Supporting Information

Synthesis of 3-CF_3-4-acyl-substituted quinoline derivatives via a cascade reaction of nitrosoarenes and *β*-CF_3-1,3-enynes

Wenhui Li[a], Shuangping Huang[a], Qiang Liu[a], Xing Li[a,*] and Wenwen Chen[b,*]

[a]Department of Biomedical Engineering, Taiyuan University of Technology, 79 West Yingze Street, Taiyuan 030024, People's Republic of China. E-mail: lixing@tyut.edu.cn
[b]School of Chemistry and Material Science, Shanxi Normal University, 339, Taiyu Road, Taiyuan 030000, People's Republic of China. Email: chenww@sxnu.edu.cn

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1. General information

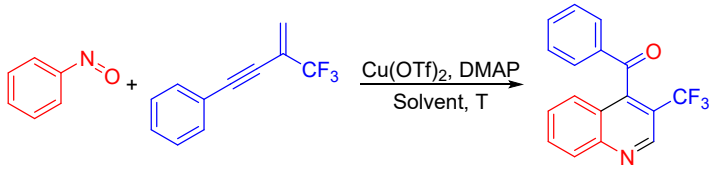
Unless otherwise indicated, all reagents were purchased from commercial sources and used without further purification. And deuterated solvents were purchased from Sigma−Aldrich. Substrates such as nitrosoarenes[1] and 2-CF_3-1,3-enynes[2] were synthesized according to the corresponding literature procedures. Unless otherwise stated, all reactions were accomplished in the reaction tubes under air atmosphere. All reactions were monitored by thin layer chromatography (TLC). Column chromatography was carried out using 200−300 mesh silica gel. ^{1}H NMR spectra were recorded on a Bruker Avance III 400 or 600 MHz NMR spectrometer and chemical shifts (in ppm) were referred to $CDCl_3$ (δ = 7.26 ppm), as an internal standard. ^{1}H NMR spectra were recorded as follows: chemical shift, multiplicity (s = singlet; d = doublet; q = quartet; m = multiplet; br = broad), coupling constant (Hz), and integral. Proton-decoupled ^{13}C NMR spectra were obtained by using the same NMR spectrometer, running at 150 or 100 MHz, respectively and were calibrated with $CDCl_3$ (δ = 77.16 ppm). The ^{19}F NMR spectra were recorded at 564 or 376 MHz. High-resolution mass spectra were performed on a micrOTOF-Q II instrument with an ESI source. Melting points were measured with an RD-II melting point apparatus and are uncorrected.

2. Optimization of reaction conditions

Next, some other reaction conditions including catalyst loading, amount of base, solvent dosage and temperature were also examined, respectively (Table 2). 30 mol% $Cu(OTf)_2$ and 0.5 equiv of DMAP were suitable for this transformation. Increasing or decreasing their amounts led to the lower yields (Table 2, entry 1 vs 2−7 and entry 1 vs 8−11). The solvent dosage had little effect on the reaction yield (Table 2, entries 12−14). It was more appropriate to use 0.8 mL EA (Table 2, entry 13). Variation of reaction temperature could not further improve the yield (Table 2, entries 13 and 15−17). The investigation of material ratio showed that the better yield (83%) was obtained when the ratio of nitrosobenzene **1a** and [3-(trifluoromethyl)but-3-en-1-yn-1-yl]benzene **2a** was 2.3:1.0 (Table 2, entry 22 vs 13, 18−21 and 23−25). After systematic optimization of the reaction conditions, the optimal condition was

determined. In the presence of $Cu(OTf)_2$ (22.0 mg, 0.06 mmol, 30 mol%) and DMAP (12.5 mg, 0.10 mmol, 0.5 equiv), the reaction of nitrosobenzene **1a** (50.8 mg, 0.46 mmol, 2.3 equiv.) and (3-(trifluoromethyl)but-3-en-1-yn-1-yl)benzene **2a** (40.5 mg, 0.20 mmol, 1.0 equiv.) was conducted in ethyl acetate (EA, 0.8 mL) at 30 °C for 12 h, affording the desired product **3aa** in 83% yield (Table 2, entry 22).

Table 2. Optimization of Other Reaction Conditions[a]



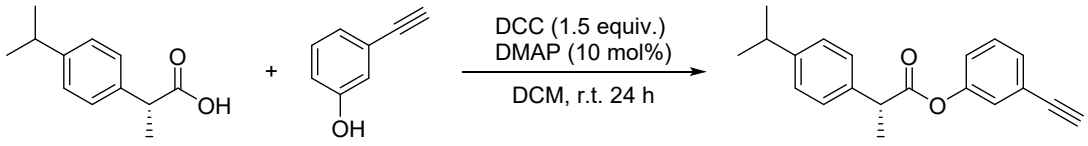
1a **2a** **3aa**

entry	catalyst (mol%)	base (equiv)	solvent (mL)	T/°C	**1a:2a**	yield[b] (%)
1	$Cu(OTf)_2$ (30)	DMAP (0.5)	DCE (1.0)	30	1.0:1.0	55
2	$Cu(OTf)_2$ (10)	DMAP (0.5)	DCE (1.0)	30	1.0:1.0	38
3	$Cu(OTf)_2$ (20)	DMAP (0.5)	DCE (1.0)	30	1.0:1.0	43
4	$Cu(OTf)_2$ (25)	DMAP (0.5)	DCE (1.0)	30	1.0:1.0	50
5	$Cu(OTf)_2$ (28)	DMAP (0.5)	DCE (1.0)	30	1.0:1.0	50
6	$Cu(OTf)_2$ (32)	DMAP (0.5)	DCE (1.0)	30	1.0:1.0	53
7	$Cu(OTf)_2$ (35)	DMAP (0.5)	DCE (1.0)	30	1.0:1.0	50
8	$Cu(OTf)_2$ (30)	DMAP (0.4)	DCE (1.0)	30	1.0:1.0	49
9	$Cu(OTf)_2$ (30)	DMAP (0.45)	DCE (1.0)	30	1.0:1.0	50
10	$Cu(OTf)_2$ (30)	DMAP (0.6)	DCE (1.0)	30	1.0:1.0	52
11	$Cu(OTf)_2$ (30)	DMAP (0.7)	DCE (1.0)	30	1.0:1.0	50
12	$Cu(OTf)_2$ (30)	DMAP (0.5)	EA (0.5)	30	1.0:1.0	67
13	$Cu(OTf)_2$ (30)	DMAP (0.5)	EA (0.8)	30	1.0:1.0	70
14	$Cu(OTf)_2$ (30)	DMAP (0.5)	EA (1.2)	30	1.0:1.0	63
15	$Cu(OTf)_2$ (30)	DMAP (0.5)	EA (0.8)	20	1.0:1.0	47
16	$Cu(OTf)_2$ (30)	DMAP (0.5)	EA (0.8)	40	1.0:1.0	70
17	$Cu(OTf)_2$ (30)	DMAP (0.5)	EA (0.8)	50	1.0:1.0	62
18	$Cu(OTf)_2$ (30)	DMAP (0.5)	EA (0.8)	30	1.3:1.0	78
19	$Cu(OTf)_2$ (30)	DMAP (0.5)	EA (0.8)	30	1.5:1.0	77
20	$Cu(OTf)_2$ (30)	DMAP (0.5)	EA (0.8)	30	1.7:1.0	75
21	$Cu(OTf)_2$ (30)	DMAP (0.5)	EA (0.8)	30	2.0:1.0	76
22	**$Cu(OTf)_2$ (30)**	**DMAP (0.5)**	**EA (0.8)**	**30**	**2.3:1.0**	**83**
23	$Cu(OTf)_2$ (30)	DMAP (0.5)	EA (0.8)	30	1.0:1.3	77
24	$Cu(OTf)_2$ (30)	DMAP (0.5)	EA (0.8)	30	1.0:1.5	78
25	$Cu(OTf)_2$ (30)	DMAP (0.5)	EA (0.8)	30	1.0:2.0	75

[a] Unless otherwise noted, all reactions were performed with nitrosobenzene **1a** (22.1 mg, 0.2 mmol, 1.0 equiv.), [3-(trifluoromethyl)-3-buten-1-ynyl]benzene **2a** (40.5 mg, 0.2 mmol, 1.0 equiv.), a catalyst (0.06 mmol, 30 mol%) and a base (0.1 mmol, 0.5 equiv.) in a solvent (1.0 mL) at 30 °C (water bath) under air atmosphere for 12 h. [b] Isolated yield after column chromatography.

3. General procedures

3.1 Operational procedure for the synthesis of compound 2n-3[3, 4]

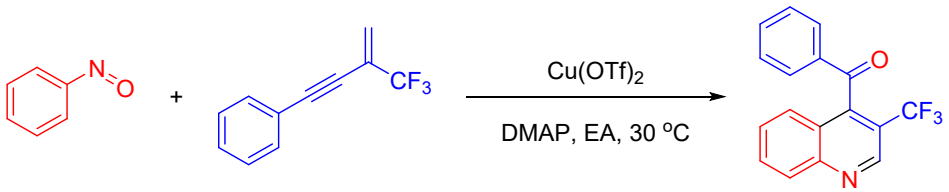


2n-1 **2n-2** **2n-3**

To a 100 mL of round-bottom flask equipped with a magnetic stir bar were added (*R*)-2-(4-isopropylphenyl)propanoic acid **2n-1** (2.5 g, 12.0 mmol, 1.2 equiv.), 3-ethynylphenol **2n-2** (1.1 mL, 10.0 mmol, 1.0 equiv.), dicyclohexylcarbodiimide (DCC, 3.1 g, 15.0 mmol, 1.5 equiv.), 4-dimethylaminopyridine (DMAP, 122.2 mg, 1.0 mmol, 10 mol%) and CH_2Cl_2 (30 mL). The mixture was then stirred at room temperature for 24 h. Finally, after the reaction mixture was evaporated, the residue was purified by column chromatography (silica gel, hexane/EtOAc) to give the 3-ethynylphenyl (*R*)-2-(4-isopropylphenyl)propanoate **2n-3**.

Subsequently, substrate **2n** was synthesized using the compound **2n-3** as a starting material via the method in the reference 2.

3.2 General procedure for the synthesis of products 3



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

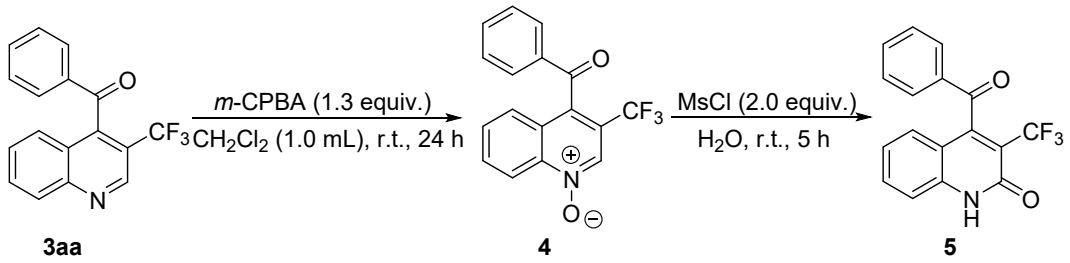
To a reaction system of nitrosobenzene **1a** (0.46 mmol, 2.3 equiv), $Cu(OTf)_2$ (0.06 mmol, 30 mol%) and DMAP (1.0 mmol, 0.5 equiv.) in ethyl acetate (EA) as a solvent (0.8 mL) was added (3-(trifluoromethyl)but-3-en-1-yn-1-yl)benzene **2a** (0.2 mmol). Then, the resultant solution was stirred under air atmosphere at 30 °C (water bath) for 12 h. Finally, the reaction mixture was purified by silica gel column chromatography (PE:EA = 15:1) to provide the corresponding product **3aa** (83% yield).

3.3 Operational procedure for 5.0 mmol-scale preparation of product 3aa

The reaction system of $Cu(OTf)_2$ (1.5 mmol, 30 mol%), DMAP (2.5 mmol, 0.5

equiv.), nitrosobenzene **1a** (11.5 mmol, 2.3 equiv.) and (3-(trifluoromethyl)but-3-en-1-yn-1-yl)benzene **2a** (5 mmol) in ethyl acetate as a solvent (20.0 mL) was stirred at 30 °C (water bath) for 15 h. At last, the reaction mixture was concentrated in vacuum and purified by silica gel column chromatography to give the desired product **3aa** (0.998 g, 67% isolated yield).

3.4 Operational procedure for the synthesis of compounds 4 and 5

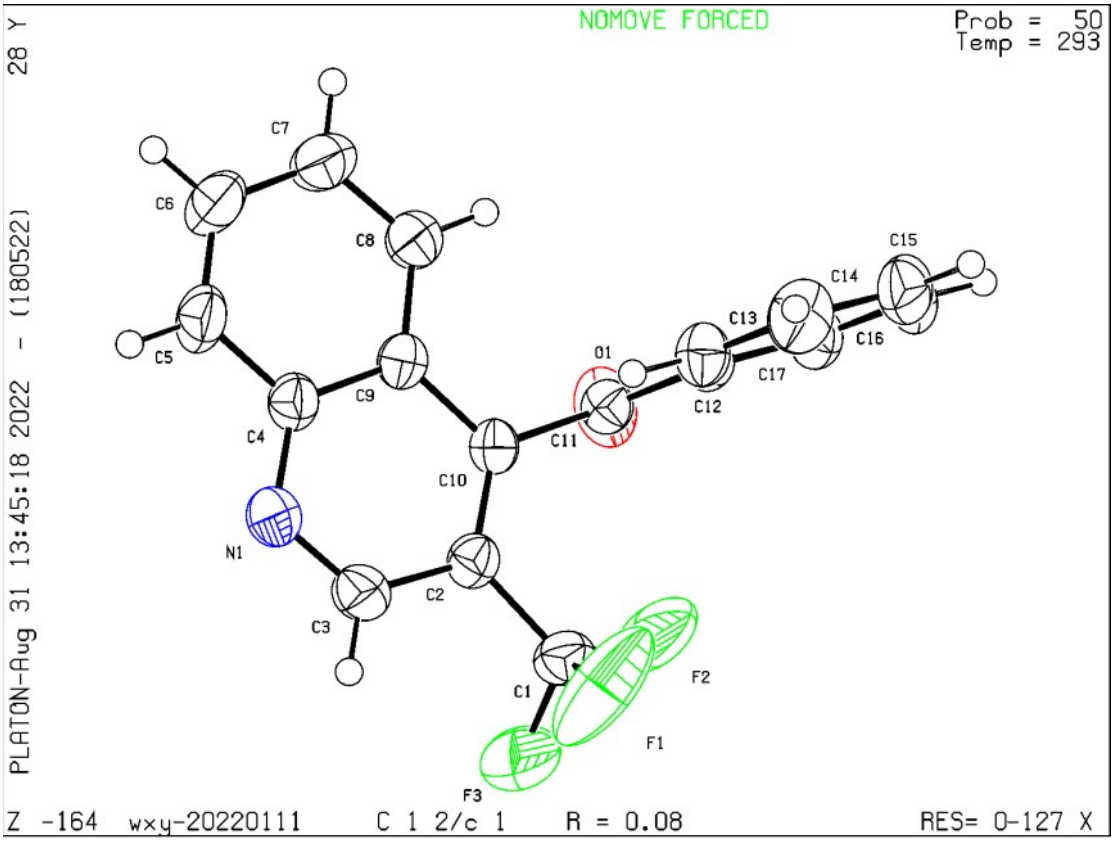


To a solution of the phenyl(3-(trifluoromethyl)quinolin-4-yl)methanone **3aa** (30.7 mg, 0.1 mmol) in CH_2Cl_2 (1.0 mL) was added *m*-chloroperoxybenzoic acid (*m*-CPBA, 28.0 mg, 0.13 mmol, 1.3 equiv.) at 0 °C. The reaction mixture was then allowed to stir at room temperature (water bath) for 24 h. Next, the reaction mixture was washed with saturated aq. $NaHCO_3$ solution (2.0 mL) and extracted with CH_2Cl_2 (5.0 mL X 3). The organic extracts were dried over anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel to obtain the pure 4-benzoyl-3-(trifluoromethyl)quinoline 1-oxide **4** (94% yield). To a 10 mL round bottom flask equipped with a magnetic stir bar were consecutively added 4-benzoyl-3-(trifluoromethyl)quinoline 1-oxide **4** (96.1 mg, 0.3 mmol), H_2O (3.0 mL) and MsCl (51.6 μL, 0.6 mmol). Subsequently, the reaction system was stirred at room temperature (water bath) for 5 h and the mixture was then extracted with CH_2Cl_2 (10.0 mL X 3). The organic extracts were dried over anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel to obtain the pure 4-benzoyl-3-(trifluoromethyl)quinolin-2(1*H*)-one **5** (94 % yield).

4. Crystal data of products 3aa, 3va and 4

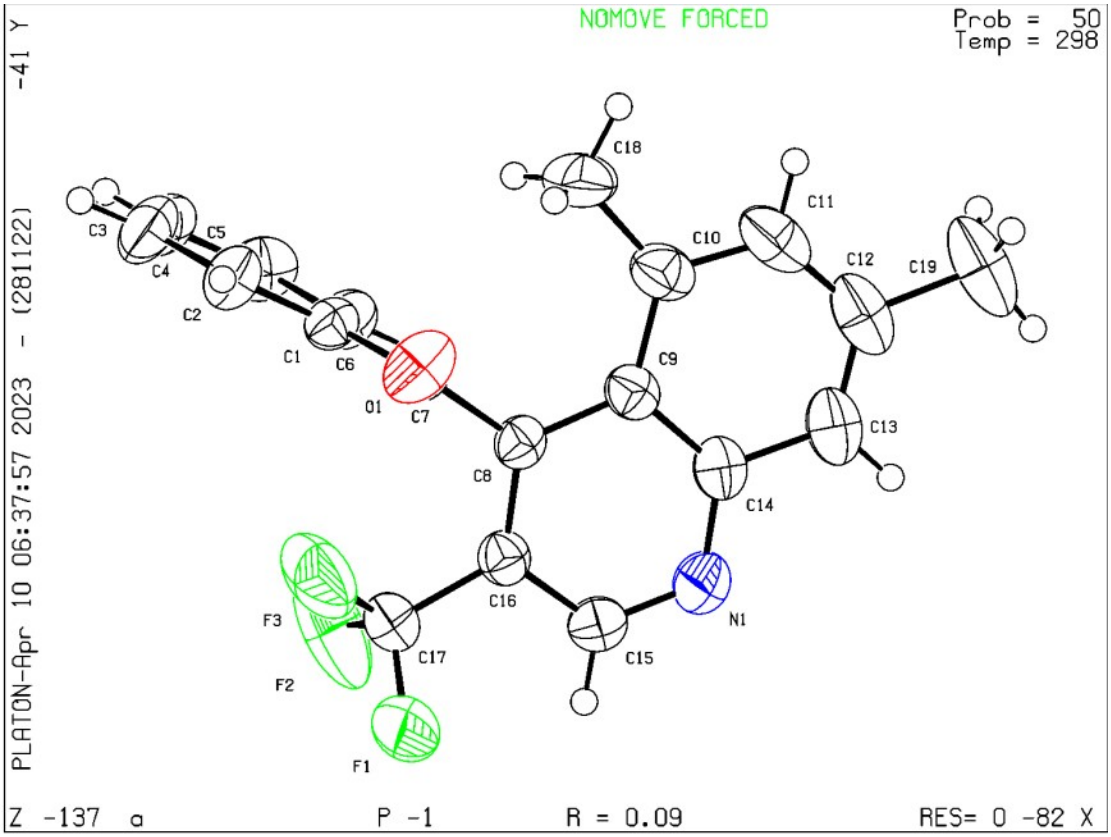
Crystallographic data for compounds **3aa** (2212193), **3va** (2255170) and **4** (2255167) have been deposited with the Cambridge Crystallographic Data Centre, Copies of the data can be obtained, free of charge, on application to CCDC (Email:

deposit@ccdc.cam.ac.uk).



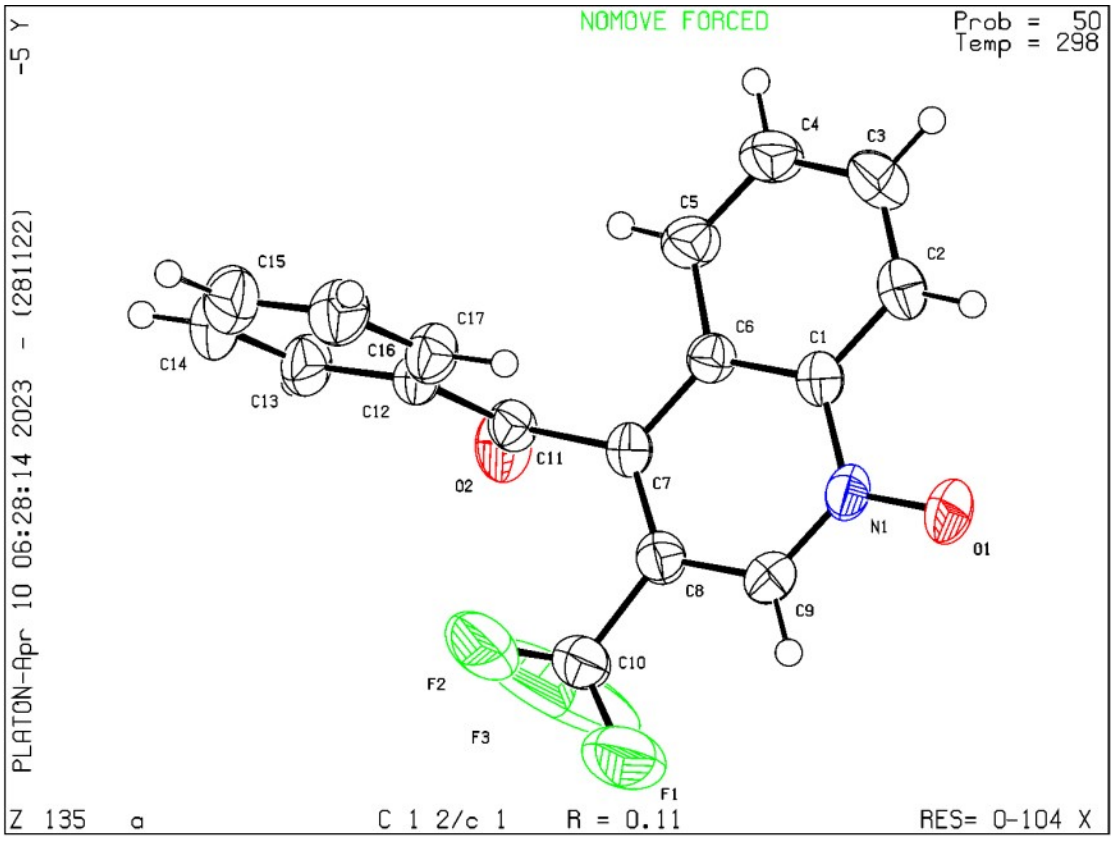
CCDC number	2212193
Identification code	**3aa**
Empirical formula	$C_{17}H_{10}F_3NO$
Formula weight	301.26
Temperature/K	293(2)
Crystal system	monoclinic
Space group	C2/c
a/Å	23.0671(4)
b/Å	7.9648(2)
c/Å	15.0332(3)
α/°	90
β/°	94.736(2)
γ/°	90
Volume/Å^3	2752.54(10)
Z	8
ρ_{calc}g/cm^3	1.454
μ/mm^{-1}	1.019
F(000)	1232.0

Crystal size/mm^3	0.29 × 0.25 × 0.2
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.692 to 143.066
Index ranges	-24 ≤ h ≤ 28, -9 ≤ k ≤ 9, -18 ≤ l ≤ 15
Reflections collected	5836
Independent reflections	2617 [R_{int} = 0.0192, R_{sigma} = 0.0247]
Data/restraints/parameters	2617/0/199
Goodness-of-fit on F^2	1.128
Final R indexes [I>=2σ (I)]	R_1 = 0.0838, wR_2 = 0.2317
Final R indexes [all data]	R_1 = 0.0962, wR_2 = 0.2380
Largest diff. peak/hole / e Å^{-3}	0.80/-0.46



CCDC number	2255170
Identification code	**3va**
Empirical formula	$C_{19}H_{14}F_3NO$
Formula weight	329.31
Temperature/K	298
Space group	P -1
a/Å	8.201(3)
b/Å	9.496(3)

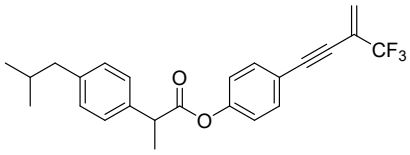
c/Å	11.840(4)
α/°	100.468 (8)
β/°	96.571 (7)
γ/°	9115.027 (8)
Volume/Å^3	802.4 (5)
Z	2
ρ_{calc}g/cm^3	1.363
μ/mm^{-1}	0.108
F(000)	340.0
Nref	4030
Tmin, Tmax	0.974, 0.984
h, k, lmax	10, 12, 15
Data completeness	0.967
Theta(max)	28.427
R(reflections)	0.0896 (2876)
wR2(reflections)	0.2929 (3895)
S	1.079
Npar	219



CCDC number	2255167
Identification code	**4**

Empirical formula	$C_{17}H_{10}F_3NO_2$
Formula weight	317.26
Temperature/K	298
Space group	C2/c
a/Å	25.164(3)
b/Å	8.0110(8)
c/Å	14.6926(14)
α/°	90
β/°	109.992 (2)
γ/°	90
Volume/Å^3	2783.4(5)
Z	8
ρ_{calc}g/cm^3	1.514
μ/mm^{-1}	0.127
F(000)	1296.0
Nref	3490
Tmin, Tmax	0.966, 0.972
h, k, lmax	33, 10, 19
Data completeness	0.993
Theta(max)	28.363
R(reflections)	0.1088(2791)
wR2(reflections)	0.4121(3464)
S	1.872
Npar	208

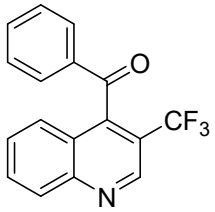
5. Characterization data for substrate 2n



White oil, Silica gel TLC R_f = 0.50 (PE); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.35−7.30 (m, 4H), 7.17−7.16 (m, 3H), 7.04−7.03 (m, 1H), 6.13 (s, 1H), 5.95 (s, 1H), 3.95 (q, J = 1.8 Hz, 1H), 2.49 (d, J = 4.2 Hz, 2H), 1.91−1.86 (m, 1H), 1.63−1.62 (m, 3H), 0.94−0.92 (m, 6H) ppm; **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$) δ 173.1, 150.8, 141.1, 137.1, 129.7, 129.5, 129.4, 127.3, 124.9, 123.0, 122.9, 122.7 (q, J = 35.3 Hz), 121.4 (q, J = 272.0 Hz), 92.3, 82.2, 45.4, 45.3, 45.2, 30.3, 22.5, 18.6 ppm; **^{19}F NMR** (564 MHz, $CDCl_3$) δ -67.9 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{24}H_{23}F_3NaO_2^+$, 423.1542; found, 423.1548.

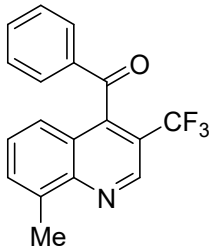
6. Characterization data for all products 3

Phenyl(3-(trifluoromethyl)quinolin-4-yl)methanone (**3aa**)



Yellow solid, 50.0 mg, 83% yield. Mp: 118−120 °C. Silica gel TLC R_f = 0.20 (PE:EA = 15:1); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.21 (s, 1H), 8.26−8.25 (m, 1H), 7.88−7.85 (m, 1H), 7.78−7.77 (m, 2H), 7.66−7.61 (m, 2H), 7.58−7.55 (m, 1H), 7.49−7.46 (m, 2H) ppm; **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$) δ 194.2, 149.4, 146.5 (q, J = 4.2 Hz), 144.9 (q, J = 2.4 Hz), 136.2, 134.9, 132.3, 130.3, 129.8, 129.2, 128.9, 126.3, 124.0, 123.5 (q, J = 273.0 Hz), 119.7 (q, J = 32.3 Hz) ppm; **^{19}F NMR** (564 MHz, $CDCl_3$) δ -57.1 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{17}H_{11}F_3NO^+$, 302.0787; found, 302.0794.

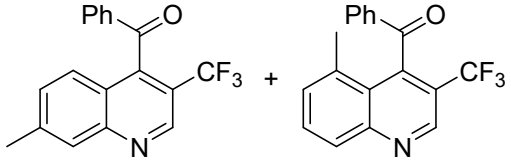
(8-Methyl-3-(trifluoromethyl)quinolin-4-yl)(phenyl)methanone (**3ba**)



Yellow oil, 35.3 mg, 56% yield. Silica gel TLC R_f = 0.20 (pure PE); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.23−9.21 (m, 1H), 7.77−7.76 (m, 2H), 7.71−7.70 (m, 1H), 7.66−7.61 (m, 1H), 7.49−7.44 (m, 4H), 2.89−2.86 (m, 3H) ppm; **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$) δ 194.5, 148.5, 145.2 (q, J = 4.1 Hz), 145.0 (q, J = 2.3 Hz), 136.4, 134.8, 132.3, 129.8, 129.1, 128.6, 124.2, 124.0, 123.6 (q, J = 272.9 Hz), 119.5 (q, J = 31.8 Hz) ppm; **^{19}F NMR** (564 MHz, $CDCl_3$) δ -57.1 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{18}H_{13}F_3NO^+$, 316.0944; found, 316.0943.

(5-Methyl-3-(trifluoromethyl)quinolin-4-yl)(phenyl)methanone (**3ca**)

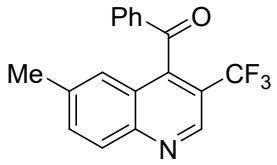
(7-Methyl-3-(trifluoromethyl)quinolin-4-yl)(phenyl)methanone (**3c'a**)



Yellow solid, 49.2 mg, 78% yield. Mp: 137−140 °C. Silica gel TLC R_f = 0.20 (PE:EA = 20:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.17 (s, 0.14H), 9.15 (s, 1H), 8.15−8.13 (m,

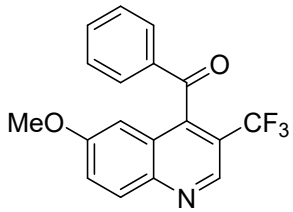
0.07H), 8.02 (s, 1H), 7.77−7.72 (m, 2.28H), 7.65−7.60 (m, 1.16H), 7.50−7.44 (m, 3.46H), 7.41 (s, 0.15H), 7.39−7.37 (m, 1H), 2.58 (s, 3H), 2.38 (s, 0.45H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 196.1, 194.3, 150.8, 149.7, 146.4 (q, J = 4.2 Hz), 145.9 (q, J = 4.8 Hz), 144.5, 143.2, 136.2, 136.0, 134.8, 134.5, 131.9, 131.1, 129.8, 129.4, 129.2, 129.1, 125.8, 123.6 (q, J = 272.7 Hz), 123.5, 122.0, 118.9 (q, J = 31.9 Hz), 23.9, 22.1 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -55.2 (s, 3F), -57.0 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{18}H_{13}F_3NO^+$, 316.0944; found, 316.0946.

(6-Methyl-3-(trifluoromethyl)quinolin-4-yl)(phenyl)methanone (**3da**)



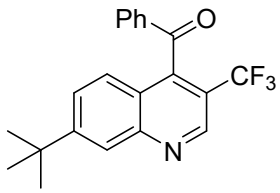
Yellow solid, 47.9 mg, 76% yield. Mp: 100−102 °C. Silica gel TLC R_f = 0.20 (PE:EA = 15:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.13 (s, 1H), 8.14−8.12 (m, 1H), 7.78−7.77 (m, 1H), 7.70−7.62 (m, 2H), 7.50−7.45 (m, 2H), 7.35 (s, 1H), 2.42 (s, 3H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 194.5, 148.1, 145.4 (q, J = 5.0 Hz), 144.0 (q, J = 3.5 Hz), 139.3, 136.2, 134.9, 134.6, 129.9, 129.8, 129.1, 124.9, 124.8, 123.1 (q, J = 277.2 Hz), 119.6 (q, J = 30.3 Hz), 21.9 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -57.0 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{18}H_{13}F_3NO^+$, 316.0944; found, 316.0945.

(6-Methoxy-3-(trifluoromethyl)quinolin-4-yl)(phenyl)methanone (**3ea**)



Yellow solid, 19.9 mg, 30% yield. Mp: 111−113 °C. Silica gel TLC R_f = 0.20 (PE:EA = 30:1); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.05 (s, 1H), 8.14−8.13 (m, 1H), 7.78−7.77 (m, 2H), 7.66−7.63 (m, 1H), 7.51−7.46 (m, 3H), 3.70 (s, 3H) ppm; **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$) δ 194.6, 159.3, 145.8, 143.8 (q, J = 4.4 Hz), 143.1 (q, J = 2.4 Hz), 136.2, 134.9, 131.6, 129.8, 129.2, 125.2, 123.6 (q, J = 273.0 Hz), 120.1 (q, J = 31.8 Hz), 103.5, 55.7 ppm; **^{19}F NMR** (564 MHz, $CDCl_3$) δ -57.0 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{18}H_{13}F_3NO_2^+$, 332.0893; found, 332.0890.

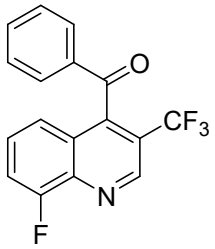
(7-(*tert*-Butyl)-3-(trifluoromethyl)quinolin-4-yl)(phenyl)methanone (**3ga**)



Yellow solid, 46.5 mg, 65% yield. Mp: 115−116 °C. Silica gel TLC R_f = 0.20 (PE:EA

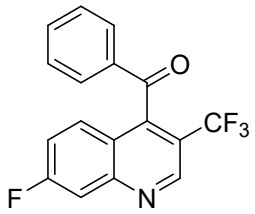
= 30:1); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.17−9.16 (m, 1H), 8.20−8.19 (m, 1H), 7.79−7.76 (m, 2H), 7.65−7.61 (m, 2H), 7.55−7.52 (m, 1H), 7.48−7.45 (m, 2H), 1.42−1.41 (m, 9H) ppm; **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$) δ 194.3, 156.1, 149.7, 146.3 (q, J = 4.1 Hz), 144.4 (q, J = 2.4 Hz), 136.3, 134.8, 129.8, 129.1, 127.9, 125.7, 125.5, 123.6 (q, J = 272.9 Hz), 121.9, 119.1 (q, J = 30.9 Hz), 35.5, 31.0 ppm; **^{19}F NMR** (564 MHz, $CDCl_3$) δ -57.0 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{19}F_3NO^+$, 358.1413; found, 358.1418.

(8-Fluoro-3-(trifluoromethyl)quinolin-4-yl)(phenyl)methanone (**3ha**)



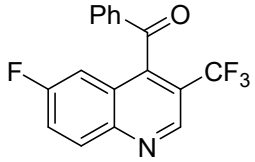
Yellow solid, 33.2 mg, 52% yield. Mp: 120−122 °C. Silica gel TLC R_f = 0.20 (PE:EA = 30:1); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.25 (s, 1H), 7.76−7.75 (m, 2H), 7.66−7.64 (m, 1H), 7.58−7.51 (m, 2H), 7.48 (t, J = 6.0 Hz, 2H), 7.41−7.40 (m, 1H) ppm; **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$) δ 193.4, 158.1 (d, J = 258.5 Hz), 146.7 (q, J = 2.4 Hz), 144.8 (q, J = 2.4 Hz), 139.8 (d, J = 11.9 Hz), 136.0 (d, J = 0.9 Hz), 135.1, 129.8, 129.3, 129.2, 129.0, 128.9, 125.6 (d, J = 1.5 Hz), 123.2 (q, J = 273.3 Hz), 122.0 (d, J = 5.0 Hz), 120.8 (q, J = 32.3 Hz) ppm; **^{19}F NMR** (564 MHz, $CDCl_3$) δ -57.3 (s, 3F), -122.7 (s, 1F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{17}H_{10}F_4NO^+$, 320.0693; found, 320.0707.

(7-Fluoro-3-(trifluoromethyl)quinolin-4-yl)(phenyl)methanone (**3ia**)



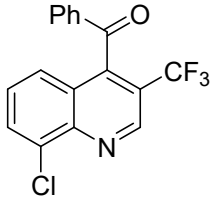
Yellow oil, 47.9 mg, 75% yield. Silica gel TLC R_f = 0.20 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.20 (s, 1H), 7.89−7.87 (m, 1H), 7.76−7.75 (m, 2H), 7.67−7.62 (m, 2H), 7.50−7.47 (m, 2H), 7.37−7.34 (m, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 193.7, 164.5 (d, J = 254.3 Hz), 150.9 (d, J = 13.2 Hz), 147.6 (q, J = 4.1 Hz), 136.0, 135.1, 129.8, 129.3, 128.6 (d, J = 10.1 Hz), 123.4 (q, J = 272.9 Hz), 121.0, 119.7, 119.5, 119.3 (q, J = 29.3 Hz), 114.2, 114.1 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -57.1 (s, 3F), -104.2 (s, 1F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{17}H_{10}F_4NO^+$, 320.0693; found, 320.0700.

(6-Fluoro-3-(trifluoromethyl)quinolin-4-yl)(phenyl)methanone (**3ja**)



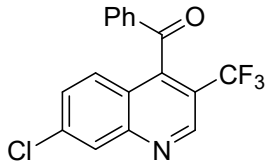
Yellow oil, 49.8 mg, 78% yield. Silica gel TLC R_f = 0.20 (PE:EA = 15:1); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.17 (s, 1H), 8.28−8.25 (m, 1H), 7.77−7.75 (m, 2H), 7.68−7.61 (m, 2H), 7.51−7.47 (m, 2H), 7.23−7.20 (m, 1H) ppm; **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$) δ 193.6, 161.5 (d, J = 376.8 Hz), 146.6, 145.8 (dt, J = 10.5 Hz, J = 4.7 Hz), 144.3 (dt, J = 5.3 Hz, J = 3.8 Hz), 135.8, 135.2, 132.9 (d, J = 14.0 Hz), 129.8, 129.3, 124.8 (d, J = 15.2 Hz), 123.3 (q, J = 273.1 Hz), 122.9, 122.7, 120.5 (q, J = 48.2 Hz), 109.8 (d, J = 35.1 Hz) ppm; **^{19}F NMR** (564 MHz, $CDCl_3$) δ -57.2 (s, 3F), -108.6 (s, 1F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{17}H_{10}F_4NO^+$, 320.0693; found, 320.0690.

(8-Chloro-3-(trifluoromethyl)quinolin-4-yl)(phenyl)methanone (**3ka**)



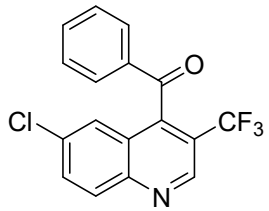
Yellow oil, 30.2 mg, 45% yield. Silica gel TLC R_f = 0.20 (PE:EA = 70:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.32 (s, 1H), 8.00−7.98 (m, 1H), 7.76−7.74 (m, 2H), 7.68−7.64 (m, 1H), 7.58−7.54 (m, 1H), 7.51−7.46 (m, 3H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 193.5, 147.0 (q, J = 4.1 Hz), 145.7, 145.5 (q, J = 2.3 Hz), 136.0, 135.2, 134.7, 132.4, 129.8, 129.3, 128.8, 128.7, 125.5, 125.3, 123.2 (q, J = 273.2 Hz), 120.7 (q, J = 32.2 Hz) ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -57.3 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{17}H_{10}ClF_3NO^+$, 336.0398; found, 336.0405.

(7-Chloro-3-(trifluoromethyl)quinolin-4-yl)(phenyl)methanone (**3la**)



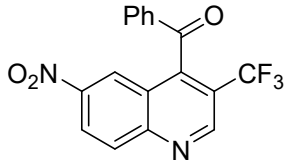
Yellow oil, 36.3 mg, 54% yield. Silica gel TLC R_f = 0.20 (PE:EA = 50:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.20 (s, 1H), 8.25 (d, J = 2.0 Hz, 1H), 7.76−7.74 (m, 2H), 7.68−7.64 (m, 1H), 7.56−7.46 (m, 4H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 193.5, 149.8, 147.0 (q, J = 4.0 Hz), 144.9 (q, J = 2.3 Hz), 138.6, 136.0, 135.2, 130.0, 129.8, 129.3, 128.6, 127.5, 123.3 (q, J = 273.0 Hz), 122.4, 119.9 (q, J = 32.2 Hz) ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -57.2 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{17}H_{10}ClF_3NO^+$, 336.0398; found, 336.0408.

(6-Chloro-3-(trifluoromethyl)quinolin-4-yl)(phenyl)methanone (**3ma**)



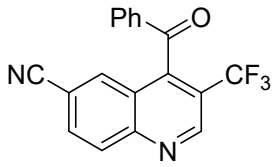
Yellow solid, 50.4 mg, 75% yield. Mp: 115−117 °C. Silica gel TLC R_f = 0.20 (PE:EA = 30:1); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.17 (s, 1H), 8.18−8.16 (m, 1H), 7.77−7.75 (m, 3H), 7.65−7.62 (m, 1H), 7.58−7.57 (m, 1H), 7.48−7.46 (m, 2H) ppm; **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$) δ 193.4, 147.8, 146.6 (q, J = 2.7 Hz), 144.0 (q, J = 2.6 Hz), 135.9, 135.2, 135.1, 133.3, 131.8, 129.8, 129.3, 124.9, 124.6, 123.2 (q, J = 273.3 Hz), 120.5 (q, J = 31.2 Hz) ppm; **^{19}F NMR** (564 MHz, $CDCl_3$) δ -57.2 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{17}H_{10}ClF_3NO^+$, 336.0398; found, 336.0404.

(6-Nitro-3-(trifluoromethyl)quinolin-4-yl)(phenyl)methanone (**3pa**)



Yellow oil, 35.3 mg, 51% yield. Silica gel TLC R_f = 0.20 (PE:EA = 20:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.36 (s, 1H), 8.64−8.61 (m, 1H), 8.54 (d, J = 2.4 Hz, 1H), 8.44−8.42 (m, 1H), 7.78−7.76 (m, 2H), 7.72−7.68 (m, 1H), 7.54−7.50 (m, 2H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 192.5, 151.1, 149.9 (q, J = 3.9 Hz), 146.9 (q, J = 2.9 Hz), 135.7, 132.4, 130.0, 129.5, 128.9, 124.3 (q, J = 272.9 Hz), 123.3, 121.5 (q, J = 32.5 Hz) ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -57.4 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{17}H_{10}F_3N_2O_3^+$, 347.0638; found, 347.0635.

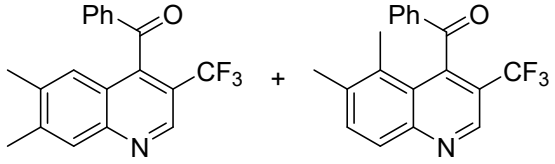
4-Benzoyl-3-(trifluoromethyl)quinoline-6-carbonitrile (**3qa**)



Yellow solid, 52.9 mg, 81% yield. Mp: 168−170 °C. Silica gel TLC R_f = 0.20 (PE:EA = 10:1); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.32 (s, 1H), 8.37−8.36 (m, 1H), 8.01−7.99 (m, 2H), 7.80−7.75 (m, 2H), 7.72−7.69 (m, 1H), 7.54−7.51 (m, 2H) ppm; **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$) δ 192.7, 150.1, 149.3 (q, J = 2.9 Hz), 145.4 (q, J = 2.6 Hz), 135.6, 133.2, 133.0, 132.8, 132.4, 131.9, 129.9, 129.5, 126.2, 123.6, 122.9 (q, J = 273.6 Hz), 121.4 (q, J = 35.7 Hz), 117.6, 112.9 ppm; **^{19}F NMR** (564 MHz, $CDCl_3$) δ -57.4 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{18}H_{10}F_3N_2O^+$, 327.0740; found, 327.0737.

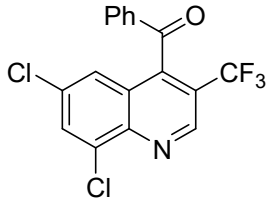
(6,7-Dimethyl-3-(trifluoromethyl)quinolin-4-yl)(phenyl)methanone (**3ra**)

(5,6-Dimethyl-3-(trifluoromethyl)quinolin-4-yl)(phenyl)methanone (**3r'a**)



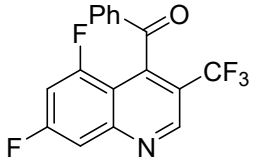
Yellow solid, 50.1 mg, 76% yield. Mp: 98−100 °C. Silica gel TLC R_f = 0.20 (PE:EA = 15:1); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.11−9.09 (m, 1.15H), 8.03 (d, J = 9.0 Hz, 0.15H), 7.99 (s, 1H), 7.77 (d, J = 7.8 Hz, 2H), 7.69 (d, J = 9.0 Hz, 0.28H), 7.64−7.59 (m, 1.16H), 7.31 (s, 1.12H), 2.48 (s, 3H), 2.41 (s, 0.45H), 2.31 (s, 3H), 2.27 (s, 0.45H) ppm; **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$) δ 196.6, 194.6, 149.7, 148.7, 145.4 (q, J = 3.9 Hz), 144.9 (q, J = 4.8 Hz), 143.7, 143.3, 139.4, 138.2, 136.3, 135.5, 134.8, 134.4, 133.0, 129.8, 129.4, 129.1, 128.5, 125.1, 123.7 (q, J = 272.7 Hz), 122.5, 118.8 (q, J = 32.0 Hz), 21.9, 20.6, 20.4, 19.0 ppm; **^{19}F NMR** (564 MHz, $CDCl_3$) δ -54.9 (s, 3F), -56.9 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{19}H_{15}F_3NO^+$, 330.1100; found, 330.1094.

(6,8-Dichloro-3-(trifluoromethyl)quinolin-4-yl)(phenyl)methanone (**3sa**)



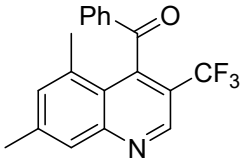
Yellow solid, 30.4 mg, 41% yield. Mp: 102−104 °C. Silica gel TLC R_f = 0.20 (PE:EA = 30:1); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.29 (s, 1H), 7.97 (d, J = 1.8 Hz, 1H), 7.75−7.72 (m, 2H), 7.70−7.68 (m, 1H), 7.52−7.50 (m, 3H) ppm; **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$) δ 192.9, 147.1 (q, J = 3.6 Hz), 144.7 (d, J = 2.3 Hz), 144.4, 136.0, 135.7, 135.5, 134.6, 133.1, 129.9, 129.4, 125.8, 124.0, 121.6 (q, J = 32.3 Hz), 123.0 (q, J = 276.6 Hz) ppm; **^{19}F NMR** (564 MHz, $CDCl_3$) δ -57.4 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{17}H_9Cl_2F_3NO^+$, 370.0008; found, 370.0010.

(5,7-Difluoro-3-(trifluoromethyl)quinolin-4-yl)(phenyl)methanone (**3ua**)



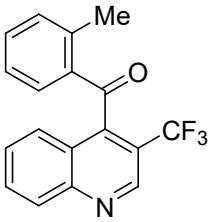
Yellow solid, 38.4 mg, 57% yield. Mp: 106−107 °C. Silica gel TLC R_f = 0.20 (PE:EA = 30:1); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.22 (s, 1H), 7.77−7.73 (m, 3H), 7.65−7.62 (m, 1H), 7.49−7.47 (m, 2H), 7.12−7.08 (m, 1H) ppm; **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$) δ 192.6, 164.0 (dd, J = 254.6 Hz, J = 14.0 Hz), 158.7 (dd, J = 261.5 Hz, J = 14.0 Hz), 150.8 (d, J = 12.6 Hz), 148.8 (q, J = 2.6 Hz), 142.6, 135.9, 134.6, 129.3, 129.1, 123.2 (q, J = 273.6 Hz), 120.5 (q, J = 31.4 Hz), 110.9 (d, J = 4.8 Hz), 110.8 (q, J = 4.4 Hz), 105.6, 105.4 (d, J = 4.5 Hz), 105.2 ppm; **^{19}F NMR** (564 MHz, $CDCl_3$) δ -62.9(s, 1F), -64.1(s, 1F), -70.1 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{17}H_9F_5NO^+$, 338.0599; found, 338.0600.

