Supporting Information for

Metal-Free Electrochemical Promoted Radical Cascade Cyclization to Access CF_3 Containing Benzimidazo[2,1-*a*]isoquinolin-6(5*H*)-ones

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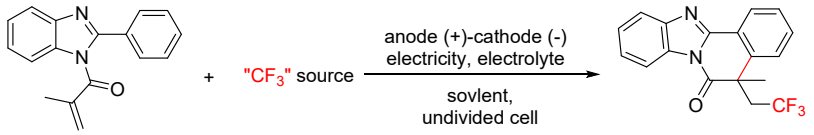
General information

All reactions were carried out in dried sealed Schlenk tubes with magnetic stirring. All anhydrous and oxygen-free environments were performed under nitrogen atmosphere in oven-dried glassware using Schlenk techniques. All the chemicals were obtained commercially and used without any prior purification. All products were isolated by short chromatography on a silica gel (200-300 mesh) column using hexane and ethyl acetate. ^{1} H, ^{13} C and ^{19} F NMR spectra were recorded on a Bruker Advance 400 spectrometer at ambient temperature with $CDCl_3$ as solvent and tetramethylsilane (TMS) as the internal standard. Analytical thin layer chromatography (TLC) was performed on Merk precoated TLC (silica gel 60 F254) plates.

Optimized reaction conditions[a]



1a **3a**

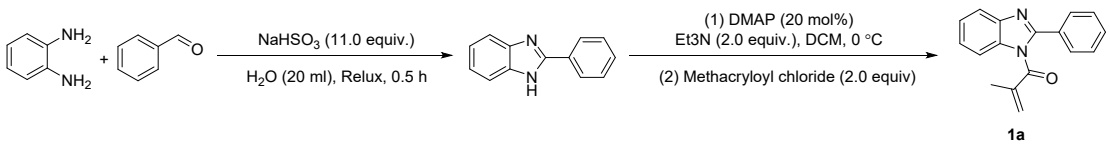
Entry	electrode	electricity	Solvent	"CF_3" source	electrolyte	electrolyte equiv.	atmosphere	Temperature(℃)	Yield(%)[b]
1	C (+)-Ni (-)	5 mA	MeCN	CF_3SO_2Na	$^{n}Bu_4NBF_4$	1.0	air	50	63
2	C (+)-C (-)	5 mA	MeCN	CF_3SO_2Na	$^{n}Bu_4NBF_4$	1.0	air	50	57
3	C (+)-Pt (-)	5 mA	MeCN	CF_3SO_2Na	$^{n}Bu_4NBF_4$	1.0	air	50	67
4	Pt (+)-Pt (-)	5 mA	MeCN	CF_3SO_2Na	$^{n}Bu_4NBF_4$	1.0	air	50	37
5[c]	C (+)-Pt (-)	3 mA	MeCN	CF_3SO_2Na	$^{n}Bu_4NBF_4$	1.0	air	50	42
6[d]	C (+)-Pt (-)	8 mA	MeCN	CF_3SO_2Na	$^{n}Bu_4NBF_4$	1.0	air	50	51
7[d]	C (+)-Pt (-)	10 mA	MeCN	CF_3SO_2Na	$^{n}Bu_4NBF_4$	1.0	air	50	30
8	C (+)-Pt (-)	0 mA	MeCN	CF_3SO_2Na	$^{n}Bu_4NBF_4$	1.0	air	50	N.D.
9	C (+)-Pt (-)	5 mA	THF	CF_3SO_2Na	$^{n}Bu_4NBF_4$	1.0	air	50	<10
10	C (+)-Pt (-)	5 mA	DMF	CF_3SO_2Na	$^{n}Bu_4NBF_4$	1.0	air	50	N.D.
11	C (+)-Pt (-)	5 mA	Acetone	CF_3SO_2Na	$^{n}Bu_4NBF_4$	1.0	air	50	21
12	C (+)-Pt (-)	5 mA	H_2O	CF_3SO_2Na	$^{n}Bu_4NBF_4$	1.0	air	50	N.D.
13	C (+)-Pt (-)	5 mA	MeCN	Togni's II	$^{n}Bu_4NBF_4$	1.0	air	50	N.D.
14	C (+)-Pt (-)	5 mA	MeCN	$TMSCF_3$	$^{n}Bu_4NBF_4$	1.0	air	50	N.D.
15	C (+)-Pt (-)	5 mA	MeCN	CF_3SO_2Na	Et_4NClO_4	1.0	air	50	64
16	C (+)-Pt (-)	5 mA	MeCN	CF_3SO_2Na	TBAB	1.0	air	50	<5
17	C (+)-Pt (-)	5 mA	MeCN	CF_3SO_2Na	TBAI	1.0	air	50	<5
18	C (+)-Pt (-)	5 mA	MeCN	CF_3SO_2Na	$^{n}Bu_4NPF_6$	1.0	air	50	63
19	C (+)-Pt (-)	5 mA	MeCN	CF_3SO_2Na	$LiClO_4$	1.0	air	50	34
20	C (+)-Pt (-)	5 mA	MeCN	CF_3SO_2Na	KI	1.0	air	50	<5
21	C (+)-Pt (-)	5 mA	MeCN	CF_3SO_2Na	KF	1.0	air	50	23
22	C (+)-Pt (-)	5 mA	MeCN	CF_3SO_2Na	$^{n}Bu_4NBF_4$	0.5	air	50	61
23	C (+)-Pt (-)	5 mA	MeCN	CF_3SO_2Na	$^{n}Bu_4NBF_4$	1.5	air	50	67

24	C (+)-Pt (-)	5 mA	MeCN	CF_3SO_2Na	$^nBu_4NBF_4$	1.0	N_2	50	65
25	C (+)-Pt (-)	5 mA	MeCN	CF_3SO_2Na	$^nBu_4NBF_4$	1.0	air	r.t.	60
26	C (+)-Pt (-)	5 mA	MeCN	CF_3SO_2Na	$^nBu_4NBF_4$	1.0	air	80	59

[a]Reaction conditions：**1a** (0.3 mmol), CF_3 source (2.0 eq.), electrolyte (1.0 eq.), solvent (6 mL) ,constant current electricity, stirred, 3 h. [b]Isolated yield. [c]5 h. [d]2 h.

Experimental Section

General procedure for the synthesis of compounds 1 (1a as an example):

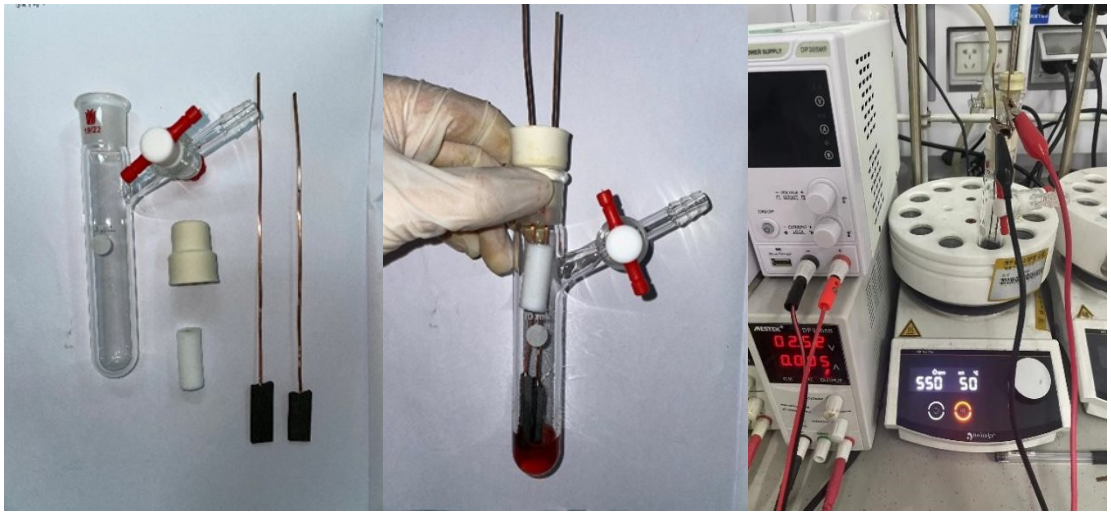


1a

Step 1: In a round-bottomed flask (50 mL) equipped with a magnetic stirrer, a mixture of benzaldehyde (5.0 mmol, 578 μL) and $NaHSO_3$ (11.0 eq, 5.73 g) in H_2O (20.0 mL) was prepared. When the mixture reached refluxing temperature, *o*-phenylenediamine (5.0 mmol, 541 mg) were added. The resulting mixture was stirred for appropriate time. After completion of the reaction, the reaction mixture was vacuum filtered after cooling to room temperature by a glass funnel. The residues were washed by water (20 mL × 2), dried in air dry oven to give the corresponding product.

Step 2: To the solution of 2-(*o*-tolyl)-1H-benzo[*d*]imidazole (3 mmol, 625 mg) and DMAP (0.6 mmol, 73 mg) in DCM (0.5 M) was added Et_3N (6 mmol, 834μL) and methacryloyl chloride (6 mmol, reaction was complete according to TLC analysis, and water (20 mL) was added to the mixture, which was extracted with CH_2Cl_2 (15 mL × 3). Then the organic solvent was concentrated in vacuo. The residue was purified by flash column chromatography with Ethyl acetate and Petroleum ether as eluent to give 1a.

Photos of the electrochemical setup

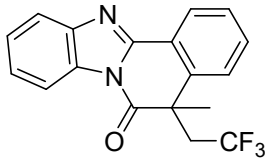


Cyclic voltammetry studies

The cyclic voltammograms experiments were conducted in a Schlenk tube that contained the

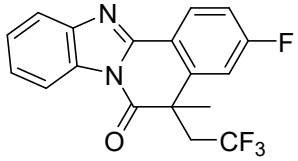
substance dissolved in a 0.1 M solution of tetrabutylammonium tetrafluoroborate in acetonitrile. A glassy carbon electrode working electrode, a platinum wire counter electrode and an Ag/Ag^+ reference electrode were used. The reference electrode was stored in silver nitrate solution for activation before use. The relevant parameters were controlled by an electrochemical workstation CHI600E.

Characterization of the products



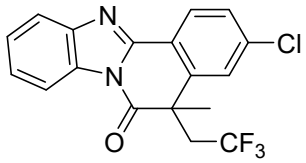
5-methyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3a)

White solid; m.p. = 128.5-129.3°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (dd, J = 7.8, 1.5 Hz, 1H), 8.39 – 8.32 (m, 1H), 7.87 – 7.80 (m, 1H), 7.62 – 7.56 (m, 1H), 7.56 – 7.49 (m, 1H), 7.49 – 7.41 (m, 3H), 3.58 – 3.36 (m, 1H), 3.02 – 2.85 (m, 1H), 1.76 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.1, 149.4, 144.1, 138.6, 131.8, 131.5, 128.6, 126.6, 126.5, 126.3, 126.0, 125.1 (q, $^1J_{C\text{-}CF3}$ = 277.0 Hz), 122.5, 120.1, 115.8, 45.4 (q, $^3J_{C\text{-}CF3}$ = 2.3 Hz), 44.1 (q, $^2J_{C\text{-}CF3}$ = 27.7 Hz), 31.1. ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.34. Spectroscopic data are in accordance with those described in the literature.[1]



3-fluoro-5-methyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3b)

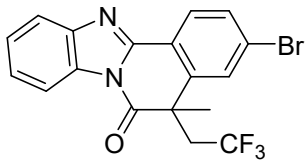
White solid; m.p. = 139.6-141.2°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (dd, J = 8.8, 5.8 Hz, 1H), 8.37 – 8.30 (m, 1H), 7.85 – 7.79 (m, 1H), 7.50 – 7.40 (m, 2H), 7.29 – 7.21 (m, 1H), 7.16 (dd, J = 9.5, 2.5 Hz, 1H), 3.56 – 3.39 (m, 1H), 2.96 – 2.79 (m, 1H), 1.77 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.5, 164.9 (d, $^1J_{C\text{-}F}$ = 252.0 Hz), 148.6, 144.0, 141.3 (d, $^3J_{C\text{-}F}$ = 8.0 Hz), 131.4, 129.1 (d, $^3J_{C\text{-}F}$ = 9.0 Hz), 126.4, 126.1, 124.9 (q, $^1J_{C\text{-}CF3}$ = 277.0 Hz), 120.1, 119.1 (d, $^4J_{C\text{-}F}$ = 3.0 Hz), 116.7 (d, $^2J_{C\text{-}F}$ = 22.0 Hz), 115.8, 113.7 (d, $^2J_{C\text{-}F}$ = 23.0 Hz), 45.6 (q, $^3J_{C\text{-}CF3}$ = 2.0 Hz; d, $^4J_{C\text{-}F}$ = 2.0 Hz), 44.2 (q, $^2J_{C\text{-}CF3}$ = 27.7 Hz), 31.0. ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.42, -106.14. Spectroscopic data are in accordance with those described in the literature.[1]



3-chloro-5-methyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3c)

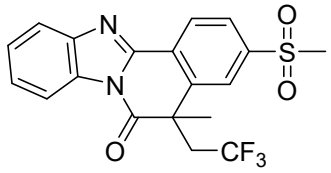
White solid; m.p. = 202.1-203.9°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (d, J = 8.5 Hz, 1H), 8.38 – 8.31 (m, 1H), 7.86 – 7.79 (m, 1H), 7.51 (dd, J = 8.5, 1.9 Hz, 1H), 7.49 – 7.42 (m, 3H), 3.57 – 3.37 (m, 1H), 2.99 – 2.80 (m, 1H), 1.77 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.4, 148.4, 144.1, 140.3, 138.1, 131.5, 129.3, 127.9, 126.9, 126.5, 126.3, 124.9 (q, $^1J_{C\text{-}CF3}$ = 277.0 Hz), 121.2, 120.2,

115.9, 45.4 (q, $^{3}J_{C\text{-}CF3}$ = 2.3 Hz), 44.2 (q, $^{2}J_{C\text{-}CF3}$ = 28.0 Hz), 30.9. ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.38. Spectroscopic data are in accordance with those described in the literature.[1]



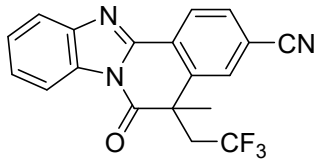
3-bromo-5-methyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3d)

White solid; m.p. = 238.1-239.6°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (d, *J* = 8.4 Hz, 1H), 8.37 – 8.31 (m, 1H), 7.87 – 7.79 (m, 1H), 7.67 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.61 (d, *J* = 1.8 Hz, 1H), 7.51 – 7.41 (m, 2H), 3.57 – 3.38 (m, 1H), 3.00 – 2.78 (m, 1H), 1.77 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.3, 148.5, 144.0, 140.3, 132.1, 131.4, 129.8, 127.9, 126.5, 126.4, 126.3, 124.9 (q, $^{1}J_{C\text{-}CF3}$ = 277.0 Hz), 121.6, 120.2, 115.8, 45.3 (q, $^{3}J_{C\text{-}CF3}$ = 2.0 Hz), 44.1 (q, $^{2}J_{C\text{-}CF3}$ = 27.7 Hz), 30.9. ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.36. Spectroscopic data are in accordance with those described in the literature.[1]



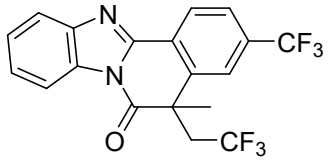
5-methyl-3-(methylsulfonyl)-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3e)

White solid; m.p. = 226.5-227.2°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 (d, *J* = 8.0 Hz, 1H), 8.43 – 8.32 (m, 1H), 8.16 – 8.01 (m, 2H), 7.93 – 7.81 (m, 1H), 7.56 – 7.43 (m, 2H), 3.66 – 3.47 (m, 1H), 3.12 (s, 3H), 3.08 – 2.95 (m, 1H), 1.81 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.0, 144.0, 143.0, 139.7, 131.5, 127.7, 127.3, 127.3, 127.8, 126.8, 126.2, 124.9 (q, $^{1}J_{C\text{-}CF3}$ = 277.0 Hz), 120.7, 116.0, 45.7 (q, $^{3}J_{C\text{-}CF3}$ = 2.0 Hz), 44.7, 43.7 (q, $^{2}J_{C\text{-}CF3}$ = 27.7 Hz), 30.9. ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.19. HRMS (ESI) m/z calculated for $C_{19}H_{16}F_3N_2O_3S^+$: 409.0828, found : 409.0845.



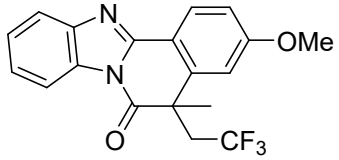
5-methyl-6-oxo-5-(2,2,2-trifluoroethyl)-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinoline-3-carbonitrile (3f)

White solid; m.p. = 258.5-259.6°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (d, *J* = 8.1 Hz, 1H), 8.40 – 8.32 (m, 1H), 7.90 – 7.84 (m, 1H), 7.82 – 7.77 (m, 2H), 7.54 – 7.47 (m, 2H), 3.60 – 3.44 (m, 1H), 3.01 – 2.85 (m, 1H), 1.80 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.8, 147.3, 144.1, 139.5, 131.7, 131.5, 130.8, 127.3, 127.1, 126.8, 126.6, 126.2 (q, $^{1}J_{C\text{-}CF3}$ = 277.0 Hz), 120.7, 117.9, 116.0, 115.2, 45.4 (q, $^{3}J_{C\text{-}CF3}$ = 2.0 Hz), 44.4 (q, $^{2}J_{C\text{-}CF3}$ = 28.0 Hz), 30.8. ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.34. Spectroscopic data are in accordance with those described in the literature.[1]



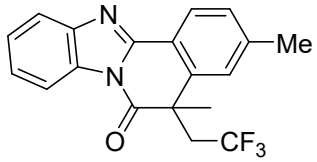
5-methyl-5-(2,2,2-trifluoroethyl)-3-(trifluoromethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3g)

White solid; m.p. = 163.7-164.6°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (d, *J* = 8.2 Hz, 1H), 8.41 – 8.33 (m, 1H), 7.90 – 7.83 (m, 1H), 7.78 (d, *J* = 8.3 Hz, 1H), 7.71 (s, 1H), 7.55 – 7.43 (m, 2H), 3.60 – 3.44 (m, 1H), 3.05 – 2.89 (m, 1H), 1.80 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.2, 147.8, 144.1, 139.2, 133.4 (q, $^{2}J_{C\text{-}CF3}$ = 32.7 Hz), 131.6, 127.2, 126.7, 126.7, 125.9, 125.5 (q, $^{3}J_{C\text{-}CF3}$ = 3.3 Hz), 124.9 (q, $^{1}J_{C\text{-}CF3}$ = 277.0 Hz), 123.8 (q, $^{4}J_{C\text{-}CF3}$ = 3.3 Hz), 123.6 (q, $^{1}J_{C\text{-}CF3}$ = 271.0 Hz), 120.5, 116.0, 45.6 (q, $^{3}J_{C\text{-}CF3}$ = 2.0 Hz), 44.1 (q, $^{2}J_{C\text{-}CF3}$ = 27.7 Hz), 30.9. ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.41, -63.03. Spectroscopic data are in accordance with those described in the literature.[1]



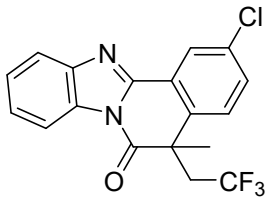
3-methoxy-5-methyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3h)

White solid; m.p. = 150.1-151.3°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (d, *J* = 8.8 Hz, 1H), 8.35 – 8.29 (m, 1H), 7.81 – 7.76 (m, 1H), 7.47 – 7.35 (m, 2H), 7.07 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.93 (d, *J* = 2.4 Hz, 1H), 3.92 (s, 3H), 3.54 – 3.37 (m, 1H), 2.98 – 2.81 (m, 1H), 1.75 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.1, 162.6, 149.6, 144.3, 140.7, 131.5, 128.5, 126.2, 125.5, 125.1 (q, $^{1}J_{C\text{-}CF3}$ = 277.0 Hz), 119.7, 115.7, 115.4, 114.2, 112.6, 55.8, 45.6 (q, $^{3}J_{C\text{-}CF3}$ = 2.0 Hz), 44.2 (q, $^{2}J_{C\text{-}CF3}$ = 27.8 Hz), 31.2. ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.28. Spectroscopic data are in accordance with those described in the literature.[1]



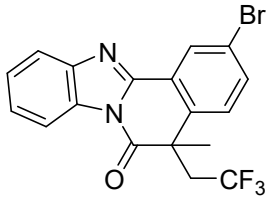
3,5-dimethyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3i)

White solid; m.p. = 203.1-203.8°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (d, *J* = 8.0 Hz, 1H), 8.37 – 8.31 (m, 1H), 7.85 – 7.78 (m, 1H), 7.49 – 7.38 (m, 2H), 7.34 (d, *J* = 8.1 Hz, 1H), 7.25 (s, 1H), 3.55 – 3.37 (m, 1H), 3.01 – 2.84 (m, 1H), 2.48 (s, 3H), 1.75 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.3, 149.6, 144.1, 142.5, 138.6, 131.4, 129.7, 127.0, 126.4, 126.2, 125.7, 125.1 (q, $^{1}J_{C\text{-}CF3}$ = 277.0 Hz), 119.9, 119.8, 115.8, 45.3 (q, $^{3}J_{C\text{-}CF3}$ = 2.0 Hz), 44.0 (q, $^{2}J_{C\text{-}CF3}$ = 27.7 Hz), 31.1, 22.1. ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.34. Spectroscopic data are in accordance with those described in the literature.[1]



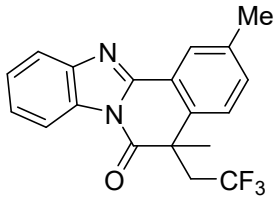
2-chloro-5-methyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3j)

White solid; m.p. = 166.2-167.3°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (d, *J* = 2.3 Hz, 1H), 8.39 – 8.31 (m, 1H), 7.88 – 7.80 (m, 1H), 7.55 (dd, *J* = 8.5, 2.3 Hz, 1H), 7.52 – 7.43 (m, 2H), 7.41 (d, *J* = 8.6 Hz, 1H), 3.56 – 3.40 (m, 1H), 2.90 (m, 1H), 1.75 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.6, 148.0, 143.9, 136.8, 134.9, 131.9, 131.5, 128.2, 126.5, 126.4, 126.2, 124.9 (q, $^{1}J_{C\text{-}CF3}$ = 277.0 Hz), 124.1, 120.3, 115.9, 45.2 (q, $^{3}J_{C\text{-}CF3}$ = 2.0 Hz), 44.0 (q, $^{2}J_{C\text{-}CF3}$ = 27.7 Hz), 31.0. ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.31. Spectroscopic data are in accordance with those described in the literature.[1]



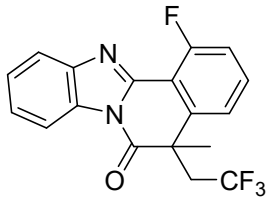
2-bromo-5-methyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3k)

White solid; m.p. = 169.0-170.8°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 2.1 Hz, 1H), 8.38 – 8.31 (m, 1H), 7.88 – 7.80 (m, 1H), 7.70 (dd, *J* = 8.5, 2.2 Hz, 1H), 7.51 – 7.43 (m, 2H), 7.34 (d, *J* = 8.5 Hz, 1H), 3.56 – 3.39 (m, 1H), 2.98 – 2.82 (m, 1H), 1.75 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.5, 147.9, 144.0, 137.3, 134.7, 131.5, 129.2, 128.3, 126.5, 126.4, 125.0 (q, $^{1}J_{C\text{-}CF3}$ = 277.0 Hz), 124.4, 122.8, 120.3, 115.9, 45.3 (q, $^{3}J_{C\text{-}CF3}$ = 2.0 Hz), 44.0 (q, $^{2}J_{C\text{-}CF3}$ = 27.7 Hz), 30.9. ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.29. HRMS (ESI) m/z calculated for $C_{18}H_{13}BrF_3N_2O^+$: 409.0158, found : 409.0173.



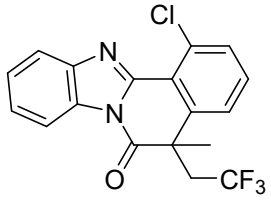
2,5-dimethyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3l)

White solid; m.p. = 131.2-131.6°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 – 8.32 (m, 2H), 7.86 – 7.80 (m, 1H), 7.49 – 7.43 (m, 2H), 7.41 (d, *J* = 7.8 Hz, 1H), 7.35 (d, *J* = 8.1 Hz, 1H), 3.54 – 3.36 (m, 1H), 3.00 – 2.84 (m, 1H), 2.48 (s, 3H), 1.73 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.4, 149.6, 144.0, 138.7, 135.7, 132.9, 131.5, 126.6, 126.5, 126.3, 125.9,125.1 (q, $^{1}J_{C\text{-}CF3}$ = 277.0 Hz), 122.1, 120.0, 115.8, 45.2 (q, $^{3}J_{C\text{-}CF3}$ = 2.0 Hz), 44.0 (q, $^{2}J_{C\text{-}CF3}$ = 27.3 Hz), 31.1, 21.1. ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.32. Spectroscopic data are in accordance with those described in the literature.[1]



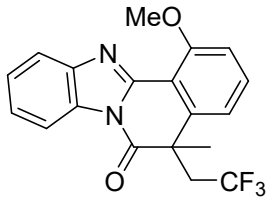
1-fluoro-5-methyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3m)

White solid; m.p. = 177.8-178.5°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 – 8.34 (m, 1H), 7.99 – 7.92 (m, 1H), 7.61 – 7.53 (m, 1H), 7.51 – 7.44 (m, 2H), 7.33 – 7.26 (m, 2H), 3.57 – 3.41 (m, 1H), 3.02 – 2.86 (m, 1H), 1.78 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.5, 160.7 (d, $^{1}J_{C\text{-}F}$ = 261.0 Hz), 145.4 (d, $^{3}J_{C\text{-}F}$ = 8.0 Hz), 144.3 (d, $^{4}J_{C\text{-}F}$ = 2.0 Hz), 141.0, 132.5 (d, $^{3}J_{C\text{-}F}$ = 10.0 Hz), 130.5, 126.6, 126.5, 125.0 (q, $^{1}J_{C\text{-}CF3}$ = 277.0 Hz), 122.6 (d, $^{3}J_{C\text{-}F}$ = 8.0 Hz), 120.9, 116.5 (d, $^{2}J_{C\text{-}F}$ = 22.0 Hz), 115.8, 112.0 (d, $^{2}J_{C\text{-}F}$ = 10.0 Hz), 45.3 (q, $^{3}J_{C\text{-}CF3}$ = 2.0 Hz; d, $^{4}J_{C\text{-}F}$ = 2.0 Hz) , 44.4 (q, $^{2}J_{C\text{-}CF3}$ = 27.7 Hz), 31.3.^{19}F NMR (376 MHz, $CDCl_3$) δ -61.27, -106.21. Spectroscopic data are in accordance with those described in the literature.[1]



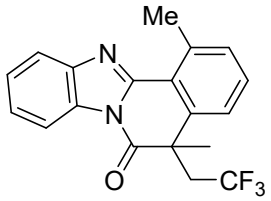
1-chloro-5-methyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3n)

White solid; m.p. = 210.4-211.3°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 – 8.35 (m, 1H), 7.98 – 7.91 (m, 1H), 7.62 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.51 – 7.45 (m, 3H), 7.42 (dd, *J* = 8.0, 1.4 Hz, 1H), 3.50 (m, 1H), 2.93 (m, 1H), 1.77 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.3, 146.7, 144.0, 141.3, 134.1, 132.2, 130.9, 130.6, 126.7, 126.3, 125.5, 125.0 (q, $^{1}J_{C\text{-}CF3}$ = 277.3 Hz), 121.0, 120.7, 115.8, 45.6 (q, $^{3}J_{C\text{-}CF3}$ = 2.0 Hz), 43.3 (q, $^{2}J_{C\text{-}CF3}$ = 27.7 Hz), 31.5. ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.17. HRMS (ESI) m/z calculated for $C_{18}H_{13}ClF_3N_2O^+$: 365.0679, found : 365.0685.



