Electronic Supplementary Material (ESI) for Chemical Communications.

Organic base-catalysed solvent-tuned chemoselective carbotrifluoromethylation and oxytrifluoromethylation of unactivated alkenes

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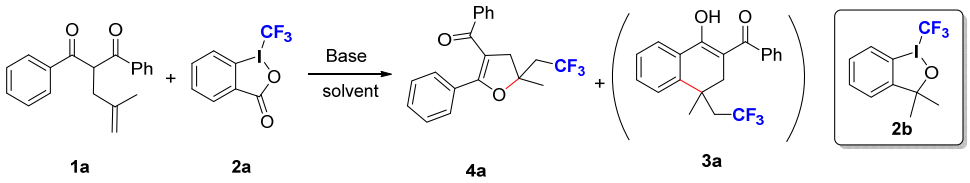
General information

All reactions were carried out under argon using Schlenk techniques. Reagents were purchased at the commercial quality and used without further purification. Analytical thin layer chromatography (TLC) was performed on precoated silica gel 60 GF254 plates. Flash column chromatography was performed using Tsingdao silica gel (60, particle size 0.040-0.063 mm). Visualization on TLC was achieved by use of UV light (254 nm) or iodine. NMR spectra were recorded on a Bruker DPX 400 spectrometer at 400 MHz for ^{1}H NMR, 100 MHz for ^{13}C NMR and 376 MHz for ^{19}F NMR in $CDCl_3$ with tetramethylsilane (TMS) as internal standard. The chemical shifts are expressed in ppm and coupling constants are given in Hz. Data for ^{1}H NMR are recorded as follows: chemical shift (ppm), multiplicity (s, singlet; d, doublet; t, triplet; q, quarter; m, multiplet), coupling constant (Hz), integration. Data for ^{13}C NMR are reported in terms of chemical shift (δ, ppm). ^{19}F NMR spectra were recorded on a Bruker DPX 400 MHz spectrometer ($CFCl_3$ as an external reference (0 ppm)). Mass spectrometric data were obtained using Bruker Apex IV RTMS.

Table S1 Screening of reaction conditions for oxytrifluoromethylation.[a]

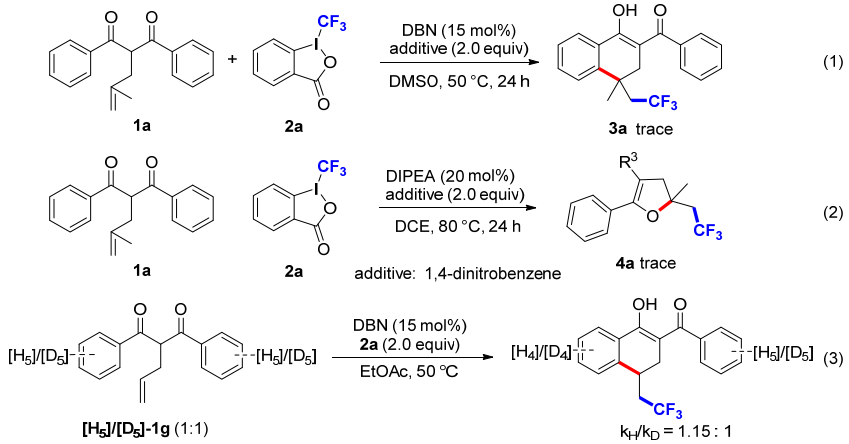


1a 2a 4a 3a

Entry	Base (X equiv)	Solvent	T (°C)	Yield(%) of **4a** (**3a**)[b]
1	DIPEA (0.2)	EtOAc	80	70 (7)
2	DIPEA (0.2)	EtOH	80	58 (17)
3	DIPEA (0.2)	CH_3CN	80	66 (21)
4	**DIPEA** (0.2)	**DCE**	**80**	**85 (10)**
5	DIPEA (0.2)	DCE	80	83 (11)[c]
5	DIPEA (0.2)	DCE	80	71 (10)[d]
6	DIPEA (0.15)	DCE	80	75 (11)[d]

[a] Unless otherwise noted, the reaction was conducted with **1a** (0.1 mmol), Togni's ester **2a** (0.2 mmol), and base (0.02 mmol) in 1.0 mL solvent for 10 h. [b] Determined by ^{19}F NMR spectroscopy using $PhCF_3$ as an internal standard. [c] **2a** (0.3 mmol) was used. [d] **2b** (0.2 mmol) was used.

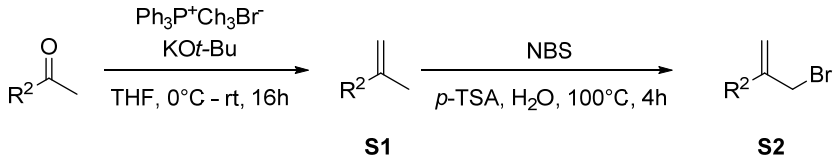
Supplementary Scheme S1: Control experiments and KIE study



Experimental procedure for synthesis of substrates

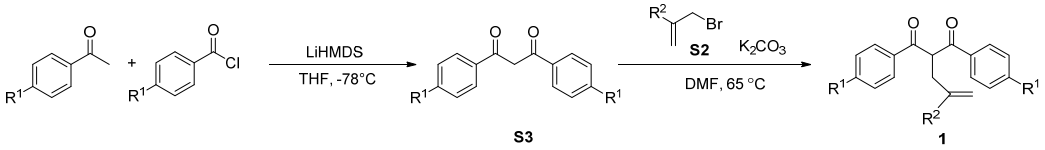
Compound 1p was synthesized following literature.[1]

General Procedure for the Synthesis of 1a-1l, 1s, 1t, and 1u-1y



Methyltriphenylphosphonium bromide (17.20g, 48 mmol) was dissolved in THF (60 mL) in a dried round bottom flask equipped with an ice water bath. Then KO*t*-Bu (5.39g, 48 mmol), the yellow suspension was stirred at 0 °C for 45 min. To this suspension was added a solution of the corresponding ketone (40 mmol) in THF (0.7 mmol/mL) dropwisely and the resulting mixture was stirred for 16 h at room temperature. The mixture was concentrated under reduced pressure and filtered. The solid was washed with petroleum ether (3 × 15 mL) and the combined organic layer was concentrated and purified by flash column chromatography (petroleum ether/EtOAc 20:1) to give the corresponding propene **S1**.

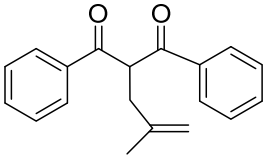
The propene **S1** (1.0 equiv) was dissolved in THF (3.0 mmol/mL) in a dried round bottom flask, followed by addition of *N*-Bromosuccinimide (1.05 equiv) and TsOH (0.1 equiv). The reaction solution was heated to 100 °C and stirred for 4 h, then cooled down to room temperature. Quenched with water (100 mL), extracted with EtOAc (3 × 50 mL). The combined organic layer was dried over Na_2SO_4, filtered and concentrated under reduced pressure to afford the residue **S2**, which could be used directly into next step without further purification.



The substituted acetophenone (10 mmol) was dissolved in THF (30 mL) in a dried round bottom flask under an Ar atmosphere. The solution was cool down to -78 °C, followed by addition of lithium bis(trimethylsilyl)amide (LiHDMS) (20 mL, 1 M in THF). This solution was stirred at -78 °C for 1 h before the corresponding benzoyl chloride (10 mmol, 1.0 equiv) was added dropwise. The mixture was allowed to warm to room temperature stirred overnight. Then quenched with 1 M HCl (30 mL, 1 M) and water (100 mL), extracted with EtOAc (3 × 50 mL). The combined organic layer was dried over Na_2SO_4, filtered and concentrated under reduced pressure to afford the crude product, which was purified by flash column chromatography (petroleum ether/EtOAc 20:1) to give the corresponding product **S3**.

The obtained **S3** (10 mmol) was dissolved in DMF (20 mL) in a dried round bottom flask, followed by addition of the corresponding allyl bromide **S2** (11 mmol) and K_2CO_3 (2.07 g, 15mmol). The mixture was stirred at 65 °C for 6 h under an Ar atmosphere. Then diluted with Water (70 mL). extracted with EtOAc (3 × 50 mL). The combined organic layer was dried over Na_2SO_4, filtered and concentrated under reduced pressure to afford the crude product, which was purified by flash column chromatography (petroleum ether/EtOAc 20:1) to give the corresponding product **1**.

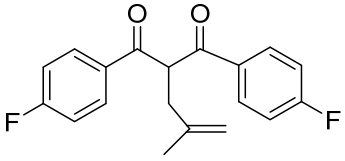
2-(2-methylallyl)-1,3-diphenylpropane-1,3-dione (1a)



1a

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (dd, *J* = 5.2, 3.4 Hz, 4H), 7.64 – 7.55 (m, 2H), 7.47 (dd, *J* = 10.6, 4.8 Hz, 4H), 5.46 (t, *J* = 6.6 Hz, 1H), 4.81 (s, 1H), 4.72 (s, 1H), 2.88 (d, *J* = 6.6 Hz, 2H), 1.81 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.53, 142.58, 136.01, 133.55, 128.90, 128.61, 112.05, 55.74, 36.57, 22.99; HRMS (ESI) m/z calcd for $C_{19}H_{19}O_2$ $[M+H]^+$ 279.1379, found 279.1374.

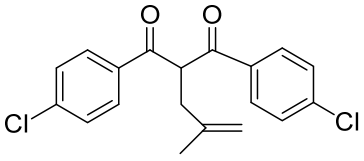
1,3-bis(4-fluorophenyl)-2-(2-methylallyl)propane-1,3-dione (1b)



1b

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 – 7.89 (m, 4H), 7.15 (dd, *J* = 11.9, 5.2 Hz, 4H), 5.31 (t, *J* = 6.7 Hz, 1H), 4.81 (s, 1H), 4.69 (s, 1H), 2.87 (d, *J* = 6.6 Hz, 2H), 1.79 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.89, 166.01 (d, $J_{C\text{-}F}$ = 255 Hz), 142.31, 132.33 (d, $J_{C\text{-}F}$ = 2.9 Hz), 131.34 (d, $J_{C\text{-}F}$ = 9.4 Hz), 116.12 (d, $J_{C\text{-}F}$ = 20.9 Hz), 112.28, 56.31, 36.62, 22.90; HRMS (ESI) m/z calcd for $C_{19}H_{17}F_2O_2$ $[M+H]^+$ 315.1191, found 315.1184.

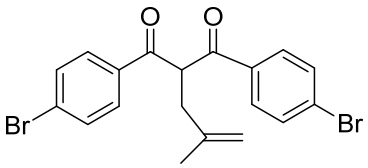
1,3-bis(4-chlorophenyl)-2-(2-methylallyl)propane-1,3-dione (1c)



1c

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.6 Hz, 4H), 7.45 (d, *J* = 8.6 Hz, 4H), 5.29 (t, *J* = 6.6 Hz, 1H), 4.81 (s, 1H), 4.68 (s, 1H), 2.85 (d, *J* = 6.6 Hz, 2H), 1.79 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.21, 142.17, 140.29, 134.20, 130.00, 129.30, 112.41, 56.28, 36.57, 22.89; HRMS (ESI) m/z calcd for $C_{19}H_{17}Cl_2O_2$ $[M+H]^+$ 347.0600, found 347.0593

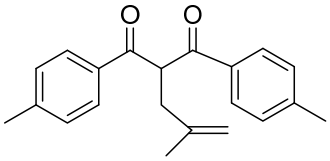
1,3-bis(4-bromophenyl)-2-(2-methylallyl)propane-1,3-dione (1d)



1d

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.6 Hz, 4H), 7.62 (d, *J* = 8.6 Hz, 4H), 5.28 (t, *J* = 6.7 Hz, 1H), 4.81 (s, 1H), 4.68 (s, 1H), 2.85 (d, *J* = 6.6 Hz, 2H), 1.79 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.39, 142.14, 134.59, 132.30, 130.07, 112.43, 56.22, 36.55, 22.89; HRMS (ESI) m/z calcd for $C_{19}H_{17}Br_2O_2$ $[M+H]^+$ 434.9590, found 434.9578.

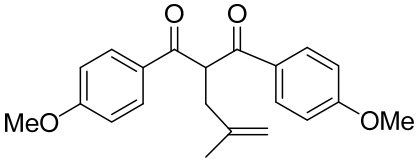
2-(2-methylallyl)-1,3-di-p-tolylpropane-1,3-dione (1e)



1e

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.2 Hz, 4H), 7.26 (d, *J* = 8.0 Hz, 4H), 5.39 (t, *J* = 6.6 Hz, 1H), 4.79 (s, 1H), 4.71 (s, 1H), 2.86 (d, *J* = 6.6 Hz, 2H), 2.41 (s, 6H), 1.79 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.23, 144.41, 142.77, 133.58, 129.55, 128.76, 111.91, 55.72, 36.66, 22.98, 21.67; HRMS (ESI) m/z calcd for $C_{21}H_{23}O_2$ $[M+H]^+$ 307.1693, found 307.1684.

1,3-bis(4-methoxyphenyl)-2-(2-methylallyl)propane-1,3-dione (1f)

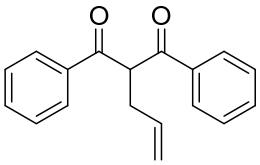


1f

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.9 Hz, 4H), 6.93 (d, *J* = 8.9 Hz, 4H), 5.30 (t, *J* = 6.7 Hz, 1H), 4.79 (s, 1H), 4.70 (s, 1H), 3.87 (s, 6H), 2.86 (d, *J* = 6.6 Hz, 2H), 1.79 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.22, 163.77, 142.89, 131.01, 129.11,

114.03, 111.87, 55.90, 55.51, 36.82, 22.97; HRMS (ESI) m/z calcd for $C_{21}H_{23}O_4$ $[M+H]^+$ 339.1591, found 339.1582.

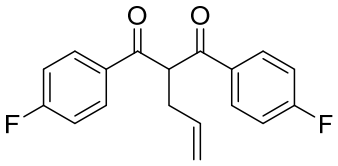
2-allyl-1,3-diphenylpropane-1,3-dione (1g)



1g

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 – 7.94 (m, 4H), 7.64 – 7.55 (m, 2H), 7.50 – 7.45 (m, 4H), 5.90 (m, 1H), 5.32 (t, *J* = 6.7 Hz, 1H), 5.13 (dq, *J* = 17.0, 1.5 Hz, 1H), 5.05 (dq, *J* = 10.1, 1.2 Hz, 1H), 2.90 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.53, 135.99, 135.09, 133.56, 128.90, 128.61, 117.25, 56.78, 33.57; HRMS (ESI) m/z calcd for $C_{18}H_{17}O_2$ $[M+H]^+$ 265.1223, found 265.1216.

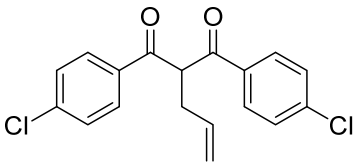
2-allyl-1,3-bis(4-fluorophenyl)propane-1,3-dione (1h)



1h

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 – 7.95 (m, 4H), 7.22 – 7.10 (m, 4H), 5.94 – 5.79 (m, 1H), 5.18 (t, *J* = 6.8 Hz, 1H), 5.15 – 5.02 (m, 2H), 2.93 – 2.84 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.86, 166.01 (d, $J_{C\text{-}F}$ = 256.4 Hz), 134.74, 132.32 (d, $J_{C\text{-}F}$ = 2.8 Hz), 131.32 (d, $J_{C\text{-}F}$ = 9.5 Hz), 117.53, 116.14 (d, $J_{C\text{-}F}$ = 22.0 Hz), 57.23, 33.58; HRMS (ESI) m/z calcd for $C_{18}H_{15}F_2O_2$ $[M+H]^+$ 301.1034, found 301.1028

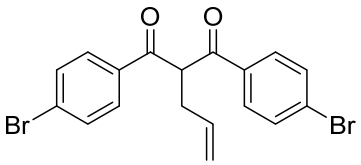
2-allyl-1,3-bis(4-chlorophenyl)propane-1,3-dione (1i)



1i

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 – 7.86 (m, 4H), 7.50 – 7.41 (m, 4H), 5.93 – 5.78 (m, 1H), 5.17 (t, *J* = 6.8 Hz, 1H), 5.14 – 5.02 (m, 2H), 2.92 – 2.83 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.19, 140.31, 134.59, 134.18, 129.98, 129.31, 117.66, 57.17, 33.51; HRMS (ESI) m/z calcd for $C_{18}H_{15}Cl_2O_2$ $[M+H]^+$ 333.0444, found 333.0440.

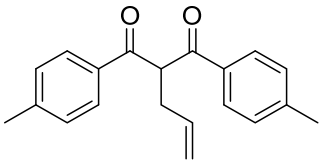
2-allyl-1,3-bis(4-bromophenyl)propane-1,3-dione (1j)



1j

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 – 7.77 (m, 4H), 7.66 – 7.58 (m, 4H), 5.93 – 5.78 (m, 1H), 5.16 (t, *J* = 6.8 Hz, 1H), 5.14 – 5.02 (m, 2H), 2.92 – 2.83 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.37, 134.58, 134.55, 132.31, 130.05, 129.09, 117.69, 57.11, 33.49; HRMS (ESI) m/z calcd for $C_{18}H_{15}Br_2O_2$ $[M+H]^+$ 420.9433, found 420.9426.

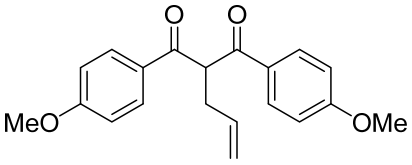
2-allyl-1,3-di-p-tolylpropane-1,3-dione (1k)



1k

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 – 7.84 (m, 4H), 7.26 (d, *J* = 7.9 Hz, 4H), 5.97 – 5.81 (m, 1H), 5.25 (t, *J* = 6.8 Hz, 1H), 5.17 – 4.99 (m, 2H), 2.92 – 2.83 (m, 2H), 2.41 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.22, 144.42, 135.31, 133.59, 129.55, 128.75, 117.04, 56.78, 33.66, 21.66; HRMS (ESI) m/z calcd for $C_{20}H_{21}O_2$ $[M+H]^+$ 293.1536, found 293.1527.

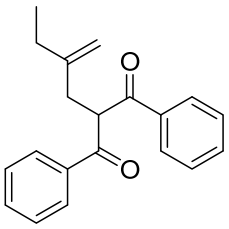
2-allyl-1,3-bis(4-methoxyphenyl)propane-1,3-dione (1l)



1l

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 – 7.92 (m, 4H), 7.03 – 6.89 (m, 4H), 5.96 – 5.83 (m, 1H), 5.17 (t, *J* = 6.8 Hz, 1H), 5.14 – 5.00 (m, 2H), 3.87 (s, 6H), 2.92 – 2.83 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.19, 163.78, 135.45, 131.00, 129.11, 116.95, 114.03, 56.93, 55.51, 33.80; HRMS (ESI) m/z calcd for $C_{20}H_{21}O_4$ $[M+H]^+$ 325.1434, found 325.1426.

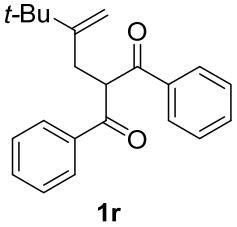
2-(2-methylenebutyl)-1,3-diphenylpropane-1,3-dione (1q)



1q

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 – 7.96 (m, 4H), 7.64 – 7.54 (m, 2H), 7.52 – 7.43 (m, 4H), 5.48 (t, *J* = 6.6 Hz, 1H), 4.81 (s, 1H), 4.73 (s, 1H), 2.89 (d, *J* = 6.6 Hz, 2H), 2.10 (q, *J* = 7.4 Hz, 2H), 1.05 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.58, 148.22, 136.01, 133.51, 128.88, 128.60, 109.50, 55.75, 35.17, 29.25, 12.18; HRMS (ESI) m/z calcd for $C_{20}H_{21}O_2$ $[M+H]^+$ 293.1536, found 293.1526.

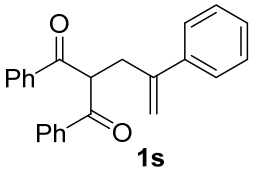
2-(3,3-dimethyl-2-methylenebutyl)-1,3-diphenylpropane-1,3-dione (1r)



1r

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 – 7.97 (m, 4H), 7.64 – 7.55 (m, 2H), 7.53 – 7.44 (m, 4H), 5.59 (t, *J* = 6.5 Hz, 1H), 4.93 (s, 1H), 4.61 (s, 1H), 2.92 (d, *J* = 6.5 Hz, 2H), 1.11 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.66, 154.99, 136.00, 133.51, 128.89, 128.59, 106.23, 55.43, 36.38, 30.39, 29.16; HRMS (ESI) m/z calcd for $C_{22}H_{25}O_2$ $[M+H]^+$ 321.1849, found 321.1841.

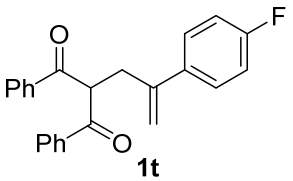
1,3-diphenyl-2-(2-phenylallyl)propane-1,3-dione (1s)



1s

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 – 7.74 (m, 4H), 7.57 – 7.52 (m, 2H), 7.45 – 7.32 (m, 9H), 5.38 (t, *J* = 6.7 Hz, 1H), 5.26 (d, *J* = 0.7 Hz, 1H), 5.12 (d, *J* = 1.1 Hz, 1H), 3.38 (dd, *J* = 6.7, 0.8 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.63, 144.98, 140.11, 136.13, 133.47, 128.77, 128.63, 128.55, 127.92, 126.55, 115.47, 55.20, 35.18; HRMS (ESI) m/z calcd for $C_{24}H_{21}O_2$ $[M+H]^+$ 341.1536,found 341.1527.

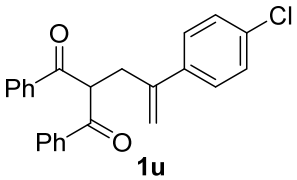
2-(2-(4-fluorophenyl)allyl)-1,3-diphenylpropane-1,3-dione (1t)



1t

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, J = 7.6 Hz, 4H), 7.56 (t, J = 7.4 Hz, 2H), 7.41 (t, J = 7.7 Hz, 4H), 7.36 – 7.27 (m, 2H), 7.03 (t, J = 8.6 Hz, 2H), 5.35 (t, J = 6.8 Hz, 1H), 5.21 (s, 1H), 5.10 (s, 1H), 3.35 (d, J = 6.7 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.50, 163.53 (d, $J_{C\text{-}F}$ = 255 Hz), 144.08, 136.22 (d, $J_{C\text{-}F}$ = 3.2 Hz), 136.07, 133.55, 128.70 (d, $J_{C\text{-}F}$ = 21.5 Hz), 128.18 (d, $J_{C\text{-}F}$ = 8.0 Hz), 115.48, 115.39, 115.27, 55.29, 35.24; HRMS (ESI) m/z calcd for $C_{24}H_{20}FO_2$ $[M+H]^+$ 359.1442, found 359.1432.

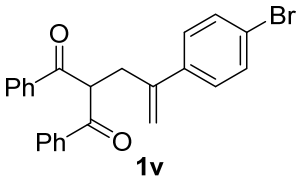
2-(2-(4-chlorophenyl)allyl)-1,3-diphenylpropane-1,3-dione (1u)



1u

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, J = 7.3 Hz, 4H), 7.56 (t, J = 7.4 Hz, 2H), 7.41 (t, J = 7.8 Hz, 4H), 7.30 (dt, J = 17.0, 5.3 Hz, 4H), 5.34 (t, J = 6.8 Hz, 1H), 5.25 (s, 1H), 5.13 (s, 1H), 3.34 (d, J = 6.7 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.45, 143.97, 138.59, 136.04, 133.76, 133.58, 128.83, 128.68, 128.60, 127.83, 115.96, 55.26, 35.03; HRMS (ESI) m/z calcd for $C_{24}H_{20}ClO_2$ $[M+H]^+$ 375.1146, found 375.1139.

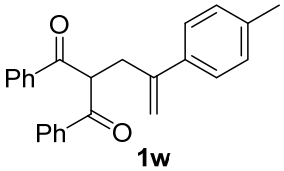
2-(2-(4-bromophenyl)allyl)-1,3-diphenylpropane-1,3-dione (1v)



1v

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (dd, J = 8.3, 1.1 Hz, 4H), 7.63 – 7.51 (m, 2H), 7.51 – 7.45 (m, 2H), 7.41 (dd, J = 10.8, 4.8 Hz, 4H), 7.26 – 7.15 (m, 2H), 5.34 (t, J = 6.8 Hz, 1H), 5.26 (s, 1H), 5.13 (s, 1H), 3.34 (d, J = 6.7 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.44, 144.02, 139.07, 136.04, 133.58, 131.64, 128.83, 128.60, 128.16, 121.93, 116.04, 55.27, 34.98; HRMS (ESI) m/z calcd for $C_{24}H_{20}BrO_2$ $[M+H]^+$ 419.0641, found 419.0630.

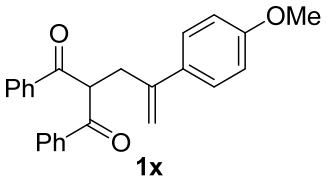
1,3-diphenyl-2-(2-(p-tolyl)allyl)propane-1,3-dione (1w)



1w

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.4 Hz, 4H), 7.55 (t, *J* = 7.4 Hz, 2H), 7.40 (t, *J* = 7.7 Hz, 4H), 7.26 (d, *J* = 8.1 Hz, 2H), 7.16 (d, *J* = 8.0 Hz, 2H), 5.37 (t, *J* = 6.7 Hz, 1H), 5.23 (s, 1H), 5.06 (s, 1H), 3.36 (d, *J* = 6.6 Hz, 2H), 2.39 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.71, 144.73, 137.73, 137.11, 136.17, 133.44, 129.24, 128.74, 128.65, 126.41, 114.73, 55.25, 35.20, 21.15; HRMS (ESI) m/z calcd for $C_{25}H_{23}O_2$ $[M+H]^+$ 355.1693, 355.1683.

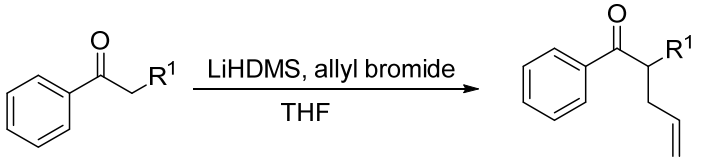
2-(2-(4-methoxyphenyl)allyl)-1,3-diphenylpropane-1,3-dione (1x)



1x

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.9 Hz, 4H), 7.55 (t, *J* = 7.4 Hz, 2H), 7.40 (t, *J* = 7.7 Hz, 4H), 7.29 (d, *J* = 8.3 Hz, 2H), 6.89 (d, *J* = 8.5 Hz, 2H), 5.38 (t, *J* = 6.7 Hz, 1H), 5.18 (s, 1H), 5.02 (s, 1H), 3.85 (s, 3H), 3.35 (d, *J* = 6.7 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.73, 159.42, 144.28, 136.17, 133.45, 132.45, 128.75, 128.63, 127.67, 114.00, 113.88, 55.33, 55.27, 35.28; HRMS (ESI) m/z calcd for $C_{25}H_{23}O_3$ $[M+H]^+$ 371.1642, found 371.1632.

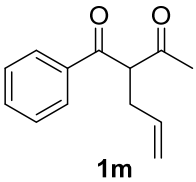
General Procedure for synthesis of 1m, 1n and 1o:



1

The corresponding ketone (10 mmol) was dissolved in THF (20 mL) in a dried round bottom flask under an Ar atmosphere. the solution was cooled to 0℃, before adding LiHDMS (1 mol/L THF solution, 20mL, 2.0 equiv.), the solution was stirred at 0℃ for 1h, then the allyl bromide (1.1g, 0.9 equiv.) was added dropwise, this solution was allowed to warm to r.t and stirred for 18h. Quenched by 1 mol/L HCl (30 mL), diluted with water (75 mL), extracted with EtOAc (3 × 20 mL). The combined organic extracts were washed with brine, dried over Na_2SO_4, filtered, and concentrated. The residue was purified by flash column chromatography (petroleum ether/EtOAc 20:1) to give the corresponding asymmetric di-keto substrate.

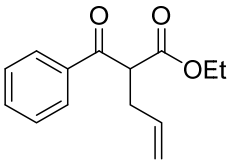
2-allyl-1-phenylbutane-1,3-dione (1m)



1m

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 – 7.97 (m, 2H), 7.67 – 7.55 (m, 1H), 7.58 – 7.46 (m, 2H), 5.85 – 5.70 (m, 1H), 5.16 – 5.00 (m, 2H), 4.56 (t, *J* = 7.2 Hz, 1H), 2.88 – 2.67 (m, 2H), 2.17 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 203.63, 195.79, 136.35, 134.35, 133.80, 128.90, 128.75, 117.50, 62.78, 33.05, 28.14; HRMS (ESI) m/z calcd for $C_{13}H_{15}O_2$ $[M+H]^+$ 203.1067, found 203.1062.

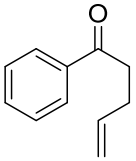
ethyl 2-benzoylpent-4-enoate (1n)



1n

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 – 7.92 (m, 2H), 7.66 – 7.55 (m, 1H), 7.55 – 7.44 (m, 2H), 5.91 – 5.75 (m, 1H), 5.28 – 5.01 (m, 2H), 4.41 (t, *J* = 7.2 Hz, 1H), 4.20 – 4.11 (m, 2H), 2.86 – 2.68 (m, 2H), 1.30 – 1.08 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.51, 169.38, 136.19, 134.50, 133.54, 128.73, 128.62, 117.41, 61.45, 53.93, 33.00, 14.02; HRMS (ESI) m/z calcd for $C_{14}H_{17}O_3$ $[M+H]^+$ 233.1172, found 233.1169.

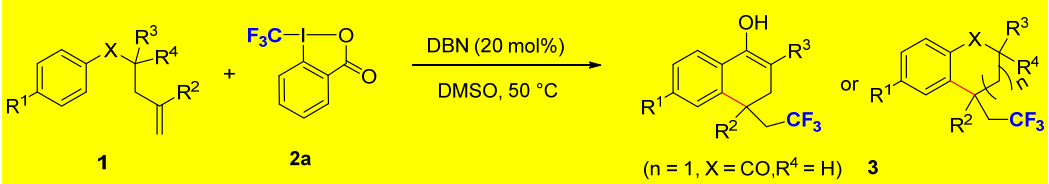
1-phenylpent-4-en-1-one (1o)



1o

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 – 7.95 (m, 2H), 7.62 – 7.53 (m, 1H), 7.53 – 7.41 (m, 2H), 6.00 – 5.85 (m, 1H), 5.15 – 5.01 (m, 2H), 3.10 (t, *J* = 6.9 Hz, 2H), 2.62 – 2.47 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.45, 137.30, 136.93, 133.02, 128.60, 128.03, 115.29, 37.75, 28.16; HRMS (ESI) m/z calcd for $C_{11}H_{13}O$ $[M+H]^+$ 161.0961, found 161.0958.

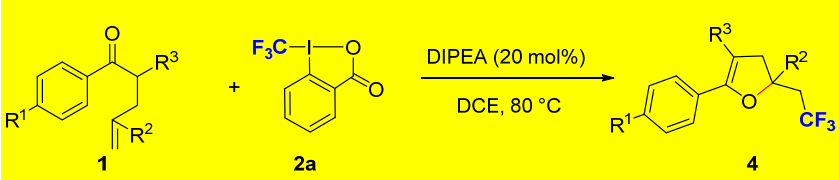
General procedure for carbotrifluoromethylation



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

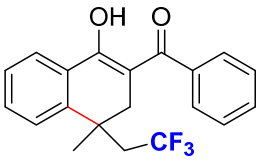
To a flame-dried Schlenk tube equipped with a magnetic stir bar were added **1** (0.2 mmol), **2a** (0.4 mmol). The tube was evacuated and backfilled with argon for three times, and then DMSO (1 mL) were added, followed by addition of DBN (0.03 mmol). The tube was stirred at 50 °C for around 10 h. the reaction mixture was purified by flash column chromatography to afford the product **3**.

General procedure for oxytrifluoromethylation



To a flame-dried Schlenk tube equipped with a magnetic stir bar were added **1** (0.2 mmol), **2a** (0.4 mmol). The tube was evacuated and backfilled with argon for three times, and then DCE (1 mL) were added, followed by the addition of DIPEA (0.04 mmol). The tube was stirred at 80 °C for 10 h. the reaction mixture was purified by flash column chromatography to afford the product **4**.

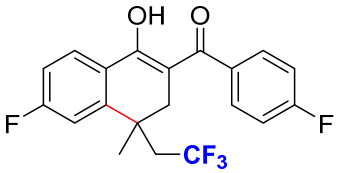
(1-hydroxy-4-methyl-4-(2,2,2-trifluoroethyl)-3,4-dihydronaphthalen-2-yl)(phenyl)methanone (3a)



3a

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (dt, *J* = 8.3, 1.5 Hz, 2H), 7.28 – 7.20 (m, 2H), 7.20 – 7.12 (m, 2H), 7.11 – 7.06 (m, 3H), 3.36 (d, *J* = 15.3 Hz, 1H), 3.22 (d, *J* = 15.3 Hz, 1H), 2.84 – 2.63 (m, 2H), 1.72 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.10, 182.52, 145.94, 135.97, 133.11, 130.80, 130.70, 128.36, 127.76, 127.59, 127.03, 126.15 (q, J_{C-F} = 278 Hz), 124.91, 103.62, 42.37 (q, J_{C-F} = 26.5 Hz), 37.54, 35.23, 25.10; ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.93; HRMS (ESI) m/z calcd. for $C_{20}H_{16}F_3O_2$ $[M-H]^-$ 345.1108, found 345.1109.

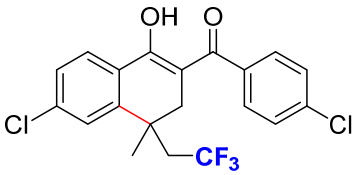
(6-fluoro-1-hydroxy-4-methyl-4-(2,2,2-trifluoroethyl)-3,4-dihydronaphthalen-2-yl)(4-fluorophenyl)methanone (3b)



3b

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (dd, J = 8.6, 6.0 Hz, 1H), 7.63 – 7.56 (m, 2H), 7.23 – 7.08 (m, 4H), 2.80 (s, 2H), 2.37 – 2.23 (m, 2H), 1.57 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 185.10, 182.23, 165.76 (d, J_{C-F} = 253 Hz), 164.10 (d, J_{C-F} = 250 Hz), 149.18 (d, J_{C-F} = 7.9 Hz), 131.83 (d, J_{C-F} = 3.3 Hz), 130.17 (d, J_{C-F} = 8.8 Hz), 130.00 (d, J_{C-F} = 9.5 Hz), 127.14 (d, J_{C-F} = 2.8 Hz), 125.96 (q, J_{C-F} = 276 Hz), 115.61 (d, J_{C-F} = 21.8 Hz), 114.96 (d, J_{C-F} = 21.8 Hz), 112.44 (d, J_{C-F} = 22.9 Hz), 102.99, 42.26 (q, J_{C-F} = 26.7 Hz), 37.45, 35.42, 25.02; ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.96, -103.86, -108.19; HRMS (ESI) m/z calcd. for $C_{20}H_{14}F_5O_2$ $[M-H]^-$ 381.0919, found 381.0918.

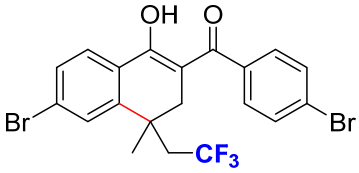
(6-chloro-1-hydroxy-4-methyl-4-(2,2,2-trifluoroethyl)-3,4-dihydronaphthalen-2-yl)(4-chlorophenyl)methanone (3c)



3c

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, J = 8.3 Hz, 1H), 7.52 (d, J = 8.7 Hz, 2H), 7.50 – 7.46 (m, 2H), 7.43 (dd, J = 8.3, 1.9 Hz, 1H), 7.38 (d, J = 1.8 Hz, 1H), 2.78 (s, 2H), 2.35 – 2.24 (m, 2H), 1.57 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 185.85, 181.64, 147.72, 139.60, 137.15, 134.10, 129.26, 129.08, 128.77, 128.68, 128.07, 125.92 (q, J_{C-F} = 277 Hz), 125.40, 103.47, 42.23 (q, J_{C-F} = 26.7 Hz), 37.17, 35.40, 24.98; ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.96; HRMS (ESI) m/z calcd. for $C_{19}H_{12}Cl_2F_3O_2$ $[M-H]^-$ 399.0172, found 399.0174.

