20 mol%), and DMSO (10 mL) and a stir bar were added to a 25 mL reaction tube under air. The mixture was stirred at 60 ℃ for 24h as monitored by TLC. After cooling down to room temperature, the solution was diluted with ethyl acetate (20 mL) and washed with 0.1 mol/L $Na_2S_2O_3$ (10 mL) aqueous solution, extracted with ethyl acetate (3×10 mL), and evaporated under vacuum. The crude reaction mixture was purified by column chromatography on silica gel (eluent: petroleum ether / ethyl acetate = 20:1) to get the desired product **1a-1m**.



Scheme S2 Preparation of the hydroxy ketone 1o

A solution of the corresponding ketone (70 mmol) in MeOH (0.2 mmol/mL) was added to a previously prepared ice-cooled solution of KOH (210 mmol) in MeOH (1.2 mmol/mL) over 5 min. Solid iodobenzene diacetate (77 mmol) was added in portions at 0 ℃ during 5 min and the resulting mixture was stirred at 0 ℃ for 1 hour and then at room temperature overnight. Organic solvents were removed under reduced pressure to give a residue which was dissolved in Et_2O, washed with water and evaporated. The residue was dissolved in EtOH (50 mL) and 6M HCl aq. (70 mL) was added. It was stirred at room temperature for 30 min, and then basified with K_2CO_3 and extracted with Et_2O. The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by flash column chromatography to give the corresponding α-hydroxy ketone **1o**.

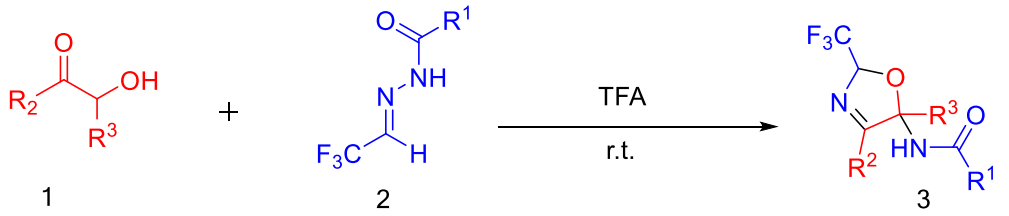
2.2. General procedure for the synthesis of trifluoromethyl N-acylhydrazones 2



Scheme S3 Preparation of the trifluoromethyl *N*-acylhydrazones 2

A solution of 1 mmol of the corresponding hydrazide and 1 mmol (116 mg) of Trifluoro acetaldehyde methyl hemiacetal in 1 mL of MeOH was placed in a glass tube. After addition of freshly dried molecular sieves (4 Å), the tube was closed and heated in an oil bath to 75 ºC for 24 h. Then, the mixture was cooled, filtered, and washed with a portion of MeOH. The solvent of the combined solutions was evaporated, and the crude products obtained were purified by column chromatography or on preparative thin layer plates (SiO_2). acylhydrazone **2** were isolated as crystalline materials. Analytically pure samples were obtained after recrystallization.

2.3. General procedure for the synthesis of compounds 3 and 4:



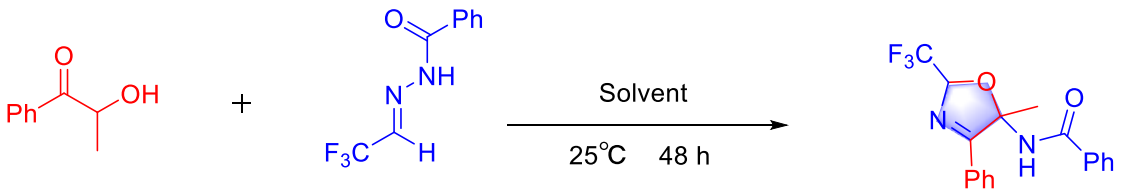
Scheme S4 Preparation of the oxazoline 3 and 4

α-Hydroxyl ketone **1** (0.6 mmol, 1.2 equiv.), trifluoromethyl *N*-acylhydrazones **2** (0.5 mmol, 1 equiv.) were added to the reaction tube under air atmosphere, and then 2.5 mL of trifluoroacetic acid was added as the solvent. The mixture was stirred at room temperature and the progress of the reaction was monitored by TLC. After the reaction was completed, the reaction was quenched with saturated $NaHCO_3$, and then the mixture was extracted with ethyl acetate (20 ml × 3). The combined organic extracts were dried over anhydrous $MgSO_4$ and concentrated in vacuum. Purification of the residue by silica gel column chromatography using petroleum ether: ethyl acetate (5:1) as eluent furnished the products **3** and **4**.

2.4. Partial condition optimization

The influence of various solvents was also examined. After stirring at 25 °C for 48 hours, none of the reactions occurred when AcOH, TFE, CH_3CN, DCE or THF were used as solvents (**Table S1**).

Table S1 Condition optimization



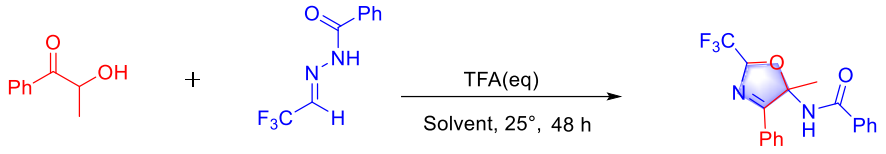
1a 2a 3a

Entry	Mole ratio of 1a/2a	Solvents	Volume of solvent(mL)	Temp. (°C)	**3a** [b] yield(%)
1	1.2: 1	AcOH	2	25	N. R
2	1.2: 1	TFE	2	25	N. R
3	1.2: 1	CH_3CN	2	25	N. R
4	1.2: 1	DCE	2	25	N. R
5	1.2: 1	THF	2	25	N. R

[a]Reaction conditions: **1a** (0.6 mmol 90 mg), **2a** (0.6 mmol 108 mg). [b]) Isolated yields. [c]) Under argon atmosphere

The influence of stoichiometric acid as the promoterwas also examined. Selected other neutral solvent such as CH_3CN, THF, TFE, DCM or DCE. After stirring at 25 °C for 48 hours, little or none of the reactions occurred (**Table S2**).

Table S2 Using TFA as a reagent for further optimization

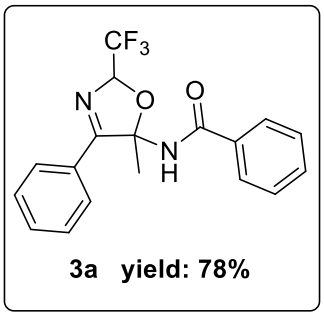


1a 2a 3a

Entry	Mole ratio of 1a/2a/TFA	Solvents	Temp. (℃)	**3a**[b] yield (%)
1	1.2: 1: 1	MeCN	25	ND
2	1.2: 1: 2	MeCN	25	ND
3	1.2: 1: 4	MeCN	25	ND
4	1.2: 1: 1	THF	25	ND
5	1.2: 1: 2	THF	25	ND
6	1.2: 1: 4	THF	25	ND
7	1.2: 1: 1	TFE	25	ND
8	1.2: 1: 2	TFE	25	ND
9	1.2: 1: 4	TFE	25	ND
10	1.2: 1: 1	DCM	25	ND
11	1.2: 1: 2	DCM	25	ND
12	1.2: 1: 4	DCM	25	trace
13	1.2: 1: 1	DCE	25	ND
14	1.2: 1: 2	DCE	25	ND
15	1.2: 1: 4	DCE	25	trace

[a]Reaction conditions: **1a** (0.6 mmol 90 mg), **2a** (0.6 mmol 108 mg). [b]) Isolated yields.

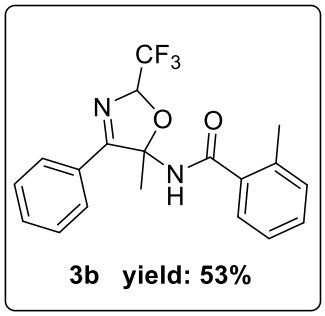
2.5. Characterization data of compounds 3 and 4



3a yield: 78%

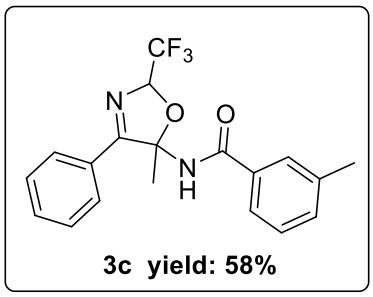
N-(5-Methyl-4-phenyl-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl) benzamide (**3a**). Purified by column chromatography (EA/PE, 1:5). White solid (131 mg, 75% yield), m.p.: 203–205 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, J = 7.2 Hz, 2H), 7.74 (d, J = 7.2 Hz, 2H), 7.55–7.38 (m, 6H), 7.11 (s, 1H), 6.28 (q, J = 5.2 Hz, 1H), 1.85 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.6 (Cq), 167.1 (Cq), 133.1 (Cq), 132.4 (Cq), 131.9 (CH), 129.3 (CH),

128.8 (CH), 128.7 (CH), 128.1 (CH), 127.1 (CH), 122.3 (q, J_{C-F} = 280.1 Hz) (Cq), 99.2 (q, J_{C-F} = 32.3 Hz) (CH), 96.0 (Cq), 26.6 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.09 (d, J = 4.9 Hz); HRMS (ESI): *m/z* calcd for chemical formula: $C_{18}H_{16}F_3N_2O_2$ $[M + H]^+$ 349.1158; found 349.1158.



3b yield: 53%

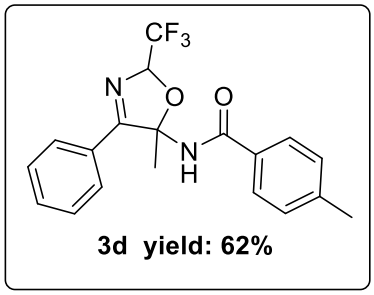
2-Methyl-N-(5-methyl-4-phenyl-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl) benzamide (**3b**). Purified by column chromatography (EA/PE, 1:5). White solid (96 mg, 53% yield), m.p.: 193–195 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, J = 7.2 Hz, 2H), 7.52 (t, J = 7.6 Hz, 1H), 7.45 (q, J = 7.2 Hz, 2H), 7.34 (t, J = 7.6 Hz, 2H), 7.21– 7.18 (m, 2H), 6.76 (s, 1H), 6.26 (q, J = 5.2 Hz, 1H), 2.27 (s, 3H), 1.81 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.5 (Cq), 169.5 (Cq), 136.7 (Cq), 134.8 (Cq), 132.0 (Cq), 131.3 (CH), 130.0 (CH), 128.7 (CH), 128.2 (CH), 126.4 (CH), 125.8 (CH), 122.3 (q, J_{C-F} = 280.5 Hz) (Cq), 99.2 (q, J_{C-F} = 31.5 Hz) (CH), 95.9 (Cq), 26.5 (CH_3), 19.0 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -79.74 (d, J = 4.5 Hz); HRMS (ESI): *m/z* calcd for chemical formula: $C_{19}H_{17}F_3N_2O_2Na$ $[M + Na]^+$ 385.1134; found 385.1133.



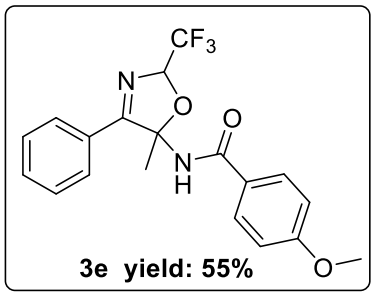
3c yield: 58%

3-Methyl-N-(5-methyl-4-phenyl-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl)benzamide (**3c**). Purified by column chromatography (EA/PE, 1:5). White solid (105 mg, 58%), m.p.: 217–219 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, J = 7.6 Hz, 2H), 7.56 (s, 1H), 7.54 (d, J = 8.0 Hz, 1H), 7.49 (t, J = 7.2 Hz, 1H), 7.41 (t, J = 7.6 Hz, 2H), 7.34 (d, J = 6.8 Hz, 2H), 6.94 (s, 1H), 6.29 (q, J = 4.8 Hz, 1H), 2.40 (s, 3H), 1.88 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.6 (Cq), 167.2 (Cq), 138.8 (Cq), 133.1 (Cq), 133.0 (Cq), 131.9 (CH), 129.4 (CH), 128.7 (CH), 128.6 (CH), 128.1 (CH), 127.9 (CH), 124.0 (CH), 121.4 (q, J_{C-F} = 279.0 Hz) (Cq), 99.2 (q, J_{C-F} = 31.5 Hz) (CH), 96.0 (Cq), 26.7 (CH_3), 21.3 (CH_3); ^{19}F NMR (376 MHz,

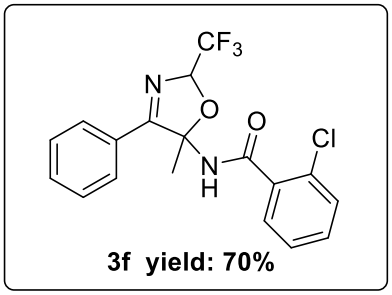
$CDCl_3$) δ -84.94 (d, J = 4.9 Hz); HRMS (ESI): *m/z* calcd for chemical formula: $C_{19}H_{18}F_3N_2O_2$ $[M + H]^+$ 363.1315; found 363.1314.



4-Methyl-*N*-(5-methyl-4-phenyl-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl)benzamide (**3d**). Purified by column chromatography (EA/PE, 1:5). White solid (112 mg, 62%), m.p.:208–210 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (dd, J = 5.6, 0.8 Hz, 2H), 7.65 (d, J = 5.6 Hz, 2H), 7.47 (t, J = 5.2 Hz, 1H), 7.39 (t, J = 5.2 Hz, 2H), 7.23 (d, J = 5.2 Hz, 2H), 6.98 (s, 1H), 6.28 (q, J = 3.2 Hz, 1H), 2.39 (s, 3H), 1.85 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.1 (Cq), 167.0 (Cq), 143.1 (Cq), 131.9 (Cq), 130.3 (Cq), 129.4 (CH), 129.4 (CH), 128.7 (CH), 128.1 (CH), 127.1 (CH), 122.3 (q, $J_{C\text{-}F}$ = 270.0 Hz) (Cq), 99.2 (q, $J_{C\text{-}F}$ = 33.0 Hz) (CH), 96.0 (Cq), 26.7 (CH_3), 21.5 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.16 (d, J = 4.9 Hz); HRMS(ESI): *m/z* calcd for chemical formula: $C_{19}H_{18}F_3N_2O_2$ $[M + H]^+$ 363.1315; found 363.1313.

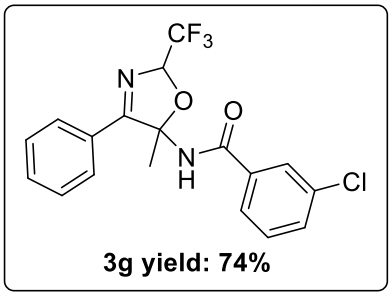


4-Methoxy-*N*-(5-methyl-4-phenyl-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl)benzamide (**3e**). Purified by column chromatography (EA/PE, 1:5). White solid (104 mg, 55%), m.p.: 262–264 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, J = 7.2 Hz, 2H), 7.73 (d, J = 9.2 Hz, 2H), 7.48 (t, J = 7.6 Hz, 1H), 7.40 (t, J = 8.0 Hz, 2H), 6.94–6.91 (m, 3H), 6.28 (q, J = 5.2 Hz, 1H), 3.85 (s, 3H), 1.86 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.7 (Cq), 166.5 (Cq), 162.9 (Cq), 131.8 (Cq), 129.5 (CH), 129.1 (CH), 128.7 (CH), 128.1 (CH), 125.3 (Cq), 122.4 (q, $J_{C\text{-}F}$ = 280.5 Hz) (Cq), 114.0 (CH), 99.3 (q, $J_{C\text{-}F}$ = 31.5.0 Hz) (CH), 96.0 (Cq), 55.5 (CH_3), 26.7 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.18 (d, J = 4.9 Hz). HRMS(ESI): *m/z* calcd for chemical formula: $C_{19}H_{16}F_3N_2O_3$ $[M – H]^+$ 377.1112; found 377.1121.



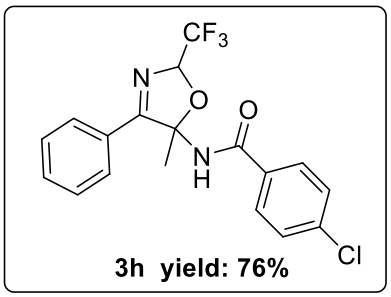
3f yield: 70%

2-Chloro-*N*-(5-methyl-4-phenyl-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl) benzamide (**3f**). Purified by column chromatography (EA/PE, 1:5). White solid (114 mg, 70%), m.p.: 182–184 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, J = 7.2 Hz, 2H), 7.63 (d, J = 8.4 Hz, 1H), 7.51 (t, J = 7.6 Hz, 1H), 7.45 – 7.36 (m, 4H), 7.33 – 7.28 (m, 2H), 6.29 (q, J = 4.8 Hz, 1H), 1.85 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.3 (Cq), 165.7 (Cq), 133.3 (Cq), 132.2 (Cq), 132.0 (CH), 130.9 (Cq), 130.5 (CH), 130.4 (CH), 129.2 (CH), 128.7 (CH), 128.4 (CH), 127.4 (CH), 122.4 (q, $J_{C\text{-}F}$ = 268.5 Hz) (Cq), 99.3 (q, $J_{C\text{-}F}$ = 33.0 Hz) (CH), 94.0 (Cq), 26.5 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -79.75 (d, J = 5.3 Hz); HRMS(ESI): *m/z* calcd for chemical formula: $C_{18}H_{15}ClF_3N_2O_2$ $[M + H]^+$ 383.0769; found 383.0769.



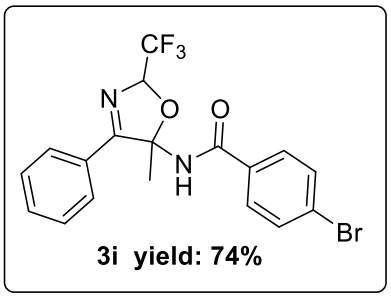
3g yield: 74%

3-Chloro-*N*-(5-methyl-4-phenyl-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl) benzamide (**3g**). Purified by column chromatography (EA/PE, 1:5). White solid (141 mg, 74%), m.p.: 187–189 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, J = 7.6 Hz, 2H), 7.58 (d, J = 6.8 Hz, 1H), 7.51 (t, J = 7.2 Hz, 1H), *7*.45 – 7.26 (m, 6H), 6.27 (q, J = 4.8 Hz, 1H), 1.82 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.3 (Cq), 165.8 (Cq), 135.0 (Cq), 134.9 (Cq), 132.4 (Cq), 130.1 (CH), 130.1 (CH), 129.2 (CH), 128.8 (CH), 128.1 (CH), 127.4 (CH), 125.2 (CH), 122.2 (q, $J_{C\text{-}F}$ = 280.2 Hz) (Cq), 99.3 (q, $J_{C\text{-}F}$ = 32.9 Hz) (CH), 96.0 (Cq), 26.6 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.14 (d, J = 4.5 Hz); HRMS(ESI): *m/z* calcd for chemical formula: $C_{18}H_{15}ClF_3N_2O_2$ $[M + H]^+$ 383.0769; found 383.0769.



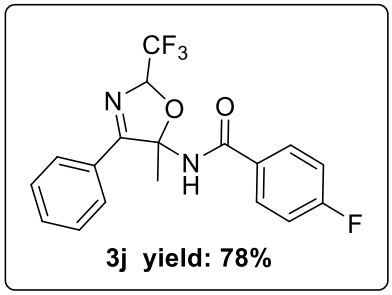
3h yield: 76%

4-Chloro-*N*-(5-methyl-4-phenyl-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl) benzamide (**3h**). Purified by column chromatography (EA/PE, 1:5). White solid (145 mg, 76%), m.p.: 212–214 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, J = 7.2 Hz, 2H), 7.69 (d, J = 8.4 Hz, 2H), 7.50 (d, J = 7.2 Hz, 1H), 7.43 – 7.39 (m, 4H), 6.95 (s, 1H), 6.28 (q, J = 4.8 Hz, 1H), 1.88 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.4 (Cq), 166.1 (Cq), 138.8 (Cq), 132.0 (Cq), 131.5 (Cq), 129.2 (CH), 129.1 (CH), 128.8 (CH), 128.5 (CH), 128.1 (CH), 122.3 (q, $J_{C\text{-}F}$ = 280.5 Hz) (Cq), 99.3 (q, $J_{C\text{-}F}$ = 33.0 Hz), 96.0 (Cq), 26.6 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.17 (d, J = 5.3 Hz); HRMS(ESI): *m/z* calcd for chemical formula: $C_{18}H_{13}ClF_3N_2O_2$ [M – H] $^{+}$ 381.0623; found 381.0623.



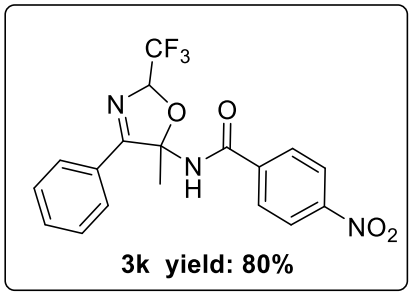
3i yield: 74%

4-Bromo-*N*-(5-methyl-4-phenyl-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl) benzamide (**3i**). Purified by column chromatography (EA/PE, 1:5). White solid (158 mg, 74%), m.p.: 218–220 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, J = 7.2 Hz, 2H), 7.61 (d, J = 8.4 Hz, 2H), 7.57 (d, J = 8.4 Hz, 2H), 7.52 – 7.48 (m, 1H), 7.41 (t, J = 7.6 Hz, 2H), 6.96 (s, 1H), 6.27 (q, J = 4.8 Hz, 1H), 1.88 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.3 (Cq), 166.1 (Cq), 132.1 (Cq), 132.0 (Cq), 131.9 (CH), 129.2 (CH), 128.8 (CH), 128.7 (CH), 128.1 (CH), 127.3 (Cq), 122.3 (q, $J_{C\text{-}F}$ = 280.5 Hz) (Cq), 99.3 (q, $J_{C\text{-}F}$ = 33.0 Hz) (CH), 96.0 (Cq), 26.6 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.16 (d, J = 4.9 Hz); HRMS(ESI): *m/z* calcd for chemical formula: $C_{18}H_{15}BrF_3N_2O_2$ [M + H] $^{+}$ 427.0264; found 427.0264.



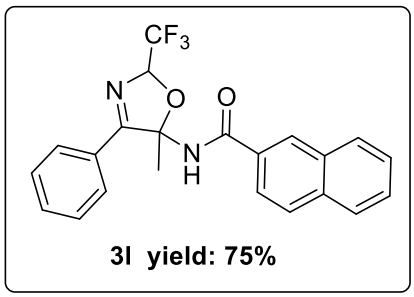
3j yield: 78%

4-fluoro-N-(5-methyl-4-phenyl-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl) benzamide (**3j**). Purified by column chromatography (EA/PE, 1:5). White solid (143 mg, 78%), m.p.: 200–202 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, J = 7.2 Hz, 2H), 7.76 – 7.73 (m, 2H), 7.49 (t, J = 7.2 Hz, 1H), 7.41 (t, J = 8.0 Hz, 2H), 7.11 – 7.06 (m, 3H), 6.27 (q, J = 4.8 Hz, 1H), 1.86 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.5 (Cq), 166.1 (Cq), 165.2 (q, $J_{C\text{-}F}$ = 253.5 Hz) (Cq), 132.0 (Cq), 129.5 (d, $J_{C\text{-}F}$ = 6.0 Hz) (CH), 129.3 (d, $J_{C\text{-}F}$ = 3.0 Hz) (Cq), 129.2 (CH), 128.8 (CH), 128.1 (CH), 122.3 (q, $J_{C\text{-}F}$ = 279.0 Hz) (CH), 115.9 (d, $J_{C\text{-}F}$ = 22.5 Hz) (CH), 99.2 (q, $J_{C\text{-}F}$ = 31.5 Hz) (CH), 95.6 (Cq), 27.3 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -79.74 (d, J = 7.5 Hz), -106.17 – -106.24 (m); HRMS(ESI): *m/z* calcd for chemical formula: $C_{18}H_{14}F_4N_2NaO_2$ $[M + Na]^+$ 389.0884; found 389.0883.



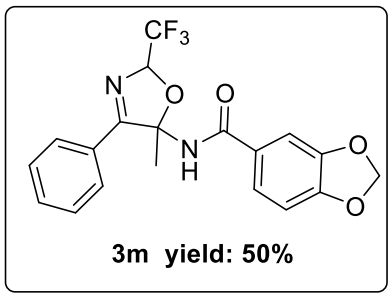
3k yield: 80%

N-(5-Methyl-4-phenyl-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl)-4-nitrobenzamide (**3k**). Purified by column chromatography (EA/PE, 1:5). White solid (157 mg, 80%), m.p.: 234–236 °C; ^{1}H NMR (400 MHz, acetone-d_6) δ 9.22 (s, 1H), 8.32 (d, J = 8.8 Hz, 2H), 8.18 – 8.16 (m, 4H), 7.56 (t, J = 7.6 Hz, 1H), 7.50 (t, J = 7.6 Hz, 2H), 6.32 (q, J = 5.2 Hz, 1H), 1.93 (s, 3H); ^{13}C NMR (150 MHz, acetone-d_6) δ 171.3 (Cq), 165.4 (Cq), 150.0 (Cq), 139.2 (Cq), 132.0 (Cq), 129.4 (CH), 129.0 (CH), 128.8 (CH), 123.5 (CH), 128.2 (CH), 120.7 (q, $J_{C\text{-}F}$ = 294.0 Hz) (Cq), 99.5 (q, $J_{C\text{-}F}$ = 33.0 Hz) (CH), 96.7 (Cq), 25.6 (CH_3); ^{19}F NMR (376 MHz, acetone-d_6) δ -80.38 (d, J = 5.3 Hz); HRMS(ESI): *m/z* calcd for chemical formula: $C_{18}H_{15}F_3N_3O_4$ $[M + H]^+$ 394.1009; found 394.1010.



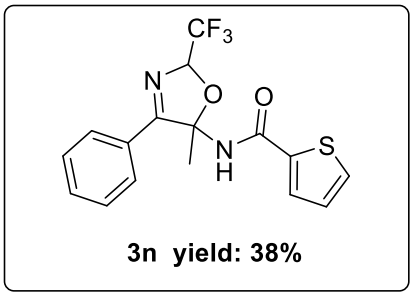
3l yield: 75%

N-(5-Methyl-4-phenyl-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl)-2-naphthamide (**3l**). Purified by column chromatography (EA/PE, 1:5). White solid (149 mg, 75%), m.p.: 206–208 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (s, 1H), 8.05 (d, J = 7.2 Hz, 2H), 7.87–7.83 (m, 3H), 7.75 (dd, J = 8.4, 1.6 Hz, 1H), 7.60 – 7.50 (m, 2H), 7.47 (t, J = 7.2 Hz, 1H), 7.39 (t, J = 7.6 Hz, 2H), 7.29 (s, 1H), 6.34 (q, J = 5.2 Hz, 1H), 1.91 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.6 (Cq), 167.2 (Cq), 135.0 (Cq), 132.4 (Cq), 131.9 (Cq), 130.3 (Cq), 129.4 (CH), 129.0 (CH), 128.8 (CH), 128.2 (CH), 127.9 (CH), 127.8 (CH), 127.0 (CH), 123.2 (CH), 122.3 (q, $J_{C\text{-}F}$ = 279.6 Hz) (Cq), 99.3 (q, $J_{C\text{-}F}$ = 33.0 Hz) (CH), 96.1 (Cq), 26.7 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.09 (d, J = 4.9 Hz). HRMS(ESI): *m/z* calcd for chemical formula: $C_{22}H_{18}F_3N_2O_2$ $[M + H]^+$ 399.1315; found 399.1313.



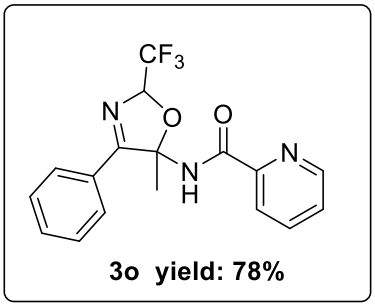
3m yield: 50%

N-(5-Methyl-4-phenyl-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl) benzo[*d*] [1,3] dioxole-5-carboxamide (**3m**). Purified by column chromatography (EA/PE, 1:5). White solid (98 mg, 50%), m.p.: 213–215 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, J = 8.0 Hz, 2H), 7.48 (t, J = 7.6 Hz, 1H), 7.40 (t, J = 8.4 Hz, 2H), 7.30 – 7.26 (m, 1H), 7.22 (d, J = 1.6 Hz, 1H), 6.88 (s, 1H), 6.82 (d, J = 8.1 Hz, 1H), 6.27 (q, J = 5.2 Hz, 1H), 6.03 (s, 2H), 1.85 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.5 (Cq), 166.2 (Cq), 151.1 (Cq), 148.2 (Cq), 131.9 (Cq), 129.4 (CH), 128.7 (CH), 128.1 (Cq), 127.3 (CH), 122.3 (q, $J_{C\text{-}F}$ = 280.5 Hz) (Cq), 121.4 (CH), 108.1 (CH), 107.7 (CH), 101.9 (CH), 99.2 (q, $J_{C\text{-}F}$ = 33.0 Hz) (CH), 96.0 (Cq), 26.7 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.17 (d, J = 5.3 Hz). HRMS(ESI): *m/z* calcd for chemical formula: $C_{19}H_{16}F_3N_2O_4$ $[M + H]^+$ 393.1057; found 393.1056.



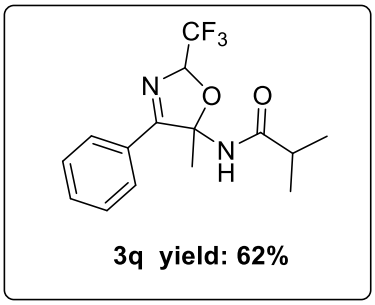
3n yield: 38%

N-(5-Methyl-4-phenyl-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl) thiophene-2 carboxamide (**3n**). Purified by column chromatography (EA/PE, 1:5). White solid (67 mg, 38%), m.p.: 214–216 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, J = 7.2 Hz, 2H), 7.56 (dd, J = 4.0, 1.2 Hz, 1H), 7.54 (dd, J = 4.8, 0.8 Hz, 1H), 7.49 (t, J = 7.6 Hz, 1H), 7.43–7.41 (m, 2H), 7.10 (dd, J = 4.8, 3.6 Hz, 1H), 6.82 (s, 1H), 6.27 (q, J = 4.8 Hz, 1H), 1.86 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.4 (Cq), 161.6 (Cq), 137.4 (Cq), 132.0 (Cq), 131.5 (CH), 129.4 (CH), 129.2 (CH), 128.8 (CH), 128.2 (CH), 127.9 (CH), 122.2 (q, $J_{C\text{-}F}$ = 280.5 Hz) (Cq), 99.2 (q, $J_{C\text{-}F}$ = 33.0 Hz) (CH), 96.1 (Cq), 26.6 (CH_3). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.18 (d, J = 5.3 Hz); HRMS(ESI): *m/z* calcd for chemical formula: $C_{16}H_{14}F_3N_2O_2S$ $[M + H]^+$ 355.0723; found 355.0723.



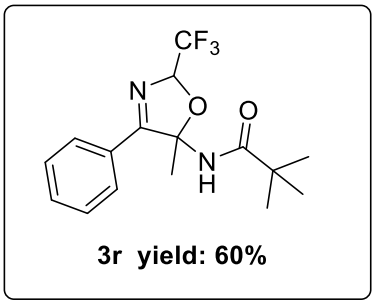
3o yield: 78%

N-(5-Methyl-4-phenyl-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl) picolinamide (**3o**). Purified by column chromatography (EA/PE, 1:5). White solid (136 mg, 78%), m.p.:137–139 °C; ^{1}H NMR (400 MHz, acetone-d_6) δ 8.68 (d, J = 4.8 Hz, 1H), 8.15 – 8.13 (m, 2H), 8.01 – 7.97 (m, 2H), 7.65 –7.62 (m, 1H), 7.55 (t, J = 7.42 Hz, 1H), 7.47 (t, J = 7.6 Hz, 2H), 6.32 (q, J = 5.2 Hz, 1H), 2.00 (s, 3H); ^{13}C NMR (150 MHz, acetone-d_6) δ 170.9 (Cq), 164.2 (Cq), 149.1 (Cq), 148.6 (CH), 137.8 (Cq), 131.9 (CH), 129.4 (CH), 128.8 (CH), 128.2 (CH), 127.1 (CH), 122.4 (q, $J_{C\text{-}F}$ = 266.7 Hz) (Cq), 122.1 (CH), 98.8 (q, $J_{C\text{-}F}$ = 33.0 Hz) (CH), 96.1 (Cq), 25.7; ^{19}F NMR (376 MHz, acetone-d_6) δ -68.14 (d, J = 3.8 Hz); HRMS (ESI): *m/z* calcd for chemical formula: $C_{17}H_{15}F_3N_3O_2$ $[M + H]^+$ 350.1111; found 350.1111.



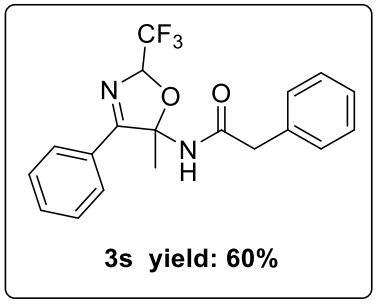
3q yield: 62%

N-(5-Methyl-4-phenyl-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl) isobutyramide (**3q**). Purified by column chromatography (EA/PE, 1:5). White solid (97 mg, 62%), m.p.: 200–202 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, J = 7.6 Hz, 2H), 7.50 (t, J = 7.2 Hz, 1H), 7.42 (t, J = 7.6 Hz, 2H), 6.30 (s, 1H), 6.18 (q, J = 4.8 Hz, 1H), 2.38 (p, J = 6.8 Hz, 1H), 1.76 (s, 3H), 1.13 (d, J = 6.8 Hz, 3H), 1.09 (d, J = 6.8 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 176.7 (Cq), 170.4 (Cq), 131.8 (Cq), 129.4 (CH), 128.6 (CH), 128.1 (CH), 122.3 (q, $J_{C\text{-}F}$ = 280.5 Hz) (Cq), 99.0 (q, $J_{C\text{-}F}$ = 32.0 Hz) (CH), 95.6 (Cq), 33.6 (CH), 26.5 (CH_3), 19.3 (CH_3), 18.9 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.23 (d, J = 4.9 Hz); HRMS(ESI): *m/z* calcd for chemical formula: $C_{15}H_{18}F_3N_2O_2$ $[M + H]^+$ 315.1315; found 315.1315.



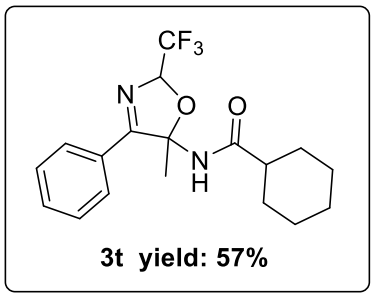
3r yield: 60%

N-(5-Methyl-4-phenyl-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl) pivalamide (**3r**). Purified by column chromatography (EA/PE, 1:5). White solid (98 mg, 60%), m.p.: 196–198 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, J = 7.2 Hz, 2H), 7.49 (t, J = 7.2 Hz, 1H), 7.41 (t, J = 7.6 Hz, 2H), 6.40 (s, 1H), 6.19 (q, J = 5.2 Hz, 1H), 1.78 (s, 3H), 1.18 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 178.1 (Cq), 171.3 (Cq), 131.8 (Cq), 129.4 (CH), 128.6 (CH), 128.0 (CH), 122.1 (q, $J_{C\text{-}F}$ = 247.5 Hz) (Cq), 99.0 (q, $J_{C\text{-}F}$ = 33.0 Hz) (CH), 95.6 (Cq), 38.6 (Cq), 27.2 (CH_3), 26.6 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -84.95 (d, J = 5.3 Hz); HRMS(ESI): *m/z* calcd for chemical formula: $C_{16}H_{20}F_3N_2O_2$ $[M + H]^+$ 329.1471; found 329.1471.



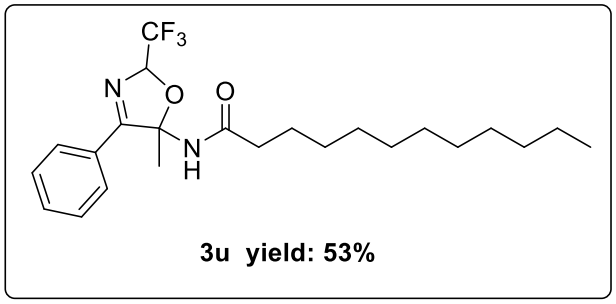
3s yield: 60%

N-(5-Methyl-4-phenyl-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl)-2-phenylacetamide(**3s**). Purified by column chromatography (EA/PE, 1:5). White solid (109 mg, 60%), m.p.: 180–182 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, J = 8.0 Hz, 2H), 7.49 (t, J = 8.0 Hz, 1H), 7.41 – 7.34 (m, 5H), 7.21 (d, J = 4.0 Hz, 2H), 6.21 – 6.17 (m, 2H), 3.55 (s, 2H), 1.62 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.6 (Cq), 170.1 (Cq), 133.9 (Cq), 131.9 (Cq), 129.3 (CH), 129.1 (CH), 128.7 (CH), 128.6 (CH), 128.1 (CH), 127.8 (CH), 122.2 (q, $J_{C\text{-}F}$ = 280.5 Hz) (Cq), 99.1 (q, $J_{C\text{-}F}$ = 33.0 Hz) (CH), 95.5 (Cq), 44.0 (CH_2), 26.2 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -79.84 (d, J = 4.9 Hz); HRMS(ESI): *m/z* calcd for chemical formula: $C_{19}H_{17}F_3N_2NaO_2$ $[M + Na]^+$ 385.1134; found 385.1133.



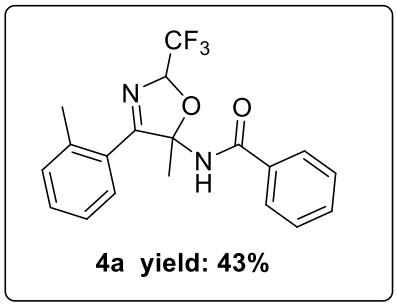
3t yield: 57%

N-(5-Methyl-4-phenyl-2-(trifluoromethyl)-2,5-dihydrooxazol-5yl) cyclohexanecarbox amide (**3t**). Purified by column chromatography (EA/PE, 1:5). White solid (101 mg, 57%), m.p.: 206–208 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, J = 8.4 Hz, 2H), 7.48 (t, J = 8.4 Hz, 1H), 7.41 (t, J = 8.0 Hz, 2H), 6.54 (s, 1H), 6.17 (q, J = 4.8 Hz, 1H), 2.10 (t, J = 11.6 Hz, 1H), 1.79 – 1.63 (m, 8H), 1.45 – 1.15 (m, 5H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 176.0 (Cq), 170.6 (Cq), 131.8 (Cq), 129.4 (CH), 128.6 (CH), 128.1 (CH), 122.3 (q, $J_{C\text{-}F}$ = 280.5 Hz), 99.0 (q, $J_{C\text{-}F}$ = 33.0 Hz) (CH), 95.6 (Cq), 45.2 (CH), 29.4 (CH_2), 28.9 (CH_2), 26.4 (CH_2), 25.5 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.19 (d, J = 7.5 Hz); HRMS(ESI): *m/z* calcd for chemical formula: $C_{18}H_{22}F_3N_2O_2$ $[M + H]^+$ 355.1628; found 355.1627.



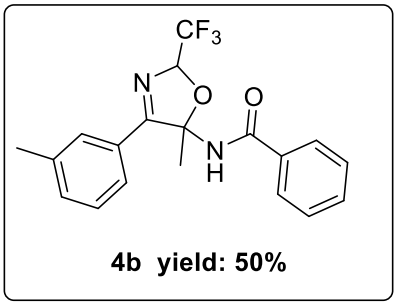
3u yield: 53%

N-(5-Methyl-4-phenyl-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl) dodecanamide (**3u**). Purified by column chromatography (EA/PE, 1:5). White solid (106 mg, 53%), m.p.: 120–122 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, J = 7.2 Hz, 2H), 7.50 (t, J = 7.6 Hz, 1H), 7.41 (t, J = 7.6 Hz, 2H), 6.45 (s, 1H), 6.17 (q, J = 5.2 Hz, 1H), 2.17 (td, J = 7.6, 3.2 Hz, 2H), 1.73 (s, 3H), 1.24–1.21 (m, 18H), 0.88 (t, J = 6.8 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 173.3 (Cq), 170.5 (Cq), 131.9 (Cq), 129.3 (CH), 128.6 (CH), 128.1 (CH), 123.0 (q, $J_{C\text{-}F}$ = 280.2 Hz) (Cq), 98.9 (q, $J_{C\text{-}F}$ = 32.9 Hz) (CH), 95.7 (Cq), 36.0 (CH_2), 31.9 (CH_2), 29.6 (CH_2), 29.5 (CH_2), 29.4 (CH_2), 29.3 (CH_2), 29.3 (CH_2), 29.1 (CH_2), 26.4 (CH_2), 25.1 (CH_2), 22.6 (CH_3), 14.1 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.23 (d, J = 4.9 Hz); HRMS (ESI): *m/z* calcd for chemical formula: $C_{23}H_{33}F_3N_2NaO_2$ $[M + Na]^+$ 449.2386; found 449.2387.



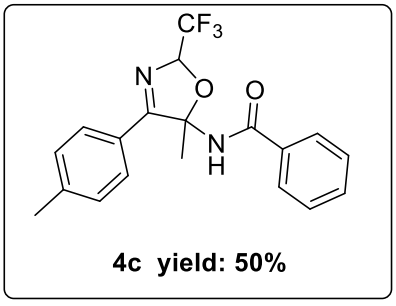
4a yield: 43%

N-(5-Methyl-4-(o-tolyl)-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl) benzamide (**4a**). Purified by column chromatography (EA/PE, 1:5). White solid (78 mg, 43%), m.p.: 274–276 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, J = 8.4 Hz, 2H), 7.55 (t, J = 7.6 Hz, 1H), 7.45 (t, J = 7.6 Hz, 2H), 7.38 (d, J = 8.0 Hz, 1H), 7.31–7.30 (m, 2H), 7.13 (t, J = 5.6 Hz, 1H), 6.93 (s, 1H), 6.35 (q, J = 5.2 Hz, 1H), 2.47 (s, 3H), 1.66 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.9 (Cq), 167.4 (Cq), 138.8 (Cq), 133.3 (Cq), 132.4 (Cq), 131.5 (CH), 130.2 (CH), 129.5 (CH), 128.8 (CH), 127.1 (CH), 127.1 (CH), 125.6 (CH), 122.4 (q, $J_{C\text{-}F}$ = 279.0 Hz (Cq)), 99.7 (q, $J_{C\text{-}F}$ = 32.9 Hz) (CH), 97.5 (Cq), 25.4 (CH_3), 20.8 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -79.83 (d, J = 5.3 Hz); HRMS (ESI): *m/z* calcd for chemical formula: $C_{19}H_{18}F_3N_2O_2$ $[M + H]^+$ 363.1315; found 363.1312.



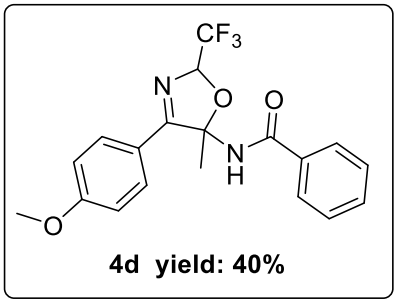
4b yield: 50%

N-(5-Methyl-4-(m-tolyl)-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl) benzamide (**4b**). Purified by column chromatography (EA/PE, 1:5). White solid (91 mg, 50%), m.p.: 200–202 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (s, 1H), 7.74–7.72 (m, 3H), 7.52 (t, J = 7.6 Hz, 1H), 7.41 (t, J = 8.0 Hz, 2H), 7.30 – 7.24 (m, 2H), 7.11 (s, 1H), 6.27 (q, J = 5.2 Hz, 1H), 2.35 (s, 3H), 1.84 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.8 (Cq), 167.2 (Cq), 138.7 (Cq), 133.2 (Cq), 132.8 (Cq), 132.3 (CH), 129.2 (CH), 129.0 (CH), 128.8 (CH), 128.5 (CH), 127.1 (CH), 124.9 (CH), 122.4 (q, $J_{C\text{-}F}$ = 280.1 Hz) (Cq), 99.1 (q, $J_{C\text{-}F}$ = 32.6 Hz) (CH), 96.1 (Cq), 26.6 (CH_3), 21.3 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -82.71 (d, J = 4.9 Hz); HRMS (ESI): *m/z* calcd for chemical formula: $C_{19}H_{18}F_3N_2O_2$ $[M + H]^+$ 363.1315; found 363.1313.



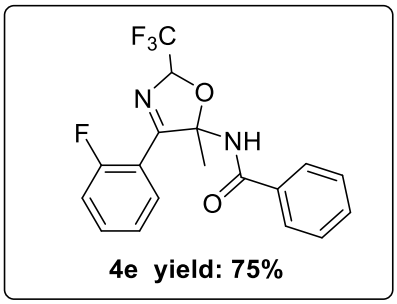
4c yield: 50%

N-(5-Methyl-4-(p-tolyl)-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl) benzamide (**4c**). Purified by column chromatography (EA/PE, 1:5). White solid (101 mg, 56%), m.p.: 201–203 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, J = 8.0 Hz, 2H), 7.73 (d, J = 7.2 Hz, 2H), 7.53 (t, J = 7.6 Hz, 1H), 7.42 (t, J = 8.0 Hz, 2H), 7.20 (d, J = 8.0 Hz, 2H), 7.03 (s, 1H), 6.26 (q, J = 5.2 Hz, 1H), 2.36 (s, 3H), 1.86 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.4 (Cq), 167.0 (Cq), 142.5 (Cq), 133.2 (Cq), 132.3 (Cq), 129.5 (CH), 128.8 (CH), 128.1 (CH), 127.1 (CH), 126.5 (CH), 123.4 (q, $J_{C\text{-}F}$ = 279.0 Hz) (Cq), 99.2 (q, $J_{C\text{-}F}$ = 33.0 Hz) (CH), 96.0 (Cq), 26.7 (CH_3), 21.5 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.20 (d, J = 4.9 Hz); HRMS(ESI): *m/z* calcd for chemical formula: $C_{19}H_{17}F_3N_2NaO_2$ $[M + Na]^+$ 385.1134; found 385.1134.



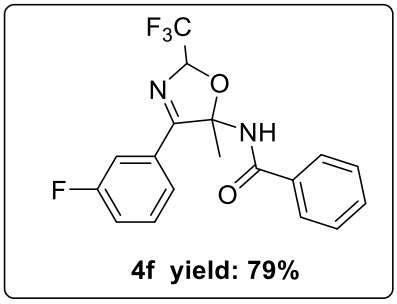
4d yield: 40%

N-(4-(4-Methoxyphenyl)-5-methyl-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl) benzamide (**4d**). Purified by column chromatography (EA/PE, 1:5). White solid (76 mg, 40%), m.p.: 207–209 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, J = 9.2 Hz, 2H), 7.73 (d, J = 7.2 Hz, 2H), 7.52 (t, J = 7.6 Hz, 1H), 7.41 (t, J = 7.6 Hz, 2H), 7.14 (s, 1H), 6.89 (d, J = 9.2 Hz, 2H), 6.23 (q, J = 5.2 Hz, 1H), 3.81 (s, 3H), 1.85 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 169.8 (Cq), 167.0 (Cq), 162.5 (Cq), 133.2 (Cq), 132.3 (Cq), 130.0 (CH), 128.7 (CH), 127.1 (CH), 122.4 (q, $J_{C\text{-}F}$ = 280.5 Hz) (Cq), 121.8 (CH), 114.1 (CH), 99.1 (q, $J_{C\text{-}F}$ = 32.9 Hz) (CH), 95.9 (Cq), 55.4 (CH_3), 26.8 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -79.85 (d, J = 5.3 Hz); HRMS(ESI): *m/z* calcd for chemical formula: $C_{19}H_{18}F_3N_2O_3$ $[M + H]^+$ 379.1264; found 379.1266.



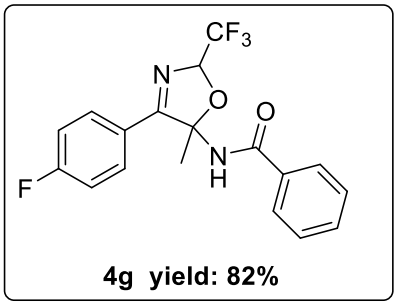
4e yield: 75%

N-(4-(2-Fluorophenyl)-5-methyl-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl) benzamide (**4e**). Purified by column chromatography (EA/PE, 1:5). White solid (248 mg, 75%), m.p.: 168–170 °C;^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (td, J = 7.6, 1.4 Hz, 1H), 7.73 (d, J = 6.8 Hz, 2H), 7.54 – 7.41 (m, 4H), 7.20 (t, J = 8.0, 1H), 7.10 (dd, J = 11.6, 8.4 Hz, 1H), 6.97 (s, 1H), 6.35 (q, J = 4.8 Hz, 1H), 1.81 (d, J = 1.6 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 168.5 (Cq), 167.1 (Cq), 160.5 (d, $J_{C\text{-}F}$ = 252.2 Hz) (Cq), 133.4 (Cq), 133.4 (d, $J_{C\text{-}F}$ = 9.0 Hz) (CH), 132.2 (CH), 131.7 (d, $J_{C\text{-}F}$ = 3.0 Hz) (CH), 128.7 (CH), 127.0 (CH), 124.7 (d, $J_{C\text{-}F}$ = 3.0 Hz) (Cq), 122.2 (q, $J_{C\text{-}F}$ = 280.5 Hz) (Cq), 116.6 (d, $J_{C\text{-}F}$ = 23.0 Hz) (CH), 99.5 (q, $J_{C\text{-}F}$ = 33.0 Hz) (CH), 96.9 (Cq), 25.2 (d, $J_{C\text{-}F}$ = 6.0 Hz) (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -79.73 (d, J = 5.3 Hz), -107.51 – -107.57 (m); HRMS(ESI): *m/z* calcd for chemical formula: $C_{18}H_{14}F_4N_2NaO_2$ $[M + Na]^+$ 389.0884; found 389.0884.



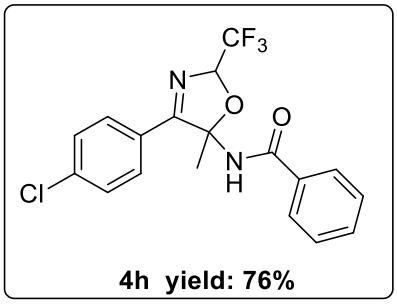
4f yield: 79%

N-(4-(3-Fluorophenyl)-5-methyl-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl) benzamide (**4f**). Purified by column chromatography (EA/PE, 1:5). White solid (145 mg, 79%), m.p.: 176–178 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 – 7.73 (m, 4H), 7.56 (t, J = 7.2 Hz, 1H), 7.46 (t, J = 7.6 Hz, 2H), 7.41 – 7.36 (m, 1H), 7.19 (td, J = 8.4, 2.4 Hz, 1H), 6.97 (s, 1H), 6.28 (q, J = 4.8 Hz, 1H), 1.87 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 169.7 (Cq), 167.3 (Cq), 162.7 (d, $J_{C\text{-}F}$ = 246.0 Hz) (Cq), 132.9 (Cq), 132.5 (Cq), 131.4 (d, $J_{C\text{-}F}$ = 7.5 Hz) (CH), 130.5 (d, $J_{C\text{-}F}$ = 7.5 Hz) (CH), 128.8 (CH), 127.1 (CH), 123.8 (CH), 122.5 (q, $J_{C\text{-}F}$ = 381.0 Hz) (Cq), 119.0 (d, $J_{C\text{-}F}$ = 21.0 Hz) (CH), 115.2 (d, $J_{C\text{-}F}$ = 22.5 Hz) (CH), 99.2 (q, $J_{C\text{-}F}$ = 31.5.0 Hz) (CH), 94.5 (Cq), 26.5 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.10 (d, J = 4.9 Hz), -111.92 – -111.98 (m); HRMS(ESI): *m/z* calcd for chemical formula: $C_{18}H_{14}F_4N_2NaO_2$ $[M + H]^+$ 389.0884; found 389.0884.



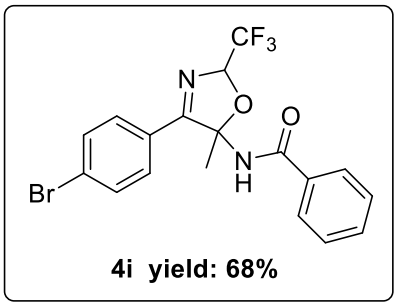
4g yield: 82%

N-(4-(4-Fluorophenyl)-5-methyl-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl) benzamide (**4g**). Purified by column chromatography (EA/PE, 1:5). White solid (150 mg, 82%), m.p.: 296–198 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 –8.01 (m, 2H), 7.72 (d, J = 6.8 Hz, 2H), 7.53 (t, J = 7.6 Hz, 1H), 7.41 (t, J = 8.0 Hz, 2H), 7.19 (s, 1H), 7.07 (t, J = 8.8 Hz, 2H), 6.23 (q, J = 4.8 Hz, 1H), 1.82 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 169.6 (Cq), 167.3 (Cq), 164.9 (d, $J_{C\text{-}F}$ = 253.5 Hz) (Cq), 133.0 (Cq), 132.5 (Cq), 130.5 (d, $J_{C\text{-}F}$ = 9.0 Hz) (CH), 128.8 (CH), 127.1 (CH), 125.6 (d, $J_{C\text{-}F}$ = 3.0 Hz) (CH), 122.3 (q, $J_{C\text{-}F}$ = 280.5 Hz) (Cq), 116.0 (d, $J_{C\text{-}F}$ = 21.0 Hz) (CH), 98.6 (q, $J_{C\text{-}F}$ = 31.5 Hz) (CH), 96.0 (Cq), 27.3 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -79.76 (d, J = 4.9 Hz), -106.66 –106.74 (m); HRMS (ESI): *m/z* calcd for chemical formula: $C_{18}H_{15}F_4N_2O_2$ $[M + H]^+$ 367.1064; found 367.1065.



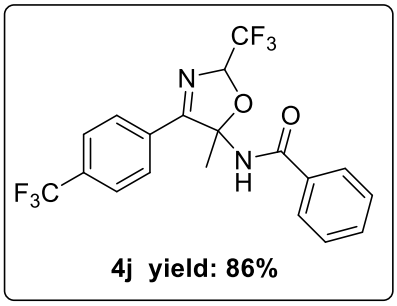
4h yield: 76%

N-(4-(4-Chlorophenyl)-5-methyl-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl) benzamide (**4h**). Purified by column chromatography (EA/PE, 1:5). White solid (145 mg, 76%), m.p.: 192–194 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 – 8.01 (m, 1H), 7.87 (dd, J = 8.0 Hz, 1.2 Hz, 1H), 7.79 –7.71 (m, 2H), 7.54 (t, J = 8.0 Hz, 1H), 7.47 – 7.42 (m, 3H), 7.34 (t, J = 8.0 Hz, 1H), 7.07 (s, 1H), 6.27 (q, J = 4.8 Hz, 1H), 1.85 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 169.6 (Cq), 167.3 (Cq), 134.9 (Cq), 132.5 (Cq), 132.0 (Cq), 130.1 (CH), 128.8 (CH), 128.3 (CH), 127.1 (CH), 126.0 (CH), 122.2 (q, $J_{C\text{-}F}$ = 280.5 Hz) (Cq), 99.2 (q, $J_{C\text{-}F}$ = 33.0 Hz) (CH), 94.6 (Cq), 26.5 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.05 (d, J = 5.3 Hz); HRMS (ESI): *m/z* calcd for chemical formula: $C_{18}H_{13}ClF_3N_2O_2$ $[M - H]^+$ 381.0623; found 381.0624.



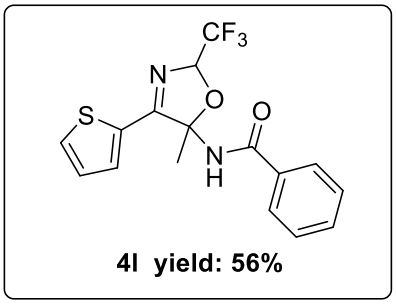
4i yield: 68%

N-(4-(4-Bromophenyl)-5-methyl-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl) benzamide (**4i**). Purified by column chromatography (EA/PE, 1:5). White solid (145 mg, 68%), m.p.: 215–217 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, J = 8.8 Hz, 2H), 7.74 (d, J = 7.2 Hz, 2H), 7.56–7.53 (m, 3H), 7.45 (t, J = 8.0 Hz, 2H), 6.97 (s, 1H), 6.25 (q, J = 5.2 Hz, 1H), 1.86 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 169.8 (Cq), 167.1 (Cq), 132.9 (Cq), 132.5 (Cq), 132.1 (CH), 129.6 (CH), 128.8 (CH), 128.2 (CH), 127.1 (CH), 126.8 (Cq), 122.2 (q, $J_{C\text{-}F}$ = 280.5 Hz) (Cq), 99.2 (q, $J_{C\text{-}F}$ = 33.0 Hz) (CH), 95.9 (Cq), 26.6 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -79.72 (d, J = 4.9 Hz); HRMS (ESI): *m/z* calcd for chemical formula: $C_{18}H_{15}BrF_3N_2O_2$ $[M + H]^+$ 427.0264; found 427.0264.



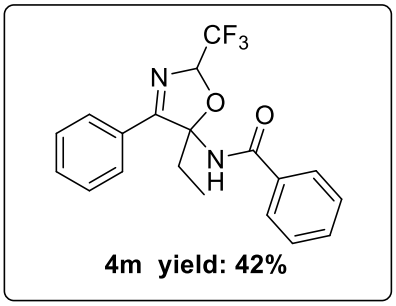
4j yield: 86%

N-(5-Methyl-2-(trifluoromethyl)-4-(4-(trifluoromethyl) phenyl)-2,5-dihydrooxazol-5-yl) benzamide (**4j**). Purified by column chromatography (EA/PE, 1:5). White solid (179 mg, 86%), m.p.: 178–180 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, J = 8.0 Hz, 2H), 7.75 (d, J = 8.0 Hz, 2H), 7.67 (d, J = 8.4 Hz, 2H), 7.56 (t, J = 7.2 Hz, 1H), 7.46 (d, J = 8.0 Hz, 2H), 7.03 (s, 1H), 6.30 (q, J = 5.2 Hz, 1H), 1.87 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 169.7 (Cq), 167.3 (Cq), 133.5 (q, $J_{C\text{-}F}$ = 33.0 Hz) (Cq), 132.8 (Cq), 132.7 (Cq), 128.9 (CH), 128.5 (CH), 127.1 (CH), 126.3 (CH), 125.8 (q, $J_{C\text{-}F}$ = 3.0 Hz) (CH), 123.6 (q, $J_{C\text{-}F}$ = 270.0 Hz) (CH), 122.1 (q, $J_{C\text{-}F}$ = 280.5 Hz) (Cq), 99.3 (q, $J_{C\text{-}F}$ = 33.0 Hz) (CH), 96.0 (Cq), 26.5 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.62 (s), -80.03 (d, J = 4.9 Hz); HRMS (ESI): *m/z* calcd for chemical formula: $C_{19}H_{15}F_6N_2O_2$ $[M + H]^+$ 417.1032; found 407.1033.



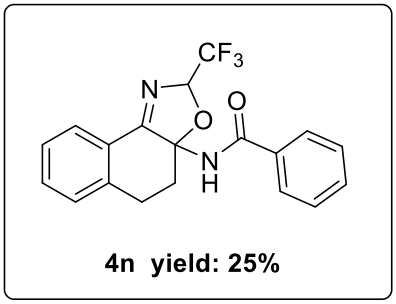
4l yield: 56%

N-(5-Methyl-4-(thiophen-2-yl)-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl) benzamide (**4l**). Purified by column chromatography (EA/PE, 1:5). White solid (99 mg, 56%), m.p.: 186–188 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 – 7.69 (m, 3H), 7.55–7.52 (m, 2H), 7.43 (t, J = 8.0 Hz, 2H), 7.07 (dd, J = 4.8, 3.6 Hz, 1H), 6.98 (s, 1H), 6.25 (q, J = 4.8 Hz, 1H), 1.93 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 166.9 (Cq), 165.7 (Cq), 133.1 (Cq), 132.4 (Cq), 132.4 (CH), 131.3 (CH), 130.5 (CH), 128.8 (CH), 127.9 (CH), 127.1 (Cq), 122.2 (q, $J_{C\text{-}F}$ = 280.5 Hz) (Cq), 99.5 (q, $J_{C\text{-}F}$ = 33.0 Hz) (CH), 96.0 (Cq), 26.9 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -79.67 (d, J = 5.3 Hz); HRMS (ESI): *m/z* calcd for chemical formula: $C_{16}H_{12}F_3N_2O_2S$ $[M – H]^+$ 353.0577; found 353.0577.



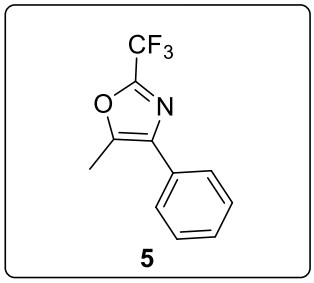
4m yield: 42%

N-(5-Ethyl-4-phenyl-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl) benzamide (**4m**). Purified by column chromatography (EA/PE, 1:5). White solid (76 mg, 42%), m.p.: 160–162 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, J = 7.2 Hz, 2H), 7.73 (d, J = 7.2 Hz, 2H), 7.54 – 7.37 (m, 6H), 7.06 (s, 1H), 6.35 (q, J = 5.2 Hz, 1H), 2.25 – 2.04 (m, 2H), 0.98 (t, J = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 169.7 (Cq), 167.3 (Cq), 133.5 (Cq), 132.5 (Cq), 132.0 (CH), 130.0 (CH), 128.9 (CH), 128.9 (CH), 128.1 (CH), 127.2 (CH), 112.5 (q, $J_{C\text{-}F}$ = 279.8 Hz) (Cq), 99.6 (q, $J_{C\text{-}F}$ = 32.9 Hz) (CH), 98.6 (Cq), 31.8 (CH_2), 7.1 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -79.05 (d, J = 5.3 Hz); HRMS (ESI): *m/z* calcd for chemical formula: $C_{19}H_{18}F_3N_2O_2$ $[M + H]^+$ 363.1315; found 363.1314.



4n yield: 25%

N-(2-(Trifluoromethyl)-4,5-dihydronaphtho[1,2-d] oxazol-3a(2H) yl) benzamide (**4n**). Purified by column chromatography (EA/PE, 1:8). Brown solid (45 mg, 25%), m.p.: 180–182 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, J = 7.6 Hz, 1H), 7.61 (d, J = 7.6 Hz, 2H), 7.48–7.42 (m, 2H), 7.35–7.29 (m, 3H), 7.23 (d, J = 7.6 Hz, 1H), 6.93 (s, 1H), 6.37 (q, J = 5.2 Hz, 1H), 3.27 – 3.10 (m, 2H), 2.71 (dd, J = 14.0, 4.4 Hz, 1H), 2.26 (td, J = 13.2, 6.4 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.0 (Cq), 167.5 (Cq), 138.6 (Cq), 133.2 (Cq), 132.3 (Cq), 132.2 (CH), 128.6 (CH), 128.6 (CH), 127.8 (CH), 127.3 (CH), 127.1 (CH), 127.0 (CH), 122.4 (q, $J_{C\text{-}F}$ = 279.0 Hz) (Cq), 101.2 (q, $J_{C\text{-}F}$ = 33.0 Hz) (CH), 93.7 (Cq), 35.1 (CH_2), 27.3 (CH_2); ^{19}F NMR (376 MHz, $CDCl_3$) δ -79.83 (d, J = 4.9 Hz); HRMS (ESI):*m/z* calcd for chemical formula: $C_{19}H_{16}F_3N_2O_2$ $[M + H]^+$ 361.1158; found 361.1157.



5

5-Methyl-4-phenyl-2-(trifluoromethyl) oxazole (**5**). Purified by column chromatography (EA/PE, 1:5). Colorless liquid (28 mg, 25%) ;^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 – 7.65 (m, 2H), 7.45 (t, J = 7.6 Hz, 2H), 7.38 – 7.34 (m, 1H), 2.61 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 148.5 (q, $J_{C\text{-}F}$ = 43.7 Hz), 136.0 (Cq), 130.1 (Cq), 128.8 (Cq), 128.1 (CH), 126.9 (CH), 126.8 (Cq), 116.6 (q, $J_{C\text{-}F}$ = 268.8 Hz) (Cq), 11.9 (CH_3); ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.43; HRMS(ESI): *m/z* calcd for chemical formula: $C_{11}H_9F_3NO$ $[M + H]^+$ 228.0629; found 228.0630.

3. References and notes

1. (a) Sai, M., *t*-KOBu/DMSO Catalytic System for Isomerization of Allylic Alcohols to Ketones. *Eur. J. Org. Chem.* **2022,** *2022* (10), e202200052. (b) Nie, X.-k.; Chen, Y.; Zhang, S.-q.; Cui, X.; Tang, Z.; Li, G.-x., Chiral Primary Amine Catalyzed Enantioselective Tandem Reactions Based on Heyns Rearrangement: Synthesis of α-Tertiary Amino Ketones. *Org. Lett.* **2022,** *24* (10), 2069-2074. (c) Liang, Y.-F.; Wu, K.; Song, S.; Li, X.; Huang, X.; Jiao, N., I_2- or NBS-Catalyzed Highly Efficient *α*-Hydroxylation of Ketones with Dimethyl Sulfoxide. *Org. Lett.* **2015,** *17*, 876-879. (d) Matsuo, K.; Shindo, M., Cu (II)-Catalyzed Acylation by Thiol Esters Under Neutral Conditions: Tandem Acylation-Wittig Reaction Leading to a One-Pot Synthesis of Butenolides. *Org. Lett.* **2010,** *12*, 5346-5349.
2. (a) Du, G.; Huang, D.; Wang, K.-H.; Chen, X.; Xu, Y.; Ma, J.; Su, Y.; Fu, Y.; Hu, Y., One-pot preparation of trifluoromethylated homoallylic *N*-acylhydrazines or α-methylene-γ-lactams from acylhydrazines, trifluoroacetaldehyde methyl hemiacetal, allyl bromide and tin. *Org. Biomol. Chem.* **2016,** *14*, 1492-1500. (b) Mlostoń, G.; Urbaniak, K.; Jacaszek, N.; Linden, A.; Heimgartner, H. J. H., Exploration of fluoral hydrazones derived from carbohydrazides for the synthesis of trifluoromethylated. *Heterocycles* **2014,** *88*, 387-401.

4. Single Crystal X-Ray Structure Determinations of Compounds 3a

Thermal ellipsoids are set at a 50% probability level. Crystal data have been deposited to CCDC, number 2156398.

Experimental

Single crystals of $C_{18}H_{15}F_3N_2O_2$ Compounds **3a** were selected and placed. A suitable crystal was selected and placed on a ROD, Synergy Custom system, HyPix diffractometer. The crystal was kept at 300.51(10) K during data collection. Using Olex2 [1], the structure was solved with the olex2.solve [2] structure solution program using Charge Flipping and refined with the olex2.refine [3] refinement package using Gauss-Newton minimisation.

Crystal structure determination of Compounds 3a.

Crystal Data for $C_{18}H_{15}F_3N_2O_2$ (M =348.32 g/mol): monoclinic, space group Cc (no. 9), a = 14.6254(2) Å, b = 14.0014(2) Å, c = 33.2503(4) Å, β = 97.3100(10) °, V = 6753.52(16) Å^3, Z = 4, T = 300.51(10) K, μ (Cu Kα) = 0.966 mm^{-1}, *Dcalc* = 1.370 g/cm^3, 57519 reflections measured (5.36° ≤ 2Θ ≤ 154.934°), 12797 unique (R_{int} = 0.0514, R_{sigma} = 0.0289) which were used in all calculations. The final R_1 was 0.0437 (I > 2σ(I)) and wR_2 was 0.1213 (all data).

Refinement model description

Number of restraints - 2, number of constraints - unknown.

Details:

1.a Ternary CH refined with riding coordinates:

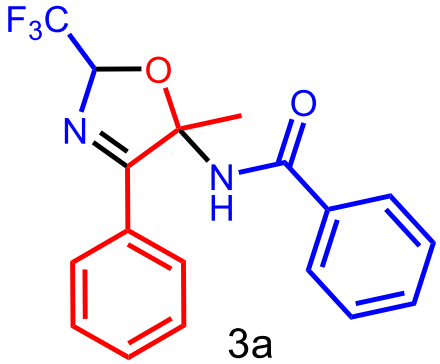
C3(H3)

1. b Aromatic/amide H refined with riding coordinates:

N4(H4), C6(H6), C7(H7), C8(H8), C9(H9), C10(H10), C12(H12), C13(H13), C14(H14), C15(H15), C16(H16)

1.c Idealised Me refined as rotating group:

C18(H18A, H18B, H18C)



3a

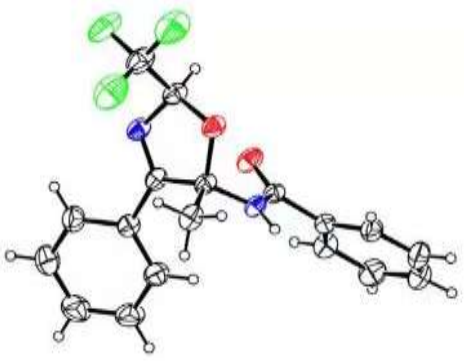


Table S2 Crystallographic Data of Compound 3a

CCDC	2156398
Empirical formula	$C_{18}H_{15}F_3N_2O_2$
Formula weight	348.32
Temperature/K	300.51(10)
Crystal system	monoclinic
Space group	Cc
a/Å	14.6254(2)
b/Å	14.0014(2)
c/Å	33.2503(2)
α/°	90
β/°	97.3100(10)
γ/°	90
Volume/Å^3	6753.52(16)
Z	4
ρ_{calc}g/cm^3	1.370
μ/mm^{-1}	0.966
F (000)	2880.0
Crystal size/mm^3	0.14 × 0.12 × 0.11
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.362 to 154.934
Index ranges	-18 ≤ h ≤ 18, -17 ≤ k ≤ 17, -39 ≤ l ≤ 41
Reflections collected	57519
Independent reflections	12797 [R_{int} = 0.0514, R_{sigma} = 0.0289]
Data/restraints/parameters	12797/2/906

Goodness-of-fit on F^2	1.031
Final R indexes [I>=2σ (I)]	R_1 = 0.0437, wR_2= 0.1181
Final R indexes [all data]	R_1 = 0.0467, wR_2 = 0.1213
Largest diff. peak/hole / e $Å^{-3}$	0.19/-0.17

Table S3 Fractional Atomic Coordinates (× 10^4) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Compound 3a. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
F^1	-2471(2)	-1880(2)	-6633.8(12)	104.7(10)
F^2	-1489.6(17)	-2995(2)	-6472.0(11)	98.4(10)
F^3	-1723(2)	-1926(3)	-6040.5(12)	114.3(13)
O^1	-3536.5(15)	-2505.7(17)	-6033.7(8)	52.5(5)
O^2	-4375.1(17)	-4504.4(17)	-5850.7(8)	57.7(6)
N^3	-3319.6(17)	-3644.9(18)	-6522.0(9)	49.2(6)
N^4	-5035.5(17)	-3057.4(18)	-5970.5(8)	44.0(5)
C^1	-4431(2)	-2724(2)	-6247.8(9)	43.6(6)
C^2	-4182(2)	-3484(2)	-6550.1(9)	44.2(6)
C^3	-2877(2)	-3086(2)	-6189.4(11)	51.0(7)
C^4	-4972.9(19)	-3926(2)	-5793.1(9)	41.6(6)
C^5	-5709(2)	-4171(2)	-5534.7(9)	44.1(6)
C^6	-5972(3)	-3530(3)	-5251.2(11)	56.1(8)
C^7	-6612(3)	-3806(4)	-5002.6(13)	74.3(12)
C^8	-7010(3)	-4685(4)	-5043.2(13)	74.2(12)
C^9	-6786(3)	-5305(3)	-5336.7(14)	70.5(10)
C^{10}	-6123(3)	-5055(2)	-5577.5(12)	56.1(8)
C^{11}	-4837(2)	-3961(2)	-6858.0(10)	46.4(6)
C^{12}	-4510(3)	-4330(3)	-7202.2(11)	62.0(9)

Atom	*x*	*y*	*z*	U(eq)
C^{13}	-5086(4)	-4836(4)	-7485.6(14)	82.2(13)
C^{14}	-6000(4)	-4985(4)	-7427.5(15)	83.4(13)
C^{15}	-6323(3)	-4618(3)	-7093.0(14)	73.7(11)
C^{16}	-5753(2)	-4107(3)	-6807.5(12)	60.7(8)
C^{17}	-2144(3)	-2469(3)	-6337.5(15)	69.9(10)
C^{18}	-4843(3)	-1830(2)	-6456.1(11)	55.8(8)

Table S4 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Compound 3a. The Anis -otropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\cdots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F^1	101(2)	82.3(18)	138(3)	17.5(18)	44(2)	-14.5(16)
F^2	53.7(13)	106(2)	143(3)	-32.7(18)	41.9(15)	-8.8(13)
F^3	82.4(18)	118(2)	147(3)	-60(2)	32.7(19)	-52.4(18)
O^1	41.8(11)	53.3(12)	63.3(14)	-17.9(10)	10.0(10)	-2.6(10)
O^2	50.1(12)	48.3(12)	77.7(15)	4.4(10)	20.4(11)	15.7(10)
N^3	40.9(13)	43.8(13)	64.6(16)	-9.7(11)	13.1(11)	0.8(10)
N^4	40.6(12)	40.5(12)	53.1(13)	-1.9(10)	14.2(10)	7.7(10)
C^1	38.5(14)	39.4(14)	54.1(16)	-6.5(12)	10.7(12)	0.4(11)
C^2	44.7(15)	36.9(14)	52.9(16)	-1.6(11)	13.3(12)	1.4(11)
C^3	39.5(15)	46.6(16)	68(2)	-9.6(14)	10.6(14)	1.1(13)
C^4	37.3(13)	39.2(14)	48.4(15)	-3.5(11)	6.3(11)	2.6(11)
C^5	38.8(14)	49.4(16)	44.1(15)	-0.6(12)	5.6(12)	5.4(12)
C^6	51.3(17)	65(2)	53.6(18)	-13.2(15)	11.4(14)	-4.7(16)
C^7	64(2)	102(3)	61(2)	-18(2)	22.6(18)	-5(2)
C^8	60(2)	102(3)	65(2)	8(2)	22.9(19)	-10(2)
C^9	66(2)	66(2)	81(3)	6(2)	17(2)	-14.6(19)
C^{10}	57.6(19)	48.1(17)	65(2)	-2.1(14)	14.9(16)	-2.3(15)
C^{11}	47.5(15)	39.3(15)	52.9(16)	-2.9(11)	7.8(13)	2.8(12)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C^{12}	64(2)	68(2)	55.3(19)	-9.8(16)	14.3(16)	-2.6(17)
C^{13}	89(3)	95(3)	63(2)	-31(2)	11(2)	-2(2)
C^{14}	78(3)	89(3)	78(3)	-29(2)	-9(2)	-9(2)
C^{15}	51(2)	81(3)	86(3)	-21(2)	-1.1(19)	-6.1(19)
C^{16}	50.2(17)	65(2)	67(2)	-18.6(16)	6.6(15)	-1.4(16)
C^{17}	54(2)	64(2)	95(3)	-17(2)	22(2)	-11.3(18)
C^{18}	62(2)	41.7(16)	67(2)	2.0(14)	19.1(16)	5.3(14)

Table S5 Bond Lengths for Compound 3a.