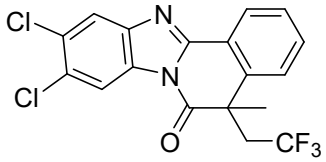
1-methoxy-5-methyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3o)

White solid; m.p. = 193.5-194.7°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 – 8.29 (m, 1H), 7.96 – 7.86 (m, 1H), 7.53 (t, *J* = 8.2 Hz, 1H), 7.47 – 7.37 (m, 2H), 7.09 (dd, *J* = 8.2, 2.9 Hz, 2H), 4.14 (s, 3H), 3.54 – 3.37 (m, 1H), 2.99 – 2.84 (m, 1H), 1.76 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 171.0, 159.0, 147.5, 144.4, 141.1, 132.2, 130.4, 126.0, 126.0, 125.0 (q, $^{1}J_{C\text{-}CF3}$ = 277.0 Hz), 120.7, 118.9, 115.6, 111.8, 111.1, 56.8, 45.2 (q, $^{3}J_{C\text{-}CF3}$ = 2.3 Hz), 44.4 (q, $^{2}J_{C\text{-}CF3}$ = 27.3 Hz), 31.4. ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.28. Spectroscopic data are in accordance with those described in the literature.[1]



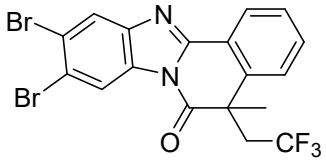
1,5-dimethyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3p)

White solid; m.p. = 166.6-168.3°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 – 8.35 (m, 1H), 7.89 – 7.81 (m, 1H), 7.50 – 7.40 (m, 3H), 7.39 – 7.31 (m, 2H), 3.59 – 3.36 (m, 1H), 3.07 (s, 3H), 3.01 – 2.87 (m, 1H), 1.76 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.3, 149.6, 144.4, 140.4, 139.7, 131.9, 130.7, 130.4, 126.0, 125.2 (q, $^{1}J_{C\text{-}CF3}$ = 277.0 Hz), 124.5, 121.2, 120.4, 115.9, 45.4 (q, $^{3}J_{C\text{-}CF3}$ = 2.3 Hz), 44.4 (q, $^{2}J_{C\text{-}CF3}$ = 27.3 Hz), 31.6, 24.9. ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.21. Spectroscopic data are in accordance with those described in the literature.[1]



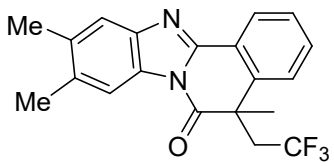
9,10-dichloro-5-methyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3q)

White solid; m.p. = 162.3-163.5°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 – 8.45 (m, 2H), 7.90 (s, 1H), 7.64 (t, *J* = 7.6 Hz, 1H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.48 (d, *J* = 7.8 Hz, 1H), 3.53 – 3.37 (m, 1H), 3.03 – 2.86 (m, 1H), 1.77 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.9, 150.9, 143.6, 138.7, 132.4, 130.5, 130.4, 129.9, 128.8, 126.7, 126.7, 124.9 (q, $^{1}J_{C\text{-}CF3}$ = 277.0 Hz), 121.9, 121.3, 117.2, 45.4 (q, $^{3}J_{C\text{-}CF3}$ = 2.0 Hz), 44.2 (q, $^{2}J_{C\text{-}CF3}$ = 27.7 Hz), 31.0. ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.42. HRMS (ESI) m/z calculated for $C_{18}H_{12}Cl_2F_3N_2O^+$: 399.0273, found : 399.0285.



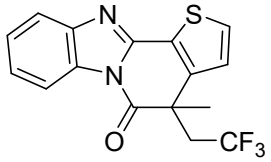
9,10-dibromo-5-methyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3r)

White solid; m.p. = 193.2-194.1°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (s, 1H), 8.49 (d, *J* = 7.8 Hz, 1H), 8.09 (s, 1H), 7.64 (t, *J* = 7.7 Hz, 1H), 7.54 (t, *J* = 7.0 Hz, 1H), 7.49 (d, *J* = 7.9 Hz, 1H), 3.54 – 3.34 (m, 1H), 3.06 – 2.83 (m, 1H), 1.77 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.0, 150.8, 144.4, 138.7, 132.5, 131.3, 128.8, 126.8, 126.7, 124.9 (q, $^{1}J_{C\text{-}CF3}$ = 277.3 Hz), 124.5, 122.0, 121.8, 121.4, 120.3, 44.4 (q, $^{3}J_{C\text{-}CF3}$ = 2.0 Hz), 44.2 (q, $^{2}J_{C\text{-}CF3}$ = 27.7 Hz), 31.0. ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.41. HRMS (ESI) m/z calculated for $C_{18}H_{12}Br_2F_3N_2O^+$: 486.9263, found : 486.9265.

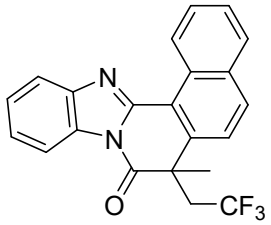


5,9,10-trimethyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3s)

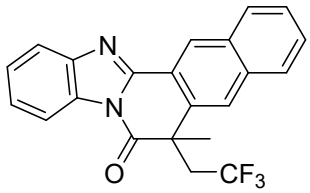
White solid; m.p. = 167.5-168.1°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, *J* = 7.8 Hz, 1H), 8.14 (s, 1H), 7.62 – 7.54 (m, 2H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.46 (d, *J* = 7.8 Hz, 1H), 3.57 – 3.36 (m, 1H), 3.03 – 2.84 (m, 1H), 2.42 (d, *J* = 6.7 Hz, 6H), 1.75 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.1, 148.6, 142.4, 138.3, 135.4, 135.4, 131.5, 129.8, 128.5, 126.6, 126.3, 125.1 (q, $^1J_{C\text{-}CF3}$ = 277.3 Hz), 122.7, 120.2, 116.1, 45.3 (q, $^3J_{C\text{-}CF3}$ = 2.0 Hz), 44.0 (q, $^2J_{C\text{-}CF3}$ = 27.7 Hz), 31.1, 20.7, 20.6. ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.41. HRMS (ESI) m/z calculated for $C_{20}H_{18}F_3N_2O^+$: 359.1366, found : 359.1369.



4-methyl-4-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[1,2-*a*]thieno[2,3-*c*]pyridin-5(4*H*)-one (3t)
White solid; m.p. = 161.0-162.5°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 – 8.27 (m, 1H), 7.84 – 7.75 (m, 1H), 7.66 (d, *J* = 5.1 Hz, 1H), 7.49 – 7.39 (m, 2H), 7.12 (d, *J* = 5.1 Hz, 1H), 3.50 – 3.32 (m, 1H), 2.93 – 2.73 (m, 1H), 1.73 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.6, 146.2, 144.3, 143.9, 131.2, 130.9, 126.3, 126.0, 125.6, 124.9 (q, $^1J_{C\text{-}CF3}$ = 277.0 Hz), 124.1, 119.9, 115.4, 45.3 (q, $^3J_{C\text{-}CF3}$ = 2.0 Hz), 44.1 (q, $^2J_{C\text{-}CF3}$ = 28.0 Hz), 29.8. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.12. Spectroscopic data are in accordance with those described in the literature.[1]



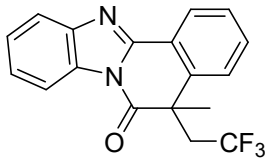
7-methyl-7-(2,2,2-trifluoroethyl)benzo[*h*]benzo[4,5]imidazo[2,1-*a*]isoquinolin-8(7*H*)-one (3u)
White solid; m.p. = 236.7-237.9°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.55 (d, *J* = 8.9 Hz, 1H), 8.49 – 8.40 (m, 1H), 8.05 (d, *J* = 8.8 Hz, 1H), 8.00 – 7.89 (m, 2H), 7.88 – 7.79 (m, 1H), 7.66 (t, *J* = 7.6 Hz, 1H), 7.59 – 7.43 (m, 3H), 3.66 – 3.46 (m, 1H), 3.15 – 2.98 (m, 1H), 1.82 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.3, 149.6, 144.2, 139.0, 133.1, 132.7, 130.5, 129.1, 128.6, 128.4, 127.5, 127.3, 126.3, 126.2, 125.1 (q, $^1J_{C\text{-}CF3}$ = 276.7 Hz), 123.2, 120.4, 118.0, 115.9, 45.7 (q, $^3J_{C\text{-}CF3}$ = 2.0 Hz), 43.8 (q, $^2J_{C\text{-}CF3}$ = 27.3 Hz), 31.0. ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.58. HRMS (ESI) m/z calculated for $C_{22}H_{16}F_3N_2O^+$: 381.1209, found : 381.1218.



7-methyl-7-(2,2,2-trifluoroethyl)benzo[*g*]benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(7*H*)-one (3v)
White solid; m.p. = 213.7-215.2°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (d, *J* = 8.6 Hz, 1H), 8.42 – 8.37 (m, 1H), 8.35 (d, *J* = 8.5 Hz, 1H), 8.01 (d, *J* = 8.6 Hz, 1H), 7.98 (d, *J* = 7.9 Hz, 1H), 7.91 – 7.84 (m, 1H), 7.69 – 7.57 (m, 2H), 7.54 – 7.43 (m, 2H), 3.91 – 3.77 (m, 1H), 3.76 – 3.62 (m, 1H),

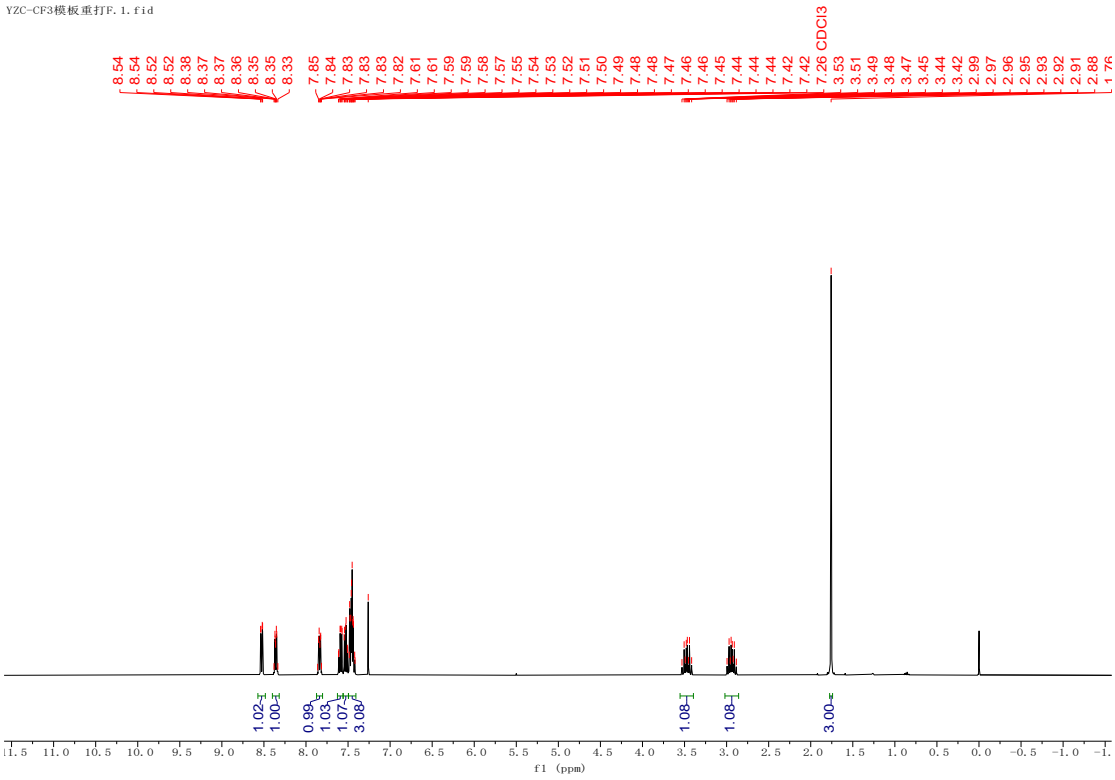
2.18 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.6, 149.9, 144.4, 136.2, 134.4, 131.3, 130.8, 130.6, 130.5, 127.3, 127.2, 126.5, 126.1, 125.2 (q, $^{1}J_{C\text{-}F}$ = 277.3 Hz), 125.2, 122.8, 121.4, 120.1, 115.8, 46.9 (q, $^{3}J_{C\text{-}F}$ = 2.0 Hz), 43.3 (q, $^{2}J_{C\text{-}F}$ = 27.7 Hz), 28.4. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.66. HRMS (ESI) m/z calculated for $C_{22}H_{16}F_3N_2O^+$: 381.1209, found : 381.1218.

Copies of NMR spectra:^{1}H-, ^{13}C- and ^{19}F-NMR spectra

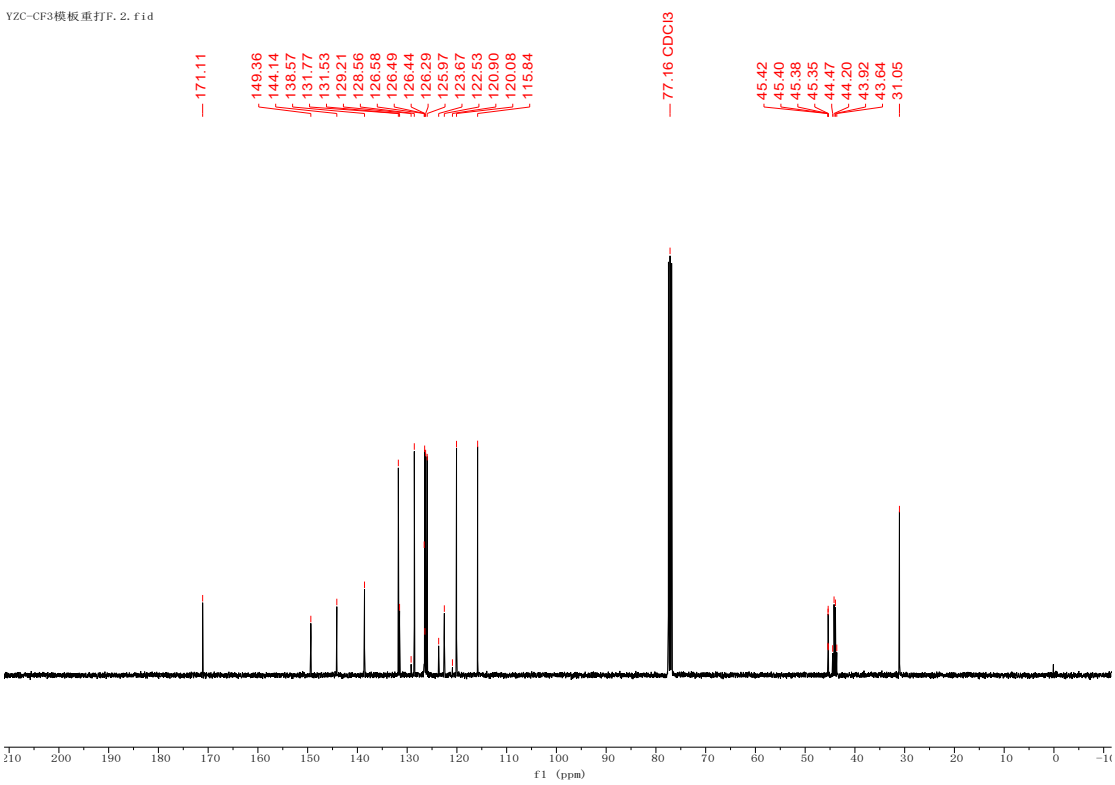


3a

^{1}H NMR



^{13}C NMR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123.67
122.53
120.90
120.08
115.84
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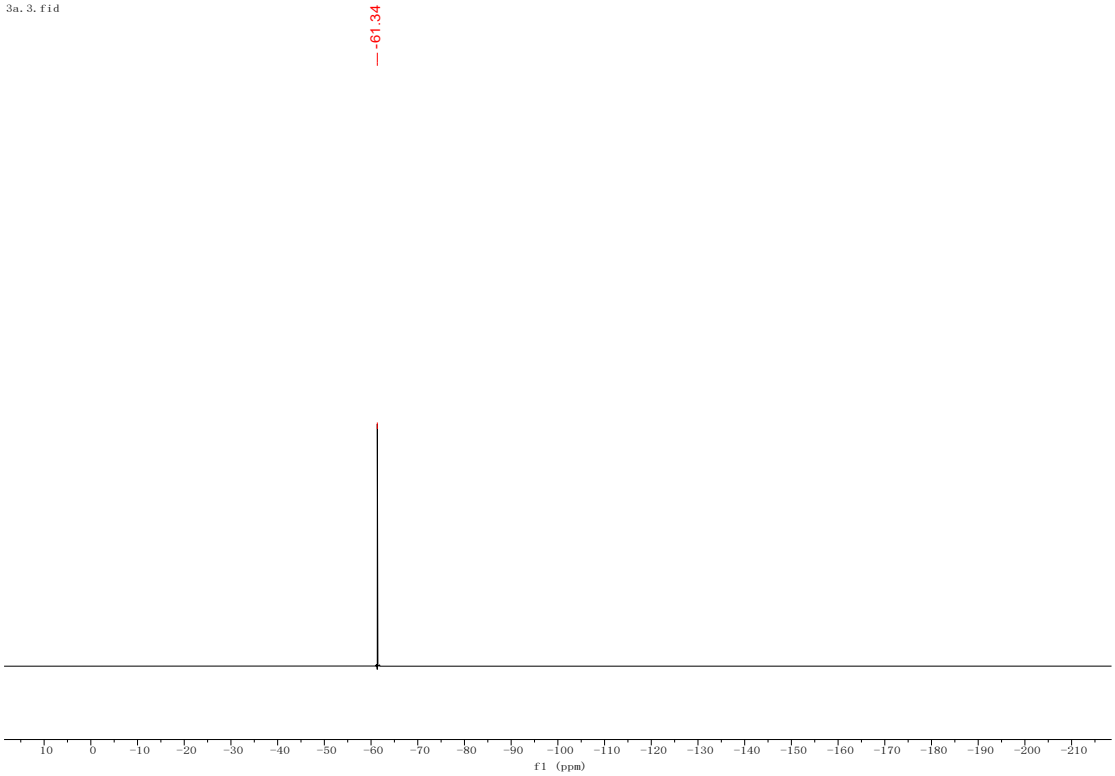
45.38
45.35
44.47
44.20
43.92
43.64
31.05
f1 (ppm)

^{19}F NMR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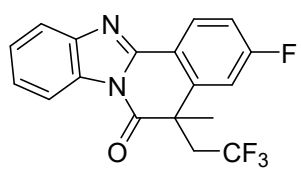
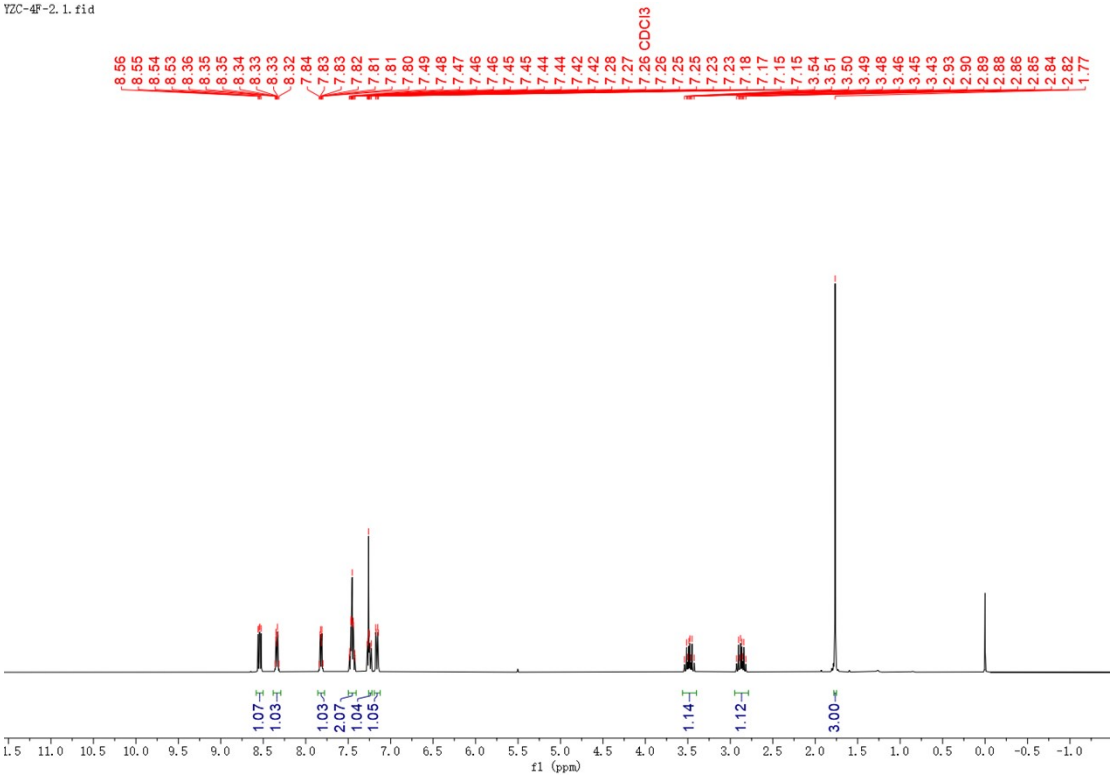
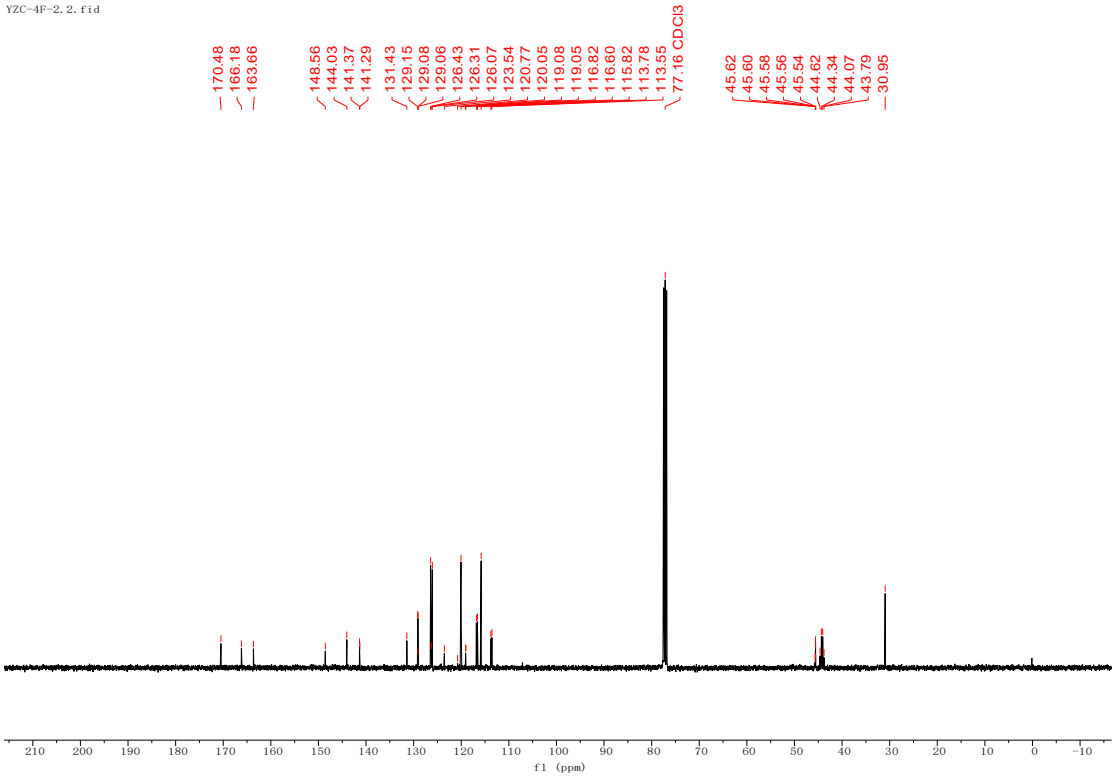

N
N
O
F
CF3

3b

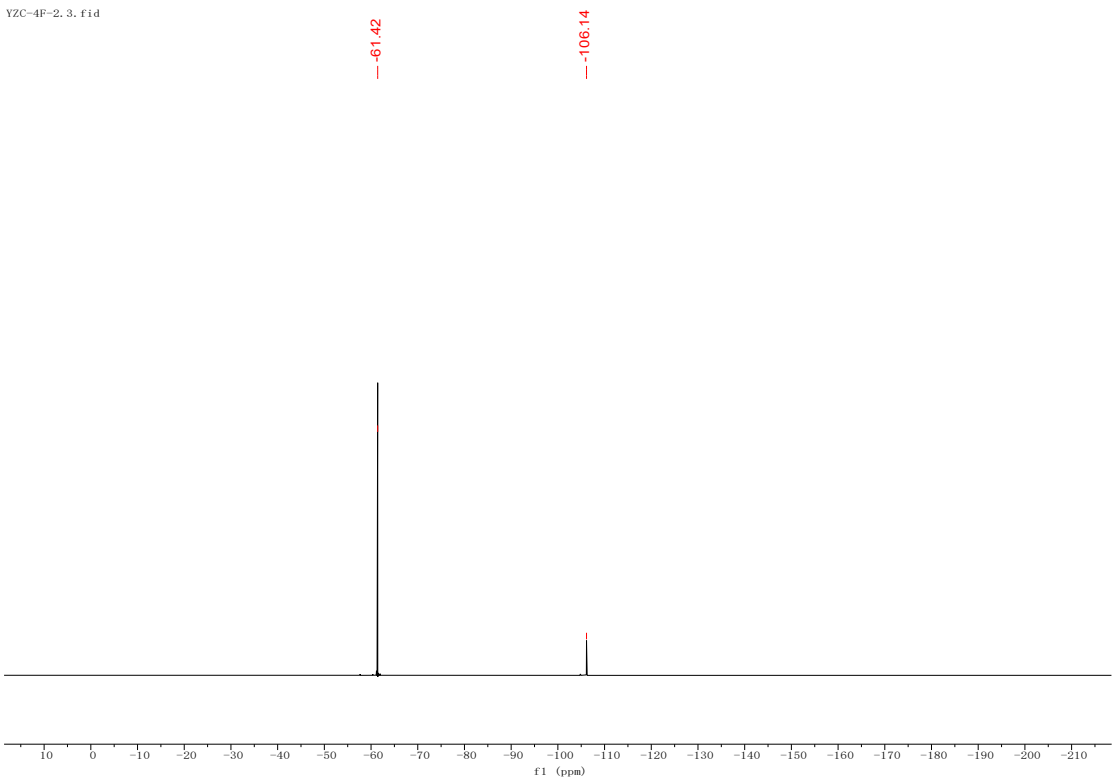
^{1}H NMR

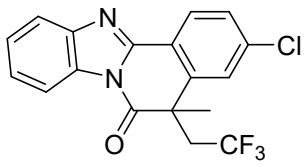


^{13}C NMR



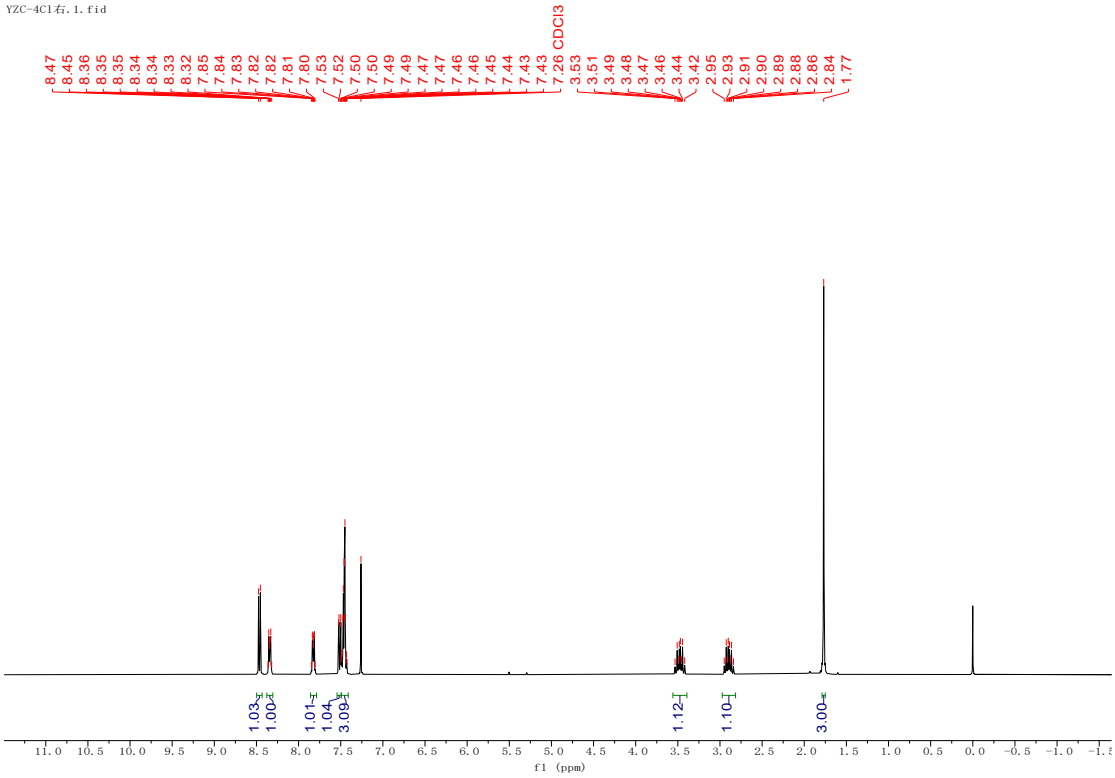
^{19}F NMR


YZC-4F-2.3.fid
-61.42
-106.14
f1 (ppm)