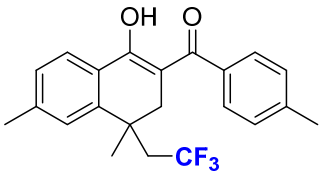
(6-bromo-1-hydroxy-4-methyl-4-(2,2,2-trifluoroethyl)-3,4-dihydronaphthalen-2-yl)(4-bromophenyl)methanone (3d)



3d

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, J = 8.3 Hz, 1H), 7.64 (d, J = 8.4 Hz, 2H), 7.59 (dd, J = 8.3, 1.6 Hz, 1H), 7.54 (d, J = 1.3 Hz, 1H), 7.44 (d, J = 8.4 Hz, 2H), 2.77 (s, 2H), 2.29 (qd, J = 11.3, 2.3 Hz, 2H), 1.57 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 186.08, 181.62, 147.78, 134.55, 131.73, 131.08, 129.46, 129.40, 128.74, 128.35, 128.33, 125.90 (q, J_{C-F} = 277 Hz), 125.59, 103.51, 42.24 (q, J_{C-F} = 26.7 Hz), 37.10, 35.36, 24.98; ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.95; HRMS (ESI) m/z calcd. for $C_{19}H_{12}Br_2F_3O_2$ $[M-H]^-$ 488.9141, found 488.9144.

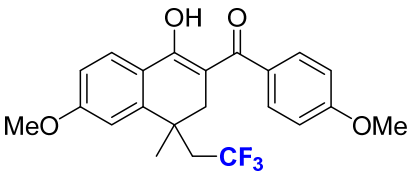
(1-hydroxy-4,6-dimethyl-4-(2,2,2-trifluoroethyl)-3,4-dihydronaphthalen-2-yl)(p-tolyl)methanone (3e)



3e

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 7.9 Hz, 1H), 7.48 (d, *J* = 8.1 Hz, 2H), 7.29 (d, *J* = 6.5 Hz, 2H), 7.25 (d, *J* = 7.9 Hz, 1H), 7.20 (s, 1H), 2.80 (d, *J* = 2.6 Hz, 2H), 2.45 (s, 3H), 2.44 (s, 3H), 2.38 – 2.23 (m, 2H), 1.56 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 186.25, 182.99, 146.12, 143.87, 141.13, 133.19, 128.99, 128.36, 128.31, 127.88, 127.13, 126.22 (q, J_{C-F} = 277 Hz), 125.53, 103.24, 42.39 (q, J_{C-F} = 26.4 Hz), 37.70, 35.20, 25.10, 22.11, 21.59; ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.89; HRMS (ESI) m/z calcd. for $C_{21}H_{18}F_3O_2$ $[M-H]^-$ 359.1264, found 359.1264.

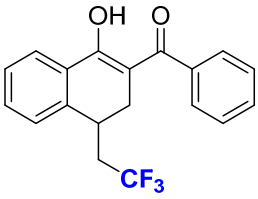
(1-hydroxy-6-methoxy-4-methyl-4-(2,2,2-trifluoroethyl)-3,4-dihydronaphthalen-2-yl)(4-methoxyphenyl)methanone (3f)



3f

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.6 Hz, 1H), 7.65 – 7.50 (m, 2H), 7.03 – 6.88 (m, 4H), 3.91 (s, 3H), 3.90 (s, 3H), 2.83 (d, *J* = 3.5 Hz, 2H), 2.40 – 2.18 (m, 2H), 1.56 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 184.48, 183.18, 163.47, 161.49, 148.40, 129.87, 129.46, 128.35, 126.22 (q, J_{C-F} = 276 Hz), 124.06, 113.62, 112.11, 111.23, 102.47, 55.52, 55.41, 42.37 (q, J_{C-F} = 26.4 Hz), 37.95, 35.39, 25.08; ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.84; HRMS (ESI) m/z calcd. for $C_{21}H_{18}F_3O_4$ [M-H]- 391.1163, found 391.1166.

(1-hydroxy-4-(2,2,2-trifluoroethyl)-3,4-dihydronaphthalen-2-yl)(phenyl)methanone (3g)

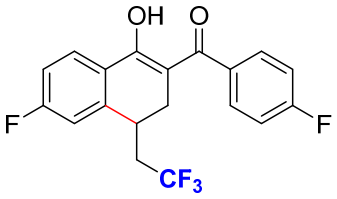


3g

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.61 – 7.57 (m, 2H), 7.55 – 7.43 (m, 5H), 7.29 (d, *J* = 6.1 Hz, 1H), 3.33 – 3.22 (m, 1H), 3.03 (dd, *J* = 15.1, 4.9 Hz, 1H), 2.85 (dd, *J* = 15.1, 3.1 Hz, 1H), 2.43 – 2.21 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 186.92, 183.06, 142.51, 135.90, 133.04, 131.10, 130.77, 128.34,

127.98, 127.73, 127.48, 126.87, 126.32 (q, J_{C-F} = 276 Hz), 102.68, 38.01 (q, J_{C-F} = 27.4 Hz), 32.61 (q, J_{C-F} = 2.5 Hz), 29.18 (q, J_{C-F} = 0.8 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.72; HRMS (ESI) m/z calcd. for $C_{19}H_{14}F_3O_2$ $[M-H]^-$ 331.0951, found 331.0945.

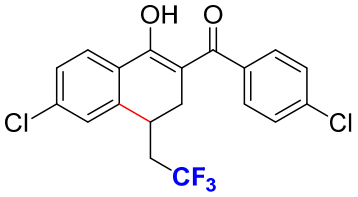
(6-fluoro-1-hydroxy-4-(2,2,2-trifluoroethyl)-3,4-dihydronaphthalen-2-yl)(4-fluoro phenyl)methanone (3h)



3h

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (dd, *J* = 8.7, 5.8 Hz, 1H), 7.66 – 7.54 (m, 2H), 7.23 – 7.11 (m, 3H), 6.99 (dd, *J* = 8.8, 2.4 Hz, 1H), 3.31 – 3.18 (m, 1H), 3.04 (dd, *J* = 15.1, 4.8 Hz, 1H), 2.83 (dd, *J* = 15.1, 3.2 Hz, 1H), 2.43 – 2.23 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 184.86, 182.79, 165.40 (d, J_{C-F} = 254 Hz), 164.08 (d, J_{C-F} = 252 Hz), 145.44 (d, J_{C-F} = 8.5 Hz), 131.73 (d, J_{C-F} = 3.3 Hz), 130.17 (d, J_{C-F} = 8.8 Hz), 129.86 (d, J_{C-F} = 9.5 Hz), 127.53 (d, J_{C-F} = 2.8 Hz), 126.12 (q, J_{C-F} = 276 Hz), 115.58 (d, J_{C-F} = 21.5Hz), 115.40 (d, J_{C-F} = 21.1Hz), 114.49 (d, J_{C-F} = 22.3Hz), 102.08, 37.83 (q, J_{C-F} = 27.6 Hz), 32.71, 29.13; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.72, -104.26, -108.20; HRMS (ESI) m/z calcd. for $C_{19}H_{12}F_5O_2$ $[M-H]^-$ 367.0762, found 367.0765.

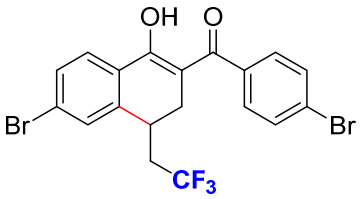
(6-chloro-1-hydroxy-4-(2,2,2-trifluoroethyl)-3,4-dihydronaphthalen-2-yl)(4-chlor ophenyl)methanone (3i)



3i

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.4 Hz, 1H), 7.54 – 7.42 (m, 4H), 7.29 – 7.28 (m, 2H), 3.27 – 3.21 (m, 1H), 3.02 (dd, *J* = 15.2, 4.8 Hz, 1H), 2.82 (dd, *J* = 15.2, 3.2 Hz, 1H), 2.44 – 2.16 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 185.59, 182.20, 144.01, 139.29, 137.13, 134.00, 129.47, 129.22, 128.73, 128.51, 128.46, 127.55, 126.06 (q, J_{C-F} = 276.0 Hz), 102.49, 37.78 (q, J_{C-F} = 27.5 Hz), 32.49 (q, J_{C-F} = 2.5 Hz), 28.90; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.72; HRMS (ESI) m/z calcd. for $C_{20}H_{16}Cl_2F_3O_2$ $[M+H]^+$ 415.0474, found 415.0659.

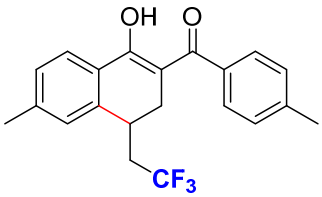
(6-bromo-1-hydroxy-4-(2,2,2-trifluoroethyl)-3,4-dihydronaphthalen-2-yl)(4-brom ophenyl)methanone (3j)



3j

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.93 (d, J = 8.3 Hz, 1H), 7.65 – 7.62 (m, 2H), 7.60 (dd, J = 8.3, 1.9 Hz, 1H), 7.48 – 7.43 (m, 3H), 3.29 – 3.21 (m, 1H), 3.01 (dd, J = 15.2, 4.9 Hz, 1H), 2.82 (dd, J = 15.2, 3.1 Hz, 1H), 2.42 – 2.20 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 185.76, 182.21, 144.09, 134.45, 131.69, 131.43, 130.50, 129.87, 129.39, 128.56, 127.96, 126.06 (q, J_{C-F} = 276 Hz), 125.55, 102.53, 37.73 (q, J_{C-F} = 27.6 Hz), 32.39 (q, J_{C-F} = 2.5 Hz), 28.84; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.71; HRMS (ESI) m/z calcd. for $C_{20}H_{15}Br_2F_3O_2$ $[M+H]^+$ 502.9464, found 502.9455.

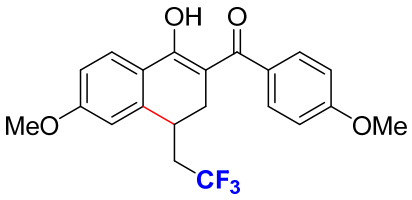
(1-hydroxy-6-methyl-4-(2,2,2-trifluoroethyl)-3,4-dihydronaphthalen-2-yl)(p-tolyl) methanone (3k)



3k

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, J = 7.9 Hz, 1H), 7.51 – 7.46 (m, 2H), 7.28 (d, J = 7.9 Hz, 2H), 7.25 (dd, J = 8.0, 1.0 Hz, 1H), 7.09 (s, 1H), 3.25 – 3.17 (m, 1H), 3.01 (dd, J = 15.0, 4.8 Hz, 1H), 2.87 (dd, J = 15.0, 3.1 Hz, 1H), 2.44 (s, 6H), 2.40 – 2.18 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 186.02, 183.57, 143.90, 142.70, 141.07, 133.10, 128.95, 128.77, 128.72, 128.02, 127.84, 126.93, 126.38 (q, J_{C-F} = 276 Hz), 102.26, 38.03 (q, J_{C-F} = 27.6 Hz), 32.66 (q, J_{C-F} = 2.5 Hz), 29.30, 21.80, 21.54; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.78; HRMS (ESI) m/z calcd. for $C_{22}H_{22}F_3O_2$ $[M+H]^+$ 375.1566, found 375.1564.

(1-hydroxy-6-methoxy-4-(2,2,2-trifluoroethyl)-3,4-dihydronaphthalen-2-yl)(4-me thoxyphenyl)methanone (3l)

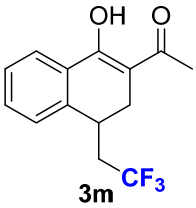


3l

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, J = 8.7 Hz, 1H), 7.57 (d, J = 8.9 Hz, 2H), 7.00 – 6.97 (m, 2H), 6.95 (dd, J = 8.7, 2.5 Hz, 1H), 6.76 (d, J = 2.5 Hz, 1H), 3.90 (s, 3H),

3.89 (s, 3H), 3.24 – 3.17 (m, 1H), 3.04 (dd, J = 15.0, 4.8 Hz, 1H), 2.89 (dd, J = 15.0, 3.1 Hz, 1H), 2.42 – 2.18 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 184.09, 183.85, 163.33, 161.46, 145.02, 129.85 ,129.19, 128.20, 126.39 (q, J_{C-F} = 276 Hz), 124.36, 113.59, 113.45, 112.53, 101.48, 55.55, 55.39, 38.03 (q, J_{C-F} = 27.6 Hz), 33.04 (q, J_{C-F} = 2.5 Hz), 29.51; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.71; HRMS (ESI) m/z calcd. for $C_{21}H_{18}F_3O_4$ $[M-H]^-$ 391.1163, found 391.1166.

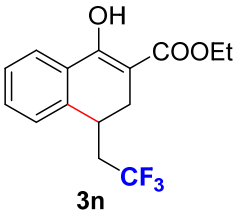
1-(1-hydroxy-4-(2,2,2-trifluoroethyl)-3,4-dihydronaphthalen-2-yl)ethan-1-one (3m)



3m

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, J = 7.7 Hz, 1H), 7.49 (t, J = 7.4 Hz, 1H), 7.41 (t, J = 7.5 Hz, 1H), 7.29 – 7.25 (m, 1H), 3.32 (dt, J = 8.4, 4.2 Hz, 1H), 2.88 – 2.77 (m, 2H), 2.52 – 2.38 (m, 1H), 2.31 – 2.17 (m, 4H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 194.01, 177.08, 142.26, 132.61, 130.31, 127.93, 127.34, 126.52, 126.42 (q, J_{C-F} = 276 Hz), 102.59, 37.66 (q, J_{C-F} = 26.5 Hz), 32.43 (q, J_{C-F} = 2.5 Hz), 26.79, 23.61; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.61; HRMS (ESI) m/z calcd. for $C_{14}H_{12}F_3O_2$ $[M-H]^-$ 269.0795, found 269.0793.

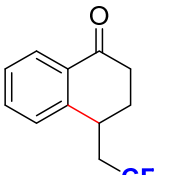
ethyl 1-hydroxy-4-(2,2,2-trifluoroethyl)-3,4-dihydronaphthalene-2-carboxylate (3n)



3n

^{1}H NMR (400 MHz, $CDCl_3$) δ 12.51 (s, 1H), 7.86 (dd, J = 7.4, 1.7 Hz, 1H), 7.44 – 7.35 (m, 2H), 7.27 – 7.23 (m, 1H), 4.39 – 4.24 (m, 2H), 3.29 – 3.20 (m, 1H), 2.86 (dd, J = 16.1, 2.9 Hz, 1H), 2.69 (dd, J = 16.0, 5.6 Hz, 1H), 2.51 – 2.17 (m, 2H), 1.37 (t, J = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.74, 164.50, 140.61, 131.10, 129.02, 127.61, 127.60, 126.58 (q, J_{C-F} = 276 Hz), 124.87, 94.00, 60.79, 37.53 (q, J_{C-F} = 26.5 Hz), 31.83 (q, J_{C-F} = 2.0 Hz), 25.08 (q, J_{C-F} = 0.9 Hz), 14.28; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.53; HRMS (ESI) m/z calcd. for $C_{15}H_{14}F_3O_3$ $[M-H]^-$ 299.0902, found 299.0900.

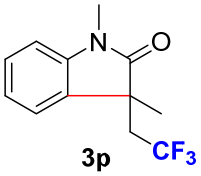
4-(2,2,2-trifluoroethyl)-3,4-dihydronaphthalen-1(2H)-one (3o)



3o

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (dd, J = 7.8, 1.4 Hz, 1H), 7.57 (td, J = 7.6, 1.5 Hz, 1H), 7.44 – 7.36 (m, 1H), 7.33 (d, J = 7.7 Hz, 1H), 3.51 – 3.36 (m, 1H), 2.84 – 2.65 (m, 2H), 2.59 – 2.46 (m, 2H), 2.44 – 2.33 (m, 1H), 2.24 (dq, J = 14.1, 4.8 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.98, 145.28, 133.99, 131.95, 128.06, 127.69, 127.65, 126.40 (q, $J_{C\text{-}F}$ = 276 Hz), 38.27 (q, $J_{C\text{-}F}$ = 26.5 Hz), 34.21, 32.53 (q, $J_{C\text{-}F}$ = 2.5 Hz), 26.53 (q, $J_{C\text{-}F}$ = 1.0 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.81; HRMS (ESI) m/z calcd. for $C_{12}H_{12}F_3O$ $[M+H]^+$ 229.0835, found 229.0833.

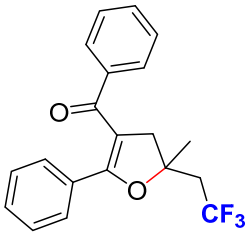
1,3-dimethyl-3-(2,2,2-trifluoroethyl)indolin-2-one (3p)[1]



3p

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (t, J = 7.7 Hz, 1H), 7.29 (d, J = 5.1 Hz, 1H), 7.12 (t, J = 7.5 Hz, 1H), 6.91 (d, J = 7.8 Hz, 1H), 3.26 (s, 3H), 2.91 – 2.79 (m, 1H), 2.73 – 2.61 (m, 1H), 1.43 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 178.53, 142.86, 131.02, 128.54, 125.25 (q, $J_{C\text{-}F}$ = 276 Hz), 123.57, 122.67, 108.48, 44.39, 40.64 (q, $J_{C\text{-}F}$ = 28.0 Hz), 26.46, 25.01; ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.95.

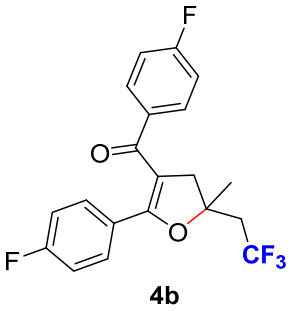
(5-methyl-2-phenyl-5-(2,2,2-trifluoroethyl)-4,5-dihydrofuran-3-yl)(phenyl)metha none (4a)



4a

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 – 7.40 (m, 2H), 7.28 – 7.17 (m, 4H), 7.13 – 7.03 (m, 4H), 3.33 (d, J = 15.2 Hz, 1H), 3.20 (d, J = 15.2 Hz, 1H), 2.79 – 2.65 (m, 2H), 1.72 (s, 3H);^{13}C NMR (101 MHz, $CDCl_3$) δ 193.37, 163.87, 138.80, 131.28, 130.13, 129.77, 129.30, 128.87, 127.70, 125.40 (q, $J_{C\text{-}F}$ = 279 Hz), 127.67, 111.42, 83.56 (q, $J_{C\text{-}F}$ = 2.1 Hz), 44.79 ($J_{C\text{-}F}$ = 1.2 Hz), 43.46 (q, $J_{C\text{-}F}$ = 27.5 Hz), 26.37($J_{C\text{-}F}$ = 1.5 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -60.89; HRMS (ESI) m/z calcd. for $C_{20}H_{18}F_3O_2$ $[M+H]^-$ 347.1253, found 347.1249.

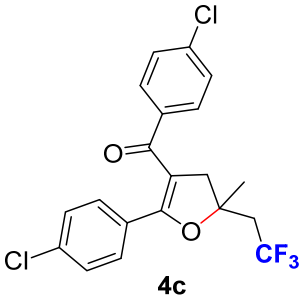
(4-fluorophenyl)(2-(4-fluorophenyl)-5-methyl-5-(2,2,2-trifluoroethyl)-4,5-dihydrofuran-3-yl)methanone (4b)



4b

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 – 7.45 (m, 2H), 7.26 – 7.16 (m, 2H), 6.90 – 6.76 (m, 4H), 3.34 (d, J = 15.3 Hz, 1H), 3.20 (d, J = 15.4 Hz, 1H), 2.84 – 2.55 (m, 2H), 1.70 (s, J = 1.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.56, 164.66 (d, $J_{C\text{-}F}$ = 252 Hz), 163.67 (d, $J_{C\text{-}F}$ = 251 Hz), 162.60, 134.90 (d, $J_{C\text{-}F}$ = 3.1 Hz), 131.46 (d, $J_{C\text{-}F}$ = 8.6 Hz), 131.29 (d, $J_{C\text{-}F}$ = 8.9 Hz), 125.83 (d, $J_{C\text{-}F}$ = 3.5 Hz), 125.37 (q, $J_{C\text{-}F}$ = 277 Hz), 115.11 (d, $J_{C\text{-}F}$ = 8.7 Hz), 114.89 (d, $J_{C\text{-}F}$ = 8.7 Hz), 111.18, 83.67 (q, $J_{C\text{-}F}$ = 2.3 Hz), 44.72 (q, $J_{C\text{-}F}$ = 1.0 Hz), 43.39 (q, $J_{C\text{-}F}$ = 27.6 Hz), 26.49 (q, $J_{C\text{-}F}$ = 1.3 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -60.93, -107.19, -108.44; HRMS (ESI) m/z calcd. for $C_{20}H_{16}F_5O_2$ $[M+H]^+$ 383.1065, found 383.1056.

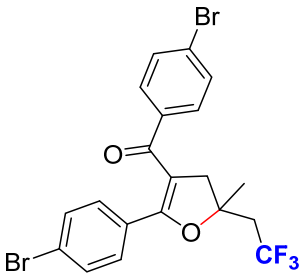
(4-chlorophenyl)(2-(4-chlorophenyl)-5-methyl-5-(2,2,2-trifluoroethyl)-4,5-dihydrofuran-3-yl)methanone (4c)



4c

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.36 (m, 2H), 7.22 – 7.07 (m, 6H), 3.33 (d, J = 15.4 Hz, 1H), 3.19 (d, J = 15.4 Hz, 1H), 2.82 – 2.61 (m, 2H), 1.70 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.57, 162.52, 137.91, 136.97, 136.64, 130.56, 130.22, 128.21, 128.16, 128.01, 125.34 (q, $J_{C\text{-}F}$ = 278 Hz), 111.51, 83.85 (q, $J_{C\text{-}F}$ = 1.0 Hz), 44.73, 43.40 (q, $J_{C\text{-}F}$ = 27.6 Hz), 26.51 (q, $J_{C\text{-}F}$ = 1.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -60.92; HRMS (ESI) m/z calcd. for $C_{20}H_{16}Cl_2F_3O_2$ $[M+H]^+$ 415.0474, found 415.0462.

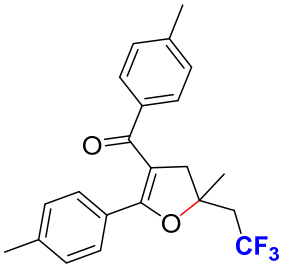
(4-bromophenyl)(2-(4-bromophenyl)-5-methyl-5-(2,2,2-trifluoroethyl)-4,5-dihydrofuran-3-yl)methanone (4d)



4d

^{1}H NMR (500 MHz, $CDCl_3$) 7.36 – 7.25 (m, 6H), 7.08 (d, J = 8.3 Hz, 2H), 3.33 (dd, J = 15.4, 1.3 Hz, 1H), 3.18 (dd, J = 15.4, 1.4 Hz, 1H), 2.77 – 2.60 (m, 2H), 1.70 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 191.72, 162.71, 137.37, 131.19, 131.14, 130.71, 130.33, 128.43, 126.46, 125.32 (q, J_{C-F} = 278 Hz), 125.05, 111.58, 83.92 (q, J_{C-F} = 1.6 Hz), 44.68 (q, J_{C-F} = 0.8 Hz), 43.41 (q, J_{C-F} = 27.6 Hz), 26.54; ^{19}F NMR (376 MHz, $CDCl_3$) δ -60.92; HRMS (ESI) m/z calcd. for $C_{20}H_{16}Br_2F_3O_2$ $[M+H]^+$ 502.9464, found 502.9444.

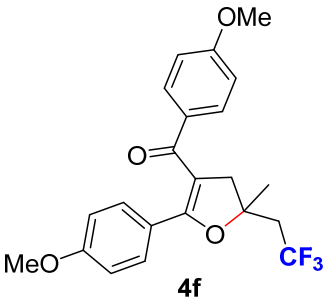
(5-methyl-2-(p-tolyl)-5-(2,2,2-trifluoroethyl)-4,5-dihydrofuran-3-yl)(p-tolyl)methanone (4e)



4e

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, J = 8.1 Hz, 2H), 7.13 (d, J = 8.1 Hz, 2H), 6.94 (d, J = 8.0 Hz, 2H), 6.91 (d, J = 8.1 Hz, 2H), 3.32 (d, J = 15.2 Hz, 1H), 3.19 (d, J = 15.2 Hz, 1H), 2.79 – 2.62 (m, 2H), 2.27 (s, 3H), 2.26 (s, 3H), 1.70 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.23, 163.29, 141.88, 140.38, 136.14, 129.24, 129.06, 128.41, 128.36, 126.98, 125.44 (q, J_{C-F} = 277.48 Hz), 110.62, 83.15 (q, J_{C-F} = 2.1 Hz), 45.12, 43.39 (q, J_{C-F} = 27.4 Hz), 26.22 (q, J_{C-F} = 0.85 Hz), 21.45, 21.38; ^{19}F NMR (376 MHz, $CDCl_3$) δ -60.88; HRMS (ESI) m/z calcd. for $C_{22}H_{22}F_3O_2$ $[M+H]^+$ 375.1566, found 375.1556.

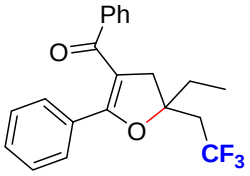
(4-methoxyphenyl)(2-(4-methoxyphenyl)-5-methyl-5-(2,2,2-trifluoroethyl)-4,5-dihydrofuran-3-yl)methanone (4f)



4f

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 – 7.48 (m, 2H), 7.27 – 7.17 (m, 2H), 6.69 – 6.60 (m, 4H), 3.76 (s, 3H), 3.74 (s, 3H), 3.29 (d, J = 15.1 Hz, 1H), 3.18 (d, J = 15.1 Hz, 1H), 2.82 – 2.54 (m, 2H), 1.68 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 192.20, 162.31, 162.28, 160.92, 131.44, 131.20, 130.98, 125.49 (q, J_{C-F} = 278 Hz), 122.27, 113.20, 113.09, 109.74, 82.83 (q, J_{C-F} = 2.1 Hz), 55.31, 55.27, 45.37, 43.32 (q, J_{C-F} = 27.4 Hz), 26.17 (q, J_{C-F} = 0.7 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -60.86; HRMS (ESI) m/z calcd. for $C_{22}H_{22}Br_2F_3O_4$ $[M+H]^+$ 407.1465, found 407.1459.

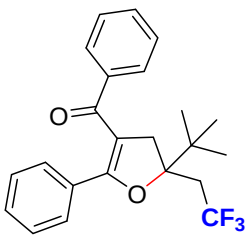
(5-ethyl-2-phenyl-5-(2,2,2-trifluoroethyl)-4,5-dihydrofuran-3-yl)(phenyl)methanone (4q)



4q

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 – 7.39 (m, 2H), 7.25 – 7.17 (m, 4H), 7.10 – 7.04 (m, 4H), 3.29 (s, 2H), 2.75 – 2.63 (m, 2H), 2.05 – 1.92 (m, 2H), 1.11 (t, J = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.40, 164.35, 138.90, 131.20, 130.07, 129.83, 129.28, 128.86, 127.68, 127.66, 125.60 (q, J_{C-F} = 278 Hz), 111.72, 86.08 (q, J_{C-F} = 1.9 Hz), 41.89. 41.47 (q, J_{C-F} = 27.1 Hz), 32.31, 7.71; ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.95; HRMS (ESI) m/z calcd. for $C_{21}H_{20}Br_2F_3O_2$ $[M+H]^+$ 361.1410, found 361.1401.

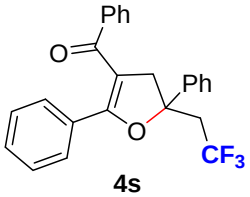
(5-(tert-butyl)-2-phenyl-5-(2,2,2-trifluoroethyl)-4,5-dihydrofuran-3-yl)(phenyl)methanone (4r)



4r

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 – 7.35 (m, 2H), 7.25 – 7.11 (m, 4H), 7.11 – 6.98 (m, 4H), 3.54 (d, J = 16.2 Hz, 1H), 3.30 (d, J = 16.1 Hz, 1H), 2.89 (dq, J = 15.4, 10.9 Hz, 1H), 2.48 (dq, J = 15.4, 10.6 Hz, 1H), 1.09 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.48, 165.31, 139.08, 130.95, 130.02, 129.84, 129.17, 128.82, 127.58, 127.55, 126.76 (q, J_{C-F} = 278.9 Hz), 112.64, 89.53 (q, J_{C-F} = 2.0 Hz), 39.03, 38.59 (q, J_{C-F} = 26.8 Hz), 37.40 (q, J_{C-F} = 6.0 Hz), 24.17; ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.81; HRMS (ESI) m/z calcd. for $C_{23}H_{24}F_3O_2$ $[M+H]^+$ 389.1723, found 389.1723.

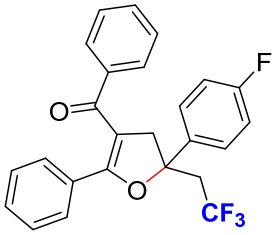
(2,5-diphenyl-5-(2,2,2-trifluoroethyl)-4,5-dihydrofuran-3-yl)(phenyl)methanone (4s)



4s

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 – 7.51 (m, 2H), 7.47 – 7.43 (m, 4H), 7.38 (dt, J = 9.4, 4.2 Hz, 1H), 7.32 (dd, J = 5.9, 2.5 Hz, 2H), 7.28 – 7.22 (m, 2H), 7.15 – 7.07 (m, 4H), 3.73 (d, J = 1.6 Hz, 2H), 3.12 – 2.90 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.18, 163.74, 143.46, 138.66, 131.43, 130.33, 129.55, 129.49, 128.92, 128.75, 128.05, 127.78, 125.11 (q, J_{C-F} = 276 Hz), 124.60, 111.43, 86.02 (q, J_{C-F} = 1.9 Hz), 45.93, 45.00 (q, J_{C-F} = 27.0 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -60.35; HRMS (ESI) m/z calcd. for $C_{25}H_{20}F_3O_2$ $[M+H]^+$ 409.1410, found 409.1409.

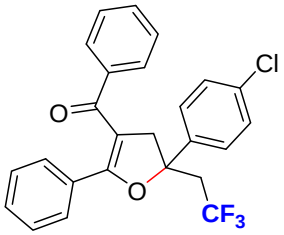
(5-(4-fluorophenyl)-2-phenyl-5-(2,2,2-trifluoroethyl)-4,5-dihydrofuran-3-yl)(phenyl)methanone (4t)



4t

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 – 7.46 (m, 2H), 7.50 – 7.40 (m, 2H), 7.34 – 7.18 (m, 4H), 7.20 – 7.06 (m, 6H), 3.70 (d, J = 1.8 Hz, 2H), 3.13 – 2.85 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.07, 163.41, 162.33 (d, J_{C-F} = 246 Hz), 139.06 (d, J_{C-F} = 3.3 Hz), 138.51, 131.50, 130.38, 129.41, 129.37, 128.89, 127.79, 126.53 (d, J_{C-F} = 8.1 Hz), 125.02 (q, J_{C-F} = 279.04 Hz), 115.60 (d, J_{C-F} = 21.5 Hz), 111.34, 85.64 (q, J_{C-F} = 2.2 Hz), 46.09, 45.02 (q, J_{C-F} = 27.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -60.36, -114.13; HRMS (ESI) m/z calcd. for $C_{25}H_{19}F_4O_2$ $[M+H]^+$ 427.1316, found 427.1314.

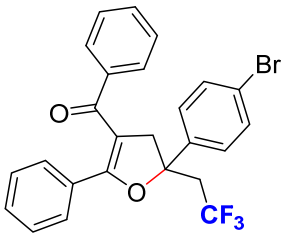
(5-(4-chlorophenyl)-2-phenyl-5-(2,2,2-trifluoroethyl)-4,5-dihydrofuran-3-yl)(phenyl)methanone (4u)



4u

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 – 7.38 (m, 6H), 7.34 – 7.19 (m, 4H), 7.12 (q, J = 8.1 Hz, 4H), 3.68 (d, J = 4.1 Hz, 2H), 3.13 – 2.84 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.06, 163.41, 141.77, 138.44, 134.00, 131.55, 130.43, 129.43, 129.28, 128.92, 128.89, 127.80, 126.16, 124.91 (q, J_{C-F} = 279.1 Hz), 111.28, 85.54 (q, J_{C-F} = 2.2 Hz), 46.07, 44.85 (q, J_{C-F} = 27.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -60.31; HRMS (ESI) m/z calcd. for $C_{25}H_{19}ClF_3O_2$ $[M+H]^+$ 443.1020, found 443.1021.

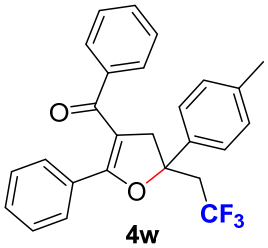
(5-(4-bromophenyl)-2-phenyl-5-(2,2,2-trifluoroethyl)-4,5-dihydrofuran-3-yl)(phenyl)methanone (4v)



4v

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 – 7.53 (m, 2H), 7.48 – 7.35 (m, 4H), 7.33 – 7.21 (m, 4H), 7.12 (q, J = 8.0 Hz, 4H), 3.75 – 3.59 (m, 2H), 3.13 – 2.84 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.04, 163.40, 142.31, 138.43, 131.88, 131.55, 130.44, 129.43, 129.26, 128.89, 127.80, 126.48, 124.90 (q, J_{C-F} = 278 Hz), 122.13, 111.27, 85.55 (q, J_{C-F} = 2.2 Hz), 46.04 , 44.80 (q, J_{C-F} = 27.4 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -60.30; HRMS (ESI) m/z calcd. for $C_{25}H_{19}BrF_3O_2$ $[M+H]^+$ 487.0515, found 487.0515.

phenyl(2-phenyl-5-(p-tolyl)-5-(2,2,2-trifluoroethyl)-4,5-dihydrofuran-3-yl)methanone (4w)

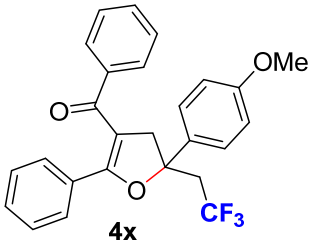


4w

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (t, J = 7.7 Hz, 4H), 7.34 – 7.22 (m, 6H), 7.11 (dt, J = 15.8, 7.7 Hz, 4H), 3.71 (s, 2H), 3.11 – 2.88 (m, 2H), 2.40 (s, 3H); ^{13}C NMR (126

MHz, $CDCl_3$) δ 193.23, 163.86, 140.46, 138.70, 137.80, 131.38, 130.28, 129.61, 129.49, 129.38, 128.92, 127.75, 125.12 (q, J_{C-F} = 278 Hz), 124.53, 111.49, 86.08 (q, J_{C-F} = 1.8 Hz), 45.80, 45.03 (q, J_{C-F} = 26.5 Hz), 21.10; ^{19}F NMR (376 MHz, $CDCl_3$) δ -60.35; HRMS (ESI) m/z calcd. for $C_{26}H_{22}F_3O_2$ $[M+H]^+$ 423.1566, found 423.1563.

(5-(4-methoxyphenyl)-2-phenyl-5-(2,2,2-trifluoroethyl)-4,5-dihydrofuran-3-yl)(phenyl)methanone (4x)

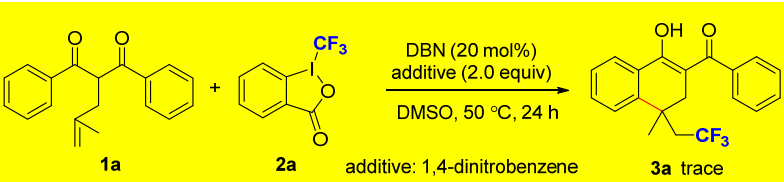


4x

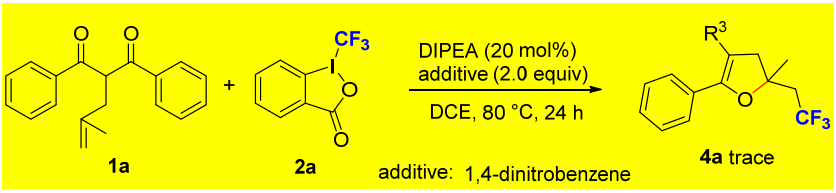
^1H NMR (500 MHz, $CDCl_3$) δ 7.48 – 7.35 (m, 4H), 7.33 – 7.20 (m, 4H), 7.15 – 7.06 (m, 4H), 7.00 – 6.93 (m, 2H), 3.85 (s, 3H), 3.70 (s, 2H), 3.06 – 2.89 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 193.23, 163.78, 159.23, 138.67, 135.29, 131.37, 130.27, 129.58, 129.45, 128.90, 127.73, 125.93, 125.07 (q, J_{C-F} = 278.3 Hz), 114.00, 111.52, 85.97 (q, J_{C-F} = 2.2 Hz), 55.33, 45.70, 45.07 (q, J_{C-F} = 27.0 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -60.40; HRMS (ESI) m/z calcd. for $C_{26}H_{22}F_3O_3$ $[M+H]^+$ 439.1516, found 439.1513.