Atom	Atom	Length/Å
F^1	C^{17}	1.326(6)
F^2	C^{17}	1.329(5)
F^3	C^{17}	1.334(5)
O^1	C^1	1.440(4)
O^1	C^3	1.409(4)
O^2	C^4	1.224(4)
N^3	C^2	1.273(4)
N^3	C^3	1.440(4)
N^4	C^1	1.434(4)
N^4	C^4	1.350(4)
C^1	C^2	1.538(4)
C^1	C^{18}	1.517(4)
C^2	C^{11}	1.471(4)

Atom	Atom	Length/Å
C^3	C^{17}	1.507(5)
C^4	C^5	1.500(4)
C^5	C^6	1.391(5)
C^5	C^{10}	1.377(5)
C^6	C^7	1.381(6)
C^7	C^8	1.361(7)
C^8	C^9	1.376(7)
C^9	C^{10}	1.379(6)
C^{11}	C^{12}	1.394(5)
C^{11}	C^{16}	1.386(5)
C^{12}	C^{13}	1.377(6)
C^{13}	C^{14}	1.391(7)
C^{14}	C^{15}	1.363(7)

Table S6 Bond Angles for Compound 3a.

Atom	Atom	Atom	Angle/°
C^3	O^1	C^1	108.5(2)
C^2	N^3	C^3	107.7(2)

Atom	Atom	Atom	Angle/°
C^{10}	C^5	C^6	119.6(3)
C^7	C^6	C^5	119.4(4)

Atom	Atom	Atom	Angle/°
C^{4}	N^{4}	C^{1}	124.1(2)
O^{1}	C^{1}	C^{2}	101.2(2)
O^{1}	C^{1}	C^{18}	109.5(3)
N^{4}	C^{1}	O^{1}	110.3(3)
N^{4}	C^{1}	C^{2}	114.3(2)
N^{4}	C^{1}	C^{18}	108.7(2)
C^{18}	C^{1}	C^{2}	112.6(3)
N^{3}	C^{2}	C^{1}	112.9(3)
N^{3}	C^{2}	C^{11}	121.5(3)
C^{11}	C^{2}	C^{1}	125.6(3)
O^{1}	C^{3}	N^{3}	109.5(3)
O^{1}	C^{3}	C^{17}	109.8(3)
N^{3}	C^{3}	C^{17}	109.2(3)
O^{2}	C^{4}	N^{4}	122.5(3)
O^{2}	C^{4}	C^{5}	121.2(3)
N^{4}	C^{4}	C^{5}	116.3(2)
C^{6}	C^{5}	C^{4}	121.4(3)
C^{10}	C^{5}	C^{4}	119.0(3)

Atom	Atom	Atom	Angle/°
C^{8}	C^{7}	C^{6}	120.6(4)
C^{7}	C^{8}	C^{9}	120.2(4)
C^{8}	C^{9}	C^{10}	120.0(4)
C^{5}	C^{10}	C^{9}	120.0(4)
C^{12}	C^{11}	C^{2}	118.6(3)
C^{16}	C^{11}	C^{2}	122.4(3)
C^{16}	C^{11}	C^{12}	118.8(3)
C^{13}	C^{12}	C^{11}	120.6(4)
C^{12}	C^{13}	C^{14}	119.8(4)
C^{15}	C^{14}	C^{13}	119.8(4)
C^{14}	C^{15}	C^{16}	120.9(4)
C^{15}	C^{16}	C^{11}	120.1(4)
F^{1}	C^{17}	F^{2}	107.6(4)
F^{1}	C^{17}	F^{3}	106.5(4)
F^{1}	C^{17}	C^{3}	113.2(3)
F^{2}	C^{17}	F^{3}	106.3(4)
F^{2}	C^{17}	C^{3}	111.4(3)
F^{3}	C^{17}	C^{3}	111.4(4)

Table S7 Torsion Angles for Compound 3a.

A	B	C	D	Angle/°
O^{1}	C^{1}	C^{2}	N^{3}	-1.6(3)
O^{1}	C^{1}	C^{2}	C^{11}	-178.8(3)

A	B	C	D	Angle/°
C^{2}	C^{11}	C^{16}	C^{15}	-175.5(4)
C^{3}	O^{1}	C^{1}	N^{4}	120.1(3)

A	B	C	D	Angle/°
O^1	C^3	C^{17}	F^1	-61.1(4)
O^1	C^3	C^{17}	F^2	177.5(3)
O^1	C^3	C^{17}	F^3	58.9(5)
O^2	C^4	C^5	C^6	136.3(4)
O^2	C^4	C^5	C^{10}	-43.0(4)
N^3	C^2	C^{11}	C^{12}	-21.8(5)
N^3	C^2	C^{11}	C^{16}	154.3(3)
N^3	C^3	C^{17}	F^1	59.0(4)
N^3	C^3	C^{17}	F^2	-62.4(5)
N^3	C^3	C^{17}	F^3	179.0(3)
N^4	C^1	C^2	N^3	-120.1(3)
N^4	C^1	C^2	C^{11}	62.7(4)
N^4	C^4	C^5	C^6	-46.6(4)
N^4	C^4	C^5	C^{10}	134.1(3)
C^1	O^1	C^3	N^3	3.5(4)
C^1	O^1	C^3	C^{17}	123.4(3)
C^1	N^4	C^4	O^2	1.2(5)
C^1	N^4	C^4	C^5	-175.8(3)
C^1	C^2	C^{11}	C^{12}	155.1(3)
C^1	C^2	C^{11}	C^{16}	-28.7(5)
C^2	N^3	C^3	O^1	-4.6(4)
C^2	N^3	C^3	C^{17}	-124.9(3)
C^2	C^{11}	C^{12}	C^{13}	175.8(4)

A	B	C	D	Angle/°
C^3	O^1	C^1	C^2	-1.3(3)
C^3	O^1	C^1	C^{18}	-120.4(3)
C^3	N^3	C^2	C^1	3.7(4)
C^3	N^3	C^2	C^{11}	-179.0(3)
C^4	N^4	C^1	O^1	-73.1(3)
C^4	N^4	C^1	C^2	40.2(4)
C^4	N^4	C^1	C^{18}	166.9(3)
C^4	C^5	C^6	C^7	-176.1(4)
C^4	C^5	C^{10}	C^9	178.5(4)
C^5	C^6	C^7	C^8	-2.4(7)
C^6	C^5	C^{10}	C^9	-0.8(6)
C^6	C^7	C^8	C^9	-0.8(7)
C^7	C^8	C^9	C^{10}	3.2(7)
C^8	C^9	C^{10}	C^5	-2.4(7)
C^{10}	C^5	C^6	C^7	3.2(6)
C^{11}	C^{12}	C^{13}	C^{14}	-0.2(7)
C^{12}	C^{11}	C^{16}	C^{15}	0.7(6)
C^{12}	C^{13}	C^{14}	C^{15}	0.8(8)
C^{13}	C^{14}	C^{15}	C^{16}	-0.6(8)
C^{14}	C^{15}	C^{16}	C^{11}	-0.1(7)
C^{16}	C^{11}	C^{12}	C^{13}	-0.5(6)
C^{18}	C^1	C^2	N^3	115.2(3)
C^{18}	C^1	C^2	C^{11}	-62.0(4)

Table S8 Hydrogen Atom Coordinates (Å × 104) and Isotropic Displacement Parameters (Å2×103) for Compound 3a.

Atom	*x*	*y*	*z*	U(eq)
H^4	-5465.08	-2680	-5913.77	53

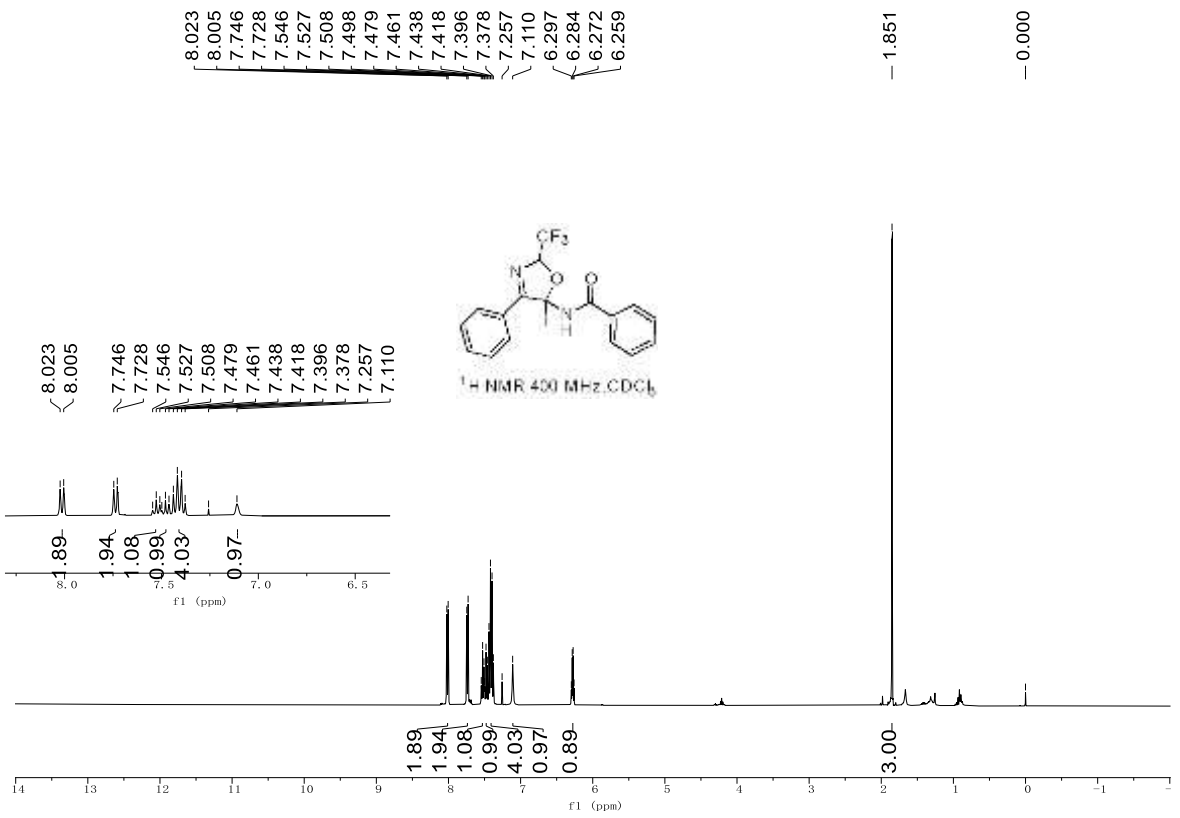
Atom	*x*	*y*	*z*	U(eq)
H^{3}	-2592.78	-3512.78	-5975.72	61
H^{6}	-5718.9	-2919.55	-5229.31	67
H^{7}	-6772.52	-3388.2	-4805.84	89
H^{8}	-7434.77	-4867.81	-4872.03	89
H^{9}	-7081.85	-5892.11	-5372.63	85
H^{10}	-5955.66	-5483.45	-5768.91	67
H^{12}	-3898.55	-4233.17	-7240.78	74
H^{13}	-4863.46	-5078.19	-7714.95	99
H^{14}	-6389.76	-5332.96	-7616.27	100
H^{15}	-6936.69	-4713.48	-7056.43	88
H^{16}	-5983.42	-3860.43	-6581.01	73
H^{18A}	-5430.16	-1980.39	-6605.74	84
H^{18B}	-4436.88	-1592.13	-6638.27	84
H^{18C}	-4921.01	-1353.1	-6256.04	84

5. Copies of NMR Spectra

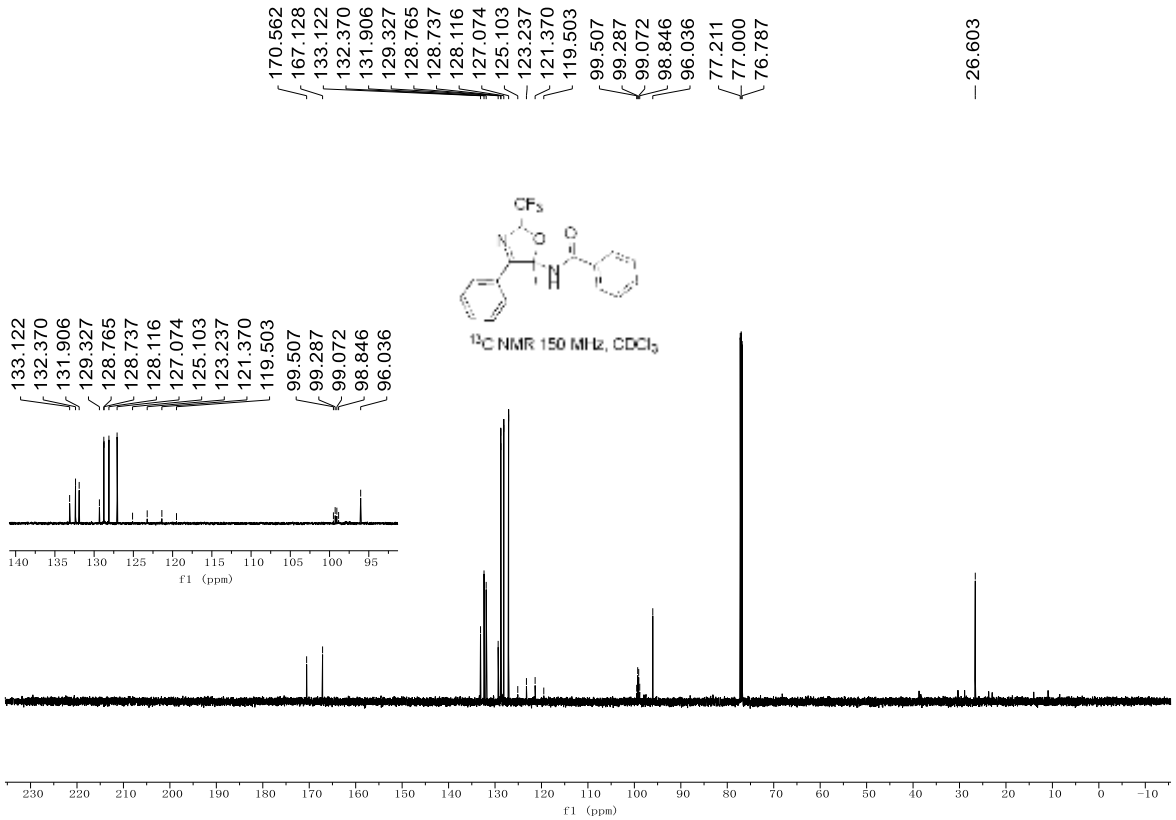
^{1}H NMR, ^{13}C NMR, ^{19}F NMR, HRMS spectra for compounds **3**, **4** and **5**

NMR copies of compound **3a**

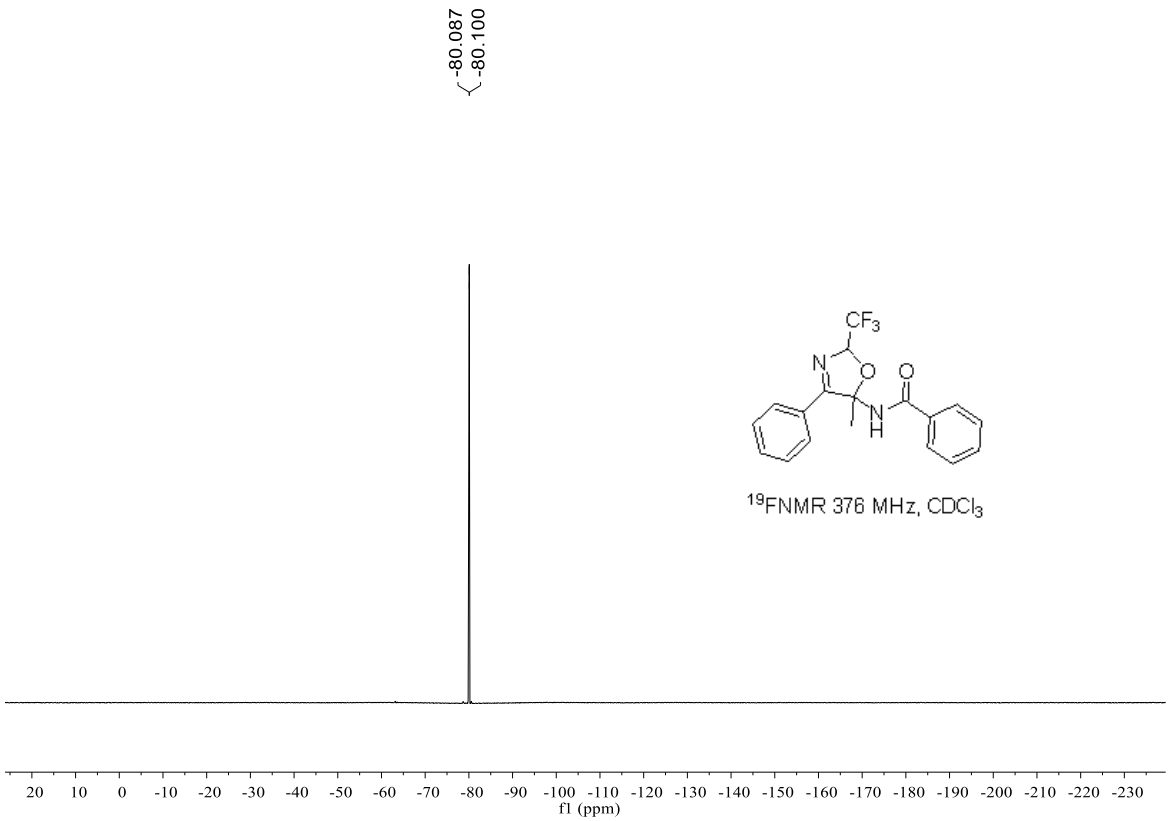
^{1}H NMR (400 MHz) spectrum of **3a** in $CDCl_3$



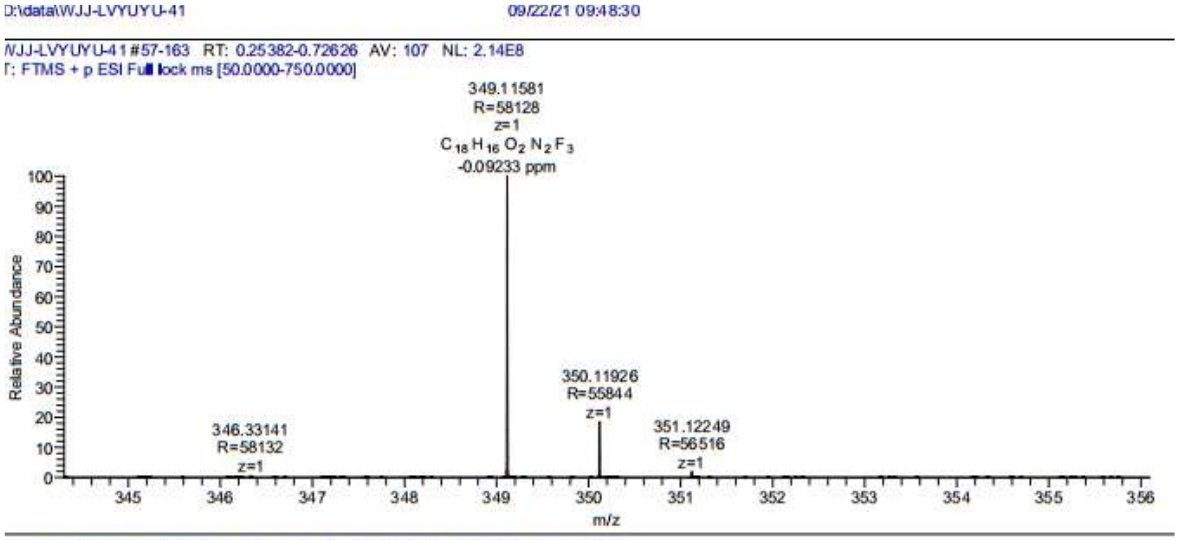
^{13}C NMR (150 MHz) spectrum of **3a** in $CDCl_3$



^{19}F NMR (376 MHz) spectrum of **3a** in $CDCl_3$



HRMS(ESI) copy of compound **3a**:

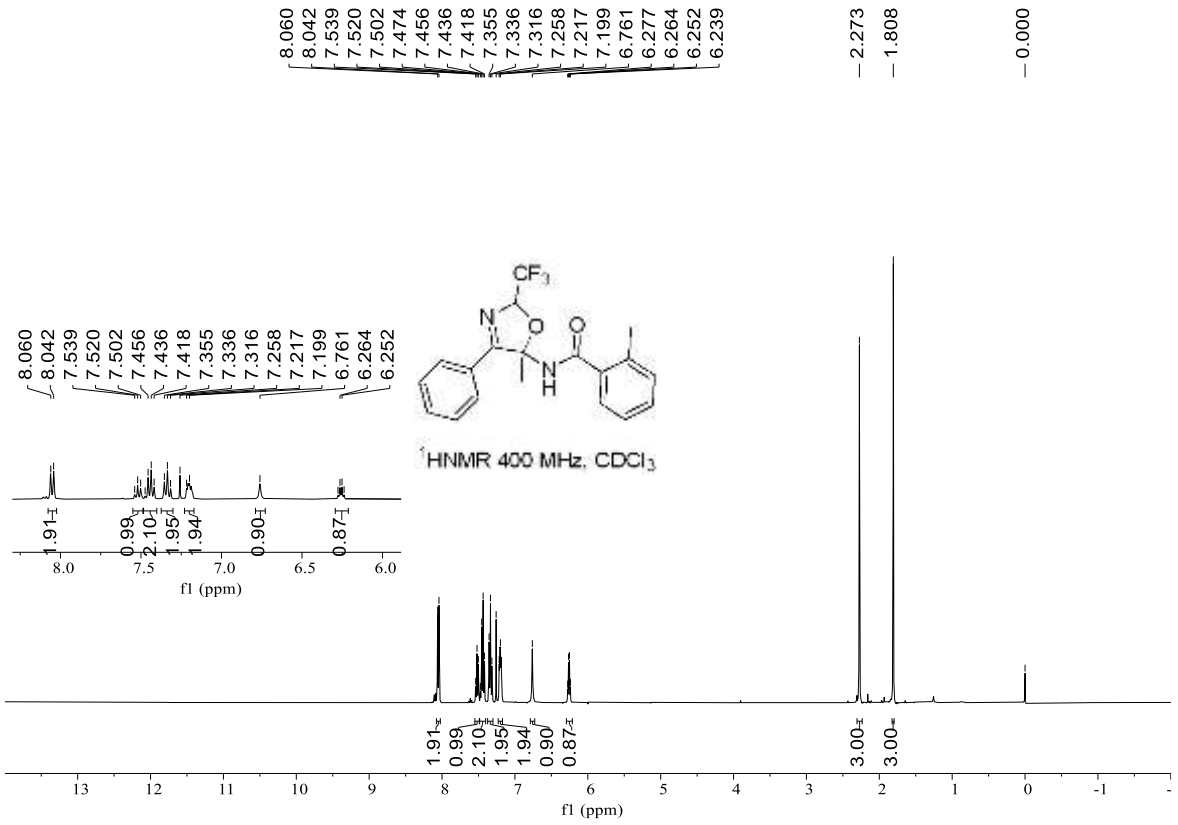


NJJ-LVYUYU-41#57-163 RT: 0.25382-0.72626 AV: 107
T: FTMS + p ESI Full lock ms [50.0000-750.0000]
m/z= 344.30123-356.09748

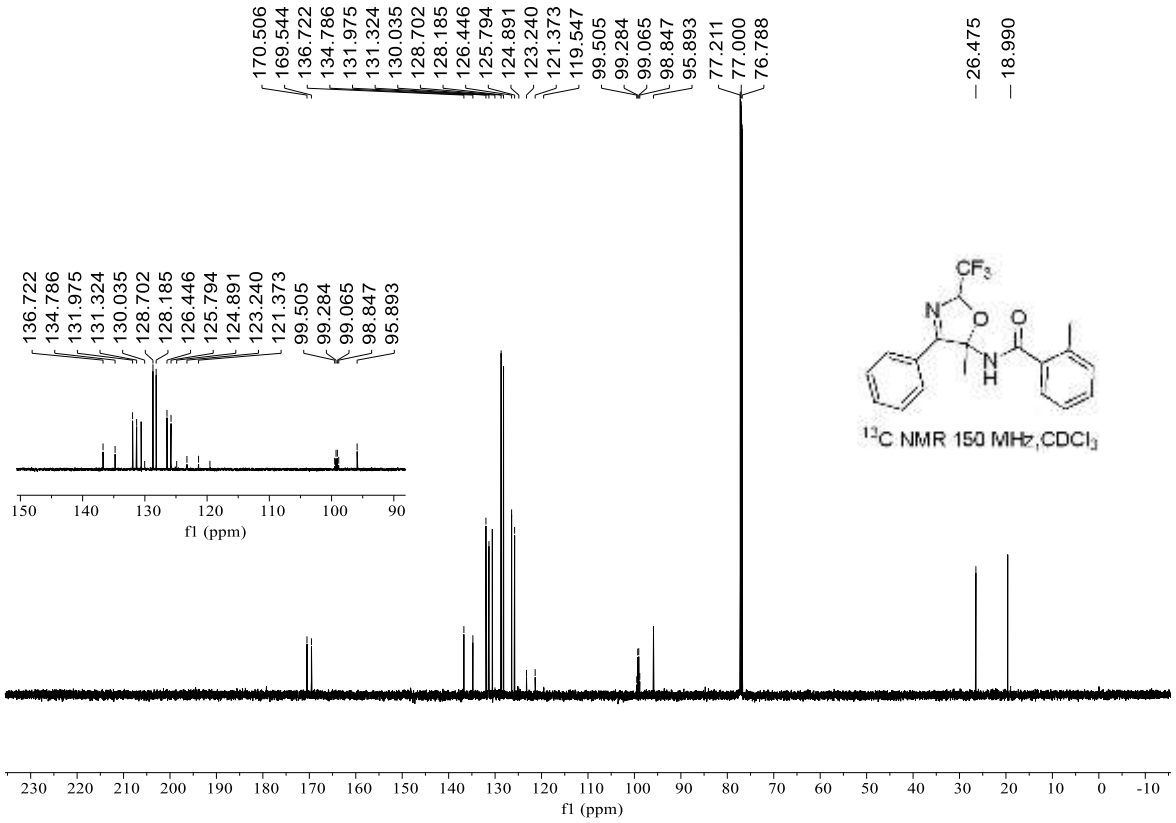
m/z	Intensity	Relative	Resolution	Charge	Delta (ppm)	Composition
346.33141	1155394.4	0.54	58132.50	1.00		
349.11581	215207664.0	100.00	58128.26	1.00	-0.09	$C_{18}H_{16}O_2N_2F_3$
349.18266	832666.8	0.39	56313.22	0.00		
350.11926	40867144.0	18.99	55843.50	1.00		
351.12249	4123196.0	1.92	56516.02	1.00		

NMR copies of compound **3b**

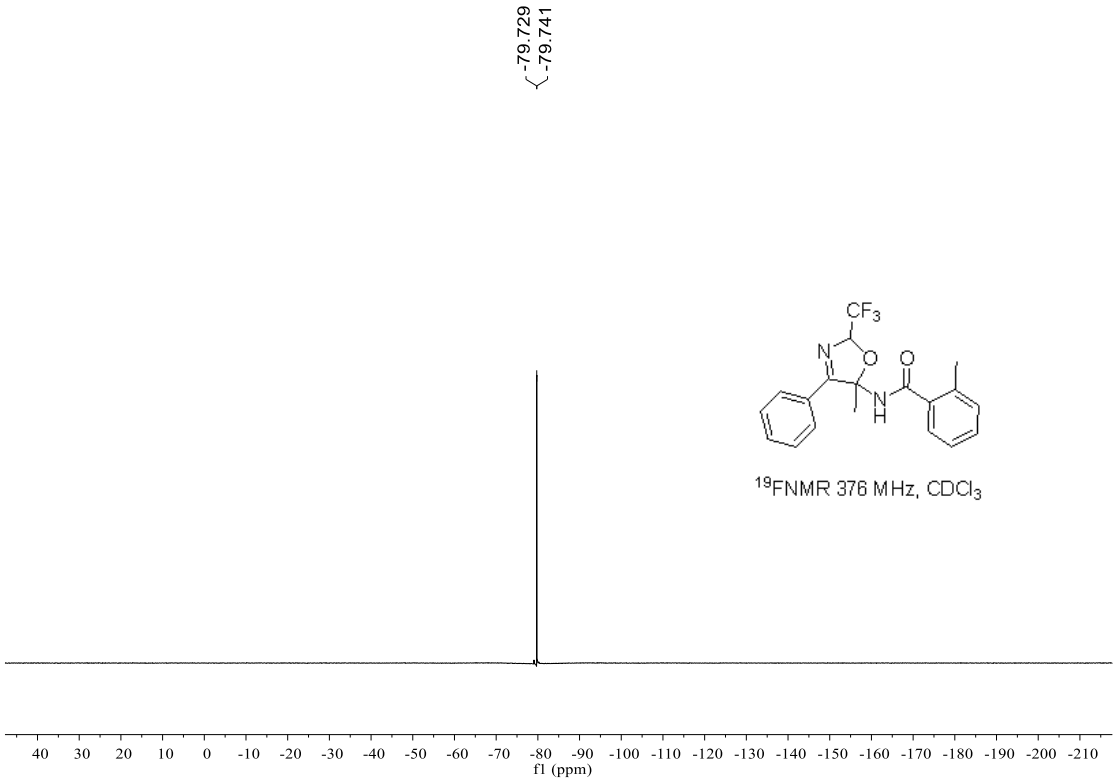
^{1}H NMR (400 MHz) spectrum of **3b** in $CDCl_3$



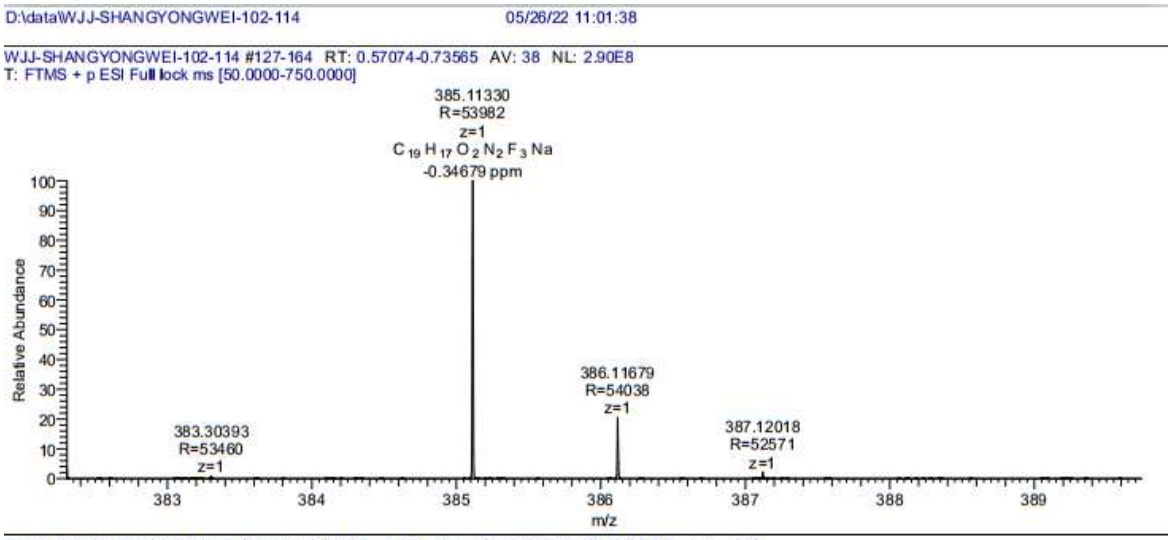
^{13}C NMR (150 MHz) spectrum of **3b** in $CDCl_3$



^{19}F NMR (376 MHz) spectrum of **3b** in $CDCl_3$



HRMS(ESI) copy of compound **3b**:

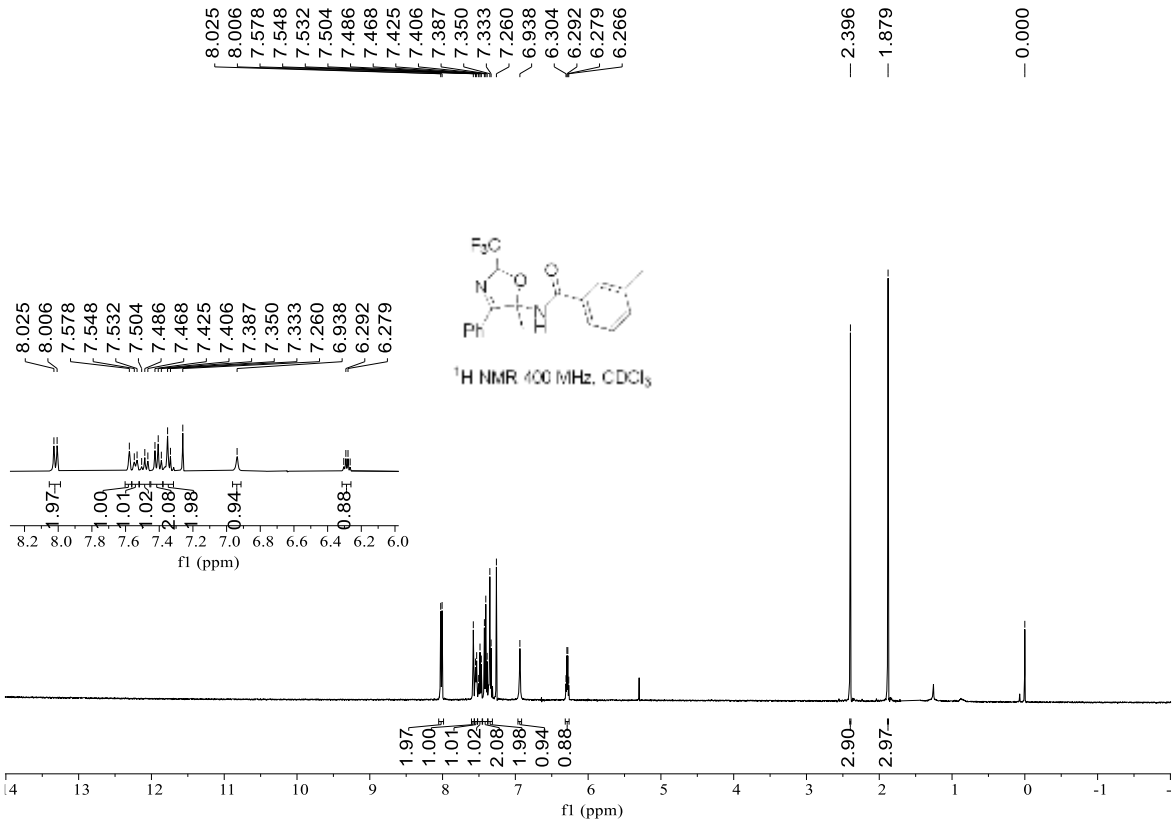


WJJ-SHANGYONGWEI-102-114#127-164 RT: 0.57074-0.73565 AV: 38
T: FTMS + p ESI Full lock ms [50.0000-750.0000]
m/z= 382.30544-389.74055

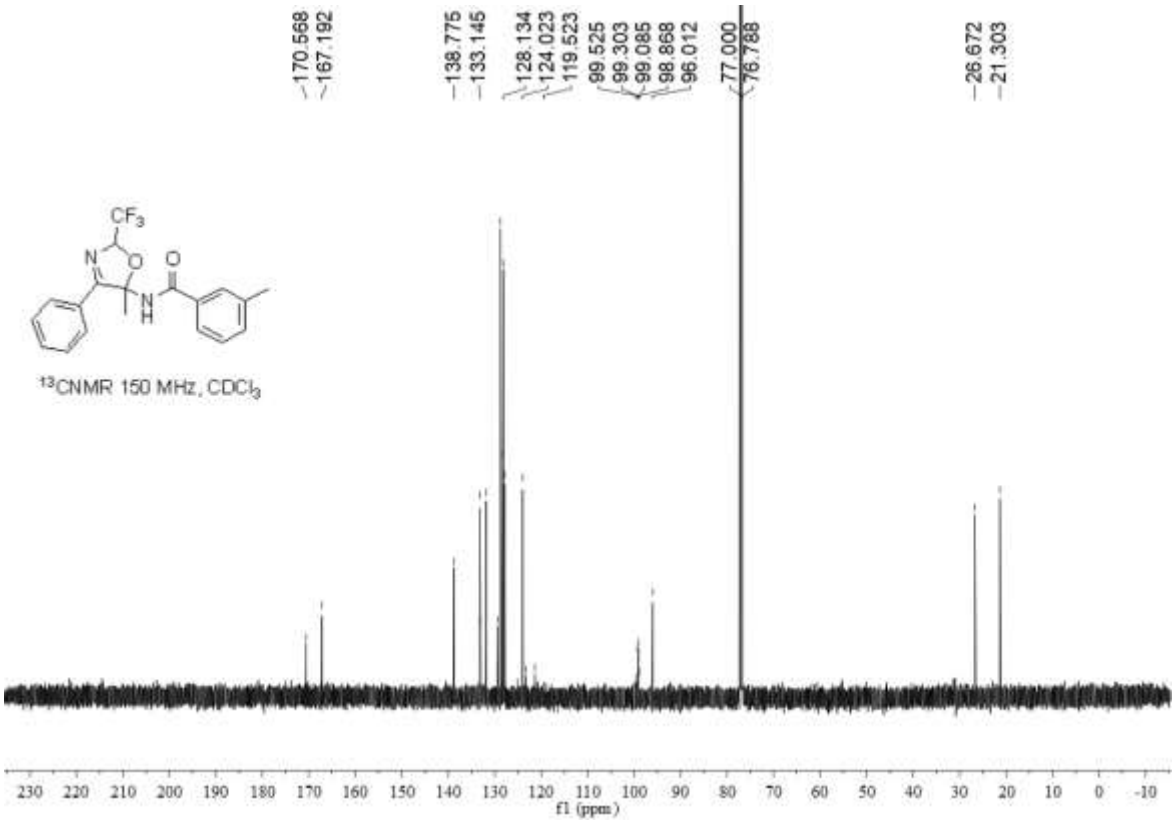
m/z	Intensity	Relative	Resolution	Charge	Delta (ppm)	Composition
383.30393	2166418.5	0.74	53460.42	1.00		
385.11330	293270720.0	100.00	53982.20	1.00	-0.35	$C_{19}H_{17}O_2N_2F_3Na$
386.11679	59565728.0	20.31	54038.04	1.00		
387.12018	6426921.5	2.19	52571.16	1.00		
388.35477	789008.3	0.27	54909.49	1.00		

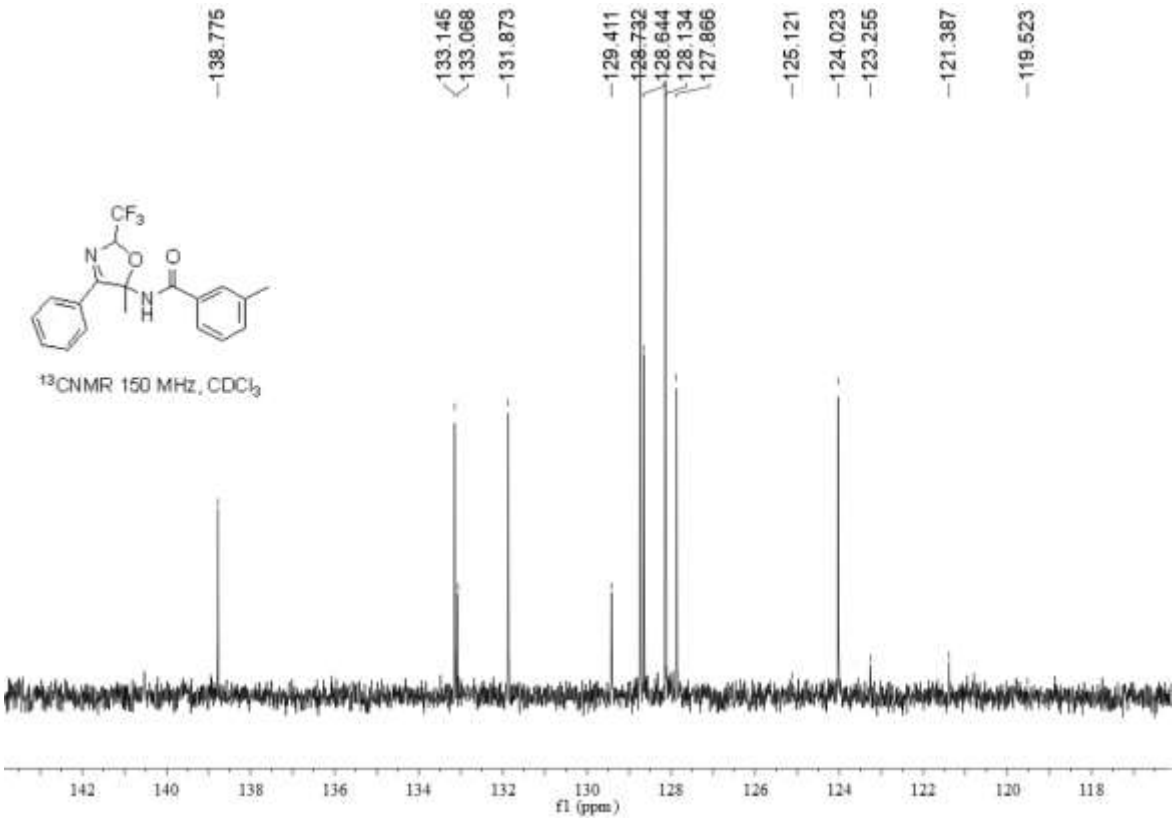
NMR copies of compound **3c**

^{1}H NMR (400 MHz) spectrum of **3c** in $CDCl_3$

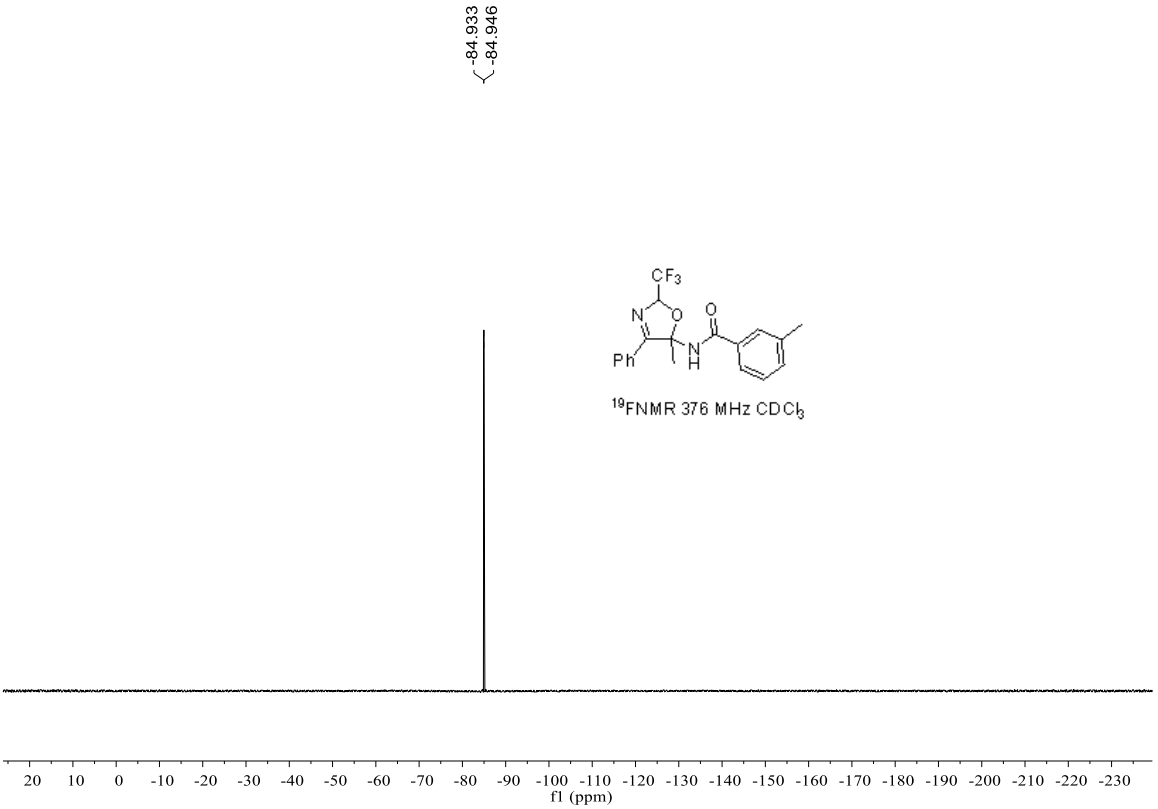


^{13}C NMR (150 MHz) spectrum of **3c** in $CDCl_3$

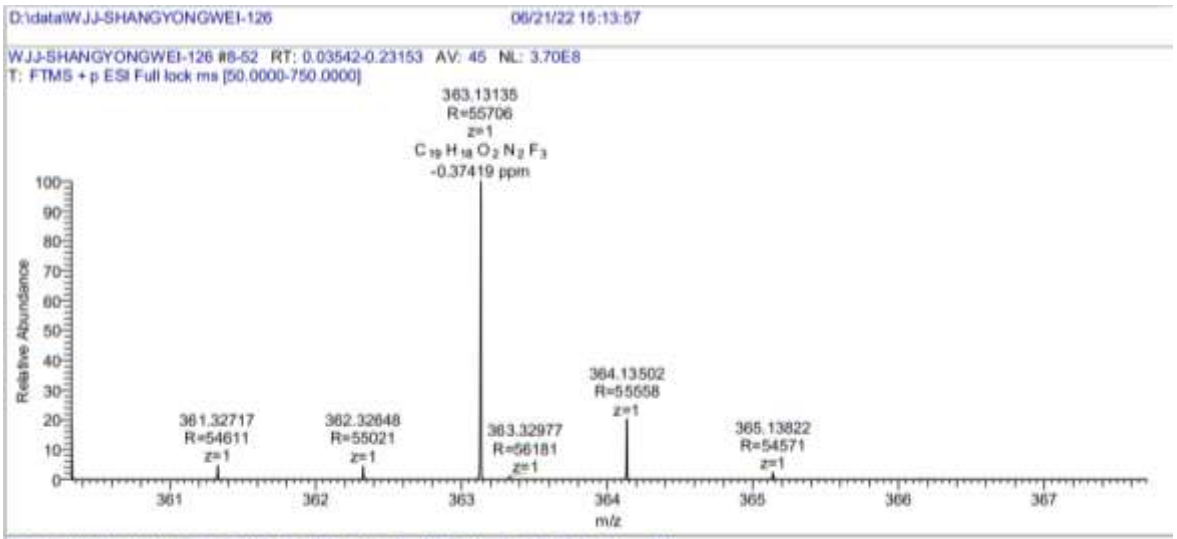




^{19}F NMR (376 MHz) spectrum of **3c** in $CDCl_3$



HRMS(ESI) copy of compound **3c**:

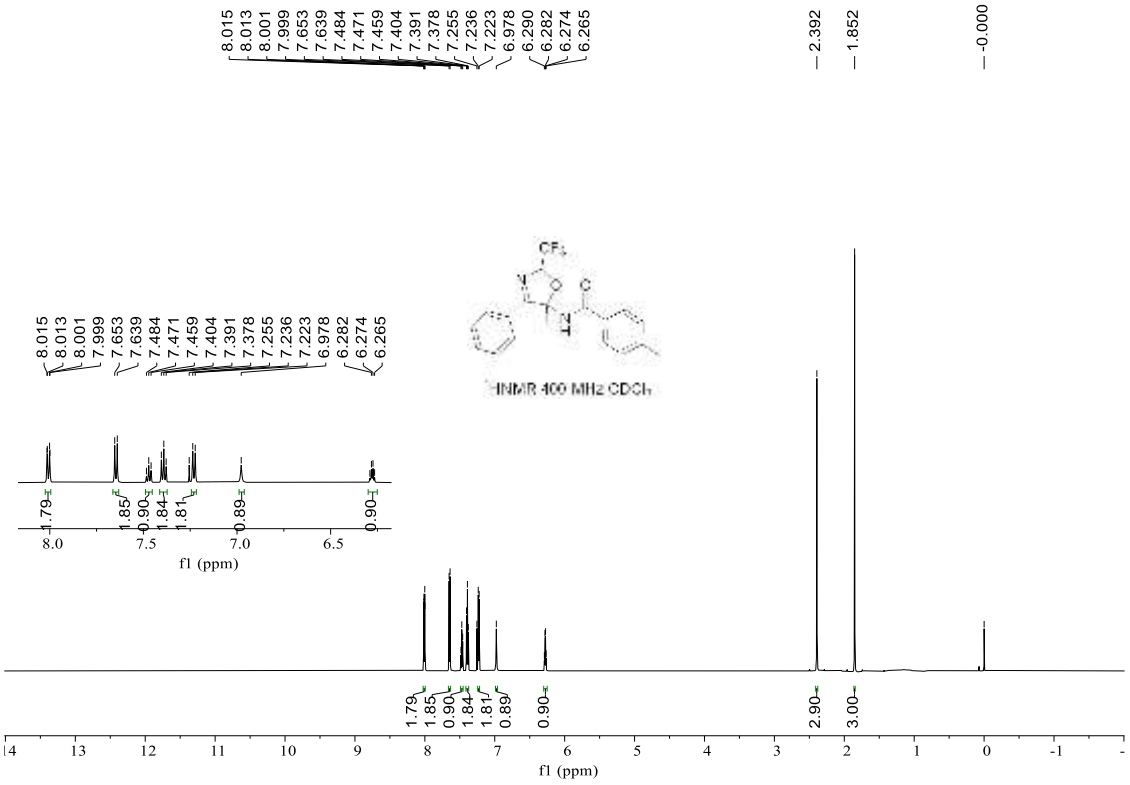


WJJ-SHANGYONGWEI-126#8-52 RT: 0.03542-0.23153 AV: 45
T: FTMS + p ESI Full lock ms [50.0000-750.0000]
m/z= 360.32286-367.70064

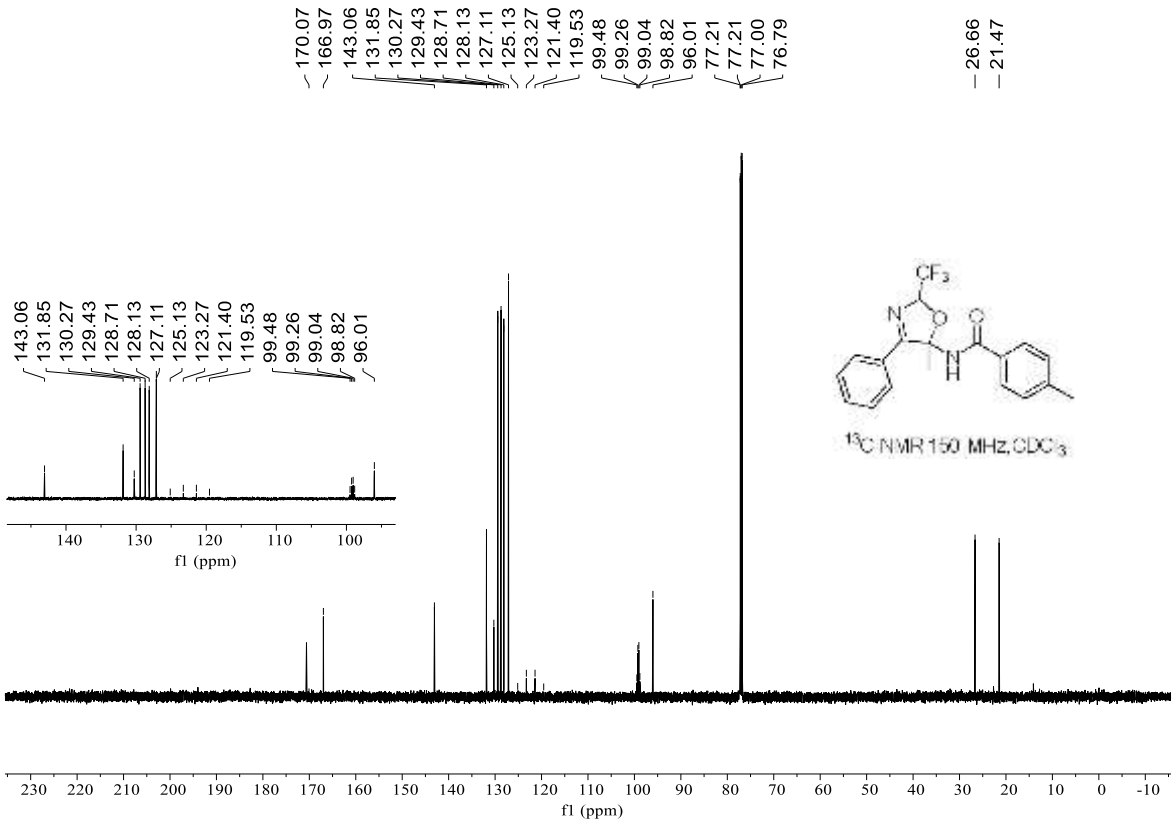
m/z	Intensity	Relative	Resolution	Charge	Delta (ppm)	Composition
360.32370	76270824.0	20.37	57067.89	1.00		
361.32717	17765272.0	4.74	54611.46	1.00		
361.72124	409708.9	0.11	55002.38	0.00		
362.32648	16638300.0	4.44	55021.12	1.00		
363.13135	374509088.0	100.00	55705.54	1.00	-0.37	$C_{19}H_{18}O_2N_2F_3$
363.32977	3517212.8	0.94	56181.02	1.00		
364.13502	75803224.0	20.24	55558.20	1.00		
365.13822	8321985.0	2.22	54570.79	1.00		
366.18156	527668.8	0.14	55480.00	0.00		

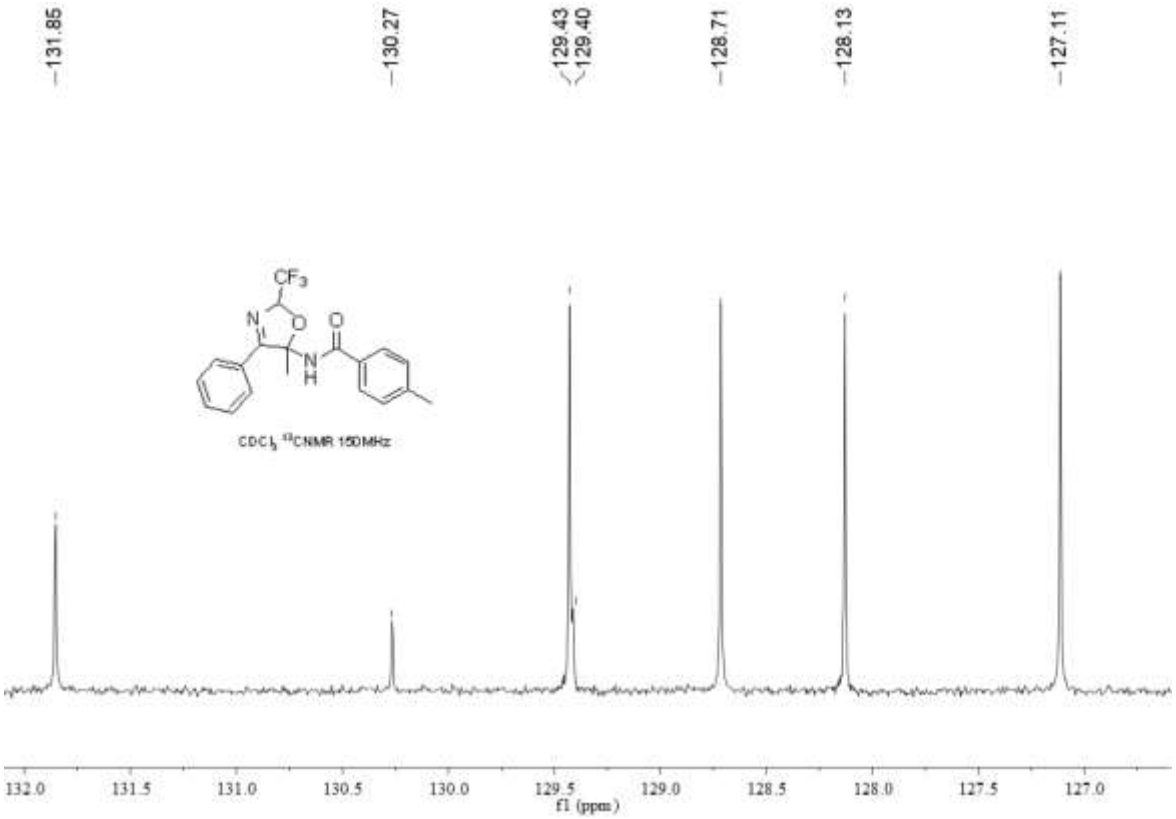
NMR copies of compound **3d**

^{1}H NMR (400 MHz) spectrum of **3d** in $CDCl_3$

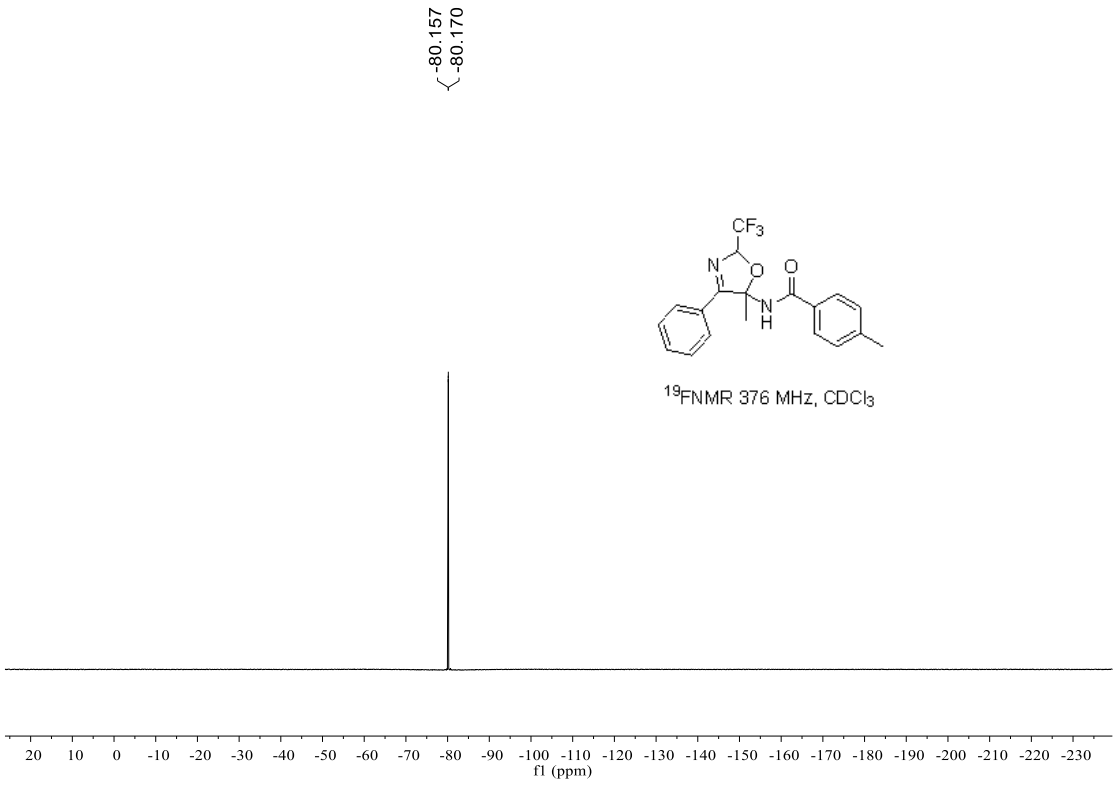


^{13}C NMR (150 MHz) spectrum of **3d** in $CDCl_3$

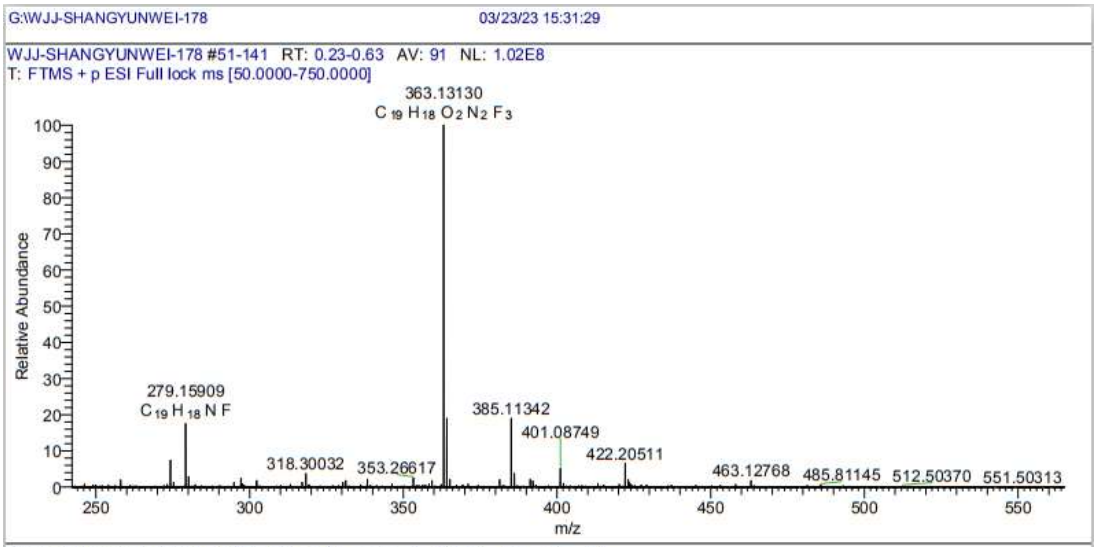




^{19}F NMR (376 MHz) spectrum of **3d** in $CDCl_3$



HRMS(ESI) copy of compound **3d**:

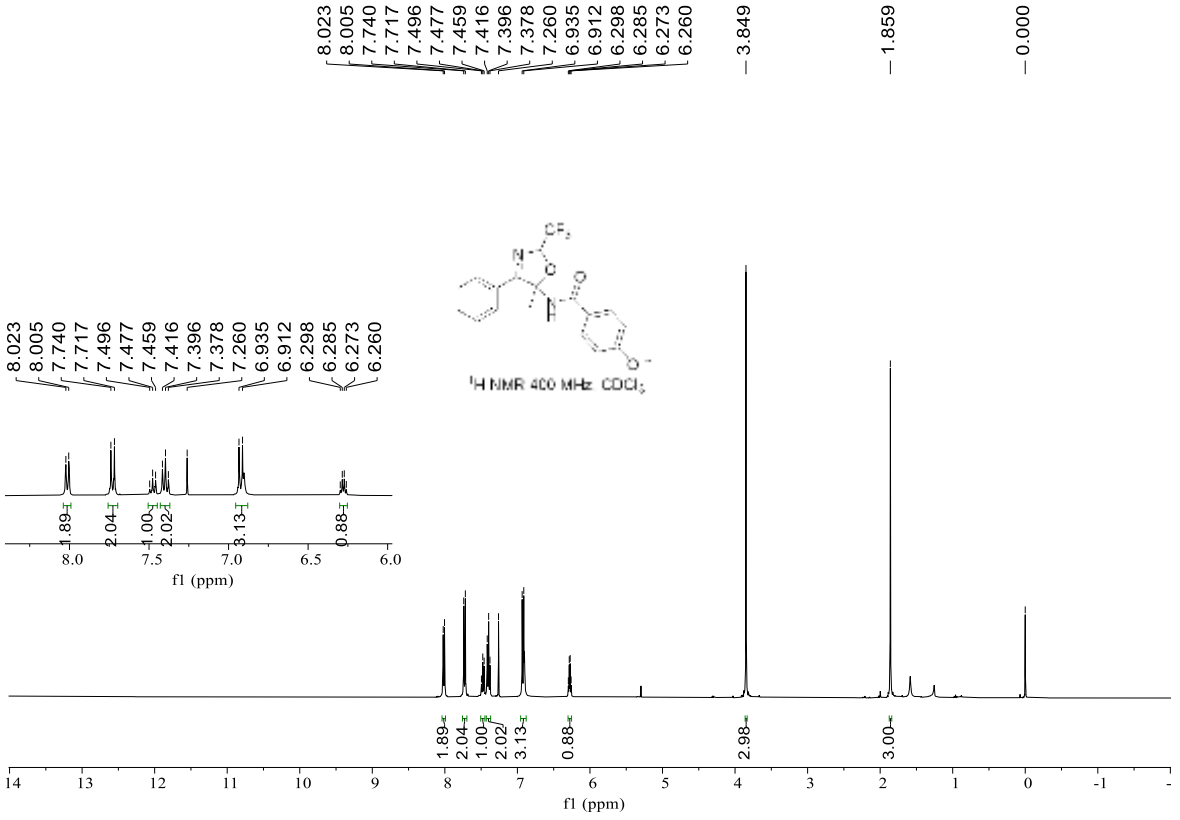


WJJ-SHANGYUNWEI-178#51-141 RT: 0.23-0.63 AV: 91
T: FTMS + p ESI Full lock ms [50.0000-750.0000]
m/z= 242.17852-564.89522

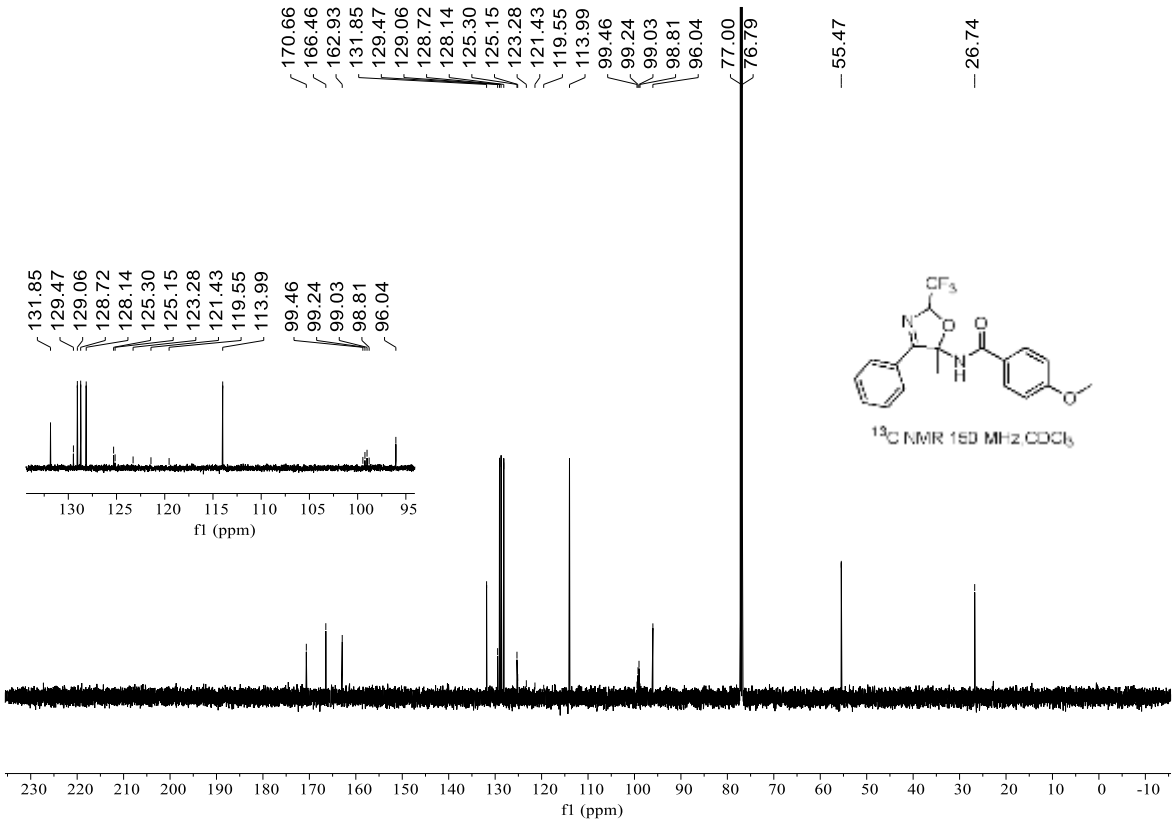
m/z	Intensity	Relative	Delta (ppm)	Composition
274.27401	7648864.0	7.42	127.56	$C_{19}H_{18}N_2$
279.15909	17970610.0	17.44	17.31	$C_{19}H_{18}NF$
363.13130	103025368.0	100.00	-0.19	$C_{19}H_{18}O_2N_2F_3$
364.13490	20029018.0	19.44		
385.11342	19992146.0	19.41		

NMR copies of compound **3e**

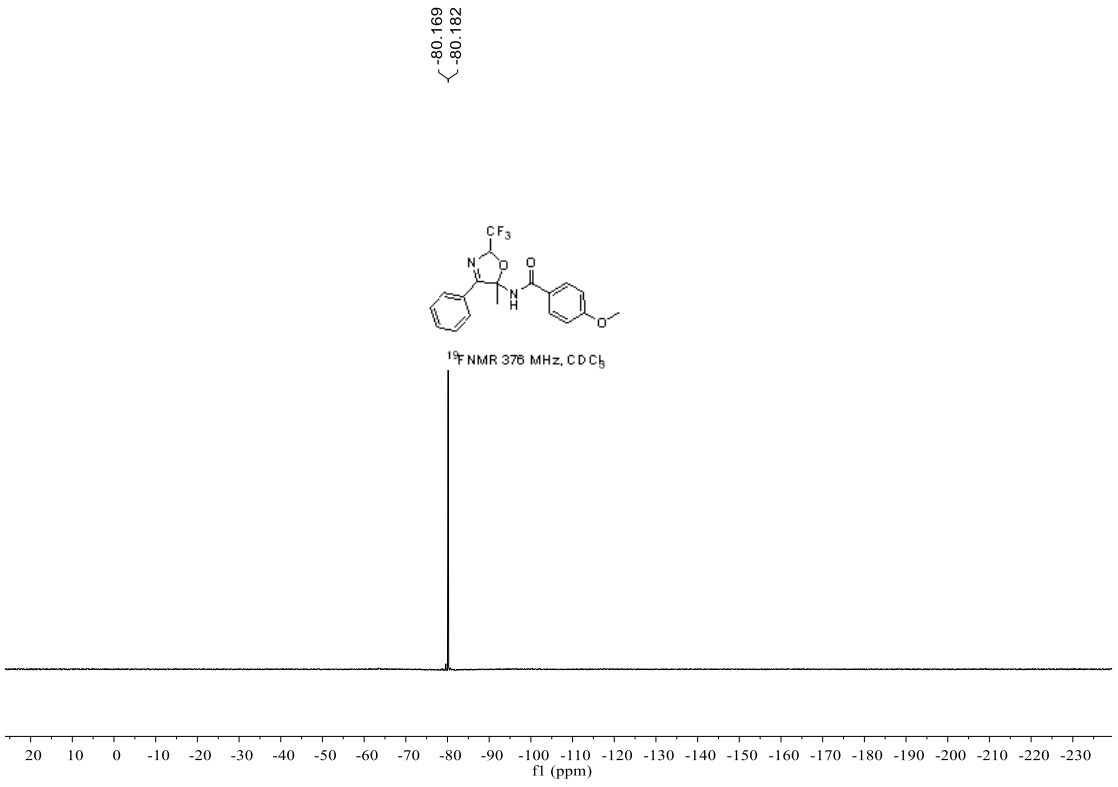
^{1}H NMR (400 MHz) spectrum of **3e** in $CDCl_3$



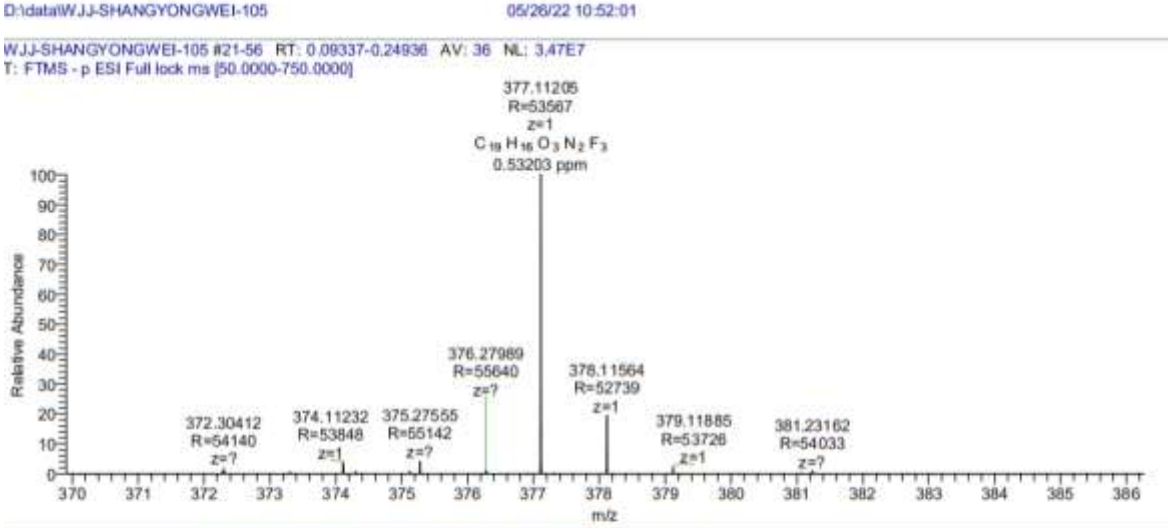
^{13}C NMR (150 MHz) spectrum of **3e** in $CDCl_3$



^{19}F NMR (376 MHz) spectrum of **3e** in $CDCl_3$



HRMS(ESI) copy of compound **3e**:

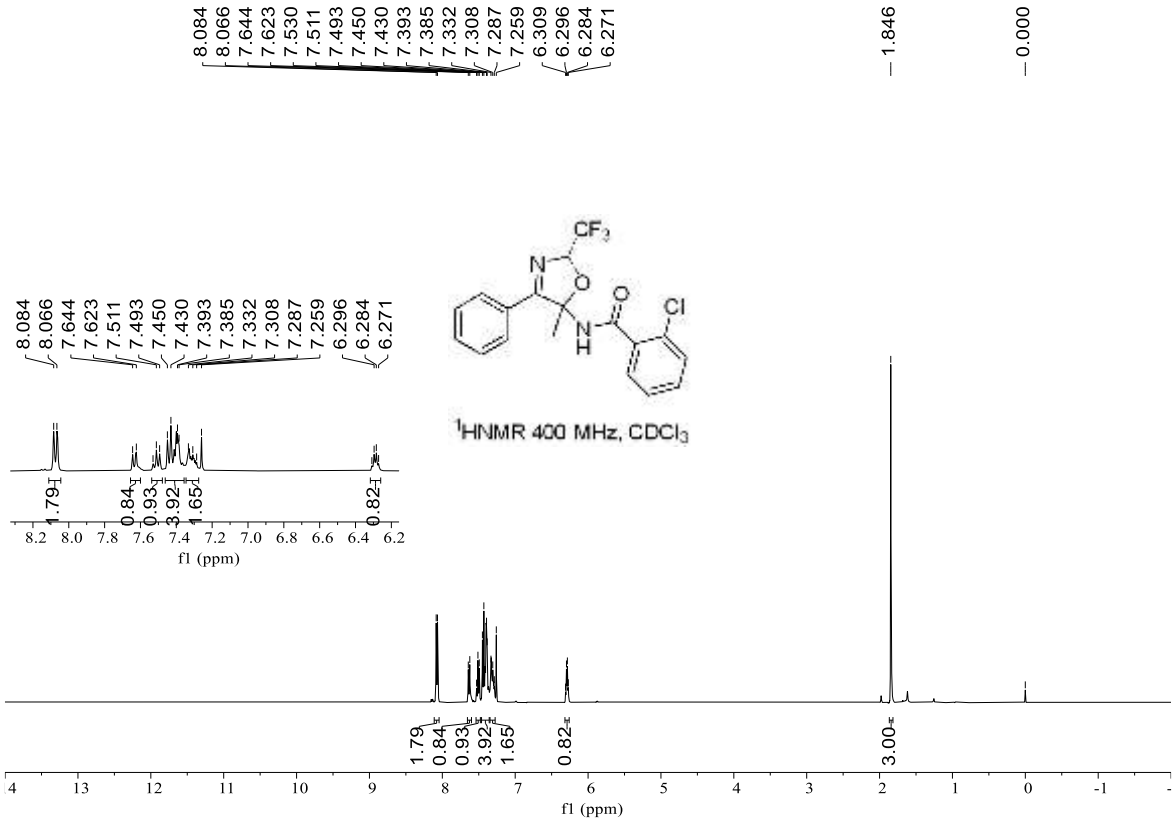


WJJ-SHANGYONGWEI-105#21-56 RT: 0.09337-0.24936 AV: 36
T: FTMS - p ESI Full lock ms [50.0000-750.0000]
m/z= 369.90846-386.26392