(5,7-Dimethyl-3-(trifluoromethyl)quinolin-4-yl)(phenyl)methanone (**3va**)



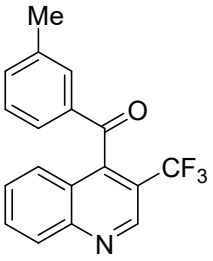
Yellow solid, 52.1 mg, 79% yield. Mp: 110−112 °C. Silica gel TLC R_f = 0.20 (PE:EA = 30:1); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.04 (s, 1H), 7.83 (s, 1H), 7.54−7.51 (m, 1H), 7.37 (s, 4H), 7.16 (s, 1H), 2.44 (s, 3H), 2.25 (s, 3H) ppm; **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$) δ 196.2, 151.2, 145.9 (q, J = 4.1 Hz), 144.5 (q, J = 3.2 Hz), 142.6, 137.6, 135.4, 134.5, 134.2, 129.1, 128.3, 123.7 (q, J = 273.8 Hz), 121.5, 119.9 (q, J = 30.9 Hz), 23.7, 21.7 ppm; **^{19}F NMR** (564 MHz, $CDCl_3$) δ -55.2 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{19}H_{15}F_3NO^+$, 330.1100; found, 330.1107.

o-Tolyl(3-(trifluoromethyl)quinolin-4-yl)methanone (**3ab**)



Yellow solid, 47.9 mg, 76% yield. Mp: 120−122 °C. Silica gel TLC R_f = 0.20 (PE:EA = 15:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.18 (s, 1H), 8.26−8.23 (m, 1H), 7.88−7.84 (m, 1H), 7.68−7.66 (m, 1H), 7.60−7.56 (m, 1H), 7.50−7.45 (m, 1H), 7.41−7.39 (m, 1H), 7.17−7.10 (m, 2H), 2.83 (s, 3H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 195.5, 149.5, 146.6 (q, J = 4.2 Hz), 146.2 (q, J = 3.6 Hz), 141.4, 134.7, 133.7, 132.8, 132.2, 130.2, 128.8, 126.4, 126.1, 124.1, 123.6 (q, J = 273.1 Hz), 119.2 (q, J = 31.9 Hz), 22.4 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -57.2 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{18}H_{13}F_3NO^+$, 316.0944; found, 316.0947.

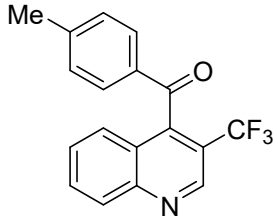
m-Tolyl(3-(trifluoromethyl)quinolin-4-yl)methanone (**3ac**)



Yellow solid, 51.7 mg, 82% yield. Mp: 102−103°C. Silica gel TLC R_f = 0.20 (PE:EA = 15:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.20 (s, 1H), 8.26−8.24 (m, 1H), 7.89−7.84 (m, 1H), 7.65−7.61 (m, 2H), 7.57−7.53 (m, 1H), 7.50−7.44 (m, 2H), 7.35−7.31 (m, 1H), 2.37 (s, 3H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 194.3, 149.4, 146.5 (q, J = 6.0 Hz), 145.1 (q, J = 3.6 Hz), 139.2, 136.2, 135.8, 132.2, 130.2, 129.9, 129.0, 128.8, 127.4, 126.3, 124.0, 123.5 (q, J = 272.9 Hz), 119.7 (q, J = 32.0 Hz), 21.4 ppm;

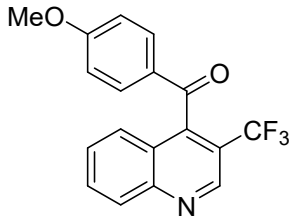
^{19}F NMR (376 MHz, $CDCl_3$) δ -57.1 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{18}H_{13}F_3NO^+$, 316.0944; found, 316.0943.

p-Tolyl(3-(trifluoromethyl)quinolin-4-yl)methanone (**3ad**)



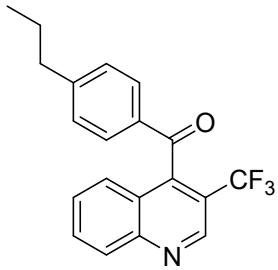
Yellow oil, 53.6 mg, 85% yield. Silica gel TLC R_f = 0.20 (PE:EA = 50:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.21 (s, 1H), 8.27−8.24 (m, 1H), 7.88−7.84 (m, 1H), 7.68−7.62 (m, 3H), 7.58−7.54 (m, 1H), 7.28−7.27 (m, 2H), 2.43 (s, 3H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 193.7, 149.3, 146.4 (q, J = 4.1 Hz), 146.3, 145.2 (q, J = 2.4 Hz), 133.9, 132.2, 130.2, 130.0, 129.9, 128.8, 126.4, 124.0, 123.5 (q, J = 272.9 Hz), 119.7 (q, J = 31.7 Hz), 22.0 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -57.1 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{18}H_{13}F_3NO^+$, 316.0944; found, 316.0951.

(4-Methoxyphenyl)(3-(trifluoromethyl)quinolin-4-yl)methanone (**3ae**)



White solid, 46.4 mg, 70% yield. Mp: 111−113 °C. Silica gel TLC R_f = 0.20 (PE:EA = 100:1); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.19 (s, 1H), 8.24−8.23 (m, 1H), 7.86−7.84 (m, 1H), 7.73 (s, 2H), 7.65−7.64 (m, 1H), 7.57−7.54 (m, 1H), 6.93−6.92 (m, 2H), 3.86 (s, 3H) ppm; **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$) δ 192.4, 165.0, 149.4, 146.5 (q, J = 4.1 Hz), 145.3 (q, J = 2.4 Hz), 132.3, 132.2, 130.2, 129.5, 128.7, 126.4, 124.1, 123.5 (q, J = 269.6 Hz), 119.6 (q, J = 32.0 Hz), 114.5, 55.8 ppm; **^{19}F NMR** (564 MHz, $CDCl_3$) δ -57.2 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{18}H_{13}F_3NO_2^+$, 332.0893; found, 332.0896.

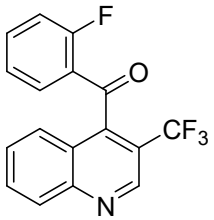
(4-Propylphenyl)(3-(trifluoromethyl)quinolin-4-yl)methanone (**3af**)



Yellow oil, 57.0 mg, 83% yield. Silica gel TLC R_f = 0.20 (PE:EA = 50:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.21 (s, 1H), 8.26−8.24 (m, 1H), 7.88−7.84 (m, 1H), 7.70−7.63

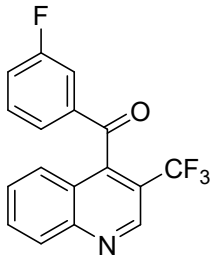
(m, 3H), 7.58−7.54 (m, 1H), 7.28−7.27 (m, 2H), 2.65 (t, *J* = 7.6 Hz, 2H), 1.71−1.62 (m, 2H), 0.95 (t, *J* = 7.6 Hz, 3H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 193.7, 150.8, 149.4, 146.4 (q, *J* = 3.7 Hz), 145.2 (q, *J* = 2.3 Hz), 134.1, 132.2, 130.2, 129.9, 129.2, 128.7, 127.6, 126.4, 124.0, 123.5 (q, *J* = 273.0 Hz), 119.6 (q, *J* = 32.1 Hz), 38.3, 24.1, 13.9 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -57.1 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{20}H_{17}F_3NO^+$, 344.1257; found, 344.1255.

(2-Fluorophenyl)(3-(trifluoromethyl)quinolin-4-yl)methanone (**3ag**)



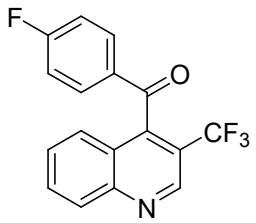
Yellow solid, 34.5 mg, 54% yield. Mp: 45−46 °C. Silica gel TLC R_f = 0.20 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.18 (s, 1H), 8.25−8.23 (m, 1H), 8.08−8.05 (m, 1H), 7.86−7.84 (m, 1H), 7.65−7.61 (m, 2H), 7.58−7.55 (m, 1H), 7.35−7.32 (m, 2H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 190.3, 162.5 (d, *J* = 259.1 Hz), 149.4, 146.4 (q, *J* = 4.1 Hz), 136.5 (d, *J* = 9.2 Hz), 132.0, 131.0, 130.2, 128.6, 125.3, 124.9 (d, *J* = 3.8 Hz), 123.1 (d, *J* = 2.0 Hz), 123.4 (q, *J* = 272.7 Hz), 118.4 (q, *J* = 29.7 Hz), 117.3, 117.1 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -57.2 (s, 3F), -108.3 (s, 1F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{17}H_{10}F_4NO^+$, 320.0693; found, 320.0701.

(3-Fluorophenyl)(3-(trifluoromethyl)quinolin-4-yl)methanone (**3ah**)



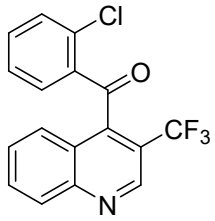
Yellow oil, 53.0 mg, 83% yield. Silica gel TLC R_f = 0.20 (PE:EA = 30:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.22 (s, 1H), 8.28−8.26 (m, 1H), 7.91−7.87 (m, 1H), 7.59−7.58 (m, 2H), 7.56−7.54 (m, 1H), 7.45−7.43 (m, 2H), 7.37−7.32 (m, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 193.0, 163.1 (d, *J* = 372.5 Hz), 149.4, 146.4 (q, *J* = 4.3 Hz), 144.1 (q, *J* = 2.1 Hz), 138.1, 132.4, 131.0 (d, *J* = 7.6 Hz), 130.4, 129.1, 126.0, 125.9 (d, *J* = 3.0 Hz), 123.8, 123.4 (q, *J* = 274.2 Hz), 122.2, 122.0, 119.8 (q, *J* = 29.7 Hz), 116.0,115.8 ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -57.0 (s, 3F), -110.6 (s, 1F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{17}H_{10}F_4NO^+$, 320.0693; found, 320.0703.

(4-Fluorophenyl)(3-(trifluoromethyl)quinolin-4-yl)methanone (**3ai**)



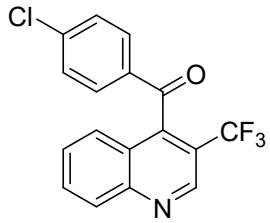
Yellow solid, 55.0 mg, 86% yield. Mp: 119−121 °C. Silica gel TLC R_f = 0.20 (PE:EA = 30:1); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.20 (s, 1H), 8.26−8.24 (m, 1H), 7.88−7.85 (m, 1H), 7.81−7.79 (m, 2H), 7.60−7.56 (m, 2H), 7.15−7.13 (m, 2H) ppm; **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$) δ 192.5, (d, J = 256.8 Hz), 149.4, 146.4 (q, J = 4.2 Hz), 144.4 (q, J = 2.4 Hz), 132.8, 132.6 (d, J = 9.8 Hz), 132.3, 130.3, 129.0, 126.1, 123.8, 123.4 (q, J = 272.9 Hz), 119.7 (q, J = 32.0 Hz), 116.6, 116.5 ppm; **^{19}F NMR** (564 MHz, $CDCl_3$) δ -57.1 (s, 3F), -101.4 (s, 1F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{17}H_{10}ClF_3NO^+$, 320.0693; found, 320.0698.

(2-Chlorophenyl)(3-(trifluoromethyl)quinolin-4-yl)methanone (**3aj**)



Yellow solid, 43.0 mg, 64% yield. Mp: 142−143 °C. Silica gel TLC R_f = 0.20 (PE:EA = 30:1); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.18 (s, 1H), 8.25−8.24 (m, 1H), 7.89−7.86 (m, 1H), 7.70−7.67 (m, 2H), 7.61−7.59 (m, 1H), 7.54−7.49 (m, 2H), 7.36−7.34 (m, 1H) ppm; **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$) δ 192.3, 149.6, 146.5 (q, J = 4.4 Hz), 134.9, 134.8, 134.4, 133.2, 132.2 (d, J = 5.6 Hz), 130.3, 129.0, 127.3, 125.8, 123.8, 123.5 (q, J = 272.9 Hz), 119.1 (q, J = 32.0 Hz) ppm; **^{19}F NMR** (564 MHz, $CDCl_3$) δ -57.1 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{17}H_{10}ClF_3NO^+$, 336.0398; found, 336.0411.

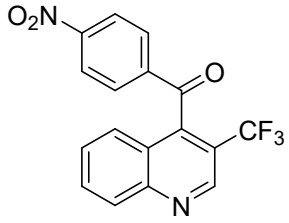
(4-Chlorophenyl)(3-(trifluoromethyl)quinolin-4-yl)methanone (**3ak**)



Yellow oil, 47.0 mg, 70% yield. Silica gel TLC R_f = 0.20 (PE:EA = 50:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.21 (s, 1H), 8.27−8.25 (m, 1H), 7.91−7.84 (m, 1H), 7.72−7.70 (m, 2H), 7.58−7.57 (m, 2H), 7.46−7.44 (m, 2H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 192.9, 149.5, 146.4 (q, J = 1.8 Hz), 146.4 (q, J = 2.3 Hz), 141.7, 134.6, 132.4, 131.1, 130.4, 129.6, 129.0, 126.0, 123.8, 123.4 (q, J = 272.9 Hz), 122.0, 119.7 (q, J = 32.2 Hz) ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -57.1 (s, 3F) ppm; **HRMS** (ESI)

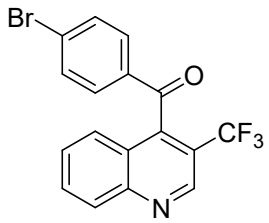
m/z: $[M + H]^+$ calcd for $C_{17}H_{10}ClF_3NO^+$, 336.0398; found, 336.0400.

(4-Nitrophenyl)(3-(trifluoromethyl)quinolin-4-yl)methanone (**3al**)



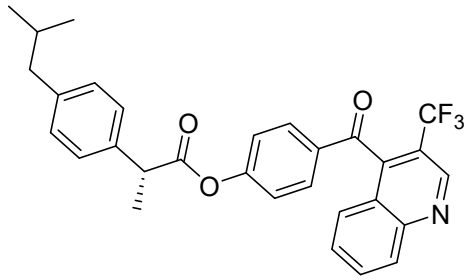
Yellow oil, 40.2 mg, 58% yield. Silica gel TLC R_f = 0.20 (PE:EA = 30:1); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.25 (s, 1H), 8.34−8.30 (m, 3H), 7.96−7.90 (m, 3H), 7.63−7.60 (m, 1H), 7.55−7.53 (m, 2H) ppm; **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$) δ 192.7, 151.3, 149.5, 146.4 (q, J = 4.1 Hz), 143.4 (q, J = 2.3 Hz), 140.1, 132.7, 130.7, 130.5, 129.4, 125.6, 125.3, 124.5, 124.0, 123.5, 123.3 (q, J = 272.9 Hz), 119.8 (q, J = 32.1 Hz) ppm; **^{19}F NMR** (564 MHz, $CDCl_3$) δ -56.9 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{17}H_{10}F_3N_2O_3^+$, 347.0638; found, 347.0640.

(4-Bromophenyl)(3-(trifluoromethyl)quinolin-4-yl)methanone (**3am**)



Yellow solid, 57.8 mg, 76% yield. Mp: 137−140 °C. Silica gel TLC R_f = 0.20 (PE:EA = 40:1); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.20 (s, 1H), 8.26 (d, J = 8.4 Hz, 1H), 7.89−7.86 (m, 1H), 7.62 (s, 4H), 7.58−7.57 (m, 2H) ppm; **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$) δ 193.1, 149.4, 146.4 (q, J = 4.1 Hz), 144.2 (q, J = 2.4 Hz), 135.0, 132.6, 132.4, 130.4, 129.0, 126.0, 123.8, 123.4 (q, J = 272.9 Hz), 119.7 (q, J = 32.0 Hz) ppm; **^{19}F NMR** (564 MHz, $CDCl_3$) δ -57.1 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{17}H_{10}BrF_3NO^+$, 379.9892; found, 379.9896.

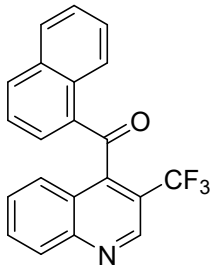
4-(3-(Trifluoromethyl)quinoline-4-carbonyl)phenyl(*R*)-2-(4-isopropylphenyl)propanoate (**3an**)



Yellow oil, 72.8 mg, 72% yield. Silica gel TLC R_f = 0.20 (PE:EA = 30:1); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.23 (s, 1H), 8.29−8.28 (m, 1H), 7.91−7.88 (m, 1H), 7.62−7.58 (m, 3H), 7.43−7.41 (m, 2H), 7.29−7.28 (m, 3H), 7.17−7.15 (m, 2H), 3.97−3.94 (m,

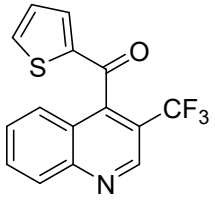
1H), 2.50−2.49 (m, 2H), 1.92−1.86 (m, 1H), 1.63−1.61 (m, 3H), 0.94−0.93 (m, 6H) ppm; **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$) δ 193.2, 172.9, 151.6, 149.4, 146.4 (q, J = 2.1 Hz), 144.3 (q, J = 2.3 Hz), 141.2, 137.4, 136.9, 132.3, 130.1, 129.7, 129.0, 128.3, 127.7, 127.3, 126.2, 123.4 (q, J = 273.0 Hz), 121.9, 45.3, 45.2, 30.3, 22.5, 18.6, 18.5 ppm; **^{19}F NMR** (564 MHz, $CDCl_3$) δ -57.0 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{29}H_{25}F_3NO_3^+$, 506.1938; found, 506.1937.

Naphthalen-1-yl(3-(trifluoromethyl)quinolin-4-yl)methanone (**3ao**)



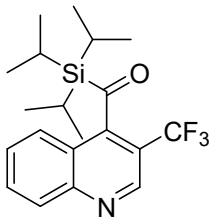
Yellow oil, 51.3 mg, 73% yield. Silica gel TLC R_f = 0.20 (PE:EA = 20:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.47 (d, 1H, J = 8.4Hz), 9.25 (s, 1H), 8.29−8.27 (m, 1H), 8.12−8.10 (m, 1H), 7.99−7.97 (m, 1H), 7.89−7.80 (m, 2H), 7.76−7.74 (m, 1H), 7.70−7.66 (m, 1H), 7.57−7.53 (m, 1H), 7.49−7.47 (m, 1H), 7.37−7.33 (m, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 195.7, 149.6 (q, J = 3.4 Hz), 146.6 (q, J = 6.3 Hz), 146.1, 136.1, 135.4, 134.2, 132.2, 132.0, 130.8, 129.9, 129.0, 128.9, 127.4, 126.5, 126.3, 125.0, 124.4, 123.6 (q, J = 273.2 Hz), 119.4 (q, J = 34.5 Hz) ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -57.0 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{13}F_3NO^+$, 352.0944; found, 352.0941.

Thiophen-2-yl(3-(trifluoromethyl)quinolin-4-yl)methanone (**3ap**)



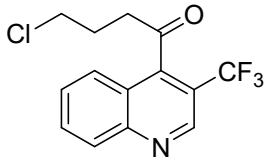
Yellow oil, 43.0 mg, 70% yield. Silica gel TLC R_f = 0.20 (PE:EA = 20:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.20 (s, 1H), 8.26−8.24 (m, 1H), 7.90−7.84 (m, 2H), 7.77−7.75 (m, 1H), 7.63−7.59 (m, 1H), 7.21−7.20 (m, 1H), 7.10−7.08 (m, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 185.7, 149.5, 146.4 (q, J = 4.0 Hz), 144.1 (q, J = 2.4 Hz), 143.6, 136.9, 136.5, 132.3, 130.1, 128.9, 127.5, 126.3, 123.8, 123.4 (q, J = 273.0 Hz), 119.5 (q, J = 31.9 Hz) ppm; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -57.1 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{15}H_9F_3NOS^+$, 308.0351; found, 308.0358.

(3-(Trifluoromethyl)quinolin-4-yl)(triisopropylsilyl)methanone (**3aq**)



Yellow oil, 32.0 mg, 42% yield. Silica gel TLC R_f = 0.20 (PE:EA = 40:1); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.01 (s, 1H), 8.21−8.20 (m, 1H), 7.86−7.84 (m, 1H), 7.68−7.66 (m, 1H), 7.62−7.60 (m, 1H), 1.04 (s, 21H) ppm; **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$) δ 191.6, 152.1, 149.5, 146.9 (q, J = 3.9 Hz), 132.1, 130.6, 128.1, 125.7, 123.8 (q, J = 273.2 Hz), 122.4, 117.0 (q, J = 32.0 Hz), 18.5, 17.8, 12.4, 11.4 ppm; **^{19}F NMR** (564 MHz, $CDCl_3$) δ -54.8 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{20}H_{27}F_3NOSi^+$, 382.1809; found, 382.1819.

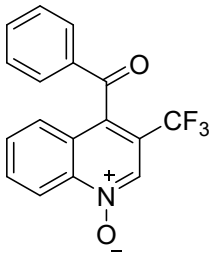
4-Chloro-1-(3-(trifluoromethyl)quinolin-4-yl)butan-1-one (**3ar**)



Yellow oil, 16.9 mg, 28% yield. Silica gel TLC R_f = 0.30 (PE:EA = 20:1); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 9.12 (s, 1H), 8.23−8.22 (m, 1H), 7.91−7.88 (m, 1H), 7.71−7.67 (m, 2H), 3.74−3.71 (m, 2H), 3.14−3.12 (m, 2H), 3.34−2.32 (m, 2H) ppm; **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$) δ 203.0, 149.6, 146.3 (q, J = 3.9 Hz), 146.1 (q, J = 2.3 Hz), 132.4, 130.5, 129.1, 125.0, 123.6 (q, J = 272.7 Hz), 122.4, 117.9 (q, J = 32.0 Hz), 43.9, 42.0, 26.0 ppm; **^{19}F NMR** (564 MHz, $CDCl_3$) δ -57.1 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{14}H_{12}ClF_3NO^+$, 302.0544; found, 302.0548.

7. Characterization data for compound 4

4-Benzoyl-3-(trifluoromethyl)quinoline 1-oxide **4**

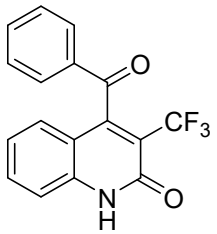


White solid, 29.8 mg, 94% yield. Mp: 172−174 °C. Silica gel TLC R_f = 0.20 (PE:EA = 1:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.83 (d, 1H, J = 8.80 Hz), 8.78 (s, 1H), 7.91−7.87 (m, 1H), 7.81−7.80 (m, 2H), 7.68−7.64 (m, 3H), 7.52−7.48 (m, 2H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 193.0, 142.7 (q, J = 2.5 Hz), 136.3 (q, J = 1.4 Hz), 135.2, 135.0, 133.3, 132.9, 131.8, 130.7, 129.9, 129.3, 127.4, 127.2, 122.1 (q, J = 273.5 Hz), 122.0 (q, J = 34.1 Hz), 120.4 ppm; **^{19}F NMR** (376MHz, $CDCl_3$) δ -58.1 (s,

3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{17}H_{11}F_3NO_2^+$, 318.0736; found, 318.0741.

8. Characterization data for compound 5

4-Benzoyl-3-(trifluoromethyl)quinolin-2(1H)-one **5**



White solid, 29.8 mg, 94% yield. Mp: 270−271 °C. Silica gel TLC R_f = 0.20 (PE:EA = 2:1); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.77 (s, 1H), 7.91−7.89 (m, 2H), 7.67−7.66 (m, 2H), 7.56−7.51 (m, 3H), 7.32−7.30 (m, 1H), 7.20−7.17 (m, 1H) ppm; **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 193.0, 160.1 (q, J = 5.2 Hz), 151.1 (q, J = 4.0 Hz), 139.4, 135.5, 135.1, 133.9, 129.4, 129.3, 127.5, 124.1, 122.4 (q, J = 272.7 Hz), 117.0, 116.3 ppm; **^{19}F NMR** (376MHz, $CDCl_3$) δ -59.0 (s, 3F) ppm; **HRMS** (ESI) *m/z*: $[M + H]^+$ calcd for $C_{17}H_{11}F_3NO_2^+$, 318.0736; found, 318.0746.

9. References

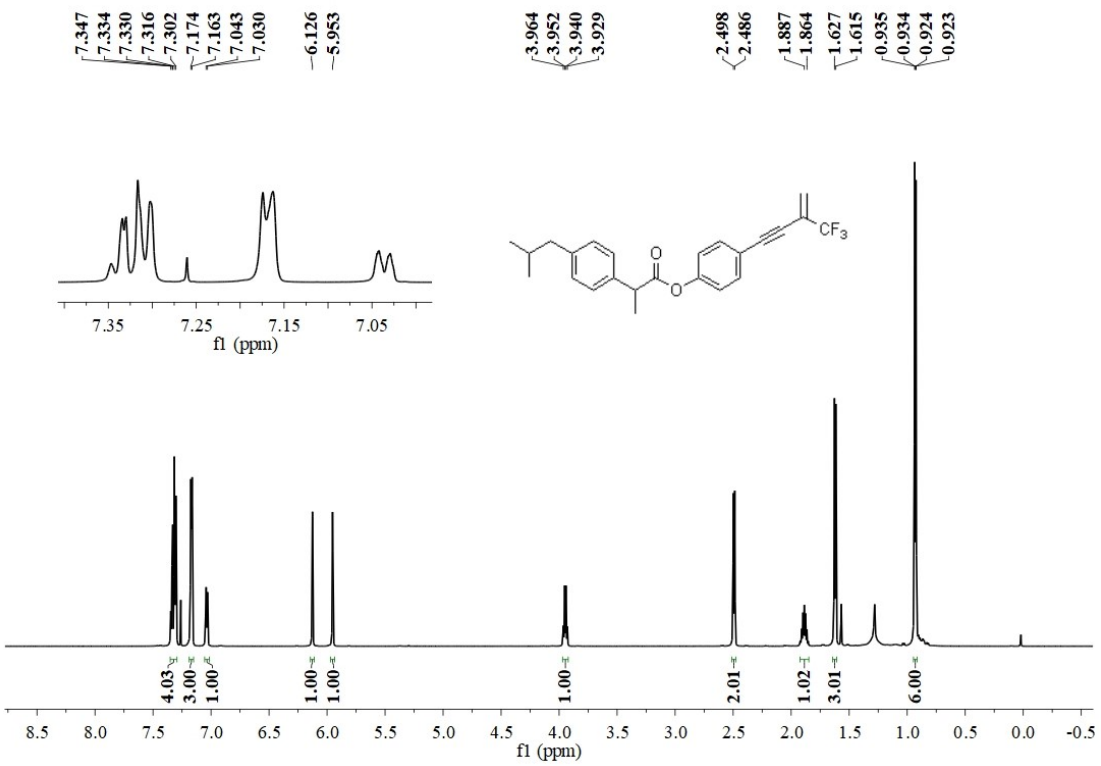
(1) (a) Priewisch, B.; Rück-Braun, K. Efficient Preparation of Nitrosoarenes for the Synthesis of Azobenzenes. *J. Org. Chem.* **2005**, *70*, 2350. (b) Hu, W.; Yu, J.-T.; Liu, S.; Jiang, Y.; Cheng, J. Copper-mediated Annulation of 2-(1-Arylvinyl) Anilines and Aryl Nitrosos towards 2,3-Diaryl-2*H*-indazoles. *Org. Chem. Front.* **2017**, *4*, 22.

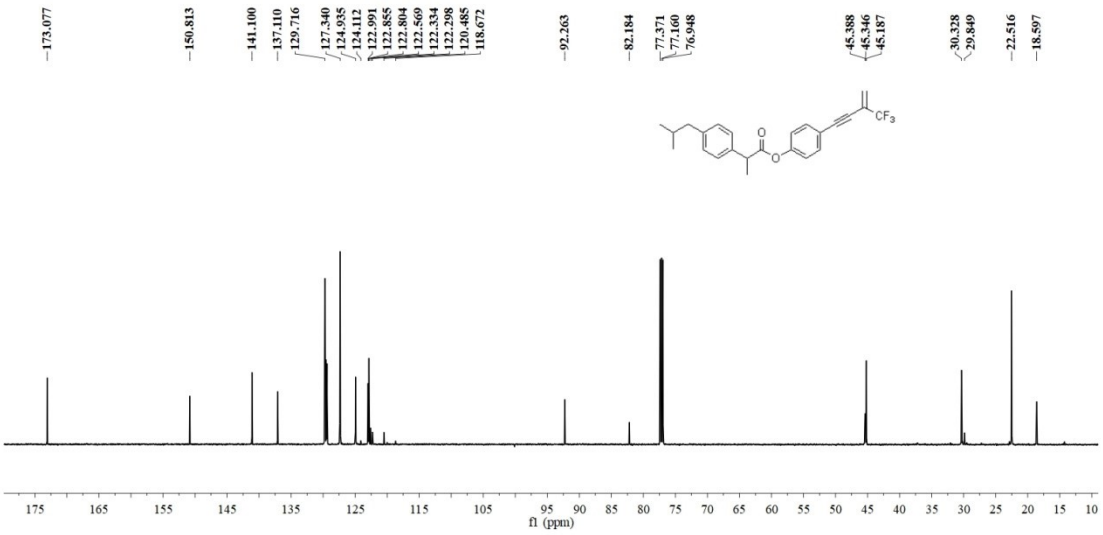
(2) Hu, C.-M.; Hong, F.; Xu, Y.-Y. Synthesis of trifluoromethyl-substituted conjugated enynes including a fluorinated siccayne. *J. Fluorine Chem*. **1993**, *64*, 1.

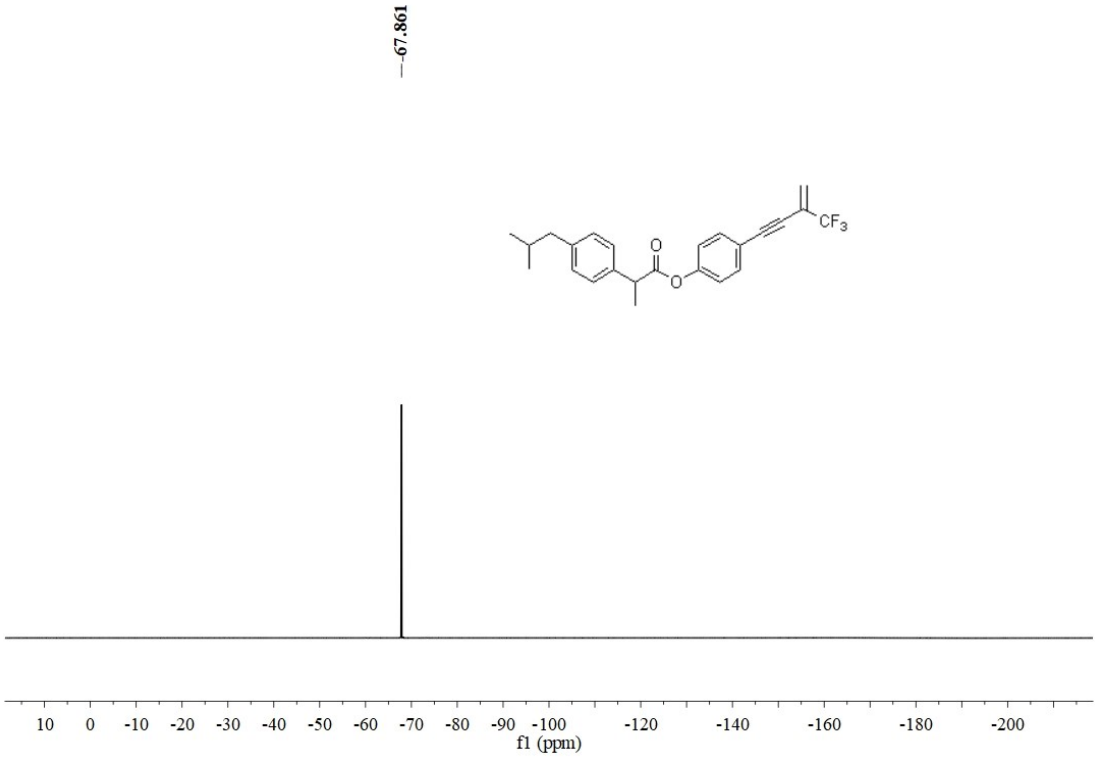
(3) März, M.; Kohout, M.; Neveselý, T.; Chudoba, J.; Prukała, D.; Niziński, S.; Sikorski, M.; Burdziński, G.; Cibulka, R. Azodicarboxylate-free esterification with triphenylphosphine mediated by flavin and visible light: method development and stereoselectivity control. *Org. Biomol. Chem.* **2018**, *16*, 6809.

(4) The information for compound **2n**, See: Zhang, J.; Ma, Z.-G.; Tian, Y.; Li, W.; Gao, W.-C.; Chang, H.-H. Divergent synthesis of fluorinated alkenes, allenes, and enynes via reaction of 2-trifluoromethyl-1,3-enynes with carbon nucleophiles. *J. Org. Chem.* **2022**, *87*, 15086.

10. ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra for substrate 2n

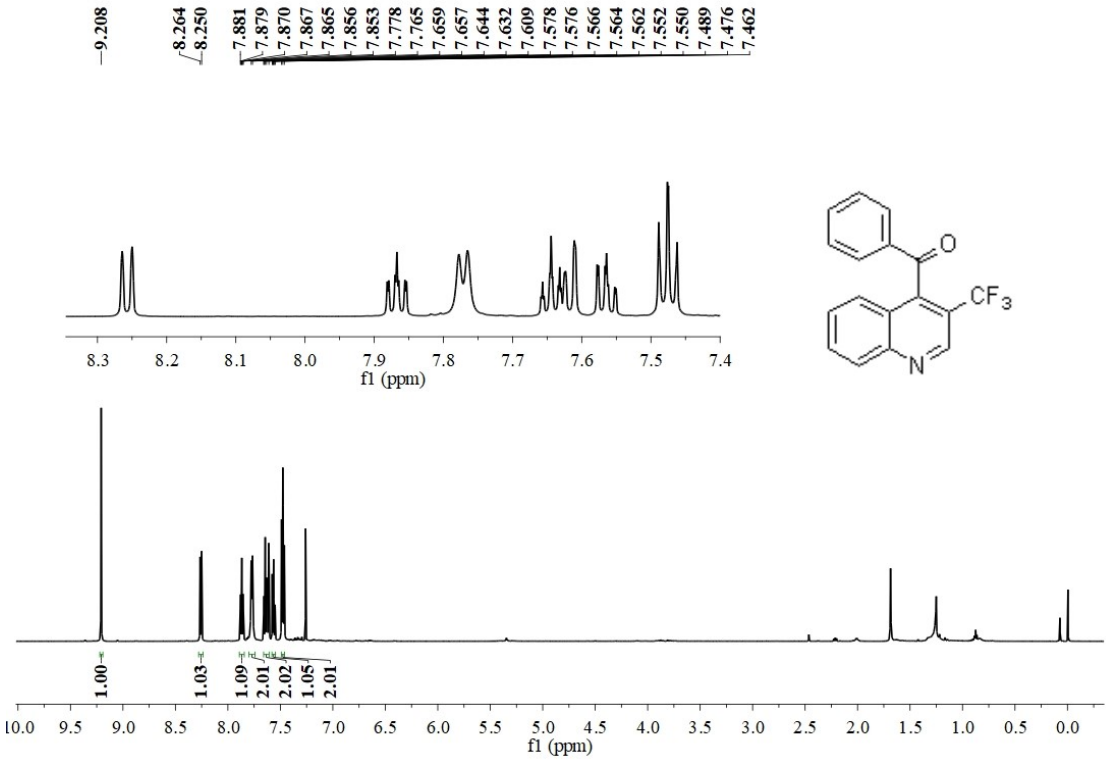


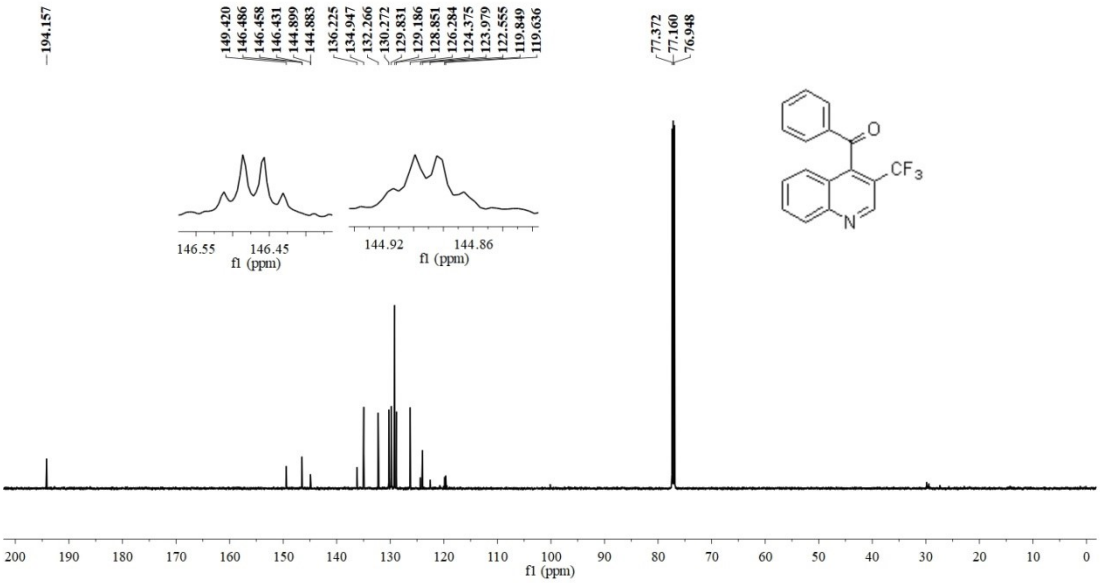


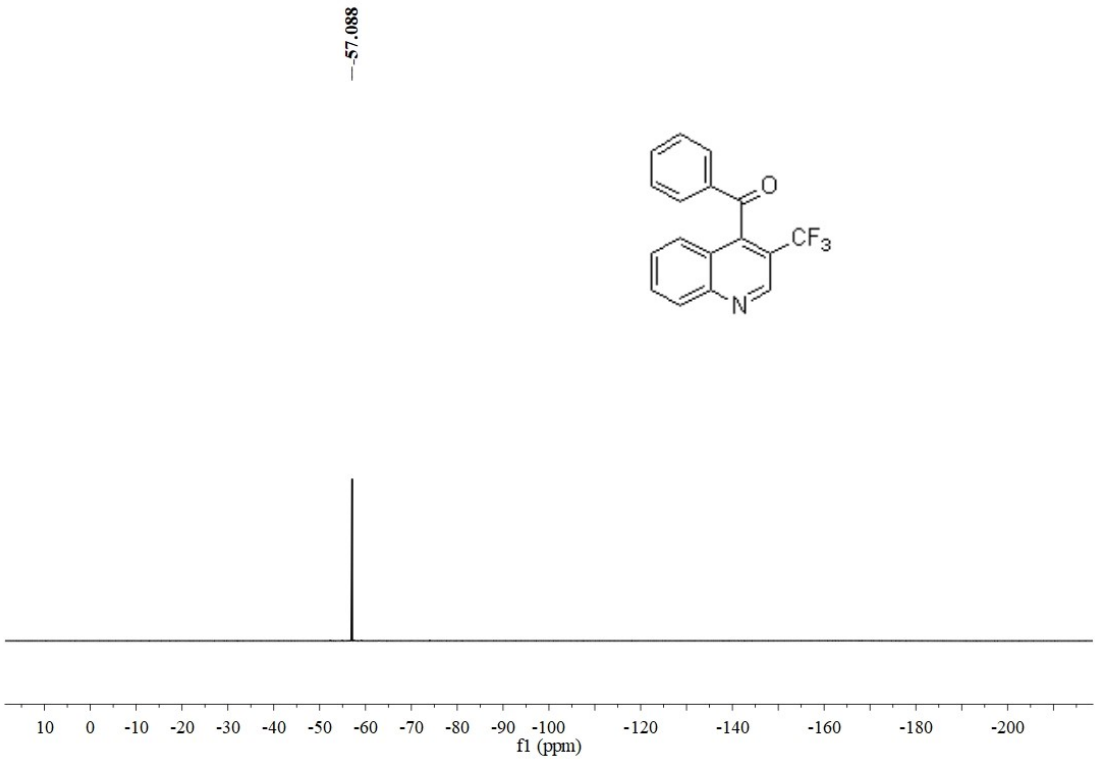


11. ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra for all products 3

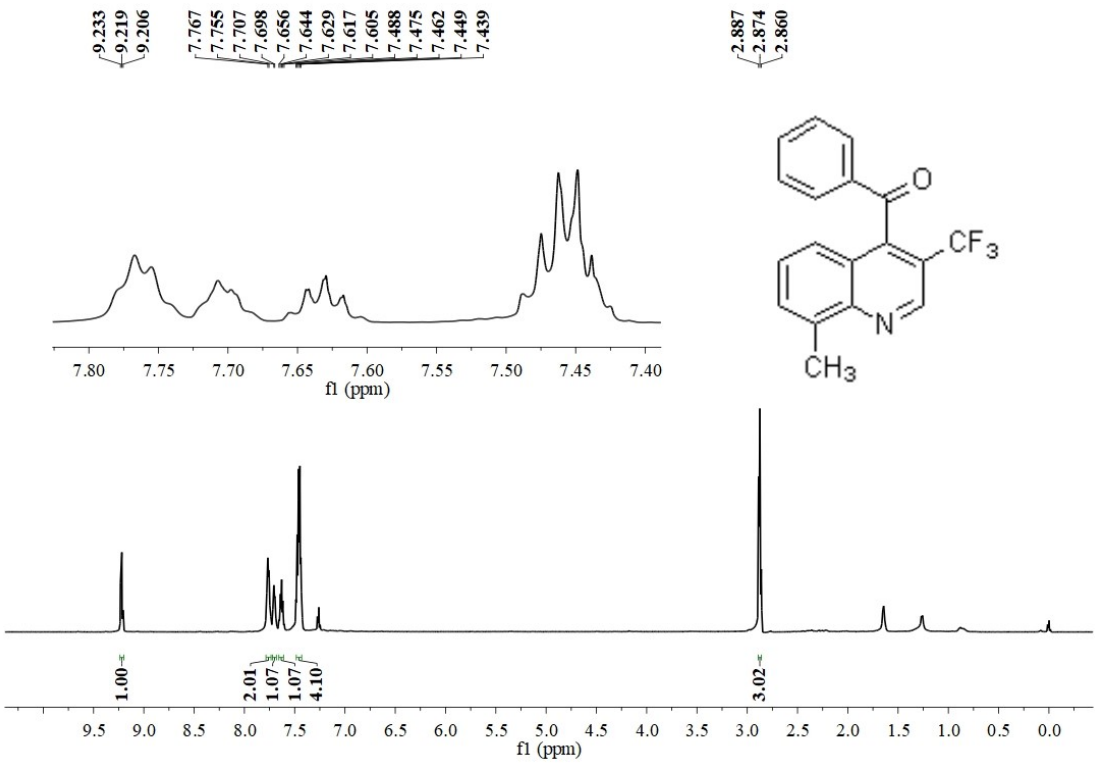
3aa

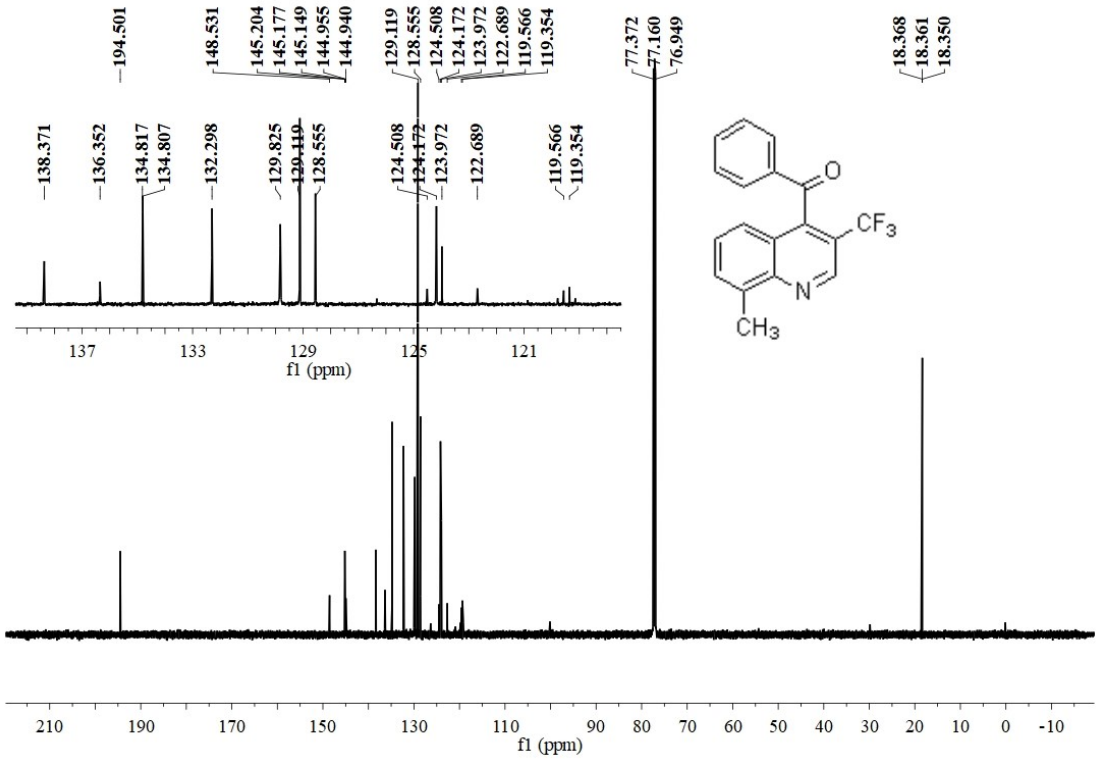


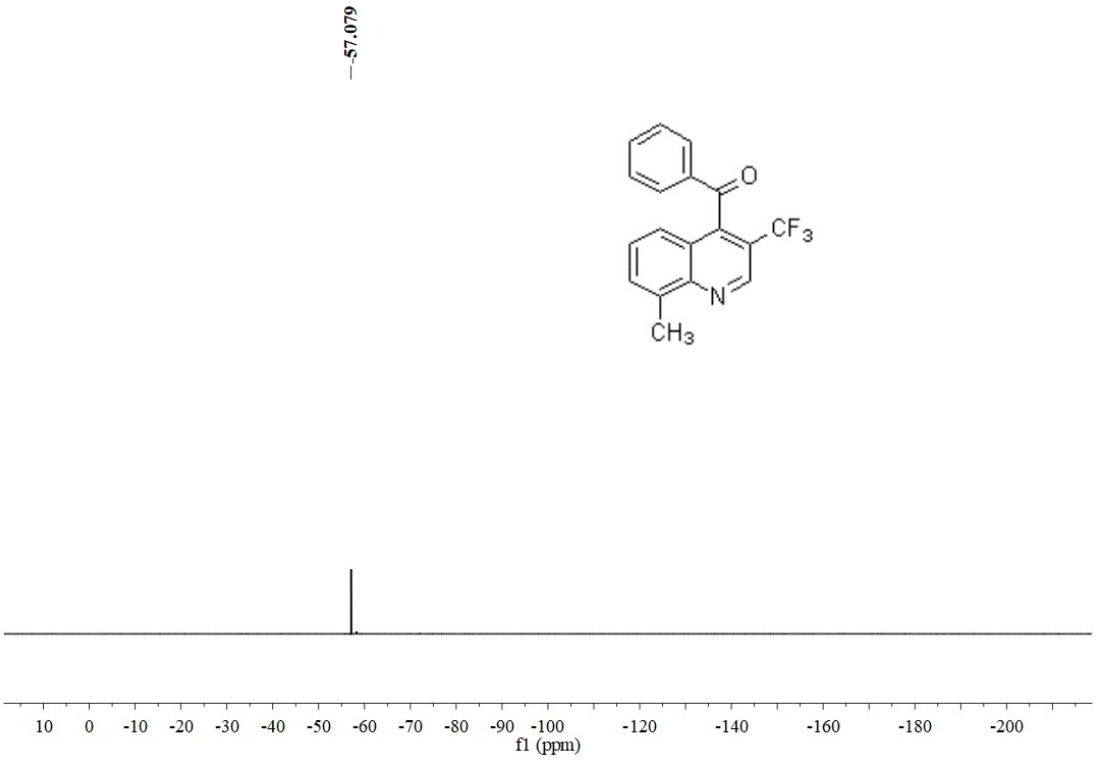

194.157
149.420
146.486
146.458
146.431
144.899
144.883
136.225
134.947
132.266
130.272
129.831
129.186
128.851
126.284
124.375
123.979
122.555
119.849
119.636
77.372
77.160
76.948
O
CF3
N
146.55
146.45
f1 (ppm)
144.92
144.86
f1 (ppm)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-57.088
O
CF3
N
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)