Mechanistic Study

Experimental procedure for control experiment

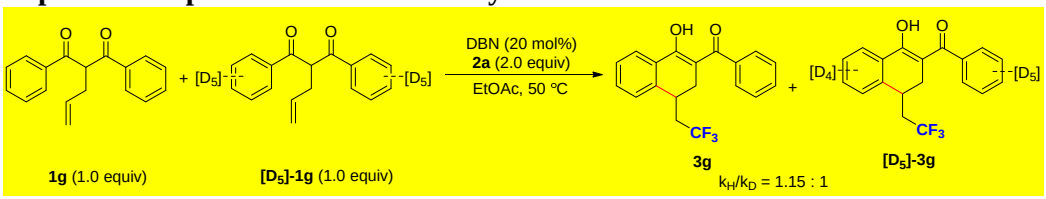


To a flame-dried Schlenk tube equipped with a magnetic stir bar were added **1** (0.2 mmol), **2a** (0.4 mmol) and 1,4-dinitrobenzene (0.4 mmol). The tube was evacuated and backfilled with argon for three times, and then DMSO (1 mL) were added, followed by DBN (0.04 mmol). The tube was stirred at 50 °C for 24 h. Trace amount of **3a** was observed from ^{19}F NMR yield.



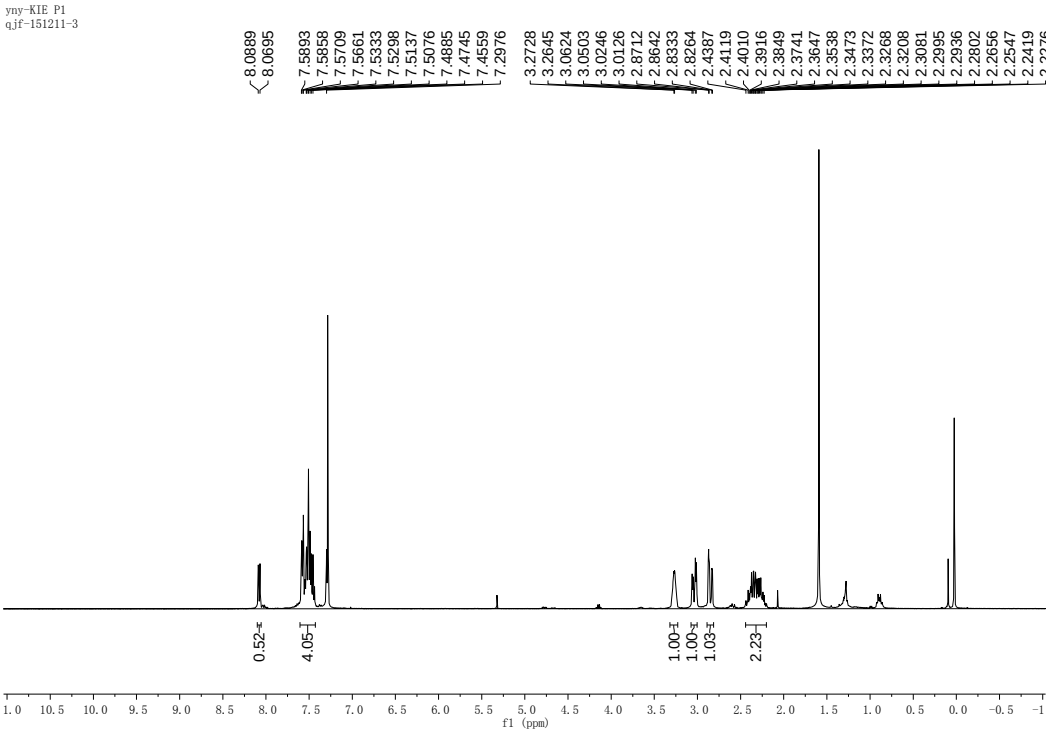
To a flame-dried Schlenk tube equipped with a magnetic stir bar were added **1** (0.2 mmol), **2a** (0.4 mmol) and 1,4-dinitrobenzene (0.4 mmol). The tube was evacuated and backfilled with argon for three times, and then DCE (1 mL) were added. followed by DIPEA (0.04 mmol). The tube was stirred at 80 °C for 24 h. Trace amount of **4a** was observed from ^{19}F NMR yield.

Experimental procedure for KIE study



The **[D$_5$]-1g** was synthesized in the same way of the general procedure.

To a flame-dried Schlenk tube equipped with a magnetic stir bar were added **1g** (0.05 mmol), **[D$_5$]-1g** (0.05 mmol), **2a** (0.2 mmol). The tube was evacuated and backfilled with argon for three times, and then EtOAc (1 mL) were added, followed by addition of DBN (0.03 mmol). The tube was stirred at 50 °C for 10 h. The reaction mixture was purified by preparative HPLC to afford the mixture of **3g** and **[D$_5$]-3g**.



Rage	Absolute value
8.13 - 8.05	80138.35
3.34 - 3.21	146474.93
3.09 - 2.99	151289.83
2.90 - 2.80	149757.77

The average absolute value of a single hydrogen was considered to be (146474.93 + 151289.83 + 149757.77) / 3 = 149174.18

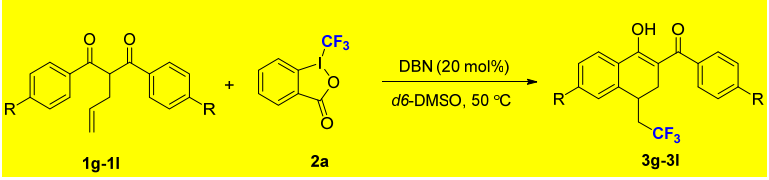
According to this average value the target peak was normalized to 80138.35/149174 18=0.537

So k_H/k_D=0.537 / (1-0.537) =1.15

Note: EtOAc, instead of DMSO, was used as the reaction solvent to prevent any loss of product.

Experimental procedure for Hammett study

Procedure for individual Hammett test:

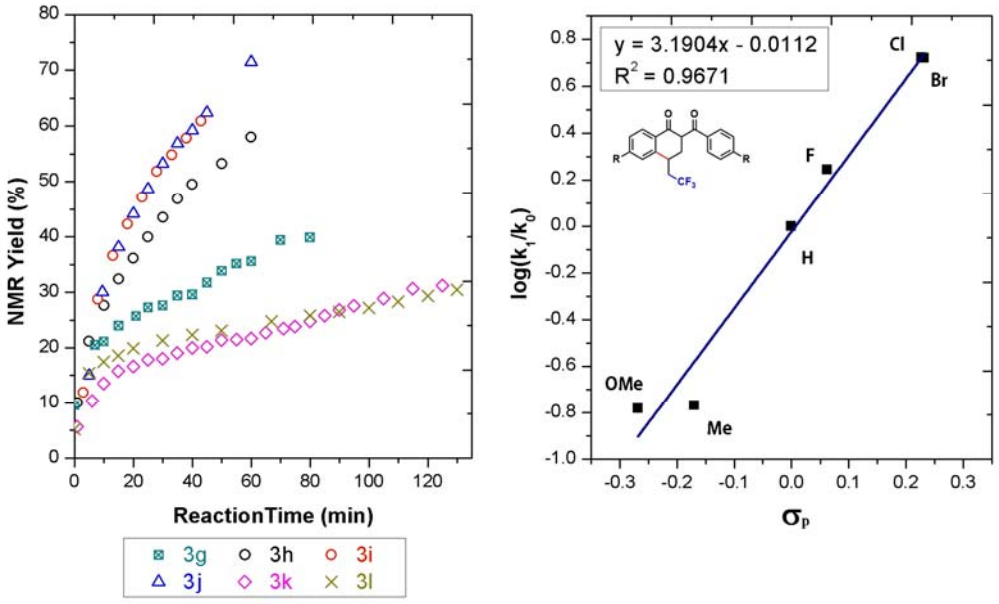


The reaction was allowed to proceed in an NMR tube. Substrate **1g-1l** (0.10 mmol),

2a (0.20 mmol), $PhCF_3$ (0.10 mmol) was dissolved in *d6*-DMSO (1.0 mL) in a round bottom flask under an Ar atmosphere. The solution was warm to 50 °C (in a sand bath), then DBN (2.5 μL, 0.02 mmol) was injected into the mixture quickly, the solution was mix thoroughly and quickly transferred enough solution into the Ar charged NMR tube, the yield was monitored by quick ^{19}F NMR for every 5 mins, after the test the NMR tube was allowed to warm to 50 °C using the sand bath.

Discussion on Hammett equation:

(1) Firstly, the Hammett plot was given in Figure S1. Using σ_p, the Hammett plot gave a good linear relationship (ρ= 3.19, R^2=0.9671). In spite of this, we assumed that it might not be suitable for disclosing this carbotrifluoromethylation reaction.



(2) As shown in Figure S2, using σ_m, however, the Hammett plot did not afford a considerable linear relationship (ρ = 2.73, R^2=0.7212), therefore ruling out the possibility of carbocation intermediate during the course of cylization.[2] This preliminary result suggested that a possible radical cyclization might be proceeded.[3]

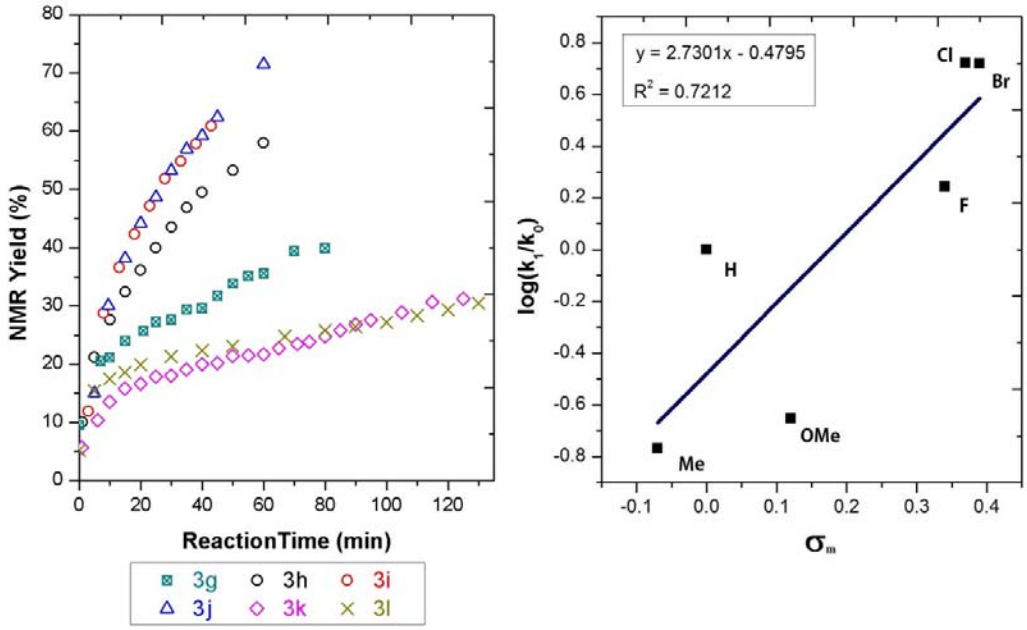
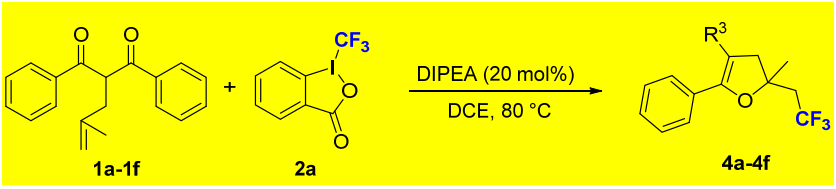


Figure S2 Hammett Study using σ_m for carbotrifluoromethylation in DMSO



In a round bottom flask, substrate **1a-1f** (0.10 mmol), **2a** (0.20 mmol) were dissolved in DCE (1.0 mL) under an Ar atmosphere, followed by addition of DIPEA (0.02 mmol) and $PhCF_3$ (0.10 mmol). The reaction mixture was heated up to 80 °C. for each 10 min, the reaction mixture (20 μL) was separated and the yield was monitored by ^{19}F NMR.

As shown in Figure S3, a negative ρ value (-0.94, R^2=0.9671) in Hammett plot was given in below, which suggested the carbocation center might occur in the cyclization step and thus a carbocation intermediate might be involved before the cyclization step for oxytrifluoromethylation.

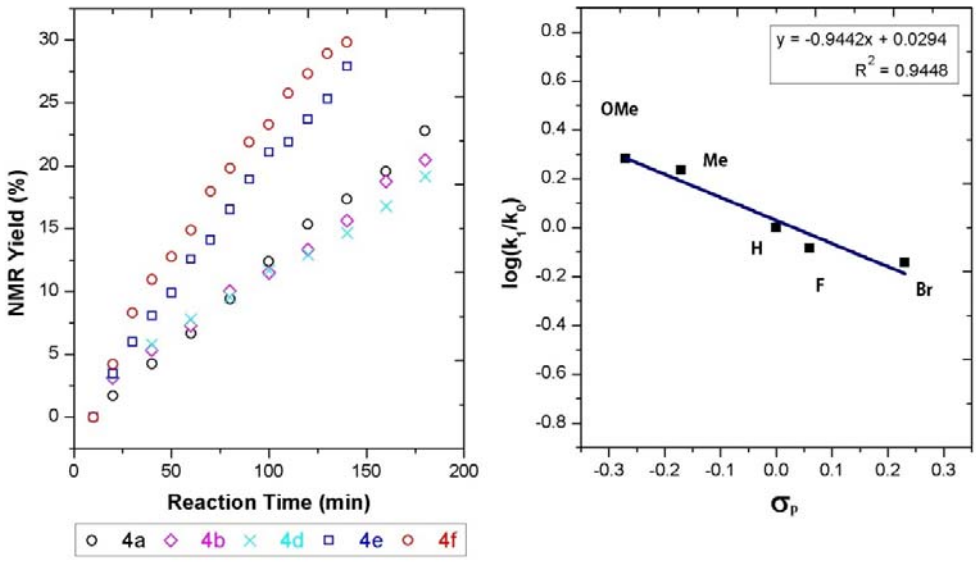
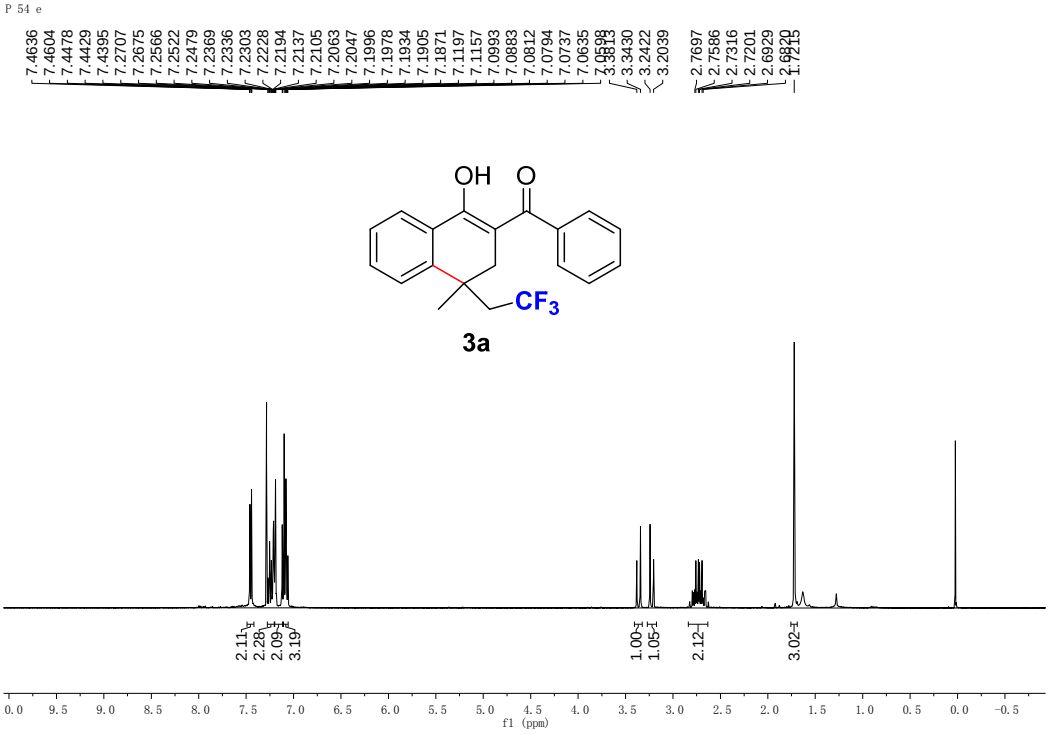
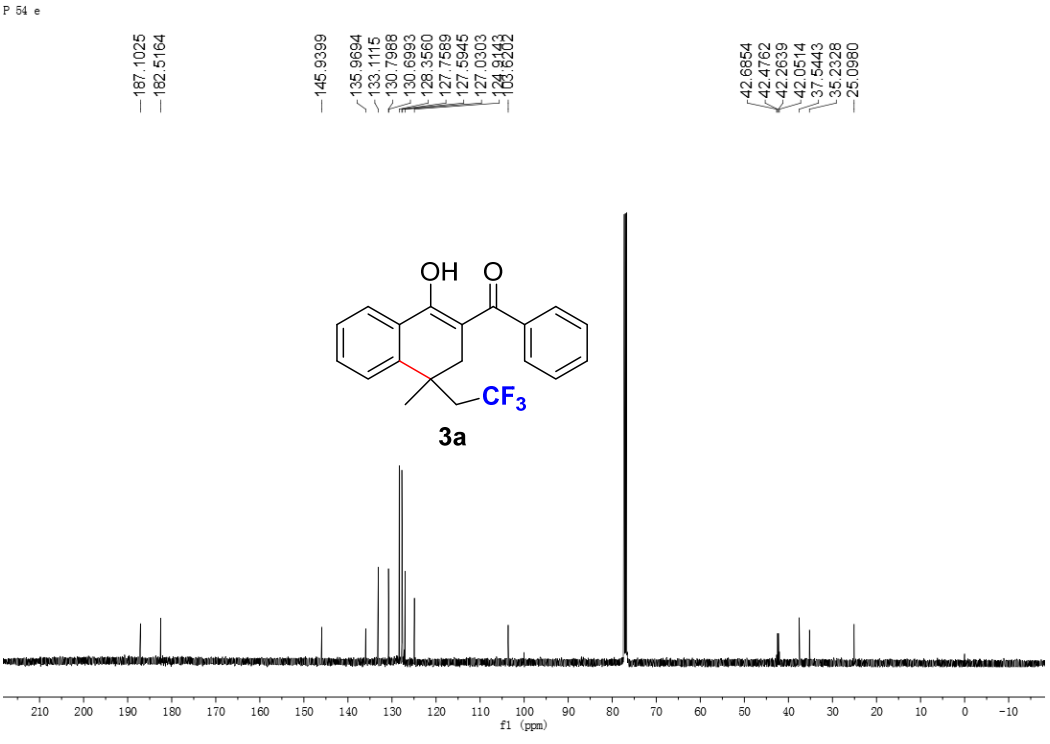


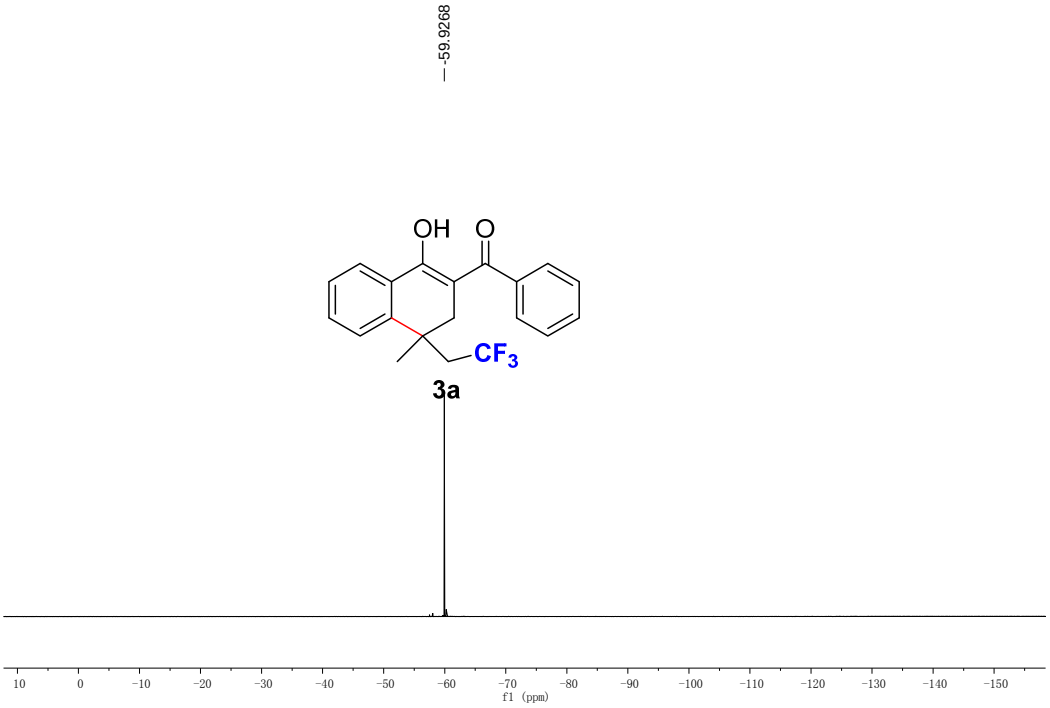
Figure S3 Hammett Study for oxytrifluoromethylation in DCE

NMR Spectrum

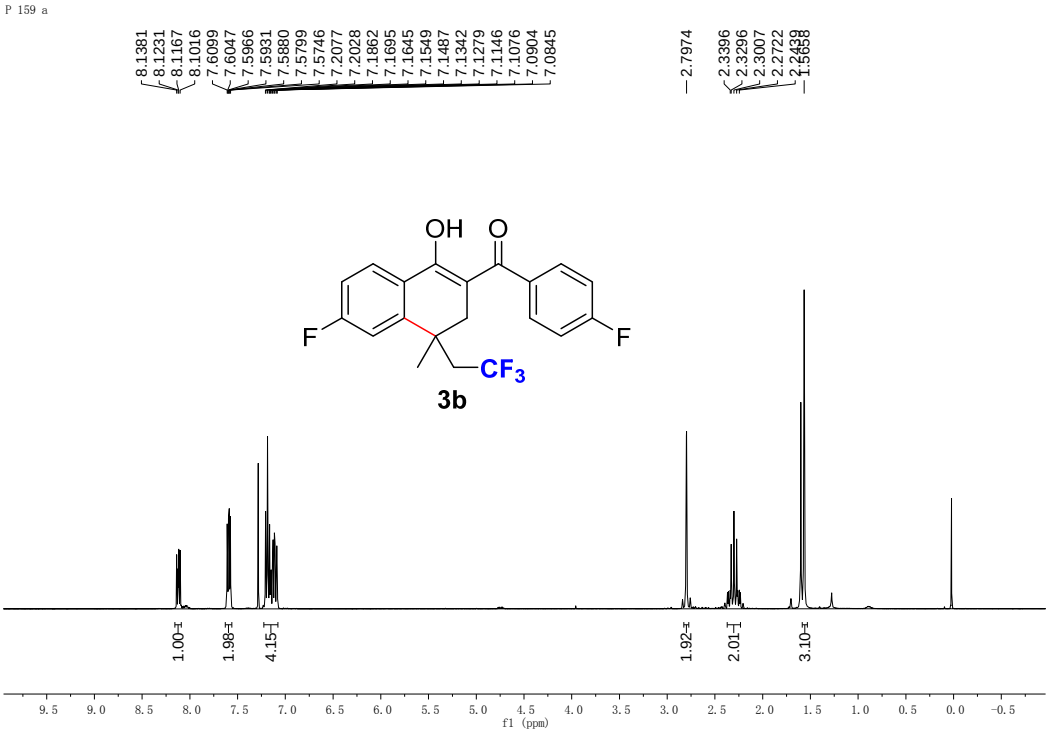


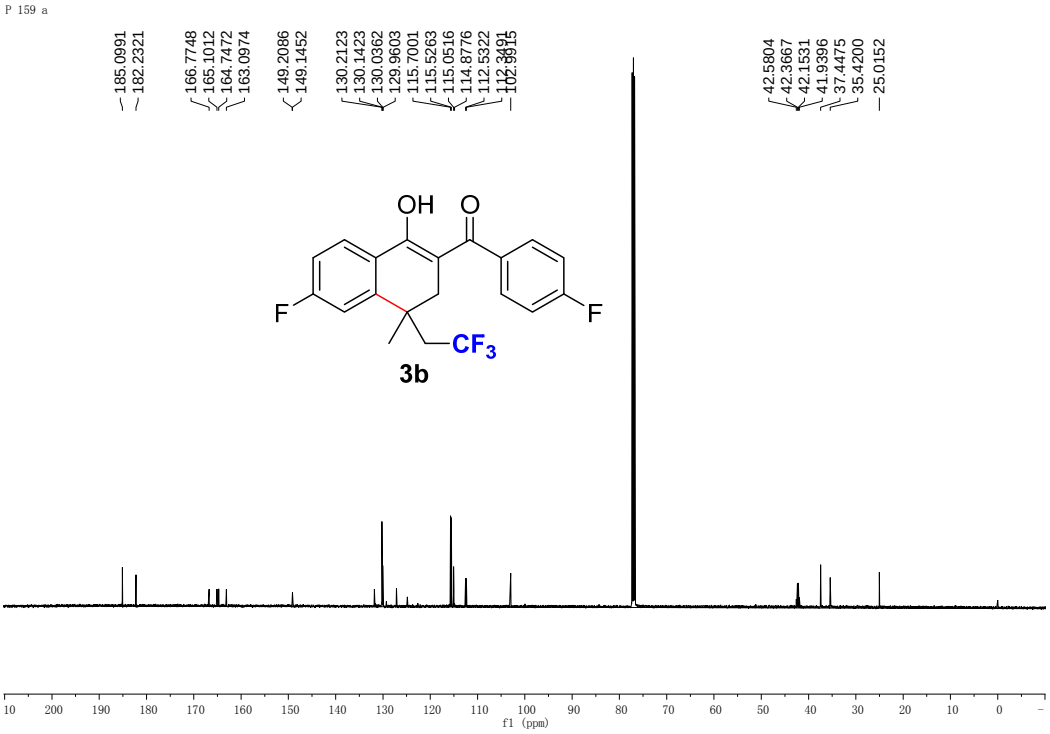


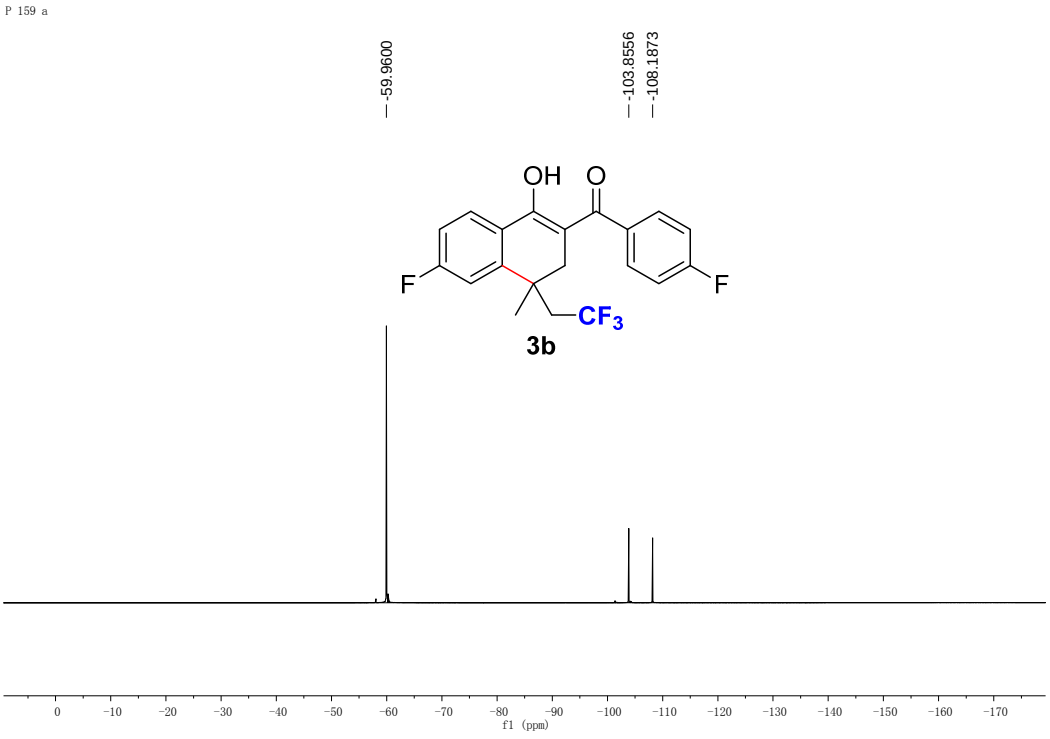
P 54 e


-59.9268
OH
O
CF3
3a
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
f1 (ppm)

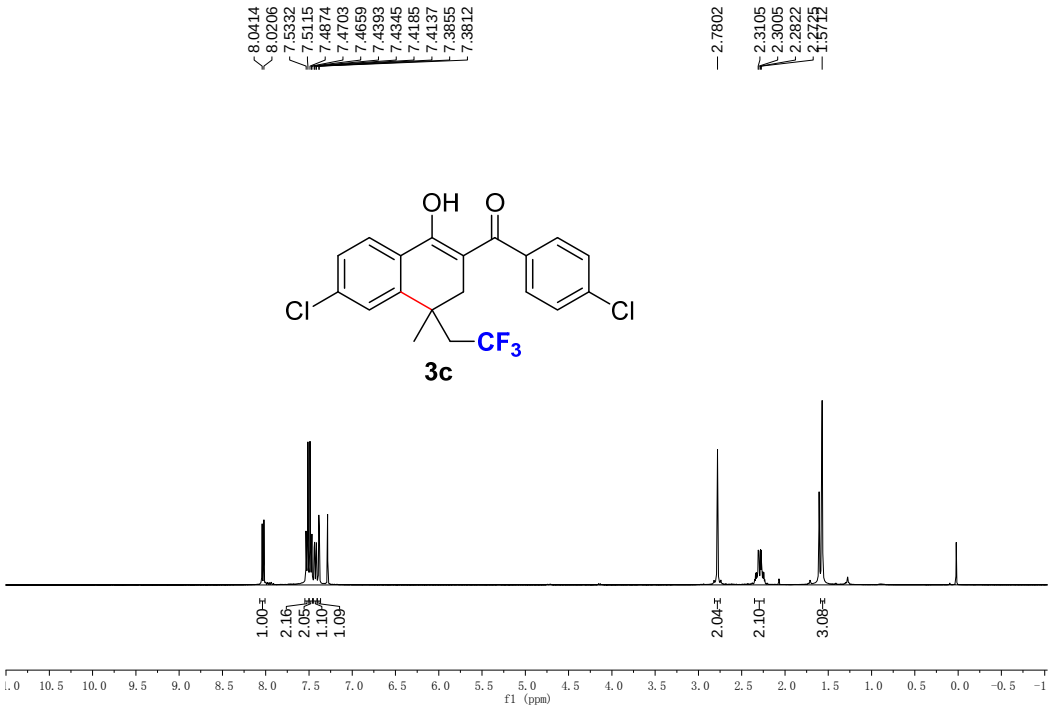
P 159 a


8.1381
8.1231
8.1167
8.1016
7.6099
7.6047
7.5966
7.5931
7.5880
7.5799
7.5746
7.2077
7.2028
7.1862
7.1695
7.1645
7.1549
7.1487
7.1342
7.1279
7.1146
7.1076
7.0904
7.0845
2.7974
2.3396
2.3296
2.3007
2.2722
2.2439
1.5658
OH
O
F
F
CF3
3b
1.00
1.98
4.15
1.92
2.01
3.10
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)

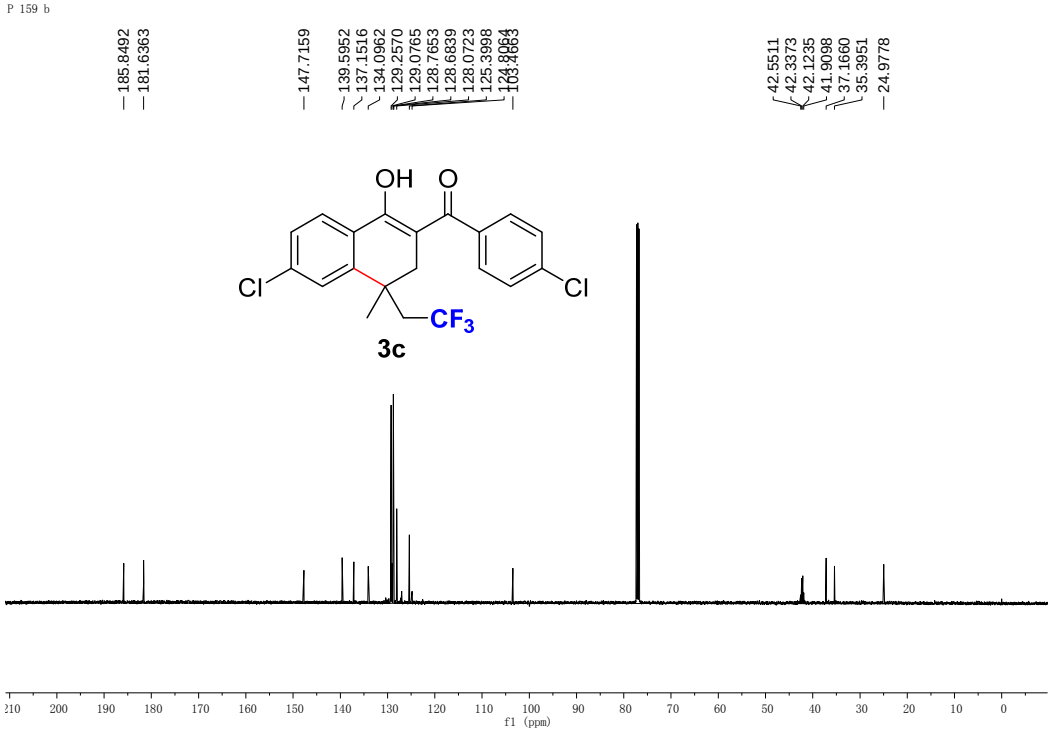

P 159 a
185.0991
182.2321
166.7748
165.1012
164.7472
163.0974
149.2086
149.1452
130.2123
130.1423
130.0362
129.9603
115.7001
115.5263
115.0516
114.8776
112.5322
42.5804
42.3667
42.1531
41.9396
37.4475
35.4200
25.0152
OH
O
F
F
CF3
3b
f1 (ppm)


P 159 a
-59.9600
-103.8556
-108.1873
OH
O
F
F
CF3
3b
f1 (ppm)

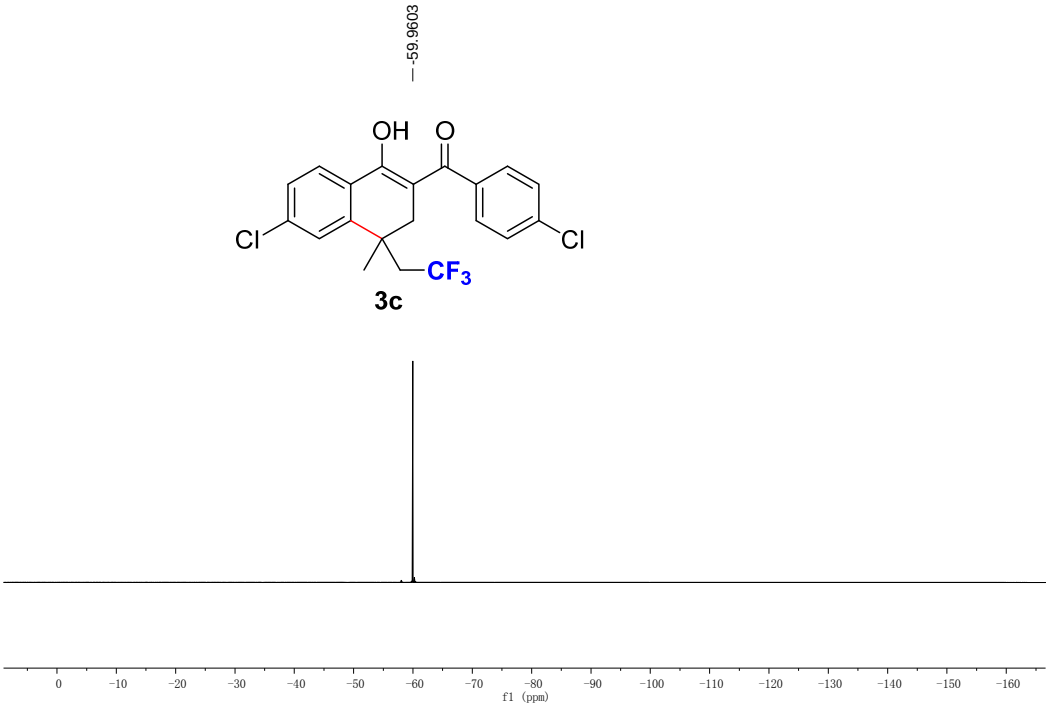
P 159 b


8.0414
8.0206
7.5332
7.5115
7.4874
7.4703
7.4659
7.4393
7.4345
7.4185
7.4137
7.3855
7.3812
2.7802
2.3105
2.3005
2.2822
2.2725
1.5712
OH
O
Cl
Cl
CF3
3c
1.00
2.16
2.05
1.10
1.09
2.04
2.10
3.08
f1 (ppm)