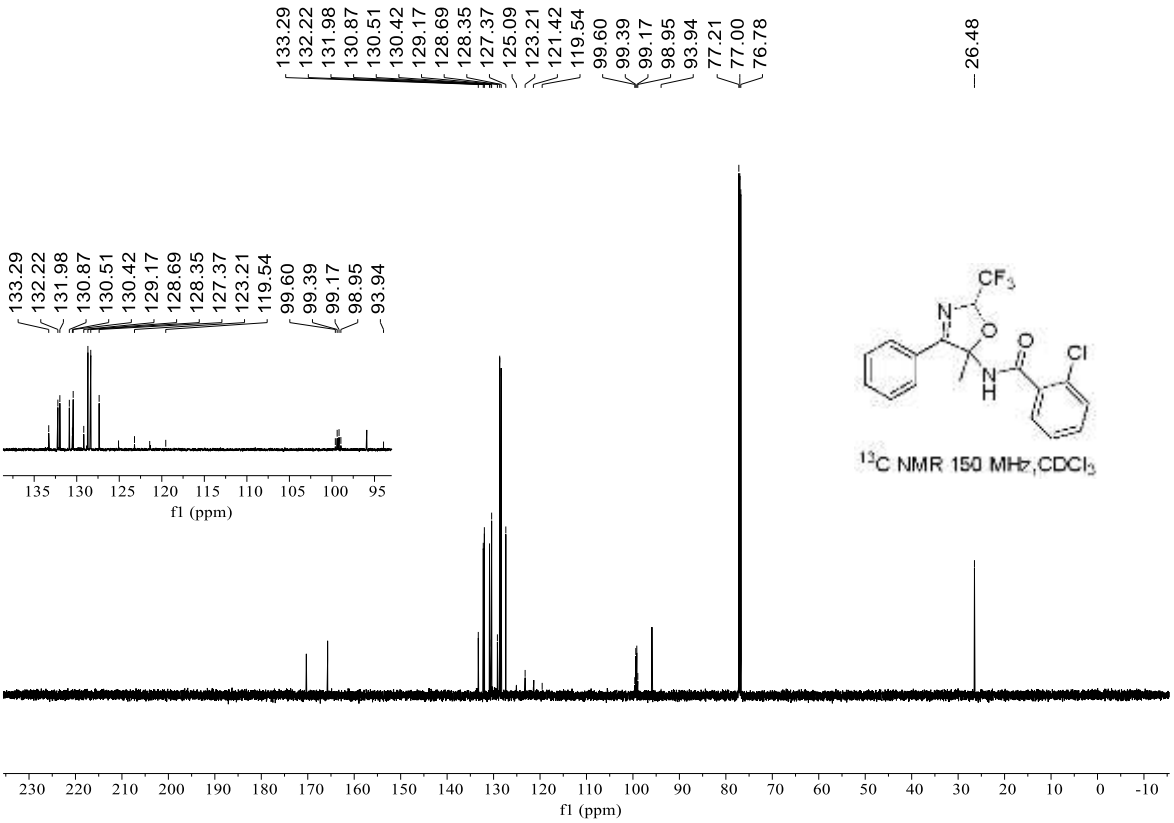
m/z	Intensity	Relative	Resolution	Charge	Delta (ppm)	Composition
374.11232	1301427.4	3.66	53848.32	1.00		
375.27555	1417542.8	3.99	55142.22	0.00		
377.11205	35527616.0	100.00	53567.28	1.00	0.53	$C_{19}H_{16}O_3N_2F_3$
378.11564	6952328.0	19.57	52739.29	1.00		
379.11885	794741.3	2.24	53726.41	1.00		

NMR copies of compound **3f**

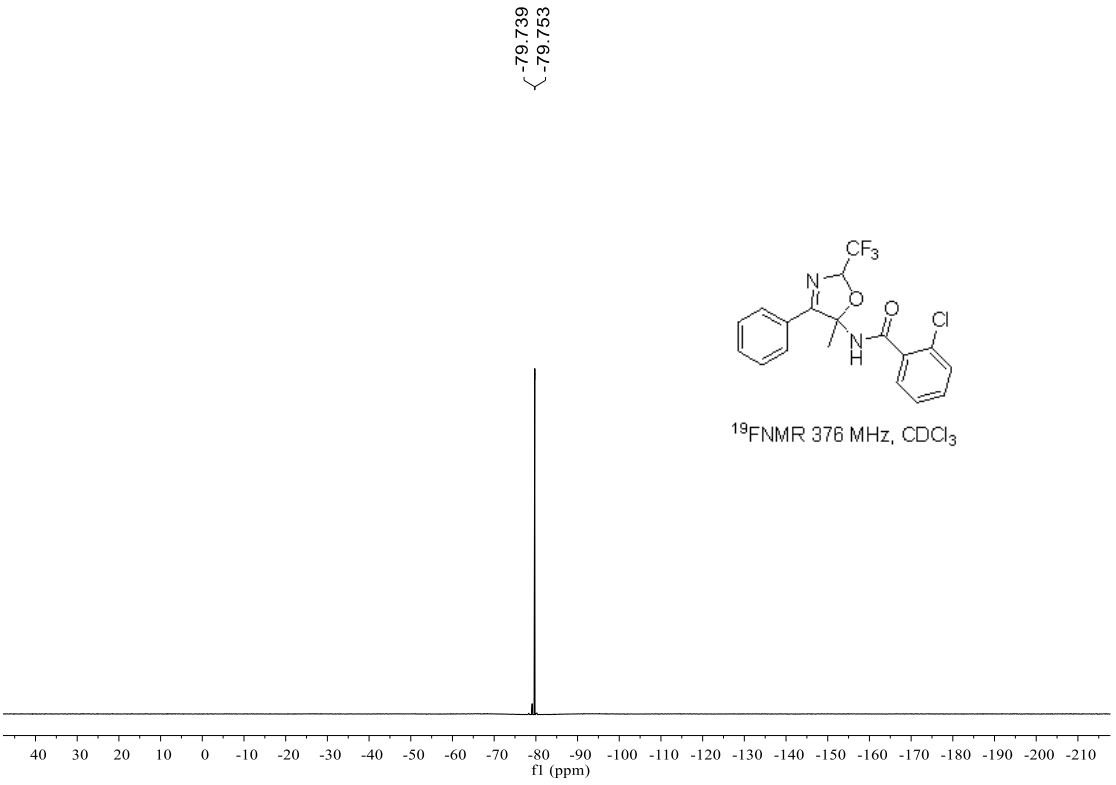
^{1}H NMR (400 MHz) spectrum of **3f** in $CDCl_3$



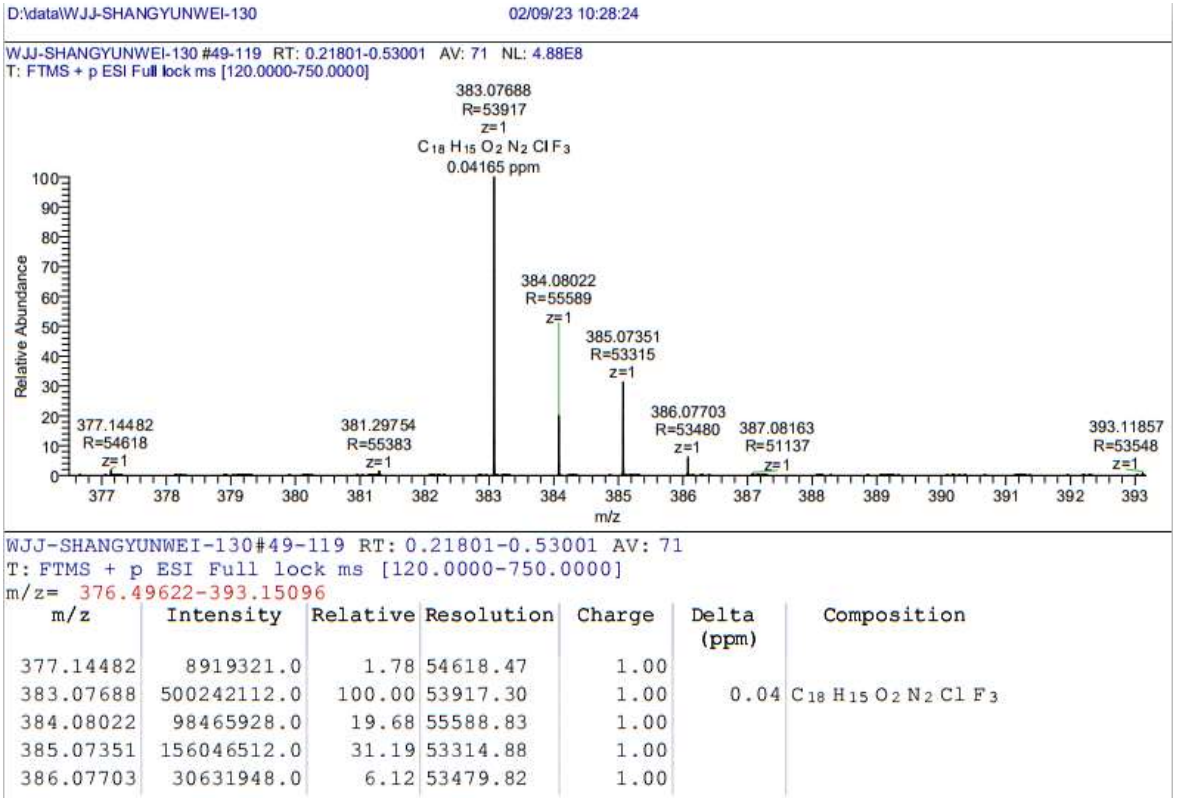
^{13}C NMR (150 MHz) spectrum of **3f** in $CDCl_3$



^{19}F NMR (376 MHz) spectrum of **3f** in $CDCl_3$



HRMS(ESI) copy of compound **3f**:

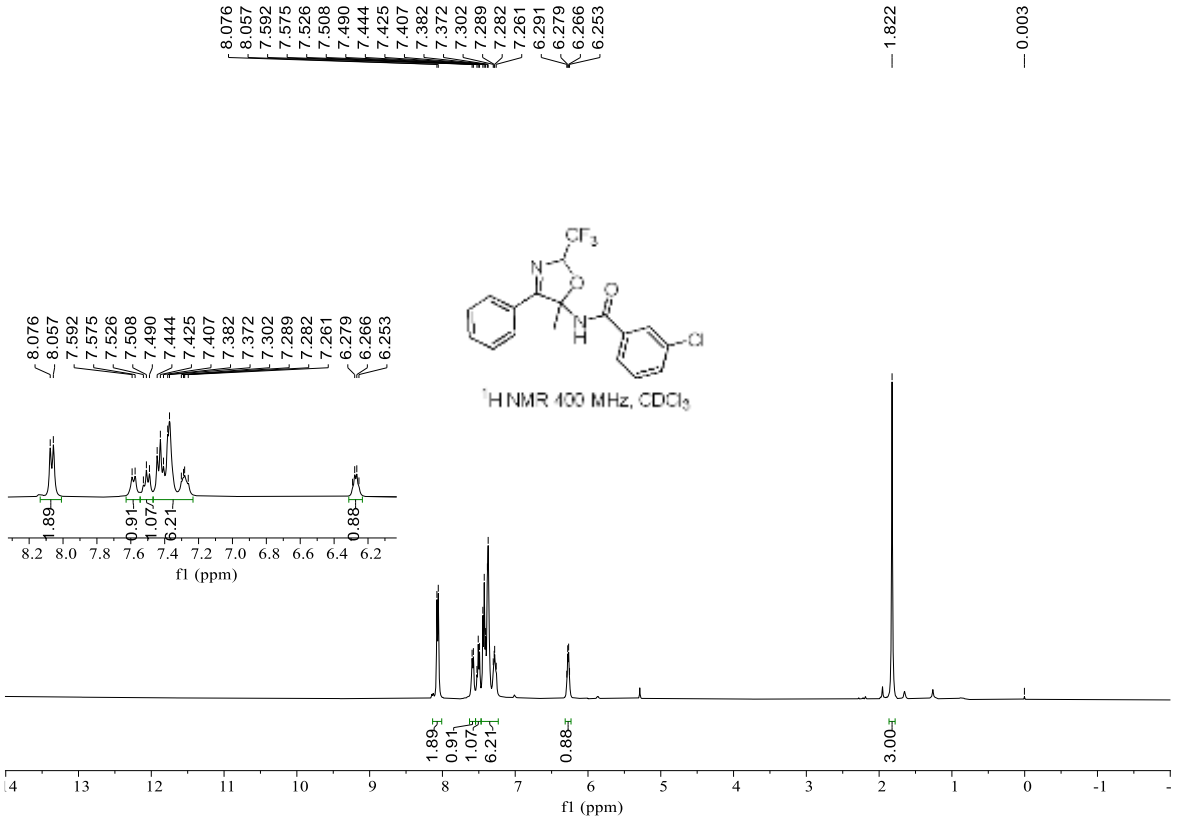


WJJ-SHANGYUNWEI-130#49-119 RT: 0.21801-0.53001 AV: 71
T: FTMS + p ESI Full lock ms [120.0000-750.0000]
m/z= 376.49622-393.15096

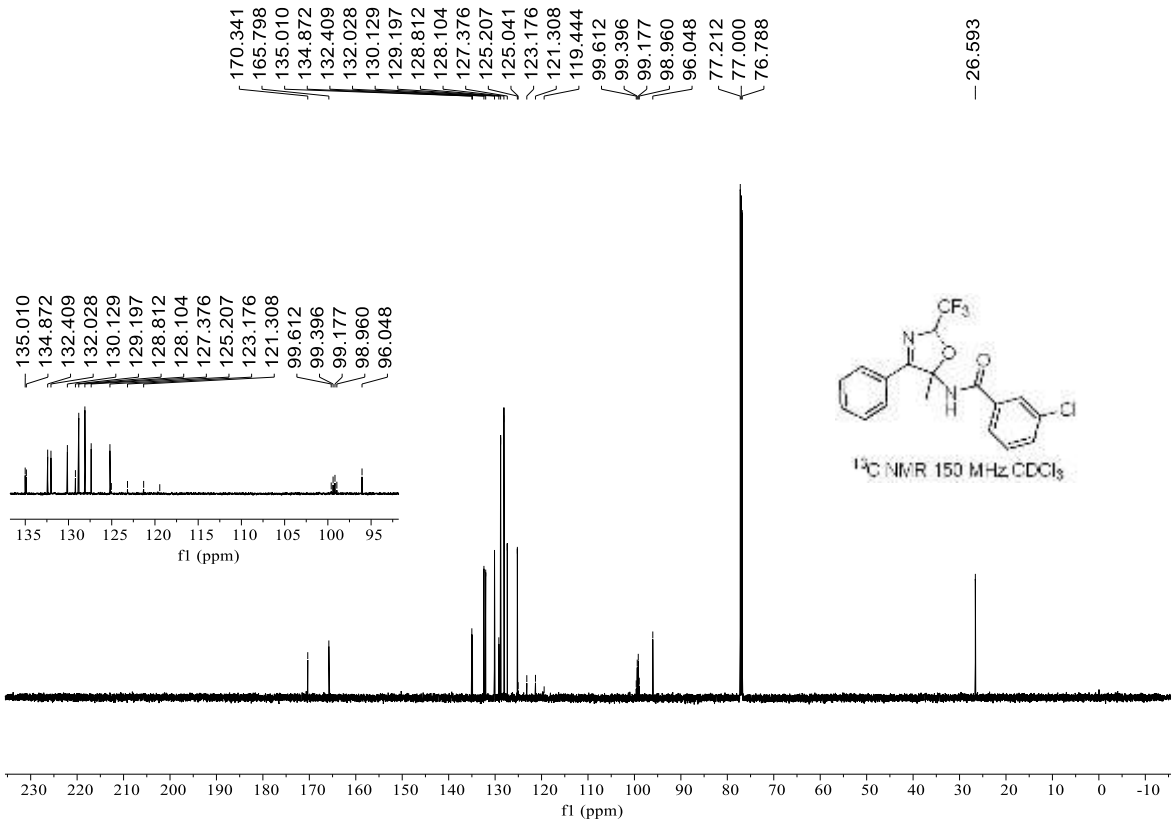
m/z	Intensity	Relative	Resolution	Charge	Delta (ppm)	Composition
377.14482	8919321.0	1.78	54618.47	1.00		
383.07688	500242112.0	100.00	53917.30	1.00	0.04	$C_{18}H_{15}O_2N_2ClF_3$
384.08022	98465928.0	19.68	55588.83	1.00		
385.07351	156046512.0	31.19	53314.88	1.00		
386.07703	30631948.0	6.12	53479.82	1.00		

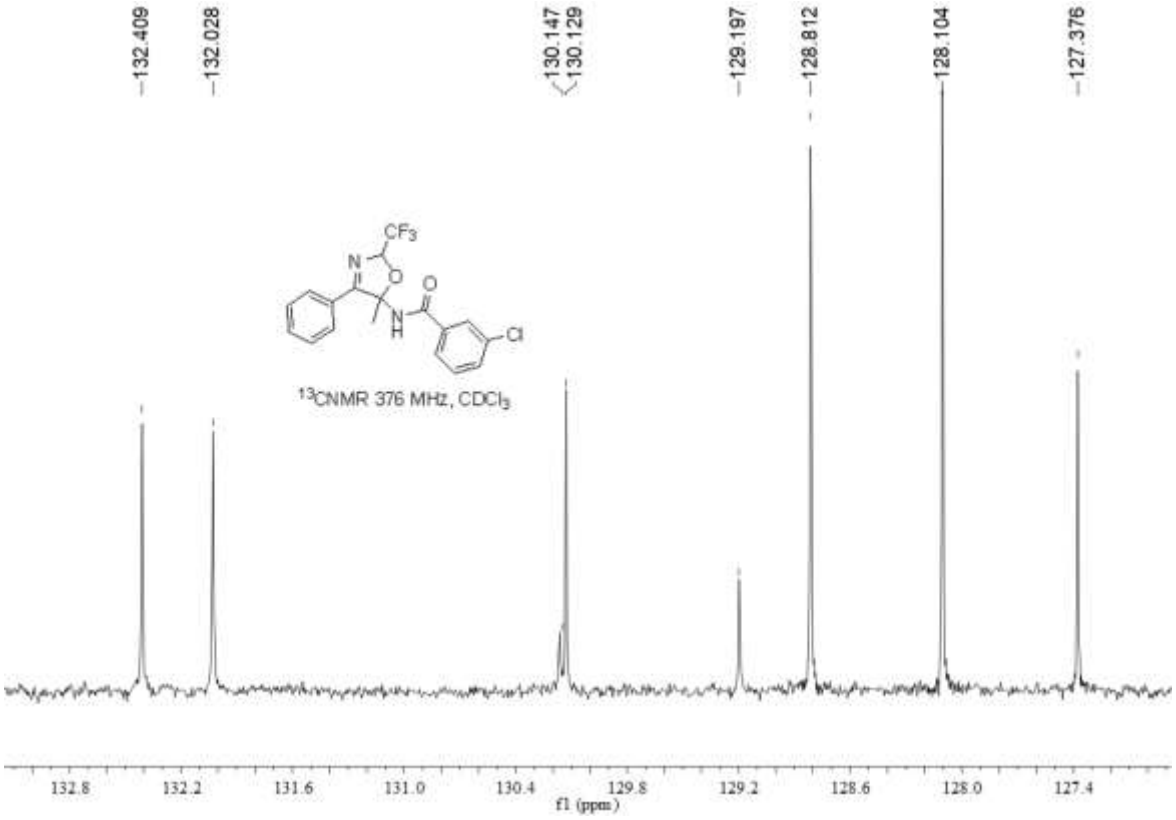
NMR copies of compound **3g**

^{1}H NMR (400 MHz) spectrum of **3g** in $CDCl_3$

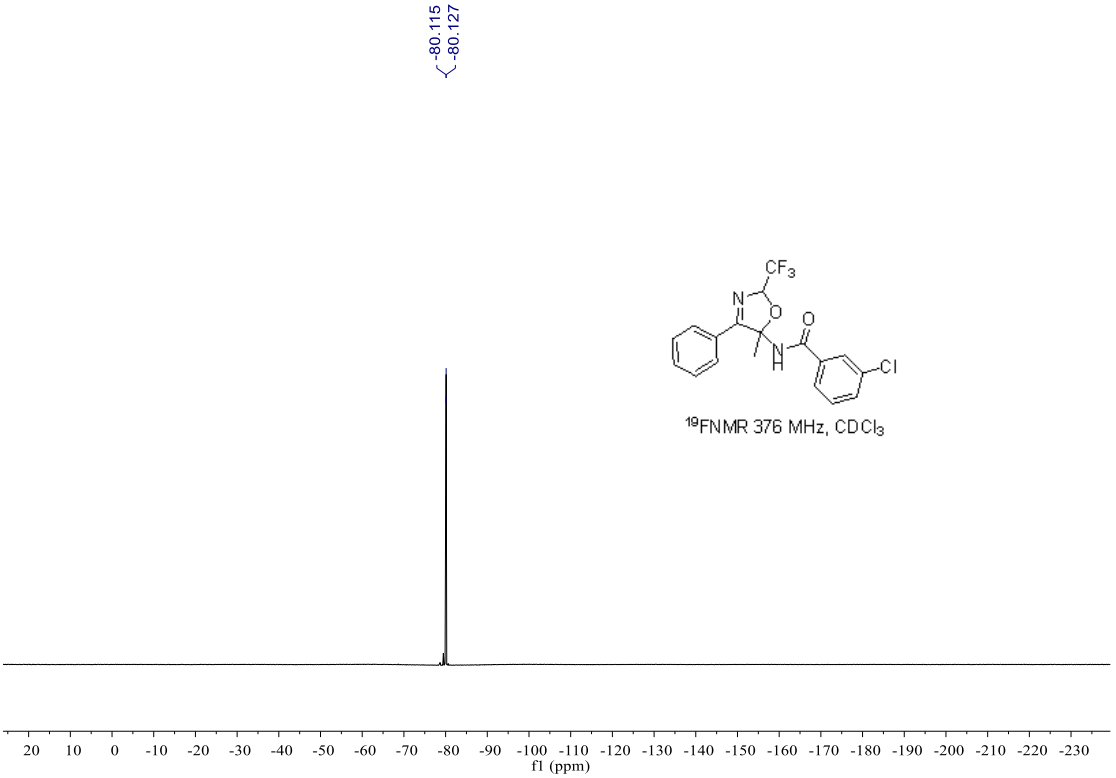


^{13}C NMR (150 MHz) spectrum of **3g** in $CDCl_3$

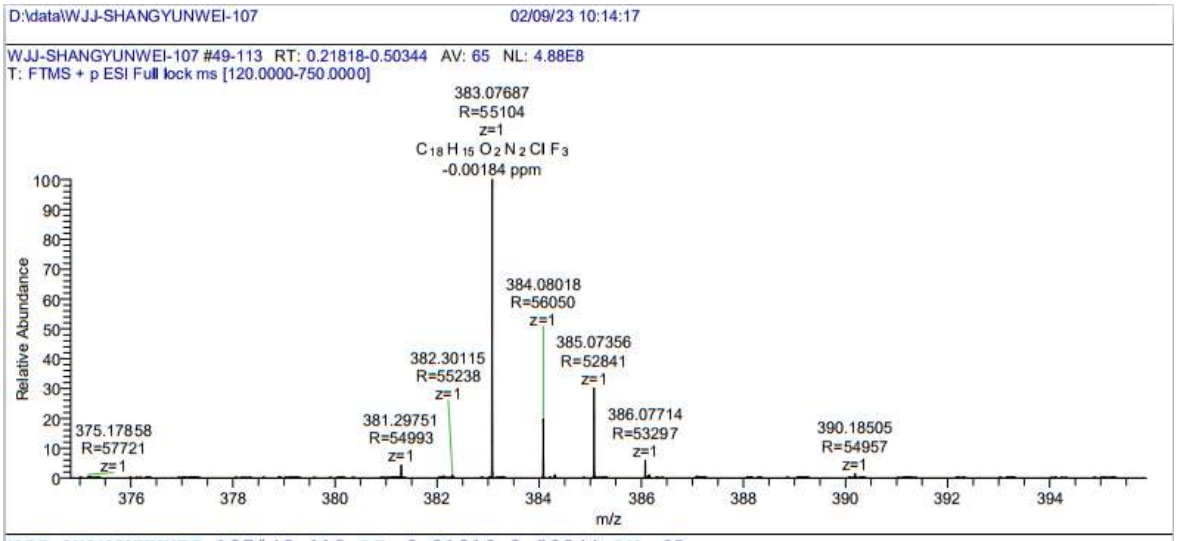




^{19}F NMR (376 MHz) spectrum of **3g** in $CDCl_3$



HRMS(ESI) copy of compound **3g**:

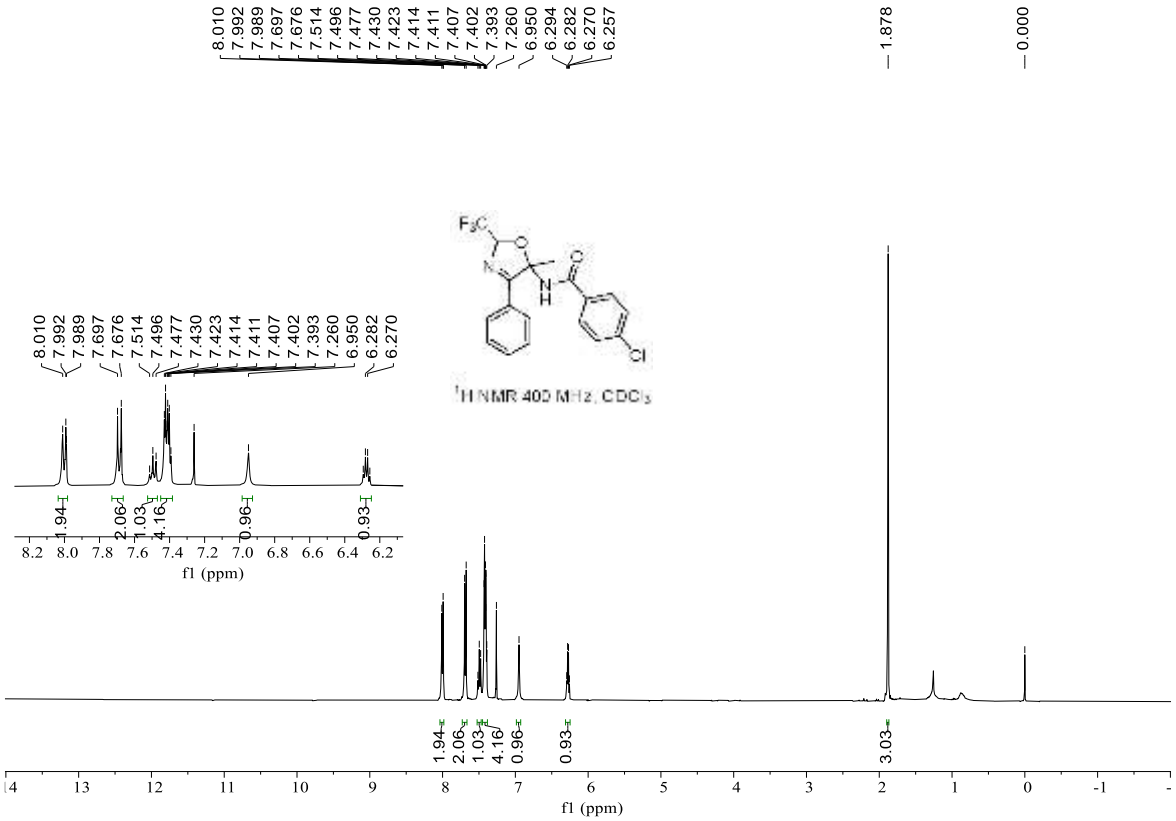


WJJ-SHANGYUNWEI-107#49-113 RT: 0.21818-0.50344 AV: 65
T: FTMS + p ESI Full lock ms [120.0000-750.0000]
m/z= 374.81919-395.88282

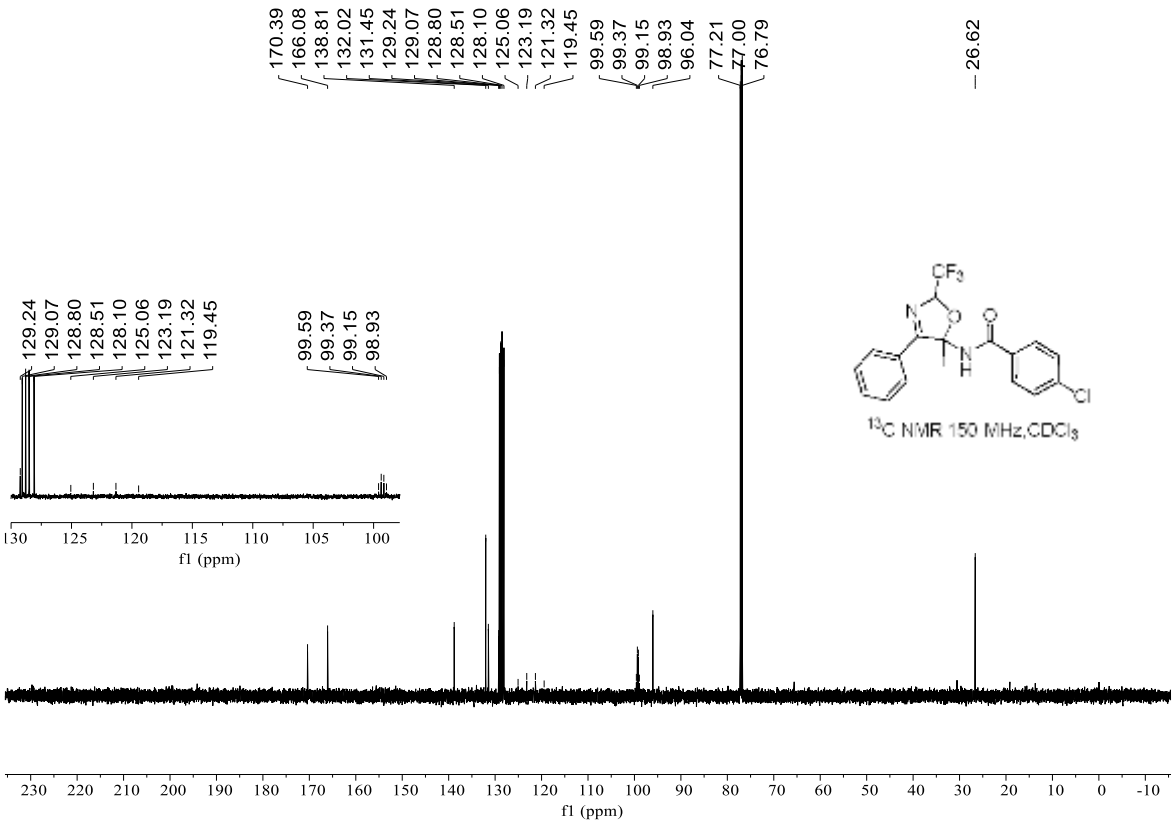
m/z	Intensity	Relative	Resolution	Charge	Delta (ppm)	Composition
381.29751	21049210.0	4.25	54993.06	1.00		
383.07687	494987552.0	100.00	55104.40	1.00	-0.00	$C_{18}H_{15}O_2N_2ClF_3$
384.08018	96638816.0	19.52	56050.45	1.00		
385.07356	151921168.0	30.69	52841.38	1.00		
386.07714	29927206.0	6.05	53297.31	1.00		

NMR copies of compound **3h**

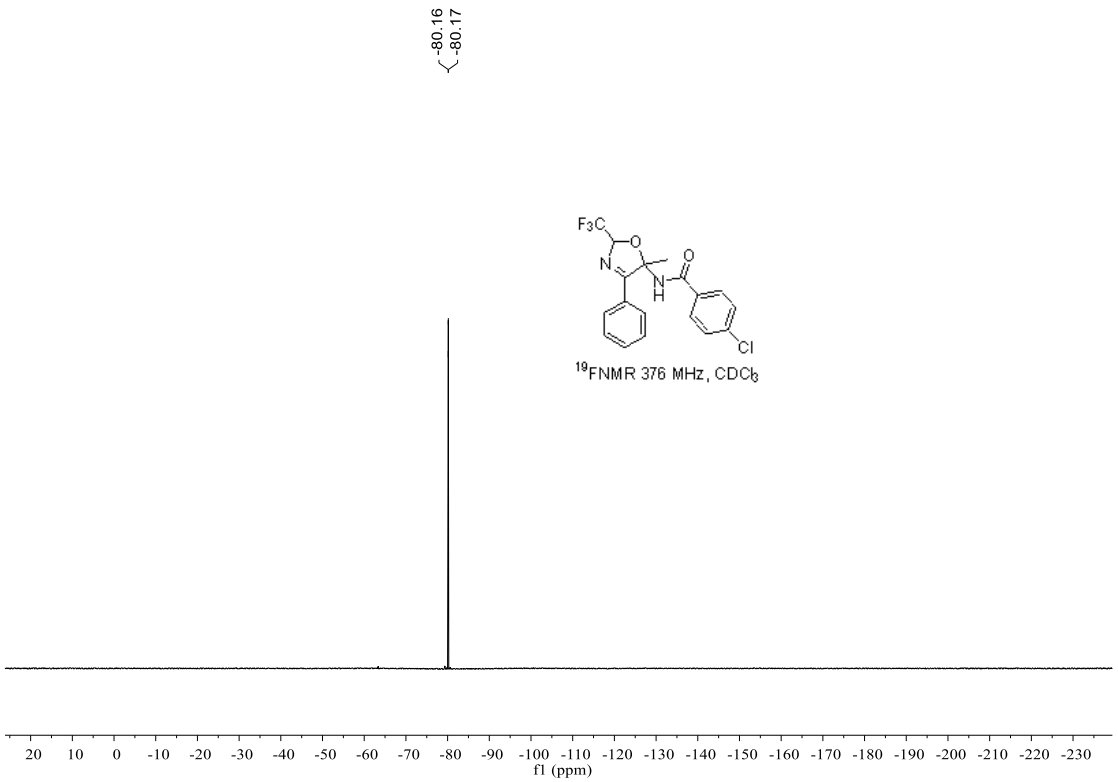
^{1}H NMR (400 MHz) spectrum of **3h** in $CDCl_3$



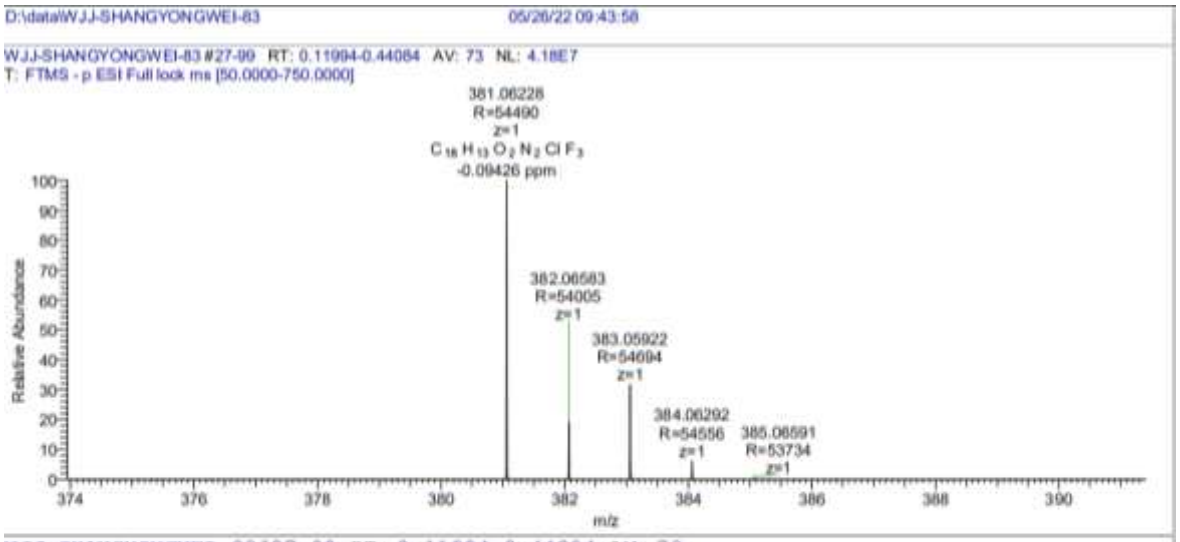
^{13}C NMR (150 MHz) spectrum of **3h** in $CDCl_3$



^{19}F NMR (376 MHz) spectrum of **3h** in $CDCl_3$



HRMS(ESI) copy of compound **3h**:

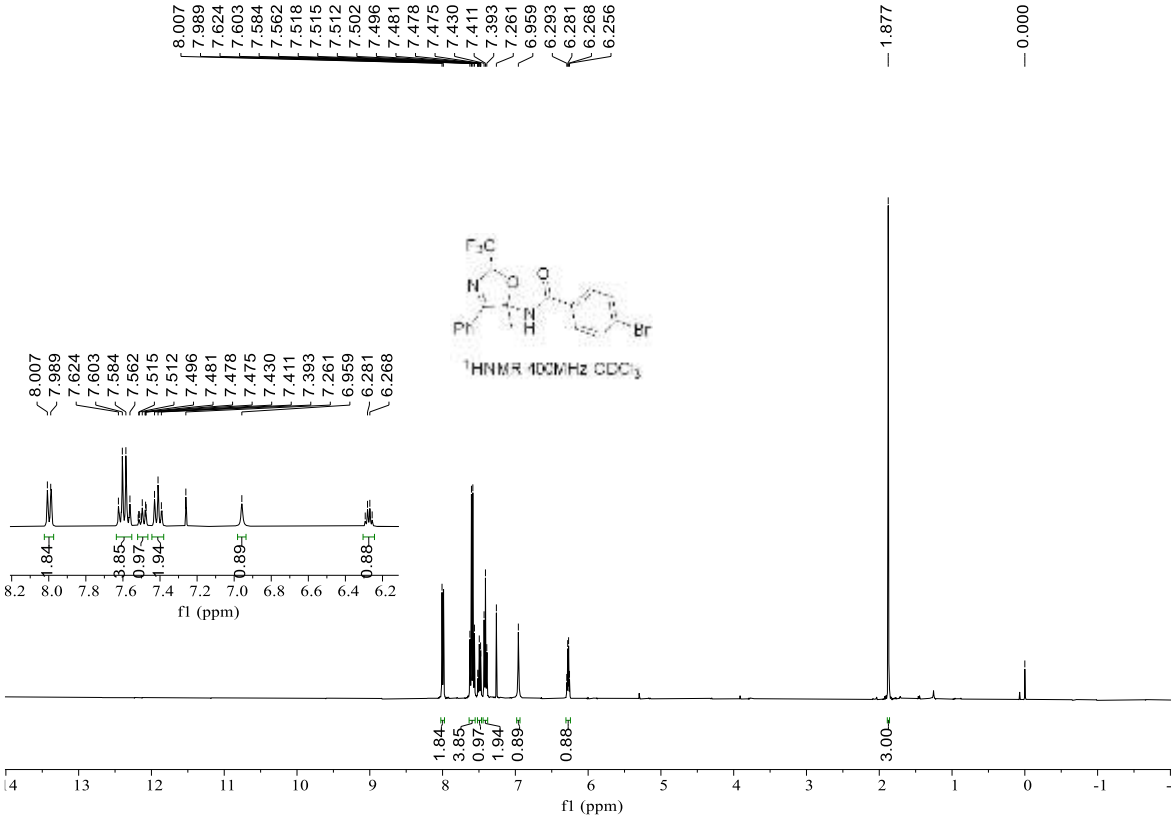


WJJ-SHANGYONGWEI-83#27-99 RT: 0.11994-0.44084 AV: 73
T: FTMS - p ESI Full lock ms [50.0000-750.0000]
m/z= 373.95480-391.39900

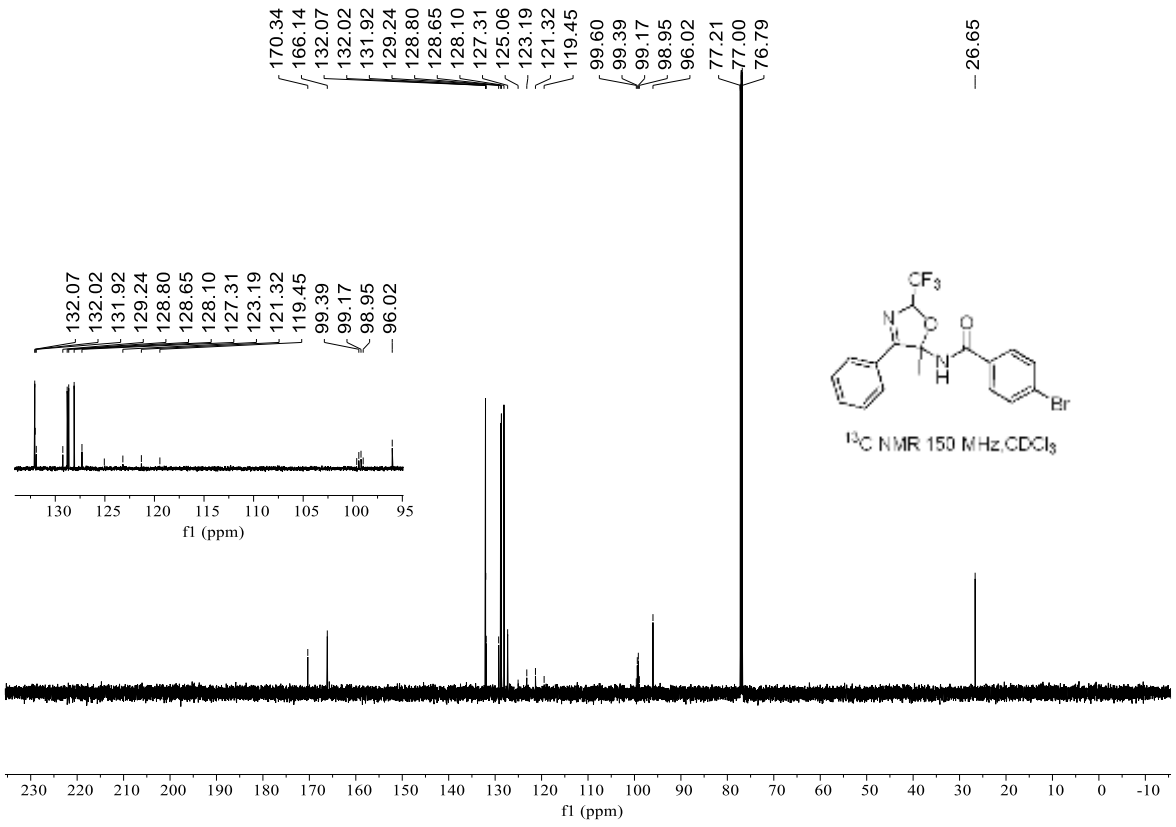
m/z	Intensity	Relative	Resolution	Charge	Delta (ppm)	Composition
381.06228	42167132.0	100.00	54490.48	1.00	-0.09	$C_{18}H_{13}O_2N_2ClF_3$
382.06583	7994935.5	18.96	54004.77	1.00		
383.05922	13319647.0	31.59	54694.17	1.00		
384.06292	2550450.0	6.05	54556.16	1.00		
385.06591	219760.3	0.52	53734.08	1.00		

NMR copies of compound **3i**

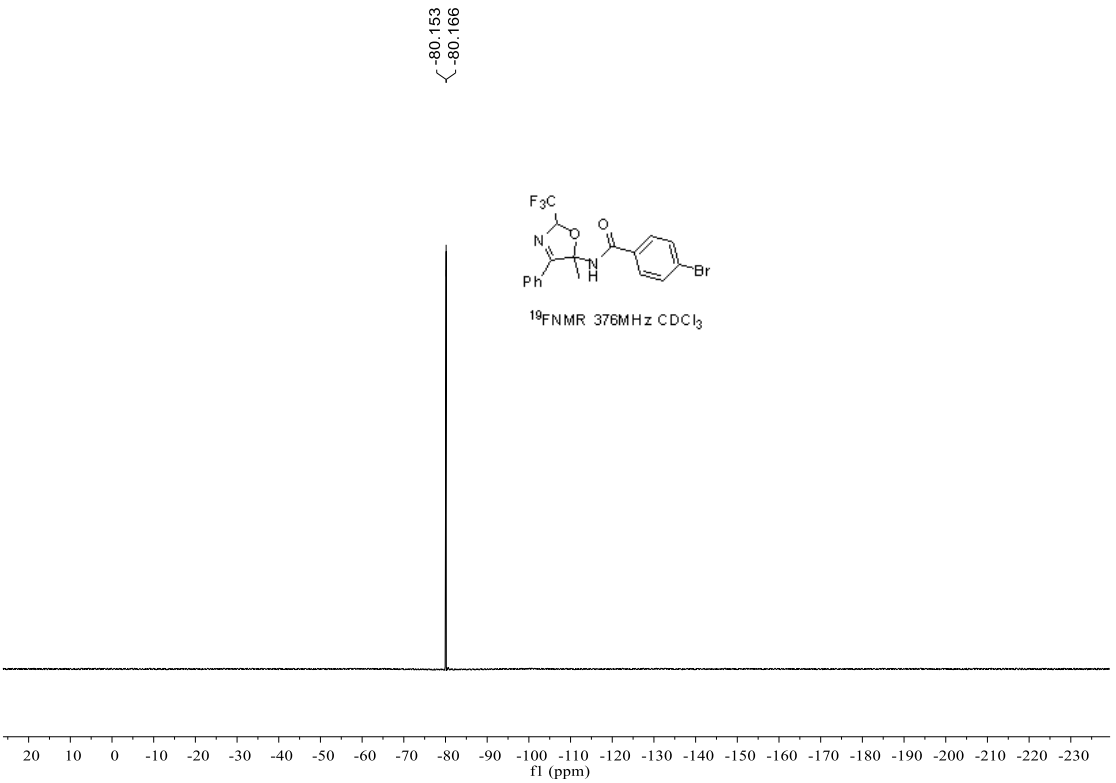
^{1}H NMR (400 MHz) spectrum of **3i** in $CDCl_3$



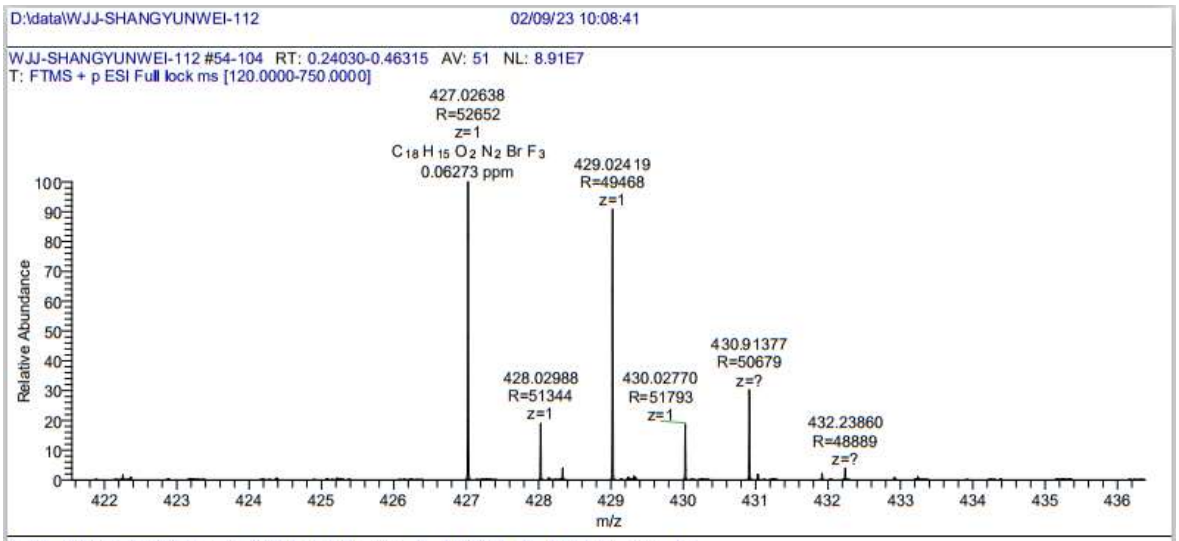
^{13}C NMR (150 MHz) spectrum of **3i** in $CDCl_3$



^{19}F NMR (376 MHz) spectrum of **3i** in $CDCl_3$



HRMS(ESI) copy of compound **3i**:

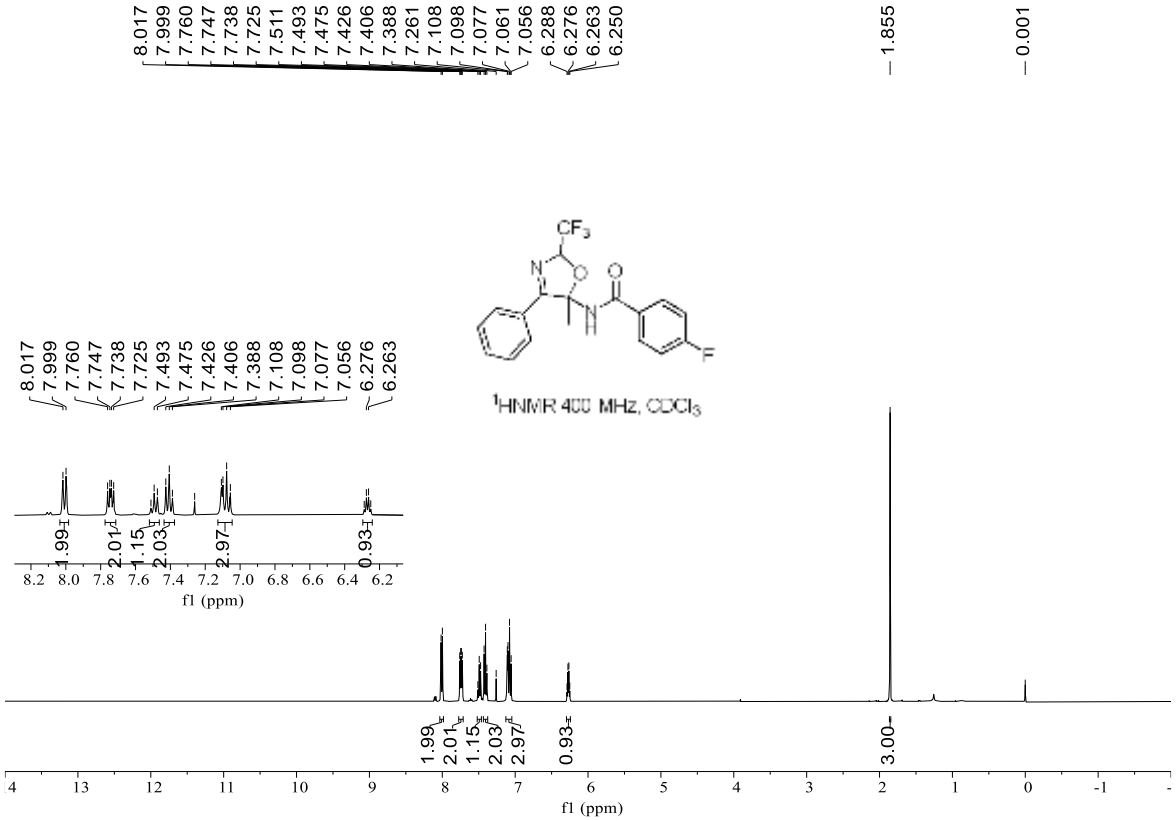


WJJ-SHANGYUNWEI-112#54-104 RT: 0.24030-0.46315 AV: 51
T: FTMS + p ESI Full lock ms [120.0000-750.0000]
m/z= 421.55170-436.38016

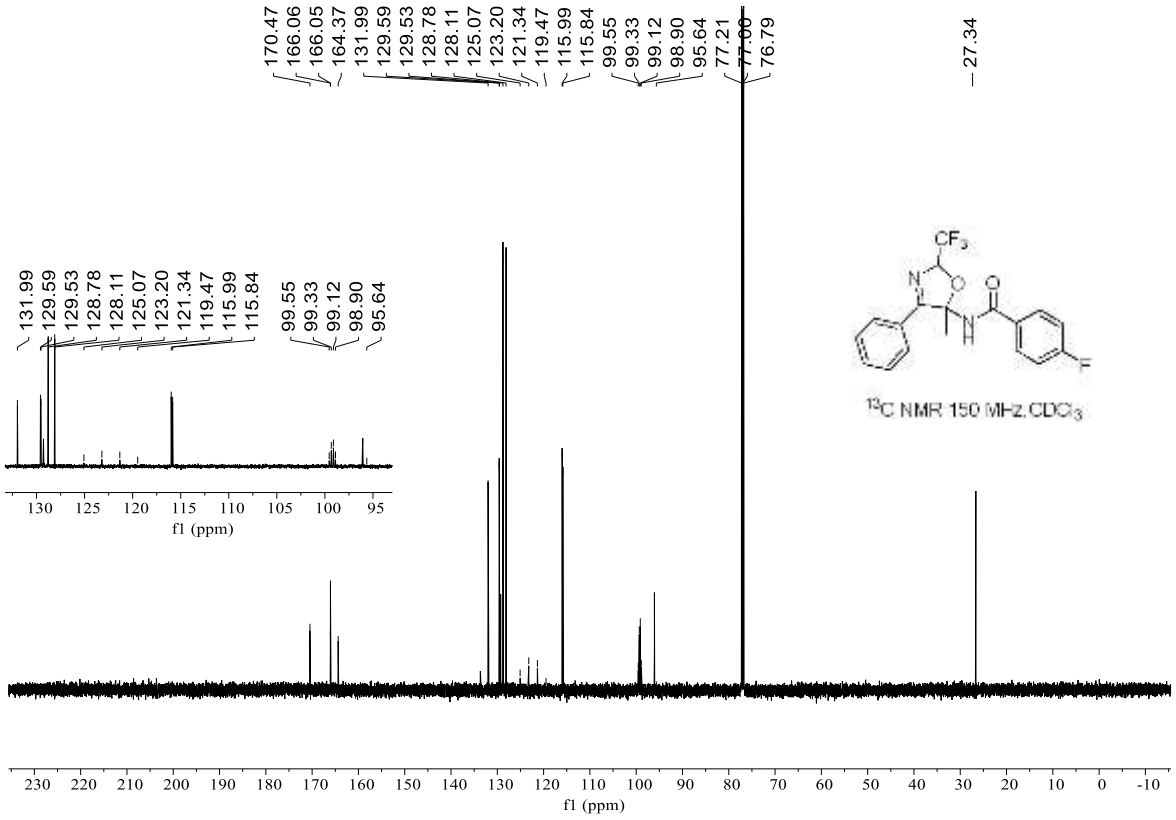
m/z	Intensity	Relative	Resolution	Charge	Delta (ppm)	Composition
427.02638	89150704.0	100.00	52651.89	1.00	0.06	$C_{18}H_{15}O_2N_2BrF_3$
428.02988	17049750.0	19.12	51343.92	1.00		
429.02419	84081136.0	94.31	49468.09	1.00		
430.02770	16679559.0	18.71	51792.79	1.00		
430.91377	27516066.0	30.86	50678.77	0.00		

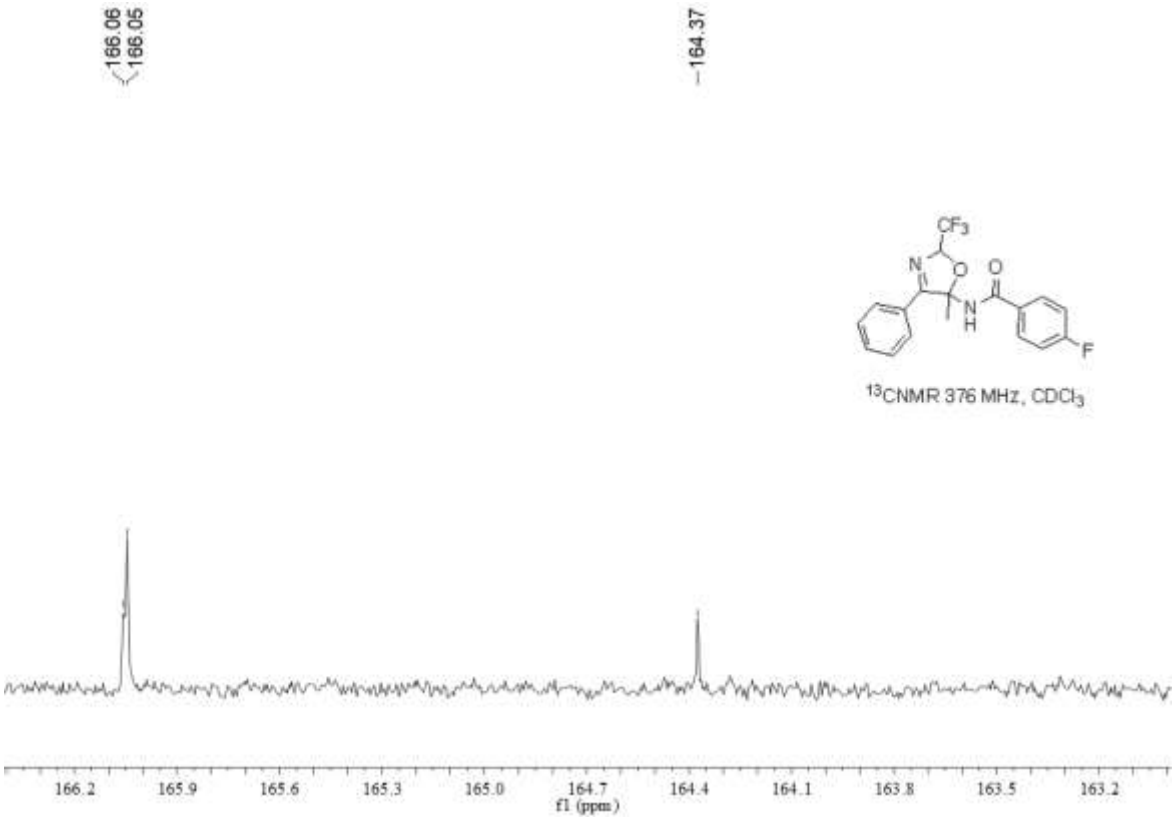
NMR copies of compound **3j**

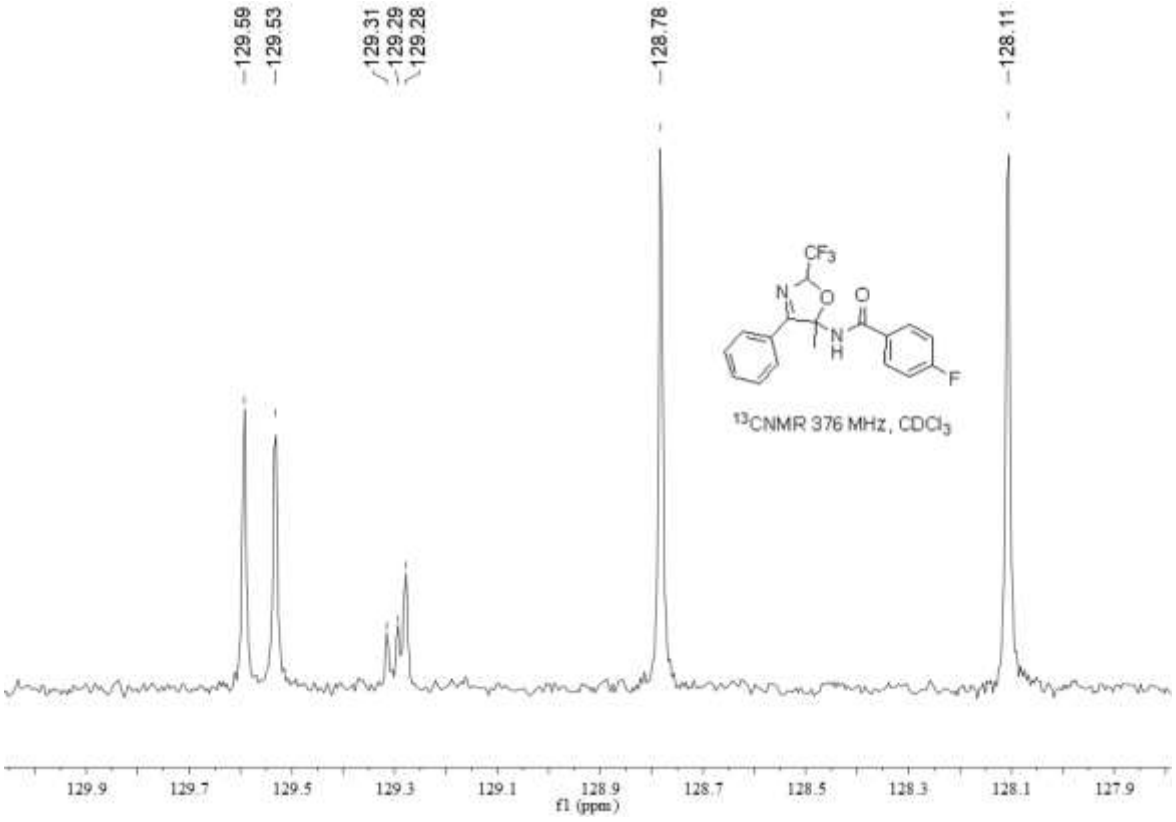
^{1}H NMR (400 MHz) spectrum of **3j** in $CDCl_3$



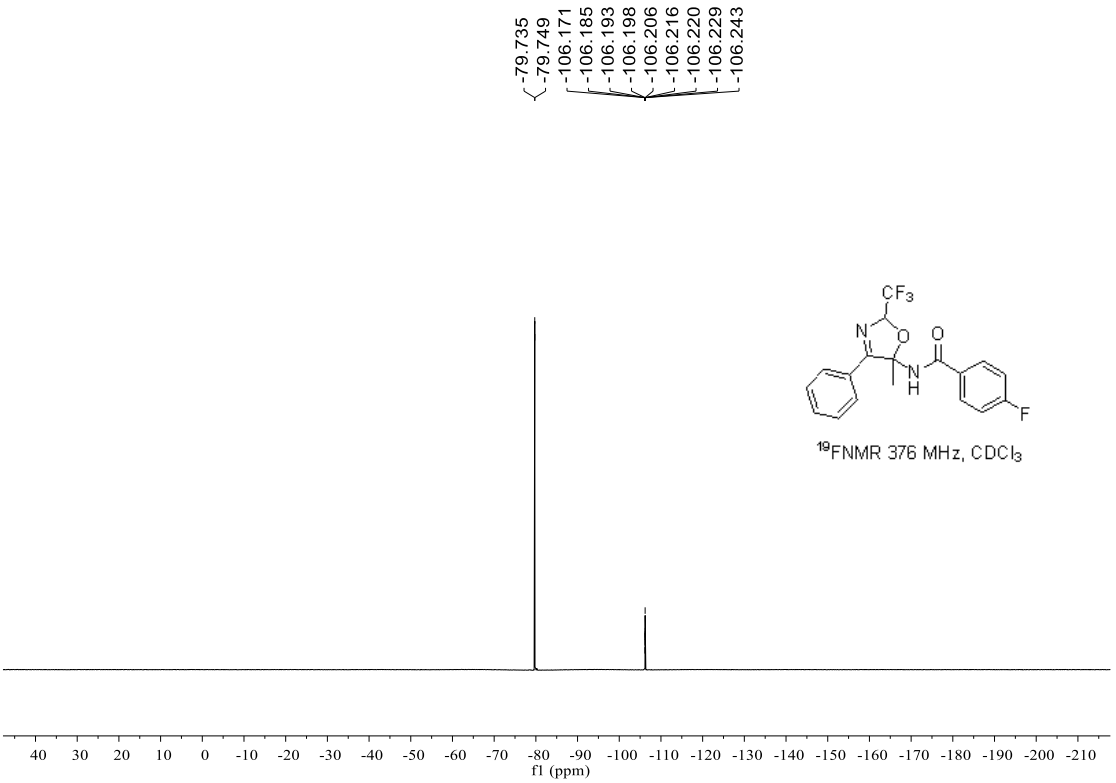
^{13}C NMR (150 MHz) spectrum of **3j** in $CDCl_3$



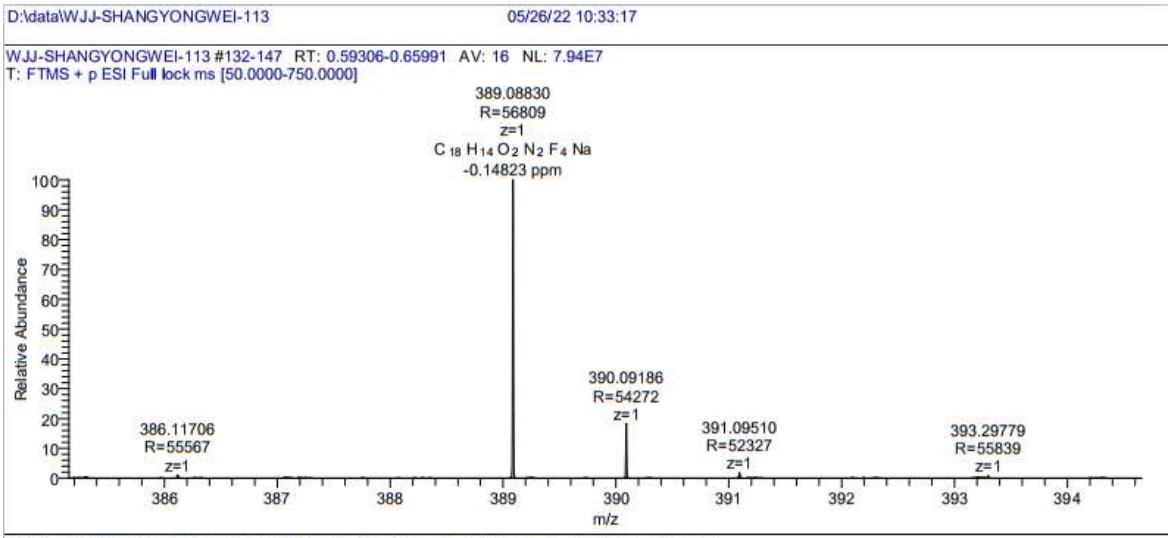

166.06
166.05
164.37
CF3
N
O
O
N
H
F
13CNMR 376 MHz, CDCl3
166.2
165.9
165.6
165.3
165.0
164.7
164.4
164.1
163.8
163.5
163.2
f1 (ppm)


129.59
129.53
129.31
129.29
129.28
128.78
128.11
CF3
N
O
O
N
H
F
13CNMR 376 MHz, CDCl3
129.9
129.7
129.5
129.3
129.1
128.9
128.7
128.5
128.3
128.1
127.9
f1 (ppm)

^{19}F NMR (376 MHz) spectrum of **3j** in $CDCl_3$



HRMS(ESI) copy of compound **3j**:

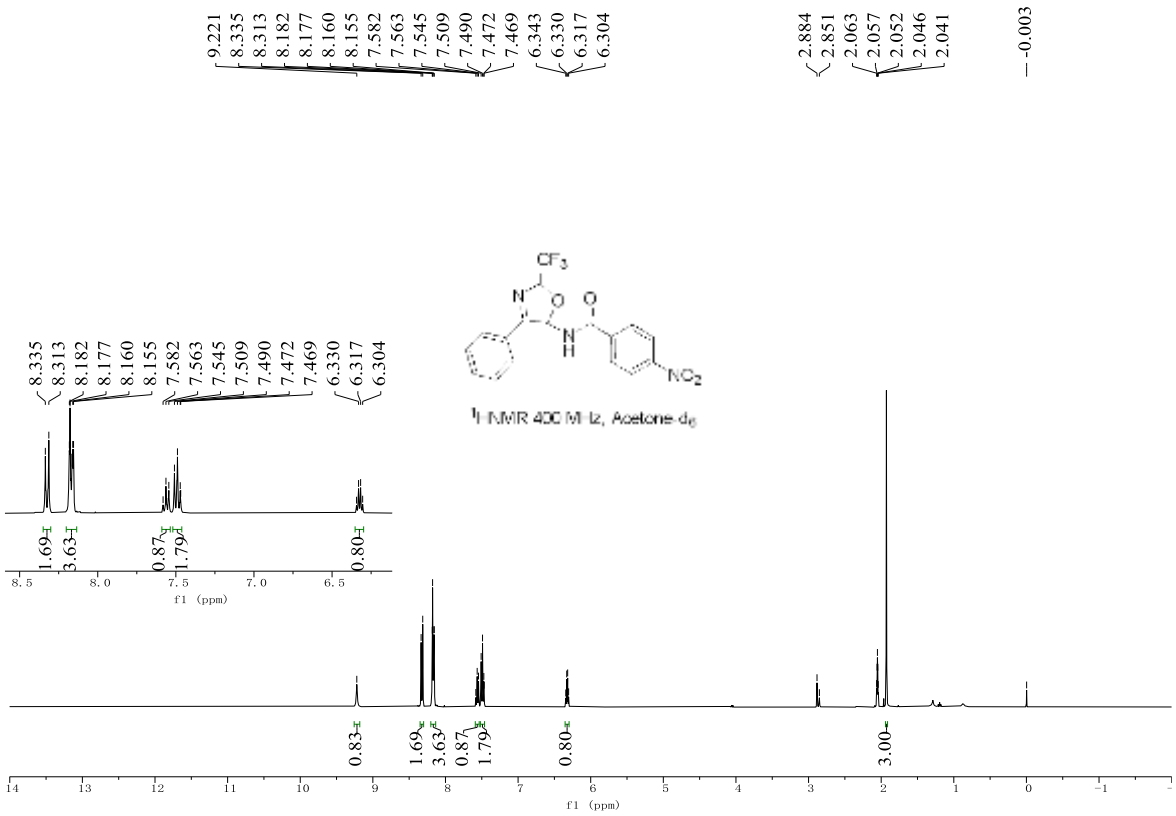


WJJ-SHANGYONGWEI-113#132-147 RT: 0.59306-0.65991 AV: 16
T: FTMS + p ESI Full lock ms [50.0000-750.0000]
m/z= 385.15349-394.65600

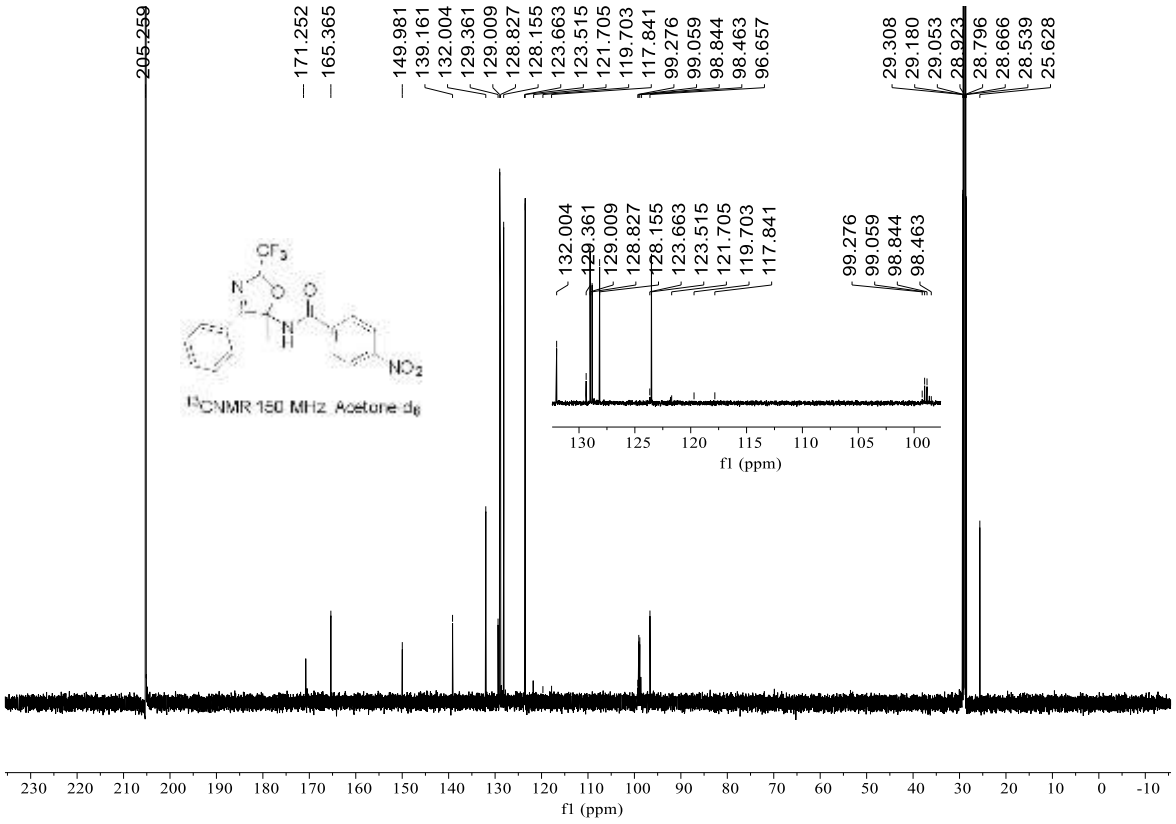
m/z	Intensity	Relative	Resolution	Charge	Delta (ppm)	Composition
386.11706	842449.1	1.06	55567.31	1.00		
389.08830	79728512.0	100.00	56809.22	1.00	-0.15	$C_{18}H_{14}O_2N_2F_4Na$
390.09186	15040360.0	18.86	54271.52	1.00		
391.09510	1459823.5	1.83	52327.50	1.00		
393.29779	604847.4	0.76	55839.39	1.00		

NMR copies of compound **3k**

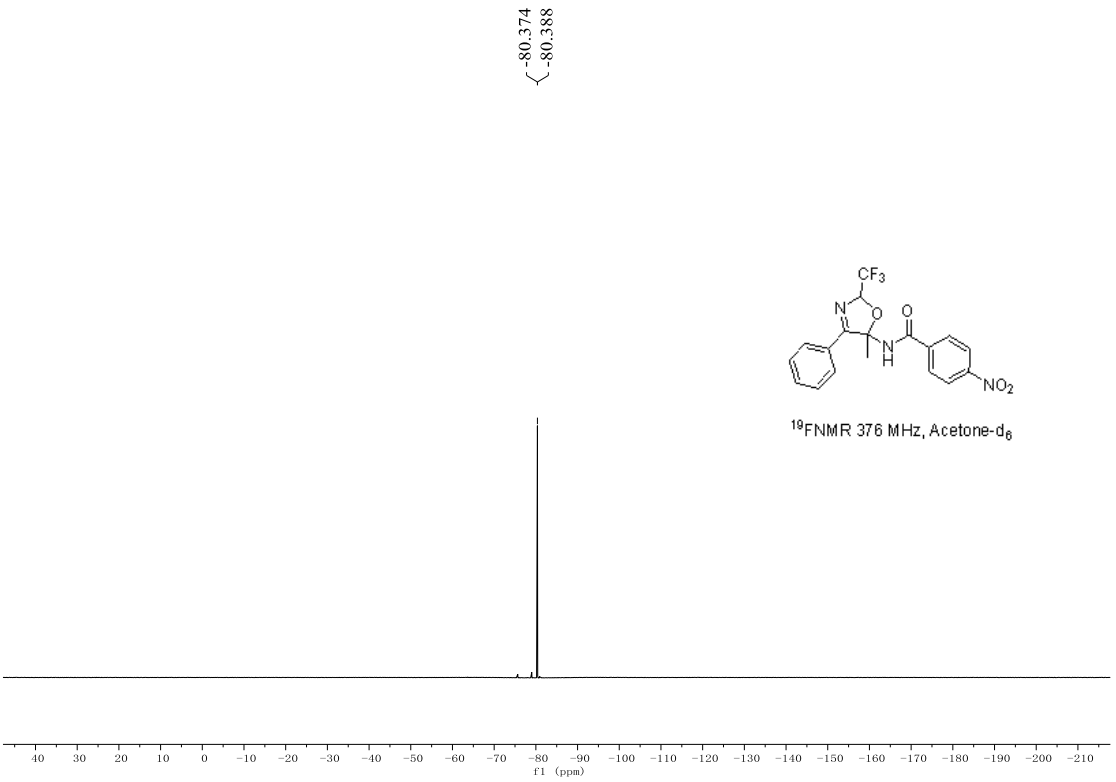
^{1}H NMR (400 MHz) spectrum of **3k** in acetone-d_6