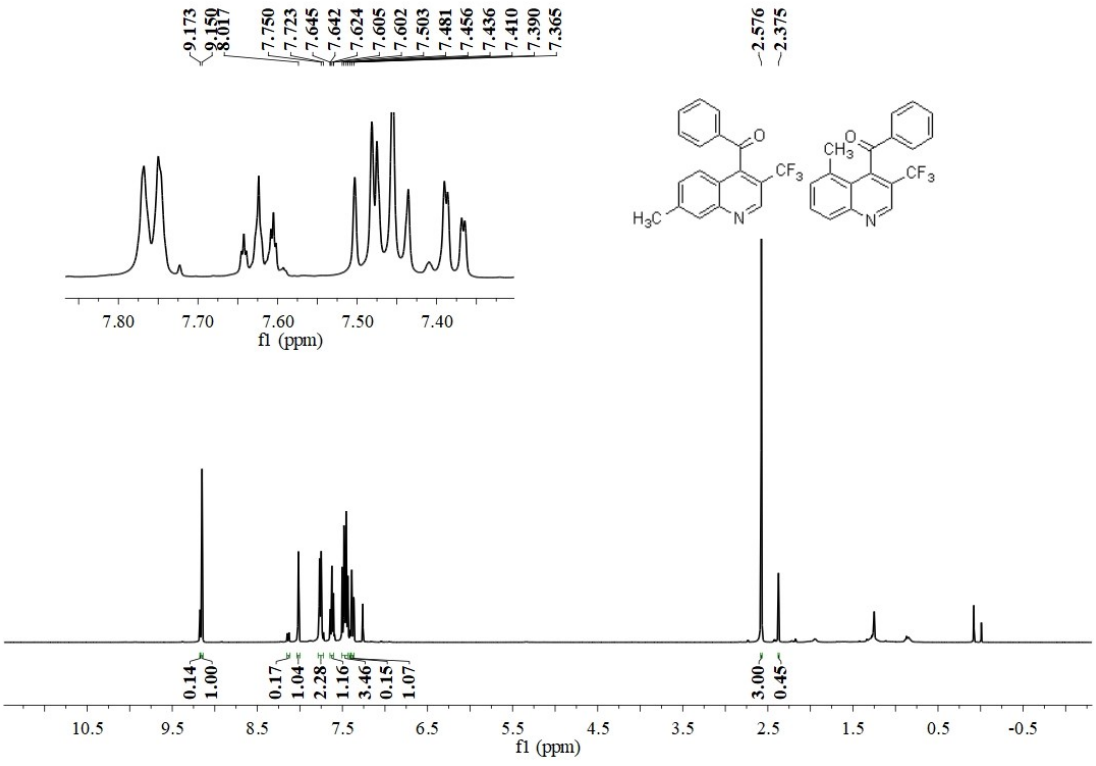
3ba

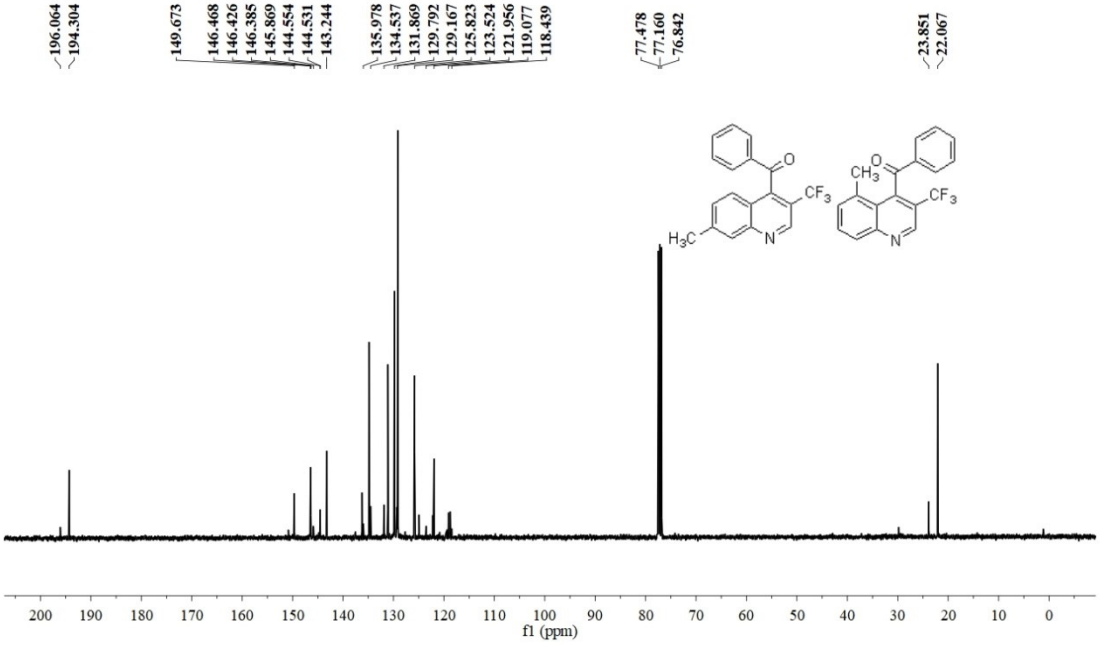

9.233
9.219
9.206
7.767
7.755
7.707
7.698
7.656
7.644
7.629
7.617
7.605
7.488
7.475
7.462
7.449
7.439
2.887
2.874
2.860
O
CF3
N
CH3
7.80 7.75 7.70 7.65 7.60 7.55 7.50 7.45 7.40
f1 (ppm)
1.00
2.01
1.07
1.07
4.10
3.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

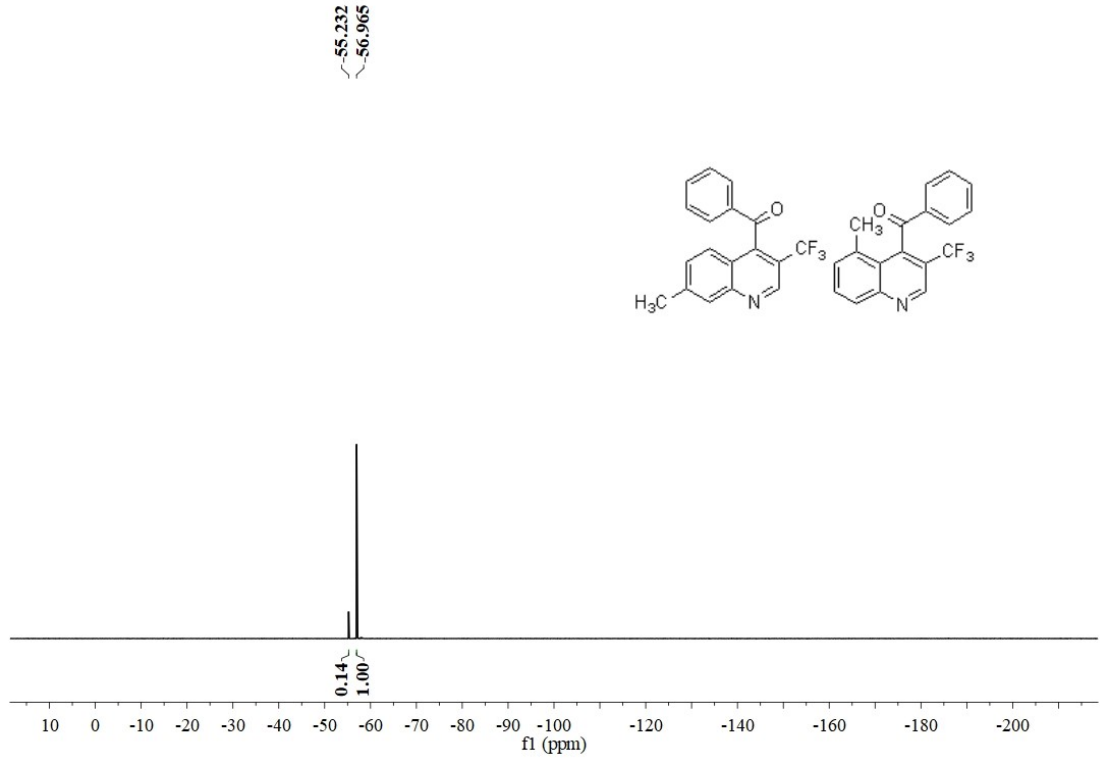

194.501
148.531
145.204
145.177
145.149
144.955
144.940
129.119
128.555
124.508
124.172
123.972
122.689
119.566
119.354
77.372
77.160
76.949
18.368
18.361
18.350
138.371
136.352
134.817
134.807
132.298
129.825
129.419
128.555
124.508
124.172
123.972
122.689
119.566
119.354
O
CF3
N
CH3
137 133 129 125 121
f1 (ppm)
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-57.079
O
CF3
N
CH3
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)

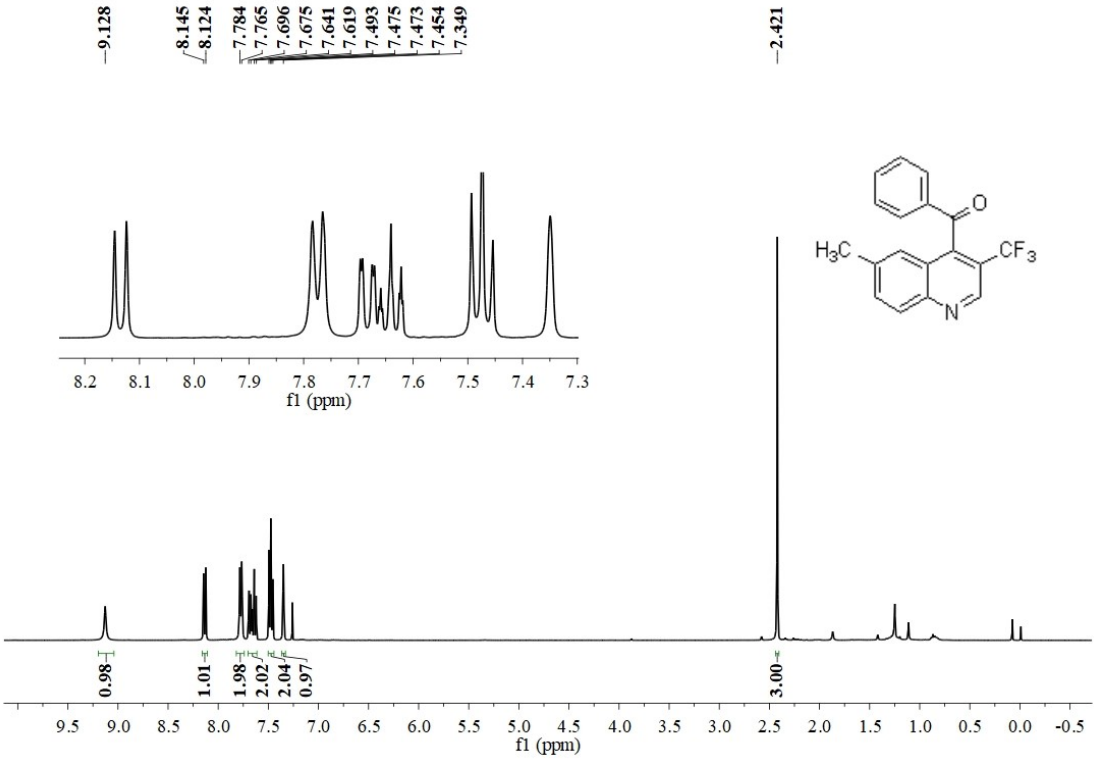
3ca + 3c'a

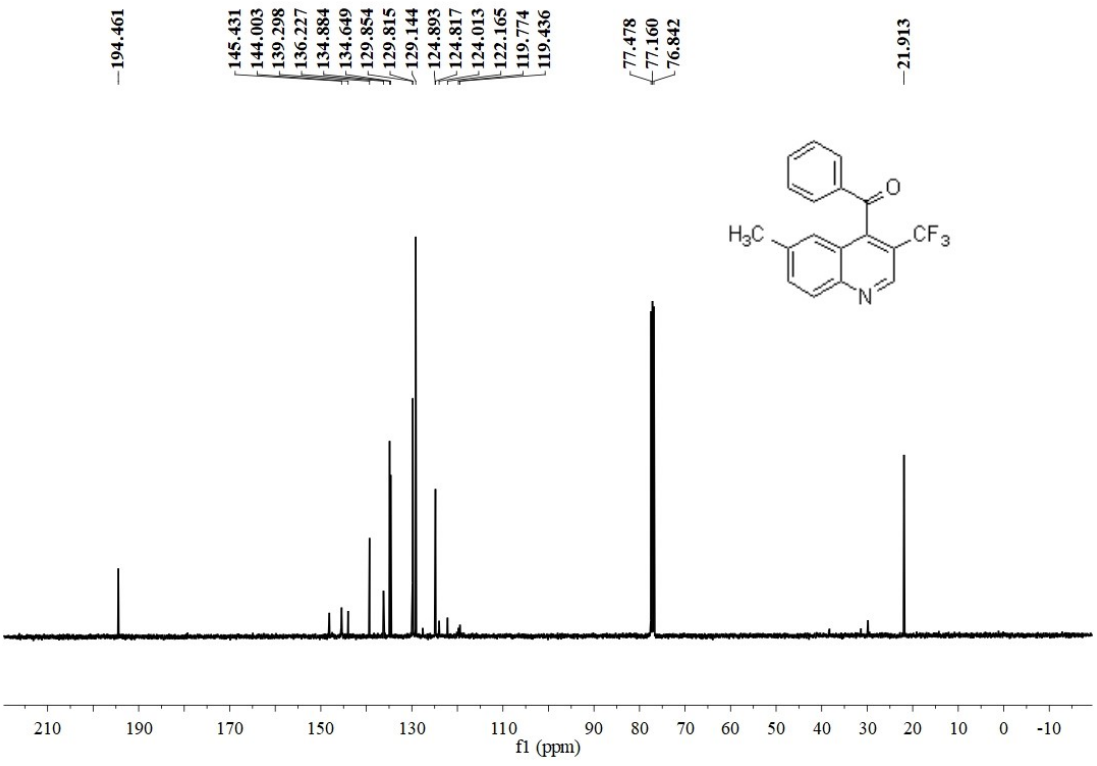

9.173
9.150
8.017
7.750
7.723
7.645
7.642
7.624
7.605
7.602
7.503
7.481
7.456
7.436
7.410
7.390
7.365
2.576
2.375
O
CF3
H3C
CH3
7.80 7.70 7.60 7.50 7.40
f1 (ppm)
0.14
1.00
0.17
1.04
2.28
1.16
3.46
0.15
1.07
3.00
0.45
10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.5
f1 (ppm)

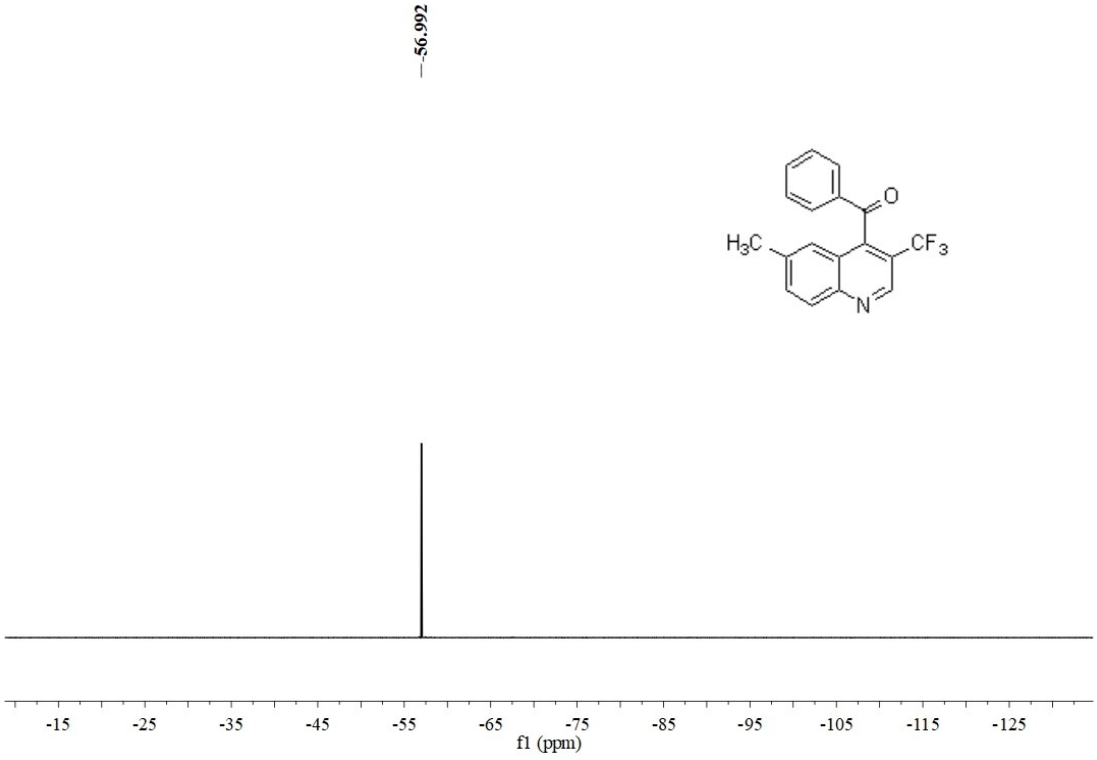

196.064
194.304
149.673
146.468
146.426
146.385
145.869
144.554
144.531
143.244
135.978
134.537
131.869
129.792
129.167
125.823
123.524
121.956
119.077
118.439
77.478
77.160
76.842
23.851
22.067
O
CF3
H3C
N
CH3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


55.232
56.965
O
CF3
H3C
N
CH3
0.14
1.00
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)

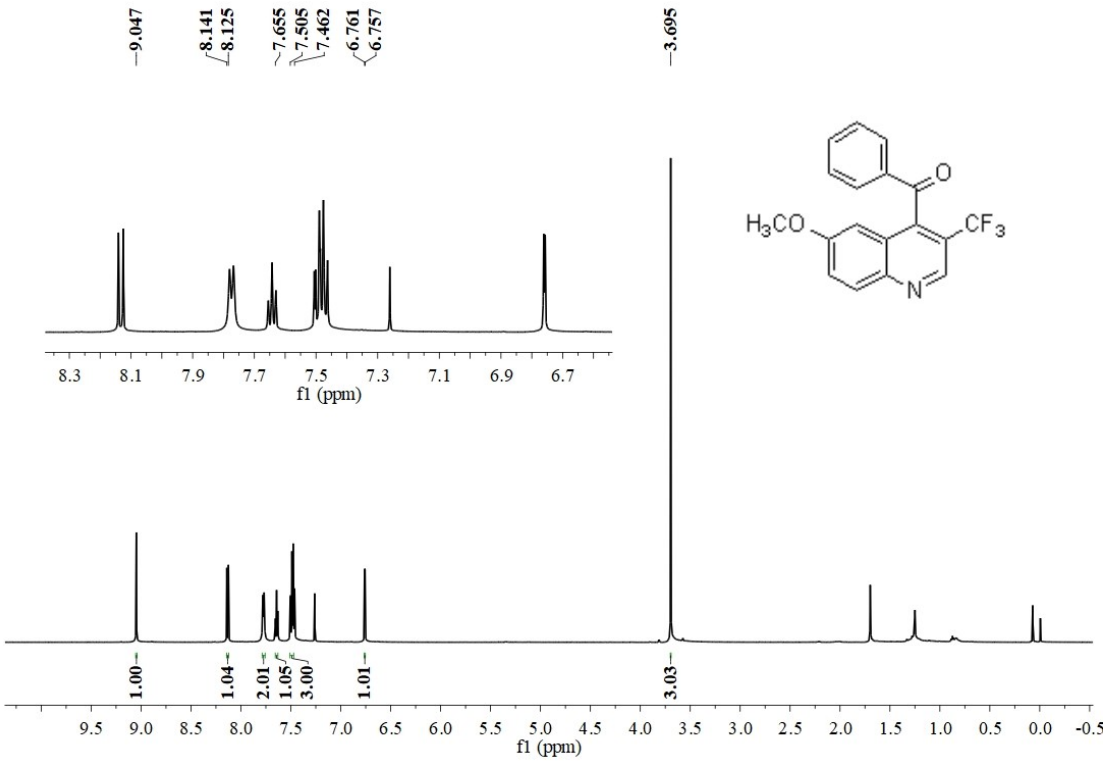
3da

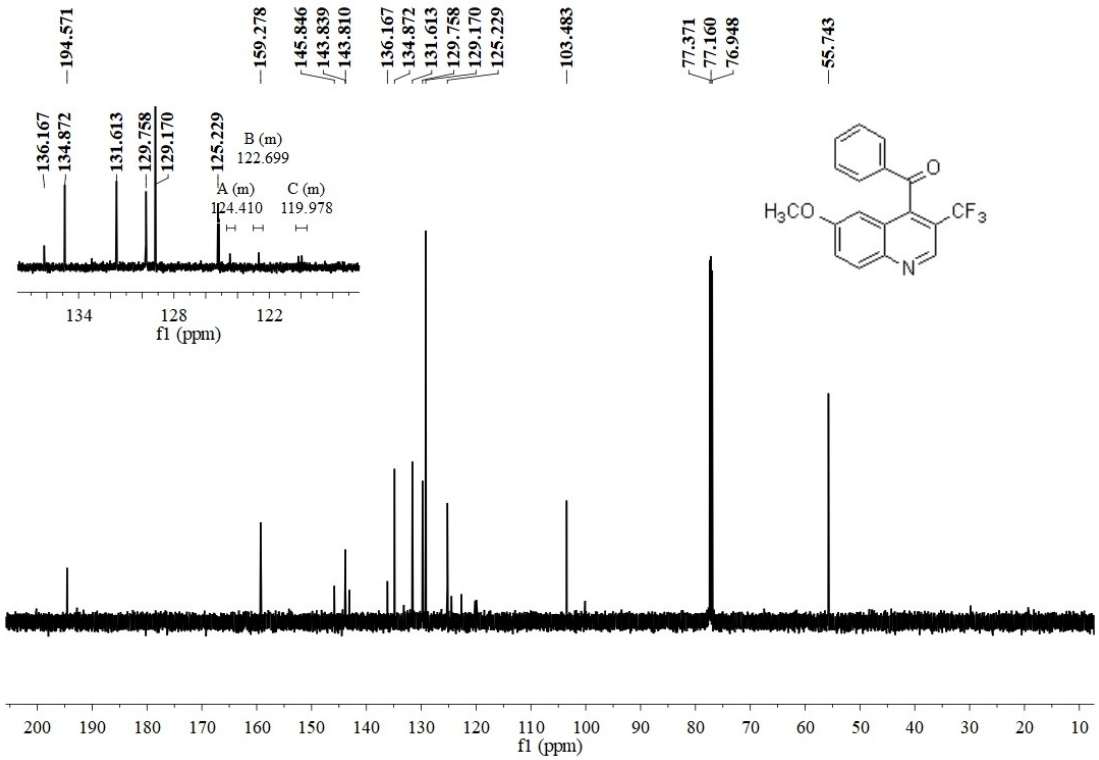

9.128
8.145
8.124
7.784
7.765
7.696
7.675
7.641
7.619
7.493
7.475
7.473
7.454
7.349
2.421
O
H3C
CF3
N
8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3
f1 (ppm)
0.98
1.01
1.98
2.02
2.04
0.97
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

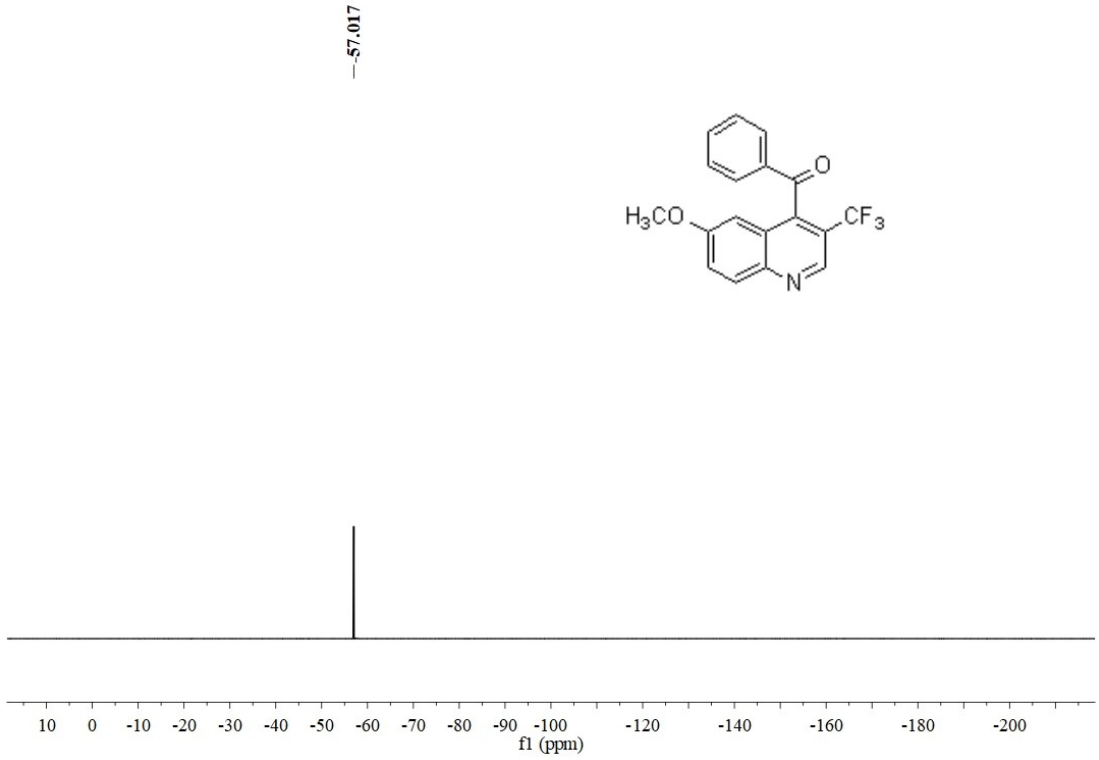

194.461
145.431
144.003
139.298
136.227
134.884
134.649
129.854
129.815
129.144
124.893
124.817
124.013
122.165
119.774
119.436
77.478
77.160
76.842
21.913
O
H3C
CF3
N
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-56.992
O
H3C
CF3
N
-15
-25
-35
-45
-55
-65
-75
-85
-95
-105
-115
-125
f1 (ppm)

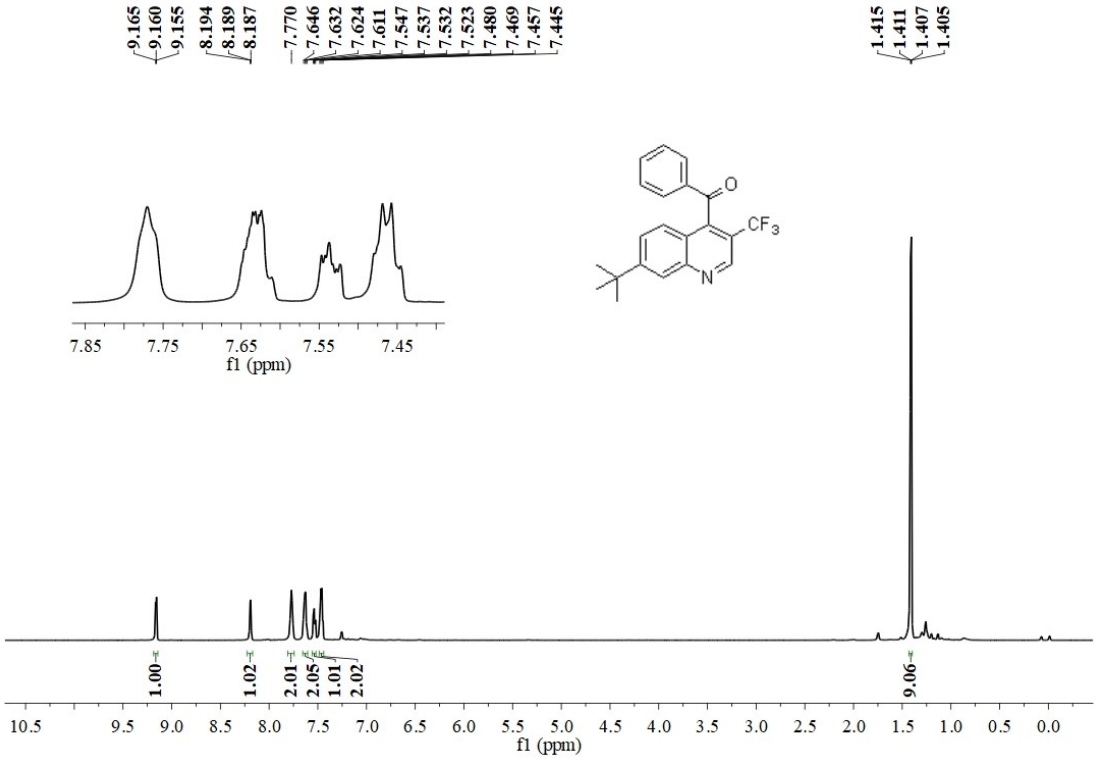
3ea

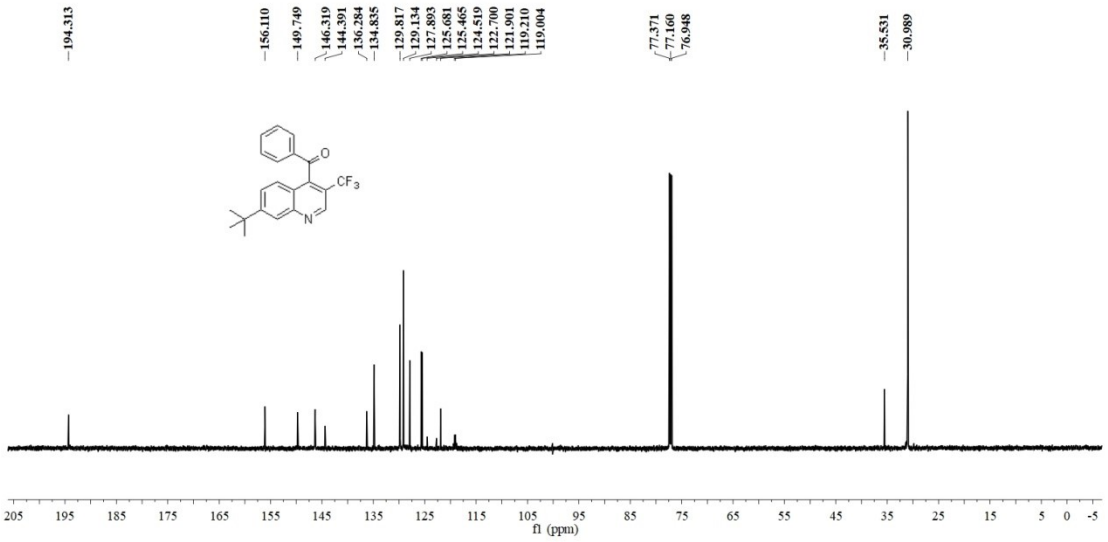

9.047
8.141
8.125
7.655
7.505
7.462
6.761
6.757
3.695
O
H3CO
CF3
N
8.3
8.1
7.9
7.7
7.5
7.3
7.1
6.9
6.7
f1 (ppm)
1.00
1.04
2.01
1.05
3.00
1.01
3.03
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

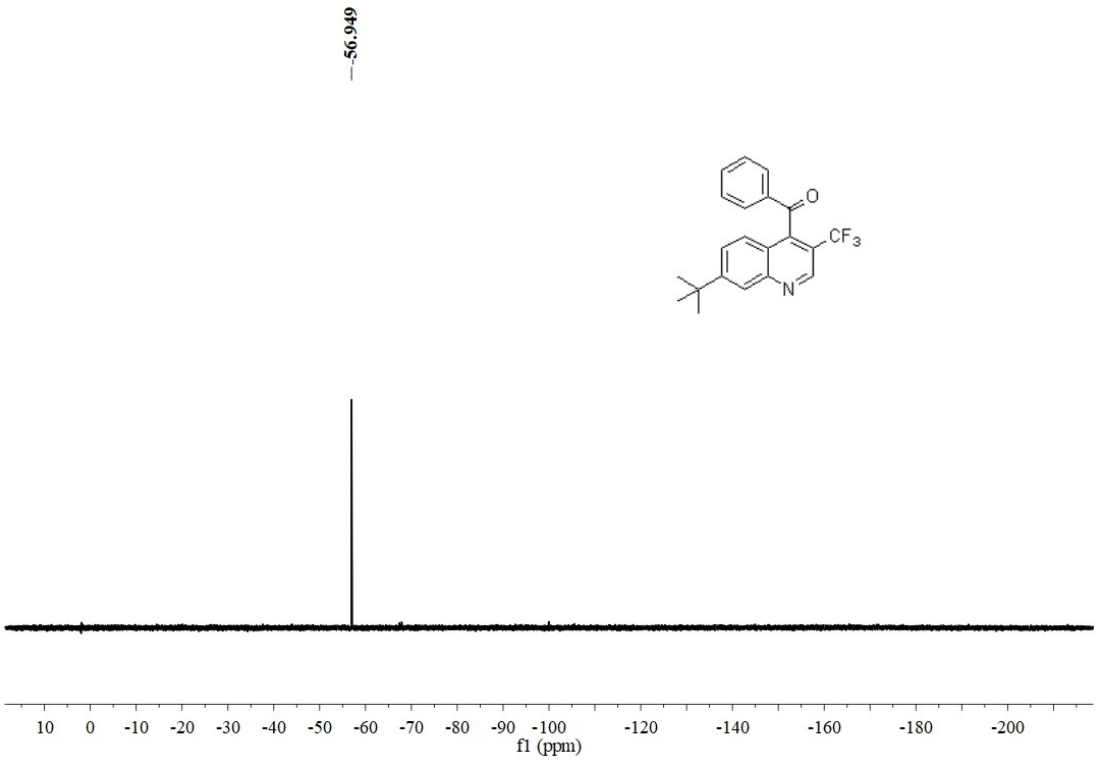

194.571
159.278
145.846
143.839
143.810
136.167
134.872
131.613
129.758
129.170
125.229
103.483
77.371
77.160
76.948
55.743
B (m)
122.699
A (m)
124.410
C (m)
119.978
f1 (ppm)
O
H3CO
CF3
N


57.017
O
H3CO
CF3
N
f1 (ppm)

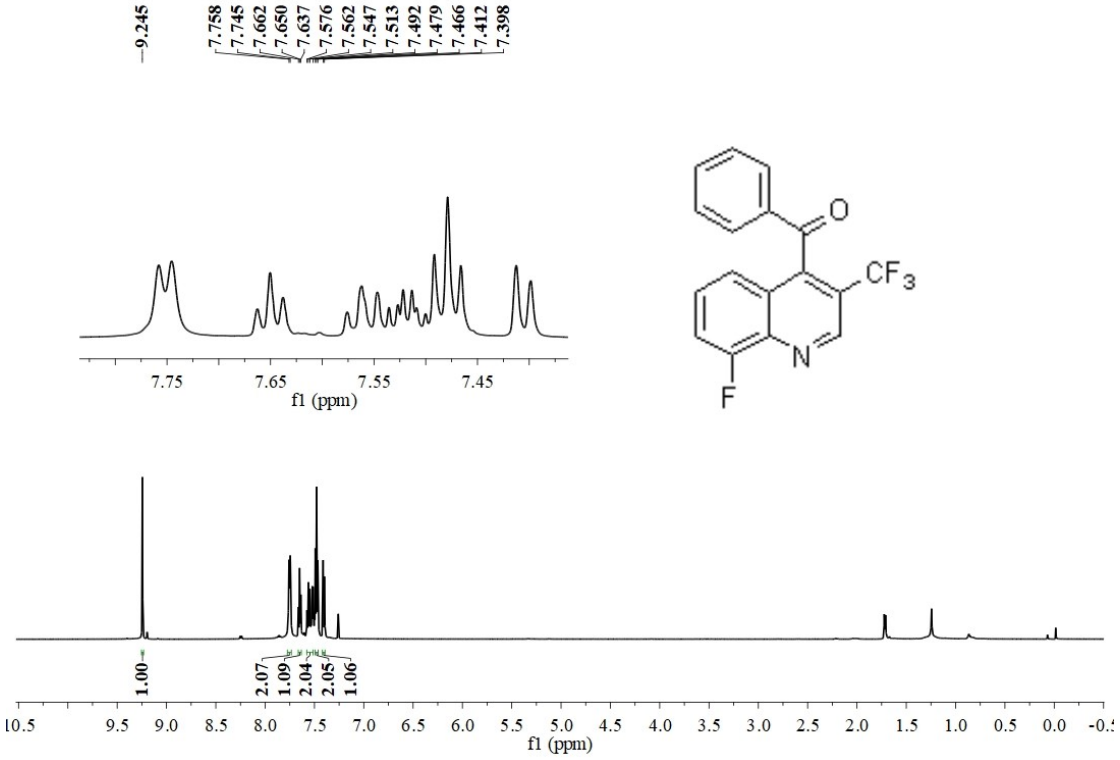
3ga

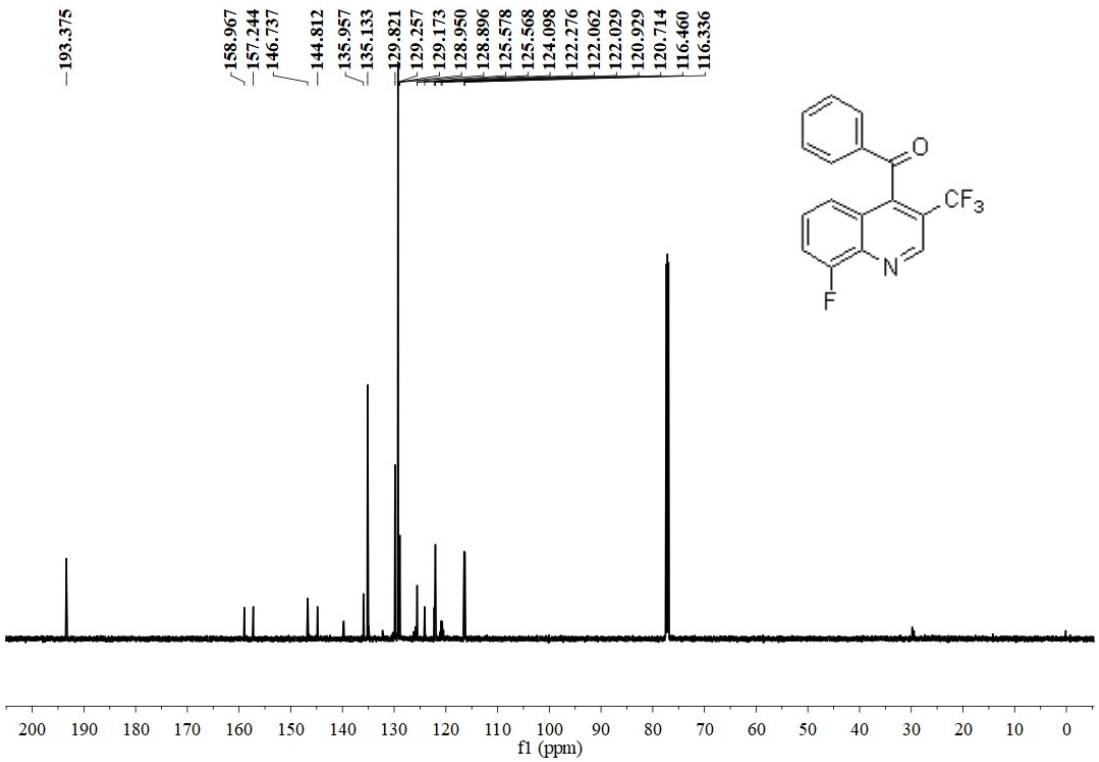

9.165
9.160
9.155
8.194
8.189
8.187
7.770
7.646
7.632
7.624
7.611
7.547
7.537
7.532
7.523
7.480
7.469
7.457
7.445
1.415
1.411
1.407
1.405
O
CF3
N
7.85
7.75
7.65
7.55
7.45
f1 (ppm)
1.00
1.02
2.01
2.05
1.01
2.02
9.06
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


194.313
156.110
149.749
146.319
144.391
136.284
134.835
129.817
129.134
127.893
125.681
125.465
124.519
122.700
121.901
119.210
119.004
77.371
77.160
76.948
35.531
30.989
O
CF3
N
205
195
185
175
165
155
145
135
125
115
105
95
85
75
65
55
45
35
25
15
5
0
-5
f1 (ppm)


-56.949
O
CF3
N
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)

3ha


9.245
7.758
7.745
7.662
7.650
7.637
7.576
7.562
7.547
7.513
7.492
7.479
7.466
7.412
7.398
O
CF3
N
F
7.75 7.65 7.55 7.45
f1 (ppm)
1.00
2.07
1.09
2.04
2.05
1.06
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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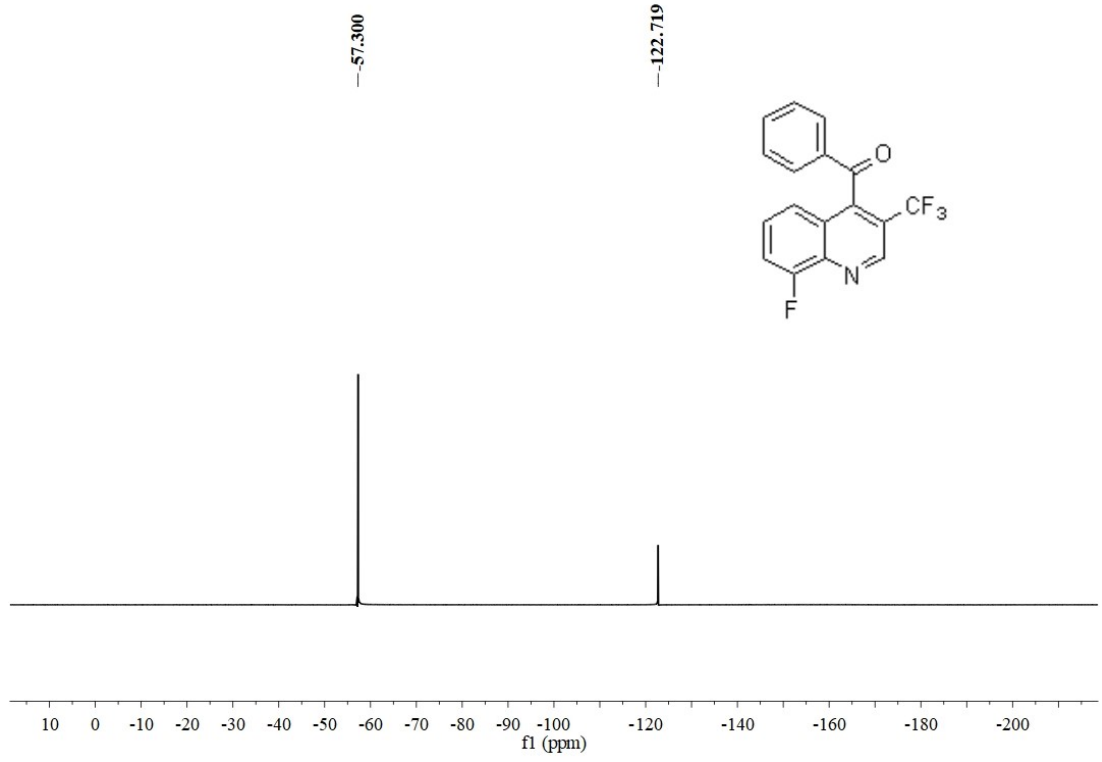
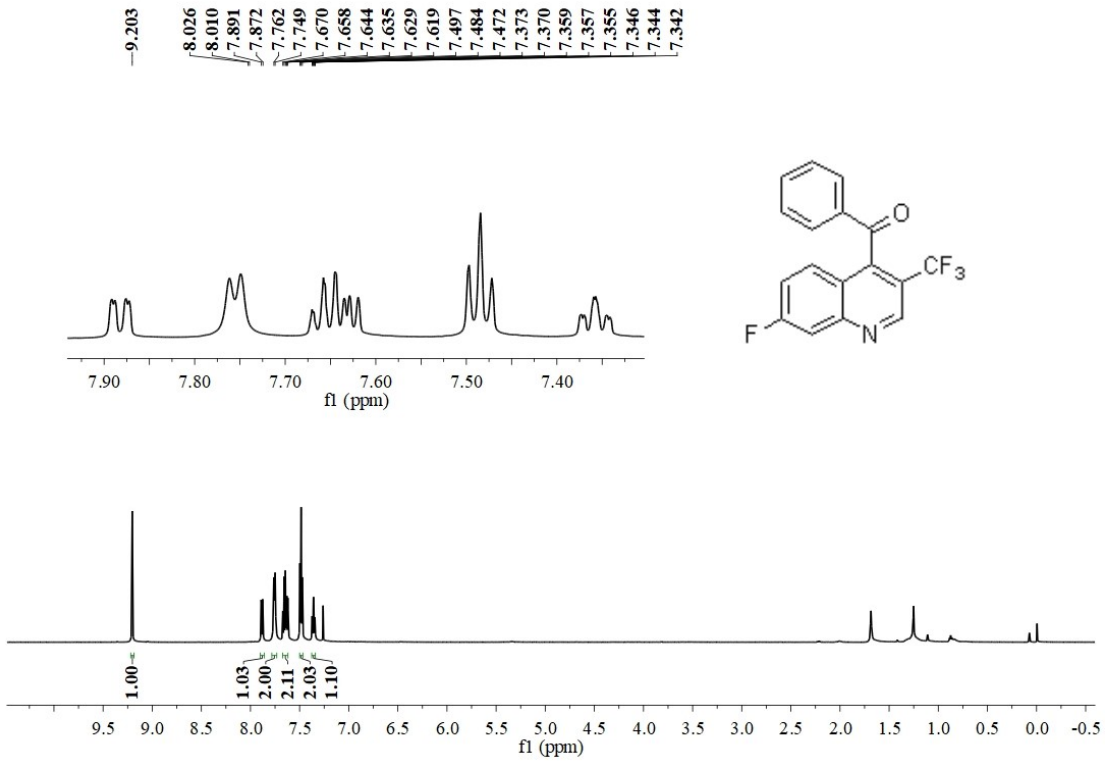
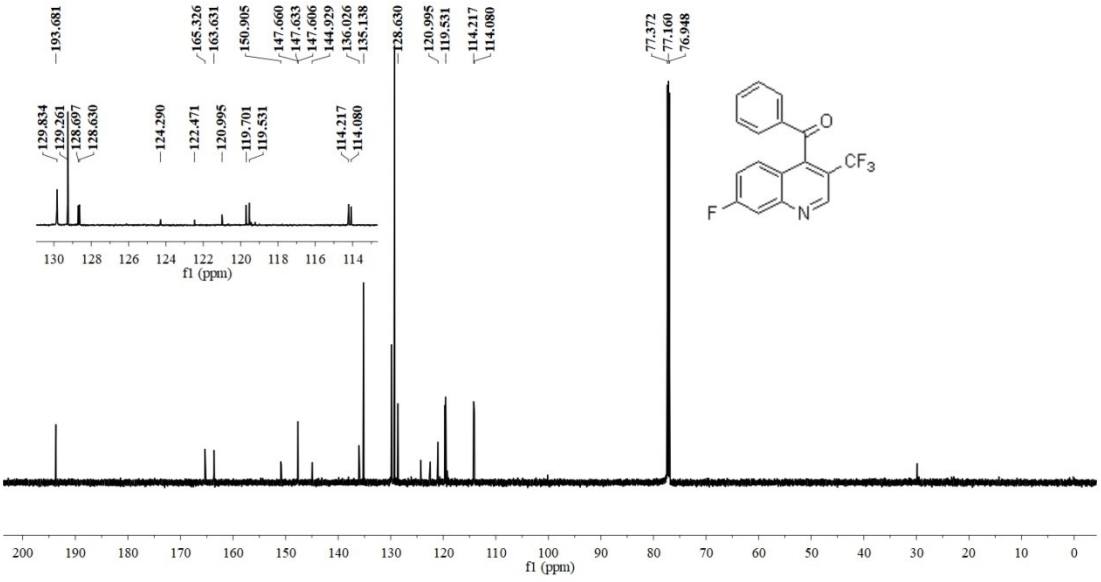
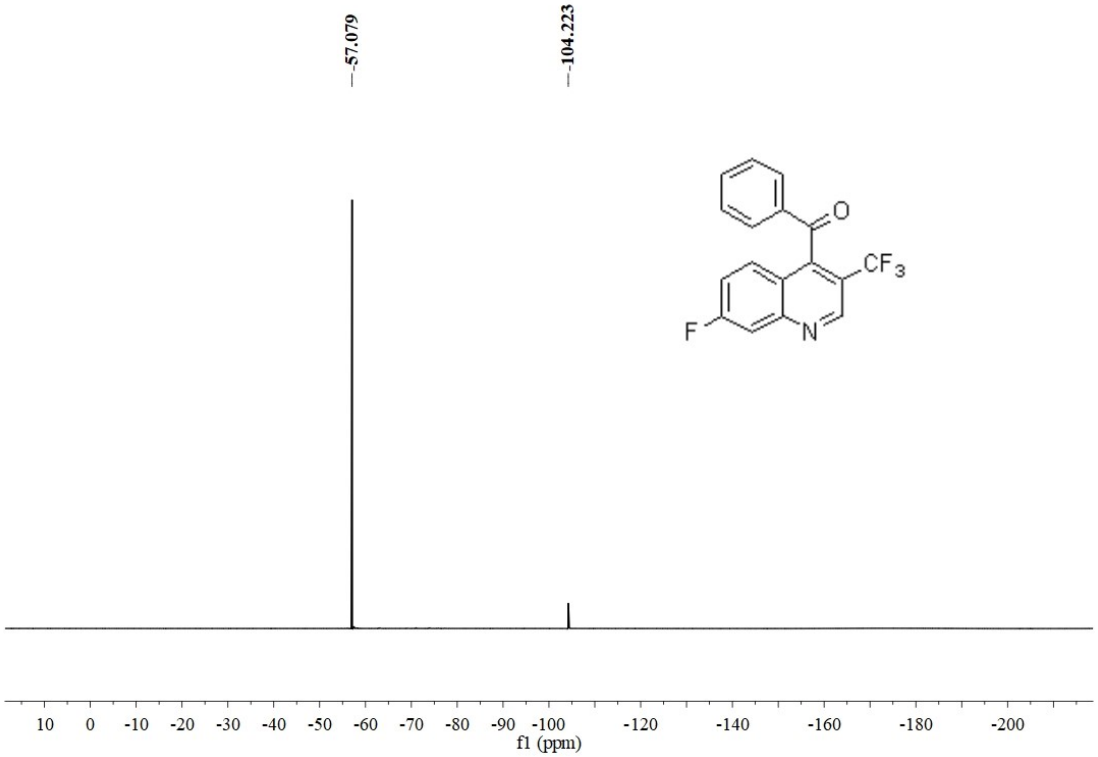
157.244
146.737
144.812
135.957
135.133
129.821
129.257
129.173
128.950
128.896
125.578
125.568
124.098
122.276
122.062
122.029
120.929
120.714
116.460
116.336
O
CF3
N
F
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-57.300
-122.719
O
CF3
N
F
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)

