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Supplementary Information

Late-Stage C-H Trifluoroacetylation of Quinoxaline-2(1*H*)-ones Using Masked Trifluoroacyl Reagents

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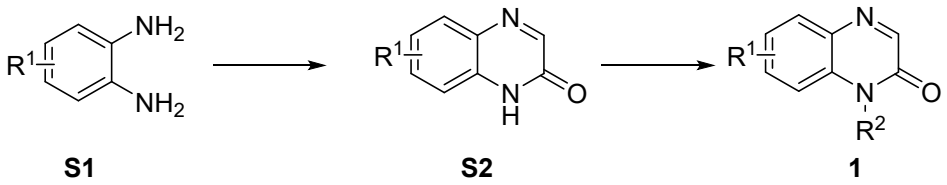
1. General information

Solvents and reagents were of reagent grade and used without purification unless otherwise noted. Anhydrous solvents were obtained as follows: DMSO was purchased directly from the reagent company-Energy-Chemical; $CHCl_3$, DMF were redistilled over CaH_2. All reactions were carried out in oven dried glassware under oxygen unless otherwise specified. Column chromatography was performed using silica gel (200-300 mesh). ^1H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded in $CDCl_3$ operating at 500/400, 126/101 and 471/376 MHz in the presence of tetramethylsilane (TMS) as an internal standard and are reported in ppm (δ). All ^1H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded on a NMR, AVANCE III 400 MHz, Bruker or JEOL 500M. Coupling constants are reported in Hertz (Hz).Spectral splitting patterns are designated as s, singlet; d, doublet; t, triplet; q, quartet; p, pentet; m, multiplet; and br, broad. High resolution mass spectroscopic data of the products were collected on a Waters Micromass GCT instrument using EI (70 eV) or an Agilent Technologies 6540 UHD Accurate-Mass Q-TOF LC/MS using ESI.

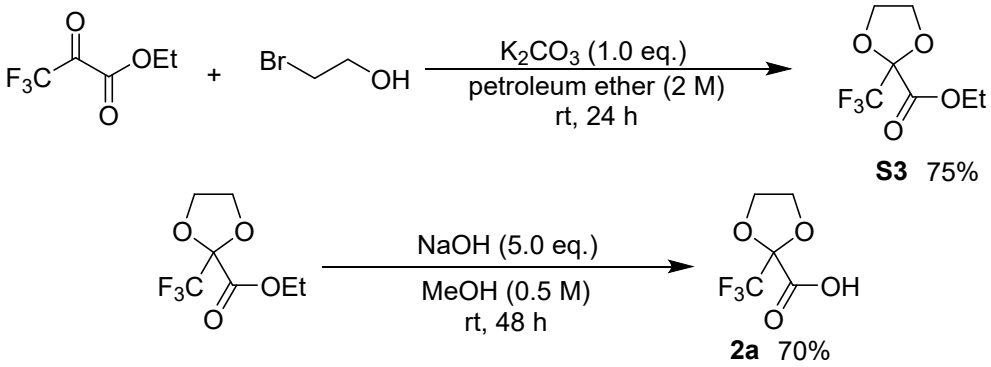
2. General Procedures for Substrates

A. General Procedure for the synthesis of compounds 1：



Following the procedure of reported literature.[1,2] To a dried round-bottom flask charged with a magnetic stirring bar, *o*-phenylenediamine **S1** (5 mmol), ethyl 2-oxoacetate (6 mmol) and ethanol (20 mL) were added successively and the mixturewas stirred at reflux for 1 h. After completion of the reaction, the reaction mixture was filtered,washed with ethanol and then dried to give quinoxalinone **S2**. Subsequently, a 50 mL oven-dried reaction vessel equipped with a magnetic stirrer bar was charged with quinoxalinone **1**, potassium carbonate (1.2 equiv.), corresponding halogenoalkane (1.6 equiv.) and DMF (20 ml). The resulting solution was stirred in air at room temperature overnight. Then the reaction mixture was diluted with ethyl acetate, washed with water, and the organic layer was separated and dried over anhydrous $NaSO_4$. The solvent was concentrated under reduced pressure and the residue was purified bycolumn chromatography on silica gel to afford the desired substrate **1**.

B. General Procedure for the synthesis of compounds 2a：

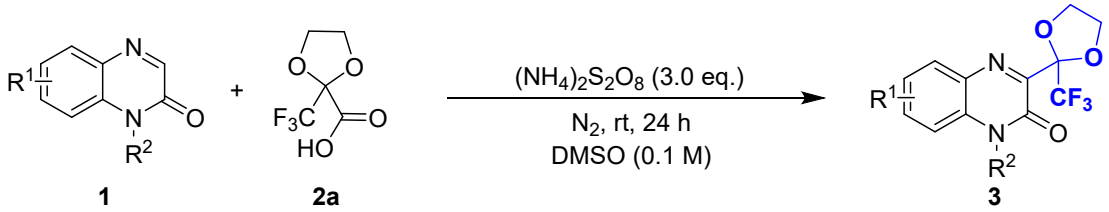


Following the procedure of reported literature.[3] Preparation method of trifluoropyruvate containing protective group: Ethyl trifluoropyruvate (10 mL, 76.0 mmol, 1 eq) and 38 mL petroleum ether were added to the mixture in a 100 mL dry round-bottom flask with magnetic stirring rod, and 2-bromoethanol (5.4 mL, 76 mmol, 1 eq) was slowly added to the mixture. The reaction mixture is stirred at room temperature for 30 minutes. Cool to 5 °C, add K_2CO_3(10.5 g, 76.0 mmol, 1 eq) and

stir vigorously. The reaction mixture is stirred at room temperature for 24 hours, diluted with 30 ml ethyl acetate and filtered. The filtrate was concentrated under reduced pressure, and the resulting substance was dissolved in ethyl acetate (30 mL) and washed with saturated sodium chloride solution. The organic layer was dried with anhydrous sodium sulfate, filtered, and the filtrate was concentrated under reduced pressure to obtain a colorless oil-like intermediate **S3** (12.2 g, 75% yield).

Dissolve sodium hydroxide solid (10.5 g, 263.5 mmo1, 5 eq.) in 40 mL water, cool to room temperature and set aside. Colorless oil intermediate and methanol (100 mL, 0.5 M) were added to the round-bottomed flask, and the prepared sodium hydroxide solution was added to the solution. The reaction mixture was rapidly stirred at room temperature for 5 min, and then stirred at room temperature for 48 h. Acidification with 1M HCl aqueous solution to pH = 2.0, then extraction with ethyl acetate. Organic extracts are washed with saturated sodium chloride solution. The organic layer was dried with anhydrous sodium sulfate, filtered, and reduced pressure to concentrate the filtrate to obtain a white solid **2a** (6.8 g, 70% yield).

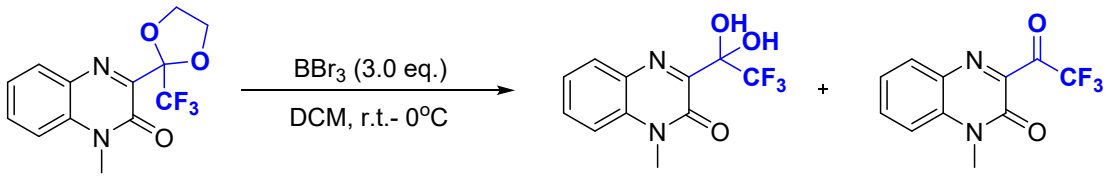
C. General Procedure for the synthesis of compounds 3:



1 **2a** **3**

To an oven dried 10.0 mL screw capped tube equipped with a magnetic stir bar, quinoxalin-2(1*H*)-one **1** (0.2 mmol, 1.0 equiv), $(NH_4)_2S_2O_8$ (0.6 mmol, 3 eq.), DMSO (0.1 M) and compound **2a** (0.5 mmol, 2.5 equiv) were placed under N_2. The resulting solution was stirred at room temperature (preheated oil bath) for 24 h (actual reaction time is mentioned in the specific reaction). Progress of the reaction was monitored by TLC analysis. After running the reaction for an appropriate time (actual time is mentioned in the specific reaction), the crude product was purified by column chromatography to afford the desired product.

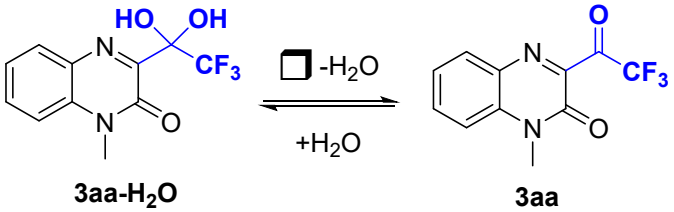
General Procedure for the deprotection of compounds 3:



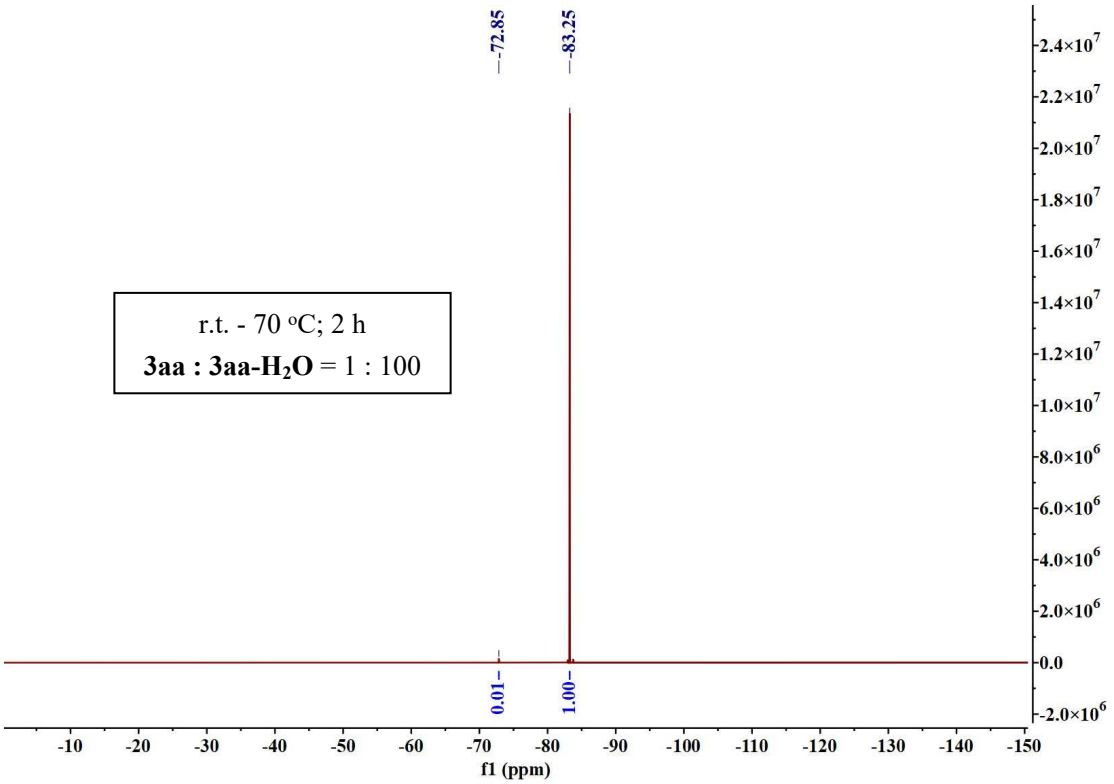
Following the modified procedure of reported literature.[4] To a 20 mL vial, BBr_3 (2.0 M in CH_2Cl_2, 1.20 mL, 1.20 mmol, 3.0 equiv) was added dropwise, at 0 °C, to compound **3a** (0.8 mmol, 1.0 equiv) The reaction mixture was stirred 2 h at 0 °C. Water (10 mL) was then slowly added and the reaction mixture was warmed to room temperature, while stirring. The mixture was extracted with $NaHCO_3$ (15 mL) and CH_2Cl_2 (3×7 mL). The combined organic layers were dried (Na_2SO_4), filtered and evaporated. The crude material was purified by flash column chromatography (hexanes/EtOAc = 2:1) to afford deprotection compounds **3aa**.

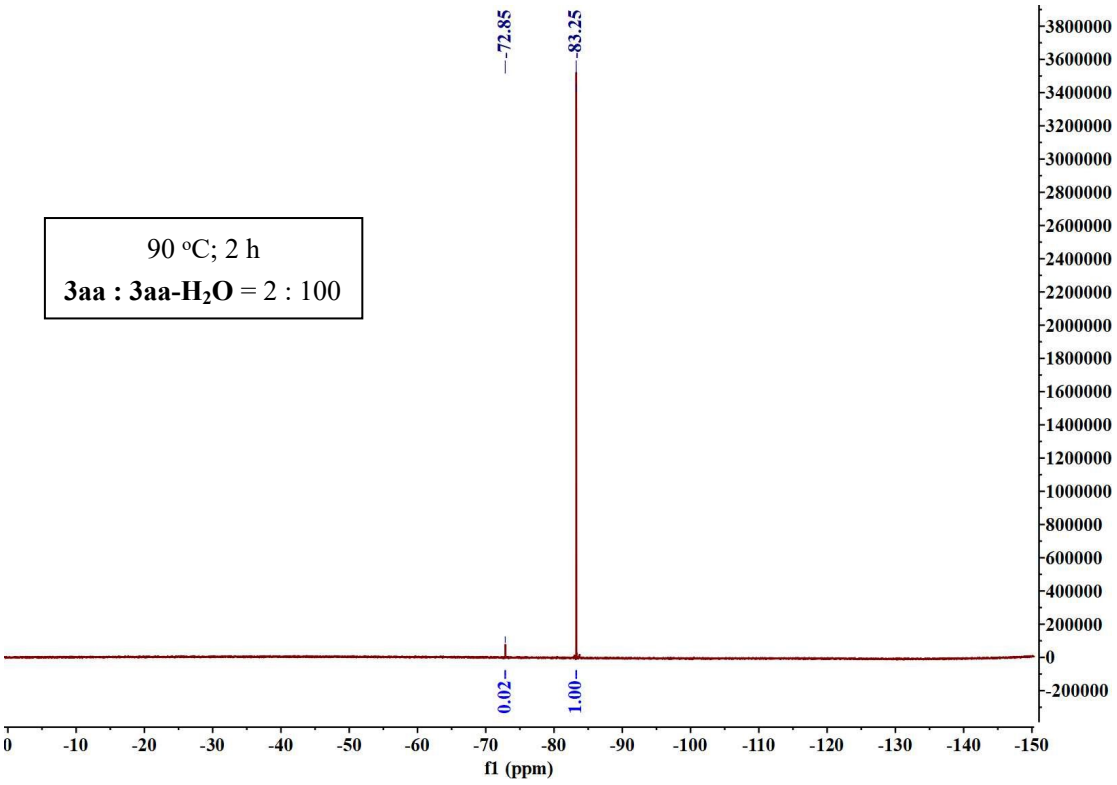
3. Heating tests of deprotection products

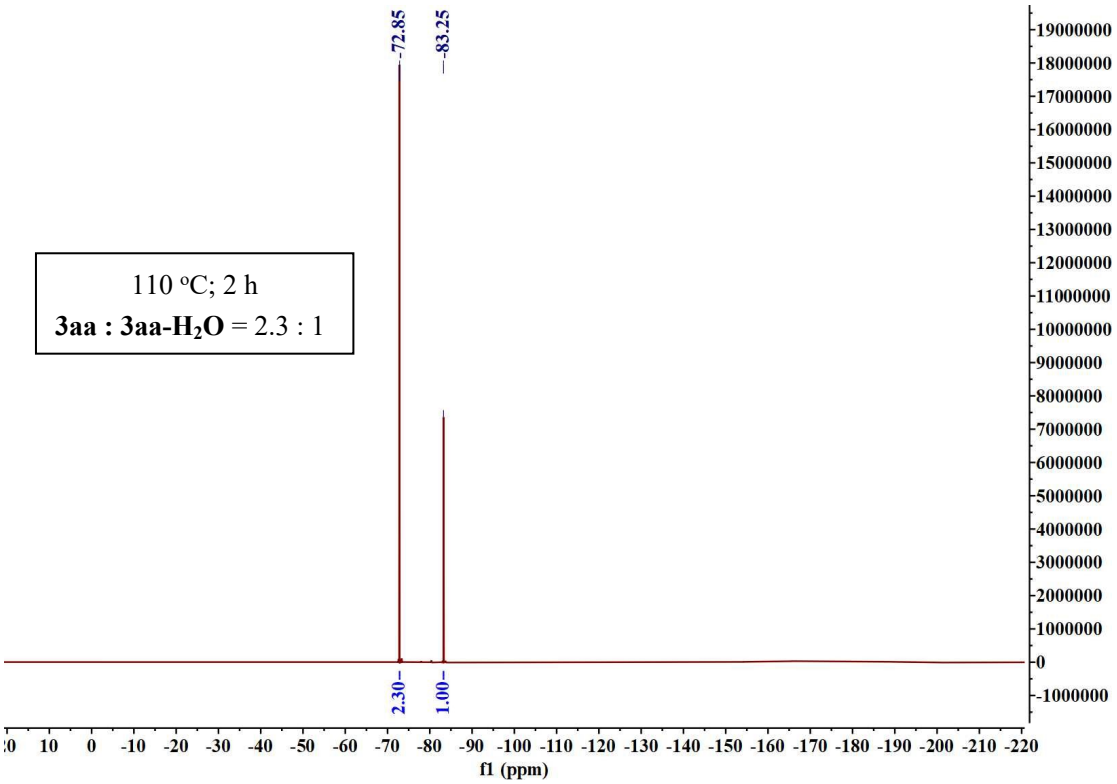
We discovered that heating can accelerate trifluoroacetyl hydrate's dehydration. Following a series of heating tests.

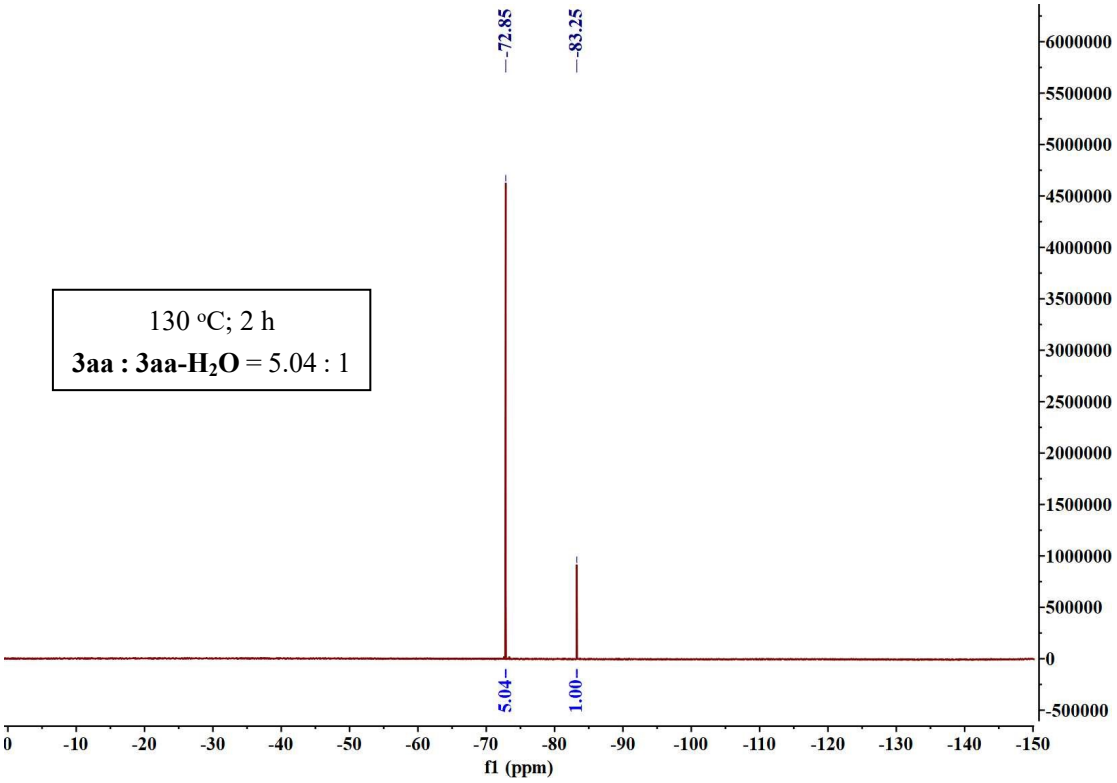


Temperature/°C	Time/h	**3aa：3aa-H_2O**
r.t. - 70	2	1：100
90	2	2：100
110	2	2.3：1
130	2	5.04：1

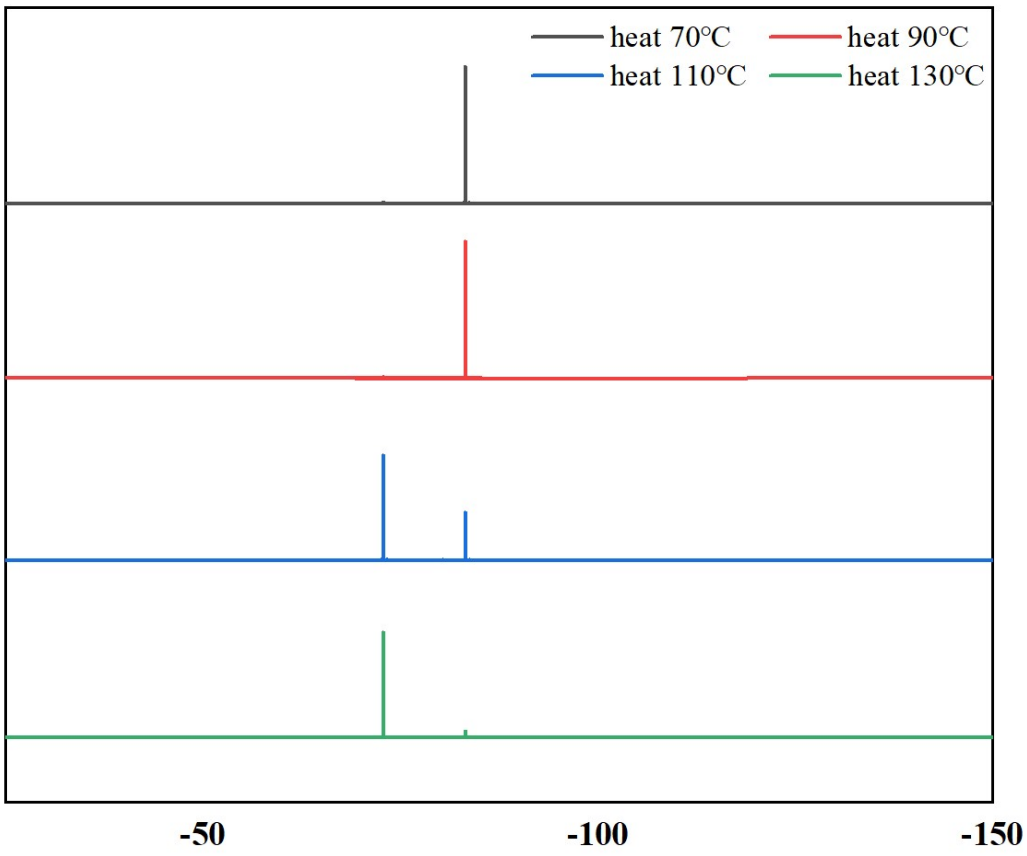

-72.85
-83.25
r.t. - 70 °C; 2 h
3aa : 3aa-H2O = 1 : 100
0.01
1.00
f1 (ppm)

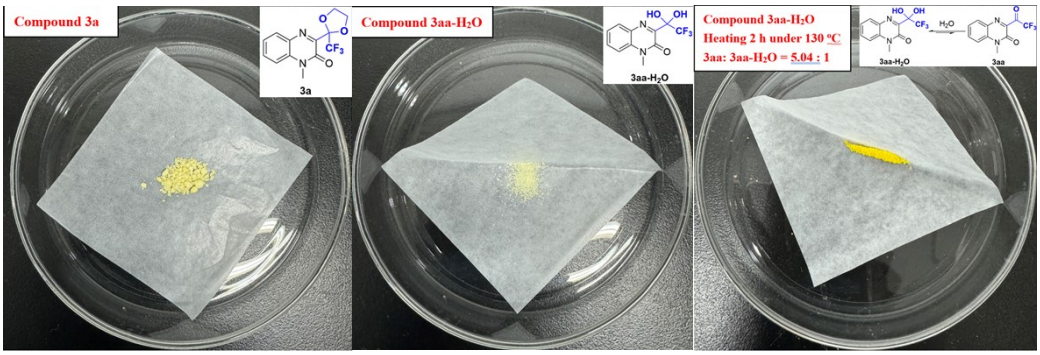

-72.85
-83.25
90 °C; 2 h
3aa : 3aa-H2O = 2 : 100
0.02
1.00
f1 (ppm)


110 °C; 2 h
3aa : 3aa-H2O = 2.3 : 1
-72.85
-83.25
2.30
1.00
f1 (ppm)

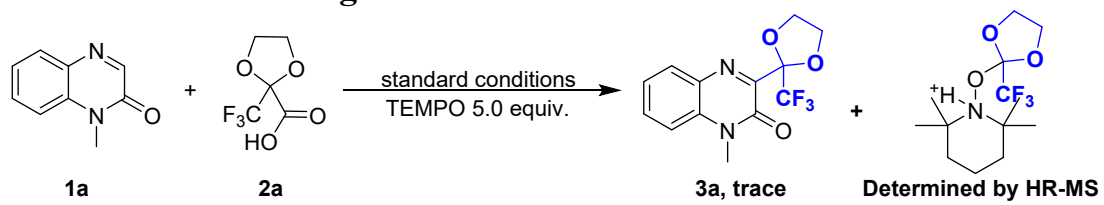

130 °C; 2 h
3aa : 3aa-H2O = 5.04 : 1
-72.85
-83.25
5.04
1.00
f1 (ppm)

^{19}F NMR of the product after heating dehydration

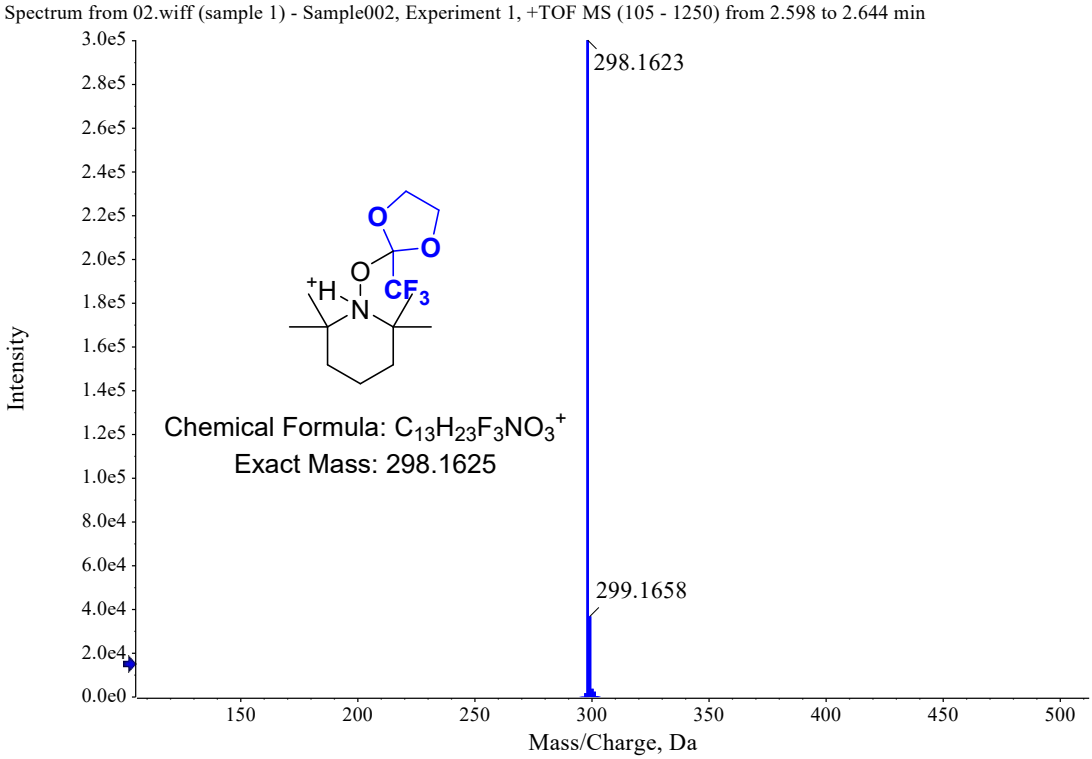


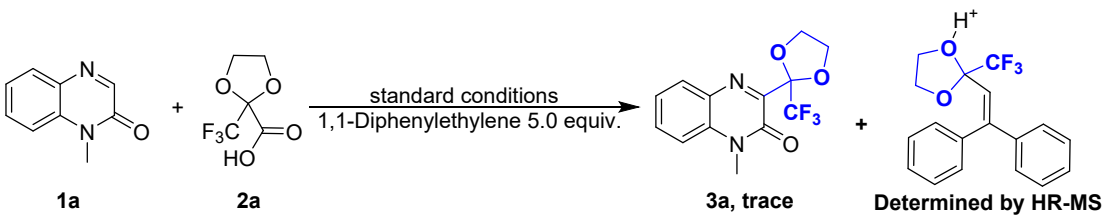


4.Mechanistic Investigation



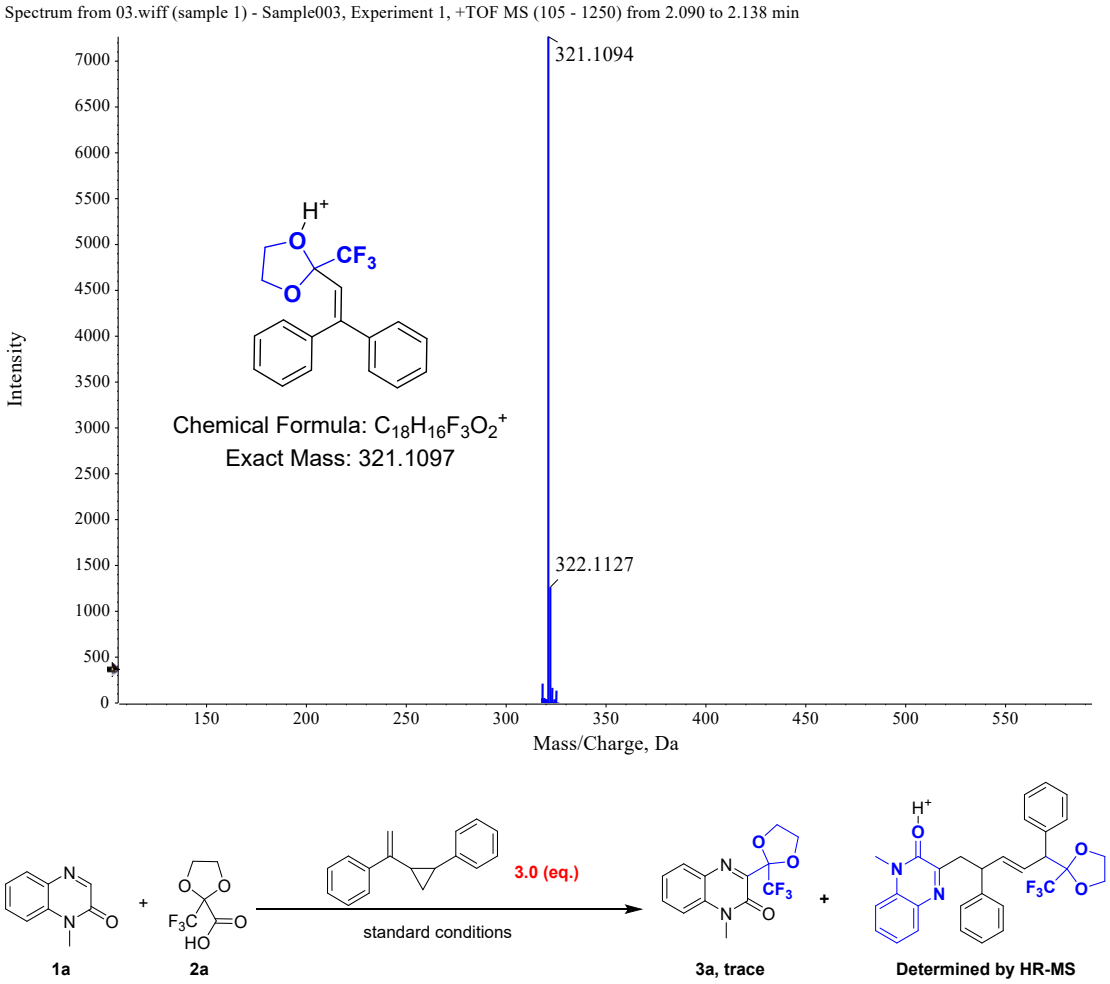
To an oven dried 10.0 mL screw capped tube equipped with a magnetic stir bar, quinoxalin-2(1*H*)-one **1a** (0.2 mmol, 1.0 equiv), $(NH_4)_2S_2O_8$ (0.6 mmol, 3 eq.), TEMPO (1.0 mmol, 5.0 equiv), DMSO (0.1 M) and compound **2a** (0.5 mmol, 2.5 equiv) were placed under N_2. The resulting solution was stirred at room temperature (preheated oil bath) for 24 h (actual reaction time is mentioned in the specific reaction). Progress of the reaction was monitored by TLC analysis. After running the reaction for an appropriate time (actual time is mentioned in the specific reaction), the crude product was detected by HR-MS.



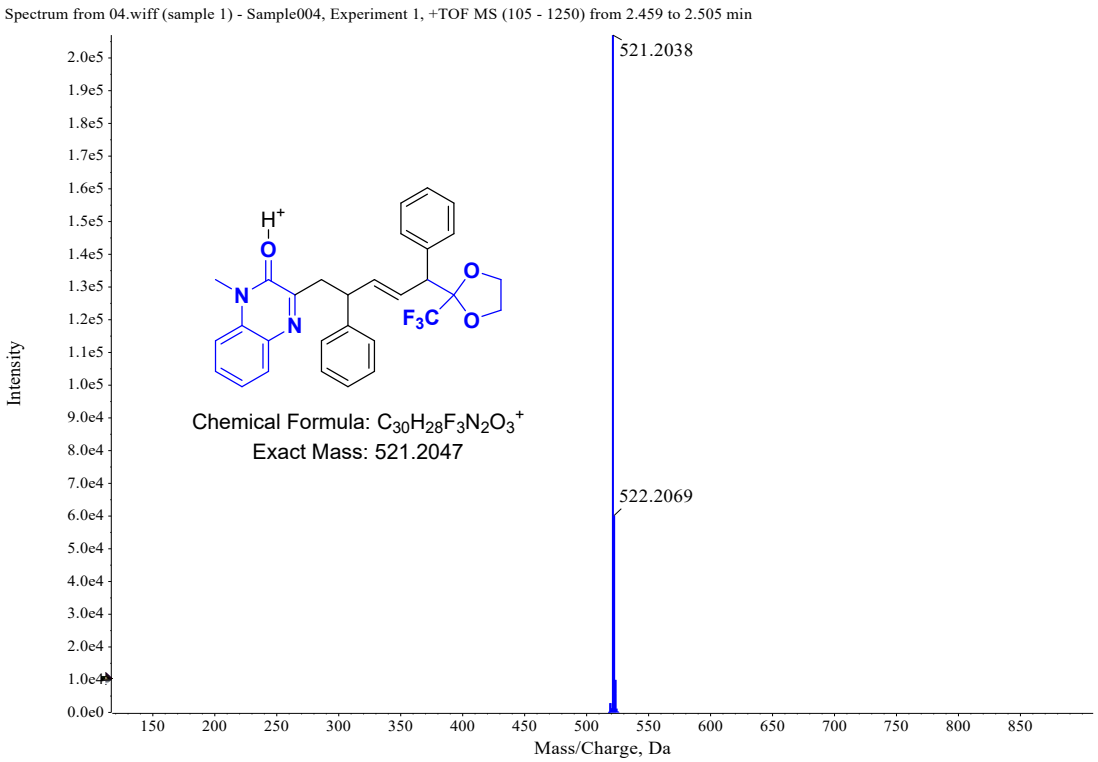


To an oven dried 10.0 mL screw capped tube equipped with a magnetic stir bar, quinoxalin-2(1*H*)-one **1a** (0.2 mmol, 1.0 equiv), $(NH_4)_2S_2O_8$ (0.6 mmol, 3 eq.), 1,1-diphenylethylene (1.0 mmol, 5.0 equiv), DMSO (0.1 M) and compound **2a** (0.5 mmol, 2.5 equiv) were placed under N_2.

The resulting solution was stirred at room temperature (preheated oil bath) for 24 h (actual reaction time is mentioned in the specific reaction). Progress of the reaction was monitored by TLC analysis. After running the reaction for an appropriate time (actual time is mentioned in the specific reaction), the crude product was detected by HR-MS.

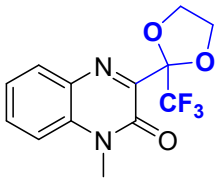


Following the procedure of reported literature.[5] To an oven dried 10.0 mL screw capped tube equipped with a magnetic stir bar, quinoxalin-2(1*H*)-one **1a** (0.2 mmol, 1.0 equiv), $(NH_4)_2S_2O_8$ (0.6 mmol, 3 eq.), (1-((1S,2R)-2-phenylcyclopropyl)vinyl)benzene (0.6 mmol, 3.0 equiv), DMSO (0.1 M) and compound **2a** (0.5 mmol, 2.5 equiv) were placed under N_2. The resulting solution was stirred at room temperature (preheated oil bath) for 24 h (actual reaction time is mentioned in the specific reaction). Progress of the reaction was monitored by TLC analysis. After running the reaction for an appropriate time (actual time is mentioned in the specific reaction), the crude product was detected by HR-MS.



5. Characterization data of products

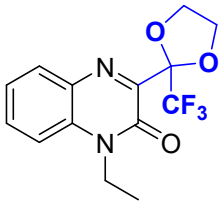
1-methyl-3-(2-(trifluoromethyl)-1,3-dioxolan-2-yl)quinoxalin-2(1*H*)-one (3a)



3a 81%

Yellow solid, *m.p.*:134.2-136.0 ℃ (48.6 mg, 81% yield). TLC (R_f = 0.2, PET/EA = 3:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.88 (d, *J* = 10.0 Hz, 1H), 7.58 (t, *J* = 5.0 Hz, 1H), 7.33 (t, *J* = 5.0 Hz, 1H), 7.27 (d, *J* = 10.0 Hz, 1H), 4.55 (t, *J* = 5.0 Hz, 2H), 4.38 (t, *J* = 5.0 Hz, 2H), 3.65 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 152.3, 149.4, 133.8, 132.1, 131.2, 130.9, 123.8, 122.9 (q, *J* = 291.1 Hz), 113.6, 105.3 (q, *J* = 30.4 Hz), 68.8, 28.8. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -77.90. **HRMS (ESI):** [M+H$^+$] Calcd for $C_{13}H_{12}F_3N_2O_3^+$: 301.0795, Found: 301.0796.

