Supporting Information

C5-regioselective C-H fluorination of 8-aminoquinoline amides and sulfonamides with selectfluor under metal-free conditions

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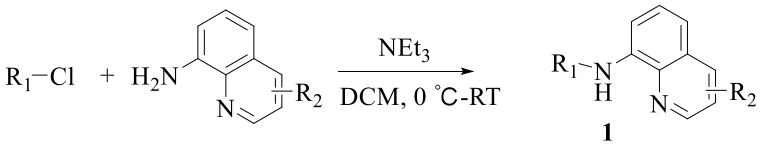
Contents

1. General information

All reagents, starting materials, and solvents were purchased from commercial sources and used without treatment, unless otherwise indicated. All the solvents were dried and newly distilled. NMR spectra were obtained on a Bruker AMX 400 system using chloroform-d as deuterated solvents. The ^{1}H-NMR spectra were recorded at 400 MHz in $CDCl_3$, the ^{13}C-NMR spectra were recorded at 100 MHz in $CDCl_3$, and the ^{19}F-NMR spectra were recorded at 376 MHz in $CDCl_3$ with TMS as internal standard. All shifts were given in ppm. All coupling constants (*J* values) were reported in Hertz (Hz). Single crystal X-ray diffraction data were collected using a Bruker-AXS SMART APEX2 CCD diffractometer (Mo Kα, λ = 0.71073 Å). High-Resolution Liquid Chromatography-Mass Spectrometry was recorded on the Bruker MicrOTOF QII. Column chromatography was performed on silica gel 100-200 mesh or 200-300 mesh. Ethyl acetate and petroleum ether were used for column chromatography.

2. Preparation of substituted amides 1a-1w.[1]

Preparation of amides **1a-1w** according to literature procedures from 8-aminoquinoline and corresponding acyl chloride: A solution of 8-aminoquinoline (1.44 g, 10.0 mmol) and NEt_3 (1.01 g, 11.0 mmol) in dichloromethane (10 mL) was added dropwise to a stirring solution of an acid chloride (11.0 mmol) in dichloromethane (40 mL) under the ice bath conditions. The resulting mixture was stirred at 25 ℃ for 10 hours. Then, the mixture was quenched with saturated aq. $NaHCO_3$ (50 mL), and was extracted with dichloromethane for three times (3 x 50 mL). The organic layer was dried over Na_2SO_4. After filtration and evaporation, the amides were purified by column chromatography (hexane: ethyl acetate 10:1-4:1) through silica gel.



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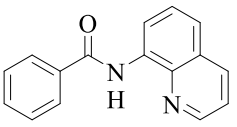

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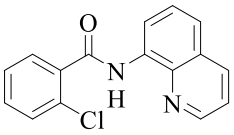

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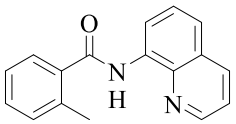

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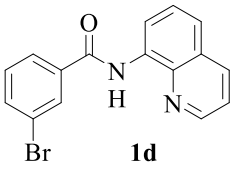

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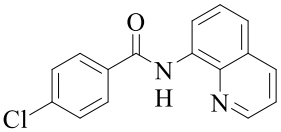

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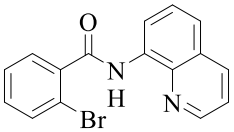

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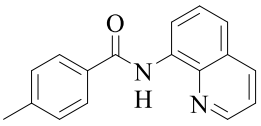

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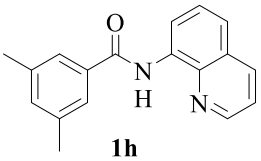

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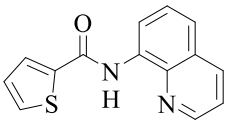

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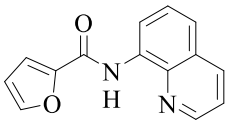

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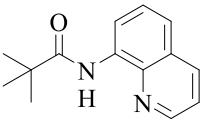

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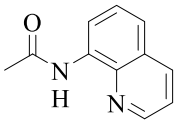

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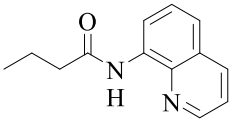

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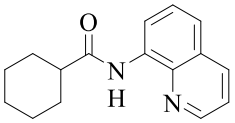

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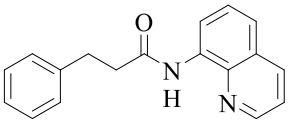

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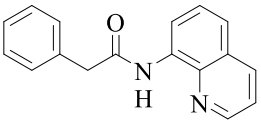

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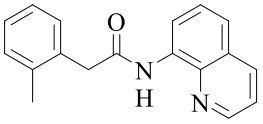

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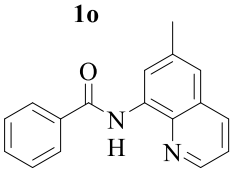

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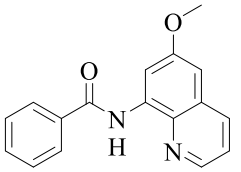

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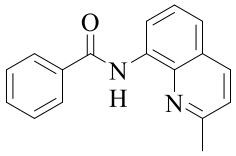

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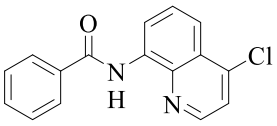

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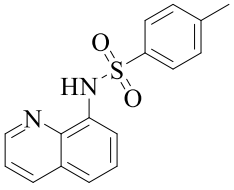

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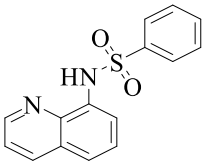

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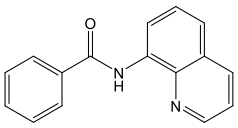

N-(Quinolin-8-yl)benzamide. This compound is known.[2]

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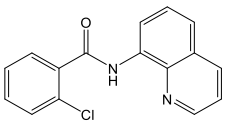
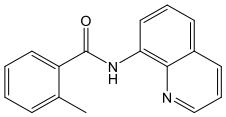


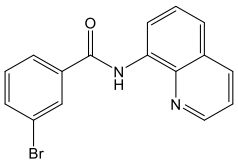
2-chloro-*N*-(8-quinolinyl)benzamide. This compound is known.[3]

1c:



2-methyl-N-(quinolin-8-yl)benzamide. This compound is known.[2]

1d:



3-bromo-N-(quinolin-8-yl)benzamide. This compound is known.[4]

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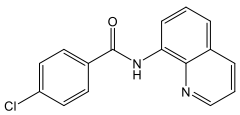
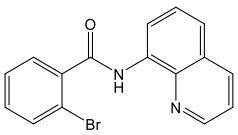


4-chloro-N-(quinolin-8-yl)benzamide. This compound is known.[3]

1f:



2-bromo-N-(quinolin-8-yl)benzamide.This compound is known.[5]

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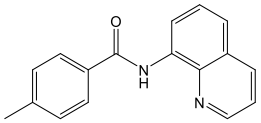
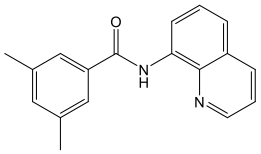


4-methyl-N-(quinolin-8-yl)benzamide. This compound is known.[3]

1h:



3,5-dimethyl-N-(quinolin-8-yl)benzamide. This compound is known.[6]

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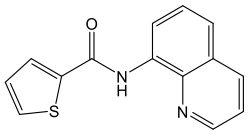

N-(quinolin-8-yl)thiophene-2-carboxamide. This compound is known.[7]

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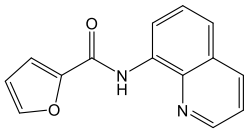

N-(quinolin-8-yl)furan-2-carboxamide. This compound is known.[2]

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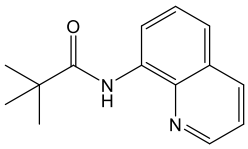

N-(quinolin-8-yl)pivalamide. This compound is known.[8]

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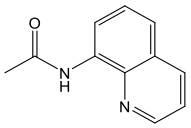

N-(quinolin-8-yl)acetamide. This compound is known.[9]

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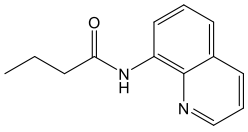

N-(quinolin-8-yl)butyramide. This compound is known.[10]

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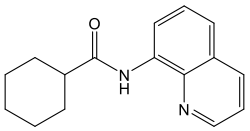

N-(quinolin-8-yl)cyclohexanecarboxamide. This compound is known.[11]

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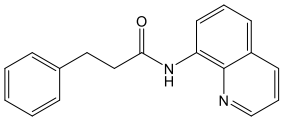

3-phenyl-N-(quinolin-8-yl)propanamide. This compound is known.[11]

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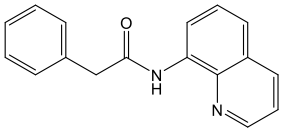

2-phenyl-N-(quinolin-8-yl)acetamide. This compound is known.[12]

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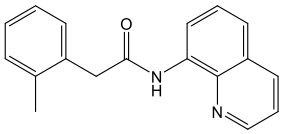
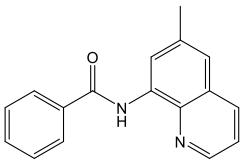


N-(quinolin-8-yl)-2-(o-tolyl)acetamide. This compound is known.[13]

1r:



N-(6-methylquinolin-8-yl)benzamide. This compound is known.[14]

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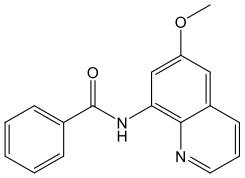

N-(6-methoxyquinolin-8-yl)benzamide. This compound is known.[8]

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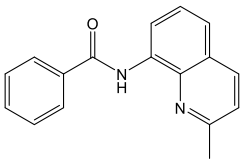

N-(2-methylquinolin-8-yl)benzamide. This compound is known.[8]

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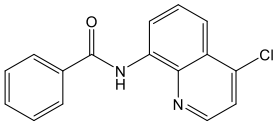
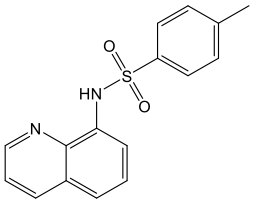


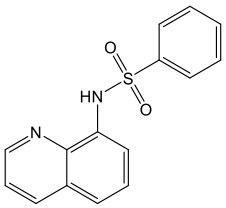
N-(4-chloroquinolin-8-yl)benzamide. This compound is known.[8]

1v:



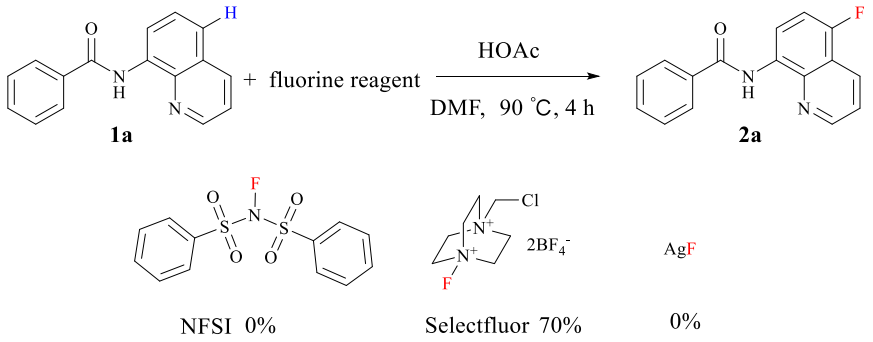
4-methyl-N-(quinolin-8-yl)benzenesulfonamide. This compound is known.[15]

1w:



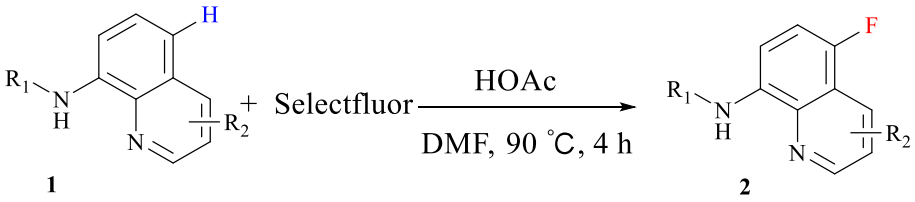
N-(quinolin-8-yl)benzenesulfonamide. This compound is known.[15]

3. Screening of fluorine reagents



N-(8-quinolinyl) benzamide **1a** (0.2 mmol, 1.0 equiv), fluorine reagent (0.4 mmol, 2.0 equiv), HOAc (0.24 mmol, 1.2 equiv) were mixed in DMF (1.5 mL) and stirred for 4 h in a sealed tube at 90 °C. The organic layer was washed with H_2O, and was extracted with dichloromethane for three times (3x10 mL). Then, the organic layer was dried over anhydrous Na_2SO_4, and resulting organic solution was concentrated under reduced pressure and further purified by flash chromatography (SiO_2, petroleum ether/ethyl acetate gradient), yielding the target product **2a**.

4. General procedure for preparation of regioselective C5 fluorinated N-(8-quinolinyl) amides and sulfonamides



1 **2**

N-(8-quinolinyl) amide or sulfonamide 1 (0.2 mmol, 1.0 equiv), Selecfluor (0.4 mmol, 2.0 equiv), HOAc (0.24 mmol, 1.2 equiv) were mixed in DMF (1.5 mL) and stirred for 4 h in a sealed tube at 90 °C. The organic layer was washed with H_2O, and was extracted with dichloromethane for three times (3 x 10mL). Then, the organic layer was dried over anhydrous Na_2SO_4, and resulting organic solution was concentrated under reduced pressure and further purified by flash chromatography (SiO_2, petroleum ether/ethyl acetate gradient), yielding the target product **2**.

5. The single crystal X-ray diffraction study of N-(5-fluoro-quinolin-8-yl) benzamide 2a and 4-chloro-N-(5-fluoroquinolin-8-yl) benzamide 2e

Single-crystal X-ray structure of **2a**

The **2a** data of single-crystal x-ray structure corresponds to our prior publication (J. S. Ding, Y. C. Zhang and J. Z. Li, *Org. Chem. Front*., 2017, **4**, 1528-1532.)

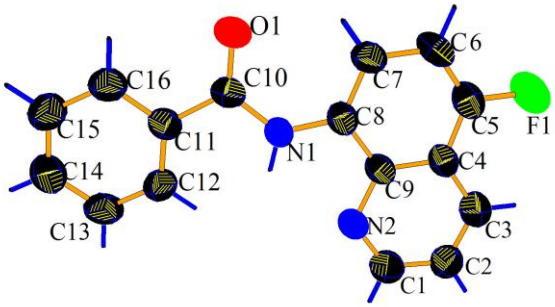


Table 1. Crystal data and structure refinement for **2a**.

Identification code	**2a**
Empirical formula	$C_{16}H_{11}FN_2O$
Formula weight	266.27
Temperature	273(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 21.229(10) A alpha = 90 deg.
	b = 3.9190(19) A beta = 105.861(11) deg.
	c = 15.628(8) A gamma = 90 deg.
Volume	1250.7(10) A^3
Z, Calculated density	4, 1.414 Mg/m^3
Absorption coefficient	0.100 mm^-1
F(000)	552

Crystal size	0.220 x 0.200 x 0.180 mm
Theta range for data collection	0.997 to 25.654 deg.
Limiting indices	-25<=h<=25, -4<=k<=4, -19<=l<=14
Reflections collected / unique	7250 / 2342 [R(int) = 0.0644]
Completeness to theta = 25.242	99.6 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2342 / 0 / 181
Goodness-of-fit on F^2	0.994
Final R indices [I>2sigma(I)]	R1 = 0.0737, wR2 = 0.2007
R indices (all data)	R1 = 0.1172, wR2 = 0.2307
Extinction coefficient	n/a
Largest diff. peak and hole	0.212 and -0.184 e.A^-3

Single-crystal X-ray structure of **2e**.

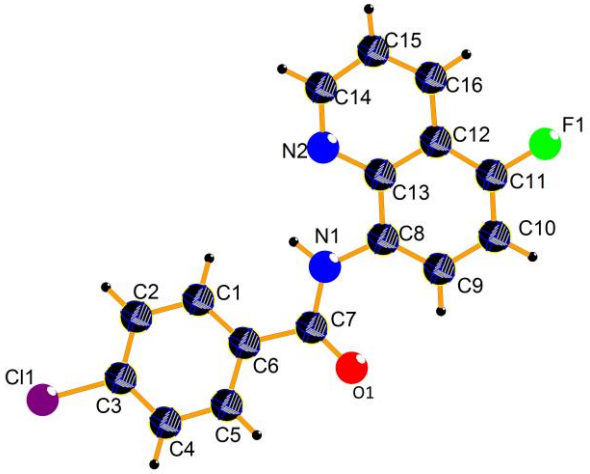
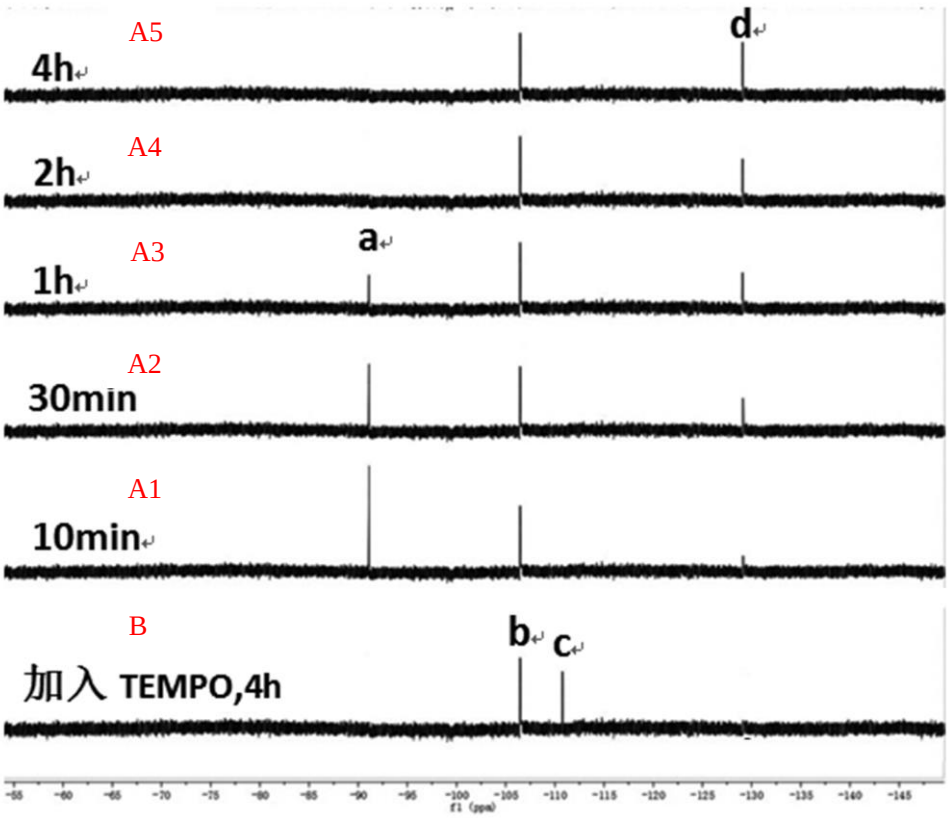


Table 2. Crystal data and structure refinement for **2e**.

Identification code	2e	
Empirical formula	$C_{16}H_{10}ClFN_2O$	
Formula weight	300.71	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.6576(13) Å	α= 115.042(4)°.
	b = 10.1949(14) Å	β= 92.445(5)°.
	c = 10.3237(15) Å	γ = 108.132(4)°.
Volume	679.55(18) $Å^3$	
Z	2	
Density (calculated)	1.470 Mg/m^3	
Absorption coefficient	0.292 mm^{-1}	
F (000)	308	
Crystal size	0.220 x 0.200 x 0.180 mm^3	
Theta range for data collection	2.224 to 24.939°.	
Index ranges	-7<=h<=9, -12<=k<=9, -12<=l<=12	
Reflections collected	4318	
Independent reflections	2337 [R(int) = 0.0231]	
Completeness to theta = 24.939°	98.4 %	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2337 / 0 / 190	
Goodness-of-fit on F^2	1.044	

Final R indices [I>2sigma(I)]	R1 = 0.0461, wR2 = 0.1166
R indices (all data)	R1 = 0.0645, wR2 = 0.1329
Extinction coefficient	n/a
Largest diff. peak and hole	0.175 and -0.264 e. $Å^{-3}$

6. ^{19}F NMR monitoring the reaction



^{19}F NMR monitoring the reaction.

Peaks are selectfluor (**a**, δ = -91.08 ppm), fluorobenzene (**b**, δ = -106.37 ppm) as an internal standard, TEMPO-F (**c**, δ = -112.80 ppm), and C5 fluorinated product (**d**, δ = -129.02 ppm). Solvent: $CDCl_3$.

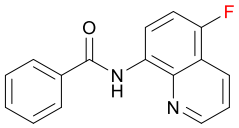
Figure A1-A5 indicated that the reaction of fluorination proceeded under standard condition without radical scavenger TEMPO (2.0 equiv), from which we can observe the changes in raw materials and target products obviously over time.

B indicated that the reaction system proceeded for 4 h under standard condition

with the addition of radical scavenger TEMPO (2.0 equiv). In addition, it can be concluded that "F" free radicals were captured by TEMPO from peak **c** in Figure B.

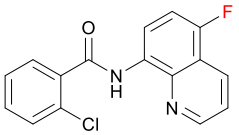
7. Characterization data of the C5 fluorinated N-(8-quinolinyl) amides and sulfonamides

2a:



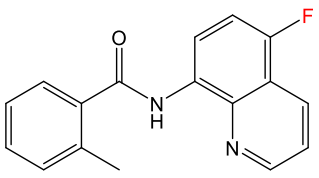
White solid, isolated yield: 70%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.55 (s, 1H), 8.91 (t, *J* = 6.6 Hz, 2H), 8.47 (d, *J* = 8.4 Hz, 1H), 8.08 (d, *J* = 7.0 Hz, 2H), 7.65-7.52 (m, 4H), 7.29 (d, *J* = 9.2 Hz, 1H).^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.34 (s), 153.01 (d, *J* = 251.2 Hz), 149.14 (s), 138.97 (d, *J* = 3.0 Hz), 134.99 (s), 131.91 (s), 131.12 (d, *J* = 4.0 Hz), 129.86 (d, *J* = 3.6 Hz), 128.83 (s), 127.24 (s), 121.77 (d, *J* = 2.6 Hz), 118.82 (d, *J* = 18.3 Hz), 116.04 (d, *J* = 7.7 Hz), 110.52 (d, *J* = 19.7 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ: -129.01 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{16}H_{11}FN_2O$: 267.0928, found: 267.0927.

2b:



White solid, isolated yield: 63%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.35 (s, 1H), 8.92 (dd, *J* = 8.6, 5.5 Hz, 1H), 8.86 (d, *J* = 3.1 Hz, 1H), 8.48 (d, *J* = 8.4 Hz, 1H), 7.82 (dd, *J* = 7.2, 1.5 Hz, 1H), 7.58-7.49 (m, 2H), 7.48-7.39 (m, 2H), 7.30 (d, *J* = 9.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 164.72 (s), 153.26 (d, *J* = 251.7 Hz), 149.23 (s), 138.92 (d, *J* = 3.2 Hz), 135.63 (s), 131.60 (s), 131.15 (s), 130.97 (d, *J* = 4.2 Hz), 130.55 (s), 130.14 (s), 129.79 (d, *J* = 3.7 Hz), 127.19 (s), 121.79 (d, *J* = 2.7 Hz), 118.81 (d, *J* = 18.1 Hz), 116.47 (d, *J* = 7.8 Hz), 110.46 (d, *J* = 19.7 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ: -128.39 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{16}H_{10}ClFN_2O$: 301.0538, found: 301.0542.

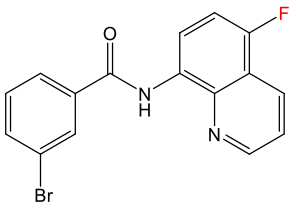
2c:



White solid, isolated yield: 67%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.03 (s, 1H), 8.90 (dd, *J* = 8.5, 5.5 Hz, 1H), 8.84 (d, *J* = 4.1 Hz, 1H), 8.48 (dd, *J* = 8.4, 1.3 Hz, 1H), 7.68 (d, *J* = 7.6 Hz, 1H), 7.55 (dd, *J* = 8.4, 4.3 Hz, 1H), 7.46-7.27 (m, 4H), 2.60 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 168.06 (s), 153.05 (d, *J* = 251.3 Hz), 149.12 (s), 138.82 (d, *J* = 3.1 Hz), 136.71 (s), 136.46 (s), 131.42 (s), 131.26 (d, *J* = 4.0 Hz), 130.41 (s), 129.81 (d, *J* = 3.6 Hz), 127.23 (s), 126.05 (s), 121.75 (d, *J* = 2.5 Hz), 118.80 (d, *J* = 18.1 Hz), 116.01 (d, *J* = 7.7 Hz), 110.46 (d, *J* = 19.6 Hz), 20.24 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ:

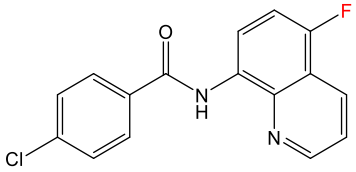
-128.93 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{17}H_{13}FN_2O$: 281.1085, found: 281.1092.

2d:



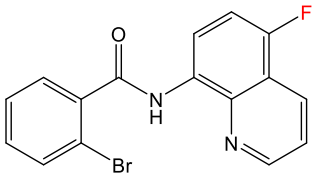
White solid, isolated yield: 55%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.49 (s, 1H), 8.93 (d, *J* = 3.0 Hz, 1H), 8.87 (dd, *J* = 8.6, 5.4 Hz, 1H), 8.48 (d, *J* = 8.5 Hz, 1H), 8.20 (s, 1H), 7.98 (d, *J* = 7.5 Hz, 1H), 7.72 (d, *J* = 7.9 Hz, 1H), 7.58 (dd, *J* = 8.4, 4.2 Hz, 1H), 7.44 (t, *J* = 7.9 Hz, 1H), 7.29 (d, *J* = 9.3 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 163.76 (s), 153.21 (d, *J* = 251.8 Hz), 149.26 (s), 138.95 (s), 136.99 (s), 134.85 (s), 130.78 (d, *J* = 4.0 Hz), 130.57 (s), 130.34 (s), 129.92 (d, *J* = 3.6 Hz), 125.66 (s), 123.08 (s), 121.85 (d, *J* = 2.5 Hz), 118.84 (d, *J* = 18.3 Hz), 116.27 (d, *J* = 7.8 Hz), 110.50 (d, *J* = 19.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ: -128.39 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{16}H_{10}BrFN_2O$: 345.0033, 347.0013, found: 345.0039, 347.0019.

2e:



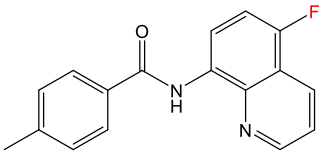
White solid, isolated yield: 71%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.51 (s, 1H), δ 8.91 (d, *J* = 4.1 Hz, 1H), 8.87 (dd, *J* = 8.6, 5.4 Hz, 1H). 8.48 (d, *J* = 8.4 Hz, 1H), 8.01 (d, *J* = 8.4 Hz, 2H), 7.60-7.51 (m, 3H), 7.29 (d, *J* = 9.1 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 164.20 (s), 153.14 (d, *J* = 251.6 Hz), 149.20 (s), 138.93 (d, *J* = 3.1 Hz), 138.19 (s), 133.38 (s), 130.88 (d, *J* = 4.0 Hz), 129.94 (d, *J* = 3.6 Hz), 129.10 (s), 128.67 (s), 121.83 (d, *J* = 2.5 Hz), 118.85 (d, *J* = 18.3 Hz), 116.15 (d, *J* = 7.7 Hz), 110.53 (d, *J* = 19.7 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ: -128.57 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{16}H_{10}ClFN_2O$: 301.0538, found: 301.0532.

2f:



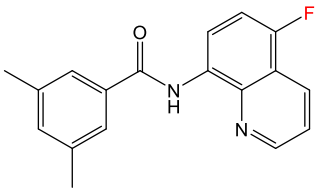
White solid, isolated yield: 57%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.11 (s, 1H), 8.99-8.81 (m, 2H), 8.46 (d, *J* = 8.4 Hz, 1H), 7.70 (t, *J* = 7.8 Hz, 2H), 7.53 (dd, *J* = 8.2, 4.1 Hz, 1H), 7.45 (t, *J* = 7.5 Hz, 1H), 7.36 (t, *J* = 7.7 Hz, 1H), 7.29 (d, *J* = 9.1 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.74 (s), 153.28 (d, *J* = 251.7 Hz), 149.20 (s), 138.88 (s), 138.17 (s), 133.70 (s), 131.55 (s), 130.88 (s), 129.84 (s), 129.71 (d, *J* = 23.0 Hz), 127.67 (s), 121.78 (s), 119.68 (s), 118.82 (d, *J* = 18.3 Hz), 116.46 (d, *J* = 7.5 Hz), 110.45 (d, *J* = 19.7 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ: -128.27 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{16}H_{10}BrFN_2O$: 345.0033, 347.0013, found: 345.0037, 347.0019.

2g:



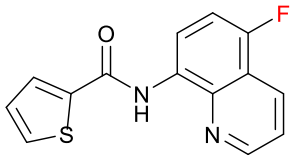
White solid, isolated yield: 59%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.52 (s, 1H), 8.96-8.86 (m, 2H), 8.47 (d, *J* = 8.4 Hz, 1H), 7.97 (d, *J* = 7.7 Hz, 2H), 7.56 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.35 (d, *J* = 7.7 Hz, 2H), 7.29 (t, *J* = 9.2 Hz, 1H),2.46 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.32 (s), 152.92 (d, *J* = 251.1 Hz), 149.08 (s), 142.40 (s), 138.97 (d, *J* = 2.8 Hz), 132.19 (s), 131.24 (d, *J* = 4.0 Hz), 129.83 (d, *J* = 3.8 Hz), 129.48 (s), 127.25 (s), 121.71 (d, *J* = 2.4 Hz), 118.82 (d, *J* = 18.1 Hz), 115.94 (d, *J* = 7.6 Hz), 110.53 (d, *J* = 19.6 Hz), 21.56 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ: -129.27 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{17}H_{13}FN_2O$: 281.1085, found: 281.1089.

2h:



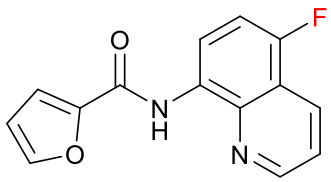
White solid, isolated yield: 62%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.46 (s, 1H), 8.98-8.86 (m, 2H), 8.47 (d, *J* = 8.4 Hz, 1H), 7.65 (s, 2H), 7.56 (dd, *J* = 8.4, 4.2 Hz, 1H), 7.28 (d, *J* = 9.2 Hz, 1H), 7.23 (d, *J* = 12.4 Hz, 1H), 2.44 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.80 (s), 152.94 (d, *J* = 251.0 Hz), 149.11 (s), 138.99 (d, *J* = 3.1 Hz), 138.51 (s), 135.05 (s), 133.53 (s), 131.25 (d, *J* = 4.2 Hz), 129.82 (d, *J* = 3.7 Hz), 124.98 (s), 121.70 (d, *J* = 2.6 Hz), 118.81 (d, *J* = 18.2 Hz), 116.04 (d, *J* = 7.7 Hz), 110.52 (d, *J* = 19.6 Hz), 21.39 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ: -129.26 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{18}H_{15}FN_2O$: 295.1241, found: 295.1238.