N
N
O
Cl
CF3

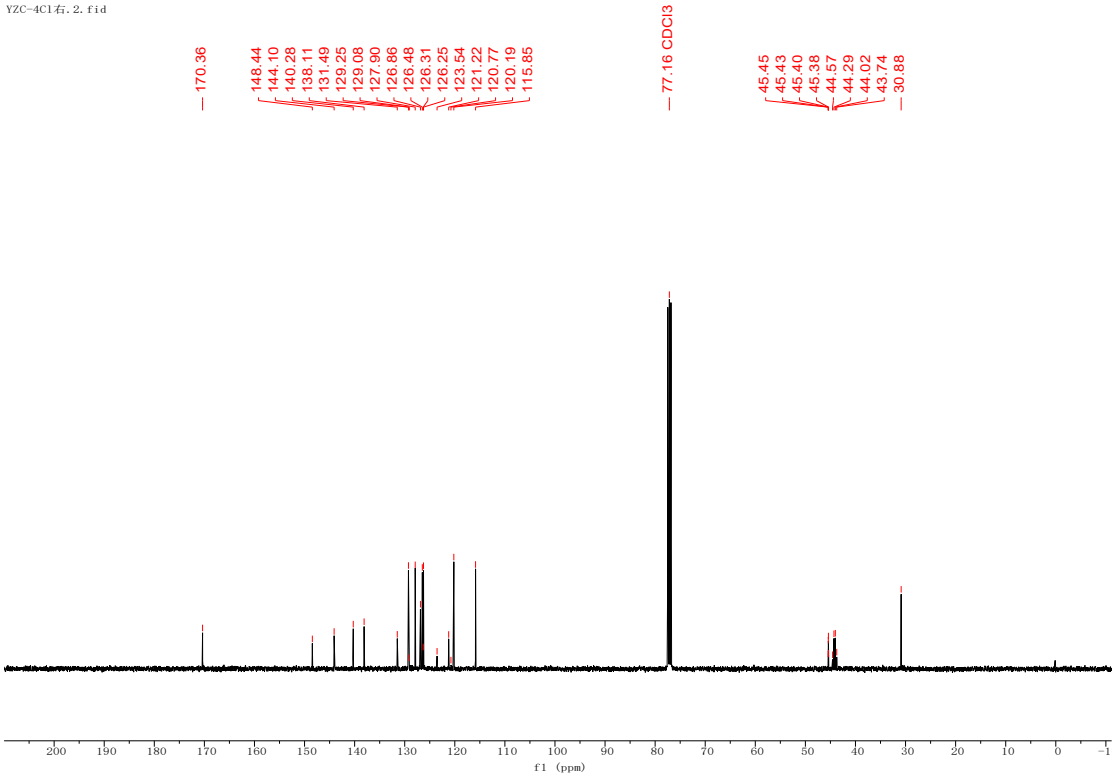
3c

^{1}H NMR


YZC-4Cl右.1.fid
CDCl3
1.03
1.00
1.01
1.04
3.09
1.12
1.10
3.00
f1 (ppm)

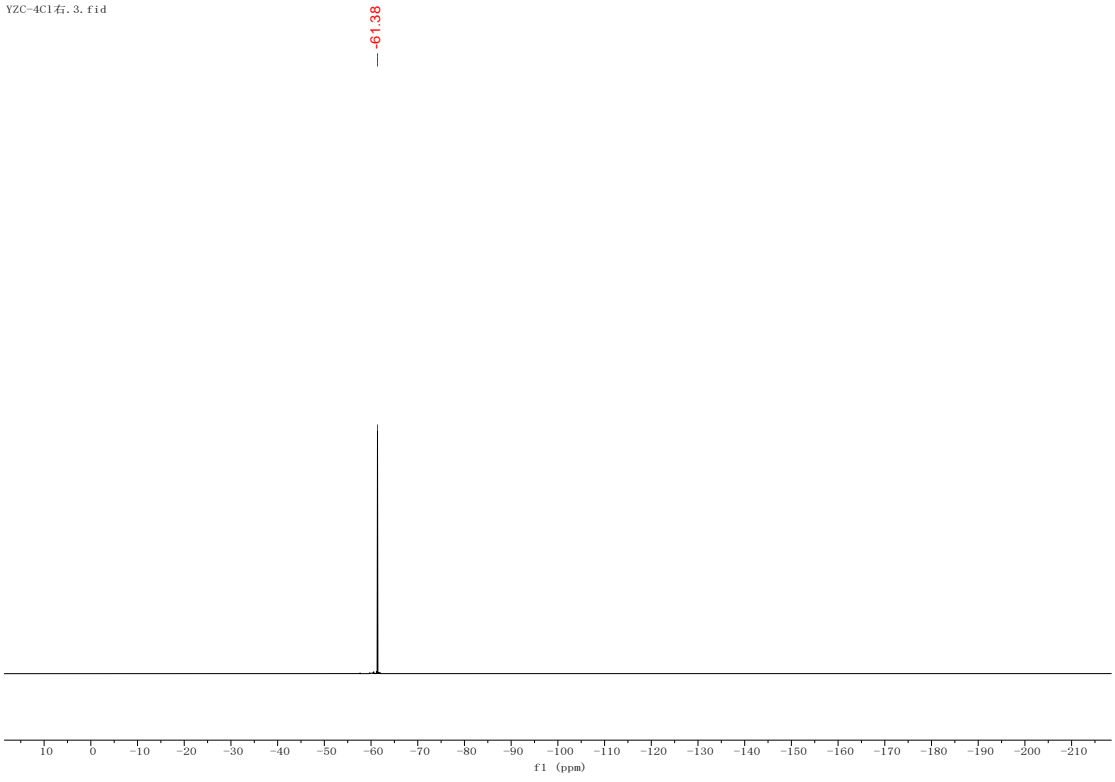
^{13}C NMR

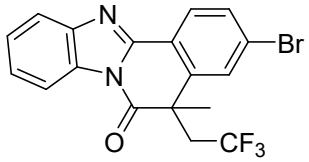
YZC-4Cl右.2.fid



^{19}F NMR

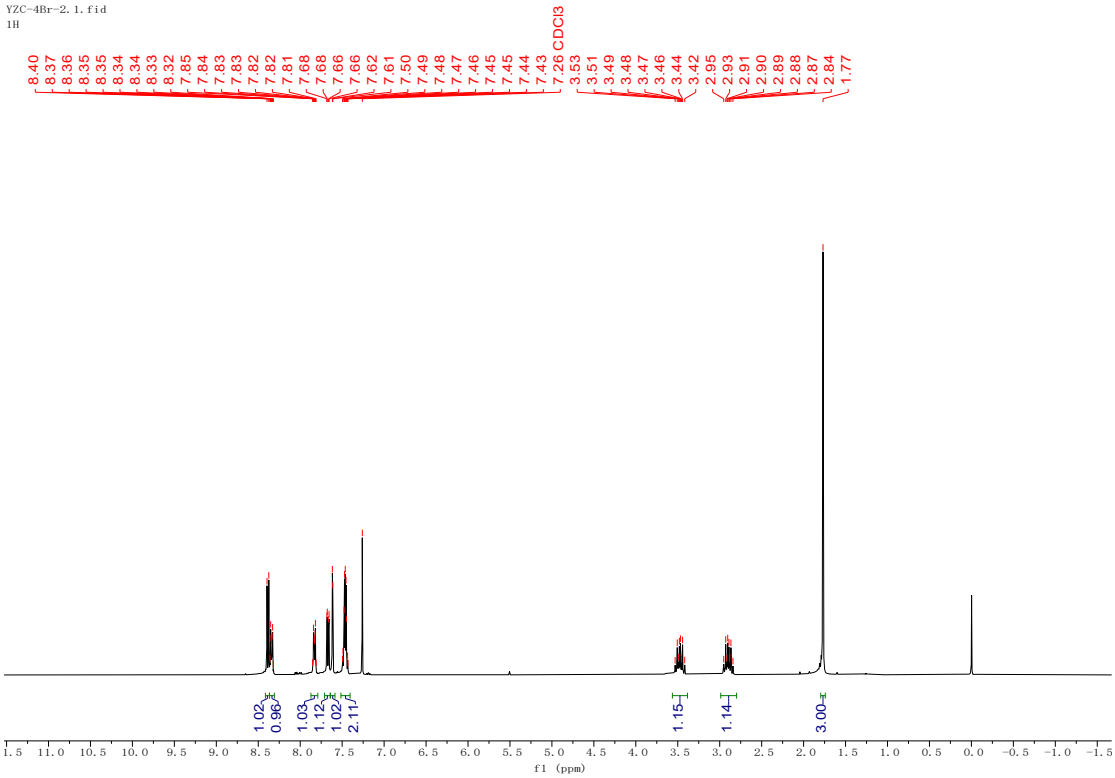
YZC-4Cl右.3.fid



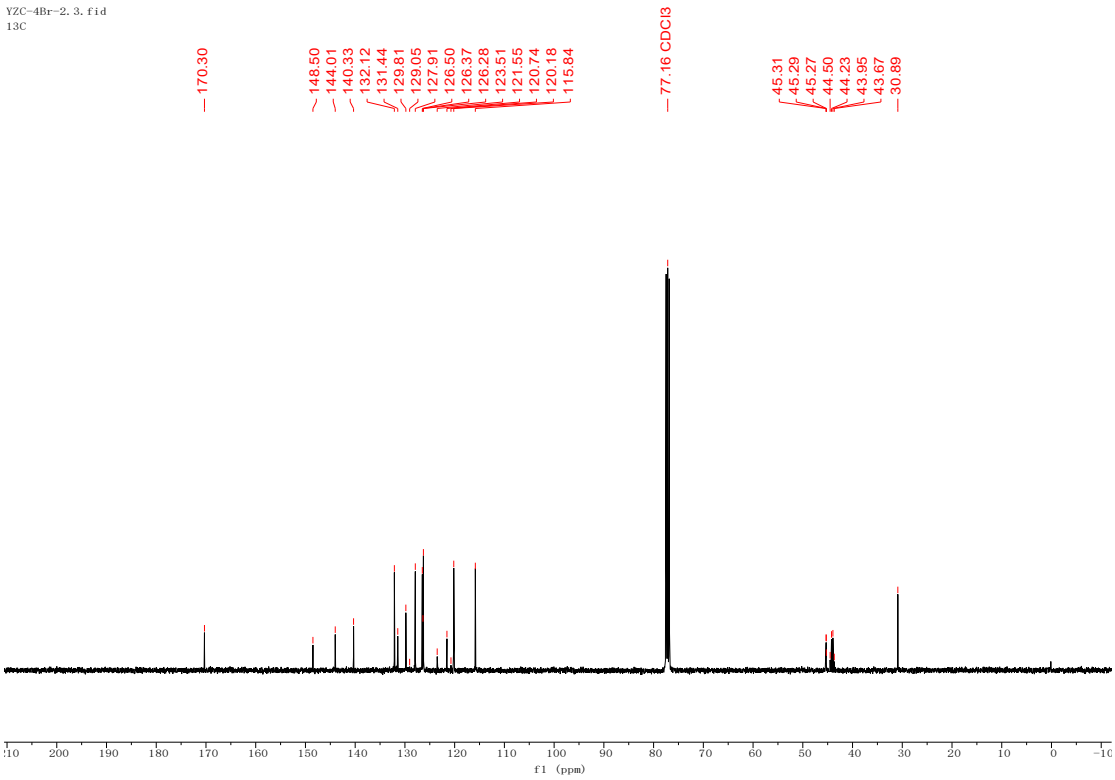


3d

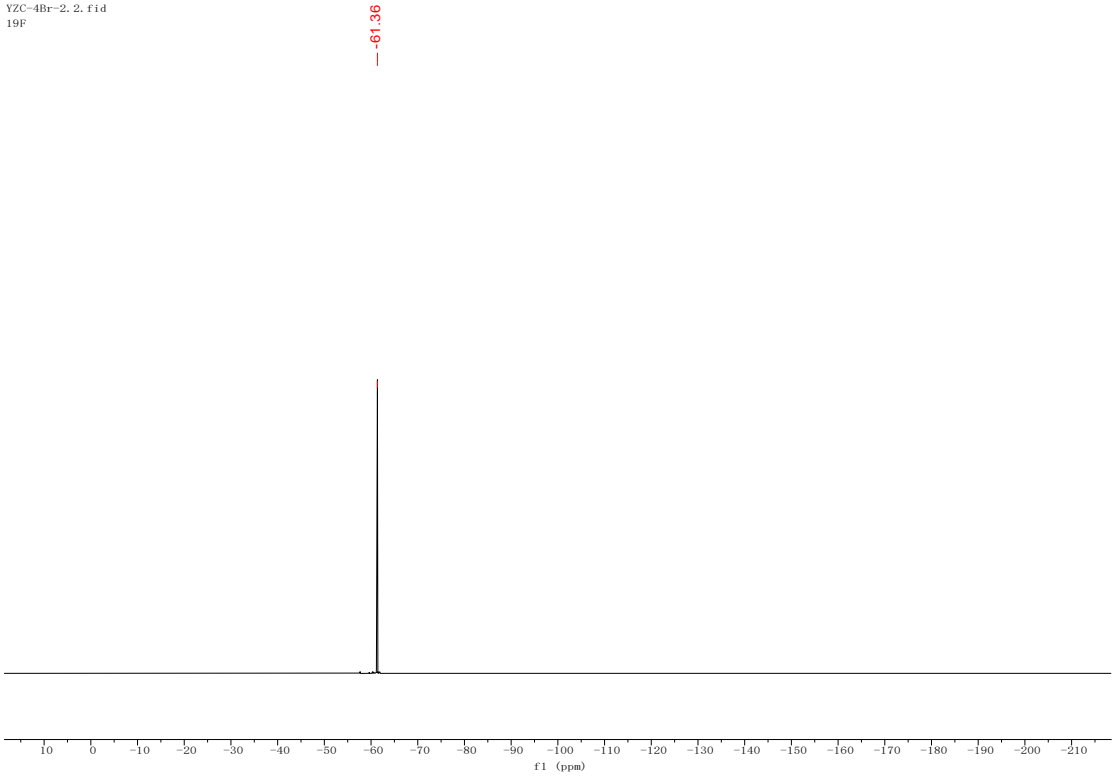
^{1}H NMR

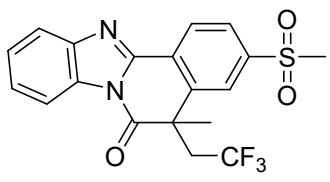


^{13}C NMR


YZC-4Br-2.3.fid
13C
170.30
148.50
144.01
140.33
132.12
131.44
129.81
129.05
127.91
126.50
126.37
126.28
123.51
121.55
120.74
120.18
115.84
77.16 CDCl3
45.31
45.29
45.27
44.50
44.23
43.95
43.67
30.89
f1 (ppm)

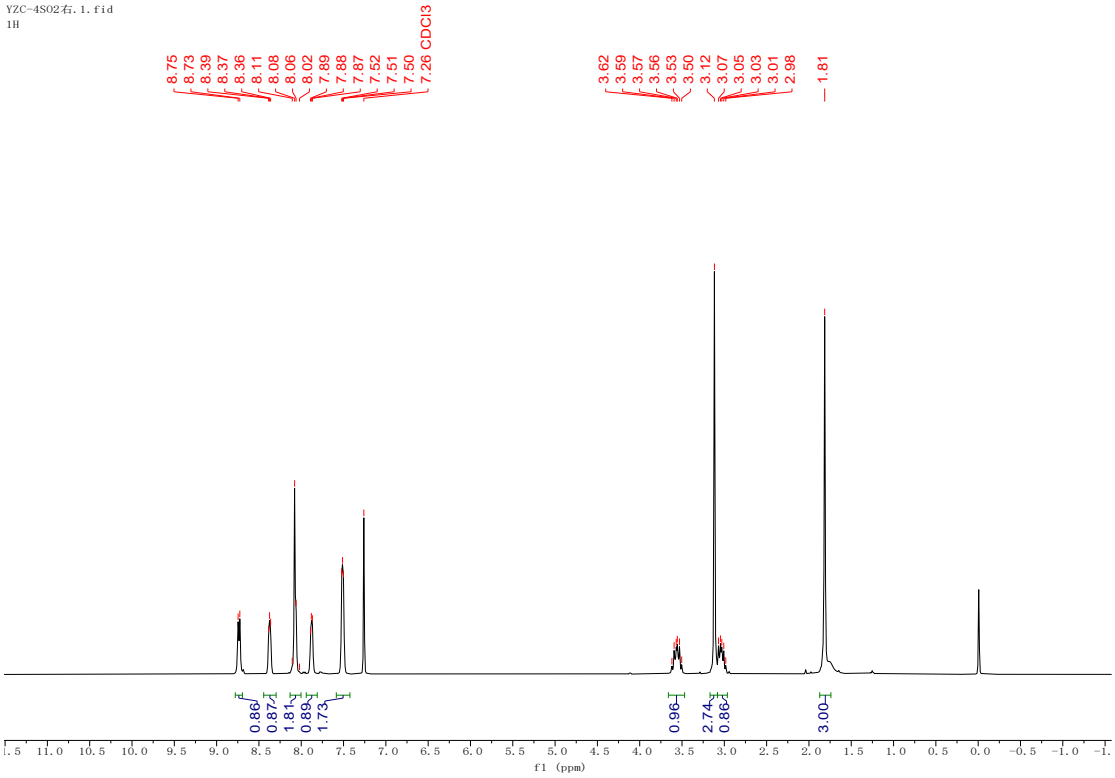
^{19}F NMR


YZC-4Br-2.2.fid
19F
-61.36
f1 (ppm)

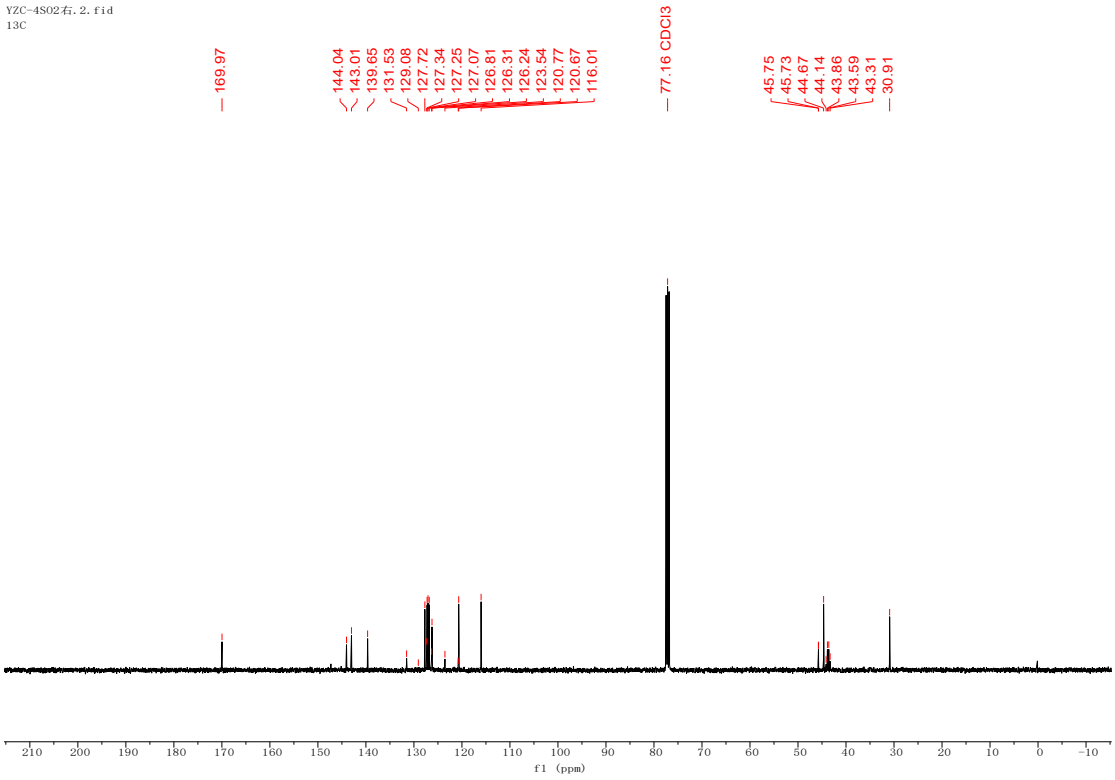

N
N
O
S
O
O
CF3

3e

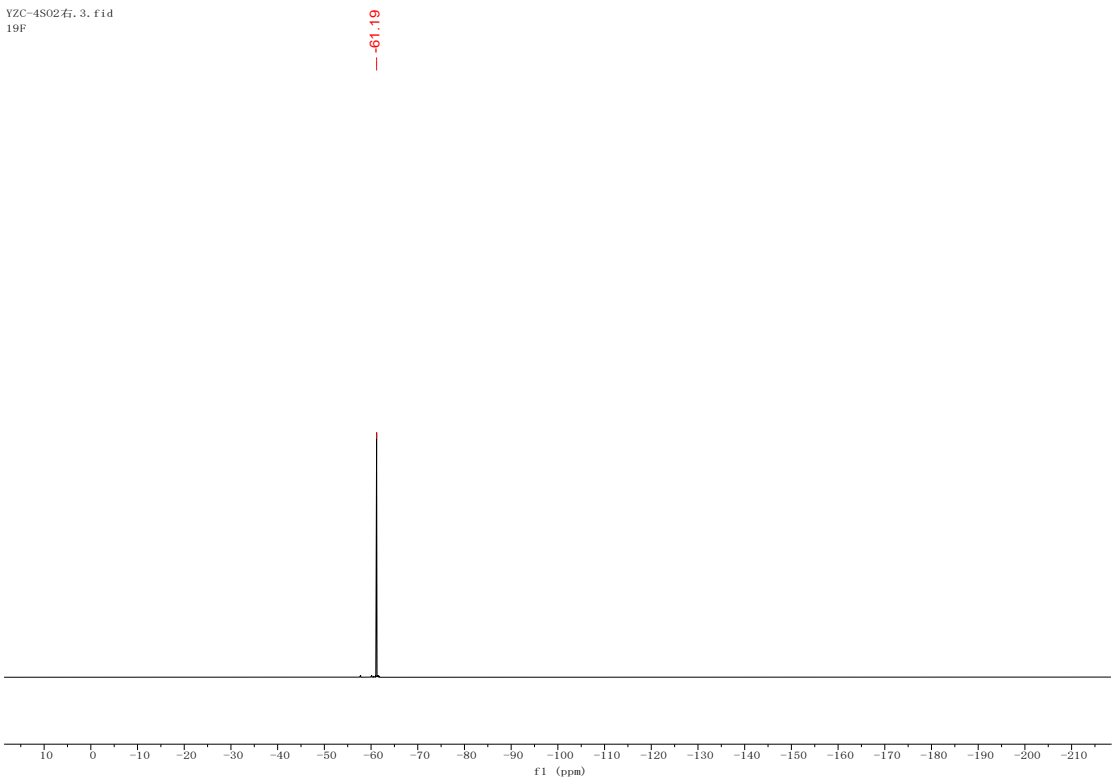
^{1}H NMR

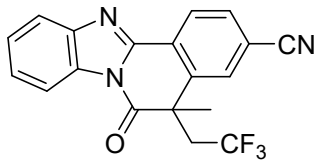


^{13}C NMR



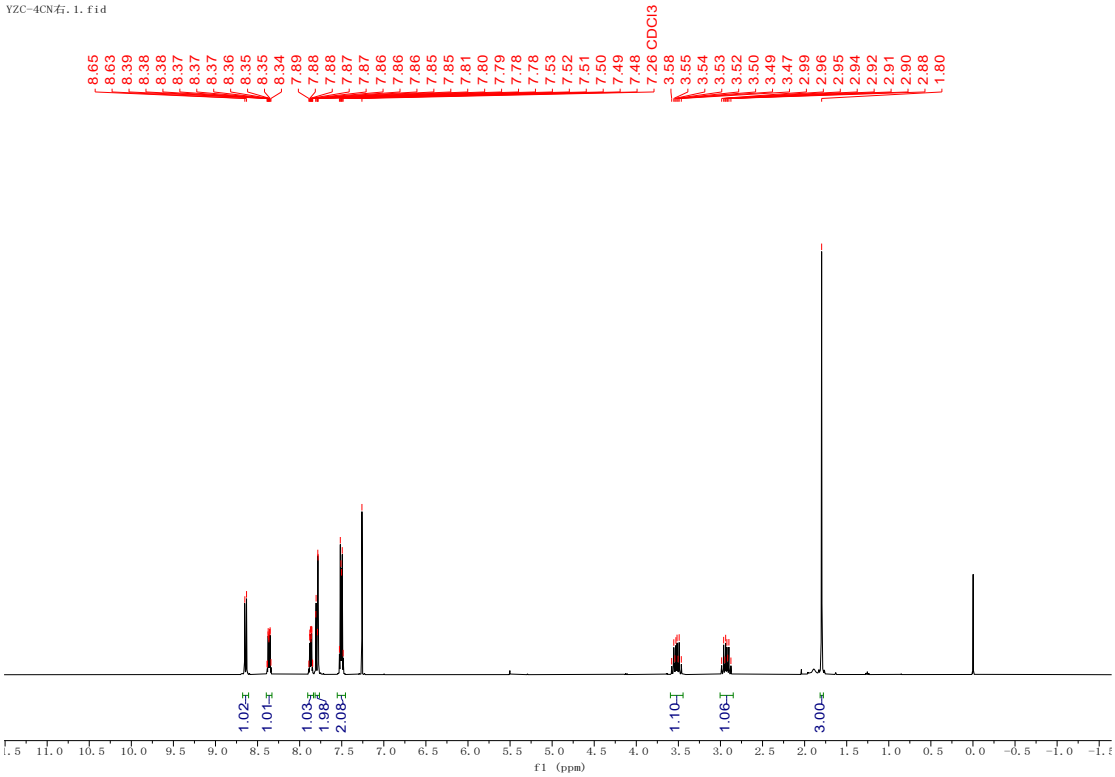
^{19}F NMR


YZC-4S02右.3.fid
19F
-61.19
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)


N
N
O
CN
CF3

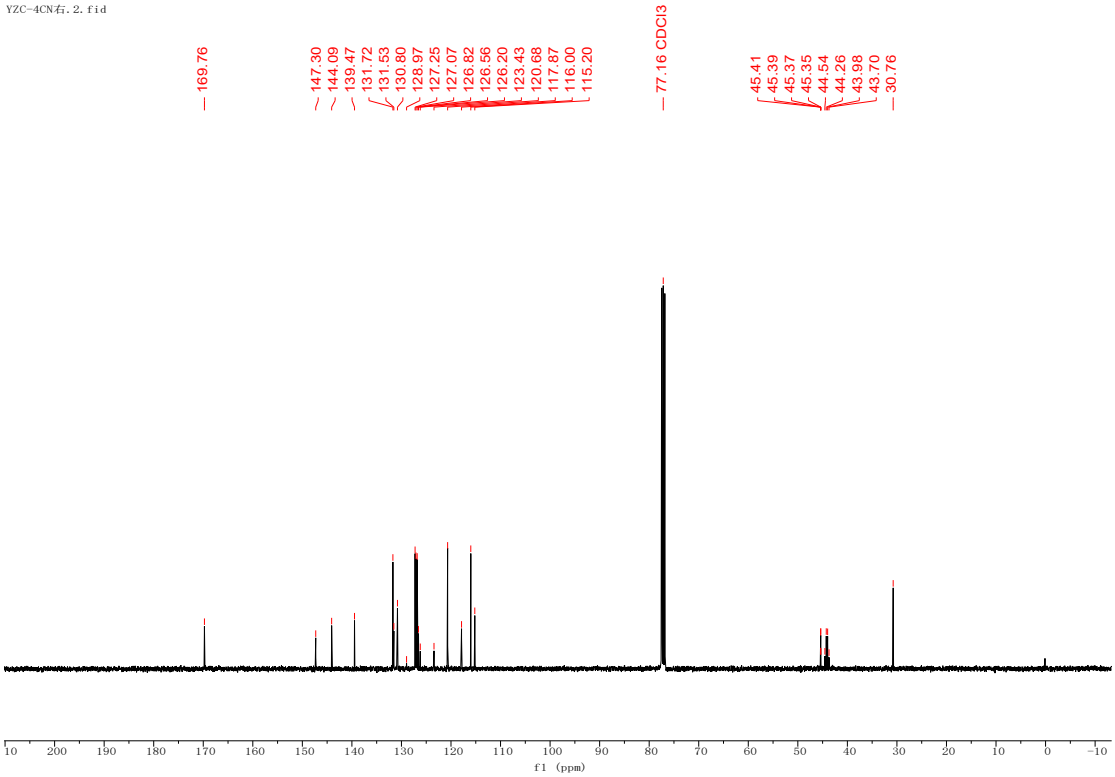
3f

^{1}H NMR


YZC-4CN右.1.fid
8.65 8.63 8.39 8.38 8.38 8.37 8.37 8.37 8.36 8.35 8.35 8.34 7.89 7.88 7.88 7.87 7.87 7.86 7.86 7.86 7.85 7.85 7.81 7.80 7.79 7.78 7.78 7.53 7.52 7.51 7.50 7.49 7.48 7.26 CDCl3 3.58 3.55 3.54 3.53 3.52 3.50 3.49 3.47 2.99 2.96 2.95 2.94 2.92 2.91 2.90 2.88 1.80
1.02 1.01 1.03 1.98 2.08 1.10 1.06 3.00
f1 (ppm)