1-ethyl-3-(2-(trifluoromethyl)-1,3-dioxolan-2-yl)quinoxalin-2(1*H*)-one (3b)

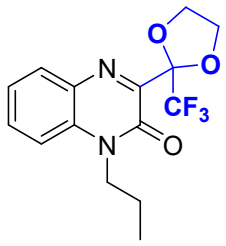


3b, 87%

Yellow solid, *m.p.*:136.7-143.1 ℃ (54.7 mg, 87% yield). TLC (R_f = 0.2, PET/EA = 3:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.85 (d, *J* = 5.0 Hz, 1H), 7.55 (t, *J* = 5.0 Hz, 1H), 7.33-7.24 (m, 2H), 4.55 (t, *J* = 5.0 Hz, 2H), 4.36 (t, *J* = 5.0 Hz, 2H), 4.24 (q, *J* = 10.0 Hz, 2H), 1.33 (t, *J* = 5.0 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 151.9, 149.4, 132.9, 132.1, 131.6, 131.3, 123.7, 123.0 (q, *J* = 291.1 Hz), 113.5, 105.3 (q, *J* = 31.2 Hz), 68.8, 37.4, 12.3. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -77.81. **HRMS (ESI):** [M+H$^+$] Calcd for $C_{14}H_{14}F_3N_2O_3^+$: 315.0951, Found:

315.0949.

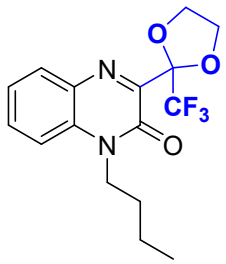
1-propyl-3-(2-(trifluoromethyl)-1,3-dioxolan-2-yl)quinoxalin-2(1*H*)-one (3c)



3c, 81%

Yellow solid, *m.p.*:138.5-143.6 ℃ (53.2 mg, 81% yield). TLC (R_f = 0.2, PET/EA = 3:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.89 (d, *J* = 10.0 Hz, 1H), 7.58 (t, *J* = 5.0 Hz, 1H), 7.31 (t, *J* = 5.0 Hz, 1H), 7.27 (d, *J* = 10.0 Hz, 1H), 4.57 (t, *J* = 5.0 Hz, 2H), 4.38 (t, *J* = 5.0 Hz, 2H), 4.19-4.12 (m, 2H), 1.82-1.71 (m, 2H), 1.05 (t, *J* = 5.0 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 152.1, 149.5, 133.3, 132.0, 131.7, 131.3, 123.7, 123.0 (q, *J* = 291.1 Hz), 105.4 (q, *J* = 30.4 Hz), 68.8, 43.9, 20.6, 11.4. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -77.83. **HRMS (ESI):** [M+H$^+$] Calcd for $C_{15}H_{16}F_3N_2O_3^+$: 329.1108, Found: 329.1105.

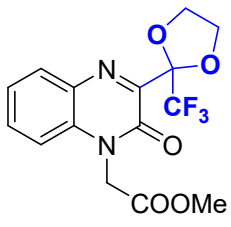
1-butyl-3-(2-(trifluoromethyl)-1,3-dioxolan-2-yl)quinoxalin-2(1*H*)-one (3d)



3d, 75%

Yellow solid, *m.p.*:184.3-186.1 ℃ (51.3 mg, 75% yield). TLC (R_f = 0.2, PET/EA = 3:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.88 (d, *J* = 10.0 Hz, 1H), 7.57 (t, *J* = 5.0 Hz, 1H), 7.31 (t, *J* = 5.0 Hz, 1H), 7.27 (d, *J* = 10.0 Hz, 1H), 4.56 (t, *J* = 5.0 Hz, 2H), 4.37 (t, *J* = 5.0 Hz, 2H), 4.18 (t, *J* = 10.0 Hz, 2H), 1.75-1.66 (m, 2H), 1.52-1.43 (m, 2H), 0.98 (t, *J* = 5.0 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 152.1, 149.5, 133.3, 132.0, 131.7, 131.3, 123.7, 123.0 (q, *J* = 291.1 Hz), 105.4 (q, *J* = 30.4 Hz), 68.8, 43.9, 20.6, 11.4. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -77.83. **HRMS (ESI):** [M+H$^+$] Calcd for $C_{15}H_{16}F_3N_2O_3^+$: 329.1108, Found: 329.1105.

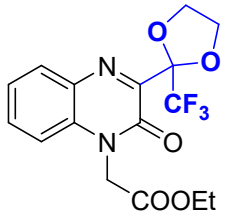
Methyl-2-(2-oxo-3-(2-(trifluoromethyl)-1,3-dioxolan-2-yl)quinoxalin-1(2*H*)-yl)acetate (3e)



3e, 62%

Yellow solid, *m.p.*:152.2-154.0 ℃ (44.4 mg, 62% yield). TLC (R_f = 0.2, PET/EA = 3:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.92 (d, *J* = 5.0 Hz, 1H), 7.57 (t, *J* = 10.0 Hz, 1H), 7.35 (t, *J* = 5.0 Hz, 1H), 7.05 (d, *J* = 5.0 Hz, 1H), 5.00 (s, 2H), 4.53 (t, *J* = 5.0 Hz, 2H), 4.37 (t, *J* = 5.0 Hz, 2H), 3.76 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 167.5, 152.0, 149.5, 133.2, 132.4, 131.8, 131.2, 124.3, 122.9 (q, *J* = 291.1 Hz), 113.2, 105.2 (q, *J* = 30.4 Hz), 68.8, 53.1, 43.3. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -77.90. **HRMS (ESI):** [M+H$^+$] Calcd for $C_{15}H_{16}F_3N_2O_3^+$: 359.0846, Found: 359.0849.

Ethyl-2-(2-oxo-3-(2-(trifluoromethyl)-1,3-dioxolan-2-yl)quinoxalin-1(2*H*)-yl)acetate (3f)

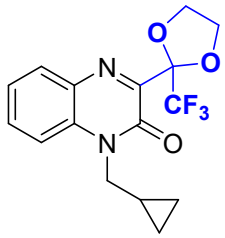


3f, 60%

Yellow solid, *m.p.*:161.7-163.0 ℃ (44.7 mg, 60% yield). TLC (R_f = 0.2, PET/EA = 3:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.93 (d, *J* = 10.0 Hz, 1H),

7.57 (t, *J* = 10.0 Hz, 1H), 7.35 (t, *J* = 5.0 Hz, 1H), 7.06 (d, *J* = 5.0 Hz, 1H), 4.99 (s, 2H), 4.53 (t, *J* = 5.0 Hz, 2H), 4.37 (t, *J* = 5.0 Hz, 2H), 4.24 (q, *J* = 5.0 Hz, 2H), 1.26 (t, *J* = 5.0 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 166.84, 151.87, 149.37, 133.15, 132.24, 131.58, 131.02, 124.13, 122.88 (q, *J* = 291.1 Hz), 113.18, 105.14 (q, *J* = 30.4 Hz), 68.74, 62.17, 43.31, 14.06. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -77.92. **HRMS (ESI):** [M+H$^+$] Calcd for $C_{15}H_{14}F_3N_2O_3^+$: 373.1006, Found: 373.1005.

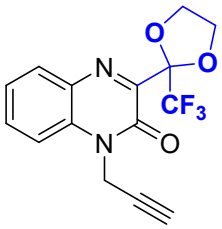
1-(cyclopropylmethyl)-3-(2-(trifluoromethyl)-1,3-dioxolan-2-yl)quinoxalin-2(1*H*)-one (3g)



3g, 90%

Yellow solid, *m.p.*:133.2-135.9 ℃ (61.3 mg, 90% yield). TLC (R_f = 0.2, PET/EA = 3:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.86 (d, *J* = 10.0 Hz, 1H), 7.56 (t, *J* = 5.0 Hz, 1H), 7.37 (d, *J* = 5.0 Hz, 1H), 7.28 (t, *J* = 5.0 Hz, 1H), 4.54 (t, *J* = 5.0 Hz, 2H), 4.36 (t, *J* = 5.0 Hz, 2H), 4.13 (d, *J* = 10.0 Hz, 2H), 0.52 (d, *J* = 10.0 Hz, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 152.3, 149.6, 133.4, 131.9, 131.5, 131.2, 123.6, 123.0 (q, *J* = 291.1 Hz), 113.9, 105.4 (q, *J* = 30.4 Hz), 68.8, 46.0, 9.6, 4.2. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -77.84. **HRMS (ESI):** [M+H$^+$] Calcd for $C_{15}H_{14}F_3N_2O_3^+$: 341.1108, Found: 373.1106.

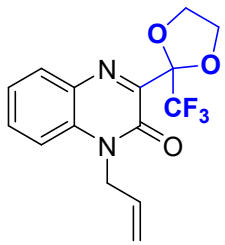
1-(prop-2-yn-1-yl)-3-(2-(trifluoromethyl)-1,3-dioxolan-2-yl)quinoxalin-2(1*H*)-one (3h)



3h, 71%

Yellow solid, *m.p.*:184.8-186.6 ℃ (46.0 mg, 71% yield). TLC (R_f = 0.2, PET/EA = 3:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.94 (d, *J* = 5.0 Hz, 1H), 7.66 (t, *J* = 5.0 Hz, 1H), 7.47 (d, *J* = 5.0 Hz, 1H), 7.40 (t, *J* = 5.0 Hz, 1H), 5.03 (d, *J* = 5.0 Hz, 2H), 4.58 (t, *J* = 5.0 Hz, 2H), 4.39 (t, *J* = 5.0 Hz, 2H), 2.30 (t, *J* = 5.0 Hz, 1H). **^{13}C NMR** (126 MHz, DMSO-D_6) δ 150.6, 149.0, 132.6, 132.3, 130.5, 130.2, 124.3, 122.8 (q, *J* = 291.1 Hz), 115.2, 104.6 (q, *J* = 30.4 Hz), 77.7, 75.4, 68.8, 31.3. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -77.91. **HRMS (ESI):** [M+H$^+$] Calcd for $C_{15}H_{12}F_3N_2O_3^+$: 325.0795, Found: 325.0793.

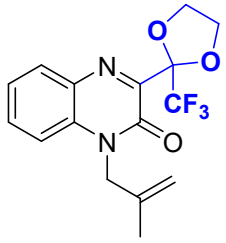
1-allyl-3-(2-(trifluoromethyl)-1,3-dioxolan-2-yl)quinoxalin-2(1*H*)-one (3i)



3i, 75%

Yellow solid, *m.p.*:145.3-147.3 ℃ (46.0 mg, 71% yield). TLC (R_f = 0.2, PET/EA = 3:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.94 (d, *J* = 5.0 Hz, 1H), 7.58 (t, *J* = 5.0 Hz, 1H), 7.35 (t, *J* = 5.0 Hz, 1H), 7.28 (d, *J* = 5.0 Hz, 1H), 5.98-5.88 (m, 1H), 5.28 (d, *J* = 10.0 Hz, 1H), 5.17 (d, *J* = 15.0 Hz, 1H), 4.91-4.87 (m, 2H), 4.58 (t, *J* = 5.0 Hz, 2H), 4.39 (t, *J* = 5.0 Hz, 2H). **^{13}C NMR** δ 152.0, 149.6, 133.3, 132.1, 131.5, 131.2, 130.4, 123.9, 123.0 (q, J = 291.1 Hz), 118.4, 114.3, 105.3 (q, J = 30.4 Hz), 68.9, 44.53. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -77.82. **HRMS (ESI):** [M+H$^+$] Calcd for $C_{15}H_{14}F_3N_2O_3^+$: 327.0951, Found: 327.0949.

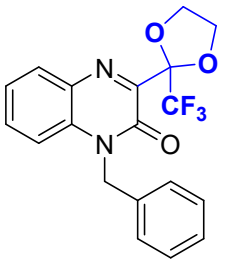
1-(2-methylallyl)-3-(2-(trifluoromethyl)-1,3-dioxolan-2-yl)quinoxalin-2(1*H*)-one (3j)



3j, 61%

Yellow solid, *m.p.*:121.5-123.7 ℃ (41.5 mg, 61% yield). TLC (R_f = 0.2, PET/EA = 3:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.91 (d, *J* = 5.0 Hz, 1H), 7.54 (t, *J* = 5.0 Hz, 1H), 7.33 (t, *J* = 5.0 Hz, 1H), 7.18 (d, *J* = 10.0 Hz, 1H), 4.91 (s, 1H), 4.76 (s, 2H), 4.57 (t, *J* = 5.0 Hz, 2H), 4.54 (s, 1H), 4.38 (t, *J* = 5.0 Hz, 2H), 1.83 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 152.0, 149.6, 137.7, 133.5, 132.0, 131.4, 131.2, 124.0, 123.0 (q, *J* = 291.1 Hz), 114.6, 111.9, 105.2(q, *J* = 30.4 Hz),, 68.9, 47.6, 20.3. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -77.82. **HRMS (ESI):** [M+H$^+$] Calcd for $C_{16}H_{16}F_3N_2O_3^+$: 341.1108, Found: 341.1106.

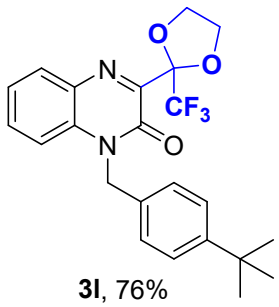
1-benzyl-3-(2-(trifluoromethyl)-1,3-dioxolan-2-yl)quinoxalin-2(1*H*)-one (3k)



3k, 84%

Yellow solid, *m.p.*:133.9-136.8 ℃ (63.2 mg, 84% yield). TLC (R_f = 0.2, PET/EA = 3:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.92 (d, *J* = 10.0 Hz, 1H), 7.46 (t, *J* = 10.0 Hz, 1H), 7.33-7.25 (m, 4H), 7.23-7.19 (m, 3H), 5.47 (s, 2H), 4.63-4.60 (t, *J* = 5.0 Hz, 2H), 4.42-4.39 (t, *J* = 5.0 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 152.4, 149.7, 134.9, 133.4, 132.1, 131.5, 131.3, 129.0, 127.8, 126.7, 123.9, 123.0 (q, *J* = 291.1 Hz), 105.4 (q, *J* = 30.4 Hz), 68.9, 45.8. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -77.73. **HRMS (ESI):** [M+H$^+$] Calcd for $C_{19}H_{16}F_3N_2O_3^+$: 377.1108, Found: 377.1105.

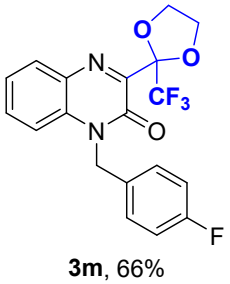
1-(4-(tert-butyl)benzyl)-3-(2-(trifluoromethyl)-1,3-dioxolan-2-yl)quinoxalin-2(1*H*)-one (3l)



3l, 76%

Yellow solid, *m.p.*:169.2-171.9 ℃ (65.7 mg, 76% yield). TLC (R_f = 0.2, PET/EA = 3:1). **^{1}H NMR** (500 MHz, $CDCl_3$). δ 7.94 (d, J = 5.0 Hz, 1H), 7.50 (t, *J* = 5.0 Hz, 1H), 7.34-7.28 (m, 4H), 7.15 (d, *J* = 10.0 Hz, 2H), 5.45 (s, 2H), 4.59 (t, *J* = 5.0 Hz, 2H), 4.40 (t, *J* = 5.0 Hz, 2H), 1.27 (s, 9H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 152.5, 150.8, 149. 8, 133.6, 132.1, 131.8, 131.6, 131.4, 126.6, 126.0, 123.9, 121.9 (q *J* = 291.1 Hz,), 114.6, 105.4 (q, *J* = 30.4 Hz), 68.9, 45.6, 34.6, 31.4. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -77.84. **HRMS (ESI):** [M+H$^+$] Calcd for $C_{23}H_{24}F_3N_2O_3^+$: 433.1734, Found: 433.1732.

1-(4-fluorobenzyl)-3-(2-(trifluoromethyl)-1,3-dioxolan-2-yl)quinoxalin-2(1*H*)-one (3m)

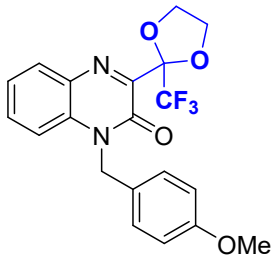


3m, 66%

Yellow solid, *m.p.*:124.3-126.7 ℃ (52.1 mg, 66% yield). TLC (R_f = 0.2, PET/EA = 3:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.89 (d, *J* = 5.0 Hz, 1H), 7.47 (t, *J* = 5.0 Hz, 1H), 7.29 (t, *J* = 10.0 Hz, 1H), 7.22-7.16 (m, 3H), 6.98 (t, *J* = 10.0 Hz, 2H), 5.41 (s, 2H), 4.58 (t, *J* = 5.0 Hz, 2H), 4.39 (t, *J* = 5.0 Hz, 2H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 152.5, 150.8, 149. 8, 133.6, 132.1, 131.8, 131.6,

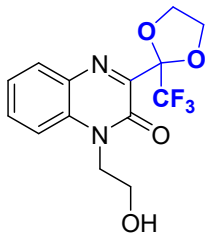
131.4, 126.6, 126.0, 123.9, 121.9 (q, J = 291.1 Hz,), 114.6, 105.4 (q, J = 30.4 Hz), 68.9, 45.6, 34.6, 31.4. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -77.77, -114.12. **HRMS (ESI):** [M+H$^+$] Calcd for $C_{23}H_{24}F_3N_2O_3^+$: 395.1013, Found: 395.1010.

1-(4-methoxybenzyl)-3-(2-(trifluoromethyl)-1,3-dioxolan-2-yl)quinoxalin-2(1*H*)-one (3n)



3n,61%

Yellow solid, *m.p.*:186.4-188.9 ℃ (49.6 mg, 61% yield). TLC (R_f = 0.2, PET/EA = 3:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.92 (d, J = 10.0 Hz, 1H), 7.49 (t, J = 5.0 Hz, 1H), 7.31 (t, J = 5.0 Hz, 1H), 7.27 (d, J = 10.0 Hz, 1H), 7.17 (d, J = 5.0 Hz, 2H), 6.84 (d, J = 10.0 Hz, 2H), 5.41 (s, 2H), 4.60 (t, J = 5.0 Hz, 2H), 4.41 (t, J = 5.0 Hz, 2H), 3.76 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 159.2, 152.5, 149.7, 133.4, 132.1, 131.6, 131.4, 128.3, 127.0, 123.9, 123.1 (q, J = 291.1 Hz), 114.5, 114.5, 105.4 (q J = 30.4 Hz,), 68.9, 55.3, 45.3. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -77.81. **HRMS (ESI):** [M+H$^+$] Calcd for $C_{20}H_{18}F_3N_2O_3^+$: 407.1213, Found: 407.1213.

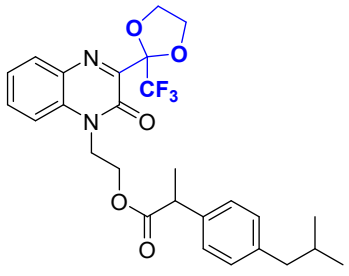


3o, 55%

1-(2-hydroxyethyl)-3-(2-(trifluoromethyl)-1,3-dioxolan-2-yl)quinoxalin-2(1*H*)-one (3o)

Yellow solid, *m.p.*:151.7-154.0 ℃ (36.3 mg, 55% yield). TLC (R_f = 0.2, PET/EA = 3:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.95 (d, J = 10.0 Hz, 1H), 7.62 (t, J = 10.0 Hz, 1H), 7.46 (d, J = 10.0 Hz, 1H), 7.38 (t, J = 5.0 Hz, 1H), 4.54 (t, J = 5.0 Hz, 2H), 4.48 (t, J = 5.0 Hz, 2H), 4.39 (t, J = 5.0 Hz, 2H), 4.05 (t, J = 5.0 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 153.1, 149.2, 133.6, 132.2, 131.6, 131.4, 124.1, 122.9 (q, J = 291.1 Hz), 114.1, 105.2 (q, J = 30.4 Hz), 68.7, 60.1, 44.8. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -77.91. **HRMS (ESI):** [M+H$^+$] Calcd for $C_{14}H_{14}F_3N_2O_3^+$: 331.0900, Found: 331.0900.

2-(2-oxo-3-(2-(trifluoromethyl)-1,3-dioxolan-2-yl)quinoxalin-1(2*H*)-yl)ethyl 2-(4-isobutylphenyl)propanoate (3p)

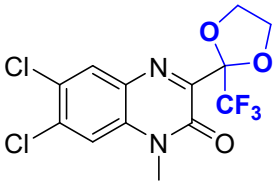


3p, 65%

Yellow solid, *m.p.*:105.7-107.2 ℃ (67.4 mg, 65% yield). TLC (R_f = 0.2, PET/EA = 3:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.90 (d, J = 5.0 Hz, 1H), 7.52 (d, J = 5.0 Hz, 1H), 7.34 (m, 2H), 7.09 (d, J = 10.0 Hz, 2H), 7.04 (d, J = 5.0 Hz, 2H), 4.58-4.49 (m, 3H), 4.44-4.36 (m, 5H), 3.59 (q, J = 10.0 Hz, 1H), 2.43 (d, J = 10.0 Hz, 2H), 1.90-1.78 (m, 1H), 1.43 (d, J = 10.0 Hz, 3H), 0.89 (d, J = 5.0 Hz, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 174.8, 152.2, 149.4, 140.8, 137.2, 133.6, 132.2, 131.7, 131.2, 129.5, 127.2, 124.0, 123.0 (q, J = 291.1 Hz), 113.9, 105.3 (q, J = 30.4 Hz), 68.9, 61.0, 45.1,45.0, 40.9, 30.2, 22.5, 18.4. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -77.86. **HRMS (ESI):** [M+H$^+$] Calcd for

$C_{27}H_{30}F_3N_2O_3^+$: 519.2101, Found: 519.2100.

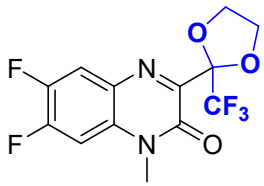
6,7-dichloro-1-methyl-3-(2-(trifluoromethyl)-1,3-dioxolan-2-yl)quinoxalin-2(1*H*)-one (3q)



3q, 57%

Yellow solid, *m.p.*:241.4-243.6 ℃ (42.1 mg, 57% yield). TLC (R_f = 0.2, PET/EA = 3:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.42 (s, 1H), 4.55 (t, *J* = 5.0 Hz, 2H), 4.39 (t, *J* = 5.0 Hz, 2H), 3.64 (s, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 151.8, 151.0, 136.5, 133.4, 132.2, 130.0, 128.0, 122.8 (q, *J* = 291.1 Hz), 115.3, 105.1 (q, *J* = 30.4 Hz,), 69.0, 29.3. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -78.02. **HRMS (ESI):** [M+H$^+$] Calcd for $C_{13}H_{10}Cl_2F_3N_2O_3^+$: 369.0015, Found: 369.0006.

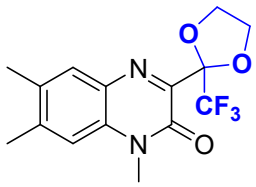
6,7-difluoro-1-methyl-3-(2-(trifluoromethyl)-1,3-dioxolan-2-yl)quinoxalin-2(1*H*)-one (3r)



3r, 63%

Orange solid, *m.p.*:188.3-190.7 ℃ (42.4 mg, 63% yield). TLC (R_f = 0.2, PET/EA = 3:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.73 (t, *J* = 5.0 Hz, 1H), 7.10 (q, *J* = 5.0 Hz, 1H), 4.54 (t, *J* = 5.0 Hz, 2H), 4.37 (t, *J* = 5.0 Hz, 2H), 3.62 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 153.8 (d, *J* = 13.7 Hz), 151.9, 151.7(d, *J* = 15.0 Hz), 150.1 (d, *J* = 3.7 Hz), 147.9 (d, *J* = 13.7 Hz), 146.0 (d, *J* = 13.7 Hz), 131.6 (d, *J* = 8.7 Hz), 127.3 (d, *J* = 10.0 Hz), 124.0, 121.7, 119.0 (d, *J* = 17.5 Hz), 105.2 (q, *J* = 30.4 Hz), 102.4 (d, *J* = 22.5 Hz), 68.9, 29.5. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -78.04, -127.08, -141.08. **HRMS (ESI):** [M+H$^+$] Calcd for $C_{13}H_{10}F_5N_2O_3^+$: 337.0606, Found: 337.0600.

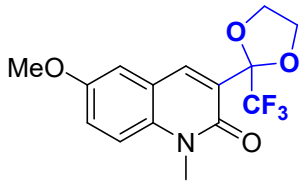
1,6,7-trimethyl-3-(2-(trifluoromethyl)-1,3-dioxolan-2-yl)quinoxalin-2(1*H*)-one (3s)



3s, 60%

Yellow solid, *m.p.*:173.0-175.2 ℃ (42.4 mg, 63% yield). TLC (R_f = 0.2, PET/EA = 3:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.62 (s, 1H), 7.02 (s, 1H), 4.56 (t, *J* = 5.0 Hz, 2H), 4.37 (t, *J* = 5.0 Hz, 1H), 4.21 (s, 1H), 3.61 (s, 3H), 2.39 (s, 3H), 2.30s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 152.6, 148.1, 142.5, 133.1, 132.0, 131.3, 129.6, 123.1 (q, *J* = 291.1 Hz), 114.1, 105.5 (q, *J* = 30.4 Hz), 68.8, 28.8, 20.8, 19.1. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -77.84. **HRMS (ESI):** [M+H$^+$] Calcd for $C_{15}H_{16}F_3N_2O_3^+$: 329.1108, Found: 329.1100.

6-methoxy-1-methyl-3-(2-(trifluoromethyl)-1,3-dioxolan-2-yl)quinolin-2(1*H*)-one (3t)

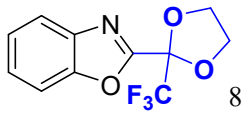


3t, 67%

White solid, m.p.:121.4-124.2 ℃ (44.1 mg, 67% yield). TLC (Rf = 0.2, PET/EA = 1:1).**^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.27 (s, 1H), 7.21 (d, *J* = 5.0 Hz, 1H), 7.20 (d, *J* = 5.0 Hz, 1H),7.04 (d, *J* = 5.0 Hz, 1H), 4.29 (t, *J* = 5.0 Hz, 2H), 4.19 (t, *J* = 5.0 Hz, 2H), 3.85 (s, 3H), 3.70 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 158.9, 154.8, 139.0, 135.4,

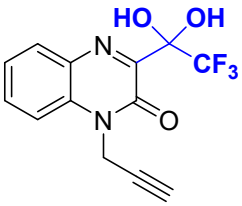
125.6, 123.0 (q, J = 291.1 Hz), 121.0, 119.7, 115.5, 111.0, 104.8 (q, J = 30.4 Hz), 67.1, 55.8, 29.8. **^{19}F NMR** (471 MHz, $CDCl_3$)δ -79.50. **HRMS (ESI):** [M+H$^+$] Calcd for $C_{15}H_{15}F_3NO_4^+$: 330.0945, Found: 330.0945.

2-(2-(trifluoromethyl)-1,3-dioxolan-2-yl)benzo[*d*]oxazole (3u)



White solid, m.p.:143.4-144.5 ℃ (124 mg, 48% yield，1 mmol reaction). TLC (Rf = 0.2, PET/EA = 4:1).**^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.82 (d, J = 8.0 Hz, 1H), 7.59 (d, J = 8.0 Hz, 1H), 7.46 -7.36 (m, 2H), 4.38 (s, 4H).**^{19}F NMR** (376 MHz, $CDCl_3$) δ -80.68.**^{13}C NMR** (101 MHz, $CDCl_3$) δ 157.91, 150.96, 140.16, 126.71, 125.26, 121.62 (q, J = 287.9 Hz), 121.35, 111.38, 100.99 (q, J = 34.8 Hz), 67.99. **HRMS (ESI)**: [M+H$^+$] Calcd for $C_{11}H_9F_3NO_3^+$: 260.0529, Found: 260.0528.

1-(prop-2-yn-1-yl)-3-(2,2,2-trifluoro-1,1-dihydroxyethyl)quinoxalin-2(1*H*)-one



3ha-H_2O, 60%

Yellow solid, m.p.:135.4-137.2 ℃ (35.8 mg, 60% yield). TLC (Rf = 0.2, PET/EA = 1:1).**^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.93 (d, J = 10.0 Hz, 1H), 7.65 (t, J = 5.0 Hz, 1H), 7.46 (d, J = 10.0 Hz, 1H), 7.39 (t, J = 5.0 Hz, 1H), 5.02 (d, J = 5.0 Hz, 2H), 4.58 (t, J = 5.0 Hz, 2H), 4.39 (t, J = 5.0 Hz, 2H), 2.30 (t, J = 5.0 Hz, 1H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 152.70, 150.69, 132.50, 131.72, 130.90, 130.49, 124.95, 122.89 (q J = 289.8 Hz), 115.47, 93.79 (q, J = 31.5 Hz), 77.58, 75.81, 31.64. **^{19}F NMR** (471 MHz, $CDCl_3$)δ -77.91. **HRMS (ESI):** [M+H$^+$] Calcd for $C_{15}H_{15}F_3NO_4^+$: 299.0638, Found: 299.0641.

6. Reference

(1) Y. Li, Z. Fu, Y. Shen, J. Zhu, K. Luo and L. Wu, *Asian J. Org. Chem.*, 2022, **11**, e202200453.

(2) X. Zhu, M. Jiang, X. Li, E. Zhu, Q. Deng, X. Song, J. Lv and D. Yang *Org. Chem. Front.*, 2022, **9**, 347-355.

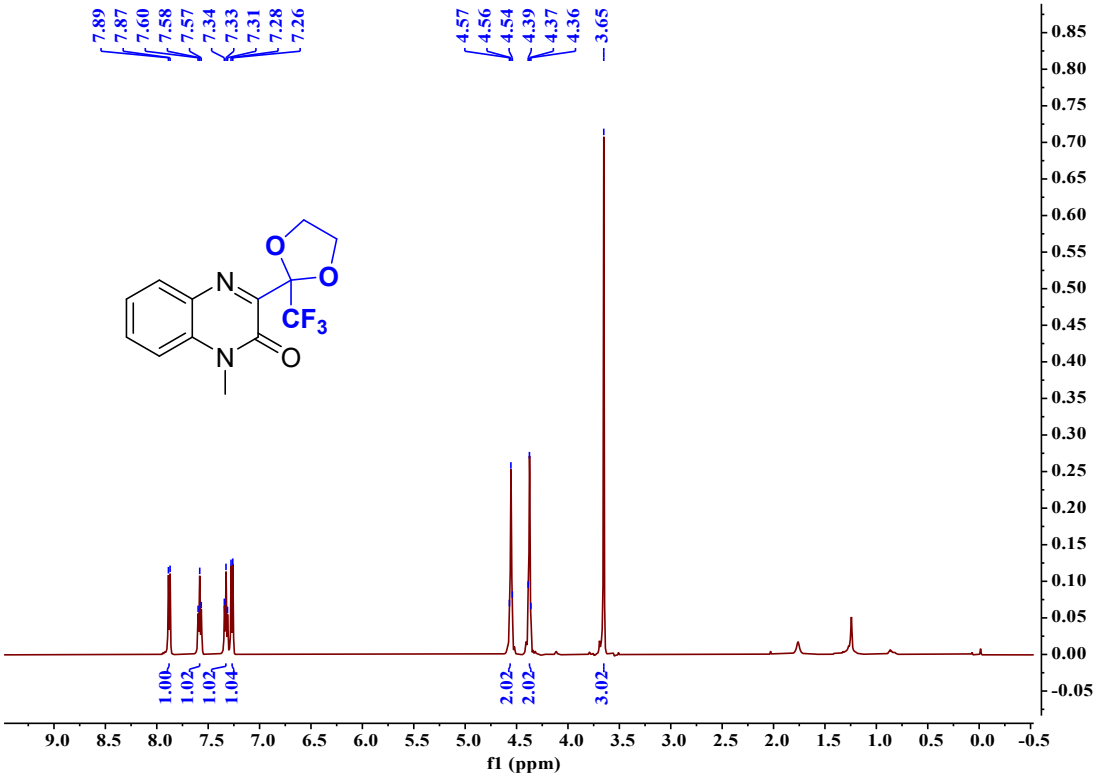
(3) S. Han, K. L. Samony, R. N. Nabi, C. A. Bache and D. K. Kim, *J. Am. Chem. Soc.*, 2023, **145**, 11530-11536.

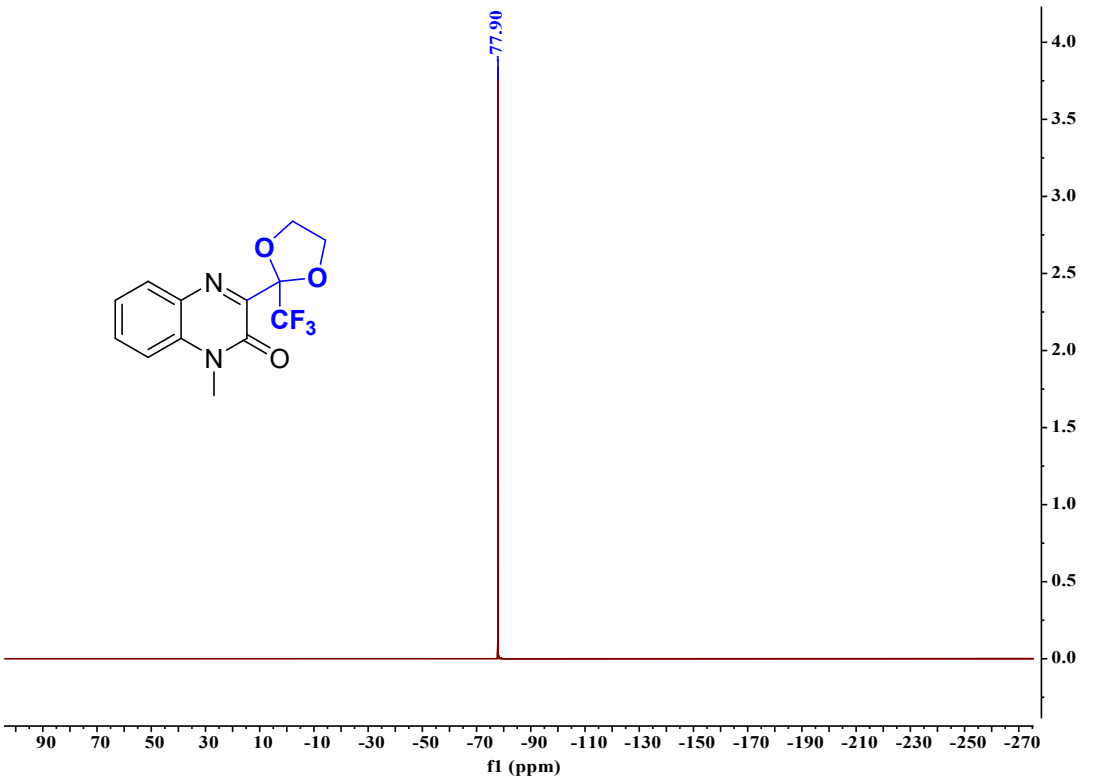
(4) C. Gong, A. Gao, Y. Zhang, M. Su, F. Chen, L. Sheng, Y. Zhou, J. Li, J. Li and F. Nan, *Eur. J. Med. Chem.* 2016, **112**, 81.

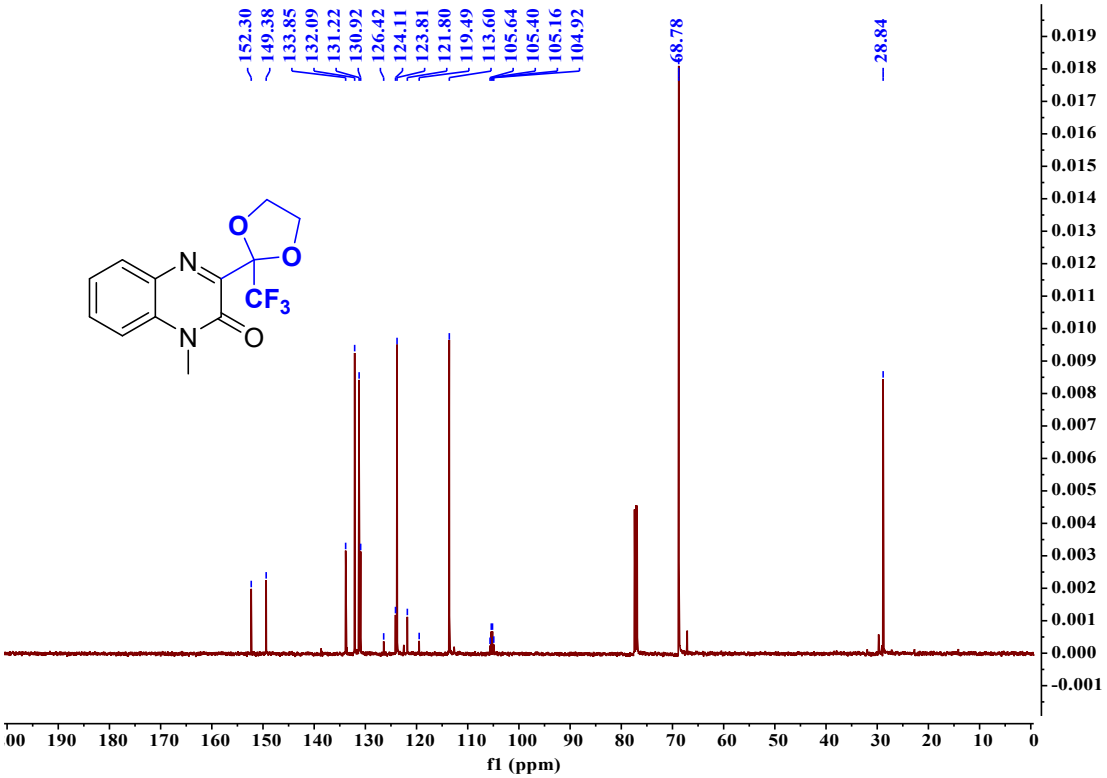
(5) S. Lu, Y. Gong and D. Zhou, *J. Org. Chem.*, 2015, **80**, 9336-9341.