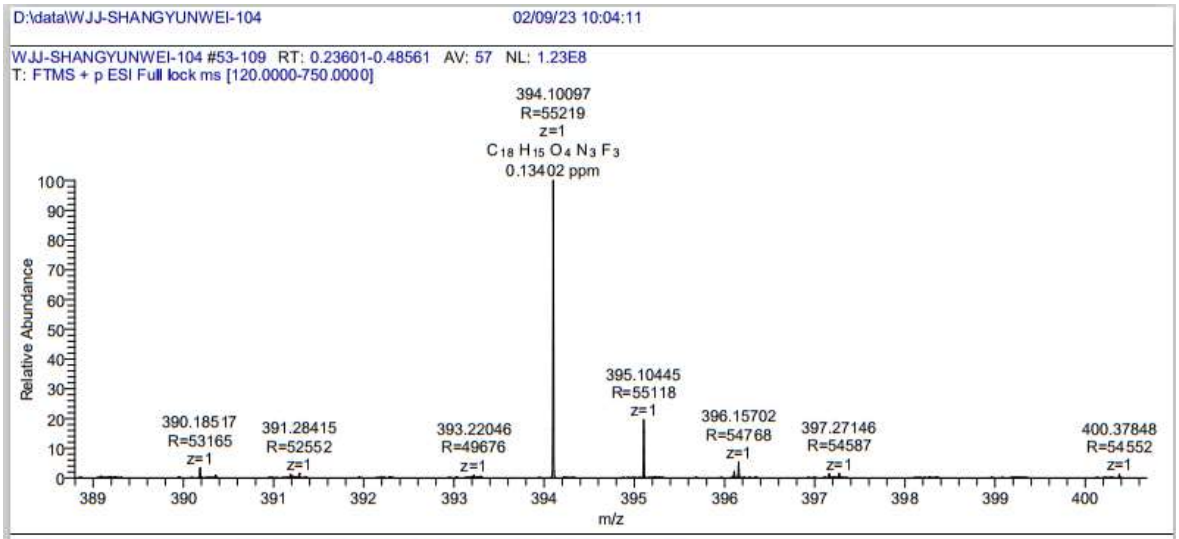
^{13}C NMR (150 MHz) spectrum of **3k** in acetone-d_6



^{19}F NMR (376 MHz) spectrum of **3k** in acetone-d_6



HRMS(ESI) copy of compound **3k**:

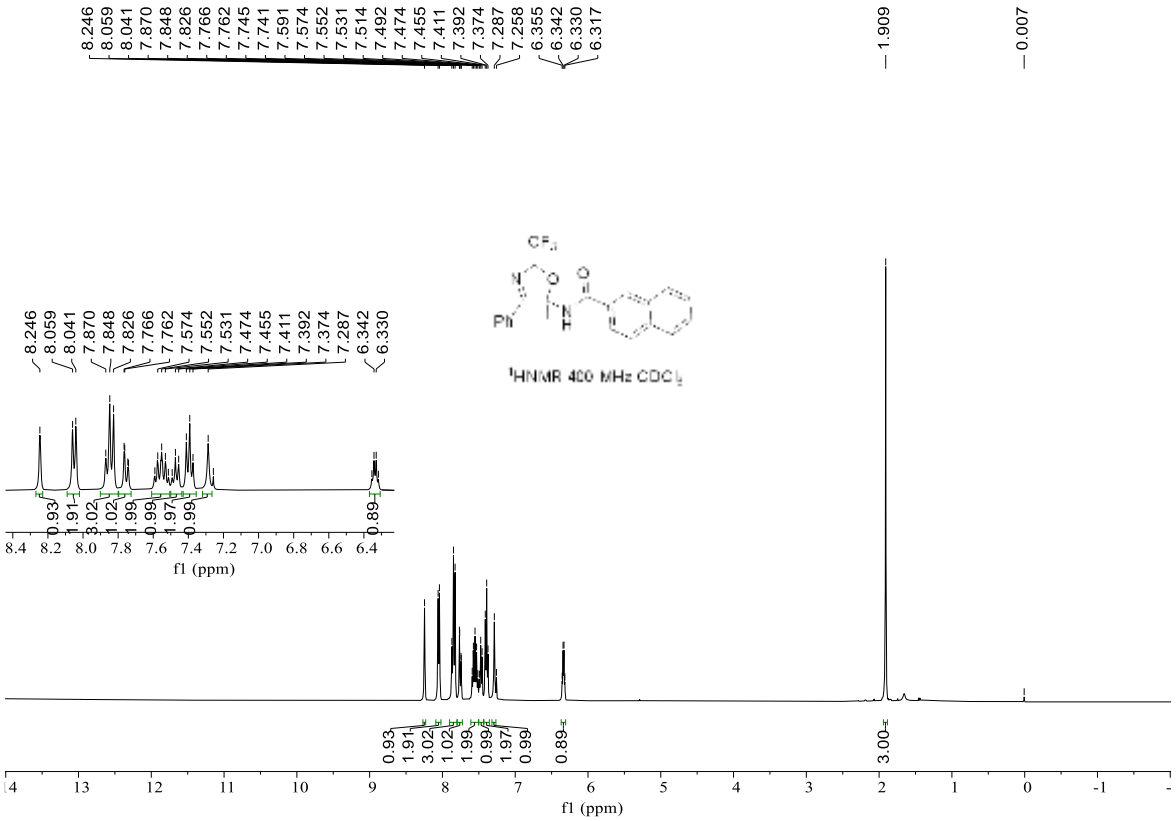


WJJ-SHANGYUNWEI-104#53-109 RT: 0.23601-0.48561 AV: 57
T: FTMS + p ESI Full lock ms [120.0000-750.0000]
m/z= 388.79535-400.67855

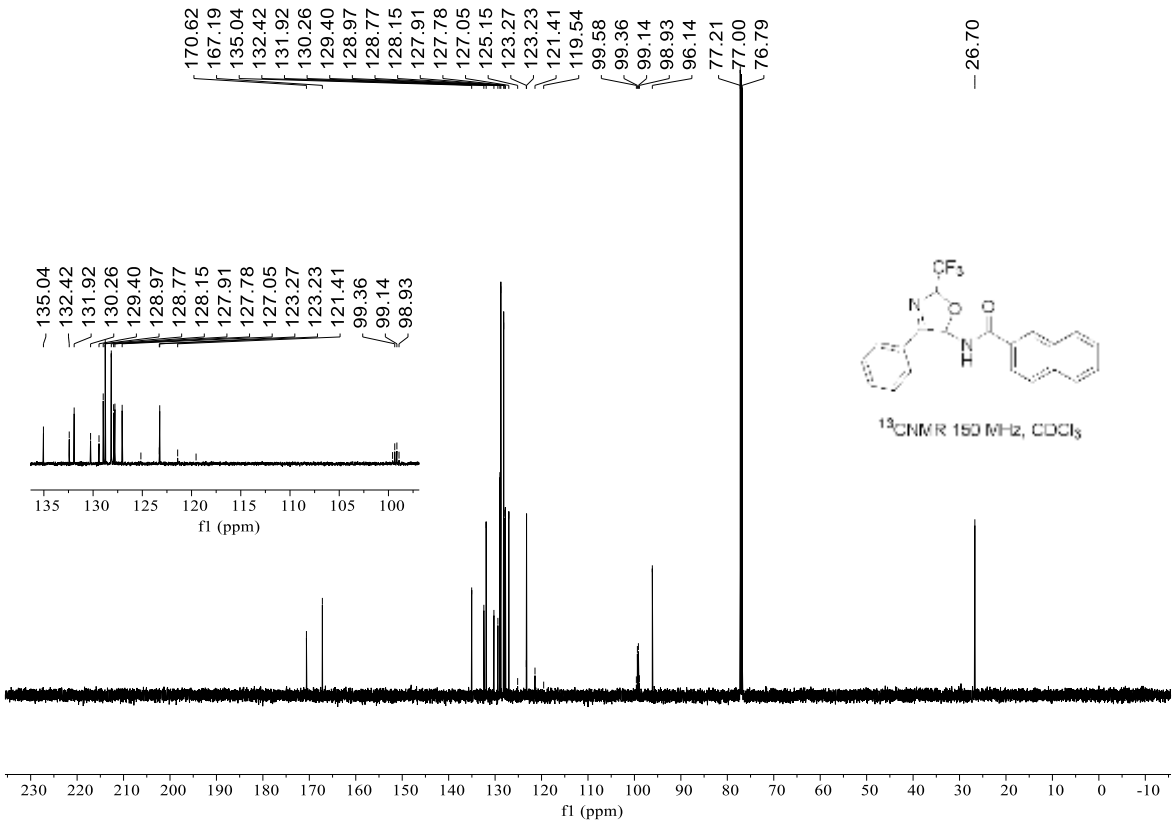
m/z	Intensity	Relative	Resolution	Charge	Delta (ppm)	Composition
390.18517	4251845.0	3.46	53165.34	1.00		
394.10097	123037960.0	100.00	55218.82	1.00	0.13	$C_{18}H_{15}O_4N_3F_3$
395.10445	24071150.0	19.56	55118.33	1.00		
396.10702	2703822.0	2.20	50914.39	1.00		
396.15702	6568107.0	5.34	54767.62	1.00		

NMR copies of compound **3l**

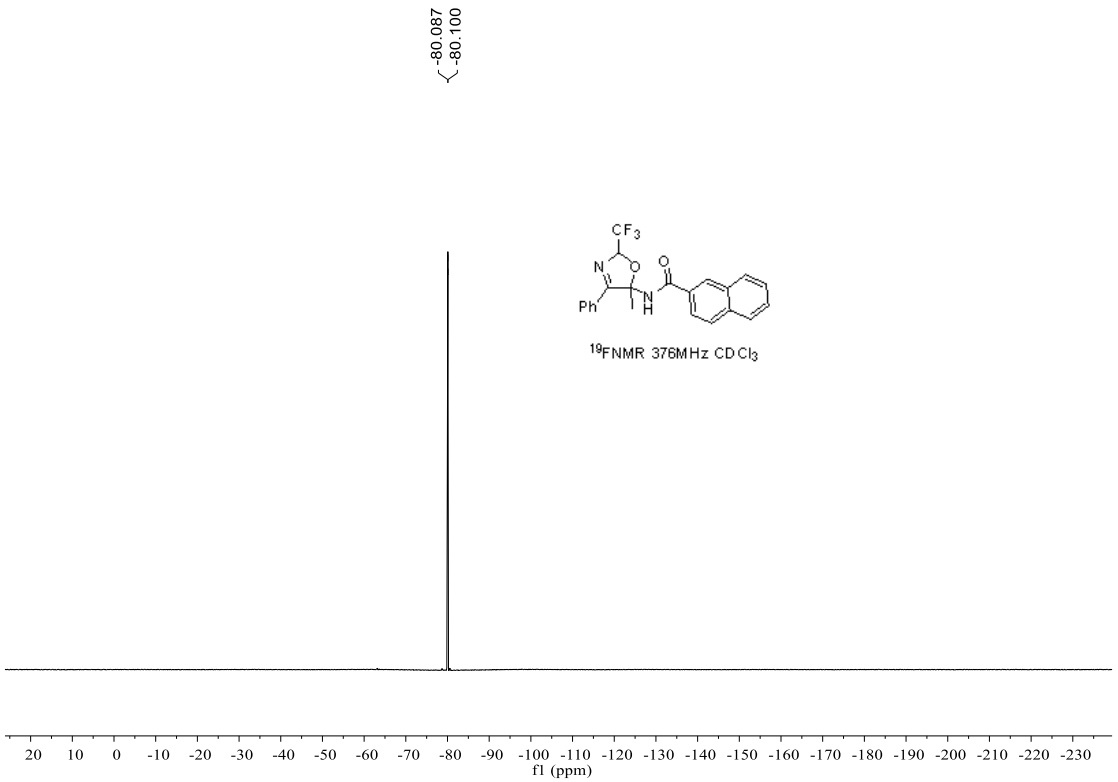
^{1}H NMR (400 MHz) spectrum of **3l** in $CDCl_3$



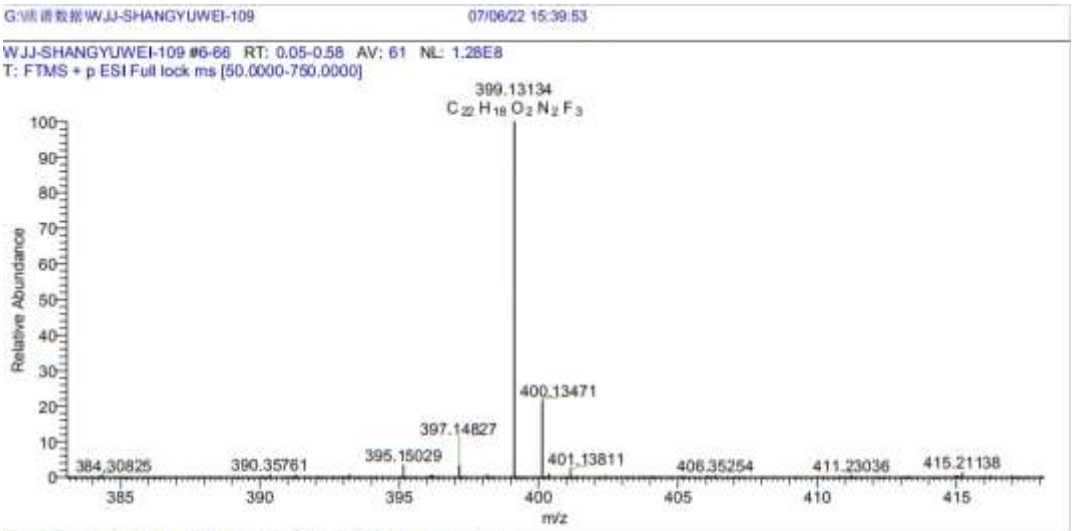
^{13}C NMR (150 MHz) spectrum of **3l** in $CDCl_3$



^{19}F NMR (376 MHz) spectrum of **3l** in $CDCl_3$



HRMS(ESI) copy of compound **3l**:

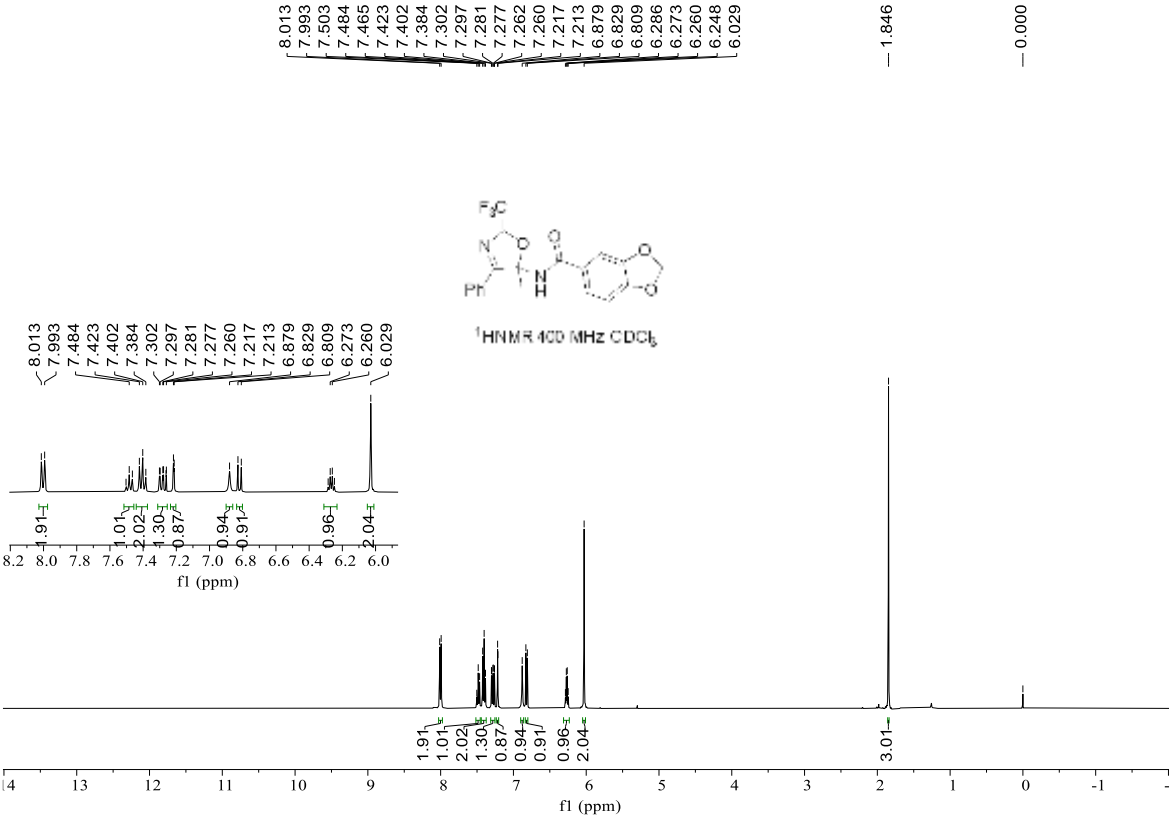


WJJ-SHANGYUWEI-109#6-66 RT: 0.05-0.58 AV: 61
T: FTMS + p ESI Full lock ms [50.0000-750.0000]
m/z= 383.07369-418.09880

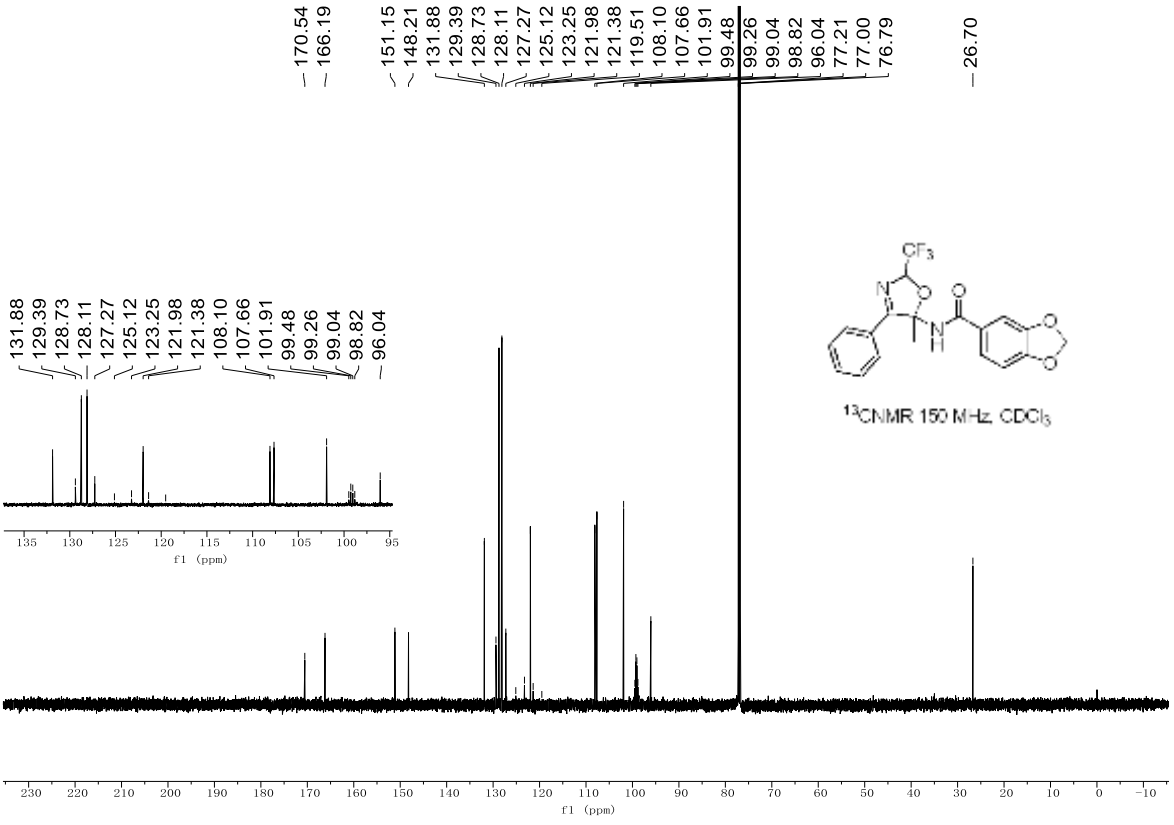
m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
395.15029	4564603.5	3.57				
397.14827	4417474.5	3.46				
399.13134	127729920.0	100.00	399.13149	-0.14	13.5	$C_{22}H_{18}O_2N_2F_3$
400.13471	28537116.0	22.34				
401.13811	2979034.8	2.33				

NMR copies of compound **3m**

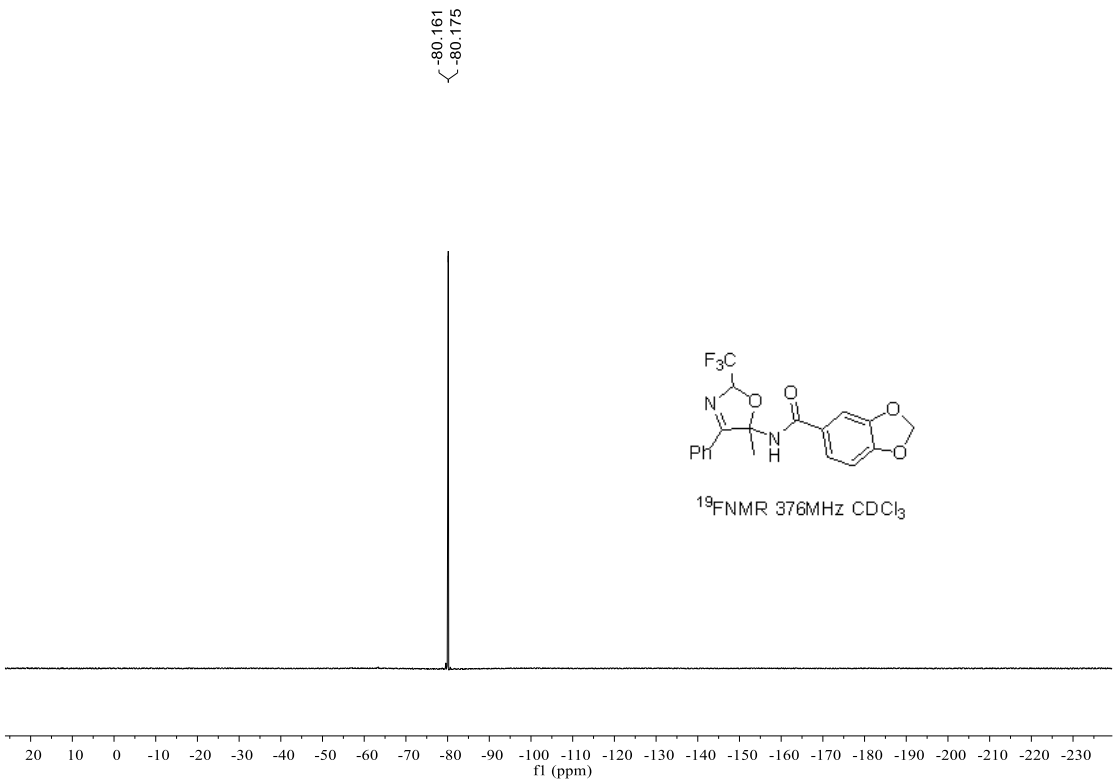
^{1}H NMR (400 MHz) spectrum of **3m** in $CDCl_3$



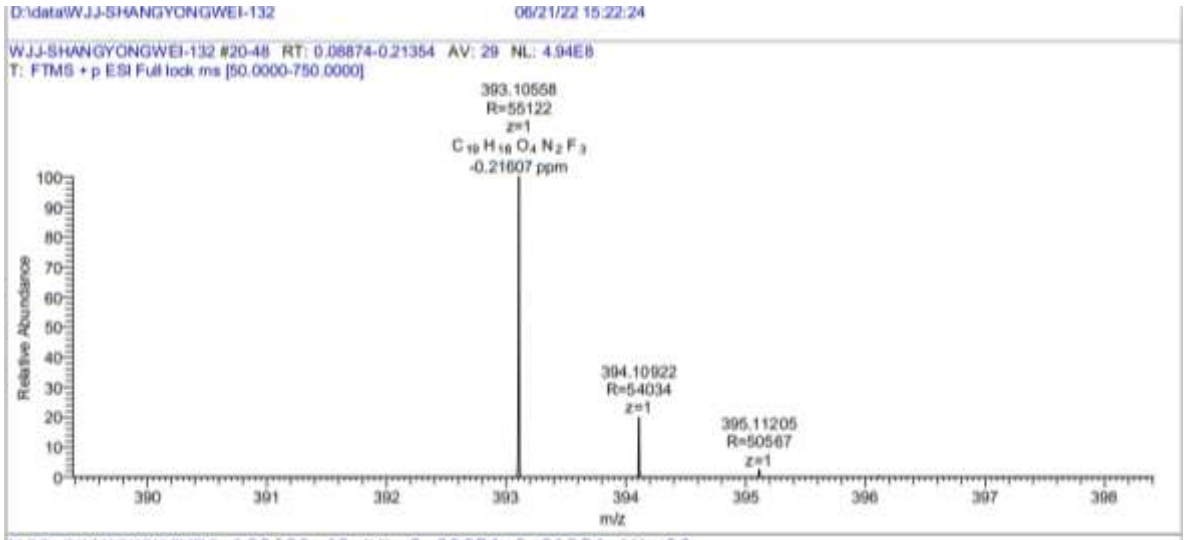
^{13}C NMR (150 MHz) spectrum of **3m** in $CDCl_3$



^{19}F NMR (376 MHz) spectrum of **3m** in $CDCl_3$



HRMS(ESI) copy of compound **3m**:

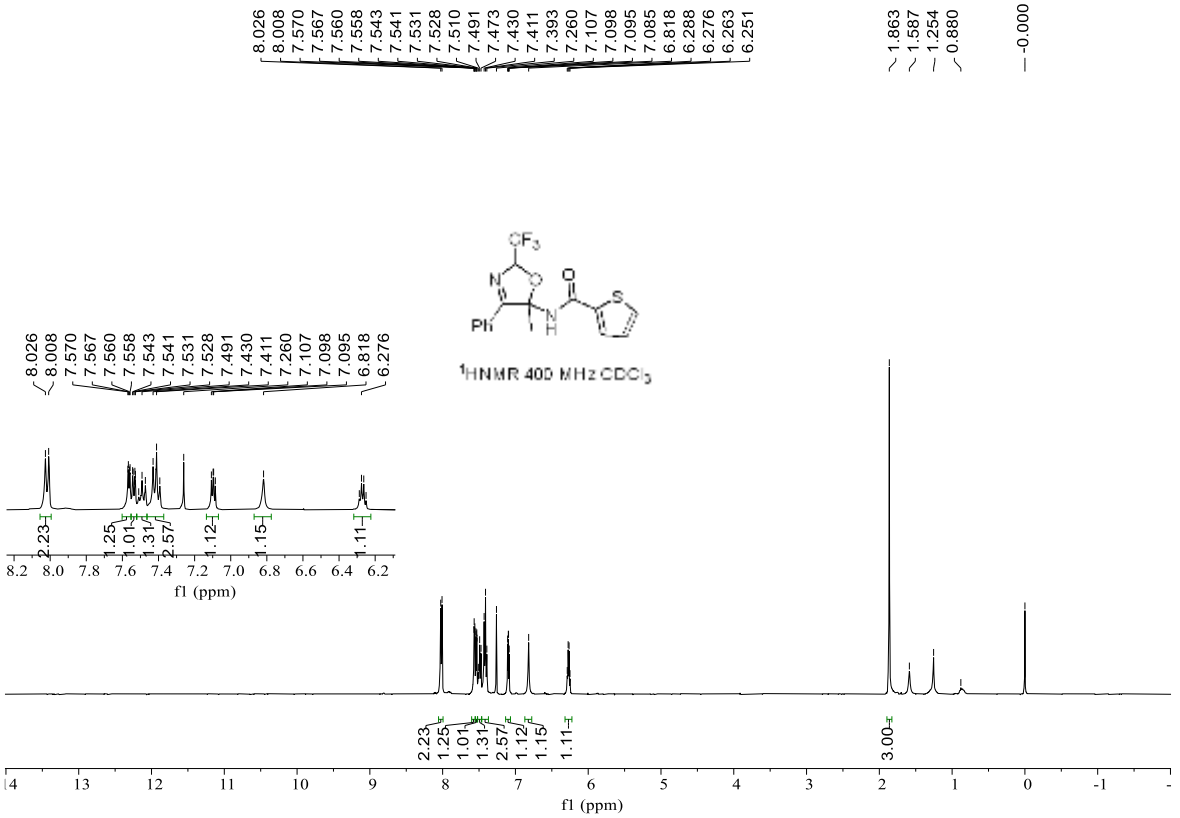


WJJ-SHANGYONGWEI-132#20-48 RT: 0.08874-0.21354 AV: 29
T: FTMS + p ESI Full lock ms [50.0000-750.0000]
m/z= 389.37710-398.41002

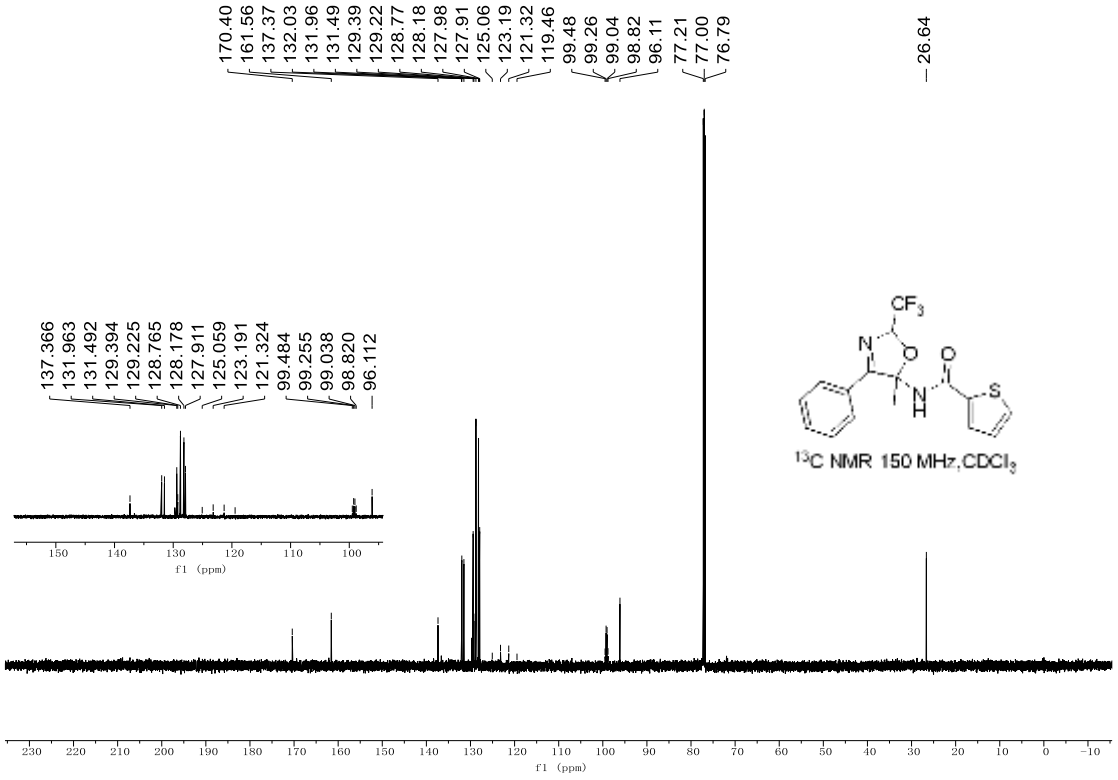
m/z	Intensity	Relative	Resolution	Charge	Delta (ppm)	Composition
393.10558	497614880.0	100.00	55122.33	1.00	-0.22	$C_{19}H_{16}O_4N_2F_3$
394.10922	98838760.0	19.86	54033.99	1.00		
395.11205	12651259.0	2.54	50567.01	1.00		
396.11400	1449083.3	0.29	51329.19	1.00		
397.27147	829902.4	0.17	56196.65	0.00		

NMR copies of compound **3n**

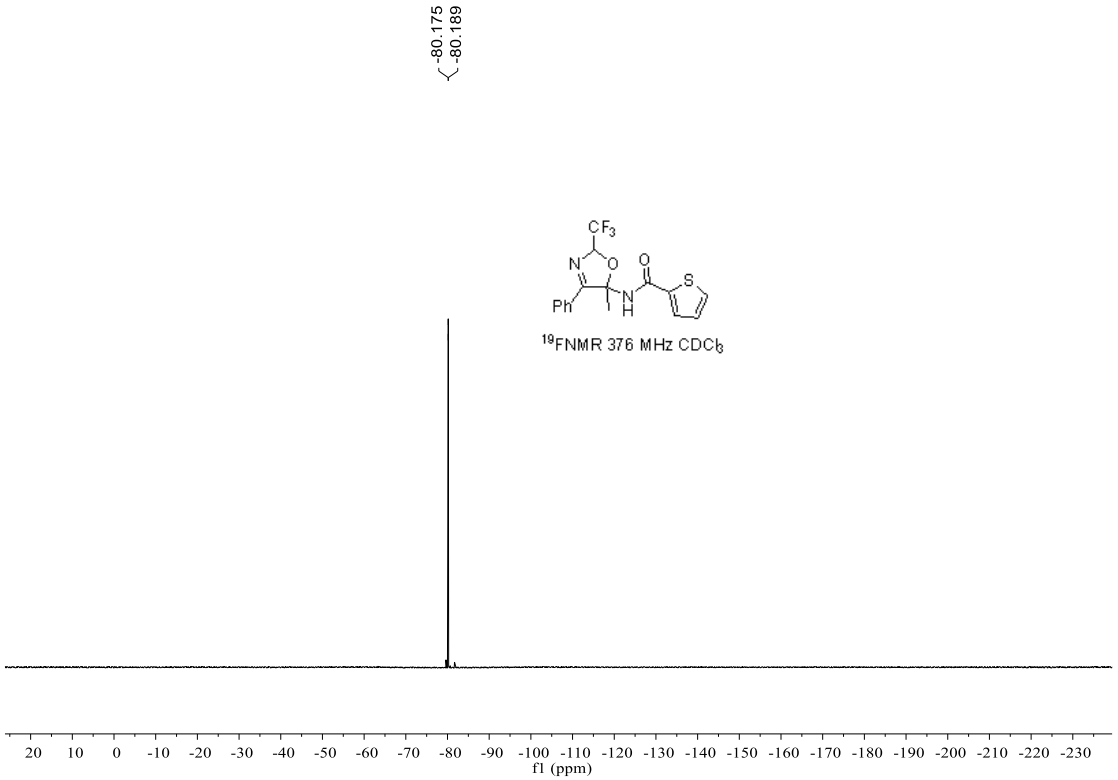
^{1}H NMR (400 MHz) spectrum of **3n** in $CDCl_3$



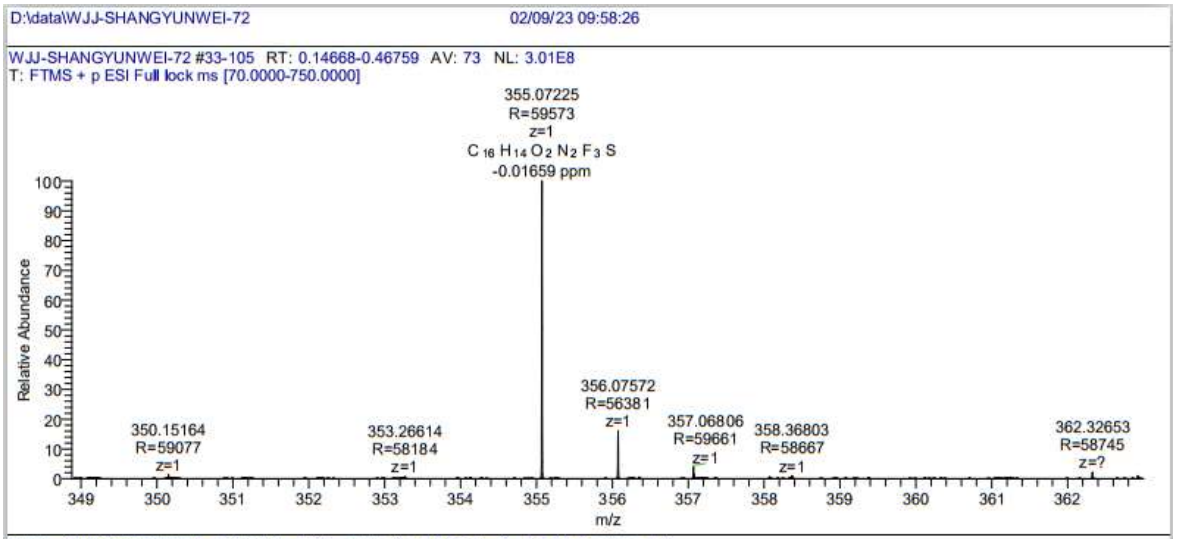
^{13}C NMR (150 MHz) spectrum of **3n** in $CDCl_3$



^{19}F NMR (376 MHz) spectrum of **3n** in $CDCl_3$



HRMS(ESI) copy of compound **3n**:

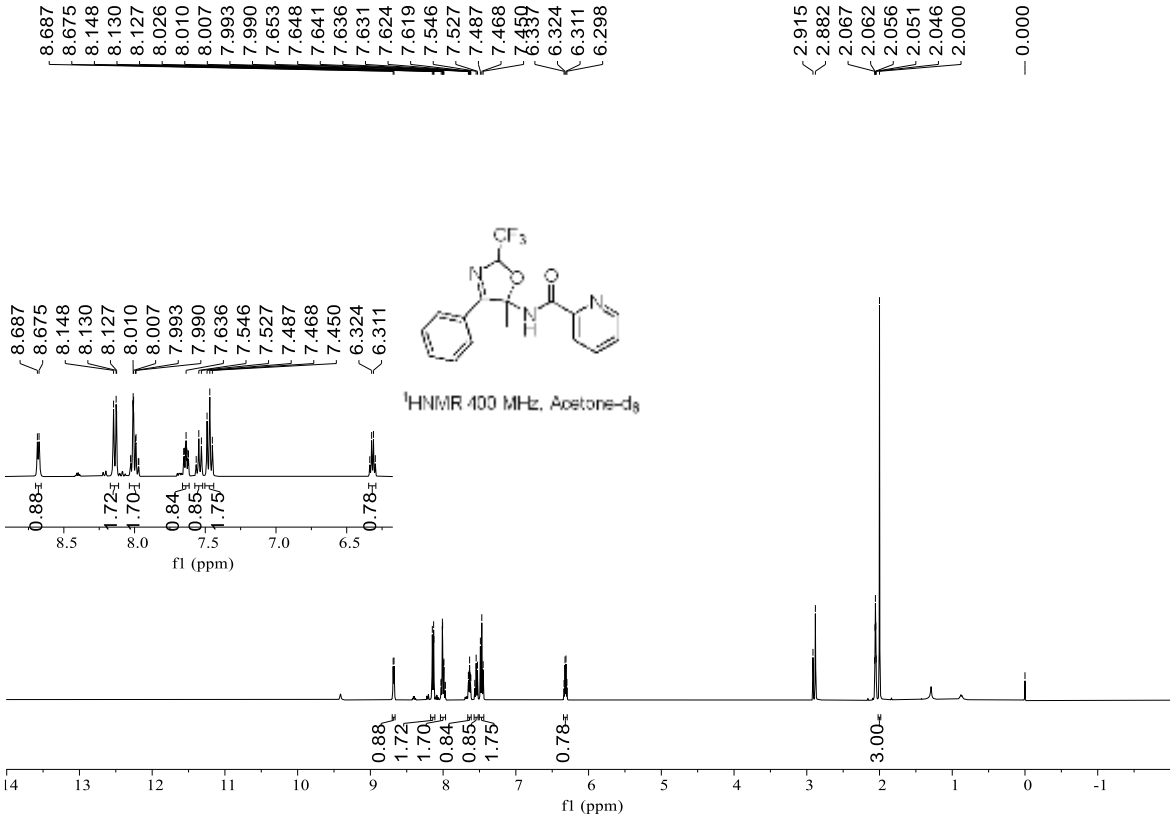


WJJ-SHANGYUNWEI-72#33-105 RT: 0.14668-0.46759 AV: 73
T: FTMS + p ESI Full lock ms [70.0000-750.0000]
m/z= 348.87689-362.99913

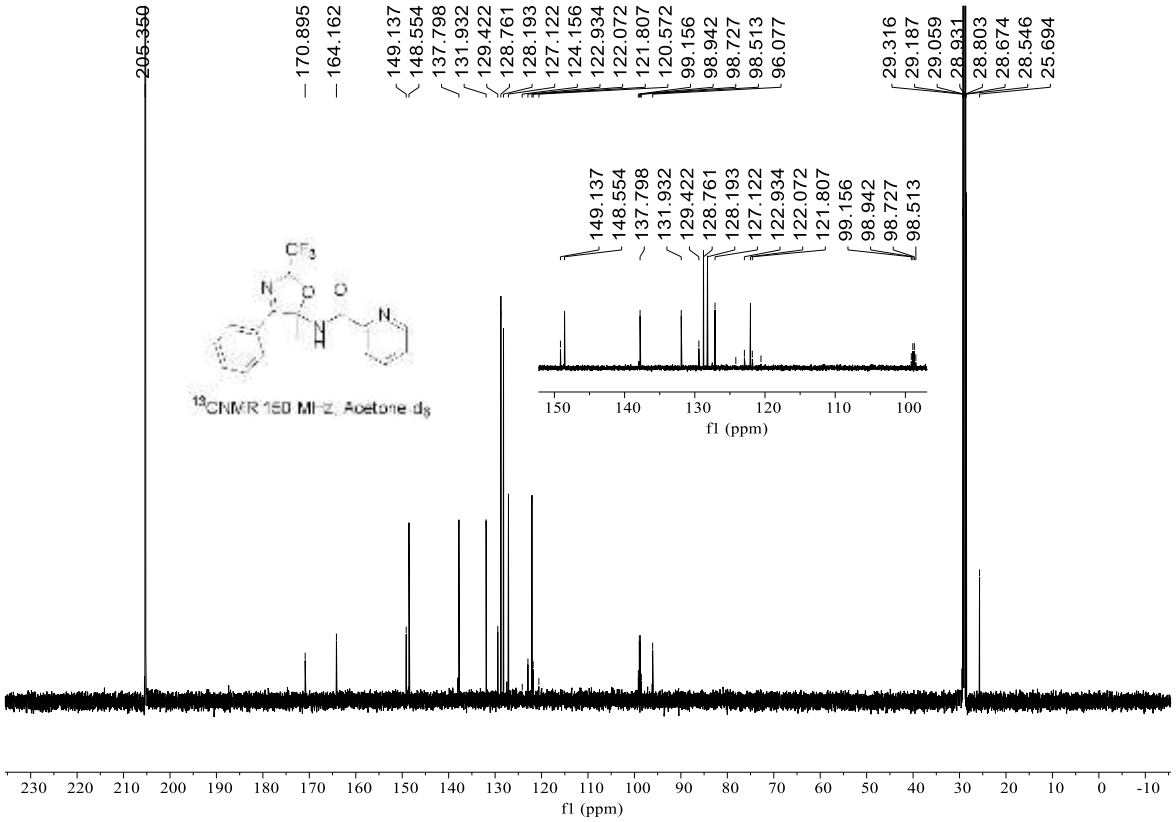
m/z	Intensity	Relative	Resolution	Charge	Delta (ppm)	Composition
355.07225	302109760.0	100.00	59573.30	1.00	-0.02	$C_{16}H_{14}O_2N_2F_3S$
356.07572	49369332.0	16.34	56381.29	1.00		
357.06806	12174908.0	4.03	59661.25	1.00		
357.07861	4258448.5	1.41	54849.52	1.00		
362.32653	6604996.0	2.19	58745.28	0.00		

NMR copies of compound **3o**

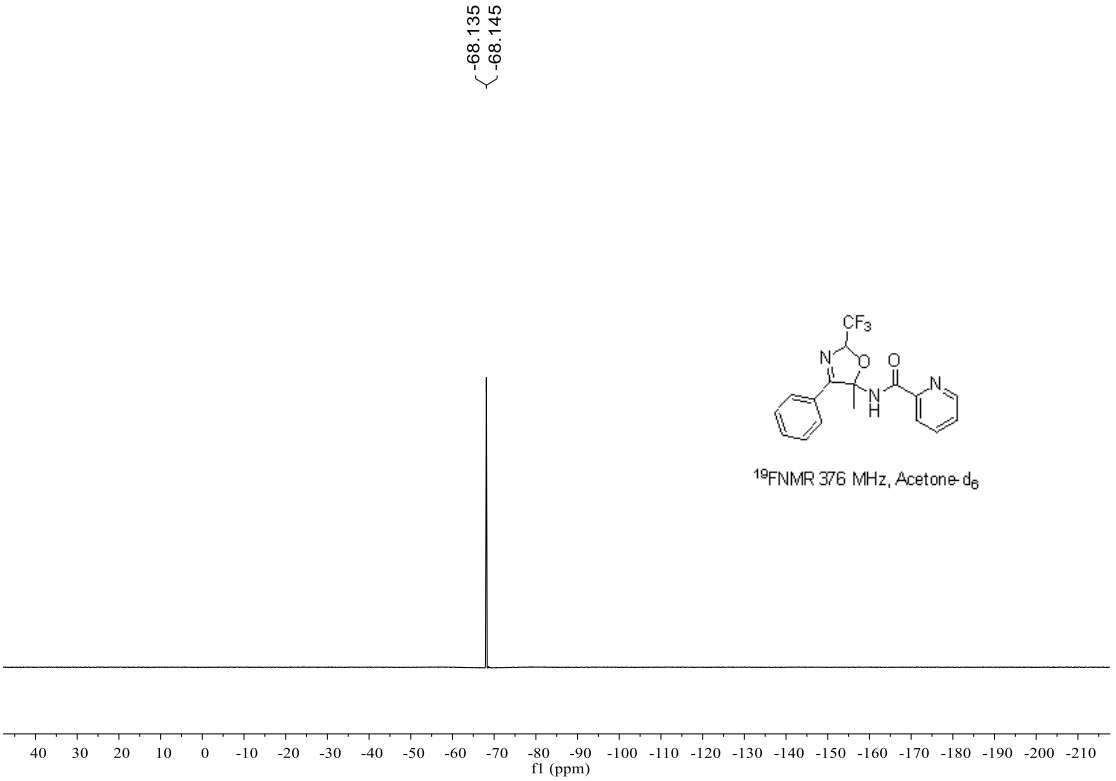
^{1}H NMR (400 MHz) spectrum of **3o** in acetone-d_6



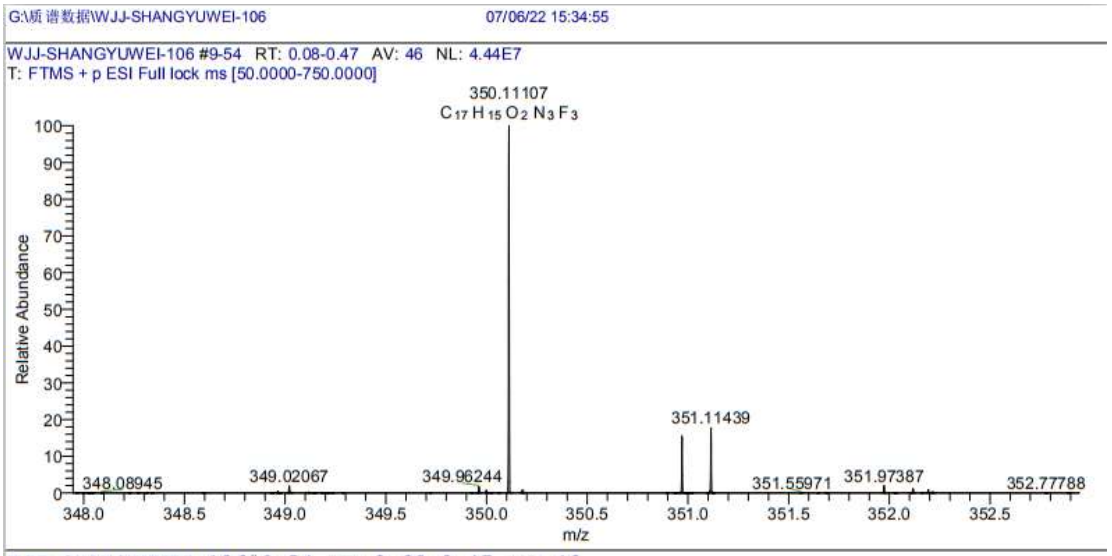
^{13}C NMR (150 MHz) spectrum of **3o** in acetone-d_6



^{19}F NMR (376 MHz) spectrum of **3o** in acetone-d_6



HRMS(ESI) copy of compound **3o**:

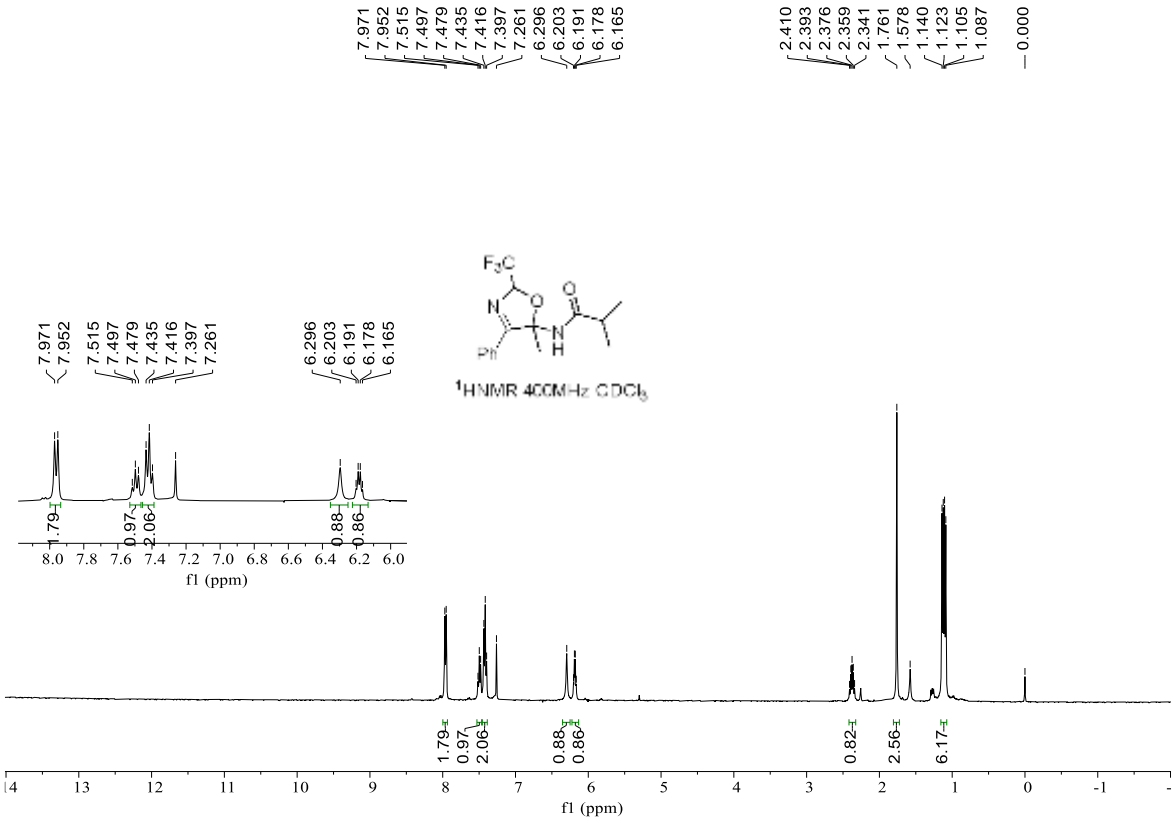


WJJ-SHANGYUWEI-106#9-54 RT: 0.08-0.47 AV: 46
T: FTMS + p ESI Full lock ms [50.0000-750.0000]
m/z= 347.94637-352.94254

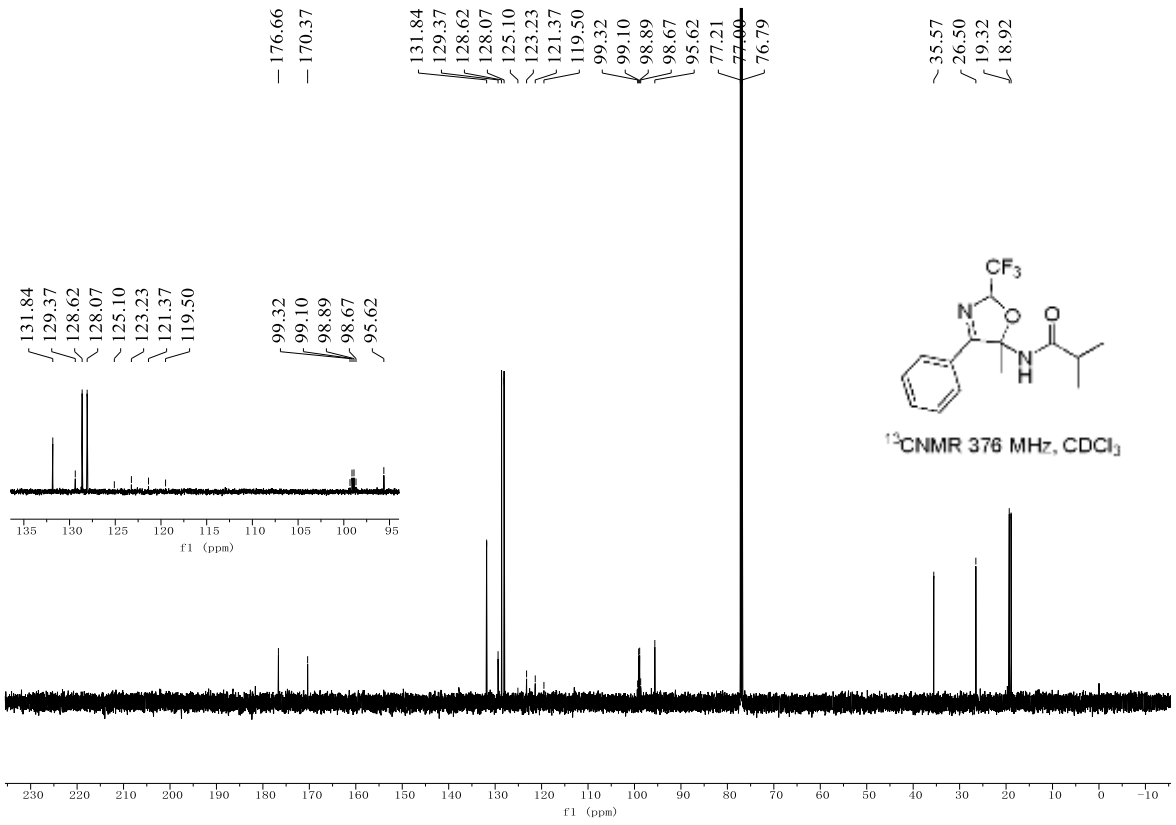
m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
349.02067	849692.1	1.89			
350.11107	44897304.0	100.00	350.11109	-0.01	$C_{17}H_{15}O_2N_3F_3$
350.97054	7008661.0	15.61			
351.11439	7916652.0	17.63			
351.97387	884980.6	1.97			

NMR copies of compound **3q**

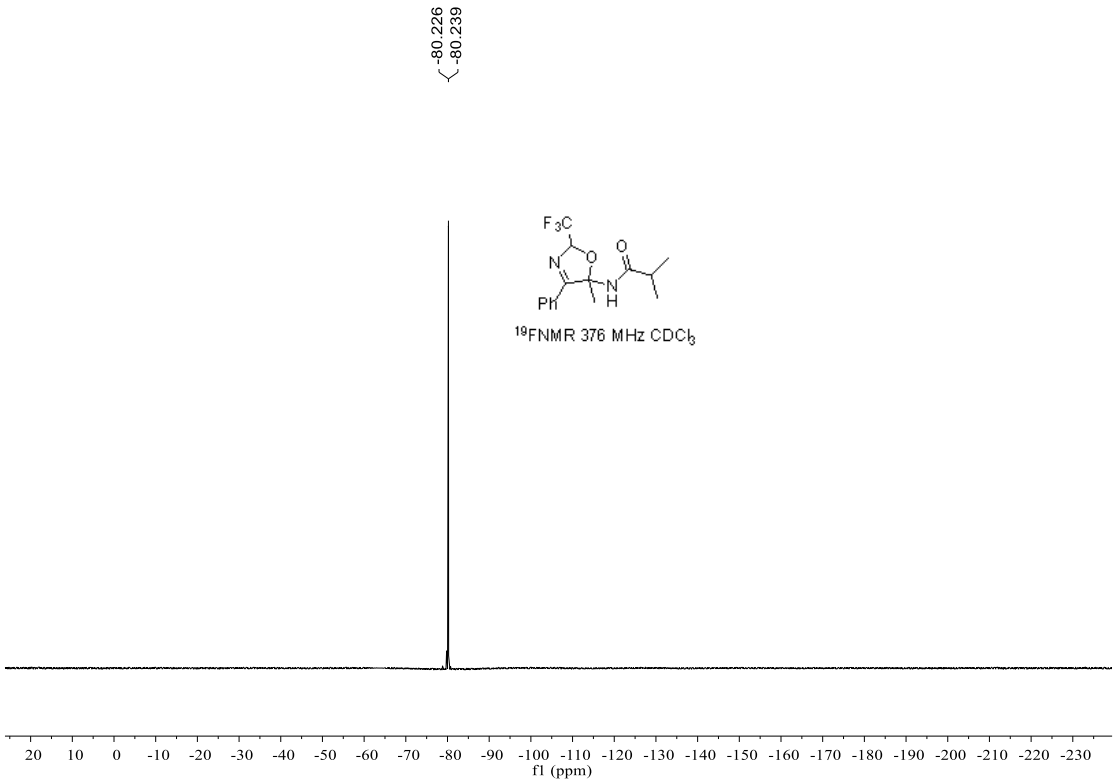
^{1}H NMR (400 MHz) spectrum of **3q** in $CDCl_3$



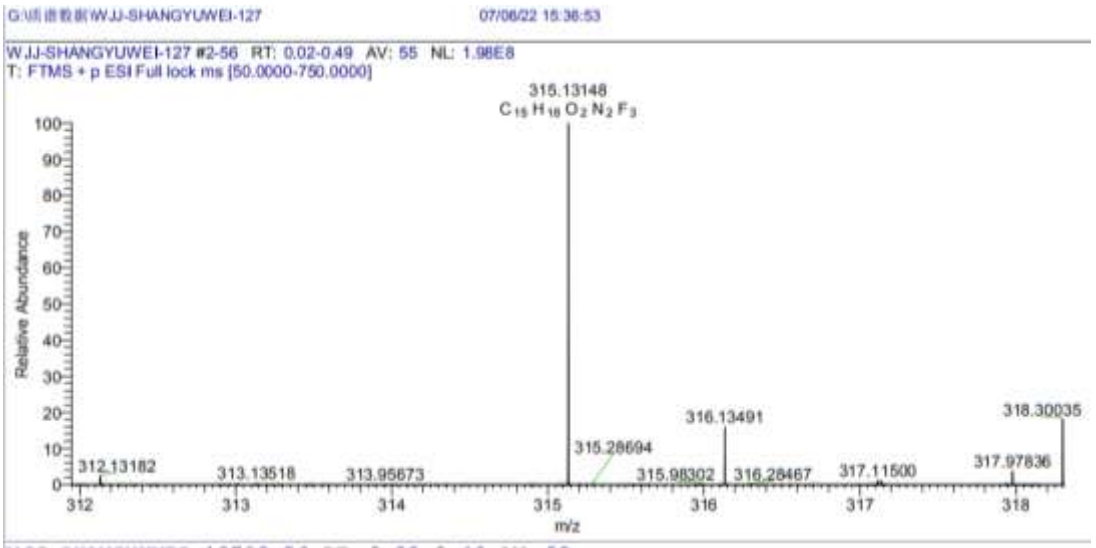
^{13}C NMR (150 MHz) spectrum of **3r** in $CDCl_3$



^{19}F NMR (376 MHz) spectrum of **3q** in $CDCl_3$



HRMS(ESI) copy of compound **3q**:

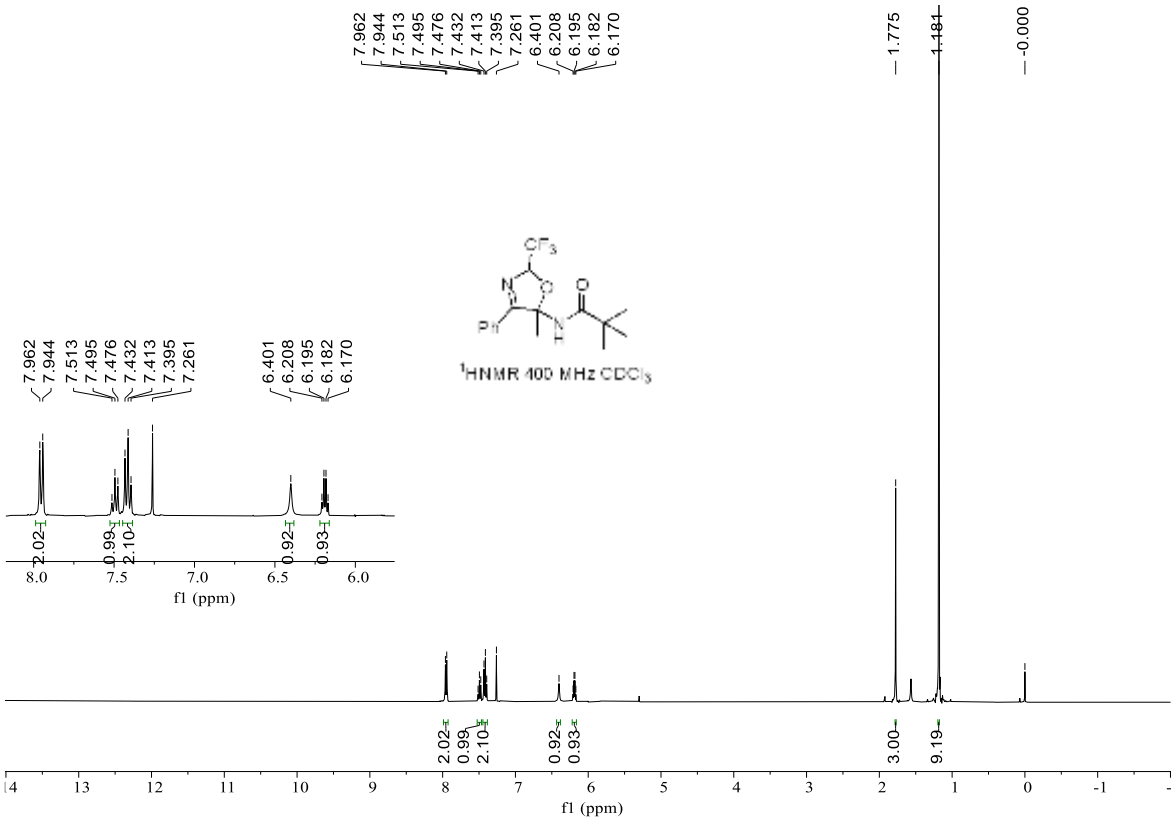


WJJ-SHANGYUWEI-127#2-56 RT: 0.02-0.49 AV: 55
T: FTMS + p ESI Full lock ms [50.0000-750.0000]
m/z= 311.94808-318.30556

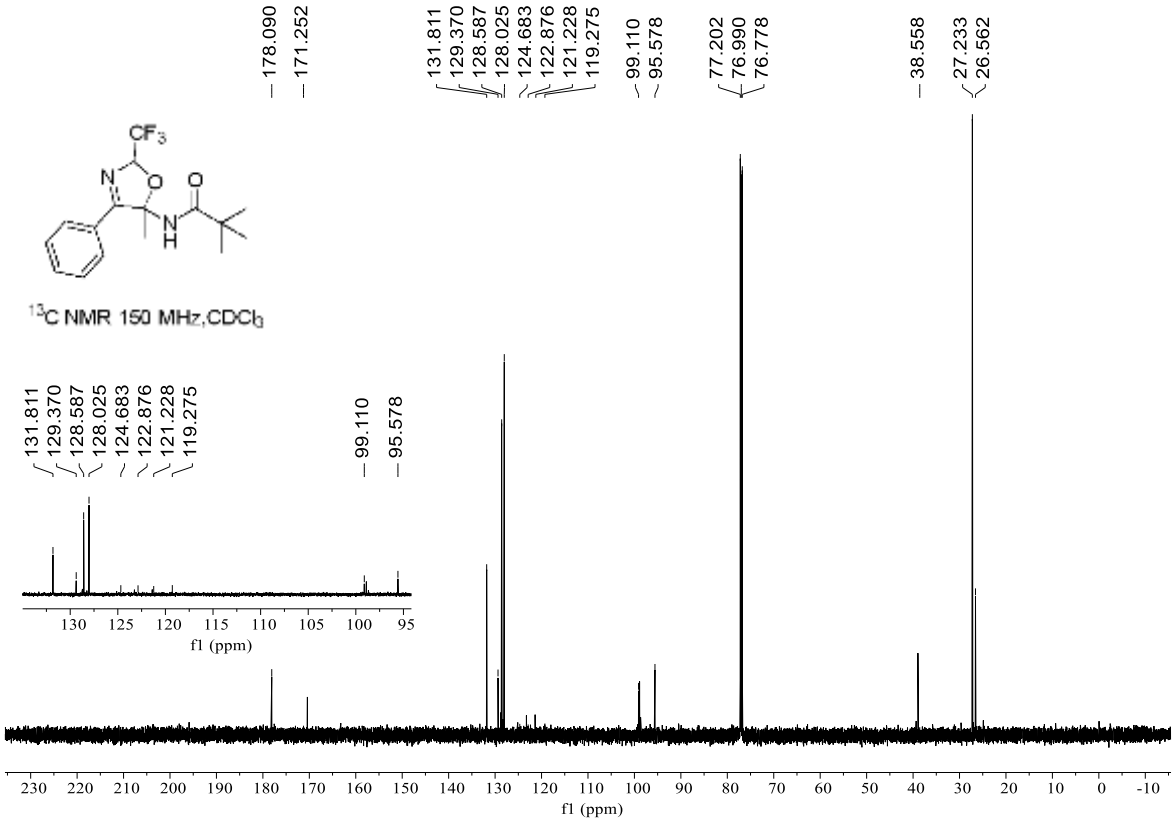
m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
312.13182	4650113.0	2.28			
315.13148	203976704.0	100.00	315.13149	-0.00	$C_{15}H_{18}O_2N_2F_3$
316.13491	31663874.0	15.52			
317.97836	7214477.5	3.54			
318.30035	36132696.0	17.71			

NMR copies of compound **3r**

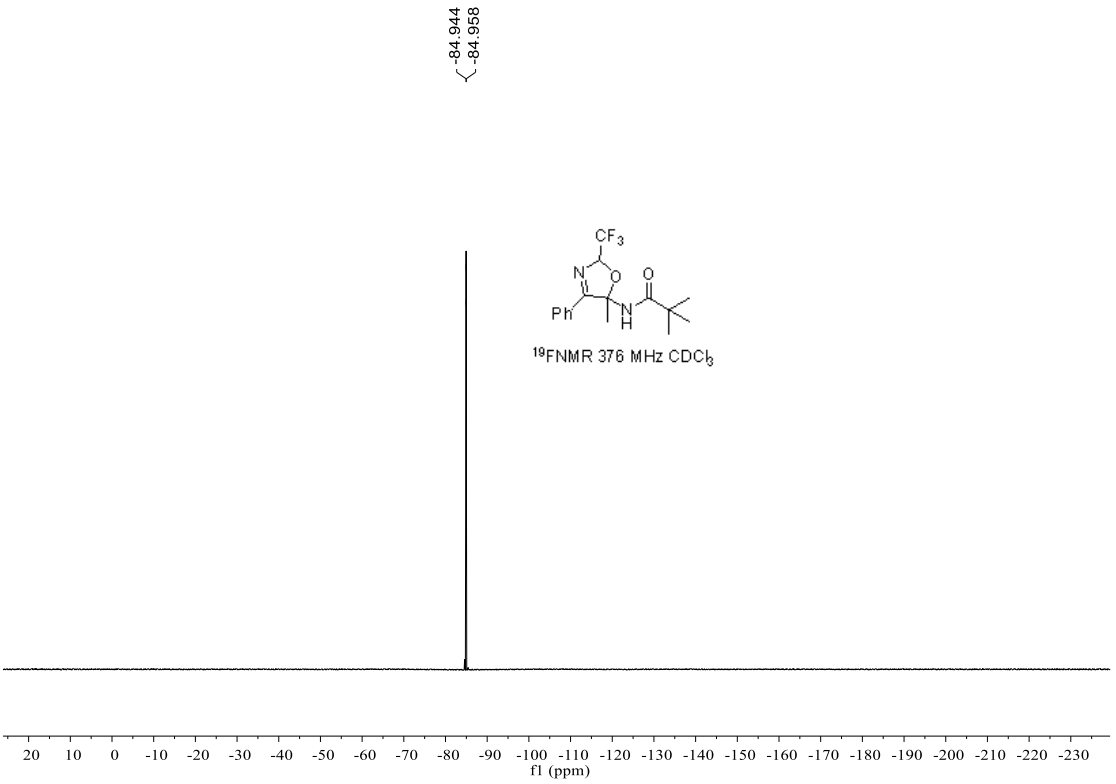
^{1}H NMR (400 MHz) spectrum of **3r** in $CDCl_3$



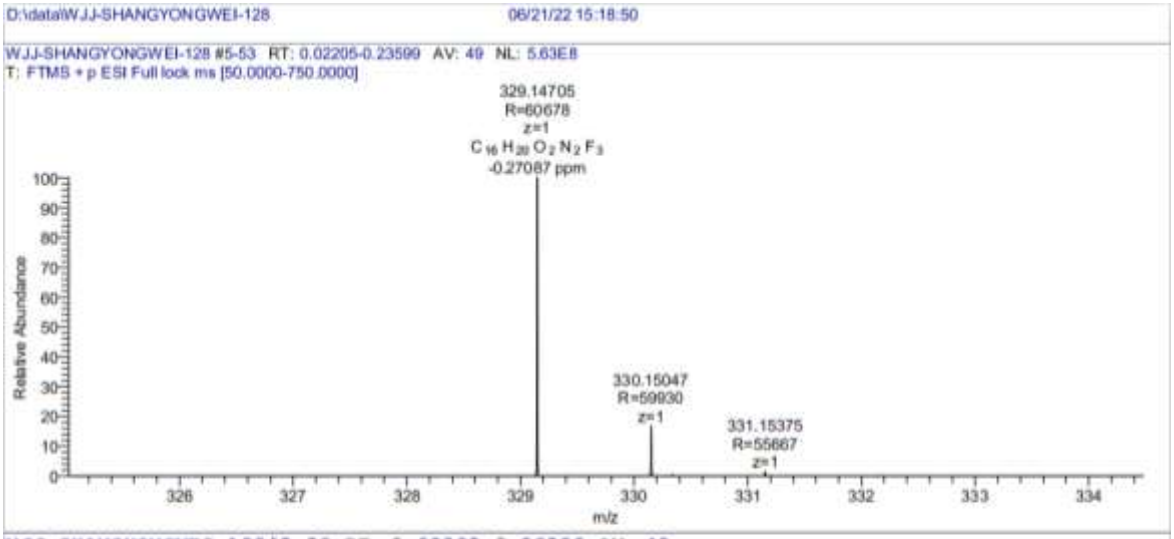
^{13}C NMR (150 MHz) spectrum of **3r** in $CDCl_3$



^{19}F NMR (376 MHz) spectrum of **3r** in $CDCl_3$



HRMS(ESI) copy of compound **3r**:

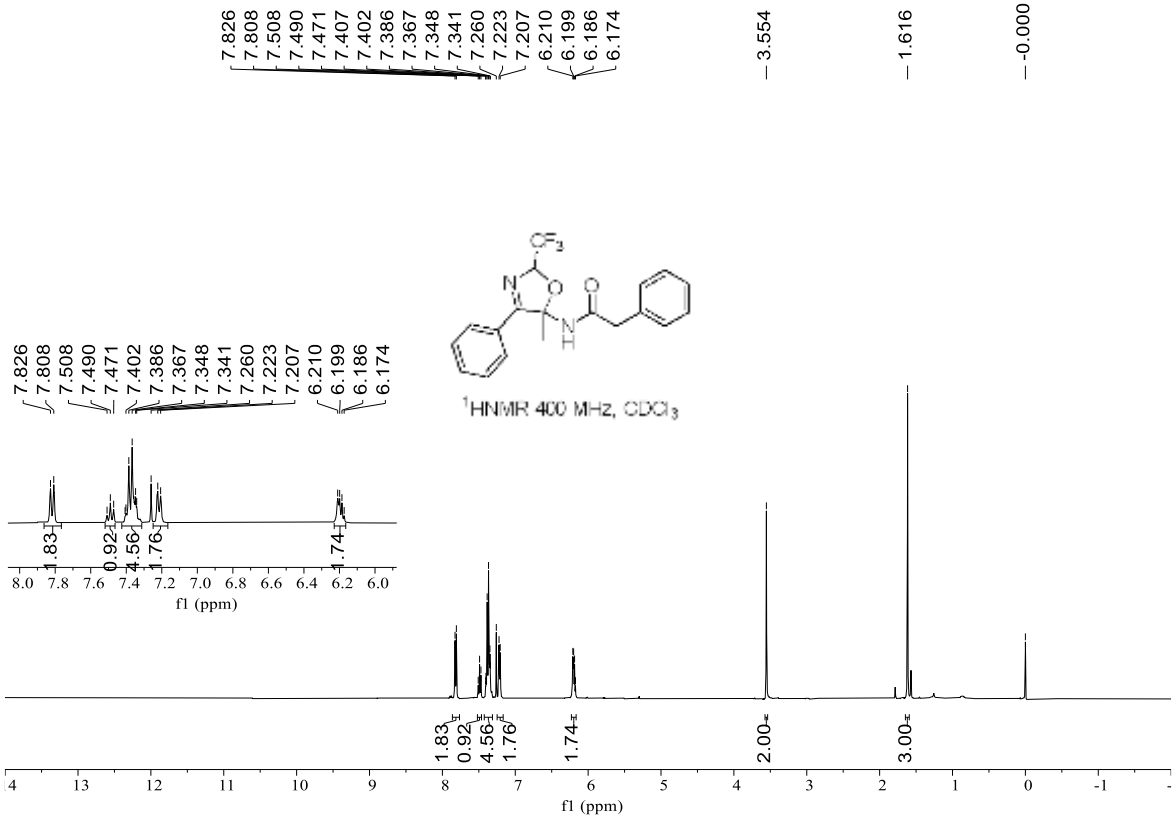


WJJ-SHANGYONGWEI-128#5-53 RT: 0.02205-0.23599 AV: 49
T: FTMS + p ESI Full lock ms [50.0000-750.0000]
m/z= 325.02583-334.47830