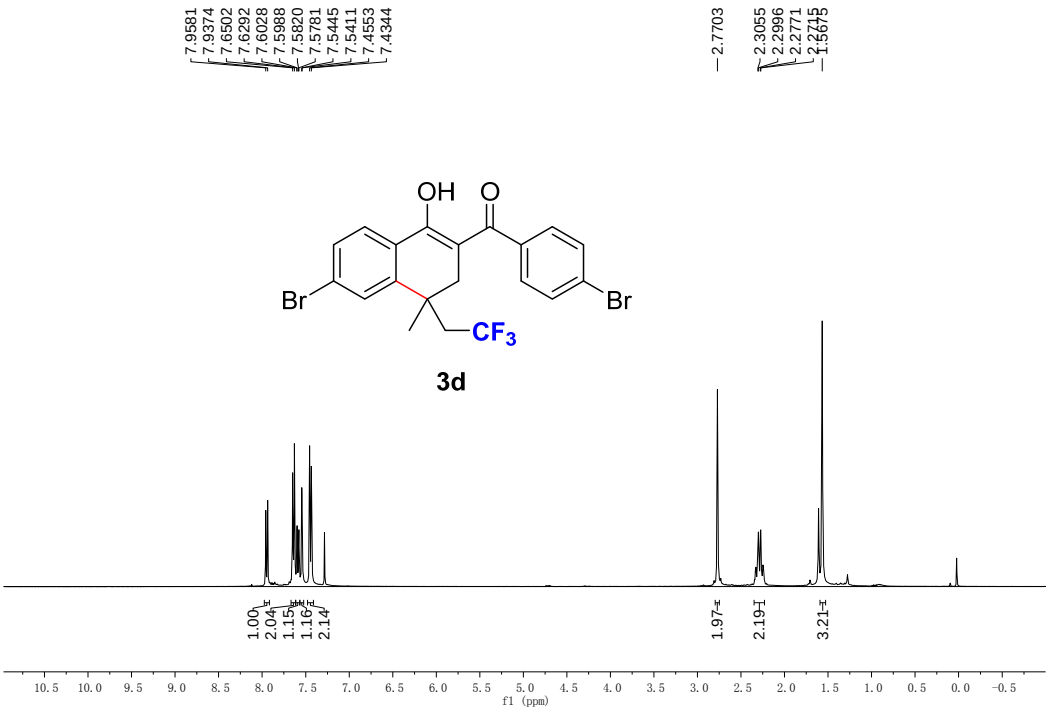
P 159 b


185.8492
181.6363
147.7159
139.5952
137.1516
134.0962
129.2570
129.0765
128.7653
128.6839
128.0723
125.3998
124.8064
103.4863
42.5511
42.3373
42.1235
41.9098
37.1660
35.3951
24.9778
OH
O
Cl
Cl
CF3
3c
f1 (ppm)

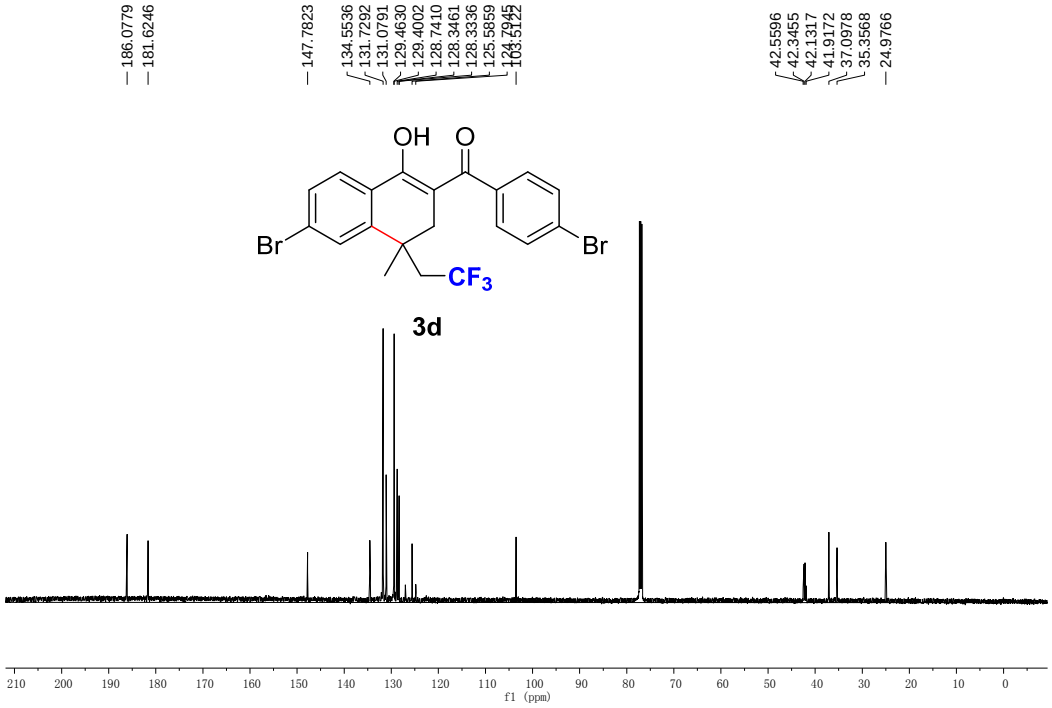
P 159 b


-59.9603
OH
O
Cl
Cl
CF3
3c
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
f1 (ppm)

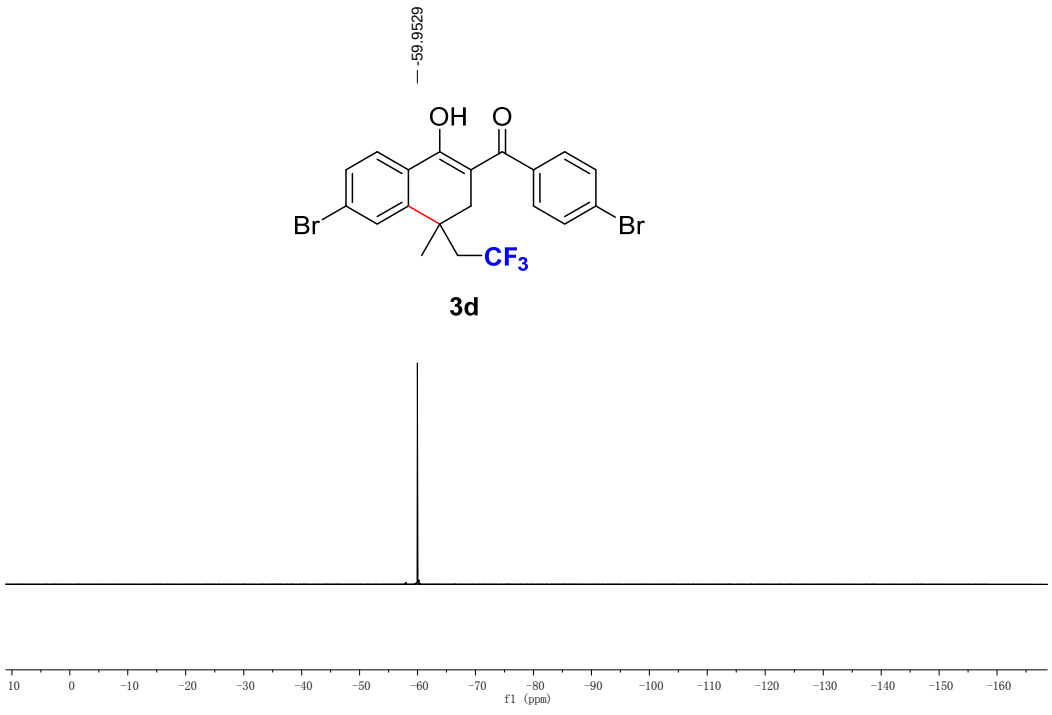
P 159 c

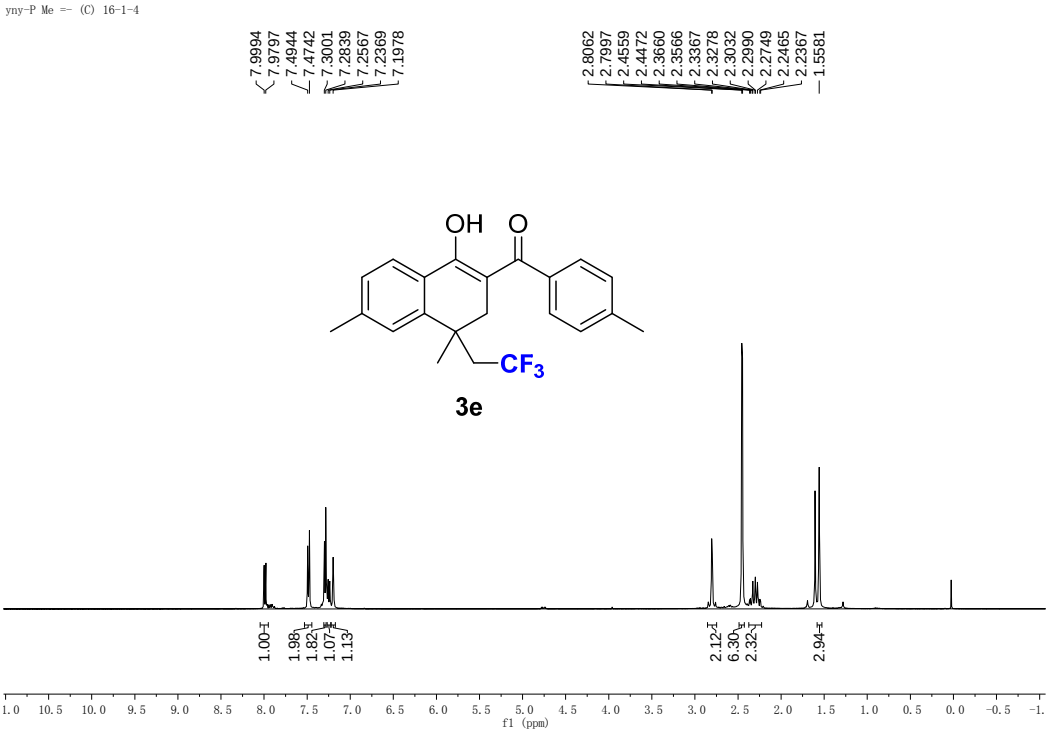

7.9581
7.9374
7.6502
7.6292
7.6028
7.5988
7.5820
7.5781
7.5445
7.5411
7.4553
7.4344
2.7703
2.3055
2.2996
2.2771
2.2715
1.5675
OH
O
Br
Br
CF3
3d
1.00
2.04
1.15
1.16
2.14
1.97
2.19
3.21
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

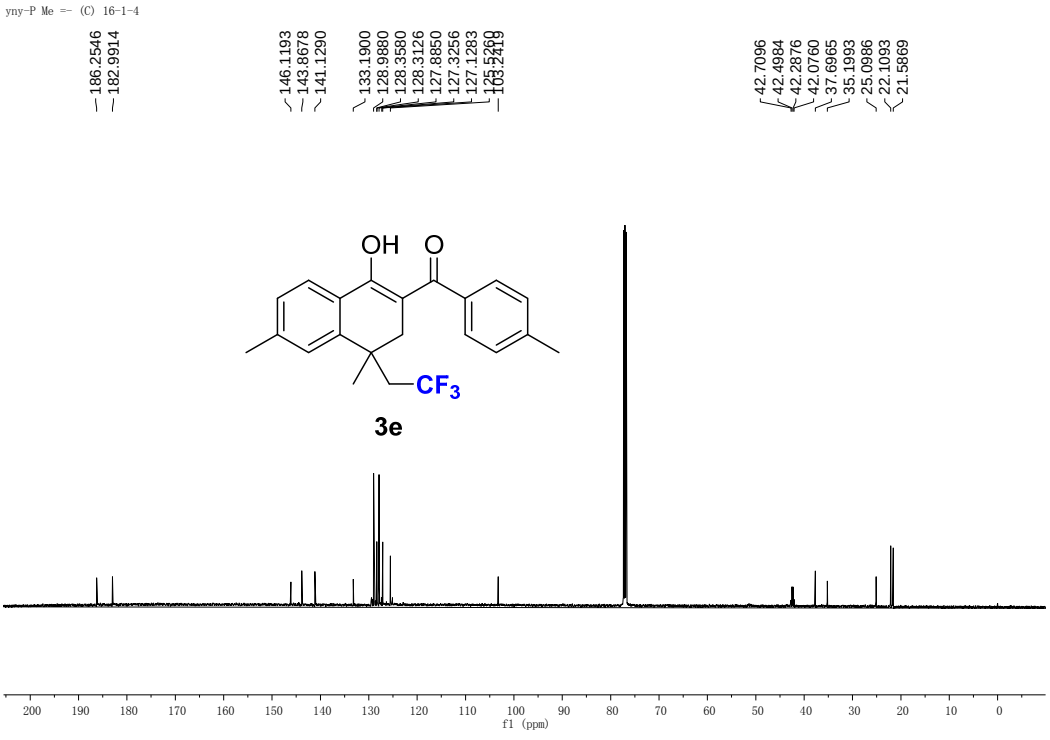
P 159 c


186.0779
181.6246
147.7823
134.5536
131.7292
131.0791
129.4630
129.4002
128.7410
128.3461
128.3336
125.5859
124.7945
103.5122
42.5596
42.3455
42.1317
41.9172
37.0978
35.3568
24.9766
OH
O
Br
Br
CF3
3d
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

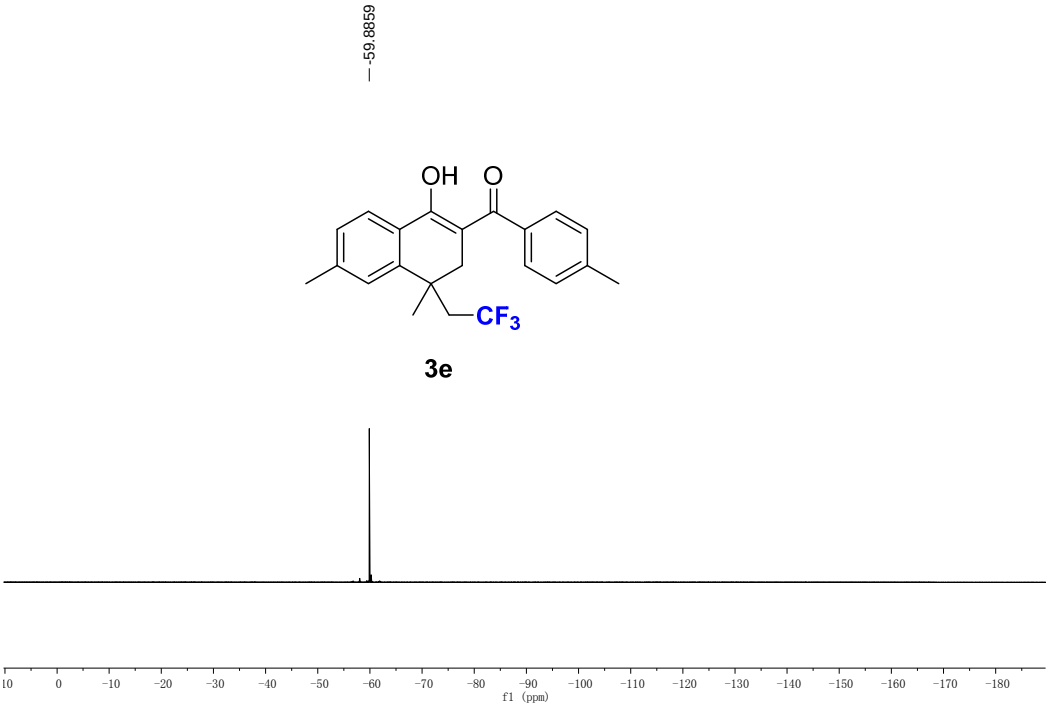
P 159 c


-59.9529
OH
O
Br
Br
CF3
3d
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
f1 (ppm)


yny-P Me =- (C) 16-1-4
7.9994
7.9797
7.4944
7.4742
7.3001
7.2839
7.2567
7.2369
7.1978
2.8062
2.7997
2.4559
2.4472
2.3660
2.3566
2.3367
2.3278
2.3032
2.2990
2.2749
2.2465
2.2367
1.5581
OH
O
CF3
3e
1.00
1.98
1.82
1.07
1.13
2.12
6.30
2.32
2.94
f1 (ppm)

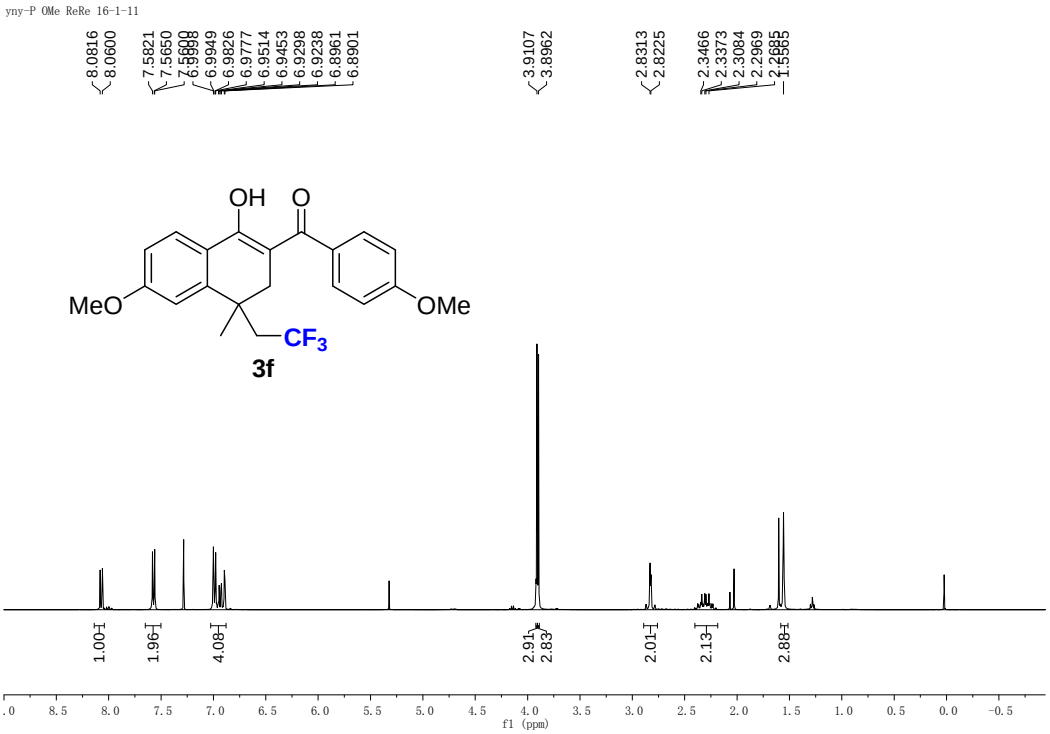

yny-P Me =- (C) 16-1-4
186.2546
182.9914
146.1193
143.8678
141.1290
133.1900
128.9880
128.3580
128.3126
127.8850
127.3256
127.1283
125.5260
103.2419
42.7096
42.4984
42.2876
42.0760
37.6965
35.1993
25.0986
22.1093
21.5869
OH
O
CF3
3e
f1 (ppm)

yny-P Me =- (C) 16-1-4

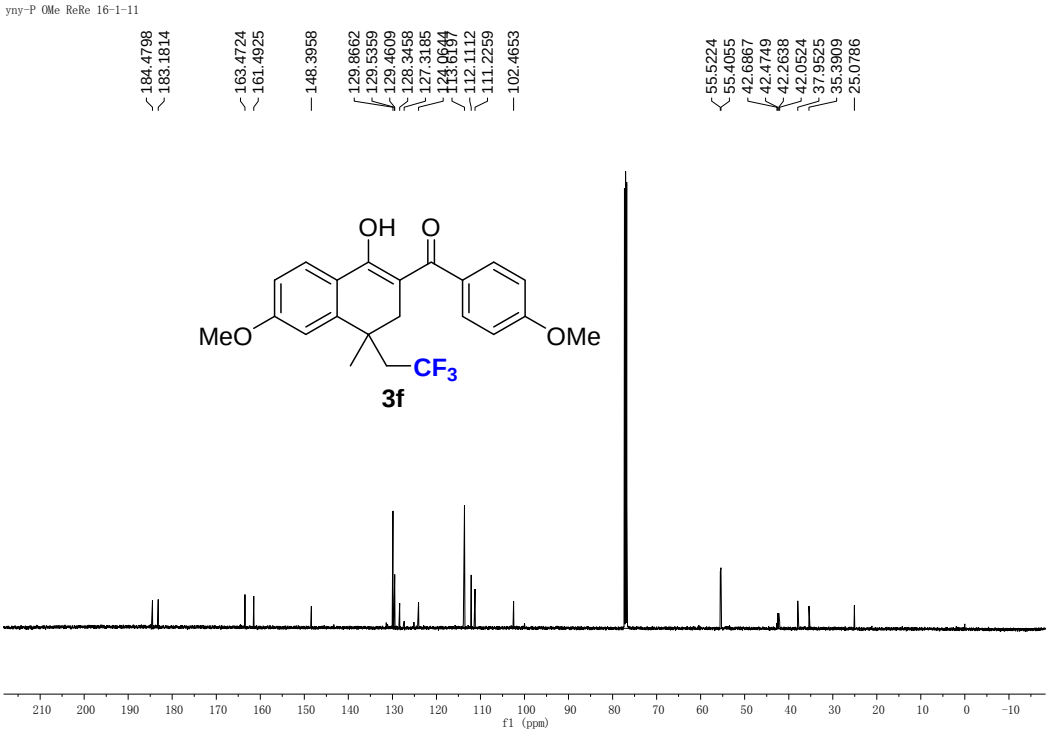


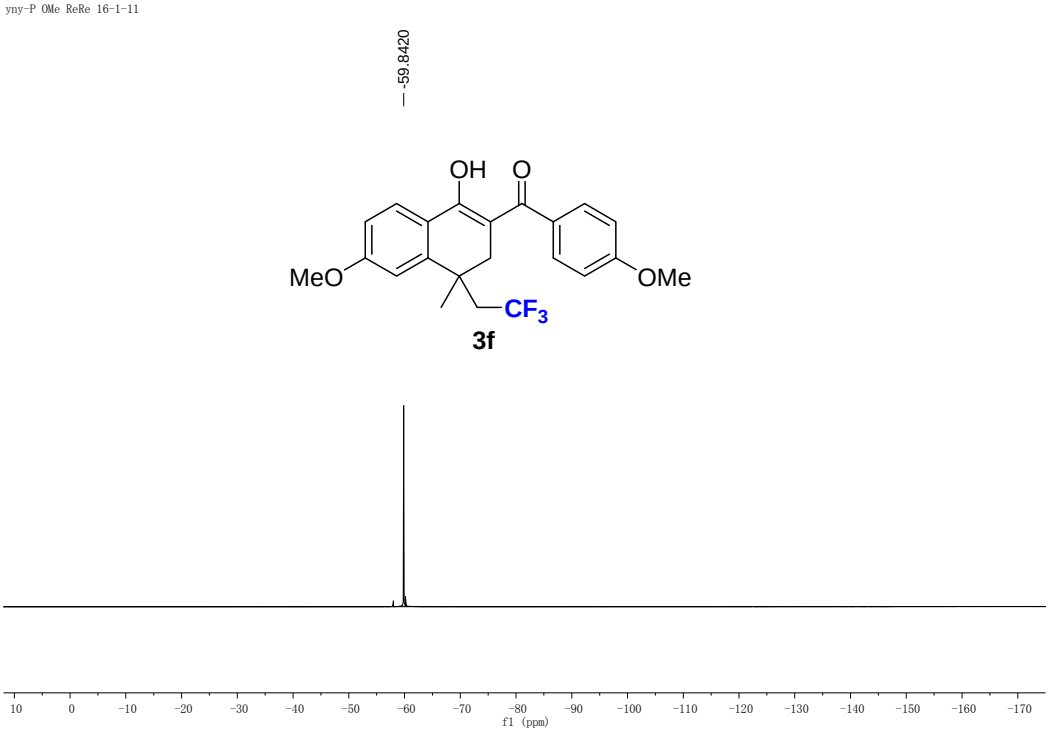
3e

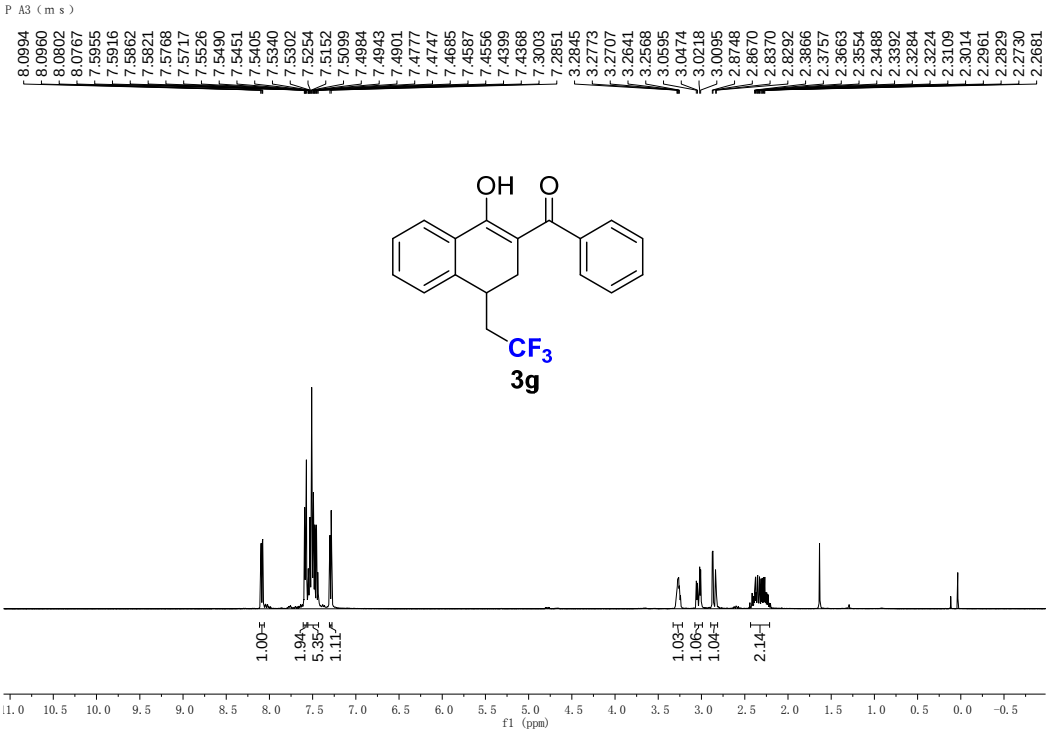
yny-P OMe ReRe 16-1-11

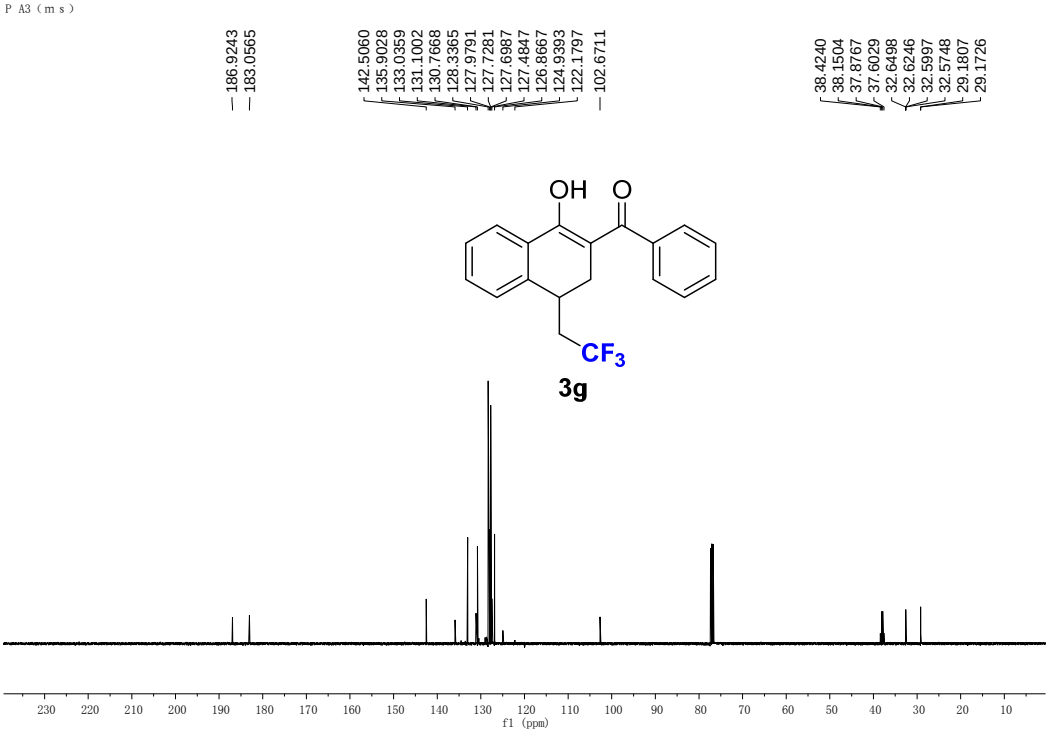


3f

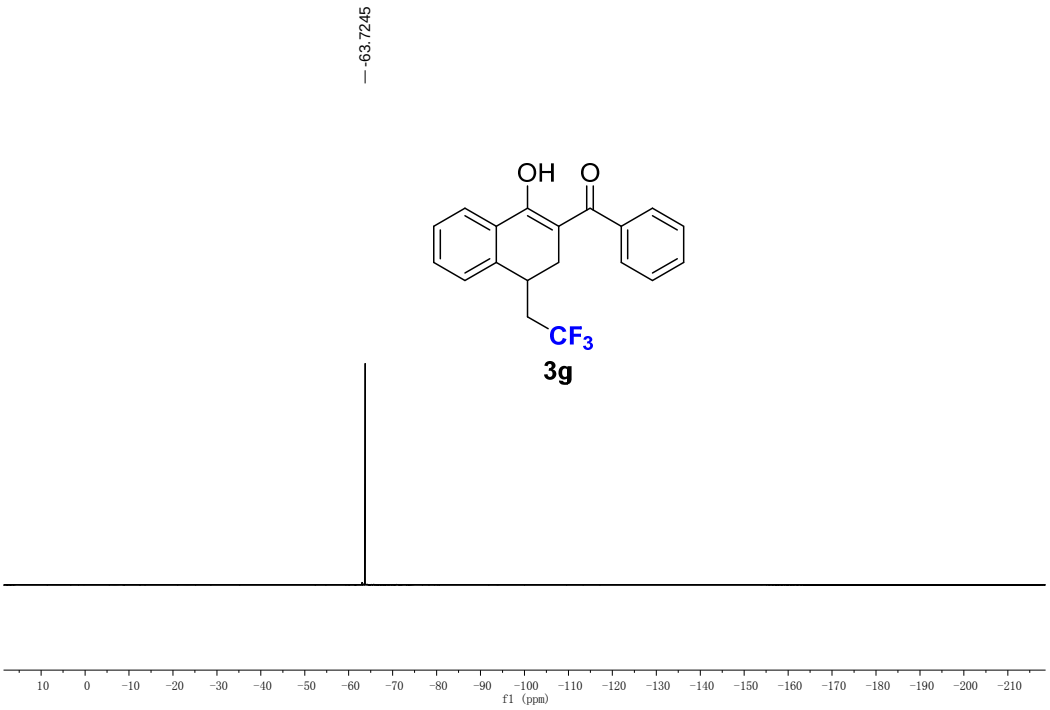

yny-P OMe ReRe 16-1-11
184.4798
183.1814
163.4724
161.4925
148.3958
129.8662
129.5359
129.4609
128.3458
127.3185
124.0644
113.6197
112.1112
111.2259
102.4653
55.5224
55.4055
42.6867
42.4749
42.2638
42.0524
37.9525
35.3909
25.0786
OH
O
MeO
OMe
CF3
3f
f1 (ppm)


yny-P OMe ReRe 16-1-11
-59.8420
OH
O
MeO
OMe
CF3
3f
f1 (ppm)

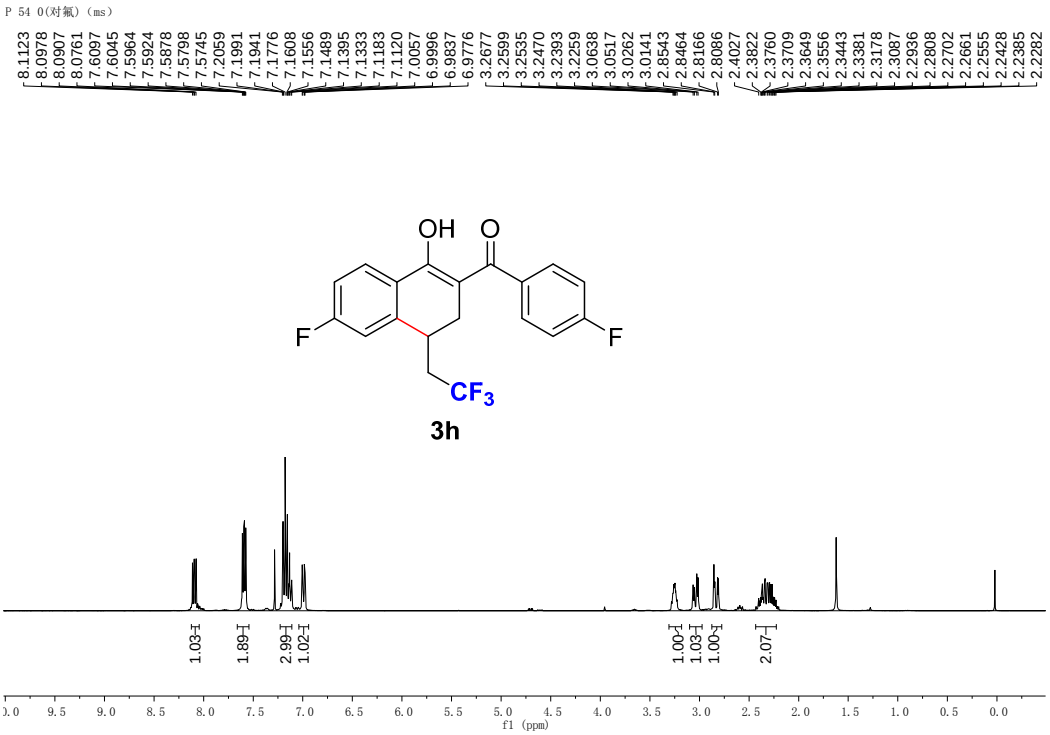

P A3 (m s)
8.0994
8.0960
8.0802
8.0767
7.5955
7.5916
7.5862
7.5821
7.5768
7.5717
7.5526
7.5490
7.5451
7.5405
7.5340
7.5302
7.5254
7.5152
7.5099
7.4984
7.4943
7.4901
7.4777
7.4747
7.4685
7.4587
7.4556
7.4399
7.4368
7.3003
7.2851
3.2845
3.2773
3.2707
3.2641
3.2568
3.0595
3.0474
3.0218
3.0095
2.8748
2.8670
2.8370
2.8292
2.3866
2.3757
2.3663
2.3554
2.3488
2.3392
2.3284
2.3224
2.3109
2.3014
2.2961
2.2829
2.2730
2.2681
OH
O
CF3
3g
1.00
1.94
5.35
1.11
1.03
1.06
1.04
2.14
f1 (ppm)


P A3 (m s)
186.9243
183.0565
142.5060
135.9028
133.0359
131.1002
130.7668
128.3365
127.9791
127.7281
127.6987
127.4847
126.8667
124.9393
122.1797
102.6711
38.4240
38.1504
37.8767
37.6029
32.6498
32.6246
32.5997
32.5748
29.1807
29.1726
OH
O
CF3
3g
f1 (ppm)