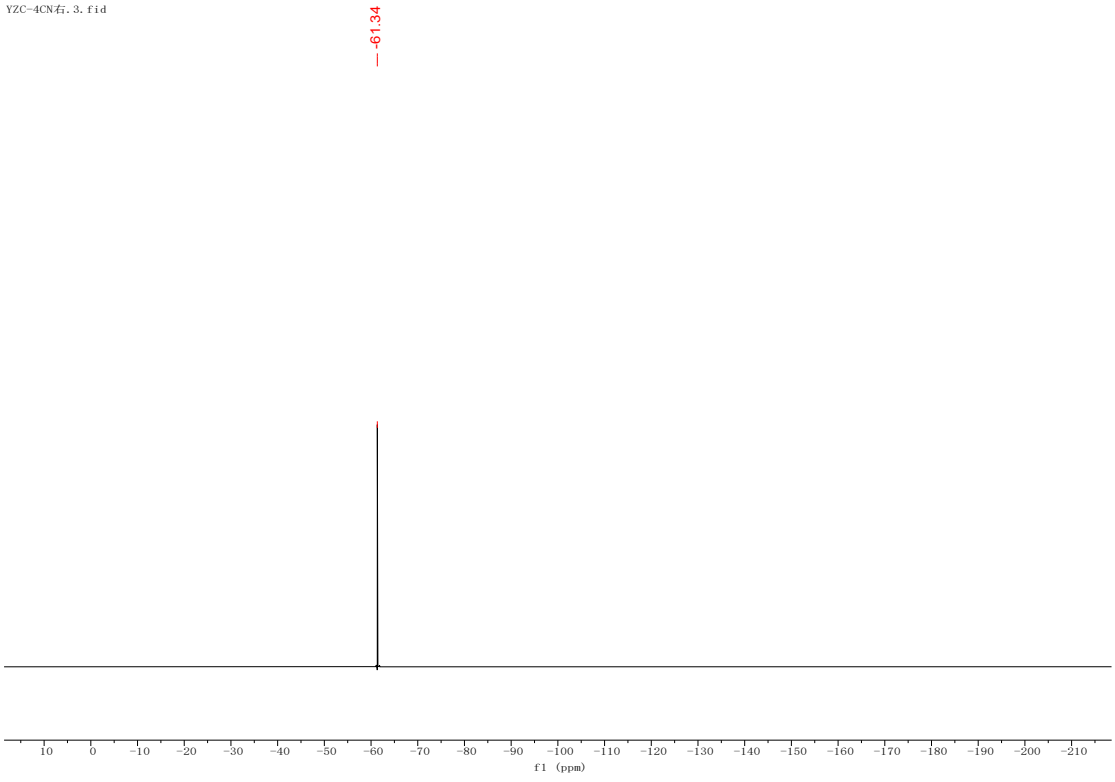
^{13}C NMR

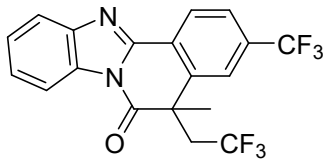
YZC-4CN石.2.fid



^{19}F NMR

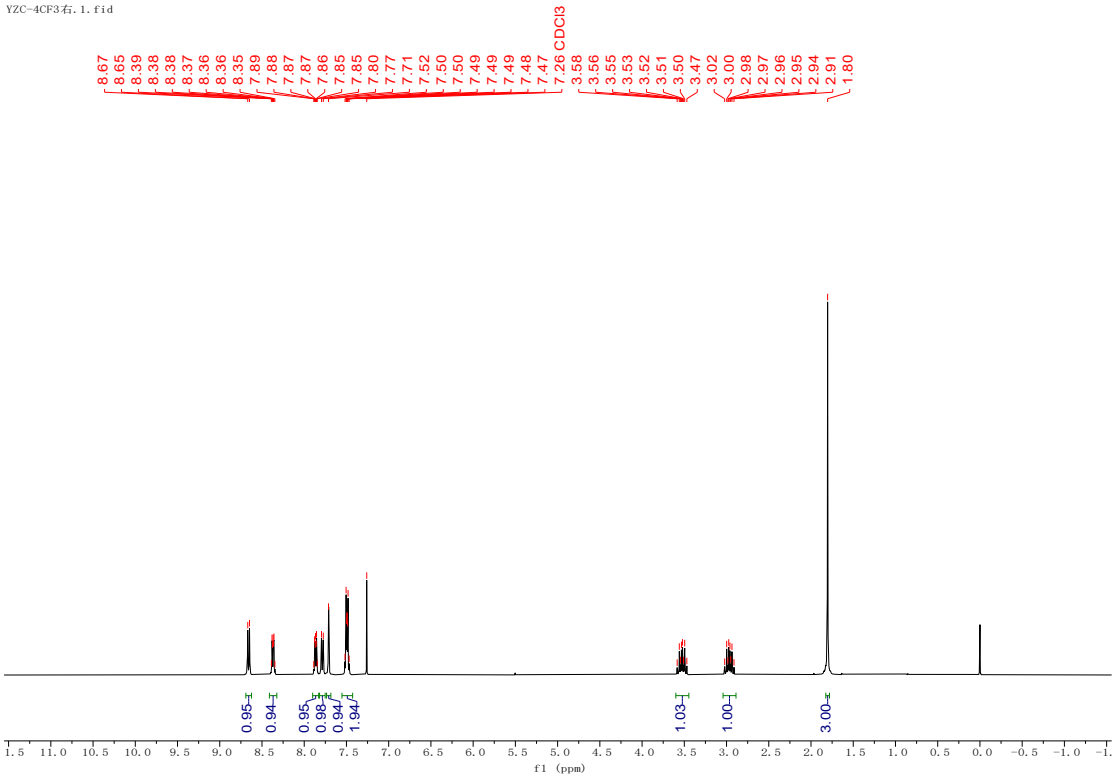
YZC-4CN石.3.fid



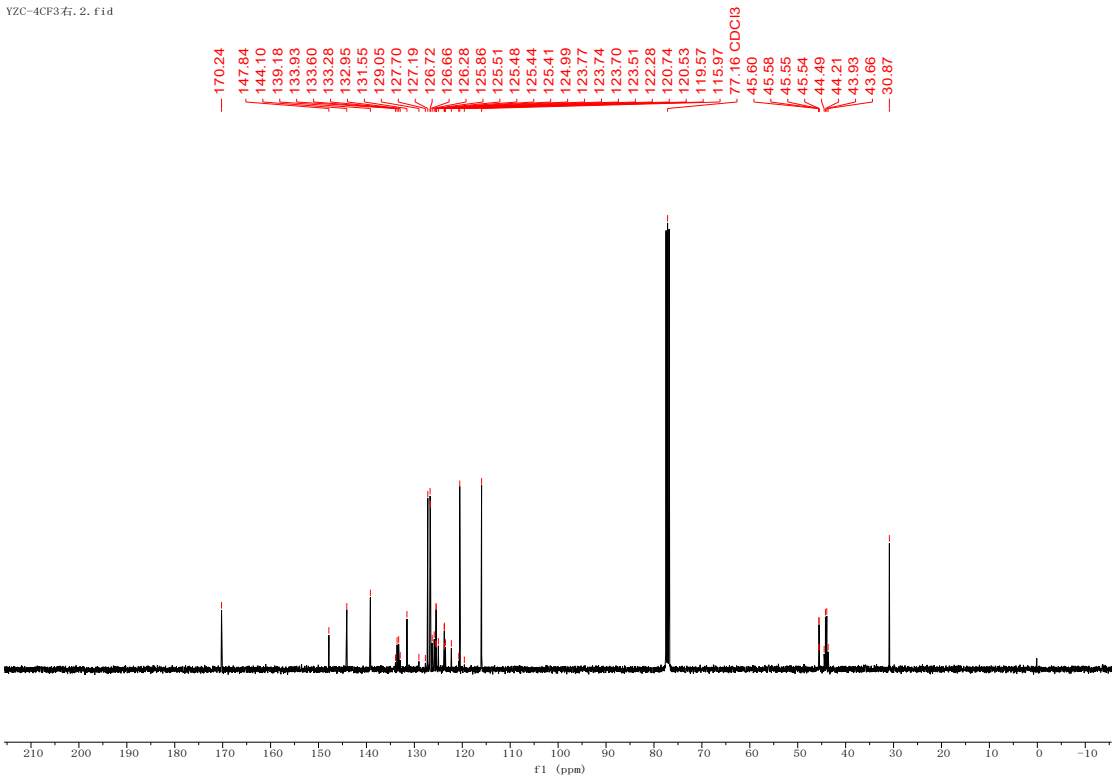


3g

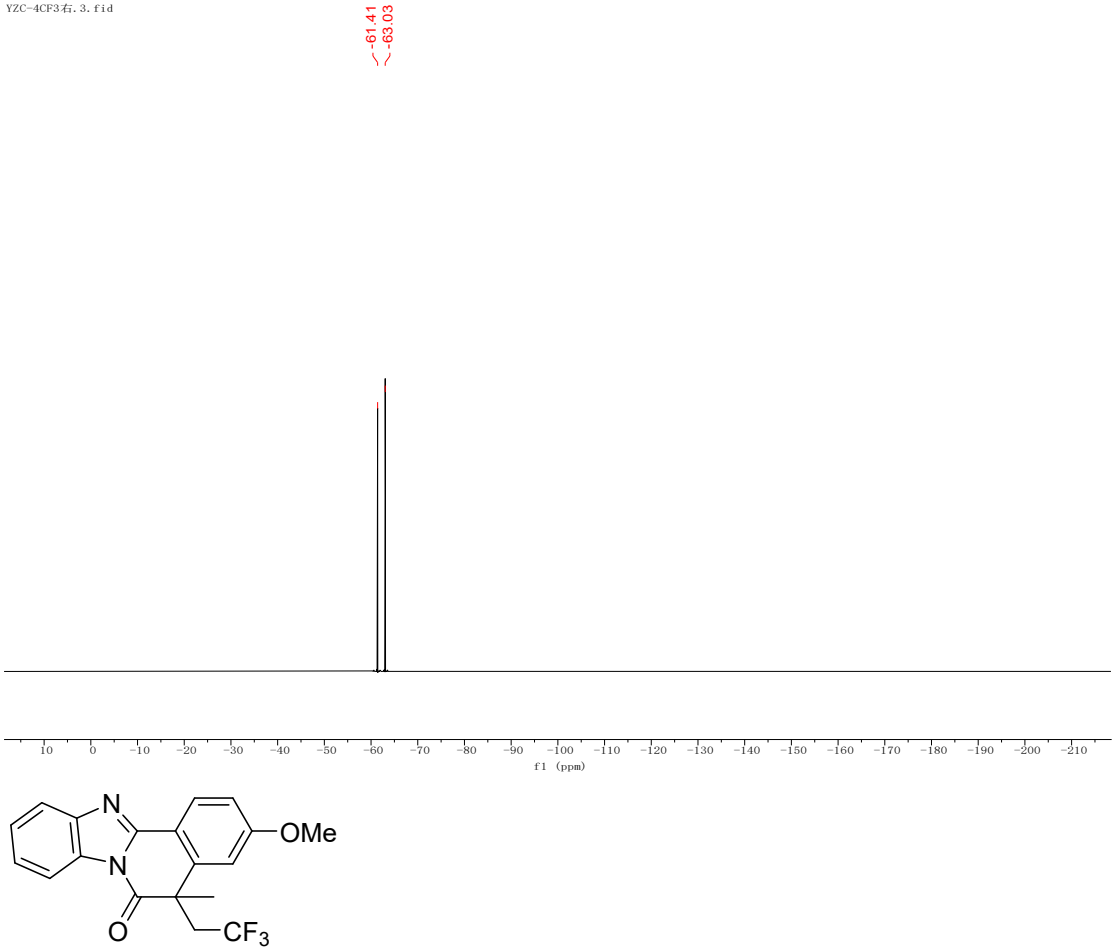
^{1}H NMR



^{13}C NMR


YZC-4CF3右.2.fid
170.24
147.84
144.10
139.18
133.93
133.60
133.28
132.95
131.55
129.05
127.70
127.19
126.72
126.66
126.28
125.86
125.51
125.48
125.44
125.41
124.99
123.77
123.74
123.70
123.51
122.28
120.74
120.53
119.57
115.97
77.16 CDCl3
45.60
45.58
45.55
45.54
44.49
44.21
43.93
43.66
30.87
f1 (ppm)

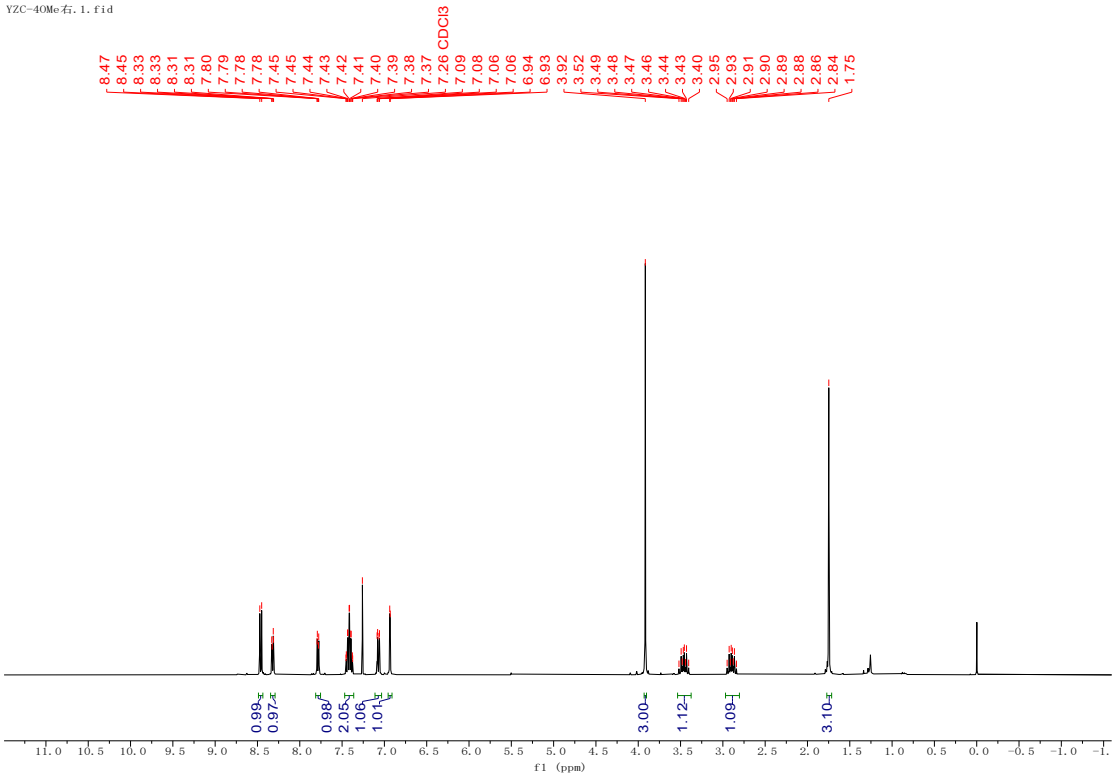
^{19}F NMR


YZC-4CF3右.3.fid
-61.41
-63.03
f1 (ppm)

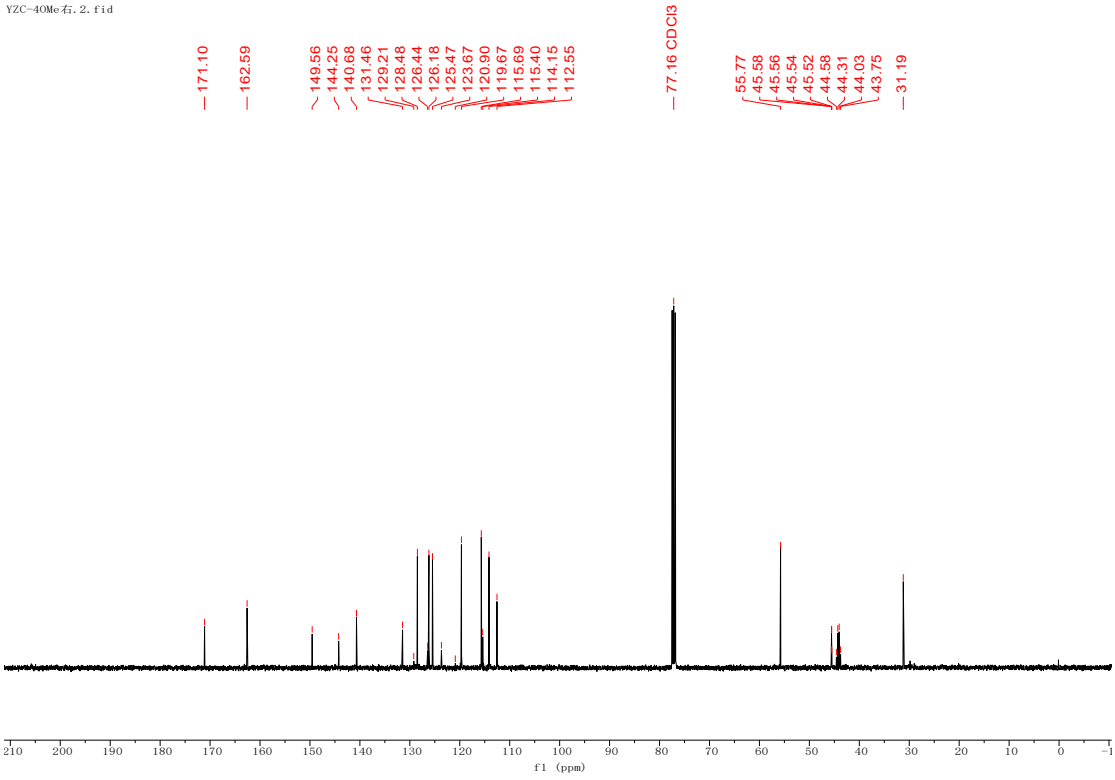
N
N
O
OMe
CF3

3h

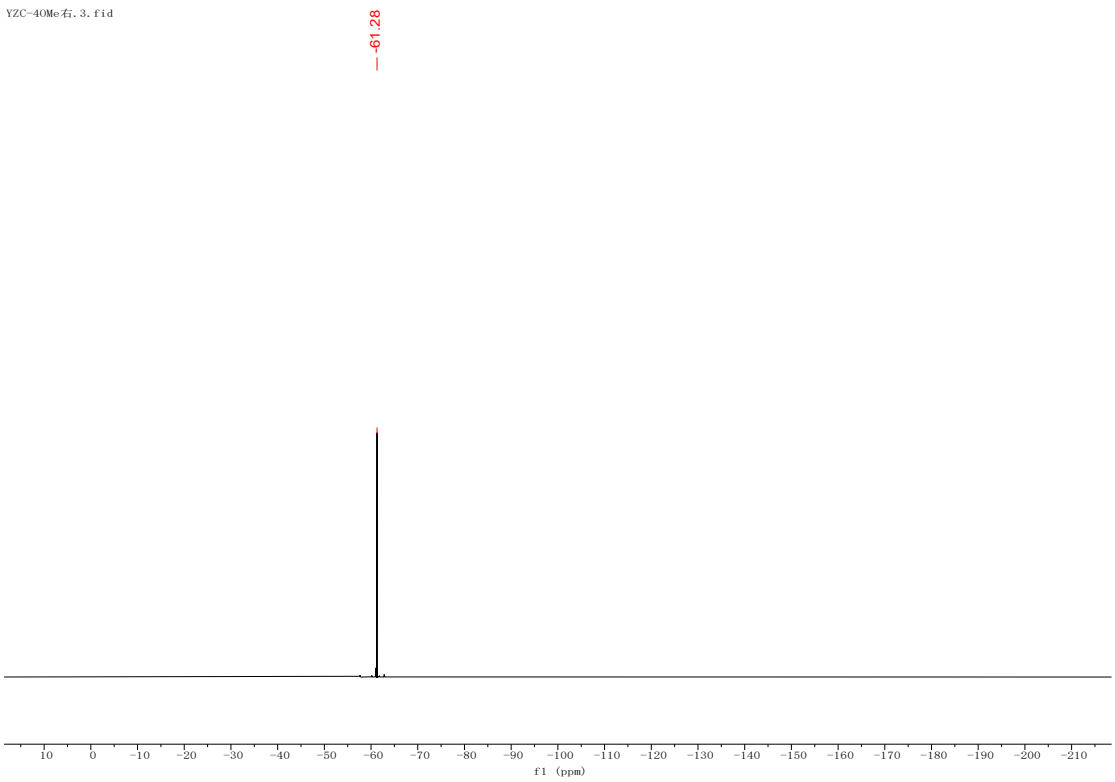
^{1}H NMR

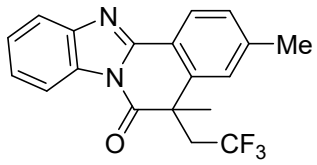


^{13}C NMR



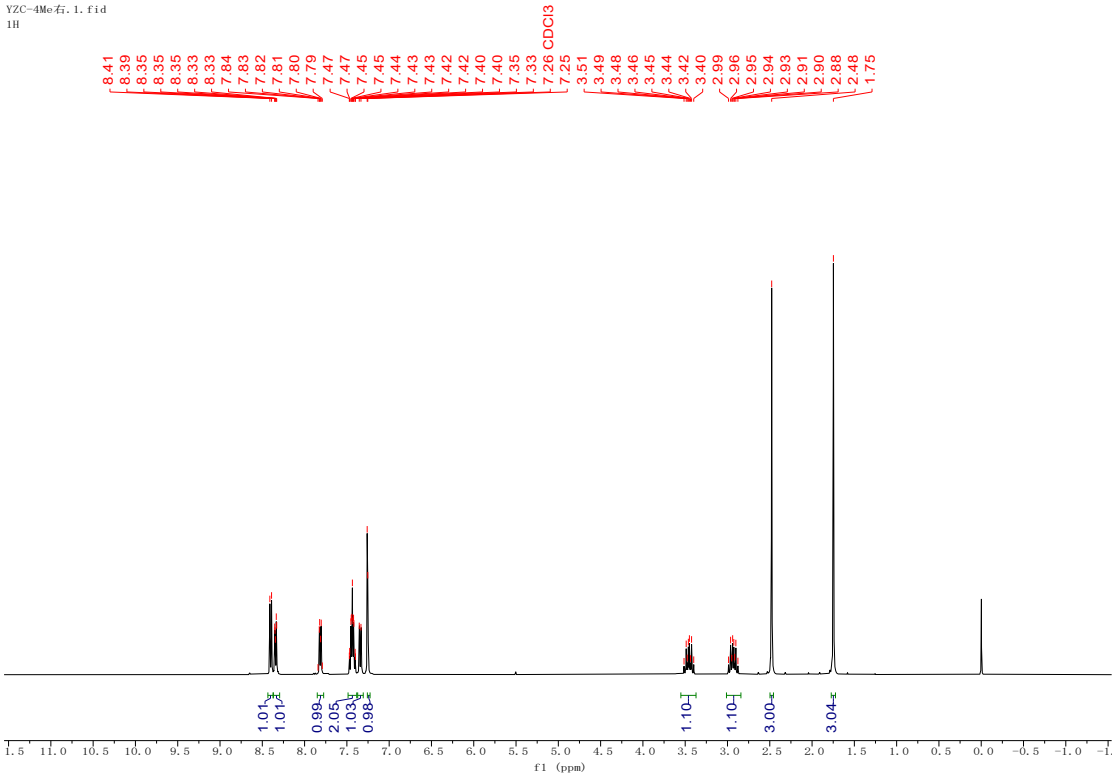
^{19}F NMR


YZC-4OMe右.3.fid
-61.28
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)

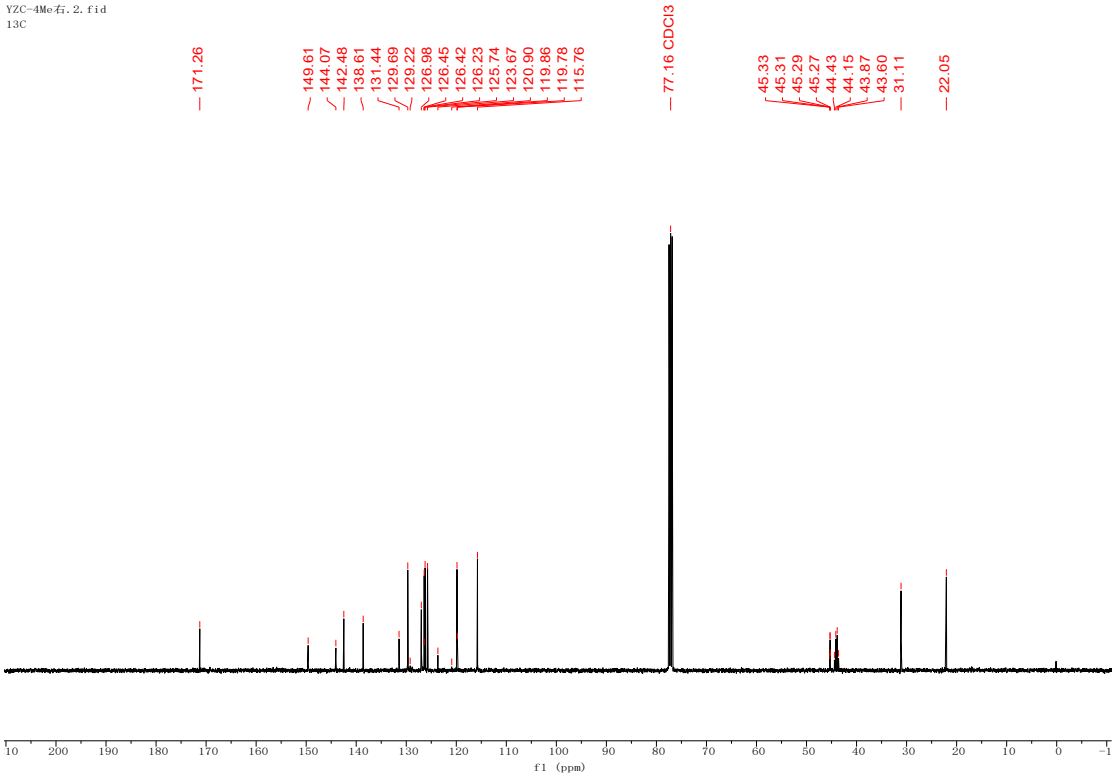

N
N
O
Me
CF3

3i

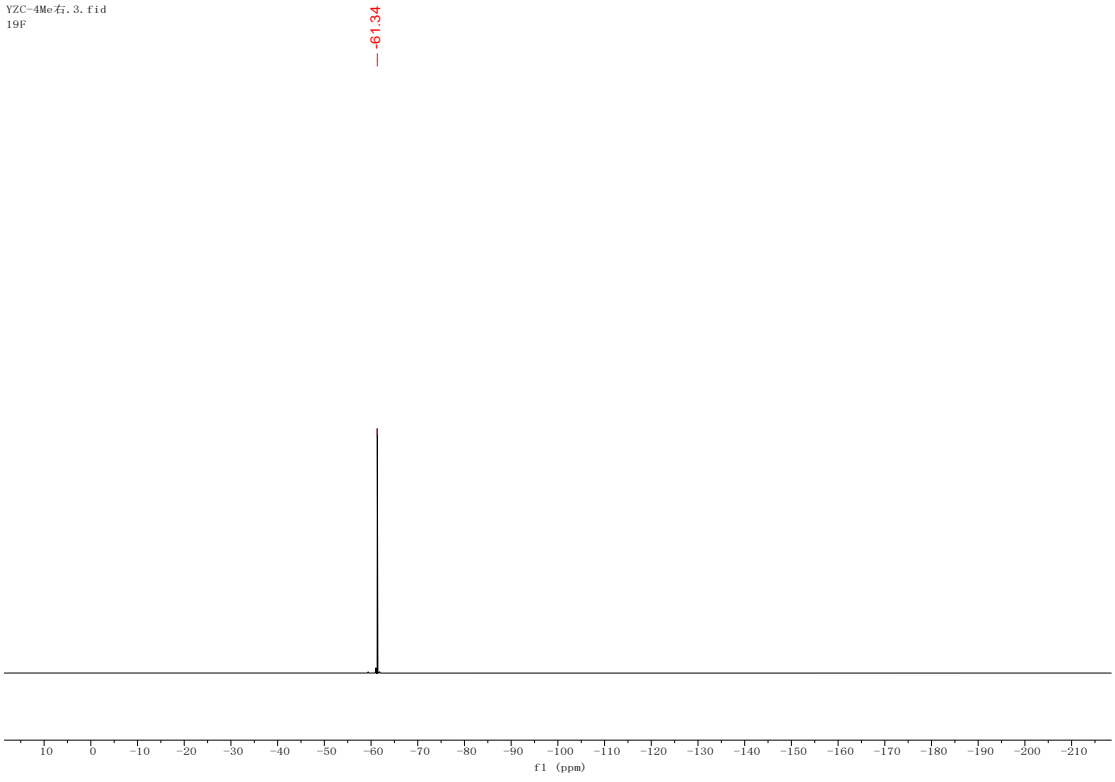
^{1}H NMR

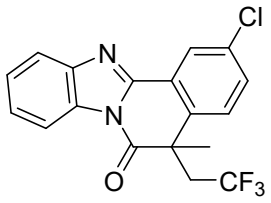

YZC-4Me右.1.fid
1H
8.41 8.39 8.35 8.35 8.35 8.33 8.33 7.84 7.83 7.82 7.81 7.80 7.79 7.47 7.47 7.45 7.45 7.44 7.43 7.43 7.42 7.42 7.40 7.40 7.35 7.33 7.26 CDCl3 7.25 3.51 3.49 3.48 3.46 3.45 3.44 3.42 3.40 2.99 2.96 2.95 2.94 2.93 2.91 2.90 2.88 2.48 1.75
1.01 1.01 0.99 2.05 1.03 0.98 1.10 1.10 3.00 3.04
f1 (ppm)