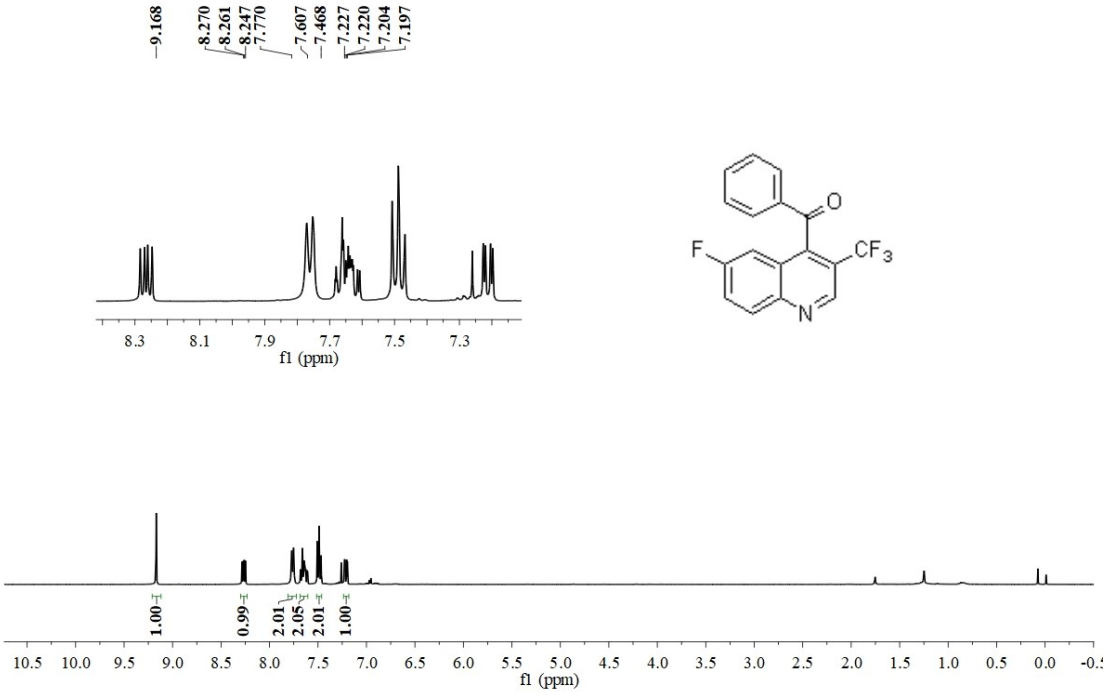
3ia

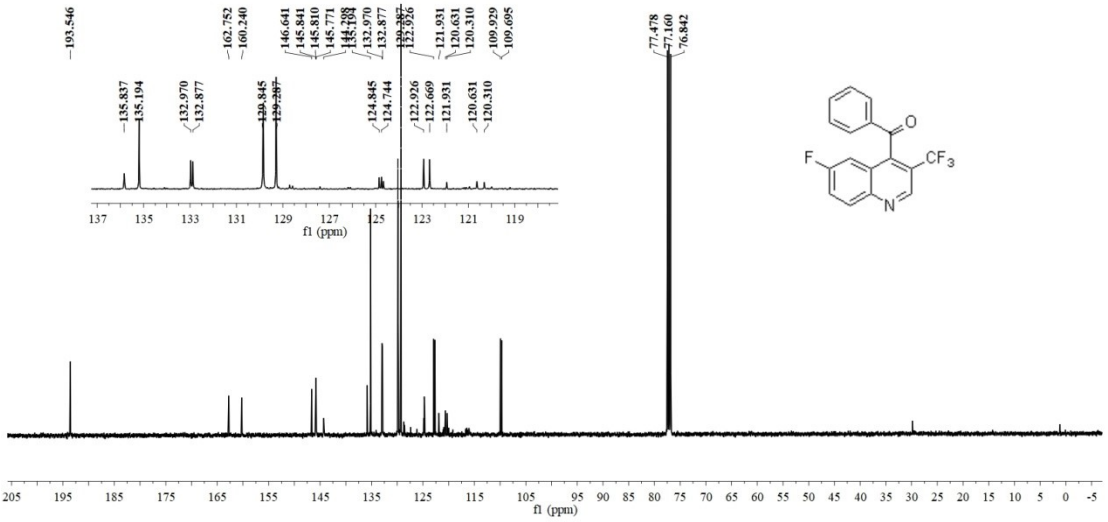

9.203
8.026
8.010
7.891
7.872
7.762
7.749
7.670
7.658
7.644
7.635
7.629
7.619
7.497
7.484
7.472
7.373
7.370
7.359
7.357
7.355
7.346
7.344
7.342
O
CF3
F
N
7.90
7.80
7.70
7.60
7.50
7.40
f1 (ppm)
1.00
1.03
2.00
2.11
2.03
1.10
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

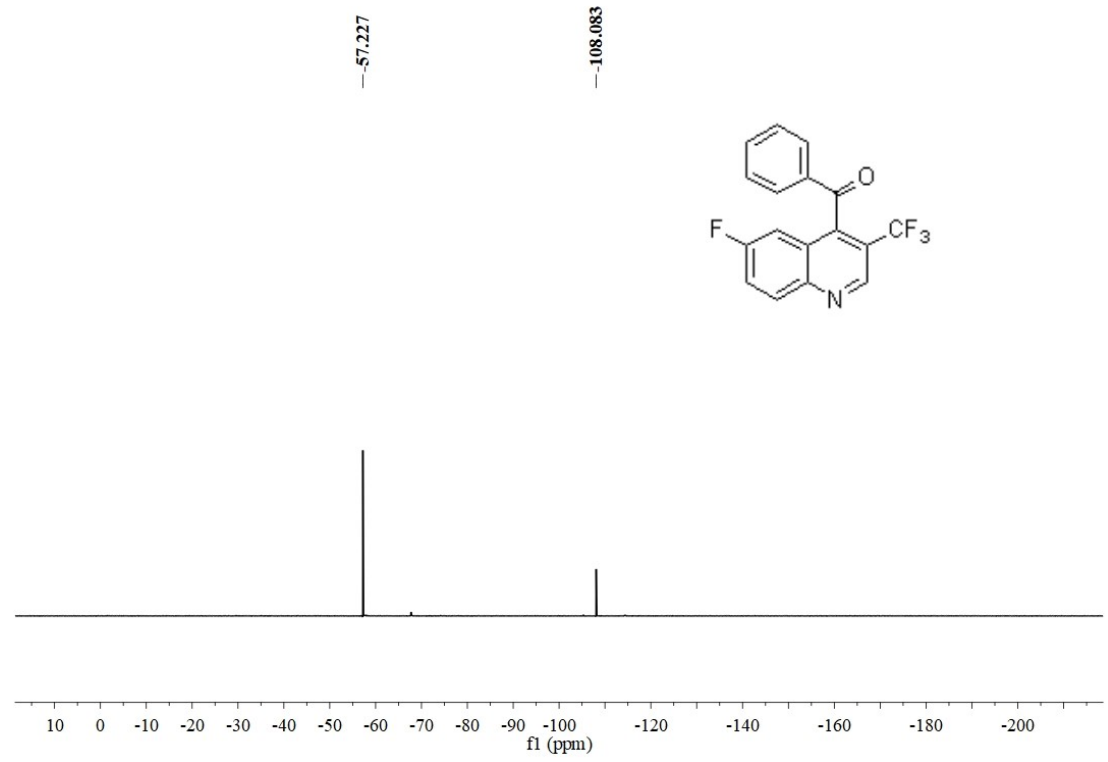

193.681
165.326
163.631
150.905
147.660
147.633
147.606
144.929
136.026
135.138
128.630
120.995
119.531
114.217
114.080
77.372
77.160
76.948
129.834
129.261
128.697
128.630
124.290
122.471
120.995
119.701
119.531
114.217
114.080
O
CF3
F
N
130
128
126
124
122
120
118
116
114
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-57.079
-104.223
O
CF3
F
N
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)

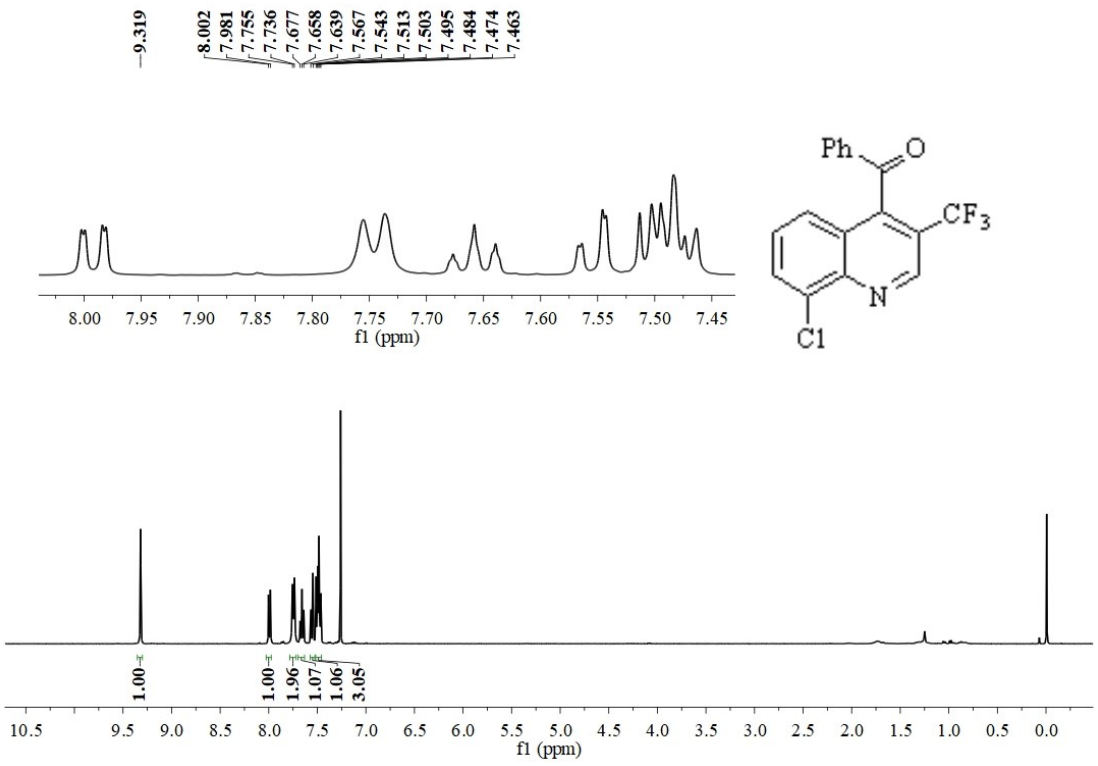
3ja

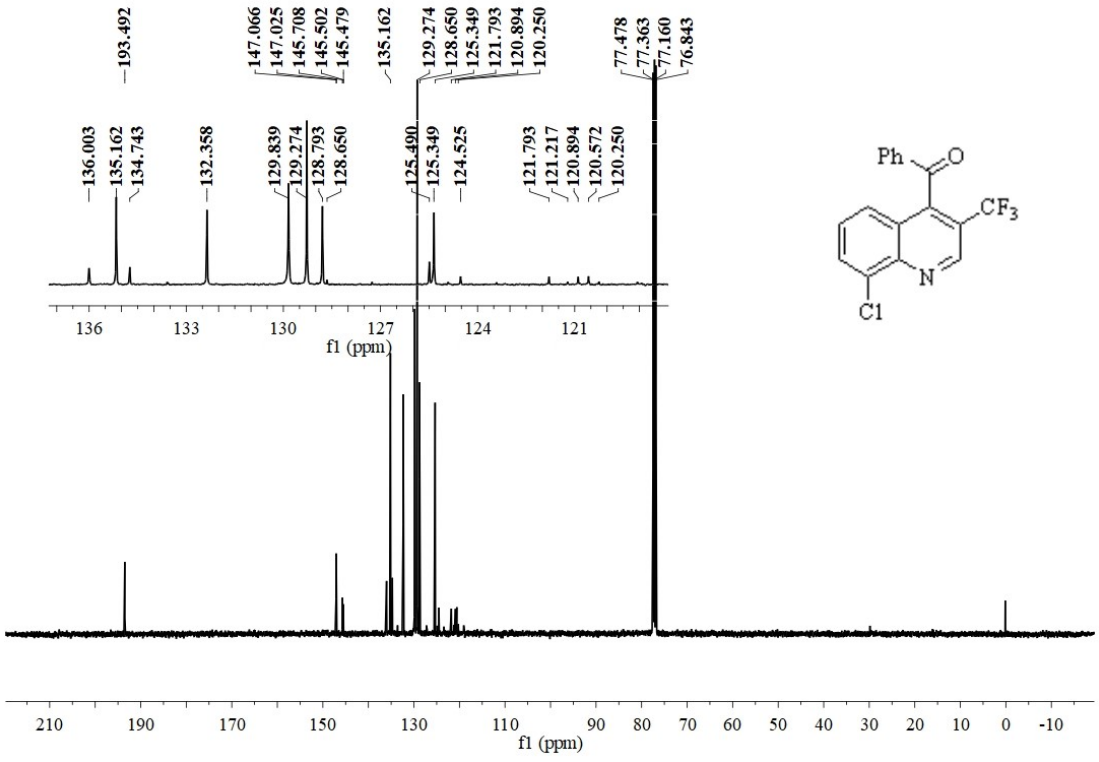

9.168
8.270
8.261
8.247
7.770
7.607
7.468
7.227
7.220
7.204
7.197
O
F
CF3
N
8.3 8.1 7.9 7.7 7.5 7.3
f1 (ppm)
1.00
0.99
2.01
2.05
2.01
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

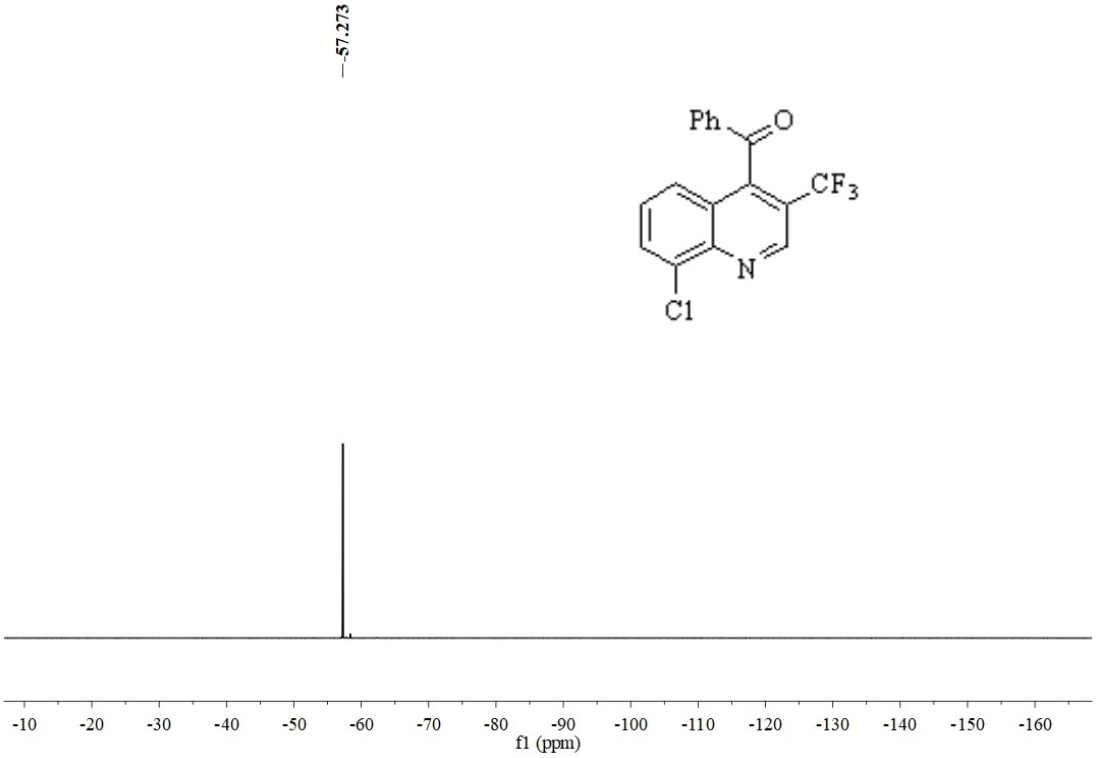

193.546
162.752
160.240
146.641
145.841
145.810
145.771
132.970
132.877
121.931
120.631
120.310
109.929
109.695
77.478
77.160
76.842
135.837
135.194
132.970
132.877
120.845
120.287
124.845
124.744
122.926
122.669
121.931
120.631
120.310
O
F
CF3
N
f1 (ppm)


-57.227
-108.083
O
F
CF3
N
f1 (ppm)

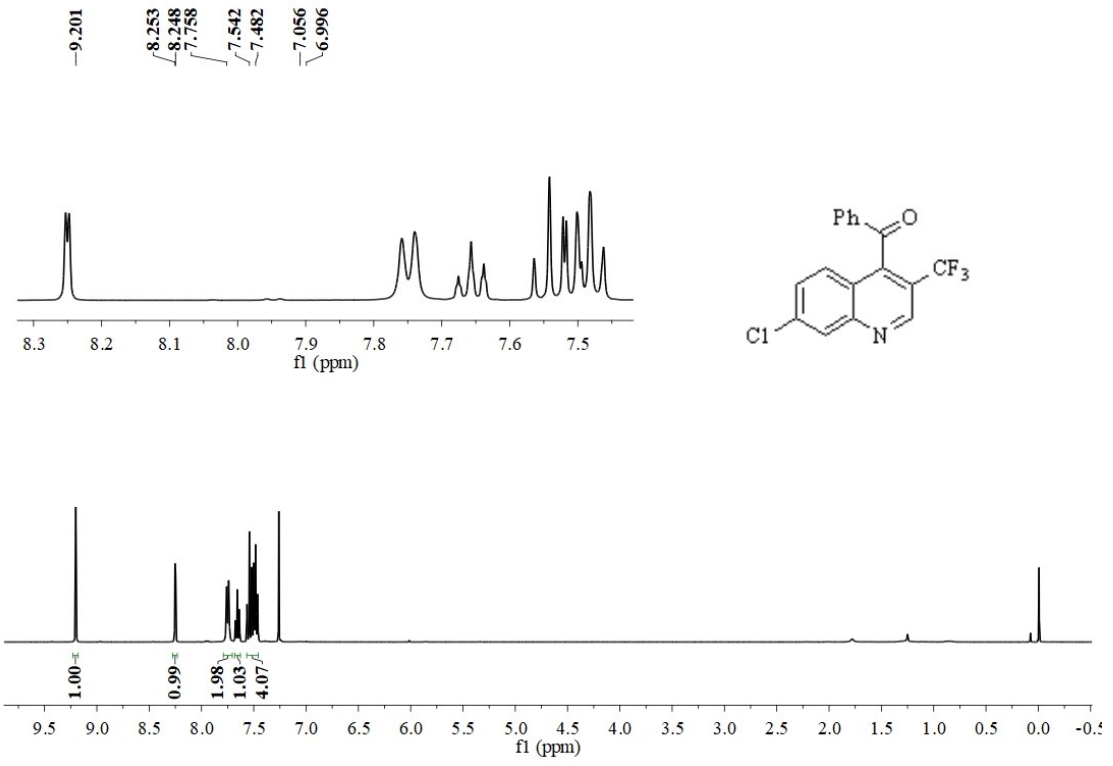
3ka

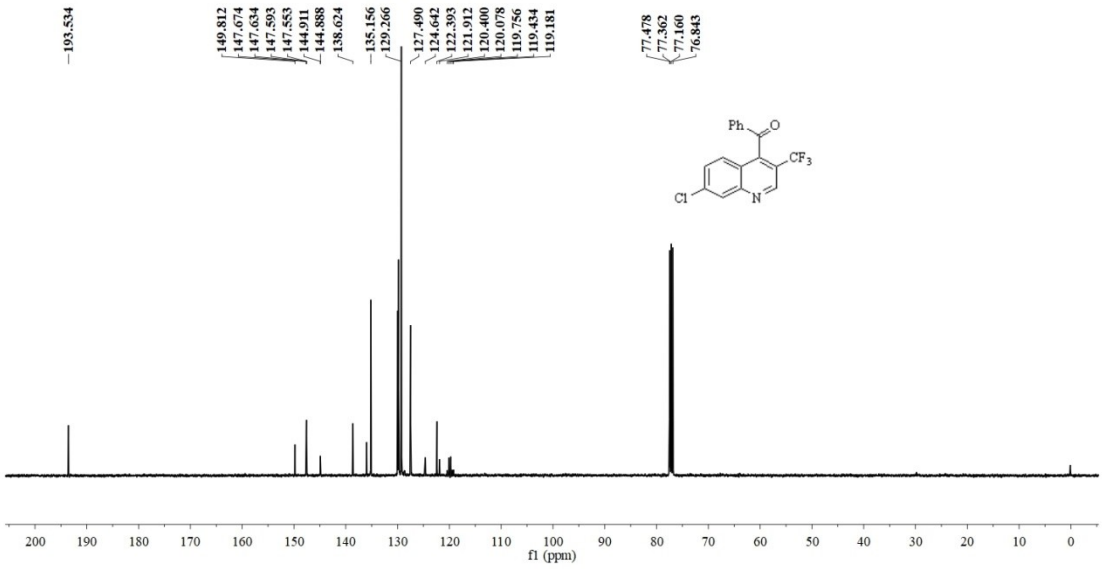

9.319
8.002
7.981
7.755
7.736
7.677
7.658
7.639
7.567
7.543
7.513
7.503
7.495
7.484
7.474
7.463
f1 (ppm)
Ph
O
CF3
N
C1
1.00
1.00
1.96
1.07
1.06
3.05
f1 (ppm)

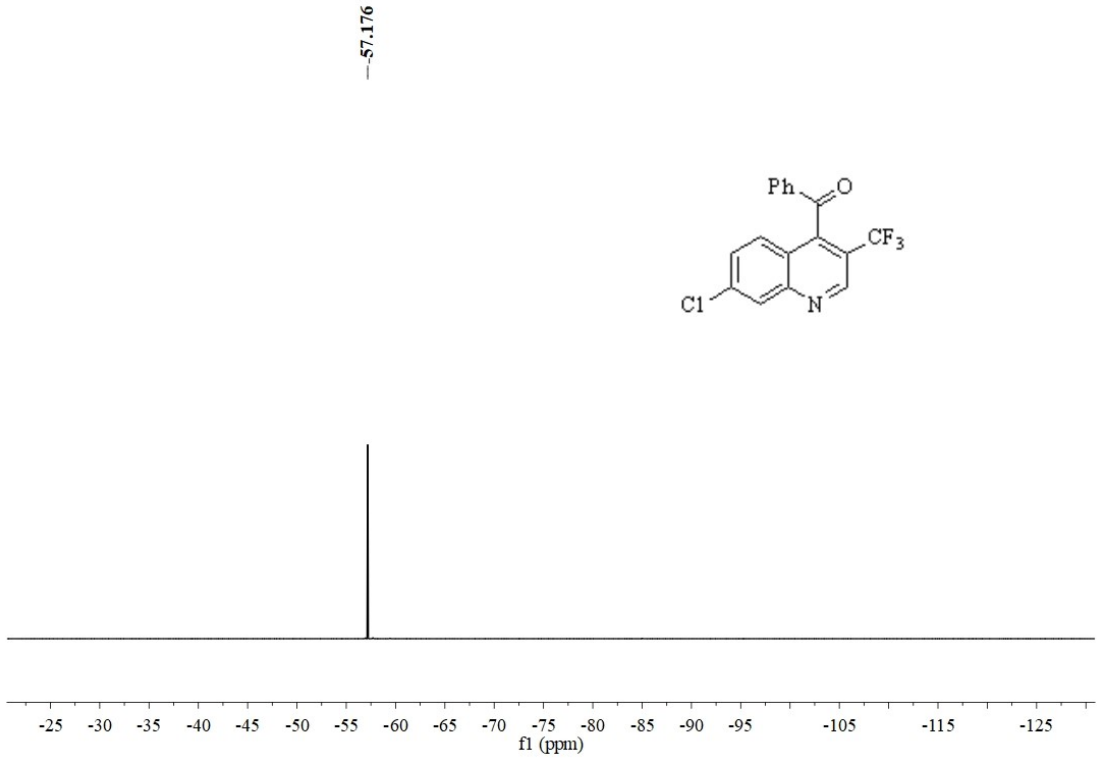

193.492
147.066
147.025
145.708
145.502
145.479
135.162
129.274
128.650
125.349
121.793
120.894
120.250
77.478
77.363
77.160
76.843
136.003
135.162
134.743
132.358
129.839
129.274
128.793
128.650
125.490
125.349
124.525
121.793
121.217
120.894
120.572
120.250
f1 (ppm)
Ph
O
CF3
N
C1
f1 (ppm)


-57.273
Ph
O
CF3
N
Cl
-10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160
f1 (ppm)

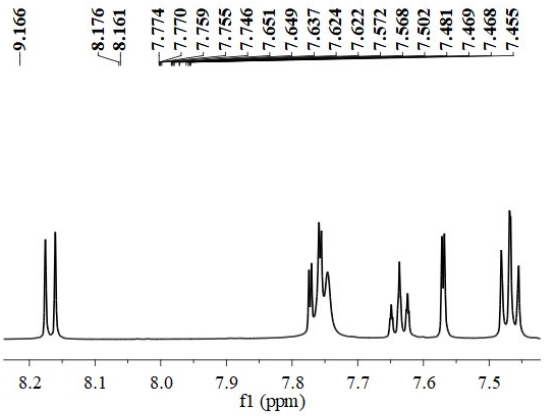
3la

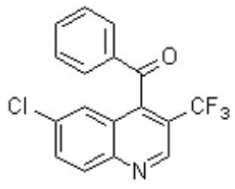

9.201
8.253
8.248
7.758
7.542
7.482
7.056
6.996
8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5
f1 (ppm)
Ph
O
CF3
Cl
N
1.00
0.99
1.98
1.03
4.07
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

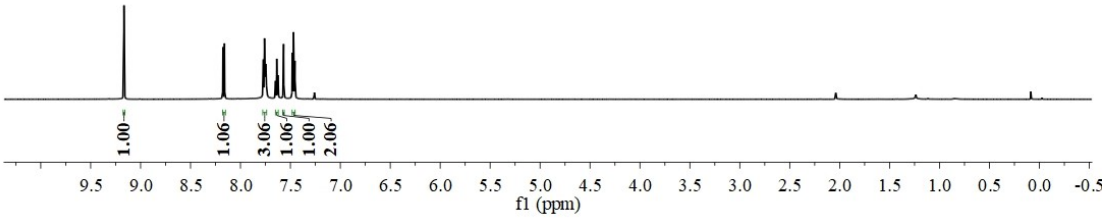

193.534
149.812
147.674
147.634
147.593
147.553
144.911
144.888
138.624
135.156
129.266
127.490
124.642
122.393
121.912
120.400
120.078
119.756
119.434
119.181
77.478
77.362
77.160
76.843
Ph
O
CF3
Cl
N
f1 (ppm)

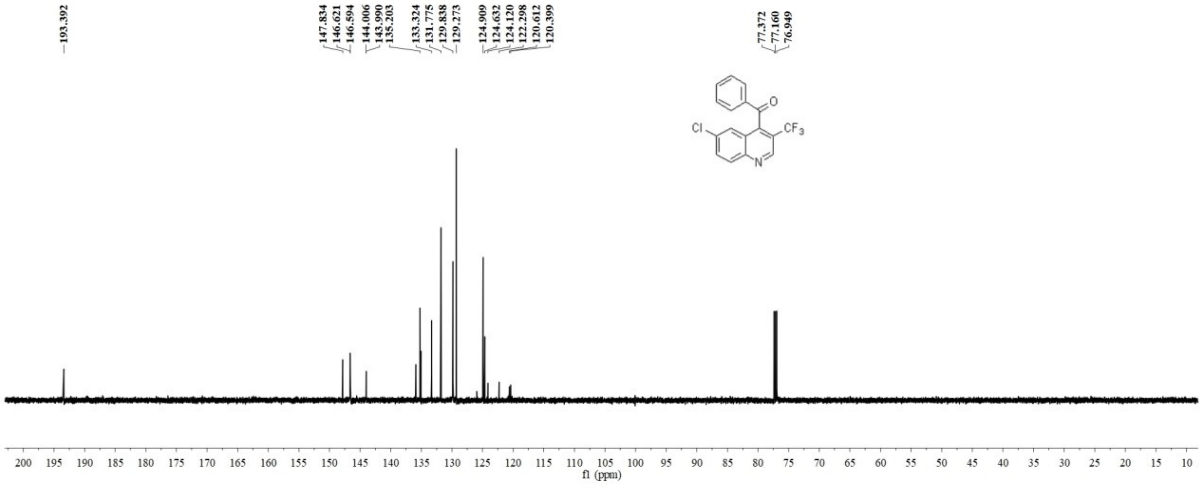

-57.176
Ph
O
CF3
Cl
N
f1 (ppm)

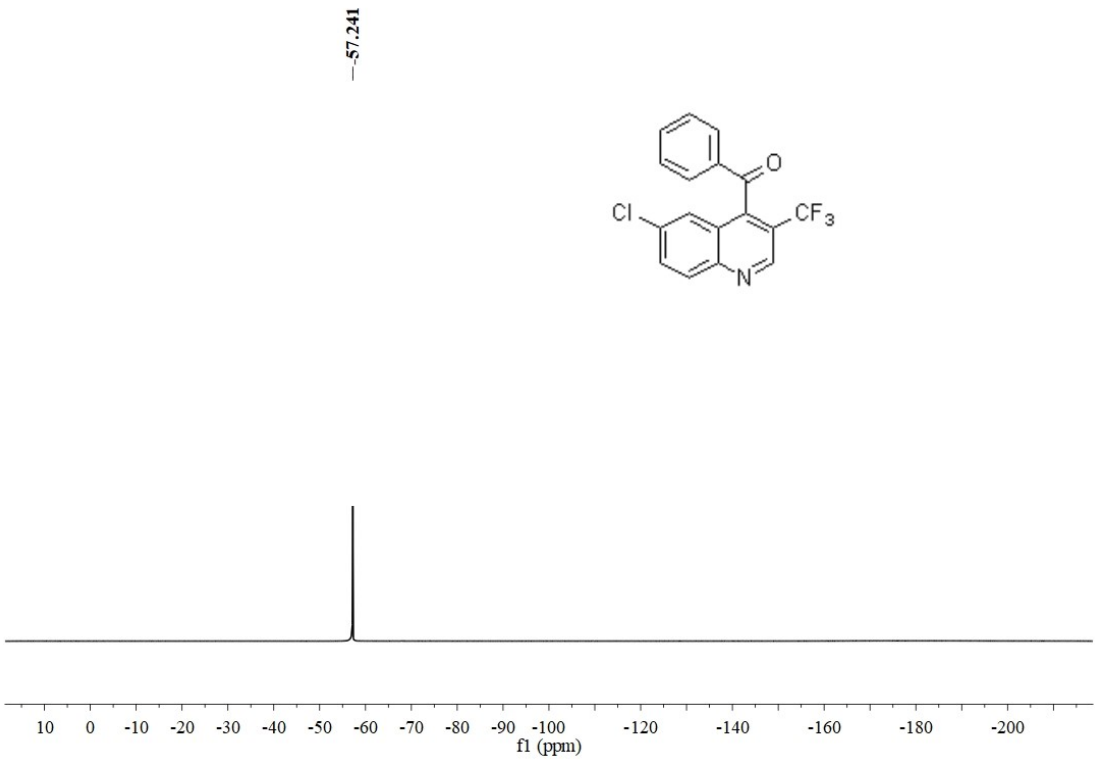
3ma


9.166
8.176
8.161
7.774
7.770
7.759
7.755
7.746
7.651
7.649
7.637
7.624
7.622
7.572
7.568
7.502
7.481
7.469
7.468
7.455
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
f1 (ppm)

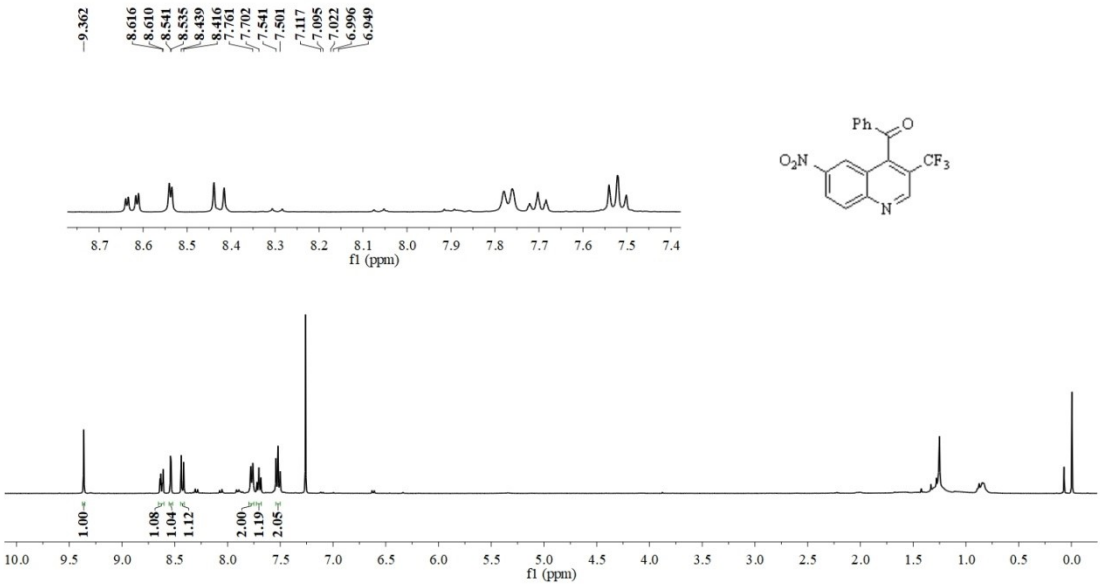

O
Cl
CF3
N

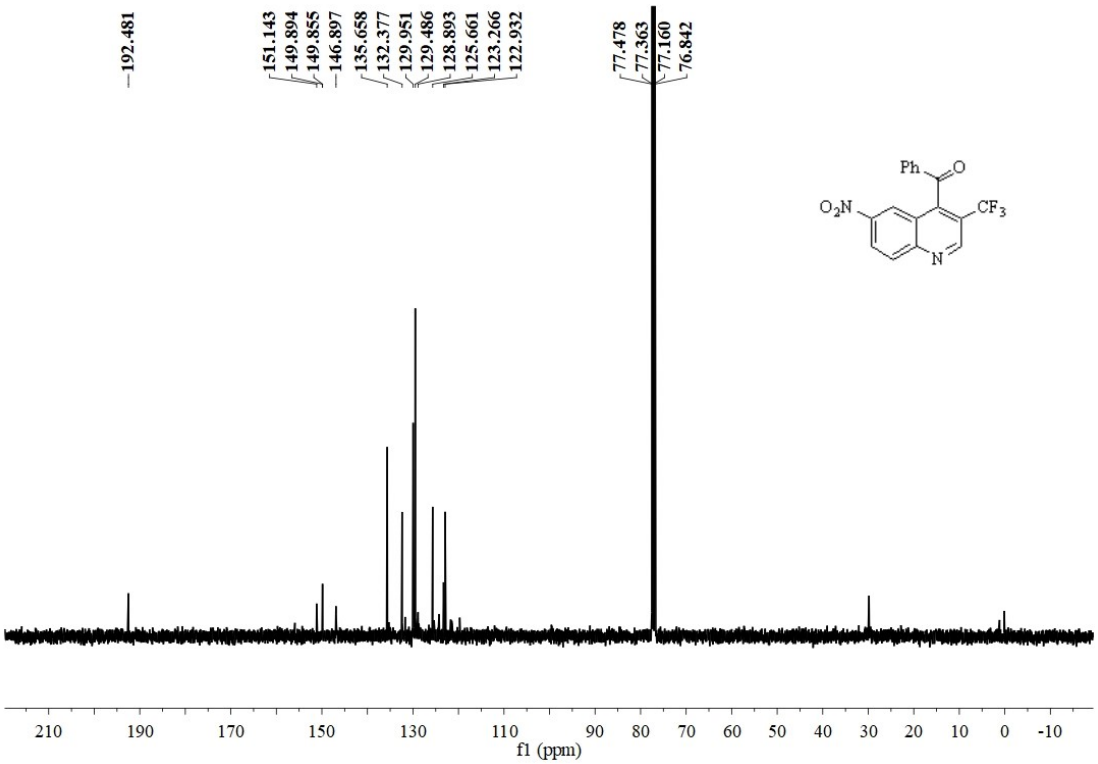

1.00
1.06
3.06
1.06
1.00
2.06
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

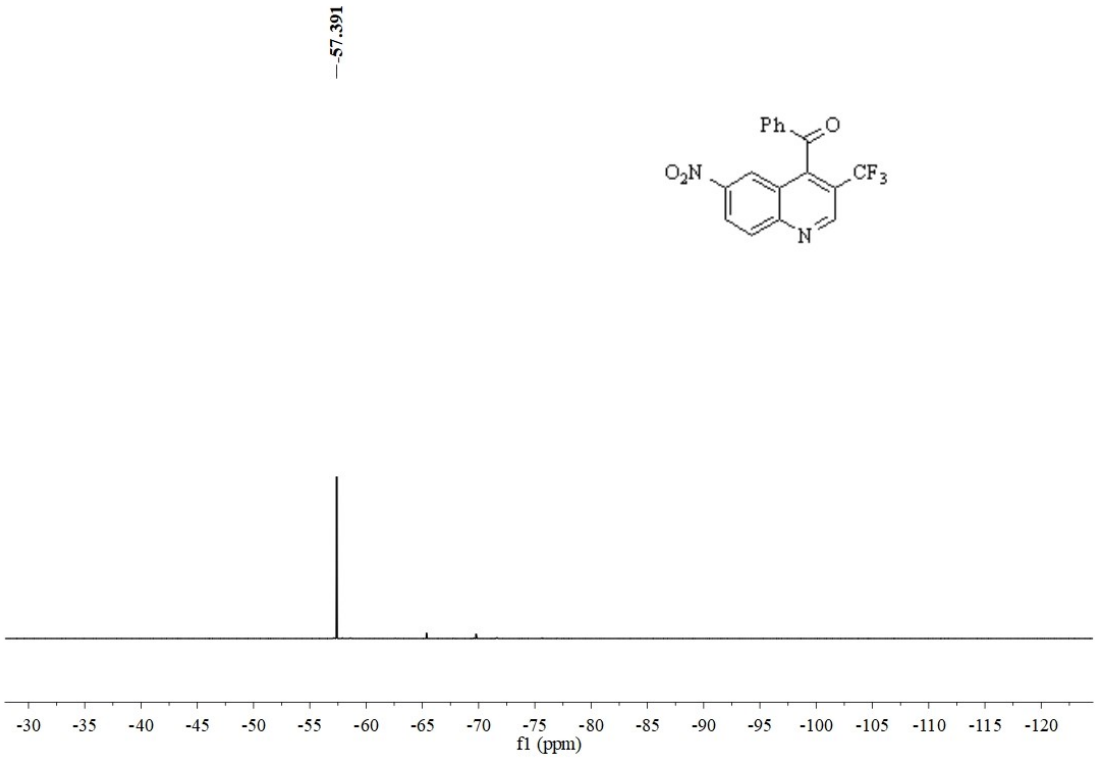

193.392
147.834
146.621
146.594
144.006
143.990
135.203
133.324
131.775
129.838
129.273
124.909
124.632
124.120
122.298
120.612
120.399
77.372
77.160
76.949
O
Cl
CF3
N
200
195
190
185
180
175
170
165
160
155
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
f1 (ppm)


-57.241
O
Cl
CF3
N
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)

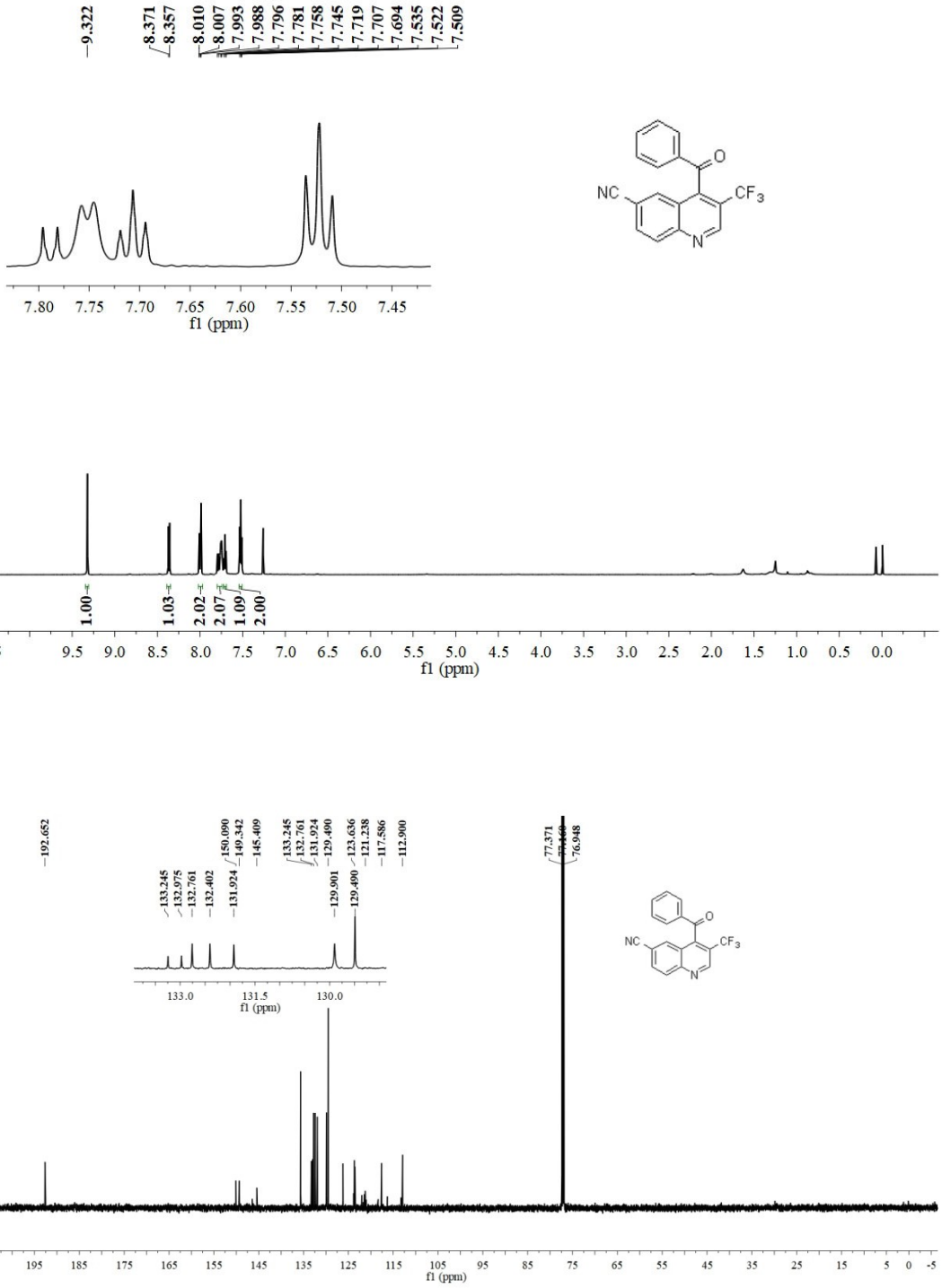
3pa

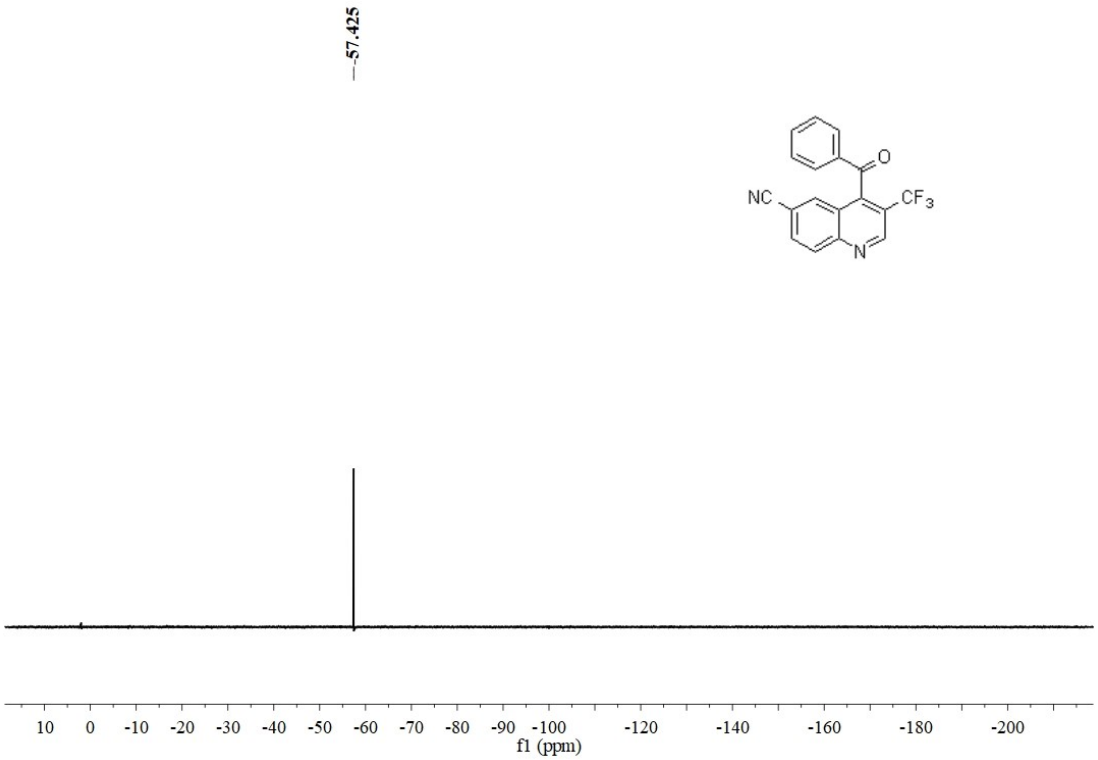

9.362
8.616
8.610
8.541
8.535
8.439
8.416
7.761
7.702
7.541
7.501
7.117
7.095
7.022
6.996
6.949
Ph
O
O2N
CF3
N
8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4
f1 (ppm)
1.00
1.08
1.04
1.12
2.00
1.19
2.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