7. ^{1}H-NMR, ^{13}C-NMR, ^{19}F-NMR and HRMS spectra

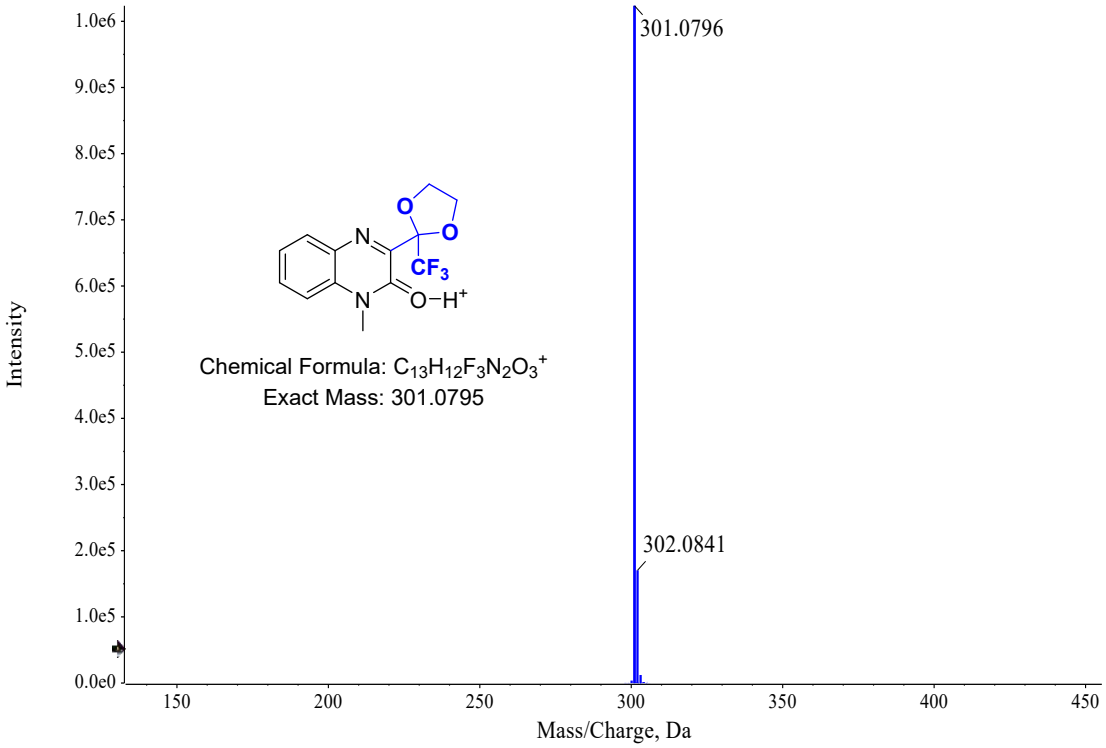
Compound 3a (^{1}H NMR, 500 Hz, $CDCl_3$; ^{19}F NMR 471 Hz, $CDCl_3$ ^{13}C NMR, 101 Hz, $CDCl_3$)



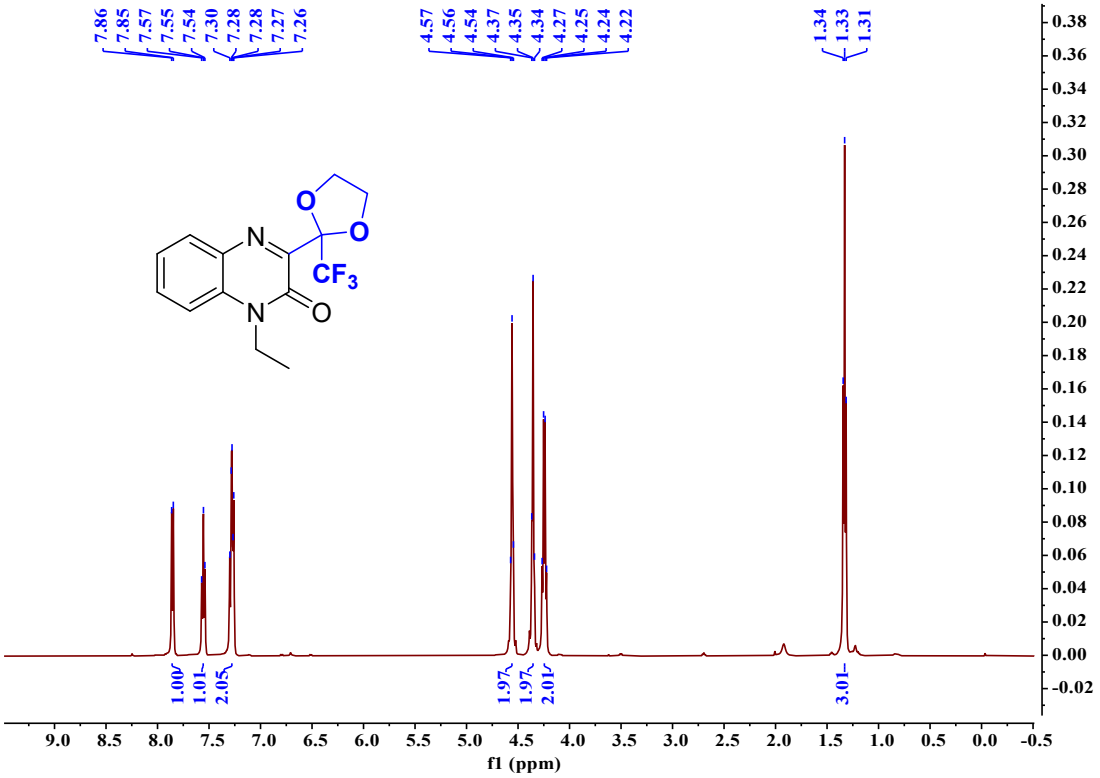


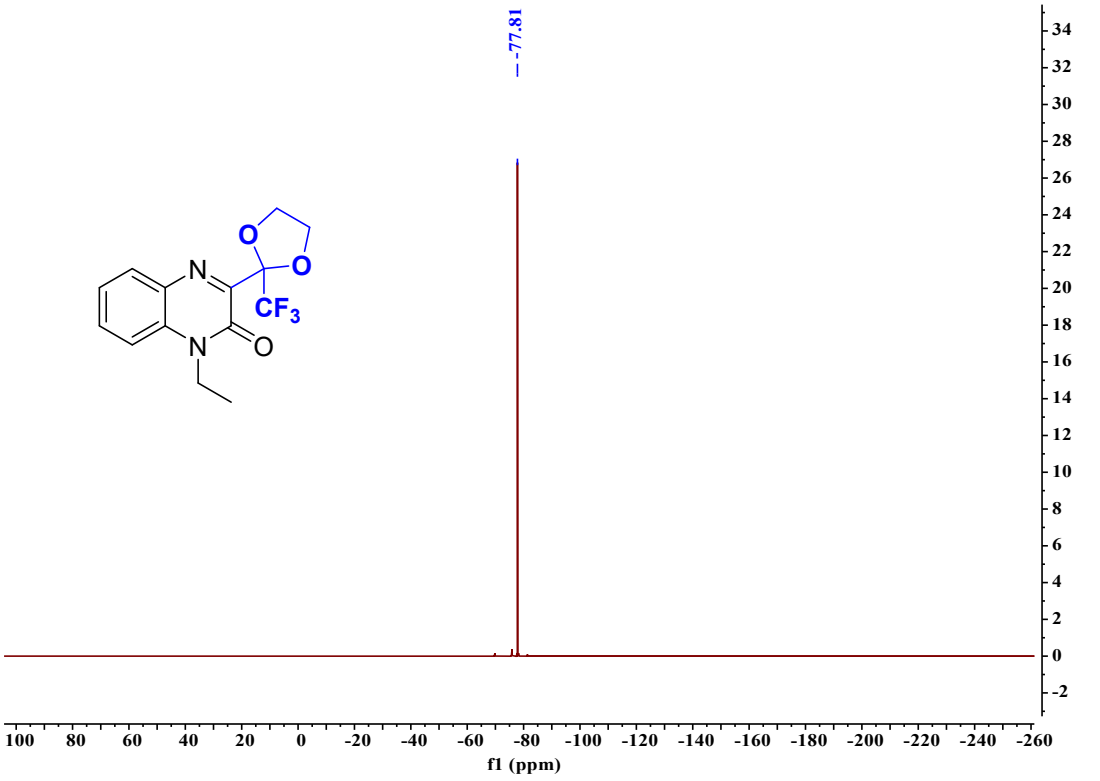


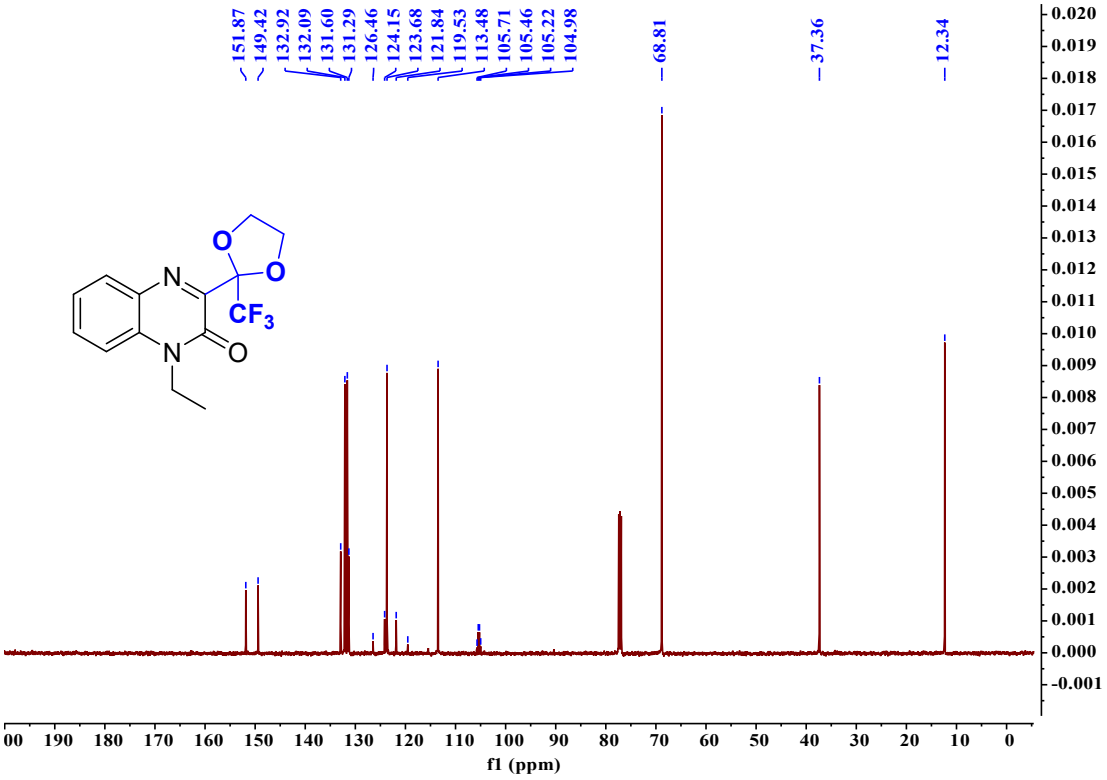
Spectrum from 01.wiff (sample 1) - Sample001, Experiment 1, +TOF MS (105 - 1250) from 2.049 to 2.097 min



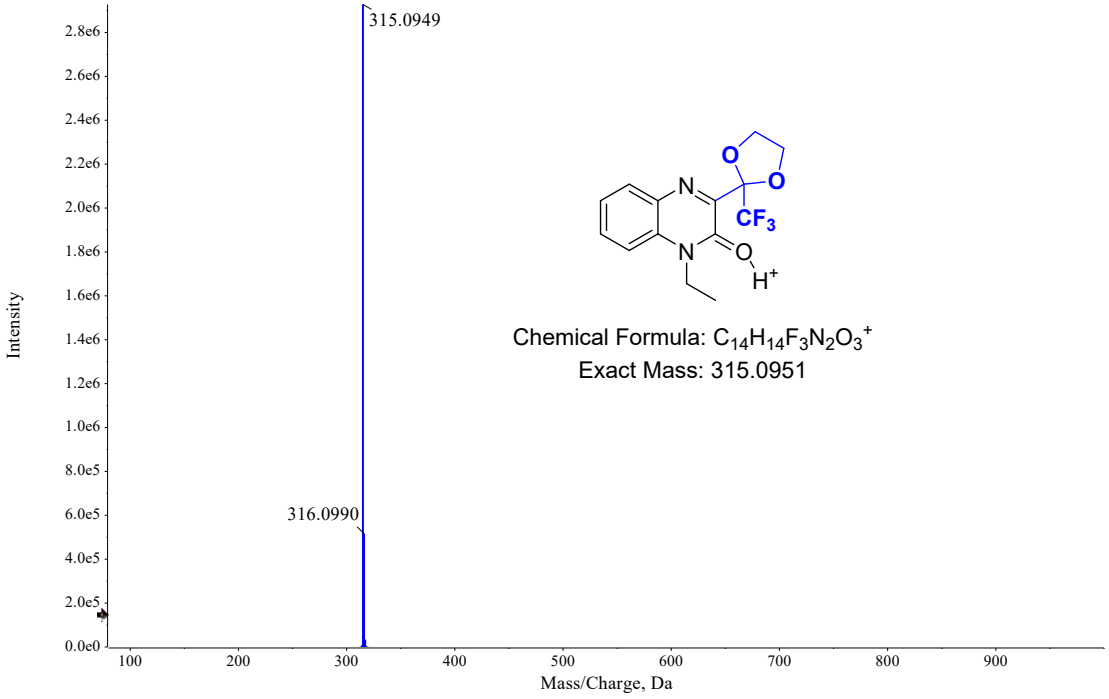
Compound 3b (^{1}H NMR, 500 Hz, $CDCl_3$; ^{19}F NMR 471 Hz, $CDCl_3$ ^{13}C NMR, 101 Hz, $CDCl_3$)







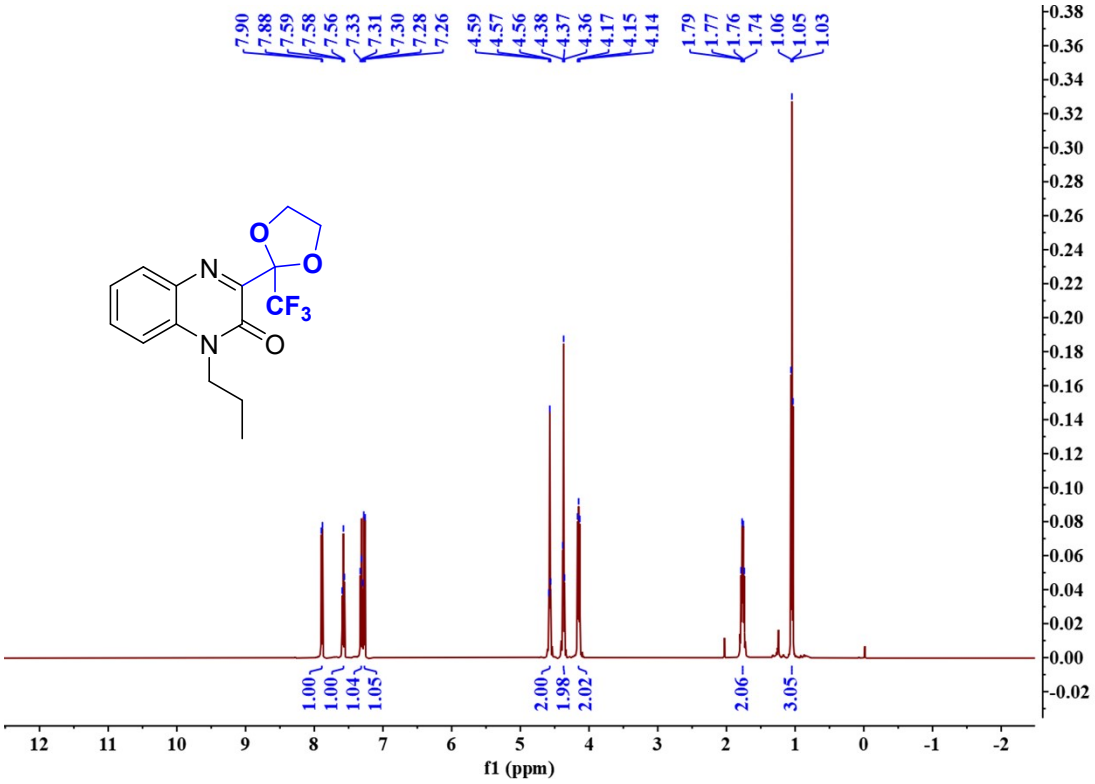
Spectrum from 1.wiff (sample 1) - Sample001, Experiment 1, +TOF MS (80 - 1000) from 0.594 to 0.638 min

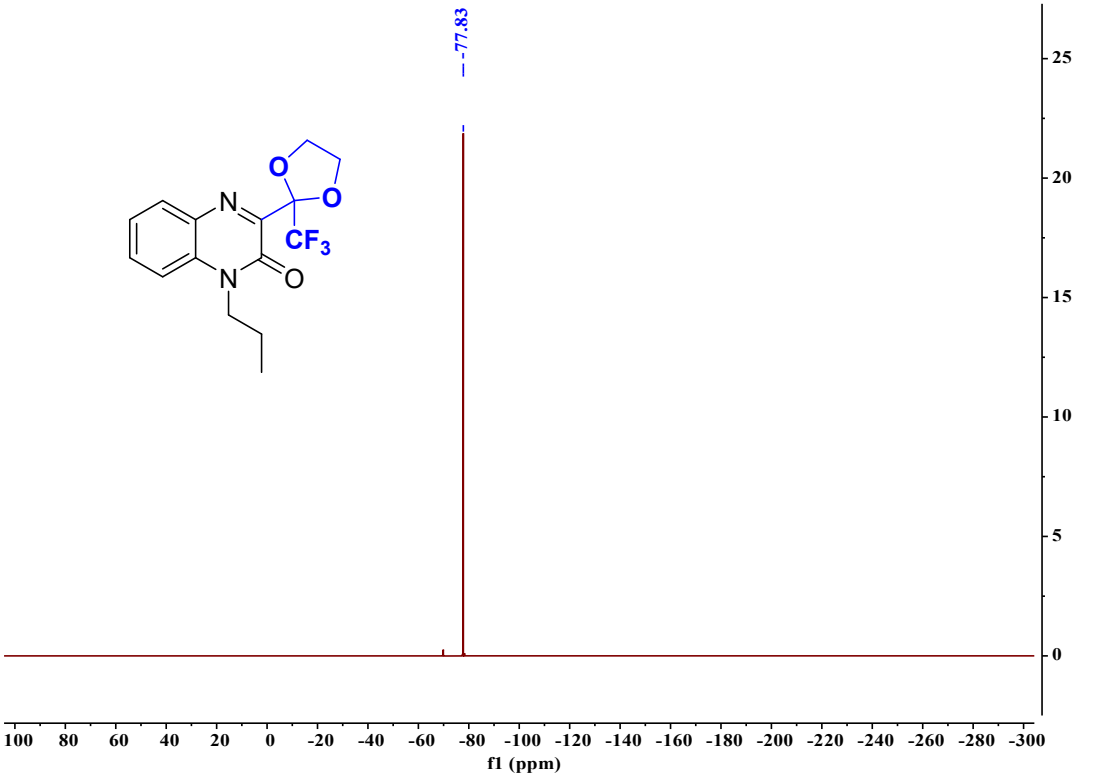


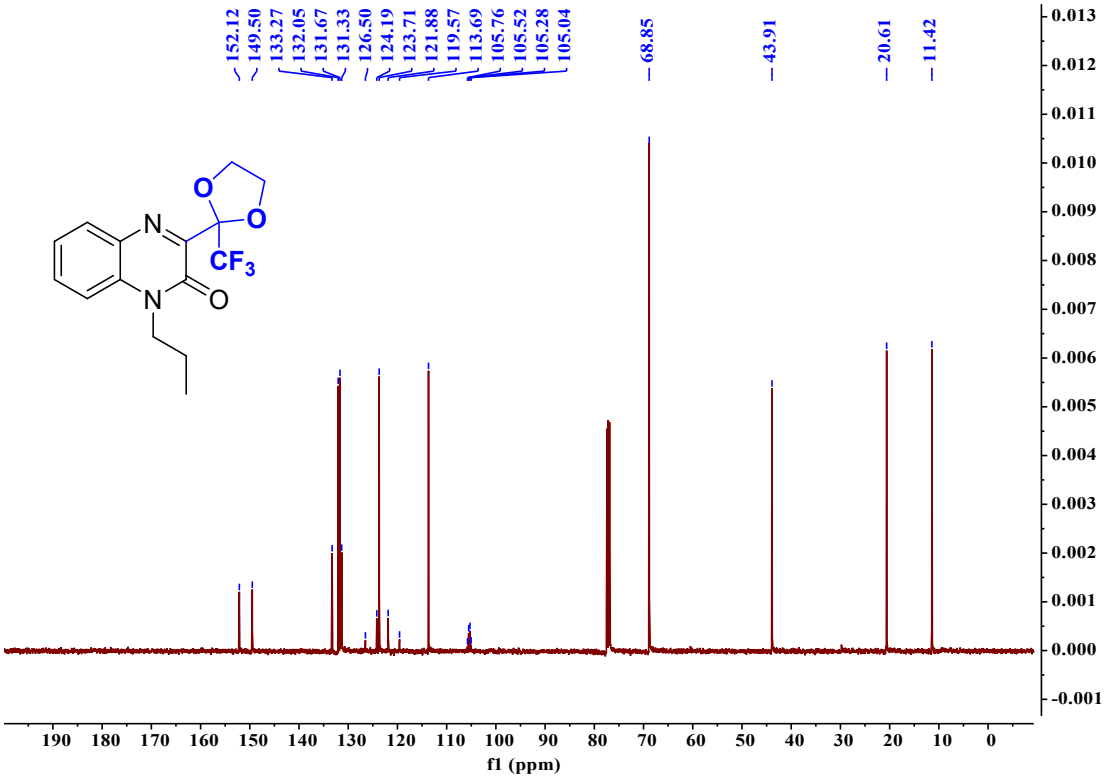
Chemical Formula: $C_{14}H_{14}F_3N_2O_3^+$

Exact Mass: 315.0951

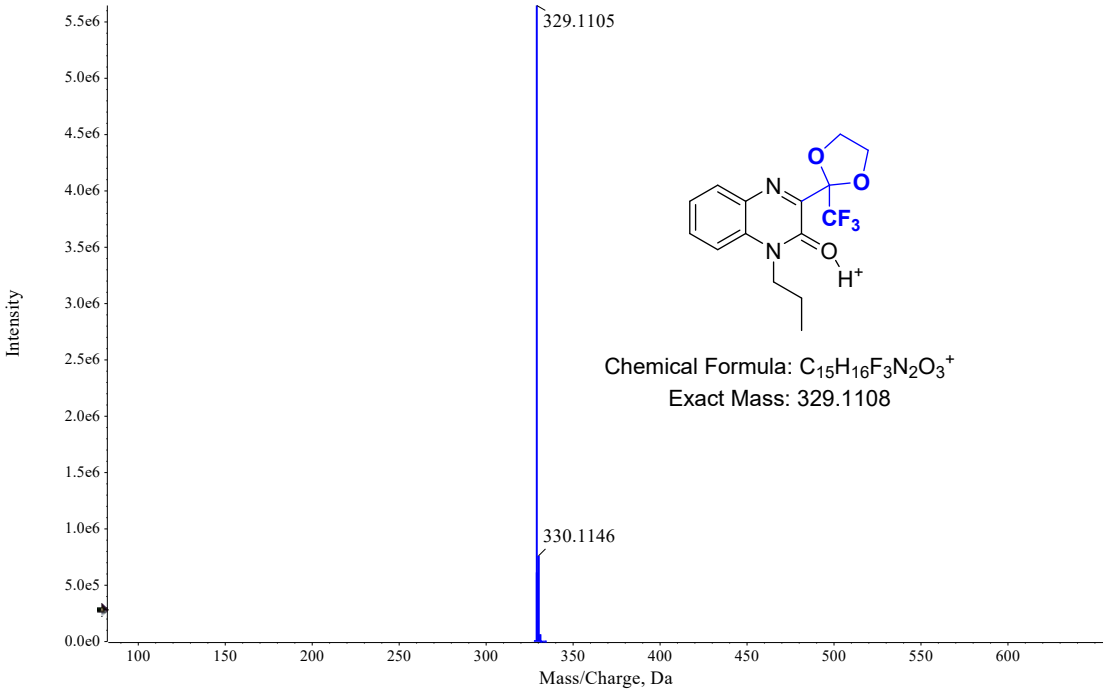
Compound 3c (^{1}H NMR, 500 Hz, $CDCl_3$; ^{19}F NMR 471 Hz, $CDCl_3$ ^{13}C NMR, 101 Hz, $CDCl_3$)



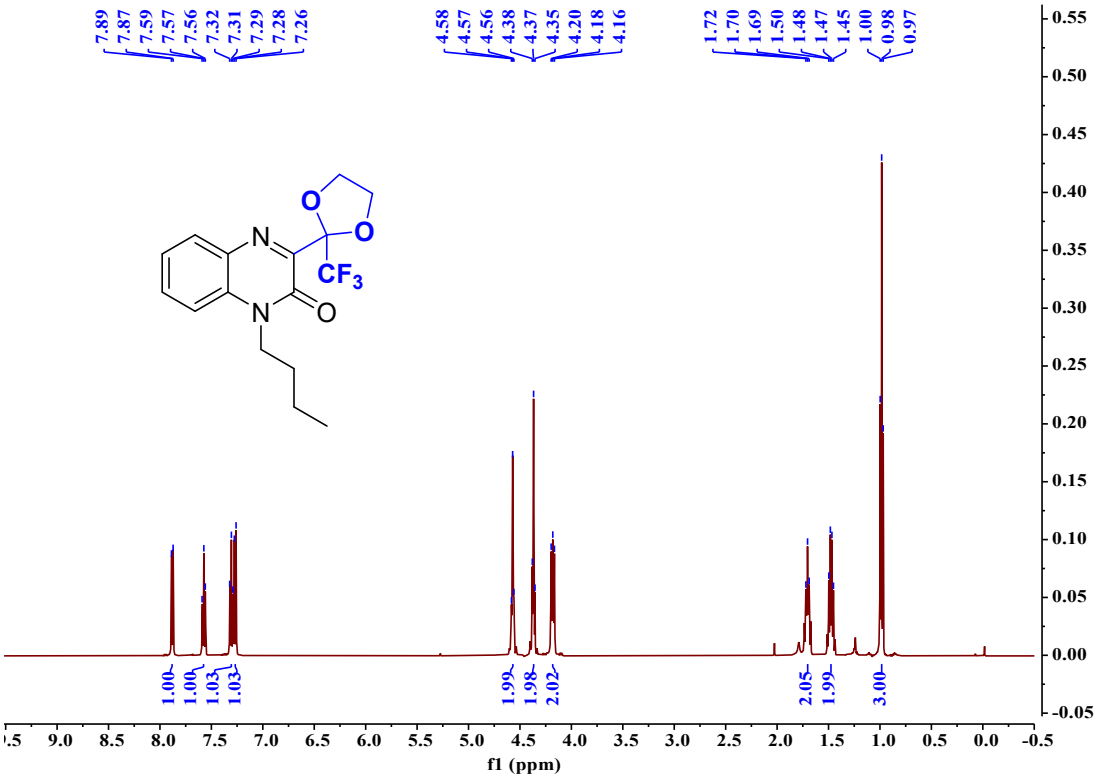


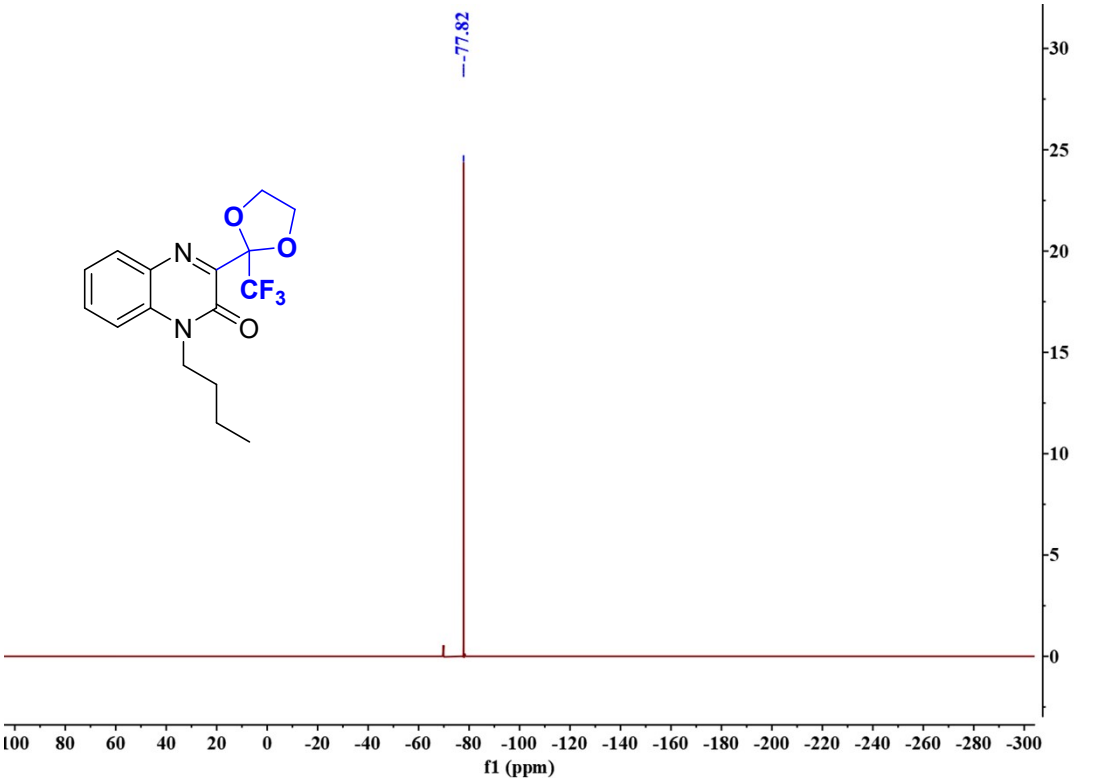


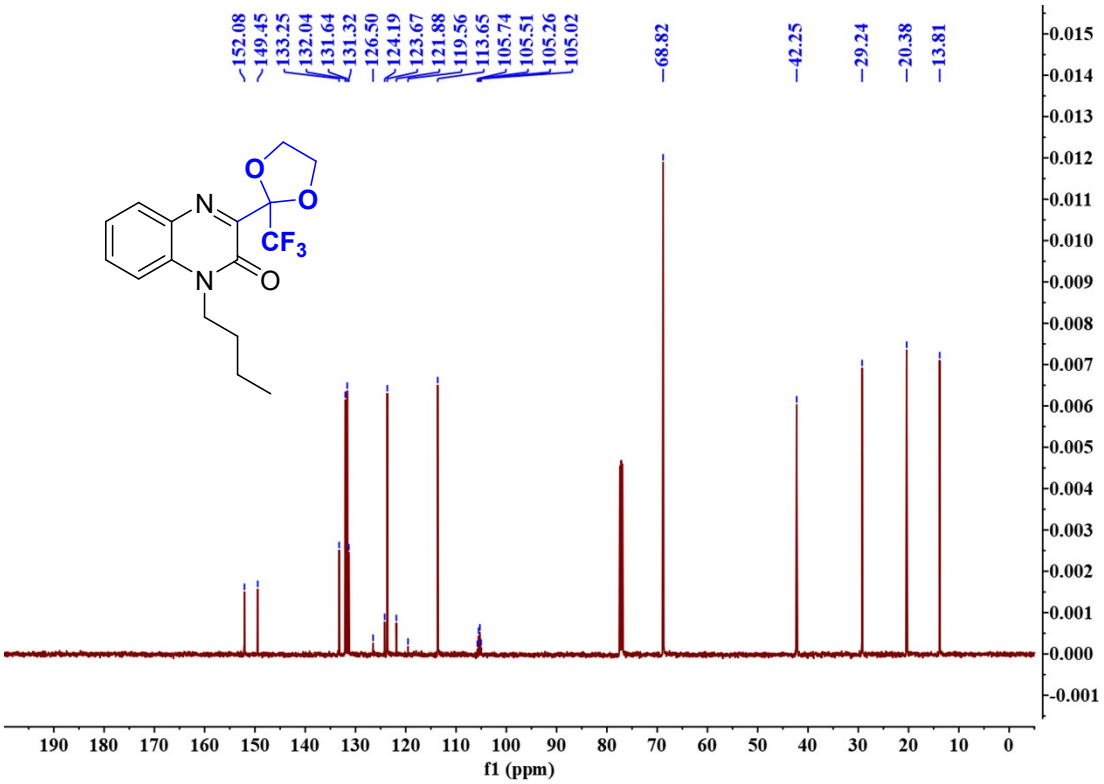
Spectrum from 2.wiff (sample 1) - Sample002, Experiment 1, +TOF MS (80 - 1000) from 0.560 to 0.604 min



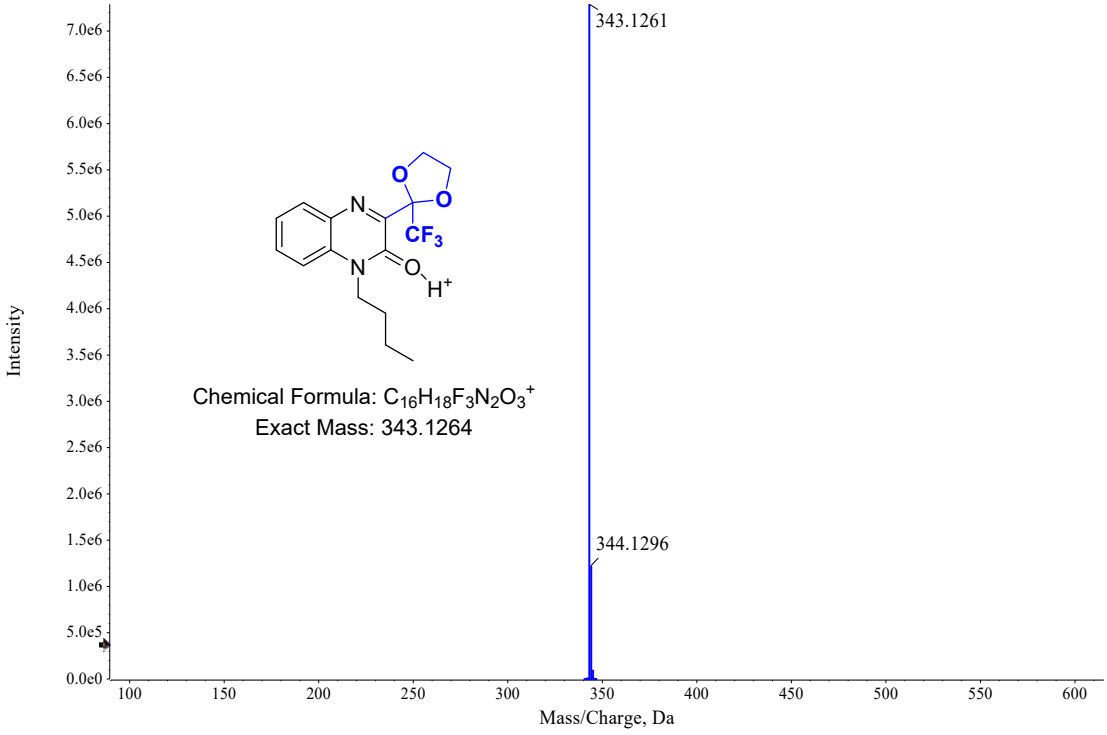
Compound 3d (^{1}H NMR, 500 Hz, $CDCl_3$; ^{19}F NMR 471 Hz, $CDCl_3$ ^{13}C NMR, 101 Hz, $CDCl_3$)



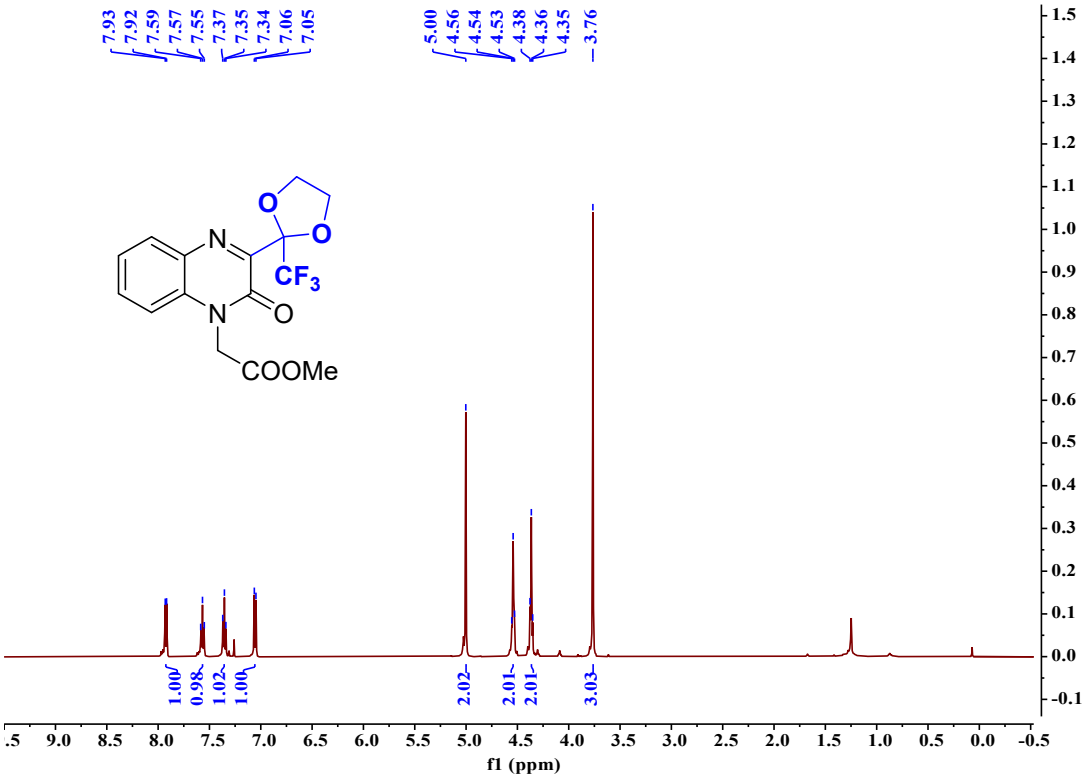


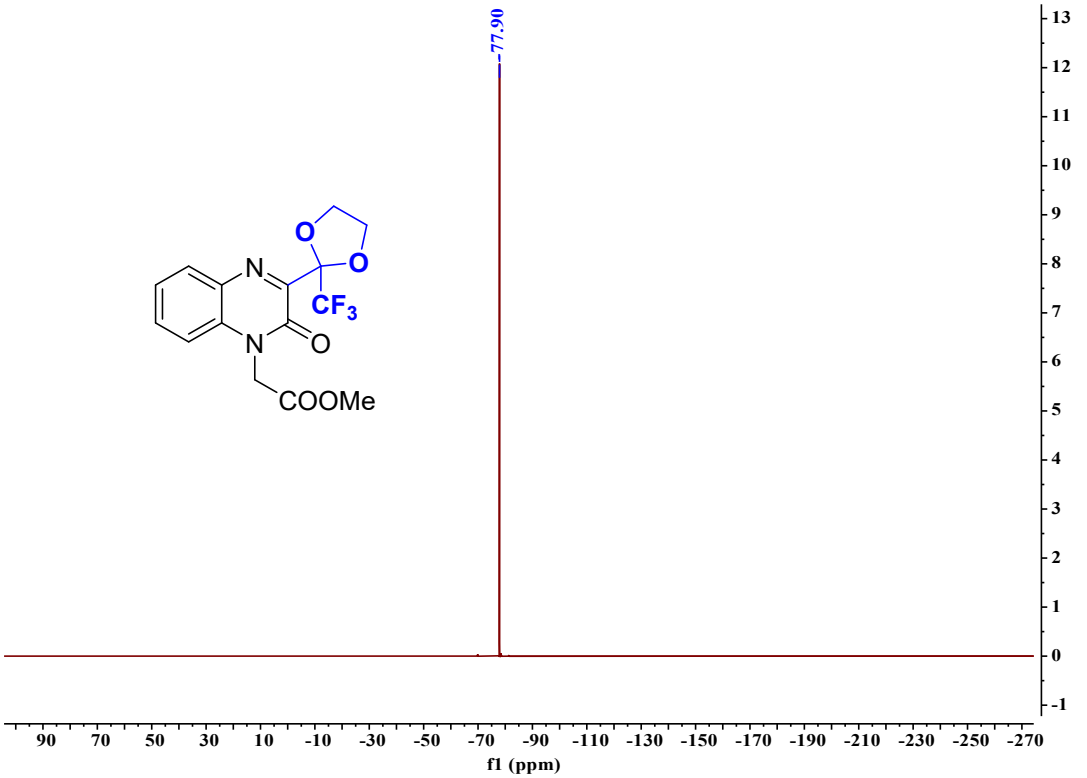


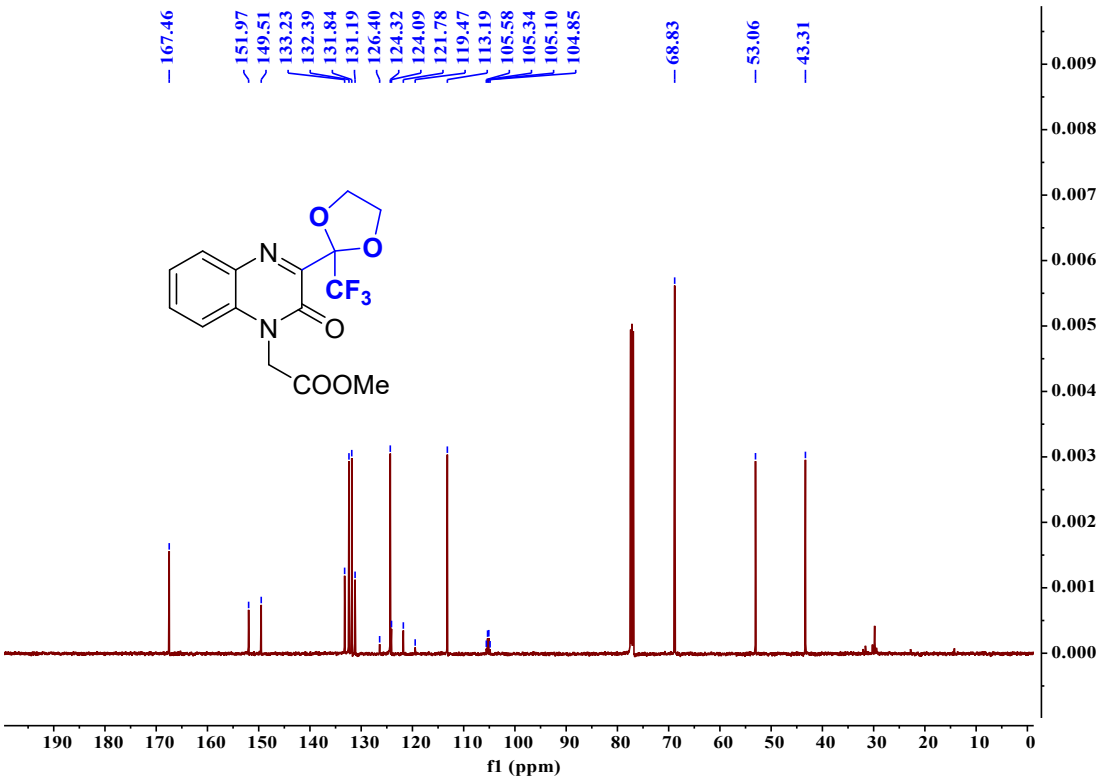
Spectrum from 3.wiff (sample 1) - Sample003, Experiment 1, +TOF MS (80 - 1000) from 0.610 to 0.654 min