^{13}C NMR



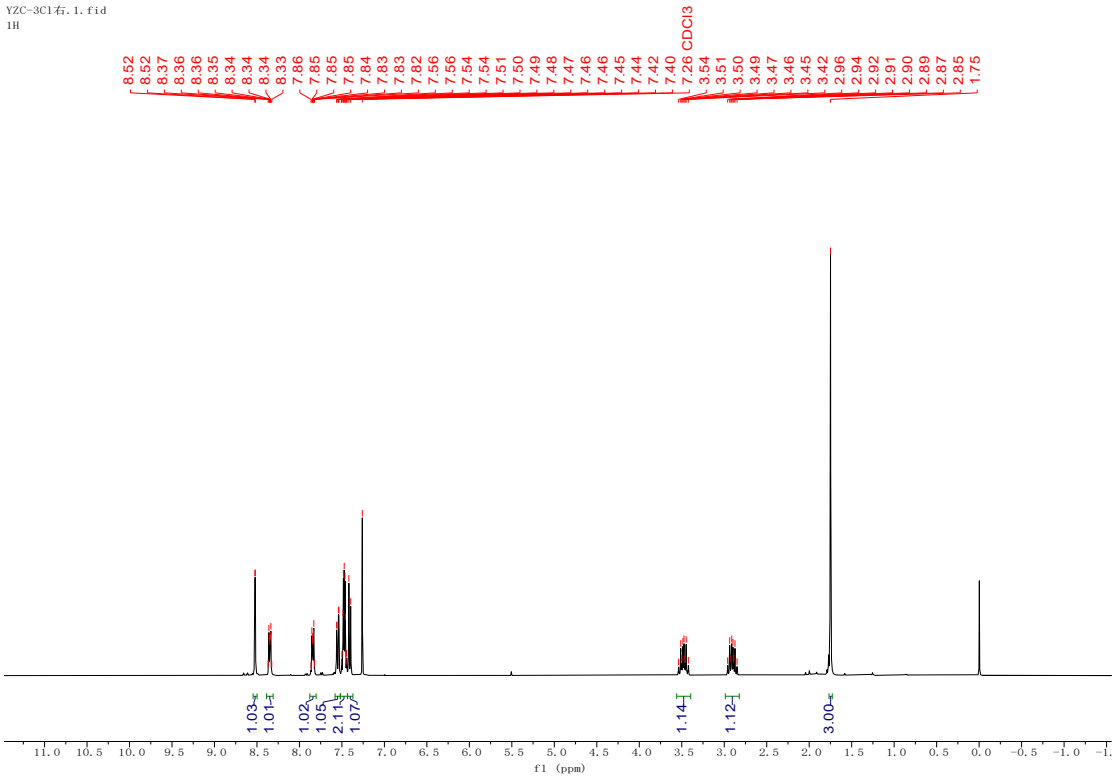
^{19}F NMR



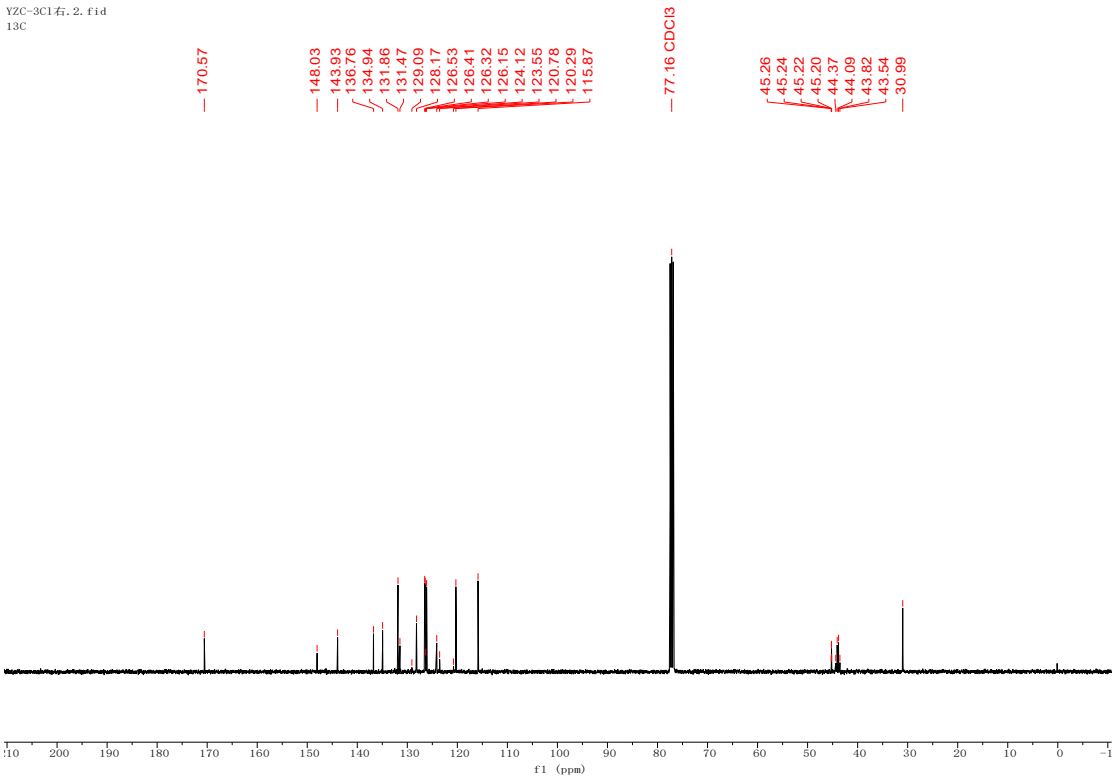


3j

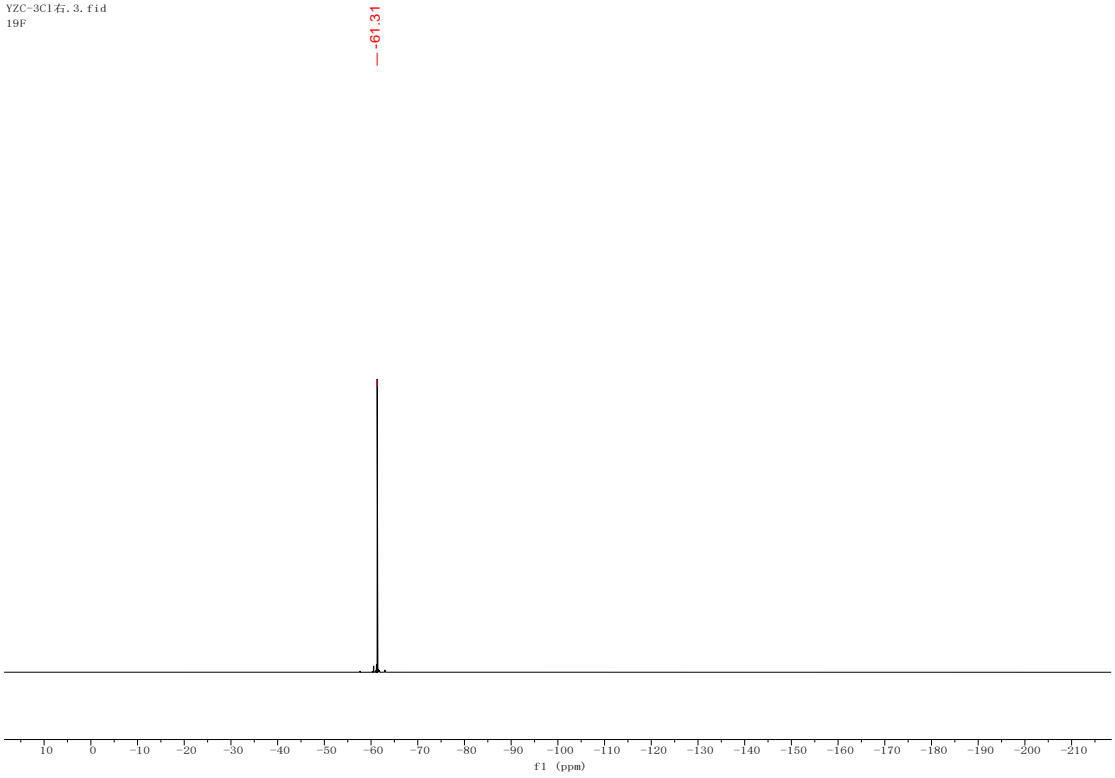
^{1}H NMR

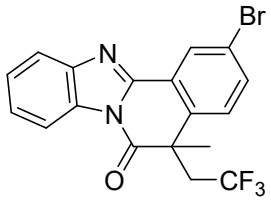


^{13}C NMR


YZC-3Cl右.2.fid
13C
170.57
148.03
143.93
136.76
134.94
131.86
131.47
129.09
128.17
126.53
126.41
126.32
126.15
124.12
123.55
120.78
120.29
115.87
77.16 CDCl3
45.26
45.24
45.22
45.20
44.37
44.09
43.82
43.54
30.99
f1 (ppm)

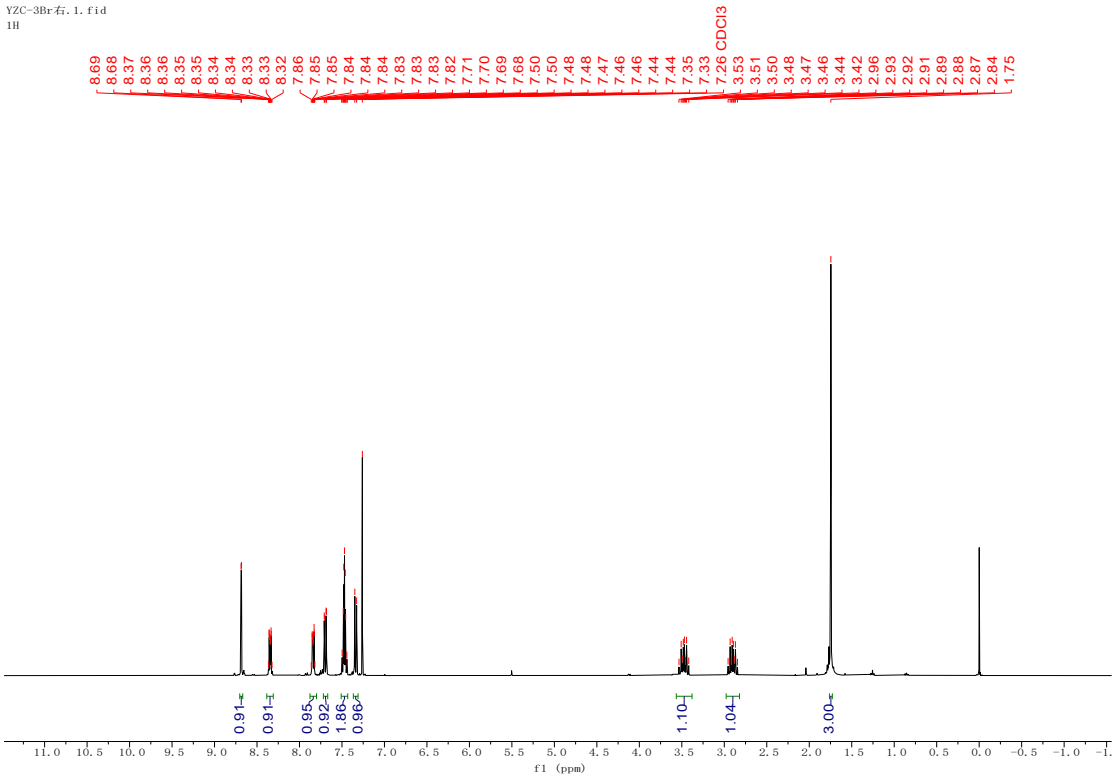
^{19}F NMR


YZC-3Cl右.3.fid
19F
-61.31
f1 (ppm)

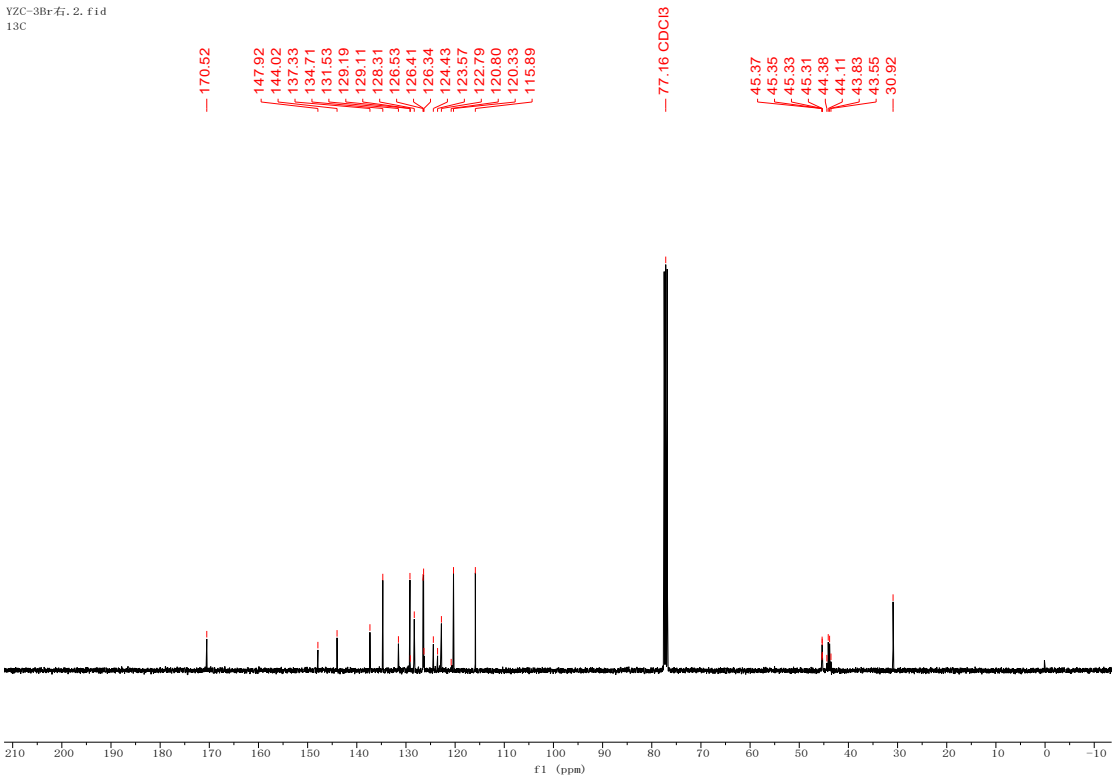


3k

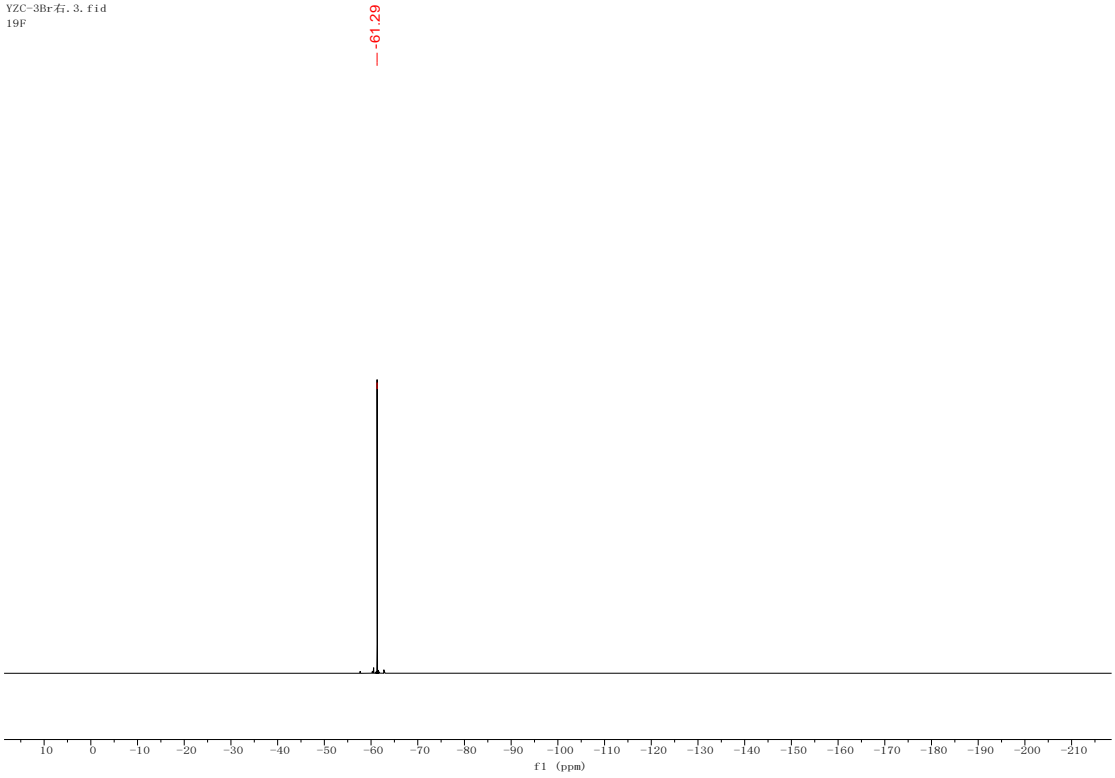
^{1}H NMR

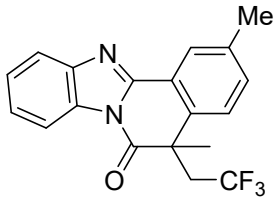


^{13}C NMR


YZC-3Br右.2.fid
13C
170.52
147.92
144.02
137.33
134.71
131.53
129.19
129.11
128.31
126.53
126.41
126.34
124.43
123.57
122.79
120.80
120.33
115.89
77.16 CDCl3
45.37
45.35
45.33
45.31
44.38
44.11
43.83
43.55
30.92
f1 (ppm)

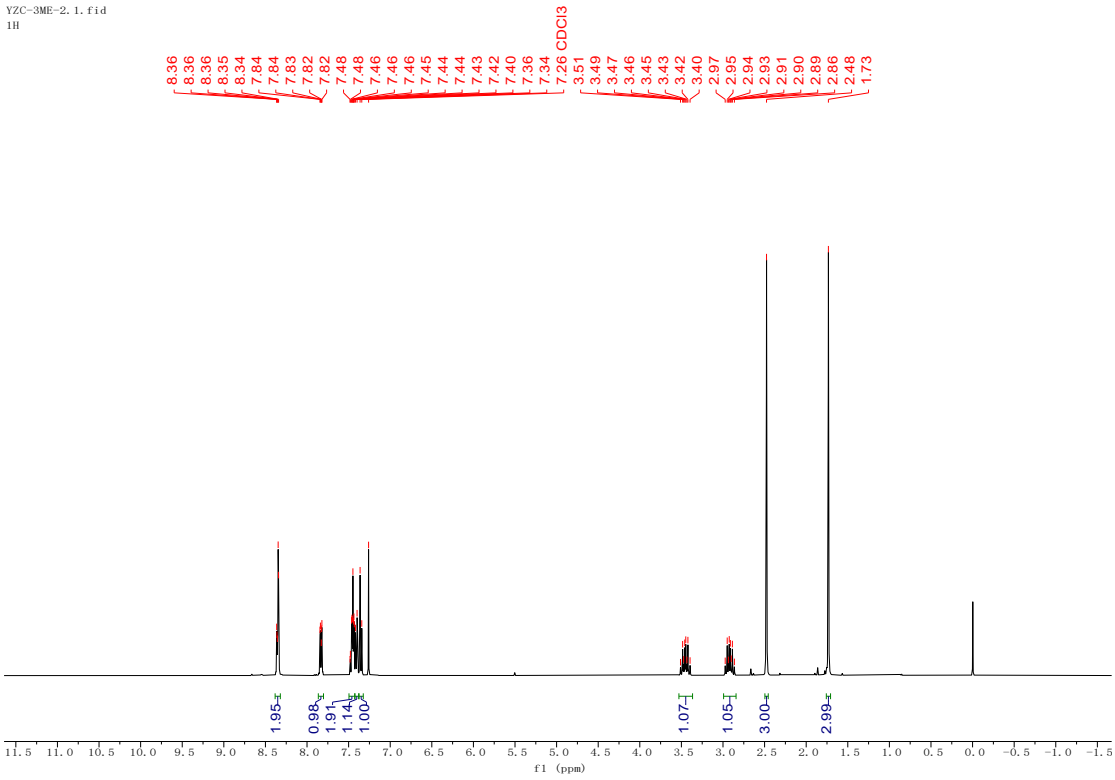
^{19}F NMR


YZC-3Br右.3.fid
19F
-61.29
f1 (ppm)

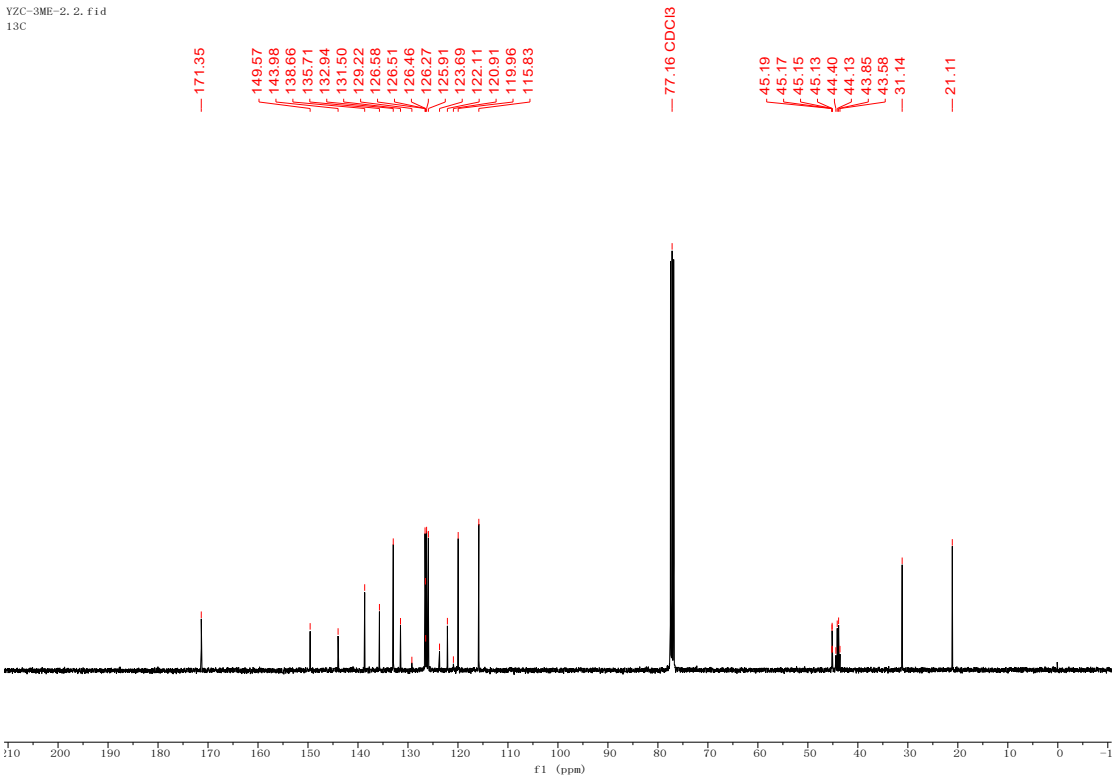


3l

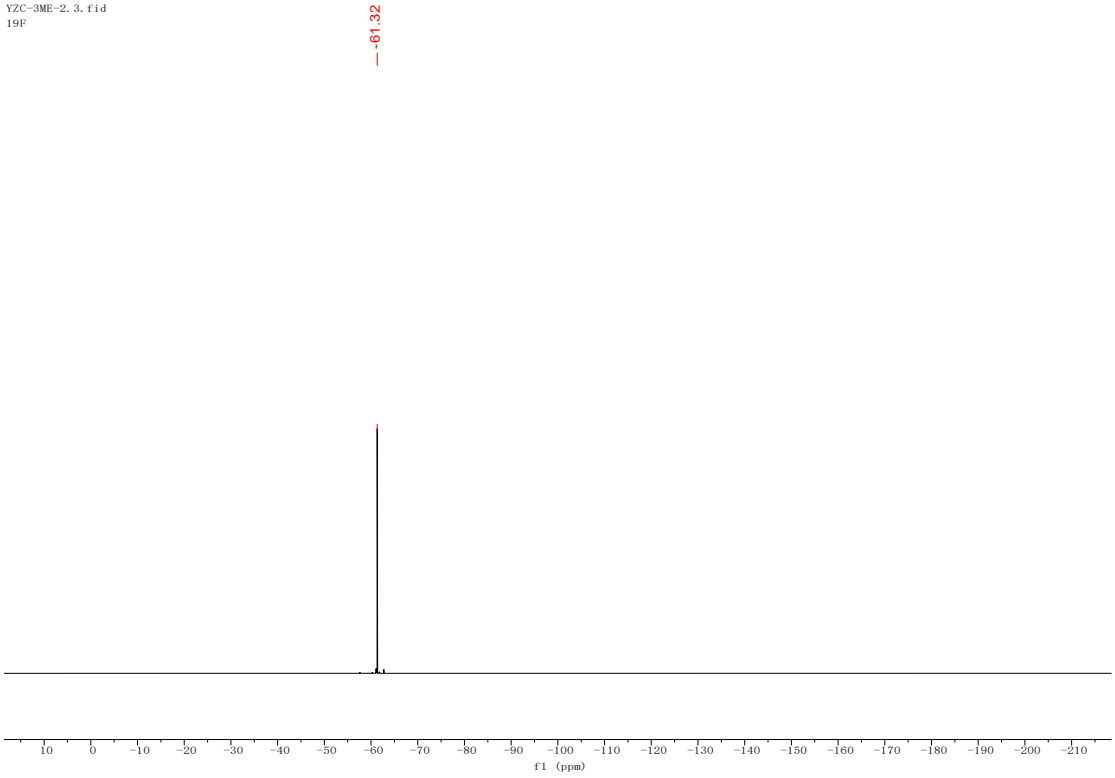
^{1}H NMR

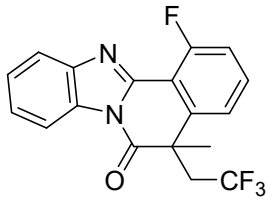


^{13}C NMR


YZC-3ME-2.2.fid
13C
171.35
149.57
143.98
138.66
135.71
132.94
131.50
129.22
126.58
126.51
126.46
126.27
125.91
123.69
122.11
120.91
119.96
115.83
77.16 CDCl3
45.19
45.17
45.15
45.13
44.40
44.13
43.85
43.58
31.14
21.11
f1 (ppm)