2i:



White solid, isolated yield: 74%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.33 (s, 1H), 8.94-8.88 (m, 1H), 8.84 (dd, *J* = 8.6, 5.4 Hz, 1H), 8.46 (d, *J* = 8.4 Hz, 1H), 8.19-8.13 (m, 1H), 7.68 (d, *J* = 5.0 Hz, 1H), 7.55 (dd, *J* = 8.4, 4.2 Hz, 1H), 7.44 (dd, *J* = 5.0, 3.0 Hz, 1H), 7.28 (t, *J* = 9.1 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 160.90 (s), 152.96 (d, *J* = 251.2 Hz), 149.11 (s), 138.79 (d, *J* = 3.0 Hz), 138.19 (s), 131.02 (d, *J* = 4.0 Hz), 129.85 (d, *J* = 3.6 Hz), 128.93 (s), 126.78 (s), 126.27 (s), 121.74 (d, *J* = 2.5 Hz), 118.82 (d, *J* = 18.2 Hz), 115.99 (d, *J* = 7.6 Hz), 110.53 (d, *J* = 19.7 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ: -129.10 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{14}H_9FN_2OS$: 273.0492, found:273.0495.

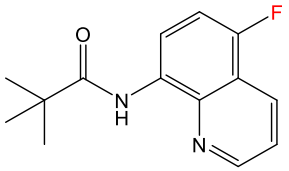
2j:



White solid, isolated yield: 59%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.59 (s, 1H), 8.95 (d, *J* = 3.8 Hz, 1H), 8.83 (dd, *J* = 8.6, 5.4 Hz, 1H), 8.47 (d, *J* = 8.4 Hz, 1H), 7.63 (s, 1H), 7.57 (dd, *J* = 8.4, 4.2 Hz, 1H),

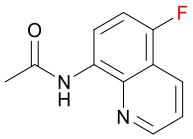
7.33-7.26 (m, 2H), 6.60 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 156.29 (s), 153.14 (d, *J* = 251.4 Hz), 149.24 (s), 148.27 (s), 144.53 (s), 138.90 (d, *J* = 3.2 Hz), 130.75 (d, *J* = 3.9 Hz), 129.83 (d, *J* = 3.8 Hz), 121.76 (d, *J* = 2.6 Hz), 118.87 (d, *J* = 18.2 Hz), 116.23 (d, *J* = 7.8 Hz), 115.15 (s), 112.46 (s), 110.51 (d, *J* = 19.7 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ: -128.74 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{14}H_9FN_2O_2$: 257.0721, found: 257.0726.

2k:



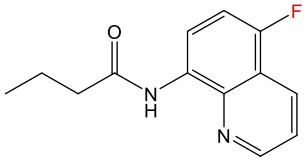
White solid, isolated yield:48%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.07 (s，1H), 8.87 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.75 (dd, *J* = 8.6, 5.5 Hz, 1H), 8.43 (dd, *J* = 8.4, 1.5 Hz, 1H), 7.52 (dd, *J* = 8.4, 4.2 Hz, 1H), 7.24 -7.13 (m, 1H), 1.42 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 177.10 (s), 152.71 (d, *J* = 250.5 Hz), 149.04 (s), 138.94 (d, *J* = 3.0 Hz), 131.22 (d, *J* = 4.1 Hz), 129.76 (d, *J* = 3.6 Hz), 121.59 (d, *J* = 2.5 Hz), 118.72 (d, *J* = 18.1 Hz), 115.65 (d, *J* = 7.6 Hz), 110.42 (d, *J* = 19.4 Hz), 40.27 (s), 27.73 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ: -129.81 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{14}H_{15}FN_2O$: 247.1241, found: 247.1245.

2l:



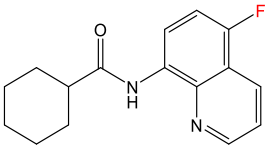
White solid, isolated yield:48%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.59 (s, 1H), 8.86 (d, *J* = 4.1 Hz, 1H), 8.72 (dd, *J* = 8.6, 5.5 Hz, 1H), 8.44 (d, *J* = 8.4 Hz, 1H), 7.53 (dd, *J* = 8.4, 4.2 Hz, 1H), 7.21 (t, *J* = 9.2 Hz, 1H), 2.34 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 168.61 (s), 152.80 (d, *J* = 250.8 Hz), 148.94 (s), 138.44 (d, *J* = 2.1 Hz), 131.04 (d, *J* = 4.1 Hz), 129.82 (d, *J* = 3.7 Hz), 121.64 (d, *J* = 2.5 Hz), 118.71 (d, *J* = 18.1 Hz), 115.94 (d, *J* = 7.6 Hz), 110.42 (d, *J* = 19.6 Hz), 25.03 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ: -129.40 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{11}H_9FN_2O$: 205.0772, found: 205.0774.

2m:



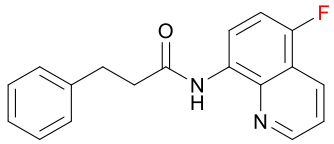
White solid, isolated yield:48%;^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.62 (s, 1H), 8.86 (d, *J* = 3.5 Hz, 1H), 8.74 (dd, *J* = 8.2, 5.8 Hz, 1H), 8.44 (d, *J* = 8.4 Hz, 1H), 7.53 (dd, *J* = 8.3, 4.1 Hz, 1H), 7.21 (t, *J* = 9.2 Hz, 1H), 2.53 (t, *J* = 7.5 Hz, 2H), 1.90-1.80 (m, 2H), 1.06 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 171.58 (s), 152.74 (d, *J* = 250.6 Hz), 148.93 (s), 138.54 (d, *J* = 2.9 Hz), 131.10 (d, *J* = 3.9 Hz), 129.78 (d, *J* = 3.6 Hz), 121.60 (d, *J* = 2.6 Hz), 118.72 (d, *J* = 18.0 Hz), 115.86 (d, *J* = 7.6 Hz), 110.43 (d, *J* = 19.6 Hz), 40.09 (s), 19.13 (s), 13.82 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ: -129.55 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{13}H_{13}FN_2O$: 233.1085, found: 233.1089.

2n:



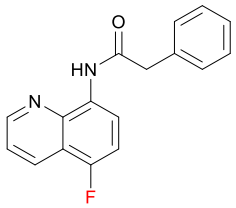
White solid, isolated yield:43%;^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.76 (s, 1H), 8.88 (dd, *J* = 4.3, 1.6 Hz, 1H), 8.77 (dd, *J* = 8.7, 5.5 Hz, 1H), 8.47 (dd, *J* = 8.4, 1.5 Hz, 1H), 7.55 (dd, *J* = 8.4, 4.3 Hz, 1H), 7.26-7.19 (m, 1H), 2.49 (m, 1H), 2.17-2.01 (m, 2H), 1.96-1.82 (m, 2H), 1.78-1.57 (m, 3H), 1.45-1.24 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 174.71 (s), 152.68 (d, *J* = 250.7 Hz), 148.89 (s), 138.61 (d, *J* = 2.6 Hz), 131.16 (d, *J* = 4.0 Hz), 129.81 (d, *J* = 3.7 Hz), 121.58 (d, *J* = 2.5 Hz), 118.71 (d, *J* = 18.0 Hz), 115.90 (d, *J* = 7.6 Hz), 110.45 (d, *J* = 19.5 Hz), 46.82 (s), 29.75 (s), 25.77 (s), 25.75 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ: -129.73 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{16}H_{17}FN_2O$: 273.1398, found: 273.1395.

2o:



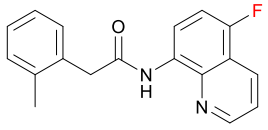
White solid, isolated yield: 58%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.59 (s, 1H), 8.82 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.74 (dd, *J* = 8.6, 5.4 Hz, 1H), 8.43 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.52 (dd, *J* = 8.4, 4.2 Hz, 1H), 7.35-7.28 (m, 4H), 7.25-7.17 (m, 2H), 3.20-3.10 (t, *J* = 7.8 Hz,, 2H), 2.93-2.83 (t, *J* = 7.8 Hz, 2H). ^{13}C NMR (100MHz, $CDCl_3$) δ: 170.57 (s), 152.82 (d, *J* = 250.9 Hz), 148.92 (s), 140.71 (s), 138.51 (d, *J* = 3.0 Hz), 130.96 (d, *J* = 4.1 Hz), 129.78 (d, *J* = 3.7 Hz), 128.57 (s), 128.39 (s), 126.27 (s), 121.63 (d, *J* = 2.5 Hz), 118.71 (d, *J* = 18.1 Hz), 115.96 (d, *J* = 7.7 Hz), 110.43 (d, *J* = 19.6 Hz), 39.66 (s), 31.48 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ: -129.34 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{18}H_{15}FN_2O$: 295.1241, found: 295.1238.

2p:



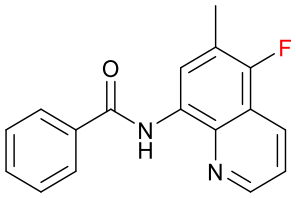
White solid, isolated yield: 48%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.82 (d, *J* = 90.9 Hz, 1H), 8.88-8.60 (m, 2H), 8.26 (dd, *J* = 8.3, 1.3 Hz, 1H), 7.51-7.39 (m, 4H), 7.33 (dd, *J* = 13.1, 6.1 Hz, 2H), 7.18 (t, *J* = 9.2 Hz, 1H), 3.88 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 169.47 (s), 153.06 (d, *J* = 251.1 Hz), 138.81 (s), 134.75 (s), 131.07 (d, *J* = 4.1 Hz), 129.84 (d, *J* = 3.6 Hz), 129.68 (s), 129.14 (s), 127.52 (s), 121.70 (d, *J* = 2.6 Hz), 118.80 (d, *J* = 18.1 Hz), 116.02 (d, *J* = 7.7 Hz), 110.50 (d, *J* = 19.6 Hz), 45.43 (s), 29.84 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ: -129.08 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{17}H_{13}FN_2O$: 281.1085, found: 281.1087.

2q:



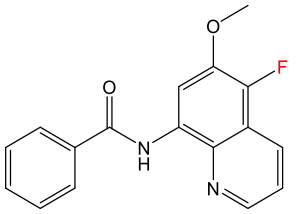
White solid, isolated yield: 67%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.64 (s, 1H), 8.73-8.66 (m, 2H), 8.38 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.45 (dd, *J* = 8.4, 4.2 Hz, 1H), 7.39-7.26 (m, 5H), 7.21-7.15 (t, *J* = 9.2 Hz, 1H), 3.89 (s, 2H), 2.40 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 169.21 (s), 152.90 (d, *J* = 250.9 Hz), 149.00 (s), 138.71 (d, *J* = 2.7 Hz), 137.25 (s), 133.09 (s), 130.91 (d, *J* = 4.0 Hz), 130.81 (s), 130.59 (s), 129.59 (d, *J* = 3.6 Hz), 127.83 (s), 126.64 (s), 121.54 (d, *J* = 2.6 Hz), 118.62 (d, *J* = 18.2 Hz), 115.75 (d, *J* = 7.8 Hz), 110.32 (d, *J* = 19.6 Hz), 43.21 (s), 19.71 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ: -129.20 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{18}H_{15}FN_2O$: 295.1241, found:295.1237.

2r:



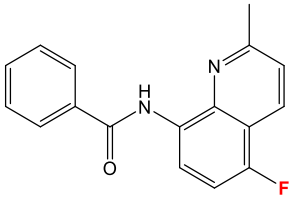
White solid, isolated yield: 49%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.52 (s, 1H), 8.83 (dd, *J* = 4.4, 2.9 Hz, 2H), 8.41 (dd, *J* = 8.4, 1.4 Hz, 1H), 8.07 (dd, *J* = 7.8, 1.4 Hz, 2H), 7.60-7.50 (m, 4H), 2.51 (d, *J* = 2.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.30 (s), 150.44 (d, *J* = 248.1 Hz), 148.09 (s), 137.79 (d, *J* = 2.8 Hz), 135.05 (s), 131.86 (s), 130.46 (d, *J* = 4.1 Hz), 129.31 (d, *J* = 4.2 Hz), 128.83 (s), 127.23 (s), 121.72 (d, *J* = 2.6 Hz), 118.82 (d, *J* = 18.2 Hz), 115.99 (d, *J* = 7.6 Hz), 110.53 (d, *J* = 19.7 Hz). 14.82 (d, *J* = 3.6 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ: -133.73 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{17}H_{13}FN_2O$: 281.1085, found: 281.1086.

2s:



White solid, isolated yield:63%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.65 (s, 1H), 9.02 (d, *J* = 8.5 Hz, 1H), 8.77 (dd, *J* = 4.2, 1.4 Hz, 1H), 8.43 (dd, *J* = 8.5, 1.4 Hz, 1H), 8.10 (d, *J* = 7.0 Hz, 2H), 7.63-7.49 (m, 4H), 4.14 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.45 (s), 146.67 (s), 143.56 (d, *J* = 9.2 Hz), 140.62 (d, *J* = 247.4 Hz), 134.76 (s), 133.48 (d, *J* = 35.8 Hz), 132.04 (s), 131.52 (s), 130.16 (s), 128.68 (dd, *J* = 22.7, 19.7 Hz), 127.23 (s), 122.11 (s), 119.41 (d, *J* = 15.1 Hz), 106.32 (s), 57.29 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ: -153.44 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{17}H_{13}FN_2O_2$: 297.1034, found: 297.1036.

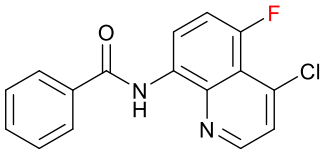
2t:



White solid, isolated yield: 48%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.60 (s, 1H), 8.85 (dd, *J* = 8.6, 5.5 Hz, 1H), 8.33 (d, *J* = 8.5 Hz, 1H), 8.07 (d, *J* = 6.9 Hz, 2H), 7.63-7.54 (m, 3H), 7.42 (d, *J* = 8.5 Hz, 1H), 7.19 (t, *J* = 9.2 Hz, 1H), 2.80 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.17 (s), 158.32 (s), 153.28 (d, *J* = 250.7 Hz), 138.52 (s), 135.19 (s), 131.79 (s), 130.46 (d, *J* = 4.2 Hz), 129.88 (d, *J* = 3.4 Hz), 128.83

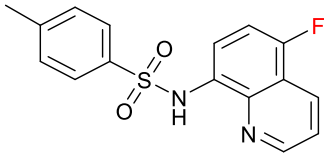
(s), 127.19 (s), 122.55 (d, *J* = 2.4 Hz), 116.87 (d, *J* = 18.2 Hz), 116.03 (d, *J* = 7.8 Hz), 109.52 (d, *J* = 19.7 Hz), 25.50 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ: -129.19 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{17}H_{13}FN_2O$: 281.1085, found: 281.1088.

2u:



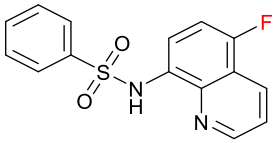
White solid, isolated yield: 49%; ^{1}H NMR (400 MHz, $CDCl_3$) δ： 10.59 (s, 1H), 9.17-8.93 (m, 1H), 8.73 (dd, *J* = 6.5, 4.9 Hz, 1H), 8.07 (dd, *J* = 6.6, 4.9 Hz, 2H), 7.66-7.55 (m, 4H), 7.37 (dd, *J* = 12.1, 8.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.24 (s), 158.39 (s), 153.34 (d, J = 251.4 Hz), 138.59 (s), 135.26 (s), 131.86 (s), 130.53 (d, J = 4.8 Hz), 129.94 (d, J = 3.9 Hz), 128.89 (s), 127.26 (s), 122.61 (d, J = 3.1 Hz), 116.93 (d, J = 17.9 Hz), 116.10 (d, J = 7.7 Hz), 109.59 (d, J = 18.6 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ: -119.89 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{16}H_{10}ClFN_2O$: 301.0538, found: 301.0538.

2v:



White solid, isolated yield: 23%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.06 (d, *J* = 87.3 Hz, 1H), 8.80 (d, *J* = 3.9, 1.6 Hz, 1H), 8.51-8.33 (m, 1H), 7.81-7.71 (m, 3H), 7.55-7.46 (m, 1H), 7.20-7.11 (m, 3H), 2.29 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 153.53 (d, *J* = 251.7 Hz), 149.37 (d, *J* = 39.5 Hz), 143.88 (d, *J* = 16.7 Hz), 139.01 (s), 136.18 (s), 133.25 (d, *J* = 22.4 Hz), 129.66 (dd, *J* = 21.7, 7.3 Hz), 127.23 (s), 126.73 (s), 122.67 (s), 121.96 (d, *J* = 2.7 Hz), 115.16 (d, *J* = 8.2 Hz)，110.18 (d, *J* = 20.4 Hz), 21.46 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ: -128.34 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{16}H_{13}FN_2O_2S$: 317.0755, found: 317.0758.

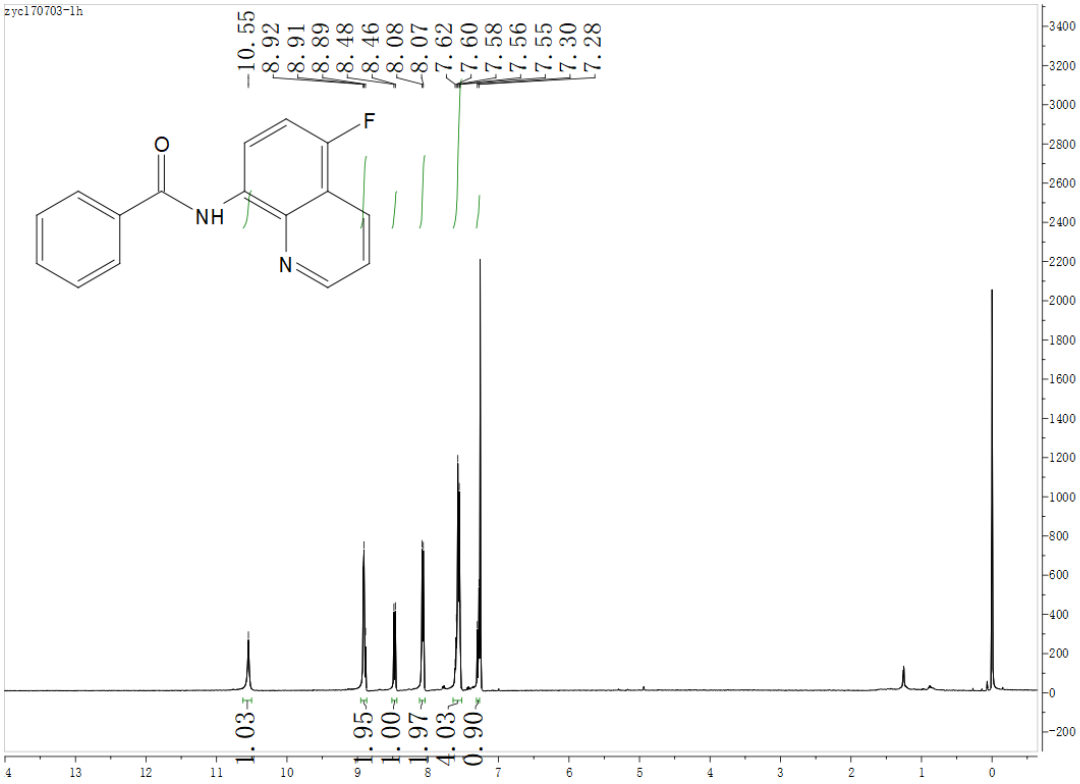
2w:

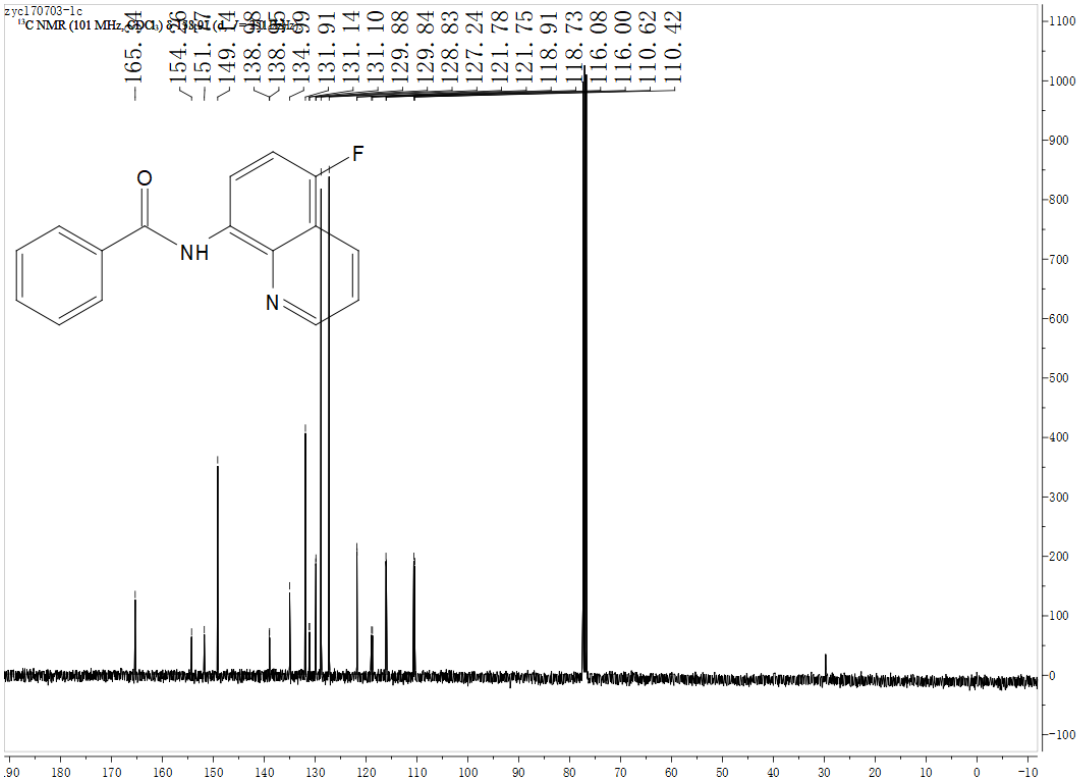


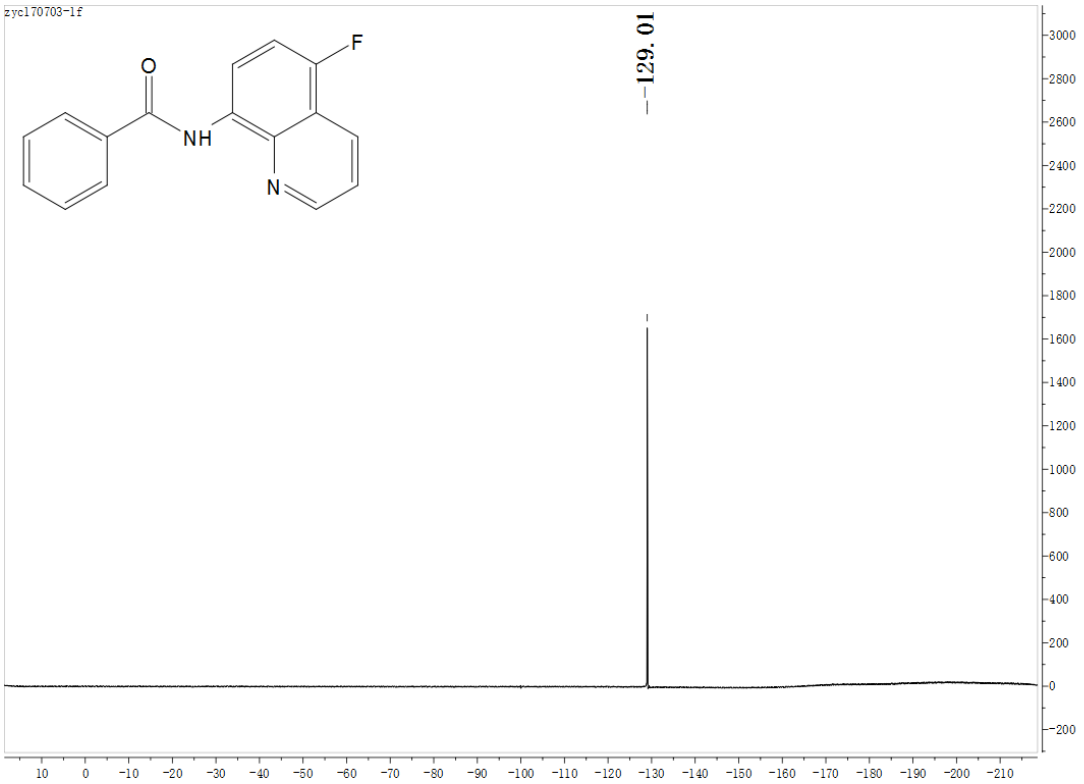
White solid, isolated yield: 28%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.19 (s, 1H), 8.79 (dd, *J* = 6.7, 2.7 Hz, 1H), 8.49-8.33 (m, 1H), 7.88 (dd, *J* = 15.2, 7.4 Hz, 2H), 7.83-7.74 (m, 1H), 7.54-7.32 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 153.69 (d, *J* = 252.5 Hz), 149.43 (d, *J* = 39.7 Hz), 139.08 (d, *J* = 9.9 Hz), 133.10 (dd, *J* = 28.0, 17.8 Hz), 129.81 (d, *J* = 3.6 Hz), 128.93 (d, *J* = 11.9 Hz), 127.17 (s), 126.72 (s), 126.23 (s), 125.26 (s), 122.37 (d, *J* = 70.5 Hz), 116.04-114.25 (m), 110.20 (d, *J* = 20.5 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ: -127.95 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{15}H_{11}FN_2O_2S$: 303.0598, found: 303.0600.

8 Spectra for C5 fluorinated N-(8-quinolinyl) amides and sulfonamides

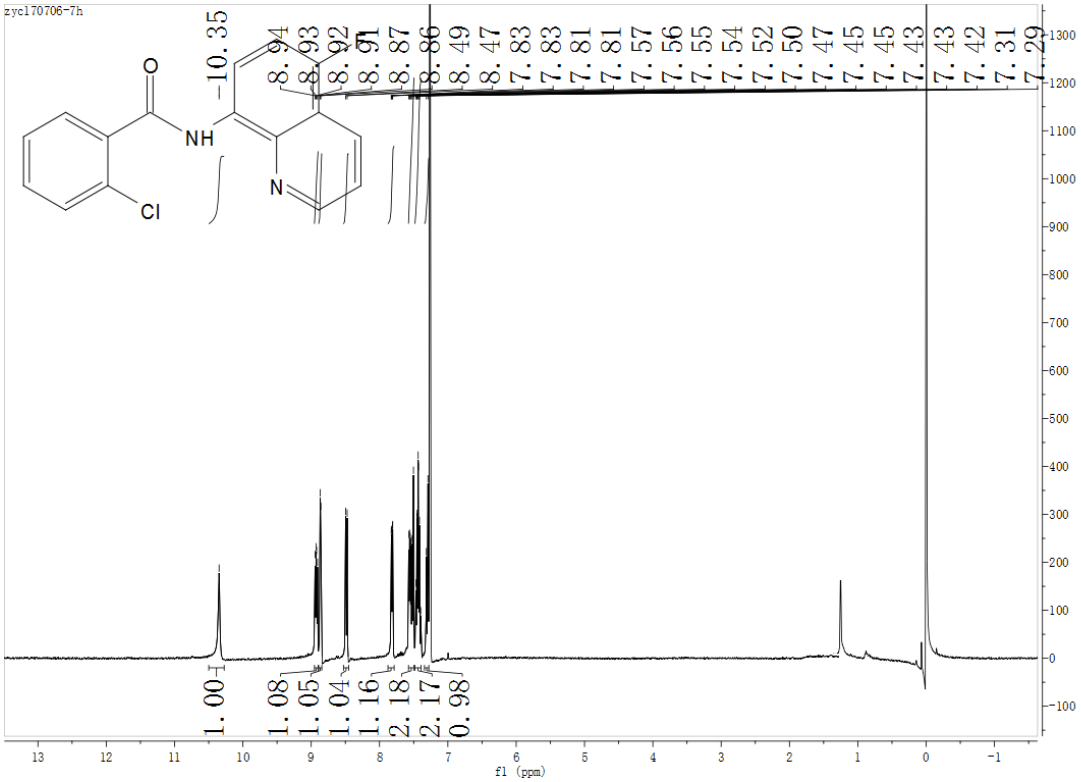
2a:

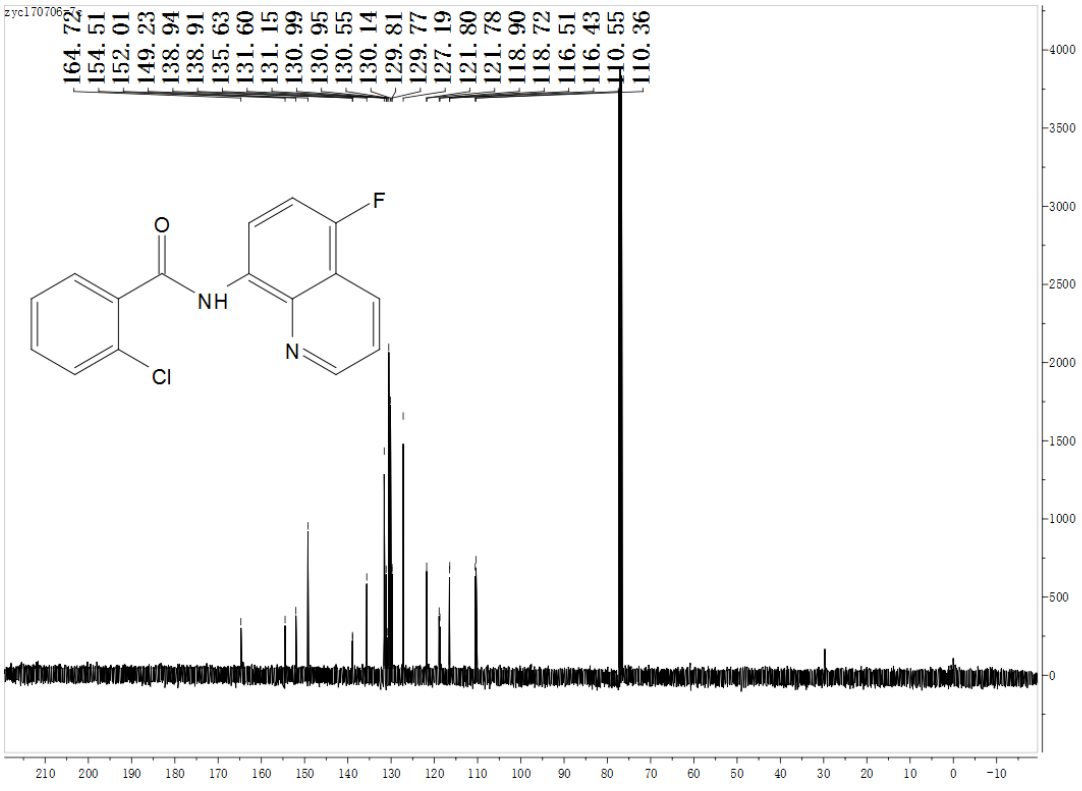


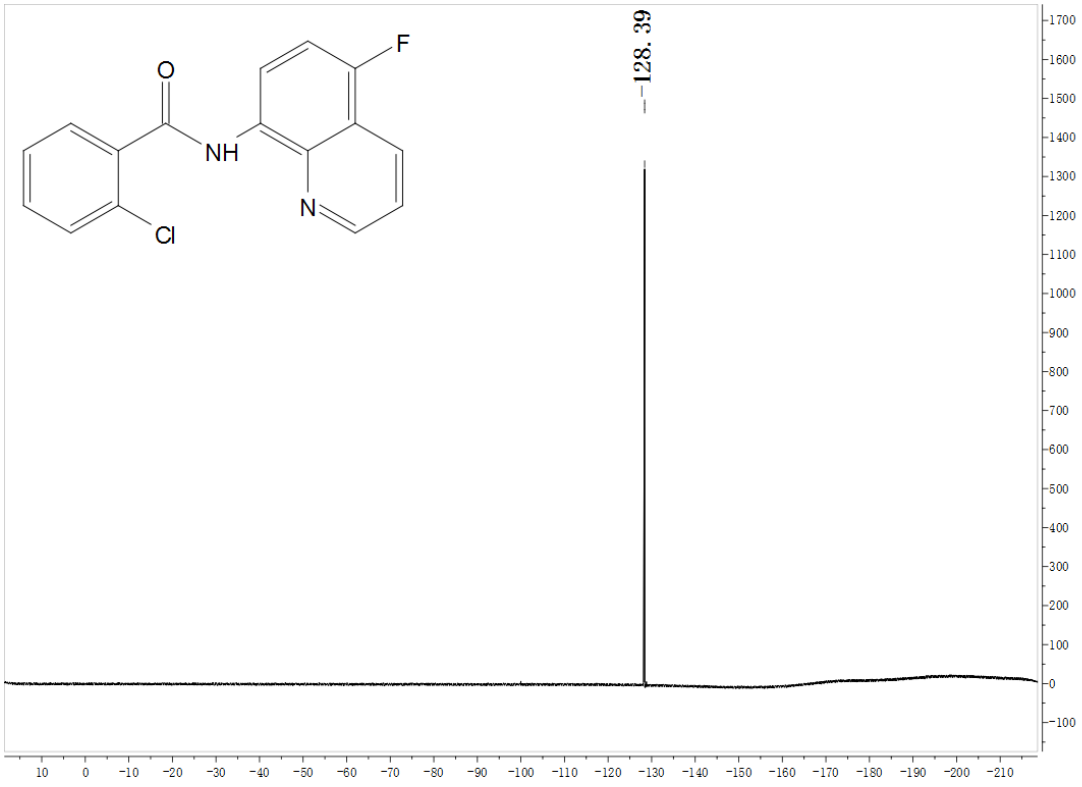



zyc170703-1f
O
NH
F
N
-129.01

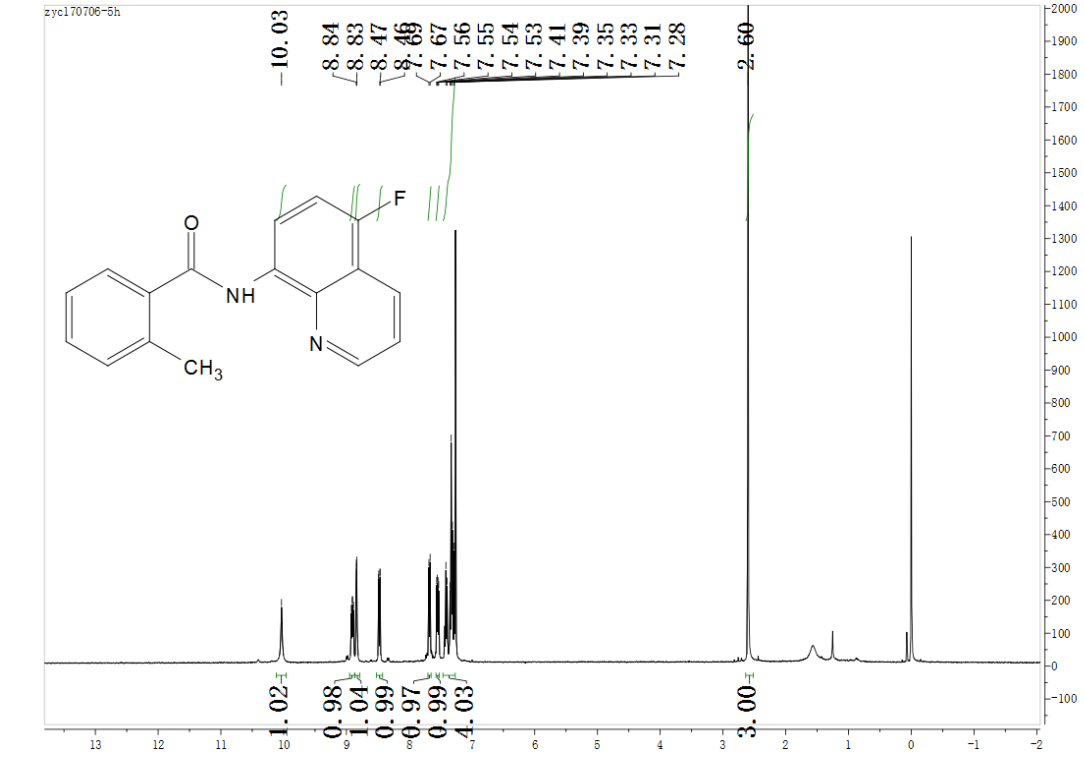
2b:

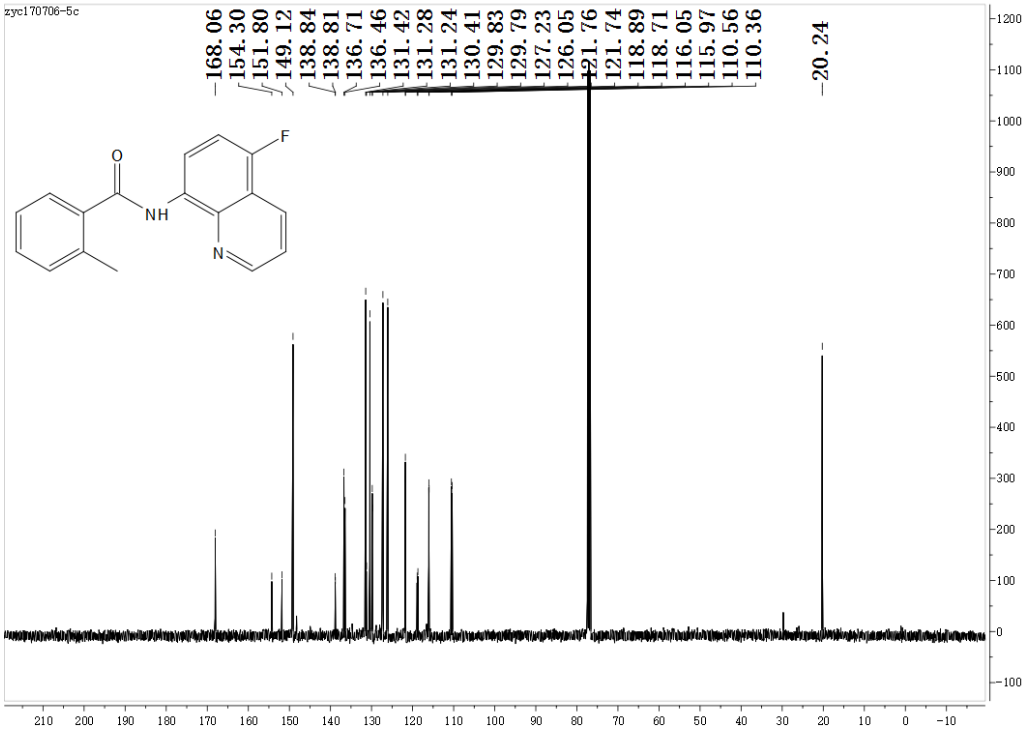

zyc170706-7h
O
NH
Cl
N
10.35
8.94
8.93
8.92
8.91
8.87
8.86
8.49
8.47
7.83
7.83
7.81
7.81
7.57
7.56
7.55
7.54
7.52
7.50
7.47
7.45
7.45
7.43
7.43
7.42
7.31
7.29
1.00
1.08
1.05
1.04
1.16
2.18
2.17
0.98
f1 (ppm)

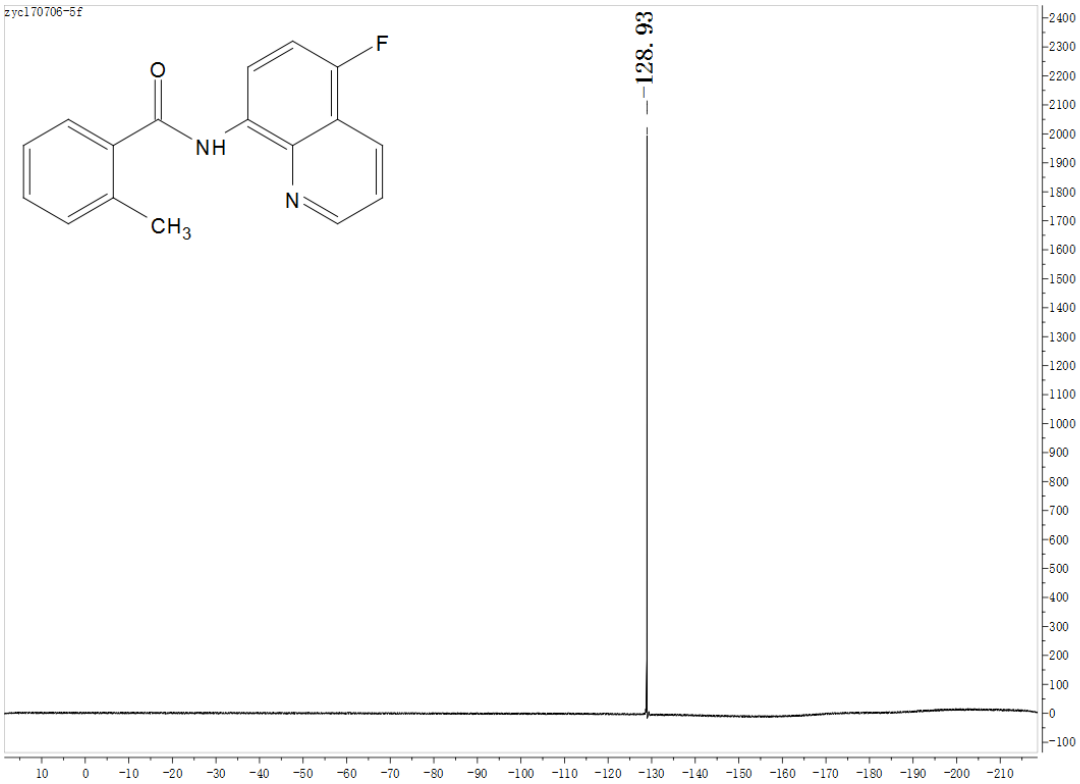

zyc170706-1s
164.72
154.51
152.01
149.23
138.94
138.91
135.63
131.60
131.15
130.99
130.95
130.55
130.14
129.81
129.77
127.19
121.80
121.78
118.90
118.72
116.51
116.43
110.55
110.36
O
NH
F
N
Cl


128.39
O
NH
F
N
Cl

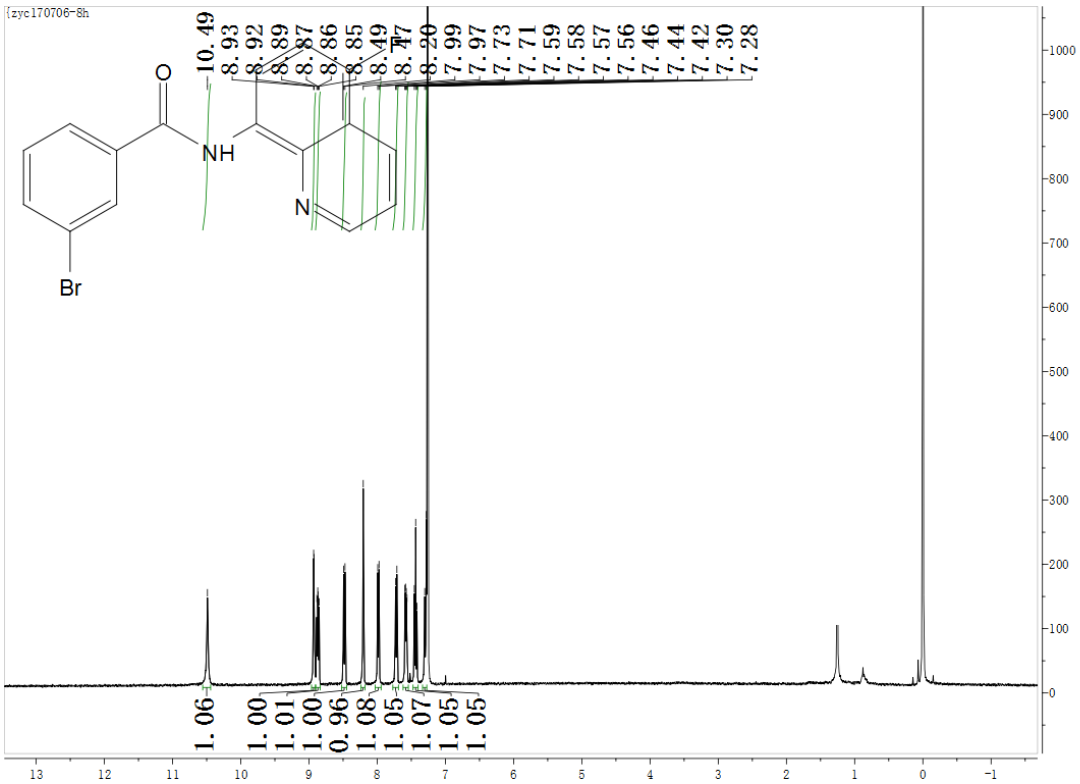
2c:

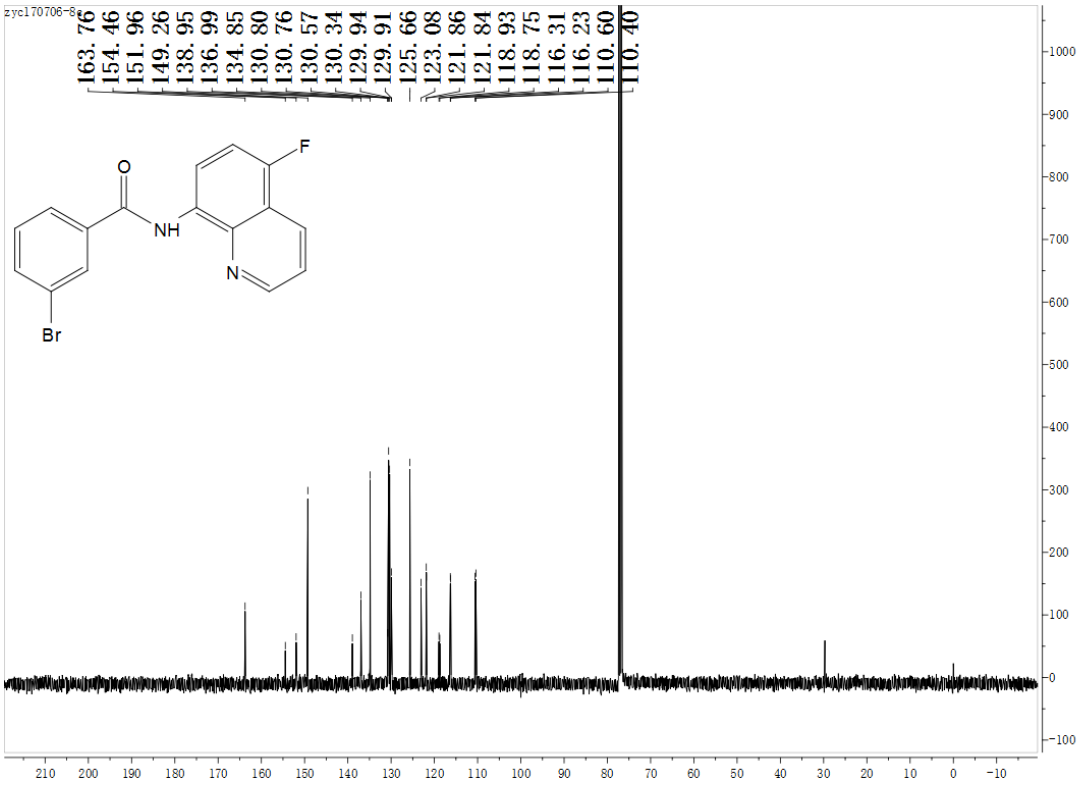

zyc170706-5h
10.03
8.84
8.83
8.47
7.67
7.56
7.55
7.54
7.53
7.41
7.39
7.35
7.33
7.31
7.28
2.60
1.02
0.98
1.04
0.99
0.97
0.99
4.03
3.00
O
NH
F
N
CH3


zyc170706-5c
168.06
154.30
151.80
149.12
138.84
138.81
136.71
136.46
131.42
131.28
131.24
130.41
129.83
129.79
127.23
126.05
121.76
121.74
118.89
118.71
116.05
115.97
110.56
110.36
20.24
O
NH
F
N


zyc170706-5f
O
NH
F
N
CH3
-128.93

2d:


zyc170706-8h
10.49
8.93
8.92
8.89
8.87
8.86
8.85
8.49
8.47
8.20
7.99
7.97
7.73
7.71
7.59
7.58
7.57
7.56
7.46
7.44
7.42
7.30
7.28
O
NH
N
Br
1.06
1.00
1.01
1.00
0.96
1.08
1.05
1.07
1.05
1.05


zyc170706-8e
163.76
154.46
151.96
149.26
138.95
136.99
134.85
130.80
130.76
130.57
130.34
129.94
129.91
125.66
123.08
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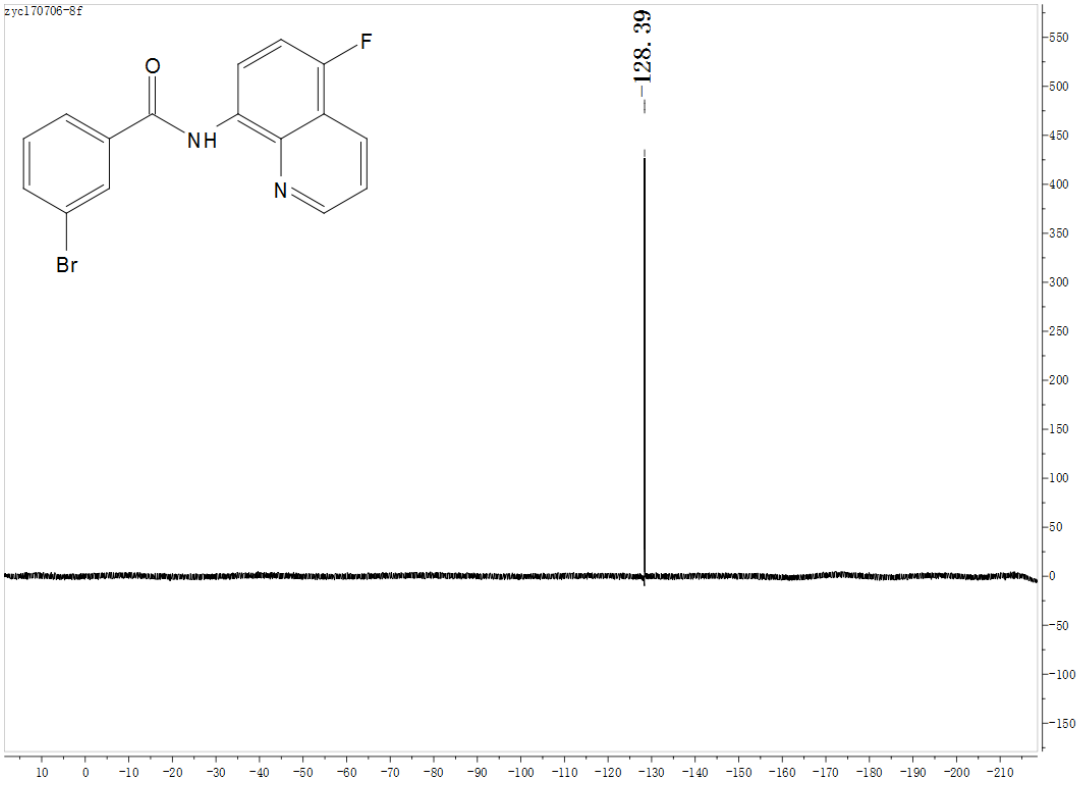
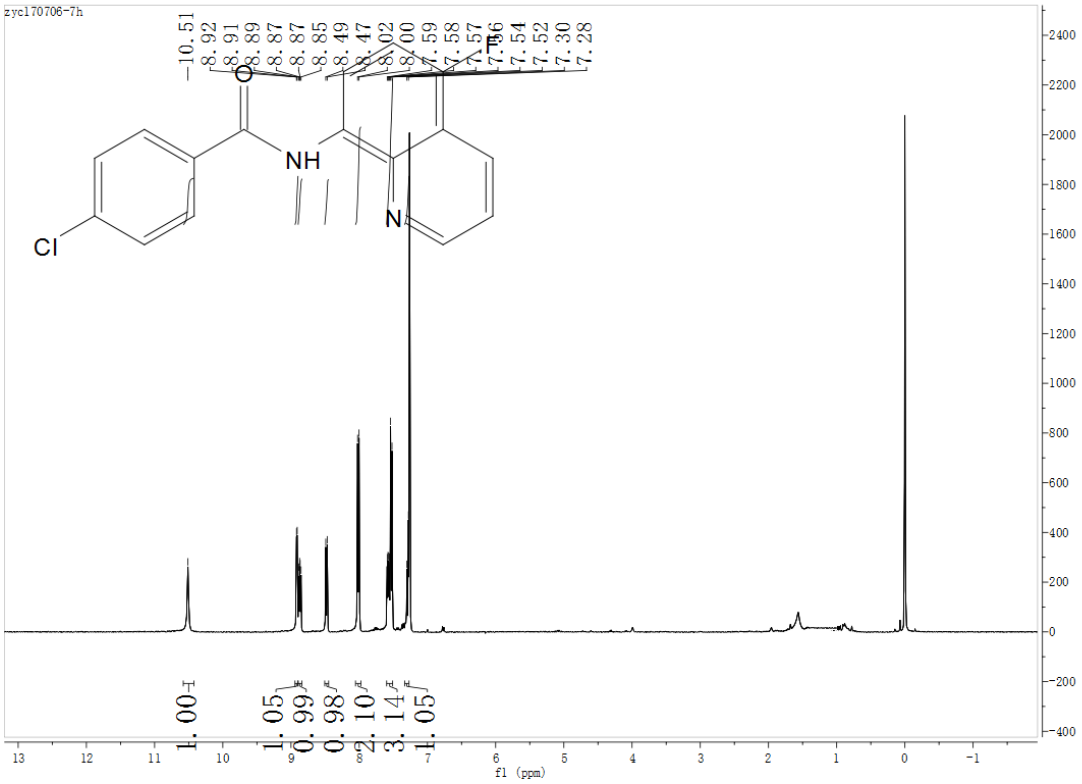
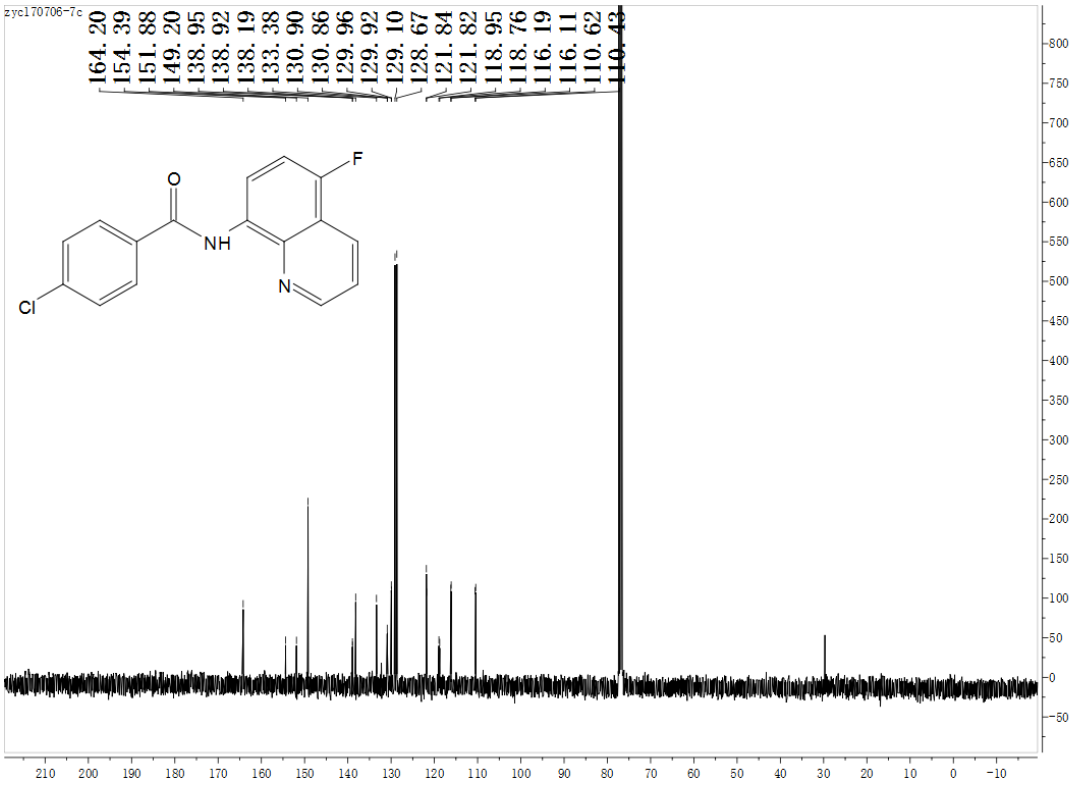
121.84
118.93
118.75
116.31
116.23
110.60
110.40
O
NH
F
N
Br


zyc170706-8f
128.39
O
NH
F
N
Br

2e:


zyc170706-7h
10.51
8.92
8.91
8.89
8.87
8.87
8.85
8.49
8.47
8.02
8.00
7.59
7.58
7.57
7.56
7.54
7.52
7.30
7.28
NH
N
Cl
1.00
1.05
0.99
0.98
2.10
3.14
1.05
f1 (ppm)


zyc170706-7c
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149.20
138.95
138.92
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133.38
130.90
130.86
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129.92
129.10
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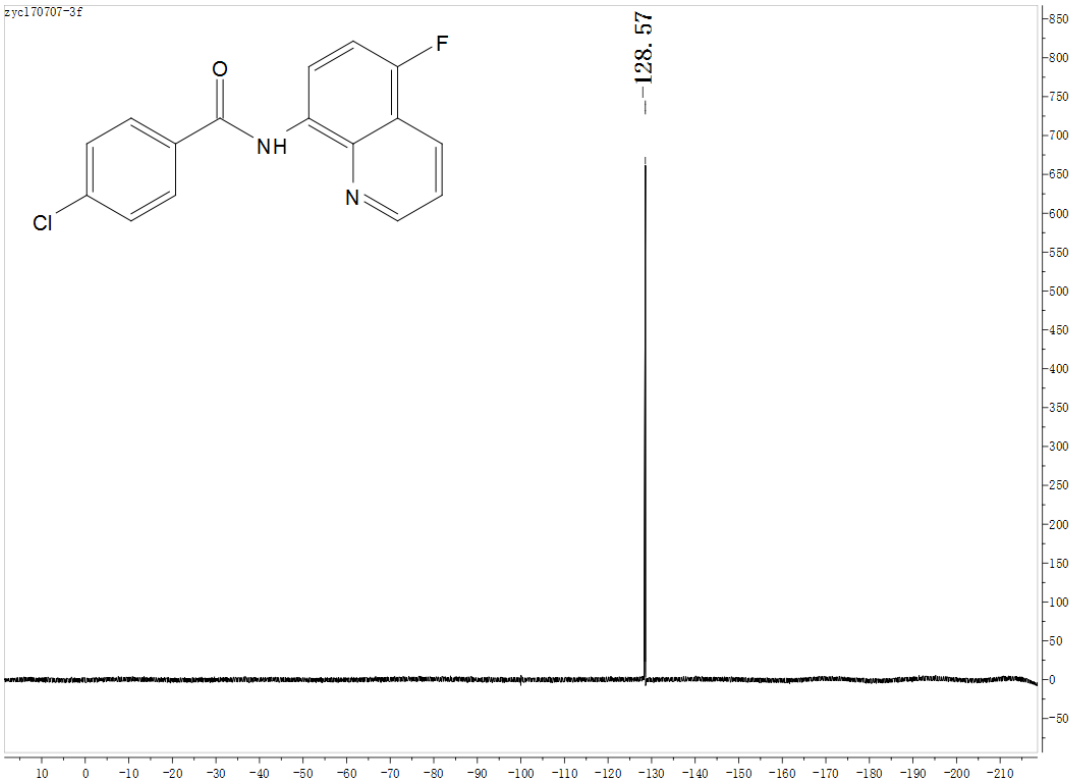
121.82
118.95
118.76
116.19
116.11
110.62
110.43
O
NH
N
F
Cl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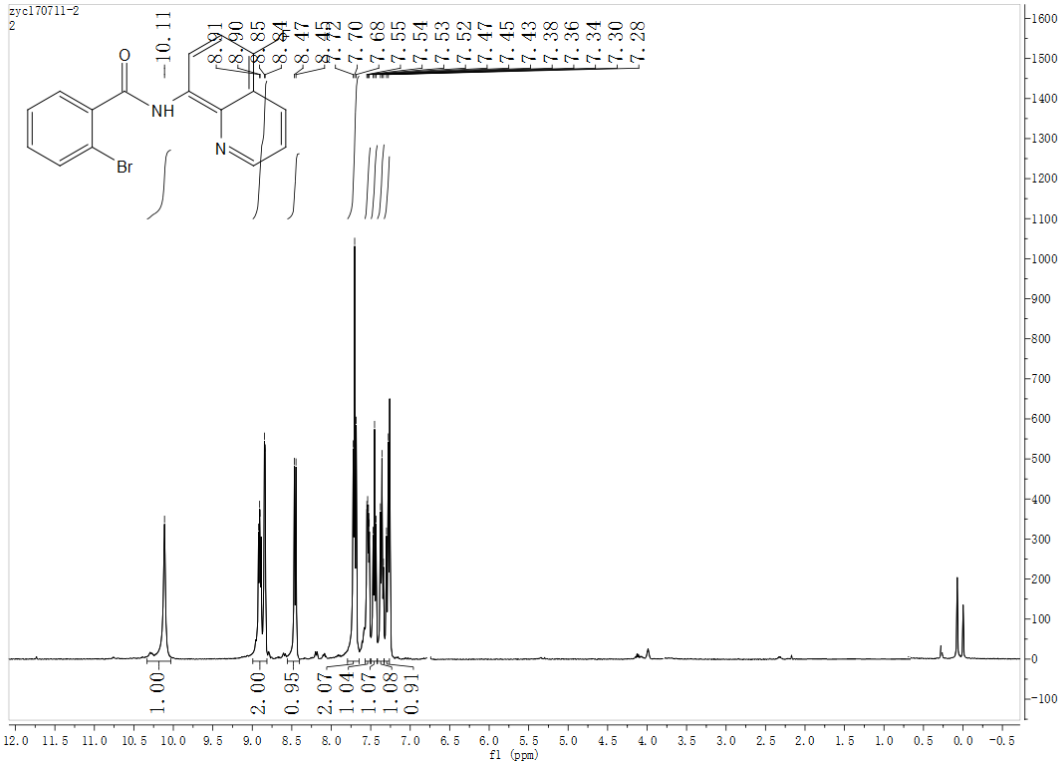
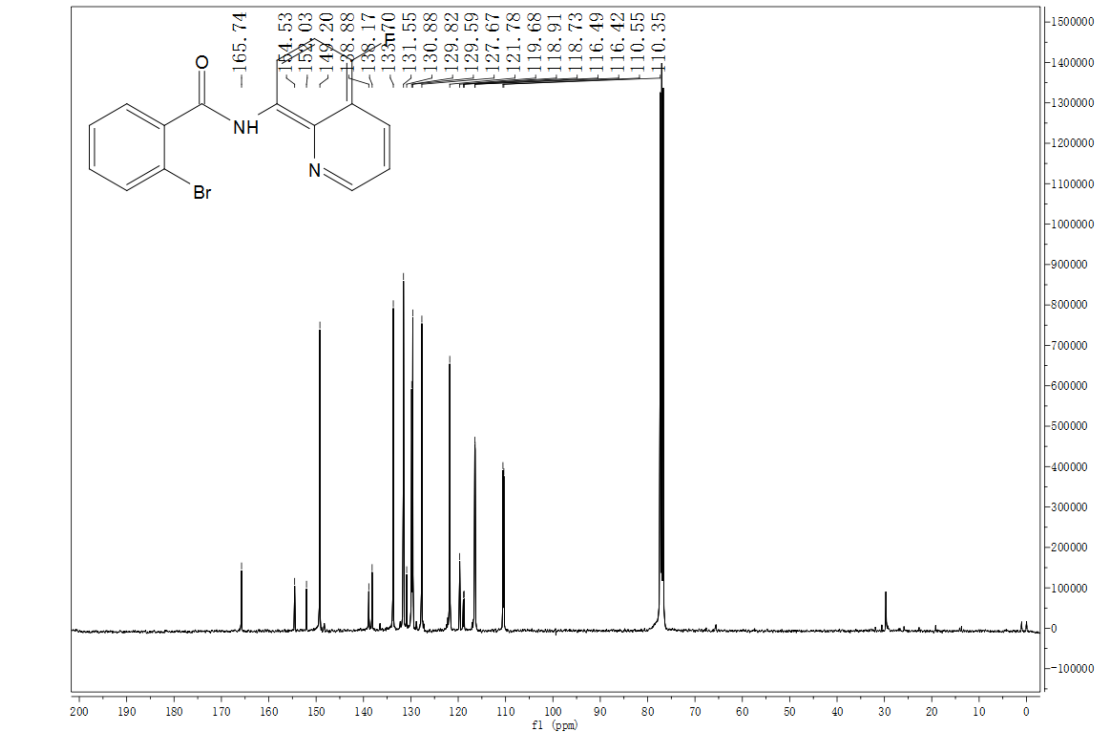
NH
F
Cl
N
-128.57