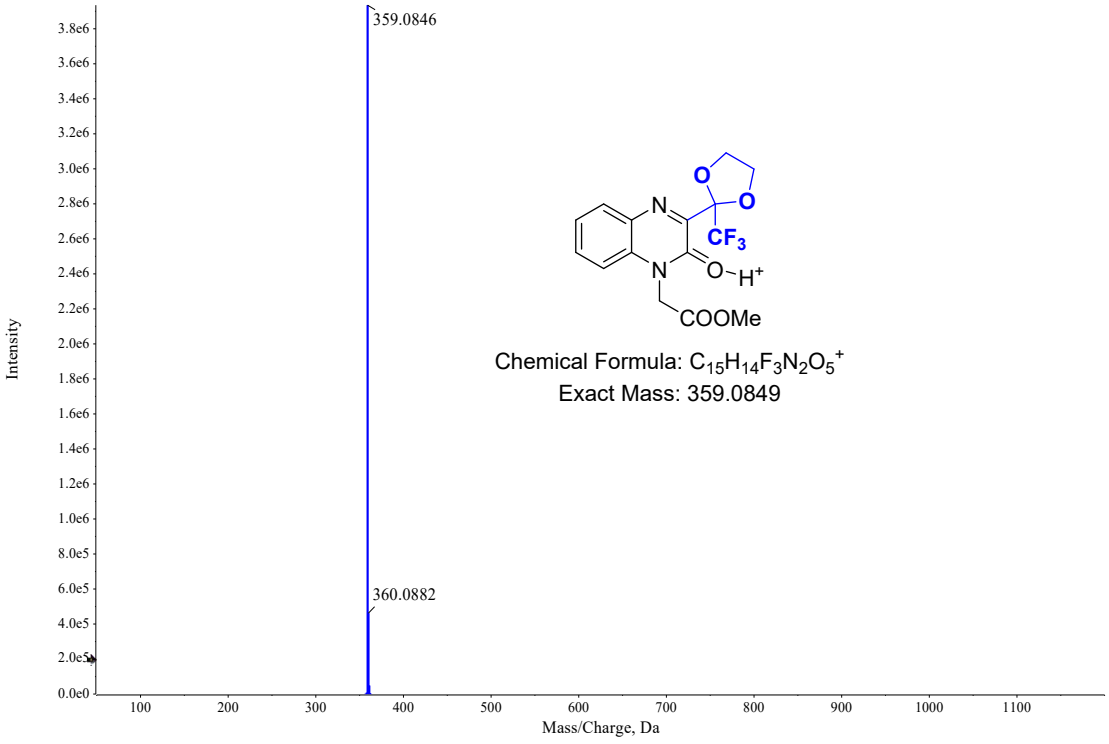
Compound 3e (^{1}H NMR, 500 Hz, $CDCl_3$; ^{19}F NMR 471 Hz, $CDCl_3$ ^{13}C NMR, 101 Hz, $CDCl_3$)







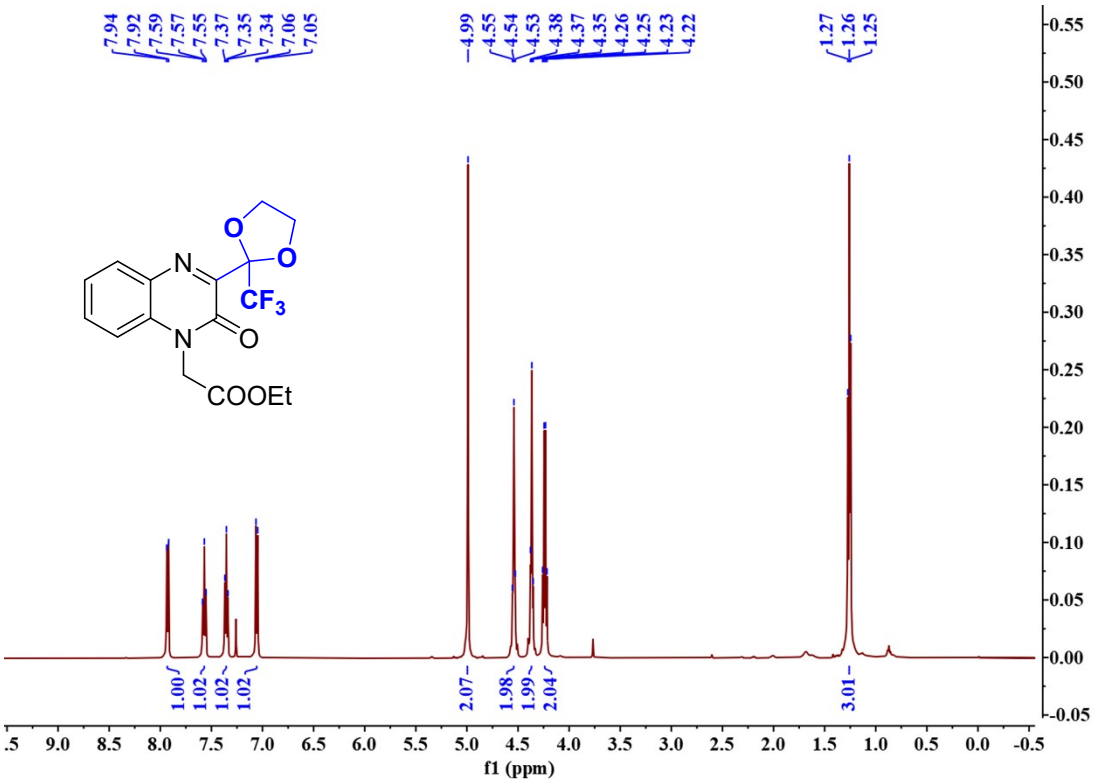
Spectrum from 9.wiff (sample 1) - Sample009, Experiment 1, +TOF MS (CE=10) (50 - 1200) from 1.237 to 1.251 min

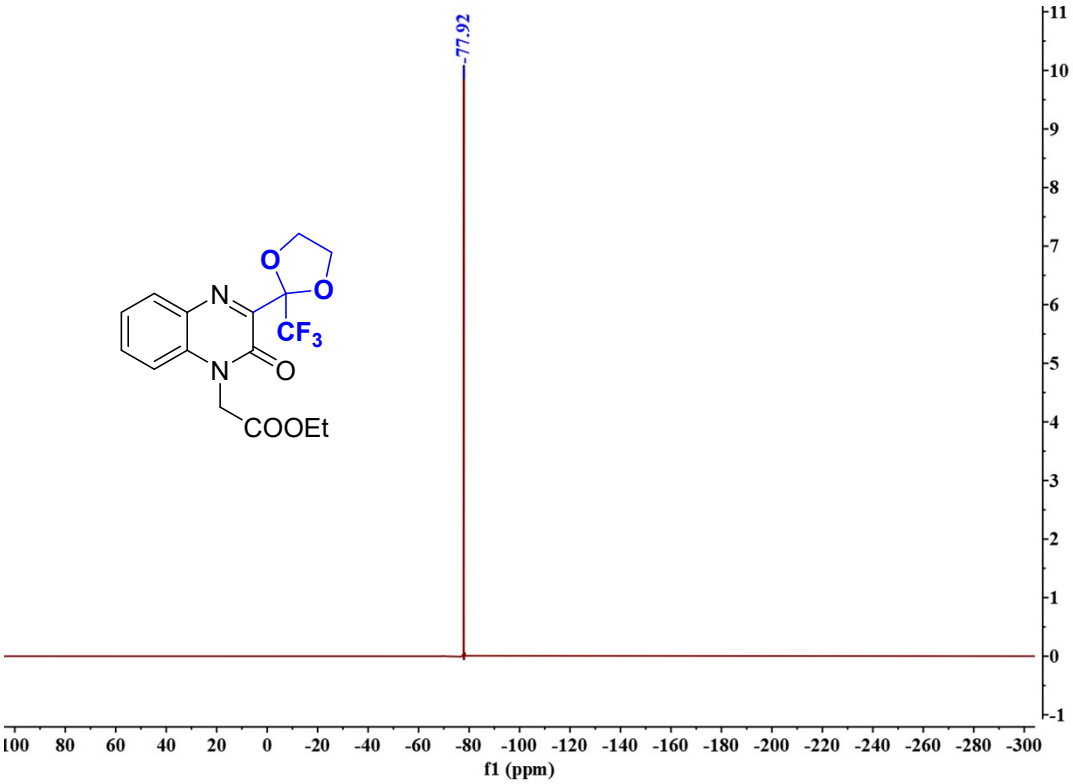


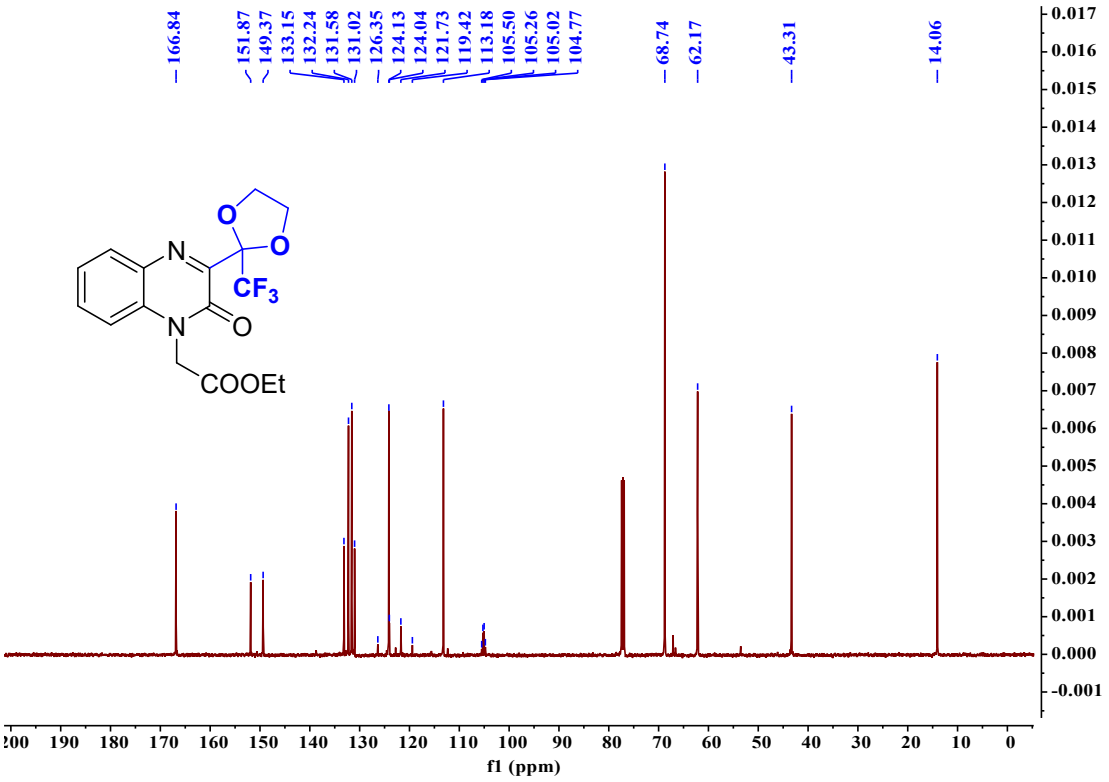
Chemical Formula: $C_{15}H_{14}F_3N_2O_5^+$

Exact Mass: 359.0849

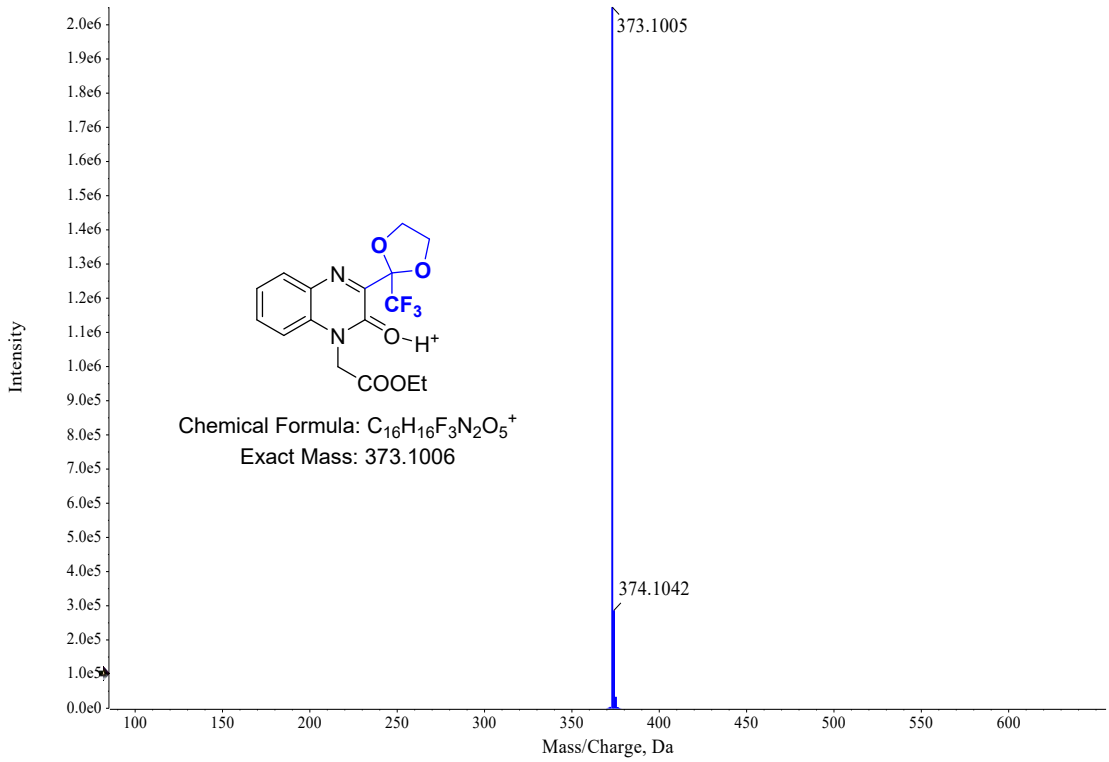
Compound 3f (^{1}H NMR, 500 Hz, $CDCl_3$; ^{19}F NMR 471 Hz, $CDCl_3$ ^{13}C NMR, 101 Hz, $CDCl_3$)



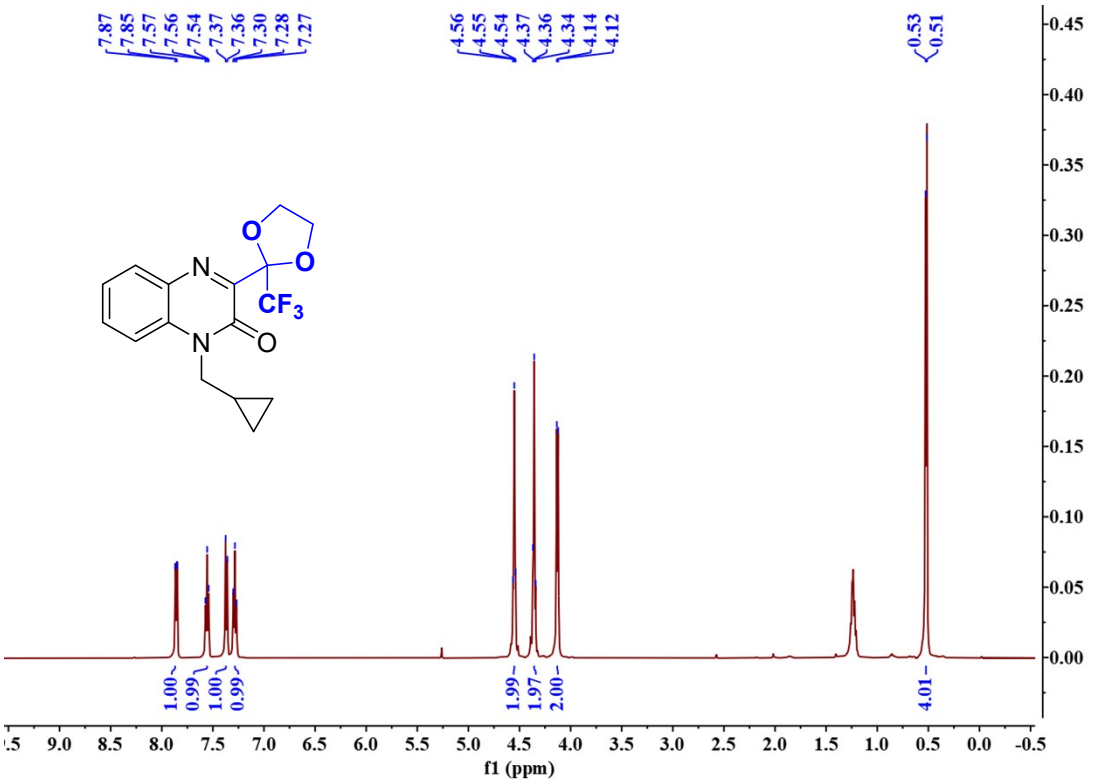


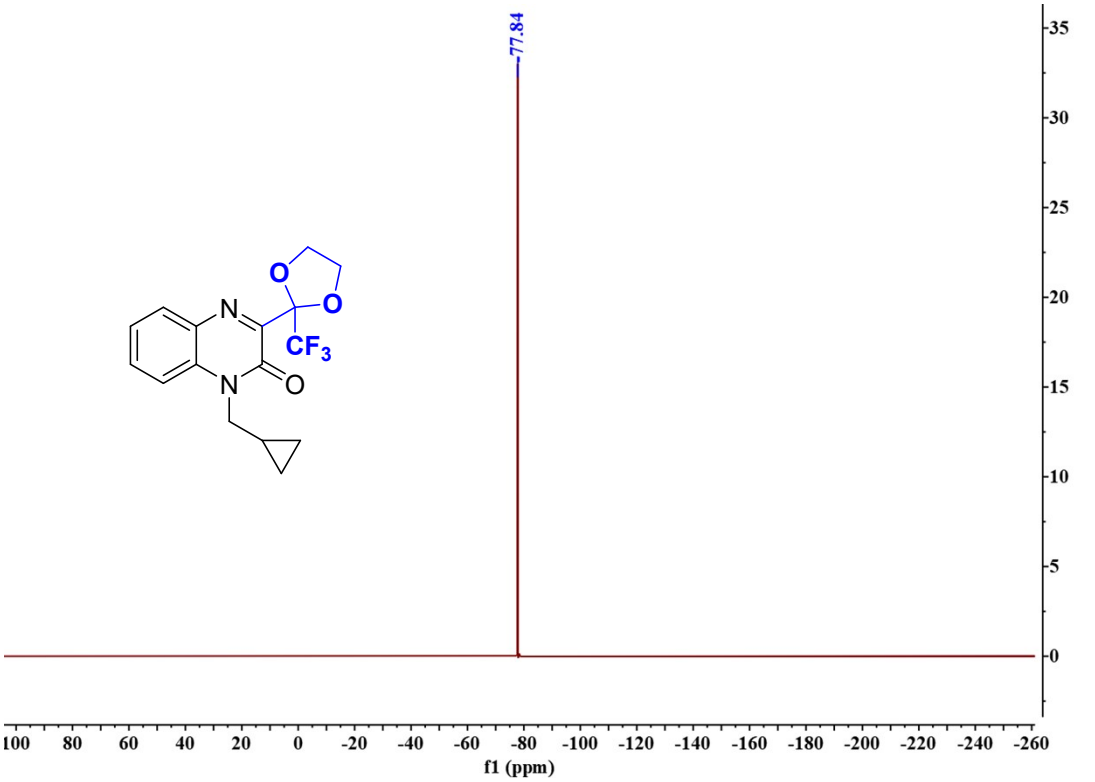


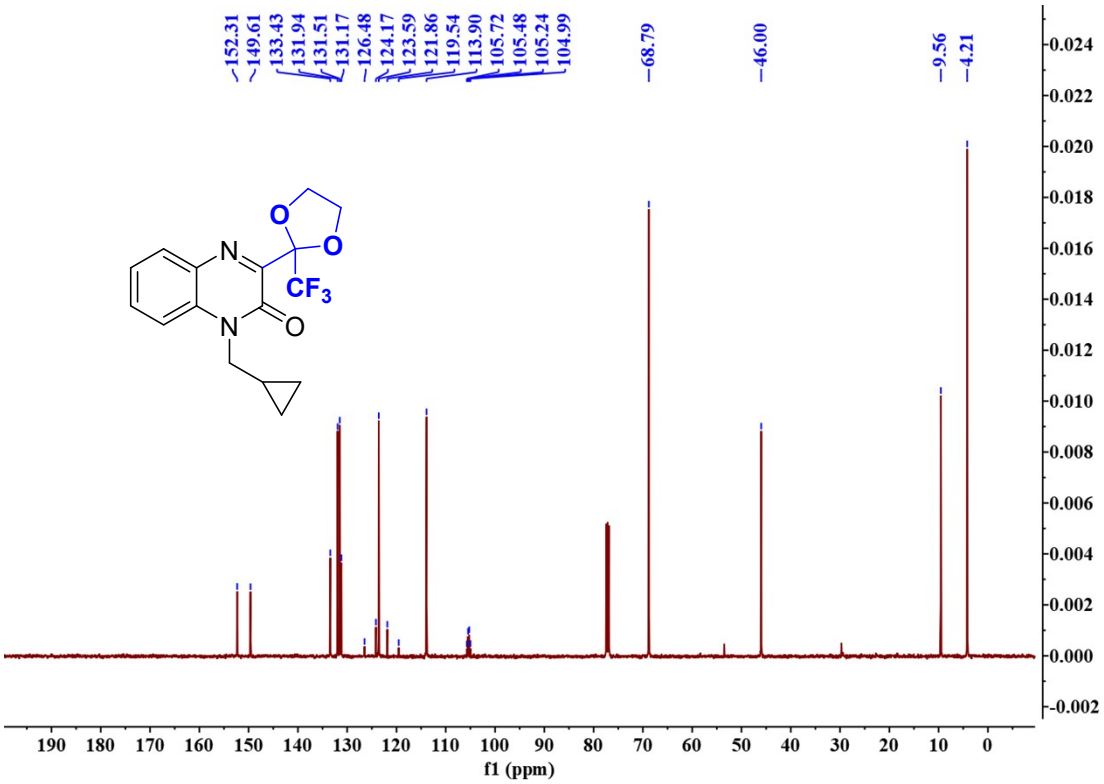
Spectrum from 5.wiff (sample 1) - Sample005, Experiment 1, +TOF MS (80 - 1000) from 0.559 to 0.604 min



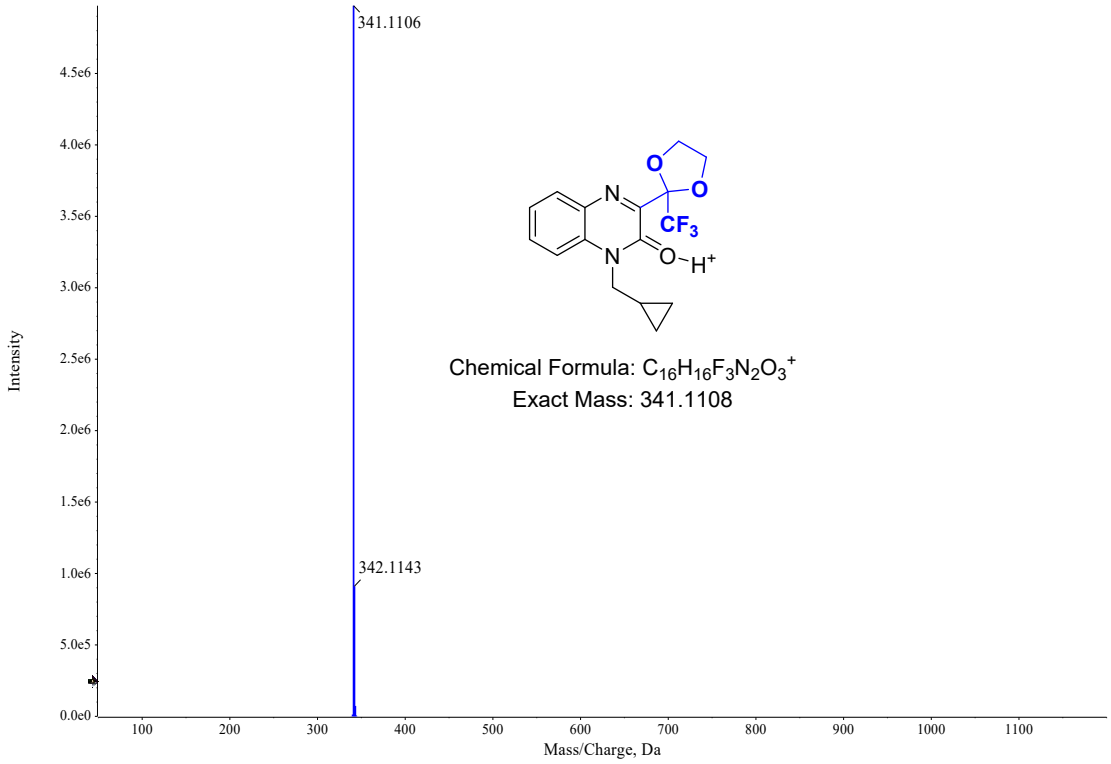
Compound 3g (^{1}H NMR, 500 Hz, $CDCl_3$; ^{19}F NMR 471 Hz, $CDCl_3$ ^{13}C NMR, 101 Hz, $CDCl_3$)







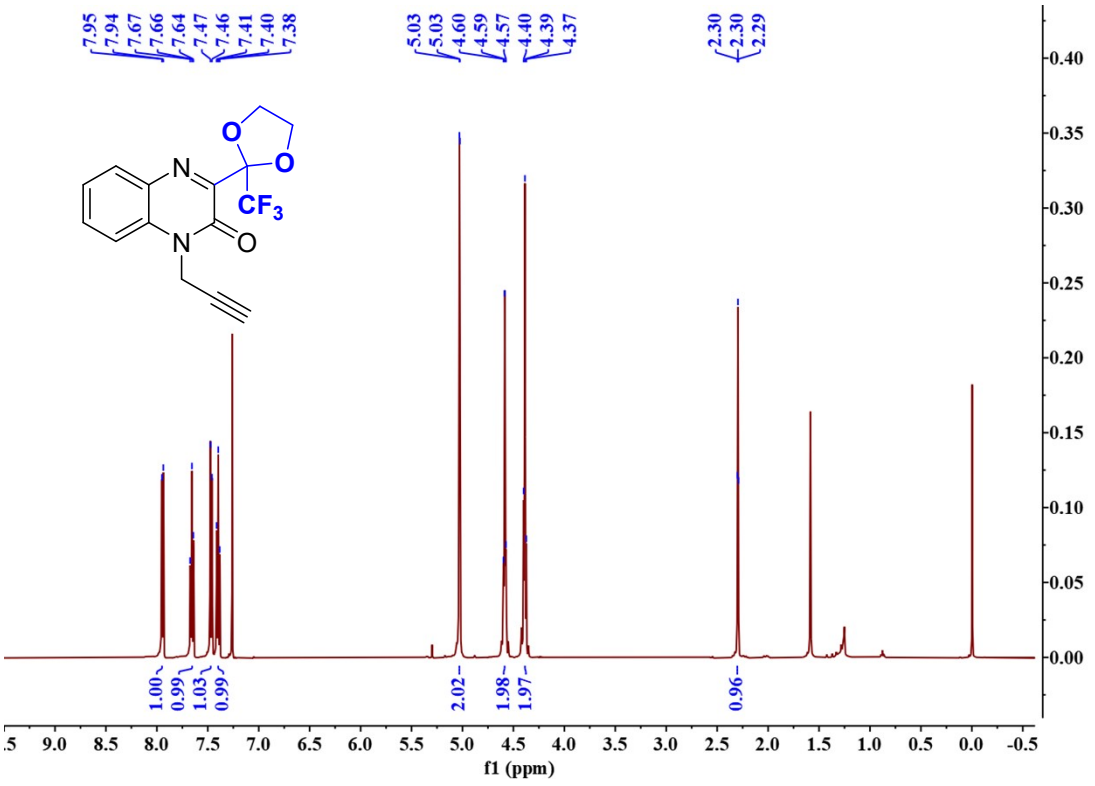
Spectrum from 12.wiff (sample 1) - Sample012, Experiment 1, +TOF MS (CE=10) (50 - 1200) from 0.584 to 0.599 min

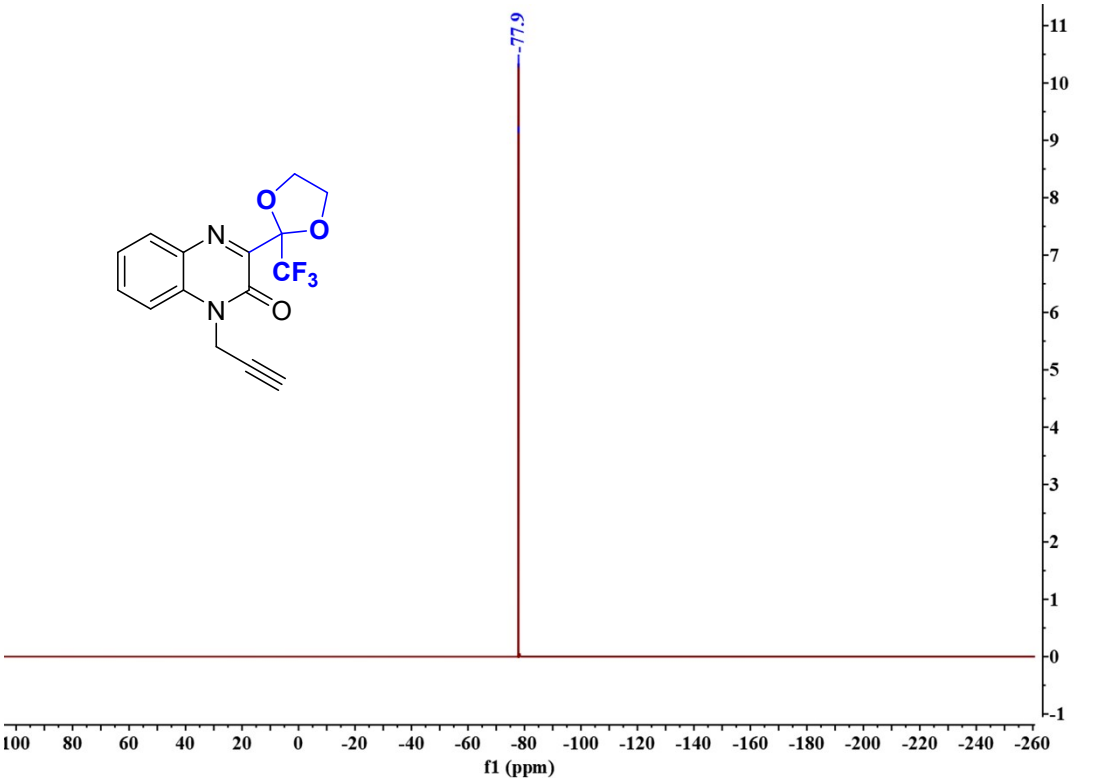


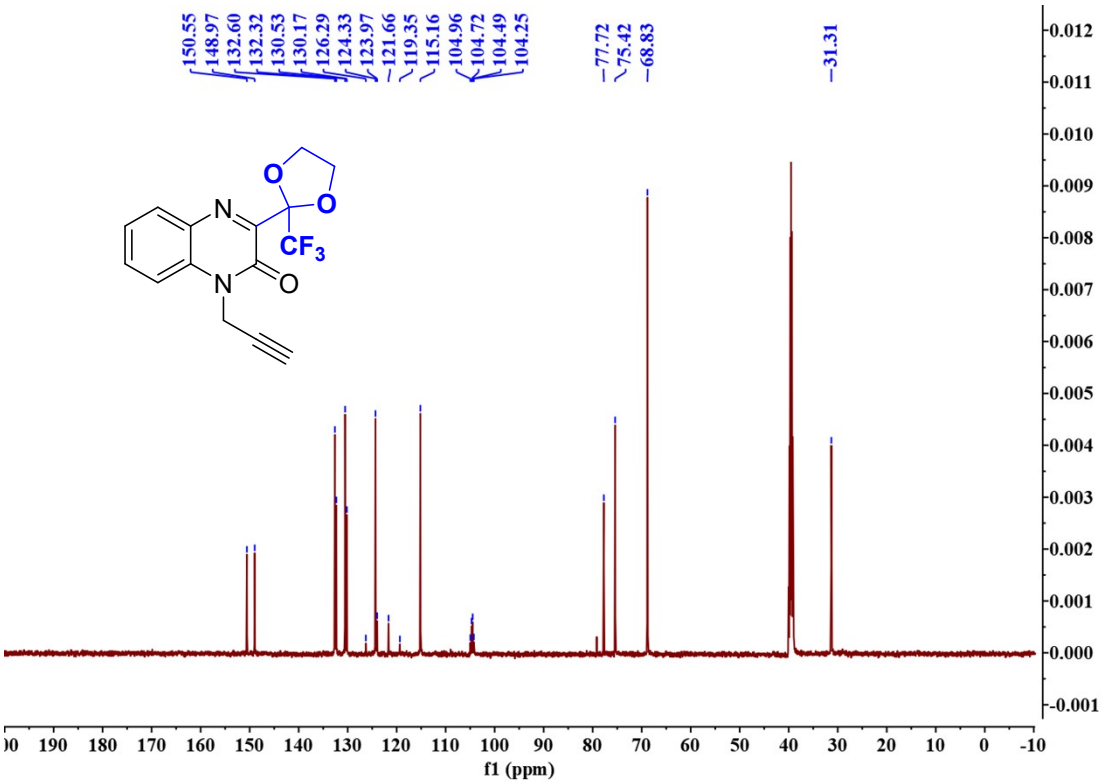
Chemical Formula: $C_{16}H_{16}F_3N_2O_3^+$

Exact Mass: 341.1108

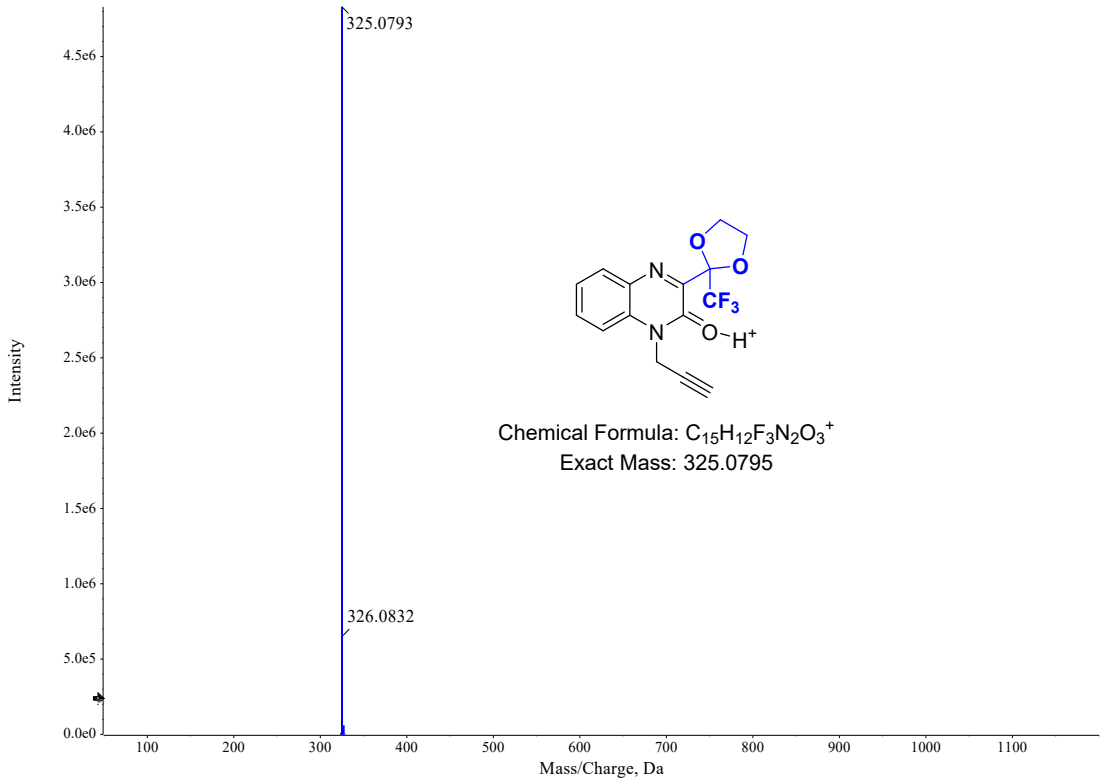
Compound 3h (^{1}H NMR, 500 Hz, $CDCl_3$; ^{19}F NMR 471 Hz, $CDCl_3$ ^{13}C NMR, 101 Hz, $CDCl_3$)