192.481
151.143
149.894
149.855
146.897
135.658
132.377
129.951
129.486
128.893
125.661
123.266
122.932
77.478
77.363
77.160
76.842
Ph
O
O2N
CF3
N
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

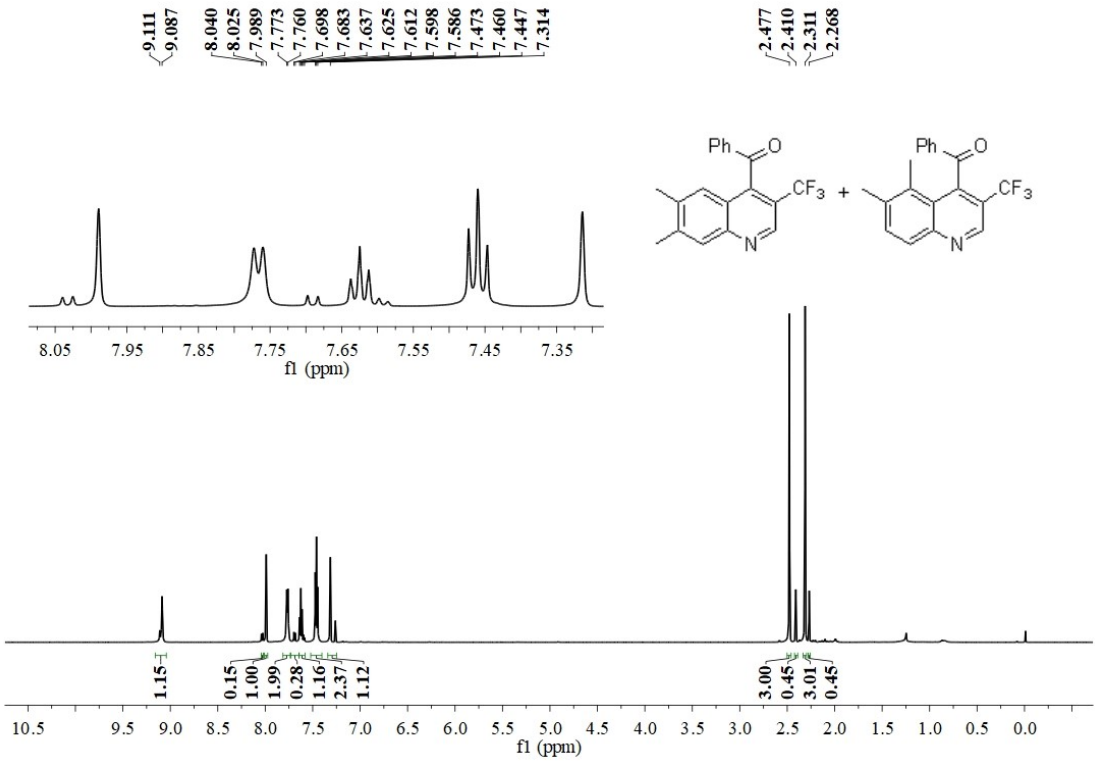

-57.391
Ph
O
O2N
CF3
N
-30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120
f1 (ppm)

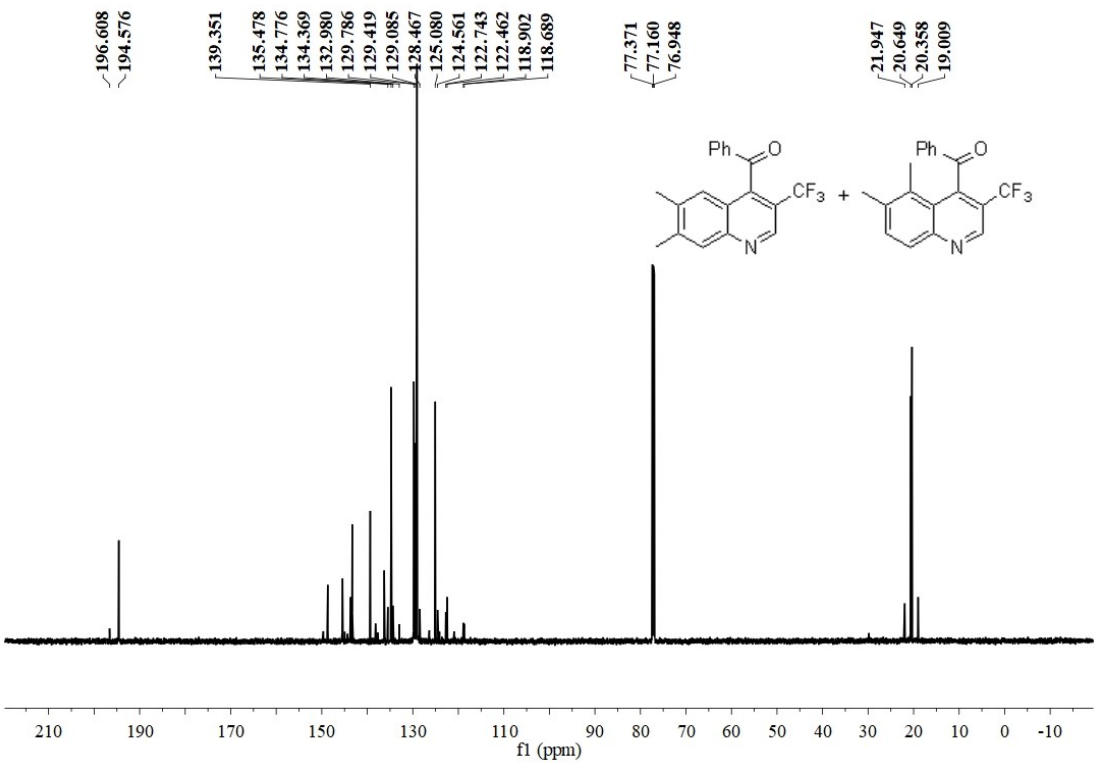
3qa

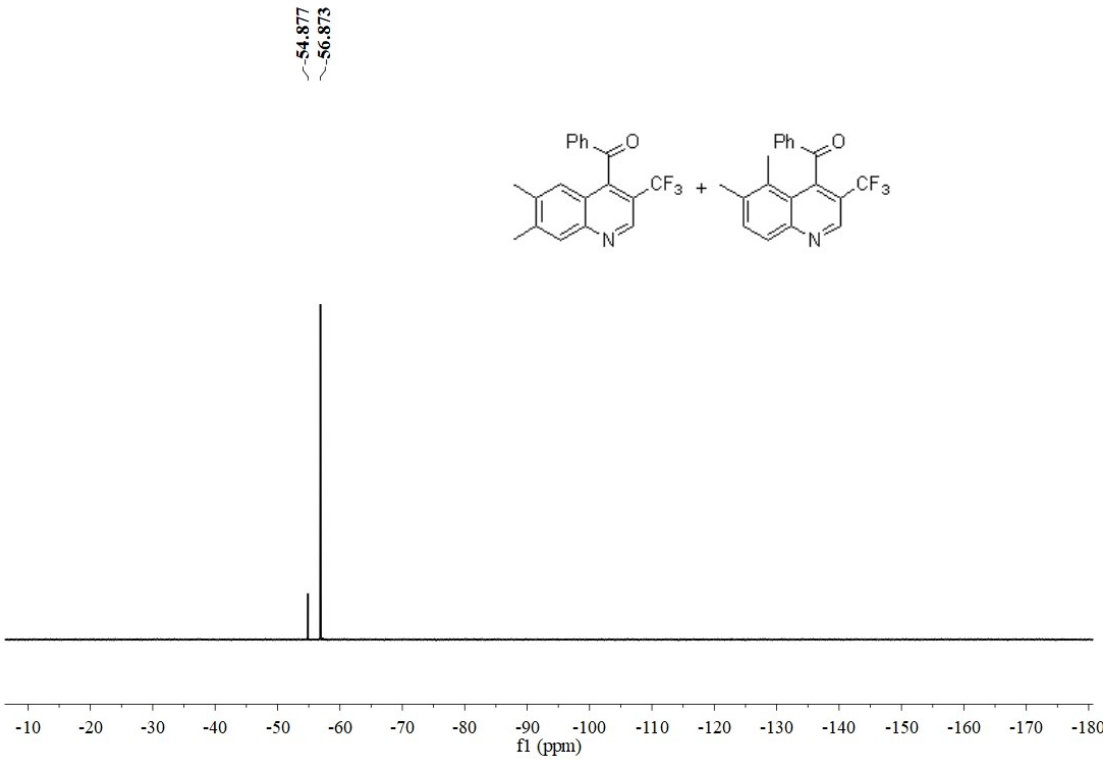

9.322
8.371
8.357
8.010
8.007
7.993
7.988
7.796
7.781
7.758
7.745
7.719
7.707
7.694
7.535
7.522
7.509
7.80 7.75 7.70 7.65 7.60 7.55 7.50 7.45
f1 (ppm)
O
NC
CF3
N
1.00
1.03
2.02
2.07
1.09
2.00
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
192.652
150.090
149.342
145.409
133.245
132.761
131.924
129.490
123.636
121.238
117.586
112.900
77.371
77.160
76.948
133.245
132.975
132.761
132.402
131.924
129.901
129.490
133.0
131.5
130.0
f1 (ppm)
205 195 185 175 165 155 145 135 125 115 105 95 85 75 65 55 45 35 25 15 5 0 -5
f1 (ppm)


-57.425
O
NC
CF3
N
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)

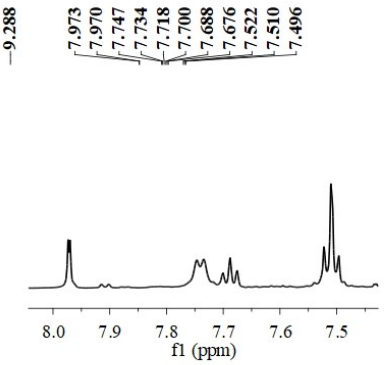
3ra + 3r'a

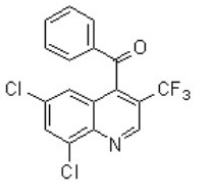

9.111
9.087
8.040
8.025
7.989
7.773
7.760
7.698
7.683
7.637
7.625
7.612
7.598
7.586
7.473
7.460
7.447
7.314
2.477
2.410
2.311
2.268
Ph
O
CF3
+
N
8.05 7.95 7.85 7.75 7.65 7.55 7.45 7.35
f1 (ppm)
1.15
0.15
1.00
1.99
0.28
1.16
2.37
1.12
3.00
0.45
3.01
0.45
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

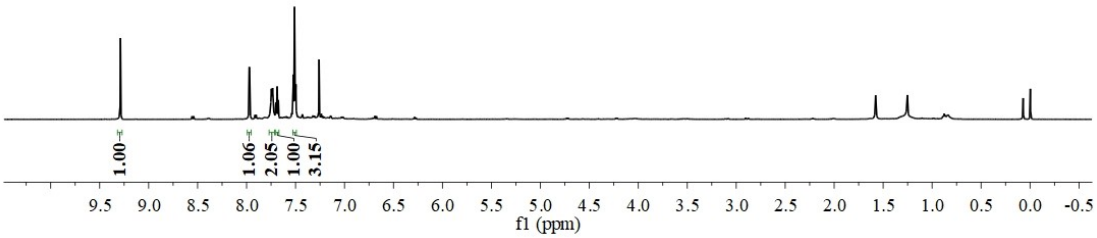

196.608
194.576
139.351
135.478
134.776
134.369
132.980
129.786
129.419
129.085
128.467
125.080
124.561
122.743
122.462
118.902
118.689
77.371
77.160
76.948
21.947
20.649
20.358
19.009
Ph
O
CF3
+
N
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

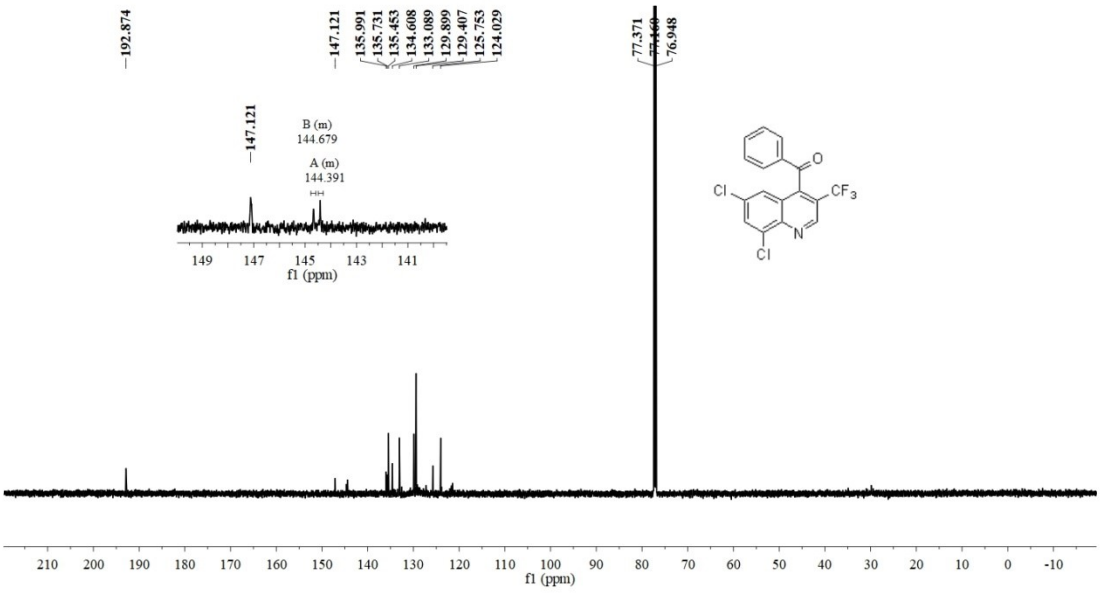

54.877
56.873
Ph
O
CF3
+
N
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
f1 (ppm)

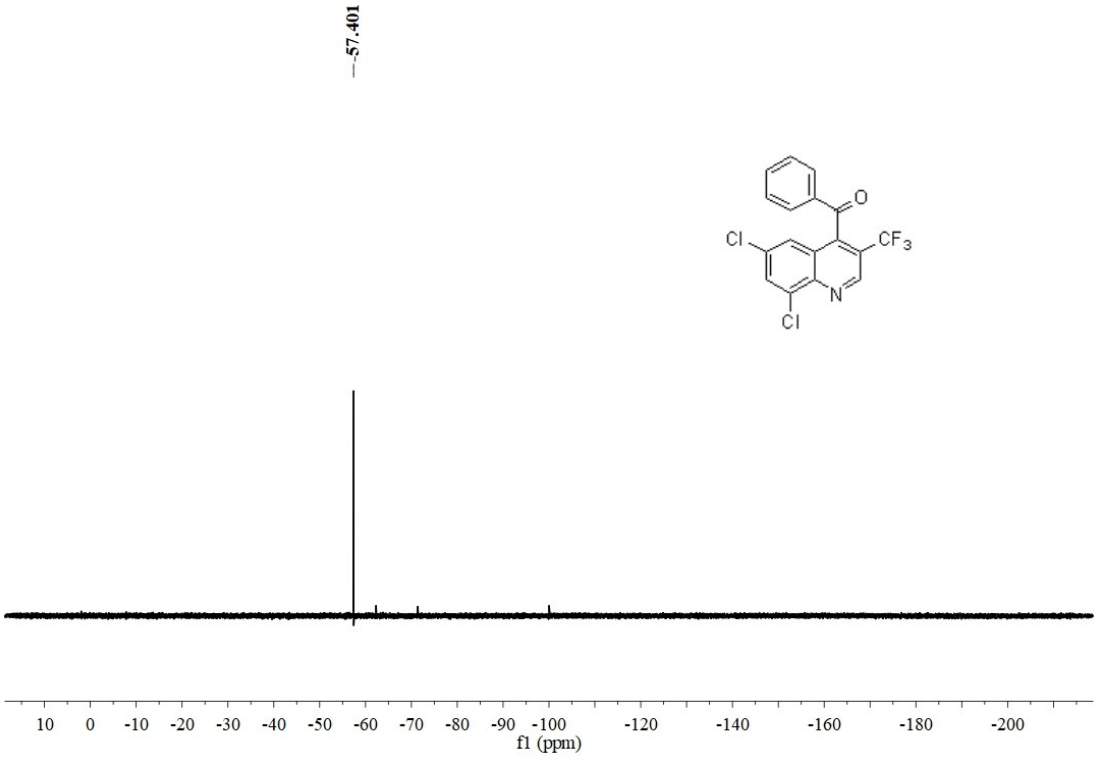
3sa


9.288
7.973
7.970
7.747
7.734
7.718
7.700
7.688
7.676
7.522
7.510
7.496
8.0 7.9 7.8 7.7 7.6 7.5
f1 (ppm)

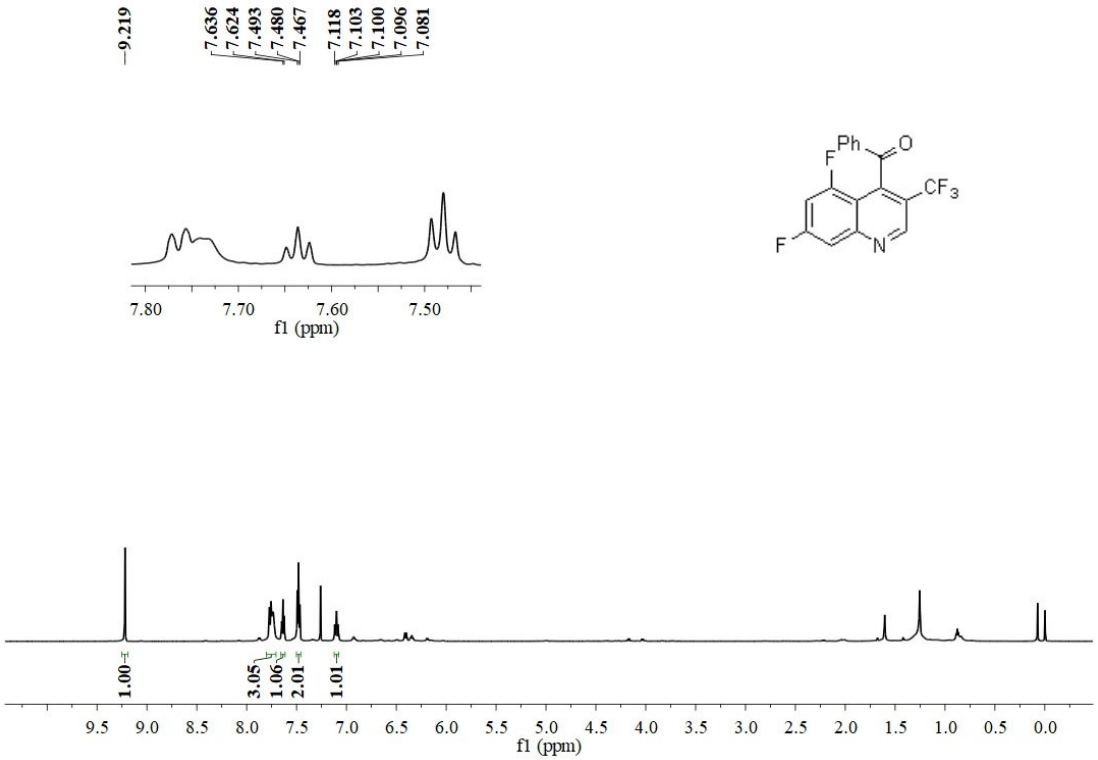

O
Cl
CF3
N
Cl

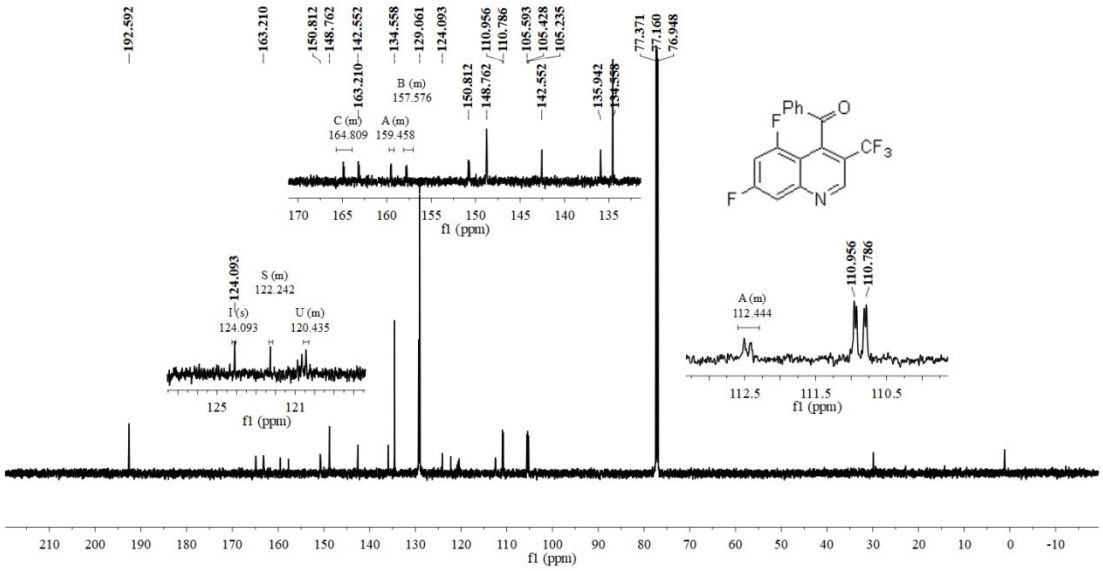

1.00
1.06
2.05
1.00
3.15
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

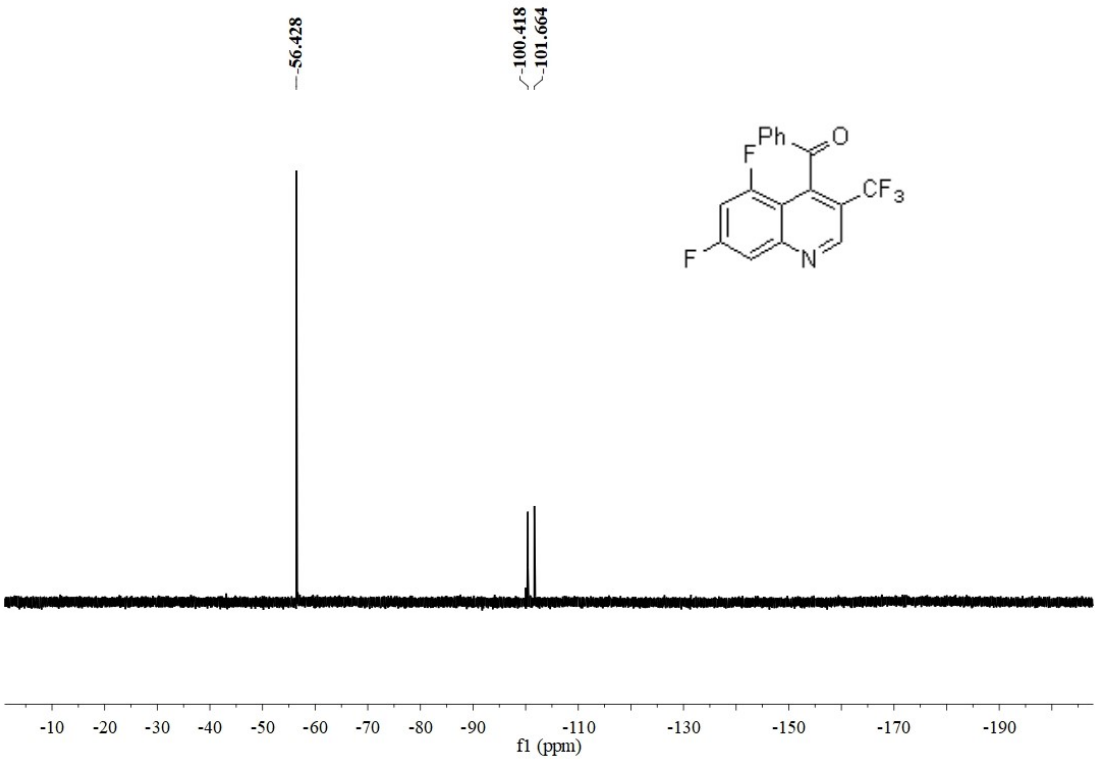

192.874
147.121
135.991
135.731
135.453
134.608
133.089
129.899
129.407
125.753
124.029
77.371
77.160
76.948
147.121
B (m)
144.679
A (m)
144.391
149 147 145 143 141
f1 (ppm)
O
Cl
CF3
N
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-57.401
O
Cl
CF3
N
Cl
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)

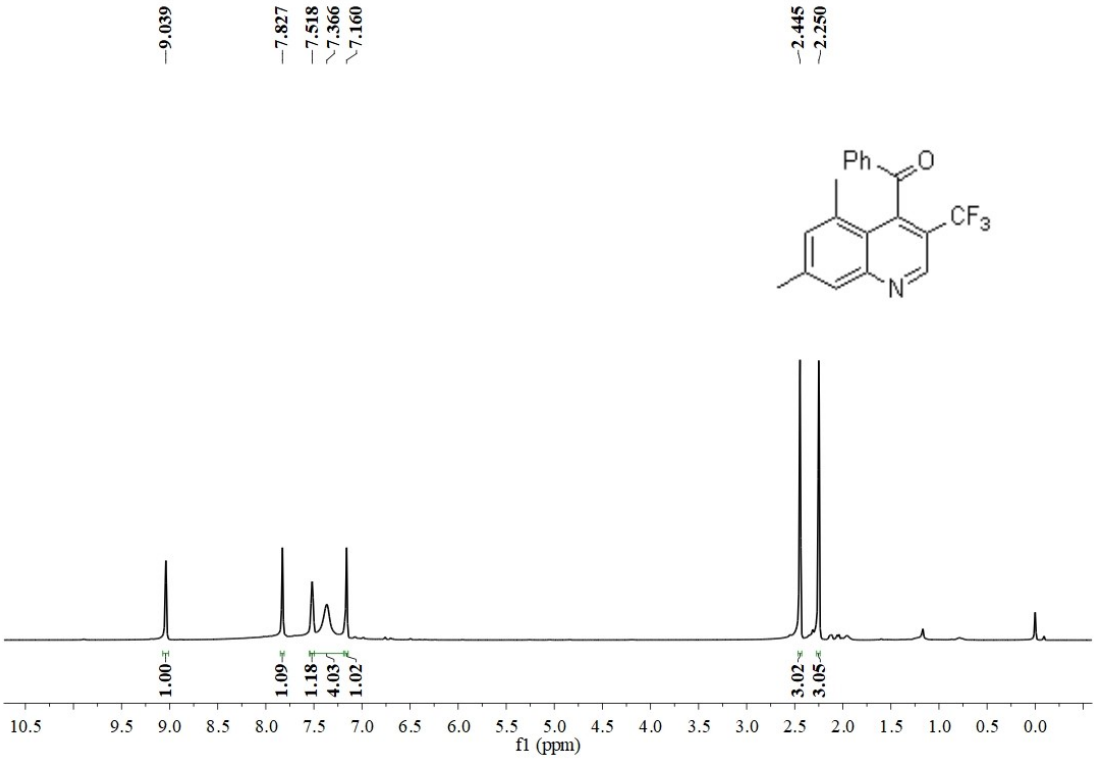
3ua

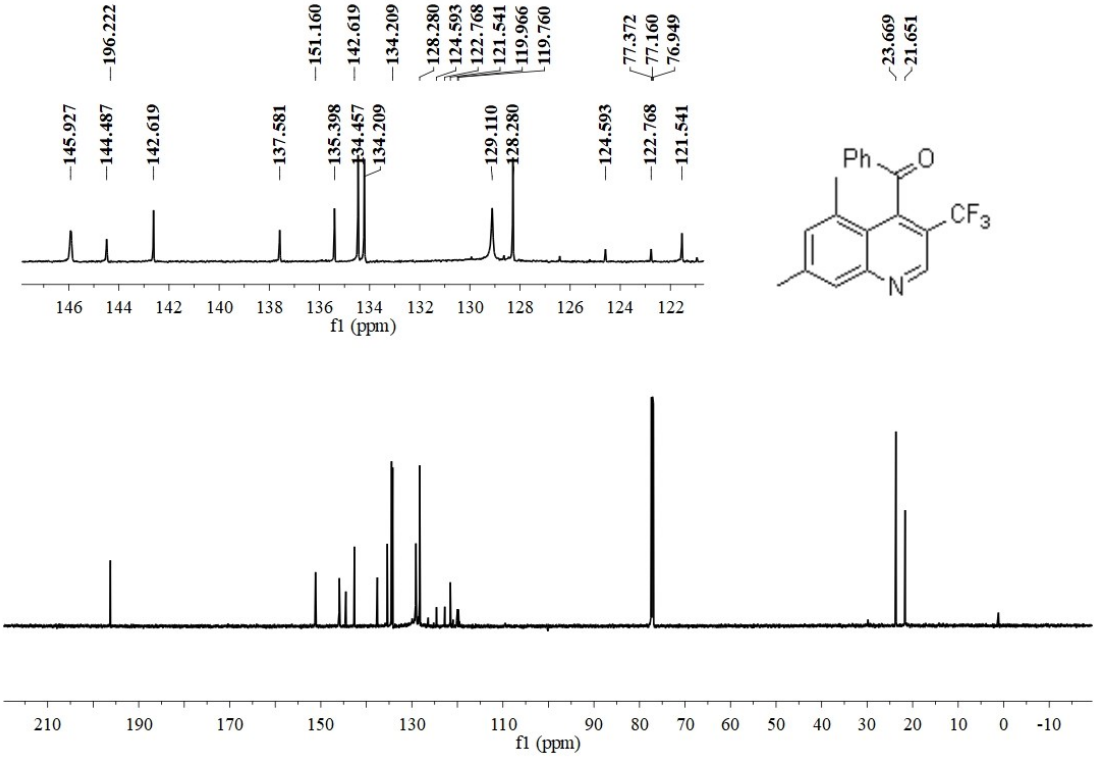

9.219
7.636
7.624
7.493
7.480
7.467
7.118
7.103
7.100
7.096
7.081
F
Ph
O
CF3
F
N
7.80 7.70 7.60 7.50
f1 (ppm)
1.00
3.05
1.06
2.01
1.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

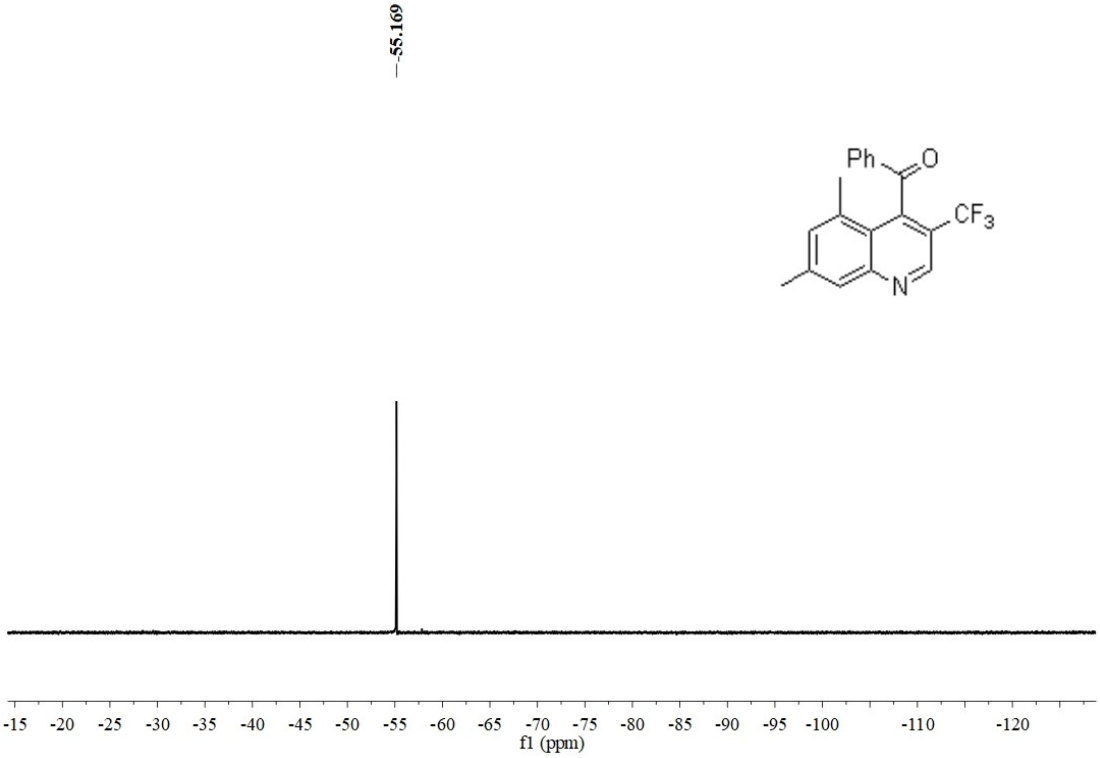

192.592
163.210
150.812
148.762
142.552
134.558
129.061
124.093
110.956
110.786
105.593
105.428
105.235
77.371
77.160
76.948
B (m)
157.576
C (m)
164.809
A (m)
159.458
f1 (ppm)
S (m)
122.242
I (s)
124.093
U (m)
120.435
A (m)
112.444
f1 (ppm)
f1 (ppm)


56.428
100.418
101.664
f1 (ppm)

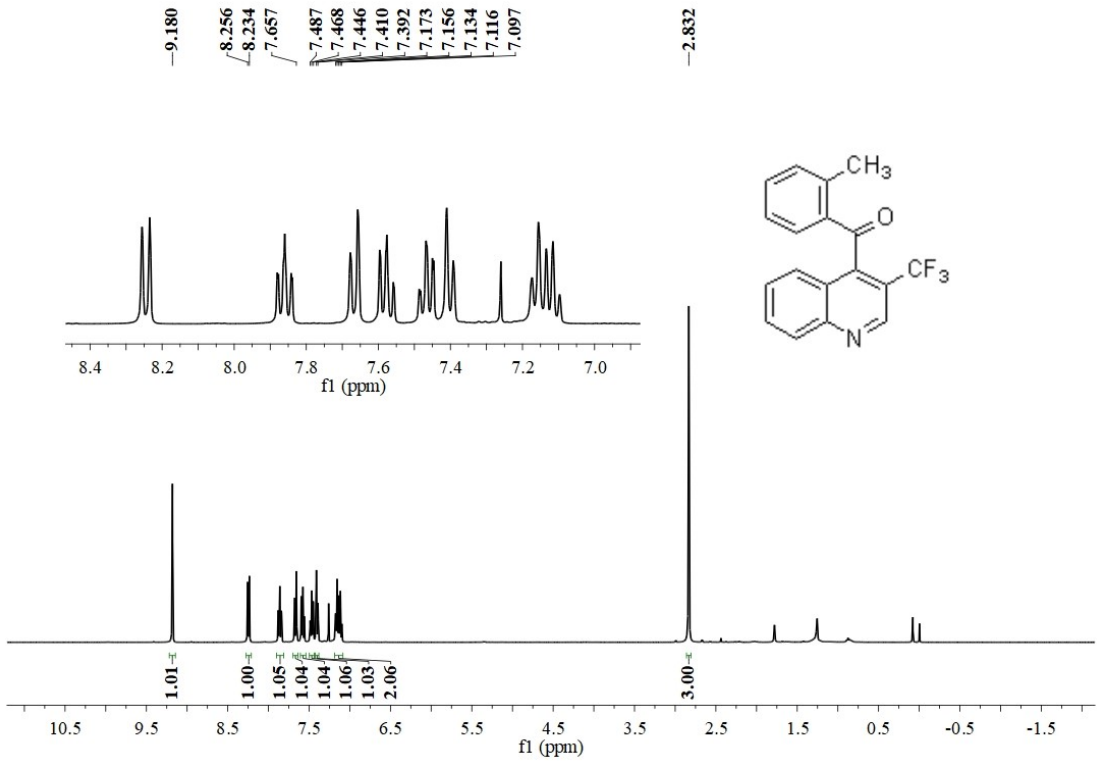
3va

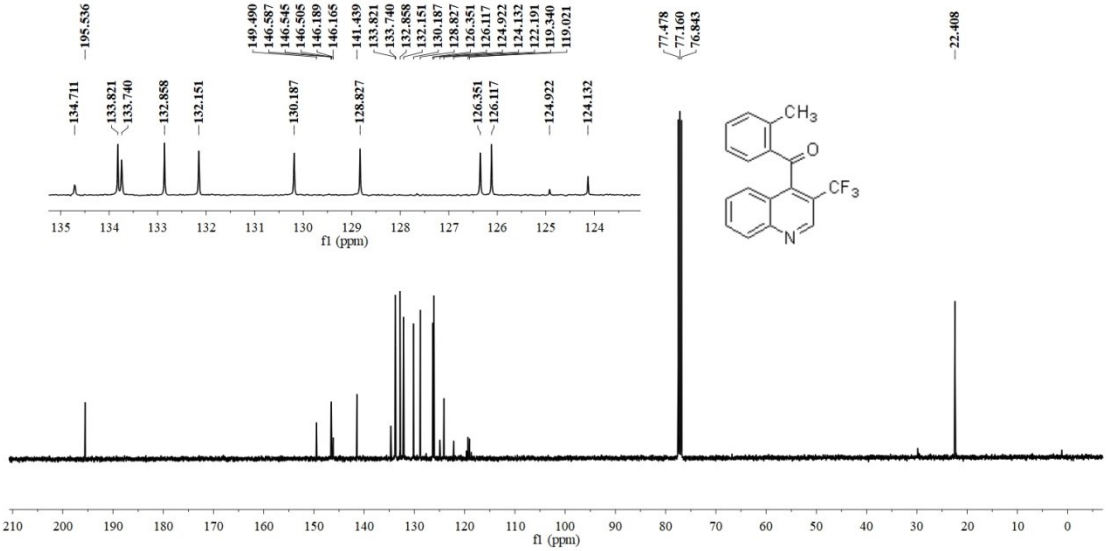

9.039
7.827
7.518
7.366
7.160
2.445
2.250
Ph
O
CF3
N
1.00
1.09
1.18
4.03
1.02
3.02
3.05
f1 (ppm)

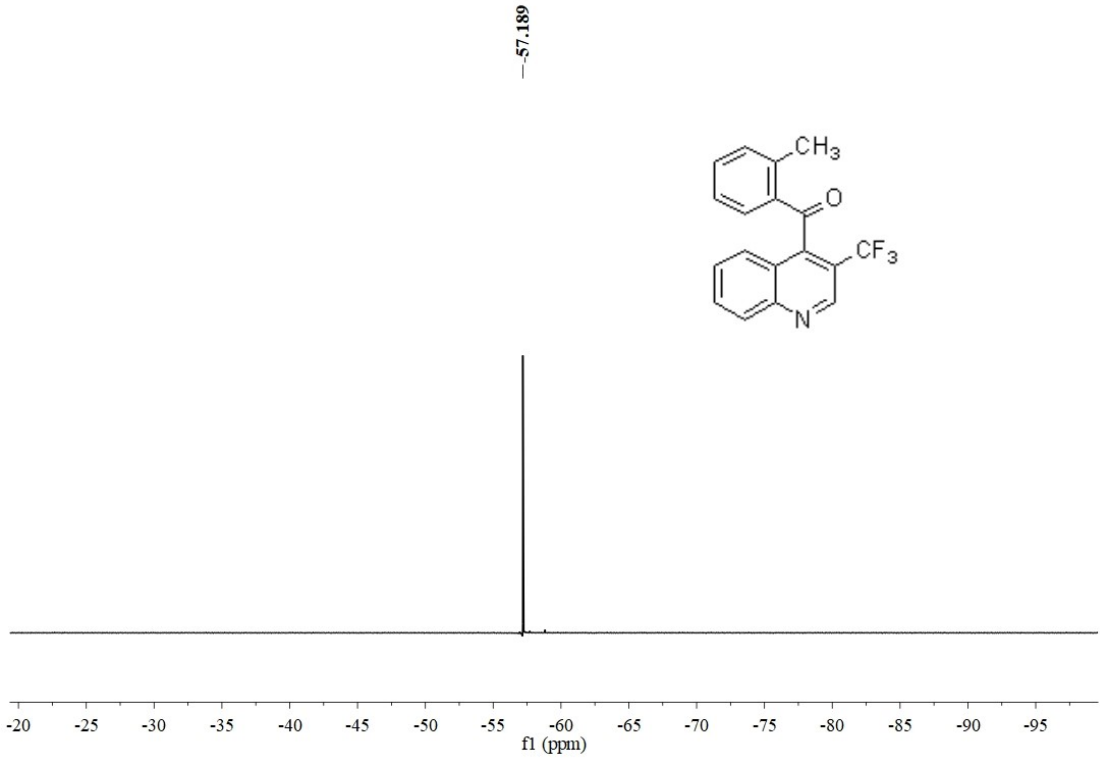

196.222
151.160
142.619
134.209
128.280
124.593
122.768
121.541
119.966
119.760
77.372
77.160
76.949
23.669
21.651
145.927
144.487
142.619
137.581
135.398
134.457
134.209
129.110
128.280
124.593
122.768
121.541
Ph
O
CF3
N
f1 (ppm)


-55.169
Ph
O
CF3
N
-15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -110 -120
f1 (ppm)

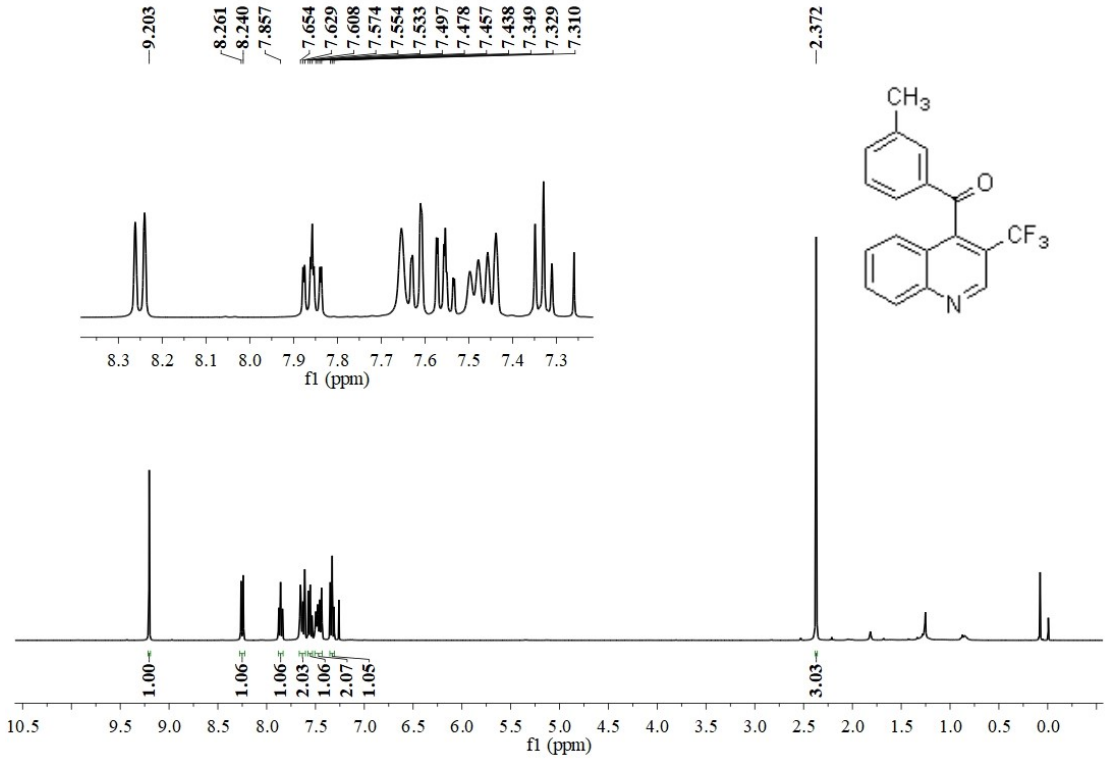
3ab

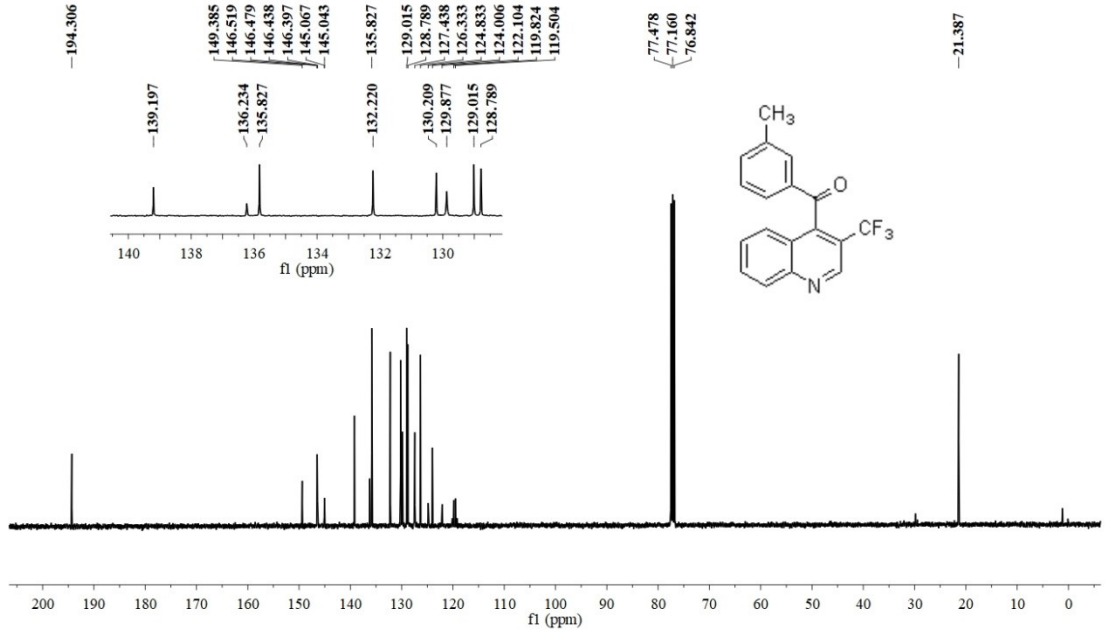

9.180
8.256
8.234
7.657
7.487
7.468
7.446
7.410
7.392
7.173
7.156
7.134
7.116
7.097
2.832
CH3
O
CF3
N
8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0
f1 (ppm)
1.01
1.00
1.05
1.04
1.04
1.06
1.03
2.06
3.00
10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.5 -1.5
f1 (ppm)