2f:


zyc170711-2
2
O
NH
Br
N
10.11
8.91
8.90
8.85
8.84
8.47
8.45
7.72
7.70
7.68
7.55
7.54
7.53
7.52
7.47
7.45
7.43
7.38
7.36
7.34
7.30
7.28
1.00
2.00
0.95
2.07
1.04
1.07
1.08
0.91
f1 (ppm)


O
NH
N
Br
165.74
154.53
152.03
149.20
138.88
138.17
133.70
131.55
130.88
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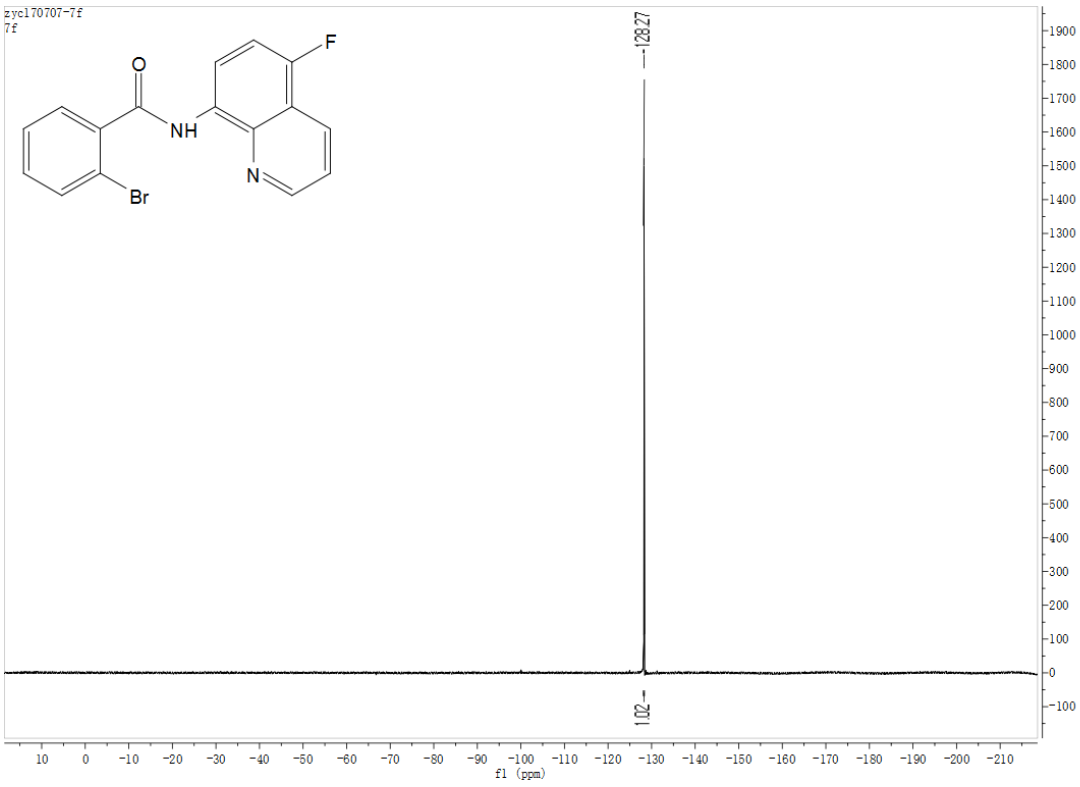
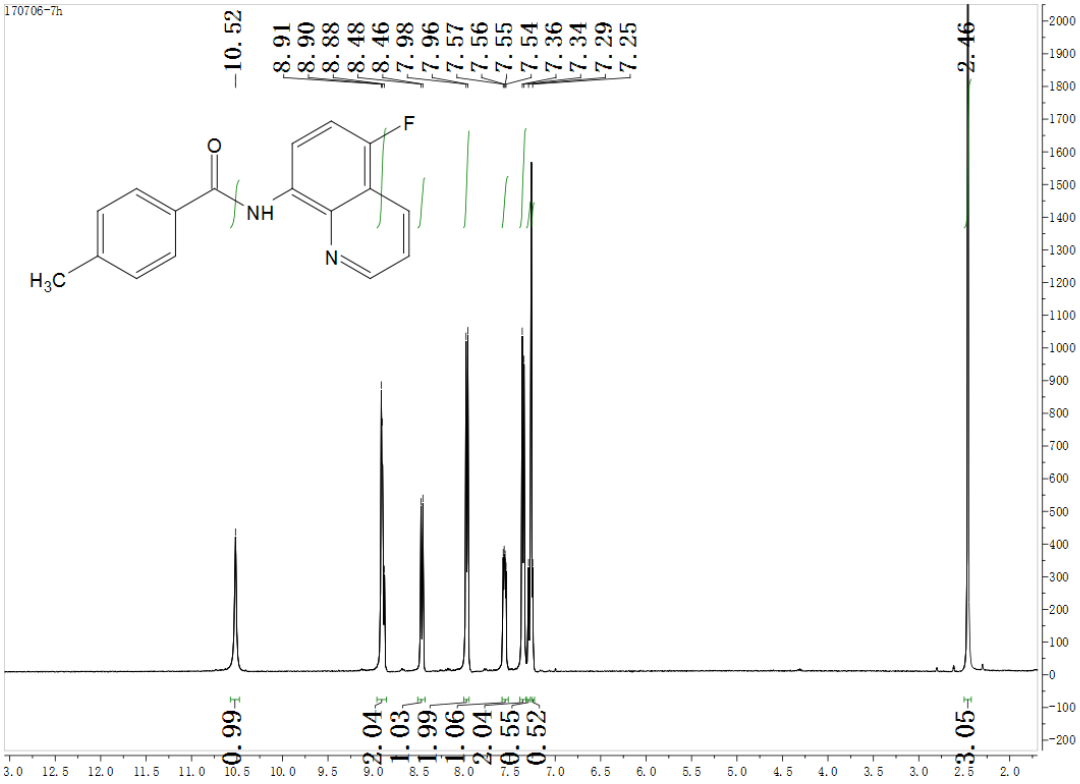
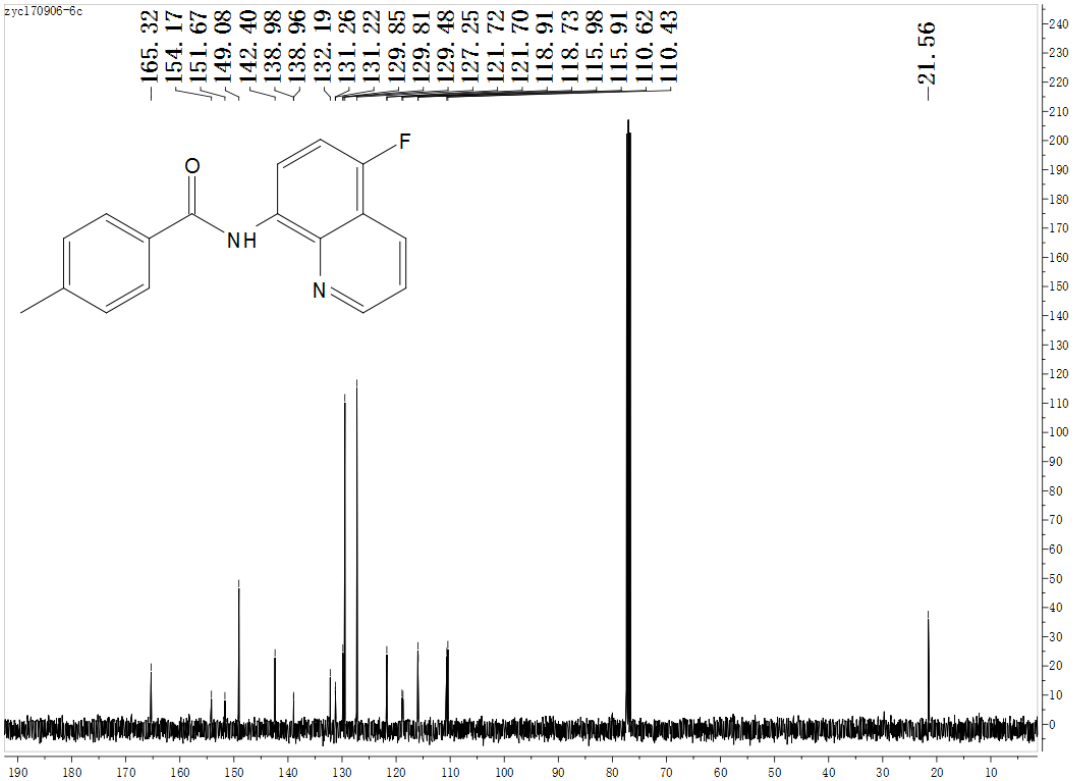
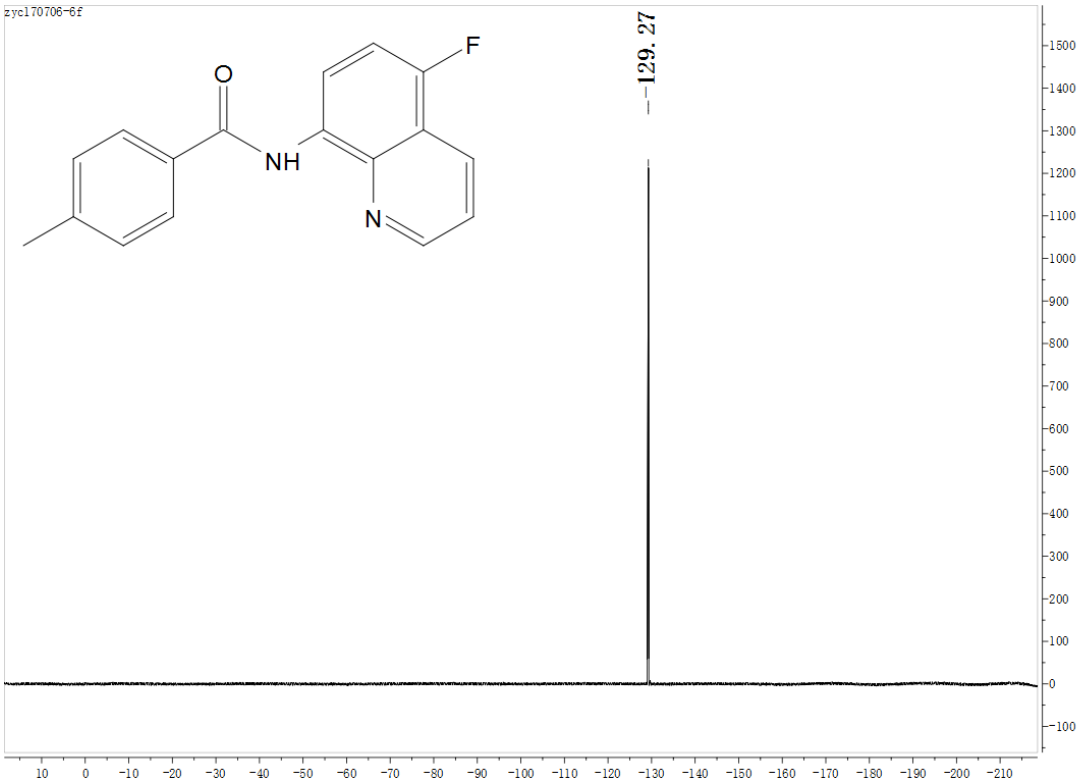
121.78
119.68
118.91
118.73
116.49
116.42
110.55
110.35
f1 (ppm)


zyc170707-7f
7f
O
NH
N
F
Br
-128.27
1.02
f1 (ppm)

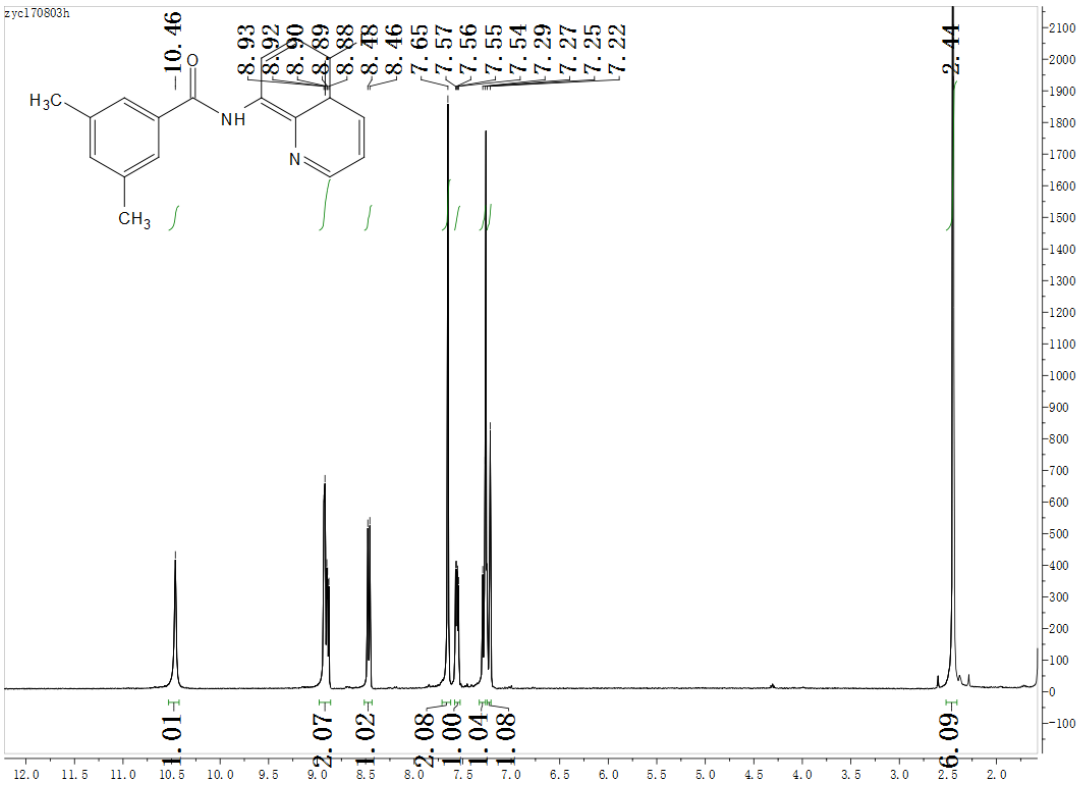
2g:


170706-7h
10.52
8.91
8.90
8.88
8.48
8.46
7.98
7.96
7.57
7.56
7.55
7.54
7.36
7.34
7.29
7.25
2.46
F
O
NH
N
H3C
0.99
2.04
1.03
1.99
1.06
2.04
0.55
0.52
3.05


zyc170906-6c
165.32
154.17
151.67
149.08
142.40
138.98
138.96
132.19
131.26
131.22
129.85
129.81
129.48
127.25
121.72
121.70
118.91
118.73
115.98
115.91
110.62
110.43
21.56
F
O
NH
N


zyc170706-6f
O
NH
F
N
-129.27

2h: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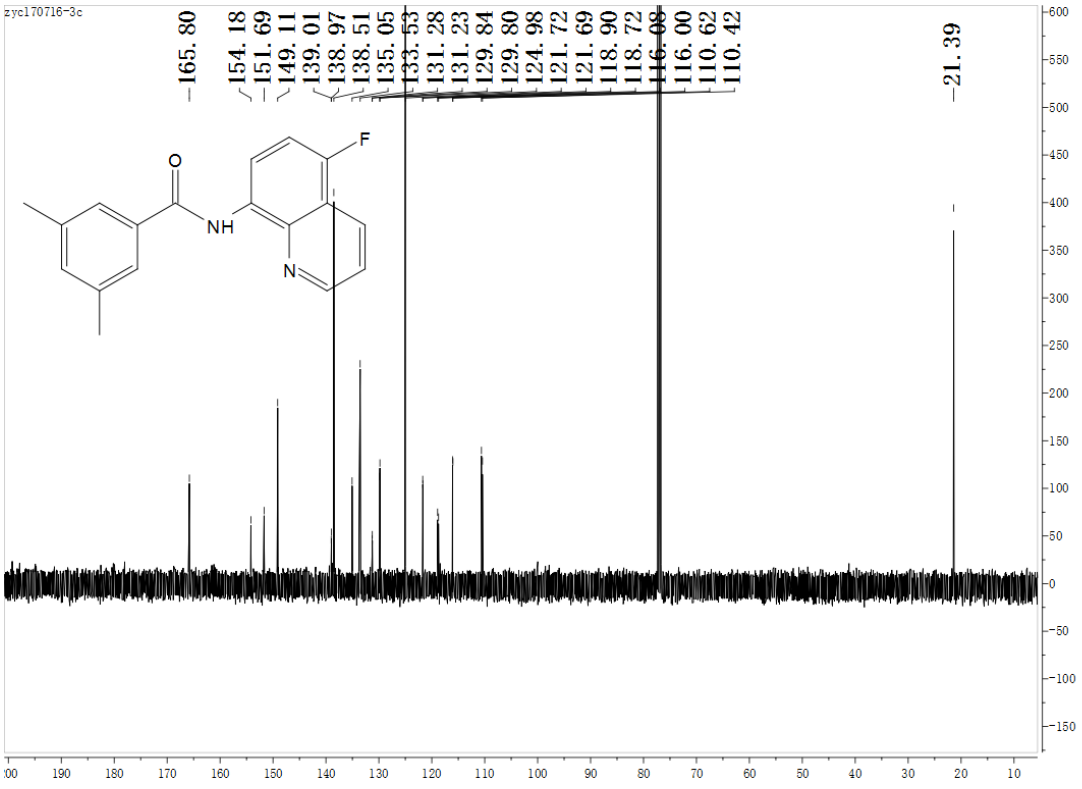
8.93
8.92
8.90
8.89
8.88
8.48
8.46
7.65
7.57
7.56
7.55
7.54
7.29
7.27
7.25
7.22
2.44
O
NH
N
H3C
CH3
1.01
2.07
1.02
2.08
1.00
1.04
1.08
6.09


zyc170716-3c
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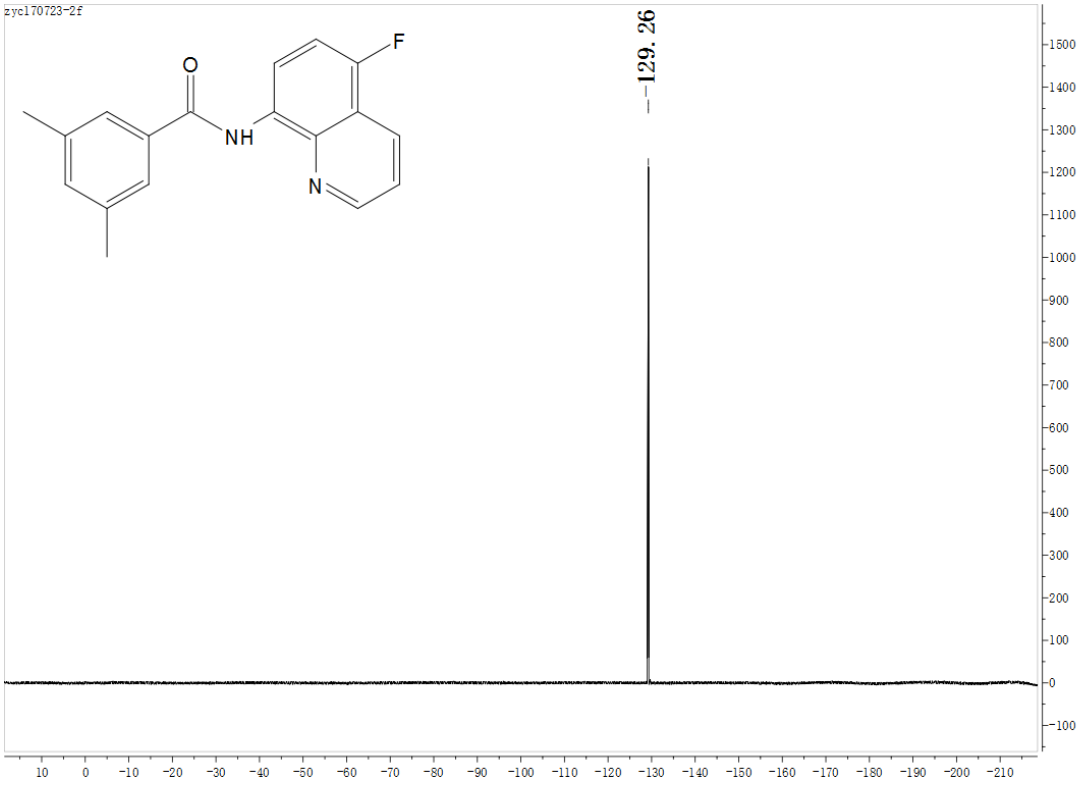
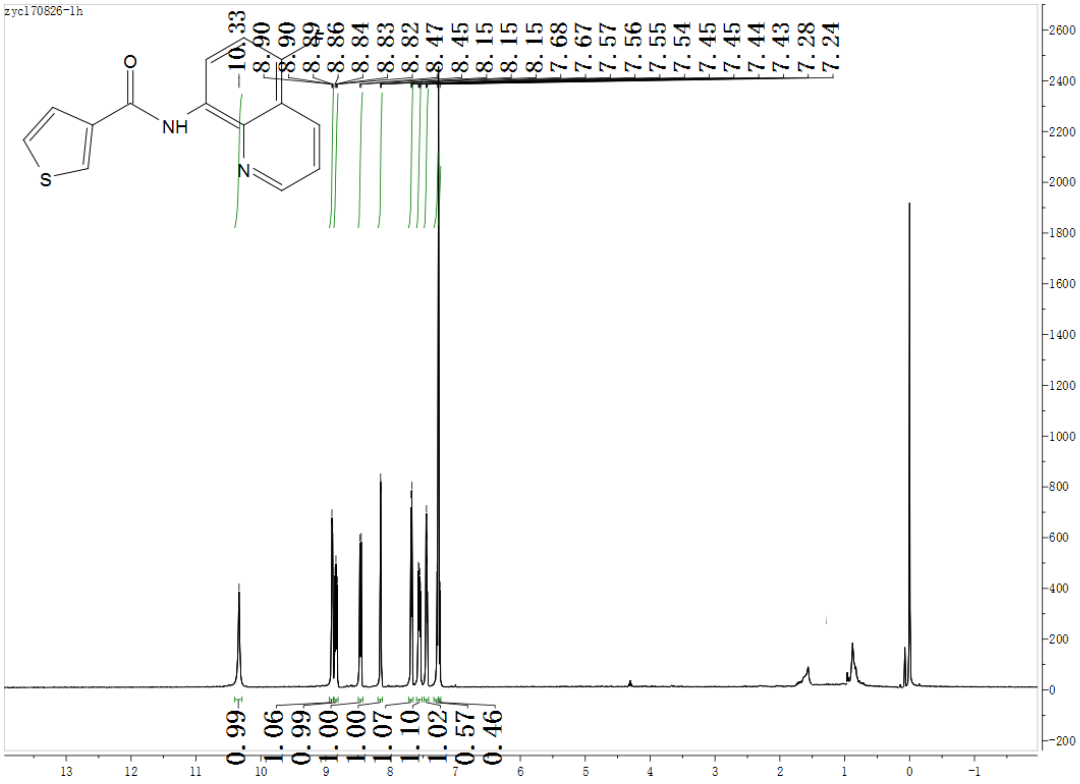
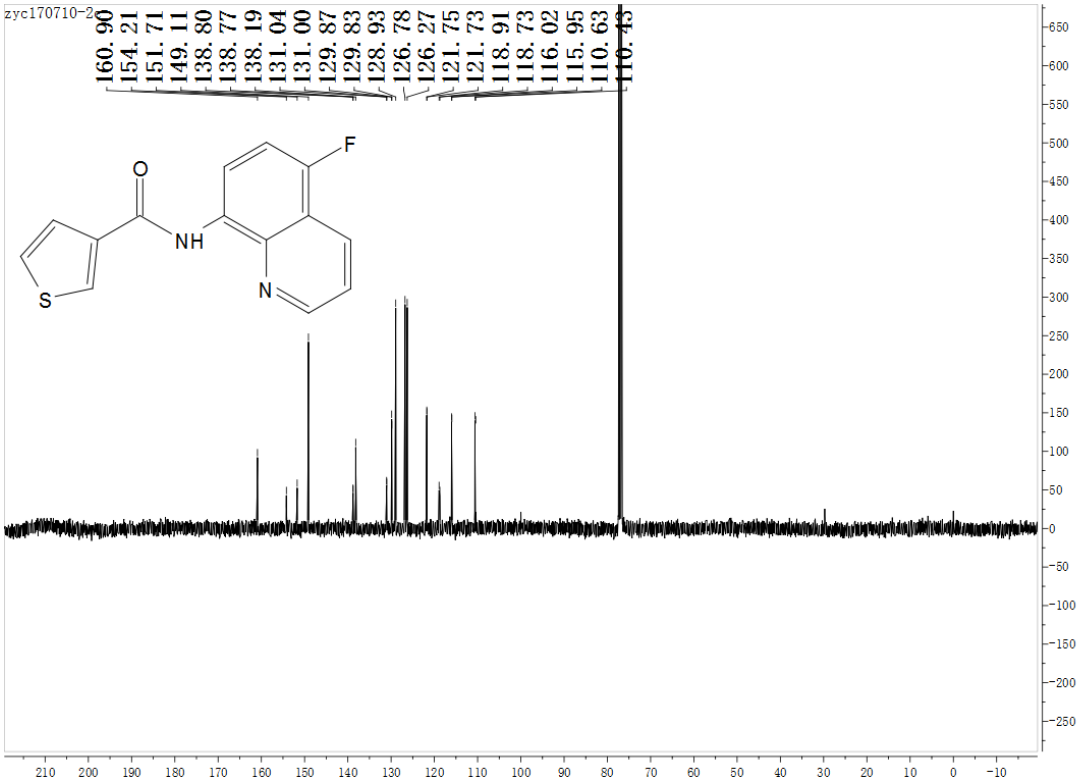
151.69
149.11
139.01
138.97
138.51
135.05
133.53
131.28
131.23
129.84
129.80
124.98
121.72
121.69
118.90
118.72
116.08
116.00
110.62
110.42
21.39
O
NH
F
N


zyc170723-2f
129.26
O
NH
F
N

2i:


zyc170826-1h
10.33
8.90
8.90
8.89
8.86
8.84
8.83
8.82
8.47
8.45
8.15
8.15
8.15
7.68
7.67
7.57
7.56
7.55
7.54
7.45
7.45
7.44
7.43
7.28
7.24
0.99
1.06
0.99
1.00
1.00
1.07
1.10
1.02
0.57
0.46
O
NH
S
N