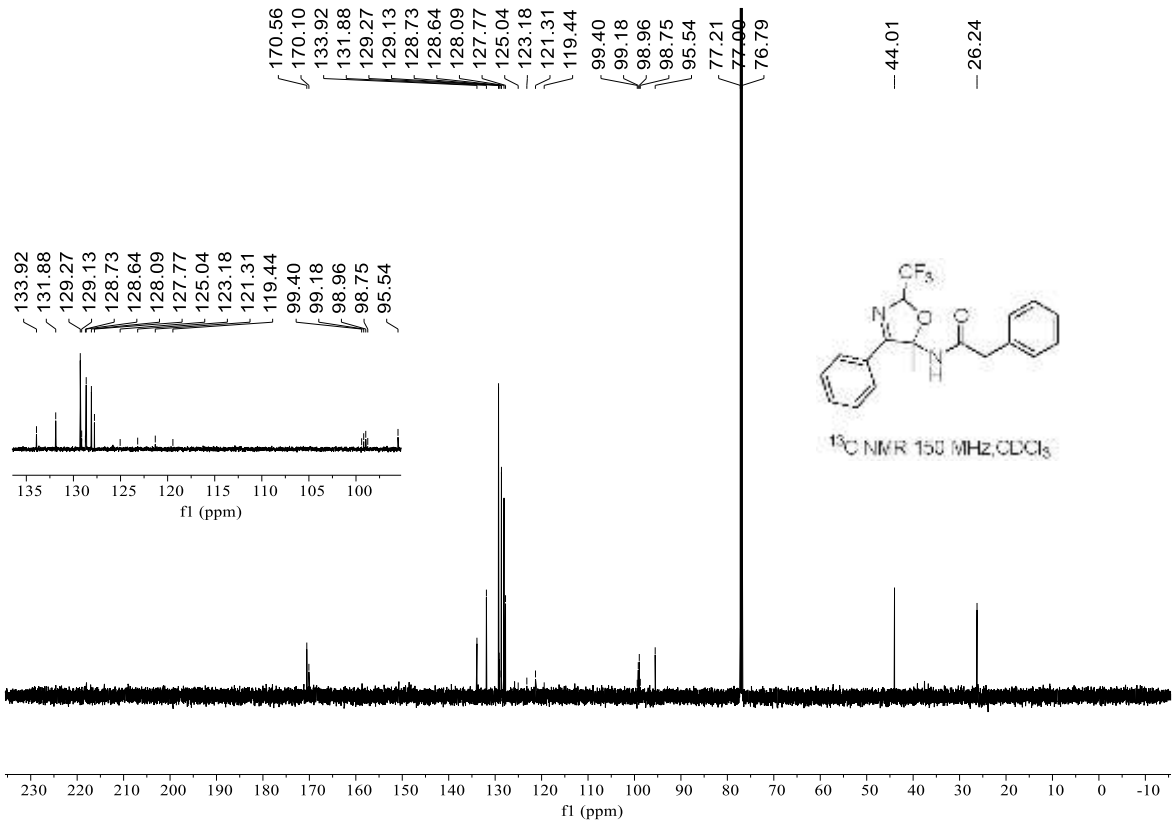
m/z	Intensity	Relative	Resolution	Charge	Delta (ppm)	Composition
329.14705	563405760.0	100.00	60677.69	1.00	-0.27	$C_{16}H_{20}O_2N_2F_3$
330.15047	94709840.0	16.81	59929.92	1.00		
330.33646	1931465.4	0.34	58930.09	1.00		
331.15375	8326552.0	1.48	55666.51	1.00		
334.29480	588149.4	0.10	56235.79	1.00		

NMR copies of compound **3s**

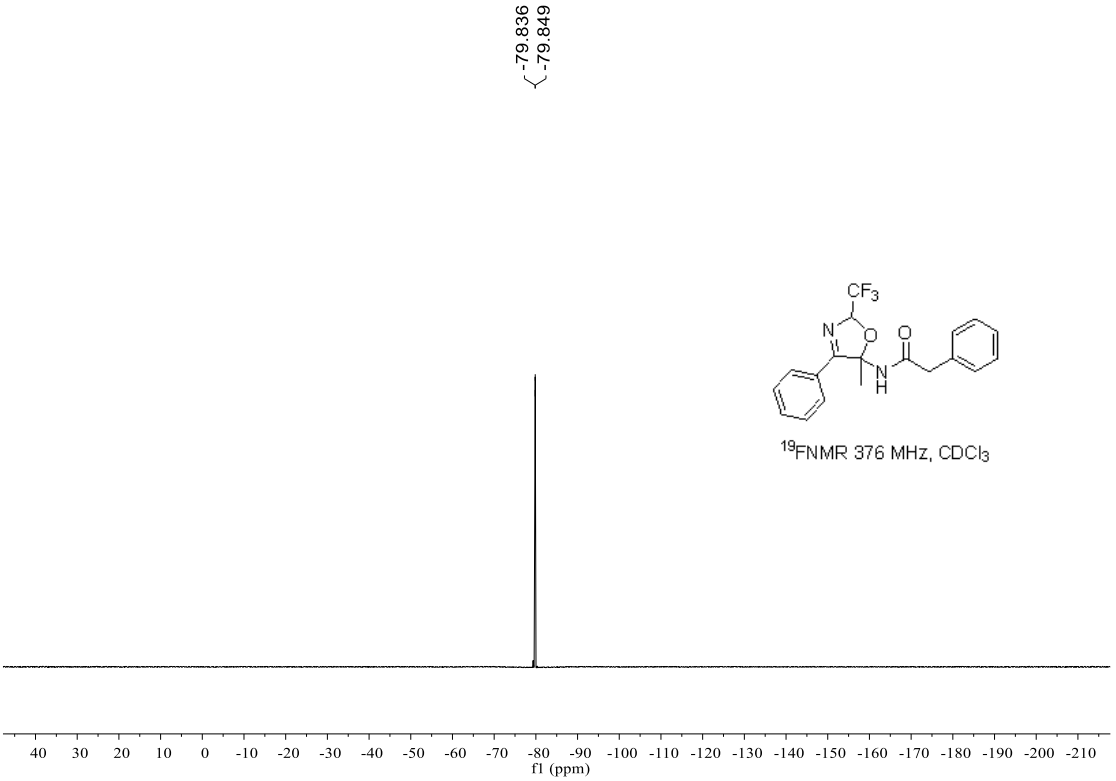
^{1}H NMR (400 MHz) spectrum of **3s** in $CDCl_3$



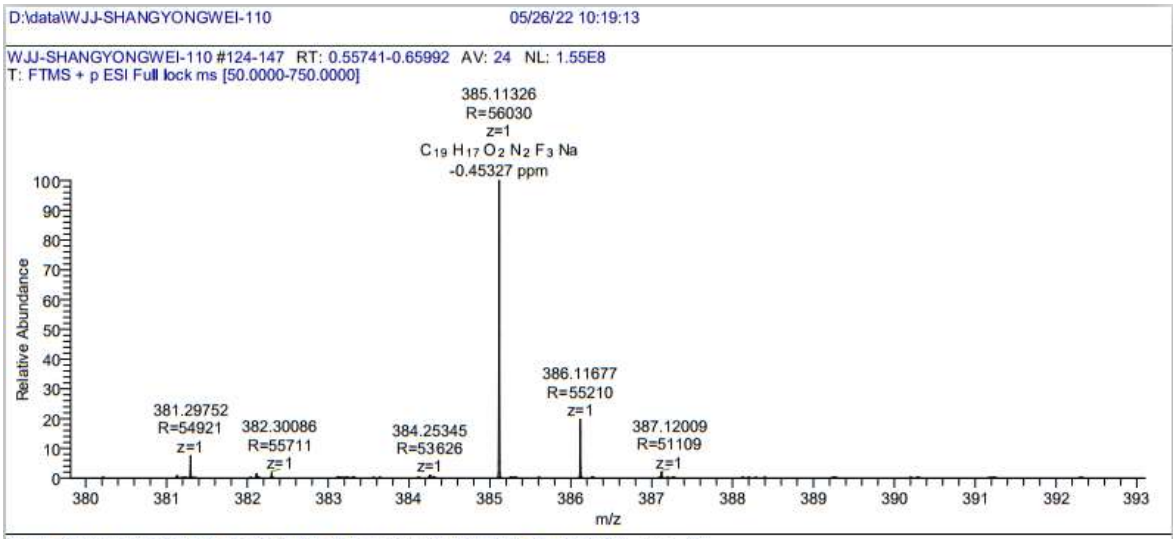
^{13}C NMR (150 MHz) spectrum of **3s** in $CDCl_3$



^{19}F NMR (376 MHz) spectrum of **3s** in $CDCl_3$



HRMS(ESI) copy of compound **3s**:

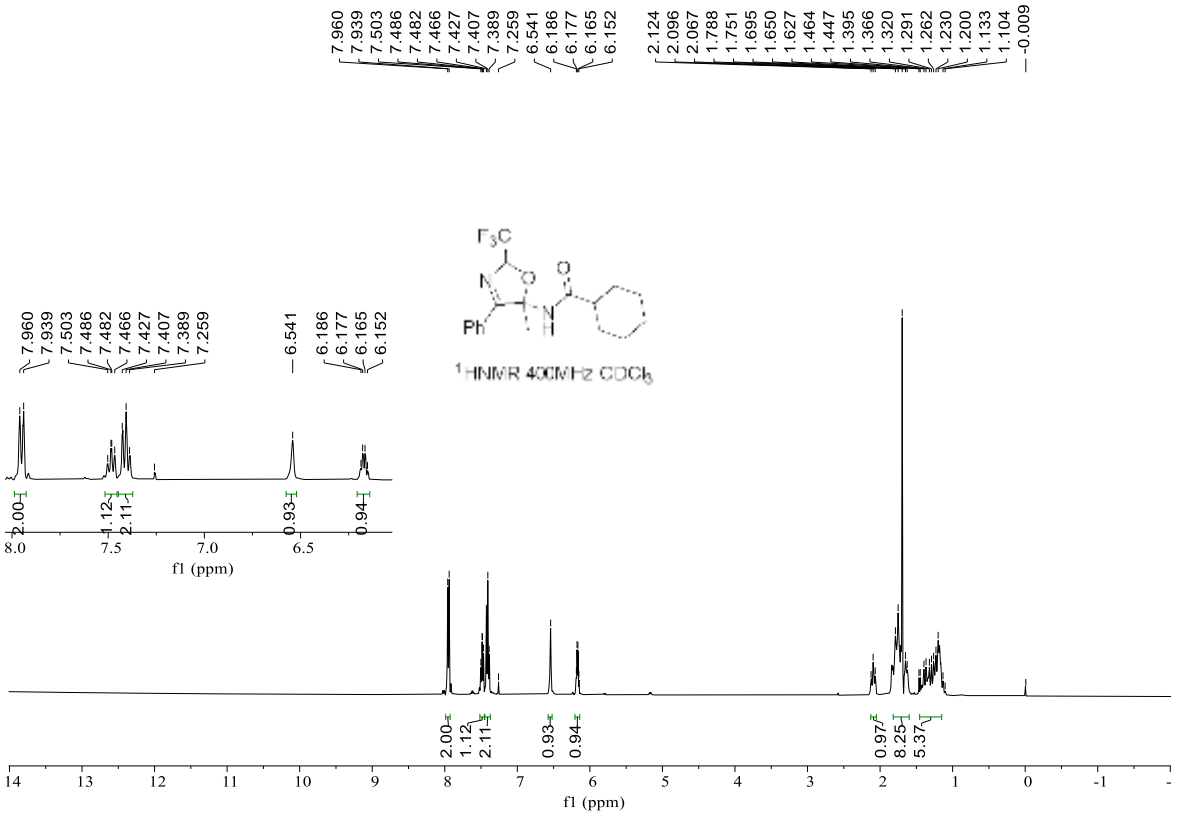


WJJ-SHANGYONGWEI-110#124-147 RT: 0.55741-0.65992 AV: 24
T: FTMS + p ESI Full lock ms [50.0000-750.0000]
m/z= 379.81237-393.09927

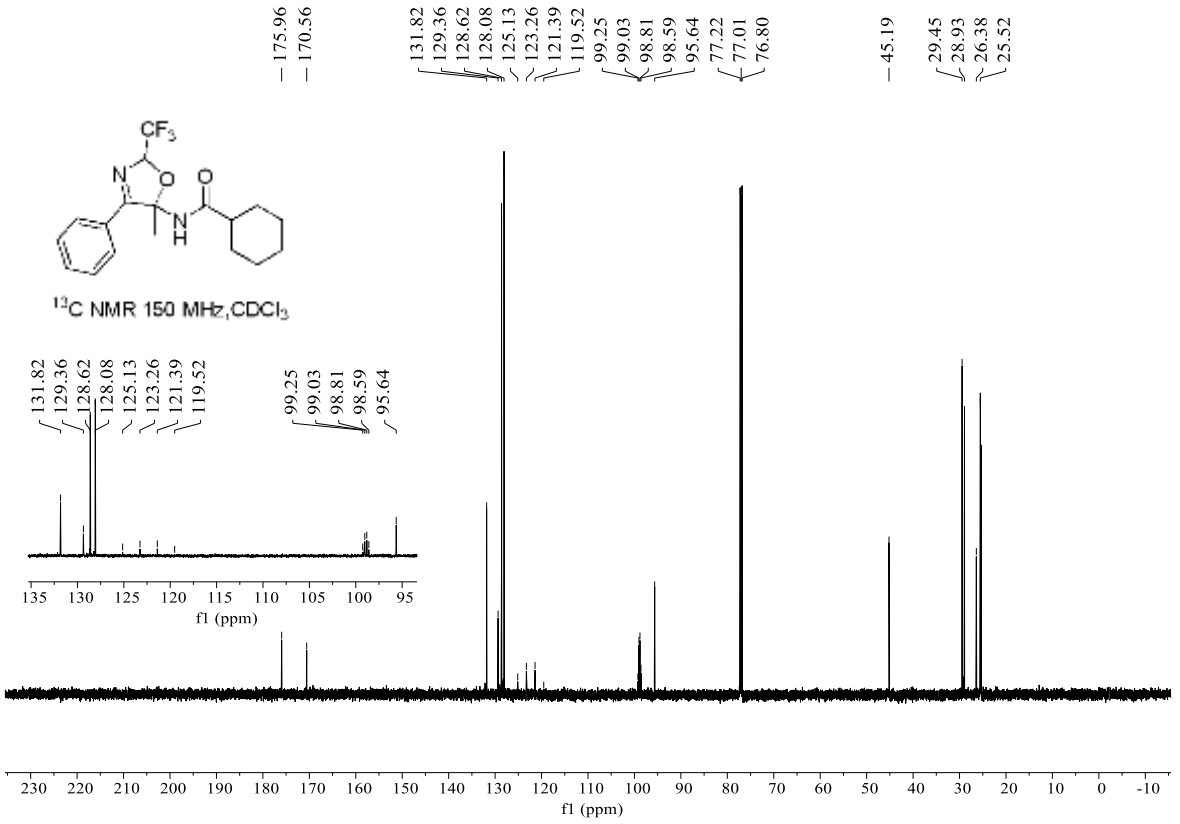
m/z	Intensity	Relative	Resolution	Charge	Delta (ppm)	Composition
381.29752	11921919.0	7.69	54921.11	1.00		
382.30086	2861770.0	1.84	55710.62	1.00		
385.11326	155112096.0	100.00	56030.40	1.00	-0.45	$C_{19}H_{17}O_2N_2F_3Na$
386.11677	30694906.0	19.79	55209.99	1.00		
387.12009	3211090.0	2.07	51108.73	1.00		

NMR copies of compound **3t**

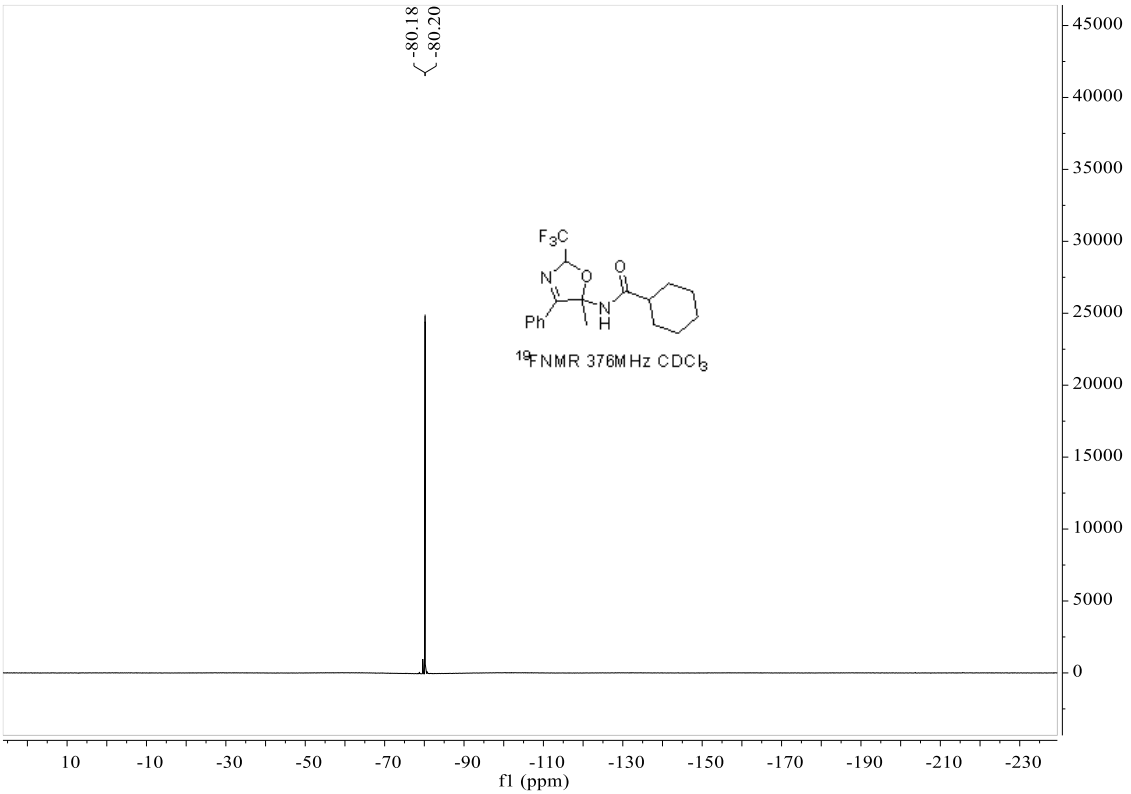
^{1}H NMR (400 MHz) spectrum of **3t** in $CDCl_3$



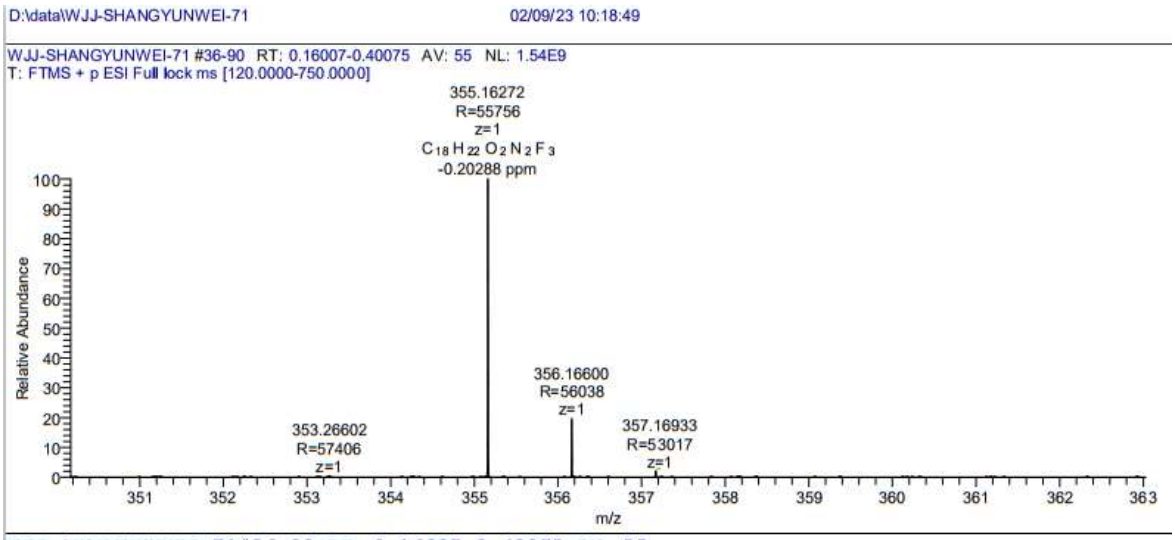
^{13}C NMR (150 MHz) spectrum of **3t** in $CDCl_3$



^{19}F NMR (376 MHz) spectrum of **3t** in $CDCl_3$



HRMS(ESI) copy of compound **3t**:

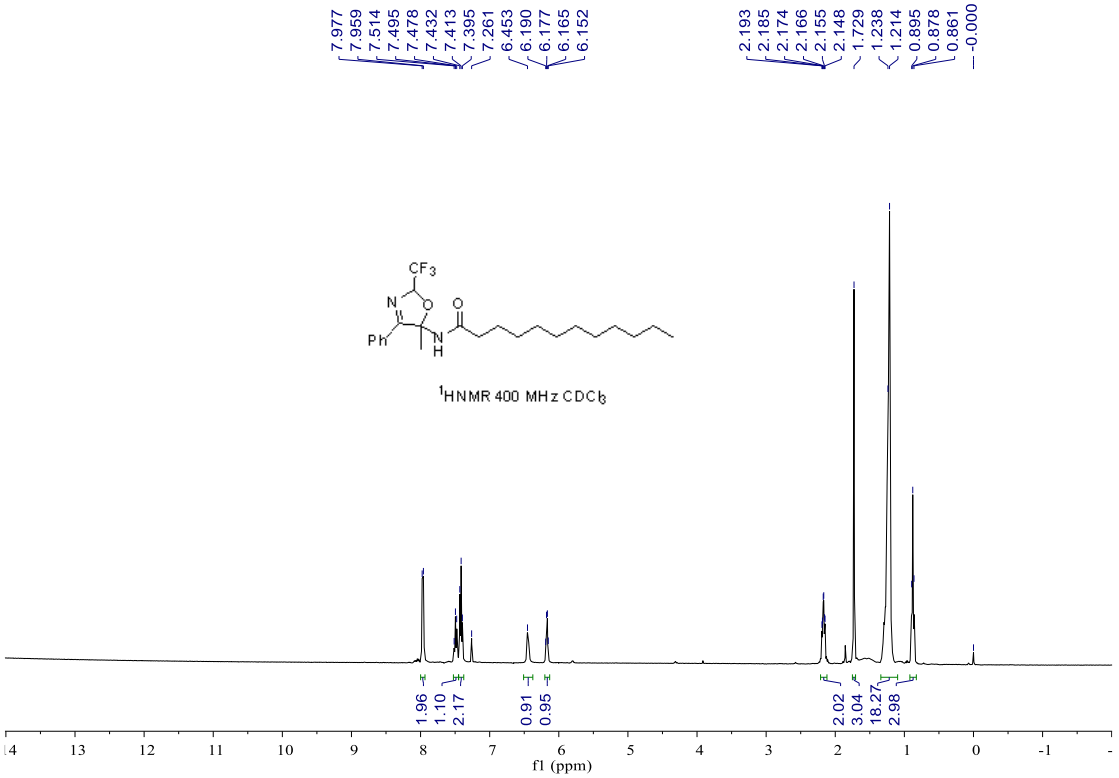


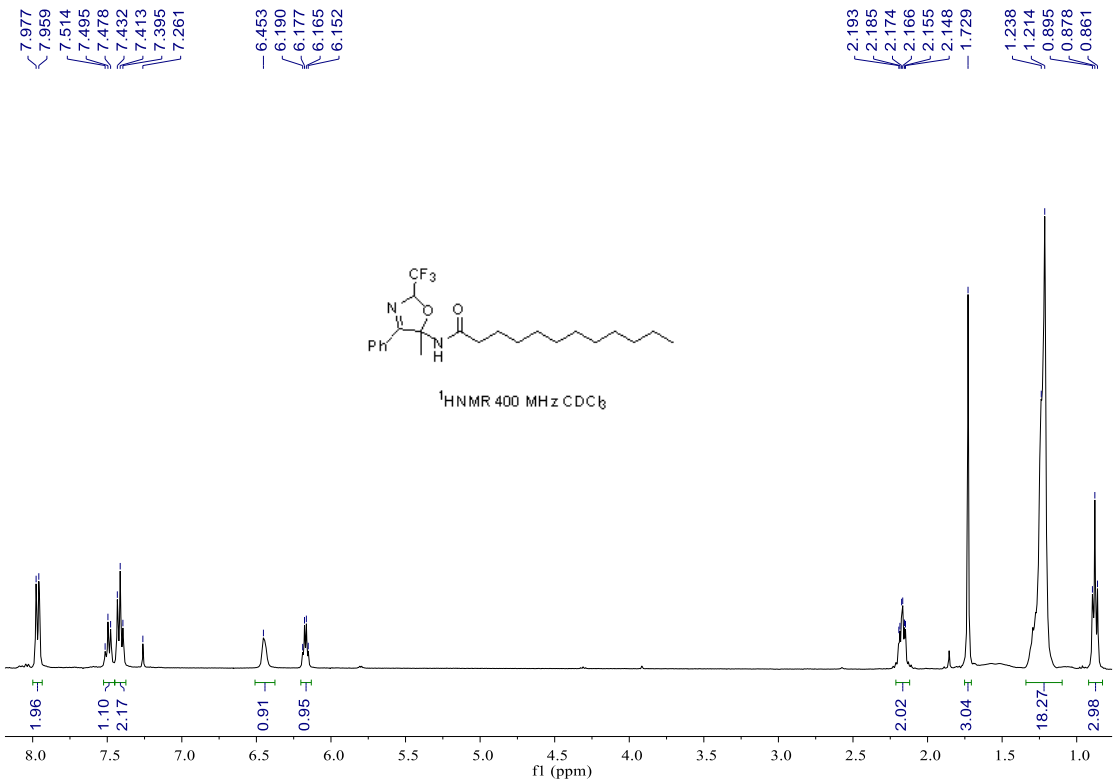
WJJ-SHANGYUNWEI-71#36-90 RT: 0.16007-0.40075 AV: 55
T: FTMS + p ESI Full lock ms [120.0000-750.0000]
m/z= 350.17140-363.02430

m/z	Intensity	Relative	Resolution	Charge	Delta (ppm)	Composition
352.24609	6173613.0	0.39	57600.57	1.00		
353.26602	7761164.5	0.49	57406.20	1.00		
355.16272	1590677760.0	100.00	55756.37	1.00	-0.20	$C_{18}H_{22}O_2N_2F_3$
356.16600	306216448.0	19.25	56037.72	1.00		
357.16933	30543262.0	1.92	53017.46	1.00		

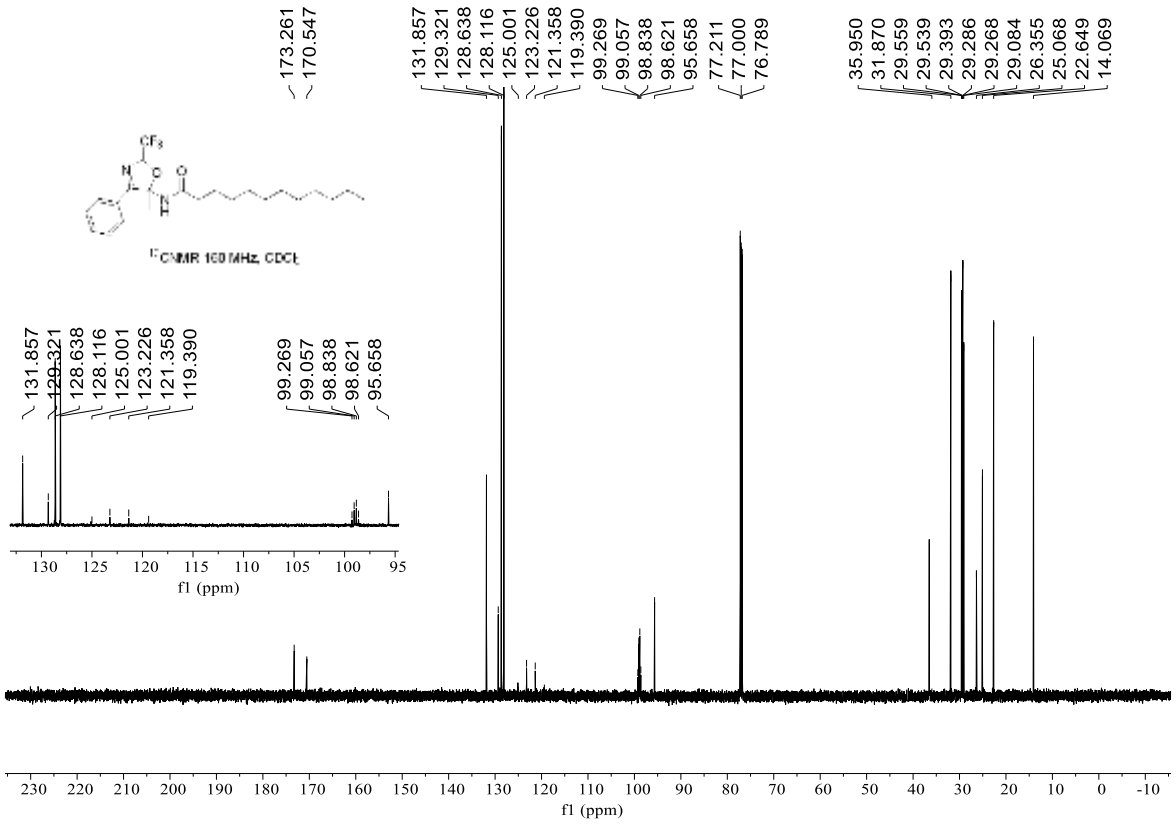
NMR copies of compound **3u**

^{1}H NMR (400 MHz) spectrum of **3u** in $CDCl_3$

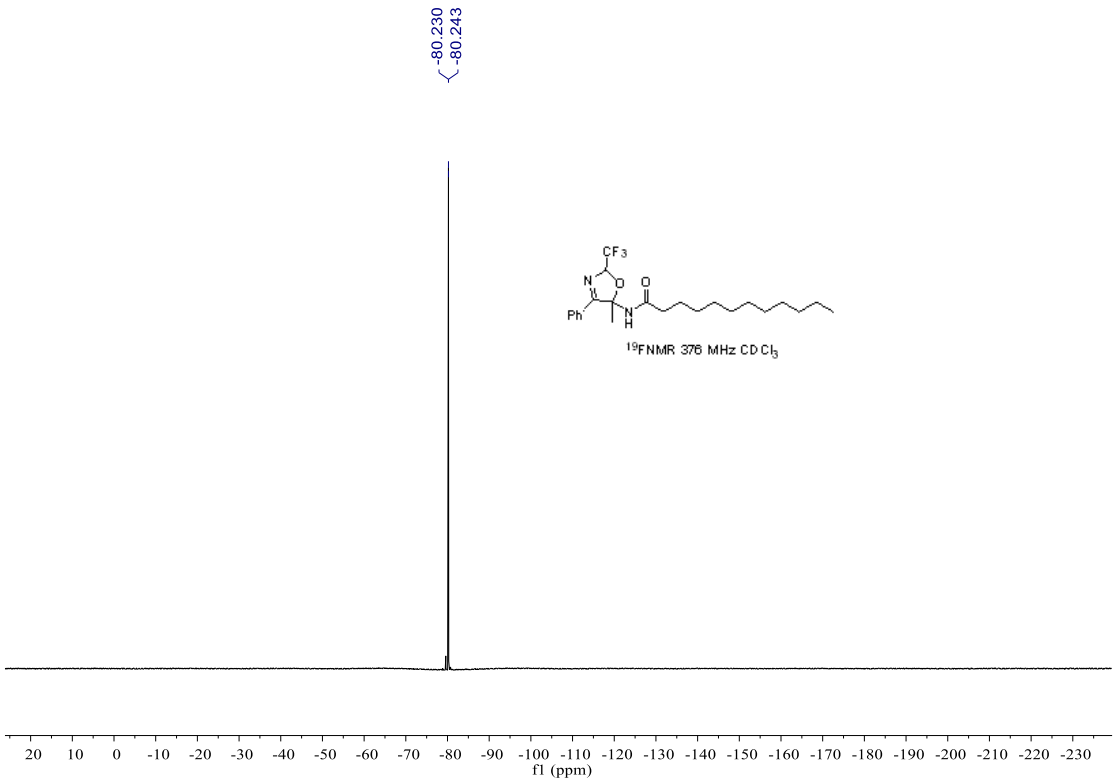




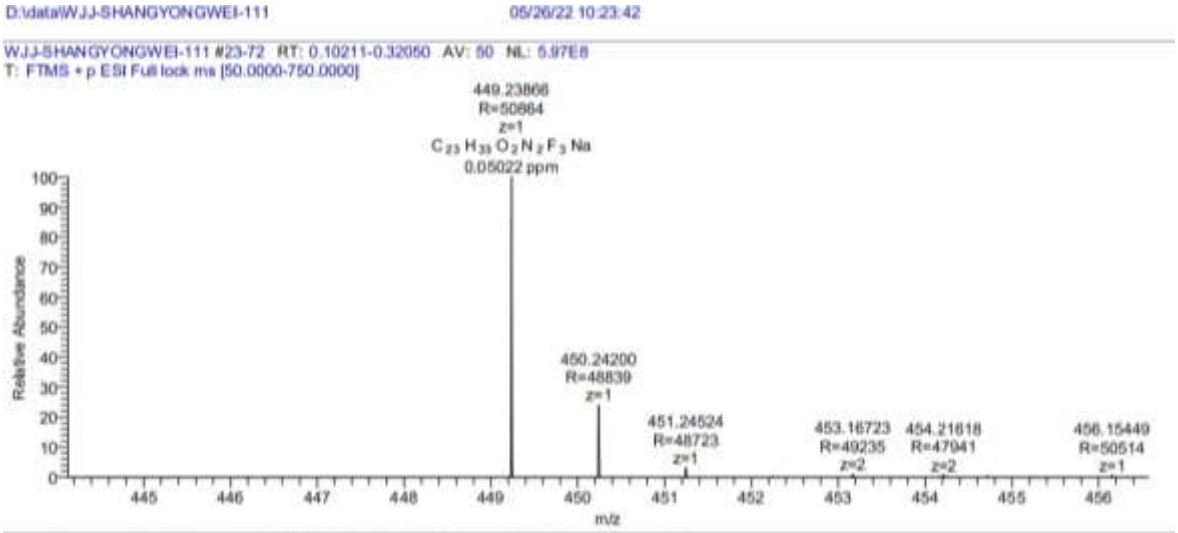
^{13}C NMR (150 MHz) spectrum of **3u** in $CDCl_3$



^{19}F NMR (376 MHz) spectrum of **3u** in $CDCl_3$



HRMS(ESI) copy of compound **3u**:

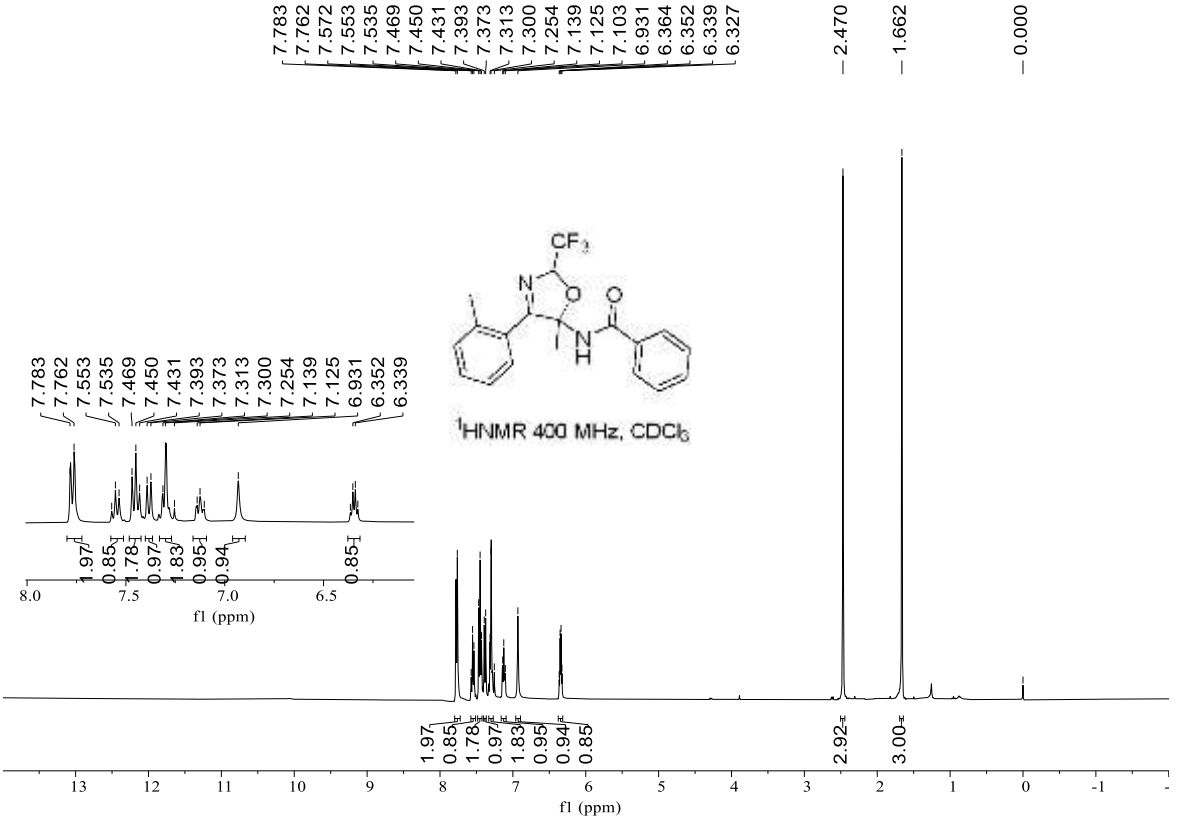


WJJ-SHANGYONGWEI-111#23-72 RT: 0.10211-0.32050 AV: 50
T: FTMS + p ESI Full lock ms [50.0000-750.0000]
m/z= 444.12853-456.56913

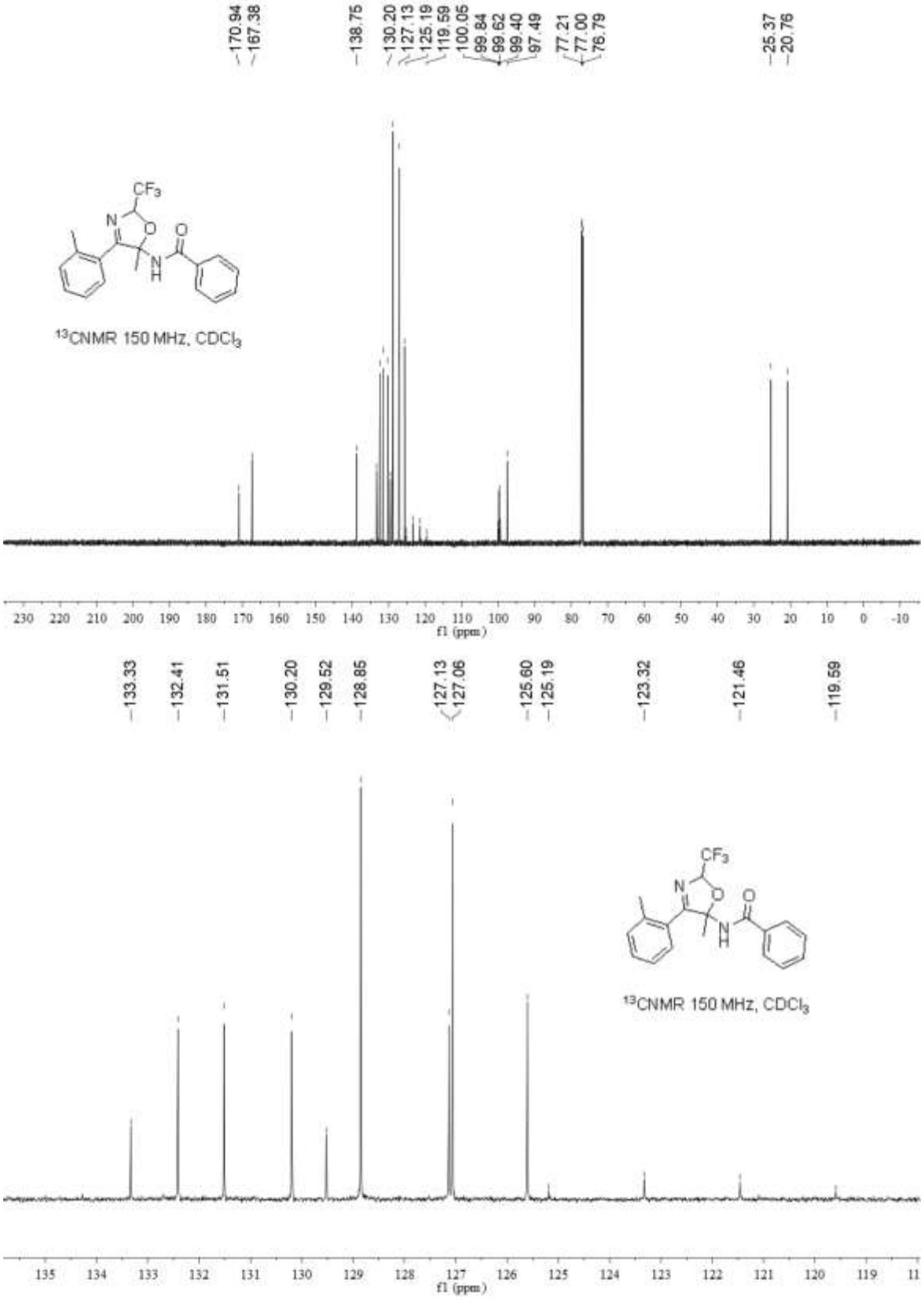
m/z	Intensity	Relative	Resolution	Charge	Delta (ppm)	Composition
449.23866	597206656.0	100.00	50863.84	1.00	0.05	$C_{23}H_{33}O_2N_2F_3Na$
450.24200	147627296.0	24.72	48838.74	1.00		
451.24524	19092064.0	3.20	48722.88	1.00		
453.16723	5897390.5	0.99	49235.32	2.00		
454.21618	4404201.0	0.74	47940.56	2.00		

NMR copies of compound **4a**

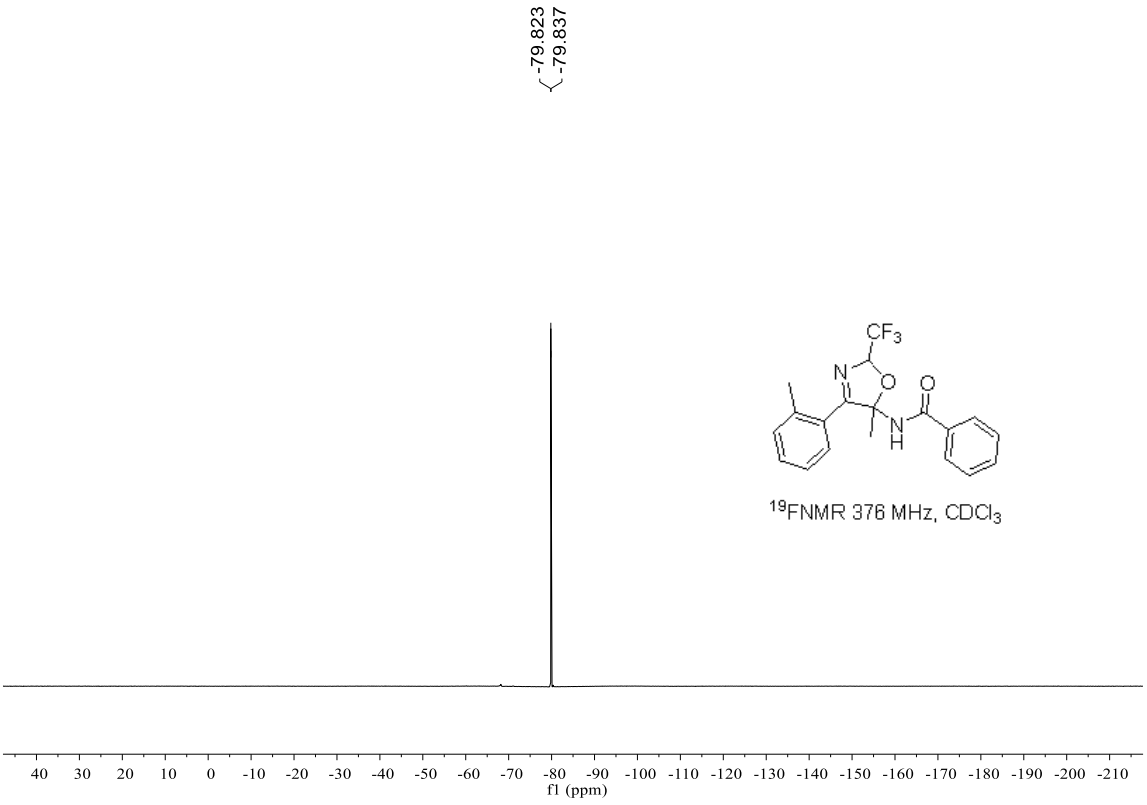
^{1}H NMR (400 MHz) spectrum of **4a** in $CDCl_3$



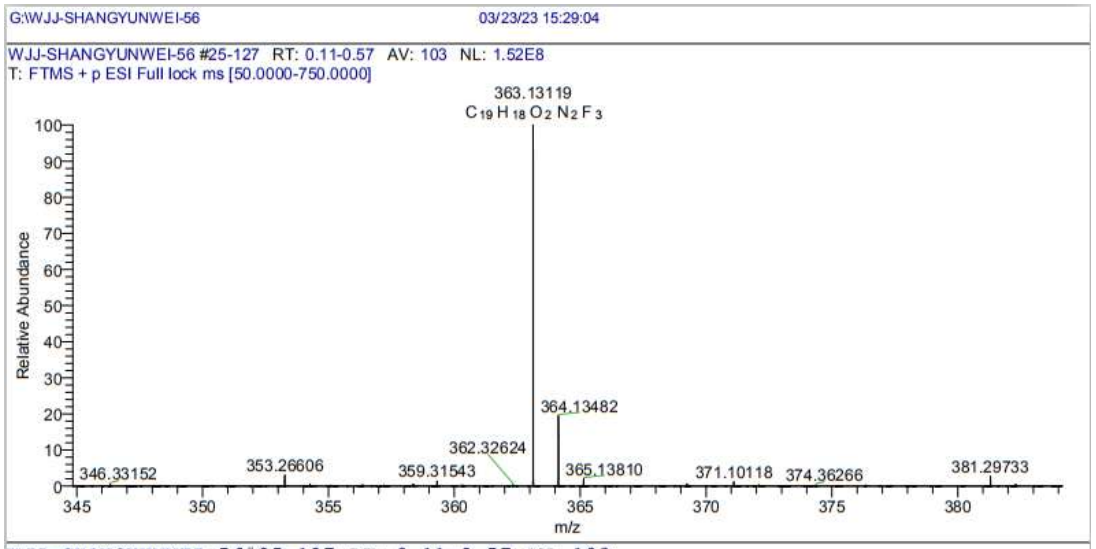
^{13}C NMR (150 MHz) spectrum of **4a** in $CDCl_3$



^{19}F NMR (376 MHz) spectrum of **4a** in $CDCl_3$



HRMS(ESI) copy of compound **4a**:

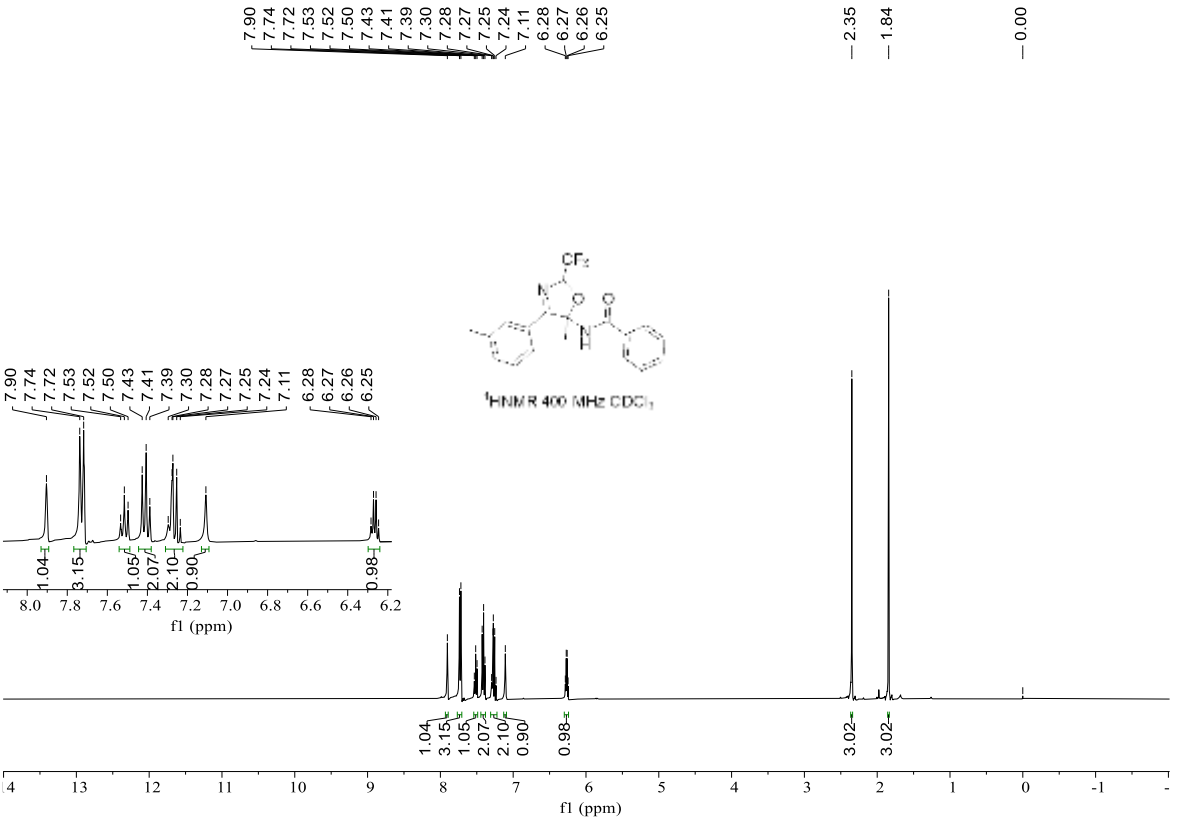


WJJ-SHANGYUNWEI-56#25-127 RT: 0.11-0.57 AV: 103
T: FTMS + p ESI Full lock ms [50.0000-750.0000]
m/z= 344.84281-384.15083

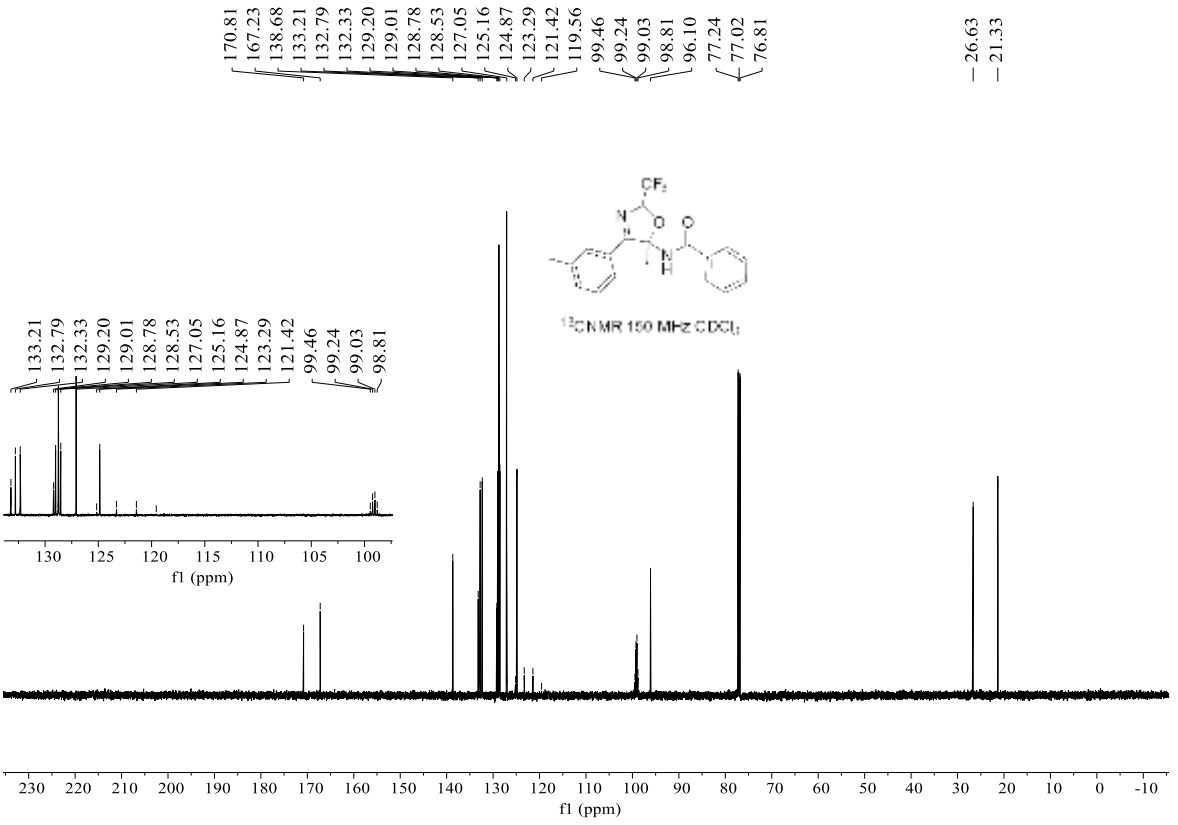
m/z	Intensity	Relative	Delta (ppm)	Composition
353.26606	4726673.5	3.09	212.82	$C_{19}H_8O_2N_2F_3$
363.13119	153018432.0	100.00	-0.30	$C_{19}H_{18}O_2N_2F_3$
364.13482	30125126.0	19.69		
365.13810	3173889.5	2.07		
381.29733	4124257.3	2.70		

NMR copies of compound **3b**

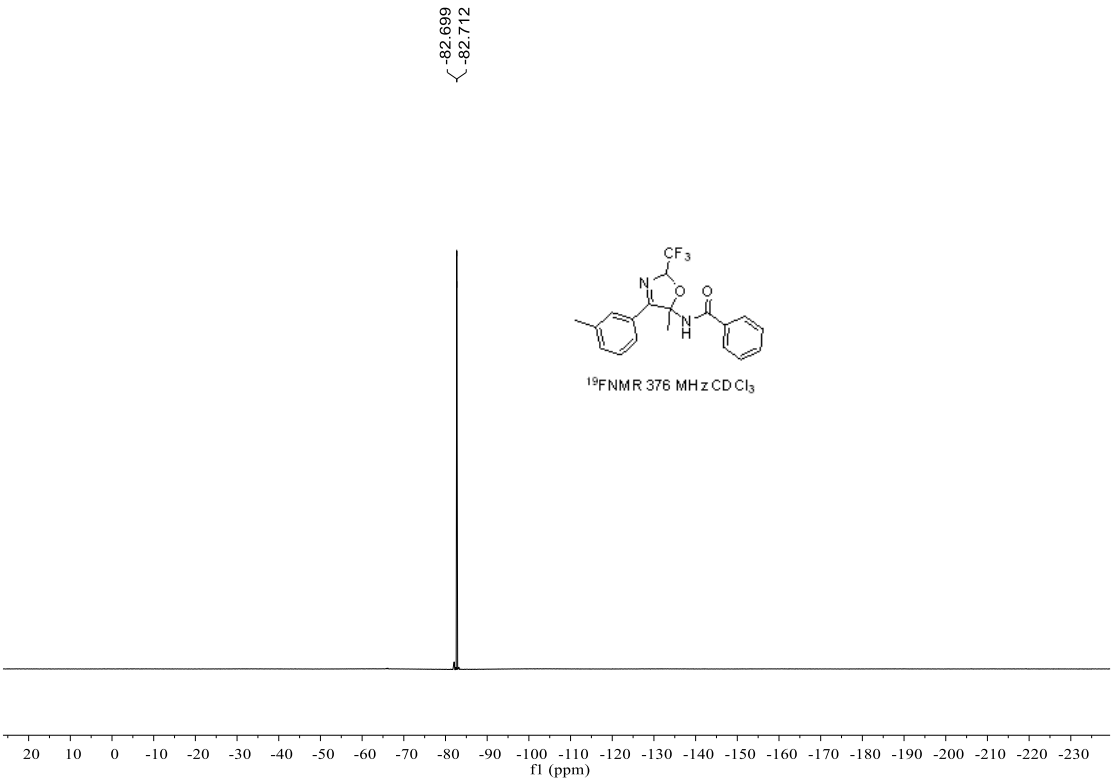
^{1}H NMR (400 MHz) spectrum of **3b** in $CDCl_3$



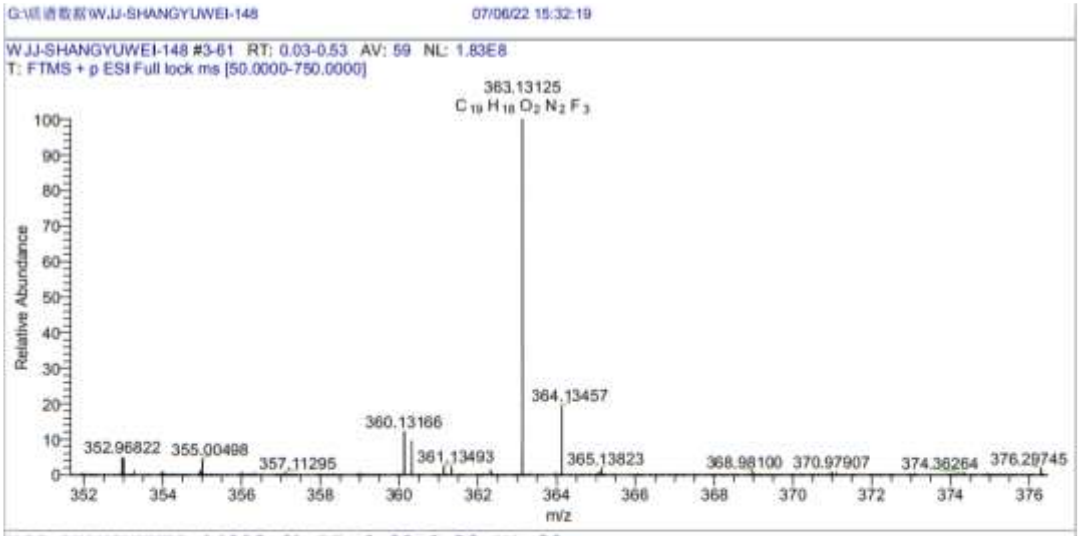
^{13}C NMR (150 MHz) spectrum of **4b** in $CDCl_3$



^{19}F NMR (376 MHz) spectrum of **4b** in $CDCl_3$



HRMS(ESI) copy of compound **4b**:

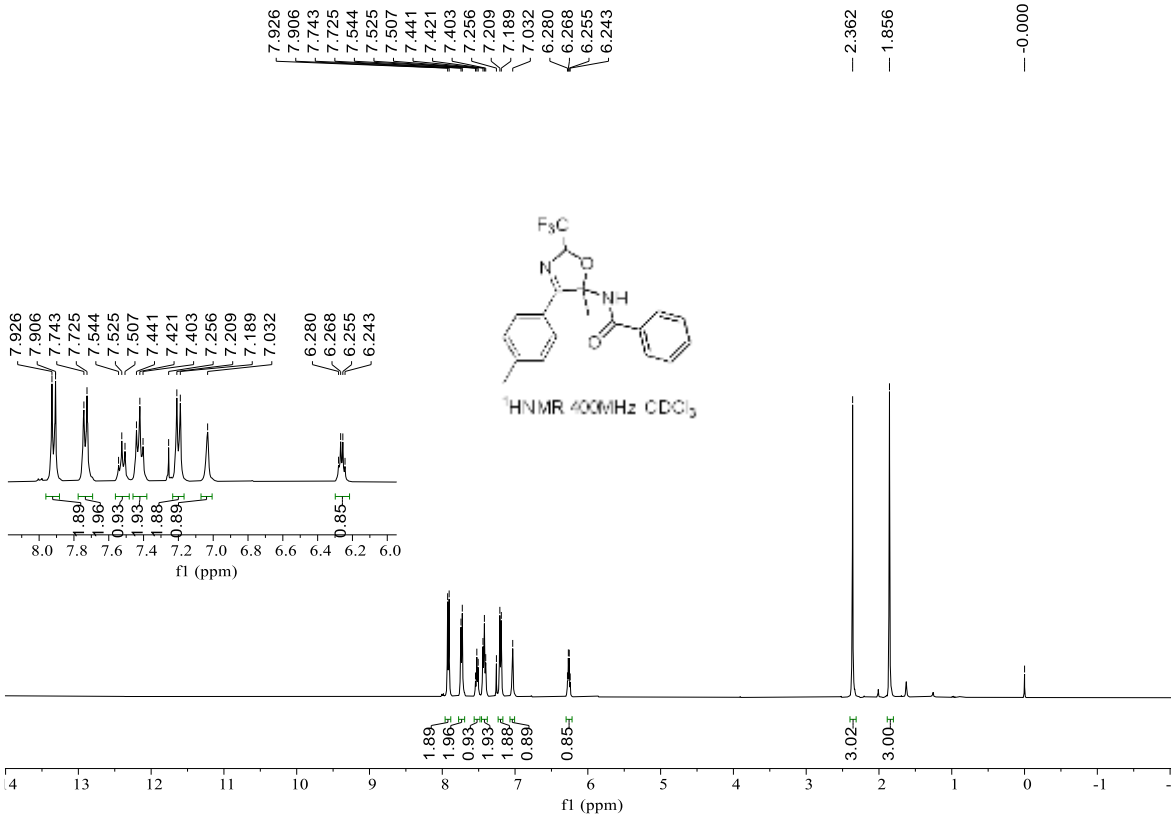


WJJ-SHANGYUWEI-148#3-61 RT: 0.03-0.53 AV: 59
T: FTMS + p ESI Full lock ms [50.0000-750.0000]
m/z= 351.65596-376.46602

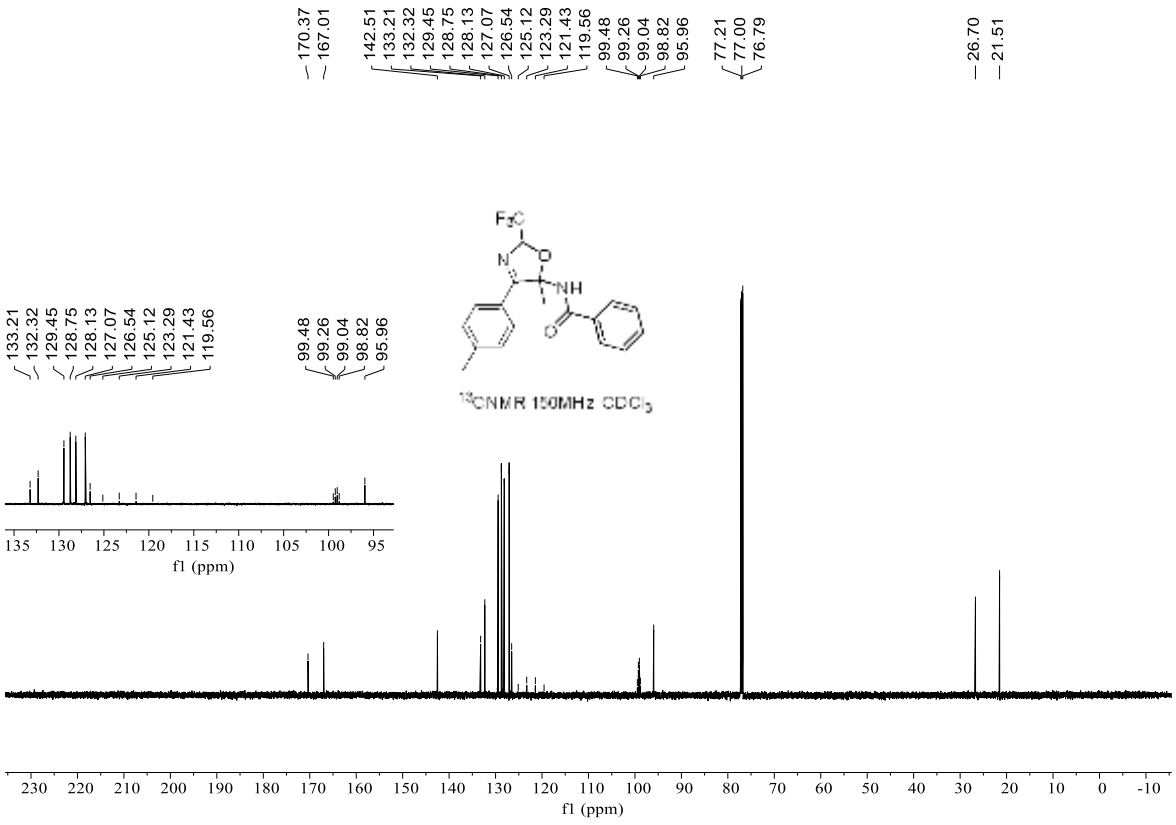
m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
352.96822	9121060.0	4.95			
360.13166	22888174.0	12.41			
360.32347	17543672.0	9.51			
363.13125	184431680.0	100.00	363.13149	-0.23	$C_{19}H_{18}O_2N_2F_3$
364.13457	36000316.0	19.52			

NMR copies of compound **4c**

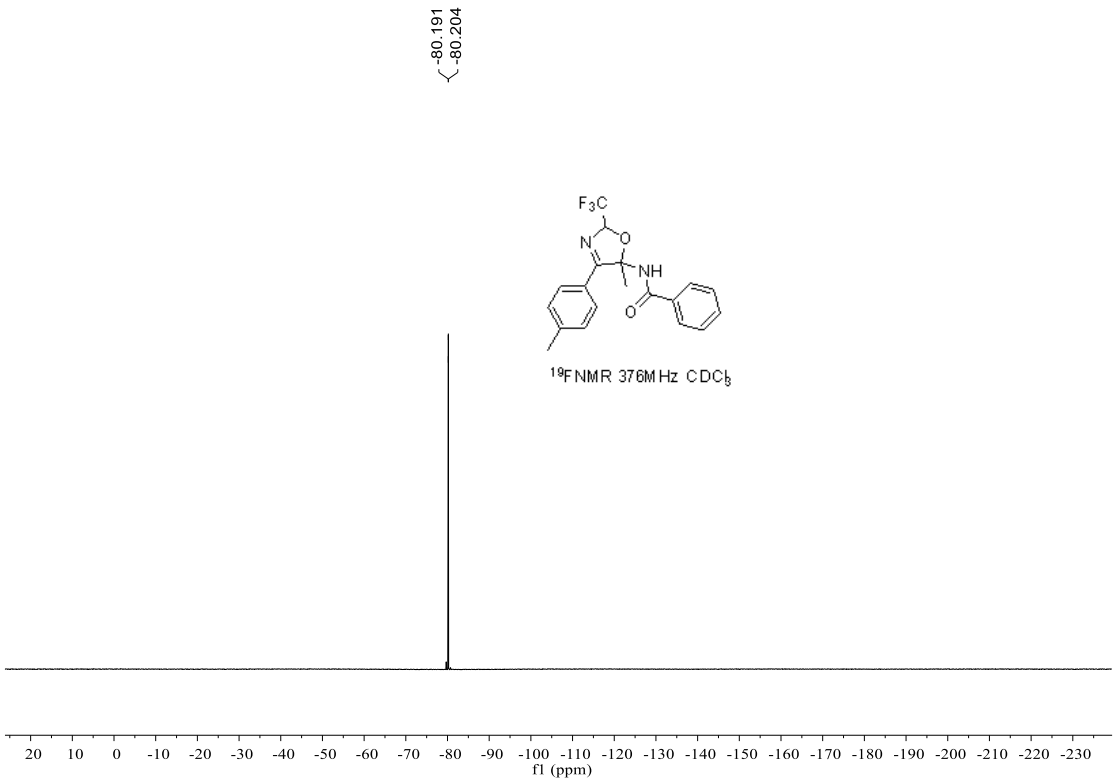
^{1}H NMR (400 MHz) spectrum of **4c** in $CDCl_3$



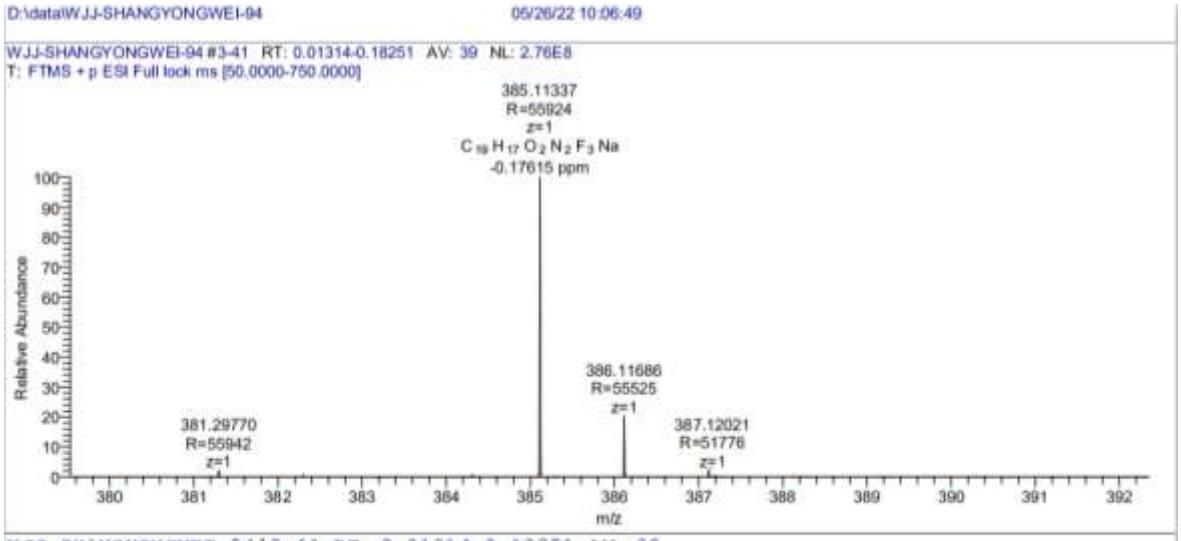
^{13}C NMR (150 MHz) spectrum of **4c** in $CDCl_3$



^{19}F NMR (376 MHz) spectrum of **4c** in $CDCl_3$



HRMS(ESI) copy of compound **4c**:

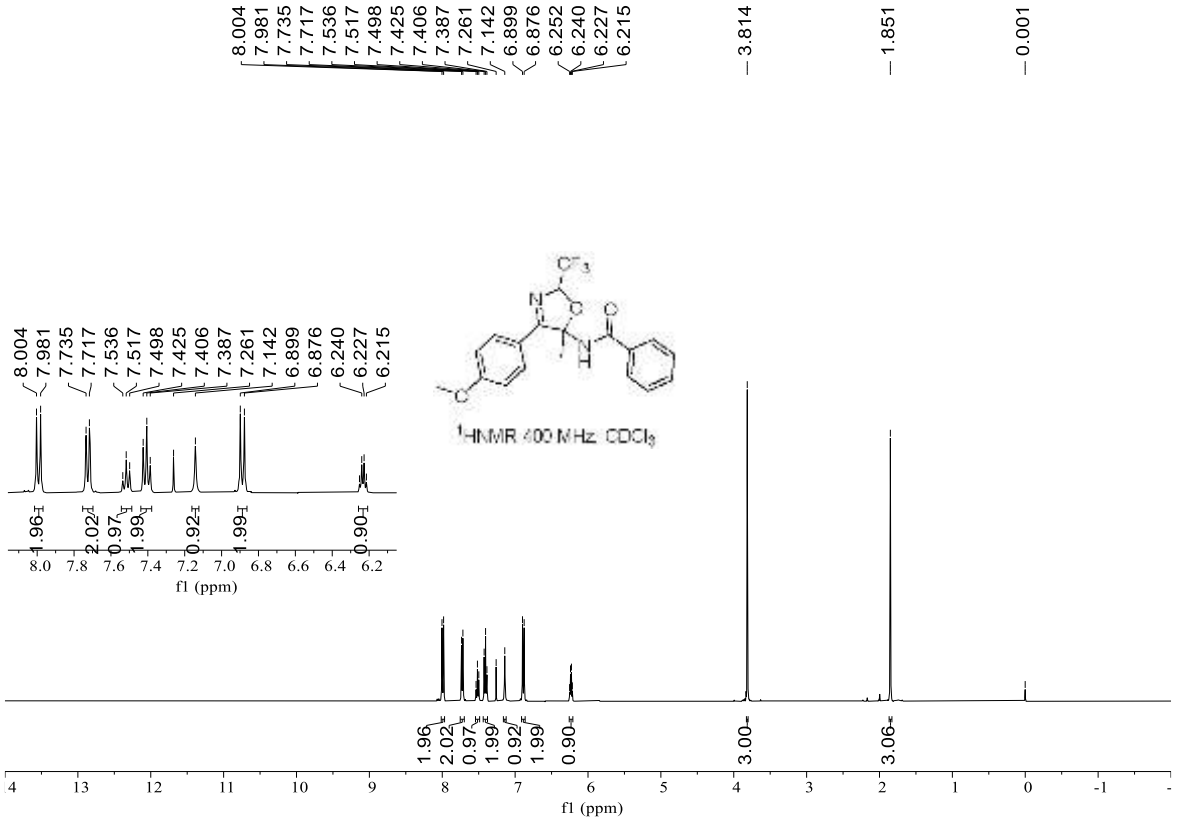


WJJ-SHANGYONGWEI-94#3-41 RT: 0.01314-0.18251 AV: 39
T: FTMS + p ESI Full lock ms [50.0000-750.0000]
m/z= 379.52951-392.34799