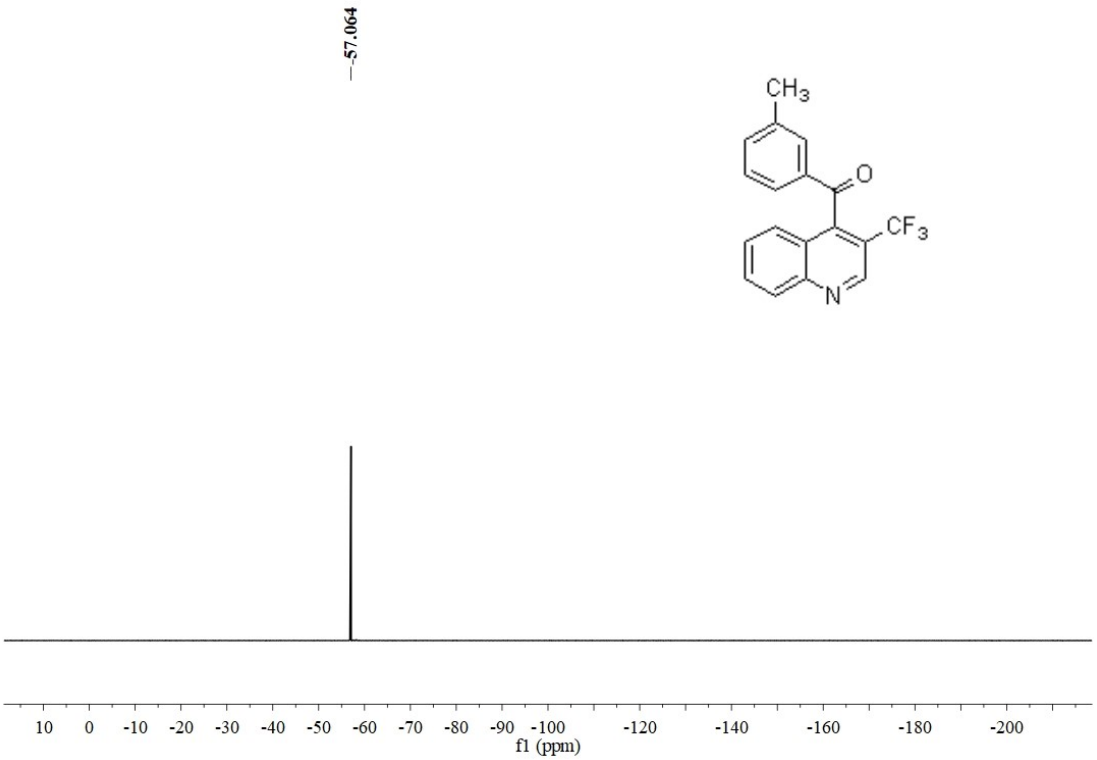

195.536
149.490
146.587
146.545
146.505
146.189
146.165
141.439
133.821
133.740
132.858
132.151
130.187
128.827
126.351
126.117
124.922
124.132
122.191
119.340
119.021
77.478
77.160
76.843
22.408
134.711
133.821
133.740
132.858
132.151
130.187
128.827
126.351
126.117
124.922
124.132
f1 (ppm)
f1 (ppm)


-57.189
f1 (ppm)

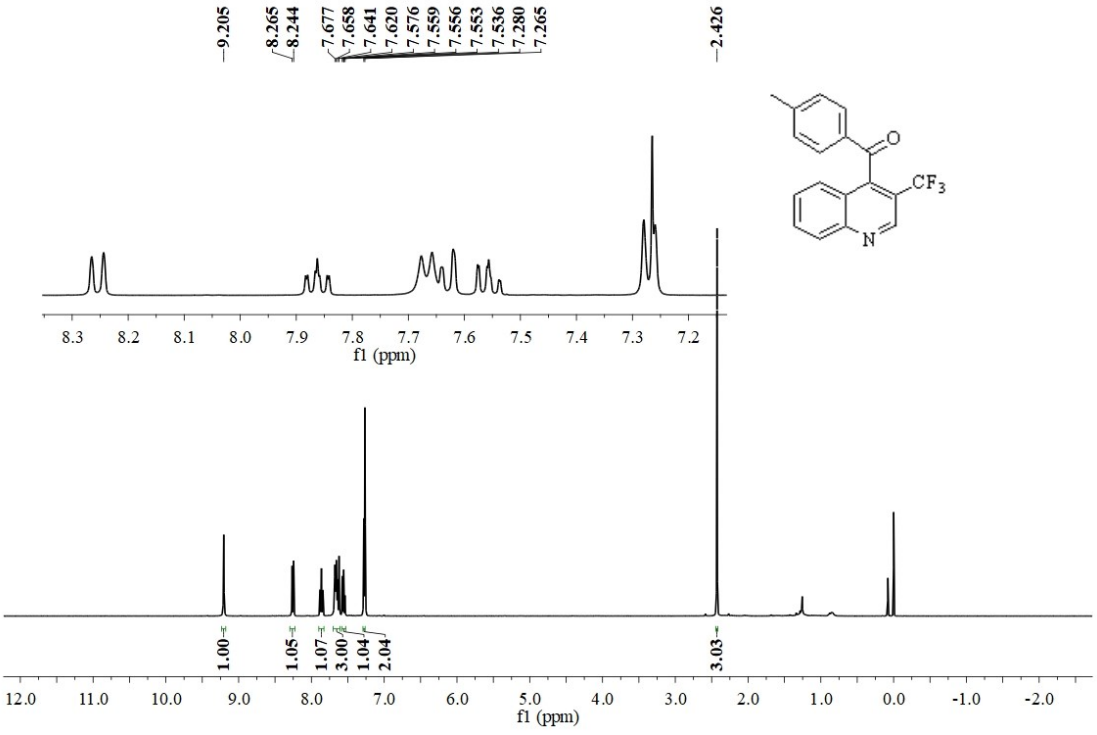
3ac

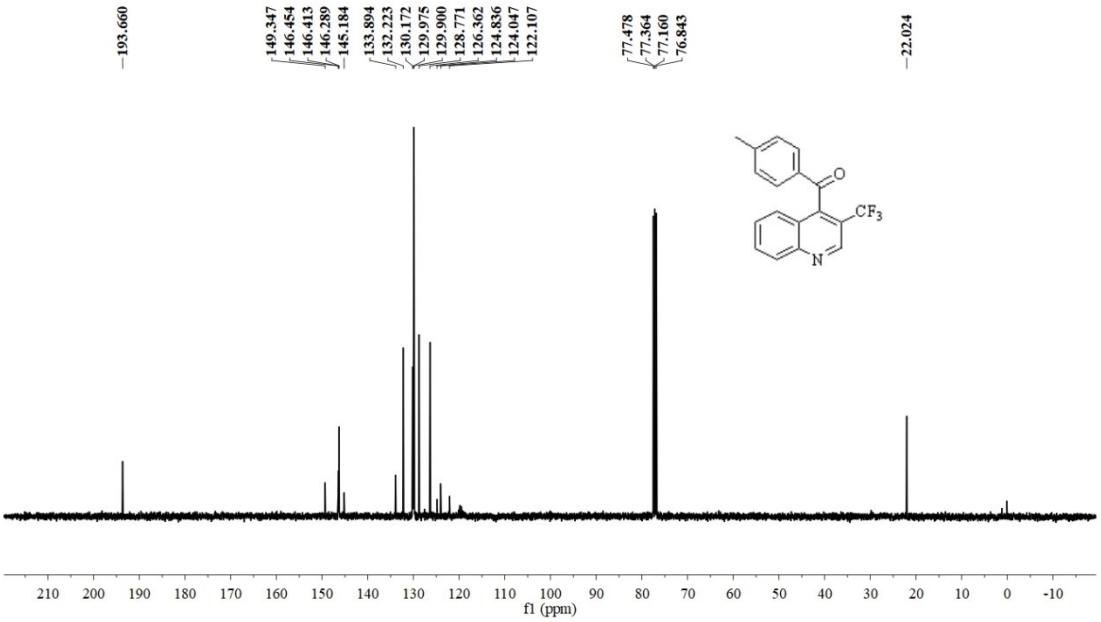

9.203
8.261
8.240
7.857
7.654
7.629
7.608
7.574
7.554
7.533
7.497
7.478
7.457
7.438
7.349
7.329
7.310
2.372
CH3
O
CF3
N
f1 (ppm)
1.00
1.06
1.06
2.03
1.06
2.07
1.05
3.03

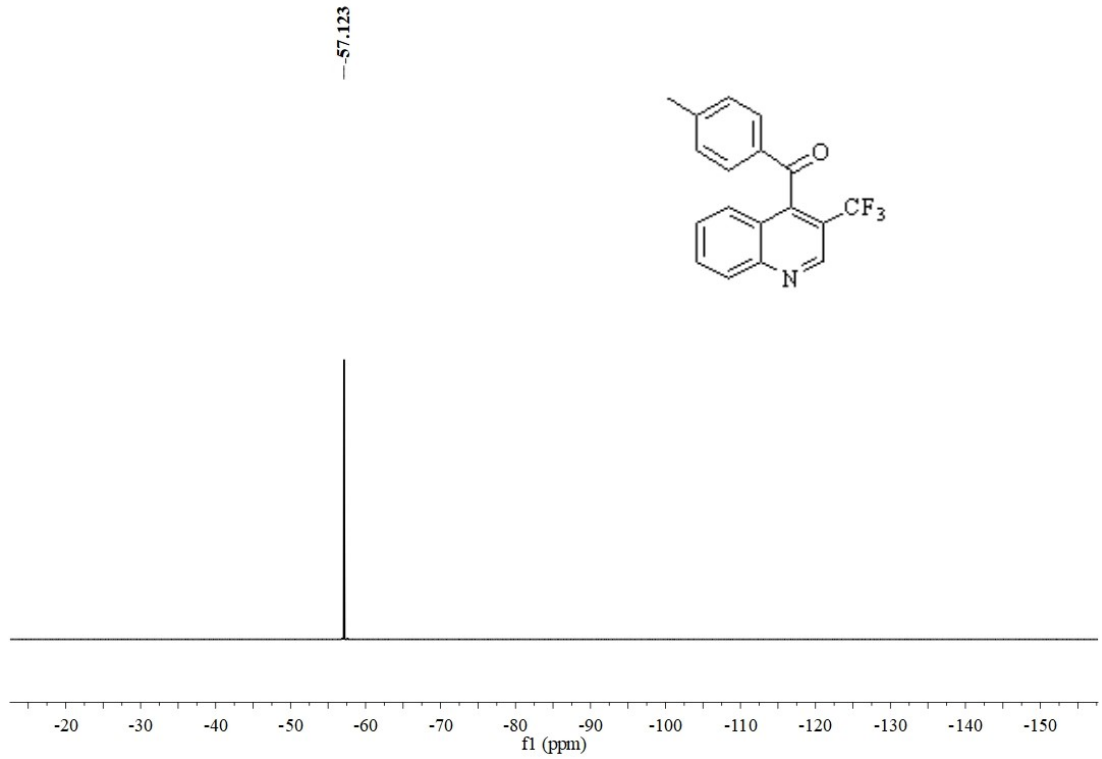

194.306
149.385
146.519
146.479
146.438
146.397
145.067
145.043
135.827
129.015
128.789
127.438
126.333
124.833
124.006
122.104
119.824
119.504
77.478
77.160
76.842
21.387
139.197
136.234
135.827
132.220
130.209
129.877
129.015
128.789
CH3
O
CF3
N
f1 (ppm)


-57.064
CH3
O
CF3
N
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)

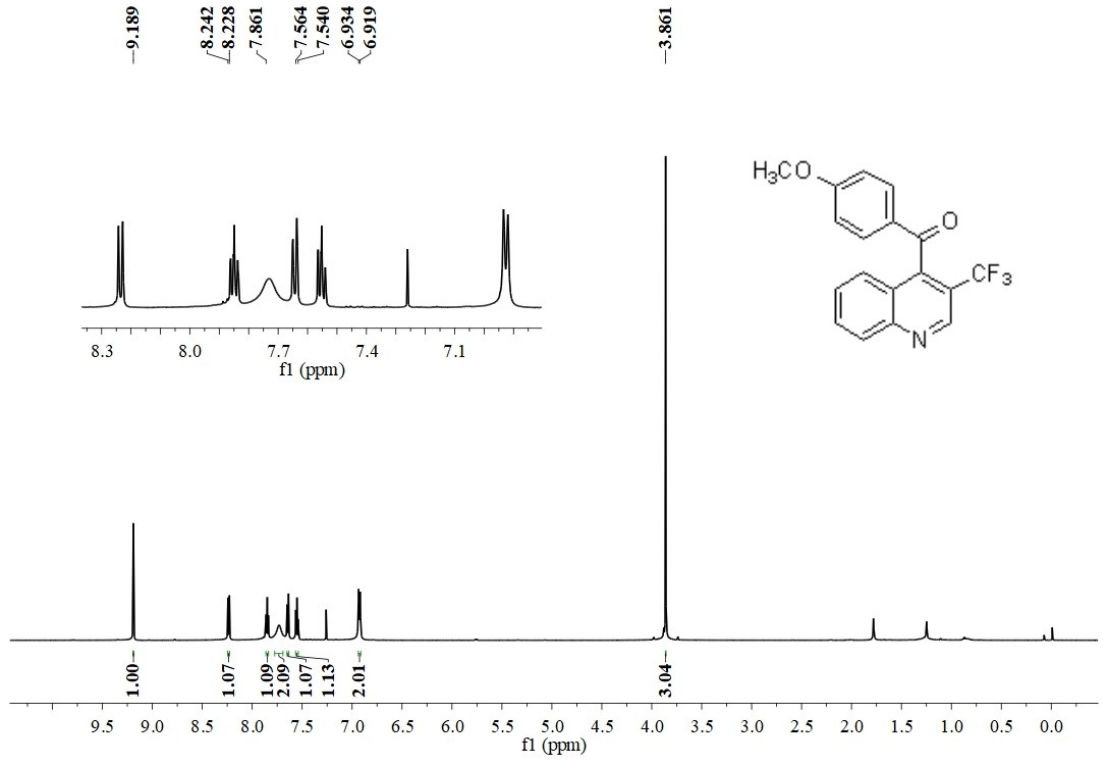
3ad

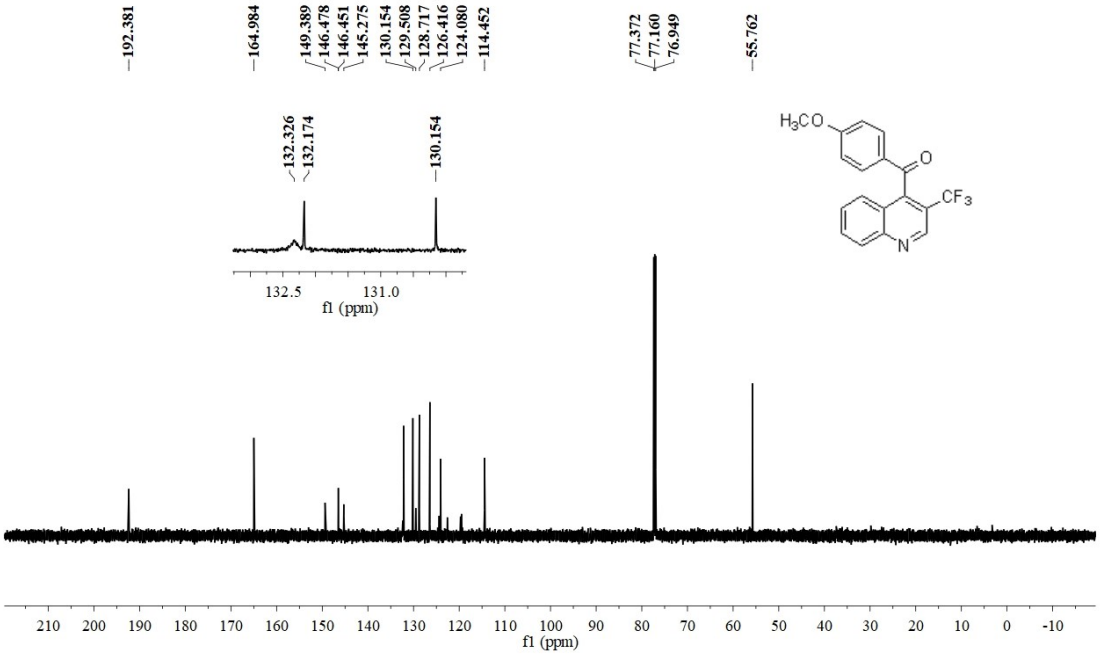

9.205
8.265
8.244
7.677
7.658
7.641
7.620
7.576
7.559
7.556
7.553
7.536
7.280
7.265
2.426
O
CF3
N
8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2
f1 (ppm)
1.00
1.05
1.07
3.00
1.04
2.04
3.03
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0 -2.0
f1 (ppm)

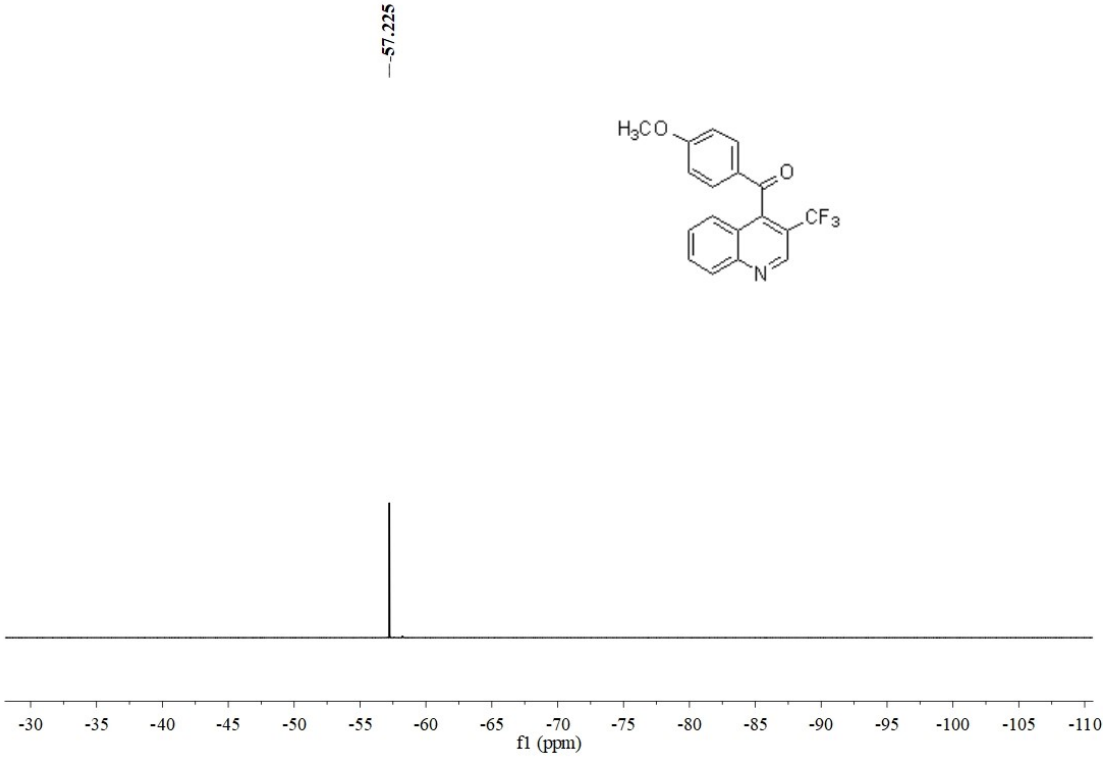

193.660
149.347
146.454
146.413
146.289
145.184
133.894
132.223
130.172
129.975
129.900
128.771
126.362
124.836
124.047
122.107
77.478
77.364
77.160
76.843
22.024
O
CF3
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-57.123
O
CF3
N
-20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150
f1 (ppm)

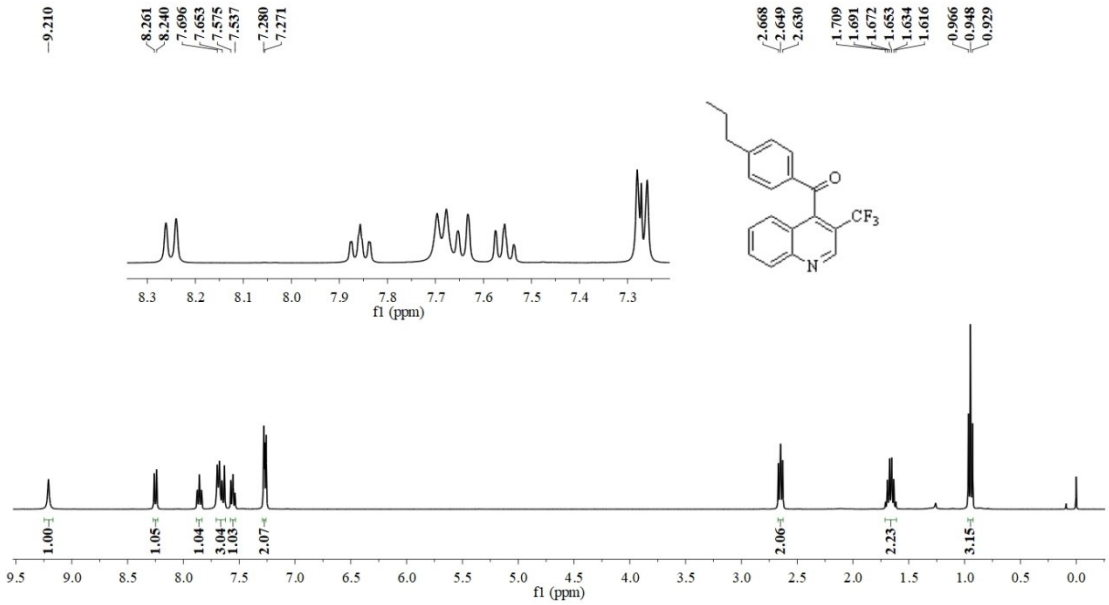
3ae

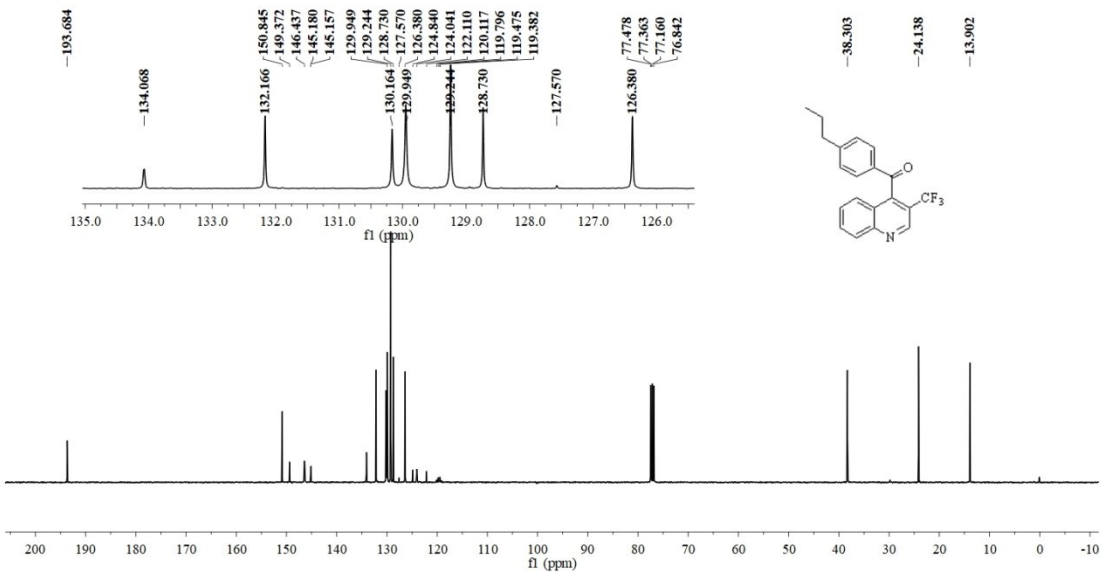

9.189
8.242
8.228
7.861
7.564
7.540
6.934
6.919
3.861
H3CO
O
CF3
N
8.3
8.0
7.7
7.4
7.1
f1 (ppm)
1.00
1.07
1.09
2.09
1.07
1.13
2.01
3.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

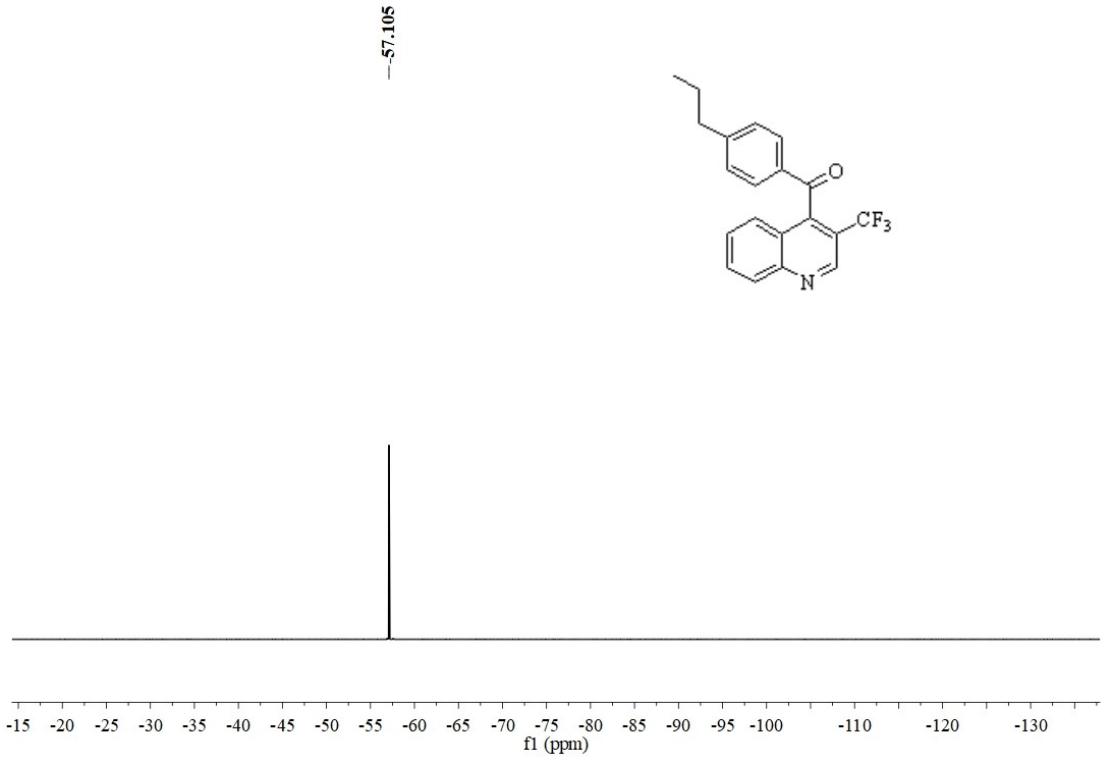

192.381
164.984
149.389
146.478
146.451
145.275
130.154
129.508
128.717
126.416
124.080
114.452
77.372
77.160
76.949
55.762
132.326
132.174
130.154
H3CO
O
CF3
N
132.5
131.0
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-57.225
H3CO
O
CF3
N
-30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110
f1 (ppm)

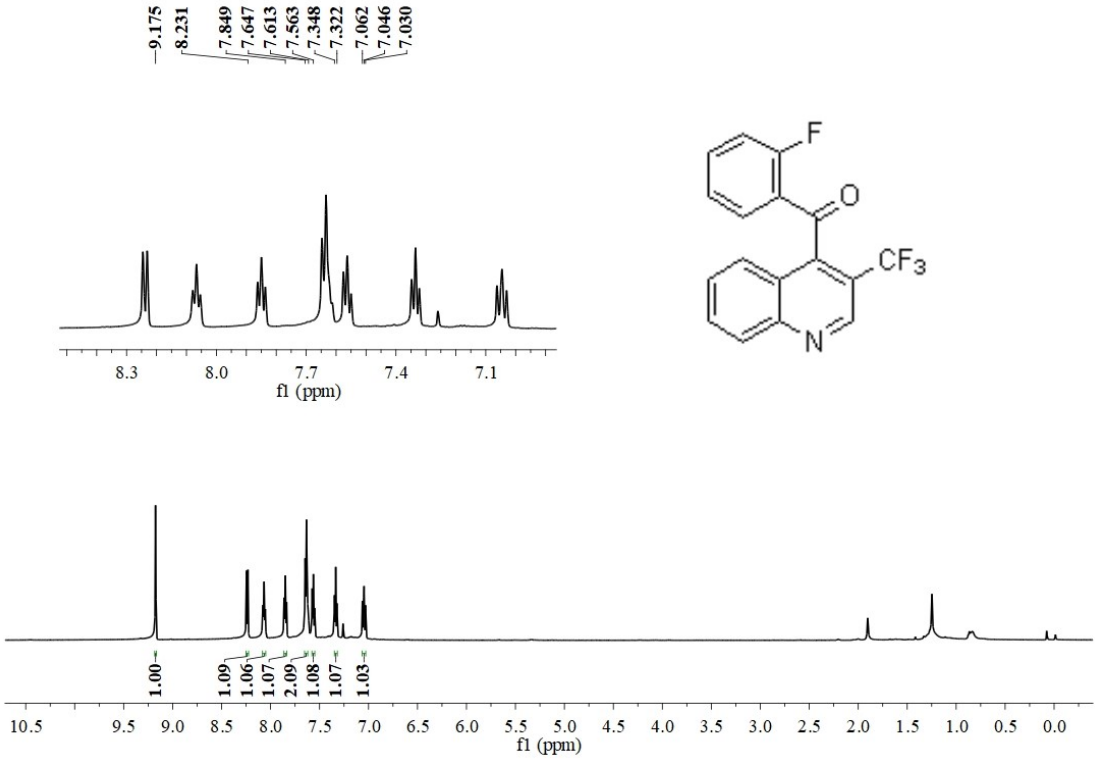
3af

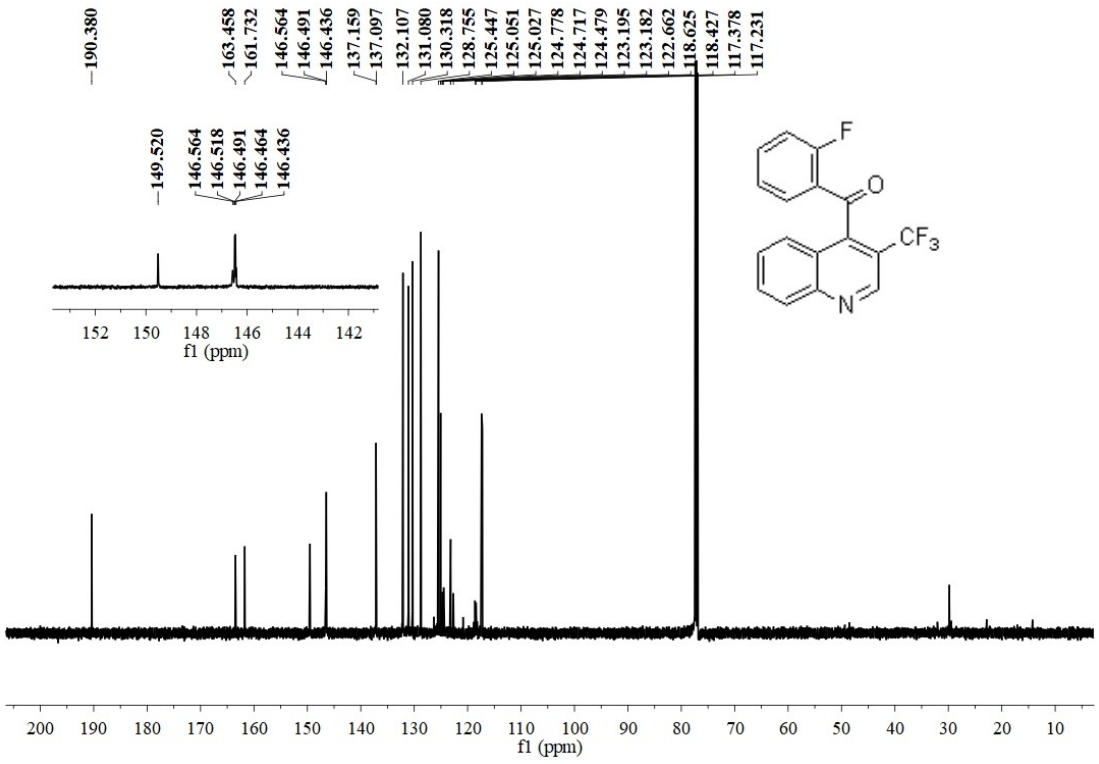

9.210
8.261
8.240
7.696
7.653
7.575
7.537
7.280
7.271
2.668
2.649
2.630
1.709
1.691
1.672
1.653
1.634
1.616
0.966
0.948
0.929
O
CF3
N
8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3
f1 (ppm)
1.00
1.05
1.04
3.04
1.03
2.07
2.06
2.23
3.15
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

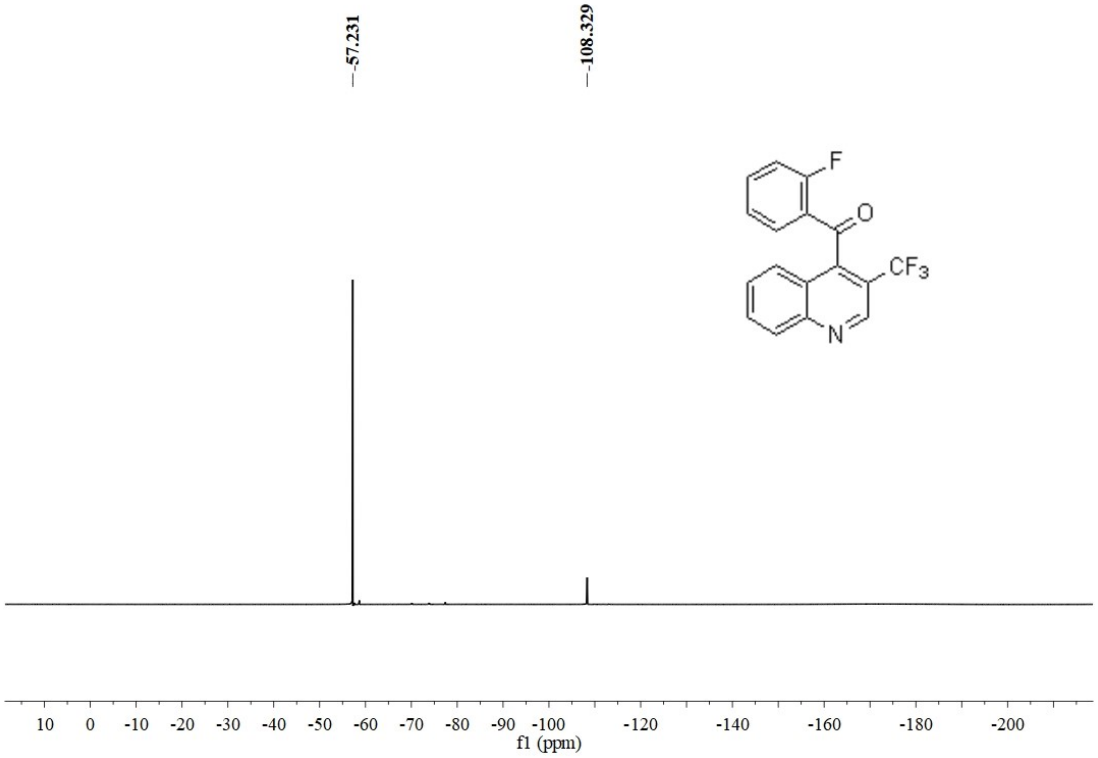

193.684
150.845
149.372
146.437
145.180
145.157
129.949
129.244
128.730
127.570
126.380
124.840
124.041
122.110
120.117
119.796
119.475
119.382
77.478
77.363
77.160
76.842
38.303
24.138
13.902
134.068
132.166
130.164
129.949
129.244
128.730
127.570
126.380
O
CF3
N
135.0 134.0 133.0 132.0 131.0 130.0 129.0 128.0 127.0 126.0
f1 (ppm)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-57.105
O
CF3
N
-15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -110 -120 -130
f1 (ppm)

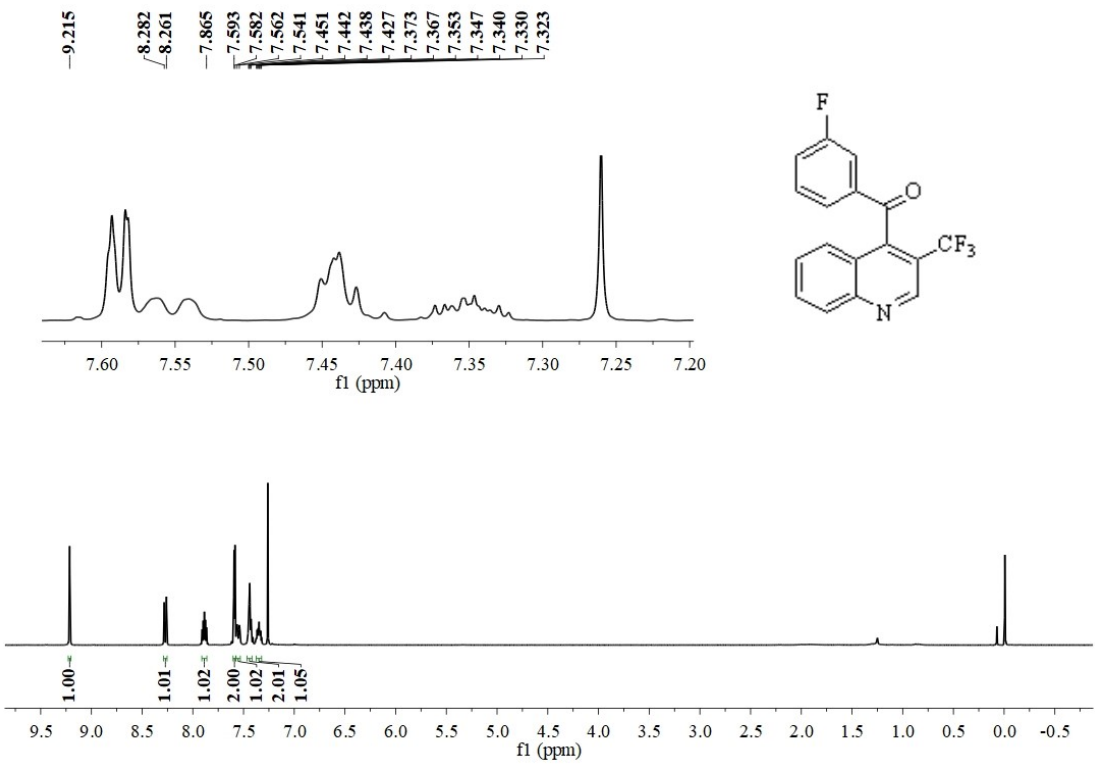
3ag

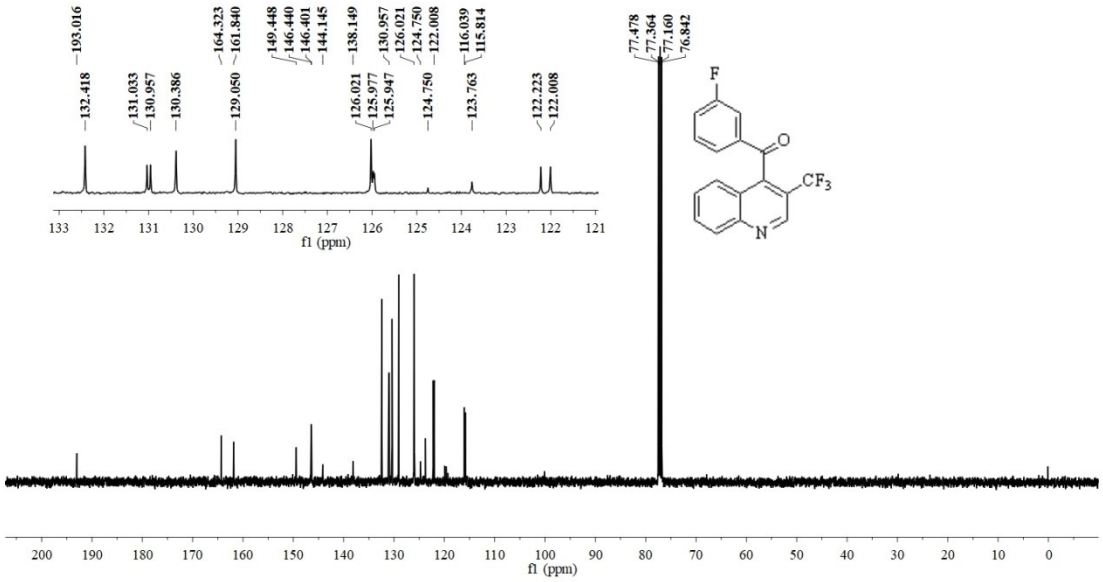

9.175
8.231
7.849
7.647
7.613
7.563
7.348
7.322
7.062
7.046
7.030
F
O
CF3
N
8.3
8.0
7.7
7.4
7.1
f1 (ppm)
1.00
1.09
1.06
1.07
2.09
1.08
1.07
1.03
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

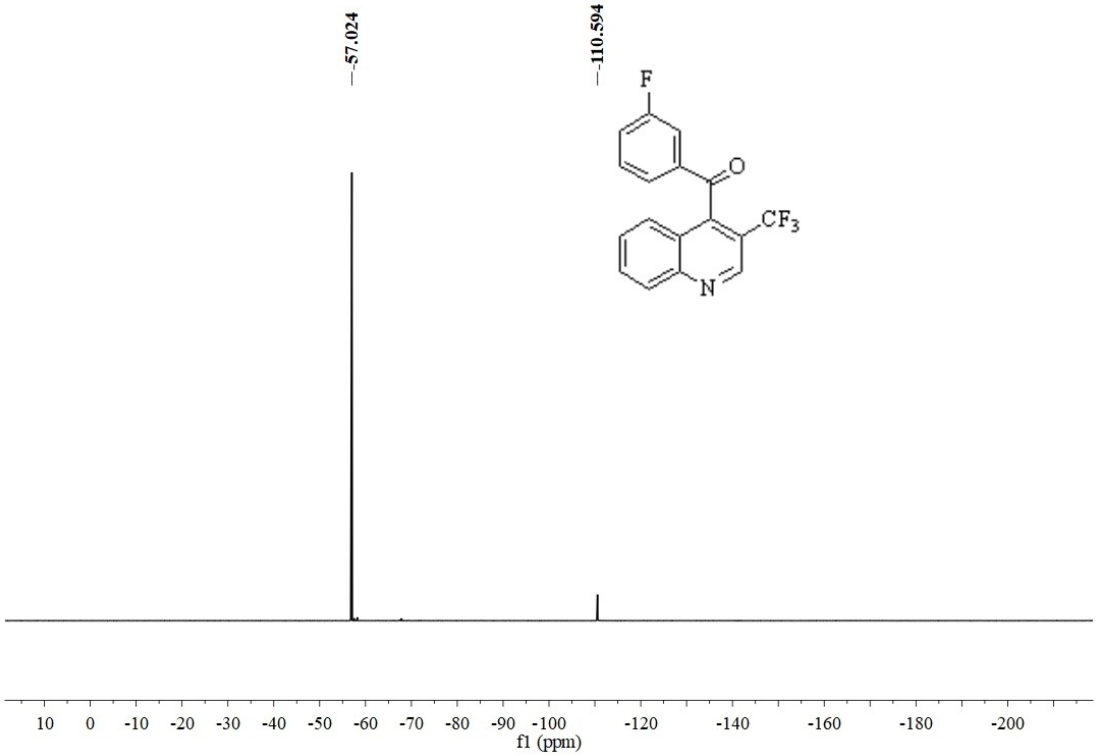

190.380
163.458
161.732
146.564
146.491
146.436
137.159
137.097
132.107
131.080
130.318
128.755
125.447
125.051
125.027
124.778
124.717
124.479
123.195
123.182
122.662
118.625
118.427
117.378
117.231
149.520
146.564
146.518
146.491
146.464
146.436
F
O
CF3
N
152
150
148
146
144
142
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


-57.231
-108.329
F
O
CF3
N
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)