zyc170710-2
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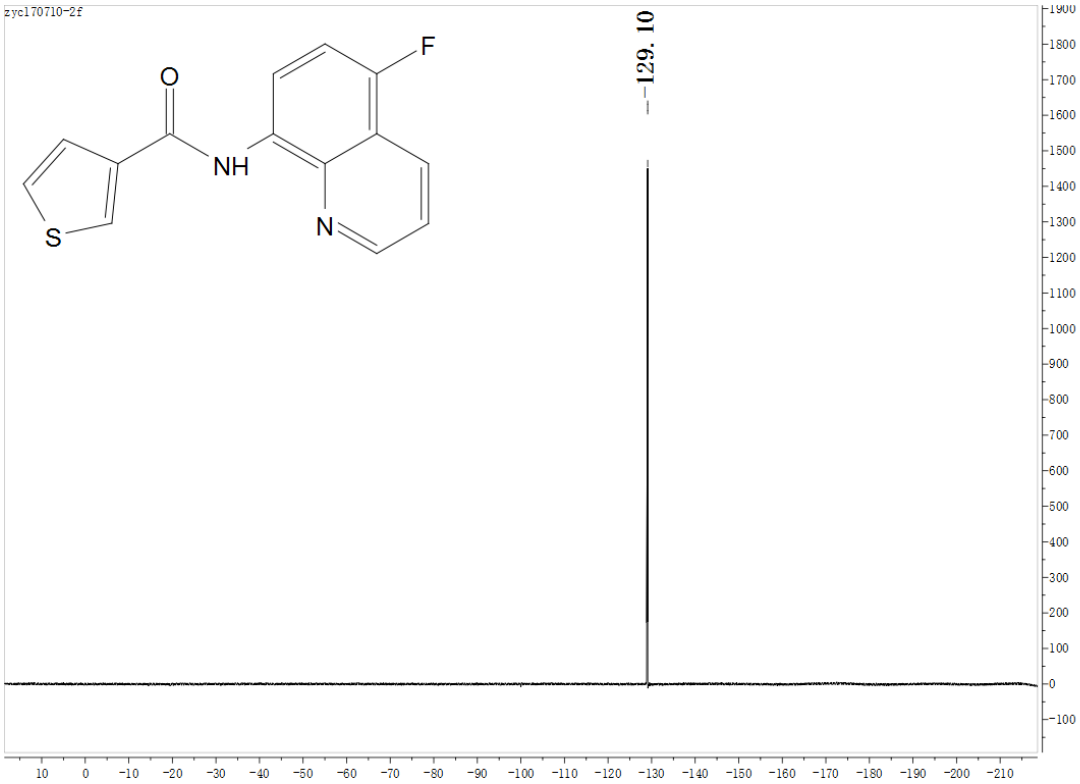
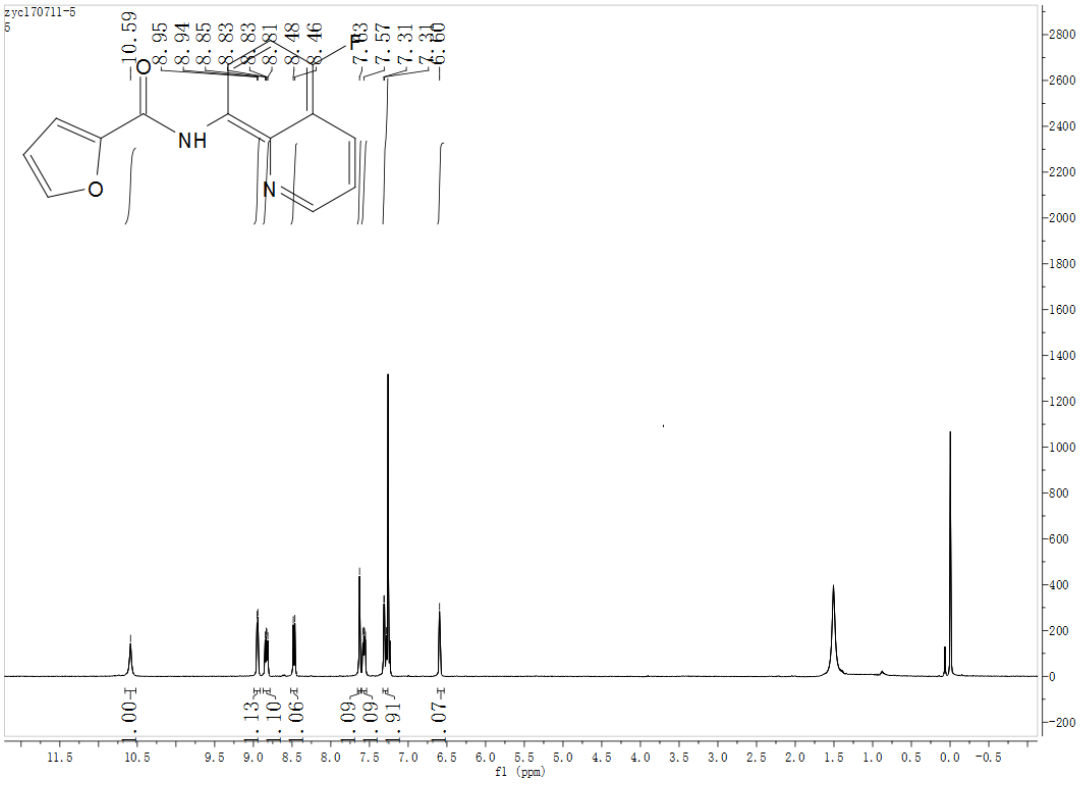
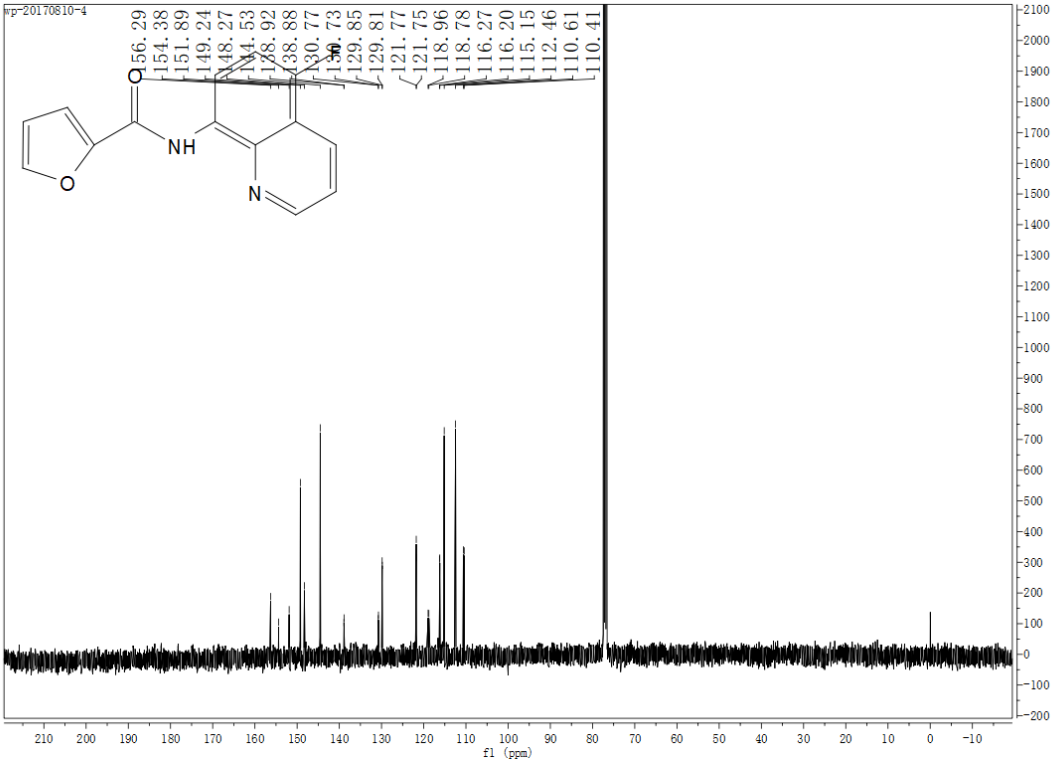
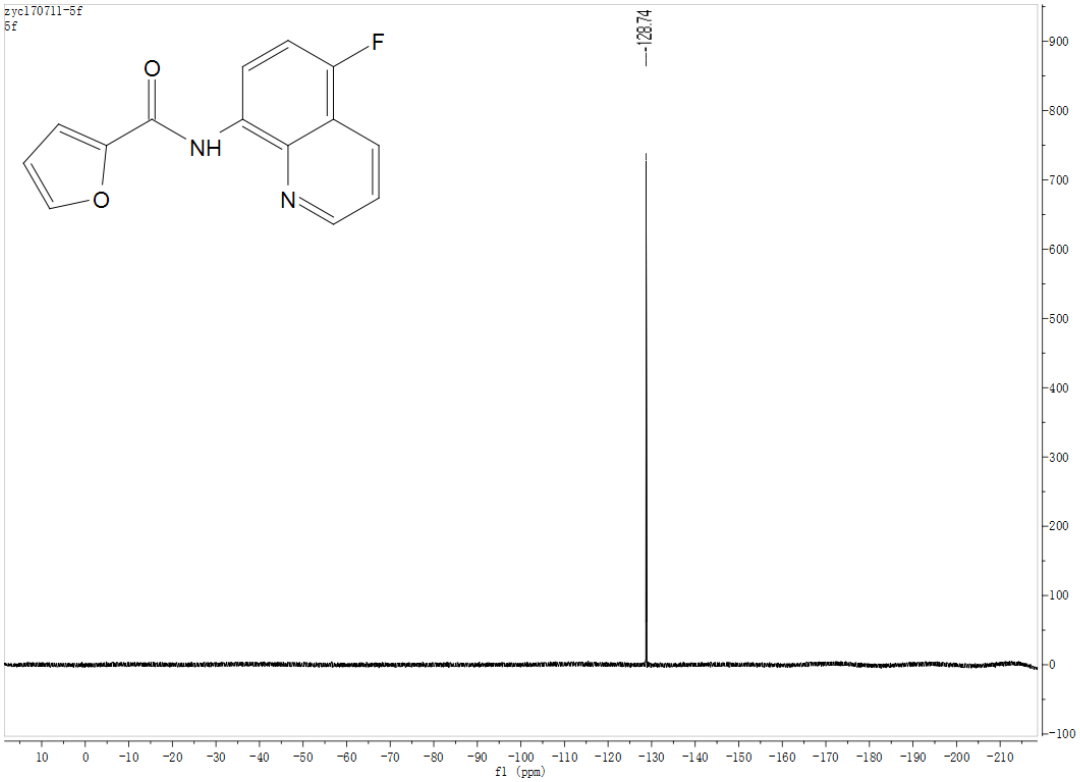
154.21
151.71
149.11
138.80
138.77
138.19
131.04
131.00
129.87
129.83
128.93
126.78
126.27
121.75
121.73
118.91
118.73
116.02
115.95
110.63
110.43
F
O
NH
S
N


zyc170710-2f
O
NH
S
F
N
-129.10

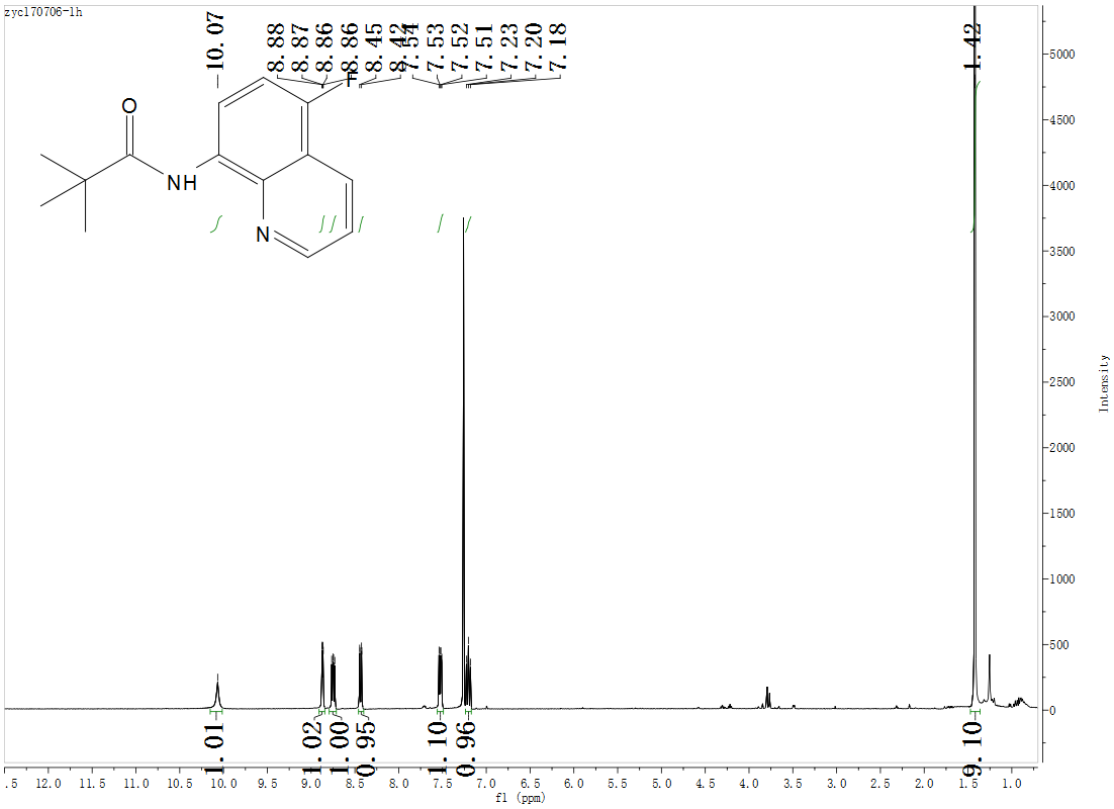
2j:

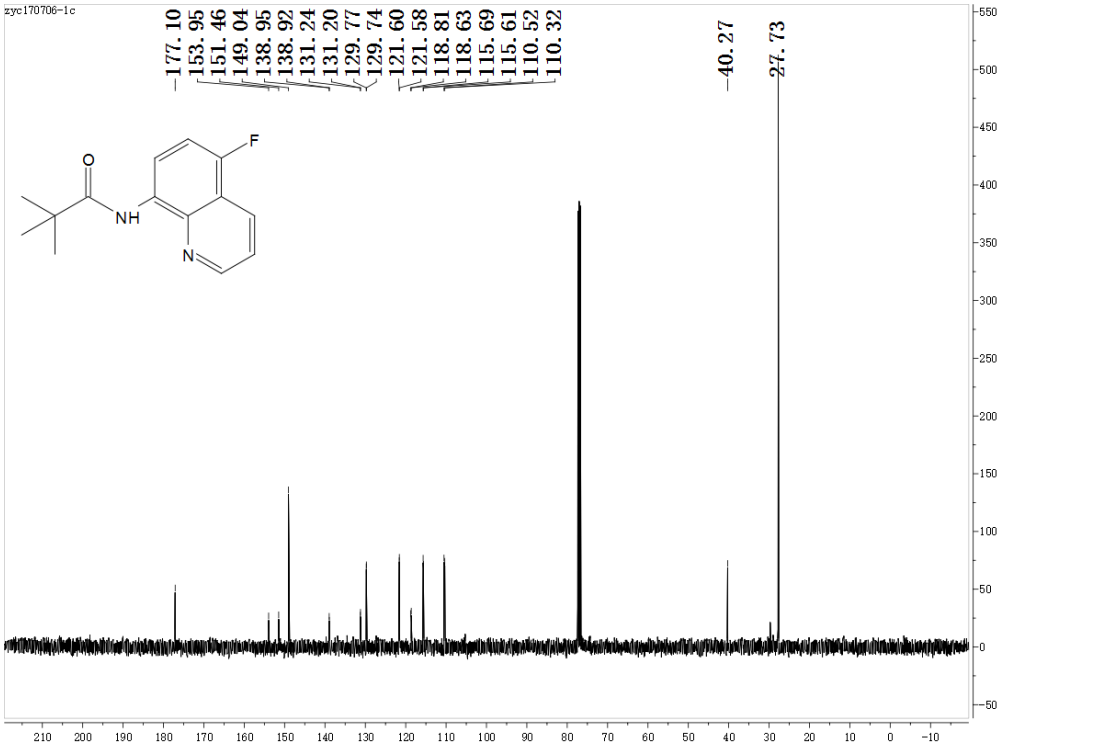

zyc170711-5
5
10.59
8.95
8.94
8.85
8.83
8.83
8.81
8.48
8.46
7.63
7.57
7.31
7.31
6.60
O
NH
O
N
F
1.00
1.13
1.10
1.06
1.09
1.09
1.91
1.07
f1 (ppm)


wp-20170810-4
156.29
154.38
151.89
149.24
148.27
144.53
138.92
138.88
130.77
130.73
129.85
129.81
121.77
121.75
118.96
118.78
116.27
116.20
115.15
112.46
110.61
110.41
O
NH
O
N
f1 (ppm)


zyc170711-5f
5f
-128.74
F
O
NH
O
N
f1 (ppm)

2k:


zyc170706-1h
10.07
8.88
8.87
8.86
8.86
8.45
8.44
7.54
7.53
7.52
7.51
7.23
7.20
7.18
1.42
1.01
1.02
1.00
0.95
1.10
0.96
9.10
O
NH
N
F
f1 (ppm)
Intensity


zyc170706-1c
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151.46
149.04
138.95
138.92
131.24
131.20
129.77
129.74
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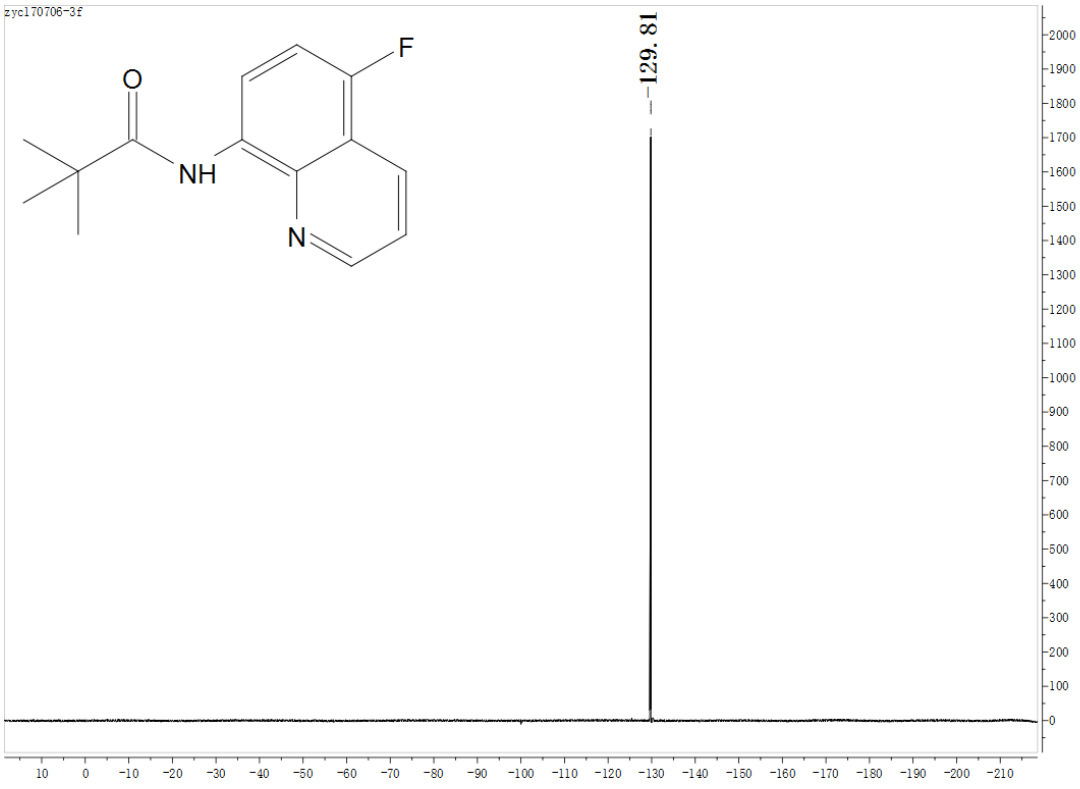
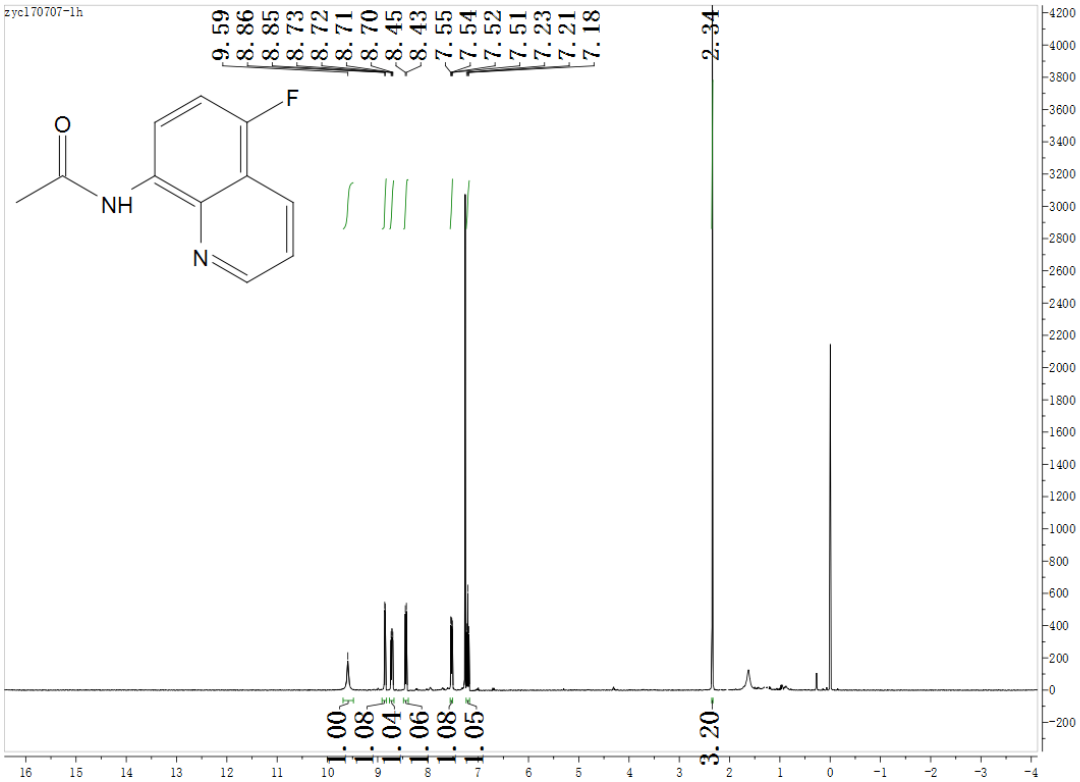
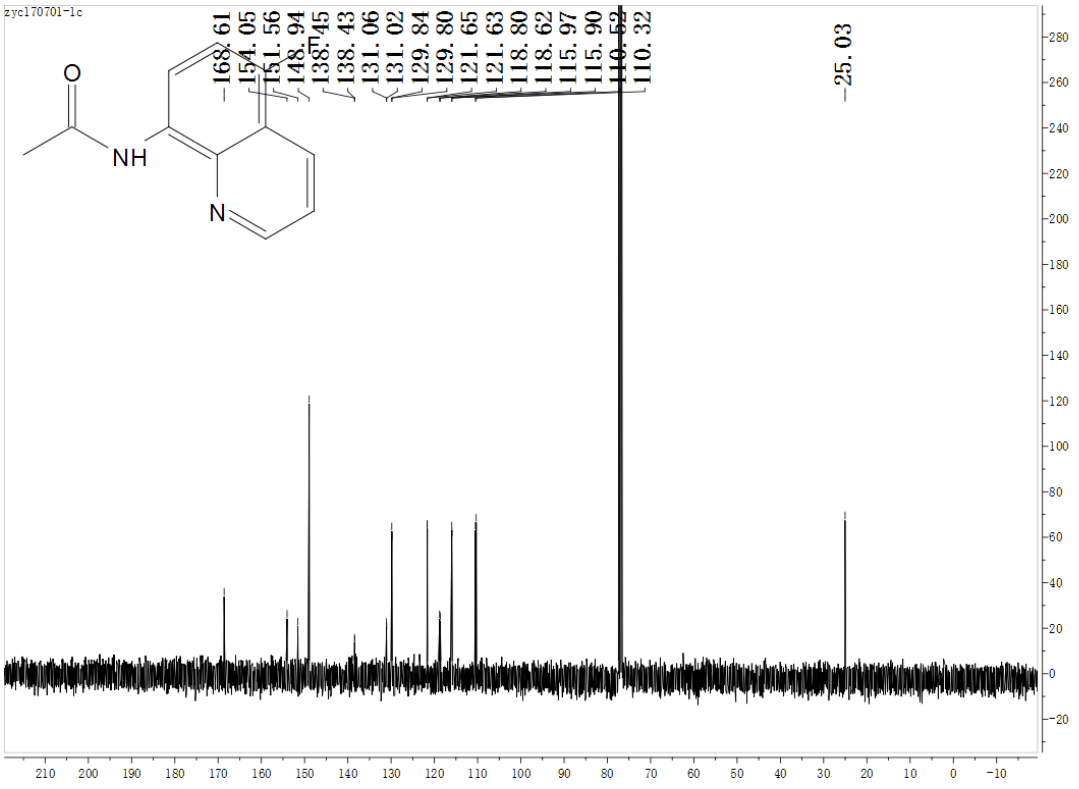
118.63
115.69
115.61
110.52
110.32
40.27
27.73
O
NH
N
F


zyc170706-3f
O
NH
F
N
-129.81

2l:


zyc170707-1h
9.59
8.86
8.85
8.73
8.72
8.71
8.70
8.45
8.43
7.55
7.54
7.52
7.51
7.23
7.21
7.18
2.34
O
NH
F
N
1.00
1.08
1.04
1.06
1.08
1.05
3.20


zyc170701-1c
O
NH
N
168.61
154.05
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138.43
131.06
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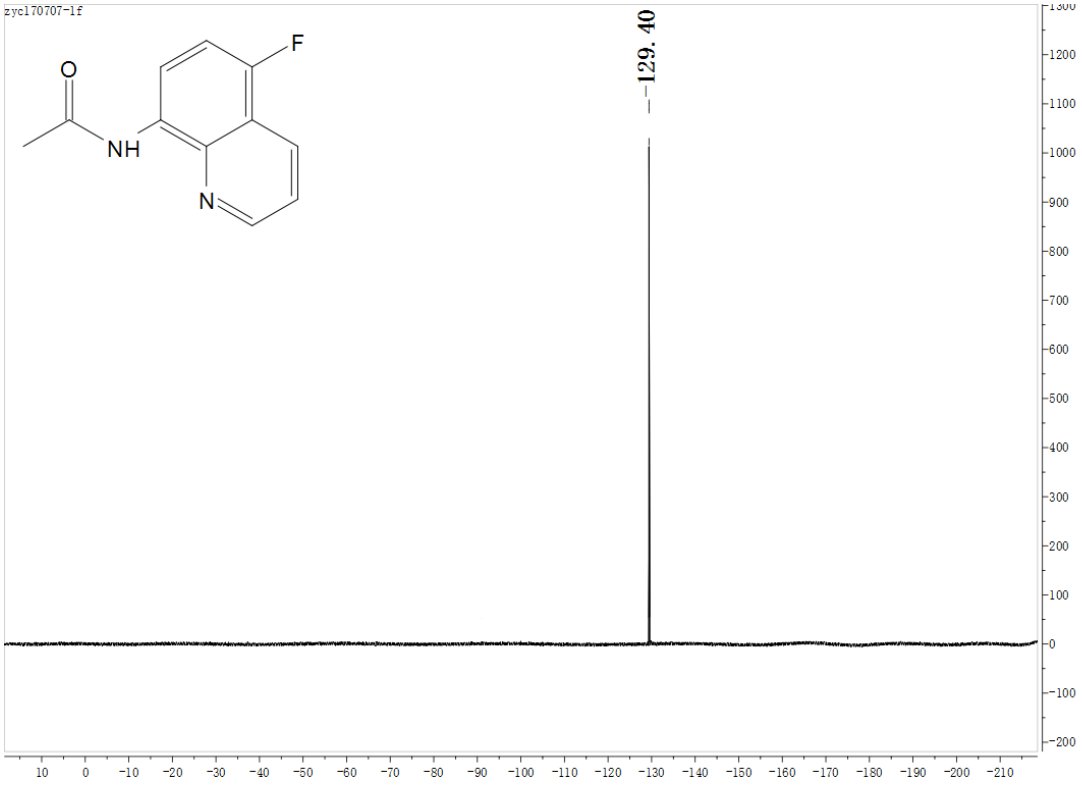
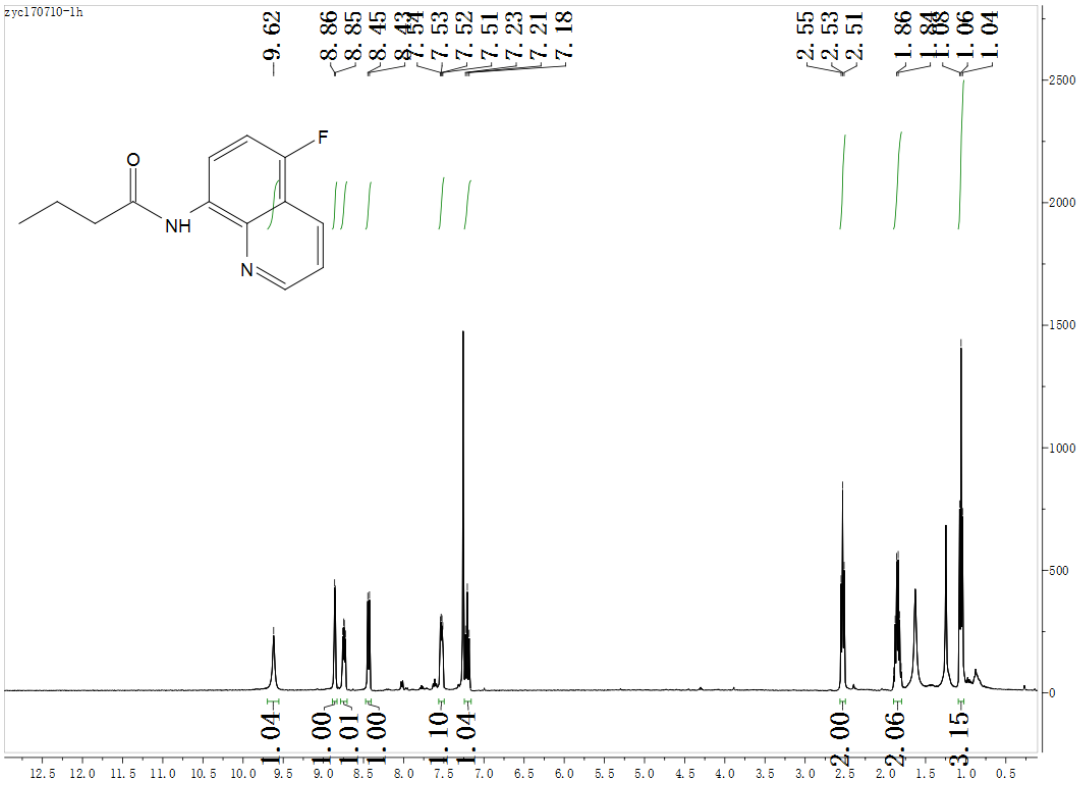
110.32
25.03