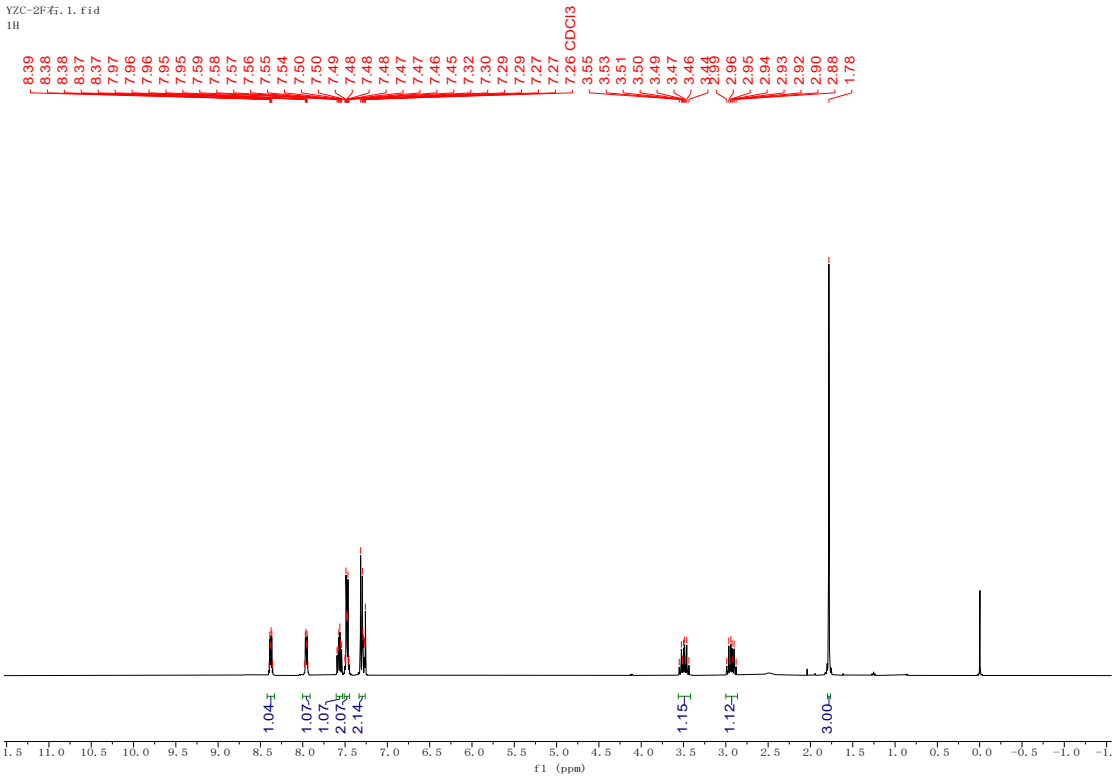
^{19}F NMR


YZC-3ME-2.3.fid
19F
-61.32
f1 (ppm)

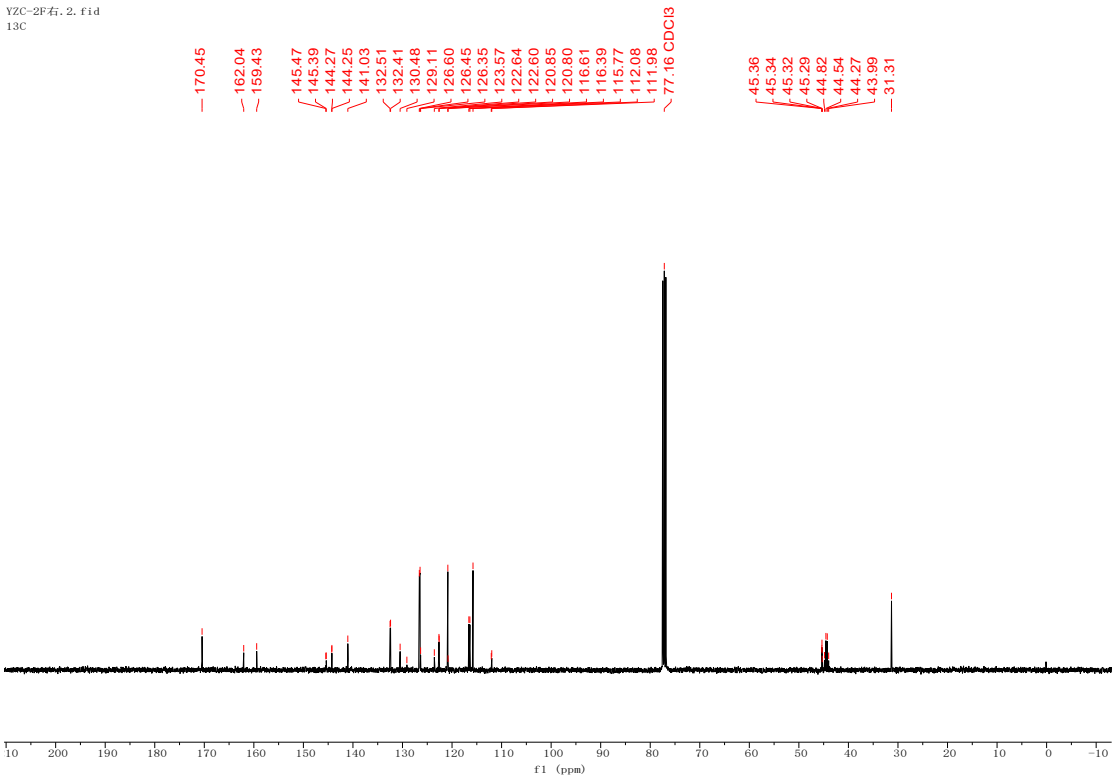


3m

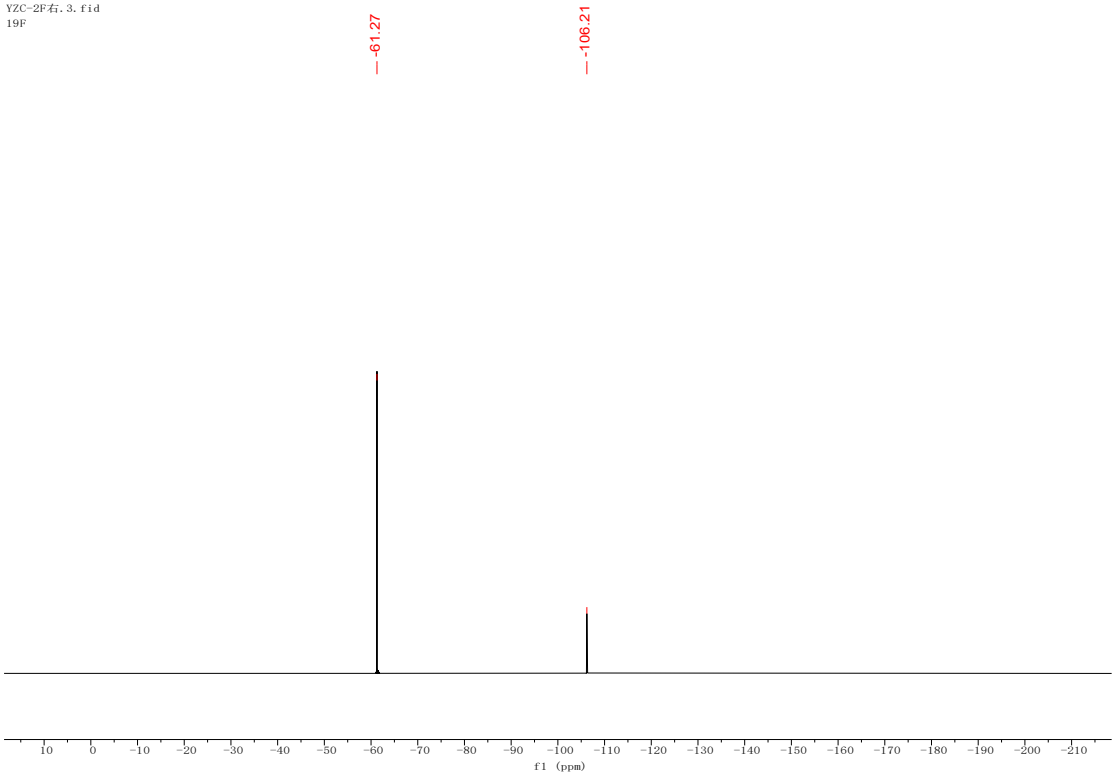
^{1}H NMR

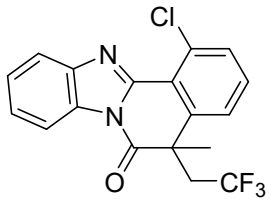


^{13}C NMR


YZC-2F右.2.fid
13C
170.45
162.04
159.43
145.47
145.39
144.27
144.25
141.03
132.51
132.41
130.48
129.11
126.60
126.45
126.35
123.57
122.64
122.60
120.85
120.80
116.61
116.39
115.77
112.08
111.98
77.16 CDCl3
45.36
45.34
45.32
45.29
44.82
44.54
44.27
43.99
31.31
f1 (ppm)

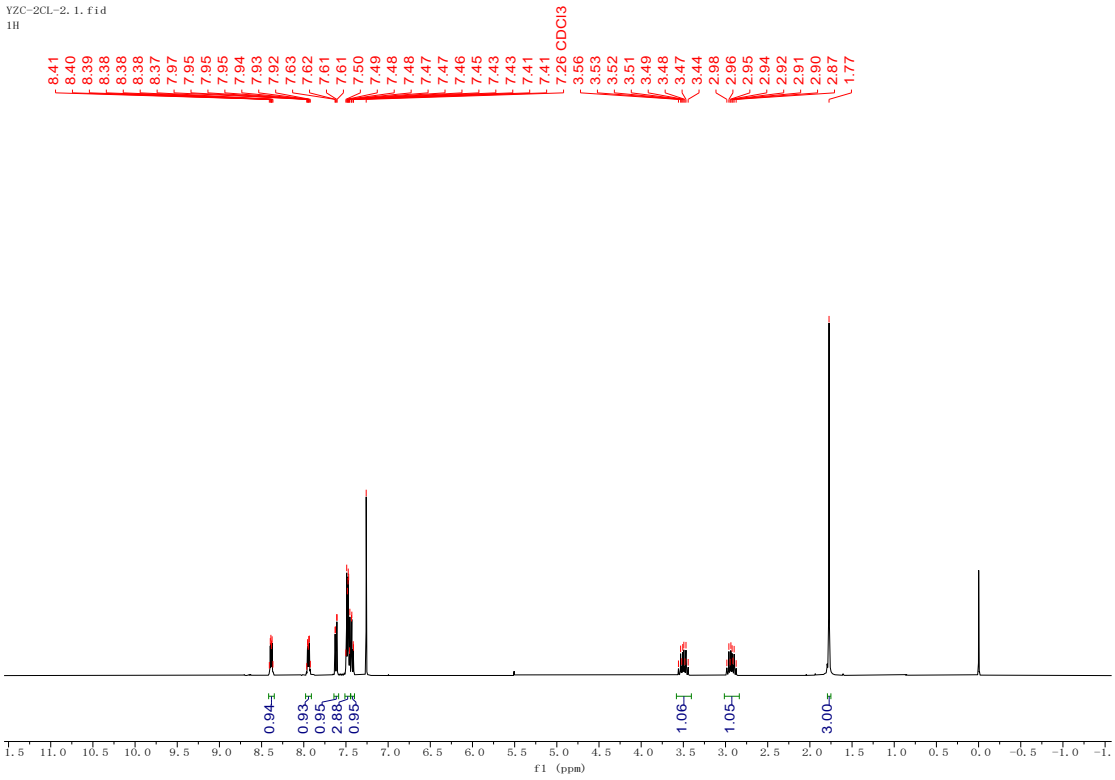
^{19}F NMR


YZC-2F右.3.fid
19F
-61.27
-106.21
f1 (ppm)

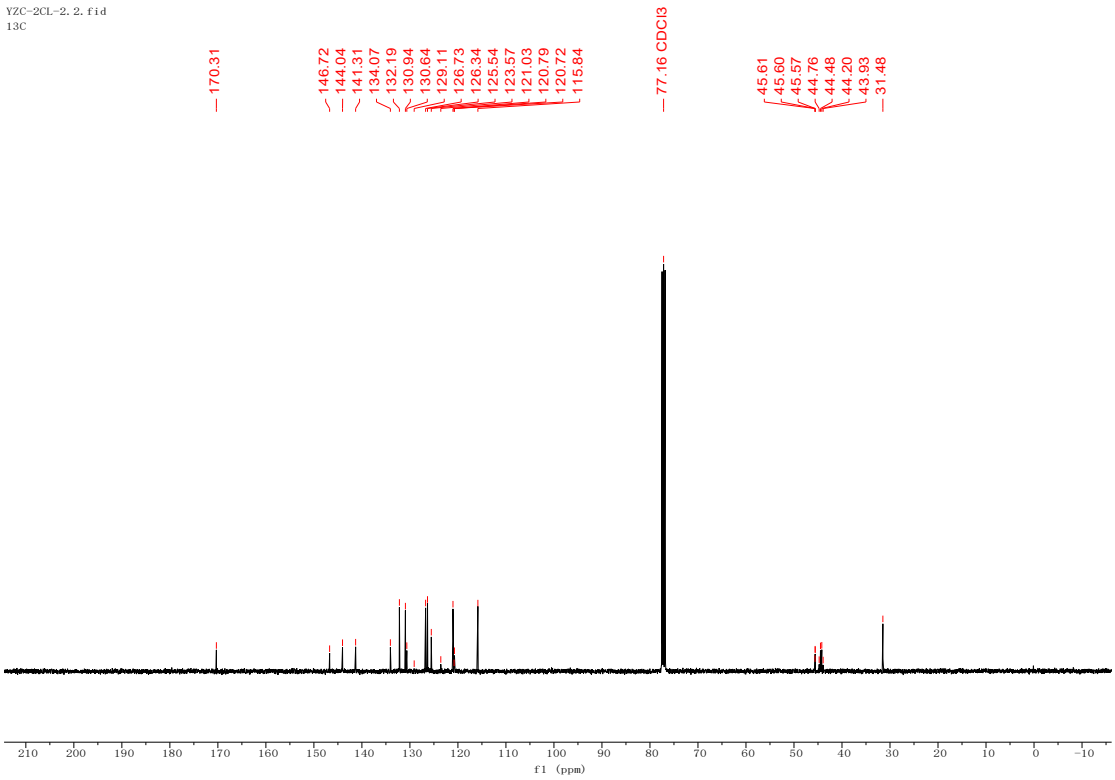


3n

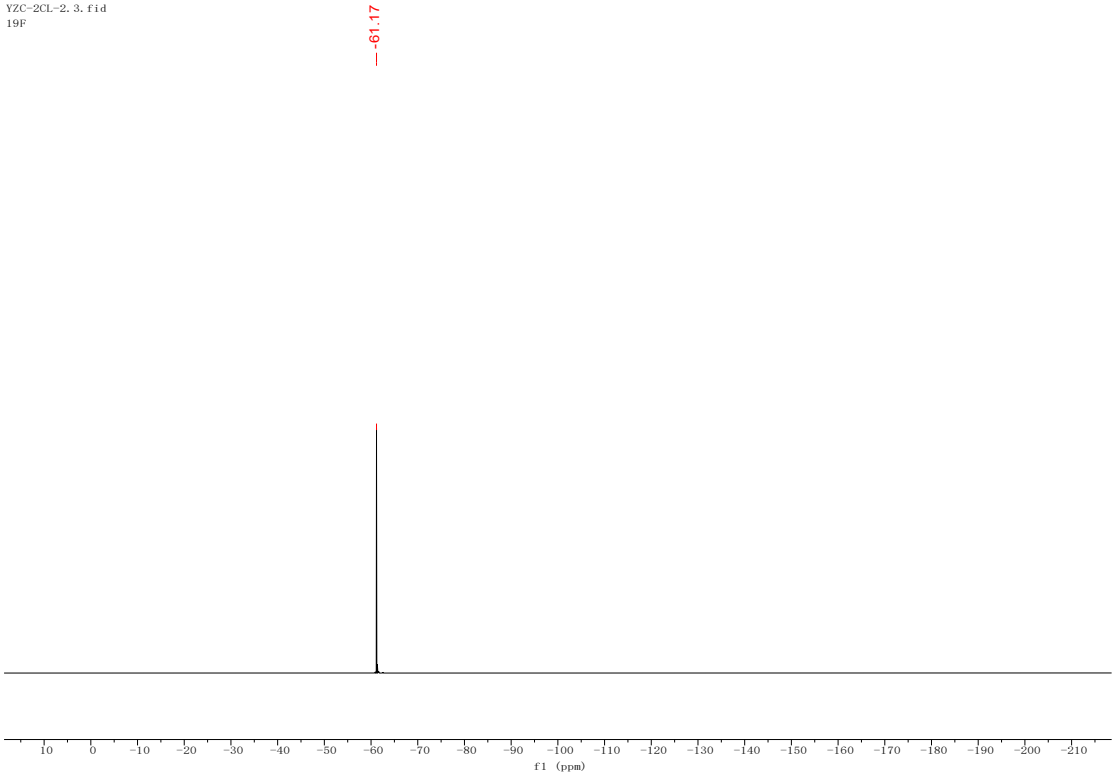
^{1}H NMR

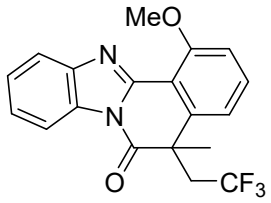


^{13}C NMR


YZC-2CL-2.2.fid
13C
170.31
146.72
144.04
141.31
134.07
132.19
130.94
130.64
129.11
126.73
126.34
125.54
123.57
121.03
120.79
120.72
115.84
77.16 CDCl3
45.61
45.60
45.57
44.76
44.48
44.20
43.93
31.48
f1 (ppm)

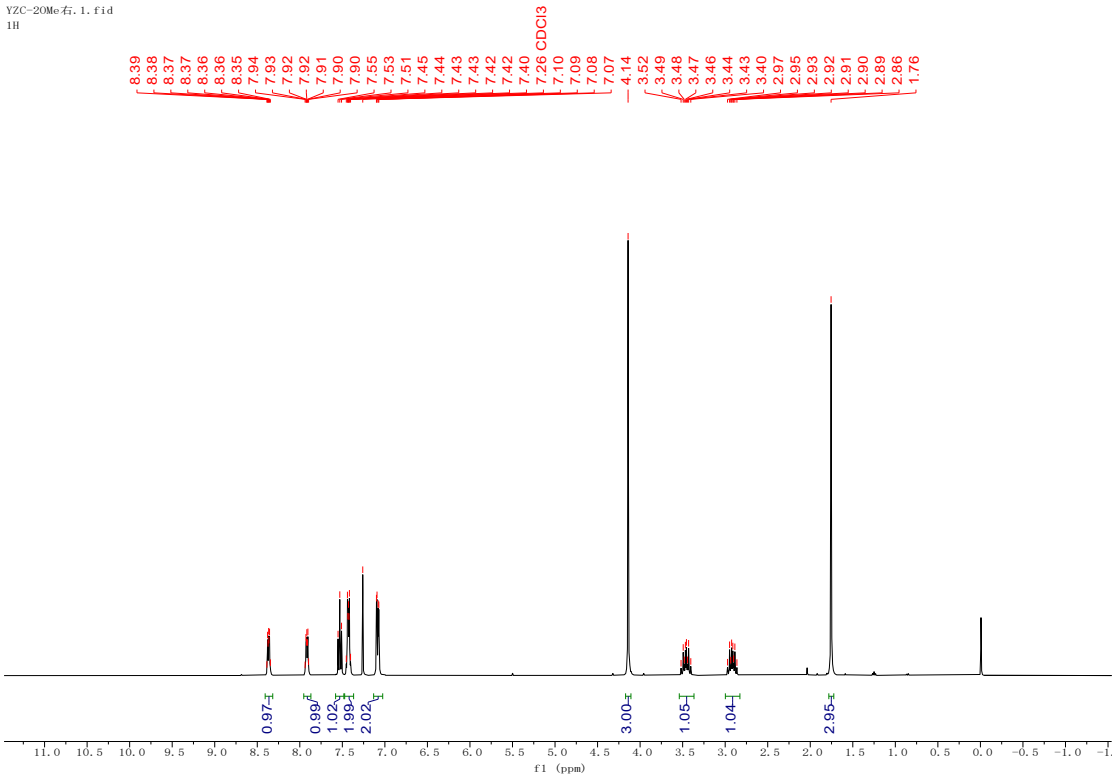
^{19}F NMR


YZC-2CL-2.3.fid
19F
-61.17
f1 (ppm)

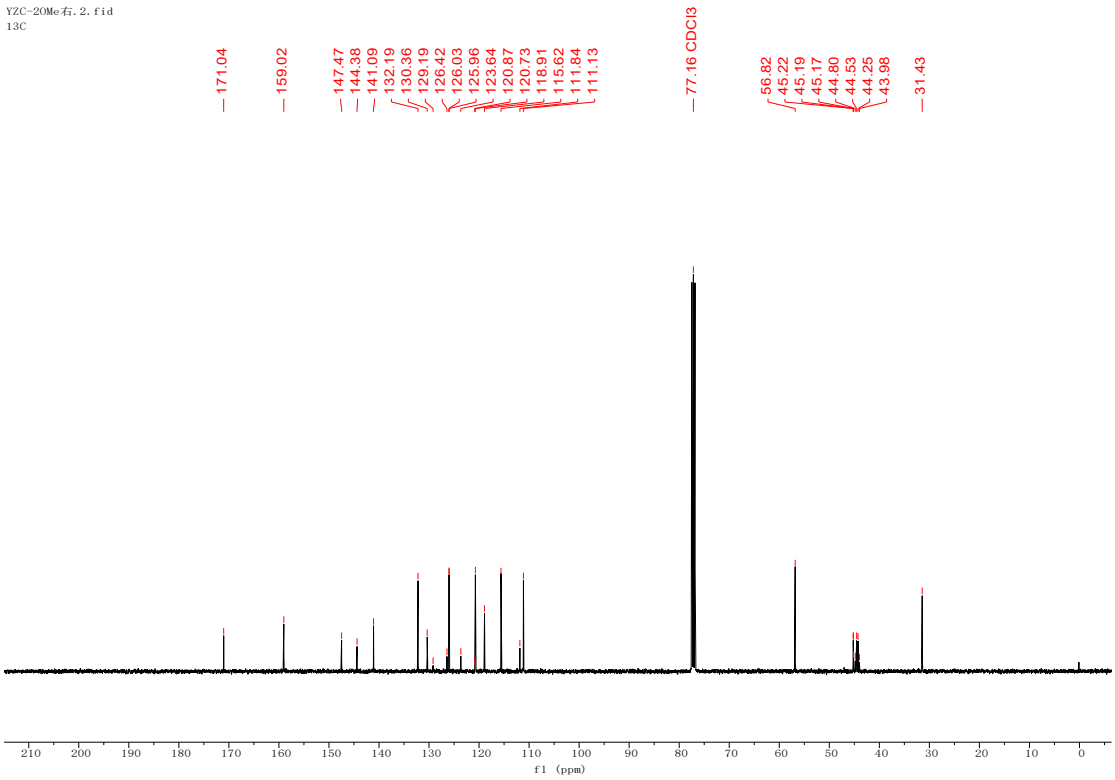


3o

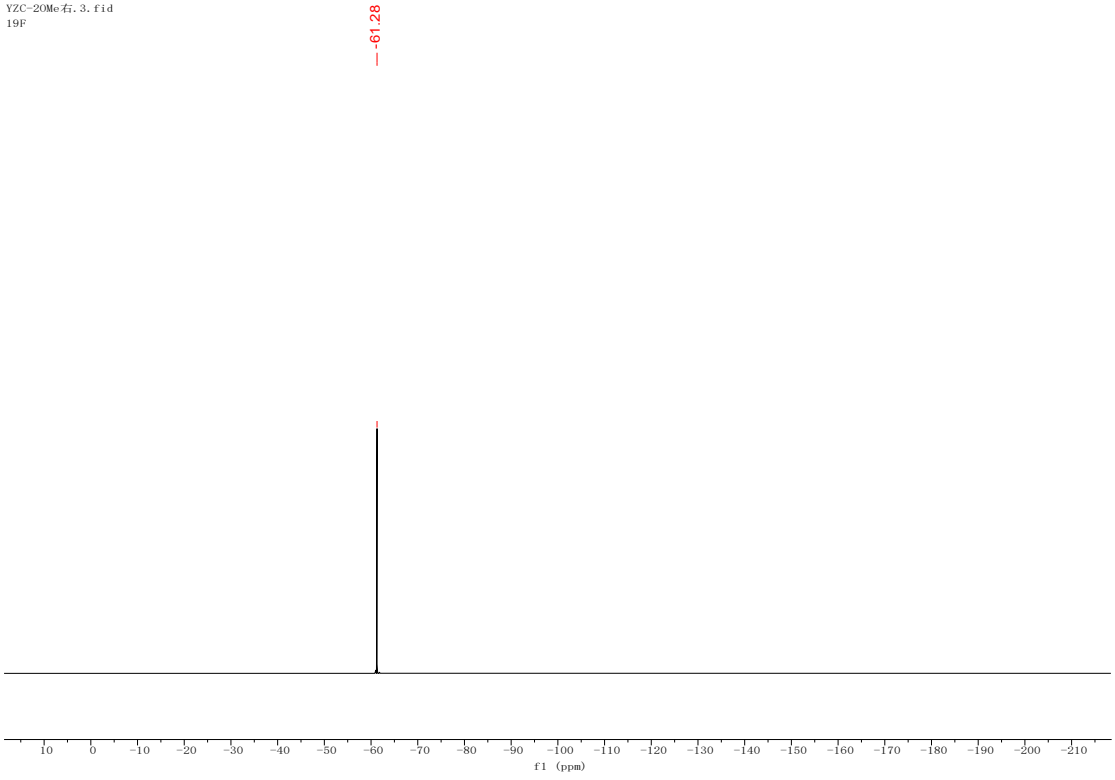
^{1}H NMR

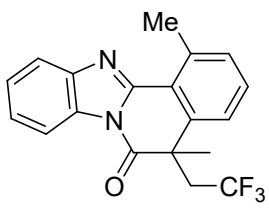


^{13}C NMR


YZC-20Me右.2.fid
13C
171.04
159.02
147.47
144.38
141.09
132.19
130.36
129.19
126.42
126.03
125.96
123.64
120.87
120.73
118.91
115.62
111.84
111.13
77.16 CDCl3
56.82
45.22
45.19
45.17
44.80
44.53
44.25
43.98
31.43
f1 (ppm)

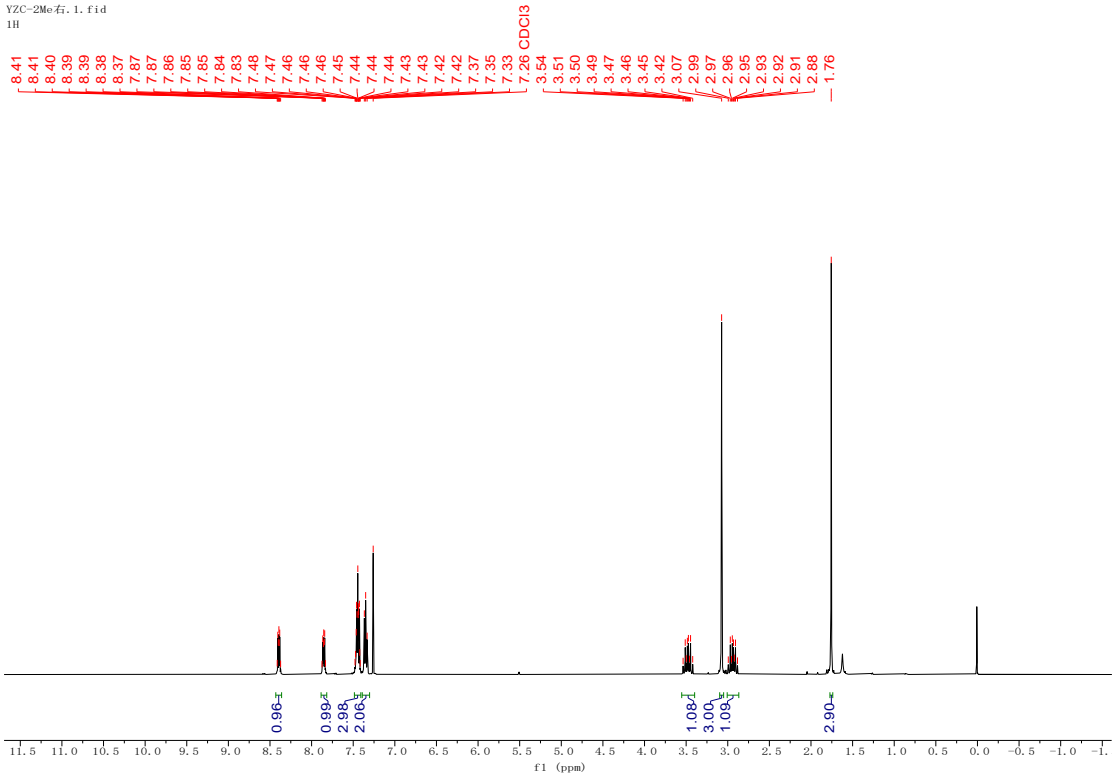
^{19}F NMR


YZC-20Me右.3.fid
19F
-61.28
f1 (ppm)