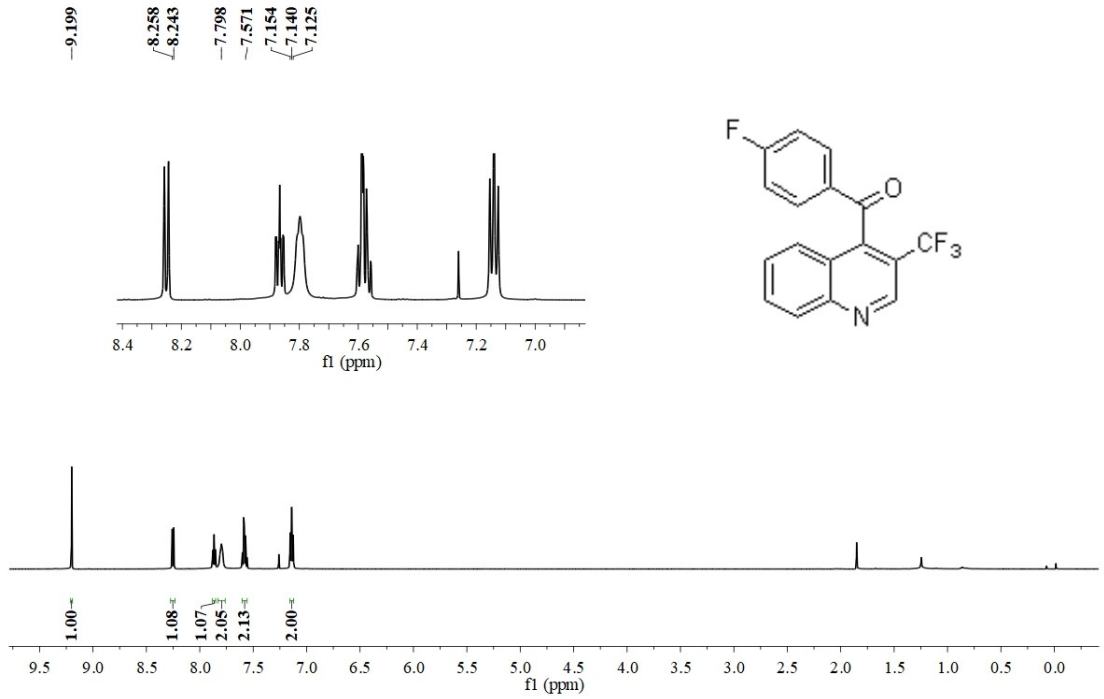
3ah

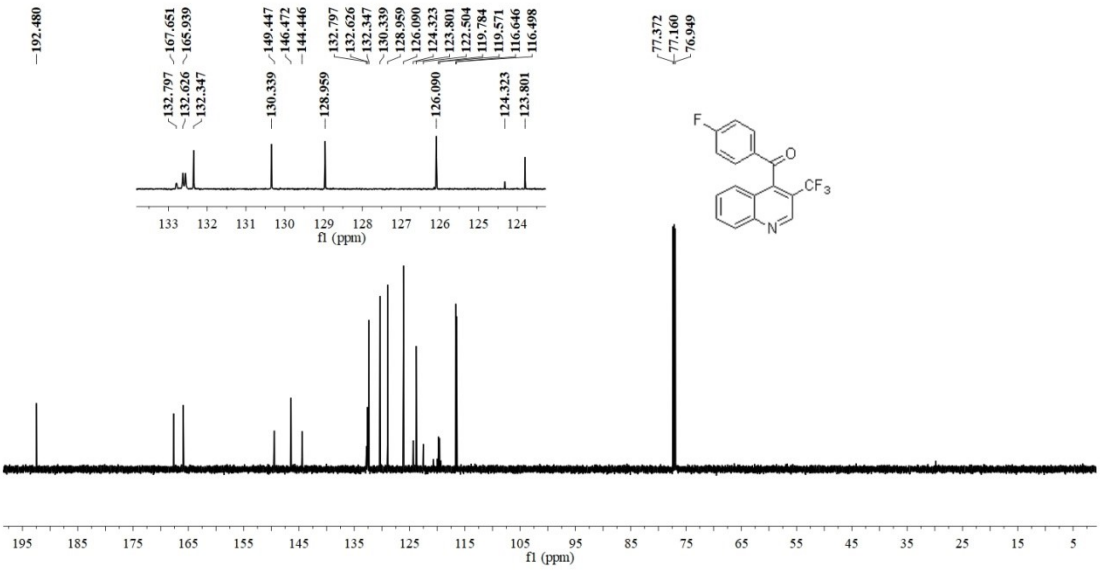

9.215
8.282
8.261
7.865
7.593
7.582
7.562
7.541
7.451
7.442
7.438
7.427
7.373
7.367
7.353
7.347
7.340
7.330
7.323
F
O
CF3
N
7.60 7.55 7.50 7.45 7.40 7.35 7.30 7.25 7.20
f1 (ppm)
1.00
1.01
1.02
2.00
1.02
2.01
1.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

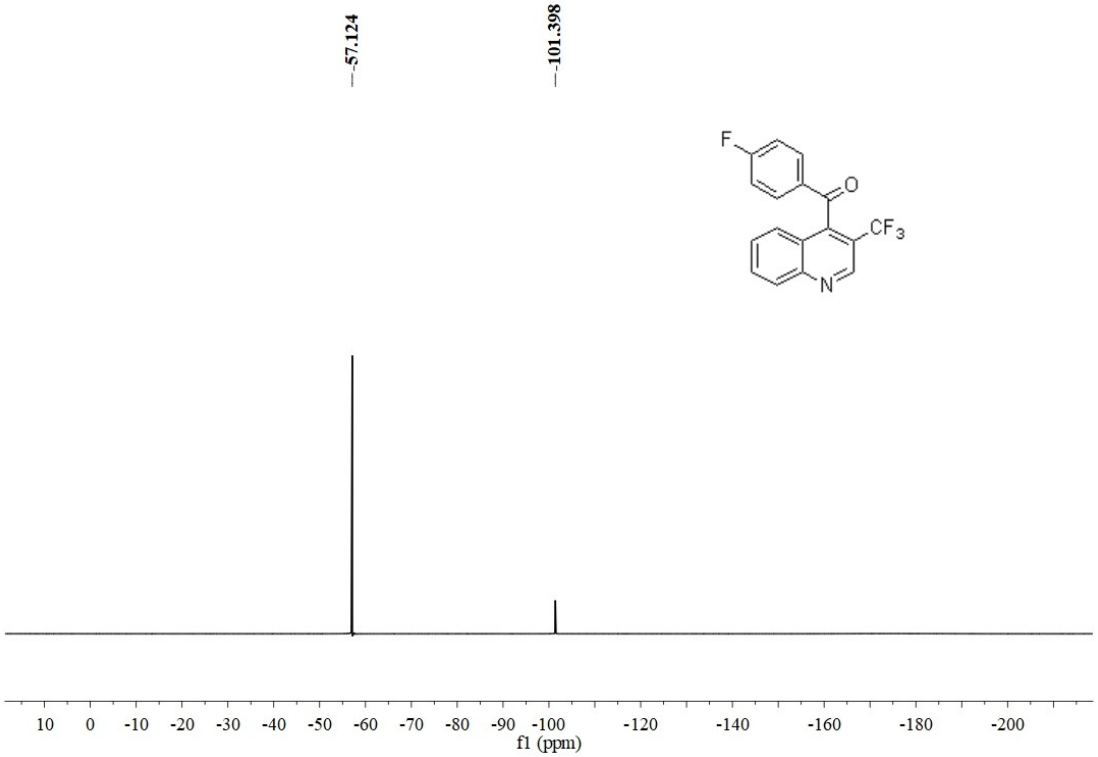

193.016
132.418
131.033
130.957
130.386
164.323
161.840
129.050
149.448
146.440
146.401
144.145
138.149
126.021
125.977
125.947
130.957
126.021
124.750
122.008
124.750
122.008
116.039
115.814
123.763
122.223
122.008
77.478
77.364
77.160
76.842
F
O
CF3
N
f1 (ppm)


-57.024
-110.594
F
O
CF3
N
f1 (ppm)

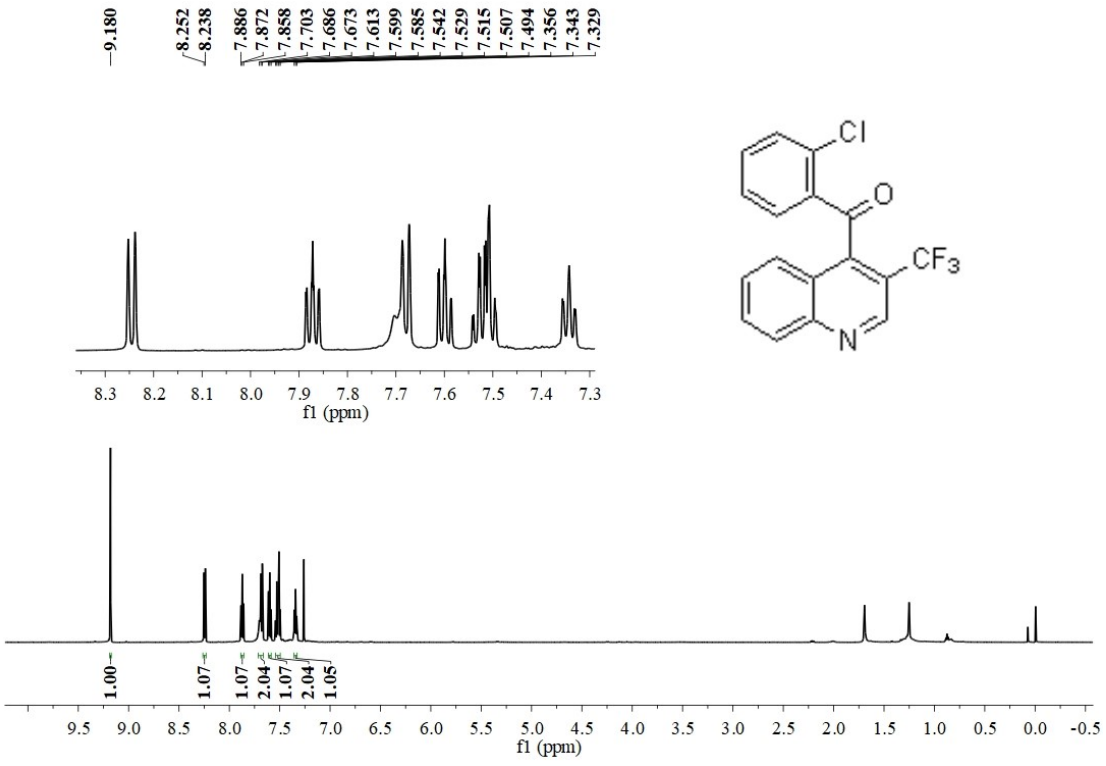
3ai

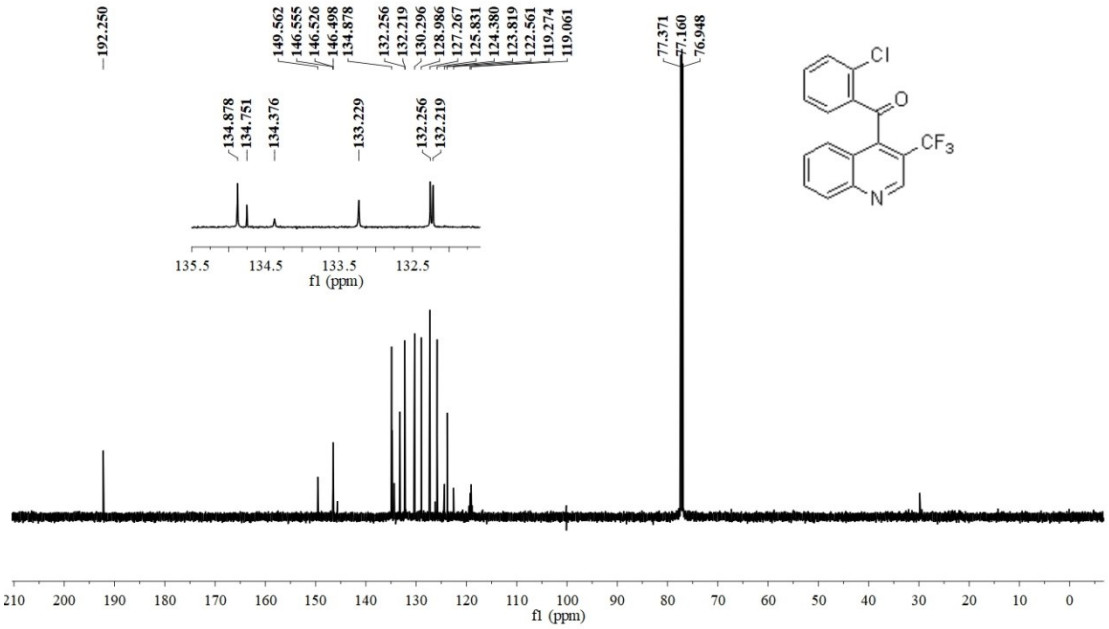

9.199
8.258
8.243
7.798
7.571
7.154
7.140
7.125
F
O
CF3
N
f1 (ppm)
1.00
1.08
1.07
2.05
2.13
2.00

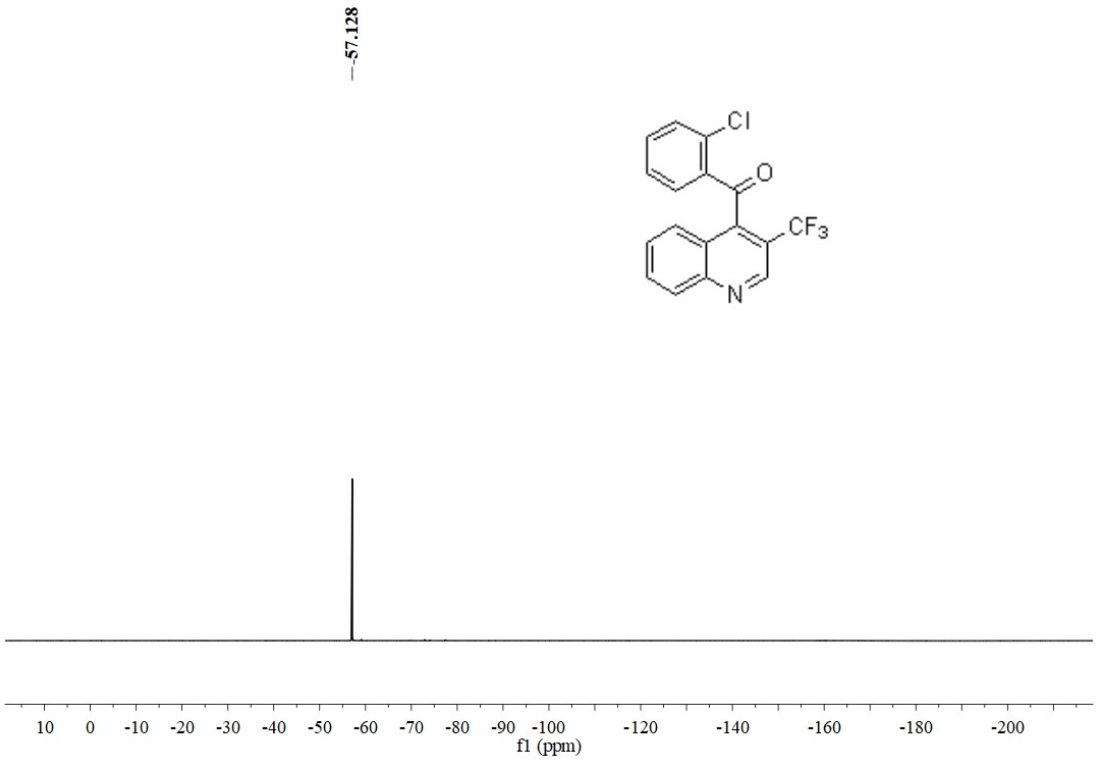

192.480
167.651
165.939
149.447
146.472
144.446
132.797
132.626
132.347
130.339
128.959
126.090
124.323
123.801
122.504
119.784
119.571
116.646
116.498
77.372
77.160
76.949
F
O
CF3
N
f1 (ppm)


-57.124
-101.398
F
O
CF3
N
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)

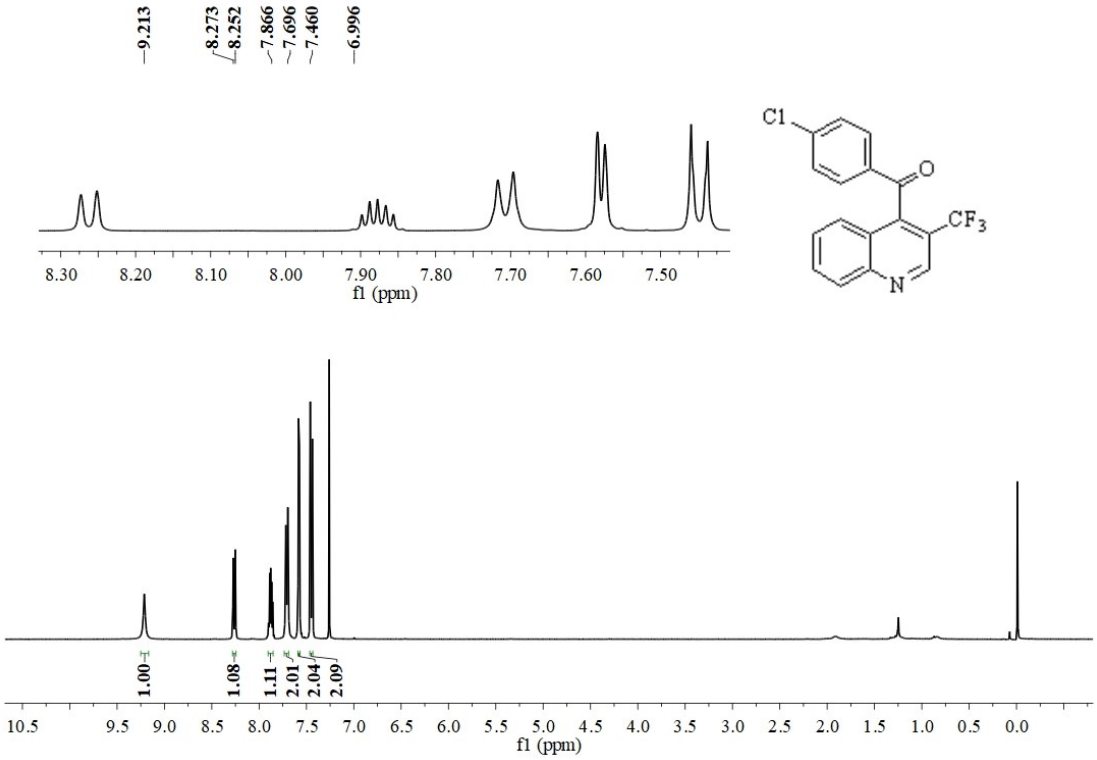
3aj

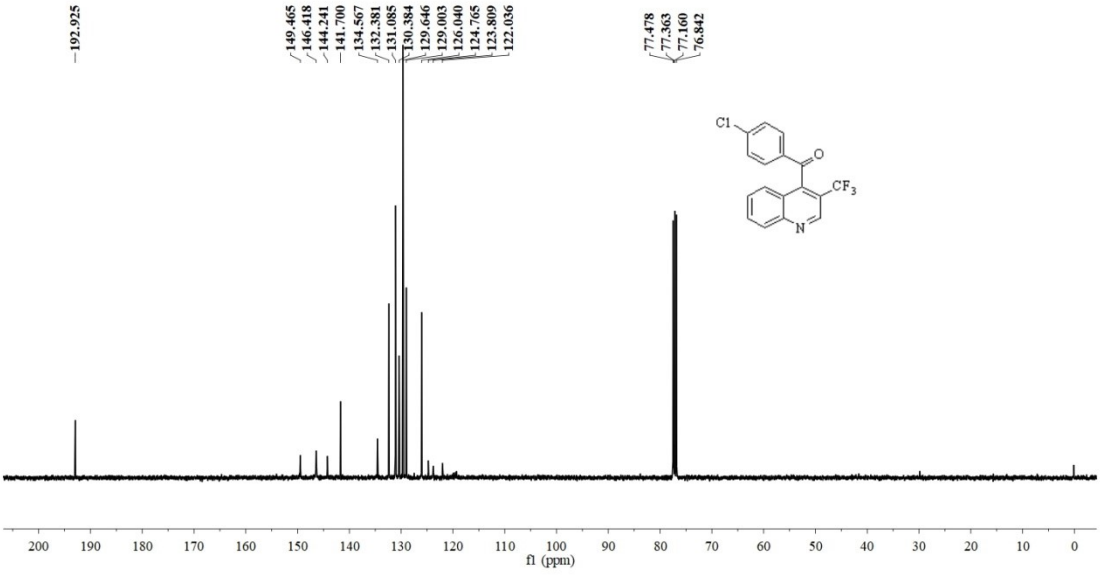

9.180
8.252
8.238
7.886
7.872
7.858
7.703
7.686
7.673
7.613
7.599
7.585
7.542
7.529
7.515
7.507
7.494
7.356
7.343
7.329
Cl
O
CF3
N
8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3
f1 (ppm)
1.00
1.07
1.07
2.04
1.07
2.04
1.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

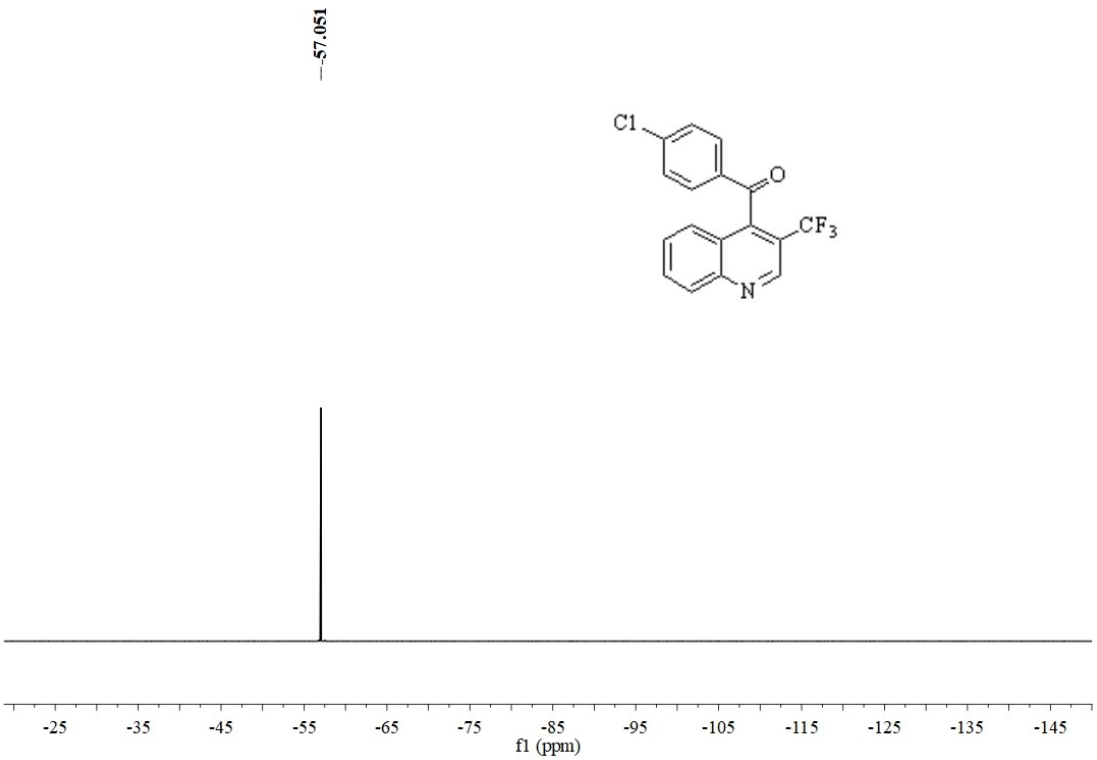

192.250
149.562
146.555
146.526
146.498
134.878
132.256
132.219
130.296
128.986
127.267
125.831
124.380
123.819
122.561
119.274
119.061
77.371
77.160
76.948
134.878
134.751
134.376
133.229
132.256
132.219
135.5
134.5
133.5
132.5
f1 (ppm)
Cl
O
CF3
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-57.128
Cl
O
CF3
N
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)

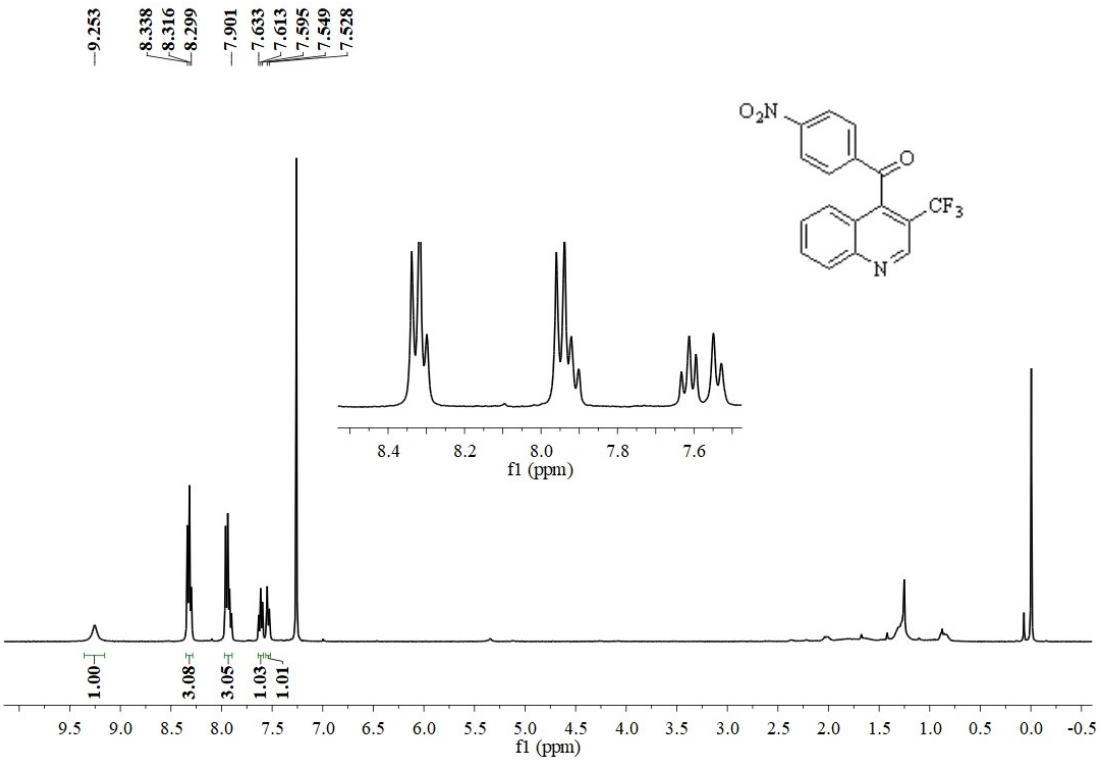
3ak

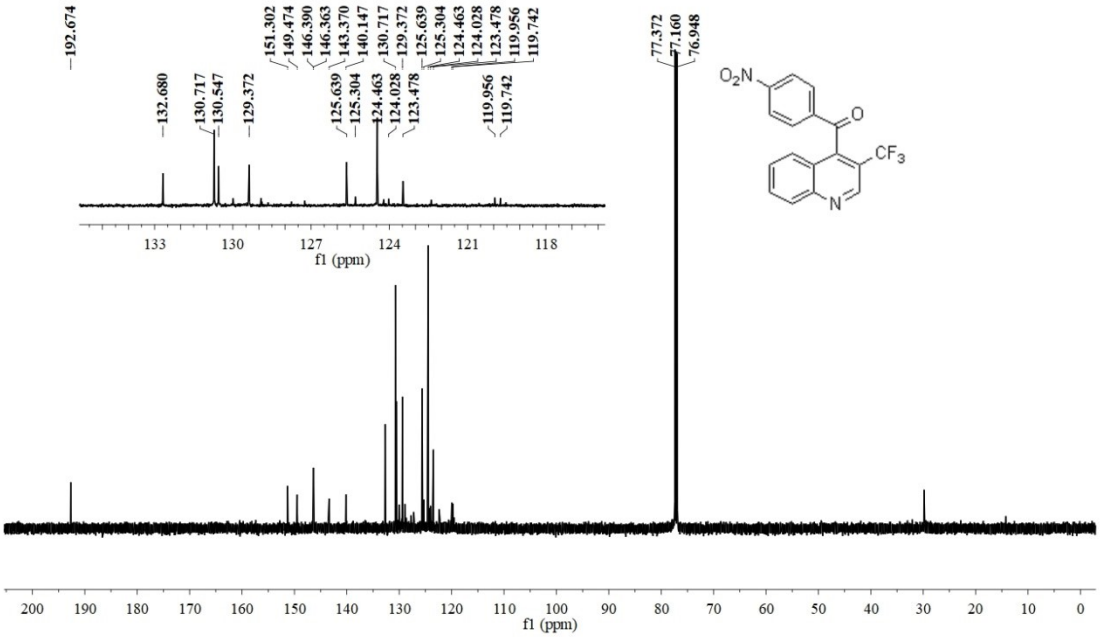

9.213
8.273
8.252
7.866
7.696
7.460
6.996
Cl
O
CF3
N
8.30 8.20 8.10 8.00 7.90 7.80 7.70 7.60 7.50
f1 (ppm)
1.00
1.08
1.11
2.01
2.04
2.09
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

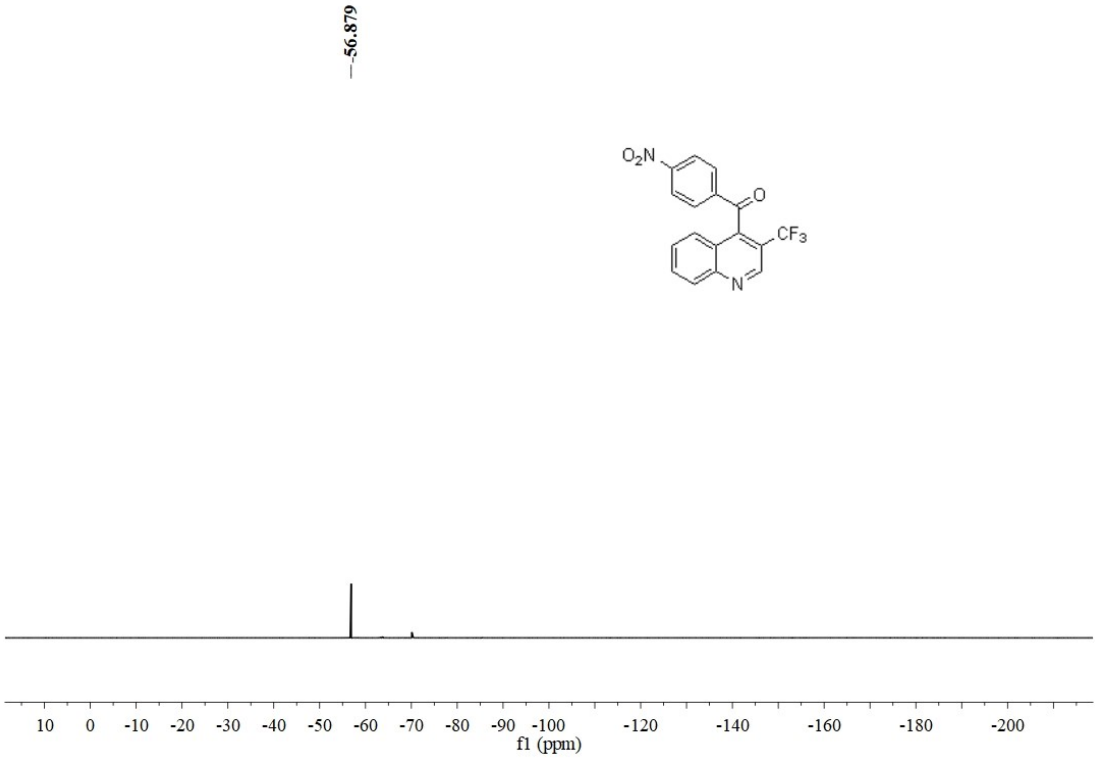

192.925
149.465
146.418
144.241
141.700
134.567
132.381
131.085
130.384
129.646
129.003
126.040
124.765
123.809
122.036
77.478
77.363
77.160
76.842
Cl
O
CF3
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-57.051
Cl
O
CF3
N
-25
-35
-45
-55
-65
-75
-85
-95
-105
-115
-125
-135
-145
f1 (ppm)

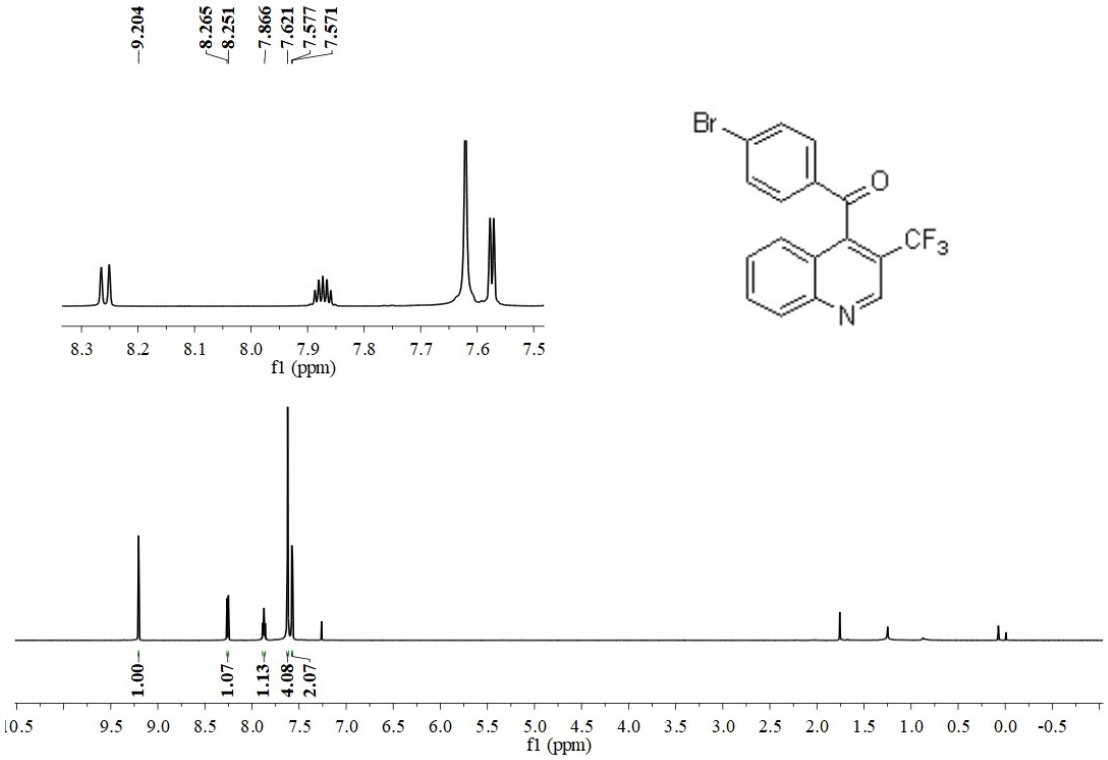
3al

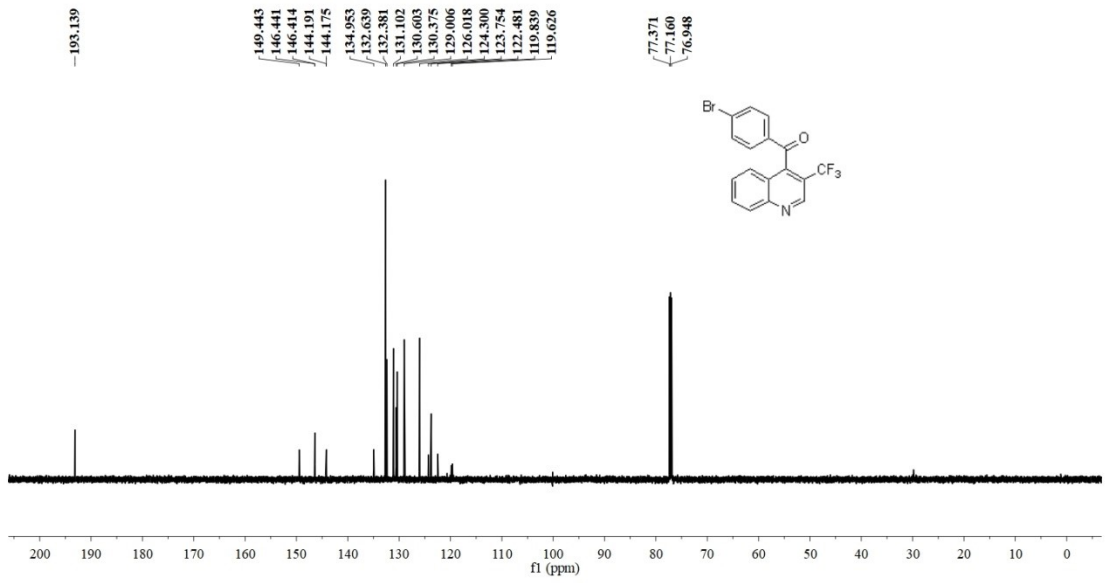

9.253
8.338
8.316
8.299
7.901
7.633
7.613
7.595
7.549
7.528
O2N
O
CF3
N
8.4
8.2
8.0
7.8
7.6
f1 (ppm)
1.00
3.08
3.05
1.03
1.01
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

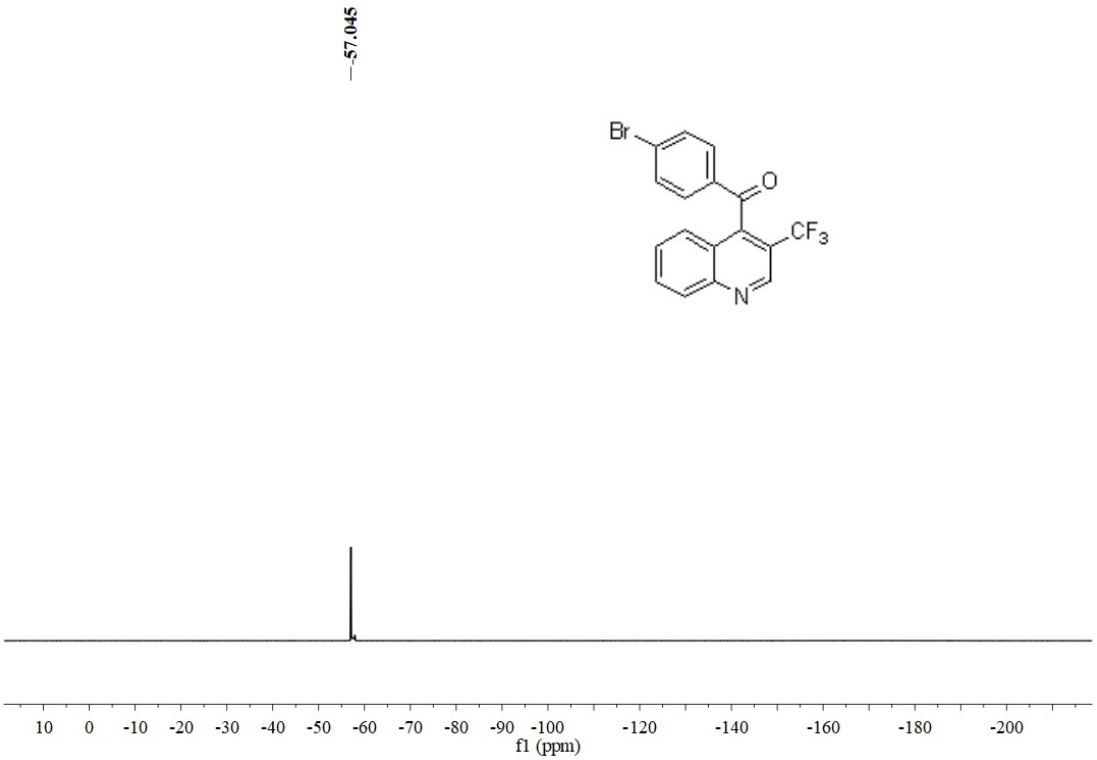

192.674
151.302
149.474
146.390
146.363
143.370
140.147
130.717
129.372
125.639
125.304
124.463
124.028
123.478
119.956
119.742
77.372
77.160
76.948
132.680
130.717
130.547
129.372
125.639
125.304
124.463
124.028
123.478
119.956
119.742
133
130
127
124
121
118
f1 (ppm)
O2N
O
CF3
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


56.879
O2N
O
CF3
N
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

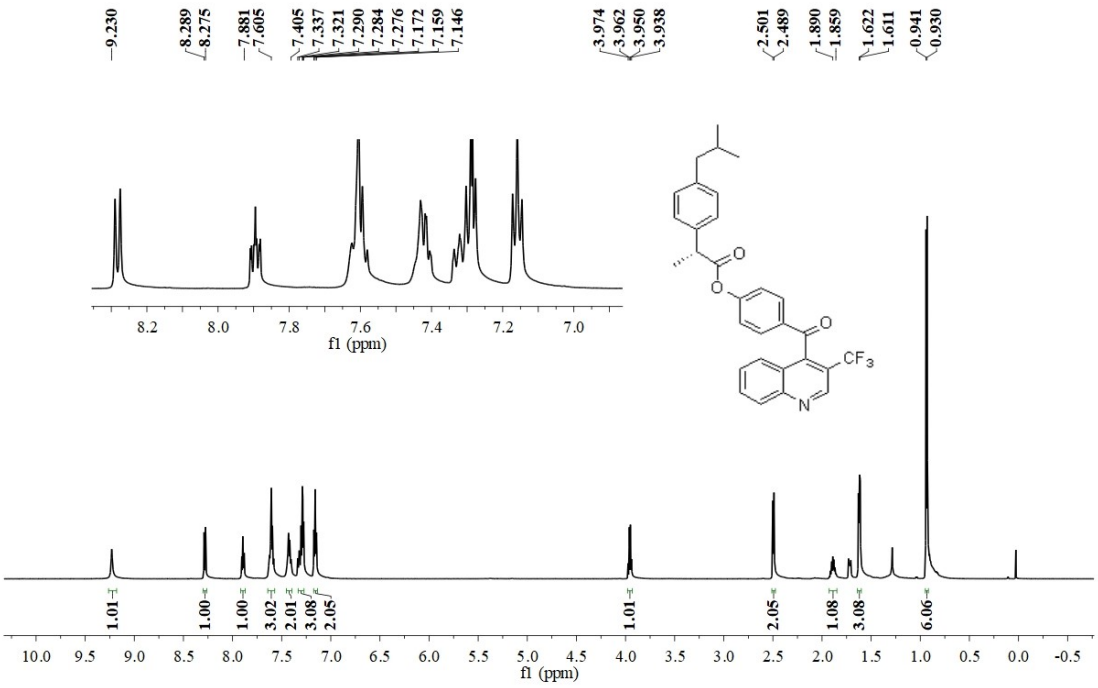
3am

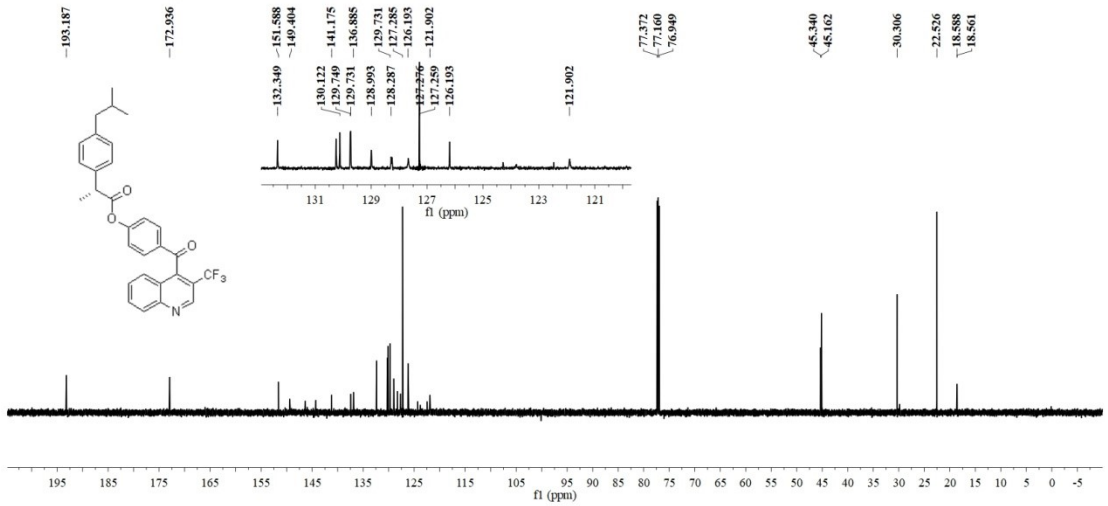

9.204
8.265
8.251
7.866
7.621
7.577
7.571
Br
O
CF3
N
f1 (ppm)
1.00
1.07
1.13
4.08
2.07
f1 (ppm)

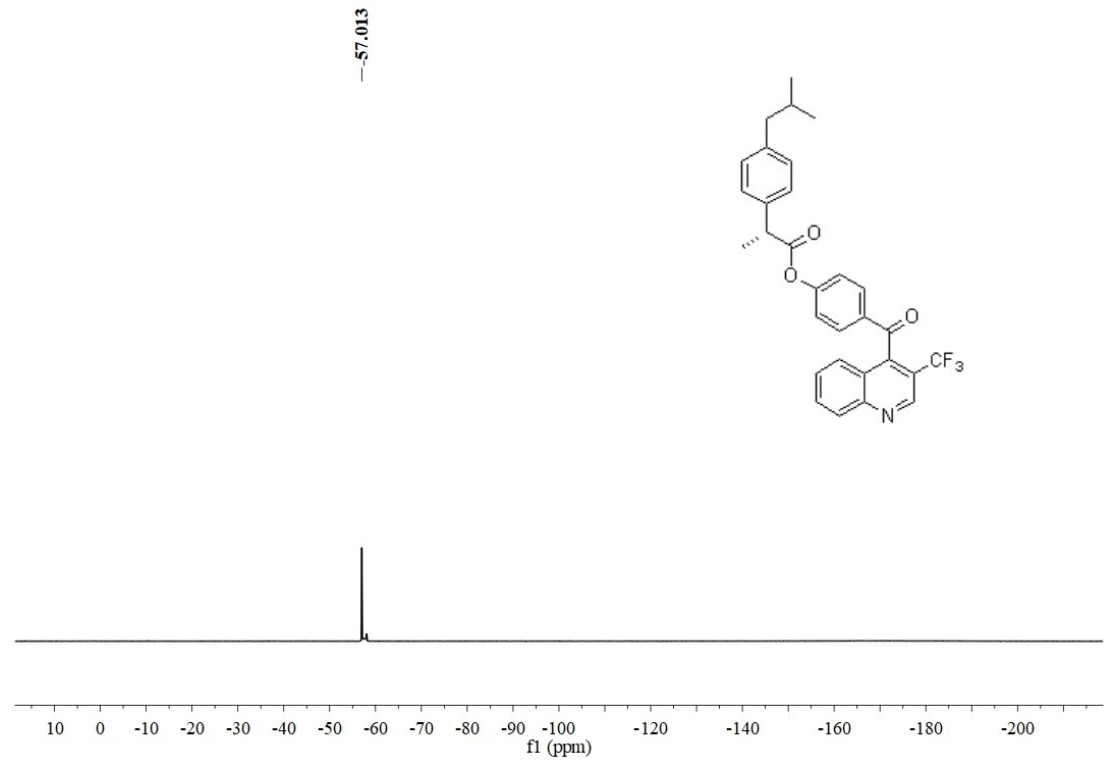

193.139
149.443
146.441
146.414
144.191
144.175
134.953
132.639
132.381
131.102
130.603
130.375
129.006
126.018
124.300
123.754
122.481
119.839
119.626
77.371
77.160
76.948
Br
O
CF3
N
f1 (ppm)


-57.045
Br
O
CF3
N
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)