zyc170707-1f
O
NH
N
F
129.40

2m: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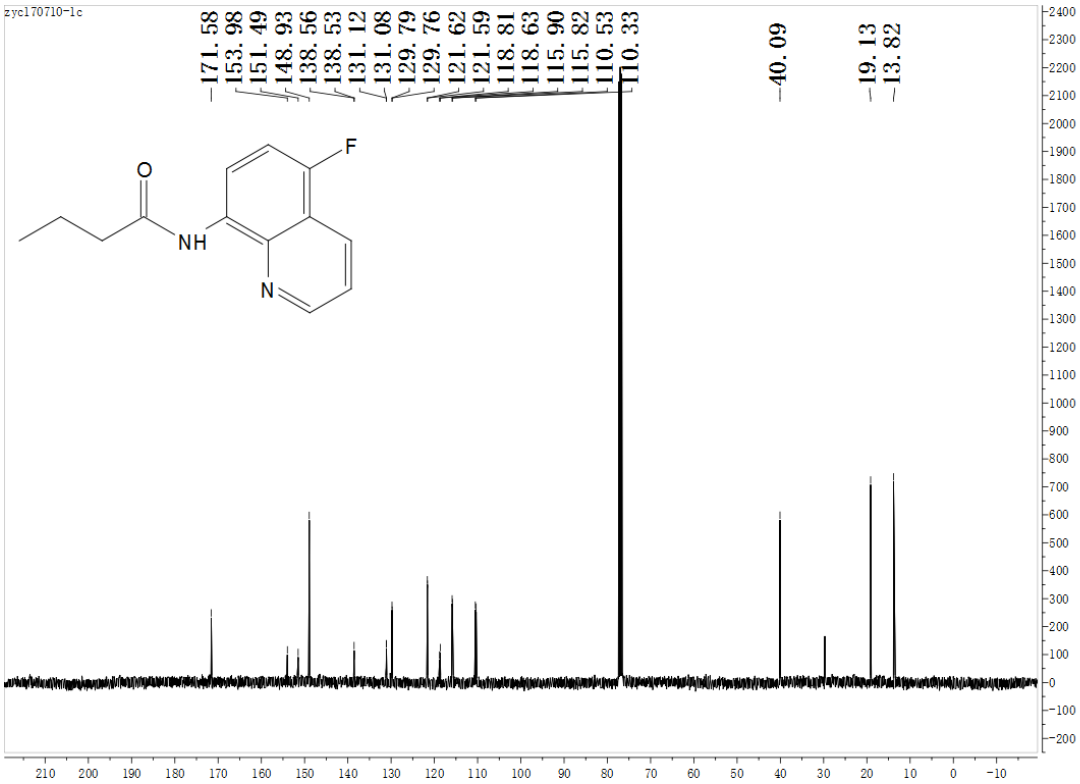
8.86
8.85
8.45
7.53
7.52
7.51
7.23
7.21
7.18
2.55
2.53
2.51
1.86
1.06
1.04
F
O
NH
N
1.04
1.00
1.01
1.00
1.10
1.04
2.00
2.06
3.15


zycl70710-1c
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151.49
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138.56
138.53
131.12
131.08
129.79
129.76
121.62
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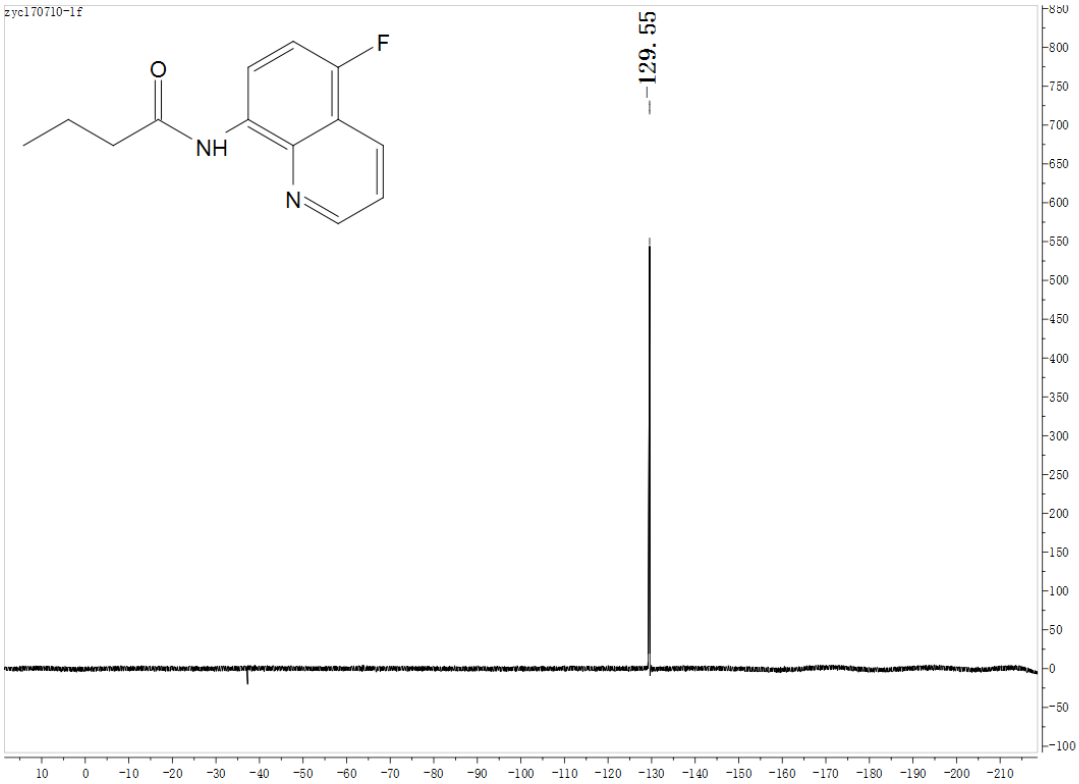
115.90
115.82
110.53
110.33
40.09
19.13
13.82
F
O
NH
N


zyc170710-1f
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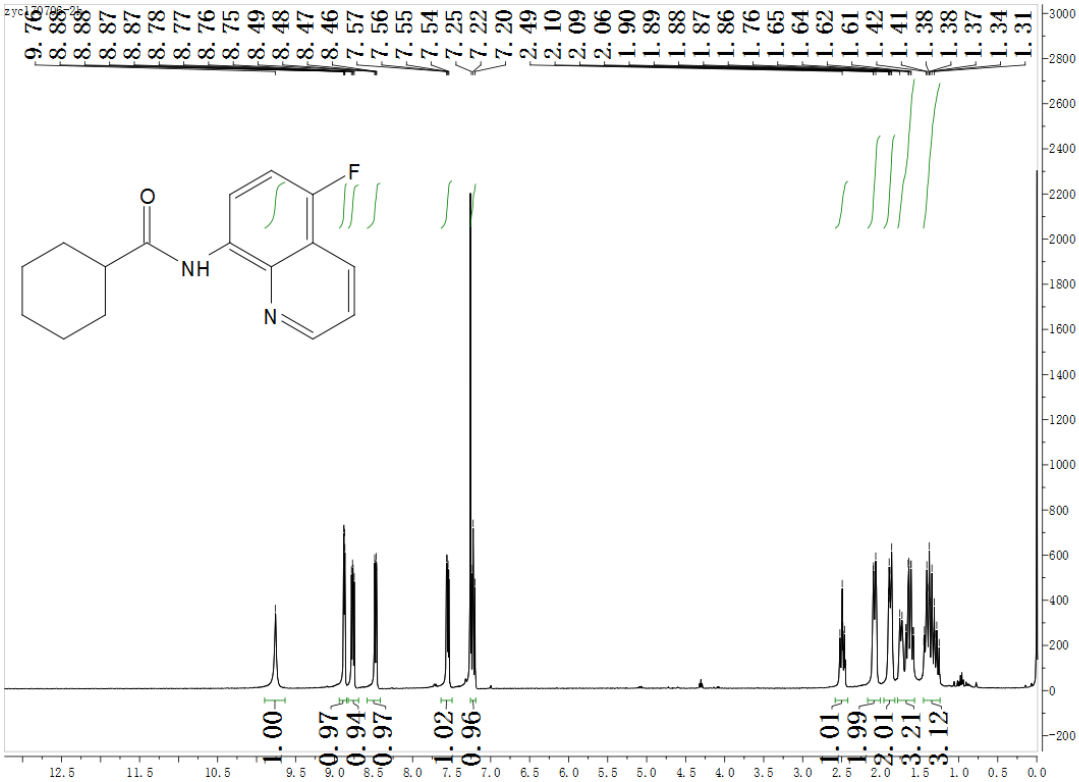
NH
N
F
-129.55

2n: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NH
N
F
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8.78
8.77
8.76
8.75
8.49
8.48
8.47
8.46
7.57
7.56
7.55
7.54
7.25
7.22
7.20
2.49
2.10
2.09
2.06
1.90
1.89
1.88
1.87
1.86
1.76
1.65
1.64
1.62
1.61
1.42
1.41
1.38
1.38
1.37
1.34
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0.94
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1.02
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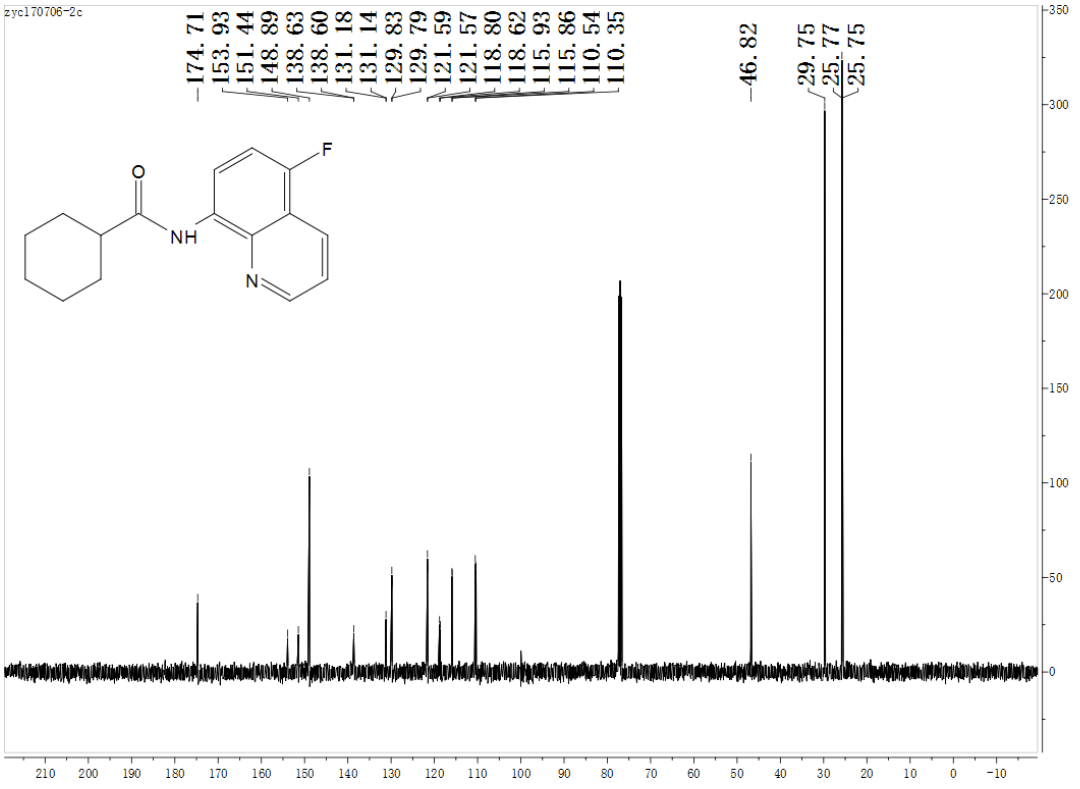
1.01
1.99
2.01
3.21
3.12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131.14
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121.57
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115.86
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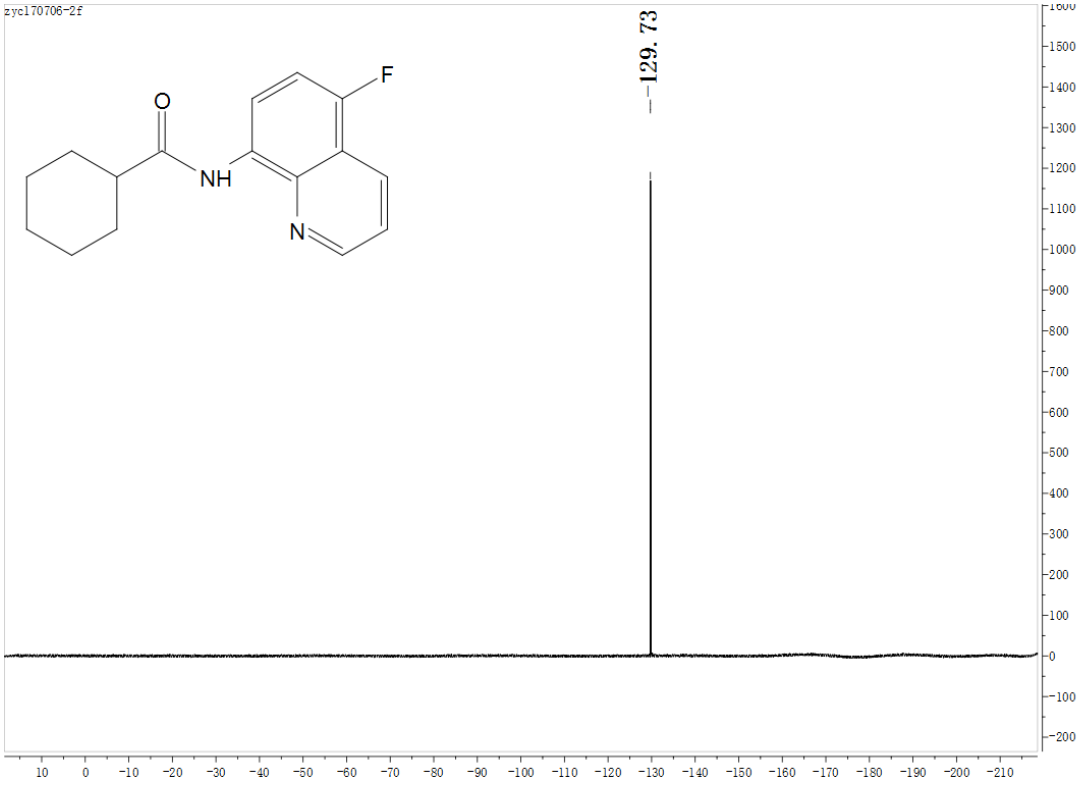
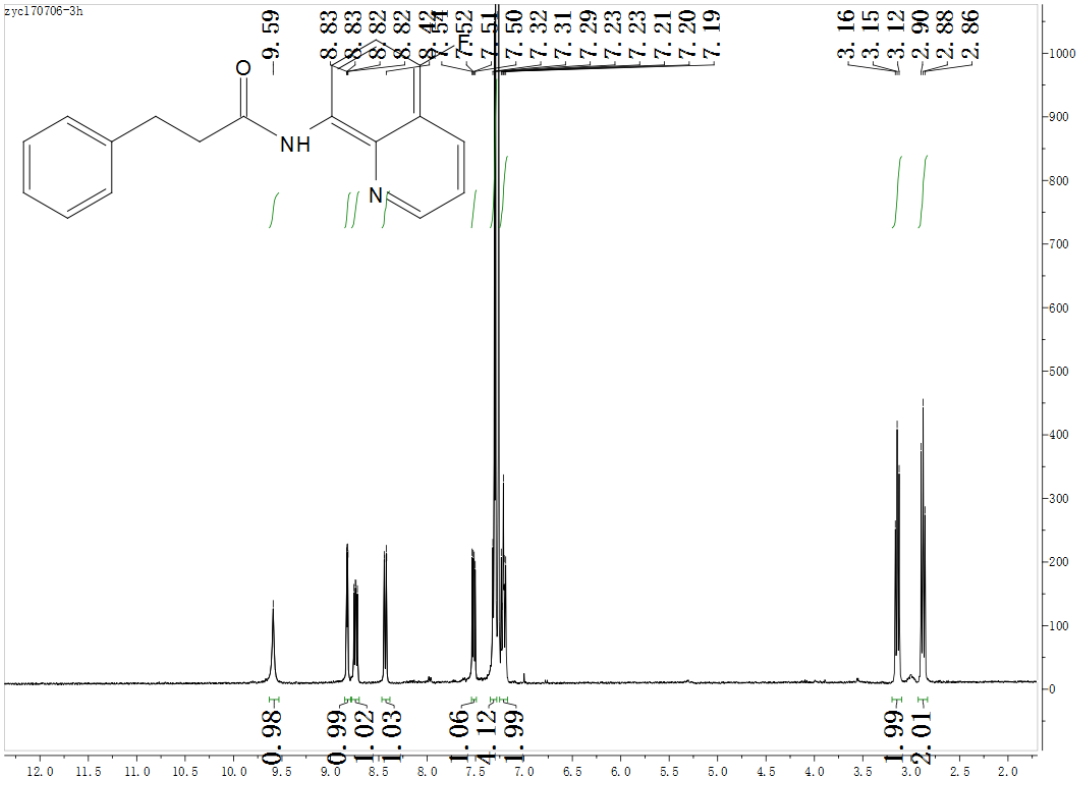
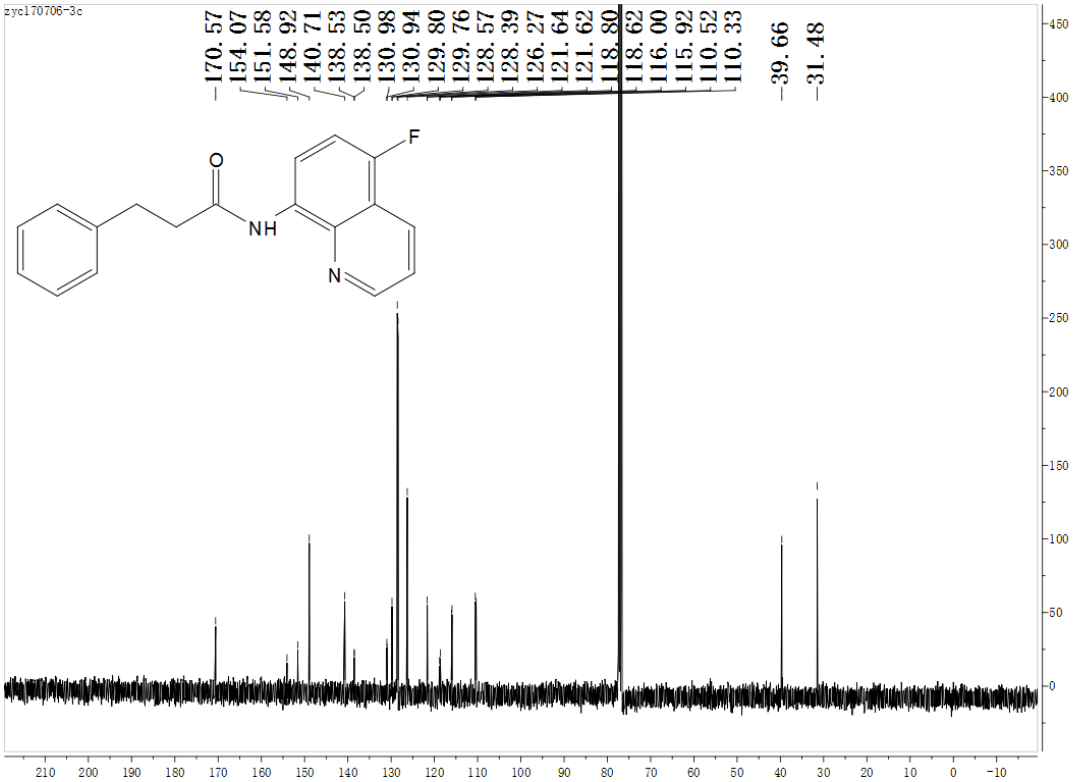
25.77
25.75
O
NH
N
F


zyc170706-2f
129.73
O
NH
N
F

2o:


zyc170706-3h
9.59
8.83
8.83
8.82
8.82
8.42
8.41
7.52
7.51
7.50
7.32
7.31
7.29
7.23
7.23
7.21
7.20
7.19
3.16
3.15
3.12
2.90
2.88
2.86
O
NH
N
0.98
0.99
1.02
1.03
1.06
4.12
1.99
1.99
2.01


zyc170706-3c
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151.58
148.92
140.71
138.53
138.50
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130.94
129.80
129.76
128.57
128.39
126.27
121.64
121.62
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F
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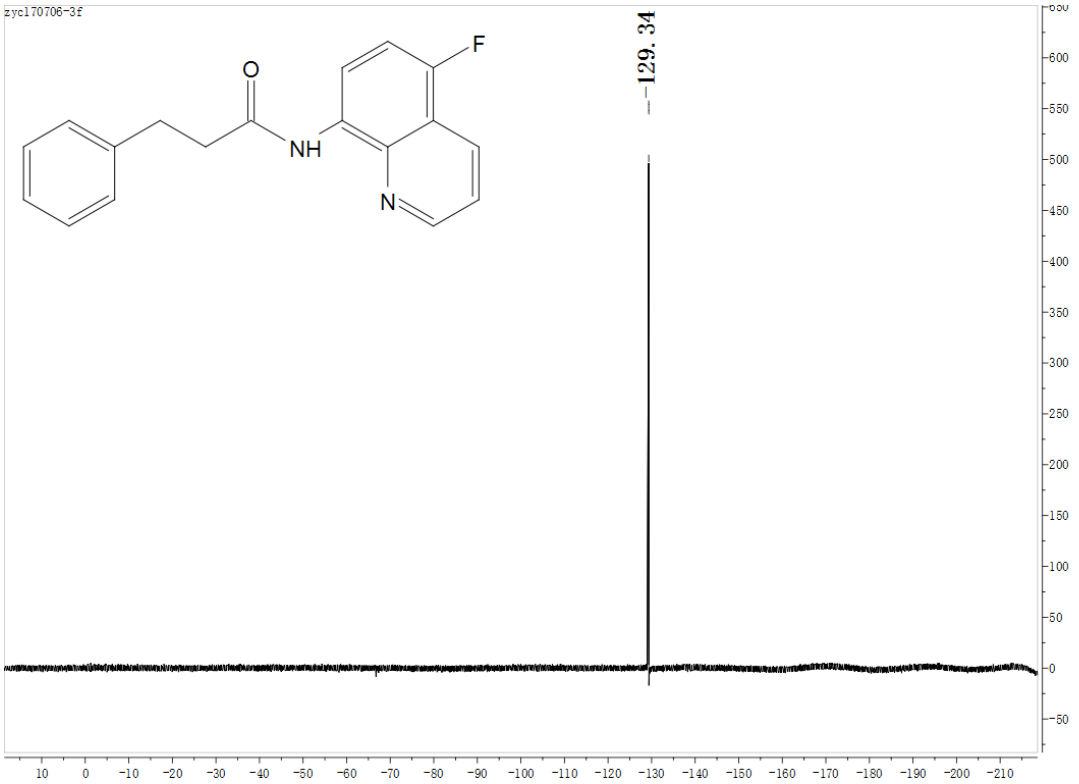
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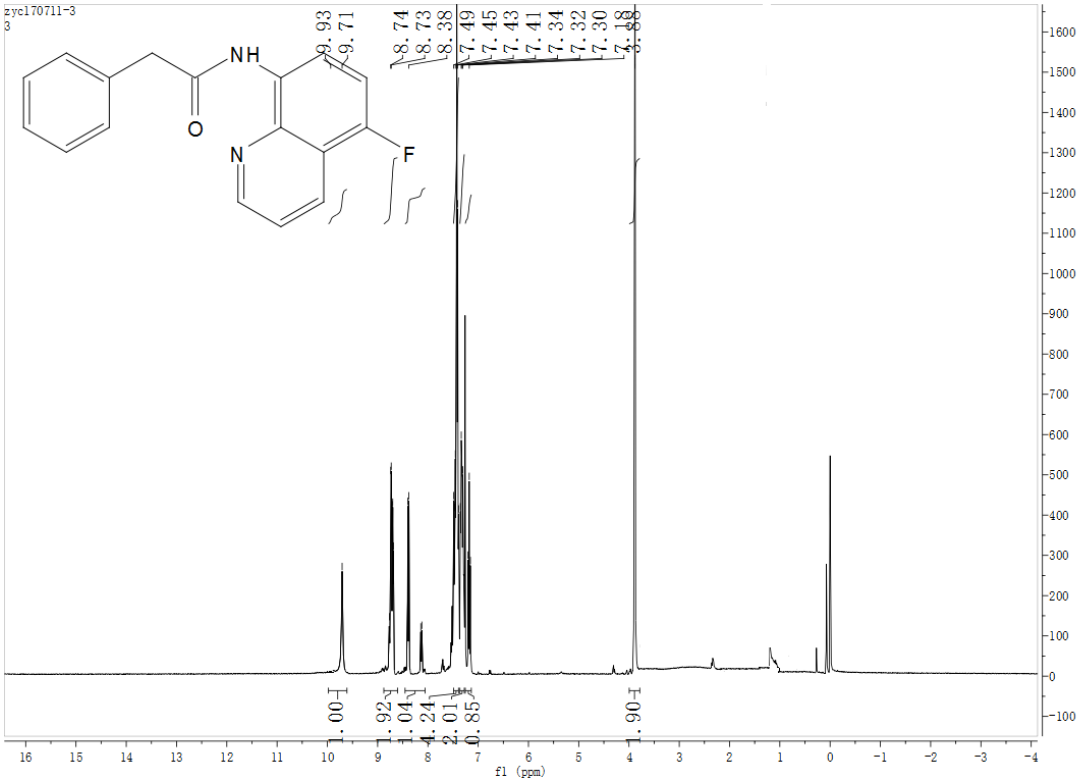
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7.43
7.41
7.34
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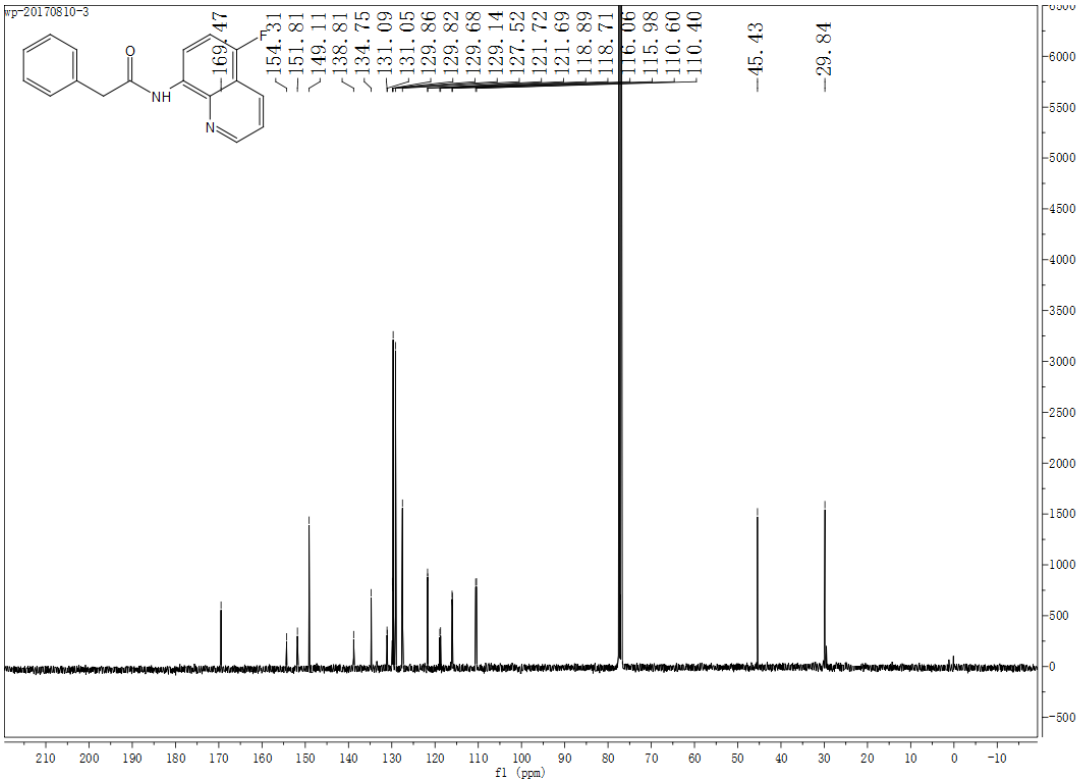
1.92
1.04
4.24
2.01
0.85
1.90
f1 (ppm)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129.82
129.68
129.14
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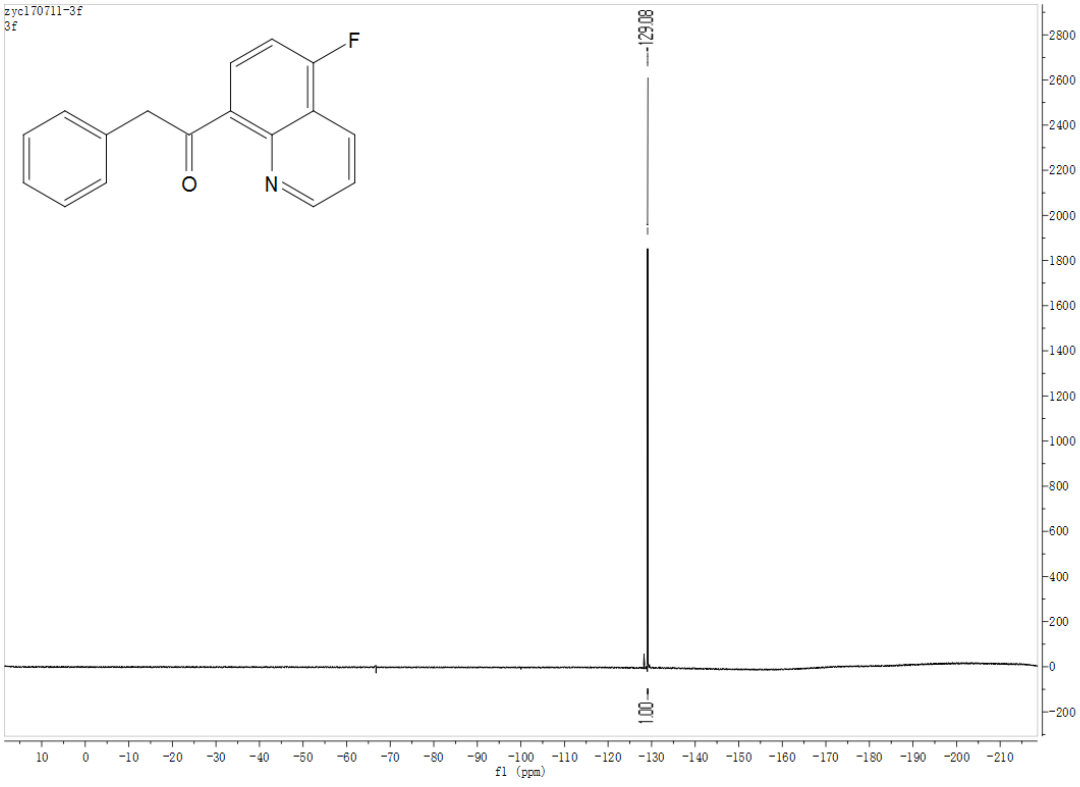
118.71
116.06
115.98
110.60
110.40
45.43
29.84
f1 (ppm)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N
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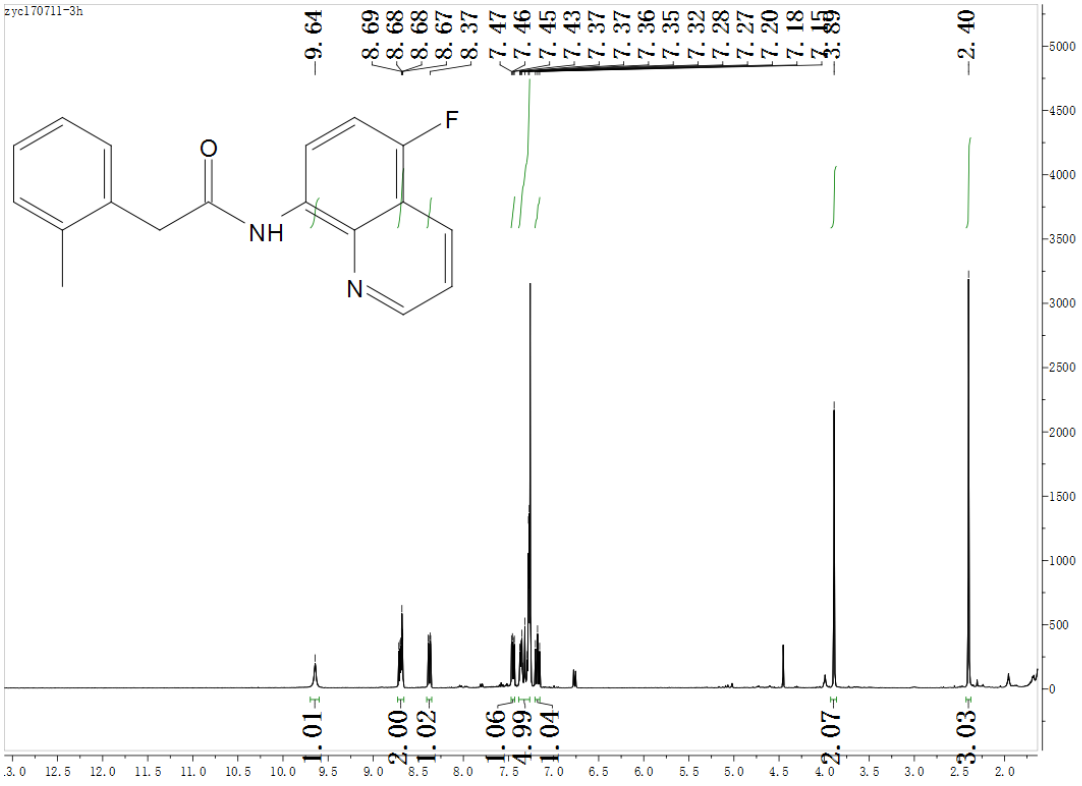
f1 (ppm)