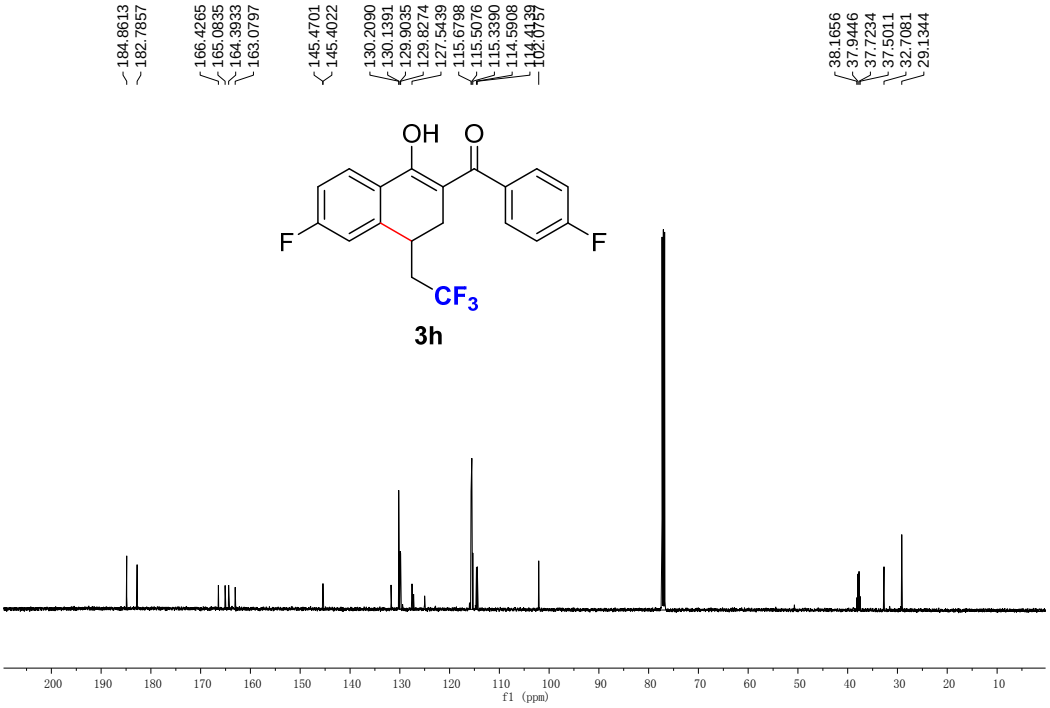
P A3（m s）



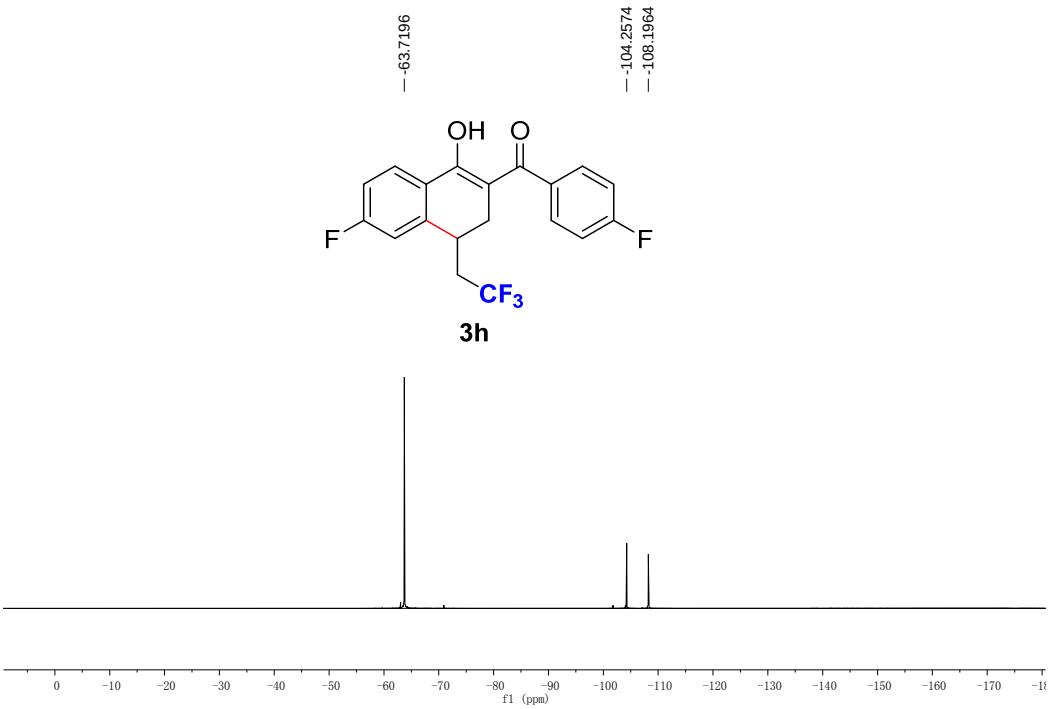
P 54 0(对氟)（ms）



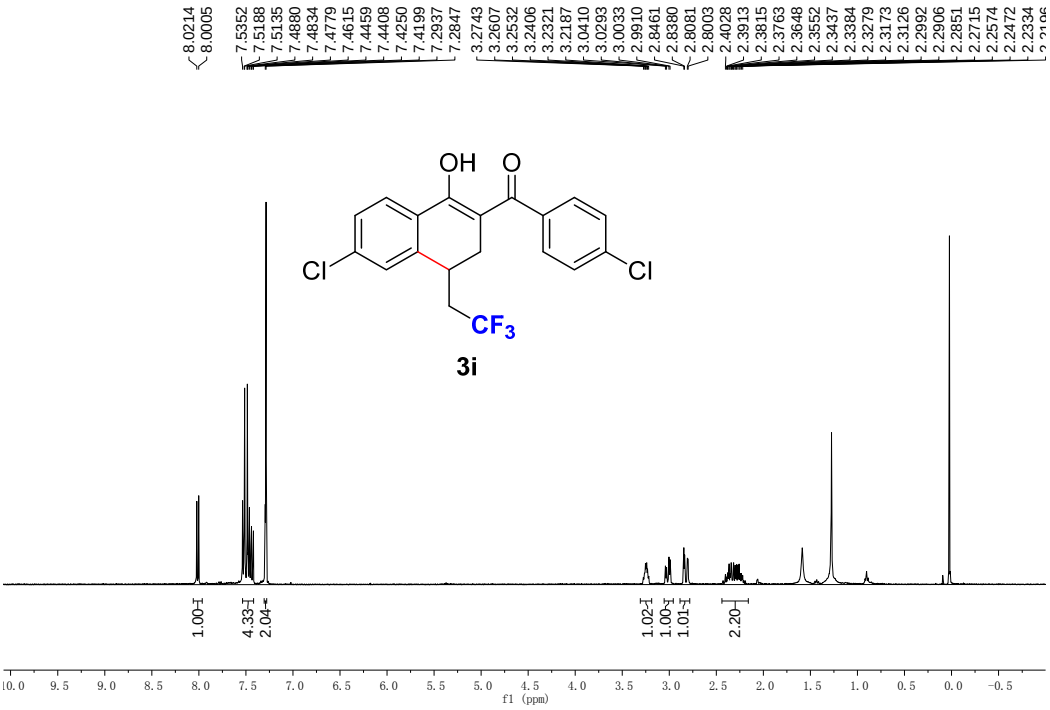
P 54 0(对氟) (ms)



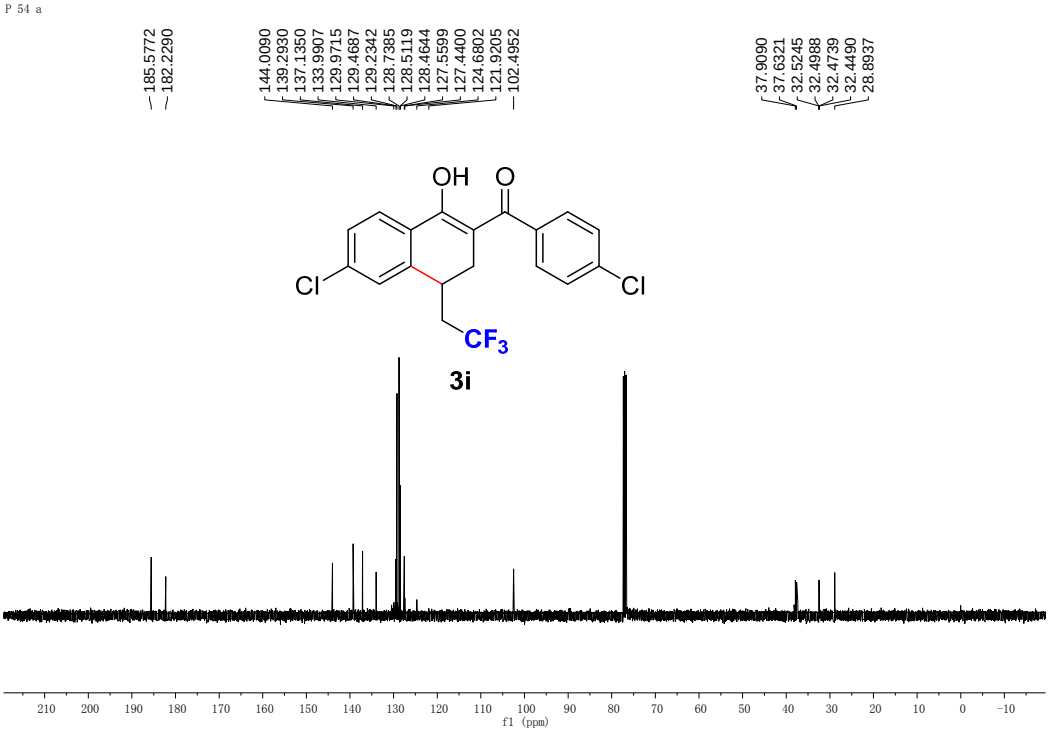
P 54 0(对氟) (ms)



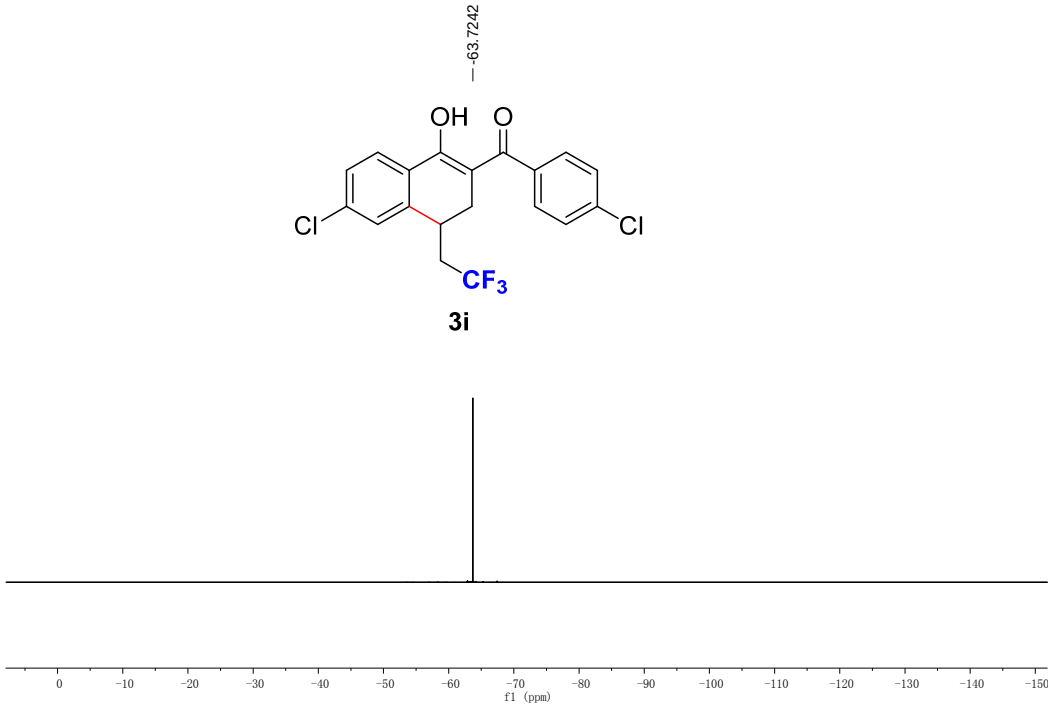
P 54 a


8.0214
8.0005
7.5352
7.5188
7.5135
7.4880
7.4834
7.4779
7.4615
7.4459
7.4408
7.4250
7.4199
7.2937
7.2847
3.2743
3.2607
3.2532
3.2406
3.2321
3.2187
3.0410
3.0293
3.0033
2.9910
2.8461
2.8380
2.8081
2.8003
2.4028
2.3913
2.3815
2.3763
2.3648
2.3552
2.3437
2.3384
2.3279
2.3173
2.3126
2.2992
2.2906
2.2851
2.2715
2.2574
2.2472
2.2334
OH
O
Cl
Cl
CF3
3i
1.00
4.33
2.04
1.02
1.00
1.01
2.20
f1 (ppm)

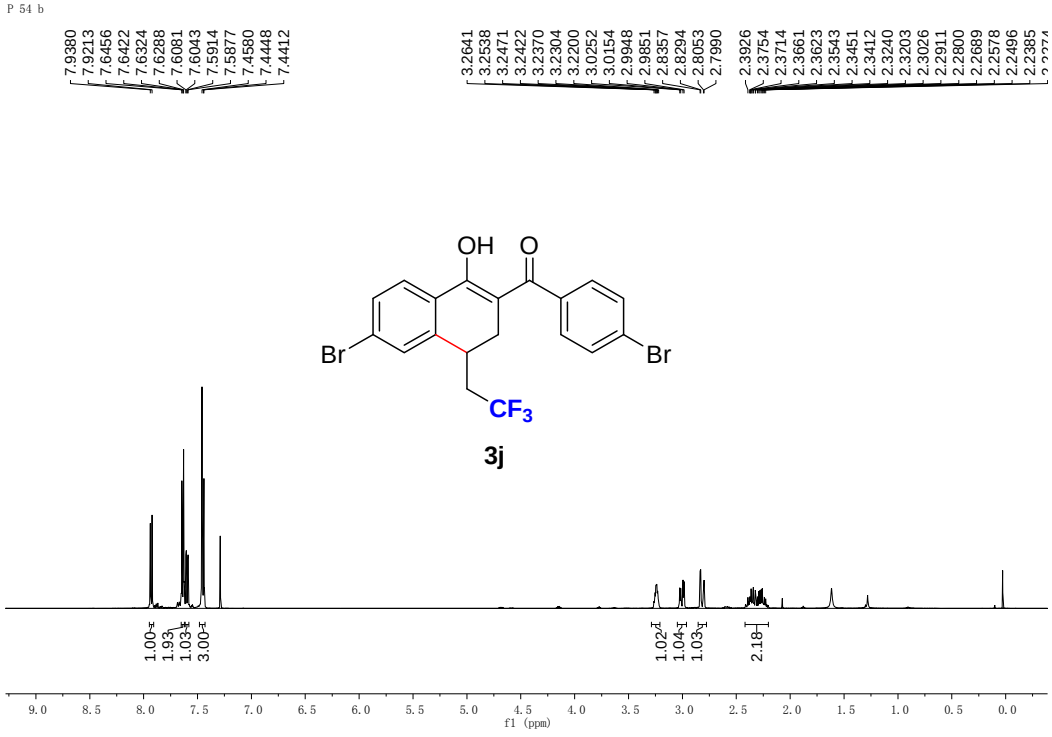
P 54 a


185.5772
182.2290
144.0090
139.2930
137.1350
133.9907
129.9715
129.4687
129.2342
128.7385
128.5119
128.4644
127.5599
127.4400
124.6802
121.9205
102.4952
37.9090
37.6321
32.5245
32.4988
32.4739
32.4490
28.8937
OH
O
Cl
Cl
CF3
3i
f1 (ppm)

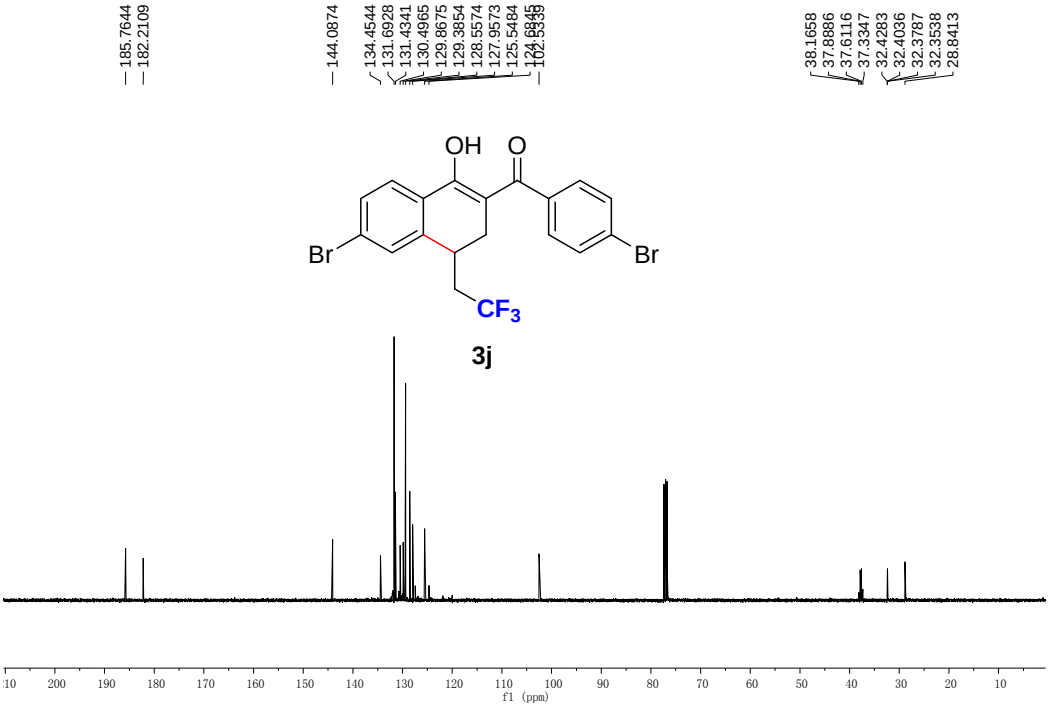
P 54 a


-63.7242
OH
O
Cl
Cl
CF3
3i
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
f1 (ppm)

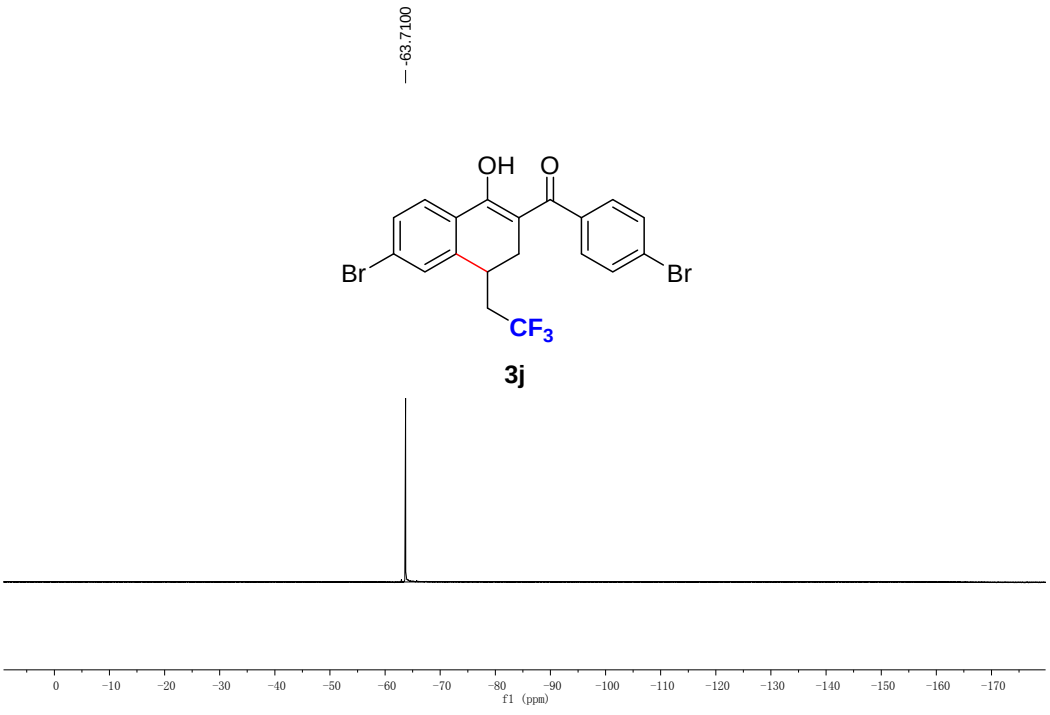
P 54 b


7.9380
7.9213
7.6456
7.6422
7.6324
7.6288
7.6081
7.6043
7.5914
7.5877
7.4580
7.4448
7.4412
3.2641
3.2538
3.2471
3.2422
3.2370
3.2304
3.2200
3.0252
3.0154
2.9948
2.9851
2.8357
2.8294
2.8053
2.7990
2.3926
2.3754
2.3714
2.3661
2.3623
2.3543
2.3451
2.3412
2.3240
2.3203
2.3026
2.2911
2.2800
2.2689
2.2578
2.2496
2.2385
OH
O
Br
Br
CF3
3j
1.00
1.93
1.03
3.00
1.02
1.04
1.03
2.18
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)

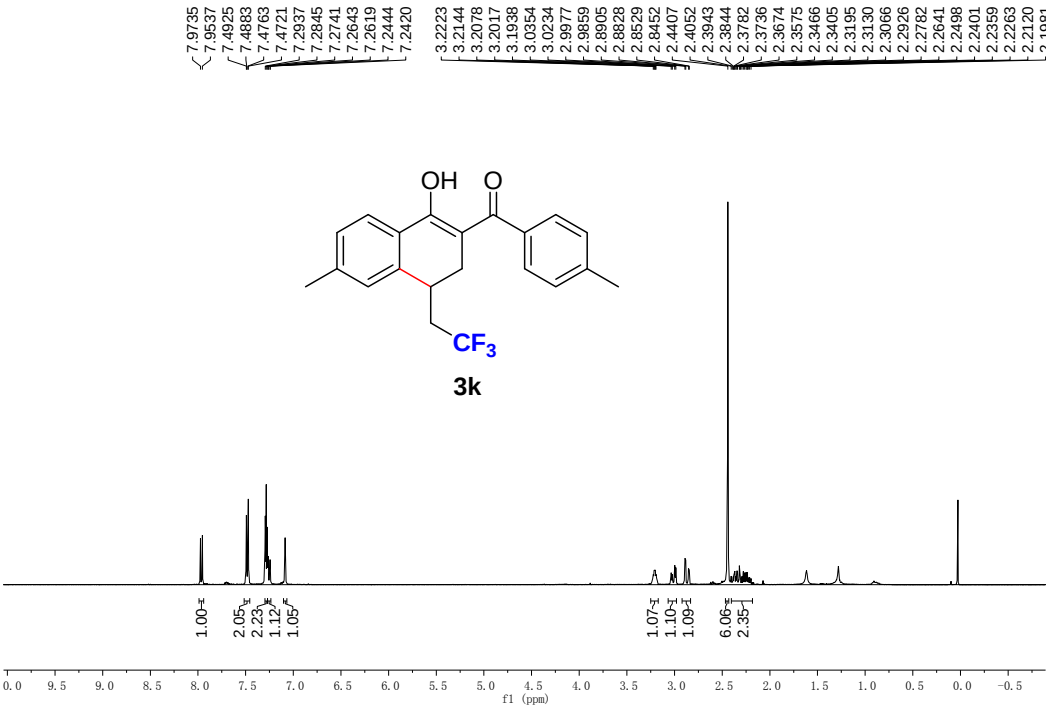
P 54 b


185.7644
182.2109
144.0874
134.4544
131.6928
131.4341
130.4965
129.8675
129.3854
128.5574
127.9573
125.5484
124.6845
102.5339
38.1658
37.8886
37.6116
37.3347
32.4283
32.4036
32.3787
32.3538
28.8413
OH
O
Br
Br
CF3
3j
f1 (ppm)

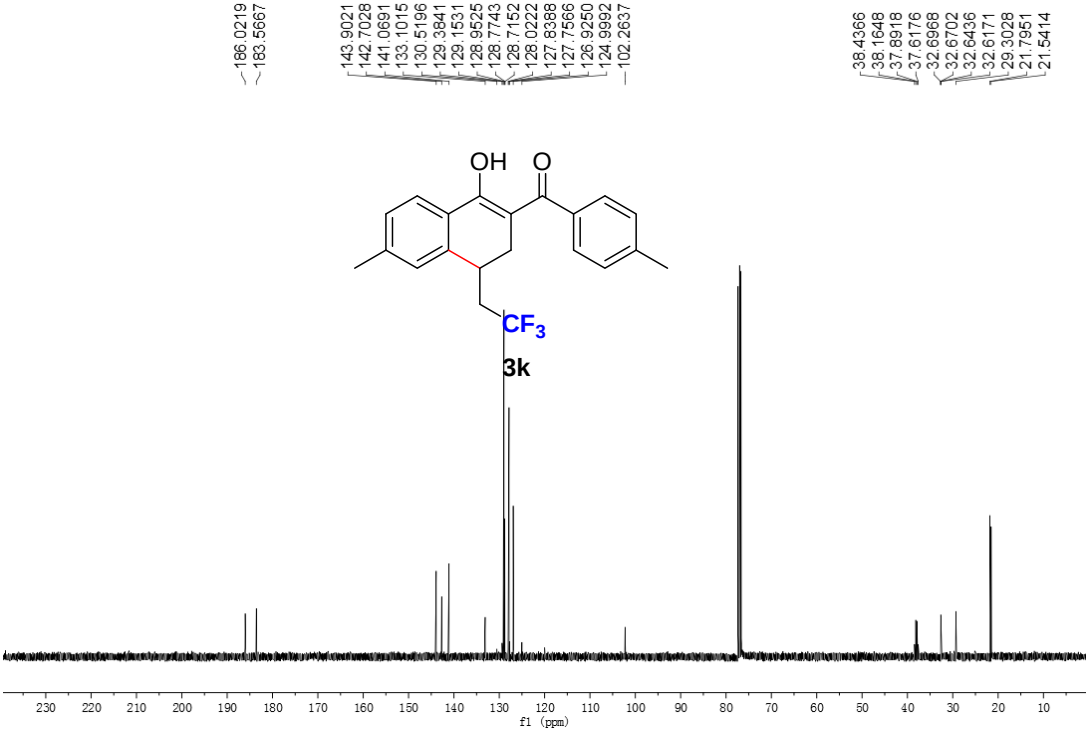
P 54 b


-63.7100
OH
O
Br
Br
CF3
3j
f1 (ppm)

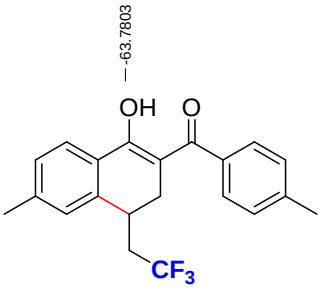
P 54 c


7.9735
7.9537
7.4925
7.4883
7.4763
7.4721
7.2937
7.2845
7.2741
7.2643
7.2619
7.2444
7.2420
3.2223
3.2144
3.2078
3.2017
3.1938
3.0354
3.0234
2.9977
2.9859
2.8905
2.8828
2.8529
2.8452
2.4407
2.4052
2.3943
2.3844
2.3782
2.3736
2.3674
2.3575
2.3466
2.3405
2.3195
2.3130
2.3066
2.2926
2.2782
2.2641
2.2498
2.2401
2.2359
2.2263
2.2120
OH
O
CF3
3k
1.00
2.05
2.23
1.12
1.05
1.07
1.10
1.09
6.06
2.35
f1 (ppm)

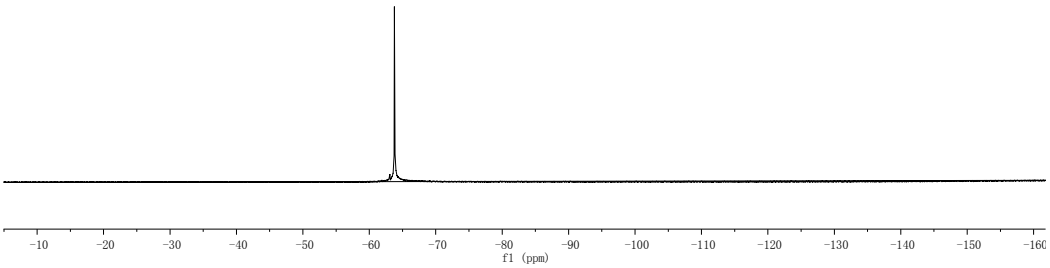
P 54 c


186.0219
183.5667
143.9021
142.7028
141.0691
133.1015
130.5196
129.3841
129.1531
128.9525
128.7743
128.7152
128.0222
127.8388
127.7566
126.9250
124.9992
102.2637
38.4366
38.1648
37.8918
37.6176
32.6968
32.6702
32.6436
32.6171
29.3028
21.7951
21.5414
OH
O
CF3
3k
f1 (ppm)

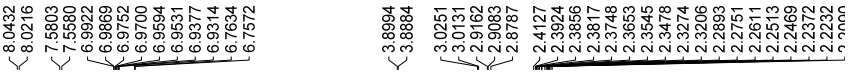
P 54 c

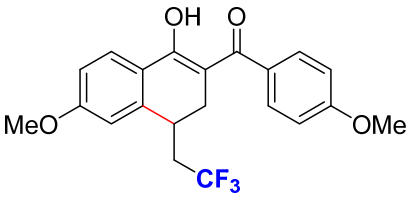


3k

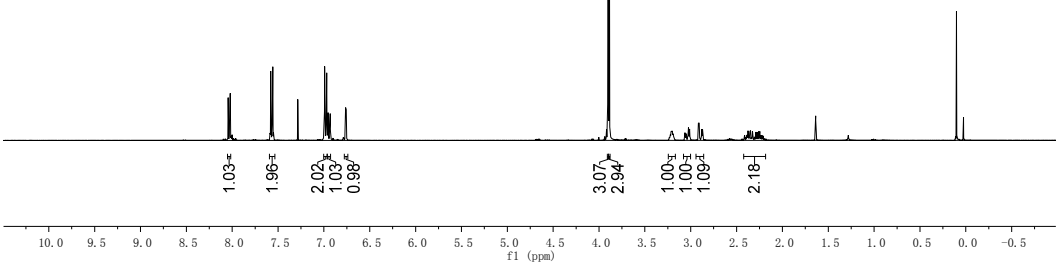


P 54 d

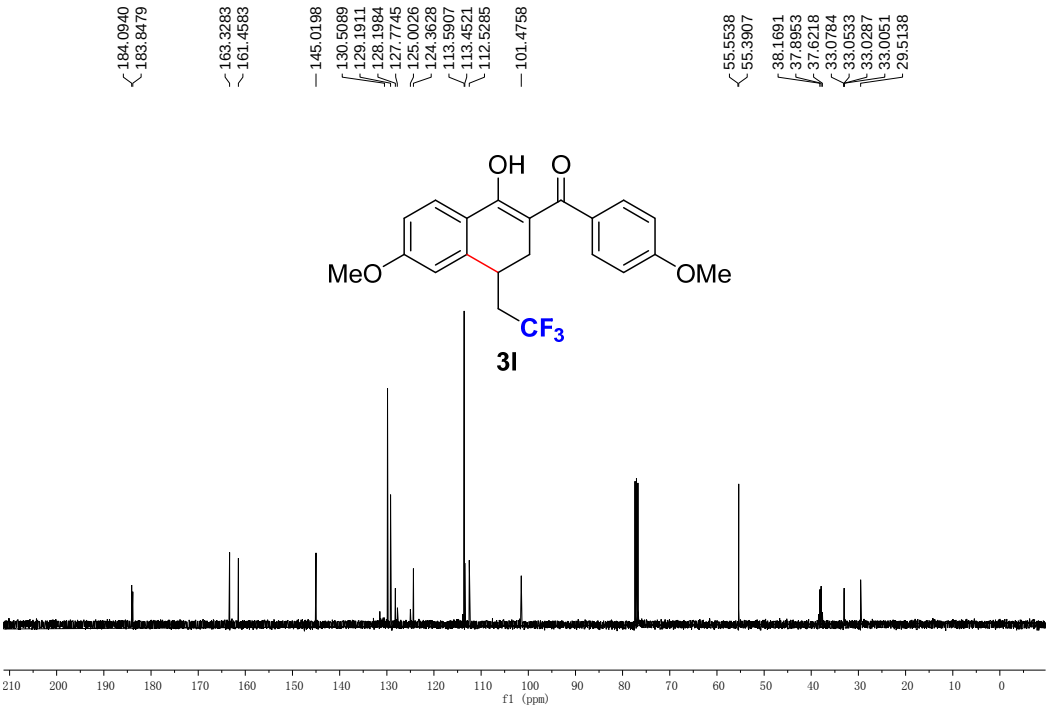




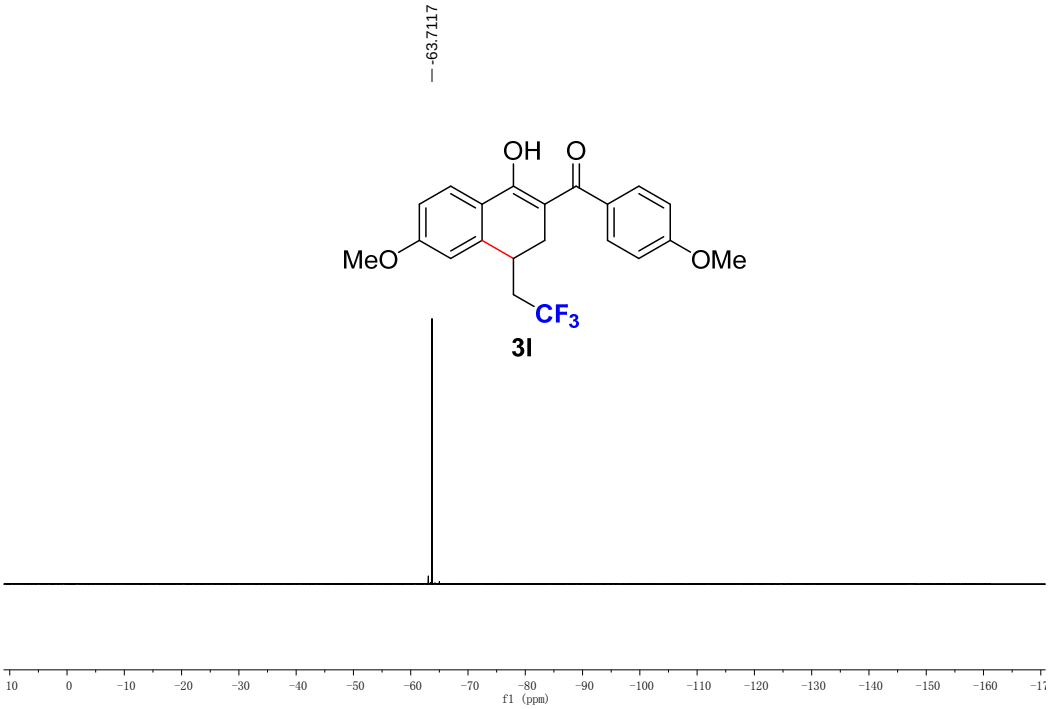
3l

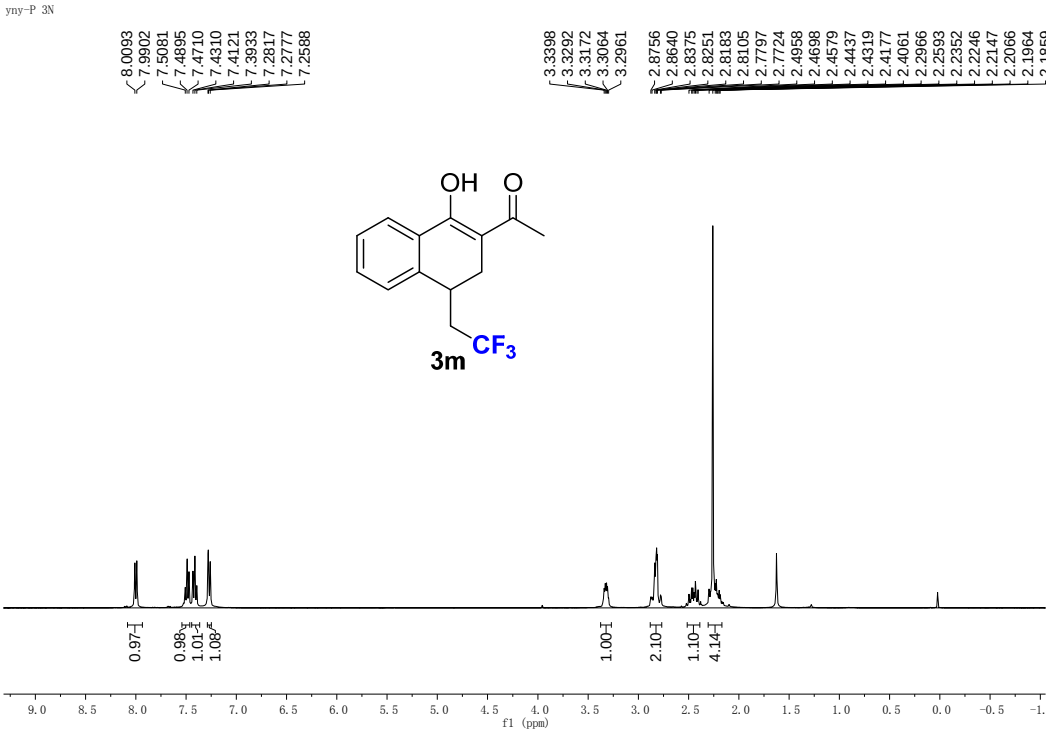


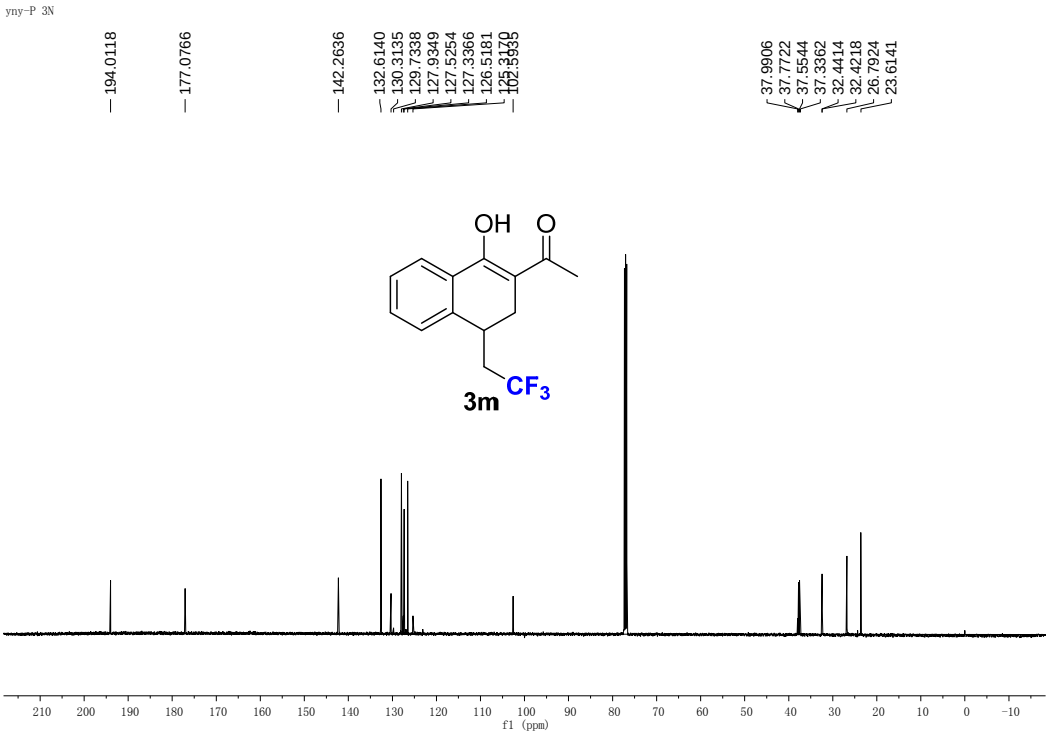
P 54 d


184.0940
183.8479
163.3283
161.4583
145.0198
130.5089
129.1911
128.1984
127.7745
125.0026
124.3628
113.5907
113.4521
112.5285
101.4758
55.5538
55.3907
38.1691
37.8953
37.6218
33.0784
33.0533
33.0287
33.0051
29.5138
OH
O
MeO
OMe
CF3
3l
f1 (ppm)