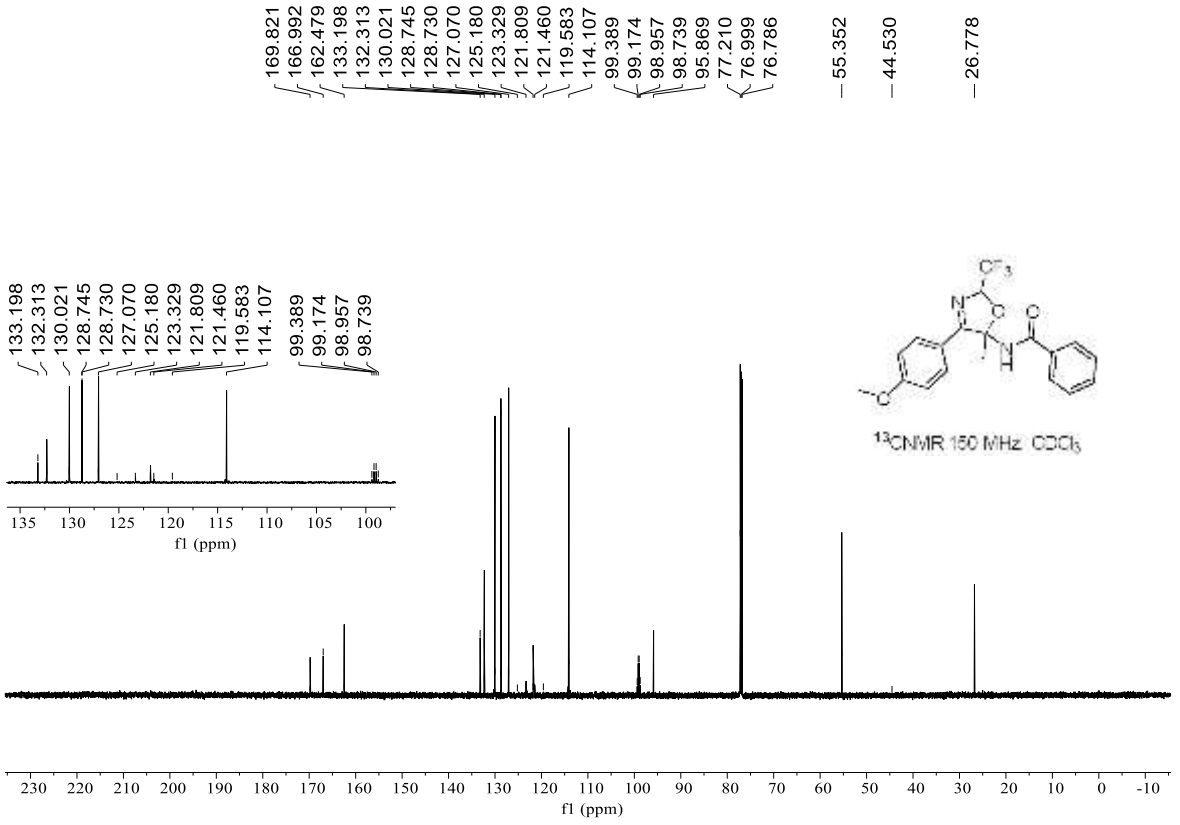
m/z	Intensity	Relative	Resolution	Charge	Delta (ppm)	Composition
381.29770	5334467.0	1.93	55942.06	1.00		
384.30844	1249897.1	0.45	54695.34	1.00		
385.11337	276727424.0	100.00	55923.50	1.00	-0.18	$C_{19}H_{17}O_2N_2F_3Na$
386.11686	55542080.0	20.07	55525.05	1.00		
387.12021	5828639.0	2.11	51776.01	1.00		

NMR copies of compound **4d**

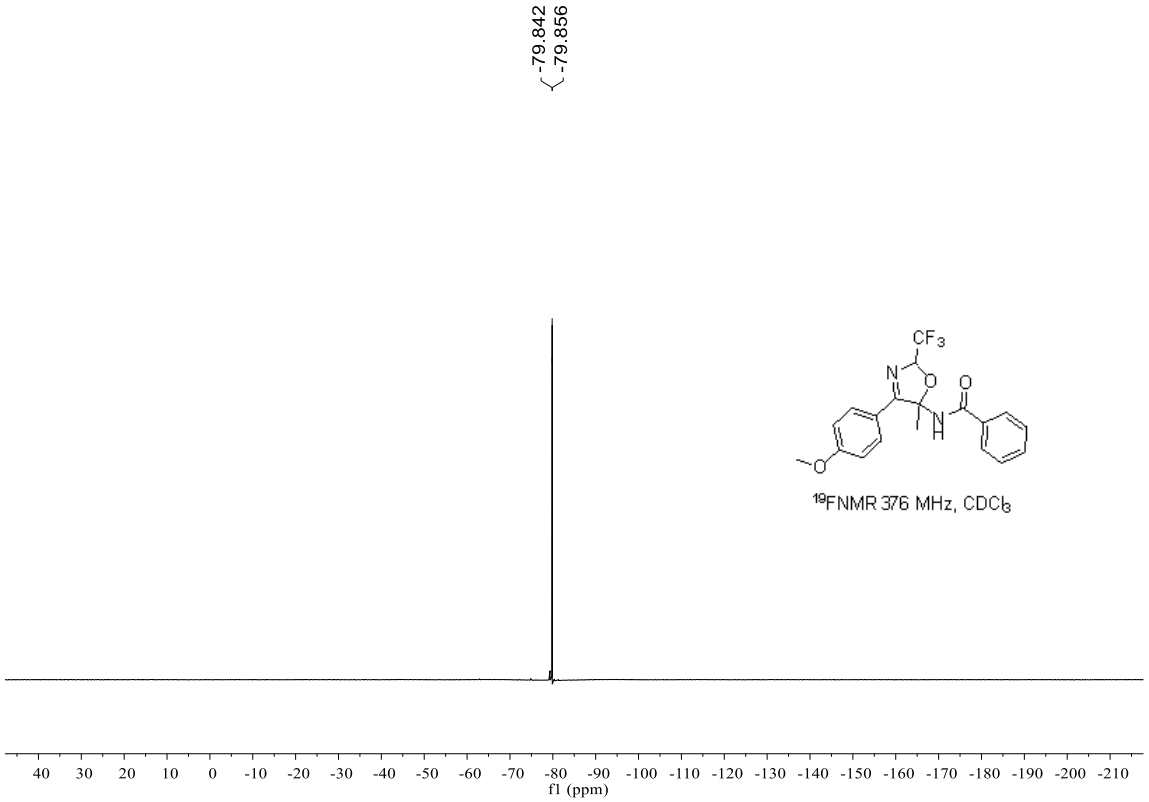
^{1}H NMR (400 MHz) spectrum of **4d** in $CDCl_3$



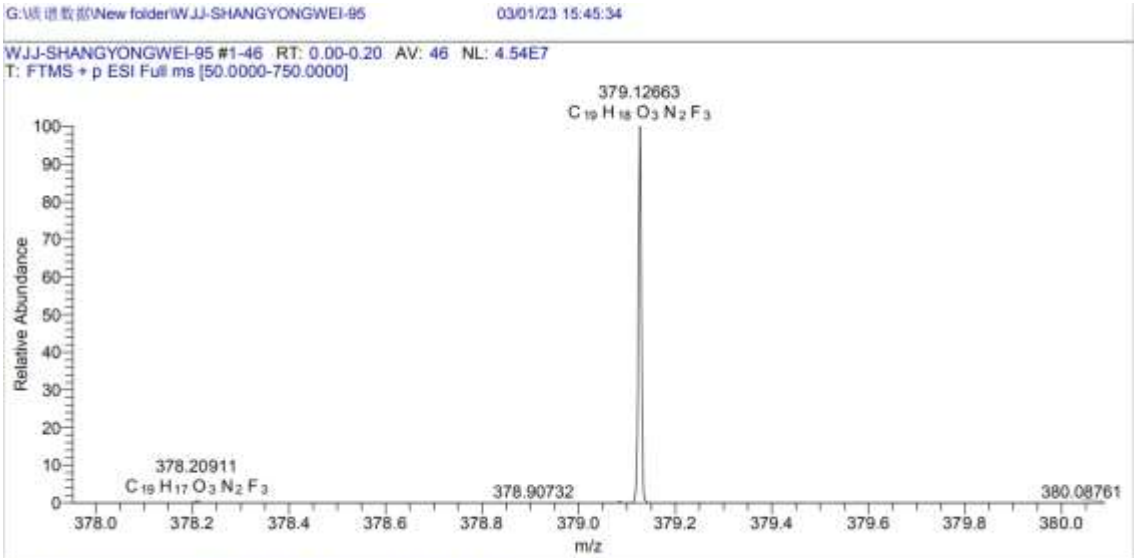
^{13}C NMR (150 MHz) spectrum of **4d** in $CDCl_3$



^{19}F NMR (376 MHz) spectrum of **4d** in $CDCl_3$



HRMS(ESI) copy of compound **4d**:

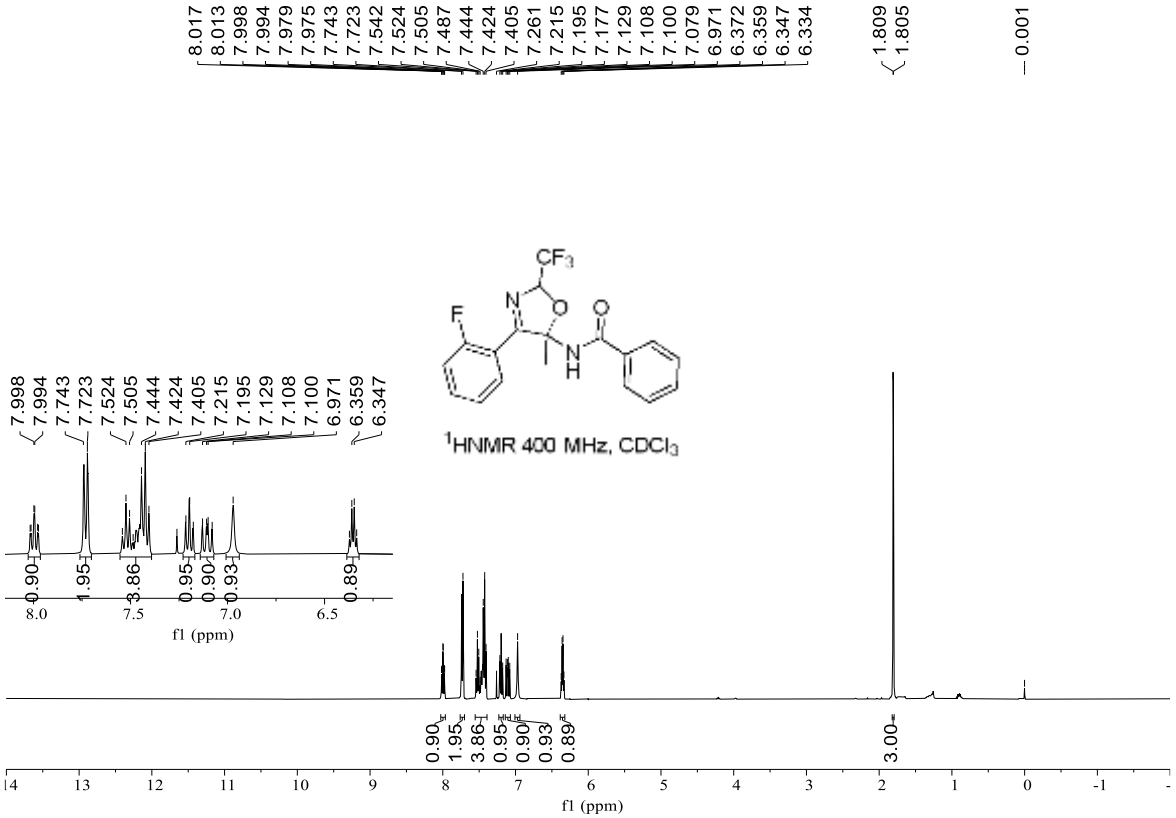


WJJ-SHANGYONGWEI-95#1-46 RT: 0.00-0.20 AV: 46
T: FTMS + p ESI Full ms [50.0000-750.0000]
m/z= 377.95202-380.08910

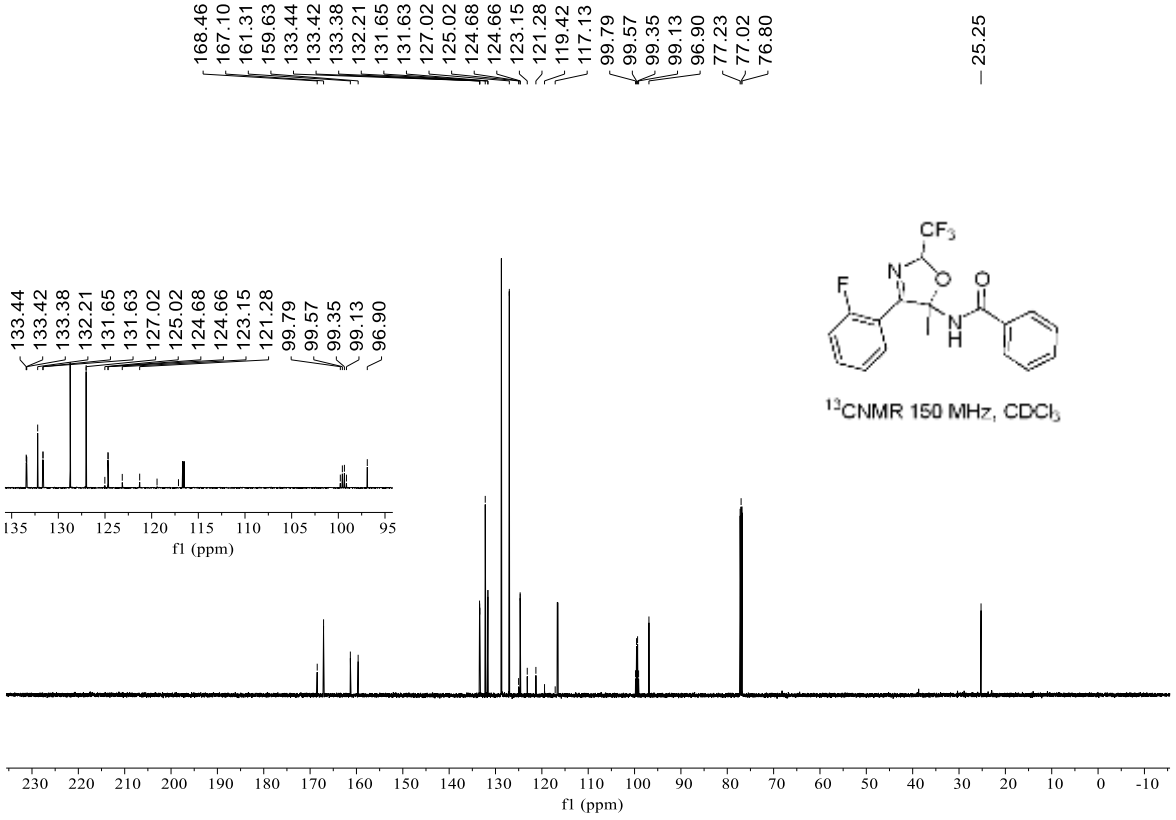
m/z	Intensity	Relative	Delta (ppm)	Composition
377.95680	17829.2	0.04	-161.78	$C_{19}H_{17}O_3N_2F_3$
378.13554	27468.5	0.06	16.96	$C_{19}H_{17}O_3N_2F_3$
378.20911	275188.8	0.61	90.53	$C_{19}H_{17}O_3N_2F_3$
379.08508	92979.8	0.20	-41.32	$C_{19}H_{18}O_3N_2F_3$
379.12663	45474024.0	100.00	0.23	$C_{19}H_{18}O_3N_2F_3$

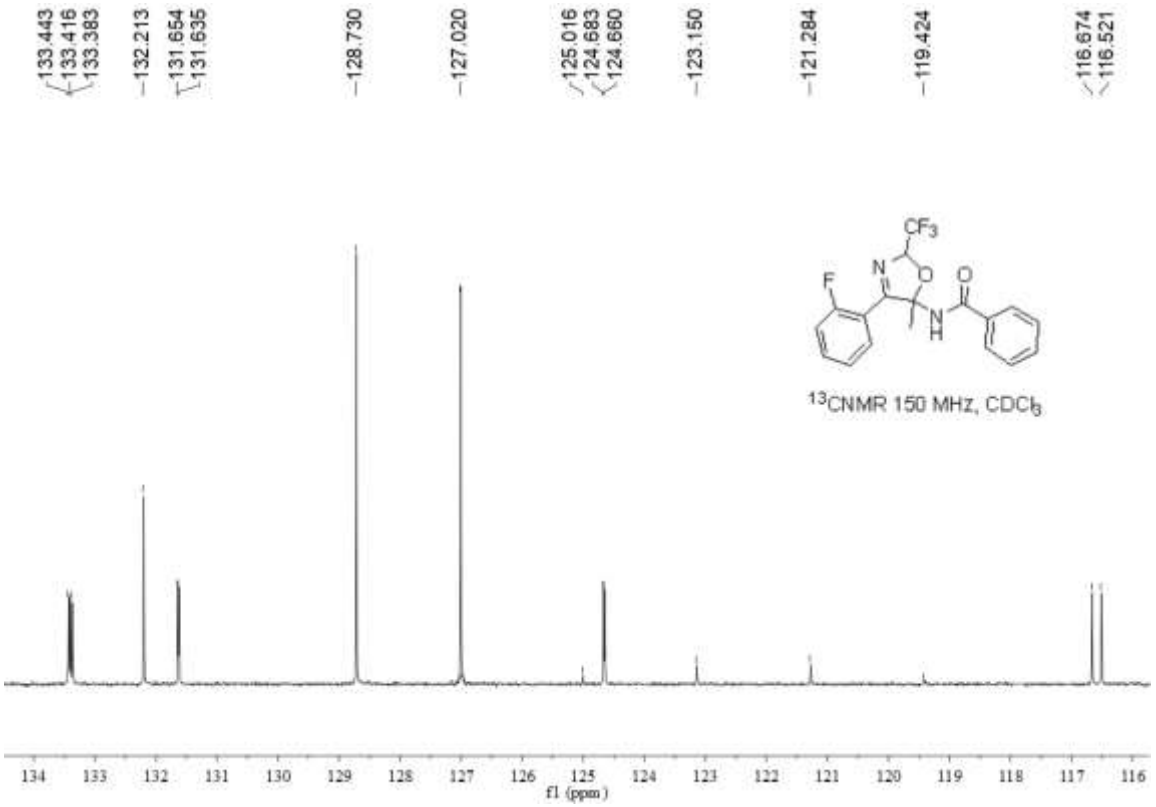
NMR copies of compound **4e**

^{1}H NMR (400 MHz) spectrum of **4e** in $CDCl_3$

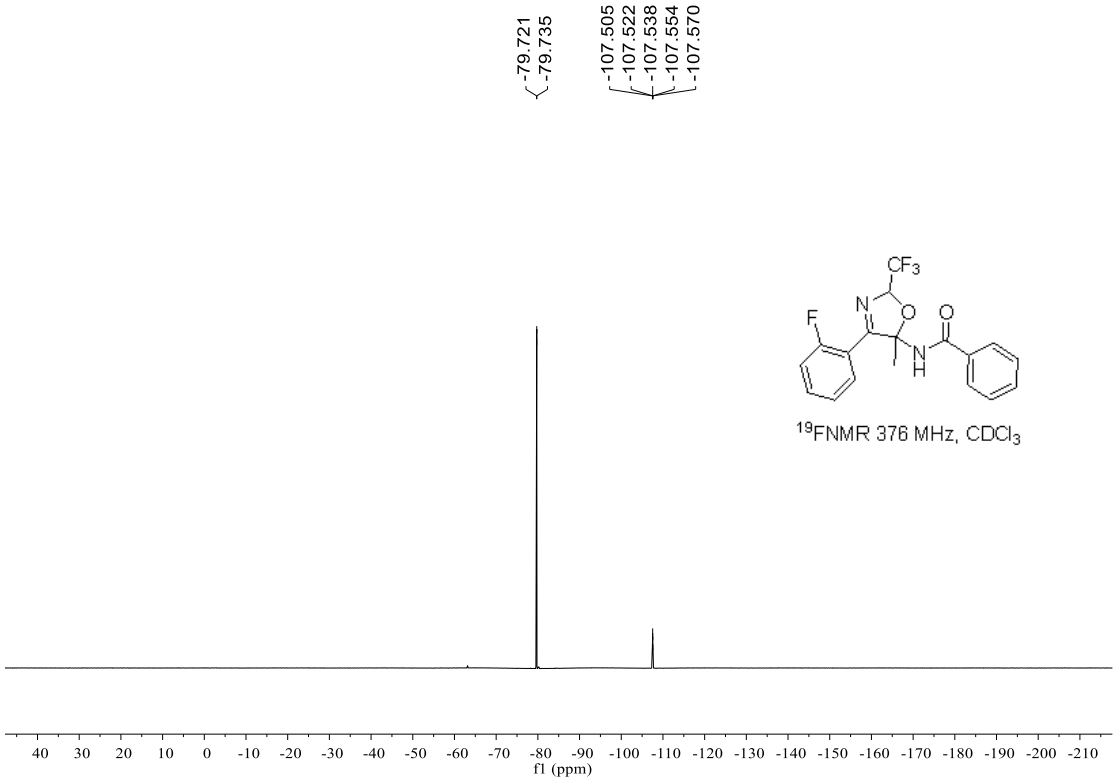


^{13}C NMR (150 MHz) spectrum of **4e** in $CDCl_3$

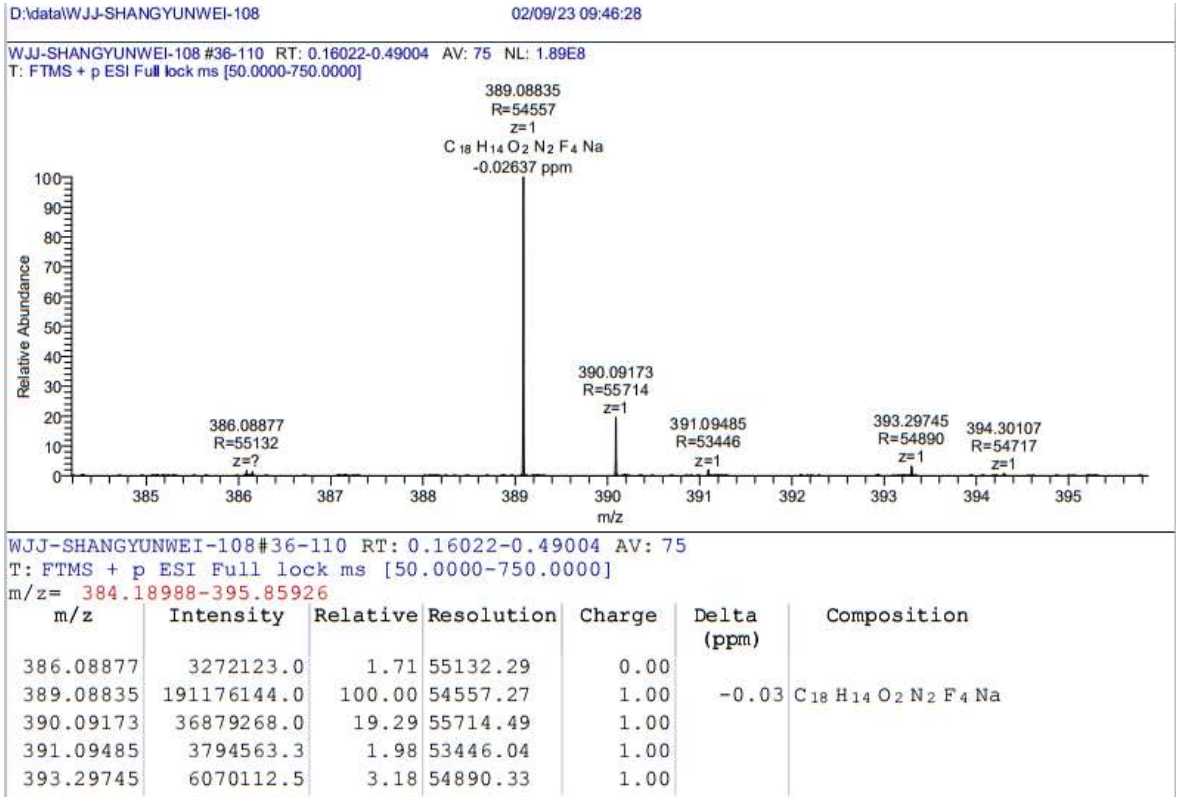




^{19}F NMR (376 MHz) spectrum of **4e** in $CDCl_3$



HRMS(ESI) copy of compound **4e**:

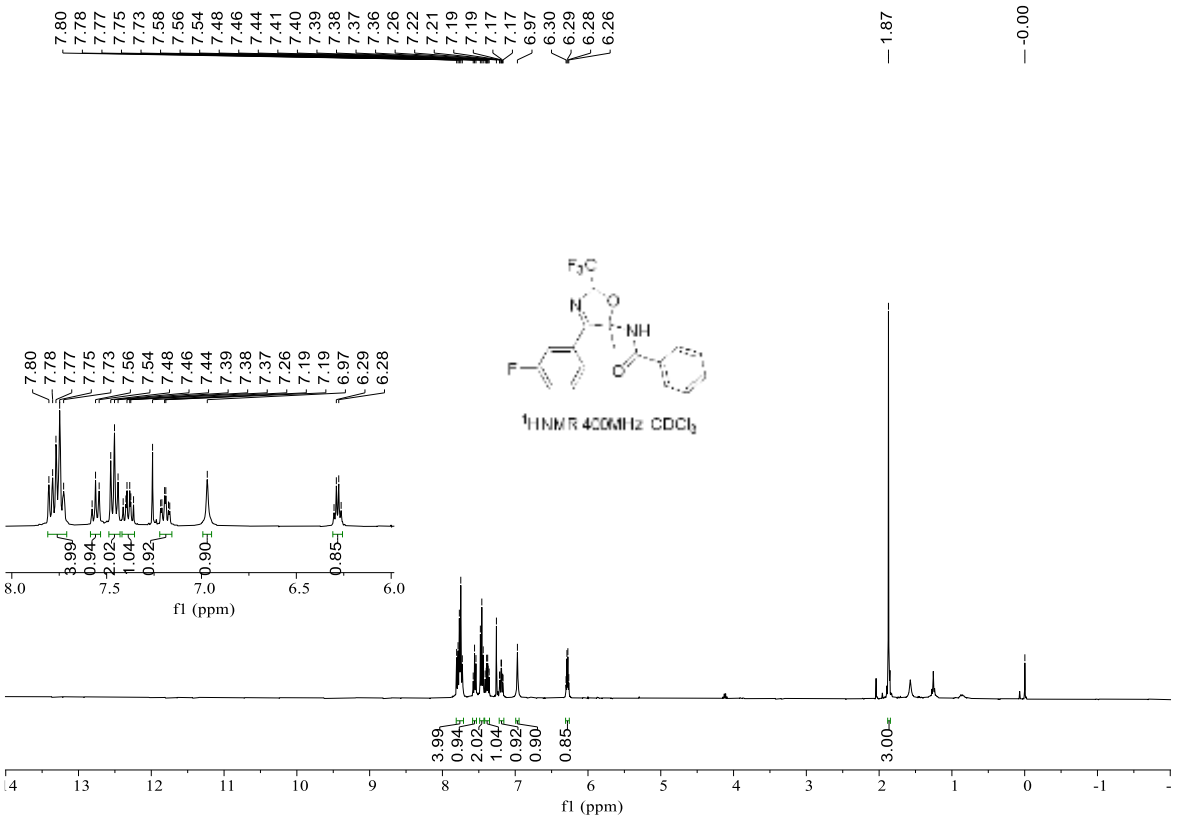


WJJ-SHANGYUNWEI-108#36-110 RT: 0.16022-0.49004 AV: 75
T: FTMS + p ESI Full lock ms [50.0000-750.0000]
m/z= 384.18988-395.85926

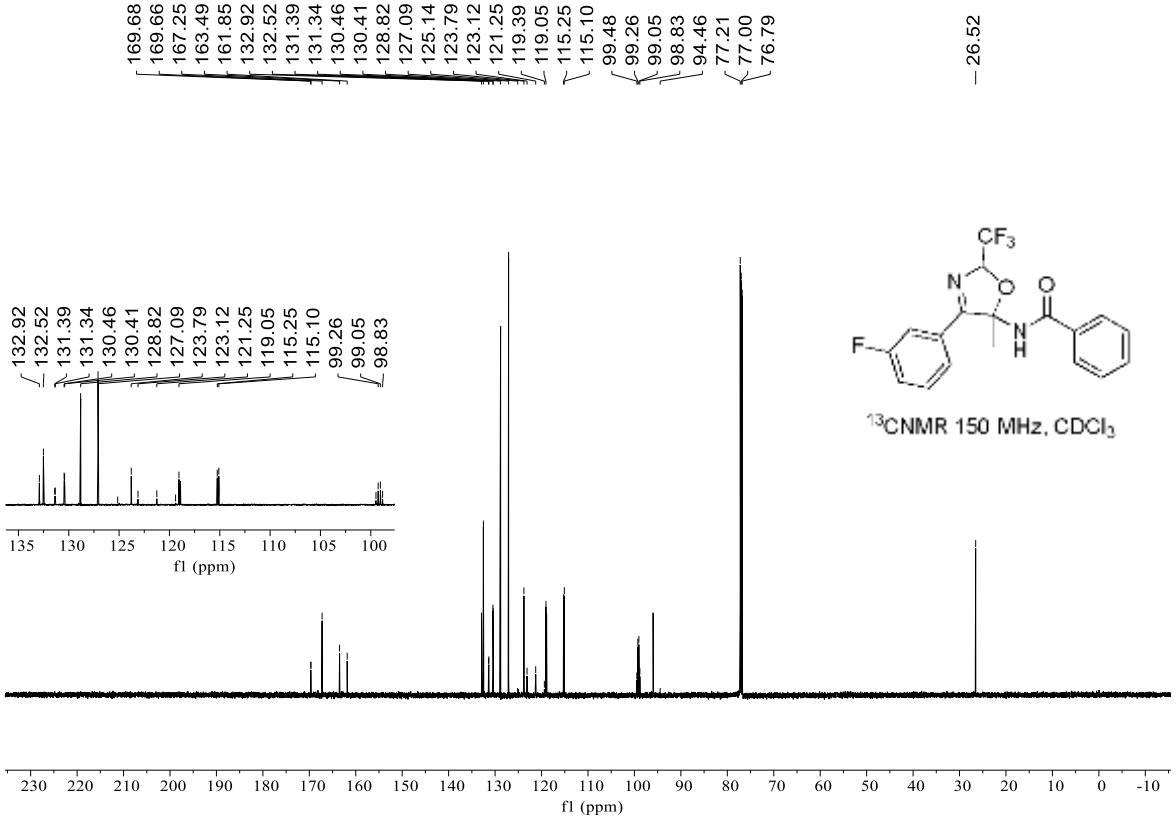
m/z	Intensity	Relative	Resolution	Charge	Delta (ppm)	Composition
386.08877	3272123.0	1.71	55132.29	0.00		
389.08835	191176144.0	100.00	54557.27	1.00	-0.03	C18 H14 O2 N2 F4 Na
390.09173	36879268.0	19.29	55714.49	1.00		
391.09485	3794563.3	1.98	53446.04	1.00		
393.29745	6070112.5	3.18	54890.33	1.00		

NMR copies of compound **4f**

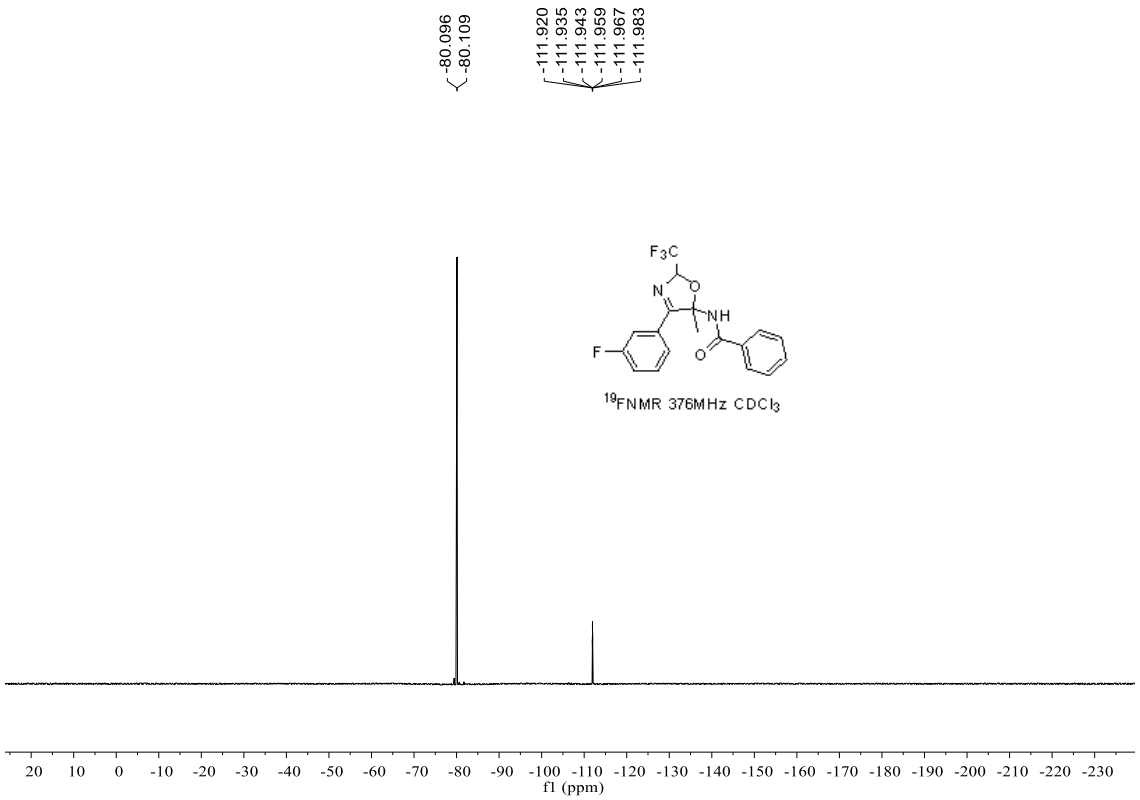
^{1}H NMR (400 MHz) spectrum of **4f** in $CDCl_3$



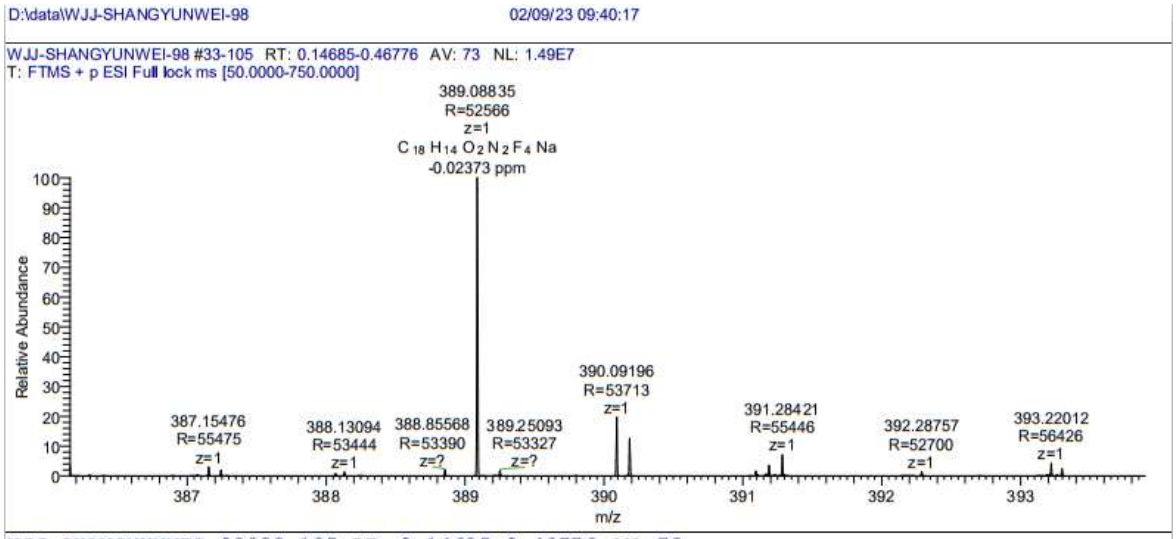
^{13}C NMR (150 MHz) spectrum of **4f** in $CDCl_3$



^{19}F NMR (376 MHz) spectrum of **4f** in $CDCl_3$



HRMS(ESI) copy of compound **4f**:

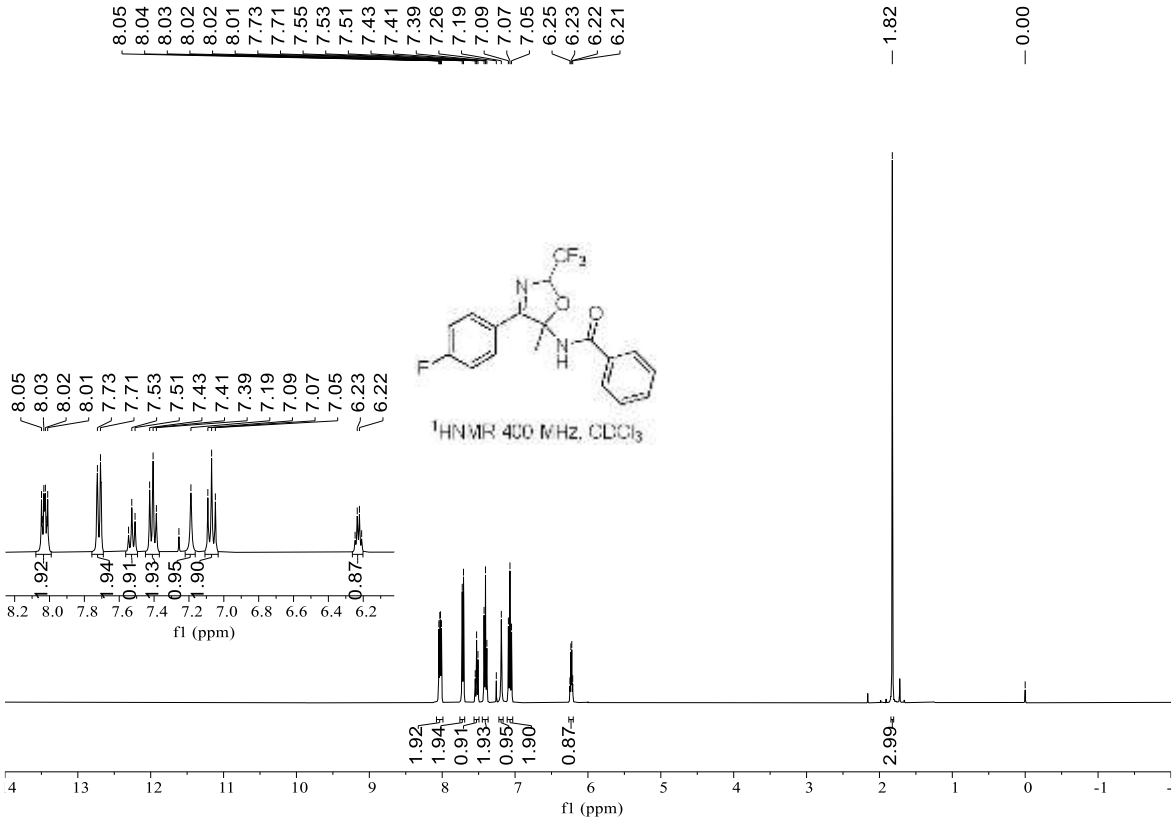


WJJ-SHANGYUNWEI-98#33-105 RT: 0.14685-0.46776 AV: 73
T: FTMS + p ESI Full lock ms [50.0000-750.0000]
m/z= 386.15631-393.89413

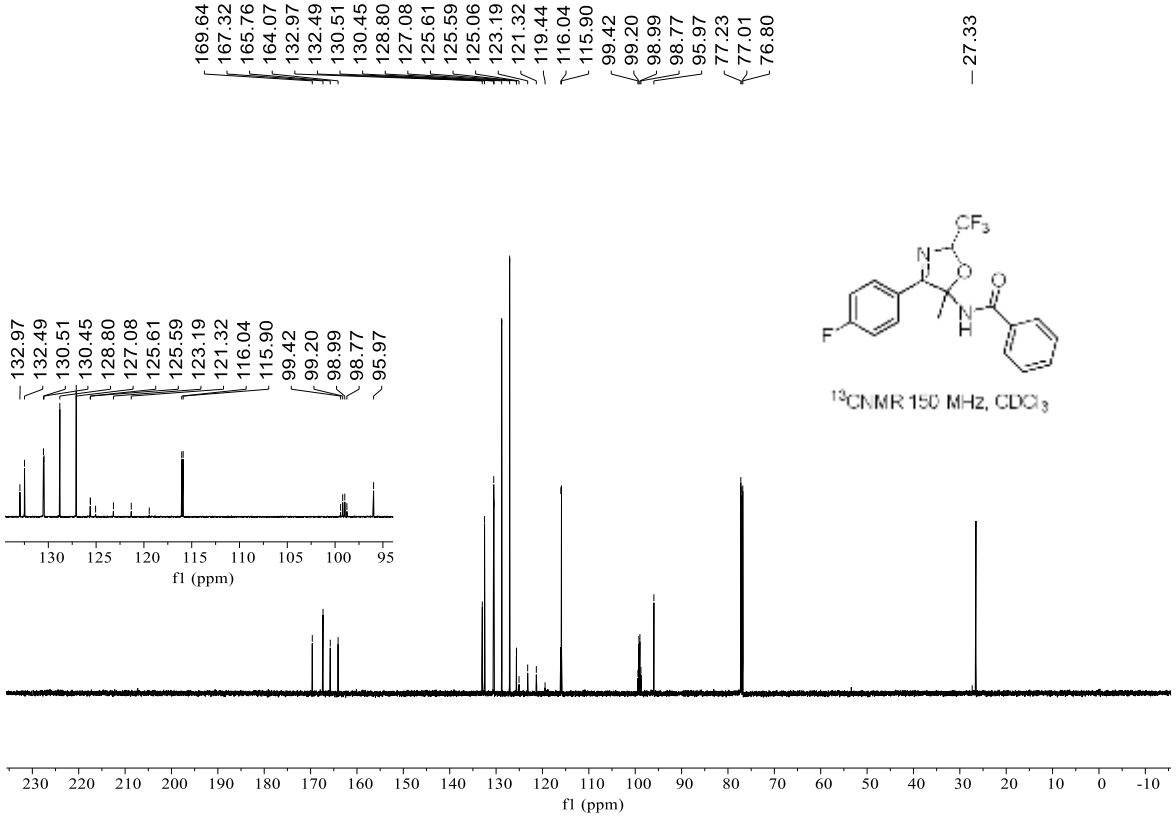
m/z	Intensity	Relative	Resolution	Charge	Delta (ppm)	Composition
389.08835	15228540.0	100.00	52566.41	1.00	-0.02	C18 H14 O2 N2 F4 Na
390.09196	2947388.0	19.35	53713.47	1.00		
390.18529	1881922.6	12.36	55119.51	1.00		
391.28421	1050648.5	6.90	55446.16	1.00		
393.22012	637490.4	4.19	56426.48	1.00		

NMR copies of compound **4g**

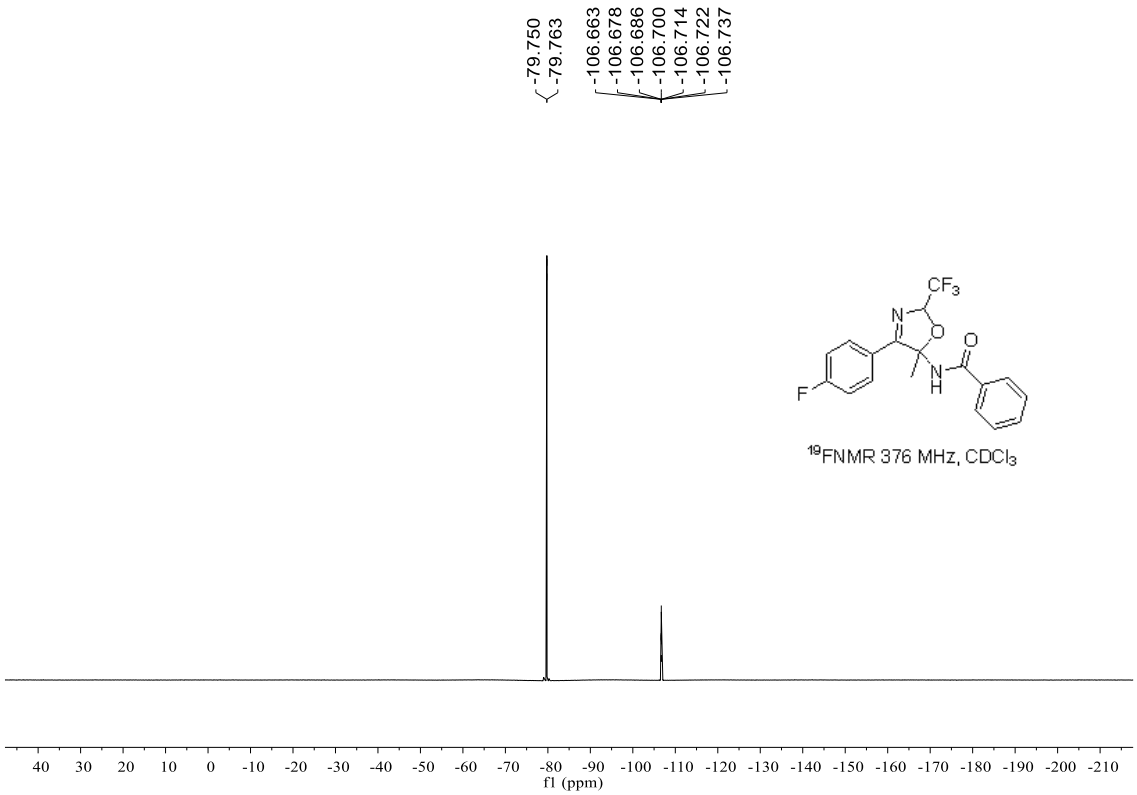
^{1}H NMR (400 MHz) spectrum of **4g** in $CDCl_3$



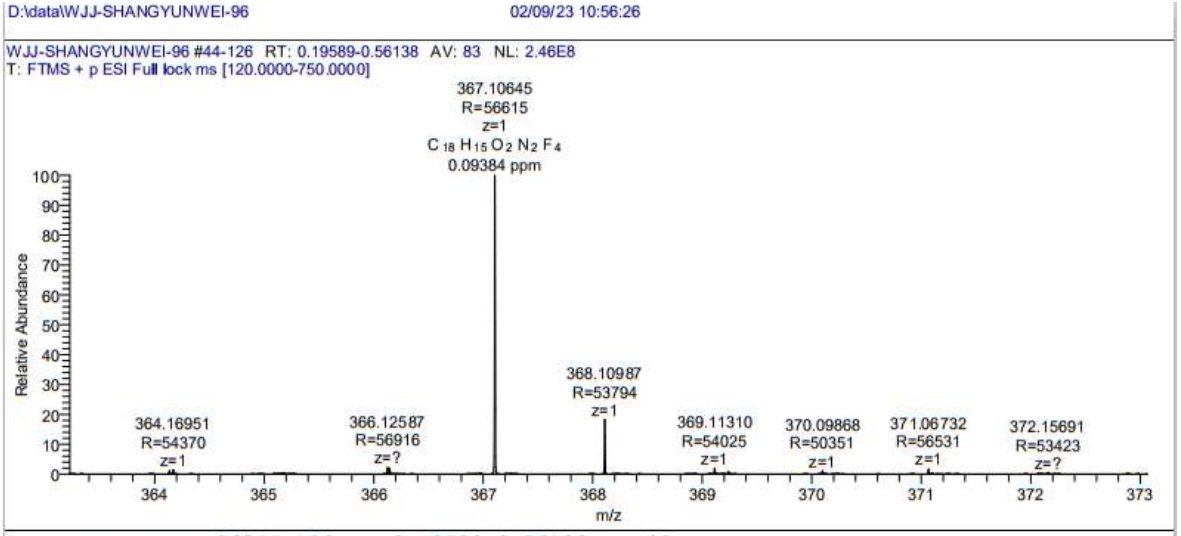
^{13}C NMR (150 MHz) spectrum of **4g** in $CDCl_3$



^{19}F NMR (376 MHz) spectrum of **4g** in $CDCl_3$



HRMS(ESI) copy of compound **4g**:

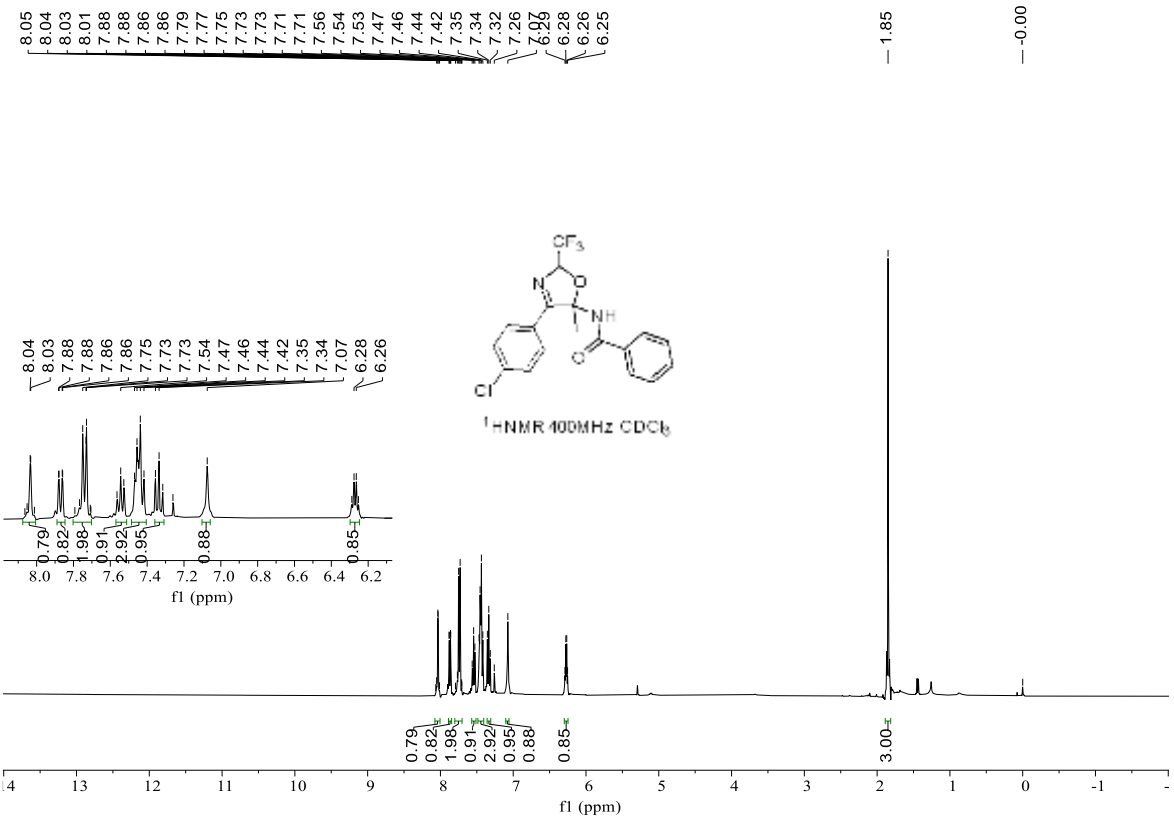


WJJ-SHANGYUNWEI-96#44-126 RT: 0.19589-0.56138 AV: 83
T: FTMS + p ESI Full lock ms [120.0000-750.0000]
m/z= 363.22320-373.05992

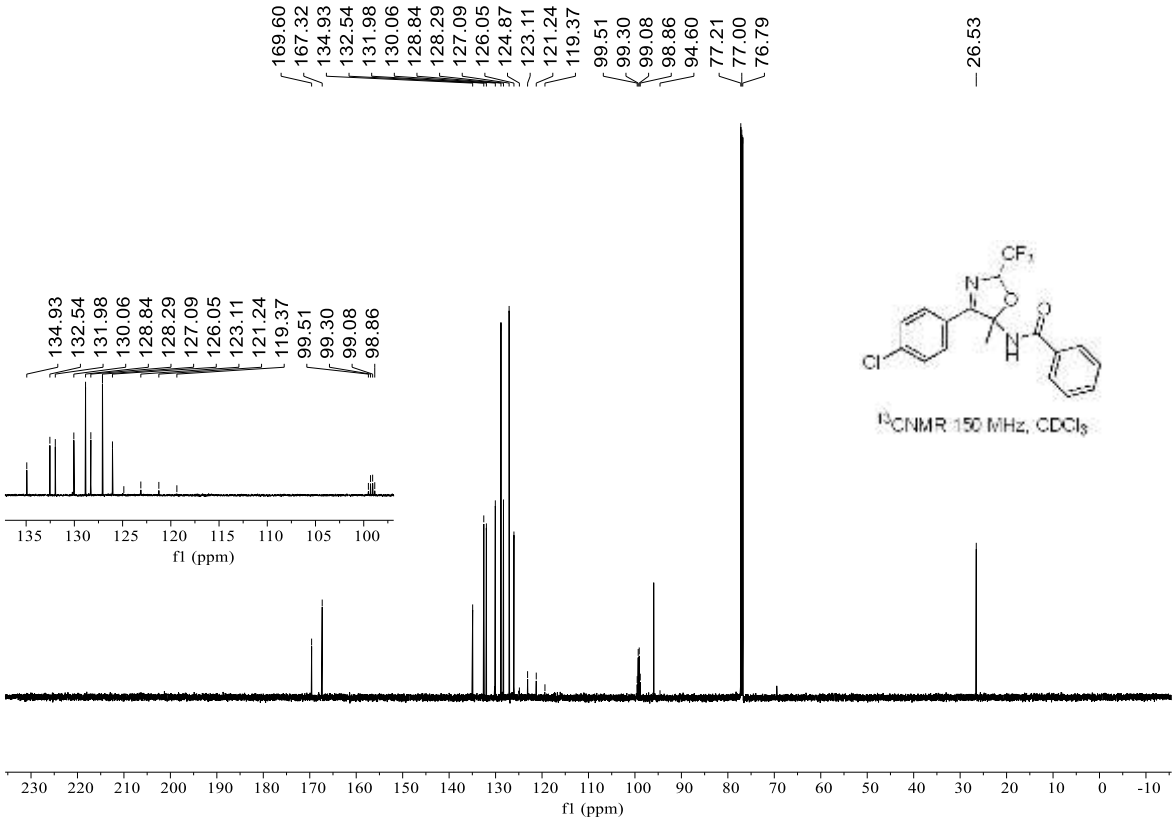
m/z	Intensity	Relative	Resolution	Charge	Delta (ppm)	Composition
366.12587	5606668.5	2.28	56916.15	0.00		
366.14594	4716604.0	1.92	54697.43	0.00		
367.10645	246143728.0	100.00	56615.12	1.00	0.09	$C_{18}H_{15}O_2N_2F_4$
368.10987	46731752.0	18.99	53794.06	1.00		
369.11310	4886686.5	1.99	54024.79	1.00		

NMR copies of compound **4h**

^{1}H NMR (400 MHz) spectrum of **4h** in $CDCl_3$

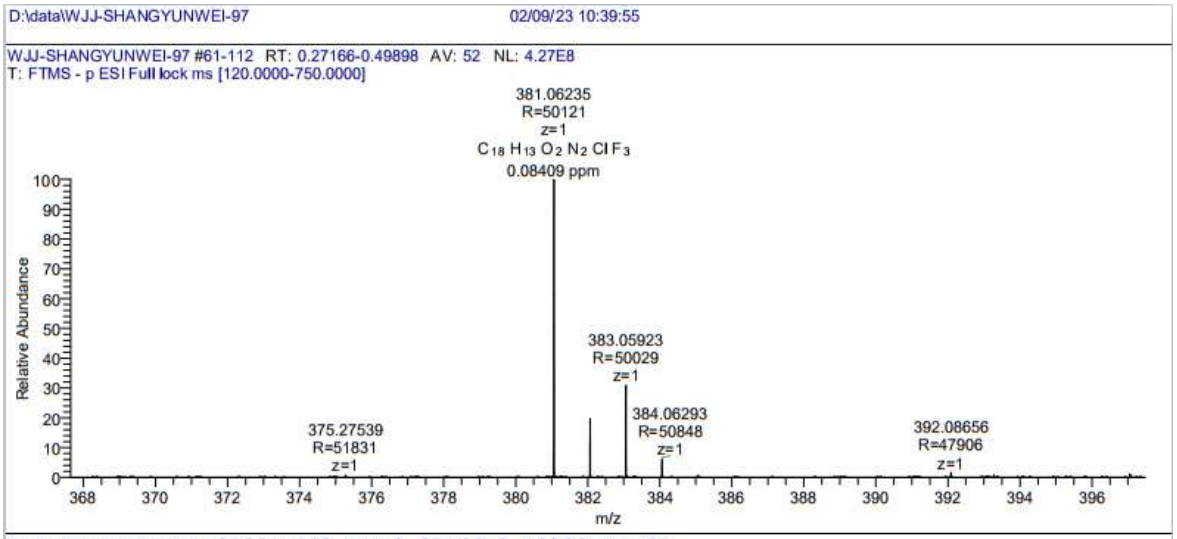


^{13}C NMR (150 MHz) spectrum of **4h** in $CDCl_3$



^{19}F NMR (376 MHz) spectrum of **4h** in $CDCl_3$

HRMS(ESI) copy of compound **4h**:

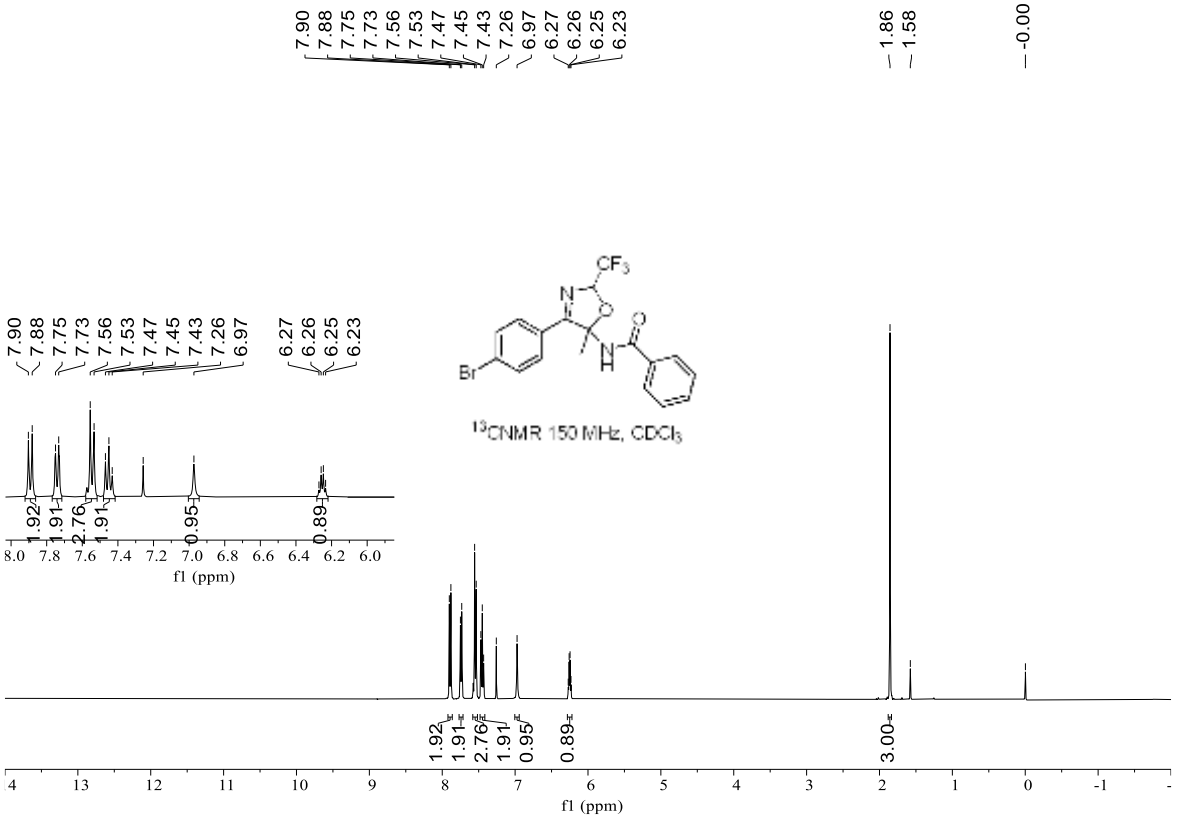


WJJ-SHANGYUNWEI-97#61-112 RT: 0.27166-0.49898 AV: 52
T: FTMS - p ESI Full lock ms [120.0000-750.0000]
m/z= 367.63845-397.46964

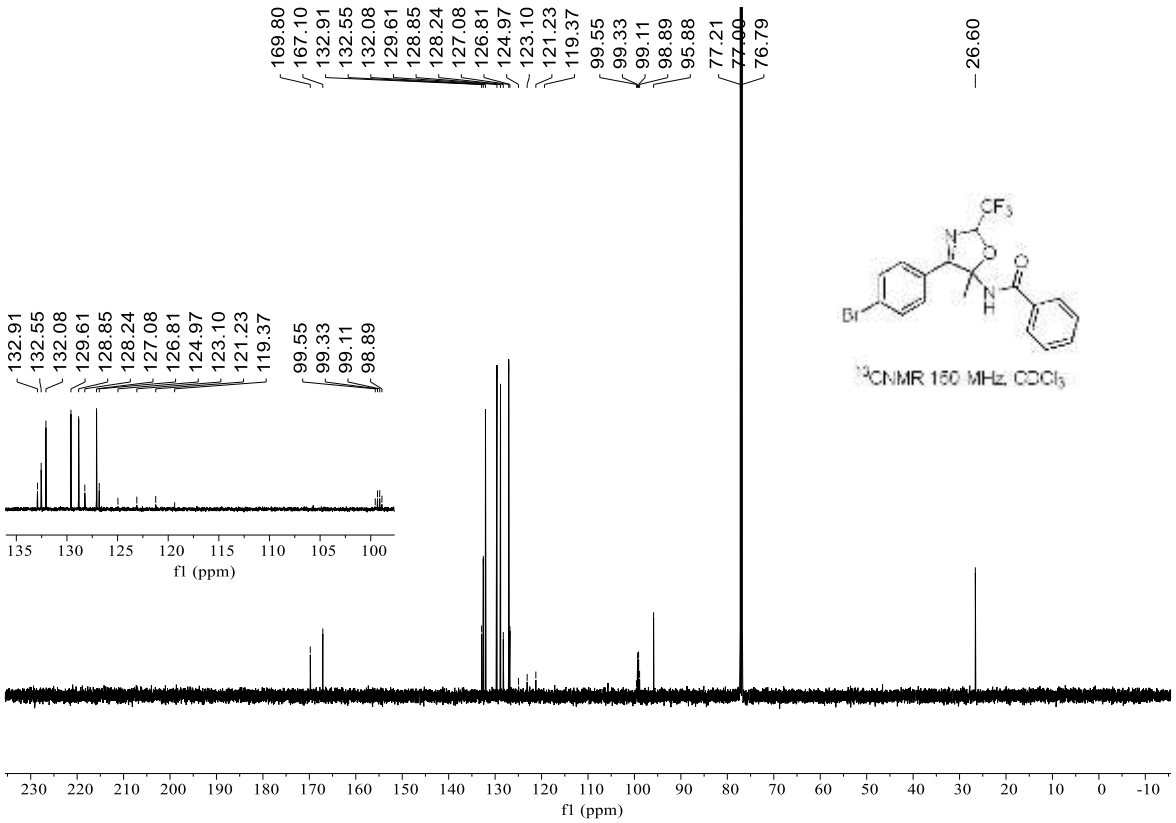
m/z	Intensity	Relative	Resolution	Charge	Delta (ppm)	Composition
381.06235	433283392.0	100.00	50120.70	1.00	0.08	$C_{18}H_{13}O_2N_2ClF_3$
382.06584	84489560.0	19.50	50488.44	1.00		
383.05923	133254368.0	30.75	50028.66	1.00		
384.06293	26369766.0	6.09	50848.25	1.00		
392.08656	7075518.5	1.63	47906.13	1.00		

NMR copies of compound **4i**

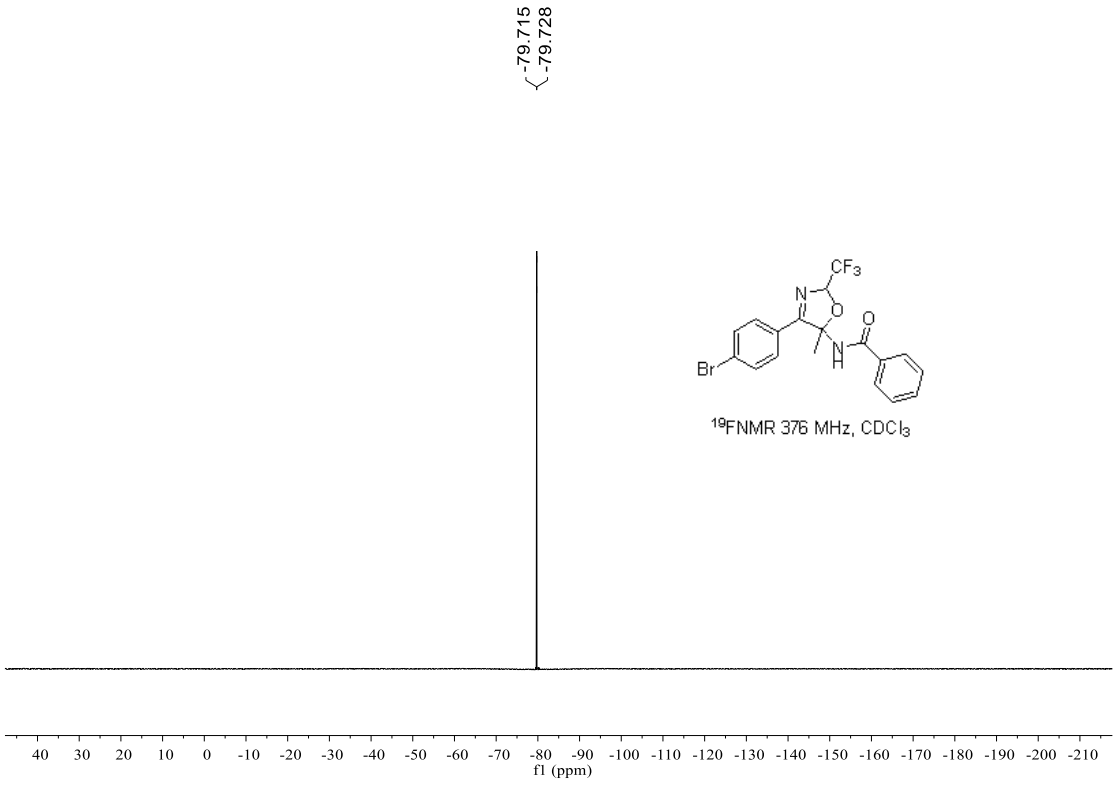
^{1}H NMR (400 MHz) spectrum of **4i** in $CDCl_3$



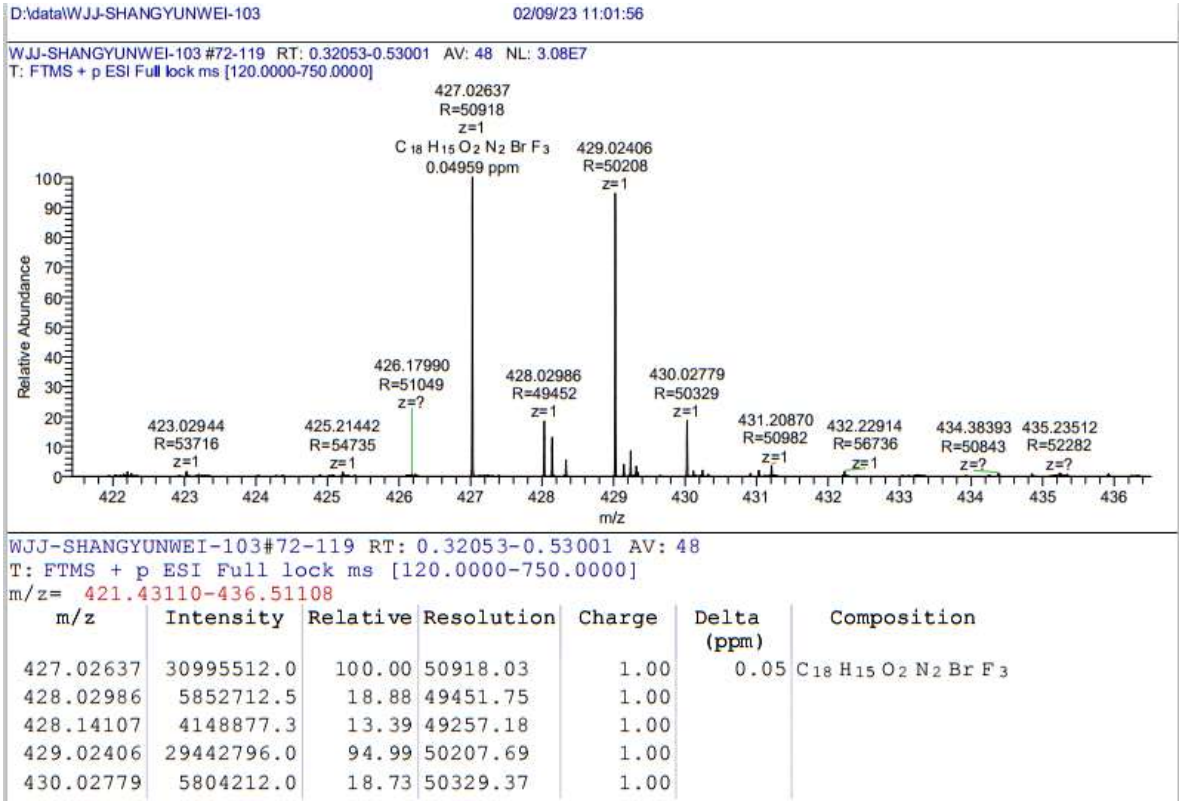
^{13}C NMR (150 MHz) spectrum of **4i** in $CDCl_3$



^{19}F NMR (376 MHz) spectrum of **4i** in $CDCl_3$



HRMS(ESI) copy of compound **4i**:



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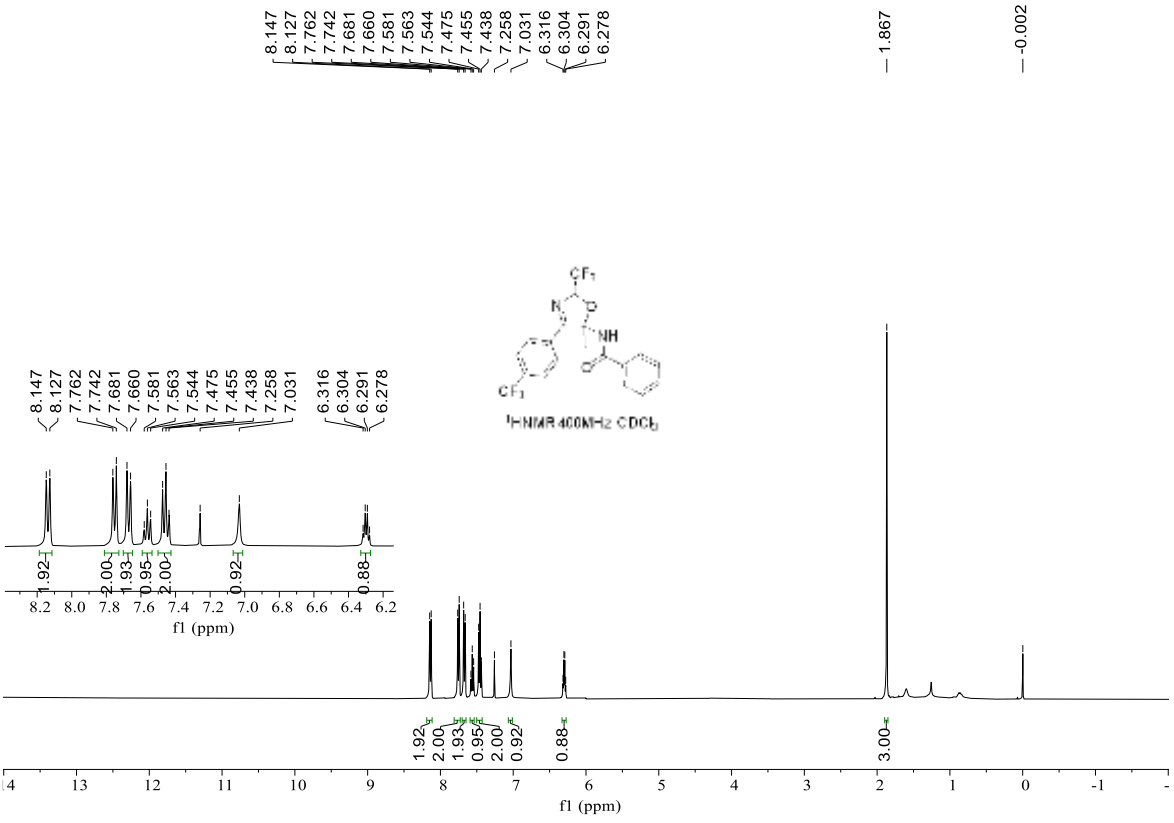
T: FTMS + p ESI Full lock ms [120.0000-750.0000]
m/z= 421.43110-436.51108

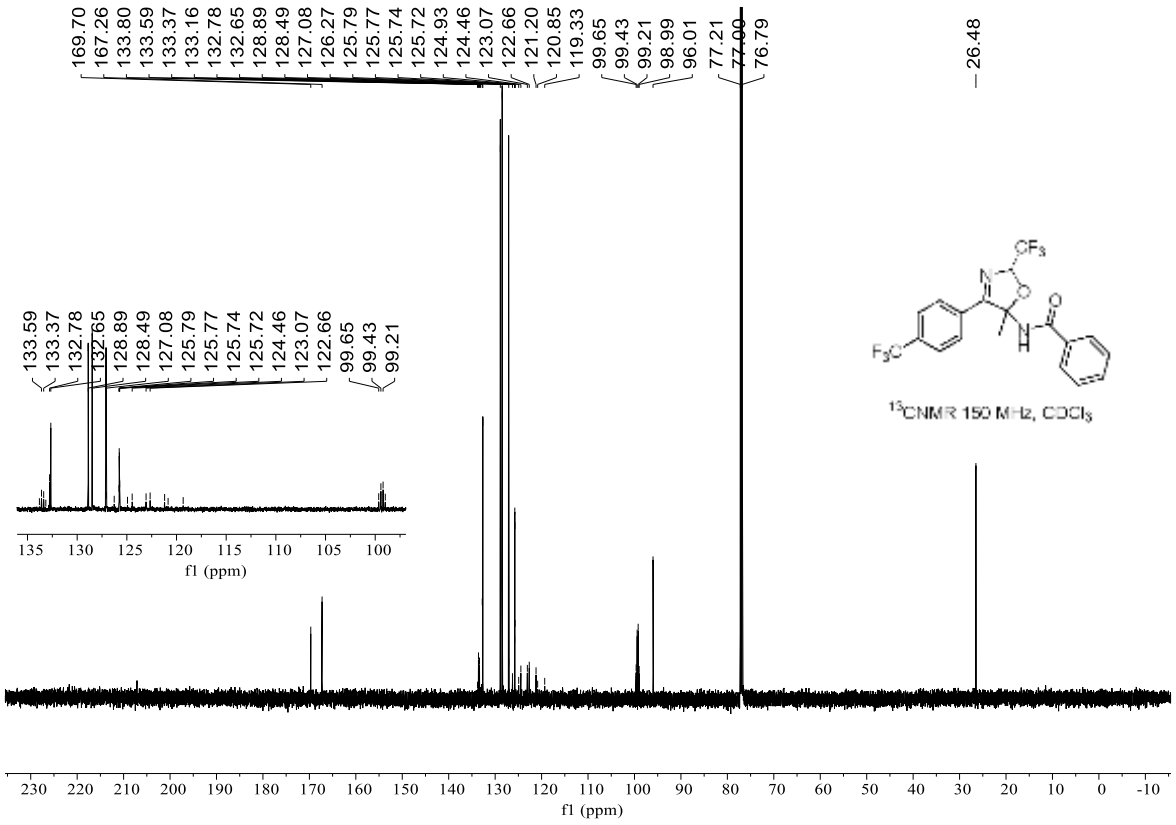
m/z	Intensity	Relative	Resolution	Charge	Delta (ppm)	Composition
427.02637	30995512.0	100.00	50918.03	1.00	0.05	C18 H15 O2 N2 Br F3
428.02986	5852712.5	18.88	49451.75	1.00		
428.14107	4148877.3	13.39	49257.18	1.00		
429.02406	29442796.0	94.99	50207.69	1.00		
430.02779	5804212.0	18.73	50329.37	1.00		