2q: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7.46
7.45
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7.37
7.37
7.36
7.35
7.32
7.28
7.27
7.20
7.18
7.15
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2.40
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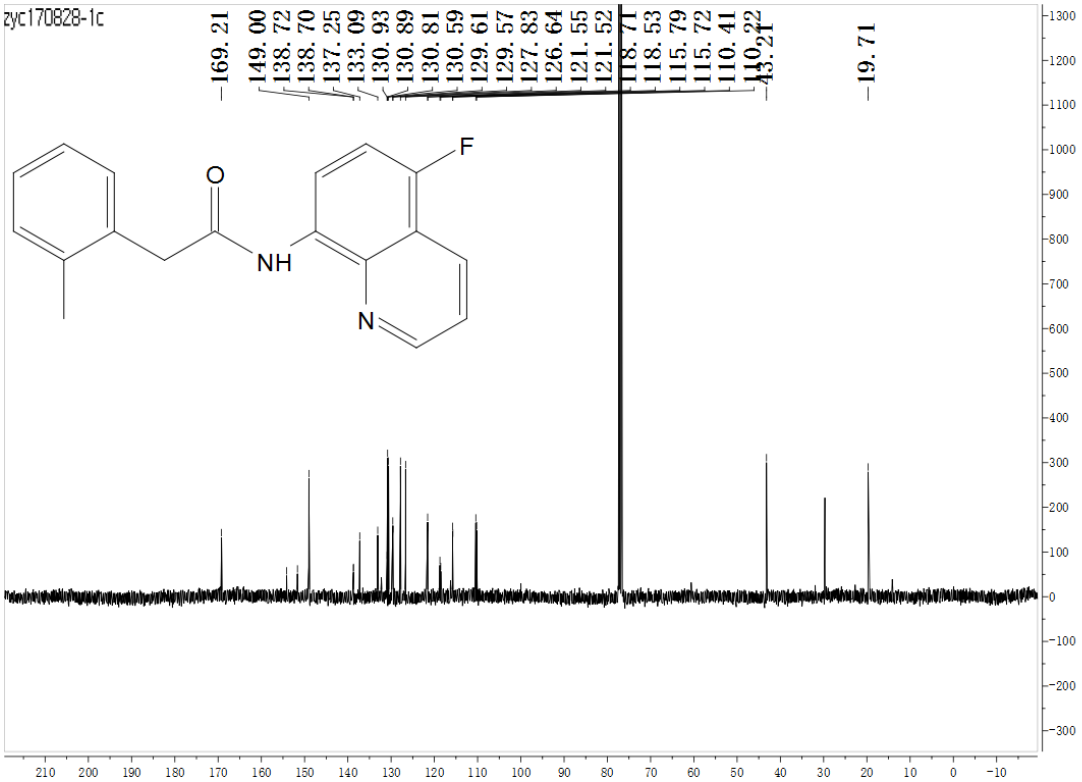
O
NH
N
1.01
2.00
1.02
1.06
4.99
1.04
2.07
3.03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127.83
126.64
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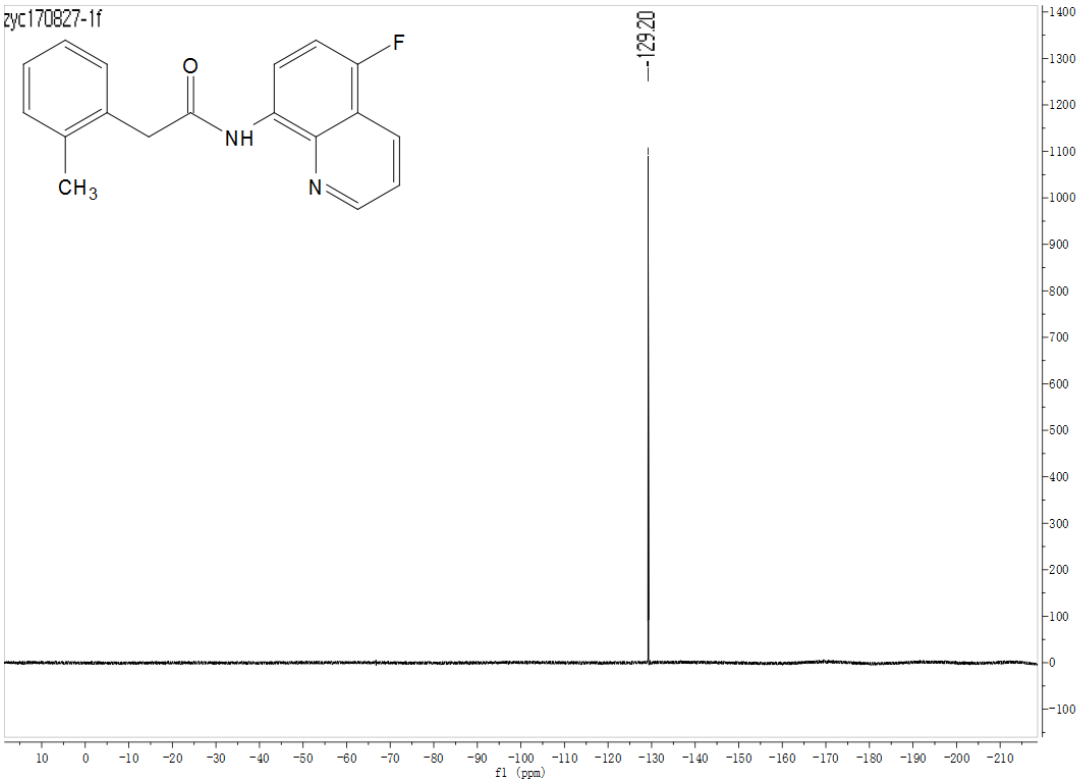
110.22
43.21
19.71
F
O
NH
N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CH3
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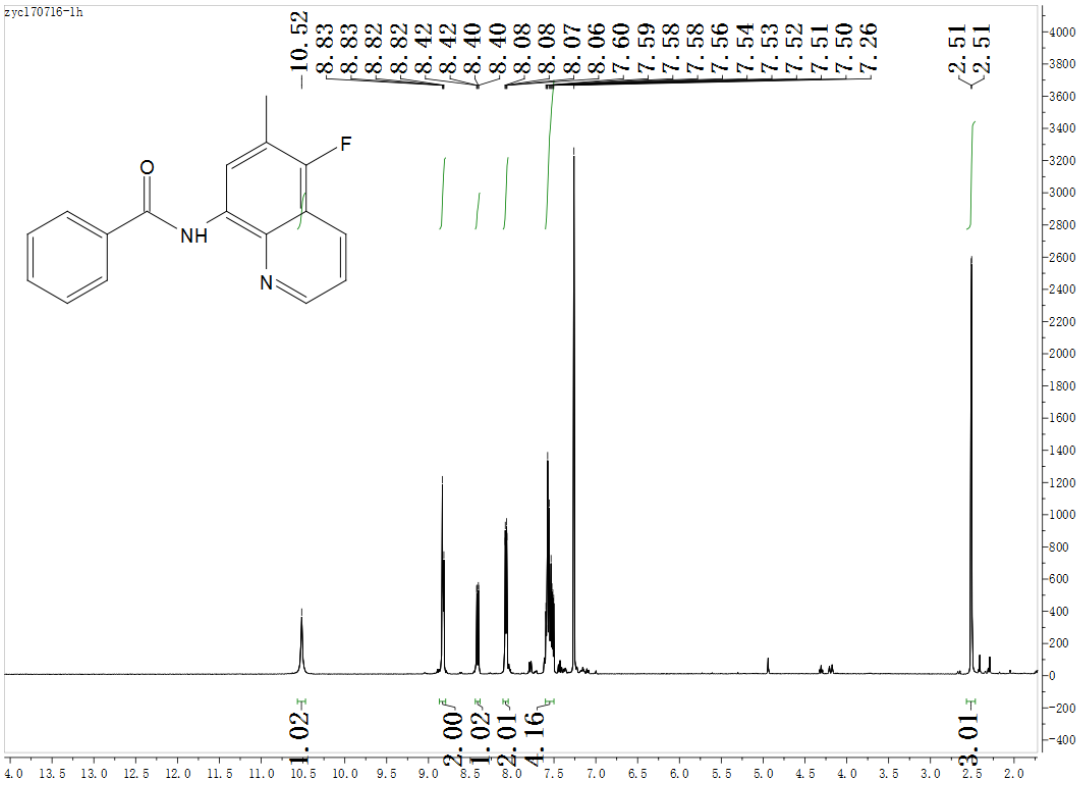
f1 (ppm)

2r: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8.82
8.42
8.42
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8.40
8.08
8.08
8.07
8.06
7.60
7.59
7.58
7.58
7.56
7.54
7.53
7.52
7.51
7.50
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2.51
O
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F
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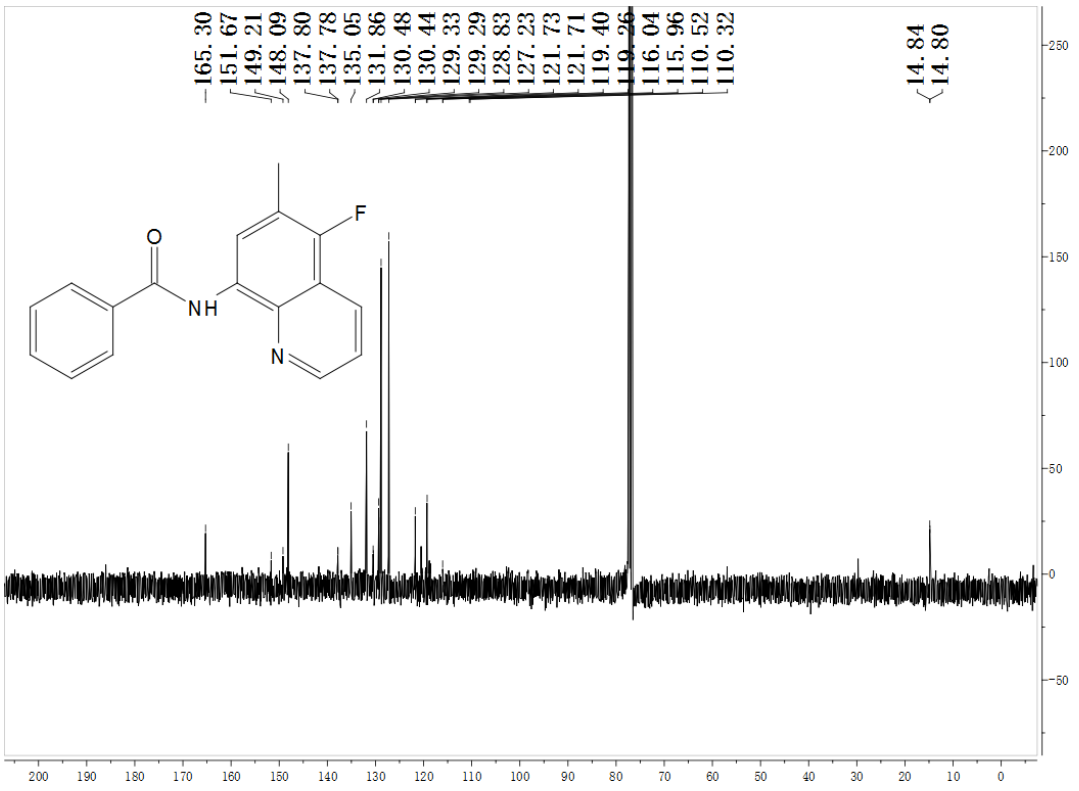
2.00
1.02
2.01
4.16
3.01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151.67
149.21
148.09
137.80
137.78
135.05
131.86
130.48
130.44
129.33
129.29
128.83
127.23
121.73
121.71
119.40
119.26
116.04
115.96
110.52
110.32
14.84
14.80
F
O
NH
N
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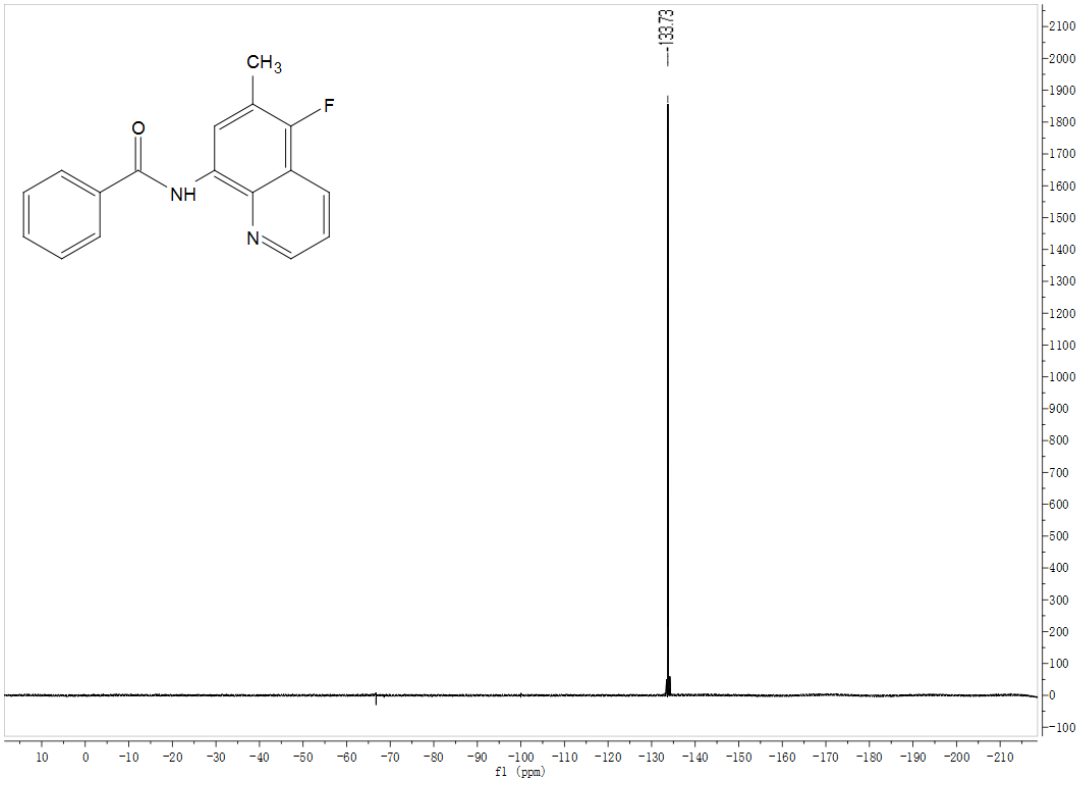
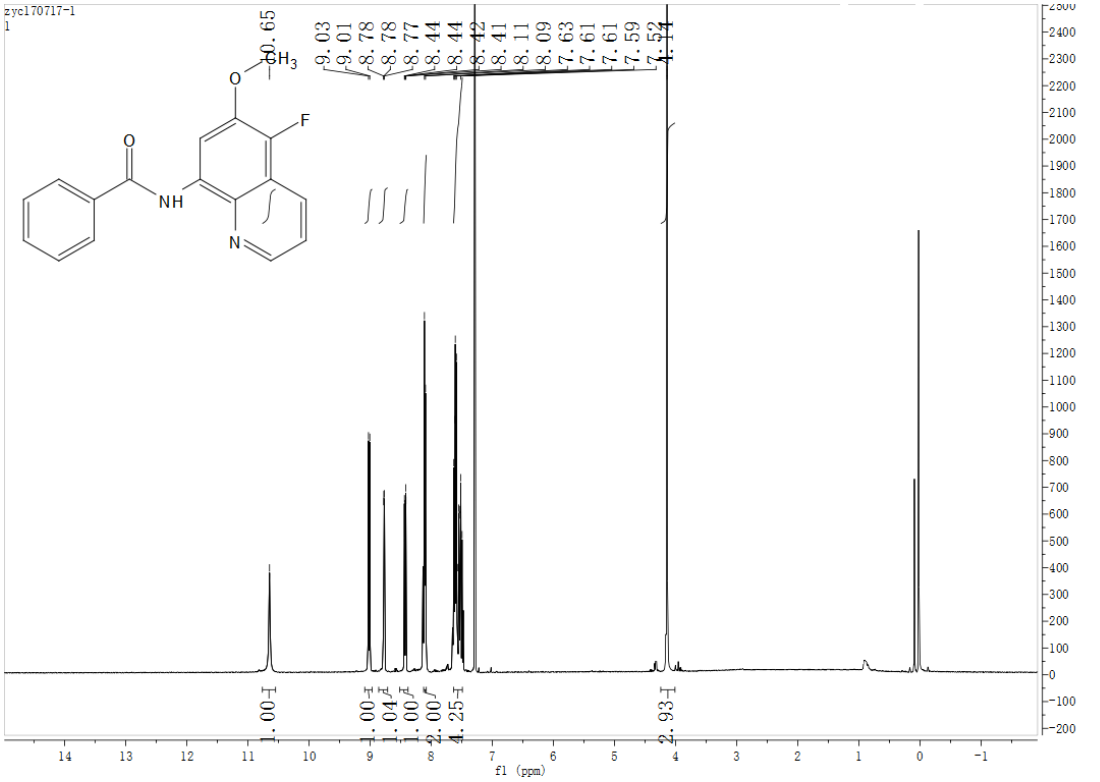
250 200 150 100 50 0 -50


-133.73
CH3
F
O
NH
N
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)
2100 2000 1900 1800 1700 1600 1500 1400 1300 1200 1100 1000 900 800 700 600 500 400 300 200 100 0 -100

2s: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1
9.03
9.01
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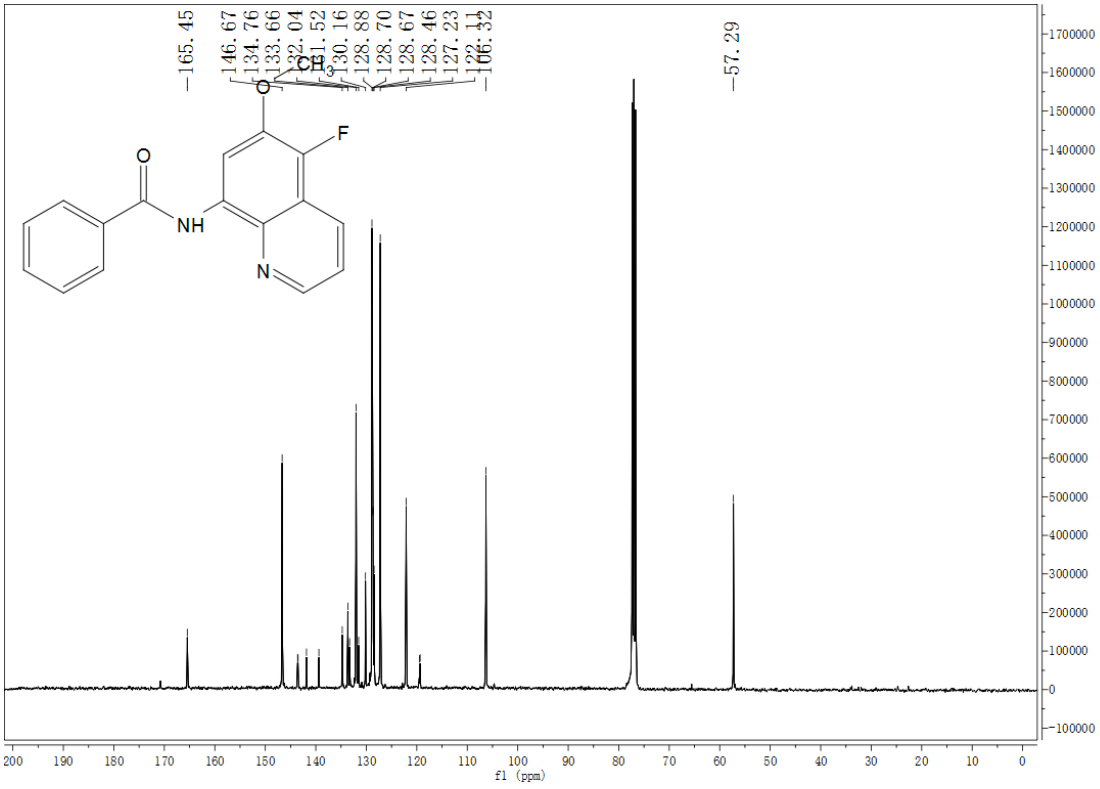
8.78
8.77
8.44
8.44
8.42
8.41
8.11
8.09
7.63
7.61
7.61
7.59
7.52
4.14
0.65
O
CH3
F
O
NH
N
1.00
1.00
1.04
1.00
2.00
4.25
2.93
f1 (ppm)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146.67
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133.66
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131.52
130.16
128.88
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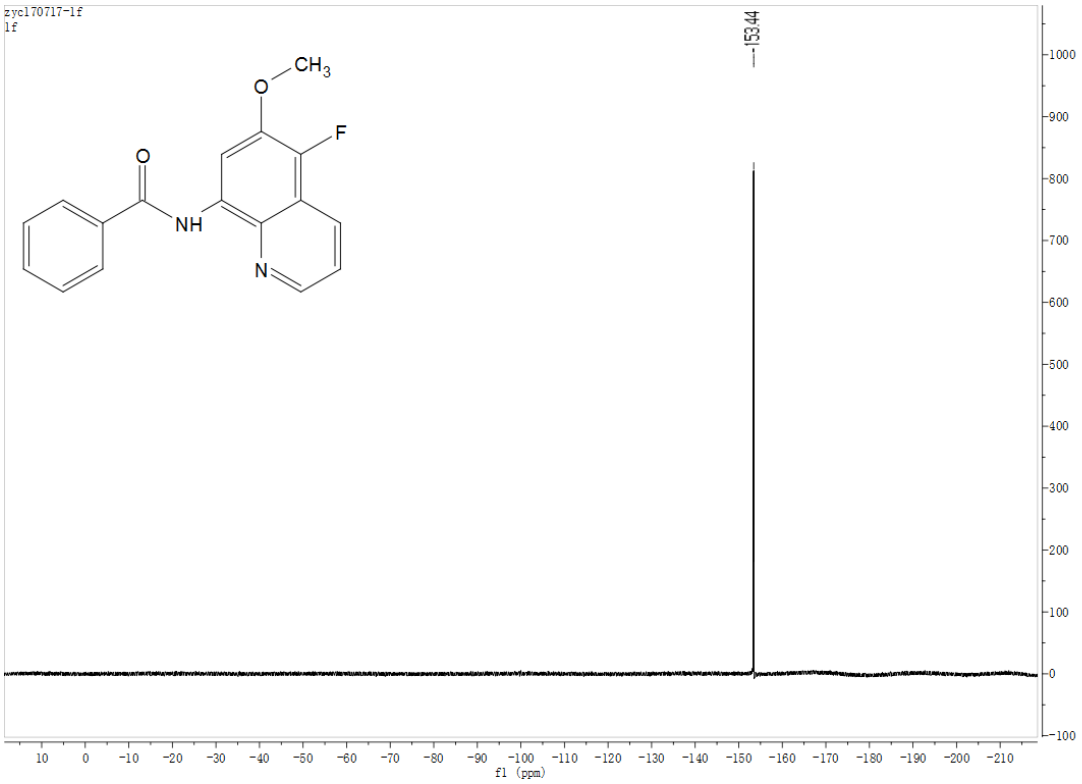
128.67
128.46
127.23
122.11
106.32
57.29
CH3
O
F
O
NH
N
f1 (ppm)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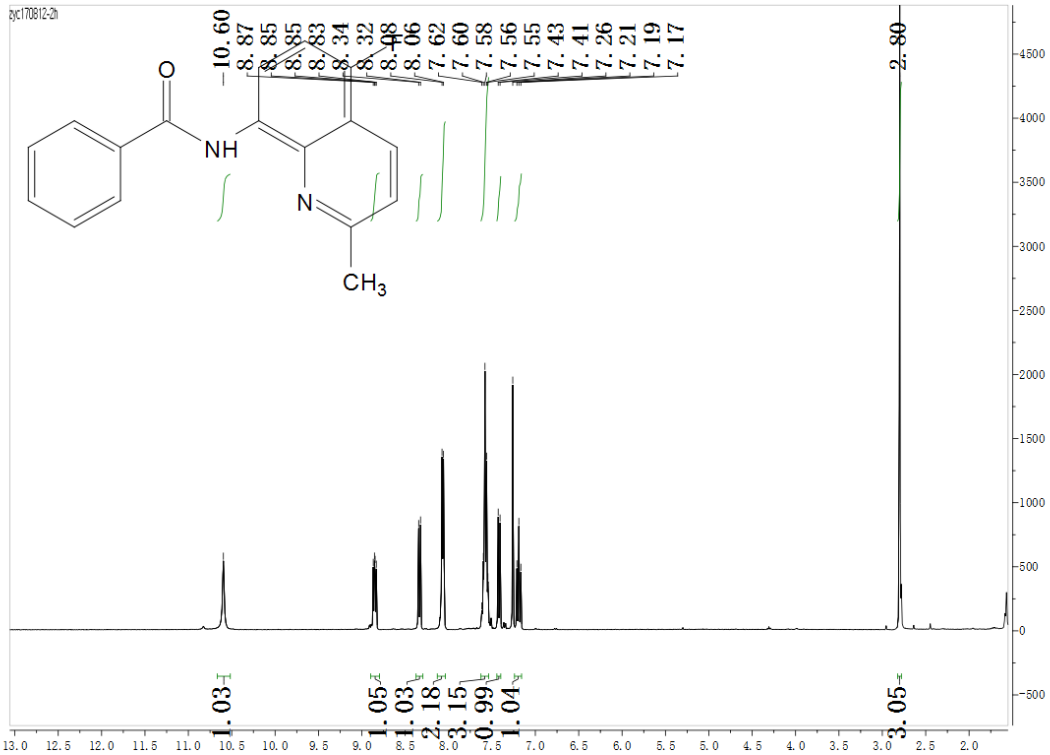
CH3
F
NH
N
-153.44
f1 (ppm)