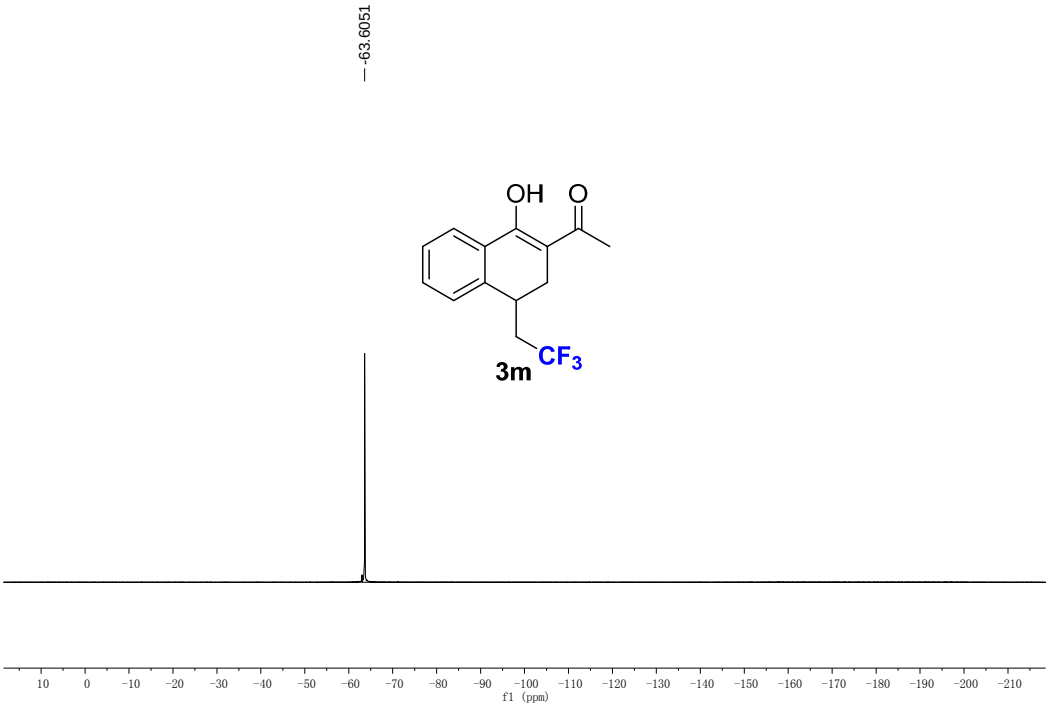
P 54 d


-63.7117
OH
O
MeO
OMe
CF3
3l
f1 (ppm)

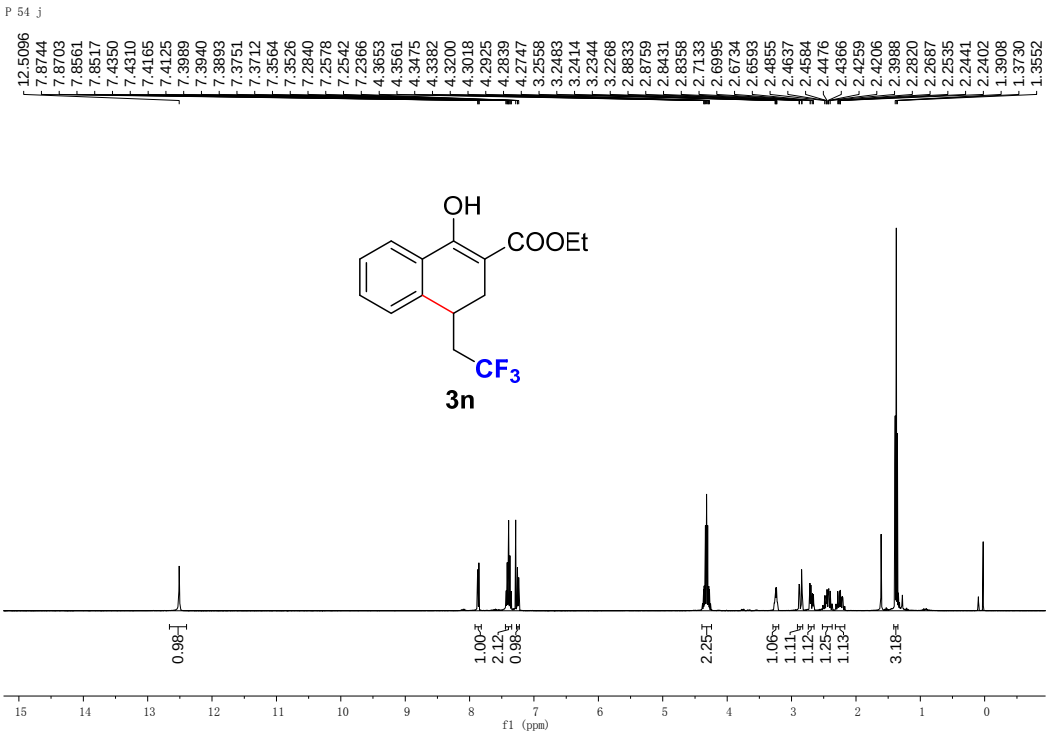

yny-P 3N
8.0093
7.9902
7.5081
7.4895
7.4710
7.4310
7.4121
7.3933
7.2817
7.2777
7.2588
3.3398
3.3292
3.3172
3.3064
3.2961
2.8756
2.8640
2.8375
2.8251
2.8183
2.8105
2.7797
2.7724
2.4958
2.4698
2.4579
2.4437
2.4319
2.4177
2.4061
2.2966
2.2593
2.2352
2.2246
2.2147
2.2066
2.1964
OH
O
CF3
3m
0.97
0.98
1.01
1.08
1.00
2.10
1.10
4.14
f1 (ppm)


yny-P 3N
194.0118
177.0766
142.2636
132.6140
130.3135
129.7338
127.9349
127.5254
127.3366
126.5181
125.3170
102.5935
37.9906
37.7722
37.5544
37.3362
32.4414
32.4218
26.7924
23.6141
OH
O
CF3
3m
f1 (ppm)

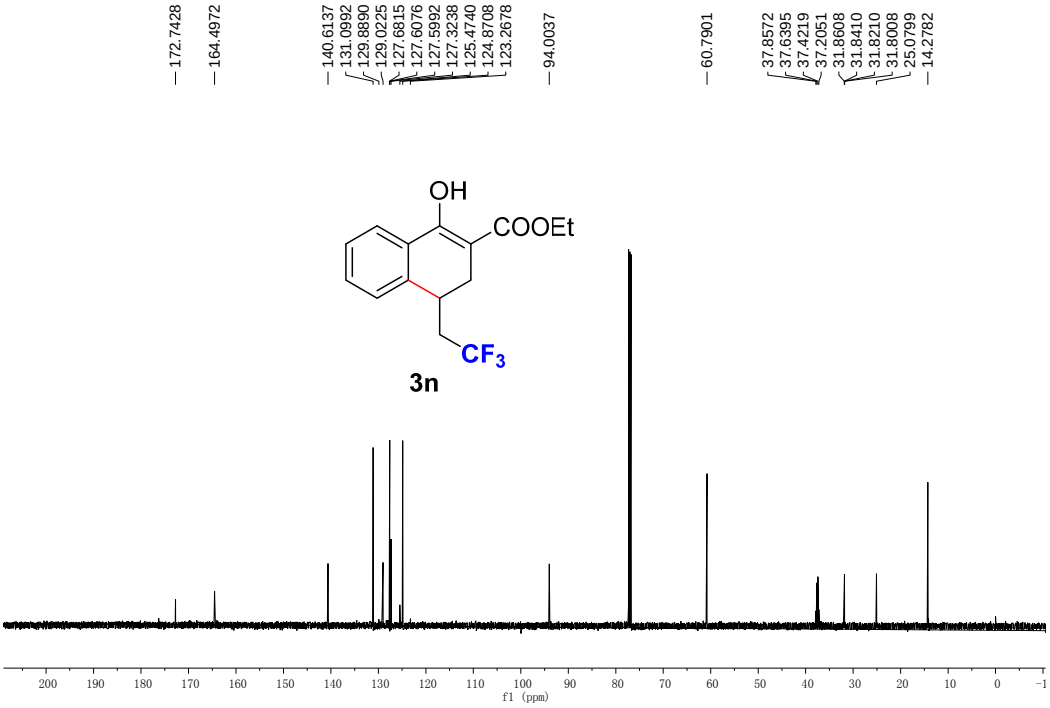
yny-P 3N


-63.6051
OH
O
CF3
3m
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

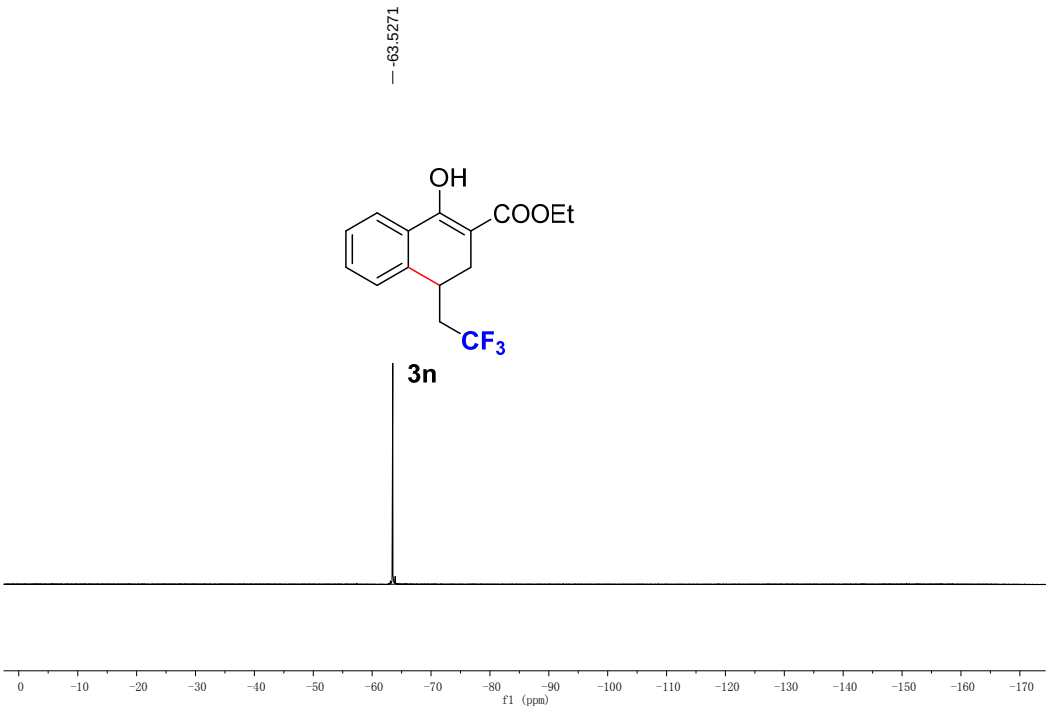
P 54 j

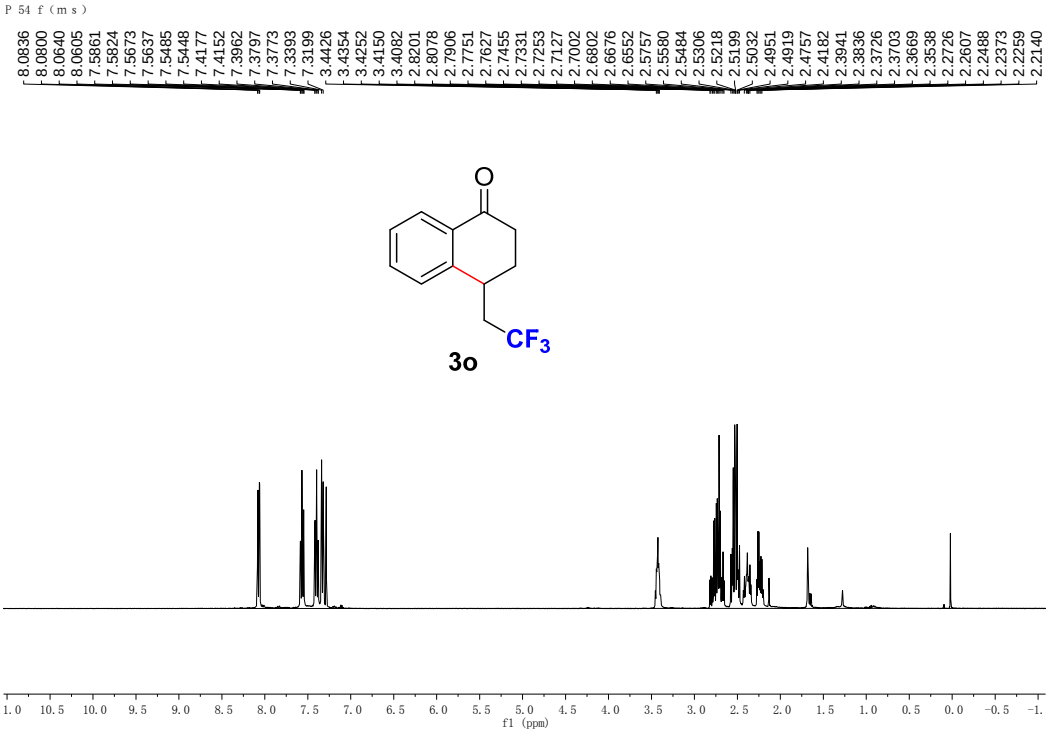

12.5096
7.8744
7.8703
7.8561
7.8517
7.4350
7.4310
7.4165
7.4125
7.3989
7.3940
7.3893
7.3751
7.3712
7.3564
7.3526
7.2840
7.2578
7.2542
7.2366
4.3653
4.3561
4.3475
4.3382
4.3200
4.3018
4.2925
4.2839
4.2747
3.2558
3.2483
3.2414
3.2344
3.2268
2.8833
2.8759
2.8431
2.8358
2.7133
2.6995
2.6734
2.6593
2.4855
2.4637
2.4584
2.4476
2.4366
2.4259
2.4206
2.3988
2.2820
2.2687
2.2535
2.2441
2.2402
1.3908
1.3730
1.3552
OH
COOEt
CF3
3n
0.98
1.00
2.12
0.98
2.25
1.06
1.11
1.12
1.25
1.13
3.18
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

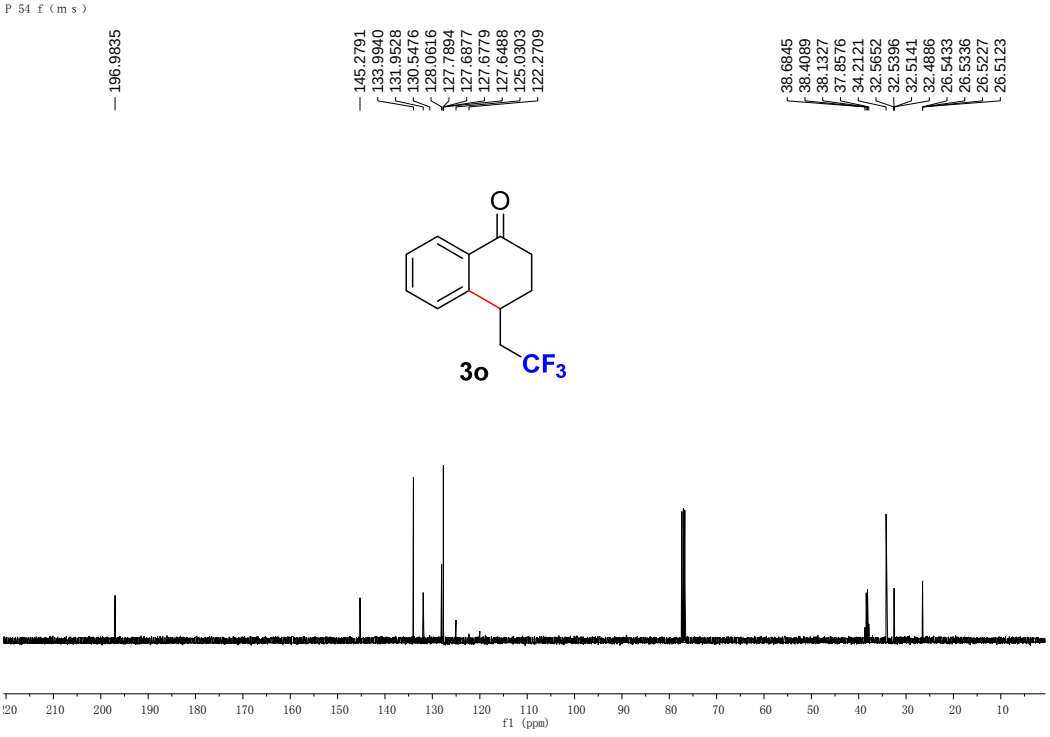
P 54 j


172.7428
164.4972
140.6137
131.0992
129.8890
129.0225
127.6815
127.6076
127.5992
127.3238
125.4740
124.8708
123.2678
94.0037
60.7901
37.8572
37.6395
37.4219
37.2051
31.8608
31.8410
31.8210
31.8008
25.0799
14.2782
OH
COOEt
CF3
3n
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

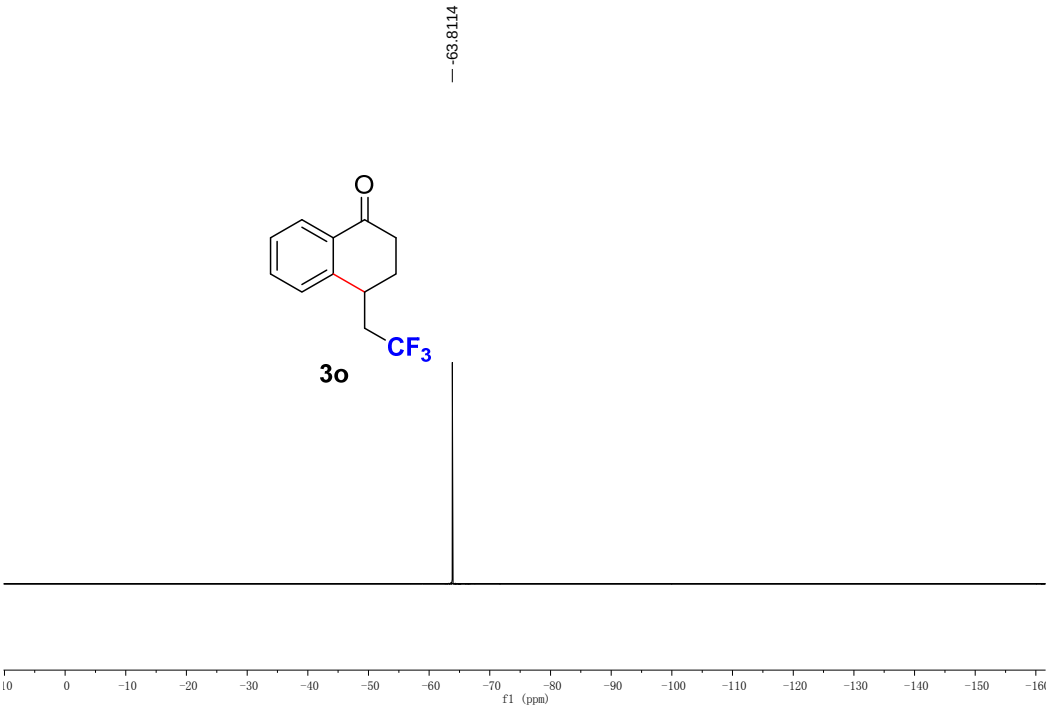
P 54 j


-63.5271
OH
COOEt
CF3
3n
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170
f1 (ppm)

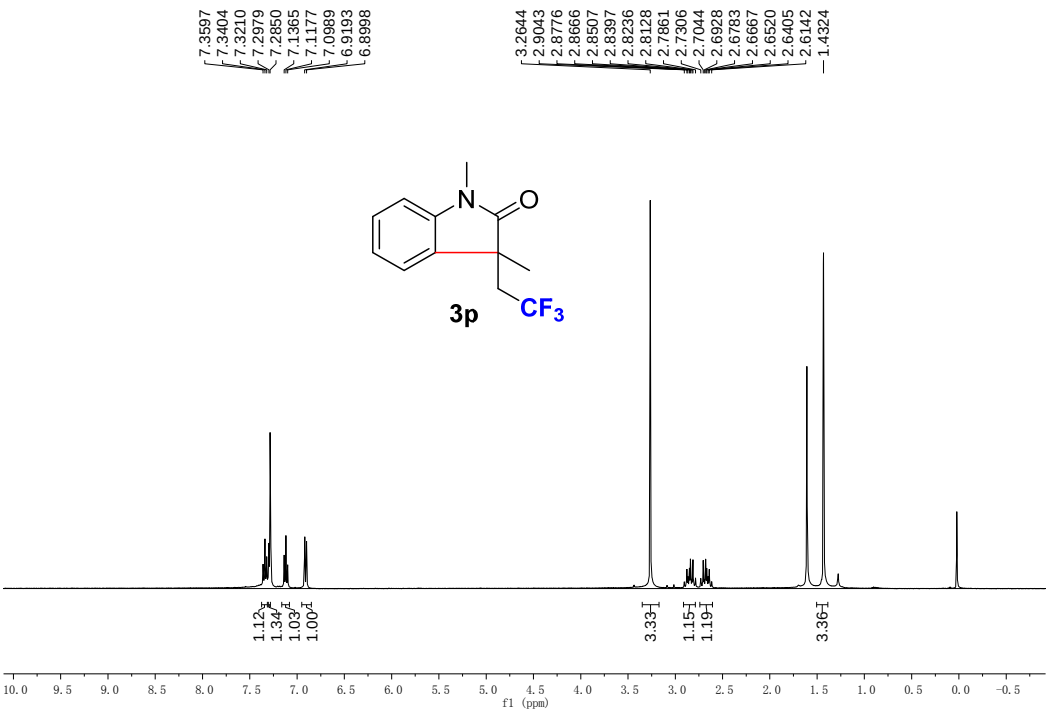

P 54 f (m s)
8.0836
8.0800
8.0640
8.0605
7.5861
7.5824
7.5673
7.5637
7.5485
7.5448
7.4177
7.4152
7.3962
7.3797
7.3773
7.3393
7.3199
3.4426
3.4354
3.4252
3.4150
3.4082
2.8201
2.8078
2.7906
2.7751
2.7627
2.7455
2.7331
2.7253
2.7127
2.7002
2.6802
2.6676
2.6552
2.5757
2.5580
2.5484
2.5306
2.5218
2.5199
2.5032
2.4951
2.4919
2.4757
2.4182
2.3941
2.3836
2.3726
2.3703
2.3669
2.3538
2.2726
2.2607
2.2488
2.2373
2.2259
2.2140
O
CF3
3o
1.0
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
−0.5
−1.
f1 (ppm)

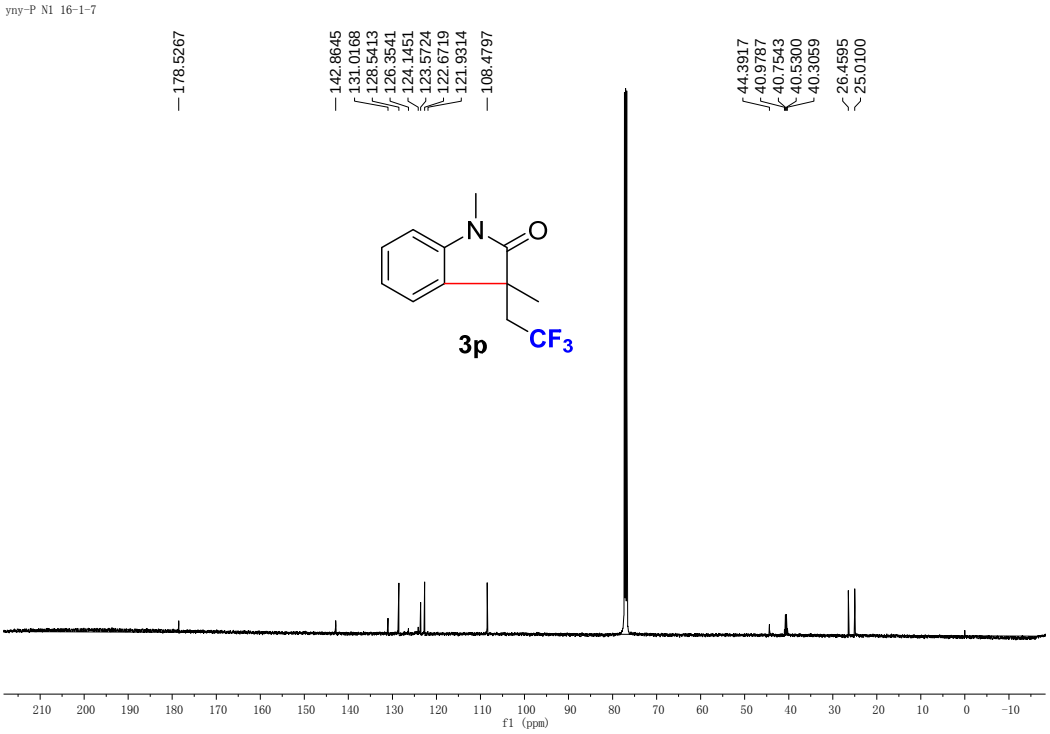

P 54 f (m s)
196.9835
145.2791
133.9940
131.9528
130.5476
128.0616
127.7894
127.6877
127.6779
127.6488
125.0303
122.2709
38.6845
38.4089
38.1327
37.8576
34.2121
32.5652
32.5396
32.5141
32.4886
26.5433
26.5336
26.5227
26.5123
O
CF3
3o
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

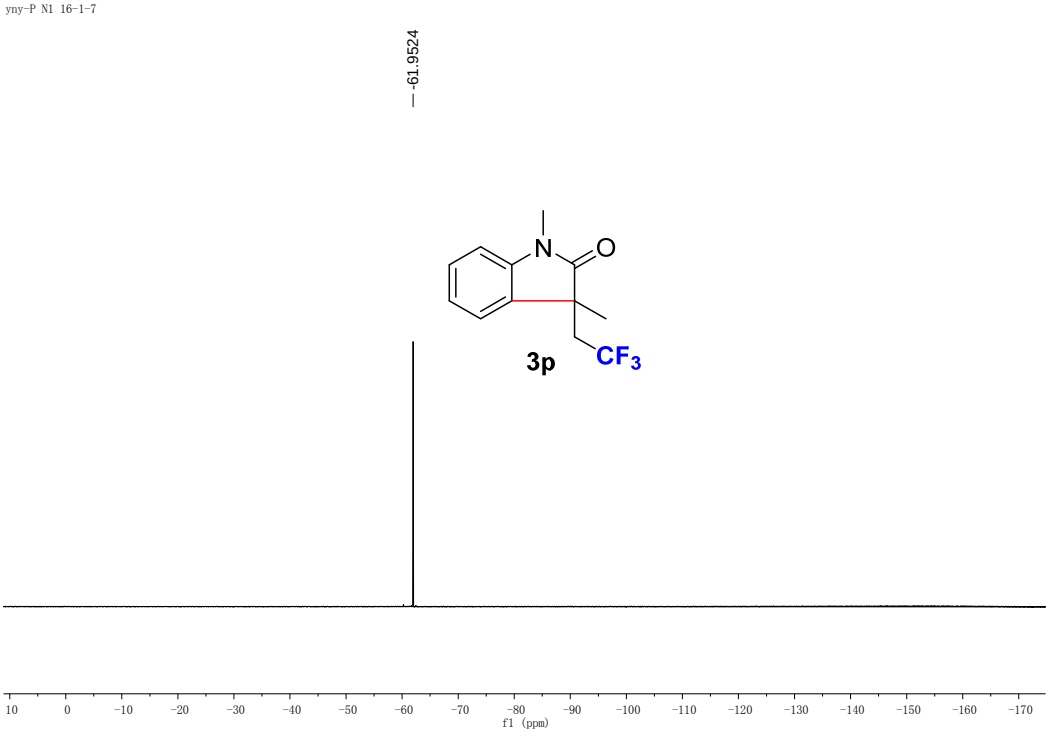
P 54 f (m s)

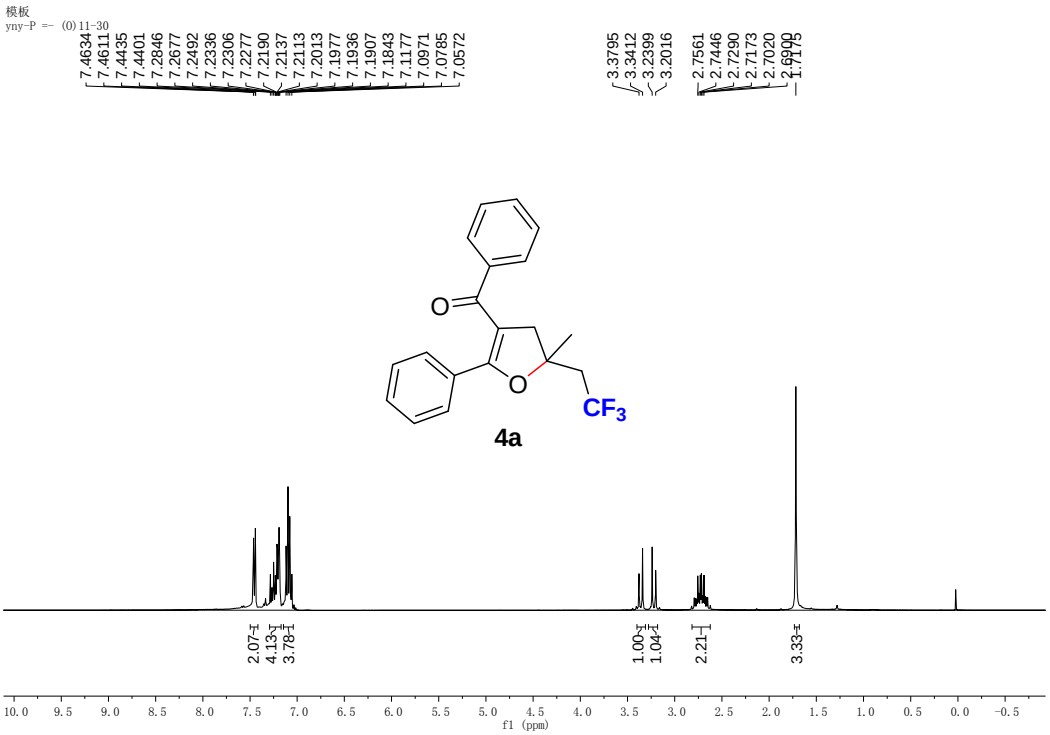


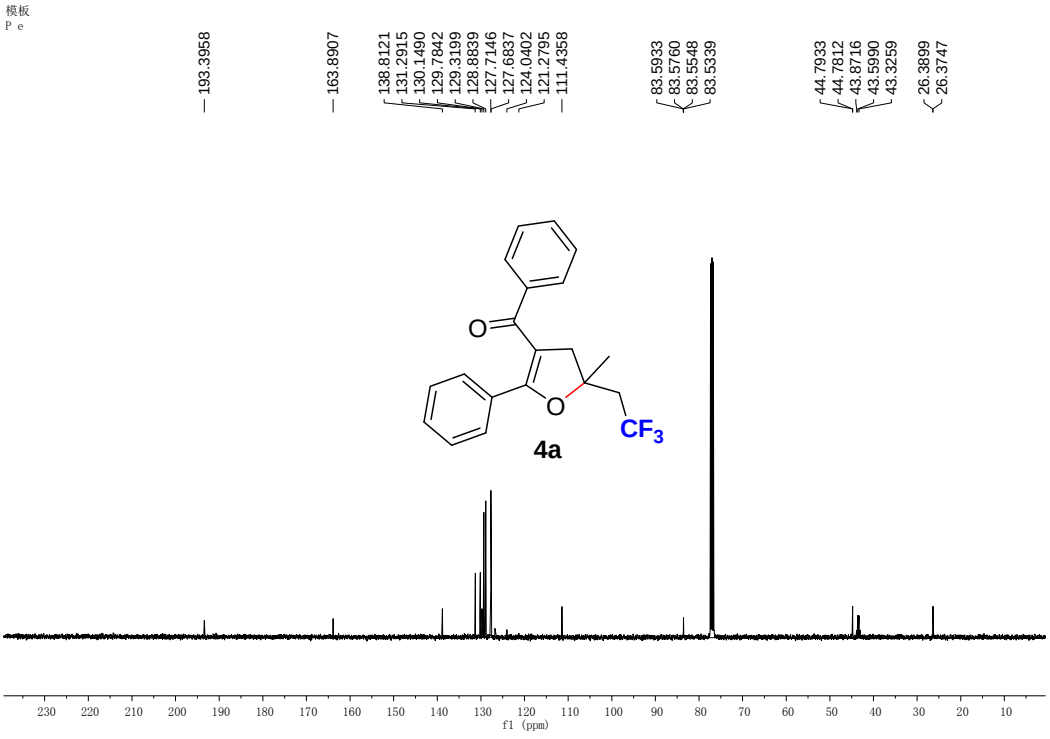
yny-P N1 16-1-7



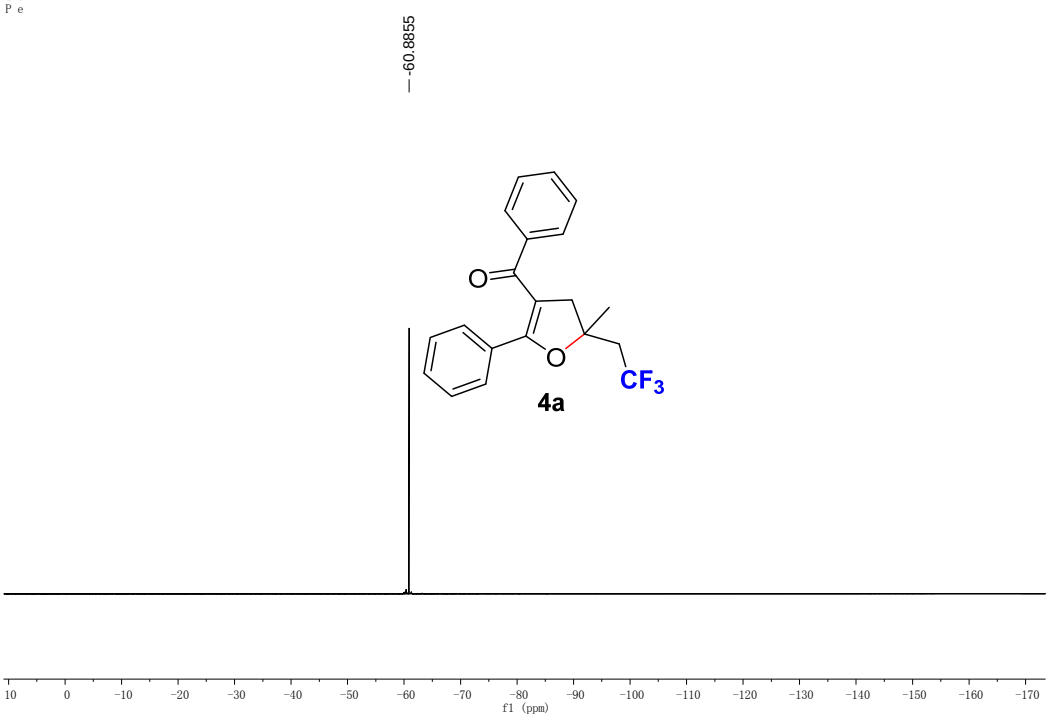

yny-P N1 16-1-7
178.5267
142.8645
131.0168
128.5413
126.3541
124.1451
123.5724
122.6719
121.9314
108.4797
44.3917
40.9787
40.7543
40.5300
40.3059
26.4595
25.0100
N
O
3p
CF3
f1 (ppm)


yny-P N1 16-1-7
-61.9524
N
O
3p
CF3
f1 (ppm)