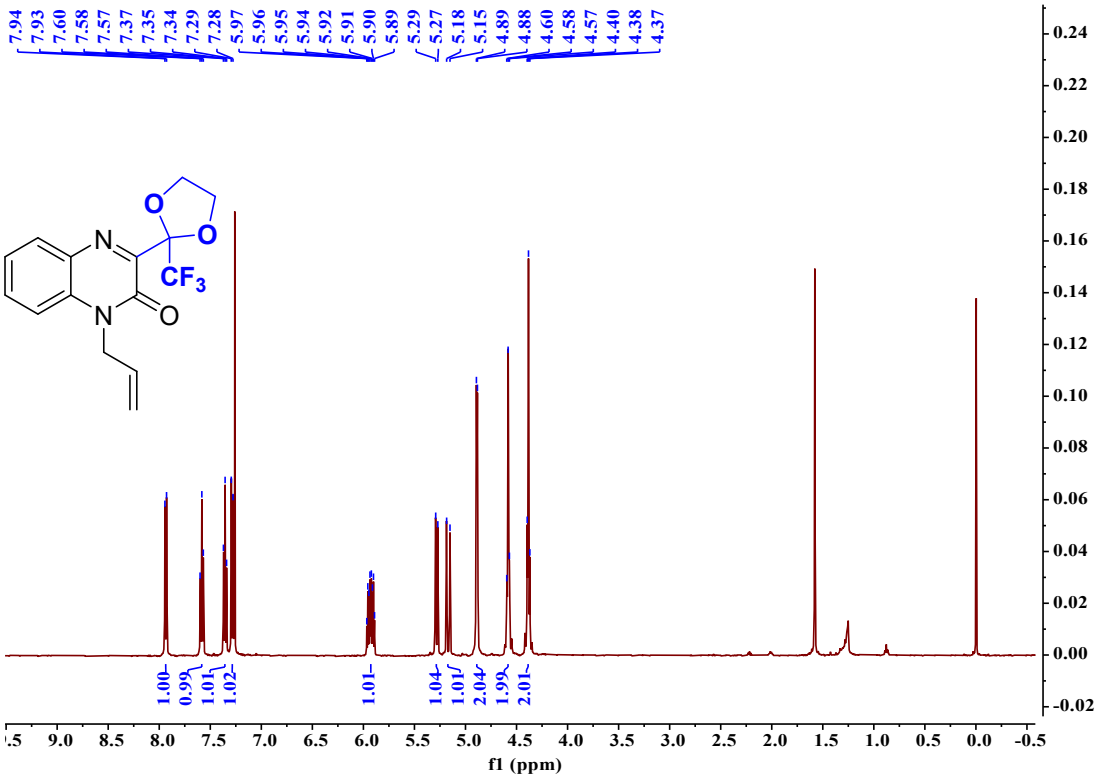


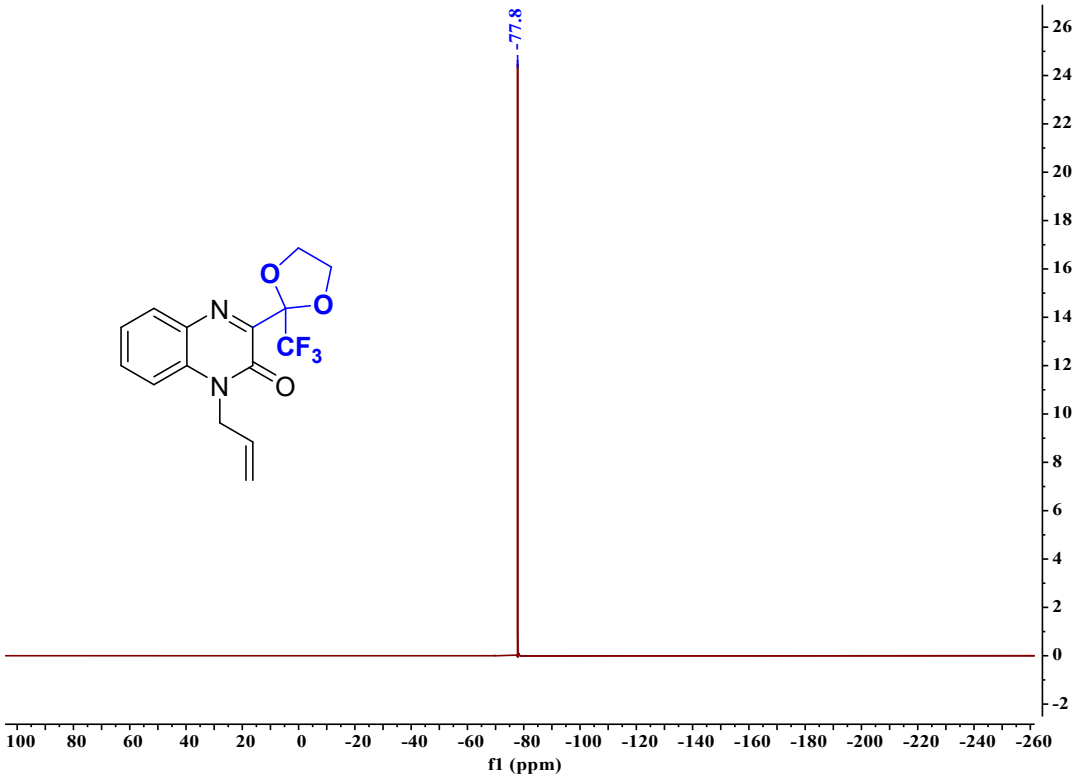
Spectrum from 10.wiff (sample 1) - Sample010, Experiment 1, +TOF MS (CE=10) (50 - 1200) from 0.518 to 0.533 min

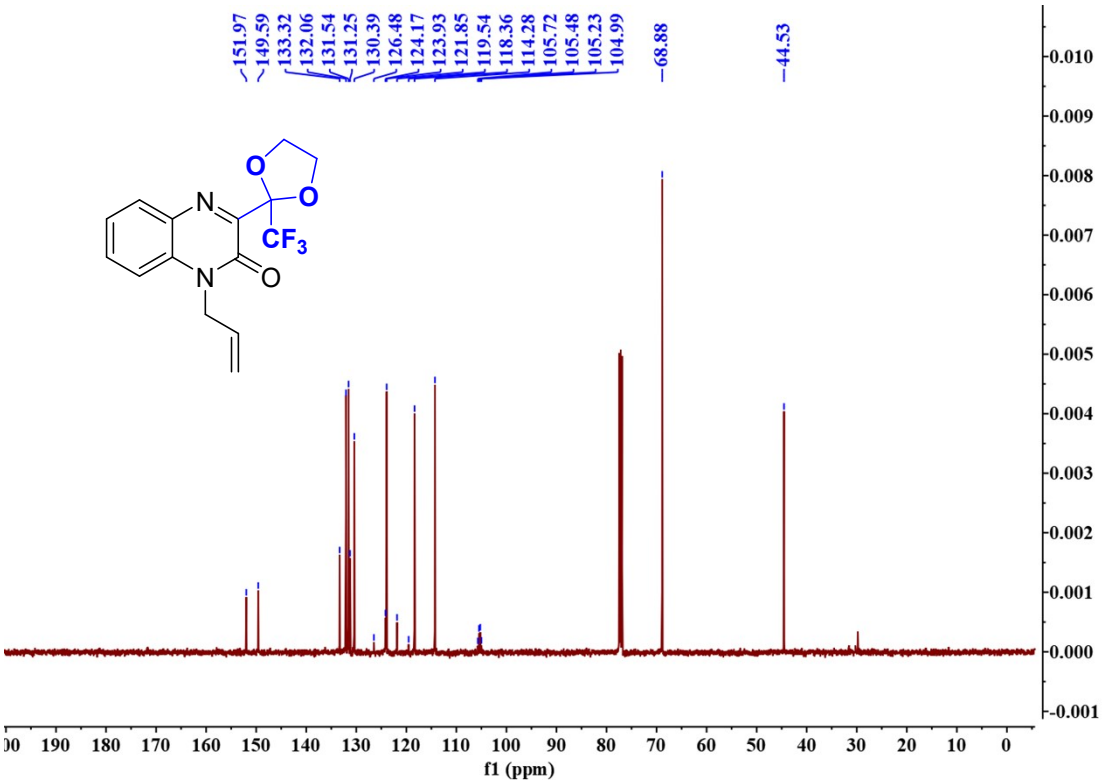


Chemical Formula: $C_{15}H_{12}F_3N_2O_3^+$
Exact Mass: 325.0795

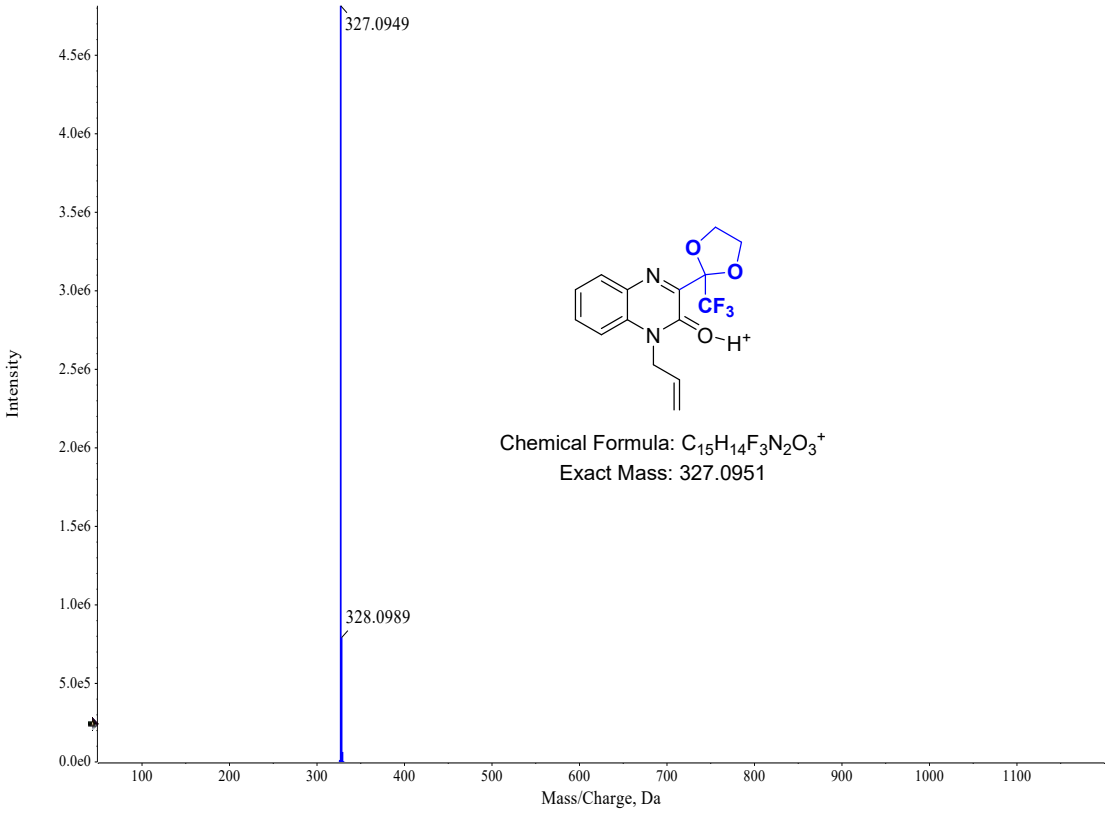
Compound 3i (^{1}H NMR, 500 Hz, $CDCl_3$; ^{19}F NMR 471 Hz, $CDCl_3$ ^{13}C NMR, 101 Hz, $CDCl_3$)





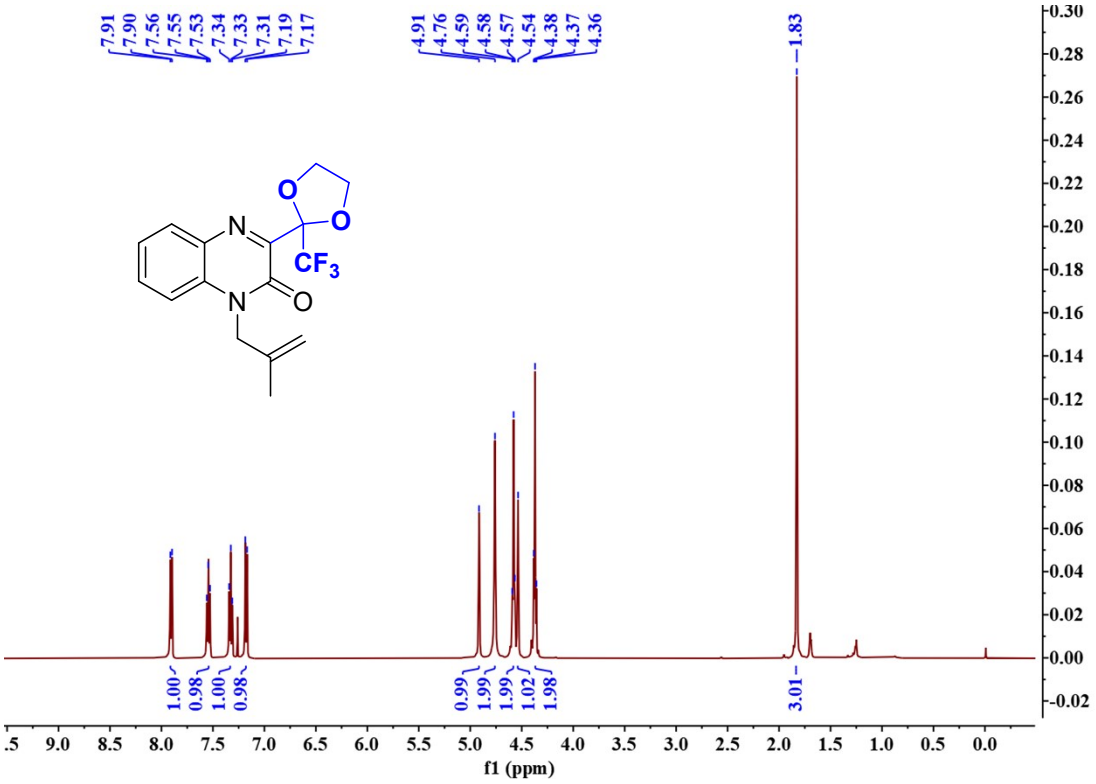


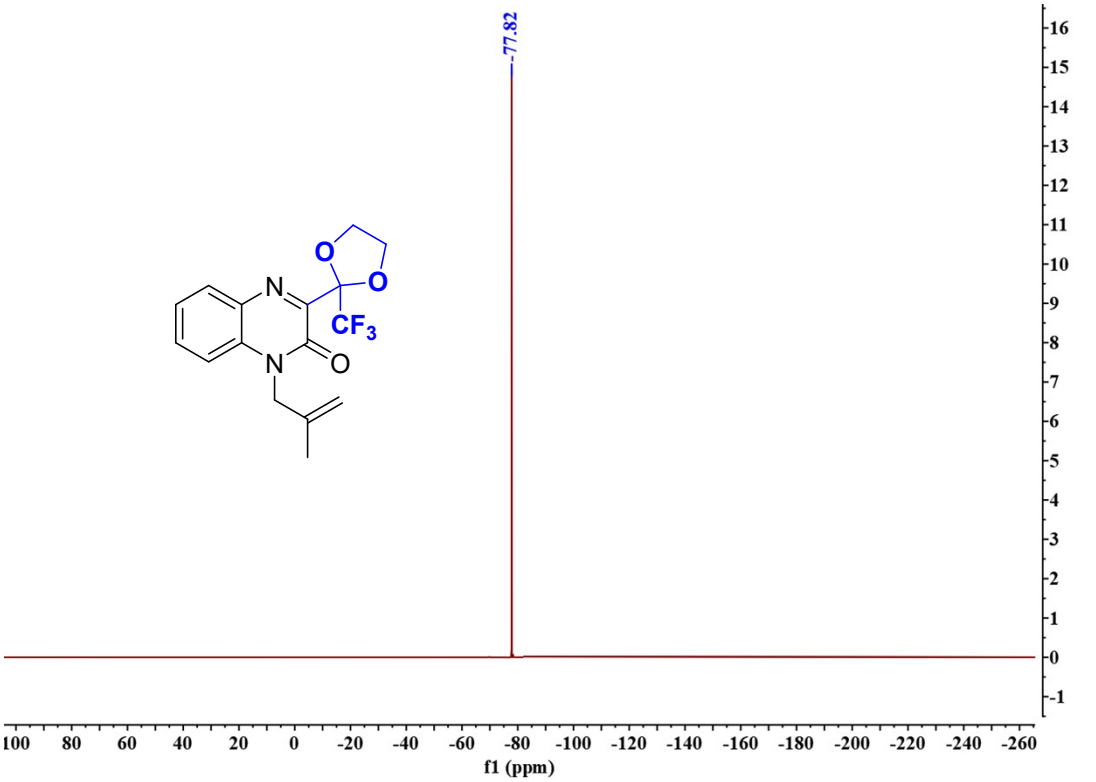
Spectrum from 11.wiff (sample 1) - Sample011, Experiment 1, +TOF MS (CE=10) (50 - 1200) from 0.599 to 0.613 min

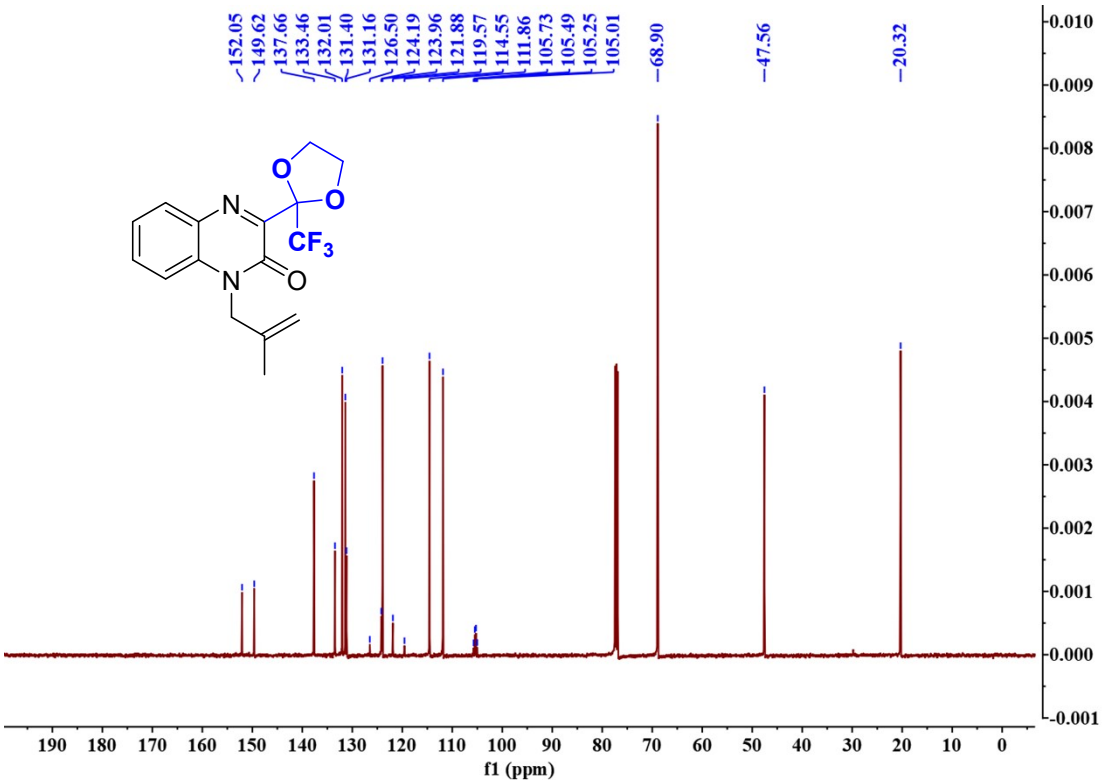


Chemical Formula: $C_{15}H_{14}F_3N_2O_3^+$
Exact Mass: 327.0951

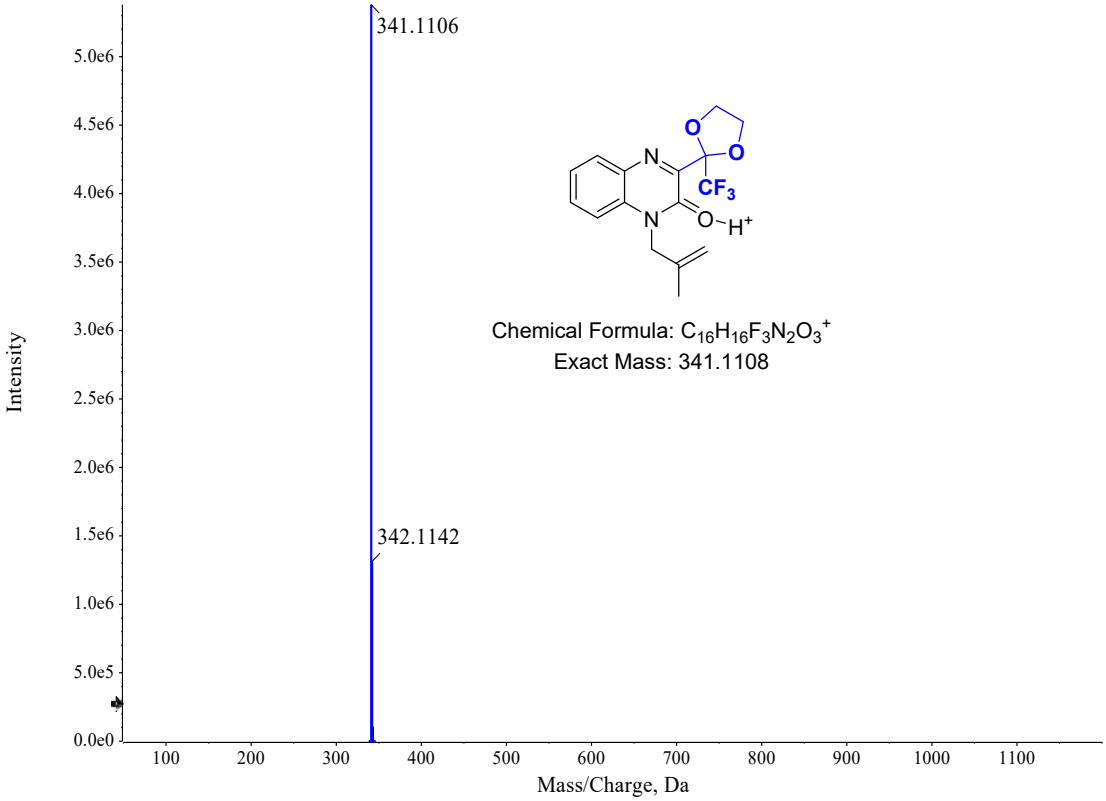
Compound 3j (^{1}H NMR, 500 Hz, $CDCl_3$; ^{19}F NMR 471 Hz, $CDCl_3$ ^{13}C NMR, 101 Hz, $CDCl_3$)



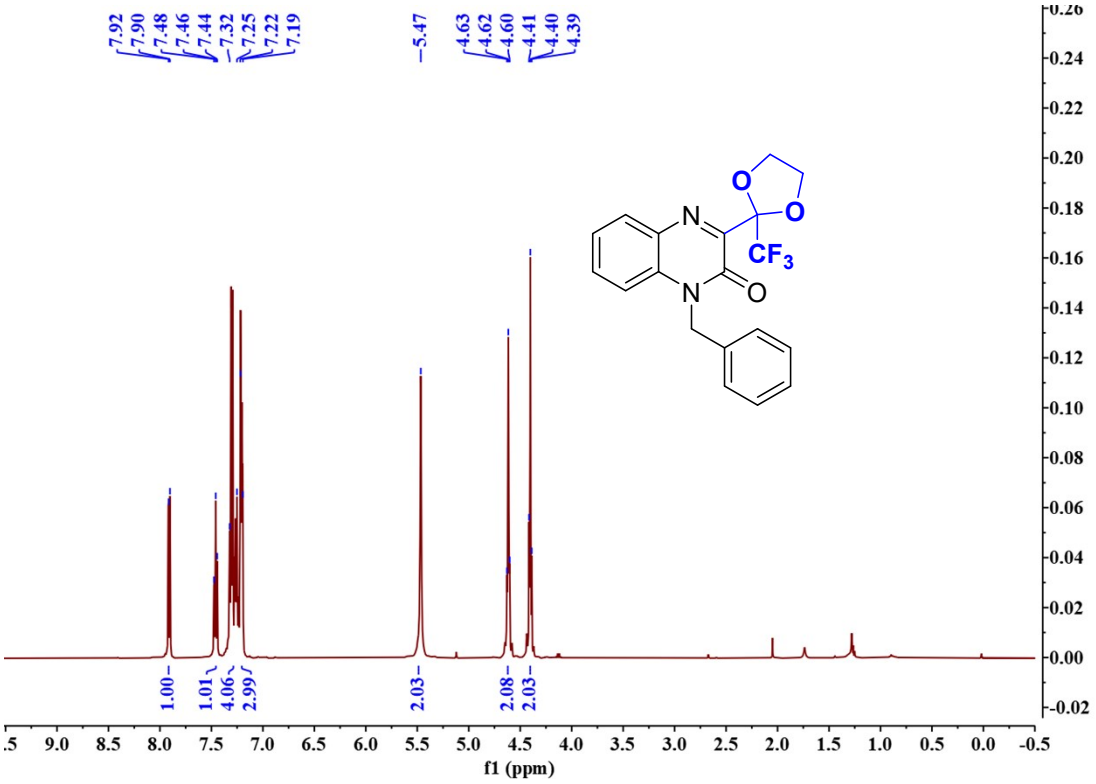


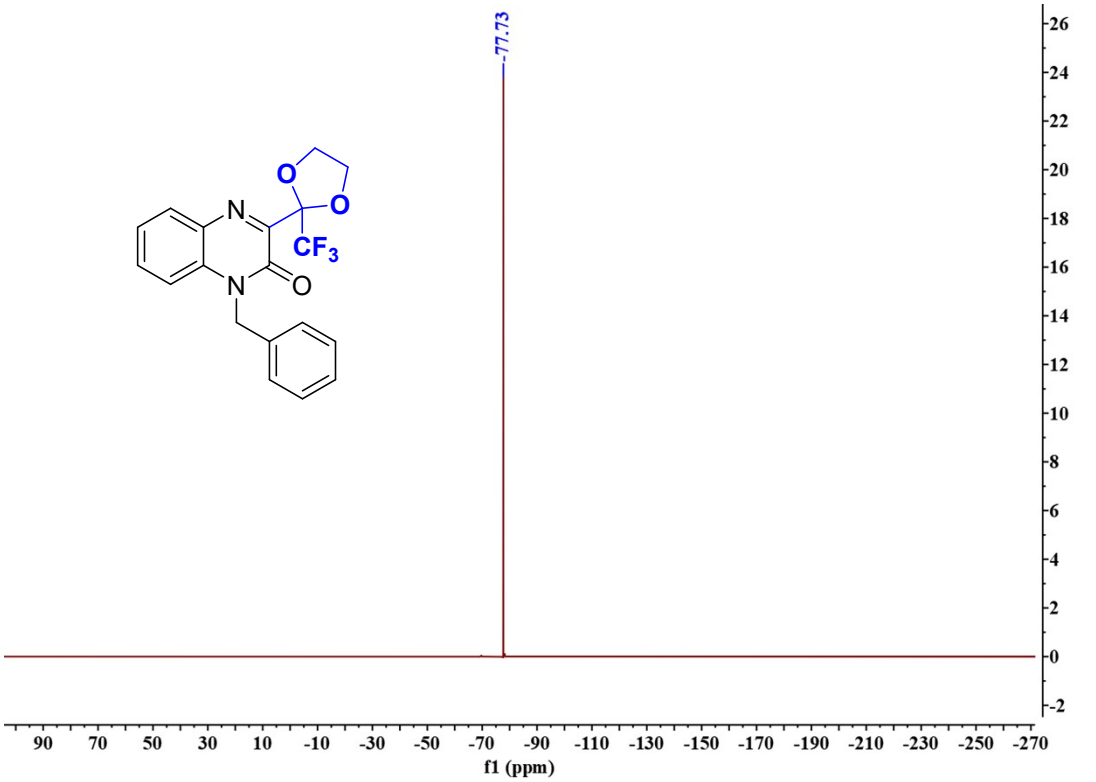


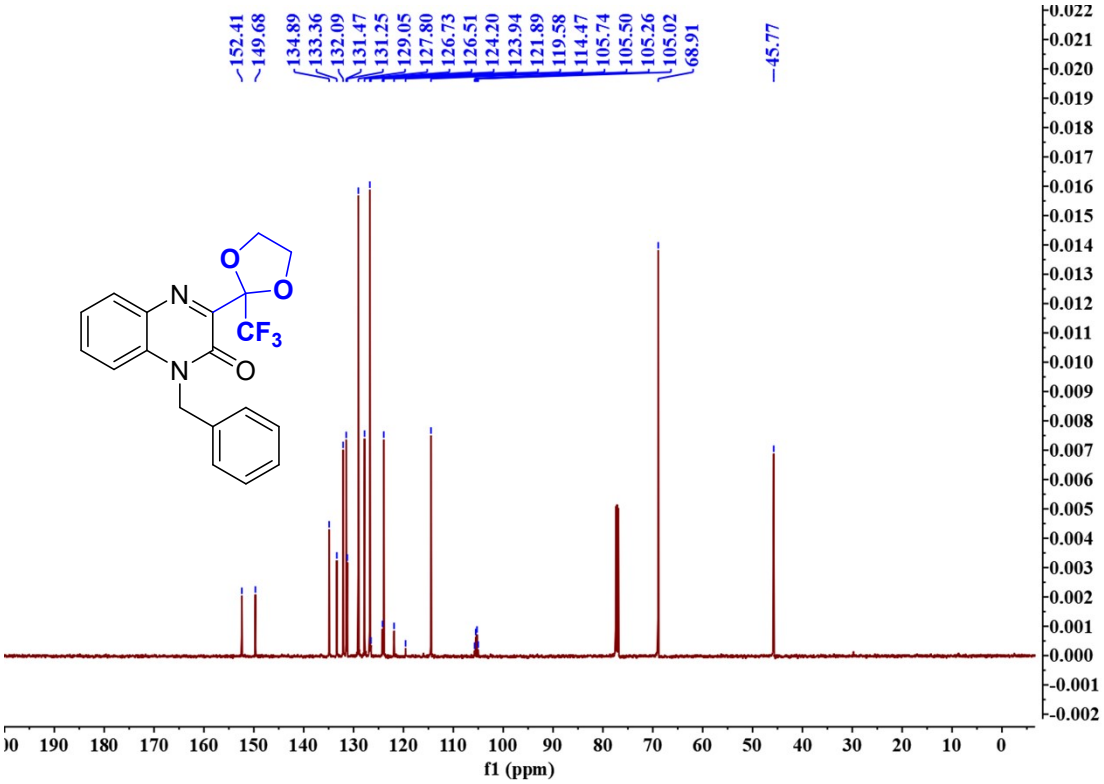
Spectrum from 15.wiff (sample 1) - Sample015, Experiment 1, +TOF MS (CE=10) (50 - 1200) from 0.621 to 0.635 min



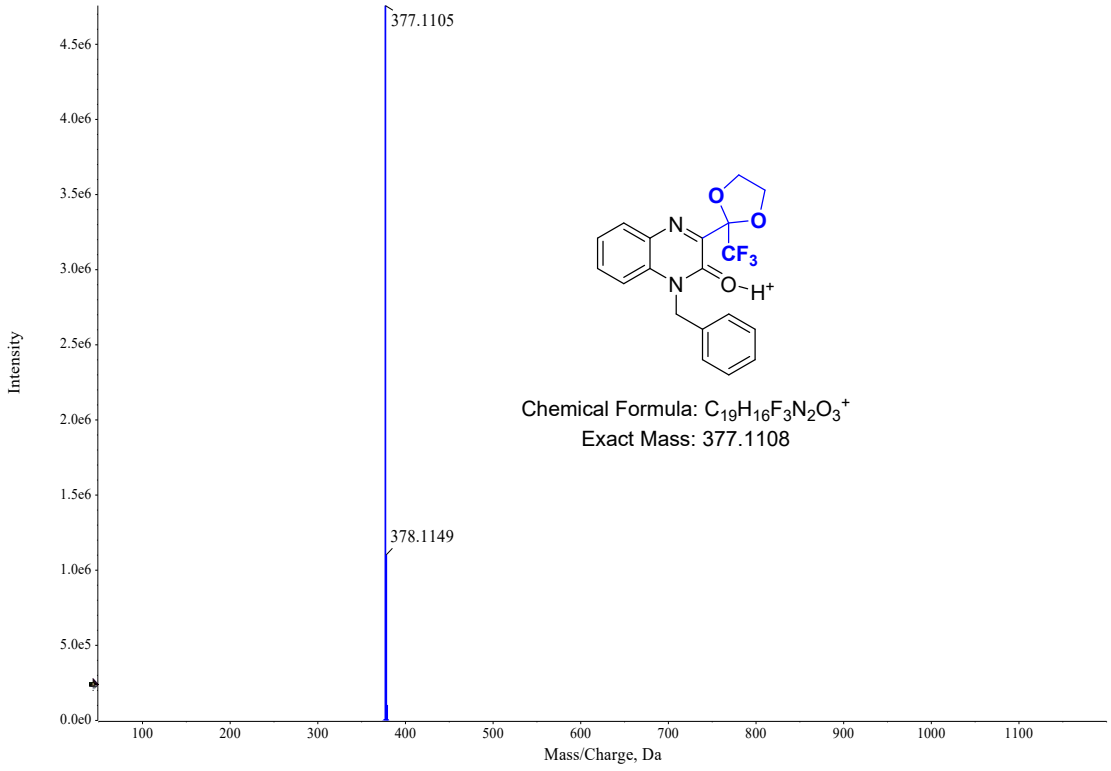
Compound 3k (^{1}H NMR, 500 Hz, $CDCl_3$; ^{19}F NMR 471 Hz, $CDCl_3$ ^{13}C NMR, 101 Hz, $CDCl_3$)





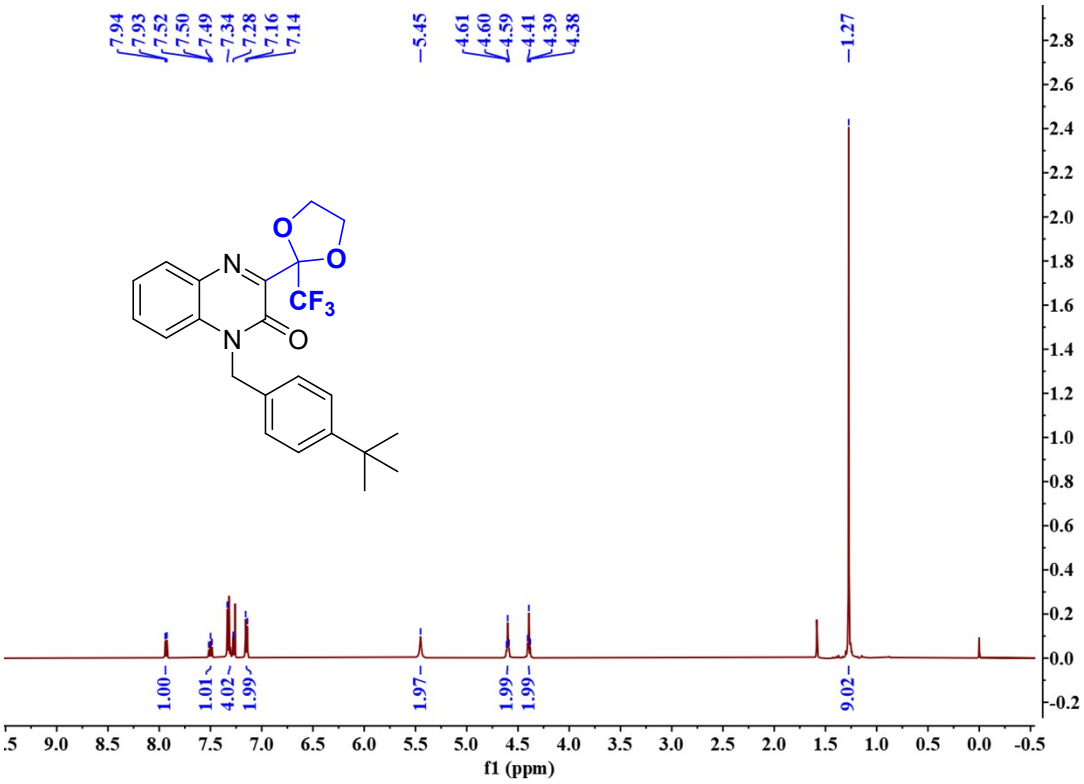


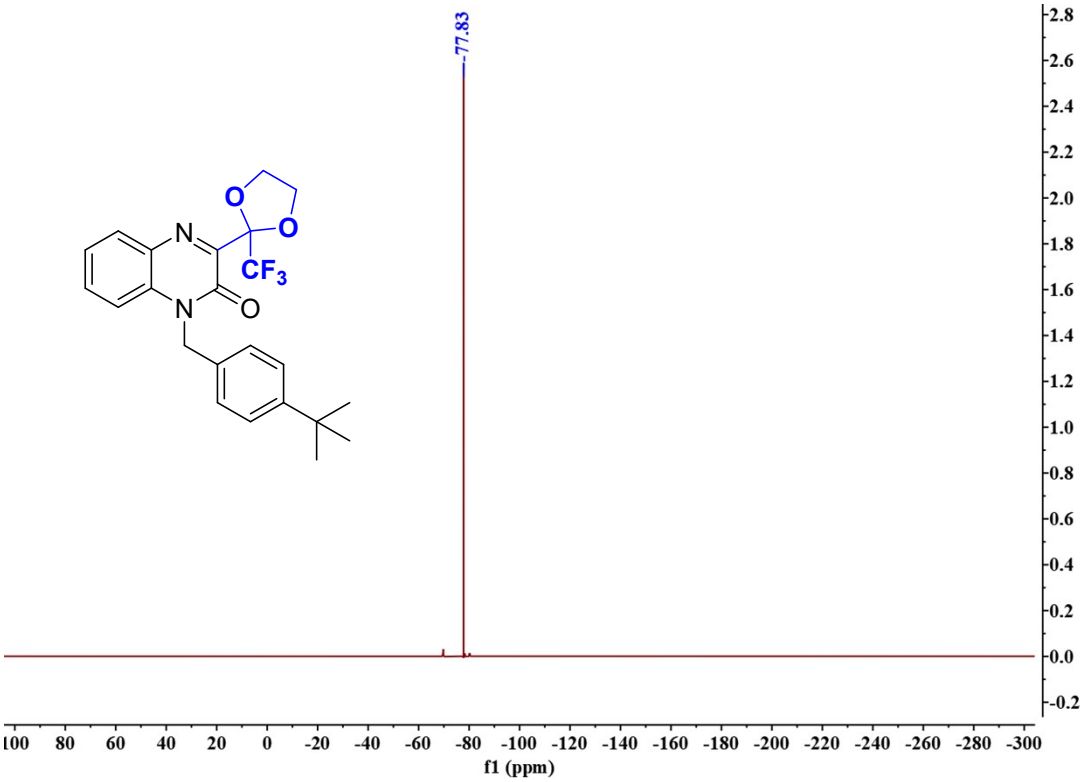
Spectrum from 13.wiff (sample 1) - Sample013, Experiment 1, +TOF MS (CE=10) (50 - 1200) from 0.591 to 0.606 min