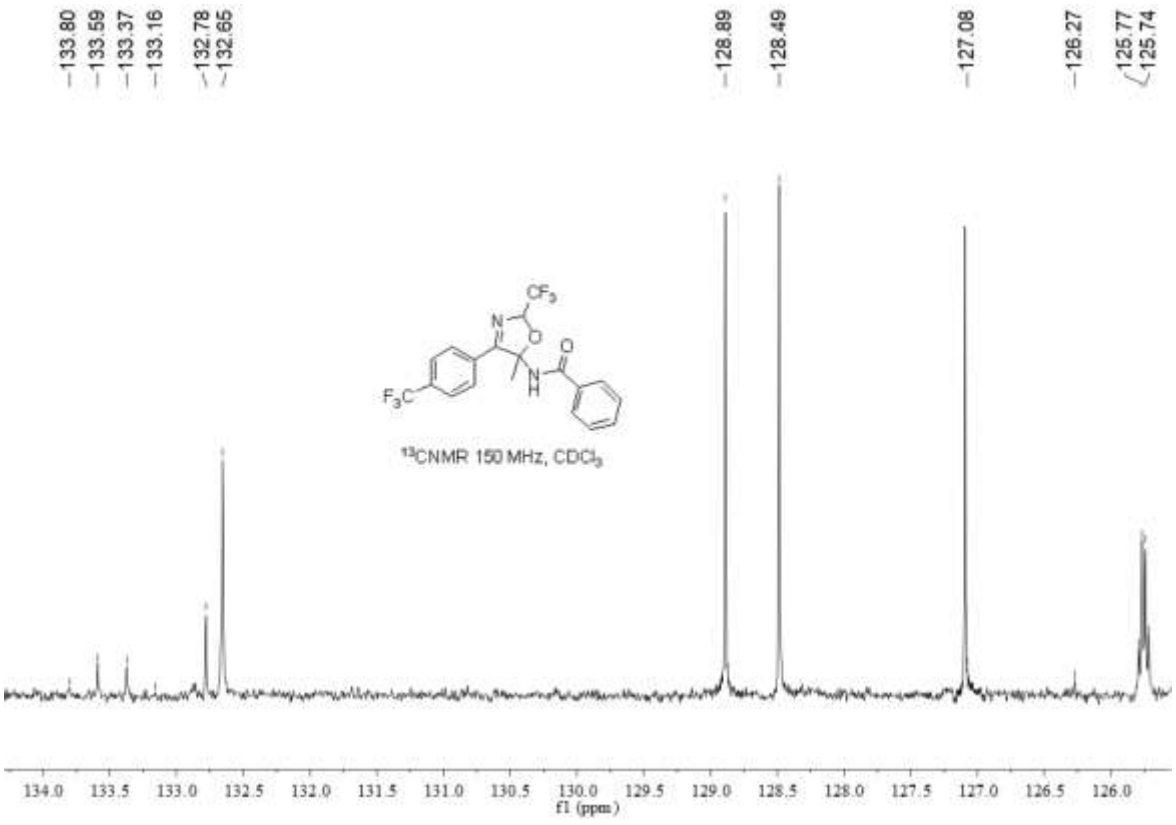
NMR copies of compound **4j**

^{1}H NMR (400 MHz) spectrum of **4j** in $CDCl_3$

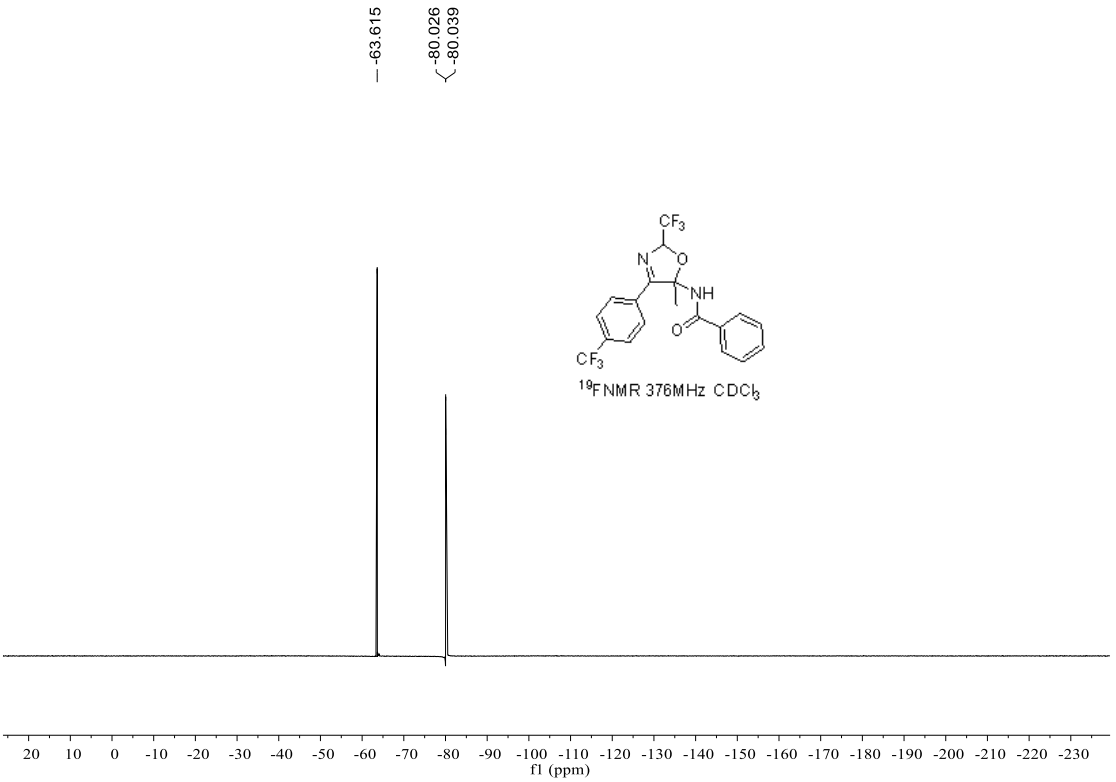


^{13}C NMR (150 MHz) spectrum of **4j** in $CDCl_3$

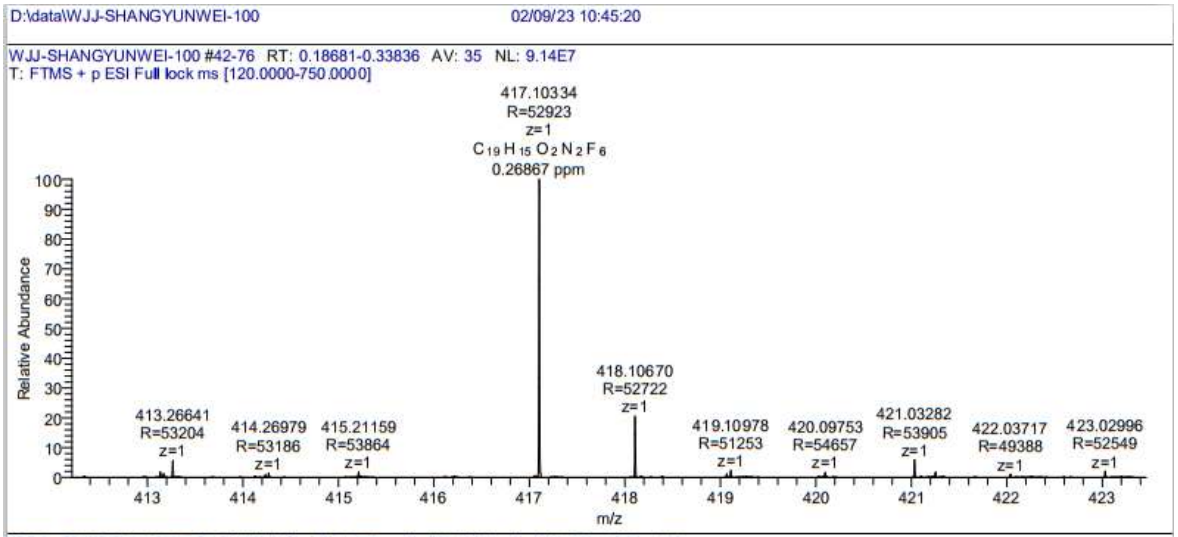




^{19}F NMR (376 MHz) spectrum of **4j** in $CDCl_3$



HRMS(ESI) copy of compound **4j**:

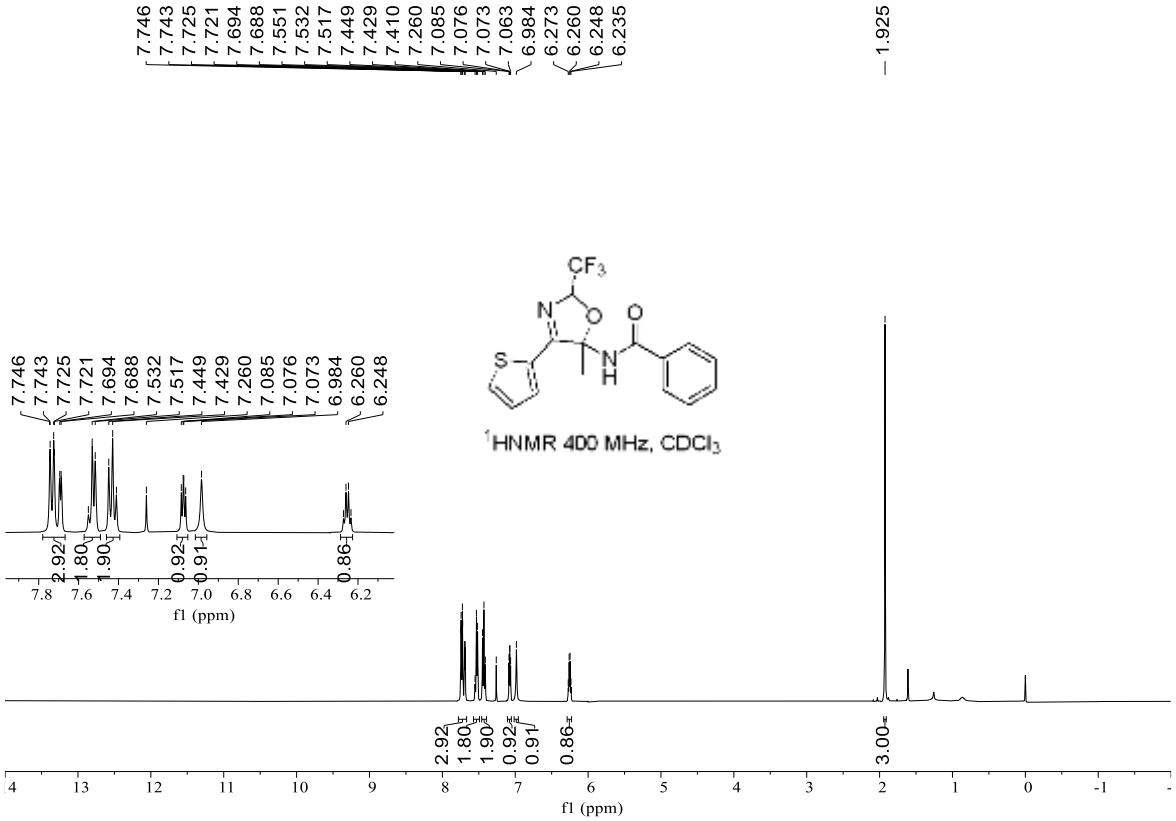


WJJ-SHANGYUNWEI-100#42-76 RT: 0.18681-0.33836 AV: 35
T: FTMS + p ESI Full lock ms [120.0000-750.0000]
m/z= 412.20944-423.45610

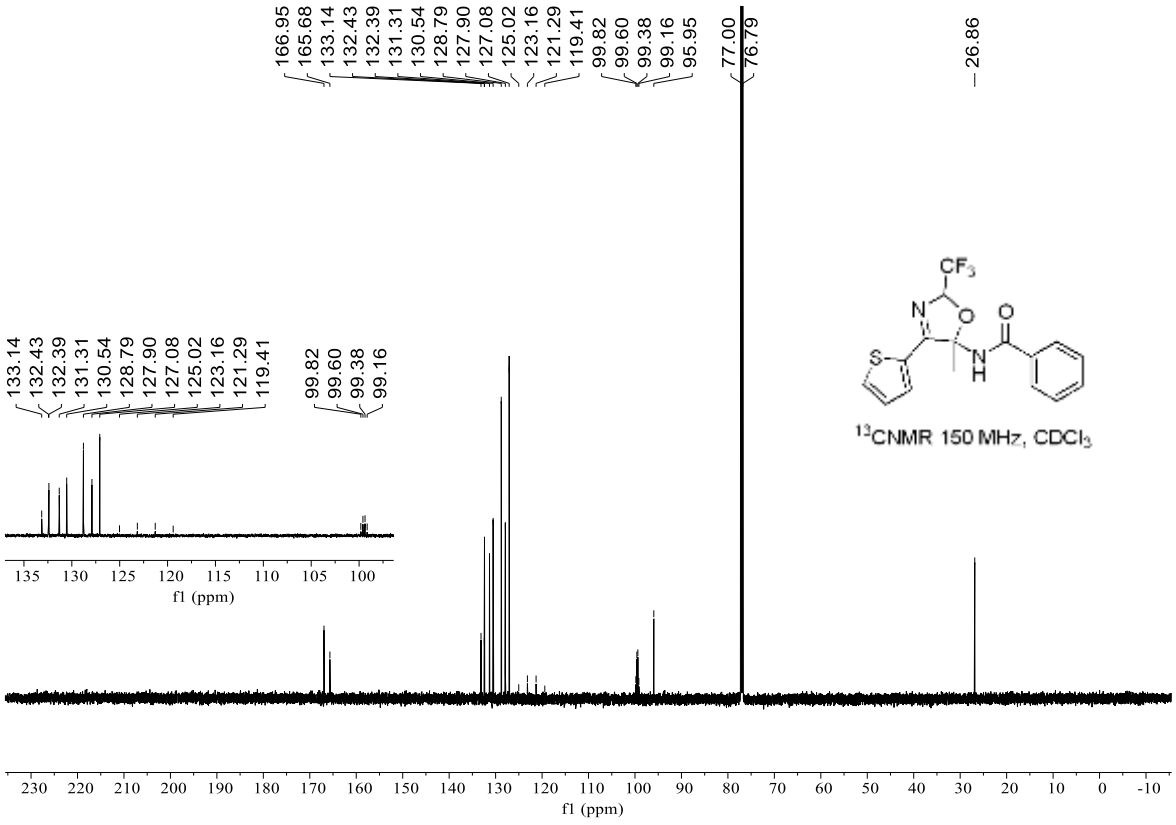
m/z	Intensity	Relative	Resolution	Charge	Delta (ppm)	Composition
413.26641	5347555.0	5.68	53204.31	1.00		
417.10334	94217864.0	100.00	52923.05	1.00	0.27	$C_{19}H_{15}O_2N_2F_6$
418.10670	18981754.0	20.15	52721.73	1.00		
419.10978	2147629.5	2.28	51252.99	1.00		
421.03282	5488066.0	5.82	53904.64	1.00		

NMR copies of compound **4l**

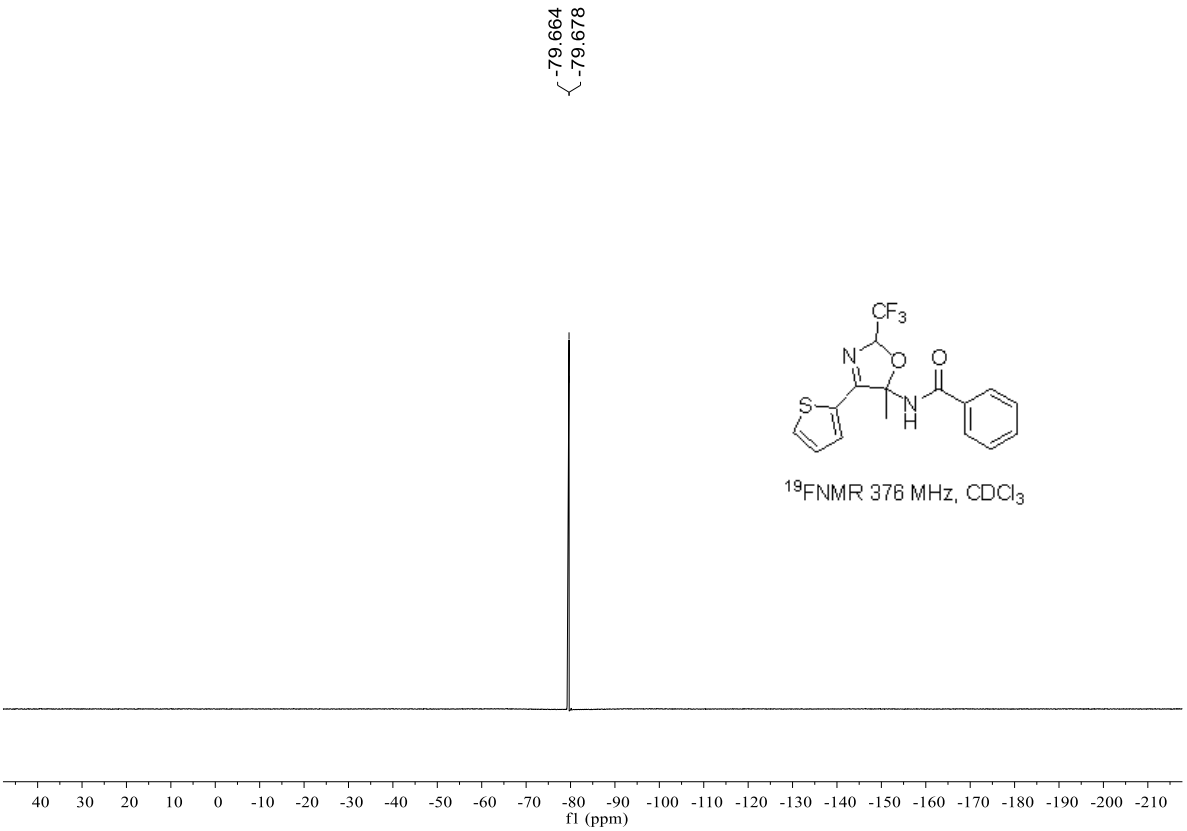
^{1}H NMR (400 MHz) spectrum of **4l** in $CDCl_3$



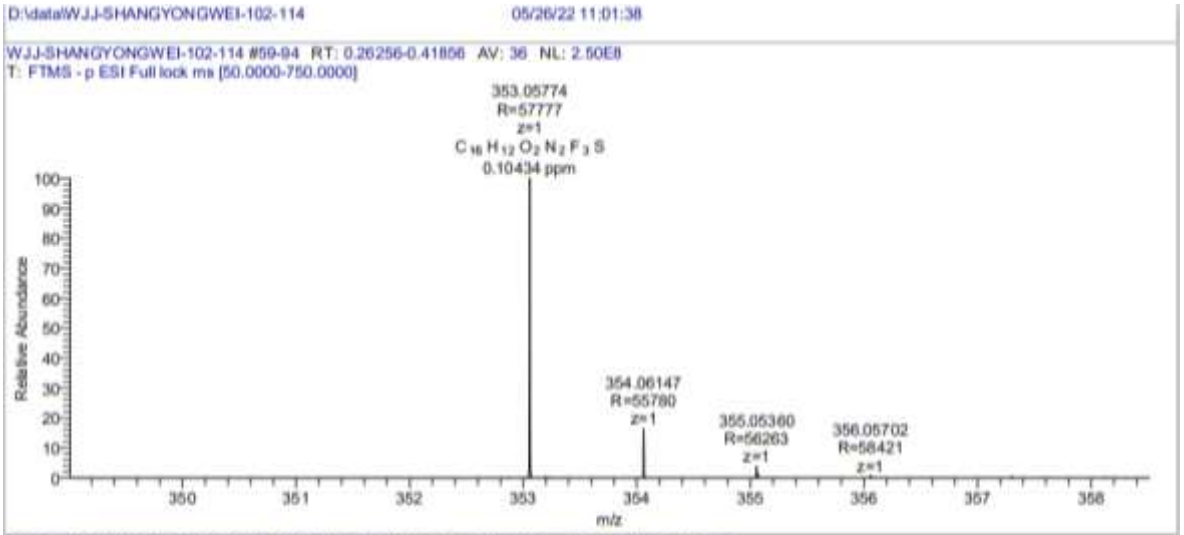
^{13}C NMR (150 MHz) spectrum of **4l** in $CDCl_3$



^{19}F NMR (376 MHz) spectrum of **4l** in $CDCl_3$



HRMS(ESI) copy of compound **4l**:

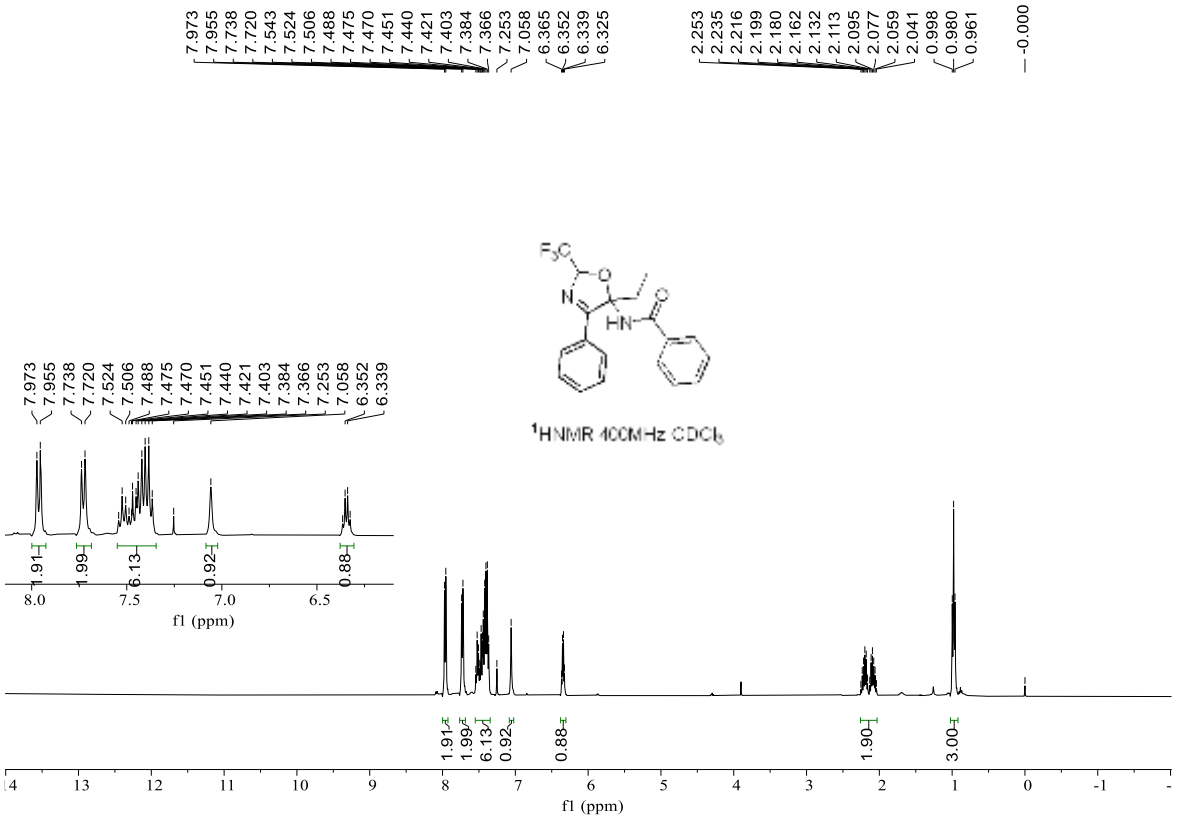


WJJ-SHANGYONGWEI-102-114#59-94 RT: 0.26256-0.41856 AV: 36
T: FTMS - p ESI Full lock ms [50.0000-750.0000]
m/z= 349.01337-358.51214

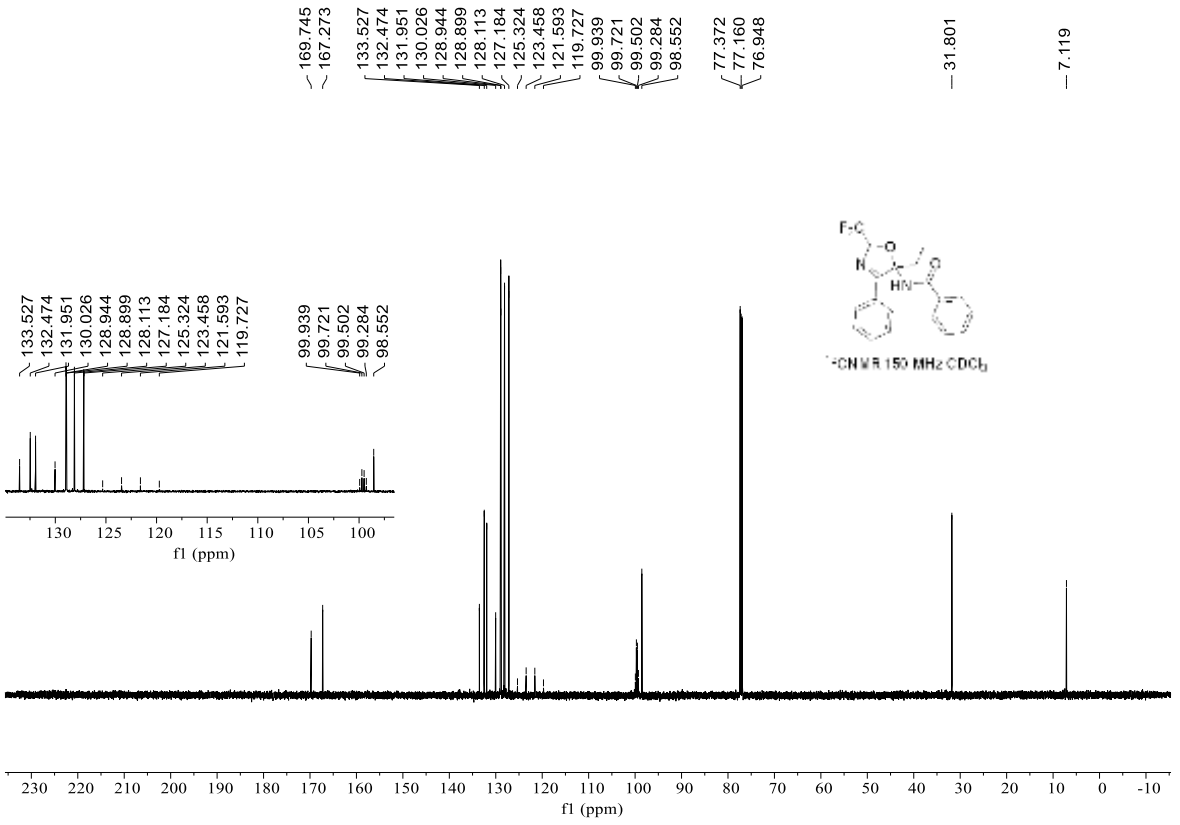
m/z	Intensity	Relative	Resolution	Charge	Delta (ppm)	Composition
353.05774	249918016.0	100.00	57777.04	1.00	0.10	$C_{16}H_{12}O_2N_2F_3S$
354.06147	41247584.0	16.50	55779.91	1.00		
355.05360	9792938.0	3.92	56263.42	1.00		
355.06407	3568369.5	1.43	53880.94	1.00		
356.05702	1758539.9	0.70	58421.24	1.00		

NMR copies of compound **4m**

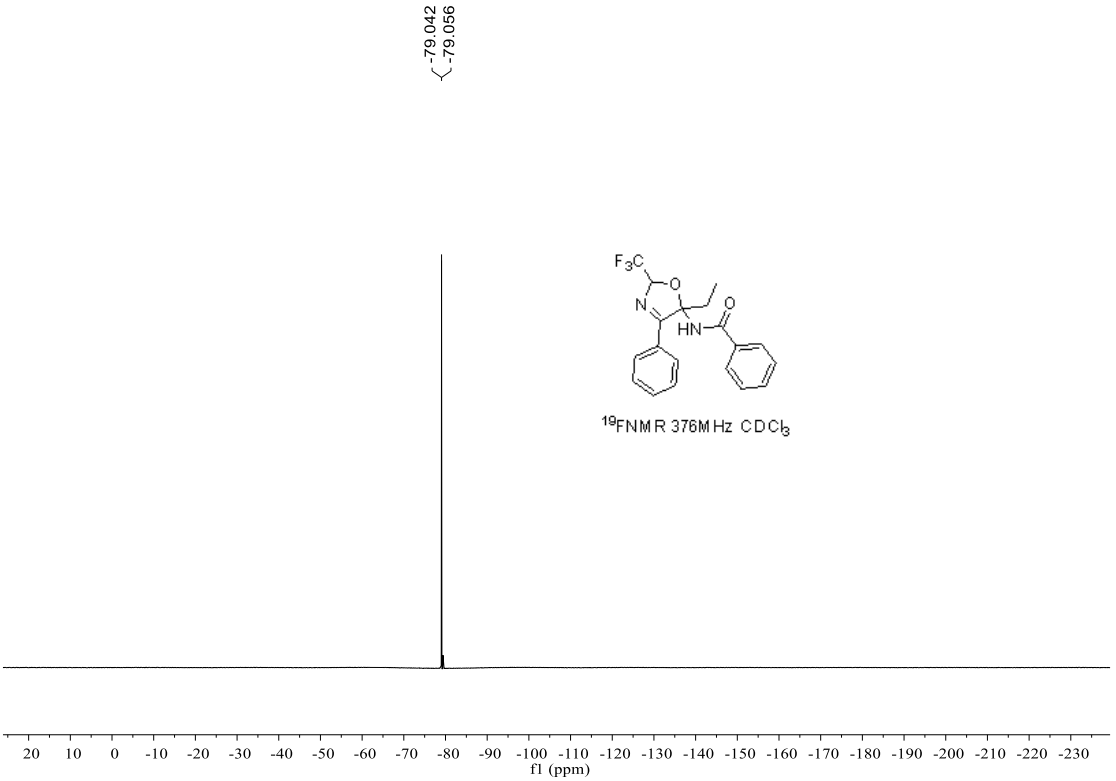
^{1}H NMR (400 MHz) spectrum of **4m** in $CDCl_3$



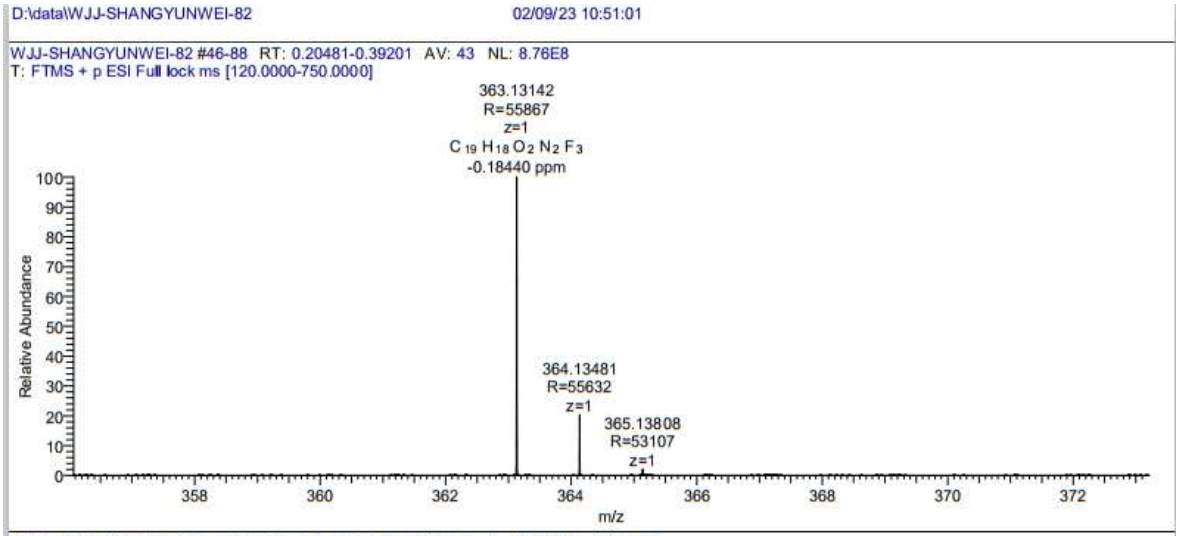
^{13}C NMR (150 MHz) spectrum of **4m** in $CDCl_3$



^{19}F NMR (376 MHz) spectrum of **4m** in $CDCl_3$



HRMS(ESI) copy of compound **4m**:

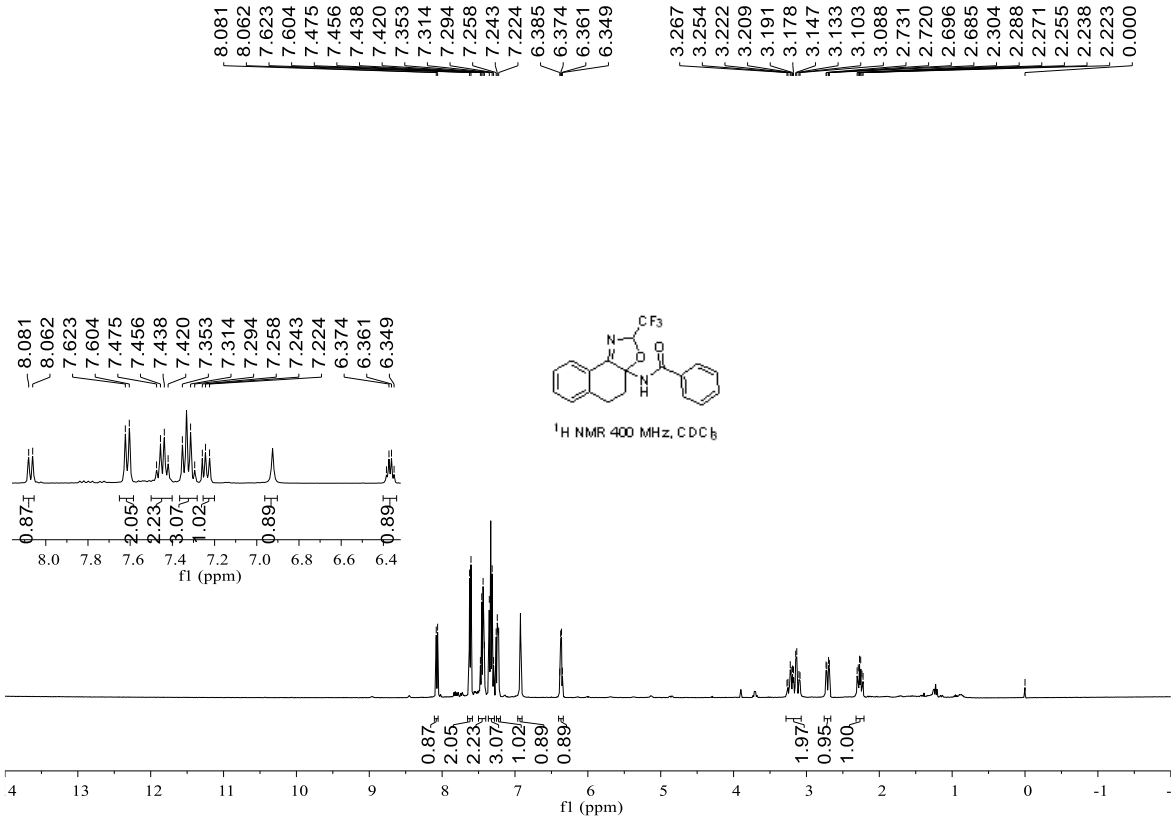


WJJ-SHANGYUNWEI-82#46-88 RT: 0.20481-0.39201 AV: 43
T: FTMS + p ESI Full lock ms [120.0000-750.0000]
m/z= 356.06797-373.18948

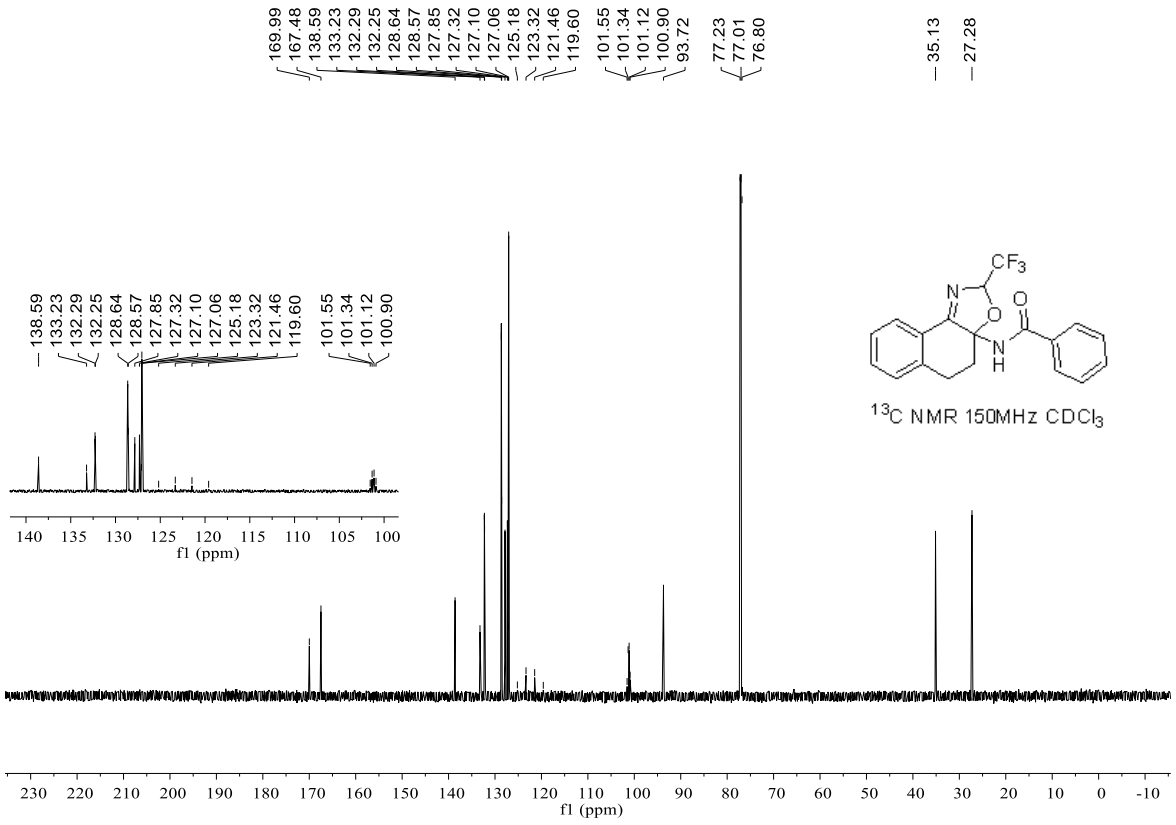
m/z	Intensity	Relative	Resolution	Charge	Delta (ppm)	Composition
362.32651	3594088.3	0.40	58919.63	1.00		
363.13142	900669248.0	100.00	55867.08	1.00	-0.18	$C_{19}H_{18}O_2N_2F_3$
364.13481	181903008.0	20.20	55631.67	1.00		
365.13808	19112984.0	2.12	53107.02	1.00		
367.10637	3611659.3	0.40	55468.24	0.00		

NMR copies of compound **4n**

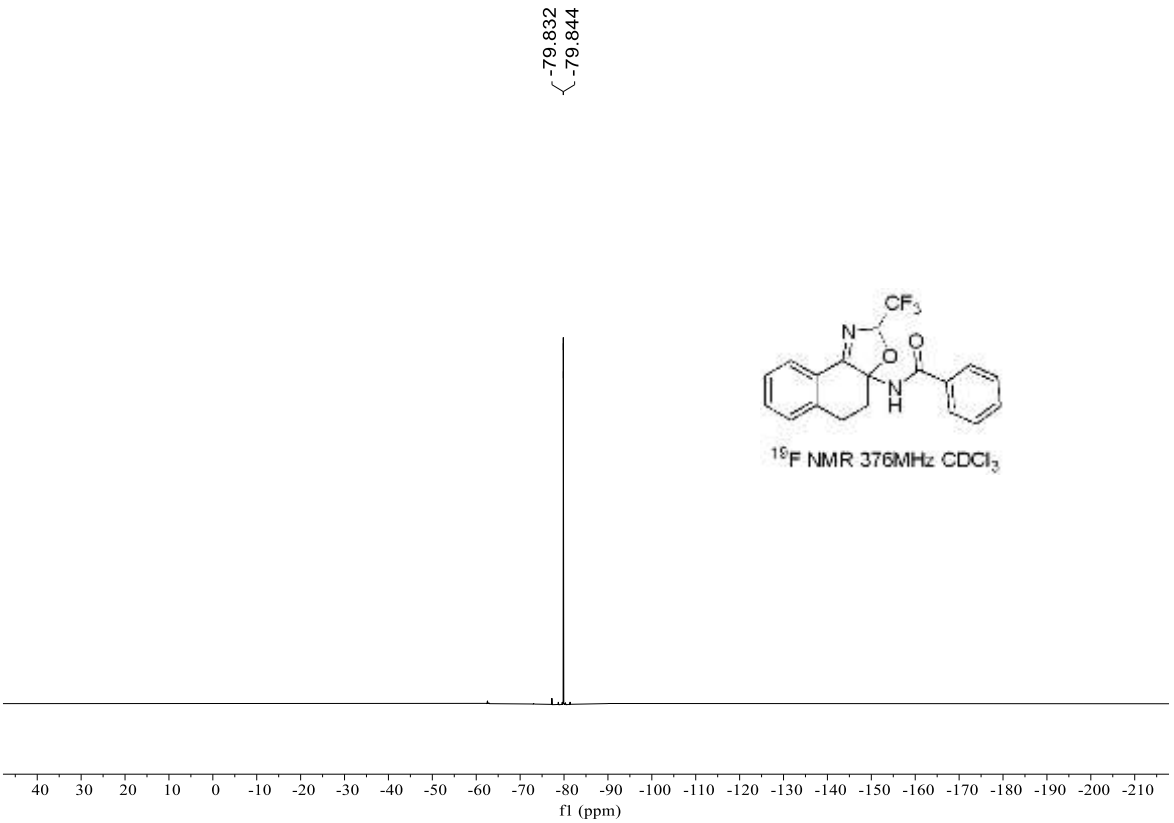
^{1}H NMR (400 MHz) spectrum of **4n** in $CDCl_3$



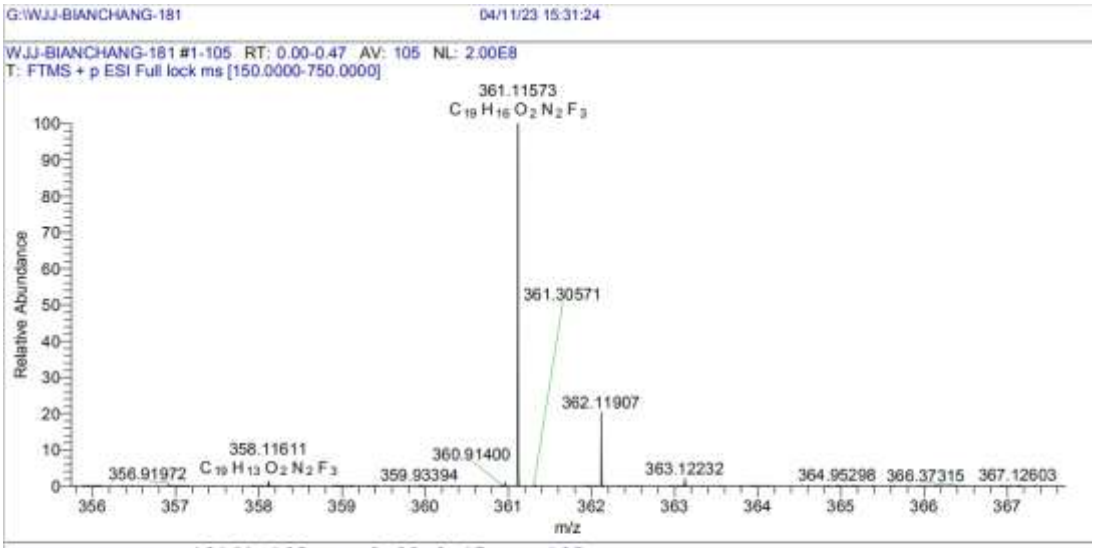
^{13}C NMR (150 MHz) spectrum of **4n** in $CDCl_3$



^{19}F NMR (376 MHz) spectrum of **4n** in $CDCl_3$



HRMS(ESI) copy of compound **4n**:

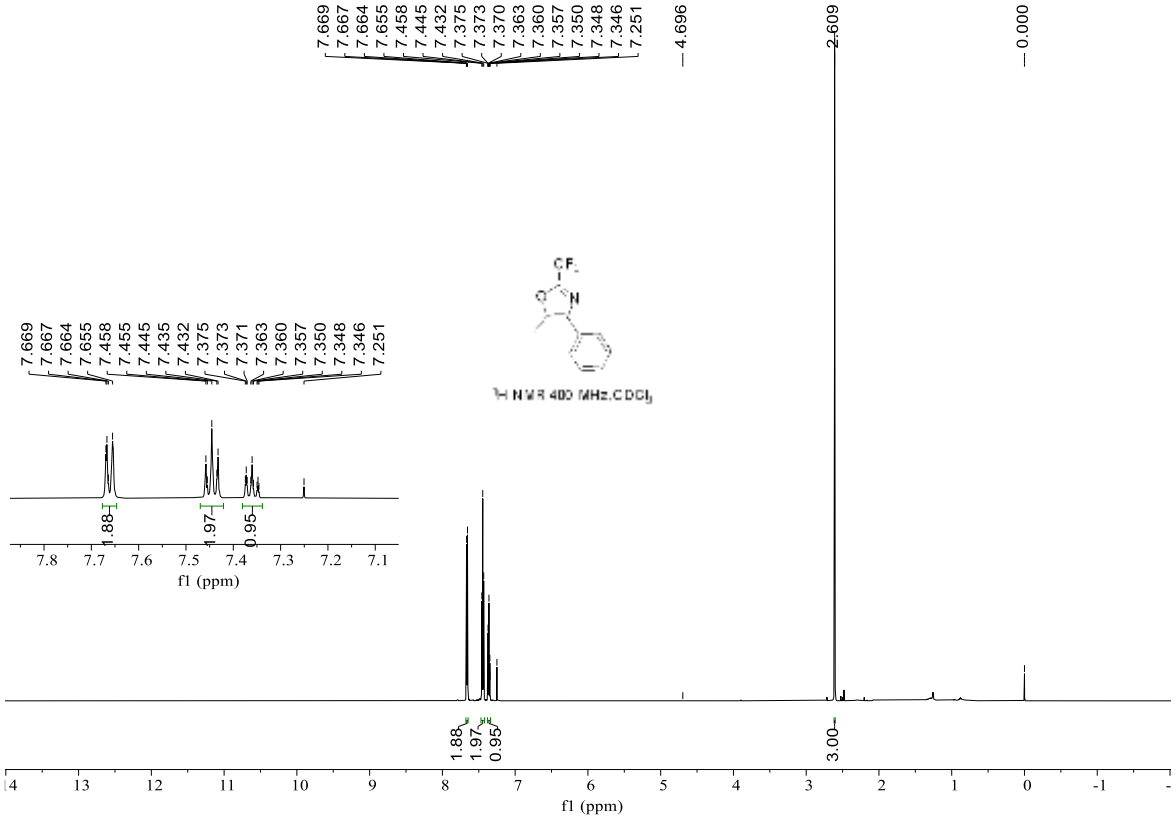


WJJ-BIANCHANG-181#1-105 RT: 0.00-0.47 AV: 105
T: FTMS + p ESI Full lock ms [150.0000-750.0000]
m/z= 355.74193-367.69857

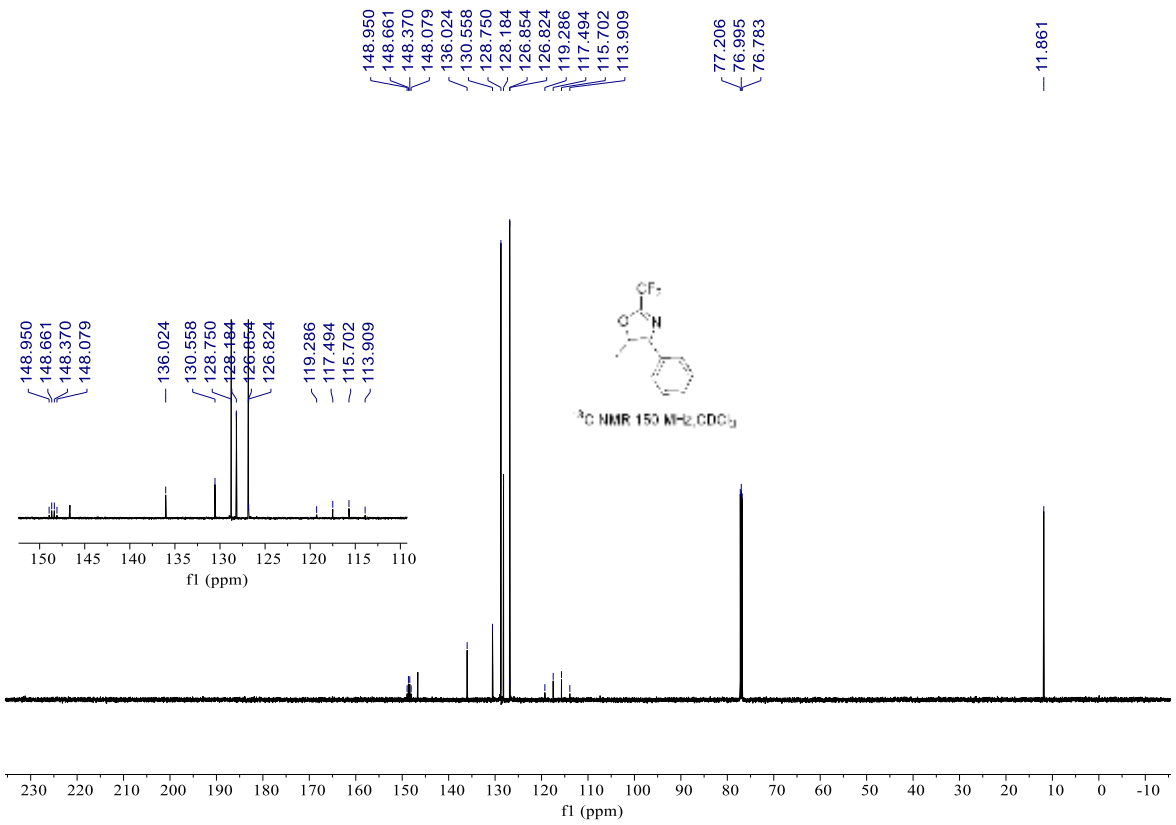
m/z	Intensity	Relative	Delta (ppm)	Composition
358.11611	2657834.0	1.31	23.75	$C_{19}H_{13}O_2N_2F_3$
360.95859	2077030.9	1.02	-157.25	$C_{19}H_{16}O_2N_2F_3$
361.11573	202769968.0	100.00	-0.11	$C_{19}H_{16}O_2N_2F_3$
362.11907	40873096.0	20.16		
363.12232	4272451.5	2.11		

NMR copies of compound **5**

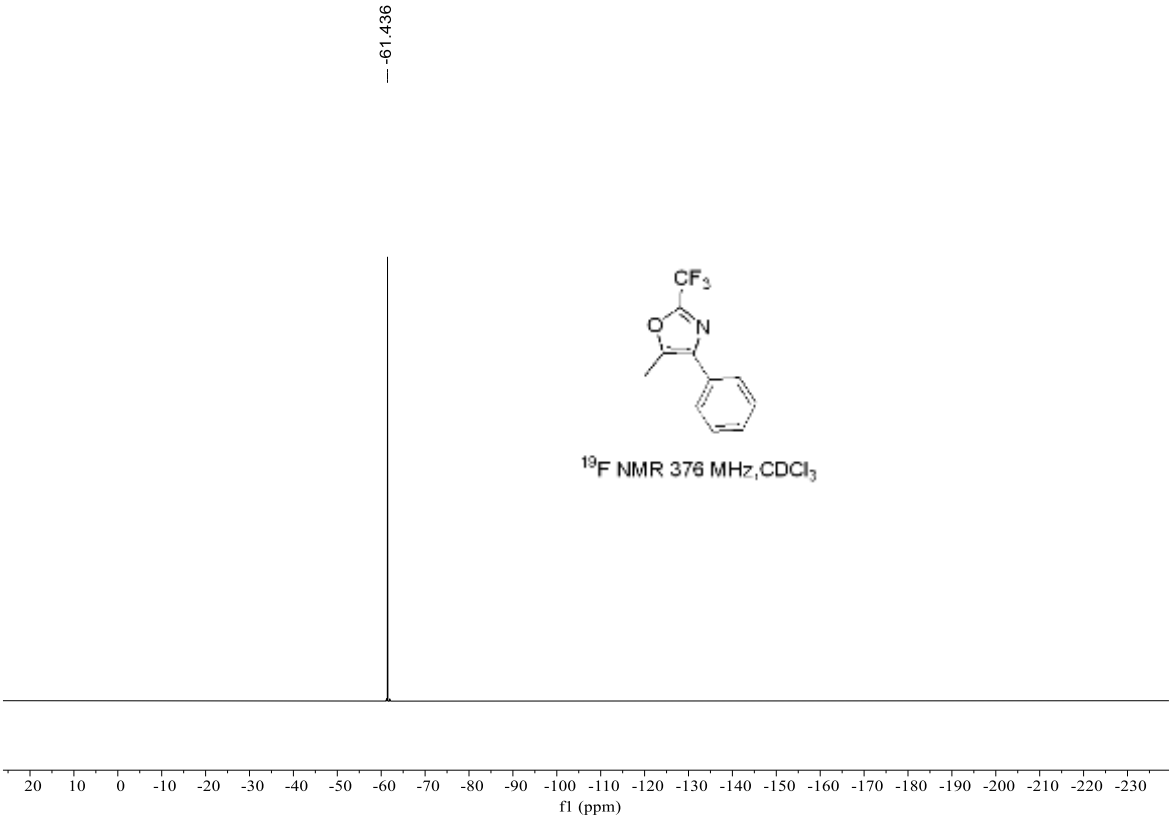
^{1}H NMR (400 MHz) spectrum of **5** in $CDCl_3$



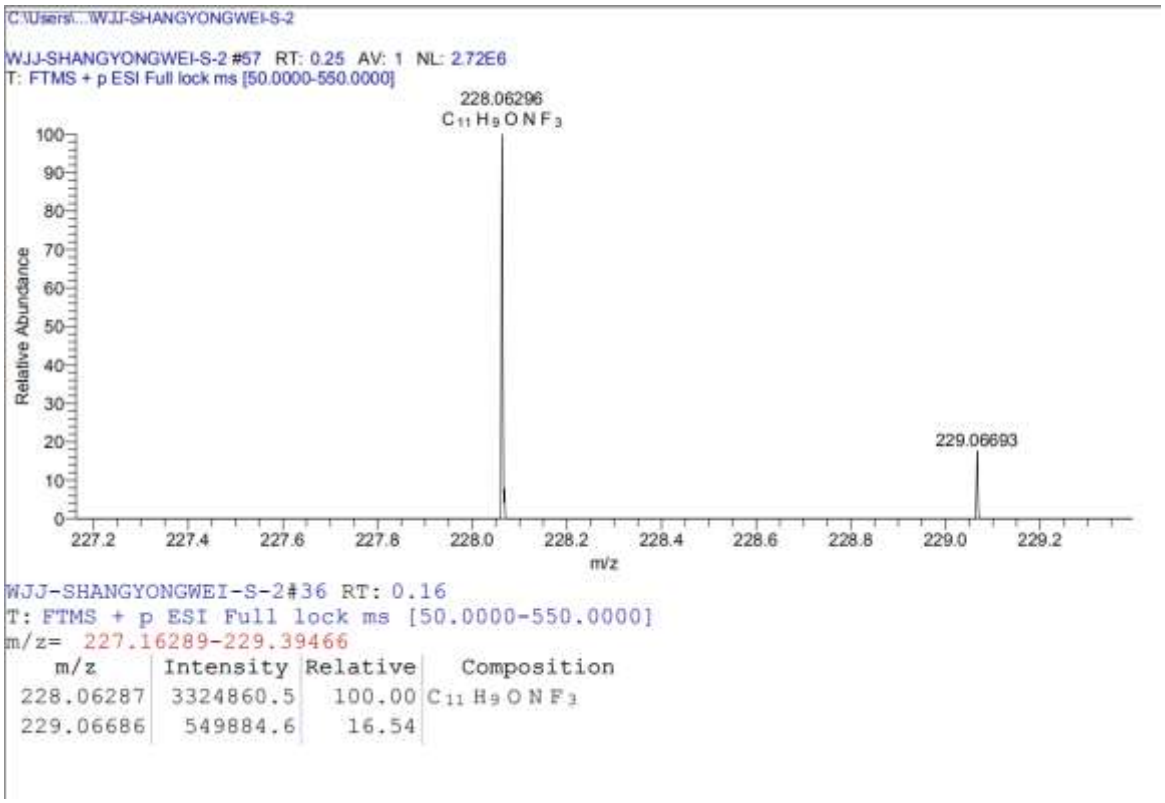
^{13}C NMR (150 MHz) spectrum of **5** in $CDCl_3$



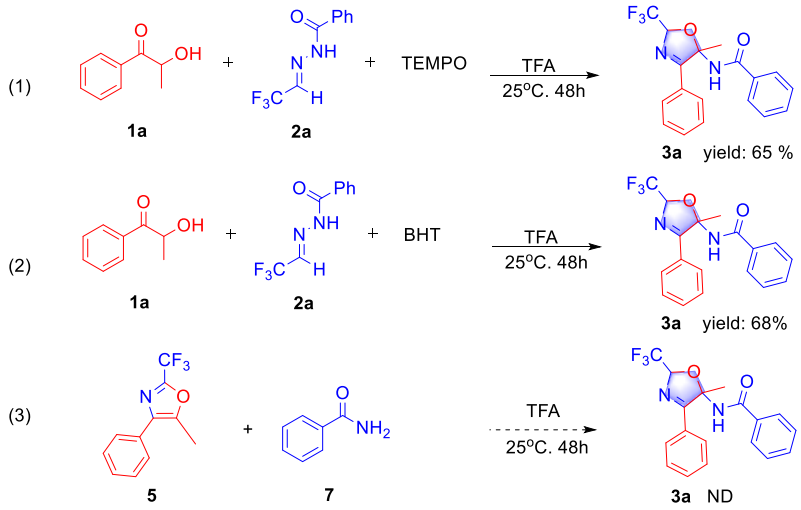
^{19}F NMR (376 MHz) spectrum of **5** in $CDCl_3$



HRMS(ESI) copy of compound **5**:



6. Control experiments



Scheme S5 Control experiments for mechanism exploration

HRMS(ESI) copies of control experiment reaction system

To elucidate the mechanism of the reaction, we carried out two free radical inhibition experiments (Scheme S5). When 1.2 equiv of free radical inhibitor TEMPO (2,2,6,6-tetramethylpiperidine-N-oxyl) and BHT (2,6-di-tert-butyl-4-methylphenol) was added to the reaction mixture containing 1a and 2a under the optimal conditions, the reaction could still work, but neither the molecular weight of Tempo adduct nor the molecular weight of

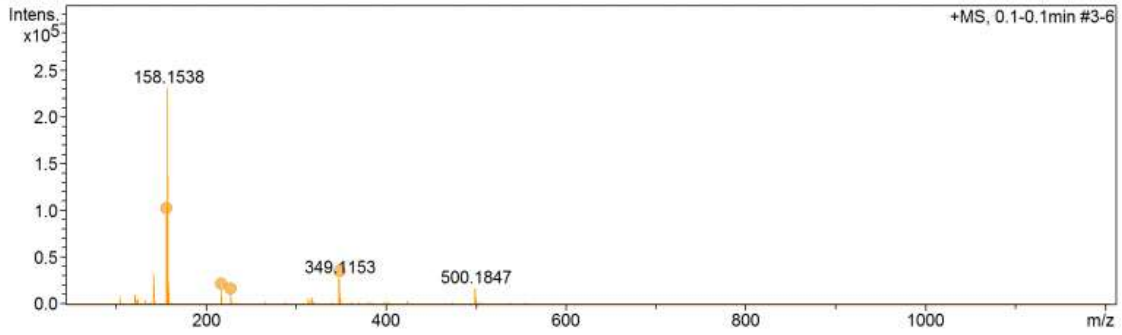
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\LICP-HY\wangjunjiao 20231020-1.d	Acquisition Date	10/20/2023 11:20:11 AM
Method	tune_pos_standard1.m	Operator	BDAL@DE
Sample Name	1	Instrument	maXis plus 1822843.21257
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¯ Conf	N-Rule
122.0597	1	C7H8NO	122.0600	2.6	6.3	1	100.00	4.5	even	ok
156.1380	1	C9H18NO	156.1383	2.1	4.2	1	100.00	1.5	even	ok
217.0575	1	C9H8F3N2O	217.0583	4.0	13.1	1	100.00	5.5	even	ok
228.0629	1	C11H9F3NO	228.0631	0.7	10.3	1	100.00	6.5	even	ok
349.1153	1	C18H16F3N2O2	349.1158	1.4	29.3	1	100.00	10.5	even	ok

BHT adduct was not found in HRMS：

The molecular weight of BHT adduct was not found in HRMS

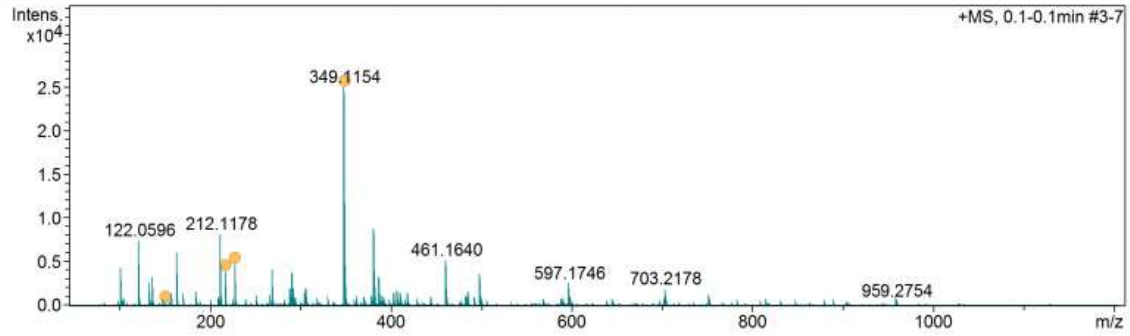
Mass Spectrum SmartFormula Report

Analysis Info

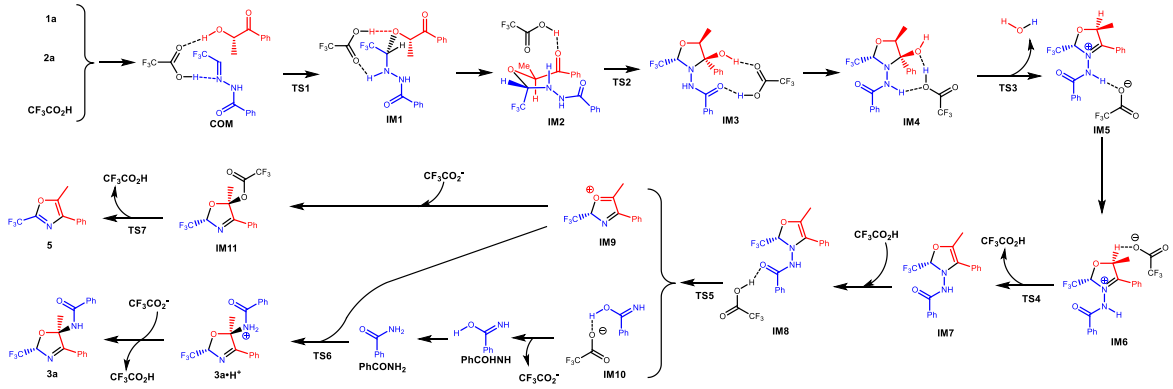
Analysis Name	D:\Data\LICP-HY\wangjunjiao 20231020-2.d	Acquisition Date	10/20/2023 11:23:09 AM
Method	tune_pos_standard1.m	Operator	BDAL@DE
Sample Name	2	Instrument	maXis plus 1822843.21257
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



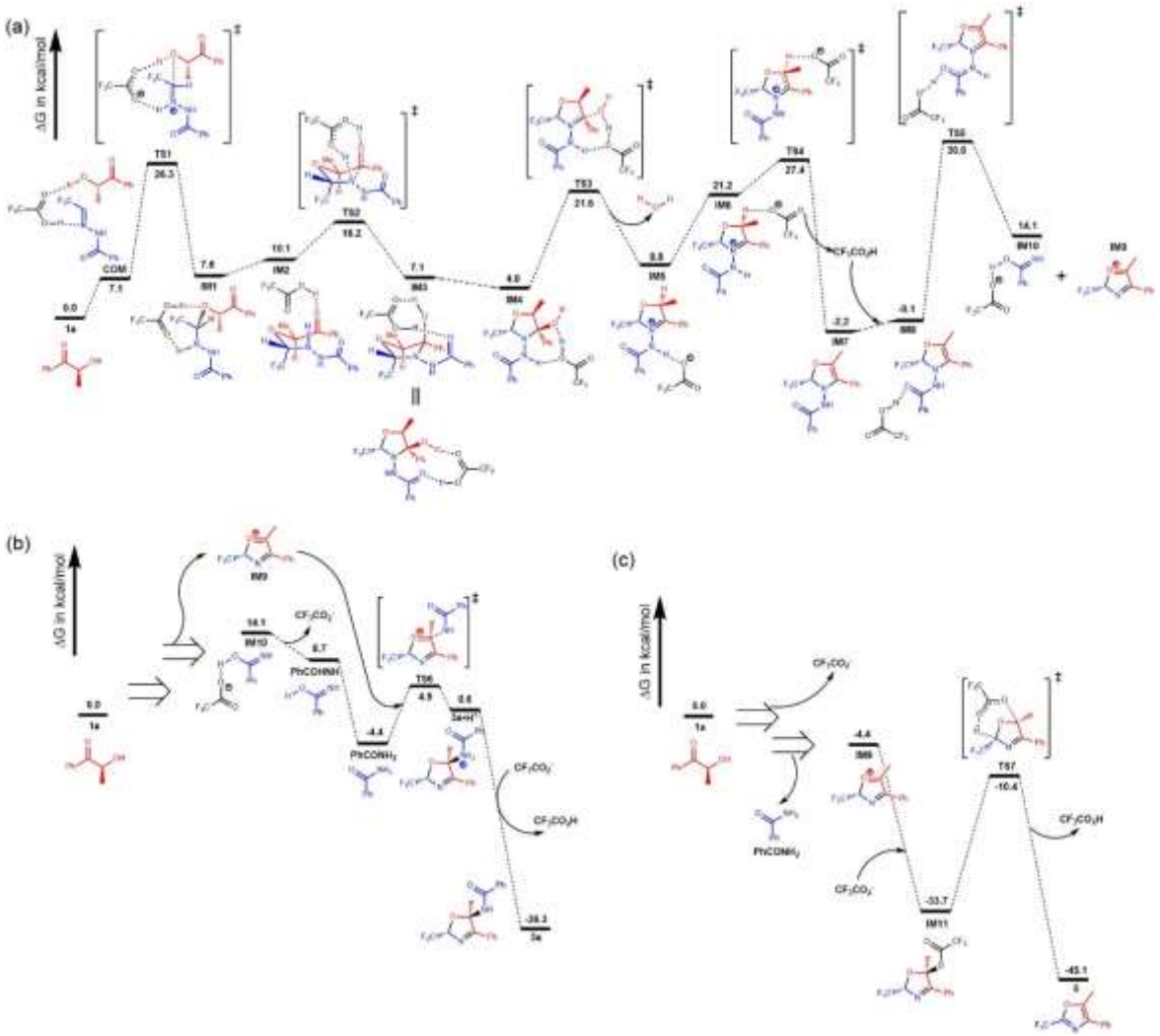
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
122.0596	1	C7H8NO	122.0600	3.3	2.9	1	100.00	4.5	even	ok
151.0754	1	C9H11O2	151.0754	-0.1	n.a.	1	100.00	4.5	even	ok
217.0577	1	C9H8F3N2O	217.0583	2.9	18.2	1	100.00	5.5	even	ok
228.0628	1	C11H9F3NO	228.0631	1.3	8.6	1	100.00	6.5	even	ok
349.1154	1	C18H16F3N2O2	349.1158	1.3	7.1	1	100.00	10.5	even	ok



Scheme S6. Proposed Reaction Mechanism.

7. Theoretical caculation

The geometry optimizations of all the intermediates, transition states, and products were carried out using M06-2X[1]-D3[2]/6-31G(d, p)/SMD[3] (CF_3CO_2H) level of theory, the solvent parameter of CF_3CO_2H was set as follows: eps=8.55, epsinf=1.69. The vibrational frequencies were computed at the same level of theory to verify whether each structure's location was at the energy minimum or first-order saddle point on the potential energy surface. The data of Gibbs free energy correction (*GFEC*) were obtained as well. Furthermore, the intrinsic reaction coordination (IRC)[4,5] calculations were performed at the same level of theory to ensure that each transition state connected the desired reactant and product. The single-point energies of the optimized structures were computed at M06-2X-D3/Def2-TZVP[6]/SMD(CF_3CO_2H) level of theory to obtain more accurate molecule energies *E*, and the Gibbs free energy *G* of each optimized structure was calculated as: *G=E+GFEC*. All calculations were performed using Gaussian 16 software package[7], and CYLview software was used to display the optimized structures[8]. The potential energy surfaces of the reactions leading to **3a** and **5** were displayed in **Scheme S7**, and the reaction mechanism was shown in **Scheme S6**.



Scheme S7. Potential energy surface of the reaction leading to intermediates IM9 and IM10 (a), 3a (b) and 5(c). The Gibbs free energies of 1a, 2a and CF_3CO_2H were set to 0.0 kcal/mol as references.

We proposed a possible reaction mechanism as follows: **1a**, **2a** and **CF_3COOH** can generate intermediates **IM9** and **IM10** (**Scheme 5(a)**), afterwards **IM9** and **IM10** can convert into **3a** and **5** in different reaction pathways (**Scheme 5(b)** and **(c)**, respectively).

In **Scheme 5(a)**, firstly **1a**, **2a** and **CF_3COOH** formed hydrogen bond complex (denoted as **COM**), then the C-O bond was formed via **TS1** to form **IM1**, subsequently **CF_3COOH** formed hydrogen bond with C=O bond of 1a moiety to form **IM2**, afterwards the C-N bond was formed via **TS2** to generate **IM3**, followed by the formation of **IM4** with different hydrogen bonds. The dehydration reaction occurred with the assistance of **CF_3COOH** via **TS3** to form ion-pair **IM5**, Afterwards the proton transfer reaction took place via **IM6→TS4→IM7→IM8** pathway, in which C=C double bond was constructed in 5-membered ring moiety. Subsequently the amide moiety was removed via **TS5** to generate

intermediates **IM9** and **IM10**.

In **Scheme 5(b)**, **IM10** released $\mathbf{CF_3COO^-}$ anion to produce **PhCOHNH**, which tautomerized to amide $\mathbf{PhCONH_2}$, afterwards the C-N bond formation occurred between **IM9** and $\mathbf{PhCONH_2}$ via **TS6** to generate $\mathbf{3a{\cdot}H^+}$, finally $\mathbf{CF_3COO^-}$ anion abstracted the proton to generate **3a**.

In **Scheme 5(c)**, after the formation of $\mathbf{PhCONH_2}$, the proton transfer reaction between $\mathbf{CF_3COO^-}$ anion and **IM9** occurred via **IM11→TS7→5** pathway.

It should be noticed that: At first, we supposed the C-O bond formation between $\mathbf{CF_3COO^-}$ anion and **IM9** should go through a transition state between **IM9** and **IM11** in **Scheme 5(c)**, however we failed to locate the transition state structure after many trials. Flexible scanning were performed to reveal the relationship between the C-O bond lengths (denoted as *l*) and energies (denoted as *E*') at M06-2X-D3/6-31G(d, p)/SMD(CF_3CO_2H) level of theory, the results were shown in **Table SX1**. It can be seen that *E*' will be lower when *l* is shorter. Therefore, we hypothesized that **IM9** and $\mathbf{CF_3COO^-}$ anion could generate **IM11** directly, however the reaction rate is hard to evaluate.

The selectivity between **3a** and **5** could be as follows: The conversion from **IM10** to **3a** only required 9.3 kcal/mol activation free energy barrier (**$\mathbf{PhCONH_2}$→TS6** procedure, **Scheme 5(b)**); however the conversion from **IM9** to **5** required 23.3 kcal/mol activation free energy barrier (**IM11→TS7** procedure, **Scheme 5(c)**), which is obviously slower.

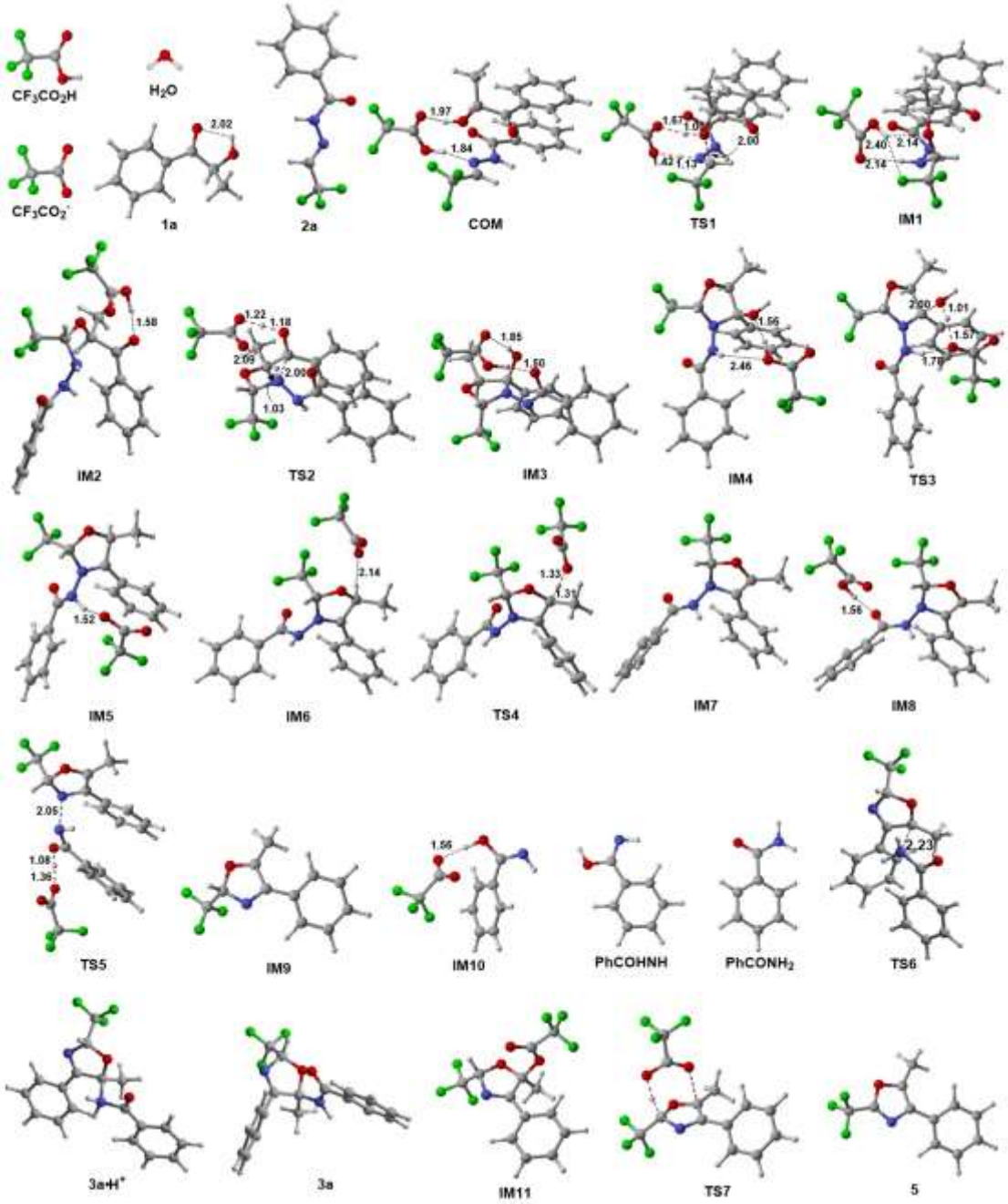


Figure S1. All optimized structures. The distance is measured in Å.