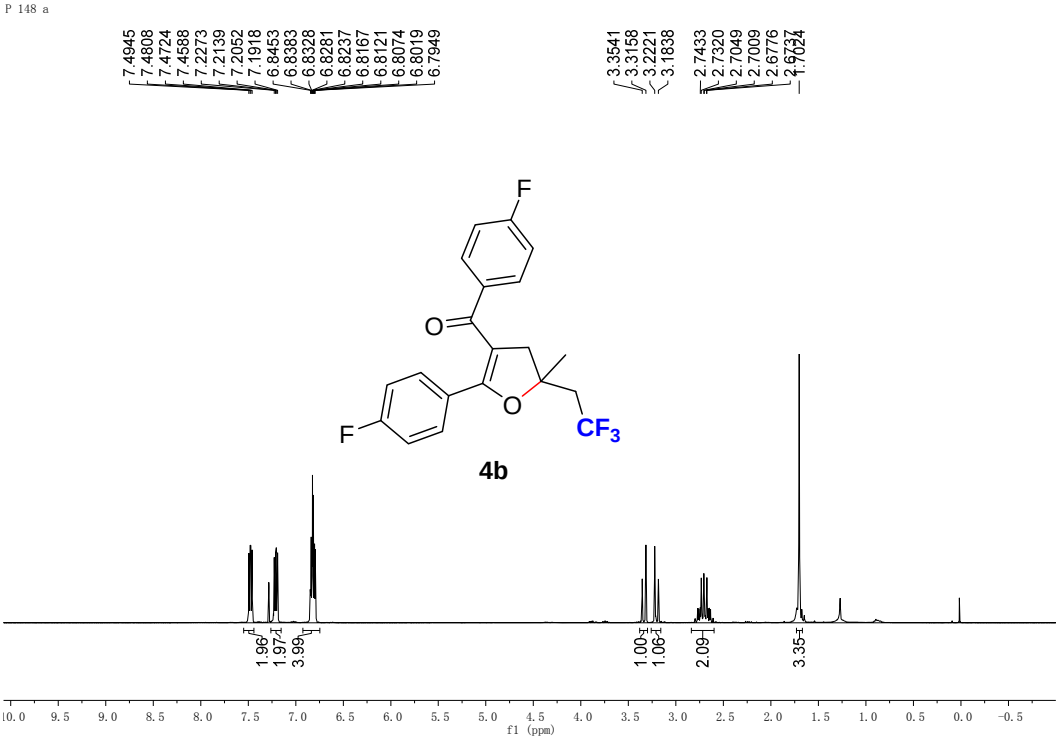

模板
yny-P =- (0) 11-30
7.4634
7.4611
7.4435
7.4401
7.2846
7.2677
7.2492
7.2336
7.2306
7.2277
7.2190
7.2137
7.2113
7.2013
7.1977
7.1936
7.1907
7.1843
7.1177
7.0971
7.0785
7.0572
3.3795
3.3412
3.2399
3.2016
2.7561
2.7446
2.7290
2.7173
2.7020
2.6900
1.7175
O
O
CF3
4a
2.07
4.13
3.78
1.00
1.04
2.21
3.33
10.0 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)


模板
P e
193.3958
163.8907
138.8121
131.2915
130.1490
129.7842
129.3199
128.8839
127.7146
127.6837
124.0402
121.2795
111.4358
83.5933
83.5760
83.5548
83.5339
44.7933
44.7812
43.8716
43.5990
43.3259
26.3899
26.3747
O
O
CF3
4a
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

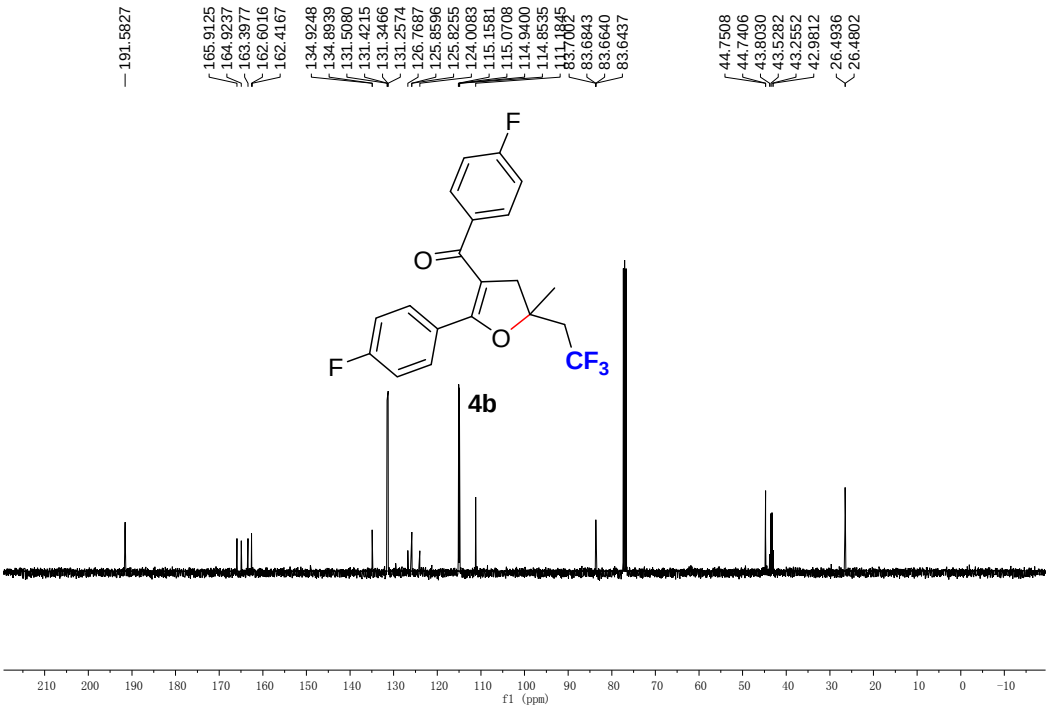
模板
P e


-60.8855
O
O
CF3
4a
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170
f1 (ppm)

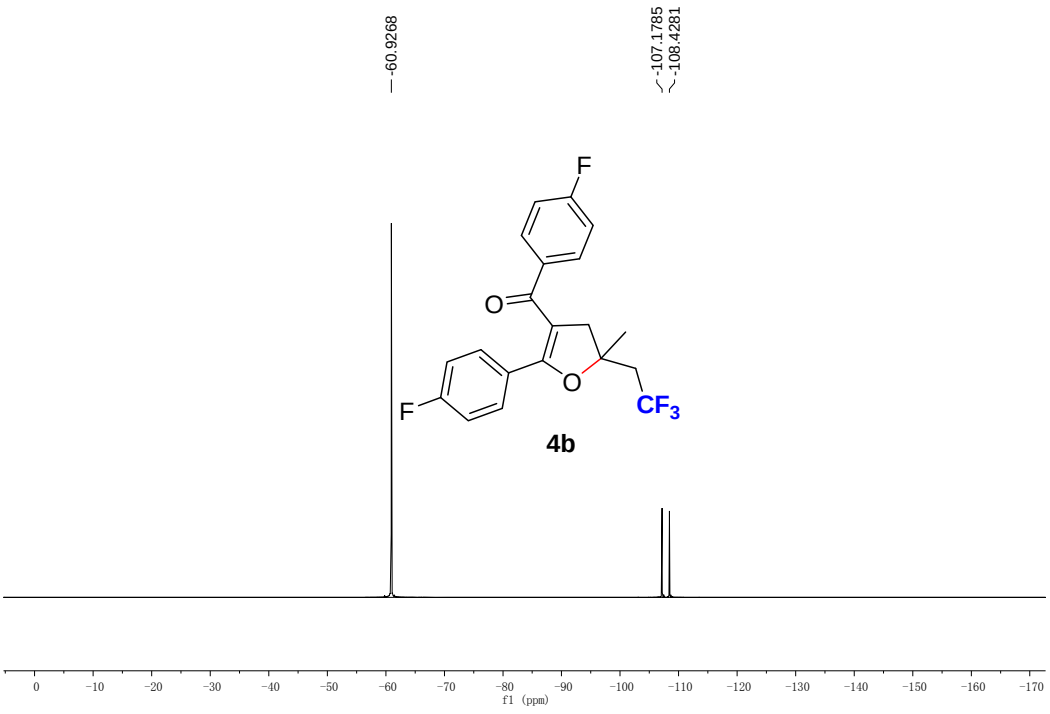
P 148 a

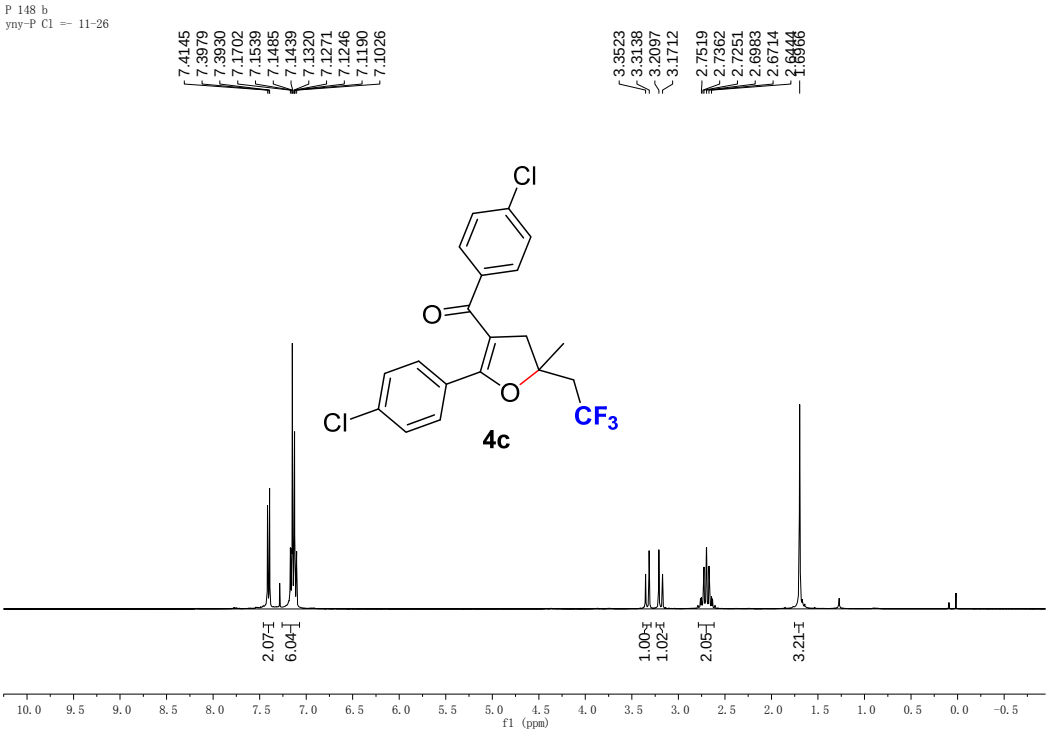

7.4945
7.4808
7.4724
7.4588
7.2273
7.2139
7.2052
7.1918
6.8453
6.8383
6.8328
6.8281
6.8237
6.8167
6.8121
6.8074
6.8019
6.7949
3.3541
3.3158
3.2221
3.1838
2.7433
2.7320
2.7049
2.7009
2.6776
1.7024
F
O
O
F
CF3
4b
1.96
1.97
3.99
1.00
1.06
2.09
3.35
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

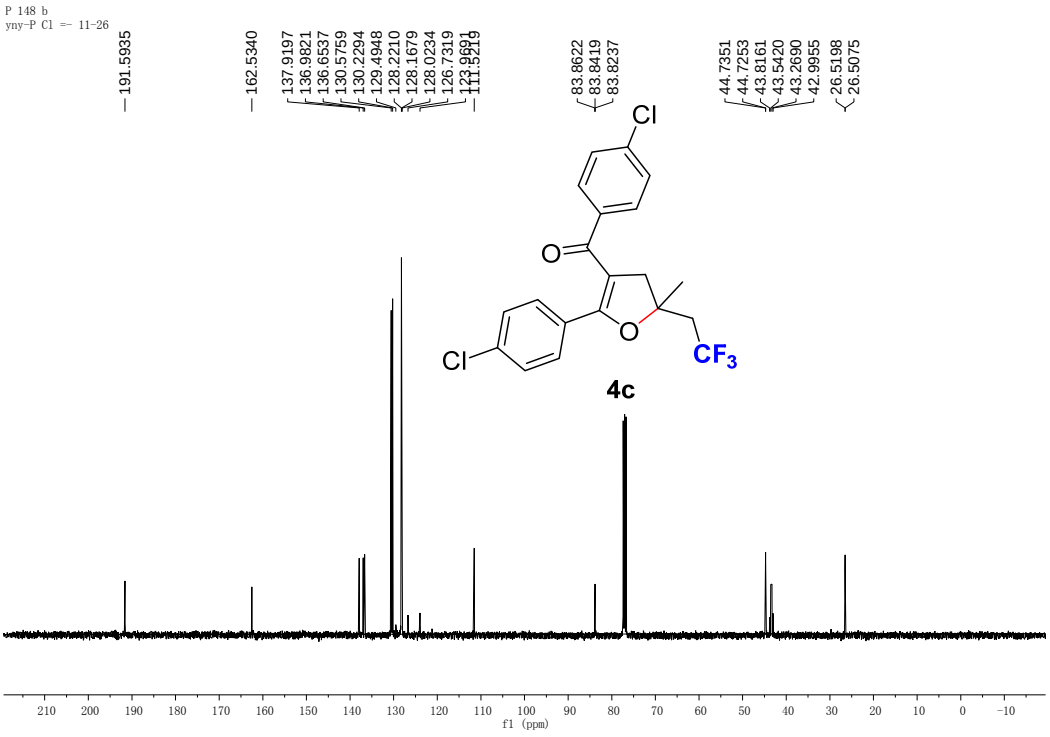
P 148 a


191.5827
165.9125
164.9237
163.3977
162.6016
162.4167
134.9248
134.8939
131.5080
131.4215
131.3466
131.2574
126.7687
125.8596
125.8255
124.0083
115.1581
115.0708
114.9400
114.8535
111.1845
83.7002
83.6843
83.6640
83.6437
44.7508
44.7406
43.8030
43.5282
43.2552
42.9812
26.4936
26.4802
F
O
O
F
CF3
4b
f1 (ppm)

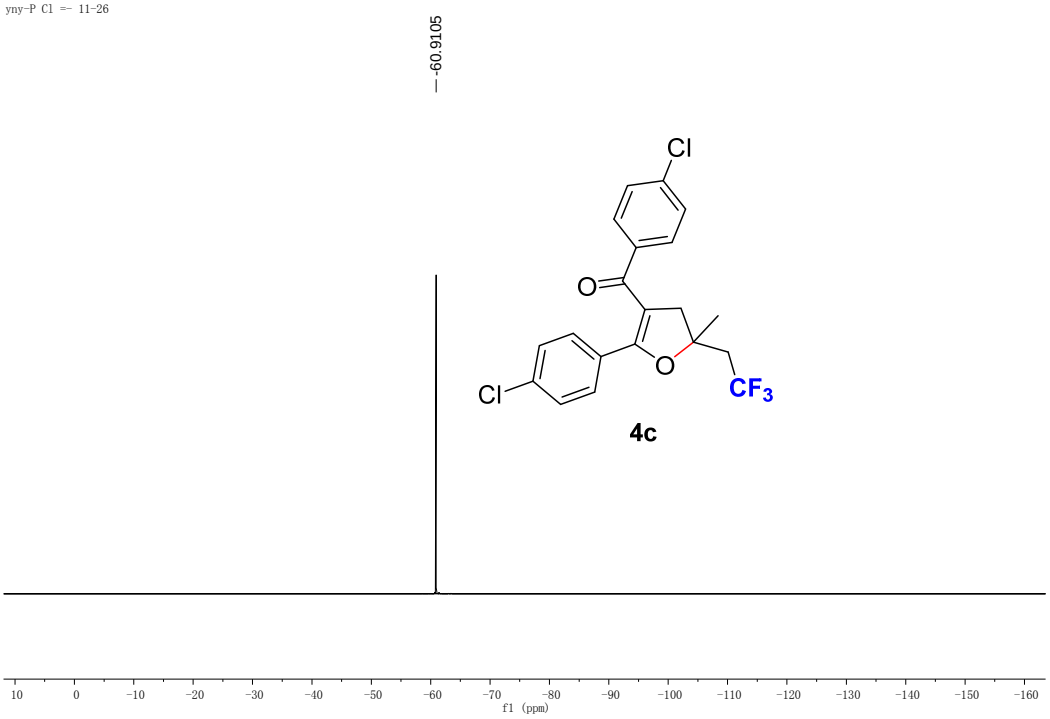
P 148 a


-60.9268
-107.1785
-108.4281
F
O
O
F
CF3
4b
f1 (ppm)

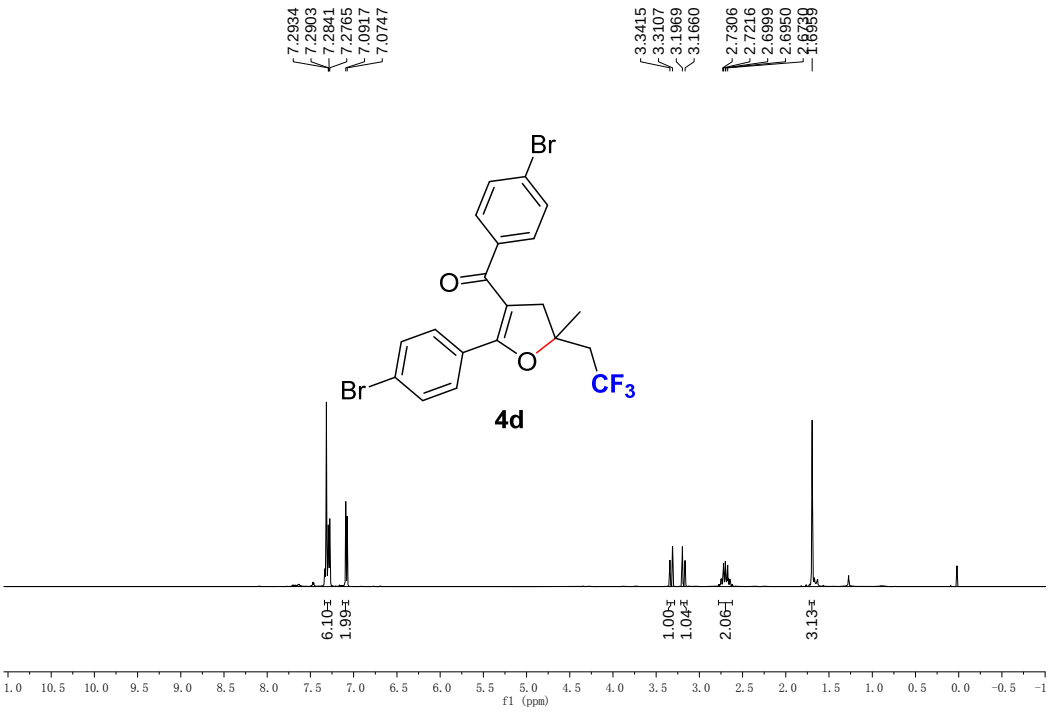

P 148 b
yny-P Cl =- 11-26
7.4145
7.3979
7.3930
7.1702
7.1539
7.1485
7.1439
7.1320
7.1271
7.1246
7.1190
7.1026
3.3523
3.3138
3.2097
3.1712
2.7519
2.7362
2.7251
2.6983
2.6714
1.6966
Cl
O
O
Cl
CF3
4c
2.07
6.04
1.00
1.02
2.05
3.21
f1 (ppm)


P 148 b
yny-P Cl =- 11-26
191.5935
162.5340
137.9197
136.9821
136.6537
130.5759
130.2294
129.4948
128.2210
128.1679
128.0234
126.7319
123.9601
111.9219
83.8622
83.8419
83.8237
44.7351
44.7253
43.8161
43.5420
43.2690
42.9955
26.5198
26.5075
Cl
O
O
Cl
CF3
4c
f1 (ppm)

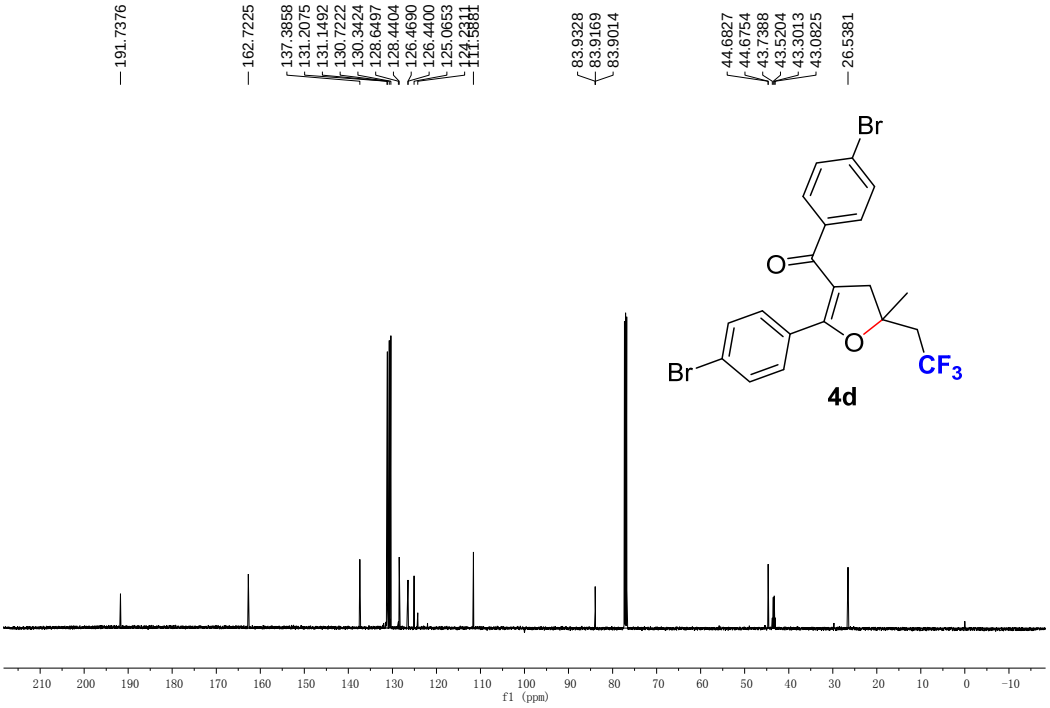
P 148 b
yny-P Cl =- 11-26



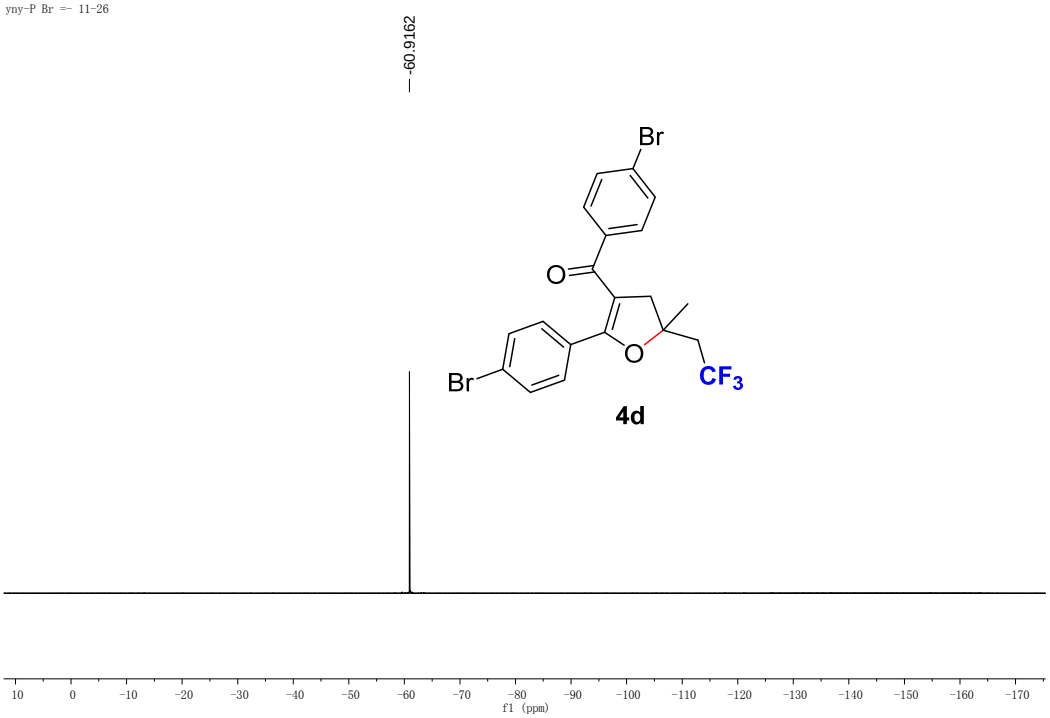
P 148 c



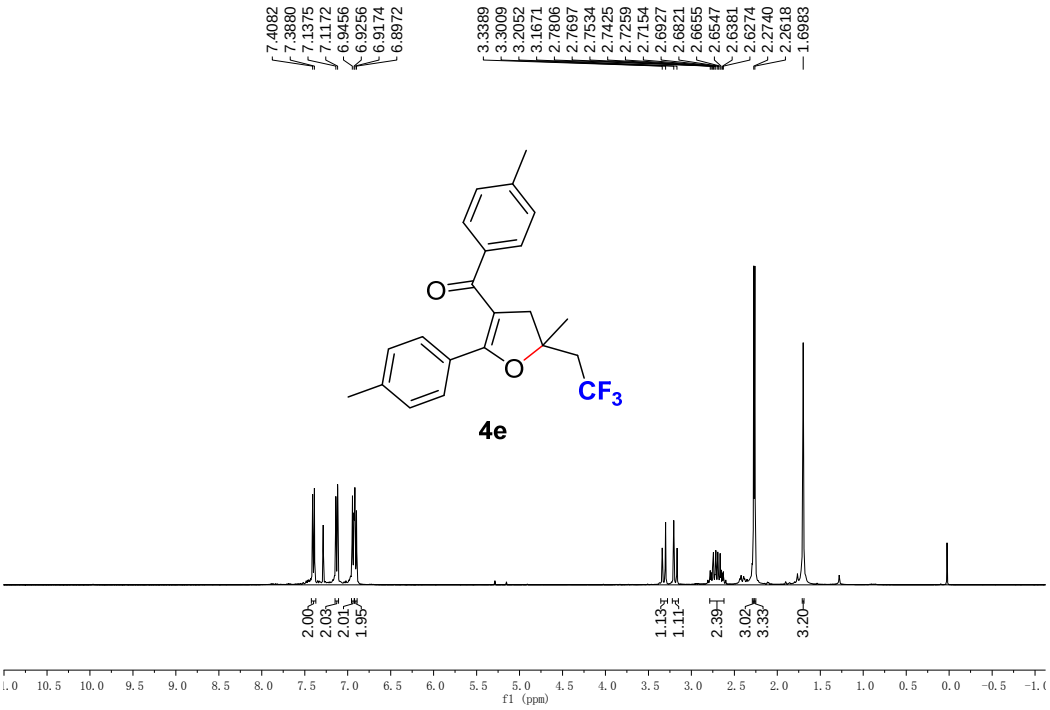
P 148 c



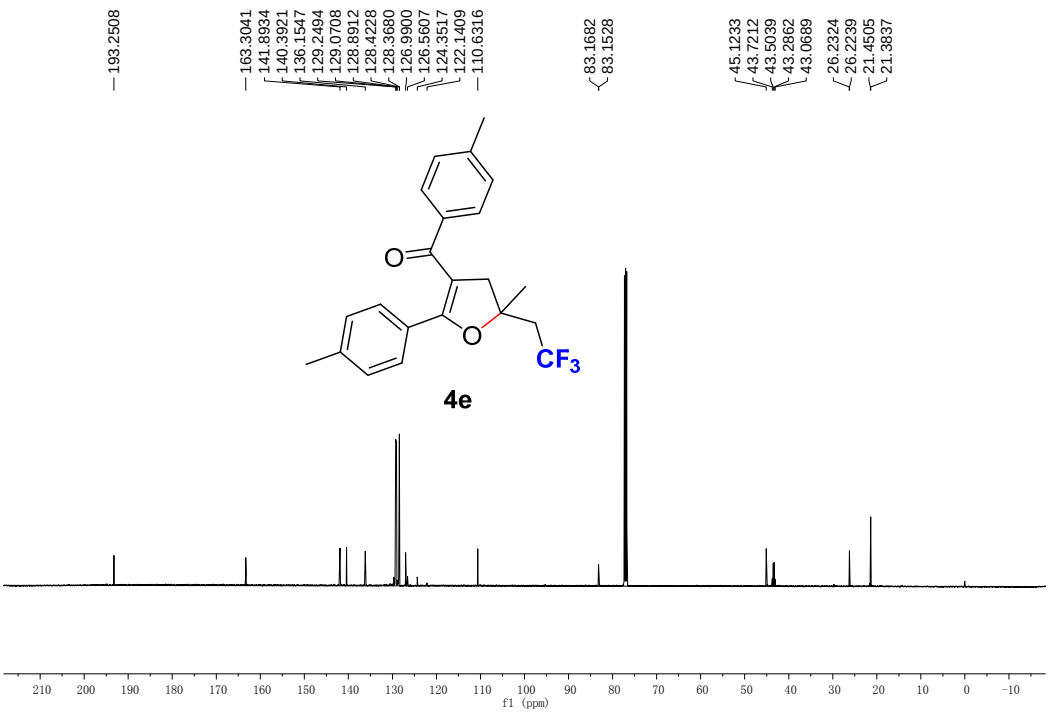
P 148 c
yny-P Br =- 11-26



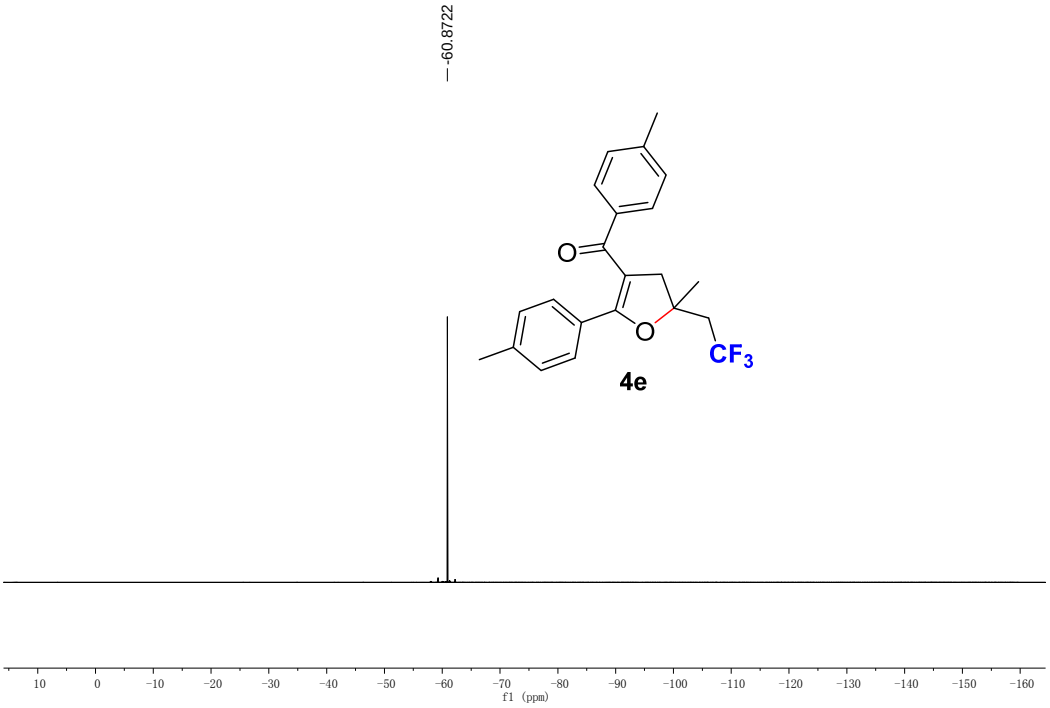
P 148 d


7.4082
7.3880
7.1375
7.1172
6.9456
6.9256
6.9174
6.8972
3.3389
3.3009
3.2052
3.1671
2.7806
2.7697
2.7534
2.7425
2.7259
2.7154
2.6927
2.6821
2.6655
2.6547
2.6381
2.6274
2.2740
2.2618
1.6983
O
O
CF3
4e
2.00
2.03
2.01
1.95
1.13
1.11
2.39
3.02
3.33
3.20
f1 (ppm)