2t: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8.85
8.83
8.34
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8.08
8.06
7.62
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7.58
7.56
7.55
7.43
7.41
7.26
7.21
7.19
7.17
2.80
O
NH
N
CH3
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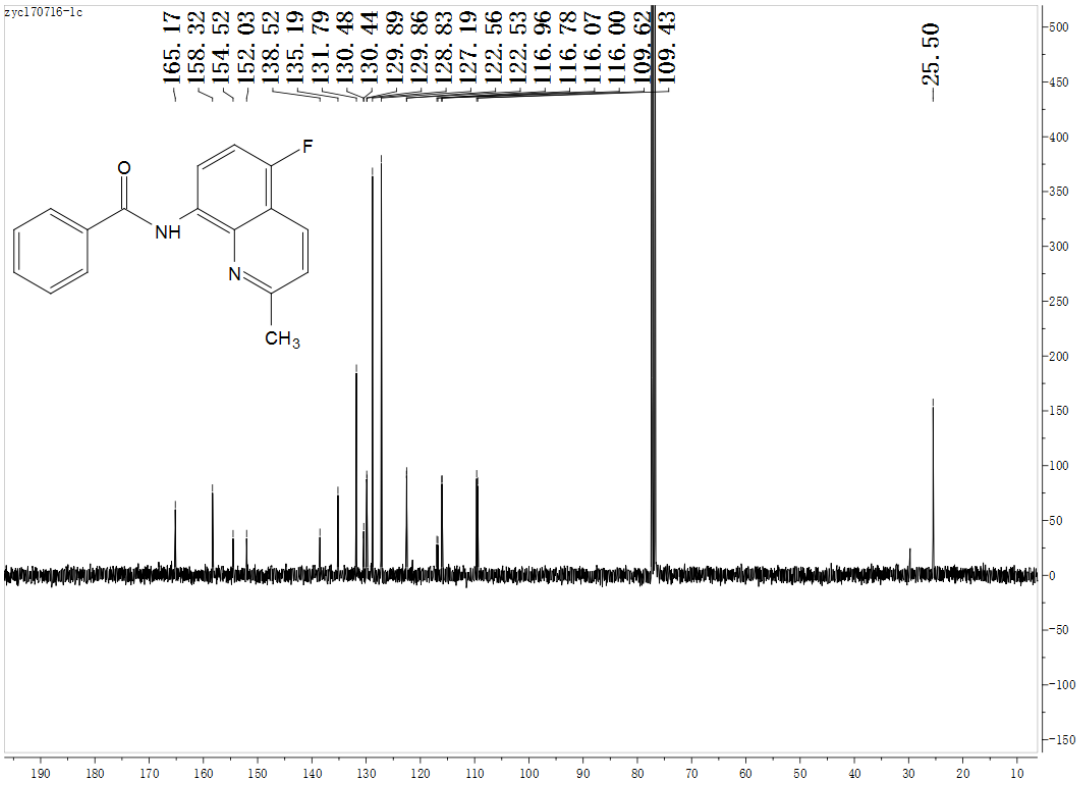
1.03
2.18
3.15
0.99
1.04
3.05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154.52
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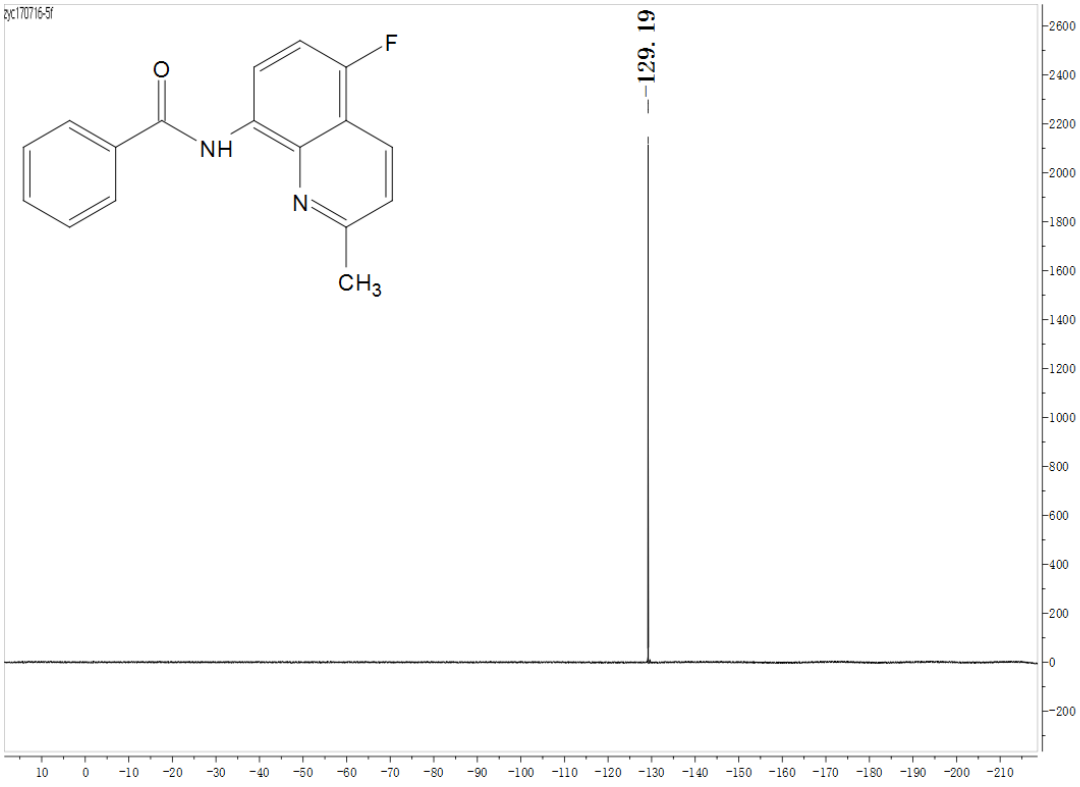
135.19
131.79
130.48
130.44
129.89
129.86
128.83
127.19
122.56
122.53
116.96
116.78
116.07
116.00
109.62
109.43
25.50
O
NH
N
F
CH3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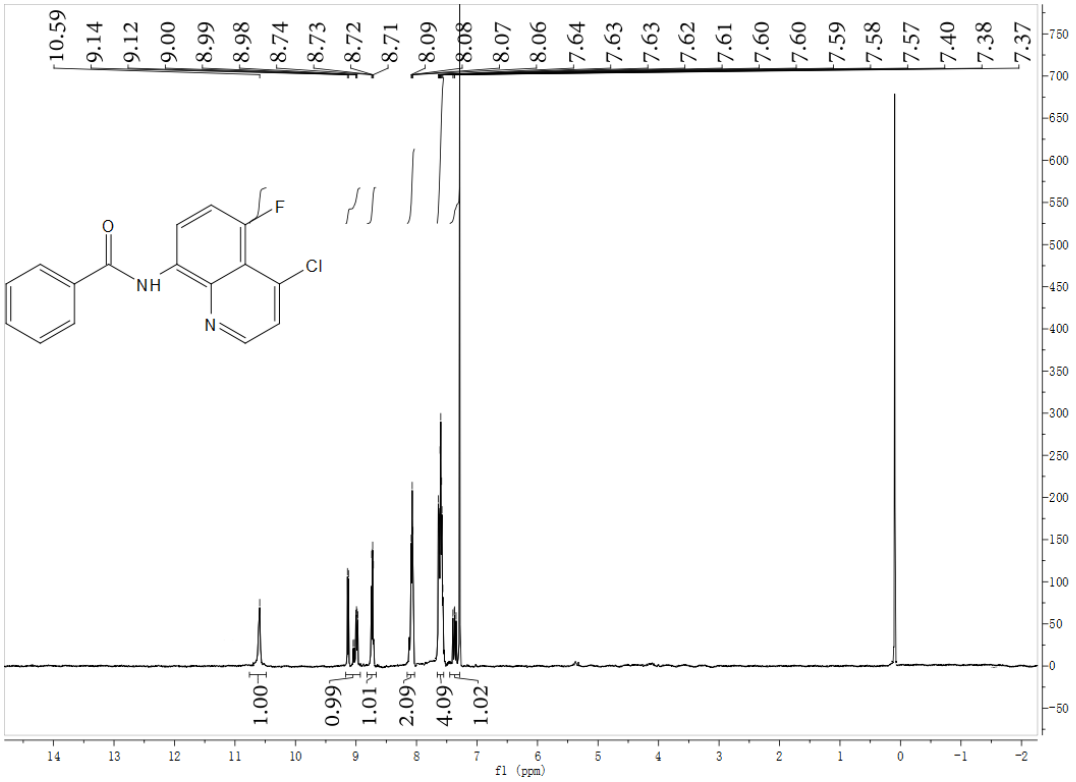
N
F
CH3

2u: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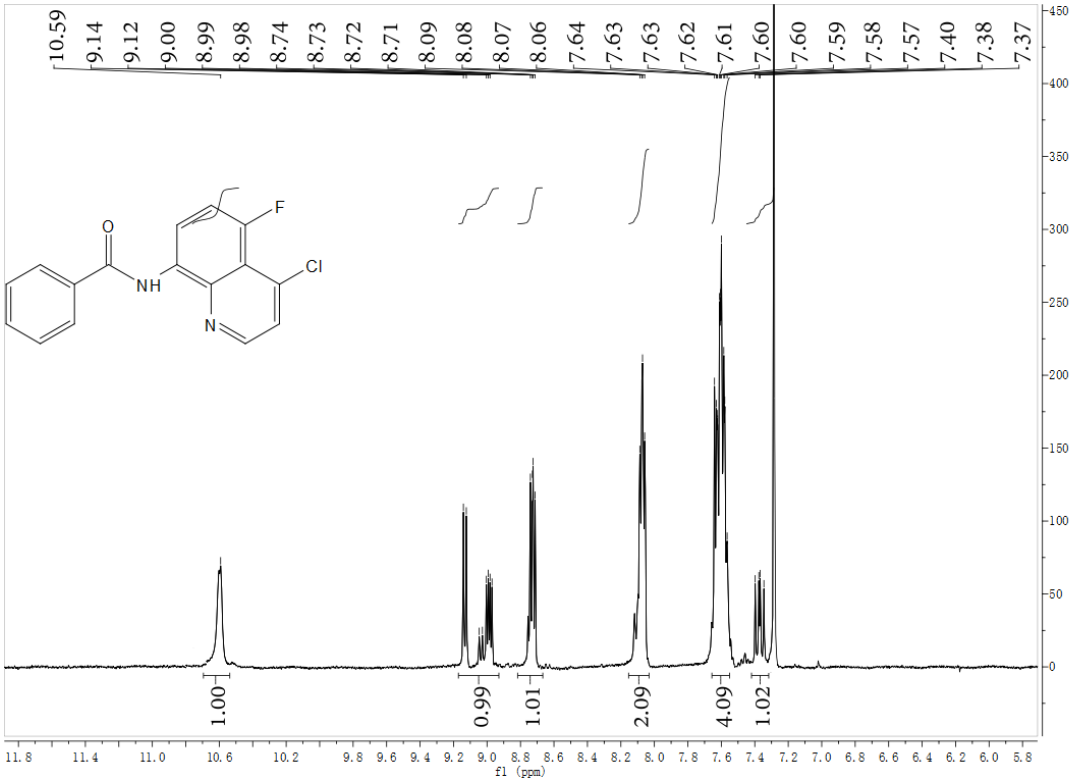
9.12
9.00
8.99
8.98
8.74
8.73
8.72
8.71
8.09
8.08
8.07
8.06
7.64
7.63
7.63
7.62
7.61
7.60
7.60
7.59
7.58
7.57
7.40
7.38
7.37
O
NH
F
Cl
N
1.00
0.99
1.01
2.09
4.09
1.02
f1 (ppm)


10.59
9.14
9.12
9.00
8.99
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8.07
8.06
7.64
7.63
7.63
7.62
7.61
7.60
7.60
7.59
7.58
7.57
7.40
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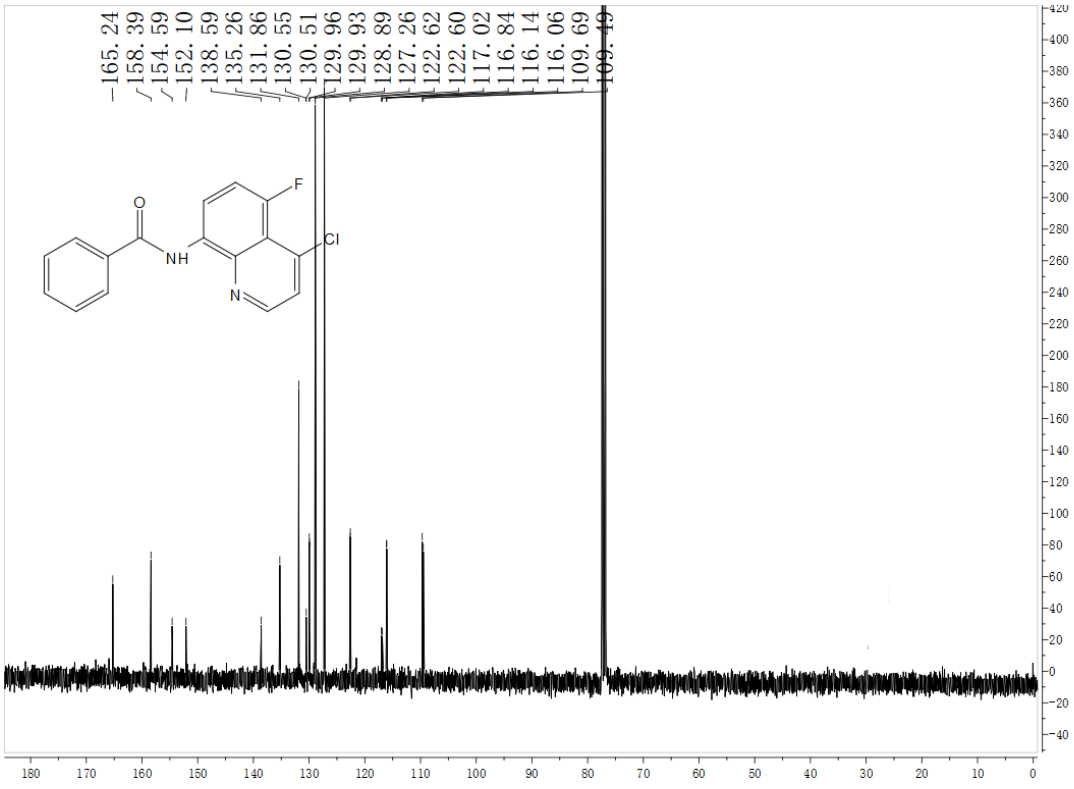
7.37
O
NH
F
Cl
N
1.00
0.99
1.01
2.09
4.09
1.02
f1 (ppm)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135.26
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130.51
129.96
129.93
128.89
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117.02
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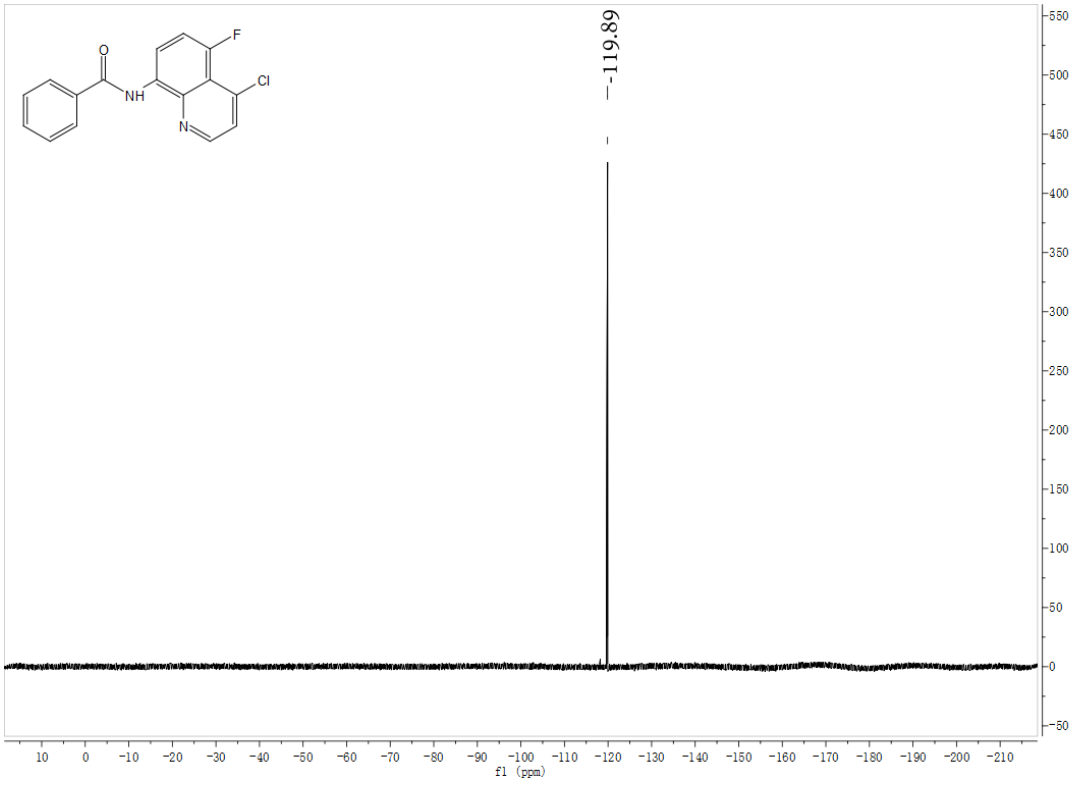
109.49
O
NH
N
F
Cl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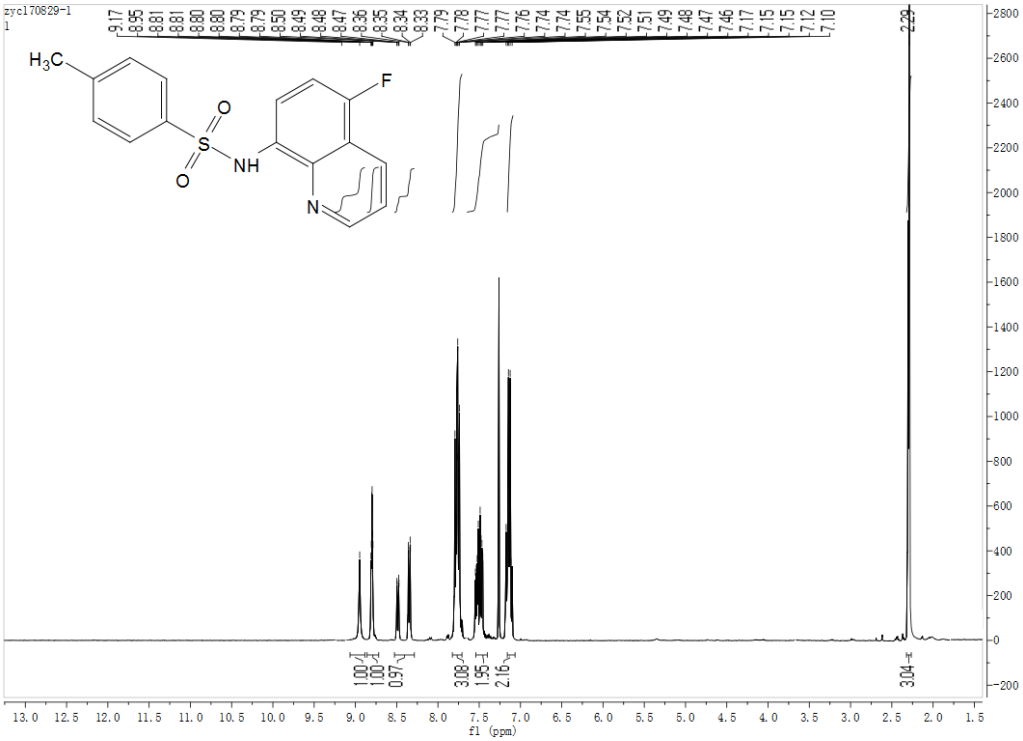
N
F
Cl
f1 (ppm)

2v: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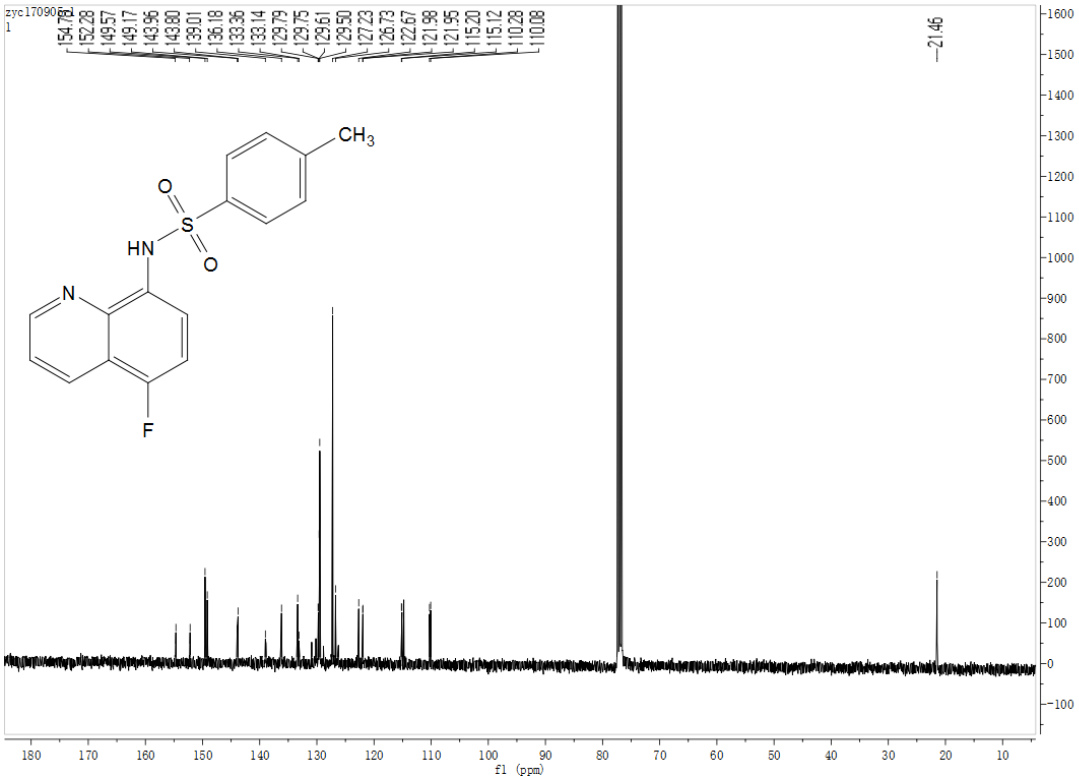
1
H3C
O
S
O
NH
F
N
f1 (ppm)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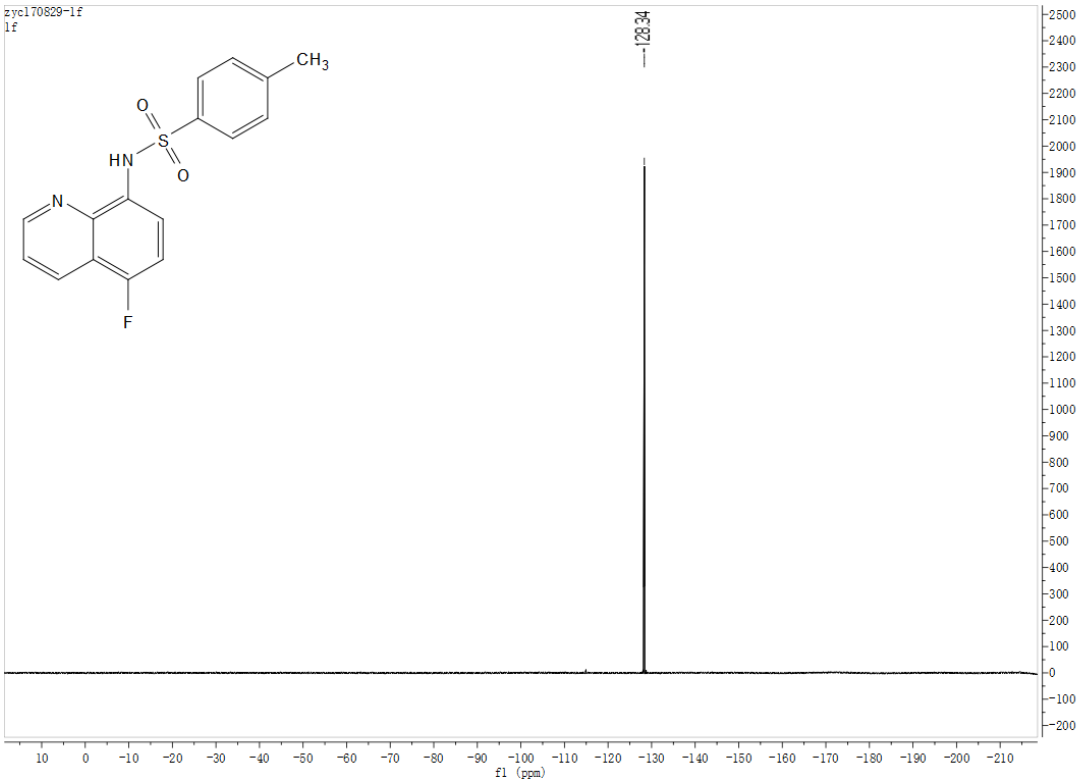
CH3
O
S
O
HN
N
F
f1 (ppm)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1f
CH3
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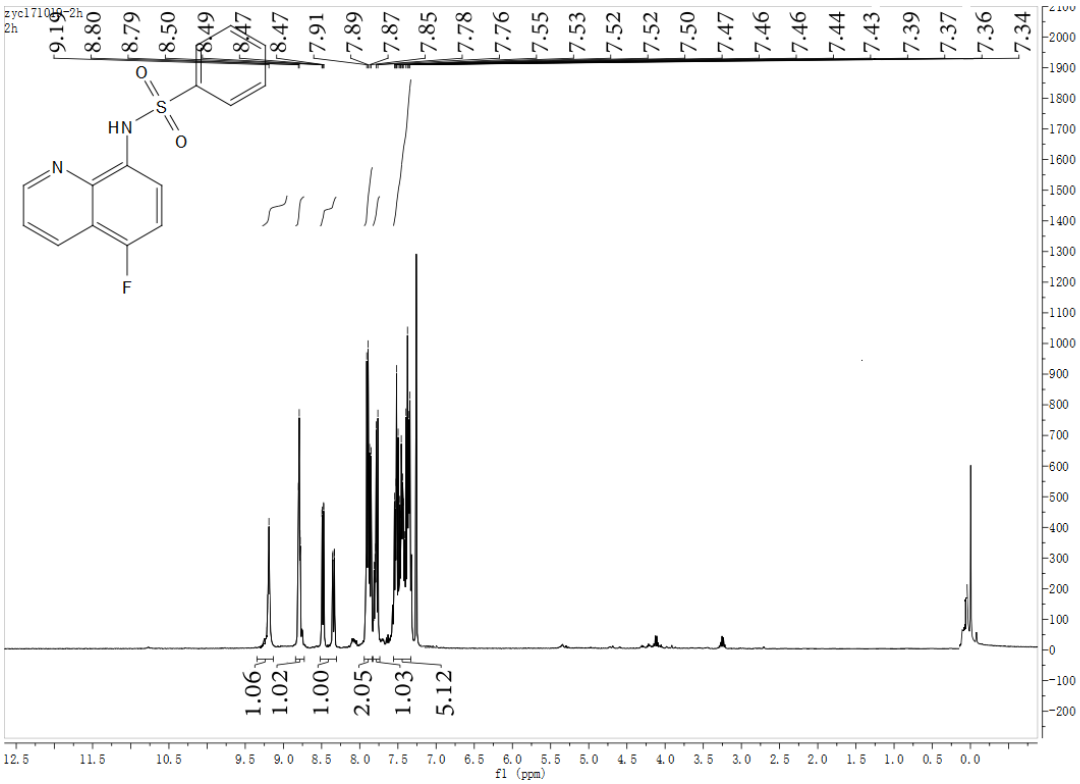
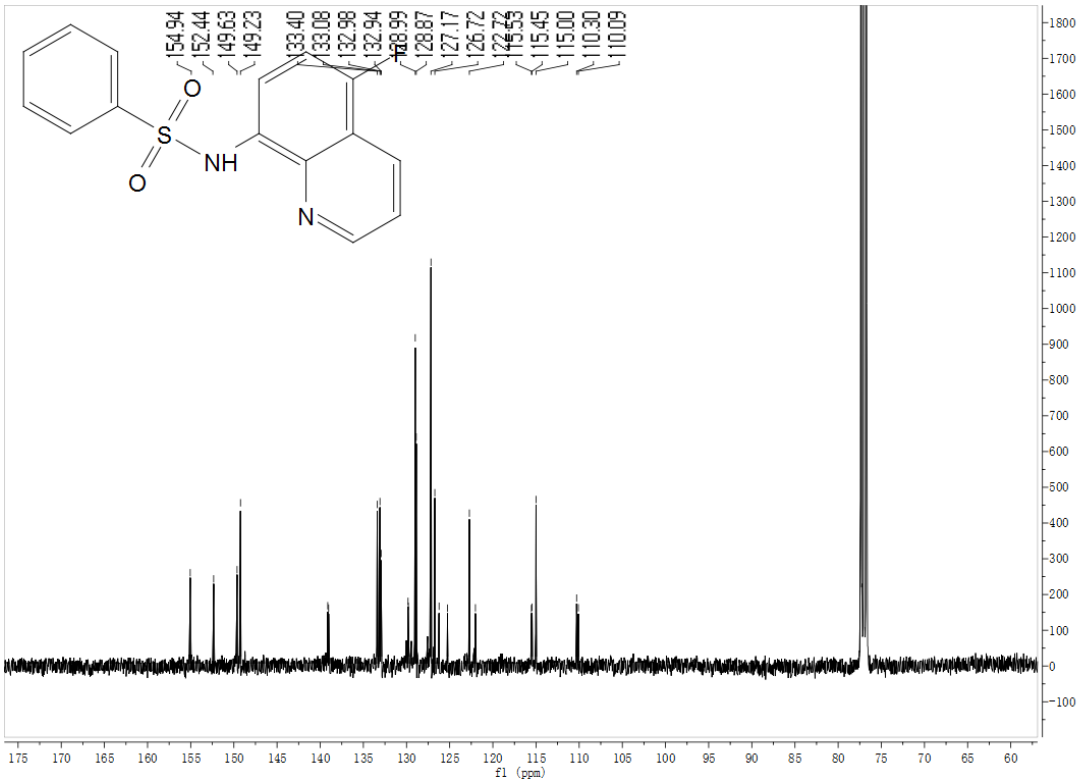
S
O
HN
N
F
128.34
f1 (ppm)

2w:


zycl71019-2h
2h
9.15
8.80
8.79
8.50
8.49
8.47
8.47
7.91
7.89
7.87
7.85
7.78
7.76
7.55
7.53
7.52
7.52
7.50
7.47
7.46
7.46
7.44
7.43
7.39
7.37
7.36
7.34
O
S
O
HN
N
F
1.06
1.02
1.00
2.05
1.03
5.12
f1 (ppm)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128.87
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126.72
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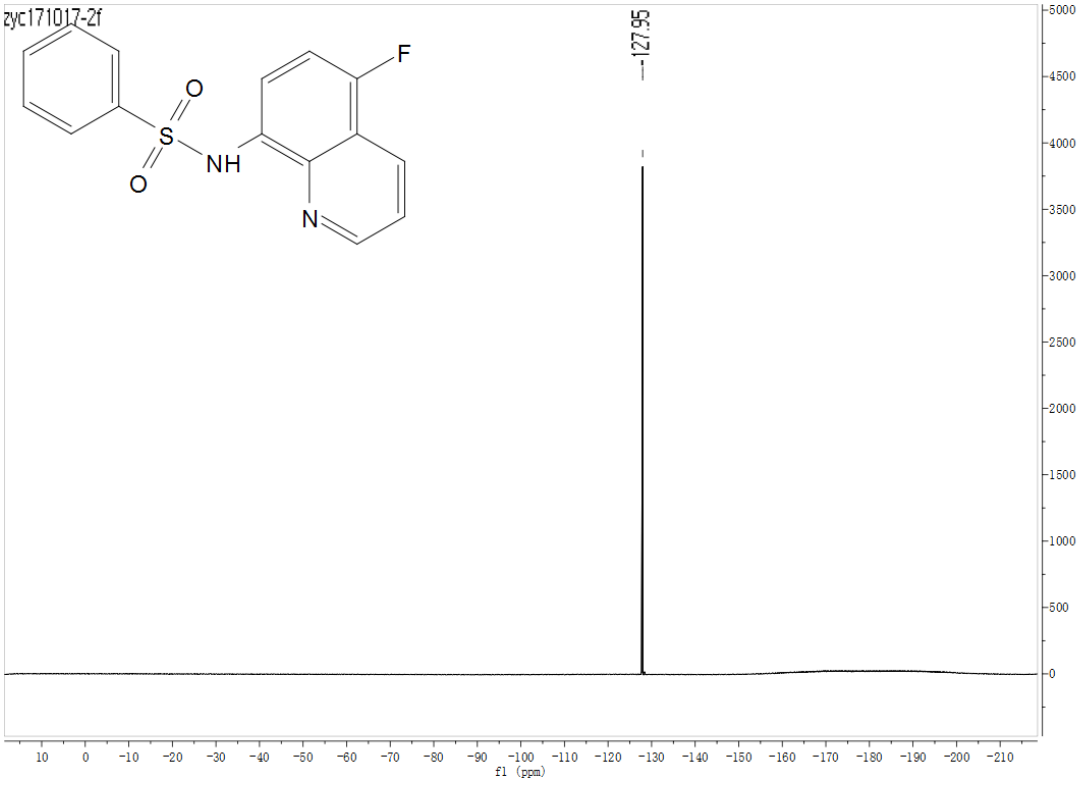
110.30
110.09
O
S
O
NH
N
f1 (ppm)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F
O
S
O
NH
N
f1 (ppm)

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