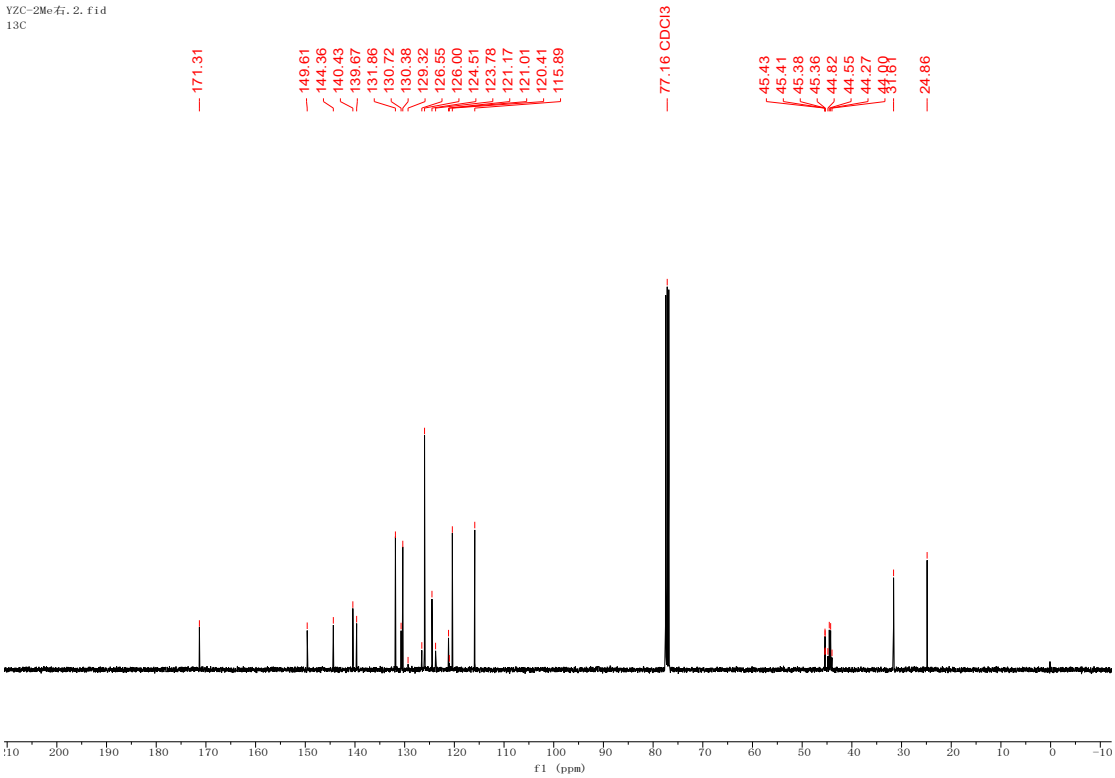

Me
N
N
O
CF3

3p

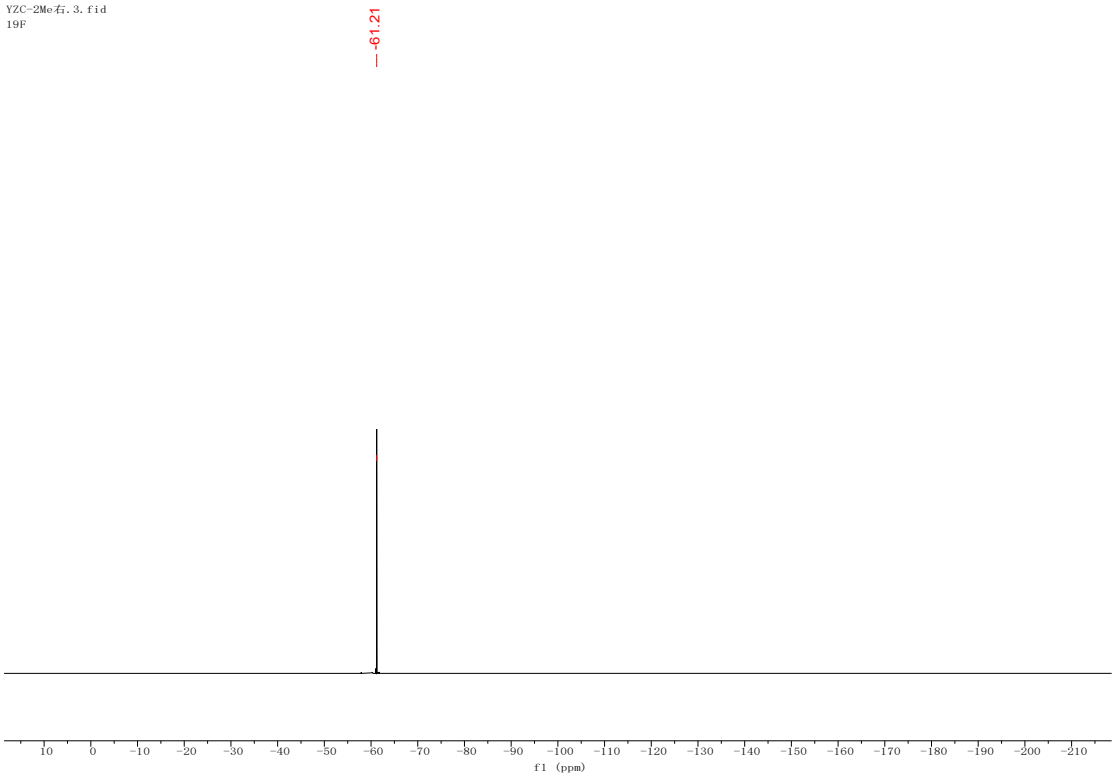
^{1}H NMR

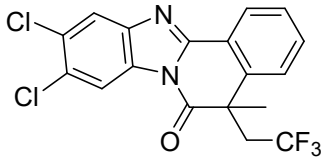


^{13}C NMR



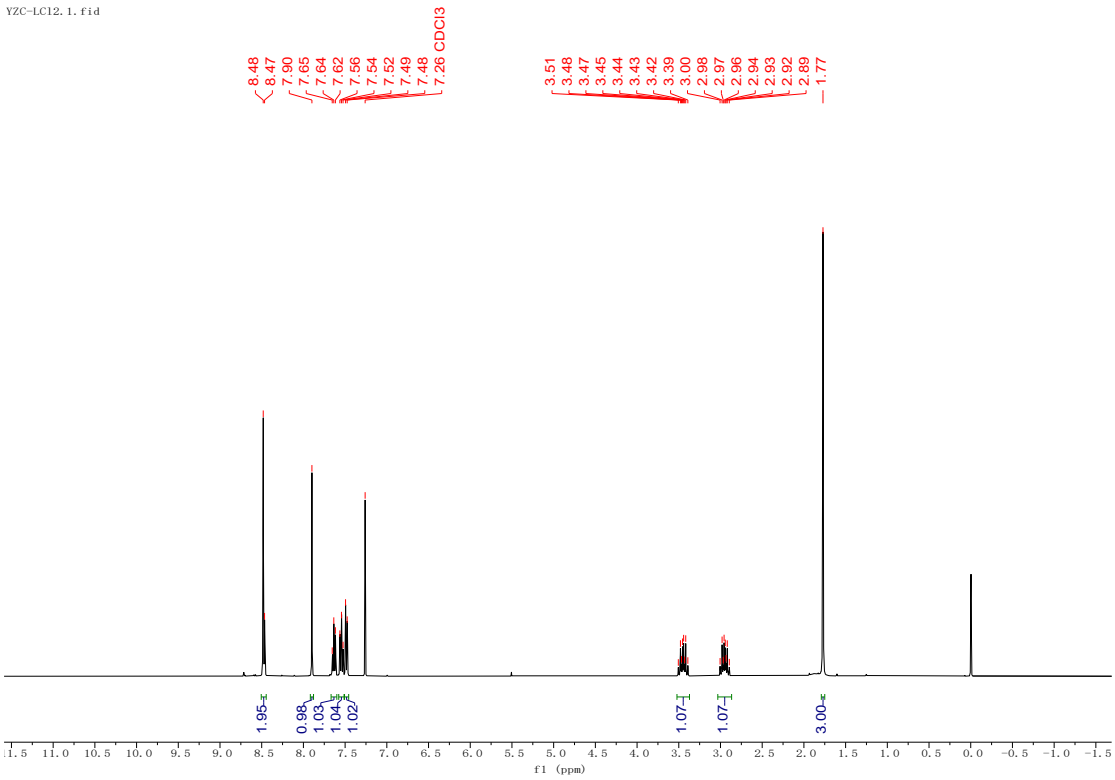
^{19}F NMR



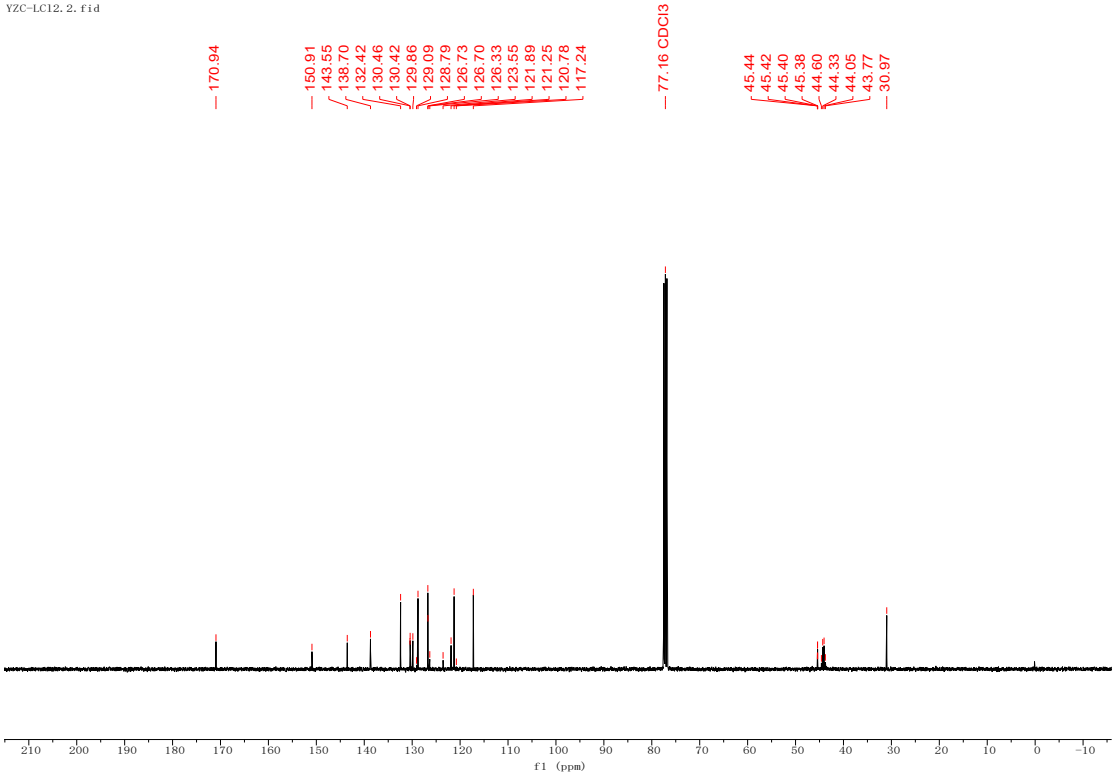


3q

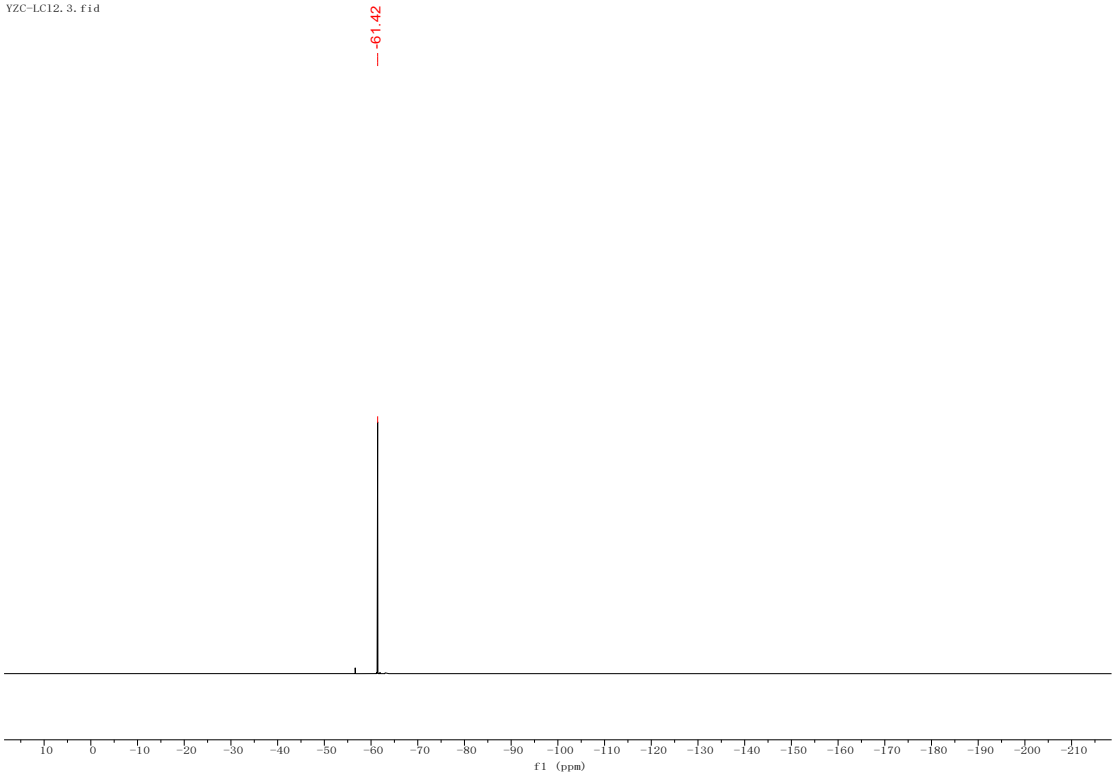
^{1}H NMR

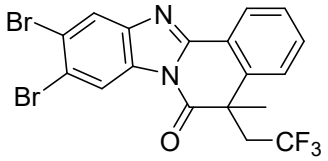

YZC-LC12.1.fid
8.48
8.47
7.90
7.65
7.64
7.62
7.56
7.54
7.52
7.49
7.48
7.26 CDCl3
3.51
3.48
3.47
3.45
3.44
3.43
3.42
3.39
3.00
2.98
2.97
2.96
2.94
2.93
2.92
2.89
1.77
1.95
0.98
1.03
1.04
1.02
1.07
1.07
3.00
f1 (ppm)

^{13}C NMR


YZC-LC12.2.fid
170.94
150.91
143.55
138.70
132.42
130.46
130.42
129.86
129.09
128.79
126.73
126.70
126.33
123.55
121.89
121.25
120.78
117.24
77.16 CDCl3
45.44
45.42
45.40
45.38
44.60
44.33
44.05
43.77
30.97
f1 (ppm)

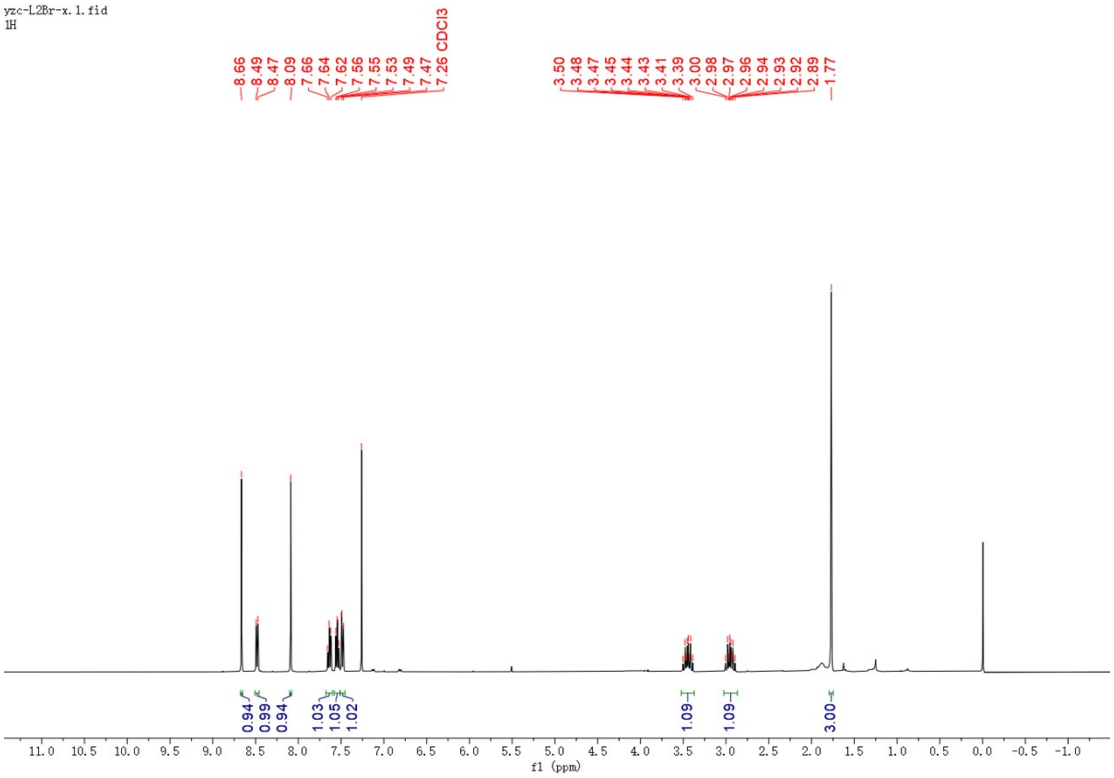
^{19}F NMR



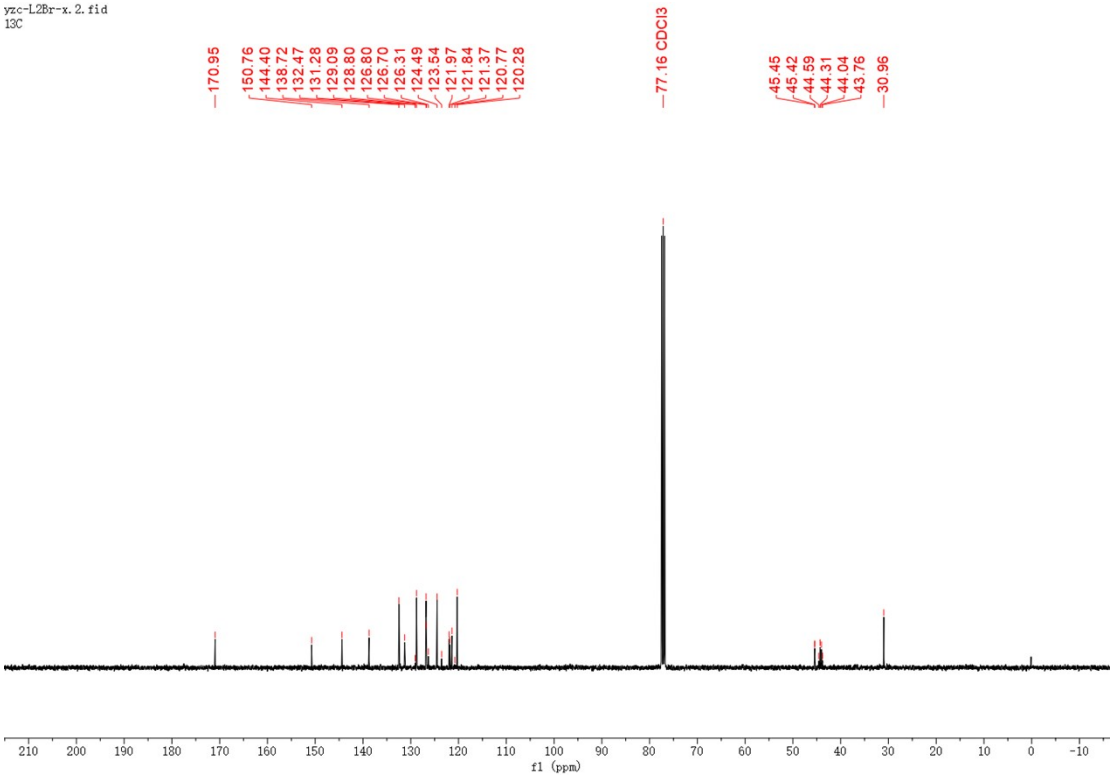


3r

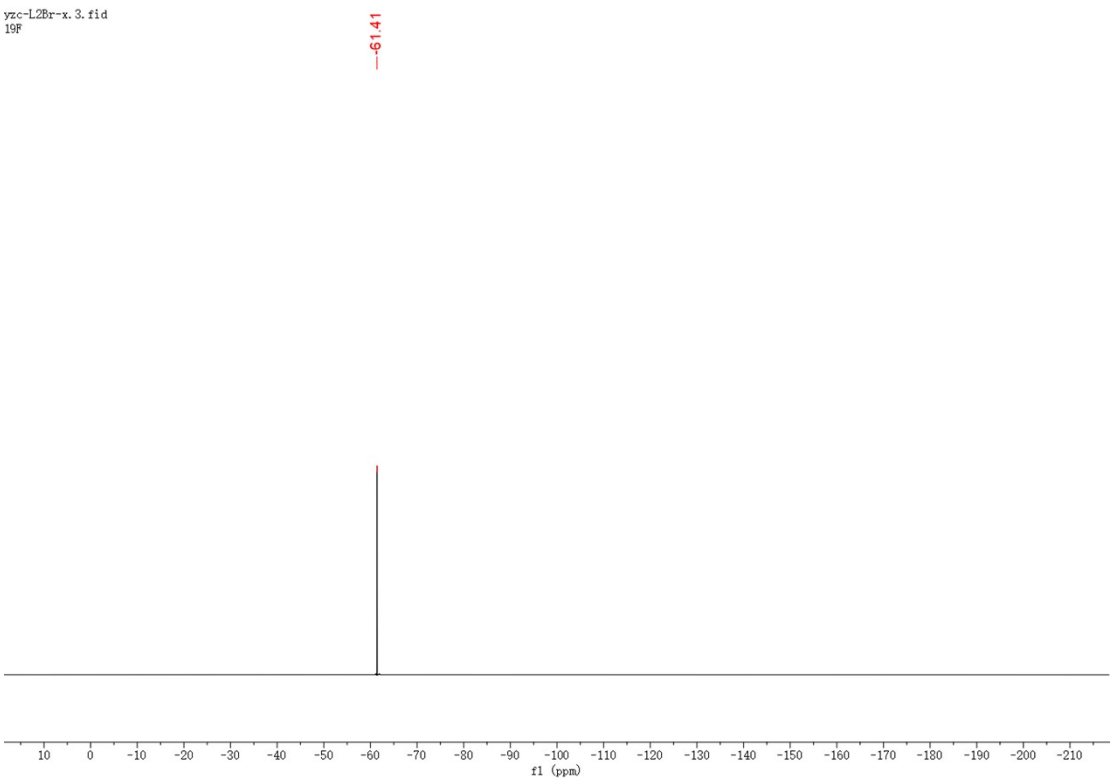
^{1}H NMR

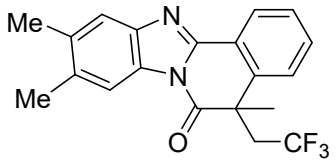


^{13}C NMR



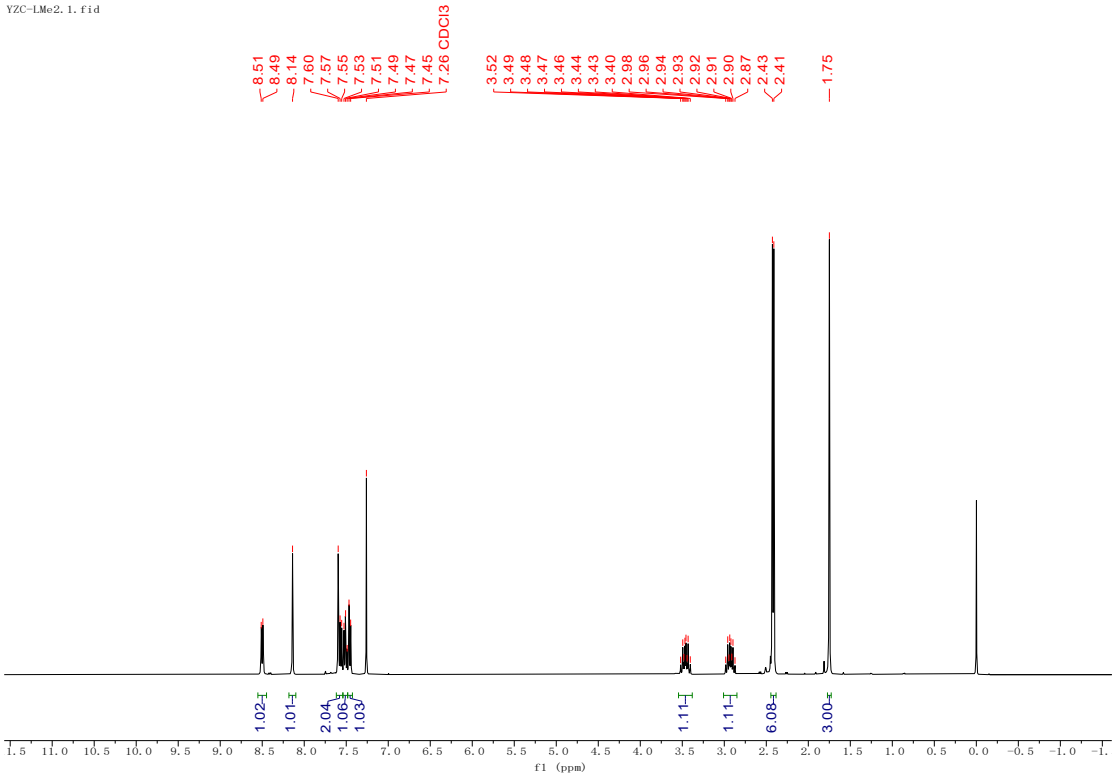
^{19}F NMR


yzc-L2Br-x.3.fid
19F
-61.41
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)

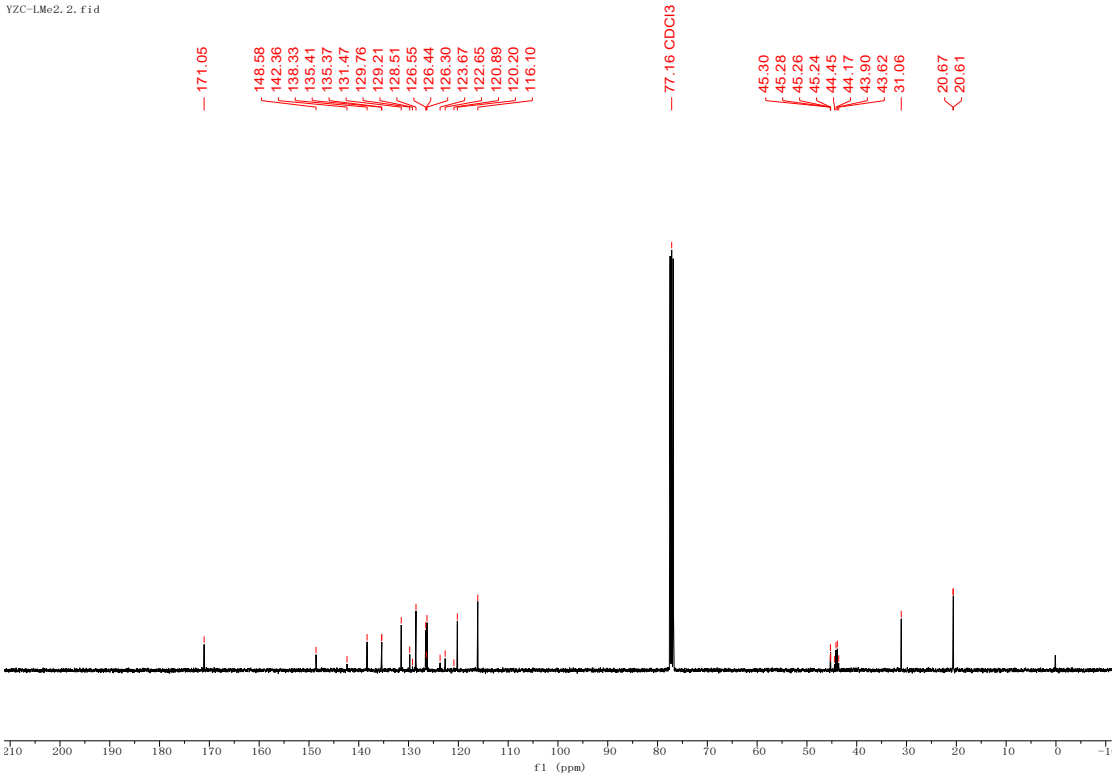

Me
Me
N
N
O
CF3

3s

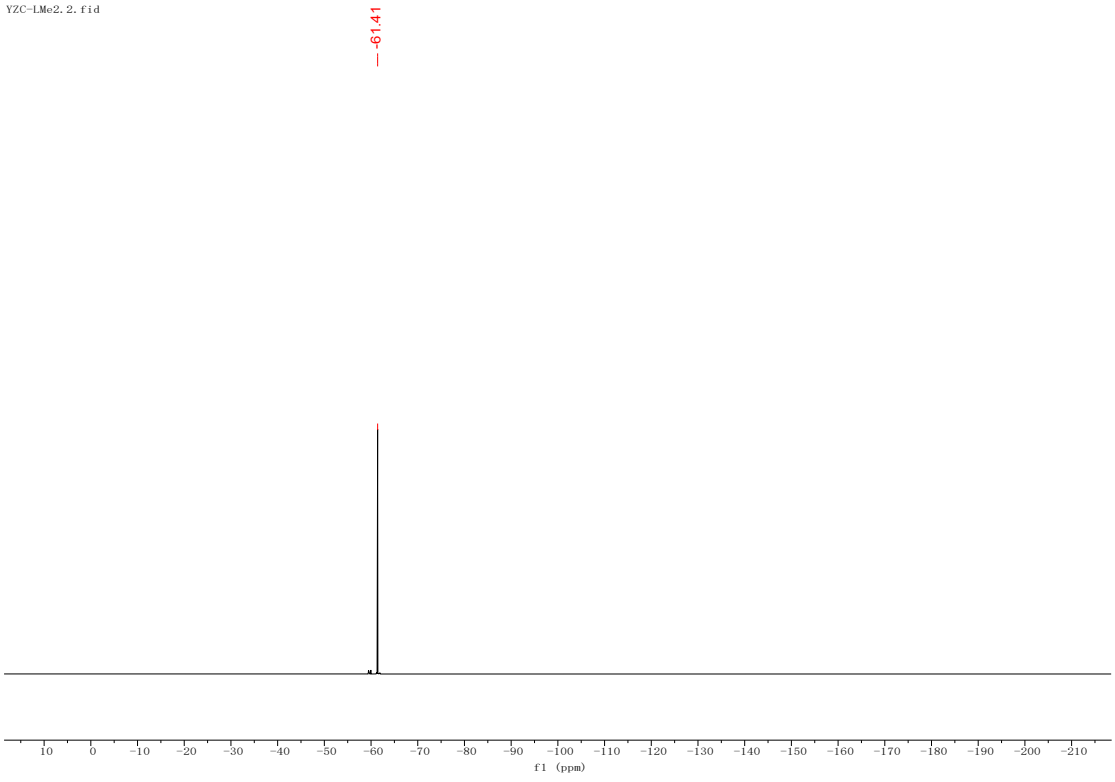
^{1}H NMR

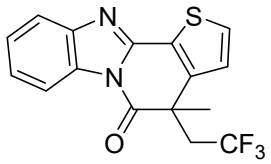

YZC-LMe2.1.fid
8.51
8.49
8.14
7.60
7.57
7.55
7.53
7.51
7.49
7.47
7.45
7.26 CDCl3
3.52
3.49
3.48
3.47
3.46
3.44
3.43
3.40
2.98
2.96
2.94
2.93
2.92
2.91
2.90
2.87
2.43
2.41
1.75
1.02
1.01
2.04
1.06
1.03
1.11
1.11
6.08
3.00
f1 (ppm)