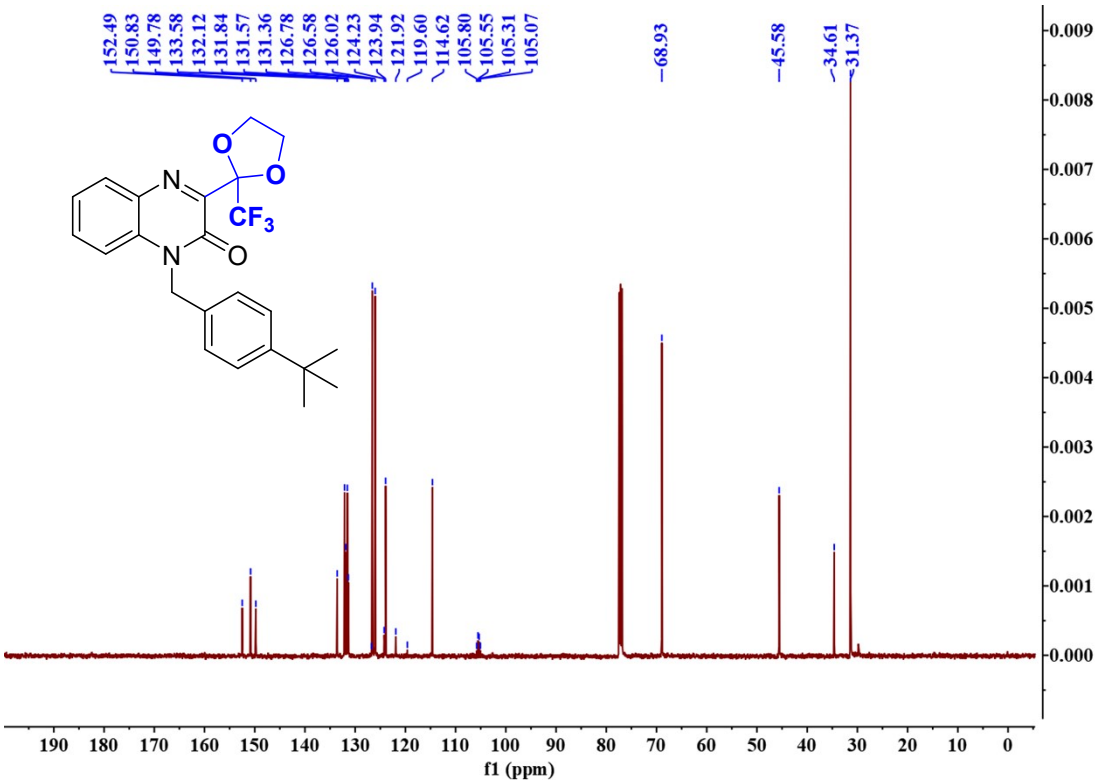


Chemical Formula: $C_{19}H_{16}F_3N_2O_3^+$
Exact Mass: 377.1108

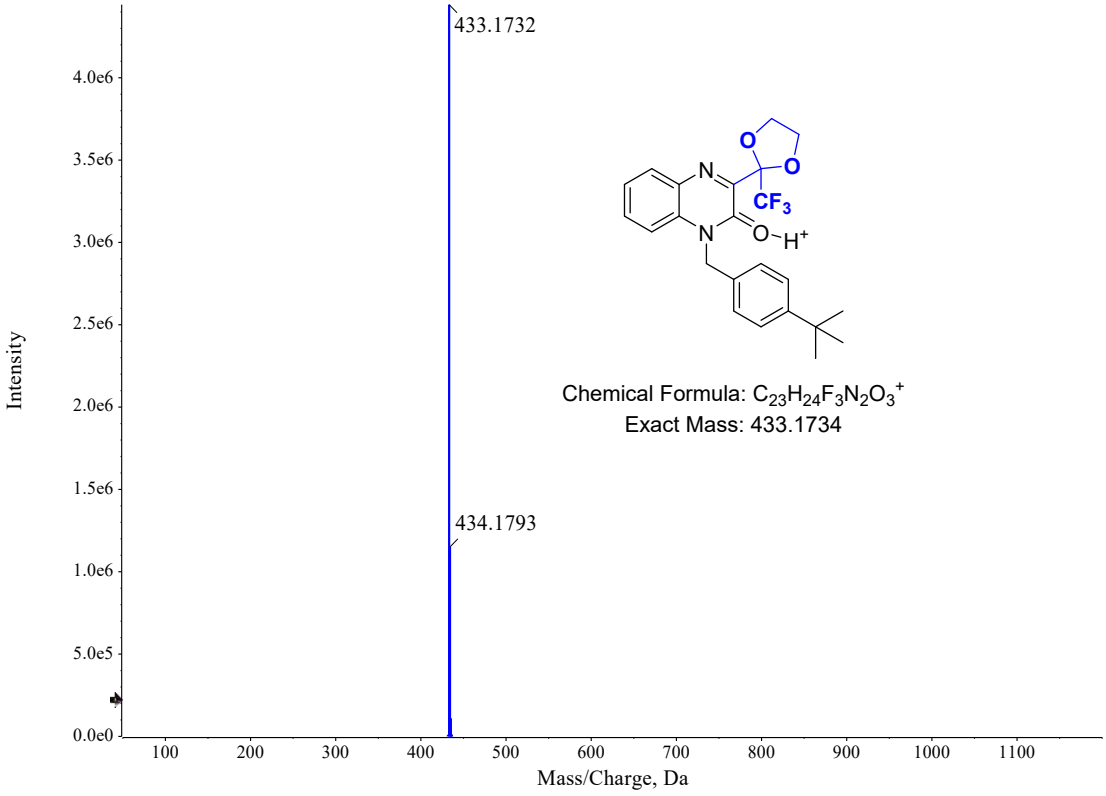
Compound 3l (^{1}H NMR, 500 Hz, $CDCl_3$; ^{19}F NMR 471 Hz, $CDCl_3$ ^{13}C NMR, 101 Hz, $CDCl_3$)



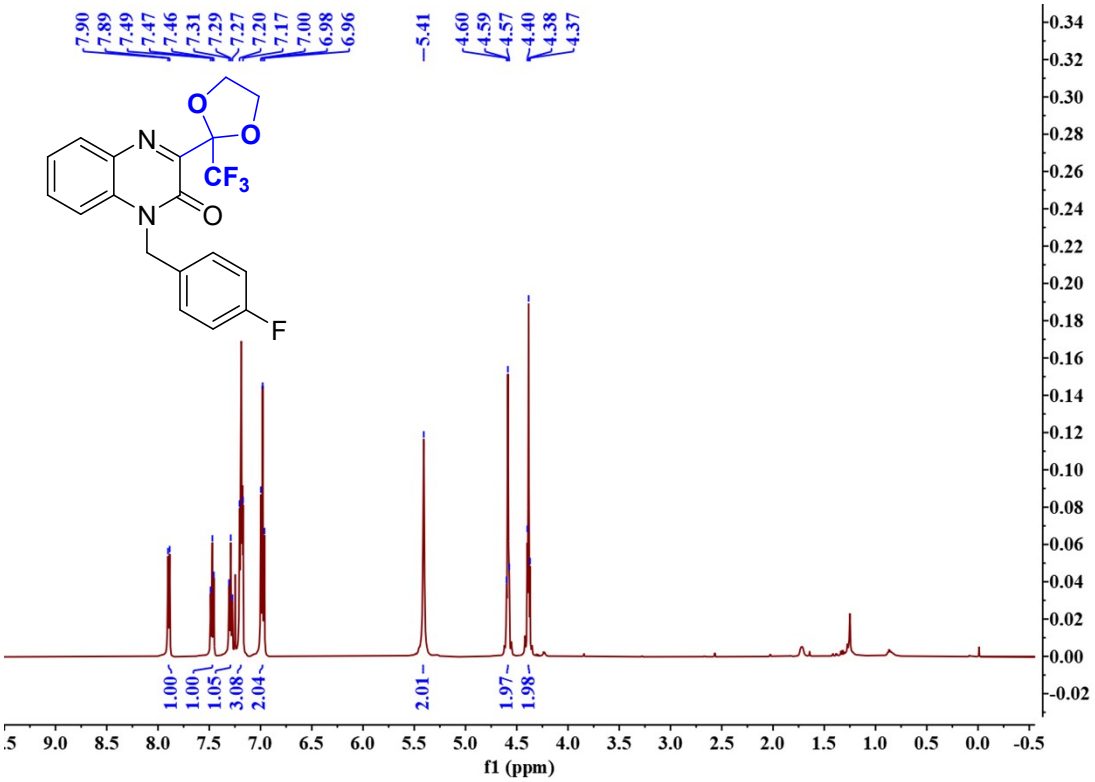


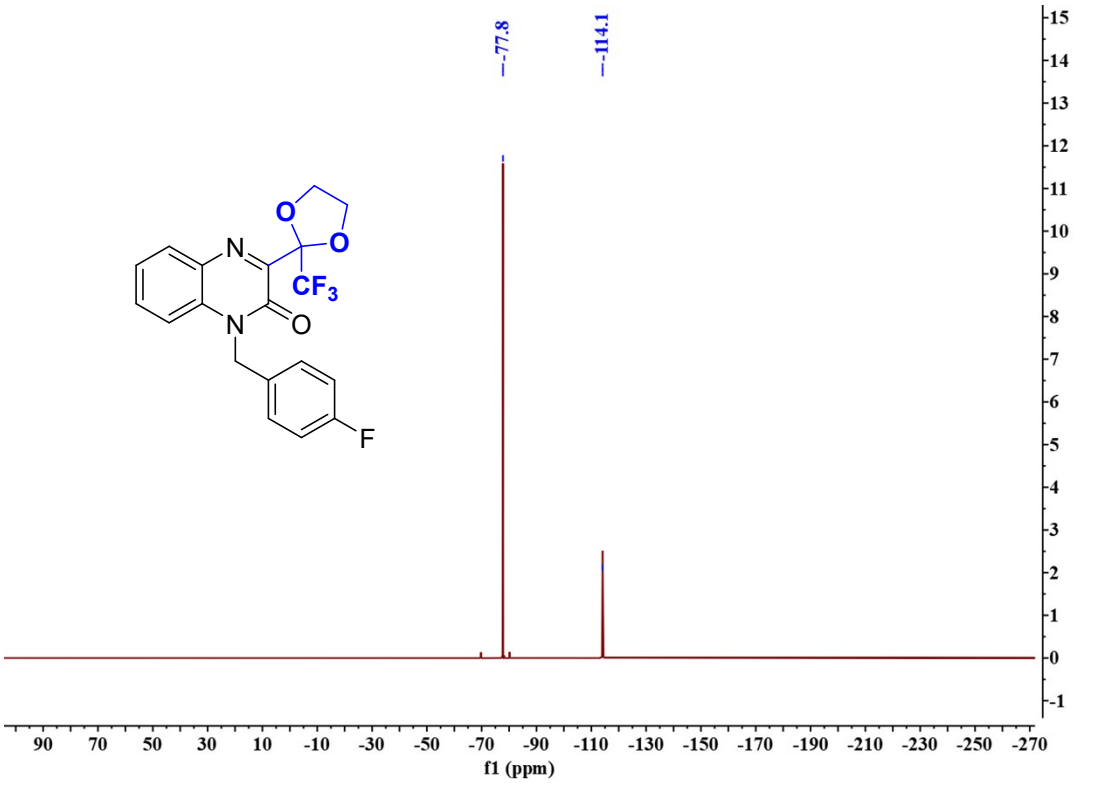


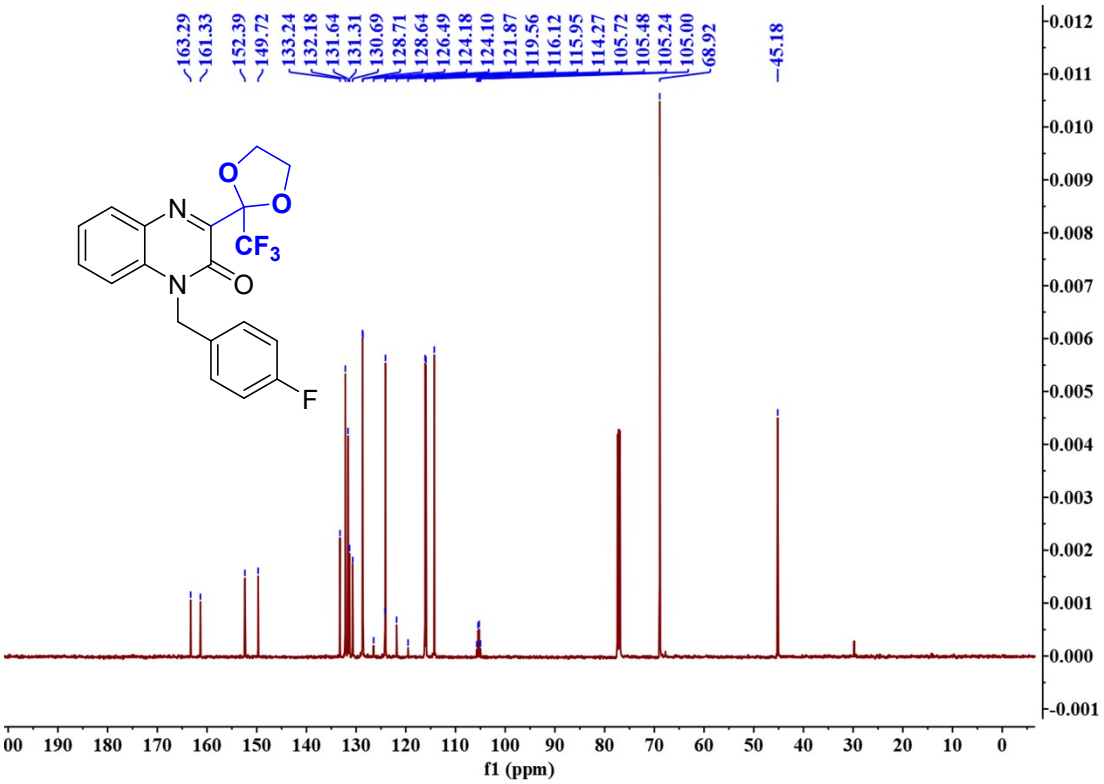
Spectrum from 14.wiff (sample 1) - Sample014, Experiment 1, +TOF MS (CE=10) (50 - 1200) from 0.826 to 0.840 min



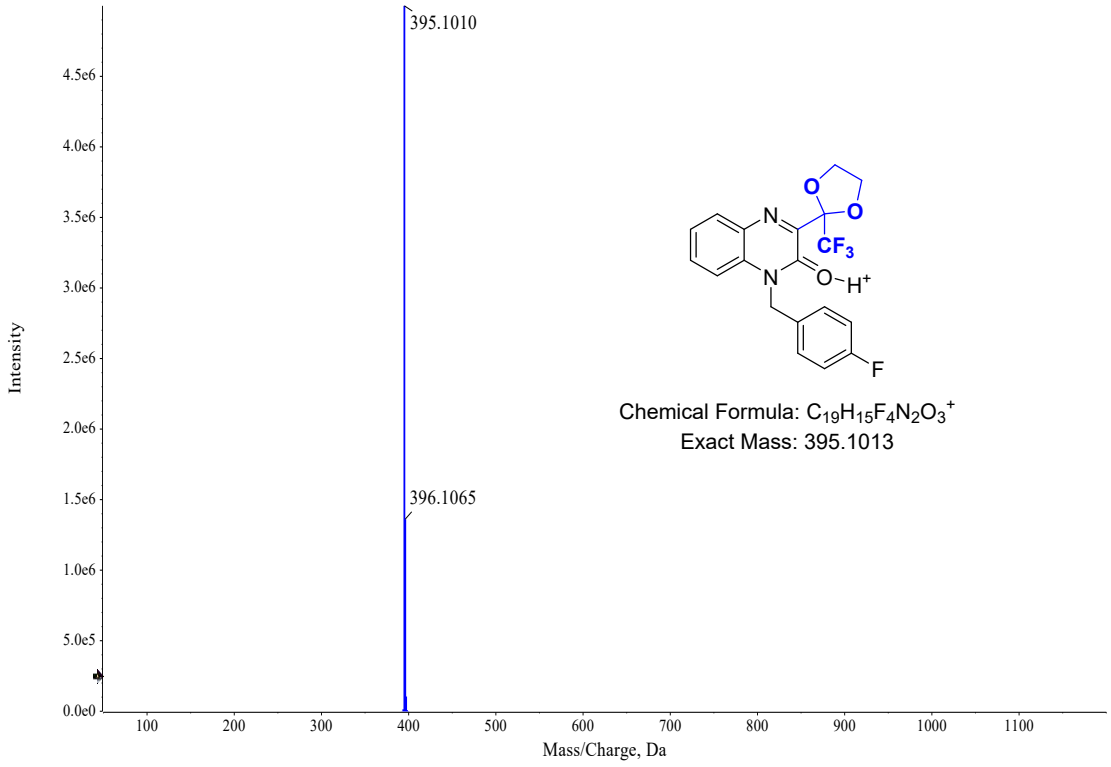
Compound 3m (^{1}H NMR, 500 Hz, $CDCl_3$; ^{19}F NMR 471 Hz, $CDCl_3$ ^{13}C NMR, 101 Hz, $CDCl_3$)





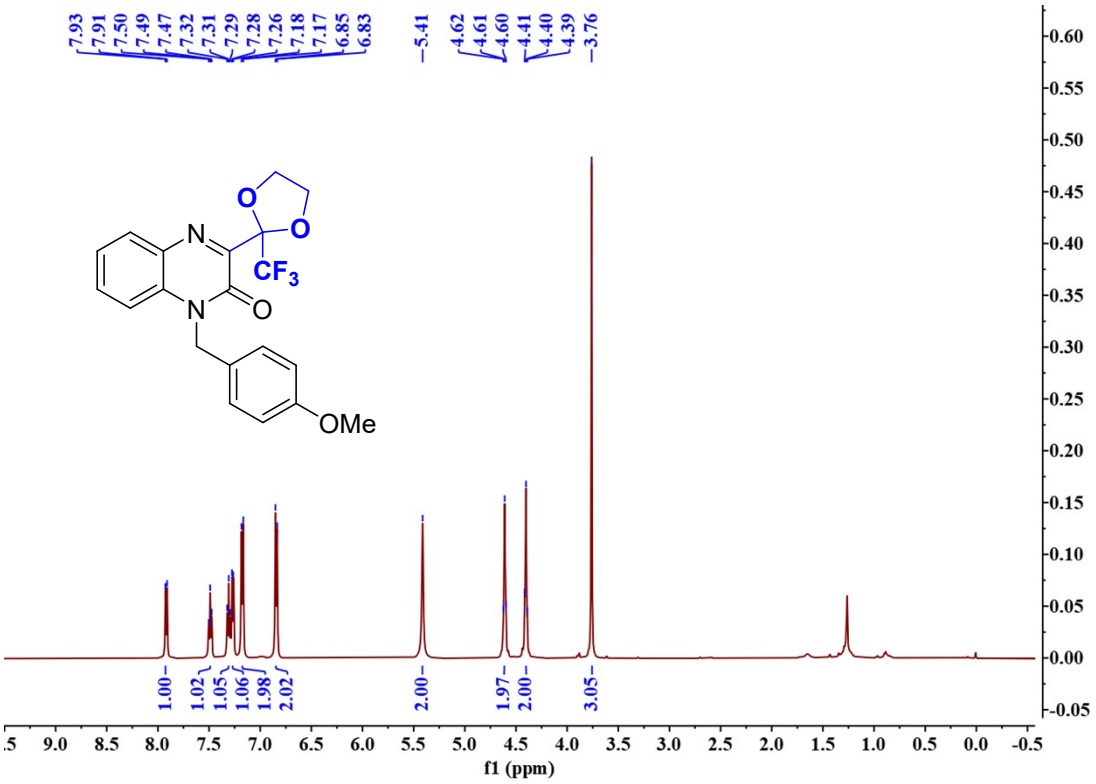


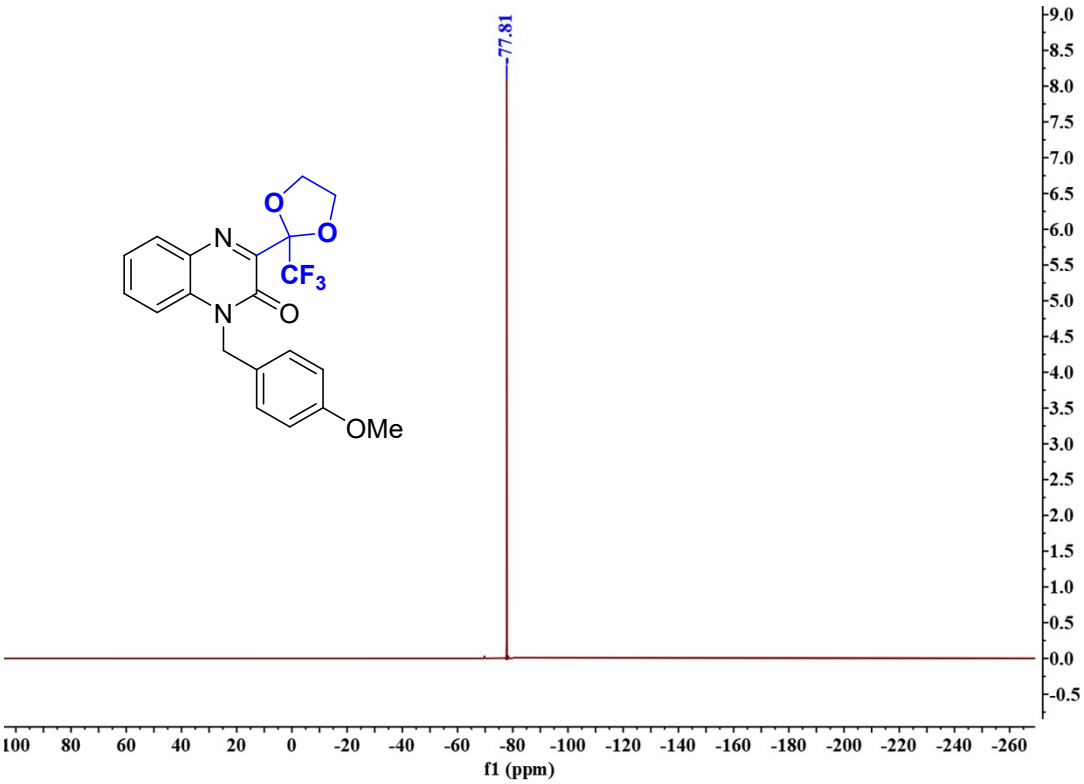
Spectrum from 16.wiff (sample 1) - Sample016, Experiment 1, +TOF MS (CE=10) (50 - 1200) from 0.620 to 0.635 min

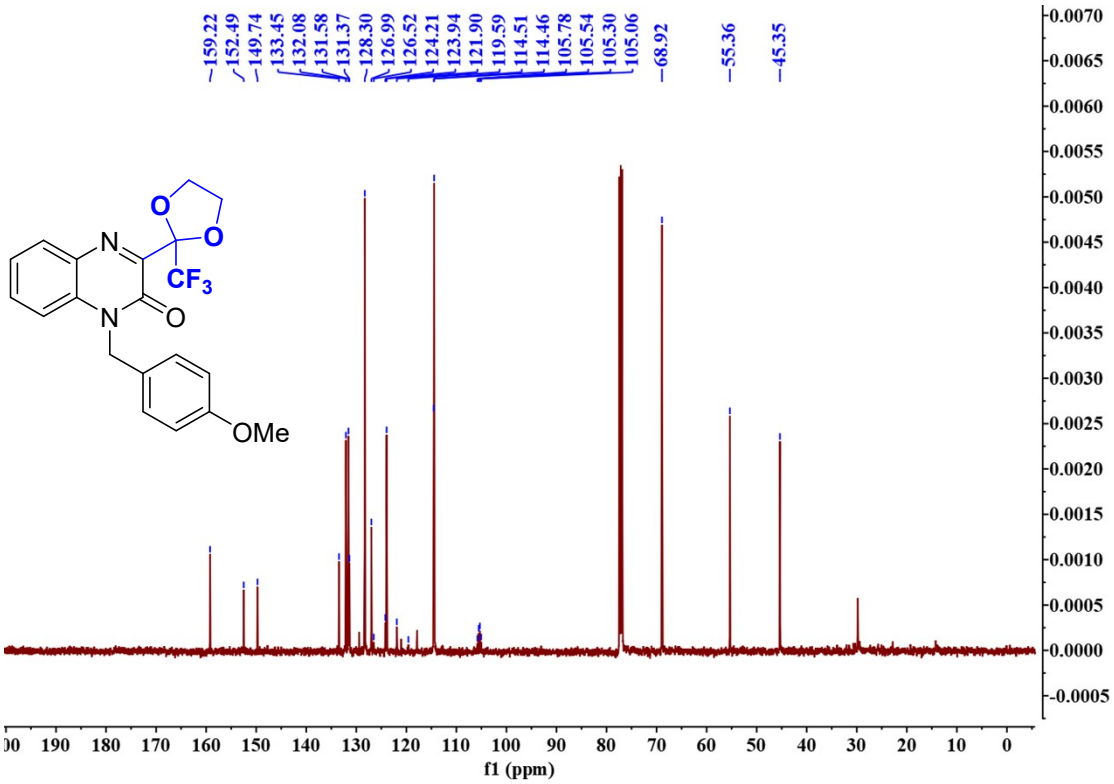


Chemical Formula: $C_{19}H_{15}F_4N_2O_3^+$
Exact Mass: 395.1013

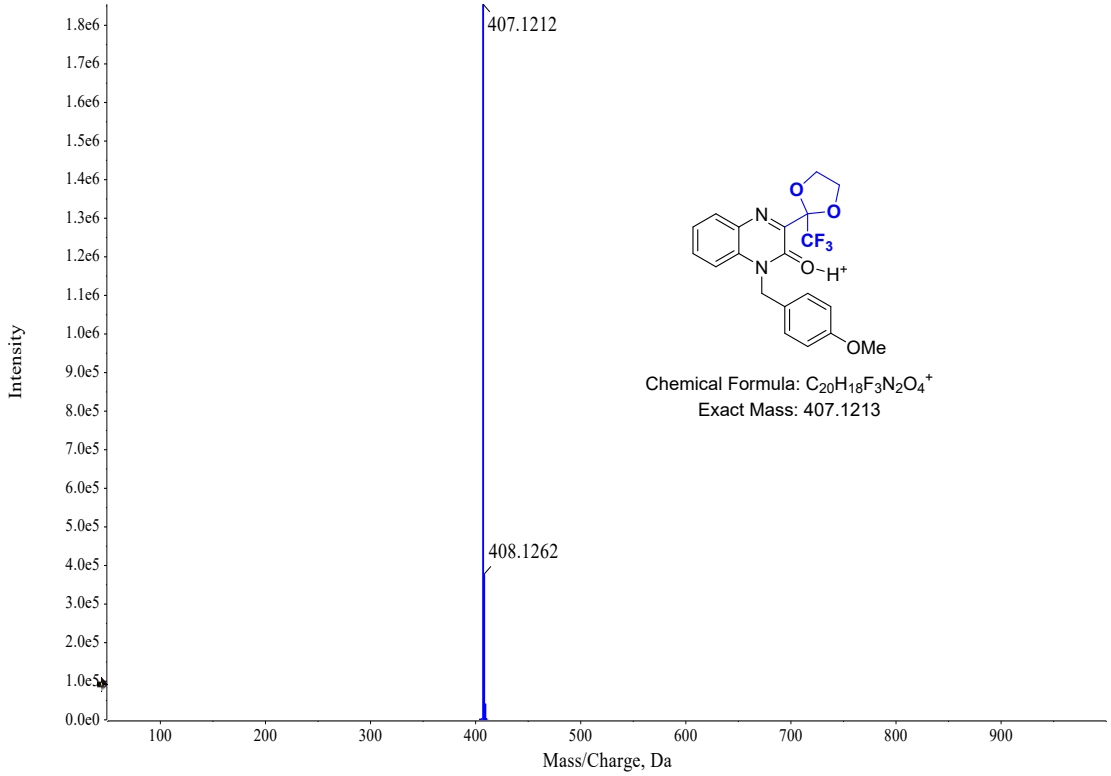
Compound 3n (^{1}H NMR, 500 Hz, $CDCl_3$; ^{19}F NMR 471 Hz, $CDCl_3$ ^{13}C NMR, 101 Hz, $CDCl_3$)



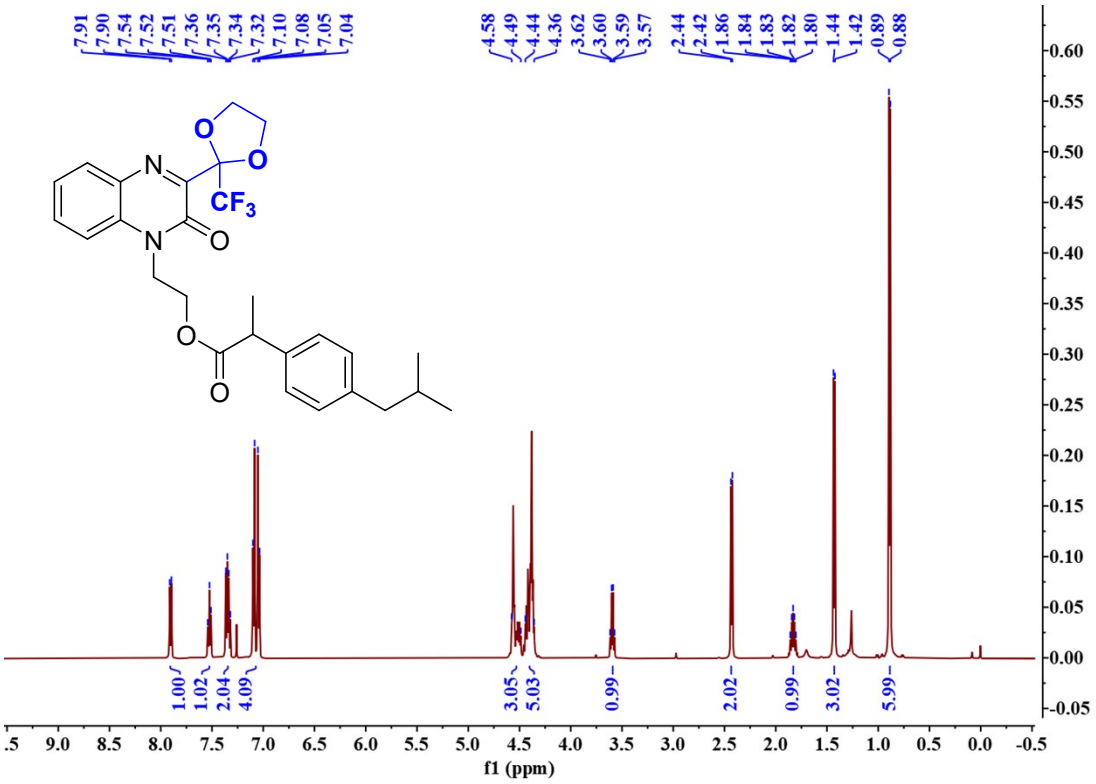


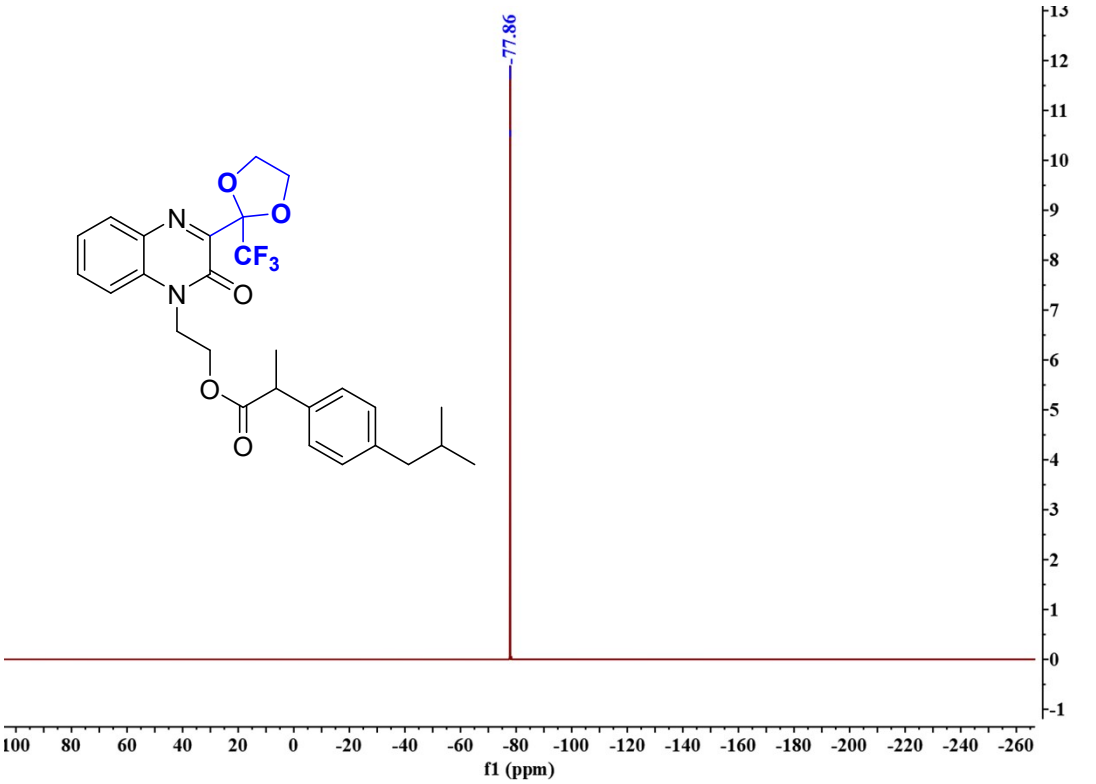


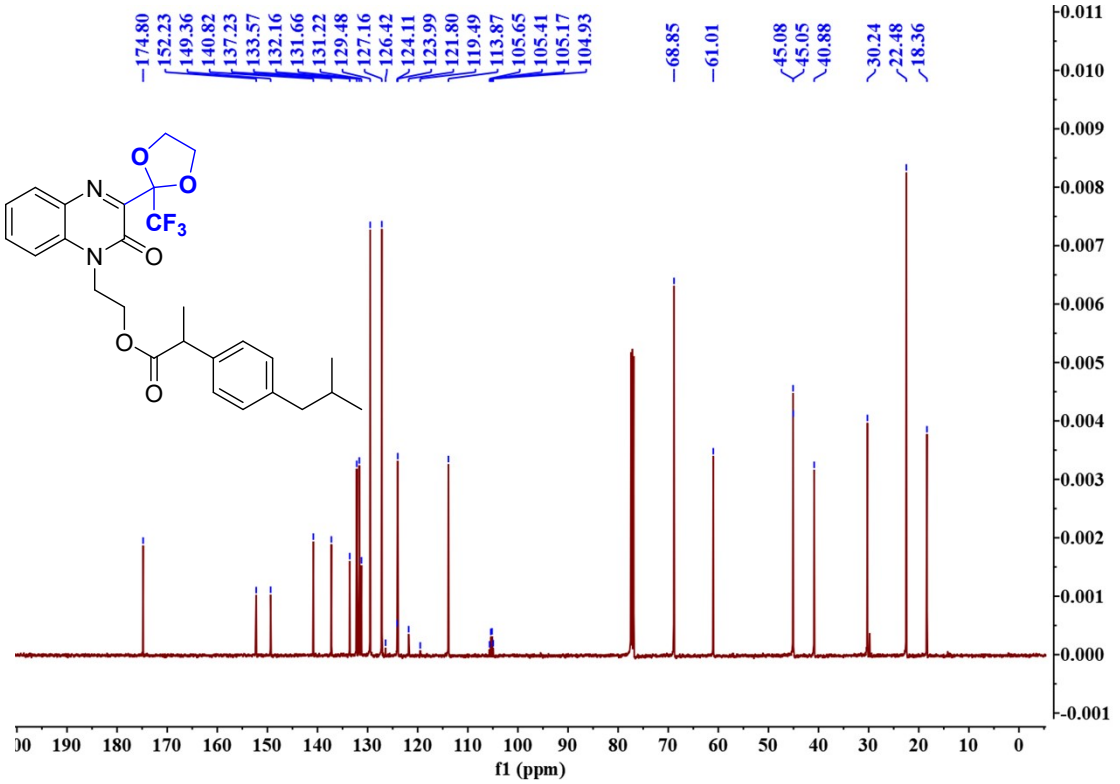
Spectrum from 4.wiff (sample 1) - Sample004, Experiment 1, +TOF MS (CE=10) (50 - 1000) from 0.599 to 0.613 min