Table SX1. The calculated C-O bond lengths (denoted as *l*) and energies (denoted as *E*').

l/Å	*E*'/a.u.	*l*/Å	*E*'/a.u.
1.8	-1379.792730	**2.4**	-1379.768043
1.9	-1379.786393	**2.5**	-1379.766177
2.0	-1379.781097	**2.6**	-1379.764547
2.1	-1379.776788	**2.7**	-1379.762956
2.2	-1379.773507	**2.8**	-1379.761338

2.3	-1379.771046	**2.9**	-1379.759879

Table S11. The calculated *GFEC*, *E*, *G* (in a.u.) of all optimized structures, and imaginary frequencies (v_is, in cm^{-1}) of all optimized transition state structures.

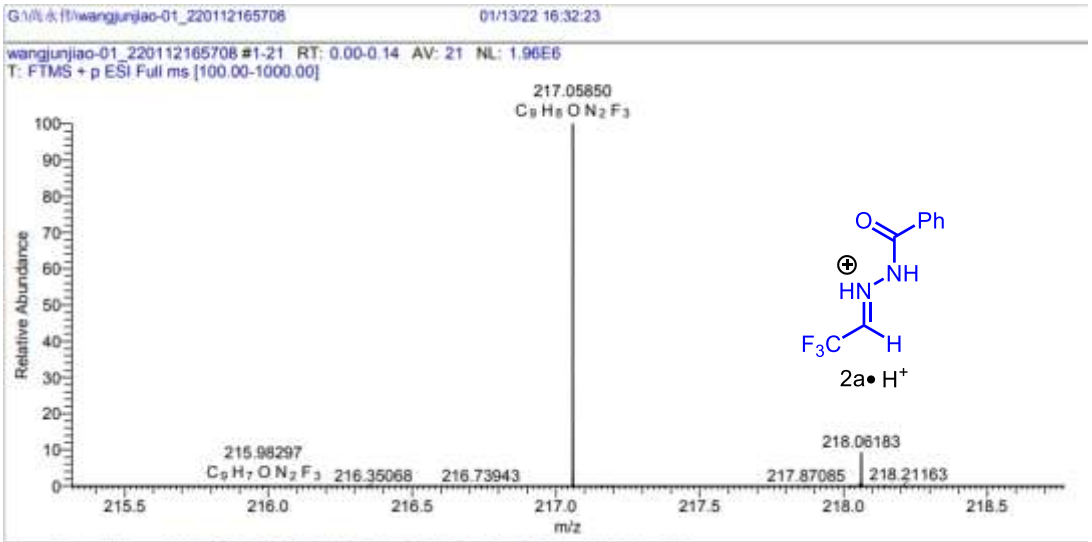
	GFEC/a.u.	*E*/a.u.	*G*/a.u.	v_i/cm^{-1}
1a	0.137610	-499.415815	-499.278205	
2a	0.115015	-831.442031	-831.327016	
CF_3CO_2H	0.008752	-526.855402	-526.846650	
$CF_3CO_2^-$	-0.003286	-526.406535	-526.409821	
H_2O	0.003847	-76.436786	-76.432939	
COM	0.304915	-1857.745413	-1857.440498	
TS1	0.308333	-1857.718348	-1857.410015	-268.7
IM1	0.315520	-1857.755238	-1857.439718	
IM2	0.310275	-1857.746068	-1857.435793	
TS2	0.310362	-1857.736391	-1857.426029	-640.4
IM3	0.316298	-1857.756851	-1857.440553	
IM4	0.313443	-1857.757527	-1857.444084	
TS3	0.314350	-1857.731850	-1857.417500	-244.5
IM5	0.287226	-1781.292100	-1781.004874	
IM6	0.286734	-1781.271899	-1780.985165	
TS4	0.281444	-1781.256658	-1780.975214	-1320.9
IM7	0.254363	-1254.430120	-1254.175757	
IM8	0.284268	-1781.303434	-1781.019166	
TS5	0.278787	-1781.249929	-1780.971142	-460.2
IM9	0.146624	-853.906803	-853.760179	
IM10	0.114650	-927.350962	-927.236312	
PhCOHNH	0.096833	-400.931837	-400.835004	
$PhCONH_2$	0.096940	-400.952898	-400.855958	
TS6	0.267876	-1254.869199	-1254.601323	-174.8
3a·H^+	0.273730	-1254.881818	-1254.608088	
3a	0.256735	-1254.486919	-1254.230184	
IM11	0.168231	-1380.384882	-1380.216651	
TS7	0.157431	-1380.336998	-1380.179567	-961.7
5	0.132315	-853.520504	-853.388189	

8. HRMS(ESI) copy of active intermediates

We carried out the model reaction under standard condition, and at the sixth hour of the reaction process, we detected a slight amount of **3a** by TLC. Then we took some reaction mixture in situ from the reaction tube and conducted the HRMS test directly.

HRMS(ESI) copy of compound **2a·H**$^{+}$

HRMS(ESI): *m/z* calcd for chemical formula: $C_9H_8O_2N_2F_3$ $[M + H]^+$ 217.0583; found 217.0585.

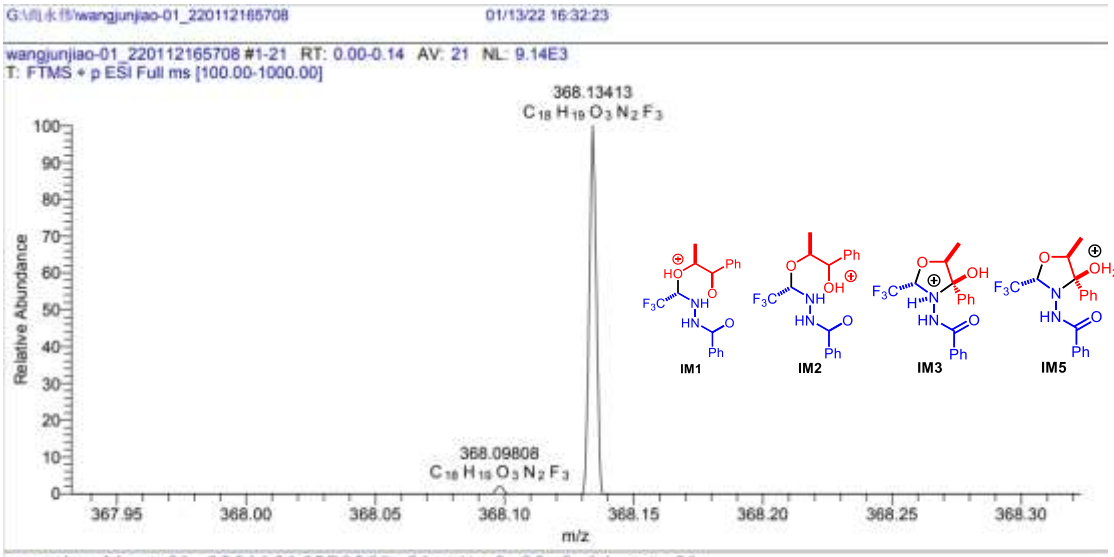


wangjunjiao-01_220112165708#1-21 RT: 0.00-0.14 AV: 21
T: FTMS + p ESI Full ms [100.00-1000.00]
m/z= 215.31556-218.76752

m/z	Intensity	Relative	Delta (ppm)	Composition
217.05850	1998628.8	100.00	0.17	C9 H8 O N2 F3
217.15897	3408.3	0.17	100.65	C9 H8 O N2 F3
218.05557	12731.7	0.64		
218.06183	184046.8	9.21		
218.21163	6793.2	0.34		

HRMS(ESI) copy of compound **IM1**, **IM2**, **IM3**, **IM5**.

HRMS(ESI): *m/z* calcd for chemical formula: $C_{18}H_{18}F_3N_2O_3$ $[M + H]^+$ 368.1342; found 368.1341.

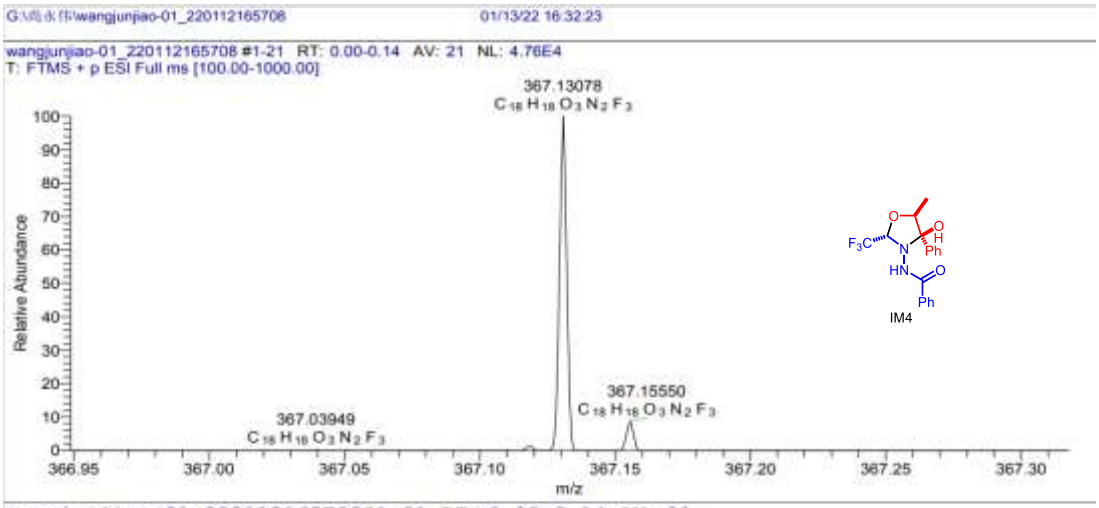


wangjunjiao-01_220112165708#1-21 RT: 0.00-0.14 AV: 21
T: FTMS + p ESI Full ms [100.00-1000.00]
m/z= 367.93230-368.32274

m/z	Intensity	Relative	Delta (ppm)	Composition
368.09808	188.1	2.06	-36.14	$C_{18}H_{19}O_3N_2F_3$
368.13413	9139.4	100.00	-0.10	$C_{18}H_{19}O_3N_2F_3$

HRMS(ESI) copy of compound **IM4**.

HRMS(ESI): *m/z* calcd for chemical formula: $C_{18}H_{18}F_3N_2O_3$ $[M + H]^+$ 367.1309; found 367.1264.

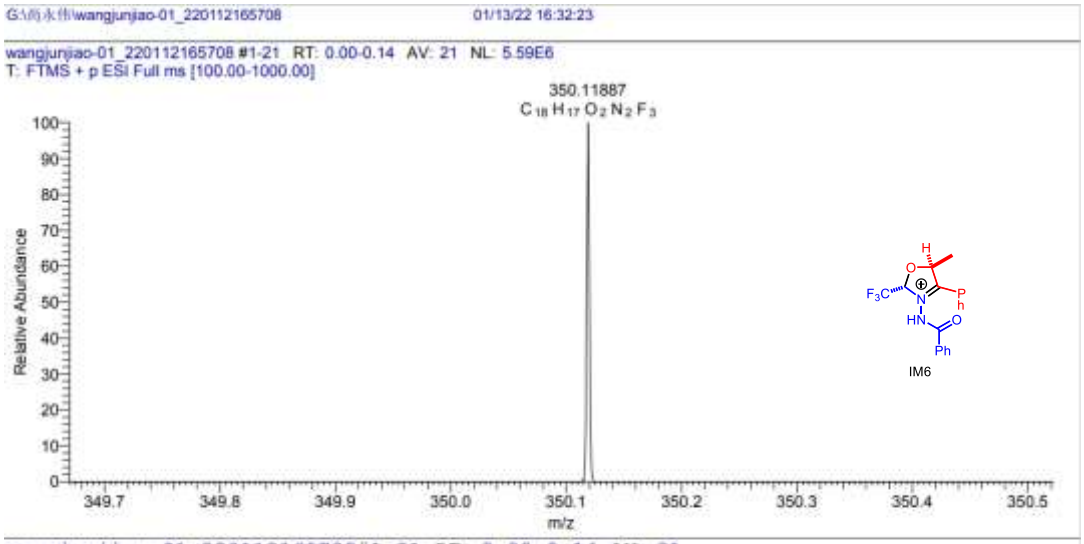


wangjunjiao-01_220112165708#1-21 RT: 0.00-0.14 AV: 21
T: FTMS + p ESI Full ms [100.00-1000.00]
m/z= 366.94880-367.31742

m/z	Intensity	Relative	Delta (ppm)	Composition
367.03949	72.4	0.15	-86.92	$C_{18}H_{18}O_3N_2F_3$
367.11848	592.1	1.24	-7.92	$C_{18}H_{18}O_3N_2F_3$
367.13078	47640.2	100.00	4.38	$C_{18}H_{18}O_3N_2F_3$
367.15550	4148.8	8.71	29.10	$C_{18}H_{18}O_3N_2F_3$

HRMS(ESI) copy of compound **IM6**.

HRMS(ESI): *m/z* calcd for chemical formula: $C_{18}H_{17}F_3N_2O_2$ $[M + H]^+$ 350.1188; found 350.1237.

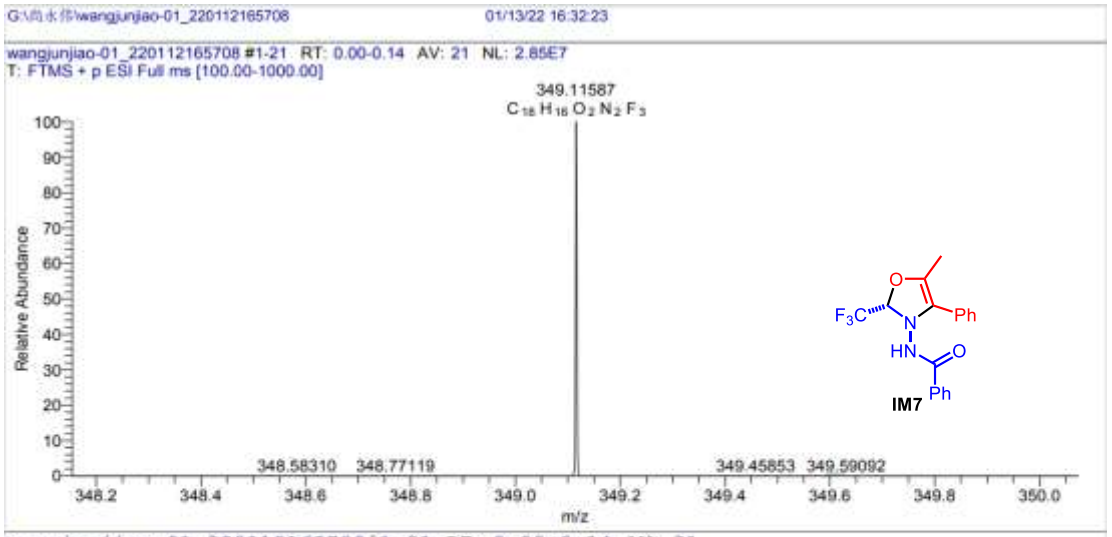


wangjunjiao-01_220112165708#1-21 RT: 0.00-0.14 AV: 21
T: FTMS + p ESI Full ms [100.00-1000.00]
m/z= 349.66959-350.52165

m/z	Intensity	Relative	Delta (ppm)	Composition
349.67621	63.0	0.00		
350.11887	5594429.5	100.00	-4.80	$C_{18}H_{17}O_2N_2F_3$
350.14140	139.7	0.00	17.74	$C_{18}H_{17}O_2N_2F_3$
350.15391	53.5	0.00	30.25	$C_{18}H_{17}O_2N_2F_3$

HRMS(ESI) copy of compound **IM7.**

HRMS(ESI): *m/z* calcd for chemical formula: $C_{18}H_{16}F_3N_2O_2$ $[M + H]^+$ 349.1158; found 349.1159.

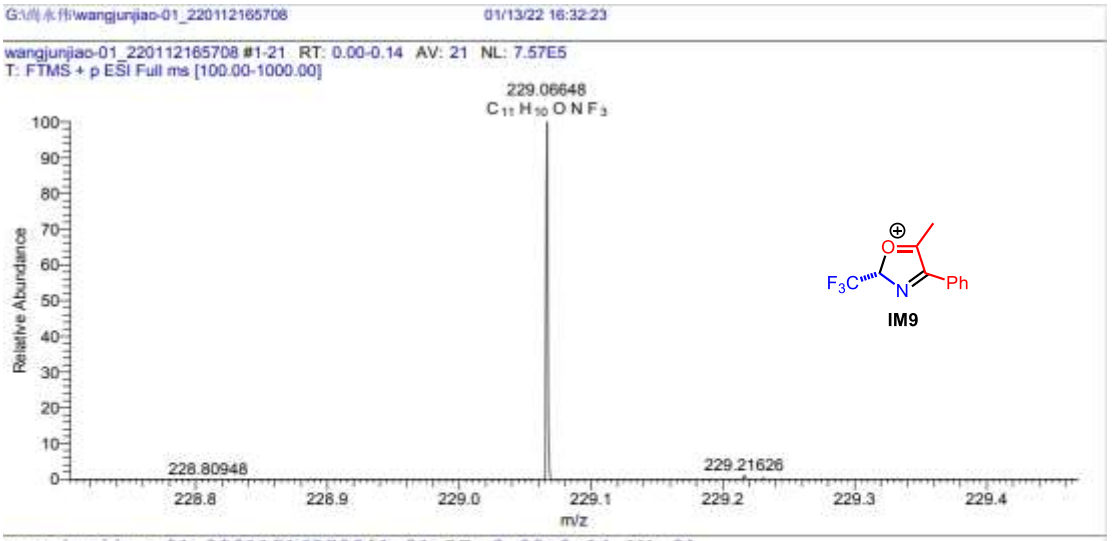


wangjunjiao-01_220112165708#1-21 RT: 0.00-0.14 AV: 21
T: FTMS + p ESI Full ms [100.00-1000.00]
m/z= 348.15416-350.07357

m/z	Intensity	Relative	Delta (ppm)	Composition
348.20641	3763.1	0.01	98.40	$C_{18}H_{15}O_2N_2F_3$
349.10808	30477.9	0.11	-7.76	$C_{18}H_{16}O_2N_2F_3$
349.11587	28731764.0	100.00	0.03	$C_{18}H_{16}O_2N_2F_3$
349.45853	1991.0	0.01	342.69	$C_{18}H_{16}O_2N_2F_3$
349.51014	1375.4	0.00	394.30	$C_{18}H_{16}O_2N_2F_3$

HRMS(ESI) copy of compound **IM9**.

HRMS(ESI): *m/z* calcd for chemical formula: $C_{11}H_{10}F_3NO$ $[M + H]^+$ 229.0710; found 229.0665.

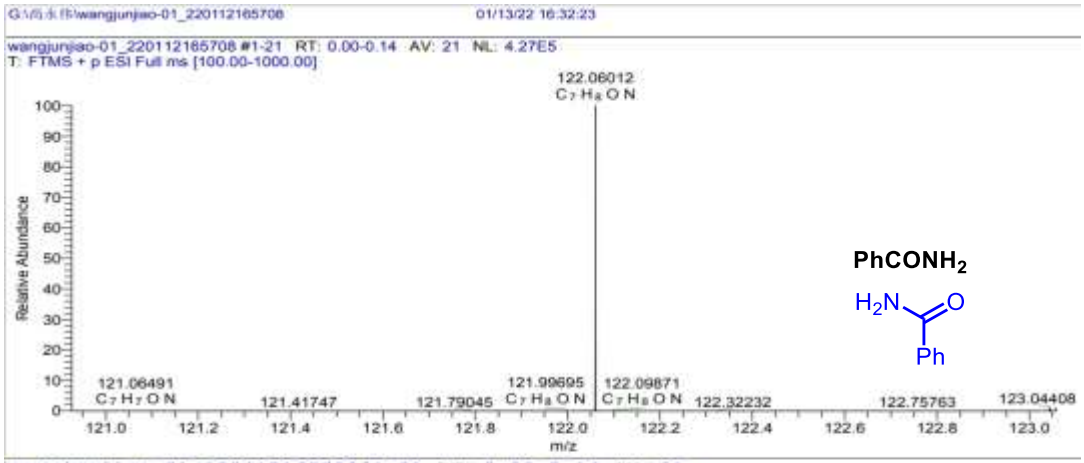


wangjunjiao-01_220112165708#1-21 RT: 0.00-0.14 AV: 21
T: FTMS + p ESI Full ms [100.00-1000.00]
m/z= 228.70489-229.46943

m/z	Intensity	Relative	Delta (ppm)	Composition
228.80948	62.1	0.01	-261.42	$C_{11}H_{10}ONF_3$
229.06242	1080.3	0.14	-8.48	$C_{11}H_{10}ONF_3$
229.06648	757913.4	100.00	-4.42	$C_{11}H_{10}ONF_3$
229.21626	7925.3	1.05	145.36	$C_{11}H_{10}ONF_3$
229.23082	2462.3	0.32	159.92	$C_{11}H_{10}ONF_3$

HRMS(ESI) copy of compound $PHCONH_2$.

HRMS(ESI): *m/z* calcd for chemical formula: C_7H_8NO $[M + H]^+$ 122.0600; found 122.0601.



wangjunjiao-01_220112165708#1-21 RT: 0.00-0.14 AV: 21
T: FTMS + p ESI Full ms [100.00-1000.00]
m/z= 120.92607-123.05716

m/z	Intensity	Relative	Delta (ppm)	Composition
121.99695	664.6	0.15	-63.09	C_7H_8ON
122.06012	435184.1	100.00	0.08	C_7H_8ON
122.09871	193.7	0.04	38.67	C_7H_8ON
123.04408	4651.5	1.07	984.04	C_7H_8ON
123.05711	4229.7	0.97	997.07	C_7H_8ON

9. References and notes

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(8) C. Y. Legault, Universite de Sherbrooke, CYLview, version 1.0b, **2009** (http://www.cylview.org/).

10. Cartesian coordinates

1a

C	0.95269500	0.58434800	-0.14003200
O	1.32245600	1.74515600	-0.03433300
C	-0.48993300	0.22472300	-0.09677800
C	-0.94463400	-1.06528900	-0.39288300
C	-1.40985100	1.22395700	0.24208800
C	-2.30570300	-1.34970500	-0.34646500
H	-0.24717800	-1.84977300	-0.66751300
C	-2.76715200	0.93586500	0.29105500
H	-1.04335900	2.21994200	0.46699200
C	-3.21550800	-0.35200500	-0.00315900
H	-2.65557800	-2.34958000	-0.57949900
H	-3.47675600	1.71173700	0.55783300
H	-4.27640800	-0.57761200	0.03405300
C	2.01879200	-0.50165900	-0.25412400
H	1.75519400	-1.19064600	-1.06369600
C	2.10931600	-1.26014000	1.07277100
H	1.17900800	-1.78054800	1.31186900
H	2.91661800	-1.99237100	1.00710700
H	2.33745800	-0.55858600	1.88050300
O	3.25708600	0.09317000	-0.57660100
H	3.18652800	1.02025600	-0.29501200

2a

C	0.91969800	0.75843500	0.20946500
O	0.70862100	1.92834300	0.48245600
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H	0.10112000	-1.06728600	-0.38670700
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C	3.31448100	1.08373200	-0.27497500
C	2.59392700	-1.14856500	0.32454800
C	4.61987300	0.62691000	-0.40841600
H	3.06751600	2.12579400	-0.44813100
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H	1.82156400	-1.84143100	0.64534300
C	4.91533000	-0.71501900	-0.17215500
H	5.40711200	1.31629500	-0.69419400
H	4.13756800	-2.63886300	0.40202600

H	5.93557600	-1.07091000	-0.27179400
C	-2.27842100	-0.58677800	-0.20907900
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C	-3.71477500	-0.18592500	-0.07680800
F	-3.86848200	1.06912000	0.33833800
F	-4.35005400	-0.98880700	0.79215900
F	-4.34815500	-0.31257600	-1.25405100

CF_3CO_2H

C	-0.93508600	0.15383800	-0.00024200
O	-1.47870000	1.22512900	-0.00009600
O	-1.50864900	-1.03806500	-0.00002400
H	-2.47669300	-0.92957000	0.00029900
C	0.59348800	-0.00193400	-0.00004900
F	1.17716400	1.18889700	-0.00229500
F	0.99064300	-0.67866200	-1.07914800
F	0.99053500	-0.67449900	1.08171100

$CF_3CO_2^-$

C	-1.02769800	0.00964500	0.00000400
O	-1.57344200	1.12782700	0.00003400
O	-1.51412600	-1.13900700	-0.00017200
C	0.52416800	0.01427600	-0.00000400
F	1.05465100	1.24455600	-0.00010600
F	1.01290900	-0.62531400	-1.07928700
F	1.01263100	-0.62525100	1.07951600

H_2O

O	0.00000000	0.00000000	0.11925000
H	0.00000000	0.75760800	-0.47700000
H	0.00000000	-0.75760800	-0.47700000

COM

C	1.03006500	0.91144700	-1.01609600
O	0.23065800	1.63857600	-0.44174500
N	0.64067400	-0.31580500	-1.49906000
H	1.29797500	-0.97310800	-1.90706700
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C	2.80913000	2.59778500	-0.87527700
C	3.43073300	0.41766900	-1.72039900
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H	3.20050500	-0.60970300	-1.98554500
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H	4.39165500	4.03918500	-0.72565200
H	5.50299600	0.16466900	-2.21389400
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C	-0.95491200	-1.88307000	-1.66556200
H	-0.25196400	-2.62454100	-2.04551800
N	-0.65129100	-0.69009300	-1.35407700
C	-2.38661700	-2.31406100	-1.54112700
F	-3.13336500	-1.43152600	-0.86900600
F	-2.47395800	-3.49381400	-0.92539100

F	-2.93484900	-2.46020800	-2.75721400
C	0.96130600	-1.86898300	1.11631300
O	0.89593100	-2.90007800	0.46585500
C	2.27699400	-1.18464900	1.32088100
C	2.38063100	0.13044600	1.78904700
C	3.43951200	-1.88836300	0.98124300
C	3.63134200	0.73124700	1.91065800
H	1.49240100	0.70601500	2.03127400
C	4.68552000	-1.29049600	1.11269700
H	3.34703600	-2.90670500	0.61827700
C	4.78214900	0.02372600	1.57410400
H	3.70303200	1.75709100	2.25646800
H	5.58238000	-1.84280100	0.85166000
H	5.75485200	0.49654100	1.66624000
C	-0.29018100	-1.25571400	1.72922000
H	-0.35725000	-0.21744100	1.36789500
C	-0.22257200	-1.26663700	3.25908700
H	0.63114100	-0.71007200	3.64924500
H	-1.14013700	-0.81945400	3.64962000
H	-0.16080600	-2.30003800	3.61059000
O	-1.40690400	-1.99725700	1.29035600
H	-2.15018000	-1.37498700	1.28540200
H	-1.81810300	0.63941100	-0.85851600
C	-3.11060900	1.22055300	0.42009000
O	-2.84020200	0.46593000	1.32577500
O	-2.56848900	1.29103200	-0.76481300
C	-4.21454200	2.27965300	0.56871400
F	-3.69630300	3.50504700	0.46226100
F	-4.81011600	2.17085300	1.74962000
F	-5.13202600	2.13277100	-0.38937600

TS1

C	0.77480100	0.89596000	-0.98145600
O	0.06766500	1.53043800	-0.21044300
N	0.32016900	-0.24733900	-1.59486900
H	0.74266400	-0.55402500	-2.46557800
C	2.19035000	1.25717500	-1.27287400
C	2.58798900	2.56630700	-0.99247000
C	3.12374300	0.31761200	-1.71987900
C	3.91383800	2.94012900	-1.17582300
H	1.85170100	3.27554700	-0.62943300
C	4.45101200	0.69581300	-1.89433600
H	2.83555500	-0.71583000	-1.88887300
C	4.84564100	2.00484300	-1.62478100
H	4.22234000	3.95832600	-0.96434600
H	5.17942100	-0.03672300	-2.22571700
H	5.88263800	2.29513300	-1.75898000
C	-1.29149200	-1.80964000	-1.10417300
H	-0.51594400	-2.56994600	-1.12883800
N	-1.02107200	-0.58733700	-1.45099900
C	-2.70591900	-2.31550500	-1.32040200
F	-3.62127800	-1.45594100	-0.87721000
F	-2.88759000	-3.48289600	-0.71520900
F	-2.89217400	-2.48988300	-2.63135700
C	0.92350500	-2.02890800	1.08036400

O	0.83132500	-3.14109700	0.58418600
C	2.24685500	-1.37133100	1.27280500
C	2.37637300	-0.05046000	1.72055700
C	3.39338100	-2.10453000	0.93810200
C	3.63860500	0.52835800	1.82259000
H	1.50419800	0.54605900	1.96876900
C	4.64970300	-1.52538100	1.04486600
H	3.27924000	-3.12654000	0.59261200
C	4.77237200	-0.20517600	1.48355900
H	3.73227900	1.55689400	2.15435200
H	5.53432000	-2.09633600	0.78308600
H	5.75402300	0.25210800	1.55672700
C	-0.32925700	-1.28679000	1.51864600
H	-0.27435300	-0.23749700	1.20917200
C	-0.50527700	-1.37349200	3.03235400
H	0.34055900	-0.91572300	3.54971600
H	-1.41763200	-0.84275500	3.31430400
H	-0.58651300	-2.42018100	3.33455700
O	-1.46894100	-1.88330100	0.88535000
H	-2.16339600	-1.16854700	0.97848900
H	-1.78793800	0.23039200	-1.34469300
C	-2.91387500	1.27038600	0.24278700
O	-2.77489900	0.38300800	1.09944500
O	-2.73009100	1.23244600	-1.00227700
C	-3.32655800	2.66424000	0.75600000
F	-2.26109500	3.47921000	0.73788100
F	-3.79320800	2.62923900	2.00474500
F	-4.26710300	3.21168900	-0.02140300

IM1

C	0.63708200	0.50666600	-1.20007200
O	0.00147900	1.37775900	-0.60549000
N	0.04673800	-0.65327000	-1.60332500
H	0.46788200	-1.15304500	-2.37838000
C	2.09302600	0.65266400	-1.48766800
C	2.63447400	1.93665600	-1.39687300
C	2.92103000	-0.44255100	-1.74906800
C	3.99896900	2.12776400	-1.58035900
H	1.97590500	2.77001000	-1.17514700
C	4.28665300	-0.24668000	-1.92626200
H	2.51753200	-1.45077000	-1.76944500
C	4.82555800	1.03617700	-1.84306300
H	4.41897100	3.12572200	-1.51315100
H	4.93217600	-1.09861000	-2.11257500
H	5.89227000	1.18427600	-1.97703500
C	-1.82289400	-1.79623400	-0.65751500
H	-1.24202500	-2.70436500	-0.83587600
N	-1.34830300	-0.77389400	-1.54828000
C	-3.27484100	-2.07035700	-1.02447300
F	-4.00820500	-0.94855600	-0.88412800
F	-3.80976900	-3.00269800	-0.23497000
F	-3.39520900	-2.48059900	-2.28614100
C	0.46106500	-2.02713400	1.15820800
O	0.24692100	-3.19348000	0.86679900
C	1.84966000	-1.51341300	1.34287500

C	2.13211600	-0.17200000	1.63232000
C	2.90407600	-2.42191000	1.18066400
C	3.45422100	0.25126100	1.74292500
H	1.33840100	0.55966100	1.75191900
C	4.22007600	-1.99661100	1.29372500
H	2.67150300	-3.45835000	0.95993300
C	4.49601800	-0.65602800	1.56990100
H	3.66757500	1.29417100	1.95182200
H	5.03211900	-2.70405100	1.16252600
H	5.52489600	-0.31914800	1.64784200
C	-0.70758200	-1.07593700	1.38744000
H	-0.46312900	-0.06894800	1.04324200
C	-1.02570600	-1.05295300	2.87797700
H	-0.16608700	-0.69066500	3.44632300
H	-1.87273200	-0.38921800	3.06102600
H	-1.27639600	-2.06204900	3.21433000
O	-1.89452200	-1.51033300	0.72777600
H	-3.00115700	0.31985900	0.88085700
H	-1.76936400	0.14104300	-1.38365200
C	-2.47312000	2.01952600	0.21495900
O	-2.62834300	1.16478600	1.20600900
O	-2.88201800	1.91021300	-0.91253000
C	-1.72069400	3.26811400	0.70127800
F	-0.74733200	2.95212700	1.55426600
F	-2.57434100	4.08184500	1.33437200
F	-1.20077000	3.92465200	-0.32732500

IM2

C	-2.15464800	-1.42120300	-0.99330100
O	-1.76610300	-2.17341300	-1.87799000
N	-1.31668600	-0.52744500	-0.37844700
H	-1.73903000	0.32755700	-0.02782800
C	-3.56259700	-1.38026900	-0.50305100
C	-4.57155600	-1.82831400	-1.35684400
C	-3.87782900	-0.91893000	0.77878700
C	-5.89704000	-1.79301700	-0.93883400
H	-4.30518200	-2.19342700	-2.34325100
C	-5.20504900	-0.89057000	1.19436900
H	-3.08678600	-0.61724500	1.45981300
C	-6.21381300	-1.32137400	0.33444100
H	-6.68328100	-2.13335500	-1.60423300
H	-5.45112100	-0.54219400	2.19182500
H	-7.24852300	-1.29702300	0.66041500
C	1.03485500	-0.94857900	-0.04815400
H	1.77517800	-1.38879000	-0.71876800
N	-0.01405700	-0.37406900	-0.85688500
C	0.60187100	-2.06863400	0.89883400
F	-0.13578100	-1.63732600	1.93476900
F	1.68963000	-2.65501600	1.41419500
F	-0.10234900	-3.00439800	0.25579300
C	0.63048500	2.10526600	0.21584500
O	1.53180700	2.53411600	-0.49969000
C	-0.74612100	2.64439600	0.07900600
C	-1.70452000	2.50412800	1.09292100
C	-1.09009600	3.27967100	-1.12054800

C	-2.99666500	2.98372200	0.89712400
H	-1.45026900	2.03689000	2.03935600
C	-2.38274200	3.74808900	-1.31326000
H	-0.33947700	3.37857100	-1.89749200
C	-3.33680400	3.59749600	-0.30645100
H	-3.73588800	2.87600800	1.68357100
H	-2.65096000	4.22539900	-2.24954000
H	-4.34816500	3.95882300	-0.46091900
C	0.93064900	1.04603300	1.28077600
H	-0.00075200	0.62532900	1.66580800
C	1.72531800	1.67801200	2.41206500
H	1.16836500	2.50947200	2.85133100
H	1.91561700	0.92854500	3.18224400
H	2.67841000	2.05047300	2.02930000
O	1.73152400	0.01145000	0.72258300
H	3.02365700	2.02480200	-0.39457600
H	0.03357300	-0.71441300	-1.81502700
C	3.87876000	0.44410600	-0.94838900
O	3.90211200	1.54360700	-0.24182900
O	3.16077900	0.18180800	-1.88580600
C	4.85767900	-0.61759800	-0.42565500
F	5.82387000	-0.10131100	0.32869700
F	5.41477300	-1.27742300	-1.43948100
F	4.17186400	-1.50007700	0.31481100

TS2

C	1.74055800	0.05763100	-1.48700700
O	1.17578200	-0.74155100	-2.21897100
N	1.01169400	0.83862800	-0.60254600
H	1.51520200	1.11753500	0.23617700
C	3.21430000	0.25067900	-1.44391900
C	4.00016800	-0.75167400	-2.01767500
C	3.81760900	1.33123500	-0.79264800
C	5.38499700	-0.68386500	-1.92579900
H	3.51188500	-1.58504500	-2.51186100
C	5.20427600	1.39568600	-0.70683500
H	3.22033700	2.13517800	-0.37203500
C	5.98659600	0.38667500	-1.26577600
H	5.99470400	-1.46698200	-2.36343300
H	5.67367300	2.23560700	-0.20636500
H	7.06789300	0.43790900	-1.19073100
C	-1.31360300	1.25502000	0.08475800
H	-2.00305700	1.43252600	-0.74353500
N	-0.25108000	0.31372100	-0.29710700
C	-0.78019500	2.62055700	0.52525300
F	0.22639300	2.52659500	1.41754900
F	-1.76199500	3.31046800	1.09969800
F	-0.32832800	3.31851900	-0.51616000
C	-0.34299200	-1.05721100	1.14956100
O	-0.94752600	-2.05119900	0.60866000
C	1.11817700	-1.25470800	1.40020400
C	1.87691000	-0.39898900	2.20844800
C	1.76116800	-2.28926000	0.70760400
C	3.25570600	-0.57274600	2.31200800
H	1.41423600	0.41435600	2.75713100

C	3.13629800	-2.45840800	0.81459300
H	1.17427600	-2.94177800	0.07127400
C	3.88846700	-1.59594000	1.61117600
H	3.83366700	0.09911300	2.93753900
H	3.62446900	-3.25508800	0.26311900
H	4.96463700	-1.71762900	1.67991700
C	-1.17151400	-0.08905100	2.00124900
H	-0.51775100	0.61720800	2.51584700
C	-2.03538800	-0.81987900	3.00703700
H	-1.39966400	-1.40839800	3.67301300
H	-2.59306100	-0.09494700	3.60215100
H	-2.73813600	-1.48414100	2.50185600
O	-2.03547000	0.63570600	1.11093600
H	-2.10276100	-1.96151700	0.36780300
H	-0.56714100	-0.25707600	-1.09563100
C	-3.39005900	-1.07653300	-0.92449100
O	-3.27919900	-1.85095400	0.08250900
O	-2.51616800	-0.69274600	-1.69765700
C	-4.79955700	-0.49241700	-1.11991900
F	-5.75150700	-1.23184500	-0.55210700
F	-5.09240300	-0.35442300	-2.41399800
F	-4.83533700	0.72867200	-0.56113800

IM3

C	-1.44576000	-1.56223500	-0.10995100
O	-0.67086900	-2.31142300	-0.72397000
N	-1.06167400	-0.37173800	0.40672100
H	-1.76742800	0.26778800	0.76199200
C	-2.87003200	-1.93514600	0.09853100
C	-3.44698200	-2.81775900	-0.81803600
C	-3.62123000	-1.44190300	1.17073700
C	-4.77914400	-3.18735000	-0.67696800
H	-2.84653700	-3.19859200	-1.63714800
C	-4.95067800	-1.82502200	1.31175600
H	-3.17110000	-0.79199300	1.91591600
C	-5.53098000	-2.69048500	0.38645300
H	-5.23019700	-3.86421800	-1.39446800
H	-5.53096000	-1.45298700	2.14904300
H	-6.56963500	-2.98377300	0.49857400
C	1.17067600	0.26603500	1.15476600
H	1.47154400	-0.70610700	1.55680600
N	0.17856400	0.12826000	0.11223100
C	0.72164400	1.10838300	2.35080900
F	0.25820400	2.31525800	1.99517700
F	1.73204300	1.29237000	3.20269800
F	-0.26770100	0.48259500	3.00758000
C	0.31884300	1.18367000	-0.91673500
O	0.33324400	0.58444400	-2.18615700
C	-0.86478900	2.15562000	-0.95186500
C	-0.85353600	3.44318300	-0.41024300
C	-2.04692600	1.69809600	-1.55411300
C	-1.99198500	4.24683600	-0.46558200
H	0.03169300	3.85311100	0.05907800
C	-3.18559000	2.49447700	-1.59595600
H	-2.06634800	0.71012800	-2.00204700

C	-3.16205900	3.77628300	-1.05044900
H	-1.95563300	5.24698400	-0.04639900
H	-4.08863400	2.11408900	-2.06213100
H	-4.04680700	4.40356600	-1.08614000
C	1.68940000	1.79031400	-0.48364600
H	1.53510700	2.73271600	0.04148900
C	2.67908500	1.99095200	-1.60324000
H	2.27023000	2.70912600	-2.31837200
H	3.60958700	2.39348500	-1.19693700
H	2.88990900	1.05492600	-2.12046900
O	2.23991300	0.85356200	0.47842400
H	0.94704900	-0.17145700	-2.16352500
H	0.80487600	-2.30995900	-0.45524200
C	2.60409000	-1.71786700	-0.86136100
O	2.40658300	-1.29174400	-1.98094300
O	1.77204800	-2.35407100	-0.09399400
C	3.98984700	-1.56946500	-0.21171100
F	4.64187000	-0.53994200	-0.74150700
F	4.70994100	-2.67671000	-0.42042500
F	3.89279400	-1.38338500	1.10550500

IM4

C	-0.47352400	1.87908800	0.54543400
O	-1.32888700	2.11292400	1.38666700
N	-0.61066600	0.89738100	-0.40255800
H	0.03832600	0.83222800	-1.18155700
C	0.80415200	2.65035800	0.46725300
C	0.78586200	3.99284900	0.85128700
C	2.00279600	2.04703800	0.08053100
C	1.95979400	4.73647600	0.81782300
H	-0.15037100	4.44043600	1.16872200
C	3.17877800	2.79131800	0.06219200
H	2.02331800	0.99266600	-0.16933000
C	3.15575400	4.13674400	0.42211100
H	1.94514100	5.78262900	1.10469200
H	4.10999600	2.31461800	-0.22589300
H	4.07186400	4.71823700	0.40384300
C	-2.75424000	0.23991100	-1.33848300
H	-2.39103400	0.55674600	-2.32507200
N	-1.69428900	0.05483400	-0.35592800
C	-3.74528900	1.27654900	-0.82688100
F	-4.20672300	0.95497100	0.38520900
F	-4.79371300	1.36712100	-1.65433900
F	-3.17621600	2.48574900	-0.75483700
C	-1.45659700	-1.35758900	-0.21238200
O	-0.66087300	-1.79620400	-1.32693700
C	-0.81661400	-1.69679900	1.11596900
C	-1.27243800	-1.05370100	2.27081200
C	0.19087700	-2.65624000	1.20902400
C	-0.71885800	-1.36919000	3.50650600
H	-2.04209500	-0.29228400	2.18609200
C	0.74426300	-2.96766500	2.45021200
H	0.56325600	-3.15608000	0.32057200
C	0.29113000	-2.32651400	3.59883700
H	-1.07123900	-0.86056300	4.39771500

H	1.53385000	-3.70932000	2.51254800
H	0.72581700	-2.56671500	4.56361900
C	-2.90083000	-1.85458000	-0.38050300
H	-3.43567100	-1.64485600	0.55298500
C	-3.06368100	-3.29896700	-0.78164800
H	-2.60029800	-3.94623000	-0.03158400
H	-4.12449500	-3.54785400	-0.84261200
H	-2.61452600	-3.48734200	-1.76049500
O	-3.39865900	-1.00466800	-1.42872700
H	-0.71160100	-2.76071400	-1.41822800
H	0.84509700	-1.37918000	-1.35771800
C	2.73630500	-1.75675100	-1.13425200
O	2.68590600	-2.95618600	-1.01132300
O	1.75276400	-0.92754400	-1.36935300
C	4.06075800	-0.98852100	-0.98068400
F	5.09831900	-1.80289500	-1.12385100
F	4.11738800	-0.43805700	0.23899000
F	4.15727400	-0.00259900	-1.87455700

TS3

C	-0.01471800	1.81680400	0.40150000
O	-0.73810800	2.12490100	1.33527500
N	-0.39921500	0.87152900	-0.53192300
H	0.29683600	0.32573200	-1.06383700
C	1.31405800	2.44855200	0.15895900
C	1.78575400	3.31962000	1.14479600
C	2.08849300	2.19536500	-0.97761000
C	3.02459700	3.93103300	0.99938100
H	1.17228900	3.50459200	2.01970800
C	3.33132100	2.80383400	-1.11463000
H	1.74569200	1.52495000	-1.75947100
C	3.79916500	3.67171400	-0.13029100
H	3.38801800	4.60567200	1.76708800
H	3.93388900	2.59694900	-1.99251000
H	4.76912200	4.14510000	-0.24317300
C	-2.83426700	0.59042600	-0.92079500
H	-2.69071200	0.82362400	-1.98071400
N	-1.56907900	0.17503200	-0.29829900
C	-3.43447800	1.80270800	-0.21410300
F	-3.56047700	1.58551400	1.09583200
F	-4.65041600	2.04016800	-0.71443900
F	-2.69027000	2.89355700	-0.40658900
C	-1.62082900	-1.09837200	0.06683300
O	-1.34428900	-1.93211300	-1.73141500
C	-0.56816900	-1.68095300	0.93288500
C	-0.24824900	-0.95660900	2.08847800
C	0.04960900	-2.90529900	0.67686400
C	0.71156100	-1.44951900	2.96451600
H	-0.75071500	-0.01671800	2.29340100
C	1.02701300	-3.37637500	1.54810700
H	-0.18755000	-3.47177300	-0.21369600
C	1.36063300	-2.65059800	2.68843300
H	0.95973700	-0.88451800	3.85640700
H	1.53209000	-4.30950300	1.32354100
H	2.12551400	-3.02154700	3.36252200

C	-3.09135800	-1.42771600	0.17750700
H	-3.35752900	-1.15257200	1.20960400
C	-3.53557600	-2.83926600	-0.11214700
H	-2.93880900	-3.53978900	0.47803400
H	-4.58187500	-2.95074700	0.17595100
H	-3.43783000	-3.06671600	-1.17351800
O	-3.68467400	-0.50800800	-0.74772400
H	-1.39442600	-2.89513100	-1.81942800
H	-0.40289900	-1.66277000	-1.98692400
C	1.85924300	-1.85739500	-1.56213000
O	1.92794200	-3.05788300	-1.80419800
O	1.02149400	-1.00457500	-2.00156400
C	2.89745900	-1.24627600	-0.59637900
F	3.64601100	-2.17442700	-0.00055100
F	2.28329400	-0.53738700	0.36563900
F	3.71971400	-0.40846900	-1.24716700

IM5

C	-0.14428900	1.71611300	0.41610700
O	-0.90186400	1.93904000	1.34867700
N	-0.44113900	0.76934300	-0.54655200
H	0.27695700	0.17802400	-1.08970800
C	1.13584100	2.44396600	0.20191200
C	1.51149900	3.37159600	1.17674400
C	1.95617900	2.21991300	-0.90816300
C	2.70468400	4.07126100	1.04507900
H	0.86140800	3.53087300	2.03020700
C	3.15369000	2.91539100	-1.02951000
H	1.68337800	1.50014700	-1.67395900
C	3.52683800	3.84152300	-0.05715100
H	2.99595600	4.79113600	1.80232600
H	3.79533200	2.73121400	-1.88443800
H	4.46169800	4.38338400	-0.15758900
C	-2.85270700	0.36345500	-1.01273500
H	-2.66611600	0.65149200	-2.05044000
N	-1.57972000	0.01735600	-0.34856700
C	-3.56067400	1.50099800	-0.27460400
F	-3.69973400	1.20976700	1.02032600
F	-4.77441800	1.66471200	-0.80034300
F	-2.89223400	2.64662700	-0.39645600
C	-1.64242800	-1.12942900	0.24485300
C	-0.54198100	-1.71995200	1.00590000
C	-0.07742900	-1.06771400	2.15365900
C	0.04347900	-2.91047900	0.56061200
C	0.97556800	-1.62815400	2.86625500
H	-0.54864300	-0.14755300	2.48220400
C	1.12628500	-3.43104800	1.25997500
H	-0.30150500	-3.38937100	-0.34962700
C	1.58284200	-2.79813200	2.41473400
H	1.33249900	-1.13890700	3.76571100
H	1.61473800	-4.32732300	0.89411000
H	2.42154700	-3.21624100	2.96135700
C	-3.01830400	-1.69662900	0.04421900
H	-3.54345100	-1.62439000	1.00678000
C	-3.05847100	-3.11234900	-0.49241400

H	-2.66636500	-3.80976800	0.24990800
H	-4.09998000	-3.36701500	-0.69552200
H	-2.48205800	-3.18805100	-1.41668900
O	-3.60670900	-0.80384100	-0.91425100
C	1.71223800	-1.75489100	-1.70570900
O	1.87718600	-2.90321000	-2.11495900
O	0.79407400	-0.93259800	-1.99644000
C	2.77932300	-1.19758800	-0.73320100
F	3.54264400	-2.15489400	-0.20335100
F	2.21321500	-0.52110200	0.28153000
F	3.59230700	-0.33919700	-1.37419200

IM6

C	2.23798600	-0.80990200	-0.21397000
O	1.45761900	-0.92894400	-1.13674900
N	1.93241000	0.01020800	0.87800800
H	2.37154000	-0.17798800	1.77604500
C	3.56993900	-1.46051100	-0.14907300
C	3.75738400	-2.59559600	-0.94249500
C	4.60973700	-0.97397200	0.64962600
C	4.97915800	-3.25613400	-0.92095900
H	2.93882900	-2.95107700	-1.55937400
C	5.83259400	-1.63586700	0.65897800
H	4.48652800	-0.06844500	1.23623900
C	6.01490100	-2.77739400	-0.11962400
H	5.12451400	-4.14301000	-1.52795300
H	6.64514900	-1.25658600	1.26886400
H	6.96959500	-3.29276300	-0.10586100
C	-0.40019700	-0.34194300	1.71696700
H	0.00877600	-0.76701300	2.63745900
N	0.63736100	0.45659200	1.01124200
C	-0.92658800	-1.47267500	0.82279400
F	-1.26724200	-1.01808900	-0.38152000
F	-1.99725000	-2.01314700	1.39522400
F	0.00088000	-2.42640200	0.67749200
C	0.16403800	1.60526000	0.61532300
C	0.92108100	2.62040200	-0.09978200
C	1.70557300	2.28281600	-1.21267000
C	0.86280100	3.94793000	0.35327700
C	2.42009000	3.27543300	-1.86879000
H	1.70587100	1.26802600	-1.59171000
C	1.61109000	4.92237200	-0.29302700
H	0.27715300	4.20781800	1.22637500
C	2.38152300	4.58942500	-1.40558500
H	3.00693300	3.02105700	-2.74415900
H	1.58597200	5.94380500	0.06918500
H	2.95014200	5.35886600	-1.91716000
C	-1.29705800	1.63668000	0.98708800
H	-1.84967800	1.35926400	0.07092500
C	-1.89922300	2.89652000	1.56139300
H	-1.90017600	3.69212300	0.81530200
H	-2.93560100	2.65483100	1.80433300
H	-1.37605000	3.21883800	2.46361500
O	-1.38527200	0.59230600	1.97296900
C	-3.93839700	0.08851700	-0.41682400

O	-4.05279700	0.32585100	0.79963300
O	-3.35821400	0.73030700	-1.31694600
C	-4.56130400	-1.25335800	-0.88453600
F	-5.57824000	-1.65082300	-0.10708200
F	-3.64026000	-2.23671400	-0.85634700
F	-5.02448200	-1.19032700	-2.14185500

TS4

C	2.20392400	-0.75103400	-0.16833500
O	1.36769600	-1.05337800	-1.00069000
N	1.87324700	0.01100600	0.93743700
H	2.49576400	0.07693500	1.73533600
C	3.63973700	-1.13305200	-0.26282400
C	3.94766600	-2.25108800	-1.04207400
C	4.65816300	-0.41280000	0.36904900
C	5.26893800	-2.66086200	-1.17175400
H	3.14421200	-2.79050500	-1.53225400
C	5.97981400	-0.82309400	0.22788900
H	4.43588800	0.48173200	0.94302900
C	6.28446000	-1.94789300	-0.53605100
H	5.50746900	-3.53433000	-1.76889600
H	6.77207900	-0.25986000	0.70887100
H	7.31653200	-2.26609300	-0.64101200
C	-0.32051800	-0.55098700	1.98860800
H	0.17397800	-0.89378600	2.90385400
N	0.56608700	0.31987400	1.19759000
C	-0.76690200	-1.78584000	1.19820700
F	-1.25104400	-1.47136500	-0.00361100
F	-1.72139900	-2.41905800	1.88084000
F	0.25983800	-2.62949300	1.03449700
C	-0.07232400	1.44328000	0.85392700
C	0.52687600	2.50656800	0.04623400
C	1.14580200	2.21543900	-1.17532000
C	0.46494700	3.82372200	0.51723800
C	1.69854500	3.24835400	-1.92219100
H	1.15426800	1.19775000	-1.55050800
C	1.04138700	4.84507500	-0.22888800
H	-0.00571200	4.04010300	1.47040300
C	1.65295600	4.55833800	-1.44765600
H	2.16383300	3.02941900	-2.87693900
H	1.00784300	5.86442600	0.13935700
H	2.09177500	5.35978800	-2.03278300
C	-1.40439600	1.36271400	1.32727200
H	-2.03536000	1.02736700	0.23184700
C	-2.23878500	2.51570200	1.81630000
H	-2.26546400	3.30366500	1.06129800
H	-3.25692000	2.14729900	1.96280500
H	-1.86171600	2.91910000	2.75997300
O	-1.41344300	0.26852800	2.26300500
C	-3.67488900	-0.17359400	-0.30586200
O	-4.01937600	-0.36592700	0.85317600
O	-2.83941000	0.67614100	-0.76703200
C	-4.24397200	-1.08850800	-1.40873300
F	-5.24828400	-1.84505900	-0.96419100
F	-3.28241800	-1.90693000	-1.86135500

F	-4.69292800	-0.37973000	-2.45256400

IM7

C	1.50779200	0.78715200	0.50031000
O	1.25897900	0.99401200	1.68172700
N	0.53578600	0.58724400	-0.43659900
H	0.76623700	0.23673300	-1.36124000
C	2.90869200	0.74034000	-0.02357700
C	3.91747600	0.39980300	0.88040900
C	3.23265800	1.03842200	-1.35031000
C	5.23941000	0.33480800	0.45610400
H	3.65073300	0.18366400	1.90943600
C	4.55864900	0.98043400	-1.76906100
H	2.46431000	1.34502800	-2.05355100
C	5.56067300	0.62359100	-0.86941500
H	6.01950700	0.06090300	1.15843200
H	4.80920500	1.22135100	-2.79666200
H	6.59326500	0.57701100	-1.19971300
C	-1.62315000	1.62772100	-0.53905200
H	-1.02801000	2.40013400	-1.03044200
N	-0.79642000	0.53751100	-0.03532800
C	-2.37543100	2.25329000	0.62704700
F	-3.14753300	1.35827300	1.25203300
F	-3.16411000	3.24882500	0.20518700
F	-1.51037600	2.75235700	1.51396000
C	-1.48304600	-0.65827000	-0.45888800
C	-1.00126500	-1.96122200	0.00343900
C	-0.30685600	-2.04744200	1.21868500
C	-1.18980500	-3.12200200	-0.75846600
C	0.15717300	-3.27641700	1.67430100
H	-0.13628100	-1.14546500	1.79901900
C	-0.73369600	-4.35025700	-0.29048400
H	-1.67106700	-3.05936600	-1.72927200
C	-0.06168600	-4.43275000	0.92728900
H	0.69079600	-3.33057500	2.61769400
H	-0.88948000	-5.24262100	-0.88805400
H	0.30055000	-5.39059400	1.28600700
C	-2.52255600	-0.31130600	-1.23045700
C	-3.62974600	-1.07263000	-1.85459700
H	-3.67012100	-2.08592400	-1.45480800
H	-4.57807500	-0.57018500	-1.64695800
H	-3.50395300	-1.12359600	-2.94059500
O	-2.57481900	1.06793000	-1.42748900

IM8

C	-0.19984700	1.24214800	0.24967100
O	-0.39295500	0.85013100	1.41360100
N	0.68836900	0.64215100	-0.56160900
H	0.88571400	1.00004600	-1.49286800
C	-0.94465400	2.39944500	-0.31432000
C	-1.35164700	3.39935400	0.57243300
C	-1.28669000	2.47456300	-1.66766600
C	-2.07091800	4.49063100	0.09999000
H	-1.09281800	3.31339100	1.62257100
C	-2.01446800	3.56509500	-2.13263600

H	-1.02275200	1.67185000	-2.34971300
C	-2.39997800	4.57424200	-1.25222900
H	-2.37831500	5.27317400	0.78523300
H	-2.29069300	3.62091900	-3.18000200
H	-2.96726000	5.42337400	-1.61920300
C	0.69480600	-1.73973300	-0.80681100
H	-0.18511500	-1.49540100	-1.40556400
N	1.26749200	-0.55890900	-0.16322300
C	0.29708800	-2.74758600	0.26369900
F	1.34667500	-3.10331700	1.01212900
F	-0.20267600	-3.85541700	-0.29440600
F	-0.63448700	-2.23280200	1.07276900
C	2.68018500	-0.64250600	-0.43407900
C	3.58365900	0.32608300	0.18851500
C	3.21307400	0.93992400	1.39369000
C	4.79985000	0.67835200	-0.41156900
C	4.06119900	1.85987100	1.99987400
H	2.25964900	0.68814500	1.84946000
C	5.64863400	1.59085100	0.20665300
H	5.06956500	0.25730700	-1.37490100
C	5.28452700	2.18238600	1.41439100
H	3.76546200	2.32576300	2.93431600
H	6.58951000	1.85273600	-0.26642100
H	5.94459800	2.90000900	1.89046200
C	2.90486100	-1.69772000	-1.22887300
C	4.13576500	-2.34925400	-1.73371500
H	5.01025500	-1.97791100	-1.19916900
H	4.06037500	-3.42956500	-1.58556600
H	4.26627200	-2.16170100	-2.80399300
O	1.71545000	-2.32355500	-1.59771700
C	-3.02922500	-0.51058700	0.36186200
O	-2.28539900	-0.53297400	-0.59167000
O	-2.81958300	0.01863700	1.53849800
H	-1.88632800	0.41377800	1.57726100
C	-4.43733600	-1.12203100	0.28550800
F	-4.59178500	-1.80182600	-0.84528400
F	-5.35817500	-0.15425100	0.32760900
F	-4.65650300	-1.94546600	1.31206300

TS5

C	-0.33784400	-0.67573600	-0.38635300
O	-0.54954300	-1.38258300	0.68310300
N	0.74165300	-0.89789500	-1.08763400
H	0.89043700	-0.16211200	-1.78201000
C	-1.30666400	0.39797500	-0.75393400
C	-1.93214700	1.12729600	0.26056800
C	-1.56321200	0.70259400	-2.09445000
C	-2.79652600	2.16761700	-0.06638000
H	-1.72929300	0.88733600	1.29863500
C	-2.43942700	1.73250800	-2.41518600
H	-1.09982100	0.11396800	-2.88086800
C	-3.05393500	2.46791000	-1.40164500
H	-3.27072700	2.73971400	0.72449800
H	-2.65104700	1.95597100	-3.45540700
H	-3.73675900	3.27249900	-1.65449500

C	3.37895700	-1.38379200	-0.63737300
H	2.98462500	-2.15495600	-1.29544400
N	2.37232800	-0.72670400	0.13541000
C	4.44536200	-1.98599900	0.28671000
F	5.00174500	-1.04759900	1.05460100
F	5.40557500	-2.54551900	-0.44707300
F	3.90294300	-2.91397200	1.06502300
C	2.62444000	0.58420900	0.02149700
C	1.79302400	1.58954300	0.69240300
C	1.27914700	1.31917000	1.96615300
C	1.43748700	2.77342000	0.03451700
C	0.44328400	2.24100600	2.58576600
H	1.53930700	0.39050400	2.46333300
C	0.59307400	3.68713800	0.65653800
H	1.79411300	2.96682400	-0.97300800
C	0.10064600	3.42510400	1.93360300
H	0.05252200	2.03131300	3.57581800
H	0.31044500	4.59725900	0.13841900
H	-0.55851300	4.13891400	2.41686200
C	3.65398300	0.78120500	-0.92211300
C	4.32124700	2.00411000	-1.39104100
H	4.19723200	2.80451500	-0.66171000
H	5.37738700	1.80297700	-1.57670300
H	3.85768800	2.31442200	-2.33553800
O	4.05999400	-0.37443500	-1.40581000
C	-3.55036300	-1.70109100	0.14242200
O	-3.11252500	-2.08561400	-0.93810700
O	-2.92955500	-1.48509700	1.23255500
H	-1.59644000	-1.42175900	0.96359800
C	-5.04865800	-1.35247200	0.24155500
F	-5.73704200	-1.76653200	-0.82384300
F	-5.20150400	-0.02064700	0.33313200
F	-5.61141100	-1.89391600	1.32995100

IM9

C	-1.80698500	0.07275700	0.83019900
H	-2.24077700	0.18995200	1.82737100
N	-0.55973100	-0.58526100	0.83679300
C	-2.81941500	-0.59261700	-0.11001900
F	-2.31858100	-0.68508300	-1.33940800
F	-3.93326700	0.12922200	-0.15439000
F	-3.10119200	-1.80767200	0.33773000
C	0.33078800	0.22004000	0.37208600
C	1.74213700	-0.10243100	0.16895400
C	2.08827400	-1.42484500	-0.13813300
C	2.73503300	0.87589900	0.30094600
C	3.42199500	-1.76028800	-0.32263400
H	1.30981700	-2.17239800	-0.24706500
C	4.06892900	0.52702000	0.12554800
H	2.47873300	1.89481300	0.56941800
C	4.41137700	-0.78587700	-0.19090000
H	3.69082500	-2.78065000	-0.57221400
H	4.84051600	1.28027600	0.23868200
H	5.45322700	-1.05160000	-0.33559400
C	-0.33721600	1.51142200	0.01715800

C	0.18772200	2.73284400	-0.58077500
H	0.91581400	2.47182300	-1.35399800
H	-0.62260600	3.34966200	-0.96581000
H	0.72906600	3.28131200	0.20308300
O	-1.57437100	1.40773700	0.29357600

IM10

C	-2.23391900	-1.27833100	0.01732900
O	-1.62062100	-2.15480800	-0.79267200
N	-3.21320600	-1.68080300	0.73290000
H	-3.60559800	-0.87789900	1.22466700
C	-1.74900100	0.13527700	-0.04495200
C	-1.37770400	0.69617400	-1.26970200
C	-1.68181600	0.90913800	1.11619100
C	-0.97318600	2.02603800	-1.33574500
H	-1.41182800	0.08698900	-2.16736300
C	-1.26127200	2.23366200	1.05106500
H	-1.93832400	0.46086300	2.07175100
C	-0.91319100	2.79593100	-0.17608100
H	-0.69726500	2.45837700	-2.29209100
H	-1.19801400	2.82481200	1.95883700
H	-0.58689600	3.82986700	-0.22672800
C	1.18382500	-1.09645700	0.07248100
O	0.70532400	-1.42767700	1.16169800
O	0.82190200	-1.40114000	-1.09710900
H	-0.66102500	-1.87374600	-0.96474400
C	2.35340600	-0.08811200	0.12287600
F	3.06396600	-0.18995900	1.25293900
F	1.87094700	1.16711300	0.06742800
F	3.20460900	-0.22988400	-0.90155900

PhCOHNH

C	3.14191300	-1.42079100	-0.79014900
O	2.79297000	-2.02434000	-1.95024900
N	2.23484500	-1.03362900	0.01701600
H	2.65445100	-0.63364400	0.85493000
C	4.61700100	-1.30674900	-0.63762300
C	5.46625000	-2.15565300	-1.35332600
C	5.16277500	-0.35370500	0.22748200
C	6.84486000	-2.06266800	-1.18977300
H	5.04434500	-2.89109500	-2.02876100
C	6.54087200	-0.25914000	0.38355200
H	4.51318600	0.33148600	0.76426000
C	7.38410400	-1.11593000	-0.32200500
H	7.49810900	-2.72989200	-1.74222500
H	6.95712800	0.48764300	1.05133800
H	8.45965500	-1.04188600	-0.19845400
H	1.82558700	-2.10193800	-1.95377200

PhCONH2

C	3.14672500	-1.43252100	-0.90363000
O	2.71211900	-1.94594400	-1.93611200
N	2.33025200	-0.95988000	0.06098700
H	2.67601600	-0.72306200	0.97806200
C	4.61963400	-1.29396500	-0.66410000

C	5.47396700	-2.15482500	-1.35626500
C	5.15315100	-0.33279900	0.19858700
C	6.84921100	-2.07329400	-1.16923500
H	5.04658700	-2.88694900	-2.03315000
C	6.53081500	-0.24657900	0.37688400
H	4.50344700	0.36982800	0.71141700
C	7.37878600	-1.11970700	-0.30120500
H	7.50853000	-2.75125500	-1.70103500
H	6.94194900	0.50658900	1.04076500
H	8.45238300	-1.05308000	-0.15744700
H	1.33672900	-1.09950700	-0.05810100

TS6

C	1.34577900	-2.07268800	-0.67806300
O	1.11337000	-3.24800100	-0.46434900
N	0.30211800	-1.25643000	-1.16084600
H	0.58830400	-0.44848200	-1.71129500
C	2.64995400	-1.42922900	-0.37463200
C	3.66779400	-2.25967700	0.10945600
C	2.88263800	-0.05691900	-0.52702300
C	4.90732900	-1.72506000	0.43213200
H	3.47192700	-3.31989300	0.22542800
C	4.12508100	0.47384400	-0.19553900
H	2.11702300	0.61727400	-0.89913000
C	5.13601500	-0.35733700	0.28140200
H	5.69500400	-2.37189600	0.80268700
H	4.29907000	1.53840500	-0.31270400
H	6.10437500	0.06084800	0.53578100
C	-2.93491400	-0.41543100	-0.63941300
H	-3.06736300	-0.89731500	-1.61217500
N	-2.25760300	0.83223100	-0.72403500
C	-4.28602100	-0.28060700	0.06219800
F	-4.13399500	0.27773500	1.26177300
F	-4.83837800	-1.48035100	0.22201700
F	-5.09702000	0.47652800	-0.66719000
C	-1.16903600	0.73886400	-0.05474400
C	-0.12556300	1.76241200	0.04491300
C	0.58269500	1.95563700	1.23664800
C	0.20201600	2.49737000	-1.10069500
C	1.62609900	2.87373400	1.27273400
H	0.30622600	1.41221600	2.13464000
C	1.25510700	3.40382300	-1.05842400
H	-0.35245000	2.33658100	-2.01964700
C	1.96973700	3.58694300	0.12525600
H	2.17233600	3.03026200	2.19630100
H	1.52016200	3.96388800	-1.94846700
H	2.79403900	4.29198100	0.15458800
C	-1.04429800	-0.65178100	0.50643600
C	-0.23024600	-1.17045100	1.61729800
H	0.77551200	-0.75102400	1.60323400
H	-0.73981700	-0.85635600	2.53749900
H	-0.20722100	-2.26125800	1.58595100
O	-2.13090900	-1.28425100	0.19817300
H	-0.38487600	-1.82372300	-1.65816100

3a·H⁺

C	1.99766100	-0.92515200	-1.14945300
O	1.87087100	-1.97868300	-1.70030500
N	0.76356900	-0.03847100	-1.15626800
H	0.99890600	0.96084500	-1.13065100
C	3.17911400	-0.41086300	-0.44911900
C	4.20635600	-1.33461900	-0.20829700
C	3.31075900	0.91965300	-0.03052700
C	5.35047000	-0.92883900	0.46208000
H	4.08773500	-2.36019800	-0.54063300
C	4.46344600	1.31776500	0.63318300
H	2.54350800	1.66260400	-0.22608800
C	5.47765800	0.39489600	0.88355100
H	6.14260400	-1.64226800	0.65856200
H	4.57017600	2.34761100	0.95402900
H	6.37307400	0.70995200	1.40890500
C	-2.04883300	-1.64839900	-0.63250000
H	-2.21817700	-2.11578600	-1.60646000
N	-2.48431100	-0.28459600	-0.60585900
C	-2.78096400	-2.45459200	0.43426500
F	-2.59259400	-1.91649800	1.64387200
F	-2.32414600	-3.70769200	0.46369200
F	-4.08985300	-2.48796300	0.18741500
C	-1.50381200	0.45399900	-0.25149100
C	-1.60196200	1.91803400	-0.12169600
C	-0.53125200	2.71870500	0.29783300
C	-2.82390600	2.52751600	-0.44582900
C	-0.68224600	4.09924500	0.38962600
H	0.42959900	2.29463300	0.57058700
C	-2.96912100	3.90310400	-0.35048900
H	-3.65343800	1.91157100	-0.77271900
C	-1.89799300	4.69332100	0.06743700
H	0.15342700	4.70727300	0.71793400
H	-3.91890600	4.36160100	-0.60317500
H	-2.01318500	5.76943100	0.14173700
C	-0.23652700	-0.38788500	-0.02395600
C	0.42116700	-0.32691300	1.33894200
H	0.97868200	0.59278200	1.51199900
H	-0.37273000	-0.41203700	2.08342900
H	1.09331100	-1.18096900	1.45012200
O	-0.66539200	-1.68190100	-0.29331300
H	0.28603400	-0.22537500	-2.04991900

3a

C	1.40938300	-0.78772900	-0.23365900
O	0.85092900	-0.81528000	-1.32926400
N	0.72445800	-0.54702500	0.91511800
H	1.22001000	-0.49745000	1.79507500
C	2.88481300	-0.99637400	-0.10121100
C	3.67624600	-0.69851200	-1.21289300
C	3.47698300	-1.49193400	1.06339800
C	5.05402100	-0.87118400	-1.15332400
H	3.19842100	-0.32759700	-2.11347100
C	4.85583500	-1.67365400	1.11577100
H	2.87136600	-1.76995900	1.92083100

C	5.64482300	-1.35812000	0.01176200
H	5.66703300	-0.62877700	-2.01494300
H	5.31260400	-2.06903900	2.01674700
H	6.71993100	-1.49833800	0.05707400
C	-2.11736300	-1.22400300	-0.68607400
H	-1.78991300	-1.79406300	-1.56183000
N	-2.00000900	0.19292100	-0.93513200
C	-3.56260600	-1.58517900	-0.38560400
F	-4.02576800	-0.90349200	0.67043800
F	-3.67494200	-2.88871300	-0.10613900
F	-4.35404600	-1.31805300	-1.42844400
C	-1.20135300	0.65662400	-0.05797600
C	-0.70706900	2.05055200	-0.05291200
C	-0.94202800	2.91426200	1.02112100
C	0.03158700	2.49220800	-1.15489700
C	-0.44578600	4.21417000	0.98506000
H	-1.53563800	2.58414300	1.86732400
C	0.53433800	3.78945700	-1.17921000
H	0.21633200	1.80902200	-1.97778400
C	0.29614400	4.65094000	-0.11047200
H	-0.64230600	4.88705400	1.81311400
H	1.11096000	4.12698900	-2.03402700
H	0.68573100	5.66346800	-0.13226900
C	-0.71181700	-0.39472300	0.94370100
C	-1.14919200	-0.13657400	2.37607700
H	-0.62742500	0.72583600	2.79591300
H	-2.22616200	0.03597300	2.40277300
H	-0.91701600	-1.02033400	2.97599100
O	-1.35143300	-1.56687400	0.45113200

IM11

C	1.98876000	0.79711100	-0.57866100
H	1.90145300	1.46625400	-1.44026900
N	1.47537400	-0.50998300	-0.88340900
C	3.45228600	0.70473900	-0.17320500
F	3.61313800	-0.11416100	0.87287900
F	3.92010300	1.90752900	0.17358300
F	4.19705000	0.24358600	-1.18050000
C	0.51564200	-0.74694000	-0.07580200
C	-0.26948600	-1.99134000	-0.07086800
C	0.26498200	-3.13535400	-0.67794000
C	-1.54154700	-2.04745700	0.51303500
C	-0.46019300	-4.31869100	-0.69529500
H	1.25211900	-3.08788800	-1.12426800
C	-2.26580400	-3.23549600	0.48586800
H	-1.98104100	-1.16474800	0.96574000
C	-1.72699400	-4.37077600	-0.11325900
H	-0.03733000	-5.20263200	-1.16060200
H	-3.25371800	-3.27065500	0.93219100
H	-2.29302100	-5.29639600	-0.12818400
C	0.30718300	0.39755000	0.92115400
C	0.44515500	0.02046300	2.37603400
H	1.41877800	-0.45169200	2.51856200
H	0.38908400	0.92697200	2.98190100
H	-0.34433300	-0.66953200	2.67631600

O	1.28496200	1.32059500	0.53810100
C	-1.38785900	1.47555400	-0.38126100
O	-1.00303800	1.00359200	0.79980300
O	-0.76562700	1.50386000	-1.40612500
C	-2.82859100	1.99913300	-0.26045800
F	-3.63786200	1.01575900	0.14117300
F	-3.25084000	2.45230800	-1.43165300
F	-2.89394200	2.98440600	0.63476000

TS7

C	-0.39393900	1.68429000	-0.08949300
H	-1.36425800	0.98238700	-0.45052400
N	0.73468300	1.16849600	-0.70293900
C	-0.67217900	3.15601300	-0.27322900
F	0.33357900	3.92062600	0.16766200
F	-1.76965400	3.50114700	0.40238400
F	-0.85950600	3.42034000	-1.56422300
C	1.32880700	0.40187900	0.16389500
C	2.50334400	-0.43630200	-0.10593700
C	3.49890400	0.02433100	-0.97335000
C	2.61378900	-1.70017400	0.48268700
C	4.60577200	-0.77283800	-1.23830900
H	3.40482900	1.00605600	-1.42562600
C	3.72327700	-2.49380500	0.20950600
H	1.82001600	-2.07698400	1.12038900
C	4.72026700	-2.02974600	-0.64545400
H	5.38093500	-0.41267700	-1.90610200
H	3.80391900	-3.47765400	0.65881200
H	5.58608300	-2.64945400	-0.85435200
C	0.64662300	0.53436500	1.44541700
C	0.91035200	-0.06515800	2.75946400
H	1.98485200	-0.19881400	2.89755900
H	0.48392900	0.55551600	3.54710500
H	0.43333900	-1.05142600	2.78112000
O	-0.30368400	1.38747100	1.30520500
C	-1.95915400	-1.06481500	-0.11294600
O	-0.93652400	-1.28846600	0.53915200
O	-2.33653000	0.00561900	-0.67839200
C	-2.96610100	-2.21879800	-0.29885200
F	-2.55524600	-3.34191000	0.28934200
F	-3.15246200	-2.47721600	-1.59872200
F	-4.15461200	-1.89063800	0.22400800

5

C	1.66029100	-0.04171000	-0.00961300
N	0.57292000	-0.72087400	-0.09188900
C	3.06895500	-0.53912400	-0.09208500
F	3.76606500	-0.18517300	0.99381900
F	3.70058700	-0.02179300	-1.15244400
F	3.09117100	-1.86405200	-0.19497400
C	-0.43345500	0.23926500	0.02470900
C	-1.85650600	-0.12022300	-0.01683800
C	-2.27029200	-1.38243200	0.42485800
C	-2.81242600	0.78169500	-0.49965500
C	-3.61685500	-1.72770100	0.39977200

H	-1.53078400	-2.08679900	0.79137000
C	-4.16008500	0.43447300	-0.51620200
H	-2.49929200	1.74597600	-0.88827700
C	-4.56644000	-0.81900500	-0.06501600
H	-3.92649400	-2.70808000	0.74707600
H	-4.89144200	1.14083600	-0.89525500
H	-5.61700100	-1.08988600	-0.08248300
C	0.14126400	1.46632100	0.18715700
C	-0.34772900	2.84720500	0.41026900
H	-1.34516600	2.81929600	0.85178500
H	0.32687700	3.37161100	1.09024200
H	-0.39801500	3.40919600	-0.52718700
O	1.50126600	1.28131900	0.15677400