^{13}C NMR



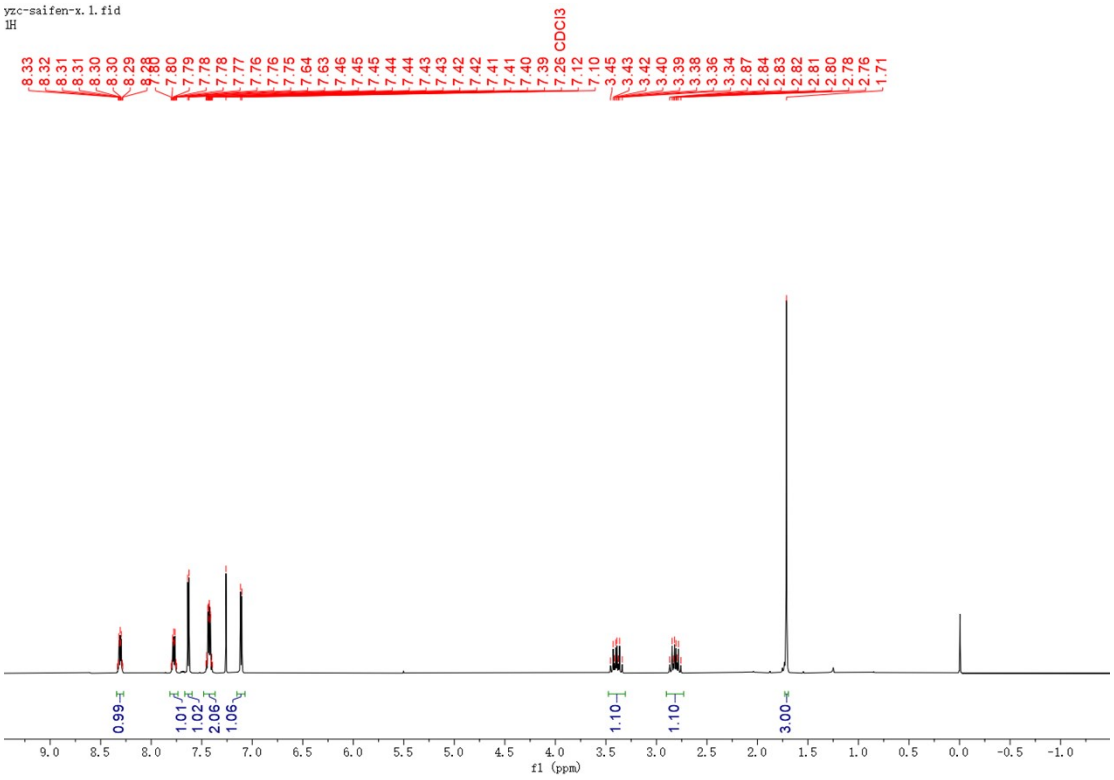
^{19}F NMR



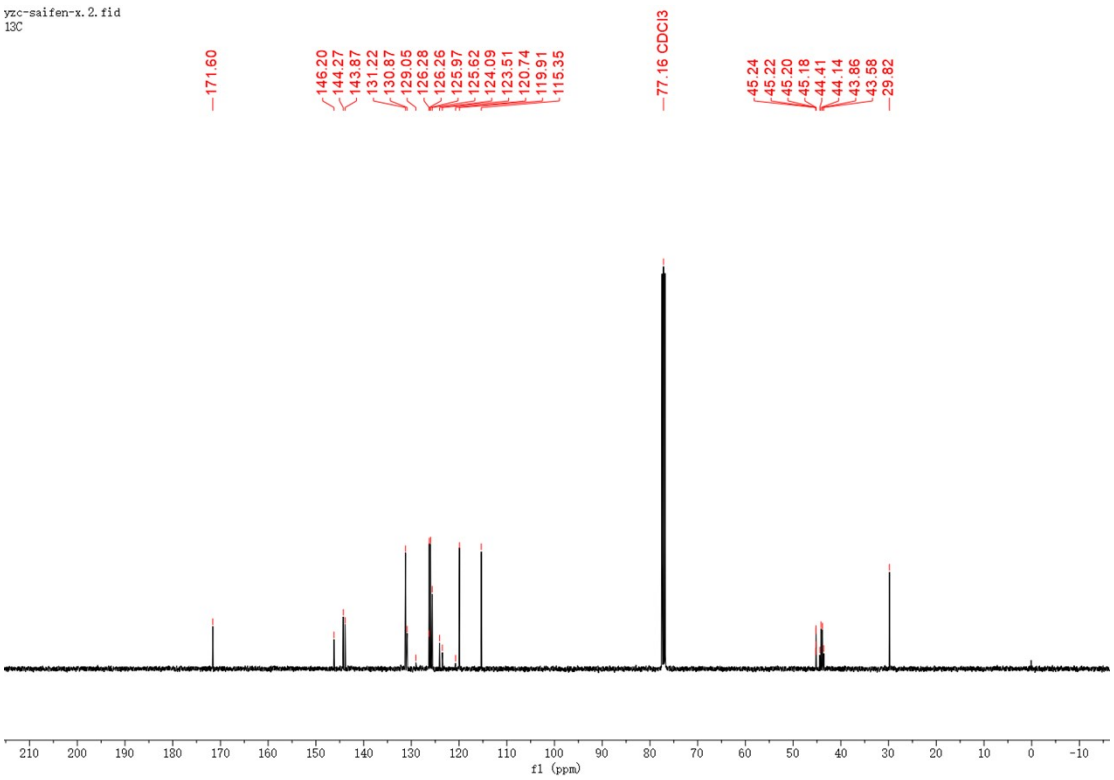


3t

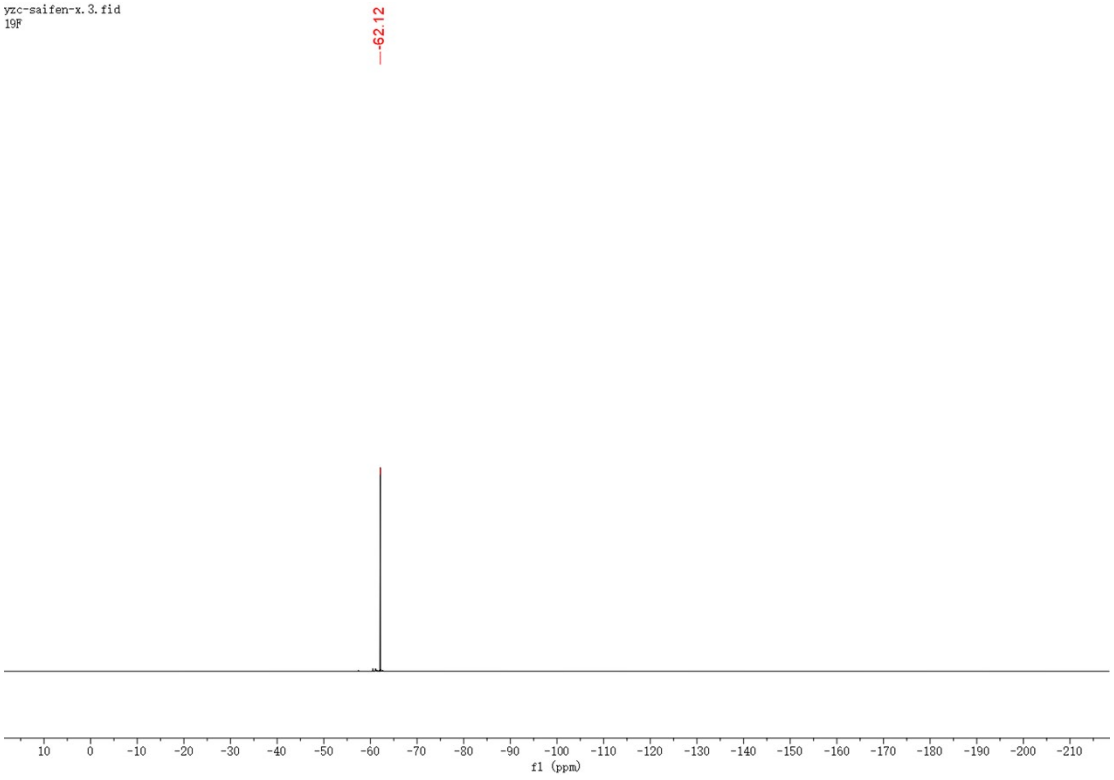
^{1}H NMR

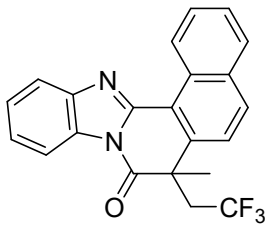


^{13}C NMR


yzc-saifen-x.2.fid
13C
171.60
146.20
144.27
143.87
131.22
130.87
129.05
126.28
126.26
125.97
125.62
124.09
123.51
120.74
119.91
115.35
77.16 CDCl3
45.24
45.22
45.20
45.18
44.41
44.14
43.86
43.58
29.82
f1 (ppm)

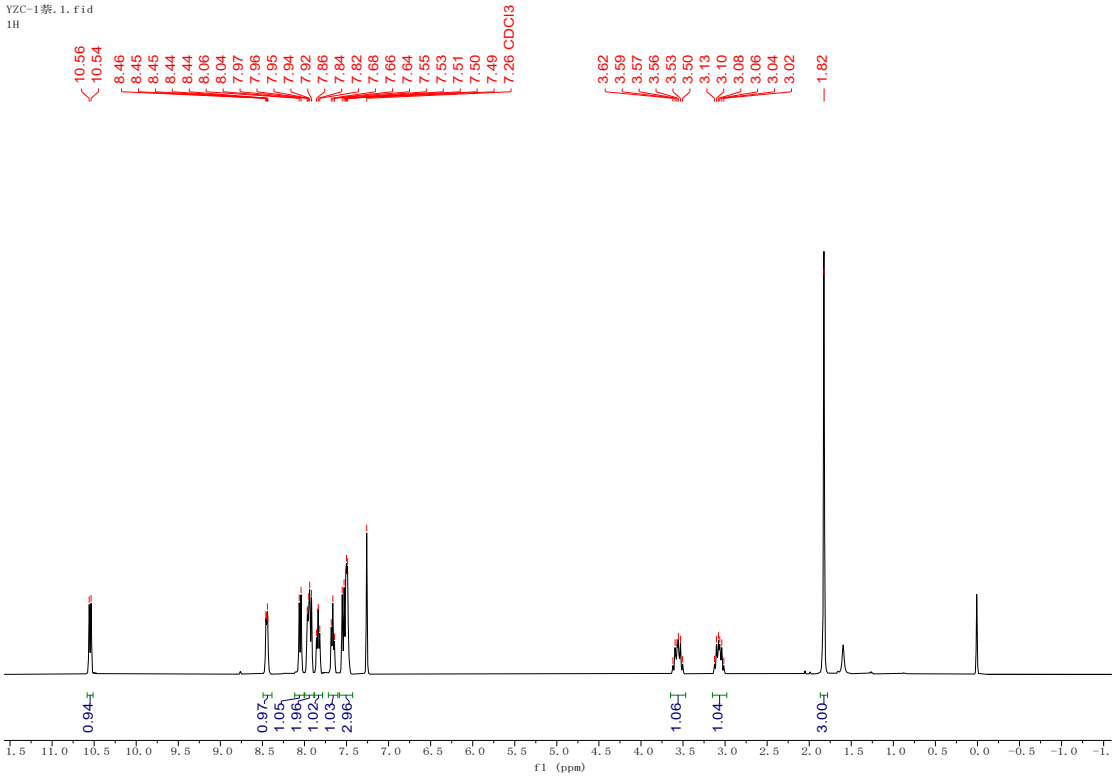
^{19}F NMR


yzc-saifen-x.3.fid
19F
-62.12
f1 (ppm)

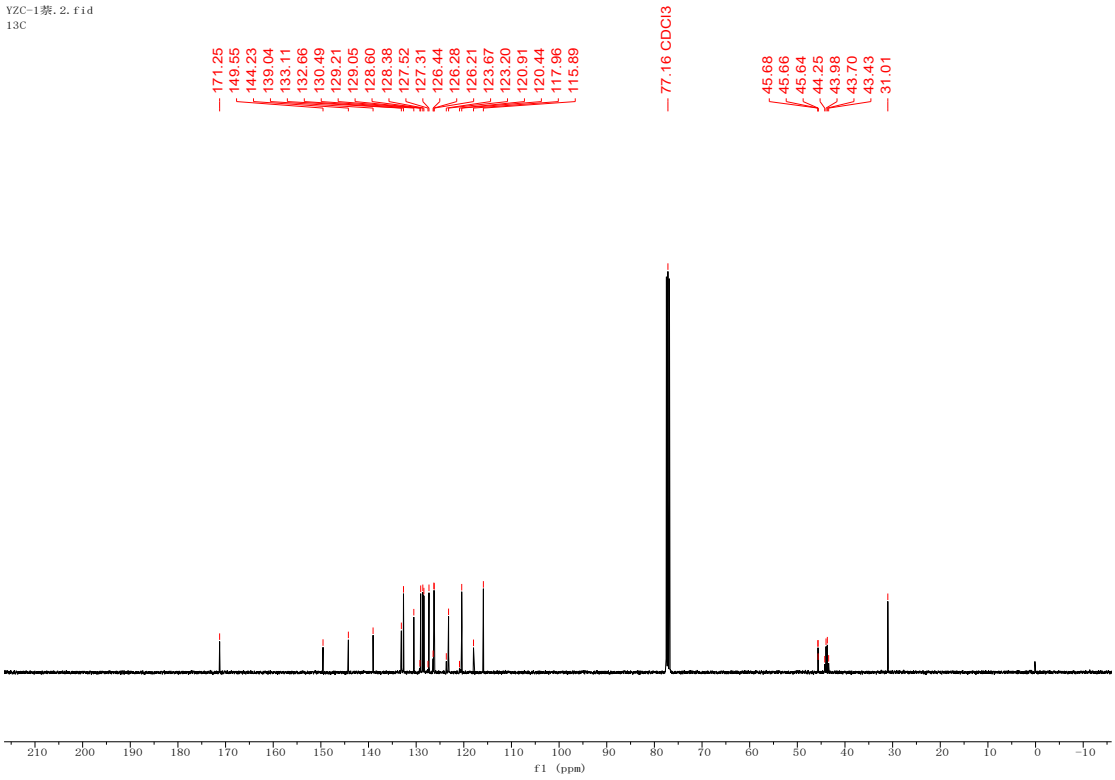

N
N
O
CF3

3u

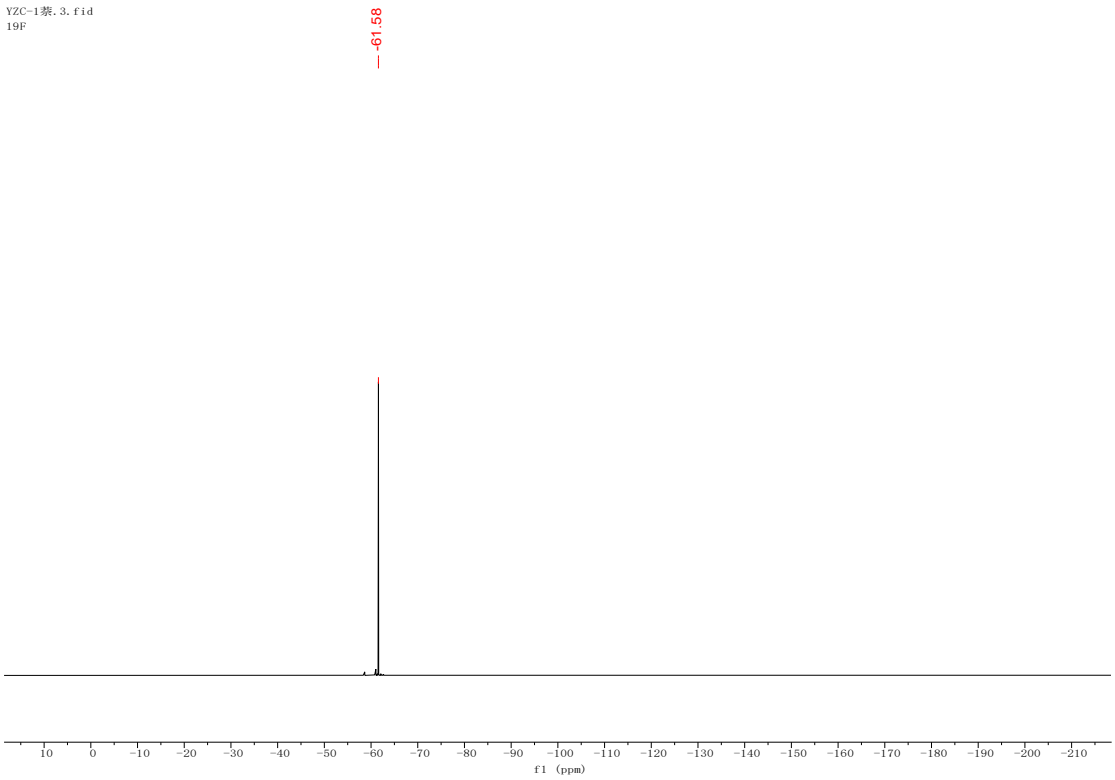
^{1}H NMR

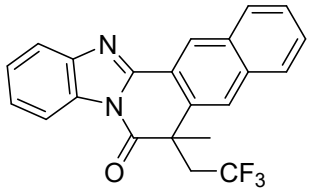


^{13}C NMR



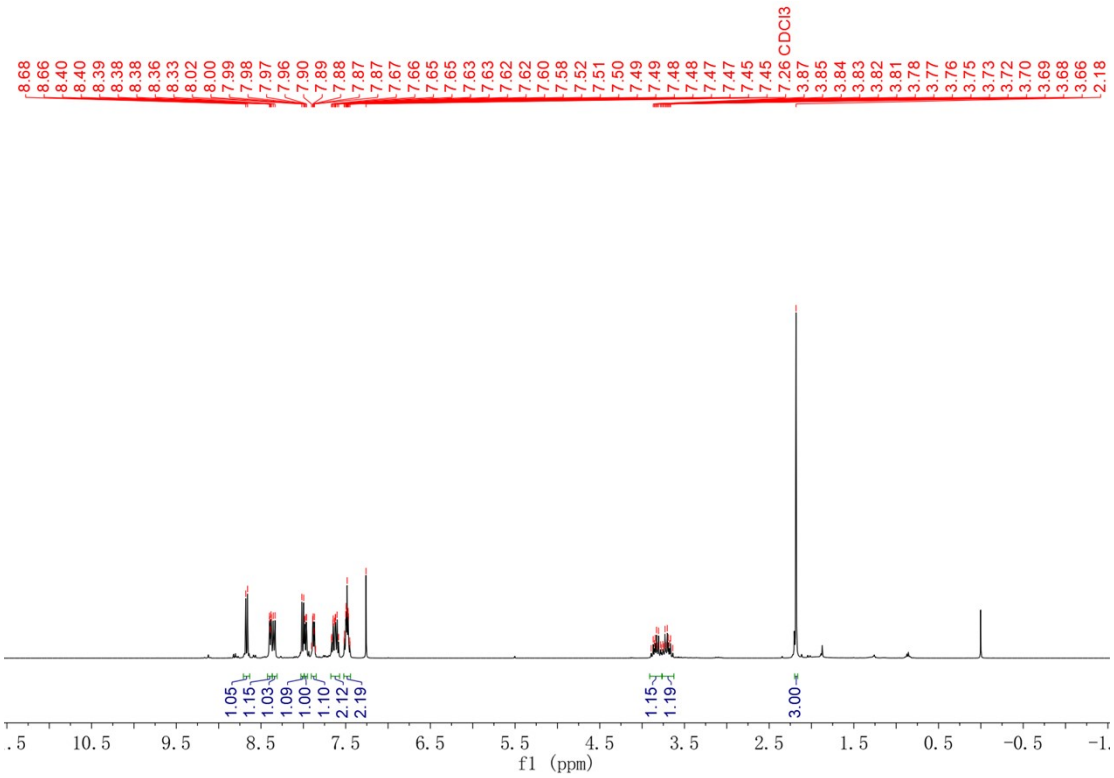
^{19}F NMR


YZC-1装.3.fid
19F
-61.58
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)

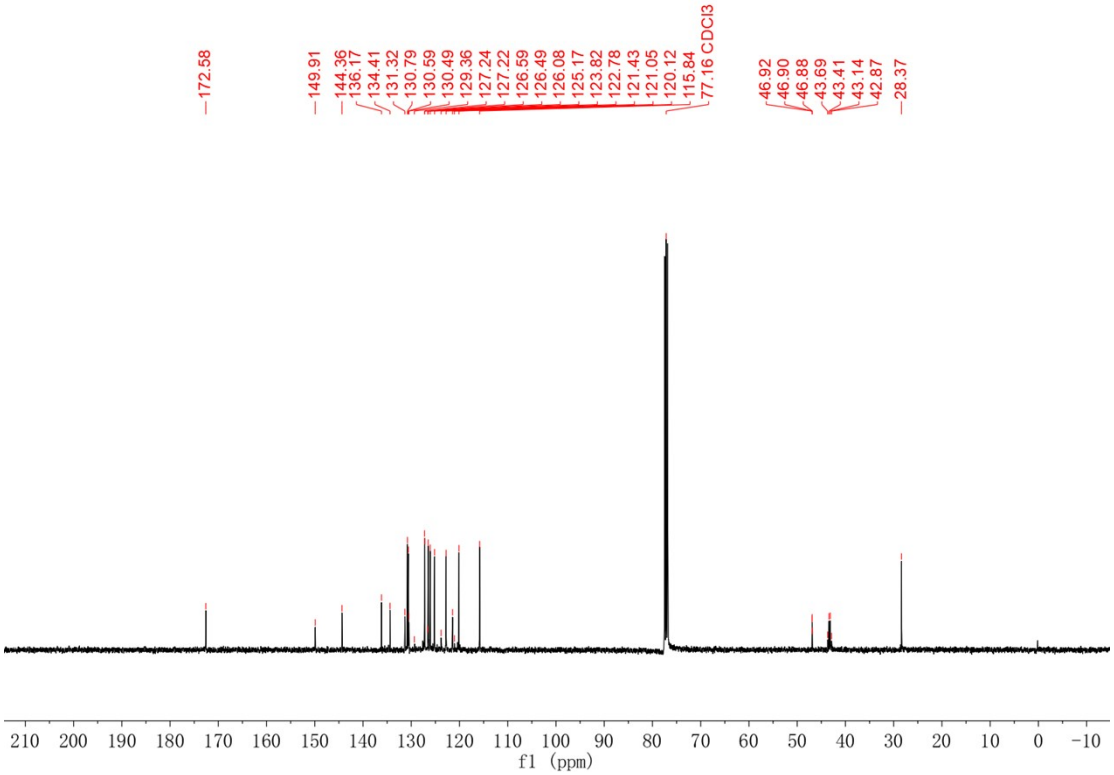

N
N
O
CF3

3v

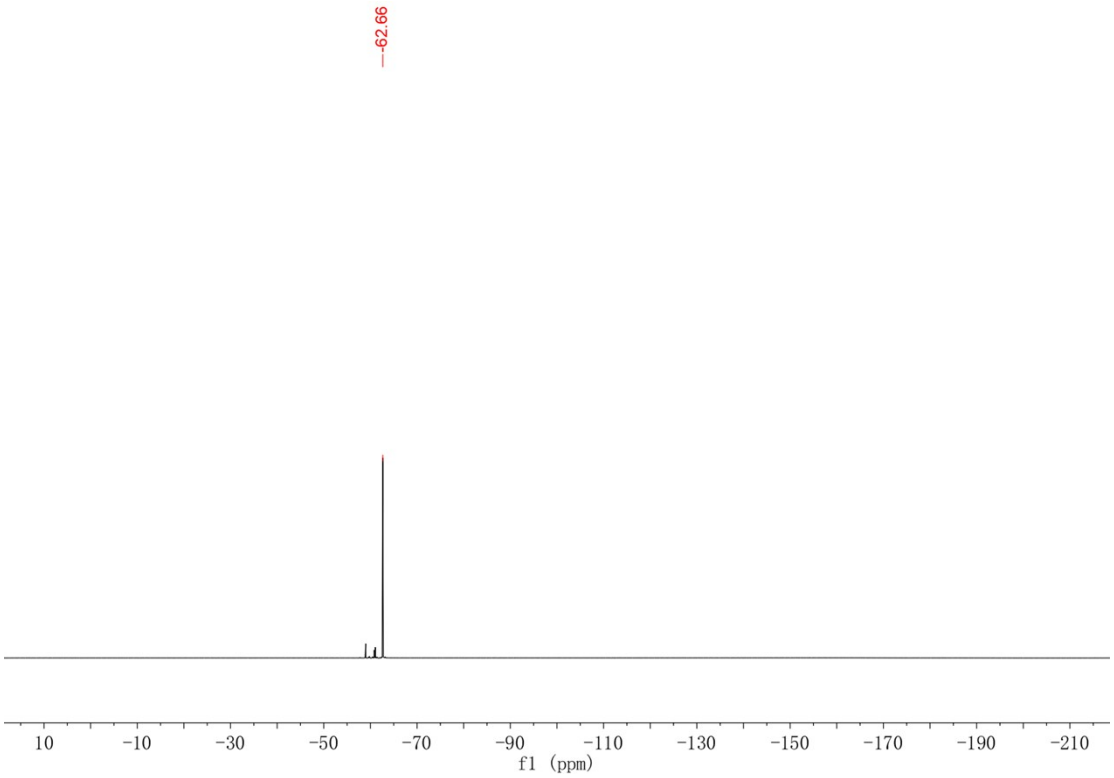
^{1}H NMR



^{13}C NMR



^{19}F NMR



Reference

[1] K. Sun, G. F. Li, S. Guo, Z. G. Zhang, G. S. Zhang, *Org*. *Biomol*. *Chem*., **2021**, 19, *375-378*.