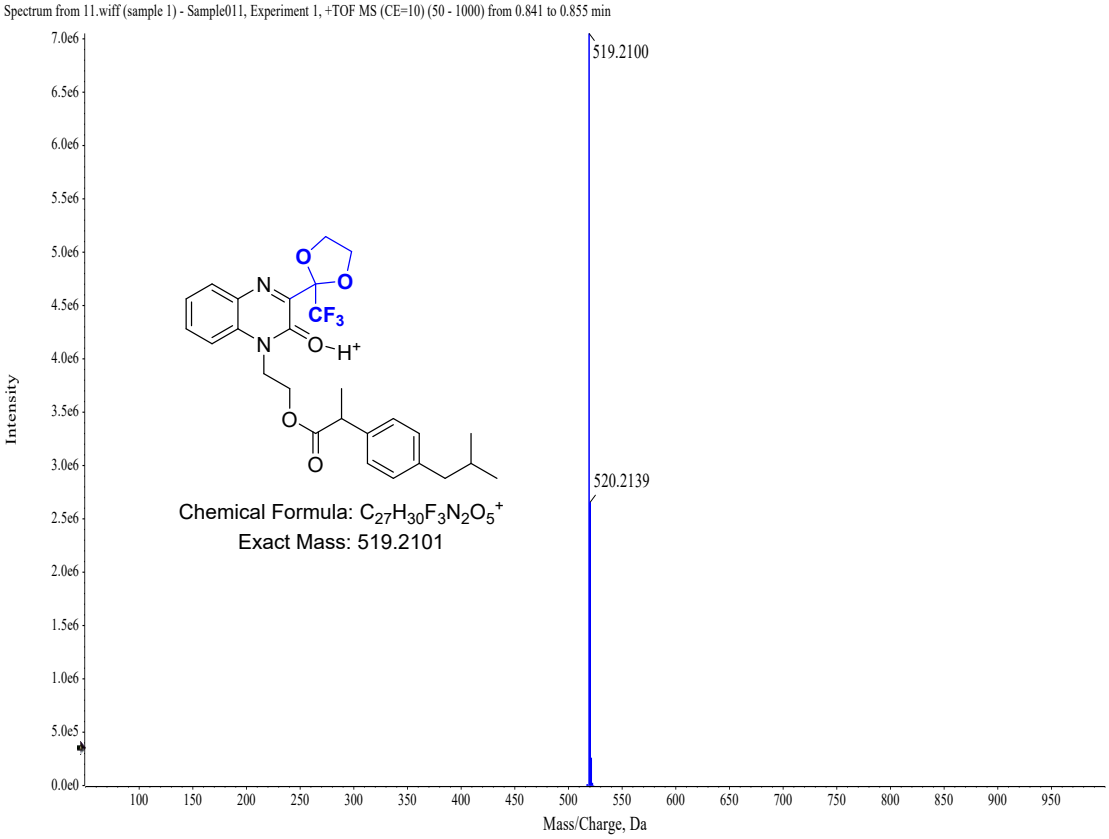


Compound 3o (^{1}H NMR, 500 Hz, $CDCl_3$; ^{19}F NMR 471 Hz, $CDCl_3$ ^{13}C NMR, 101 Hz, $CDCl_3$)

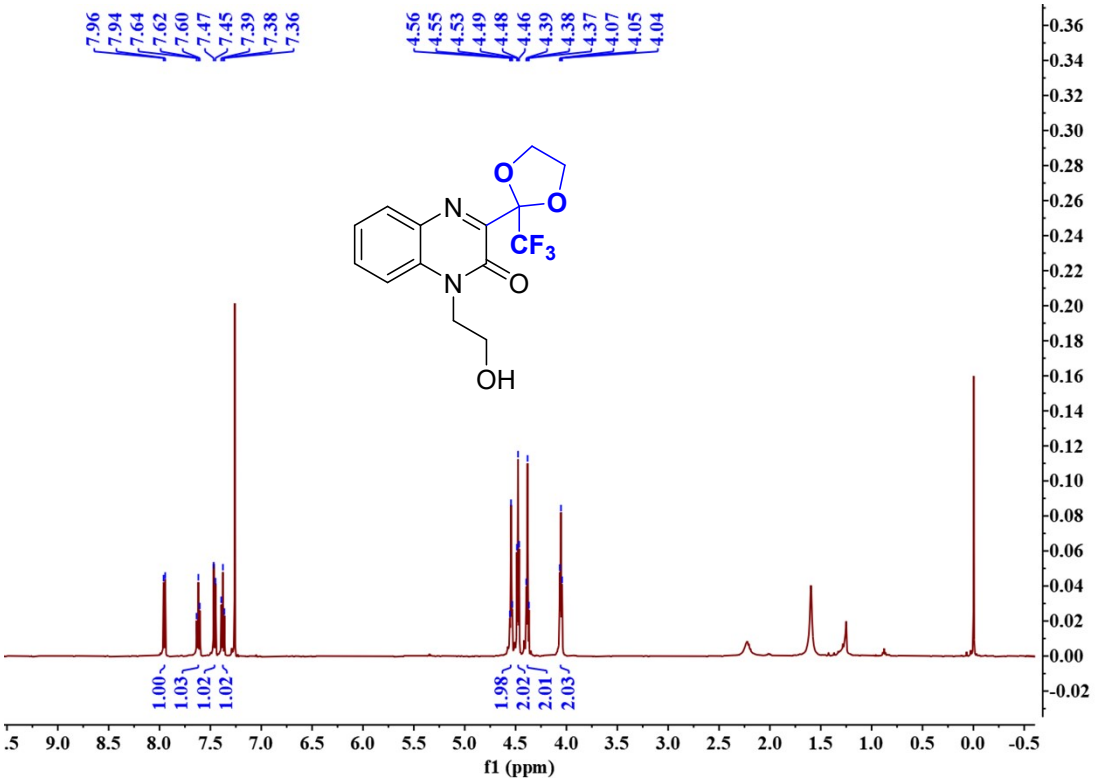


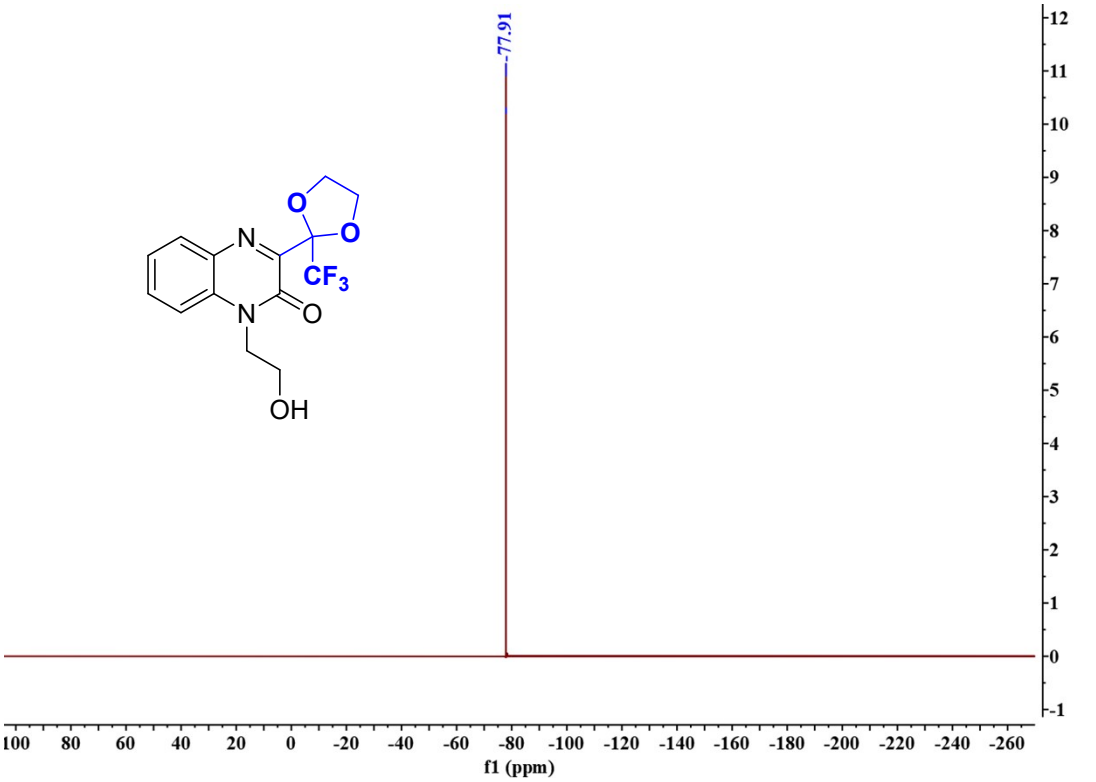


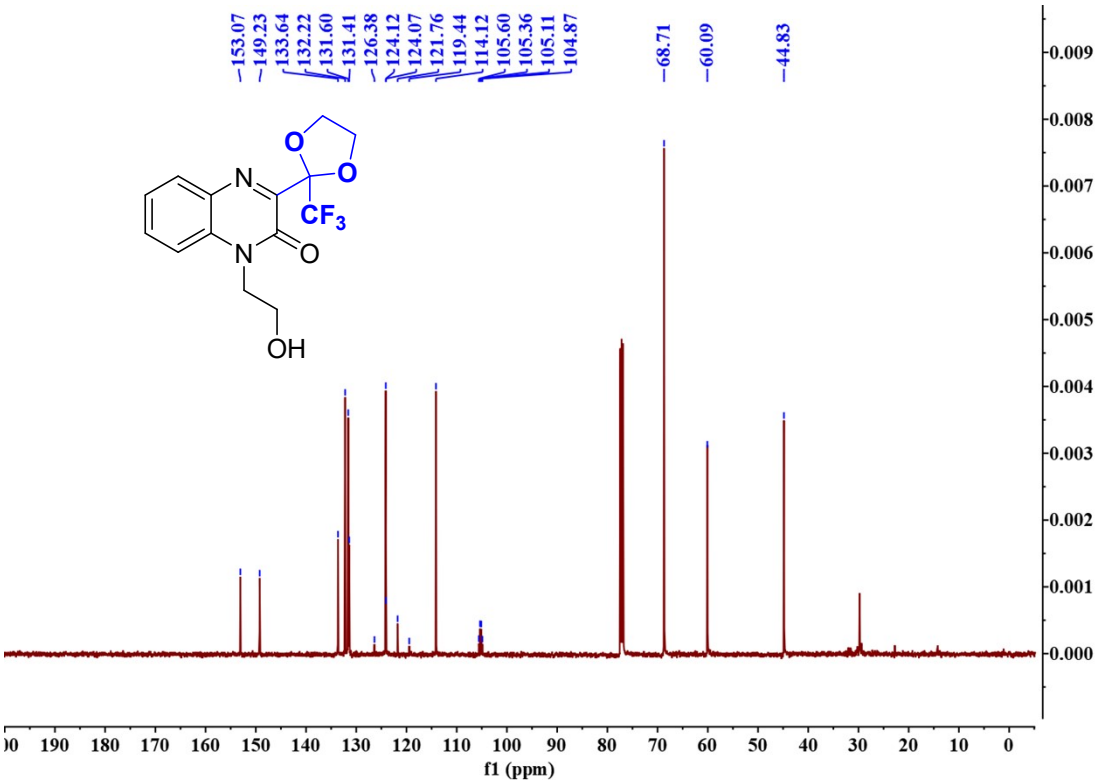

174.80
152.23
149.36
140.82
137.23
133.57
132.16
131.66
131.22
129.48
127.16
126.42
124.11
123.99
121.80
119.49
113.87
105.65
105.41
105.17
104.93
68.85
61.01
45.08
45.05
40.88
30.24
22.48
18.36
O
O
N
CF3
N
O
O
O
0.011
0.010
0.009
0.008
0.007
0.006
0.005
0.004
0.003
0.002
0.001
0.000
-0.001
f1 (ppm)


Spectrum from 11.wiff (sample 1) - Sample011, Experiment 1, +TOF MS (CE=10) (50 - 1000) from 0.841 to 0.855 min
519.2100
520.2139
Intensity
Mass/Charge, Da
O
O
N
CF3
N
O-H+
O
O
Chemical Formula: C27H30F3N2O5+
Exact Mass: 519.2101

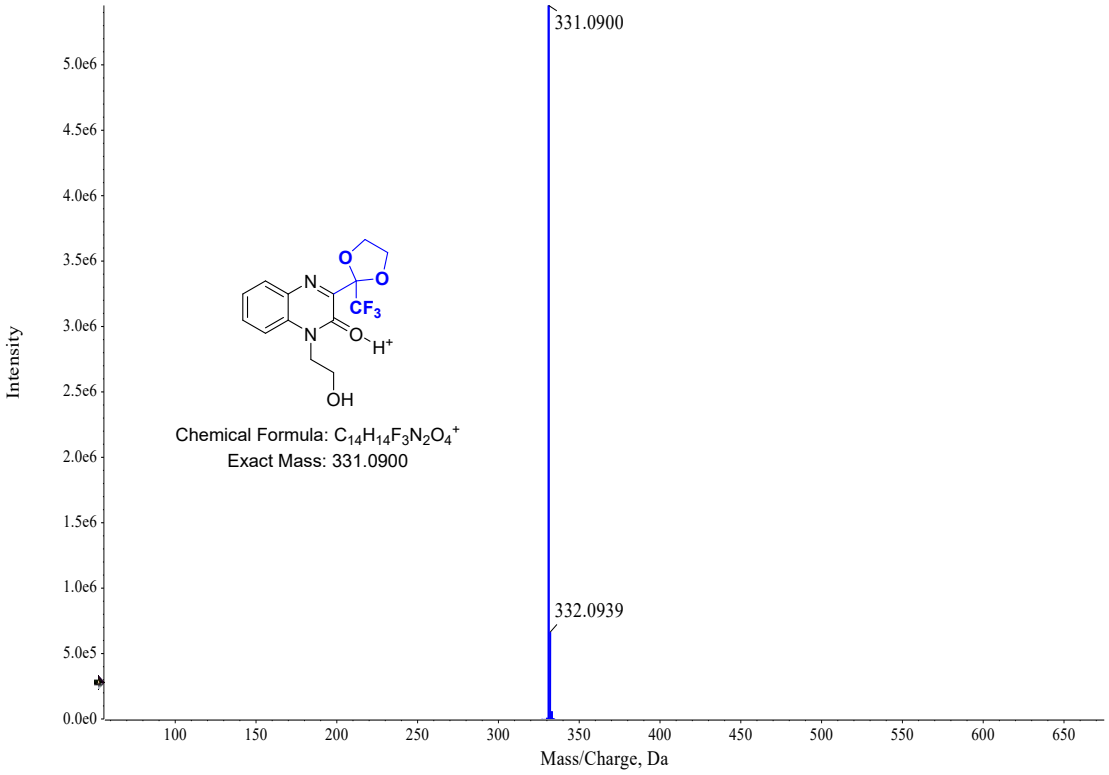
Compound 3p (^{1}H NMR, 500 Hz, $CDCl_3$; ^{19}F NMR 471 Hz, $CDCl_3$ ^{13}C NMR, 101 Hz, $CDCl_3$)



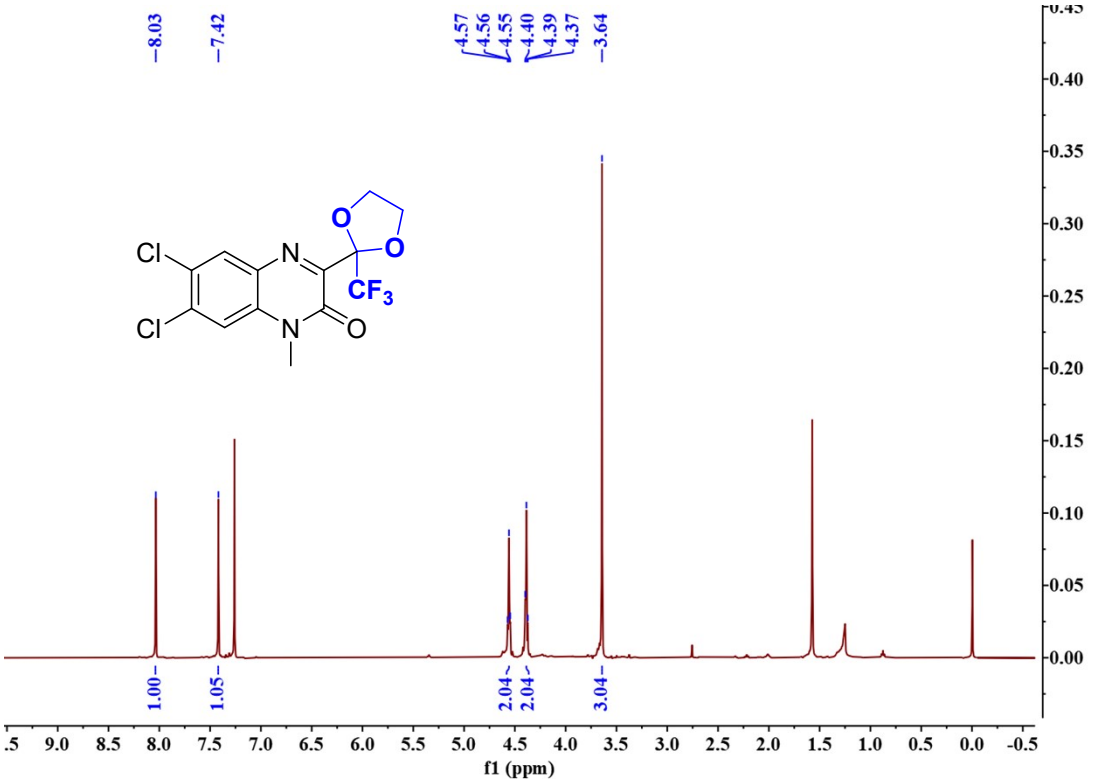


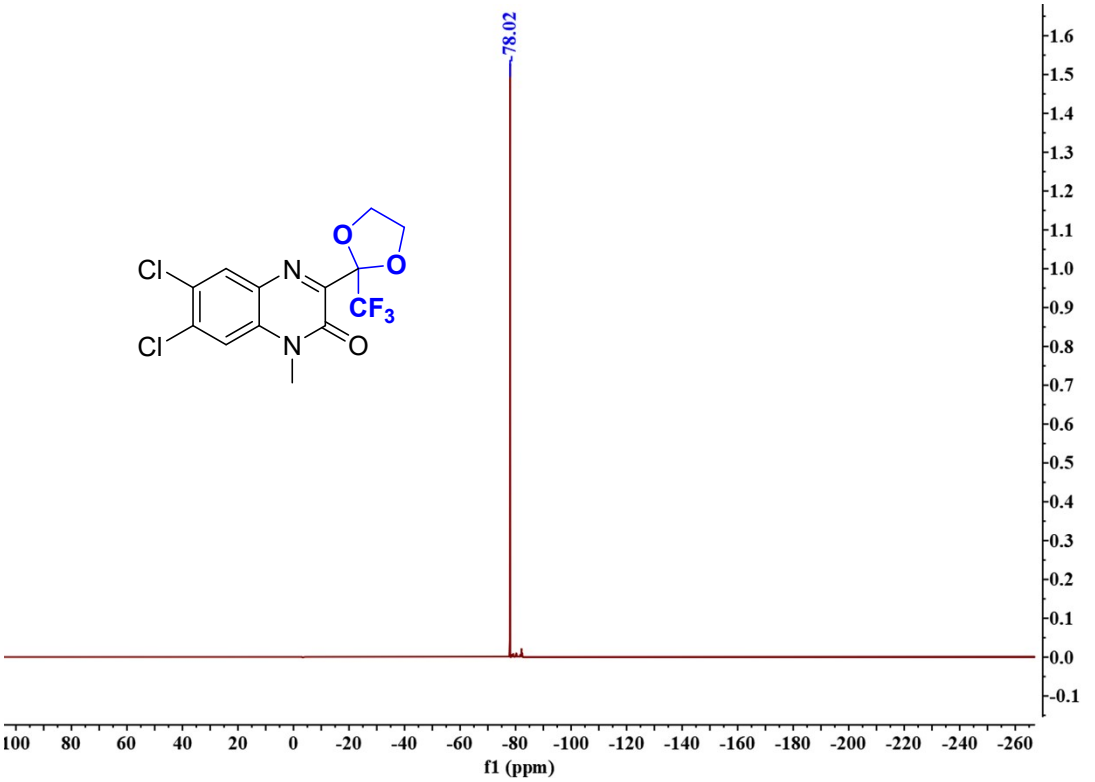


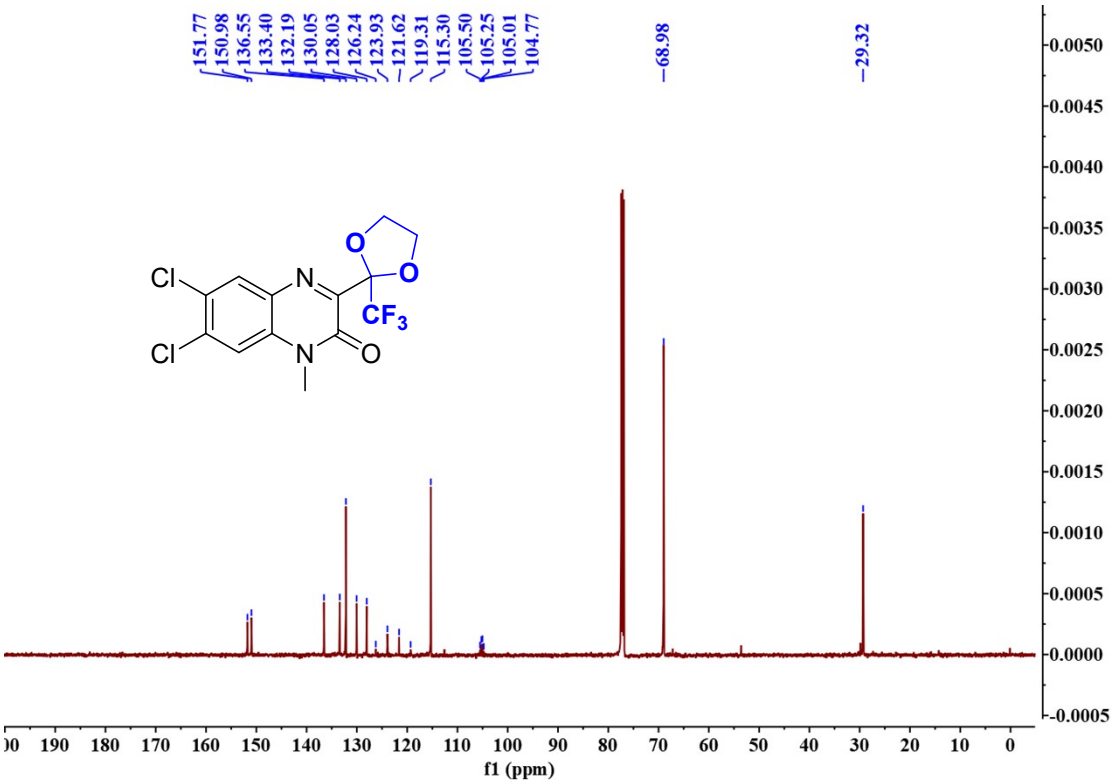
Spectrum from 3.wiff (sample 1) - Sample003, Experiment 1, +TOF MS (CE=10) (50 - 1000) from 0.533 to 0.547 min



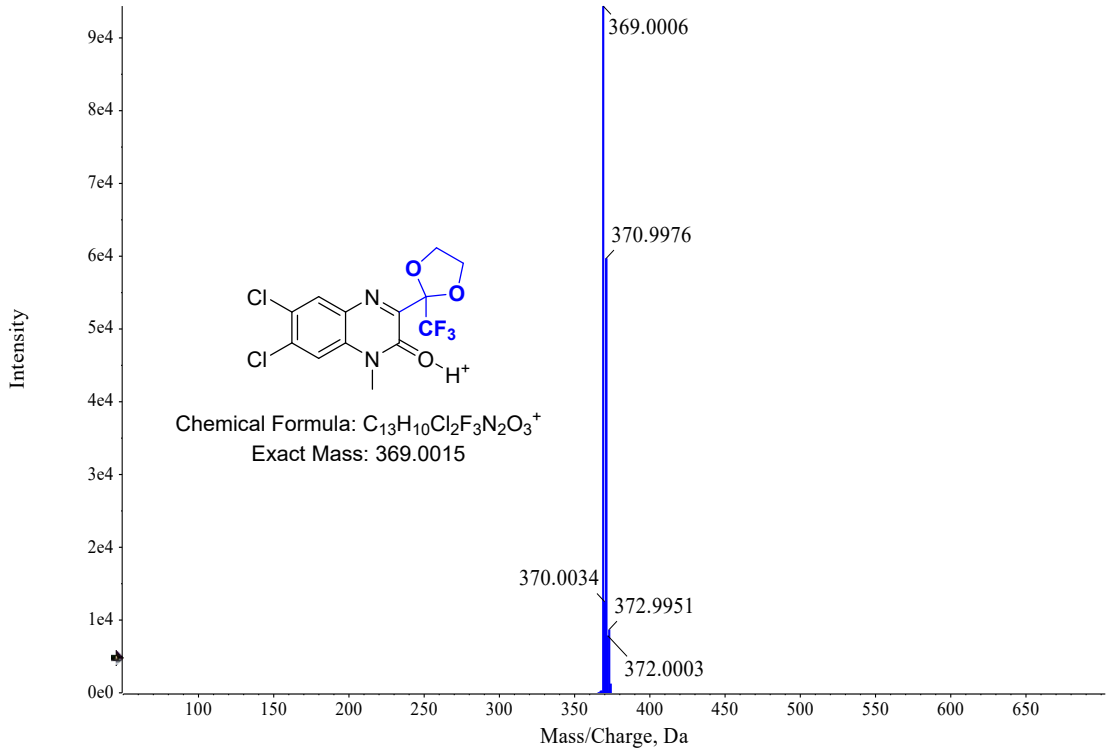
Compound 3q (^{1}H NMR, 500 Hz, $CDCl_3$; ^{19}F NMR 471 Hz, $CDCl_3$ ^{13}C NMR, 101 Hz, $CDCl_3$)



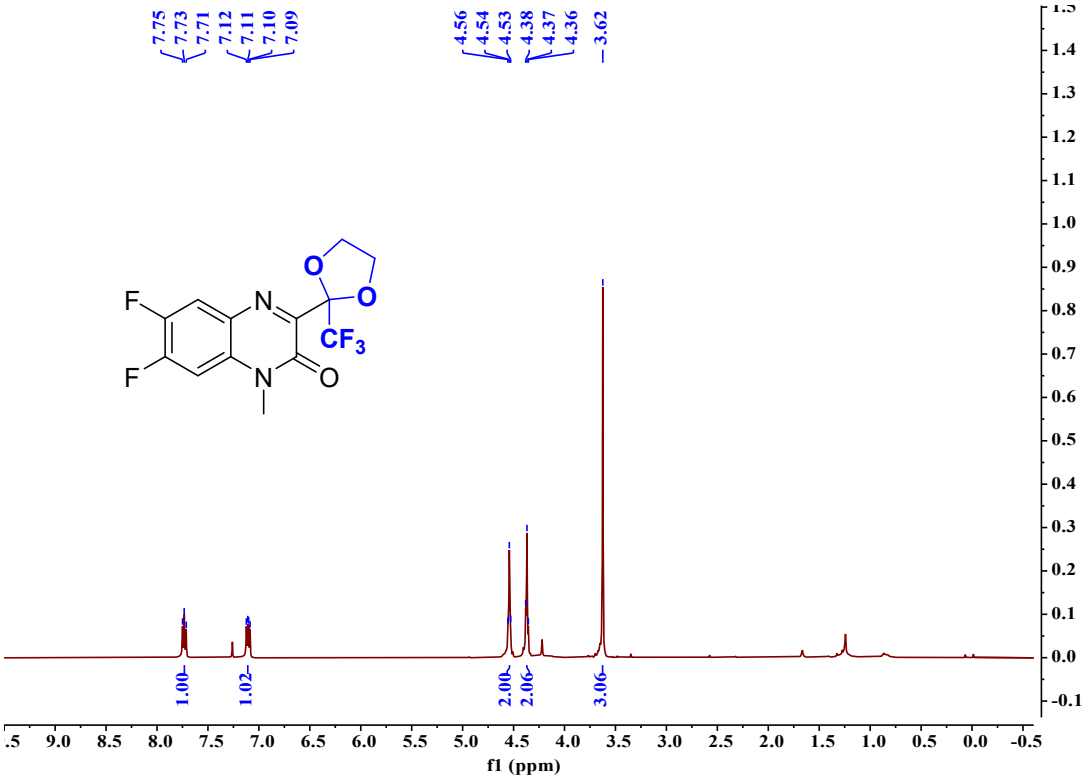


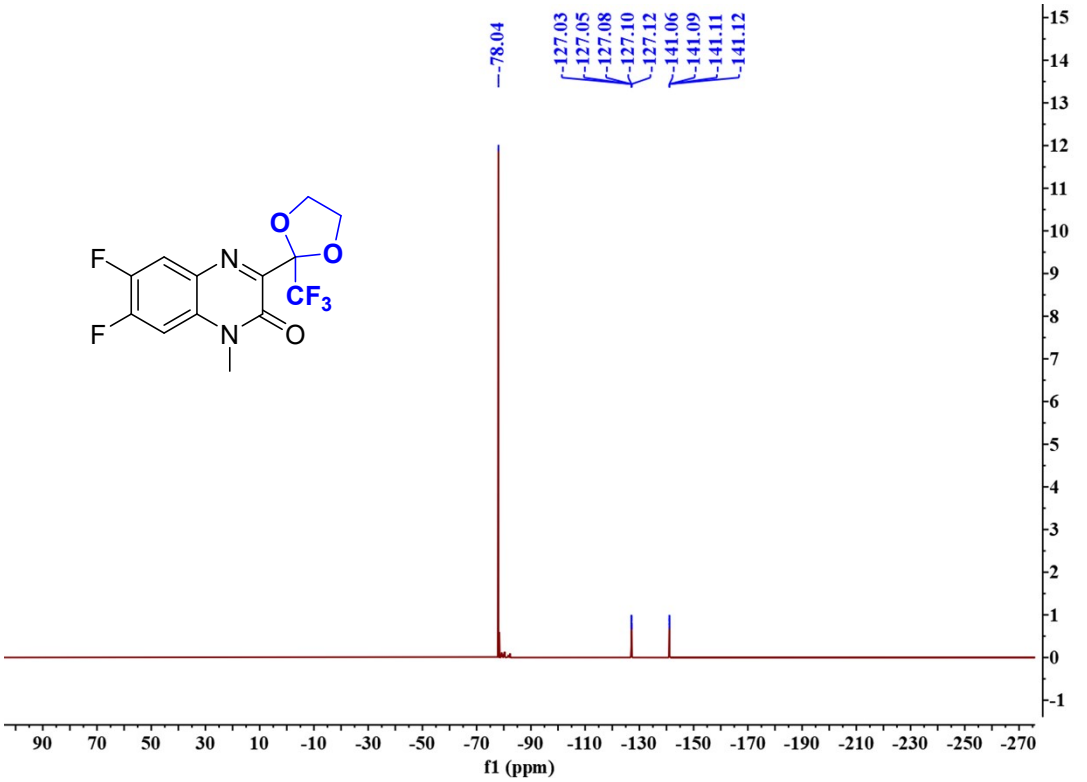


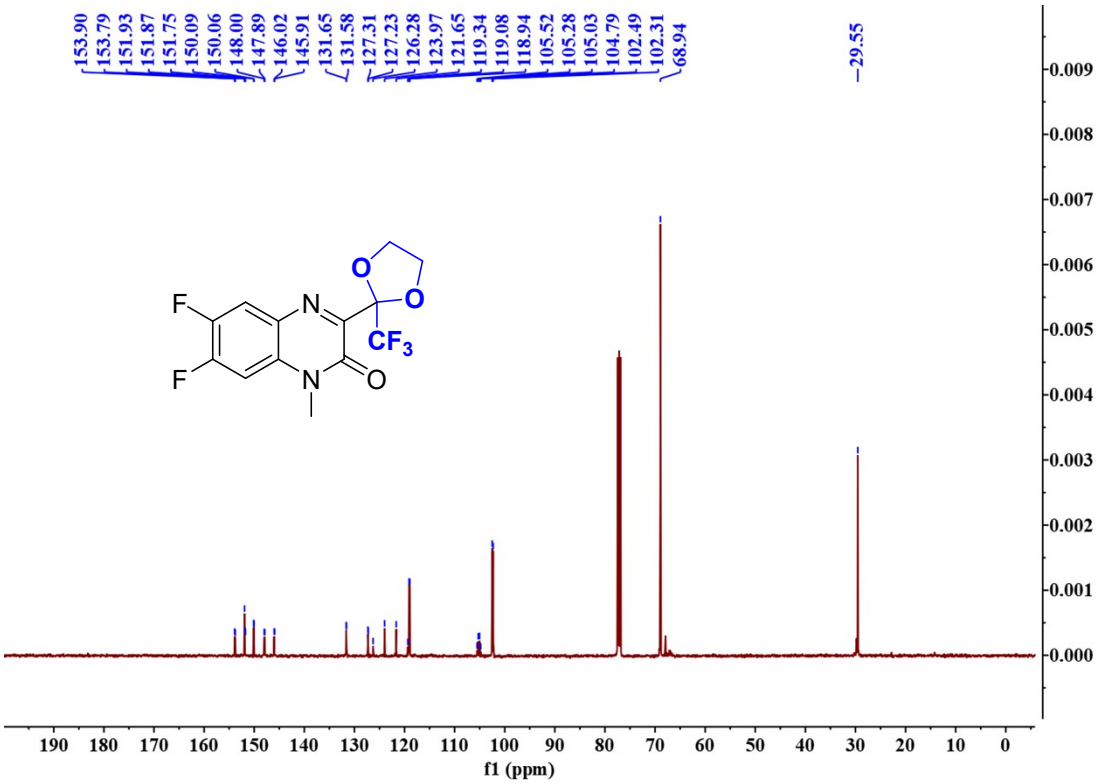
Spectrum from 21.wiff (sample 1) - Sample021, Experiment 1, +TOF MS (CE=10) (50 - 1000) from 0.752 to 0.767 min



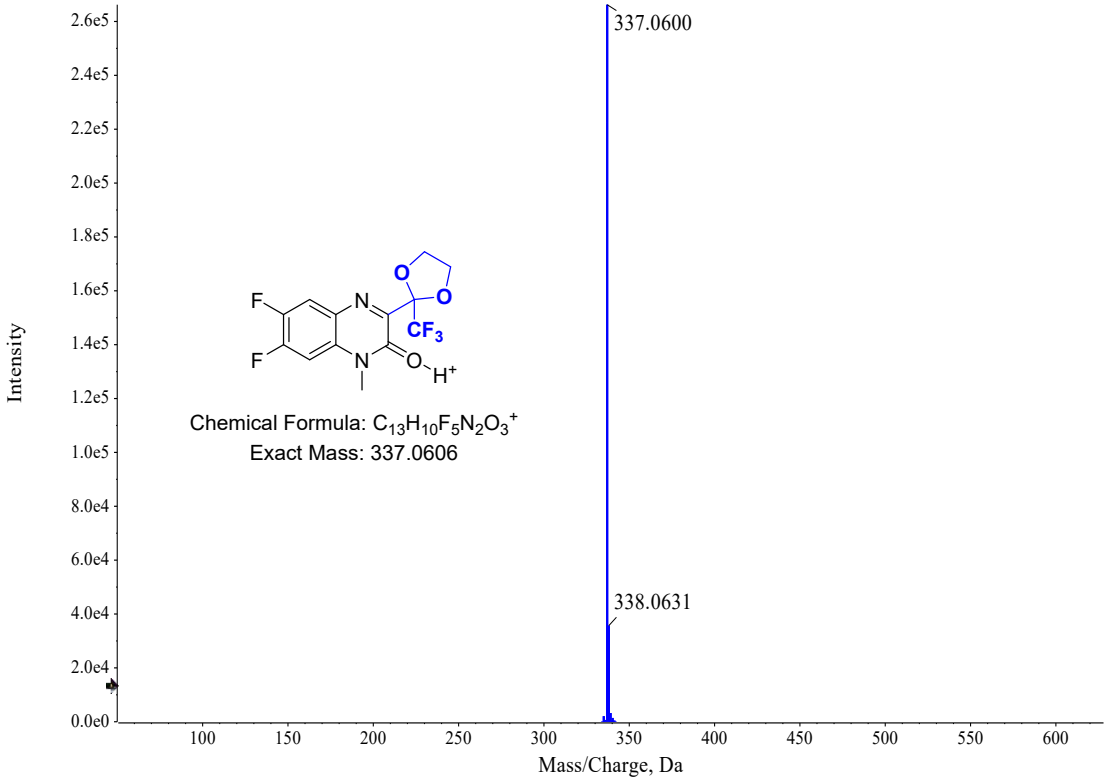
Compound 3r (^{1}H NMR, 500 Hz, $CDCl_3$; ^{19}F NMR 471 Hz, $CDCl_3$ ^{13}C NMR, 101 Hz, $CDCl_3$)