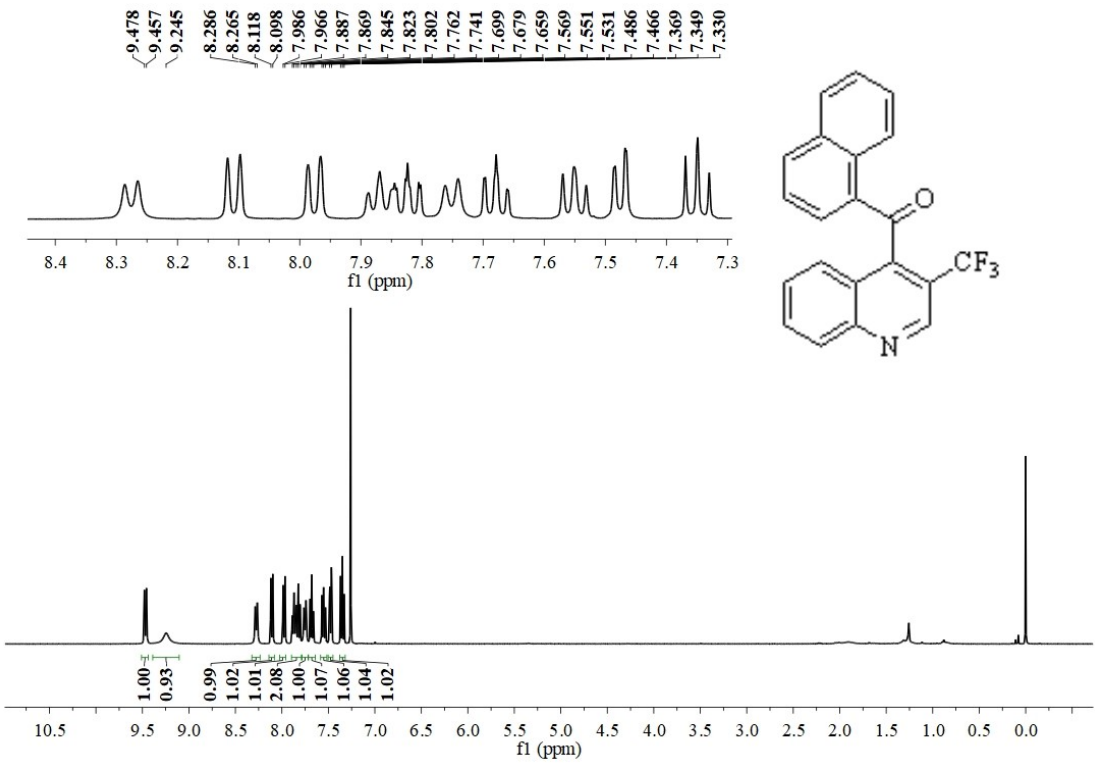
3an

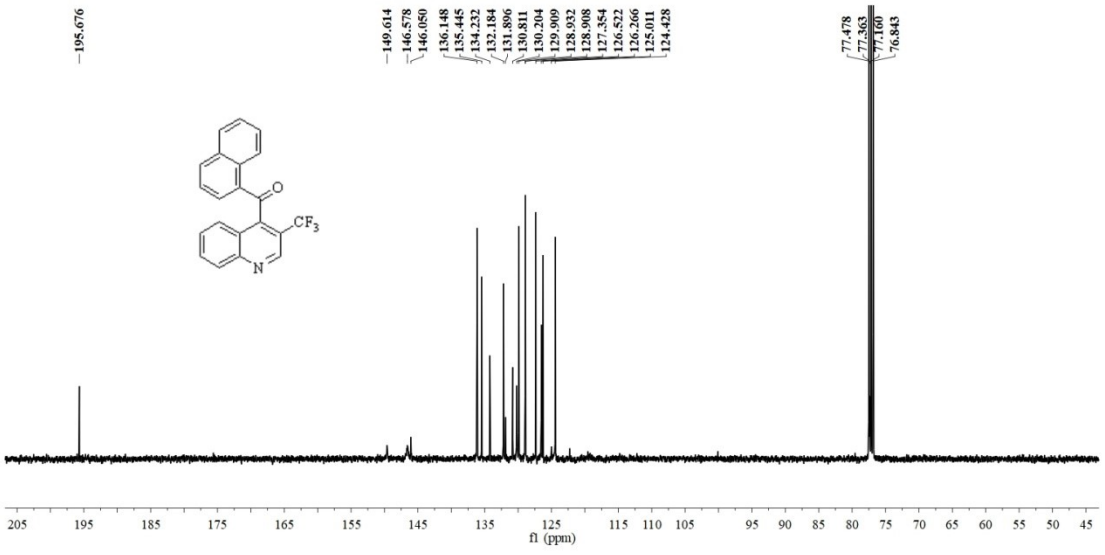

9.230
8.289
8.275
7.881
7.605
7.405
7.337
7.321
7.290
7.284
7.276
7.172
7.159
7.146
3.974
3.962
3.950
3.938
2.501
2.489
1.890
1.859
1.622
1.611
0.941
0.930
8.2 8.0 7.8 7.6 7.4 7.2 7.0
f1 (ppm)
O
O
O
CF3
N
1.01
1.00
1.00
3.02
2.01
3.08
2.05
1.01
2.05
1.08
3.08
6.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

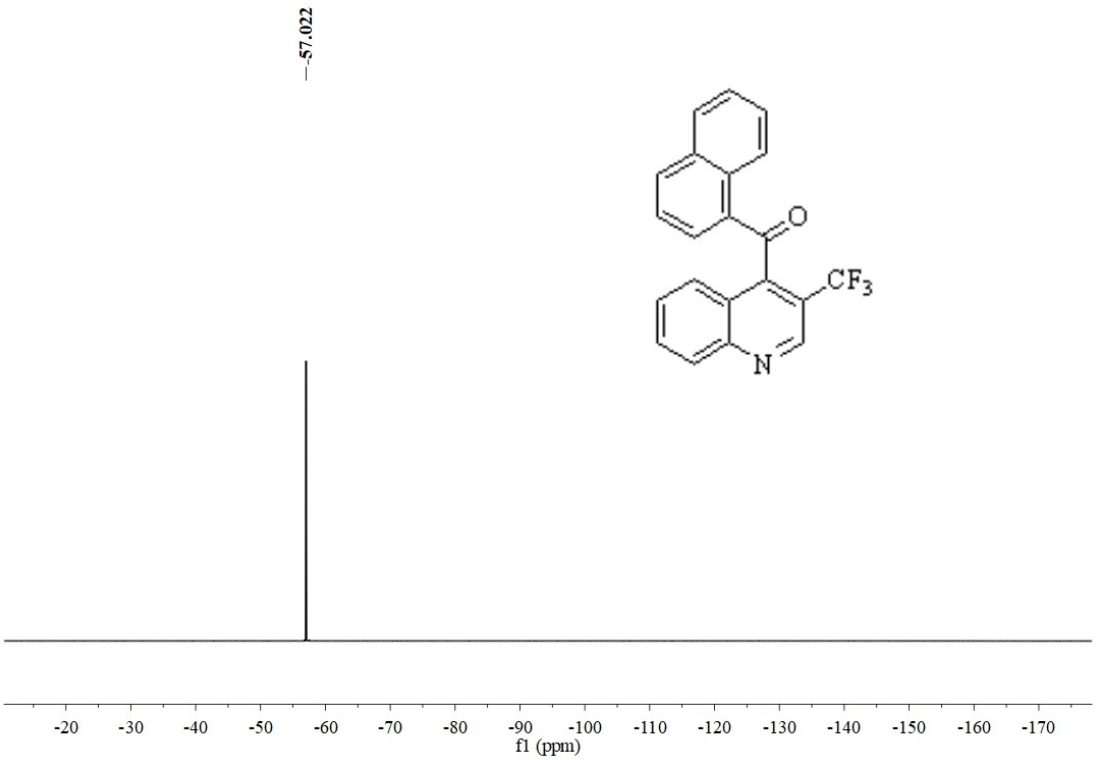

193.187
172.936
151.588
149.404
141.175
136.885
129.731
127.285
126.193
121.902
77.372
77.160
76.949
45.340
45.162
30.306
22.526
18.588
18.561
132.349
130.122
129.749
129.731
128.993
128.287
127.276
127.259
126.193
121.902
131
129
127
125
123
121
f1 (ppm)
O
O
CF3
N
195 185 175 165 155 145 135 125 115 105 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5
f1 (ppm)


-57.013
O
O
O
CF3
N
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)

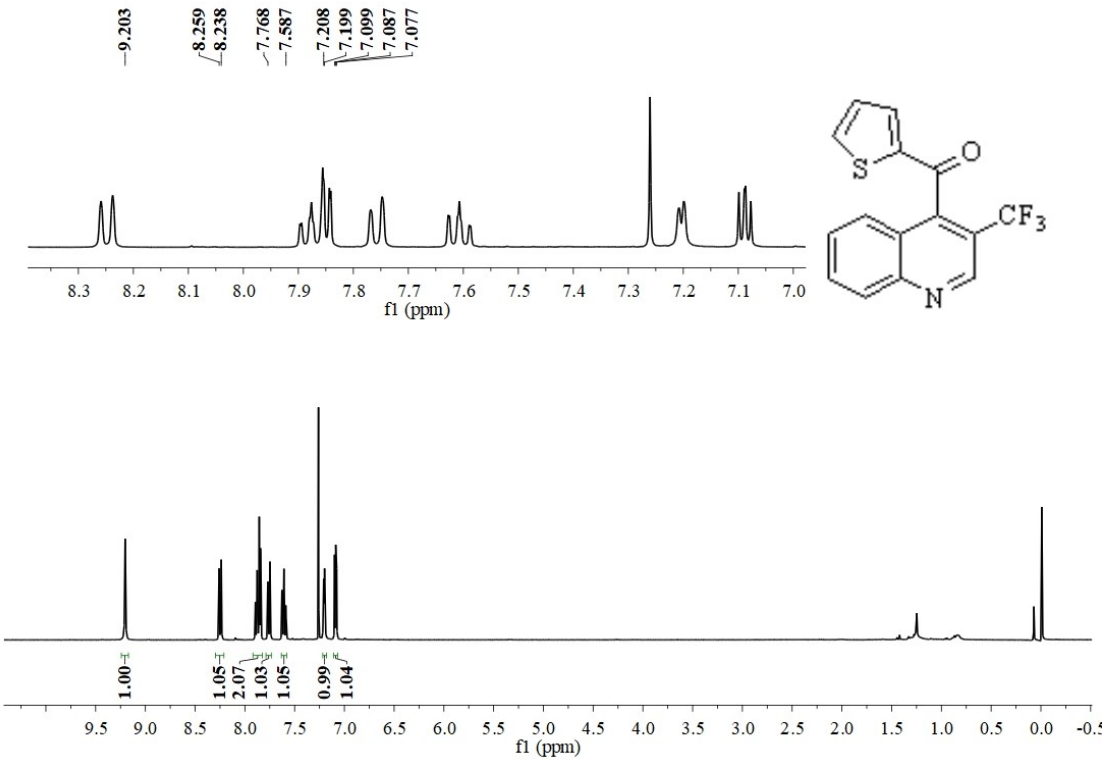
3ao

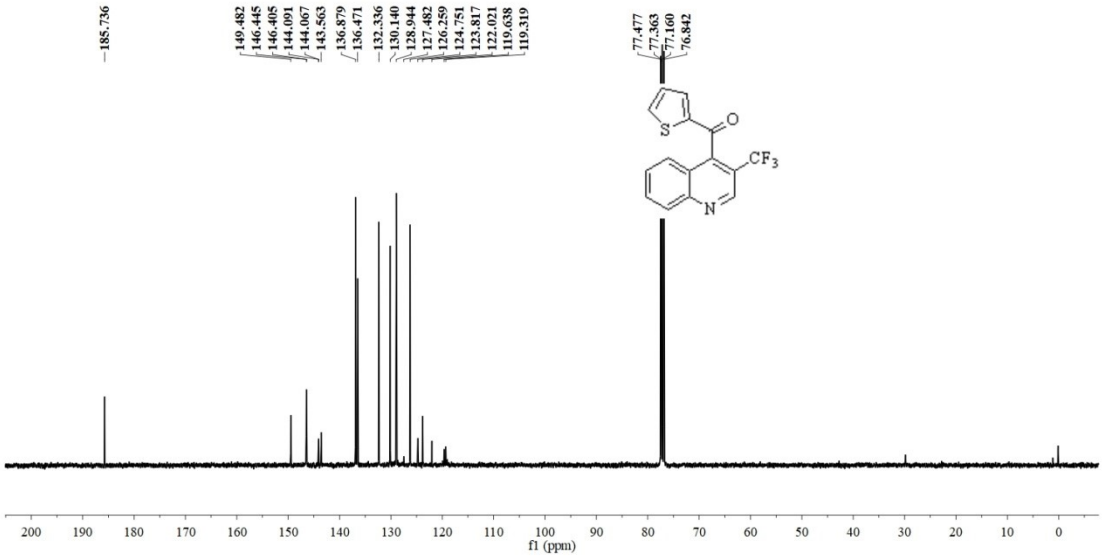

9.478
9.457
9.245
8.286
8.265
8.118
8.098
7.986
7.966
7.887
7.869
7.845
7.823
7.802
7.762
7.741
7.699
7.679
7.659
7.569
7.551
7.531
7.486
7.466
7.369
7.349
7.330
f1 (ppm)
O
CF3
N
1.00
0.93
0.99
1.02
1.01
2.08
1.00
1.07
1.06
1.04
1.02
f1 (ppm)

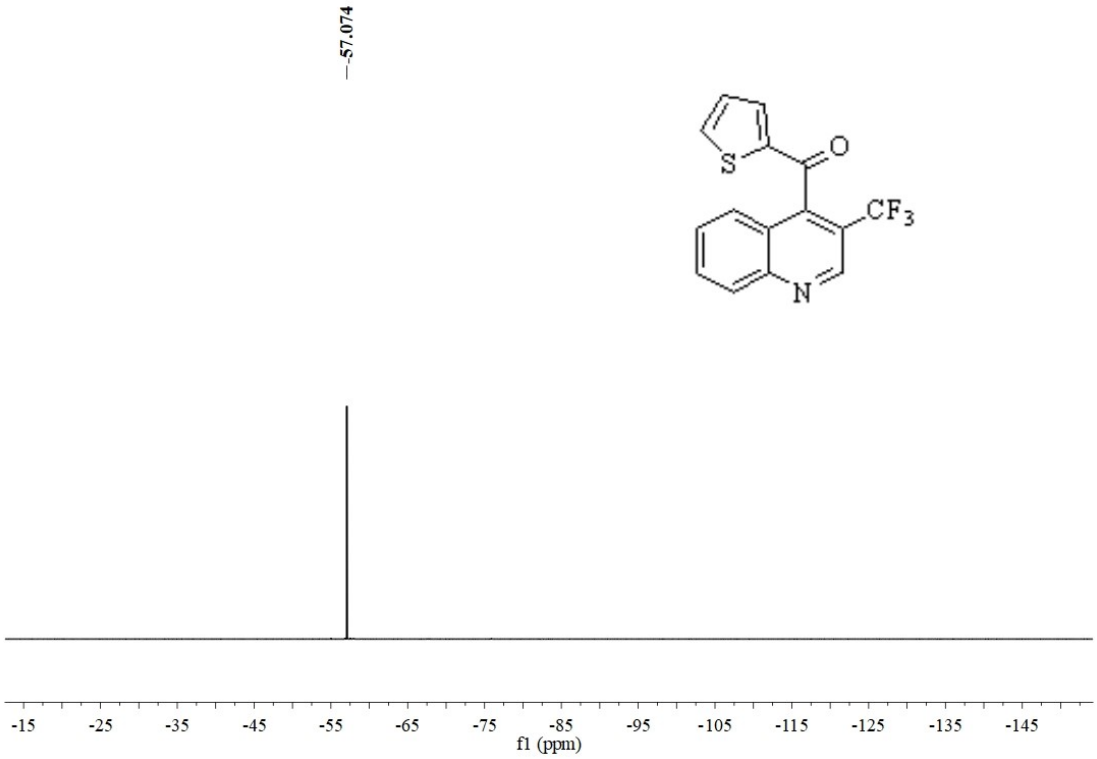

195.676
149.614
146.578
146.050
136.148
135.445
134.232
132.184
131.896
130.811
130.204
129.909
128.932
128.908
127.354
126.522
126.266
125.011
124.428
77.478
77.363
77.160
76.843
O
CF3
N
f1 (ppm)


-57.022
O
CF3
N
-20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170
f1 (ppm)

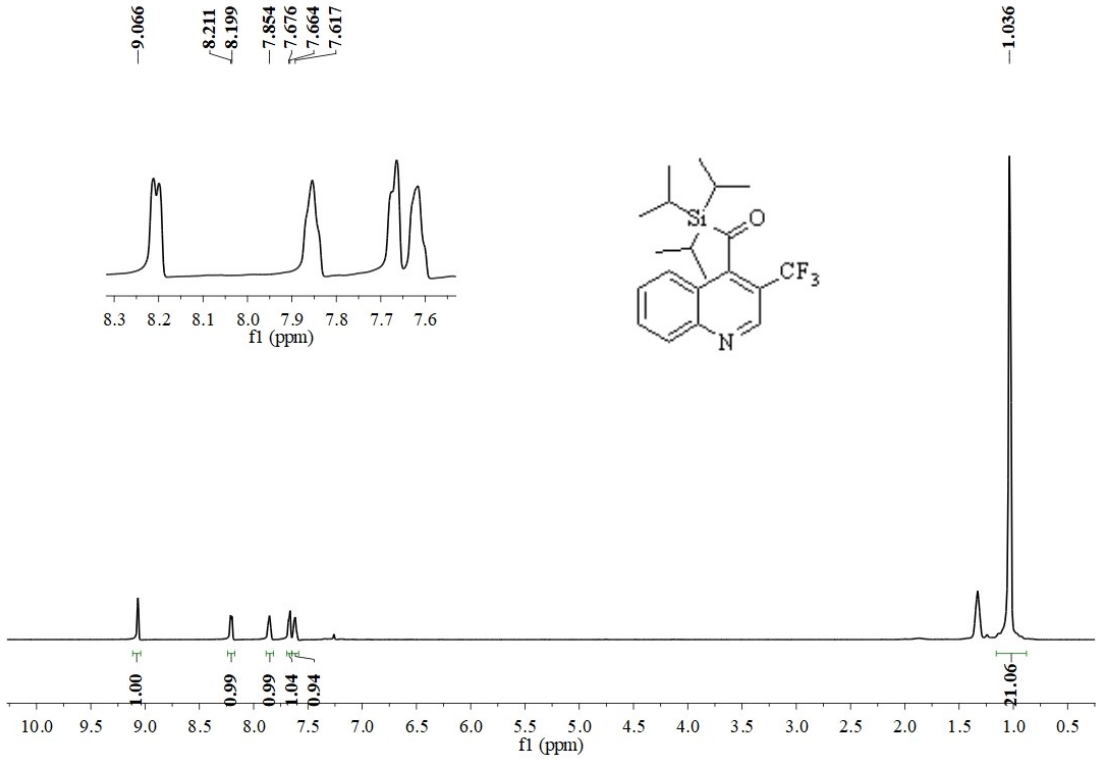
3ap

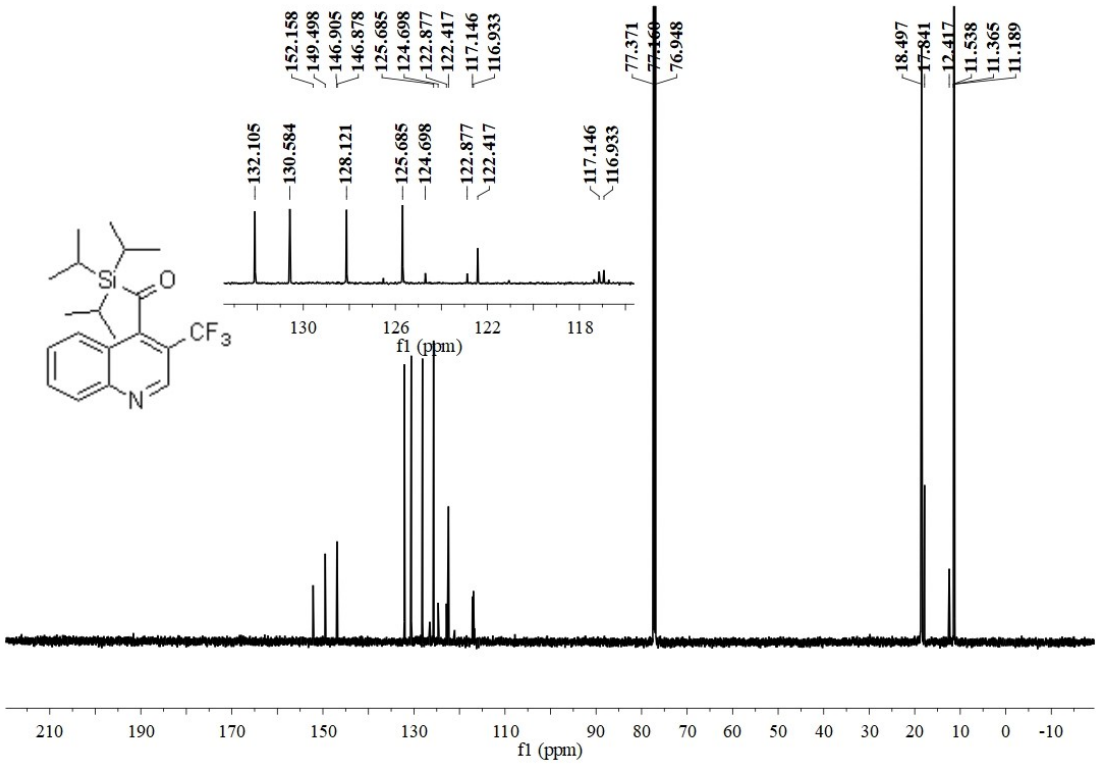

9.203
8.259
8.238
7.768
7.587
7.208
7.199
7.099
7.087
7.077
S
O
CF3
N
8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0
f1 (ppm)
1.00
1.05
2.07
1.03
1.05
0.99
1.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

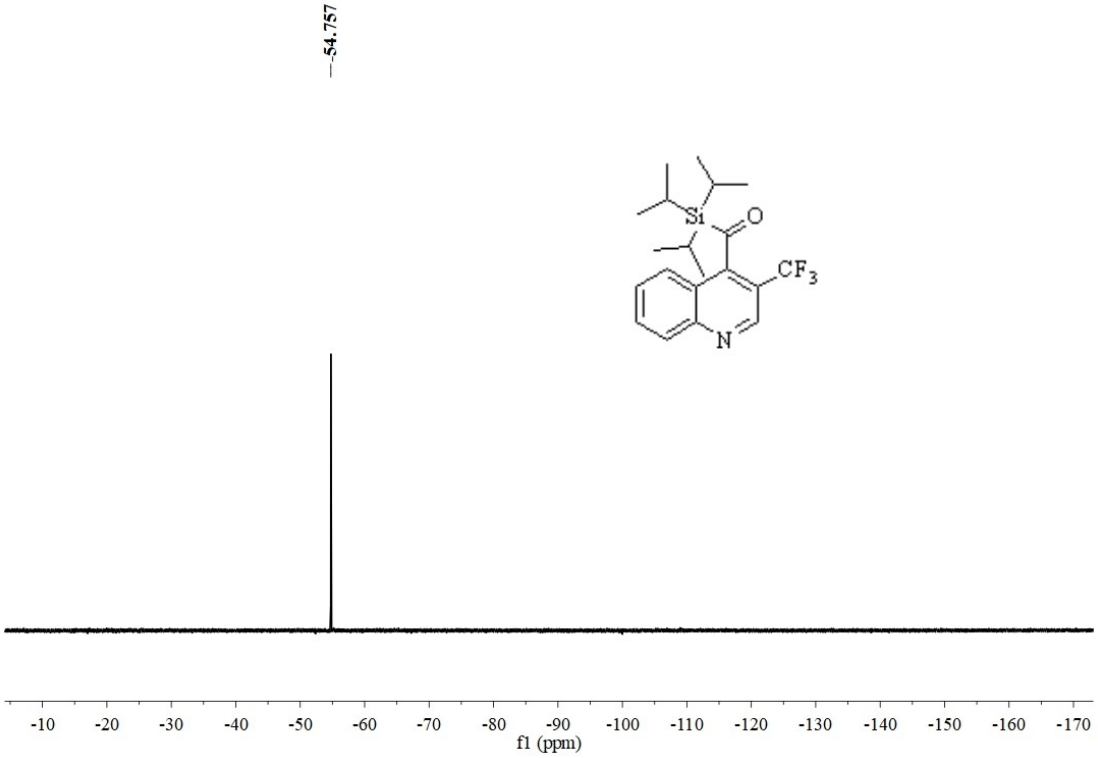

185.736
149.482
146.445
146.405
144.091
144.067
143.563
136.879
136.471
133.336
130.140
128.944
127.482
126.259
124.751
123.817
122.021
119.638
119.319
77.477
77.363
77.160
76.842
S
O
CF3
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-57.074
S
O
CF3
N
-15 -25 -35 -45 -55 -65 -75 -85 -95 -105 -115 -125 -135 -145
f1 (ppm)

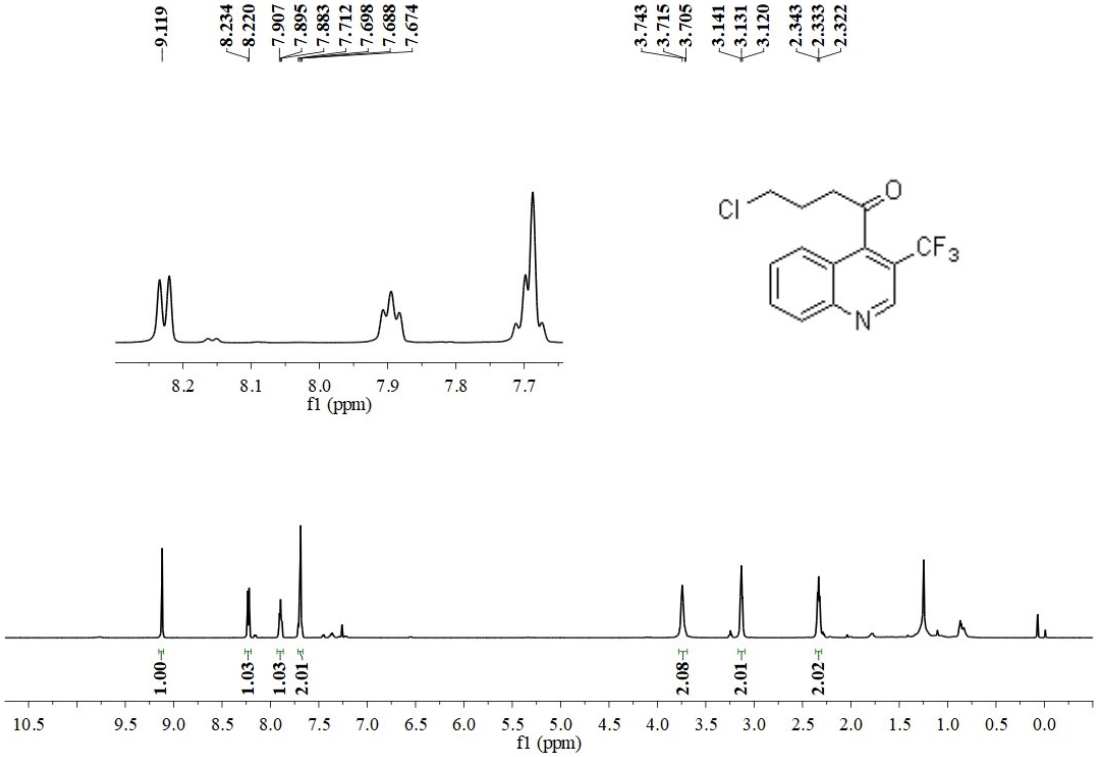
3aq

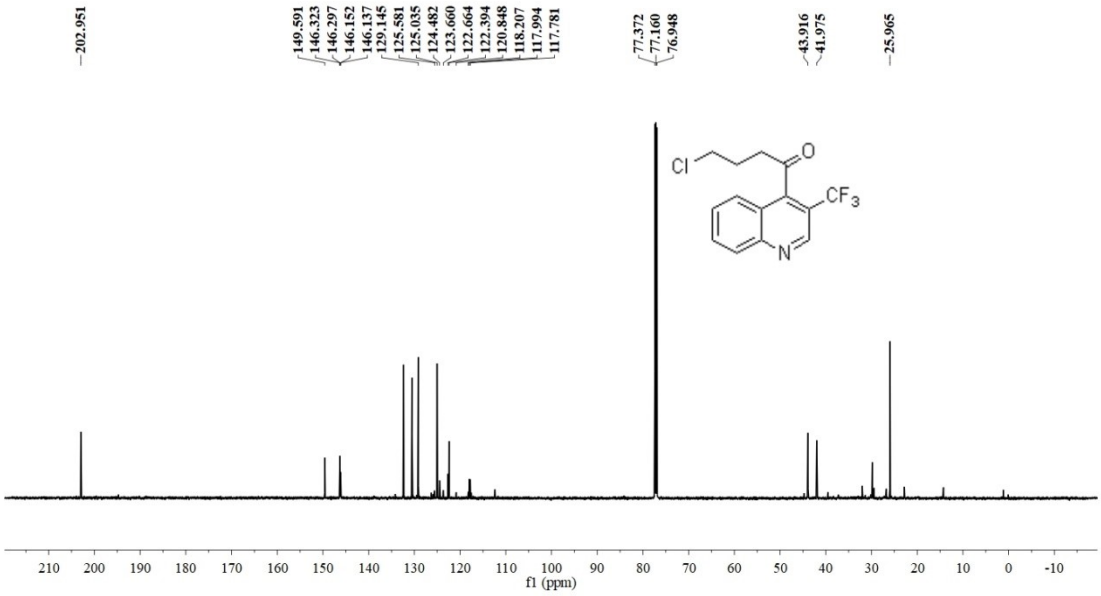

9.066
8.211
8.199
7.854
7.676
7.664
7.617
1.036
Si
O
CF3
N
8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6
f1 (ppm)
1.00
0.99
0.99
1.04
0.94
21.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

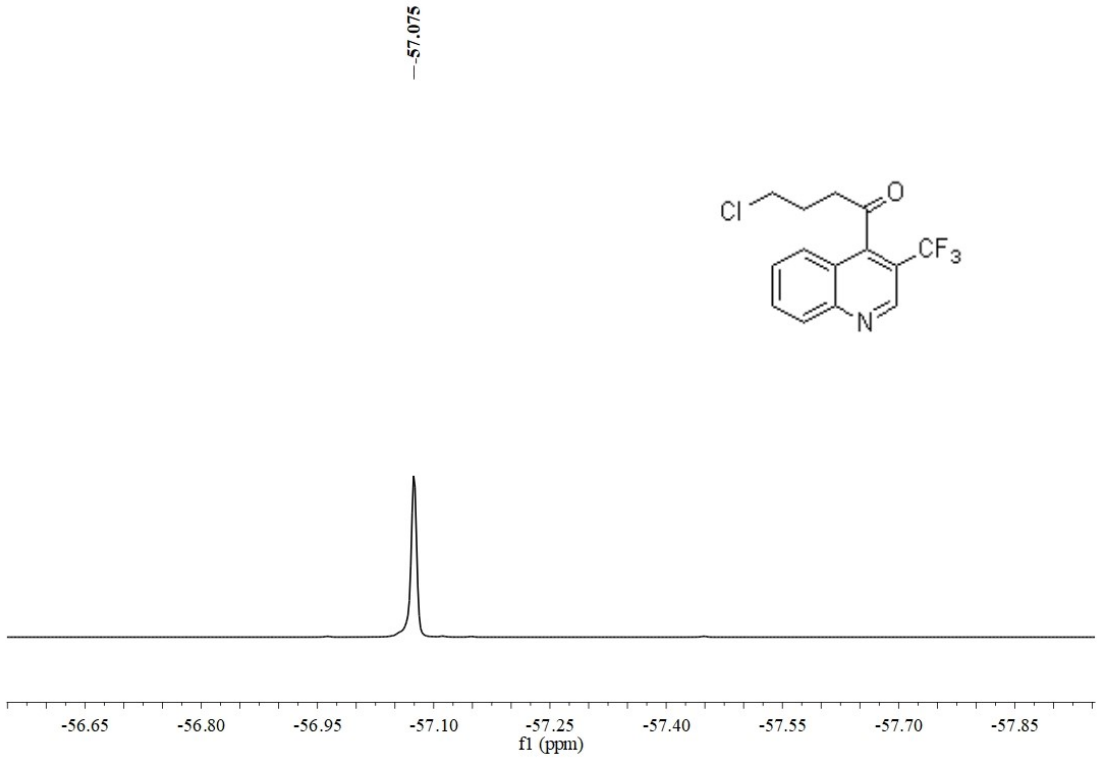

152.158
149.498
146.905
146.878
125.685
124.698
122.877
122.417
117.146
116.933
77.371
77.160
76.948
18.497
17.841
12.417
11.538
11.365
11.189
132.105
130.584
128.121
125.685
124.698
122.877
122.417
117.146
116.933
Si
O
CF3
N
130 126 122 118
f1 (ppm)
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-54.757
Si
O
CF3
N
-10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170
f1 (ppm)

4ar

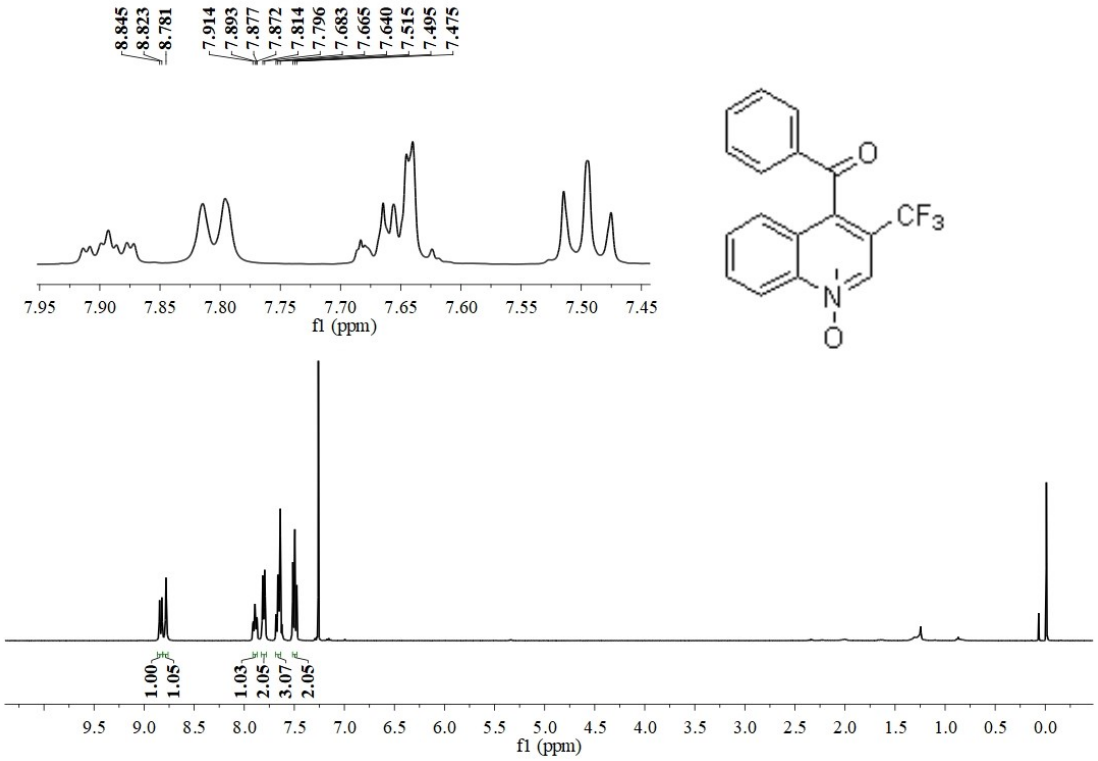

9.119
8.234
8.220
7.907
7.895
7.883
7.712
7.698
7.688
7.674
3.743
3.715
3.705
3.141
3.131
3.120
2.343
2.333
2.322
Cl
O
CF3
N
8.2 8.1 8.0 7.9 7.8 7.7
f1 (ppm)
1.00
1.03
1.03
2.01
2.08
2.01
2.02
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

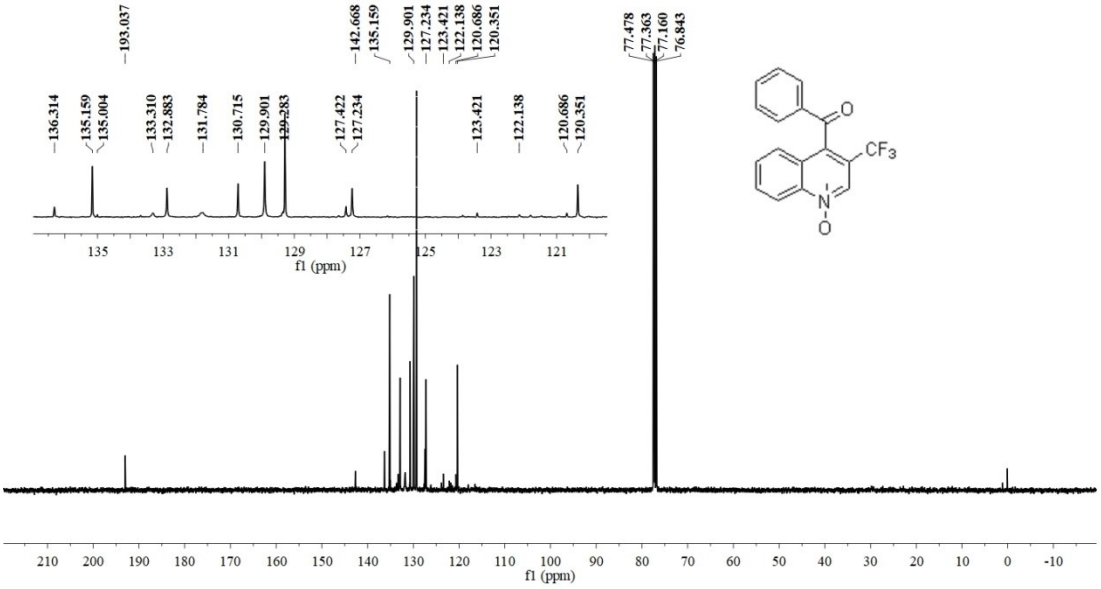

202.951
149.591
146.323
146.297
146.152
146.137
129.145
125.581
125.035
124.482
123.660
122.664
122.394
120.848
118.207
117.994
117.781
77.372
77.160
76.948
43.916
41.975
25.965
Cl
O
CF3
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

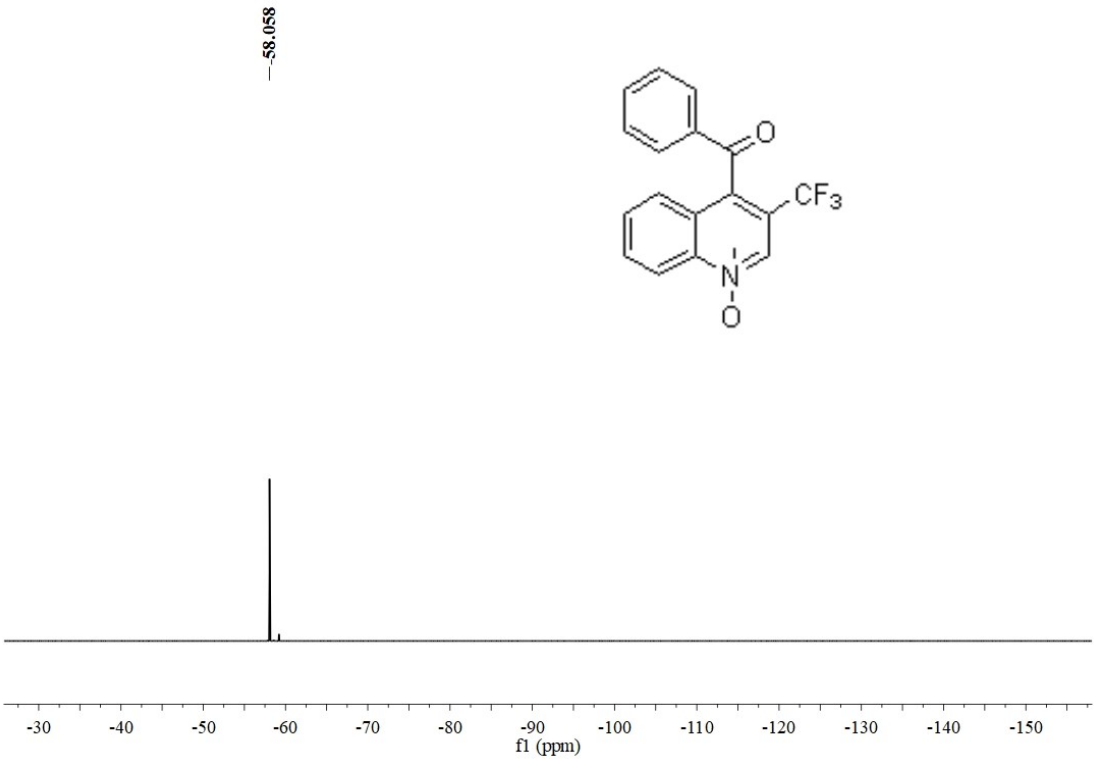

-57.075
Cl
O
CF3
N
-56.65 -56.80 -56.95 -57.10 -57.25 -57.40 -57.55 -57.70 -57.85
f1 (ppm)

12. ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra for compound 4

4

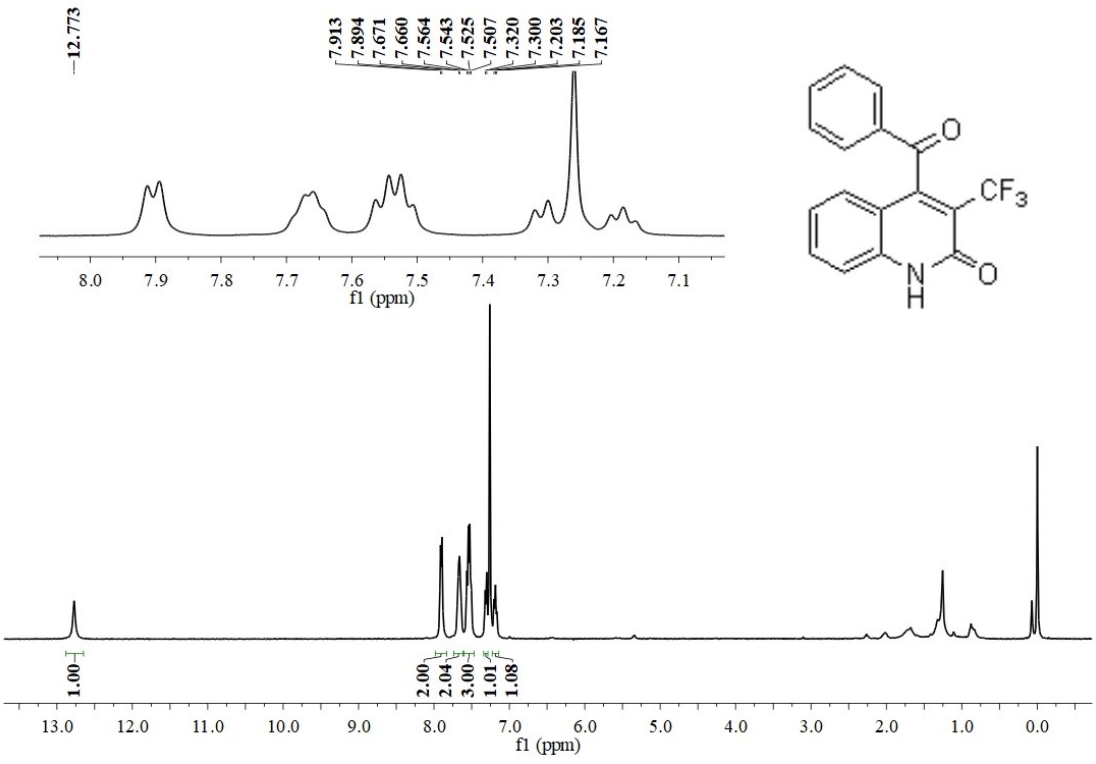


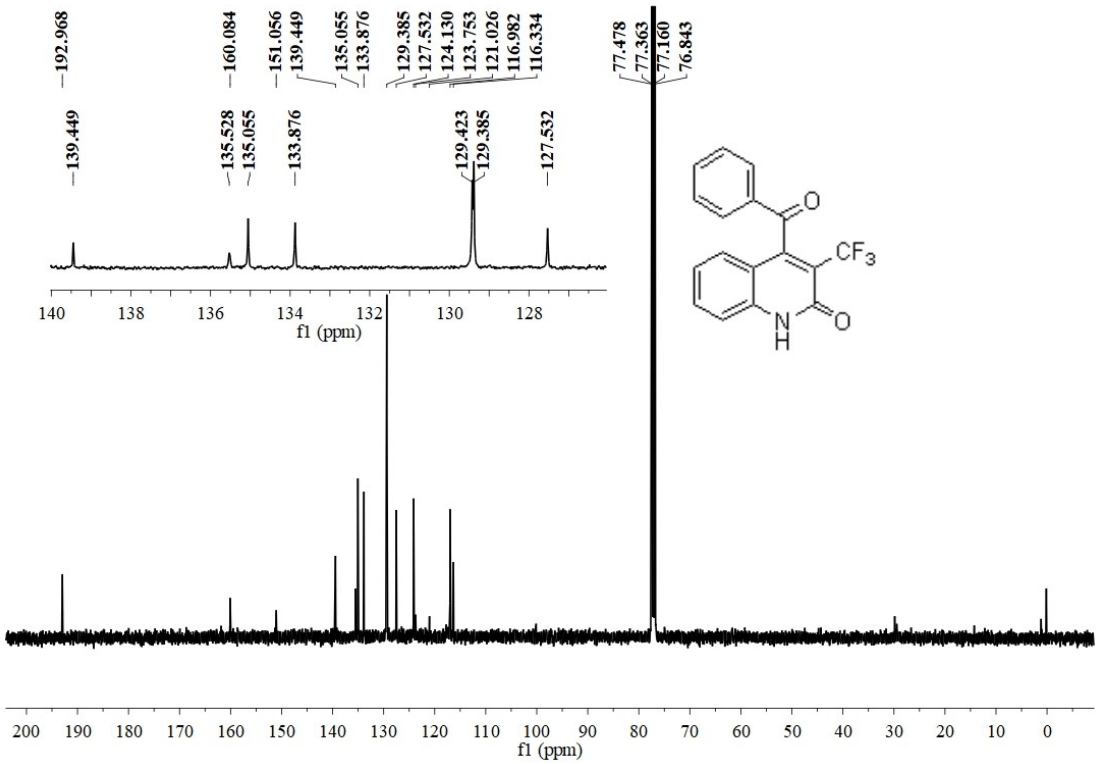


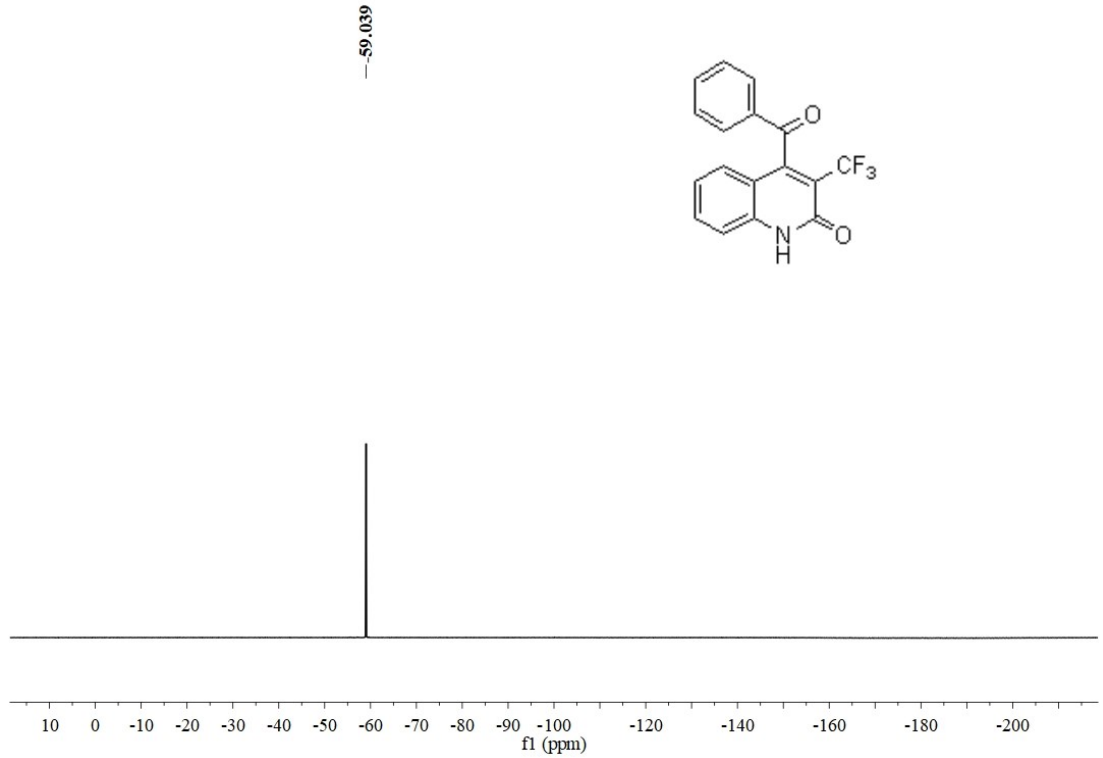


13. ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra for compound 5

5




192.968
160.084
151.056
139.449
135.055
133.876
129.385
127.532
124.130
123.753
121.026
116.982
116.334
77.478
77.363
77.160
76.843
139.449
135.528
135.055
133.876
129.423
129.385
127.532
O
CF3
N
H
O
140 138 136 134 132 130 128
f1 (ppm)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


59.039
O
CF3
N
H
O
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)