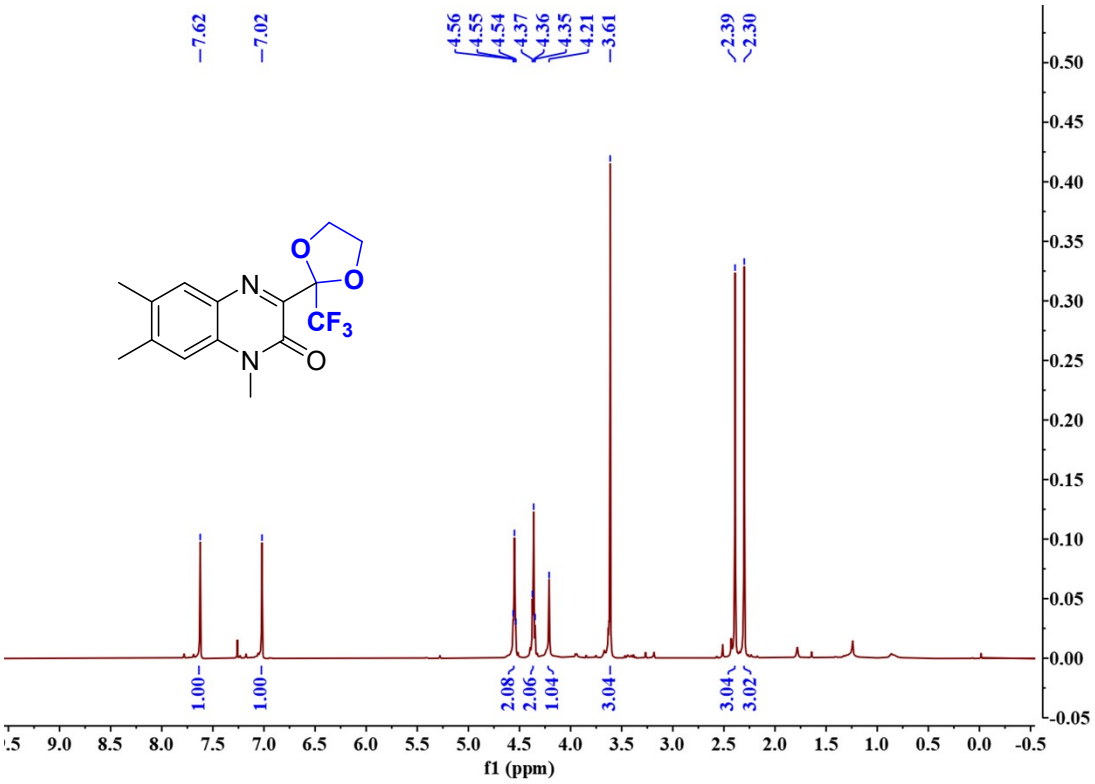


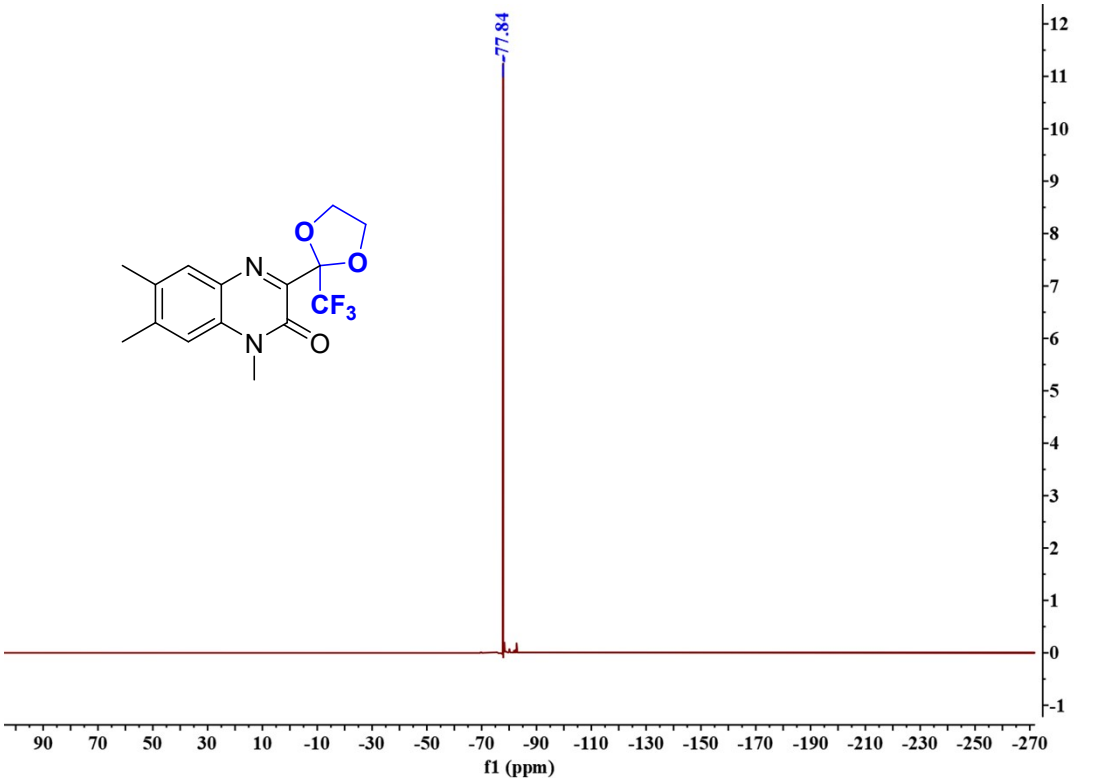


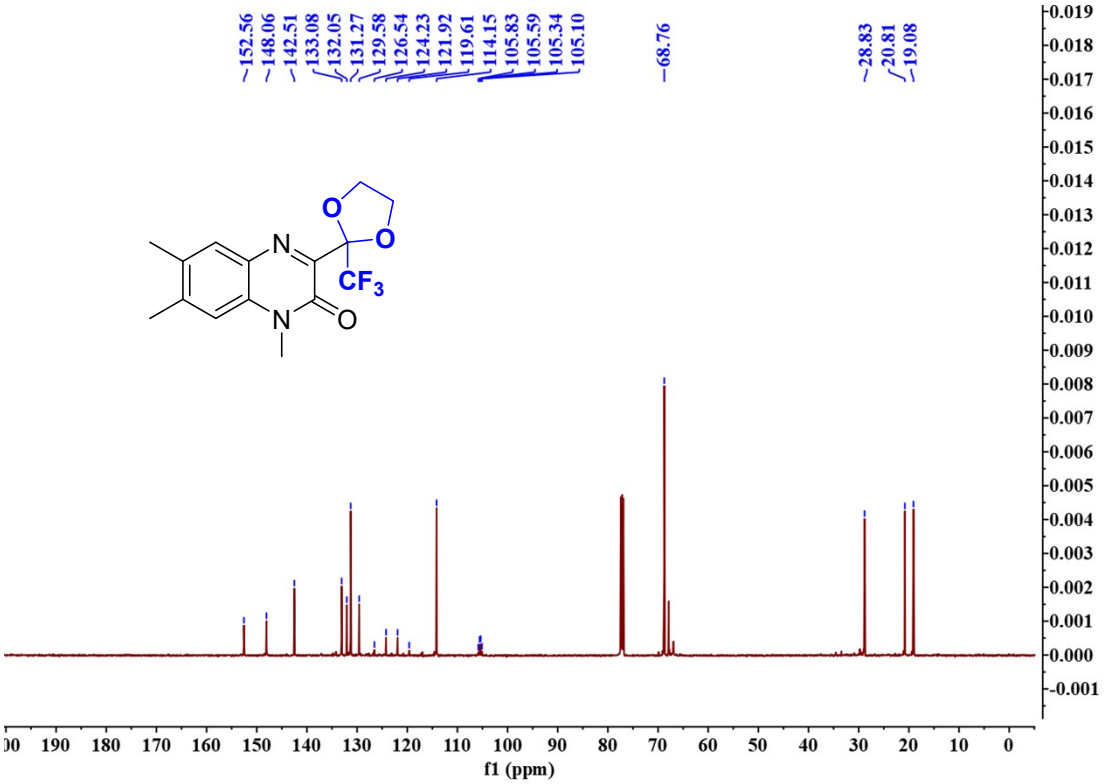
Spectrum from 22.wiff (sample 1) - Sample022, Experiment 1, +TOF MS (CE=10) (50 - 1000) from 0.606 to 0.621 min



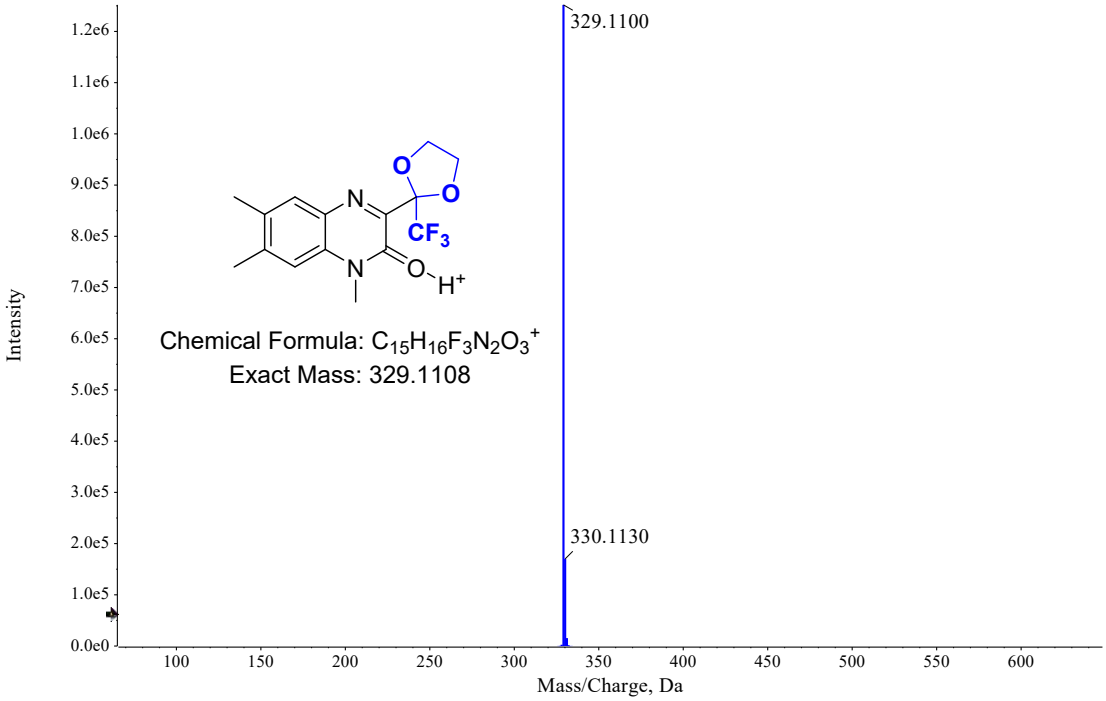
Compound 3s (^{1}H NMR, 500 Hz, $CDCl_3$; ^{19}F NMR 471 Hz, $CDCl_3$ ^{13}C NMR, 101 Hz, $CDCl_3$)



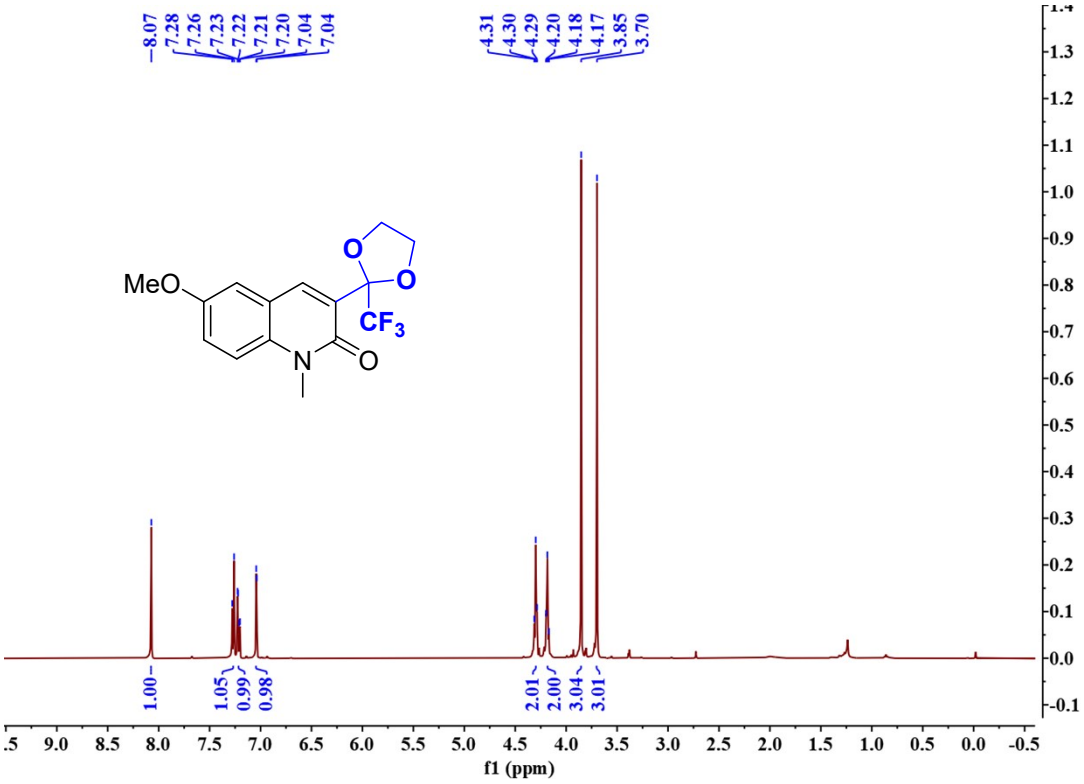


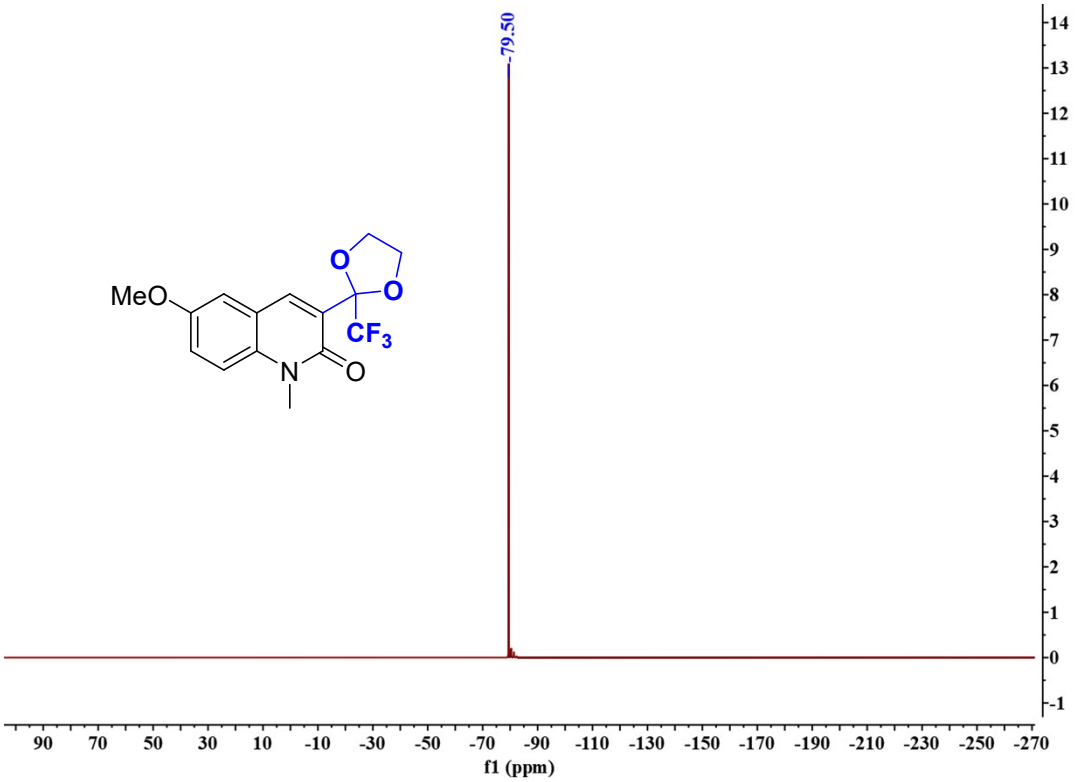


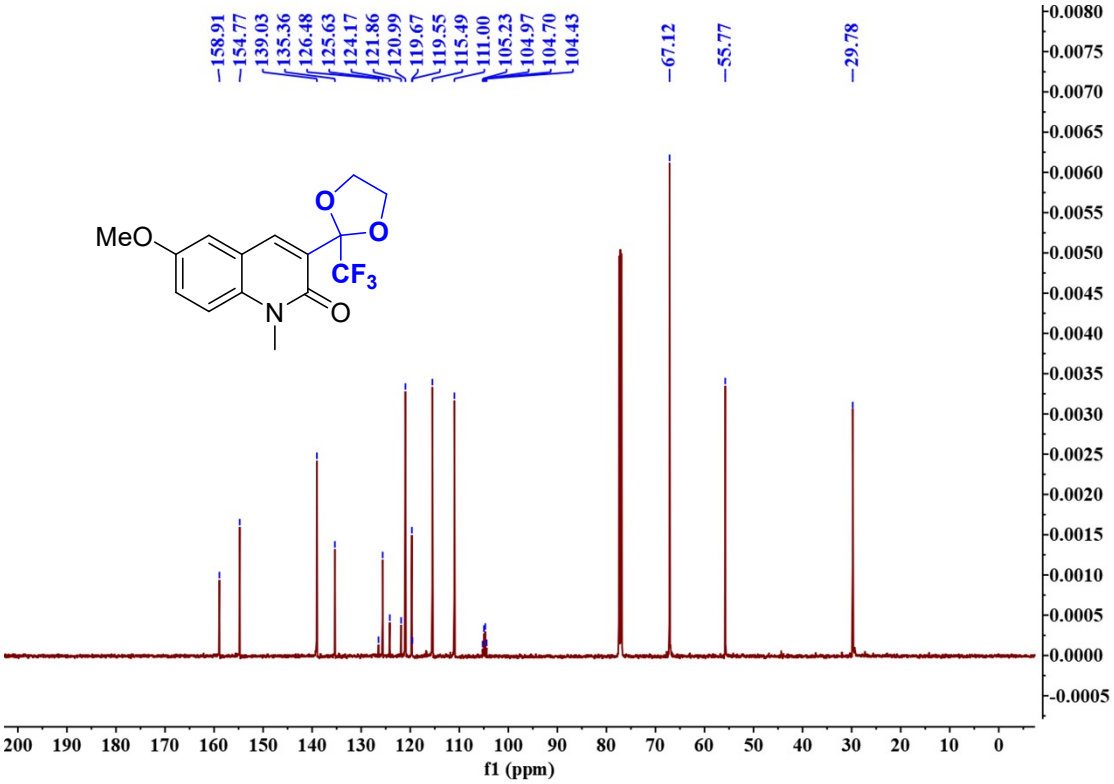
Spectrum from 19.wiff (sample 1) - Sample019, Experiment 1, +TOF MS (CE=10) (50 - 1000) from 0.694 to 0.709 min



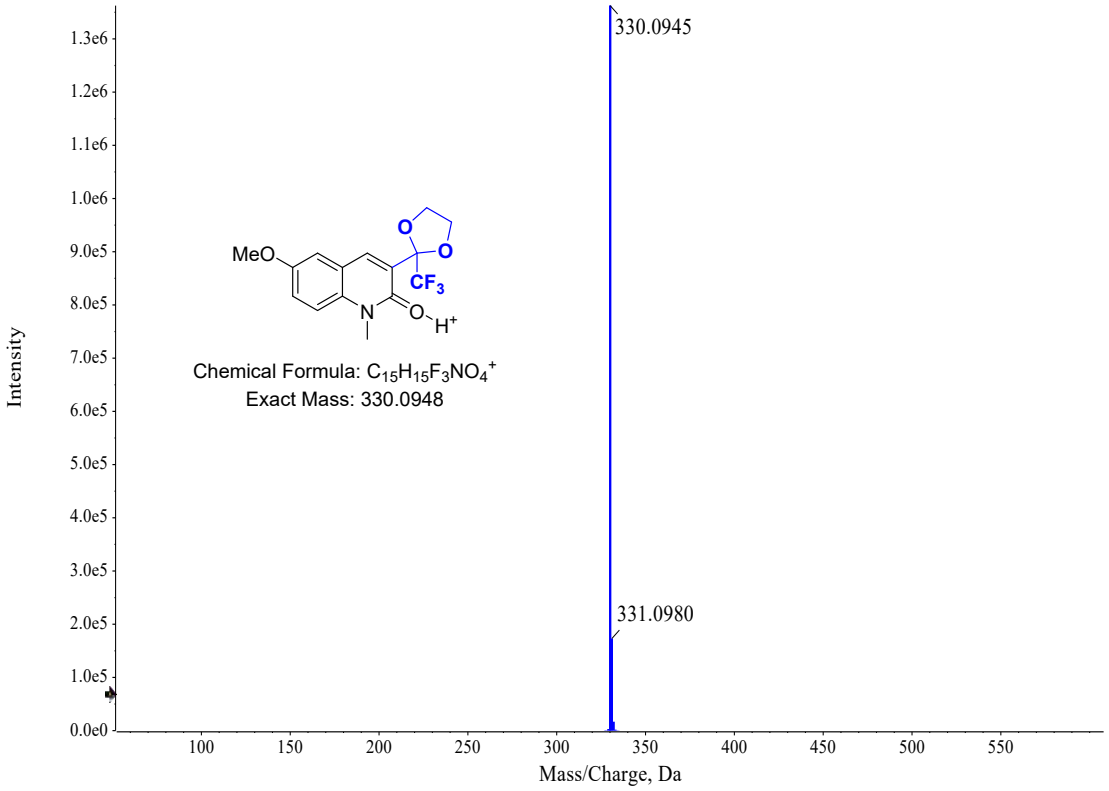
Compound 3t (^{1}H NMR, 500 Hz, $CDCl_3$; ^{19}F NMR 471 Hz, $CDCl_3$ ^{13}C NMR, 101 Hz, $CDCl_3$)



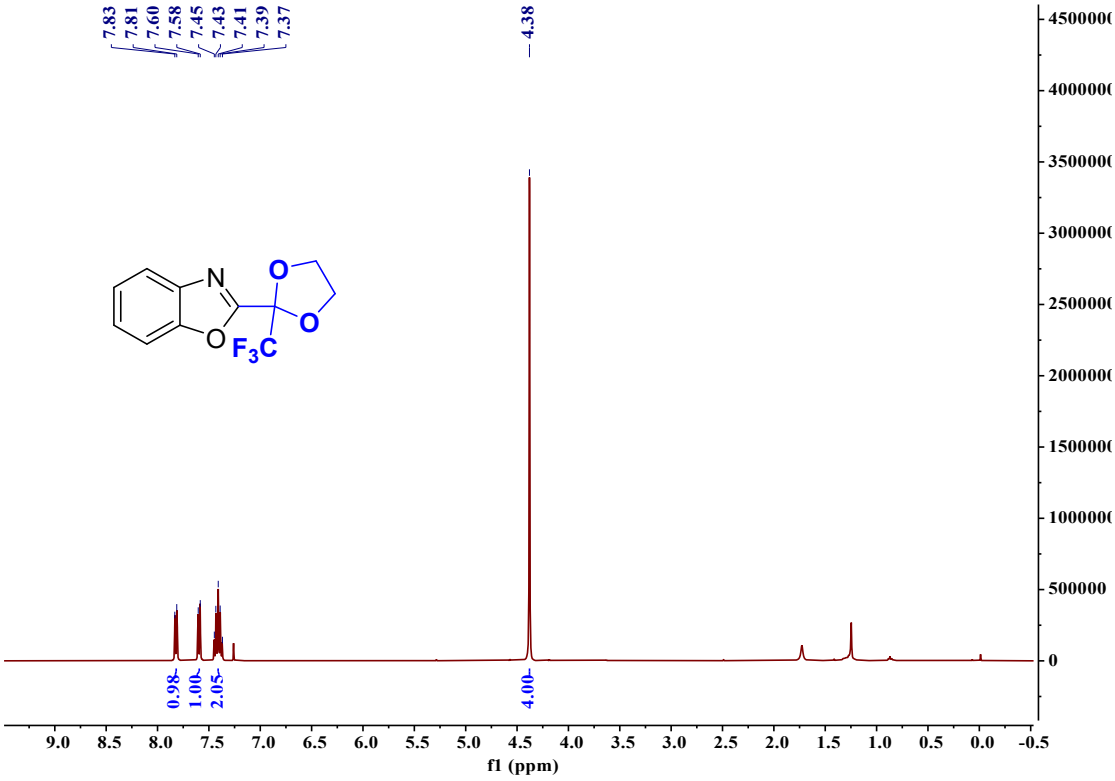


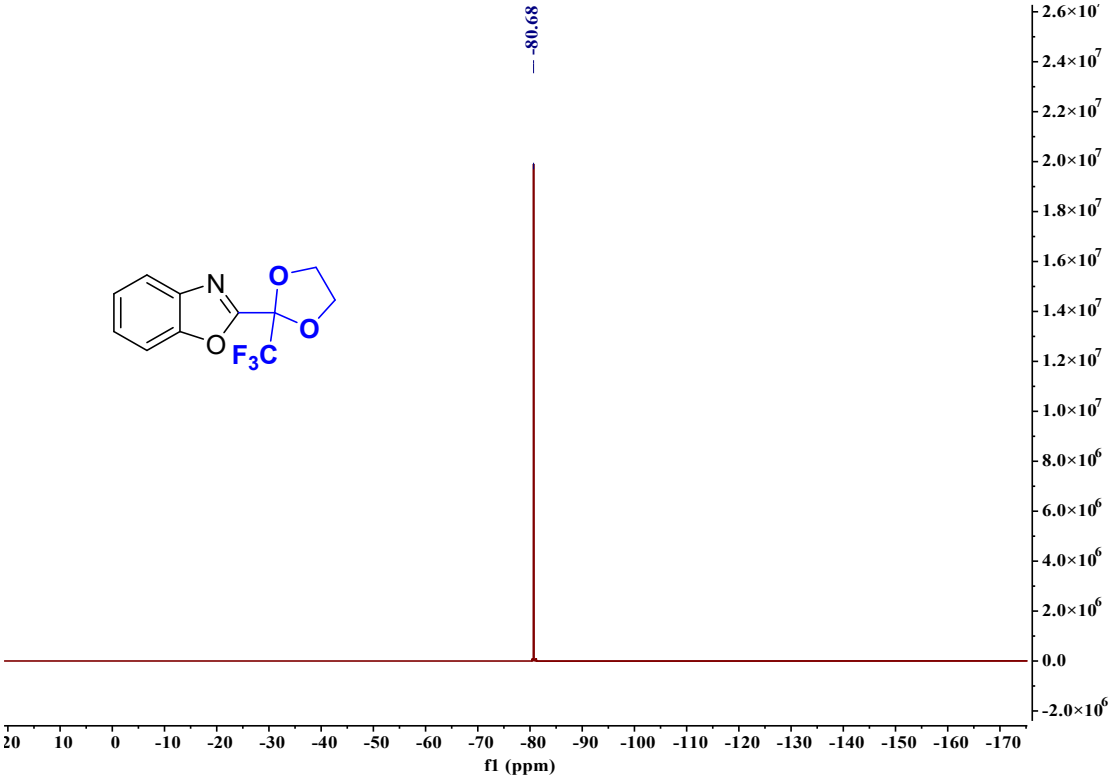


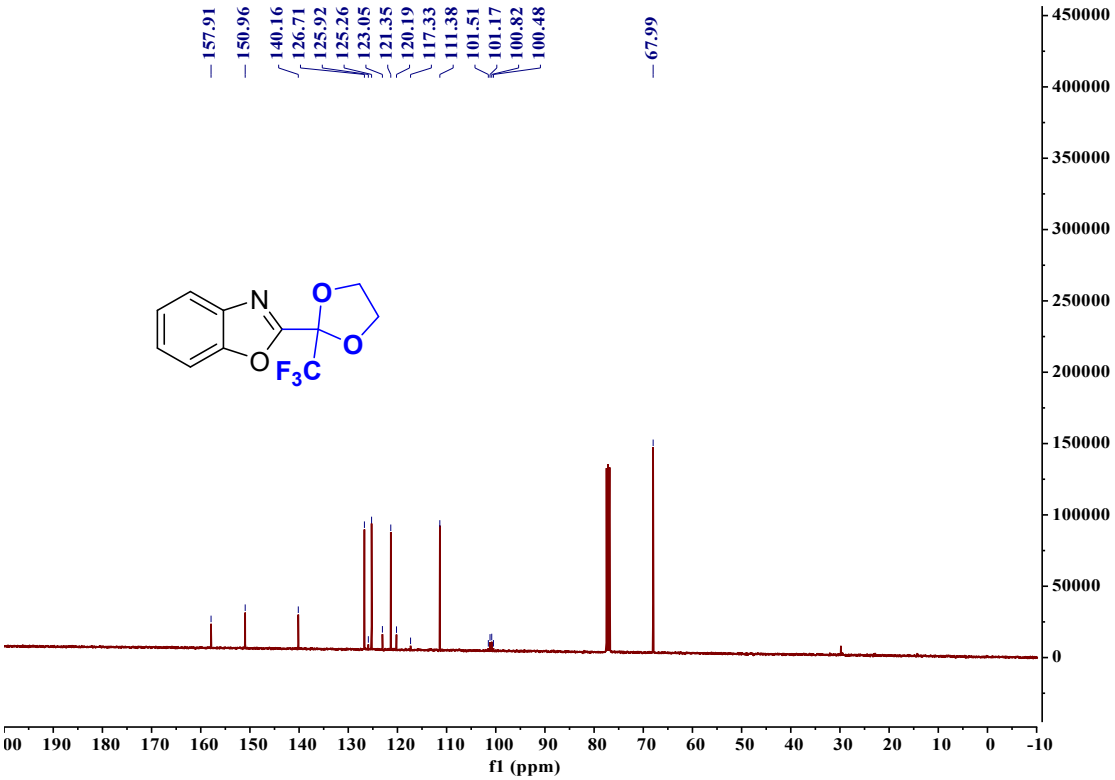
Spectrum from 26.wiff (sample 1) - Sample026, Experiment 1, +TOF MS (CE=10) (50 - 1000) from 0.562 to 0.577 min



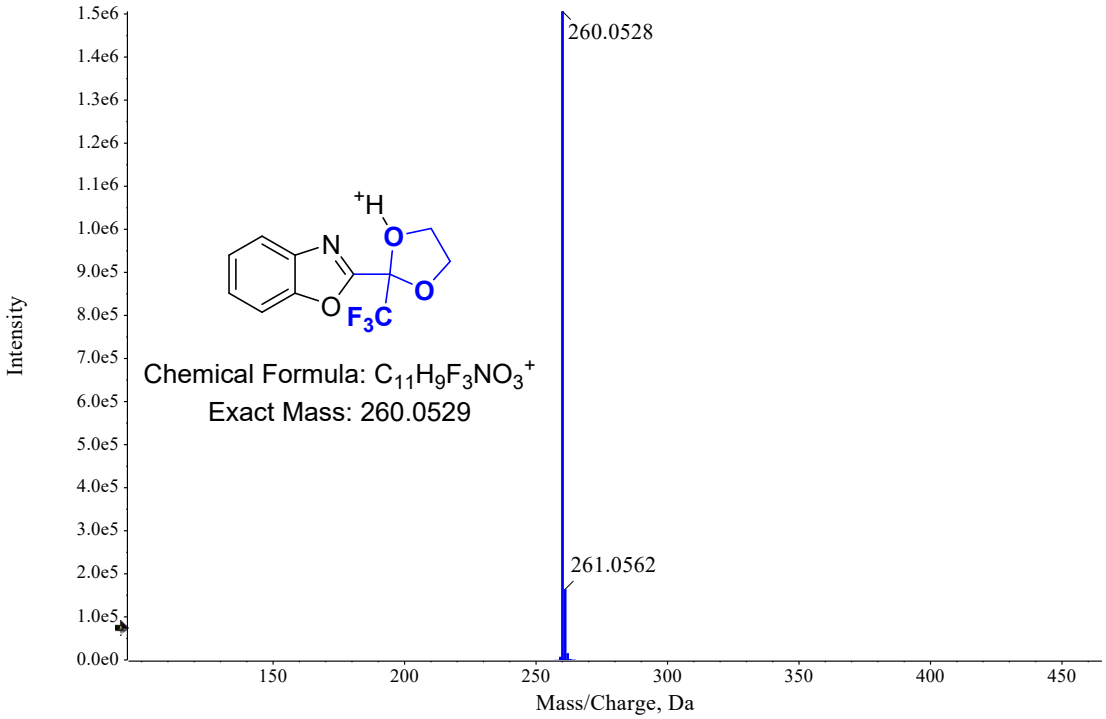
Compound 3u (^{1}H NMR, 400 Hz, $CDCl_3$; ^{19}F NMR 376 Hz, $CDCl_3$ ^{13}C NMR, 101 Hz, $CDCl_3$)



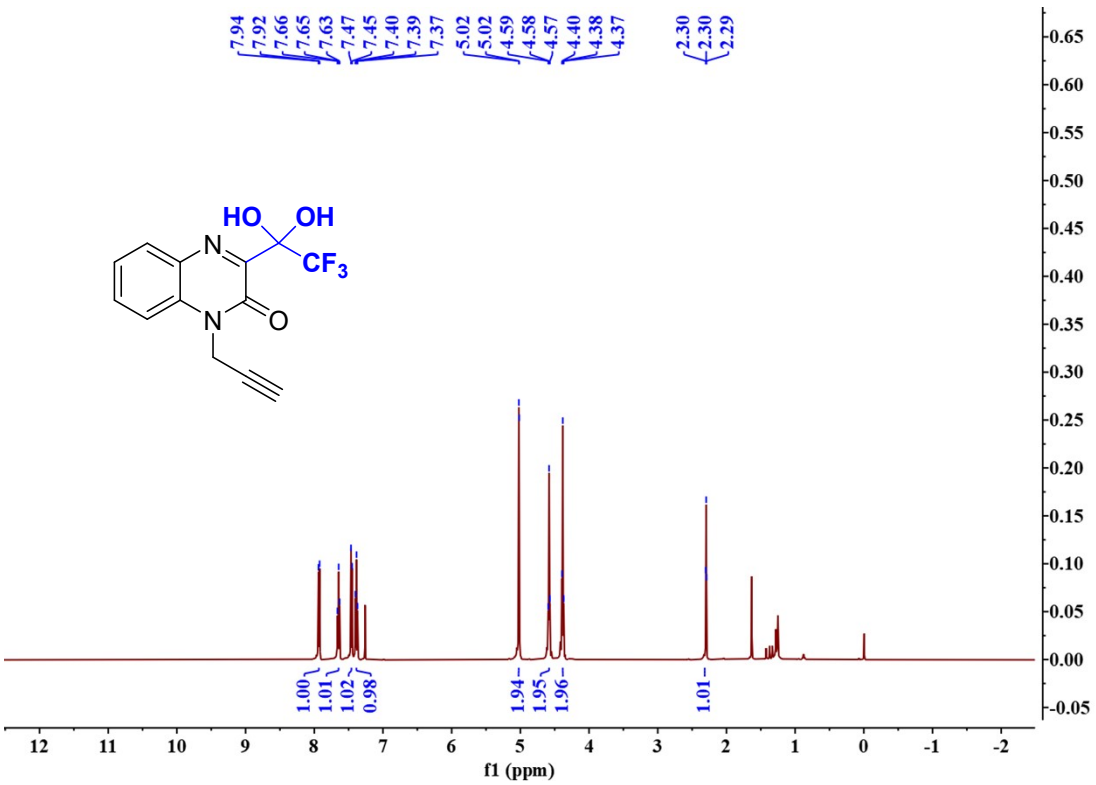


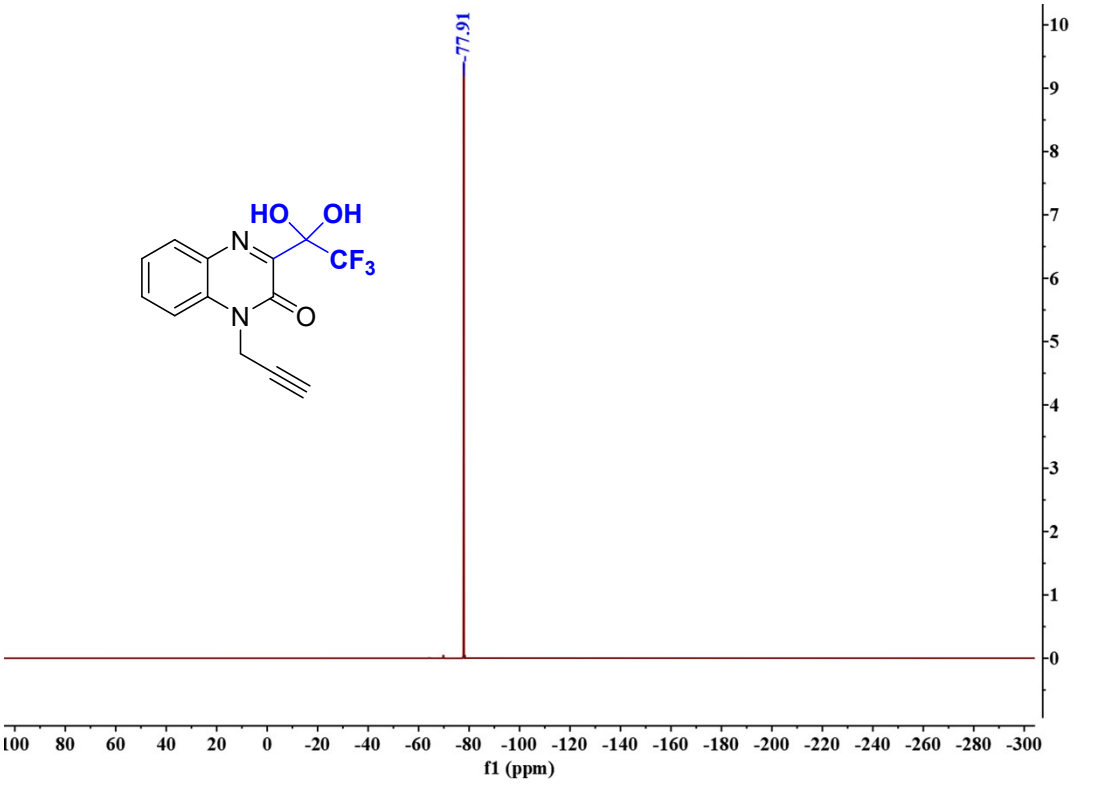


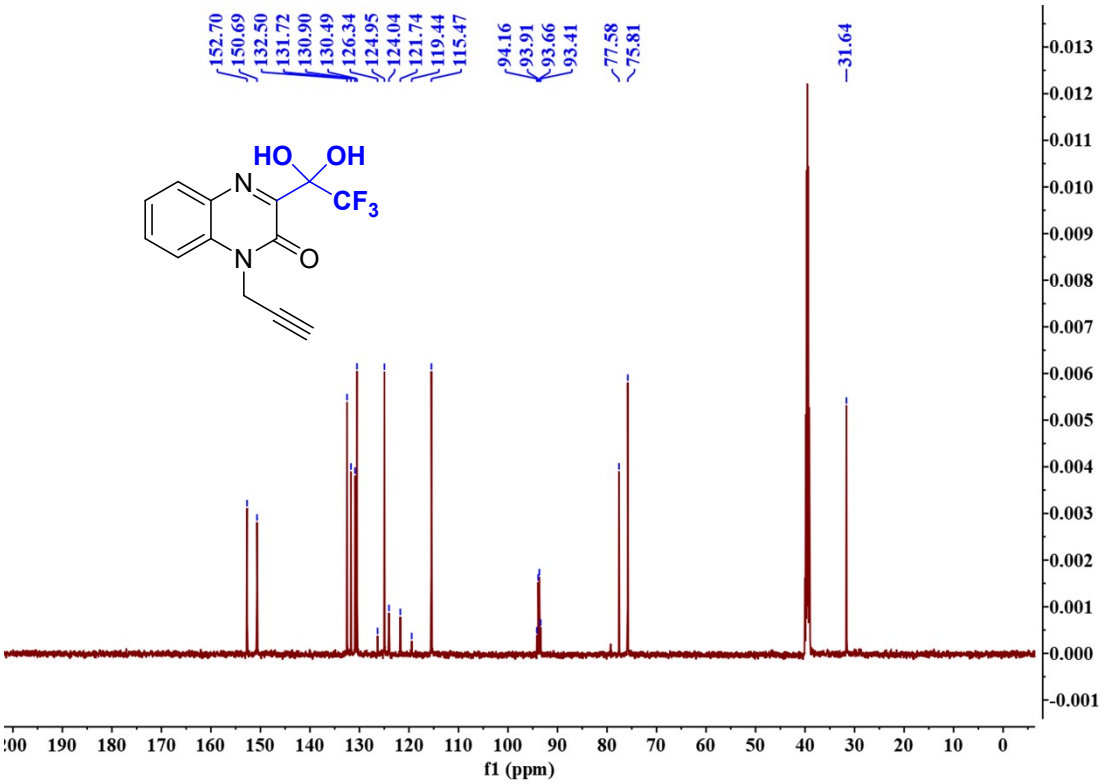
Spectrum from 30.wiff (sample 1) - Sample030, Experiment 1, +TOF MS (CE=10) (50 - 1000) from 0.613 to 0.628 min



Compound 3aa (^{1}H NMR, 500 Hz, $CDCl_3$; ^{19}F NMR 471 Hz, $CDCl_3$ ^{13}C NMR, 101 Hz, $CDCl_3$)







Spectrum from 1.wiff (sample 1) - Sample001, Experiment 1, +TOF MS (CE=10) (50 - 1000) from 1.134 to 1.149 min