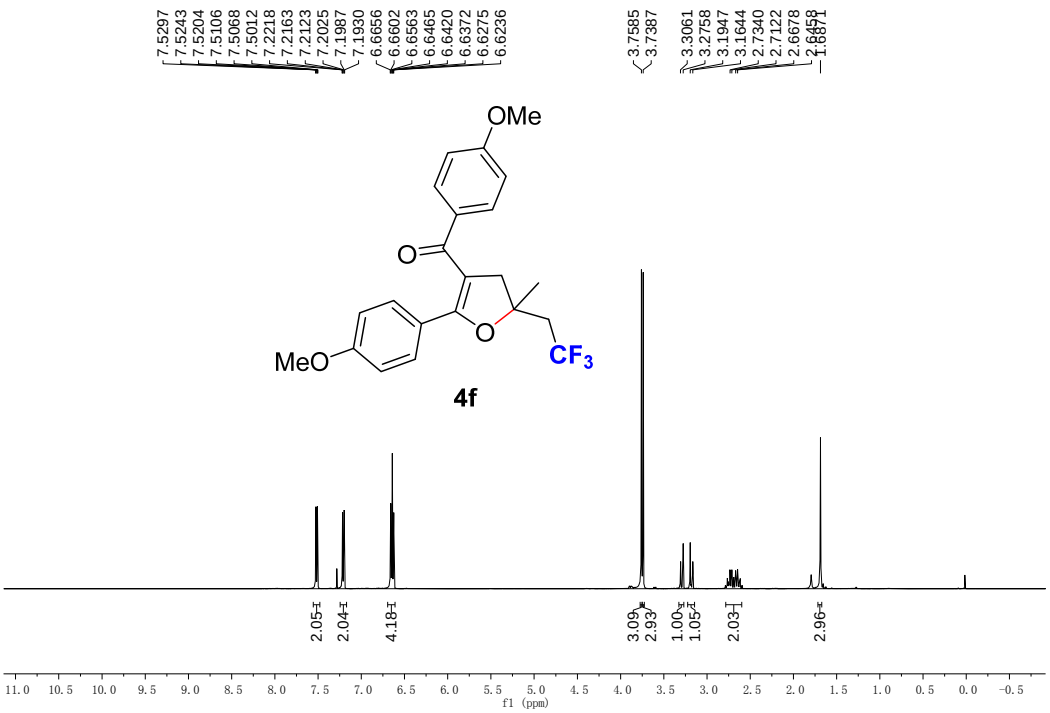
P 148 d


193.2508
163.3041
141.8934
140.3921
136.1547
129.2494
129.0708
128.8912
128.4228
128.3680
126.9900
126.5607
124.3517
122.1409
110.6316
83.1682
83.1528
45.1233
43.7212
43.5039
43.2862
43.0689
26.2324
26.2239
21.4505
21.3837
O
O
CF3
4e
f1 (ppm)

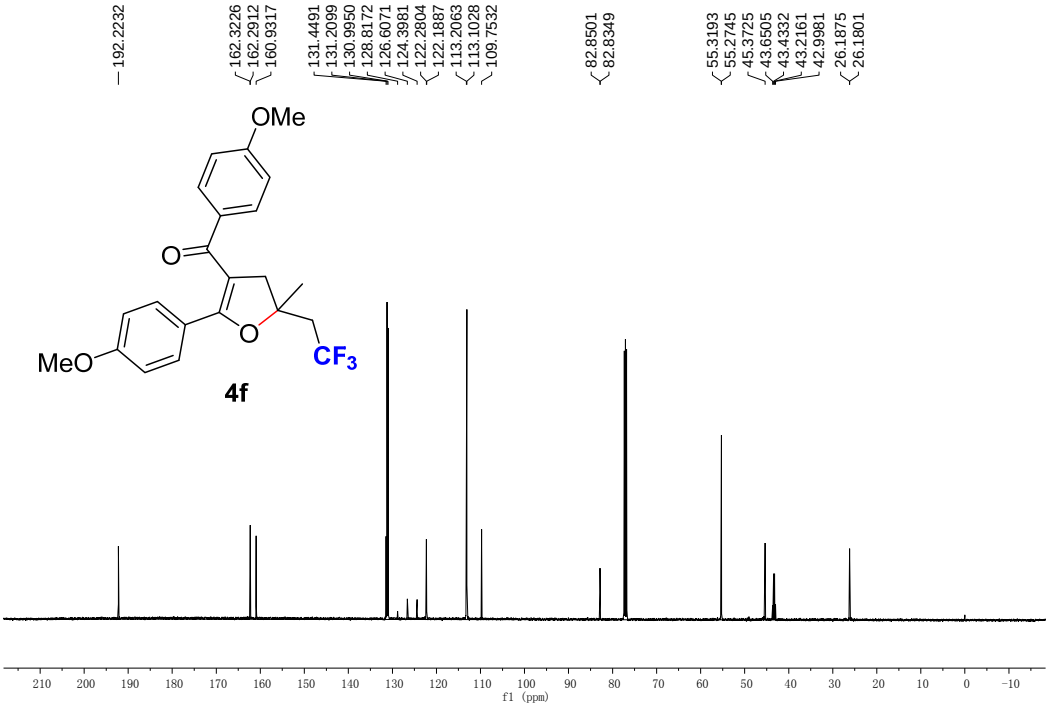
P 148 d


-60.8722
O
O
CF3
4e
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
f1 (ppm)

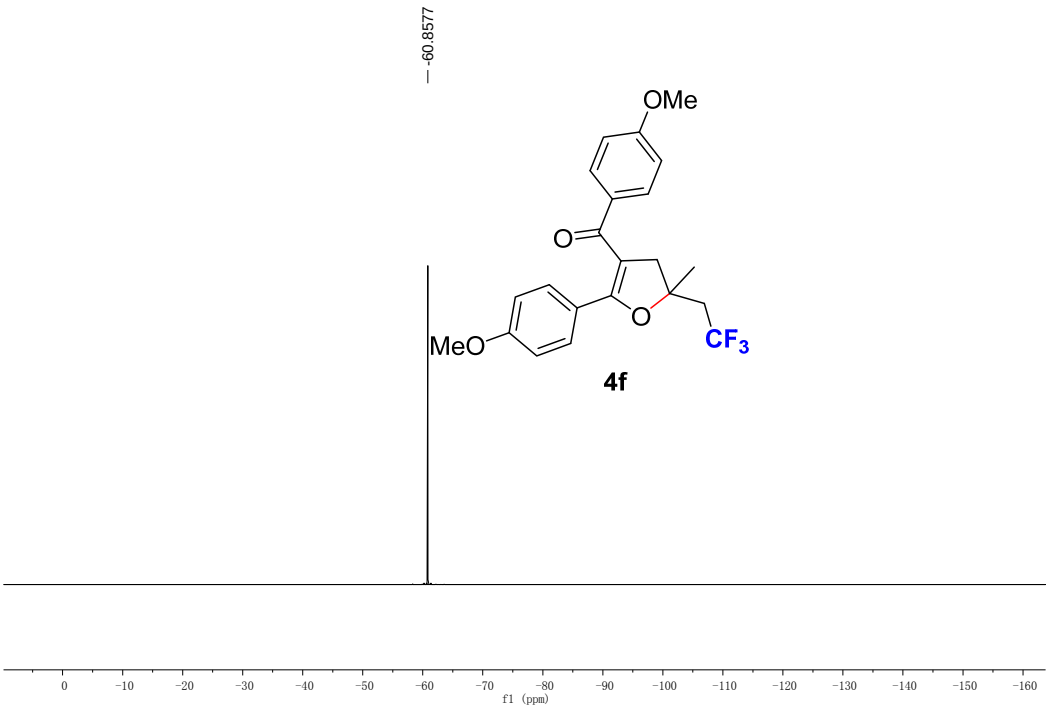
P 148 e

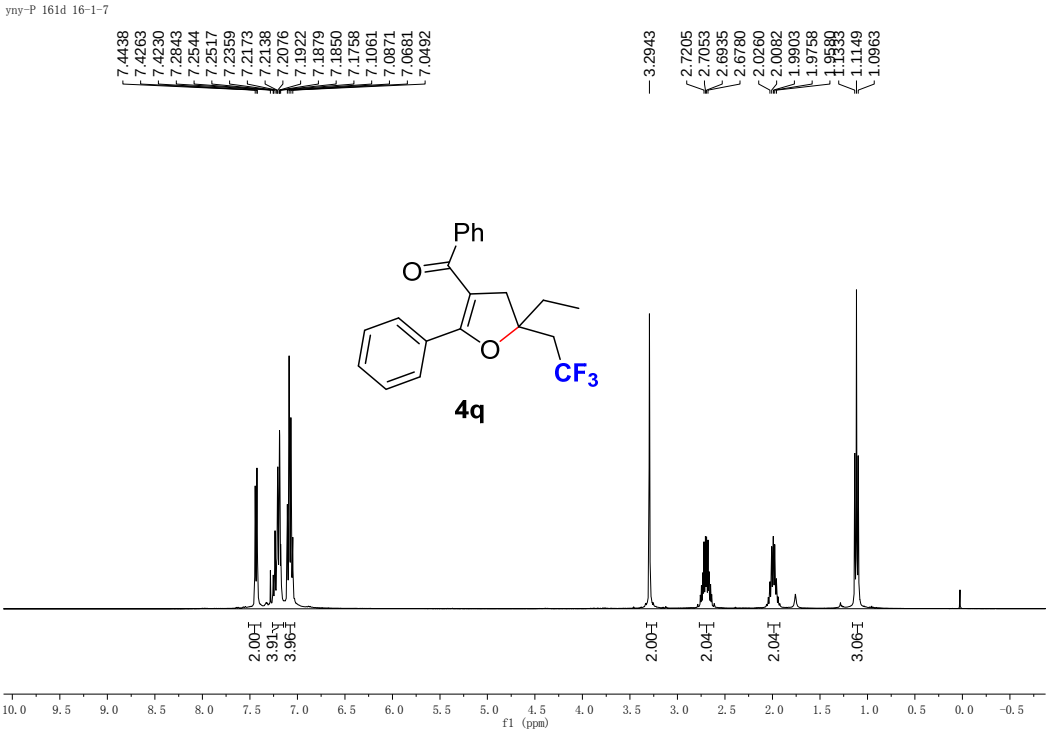

7.5297
7.5243
7.5204
7.5106
7.5068
7.5012
7.2218
7.2163
7.2123
7.2025
7.1987
7.1930
6.6656
6.6602
6.6563
6.6465
6.6420
6.6372
6.6275
6.6236
3.7585
3.7387
3.3061
3.2758
3.1947
3.1644
2.7340
2.7122
2.6678
2.6458
1.6871
OMe
O
O
MeO
CF3
4f
2.05
2.04
4.18
3.09
2.93
1.00
1.05
2.03
2.96
11.0
10.5
10.0
9.5
9.0
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
−0.5
f1 (ppm)

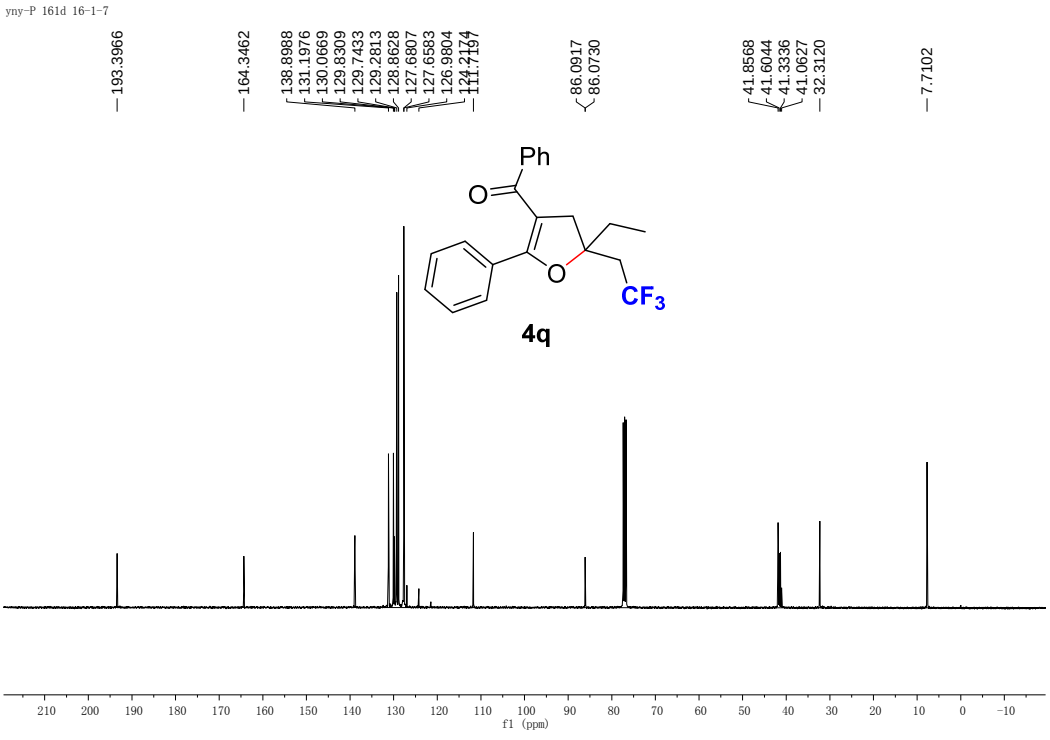
P 148 e


192.2232
162.3226
162.2912
160.9317
131.4491
131.2099
130.9950
128.8172
126.6071
124.3981
122.2804
122.1887
113.2063
113.1028
109.7532
82.8501
82.8349
55.3193
55.2745
45.3725
43.6505
43.4332
43.2161
42.9981
26.1875
26.1801
OMe
O
MeO
O
CF3
4f
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)

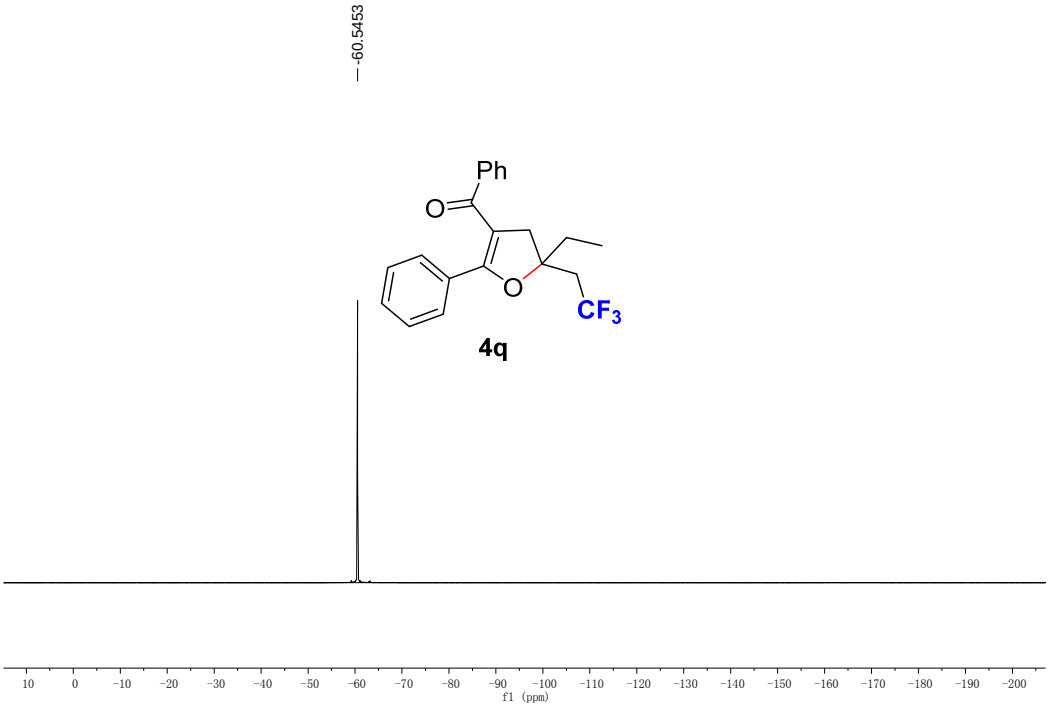
P 148 e


−60.8577
OMe
O
MeO
O
CF3
4f
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
f1 (ppm)

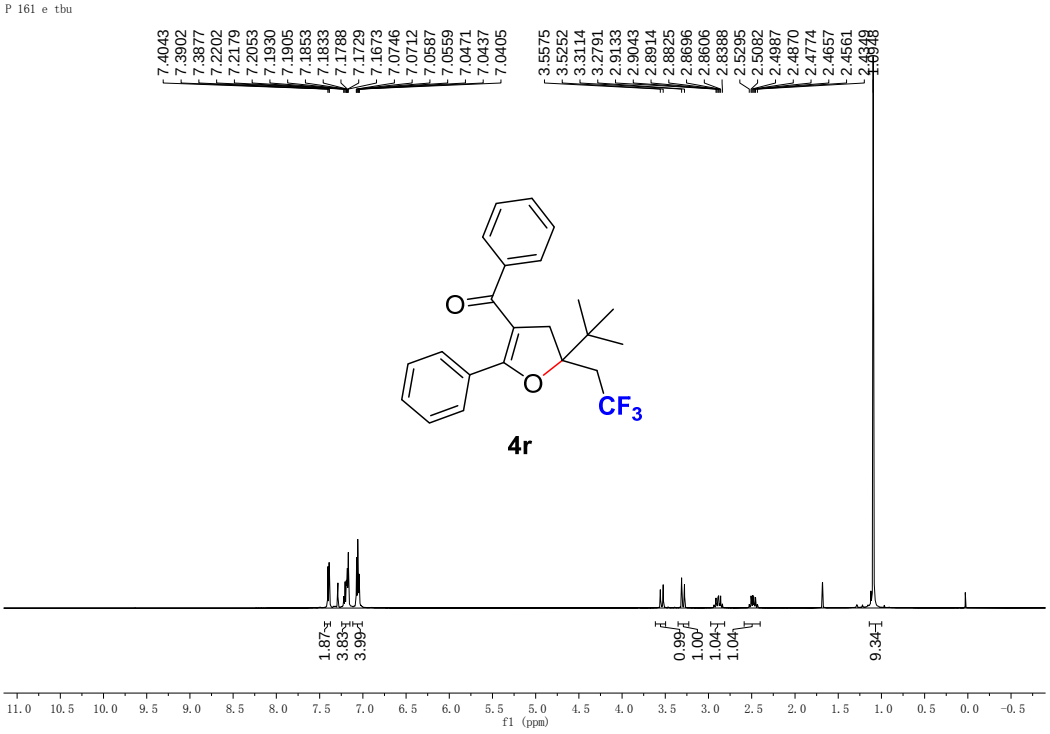

yny-P 161d 16-1-7
7.4438
7.4263
7.4230
7.2843
7.2544
7.2517
7.2359
7.2173
7.2138
7.2076
7.1922
7.1879
7.1850
7.1758
7.1061
7.0871
7.0681
7.0492
3.2943
2.7205
2.7053
2.6935
2.6780
2.0260
2.0082
1.9903
1.9758
1.1149
1.0963
Ph
O
O
CF3
4q
2.00
3.91
3.96
2.00
2.04
2.04
3.06
f1 (ppm)


yny-P 161d 16-1-7
193.3966
164.3462
138.8988
131.1976
130.0669
129.8309
129.7433
129.2813
128.8628
127.6807
127.6583
126.9804
124.2174
111.7197
86.0917
86.0730
41.8568
41.6044
41.3336
41.0627
32.3120
7.7102
Ph
O
O
CF3
4q
f1 (ppm)

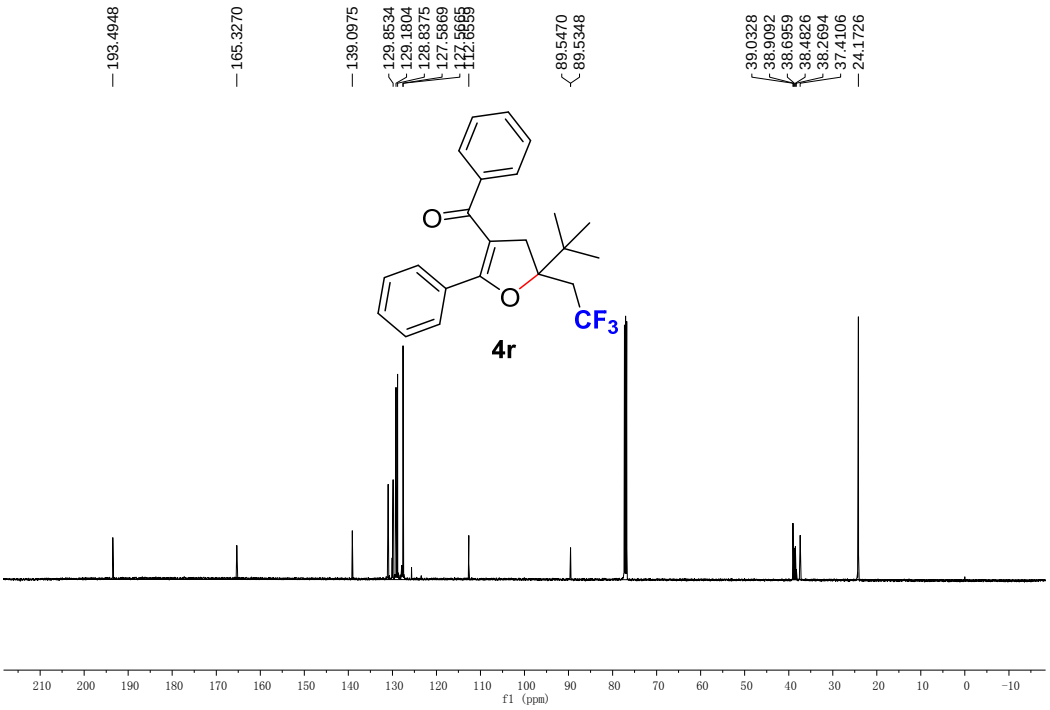
yny-P 161d 16-1-7



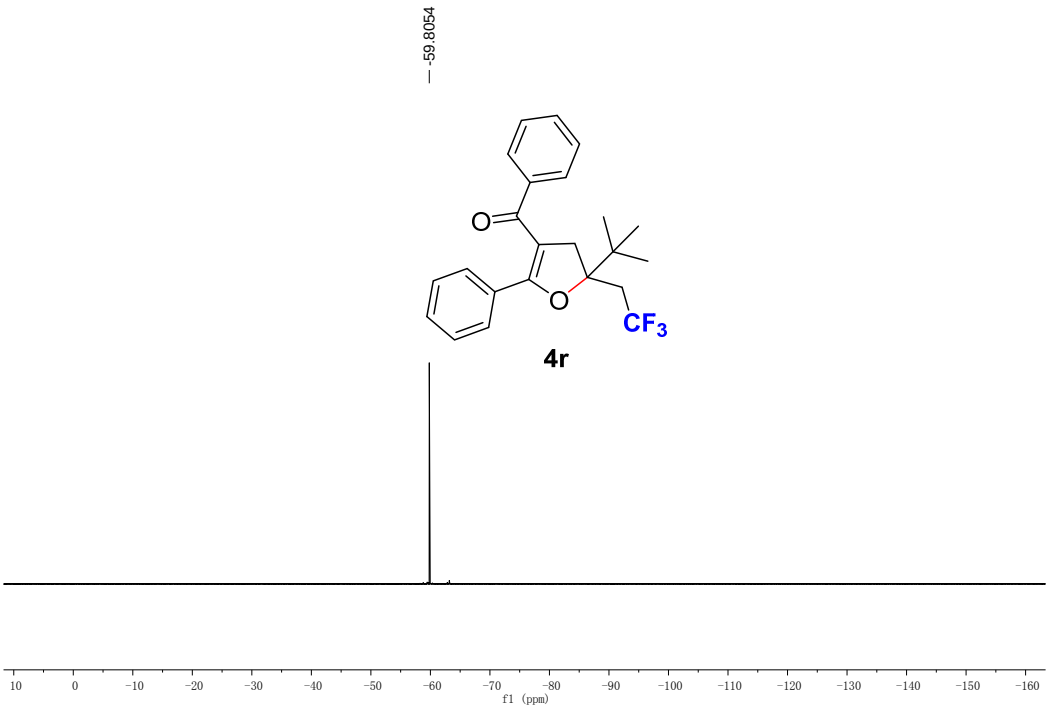
P 161 e tbu

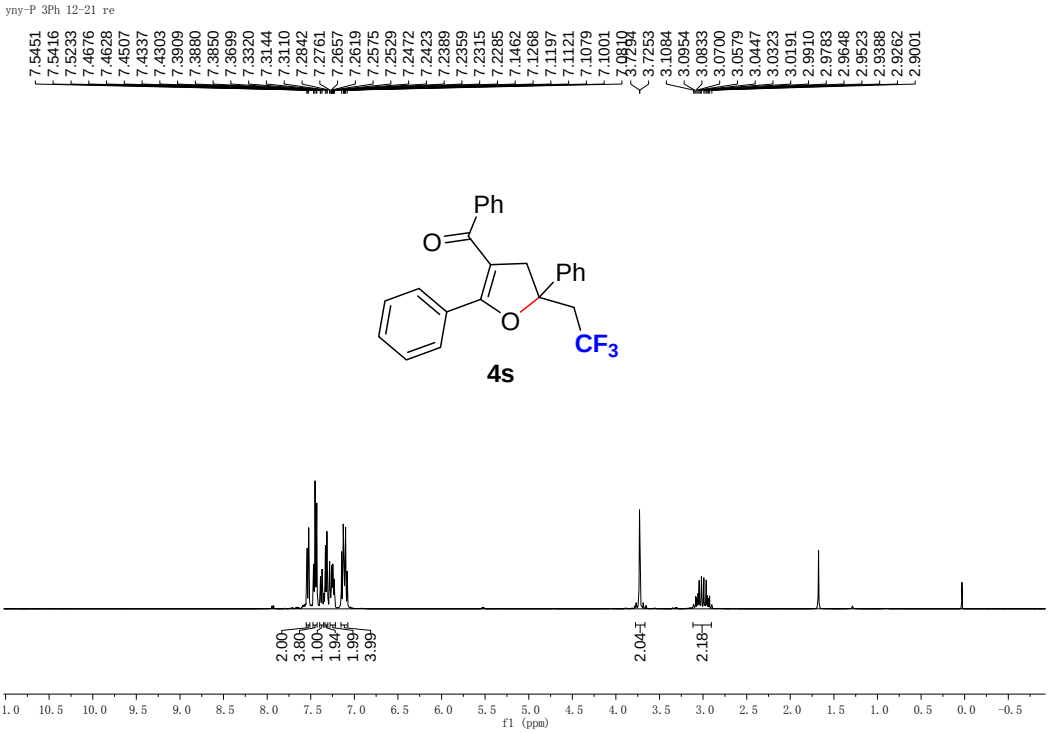


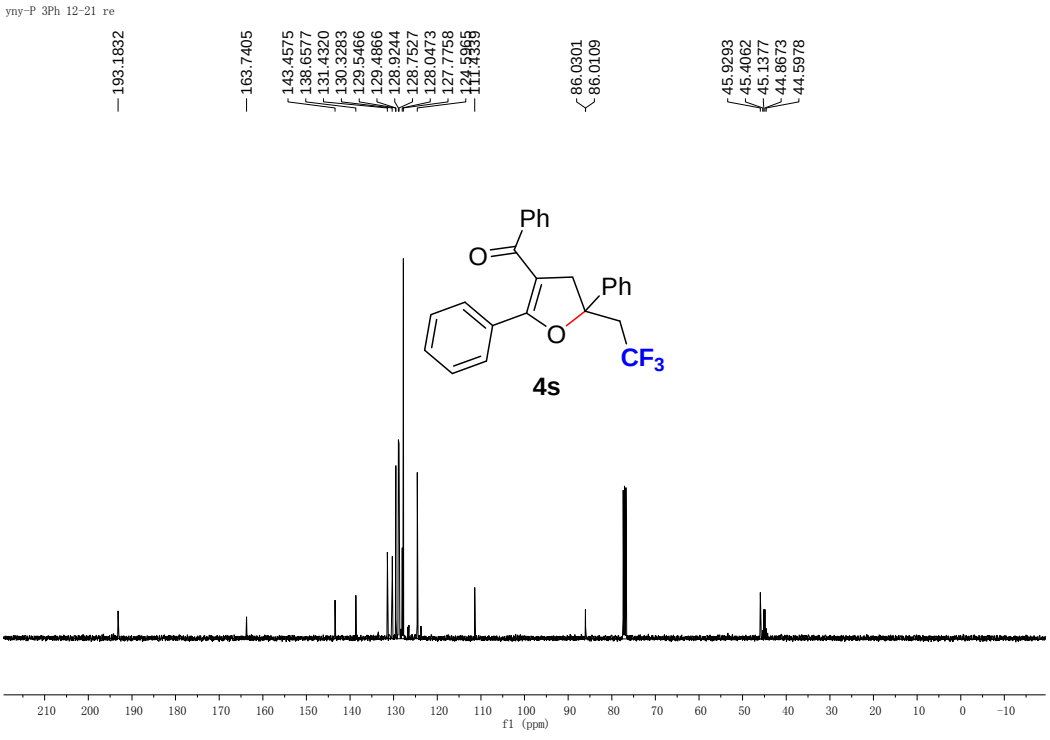
P 161 e tbu



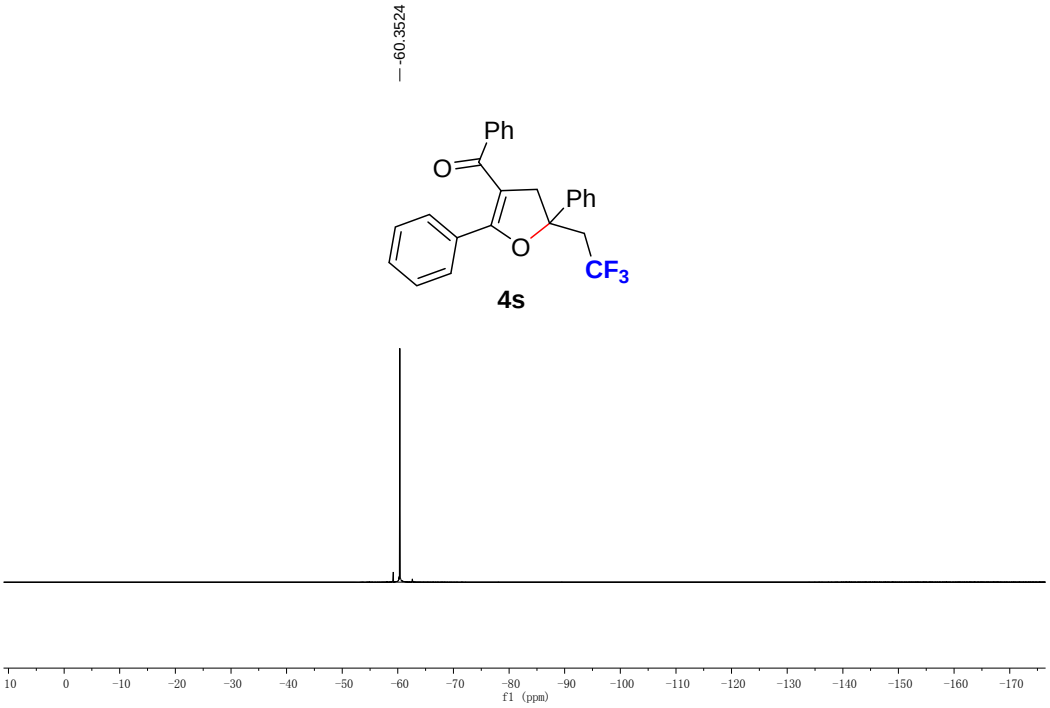
P 161 e tbu



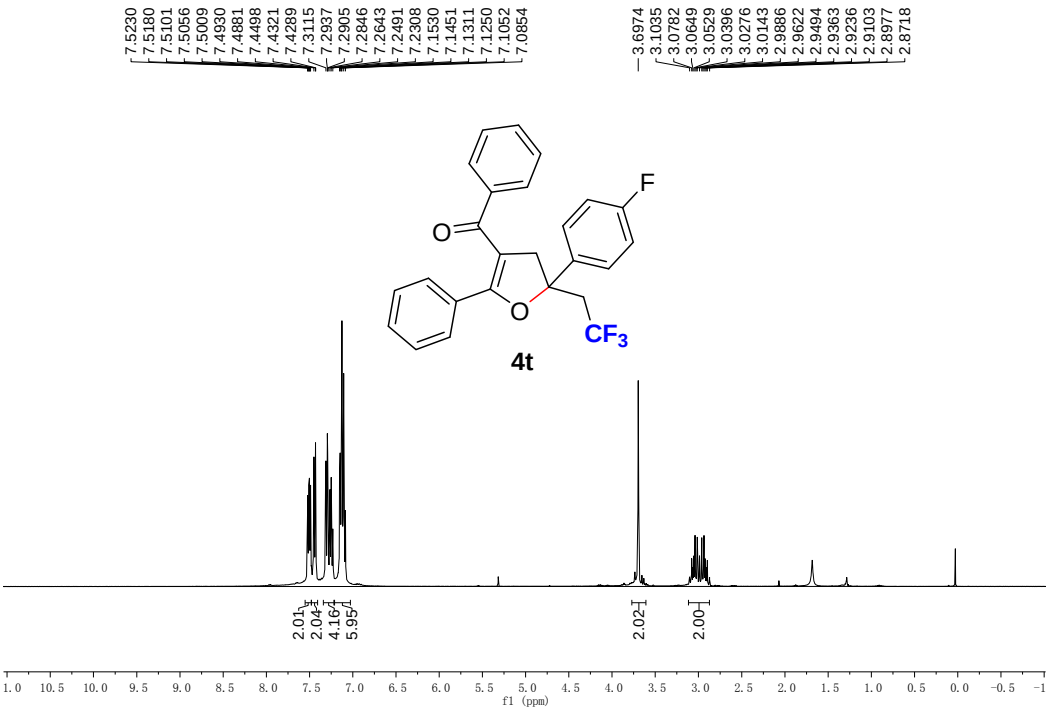

yny-P 3Ph 12-21 re
7.5451
7.5416
7.5233
7.4676
7.4628
7.4507
7.4337
7.4303
7.3909
7.3880
7.3850
7.3699
7.3320
7.3144
7.3110
7.2842
7.2761
7.2657
7.2619
7.2575
7.2529
7.2472
7.2423
7.2389
7.2359
7.2315
7.2285
7.1462
7.1268
7.1197
7.1121
7.1079
7.1001
3.7294
3.7253
3.1084
3.0954
3.0833
3.0700
3.0579
3.0447
3.0323
3.0191
2.9910
2.9783
2.9648
2.9523
2.9388
2.9262
2.9001
Ph
O
Ph
O
CF3
4s
2.00
3.80
1.00
1.94
1.99
3.99
2.04
2.18
f1 (ppm)

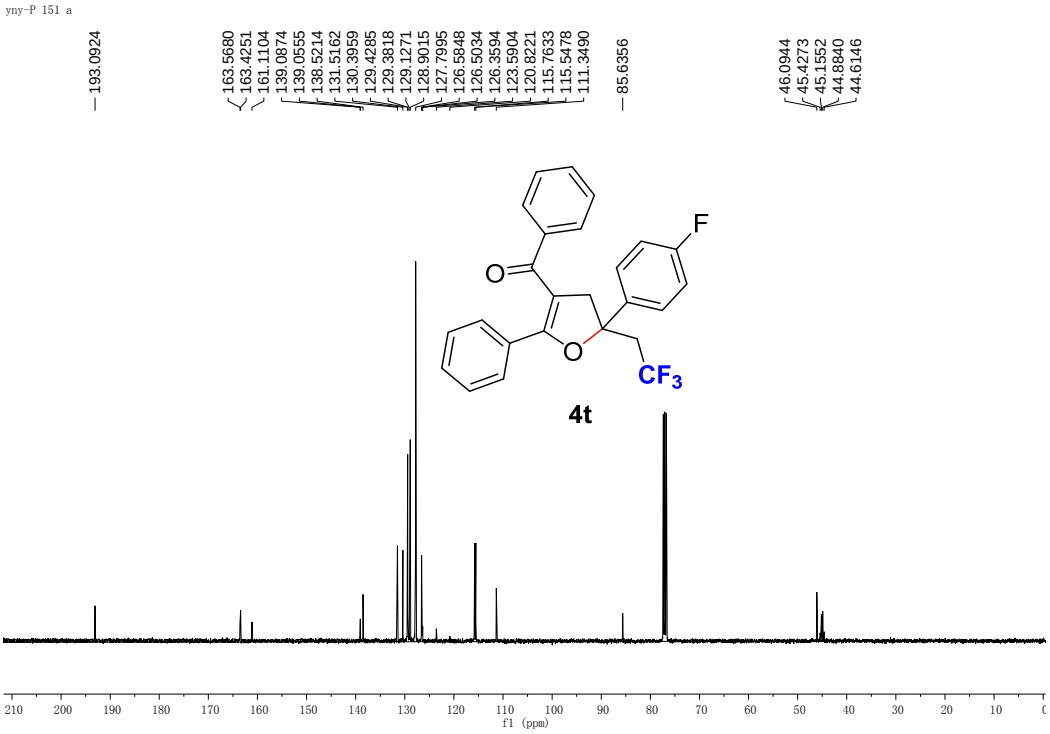

yny-P 3Ph 12-21 re
193.1832
163.7405
143.4575
138.6577
131.4320
130.3283
129.5466
129.4866
128.9244
128.7527
128.0473
127.7758
86.0301
86.0109
45.9293
45.4062
45.1377
44.8673
44.5978
Ph
O
Ph
O
CF3
4s
f1 (ppm)

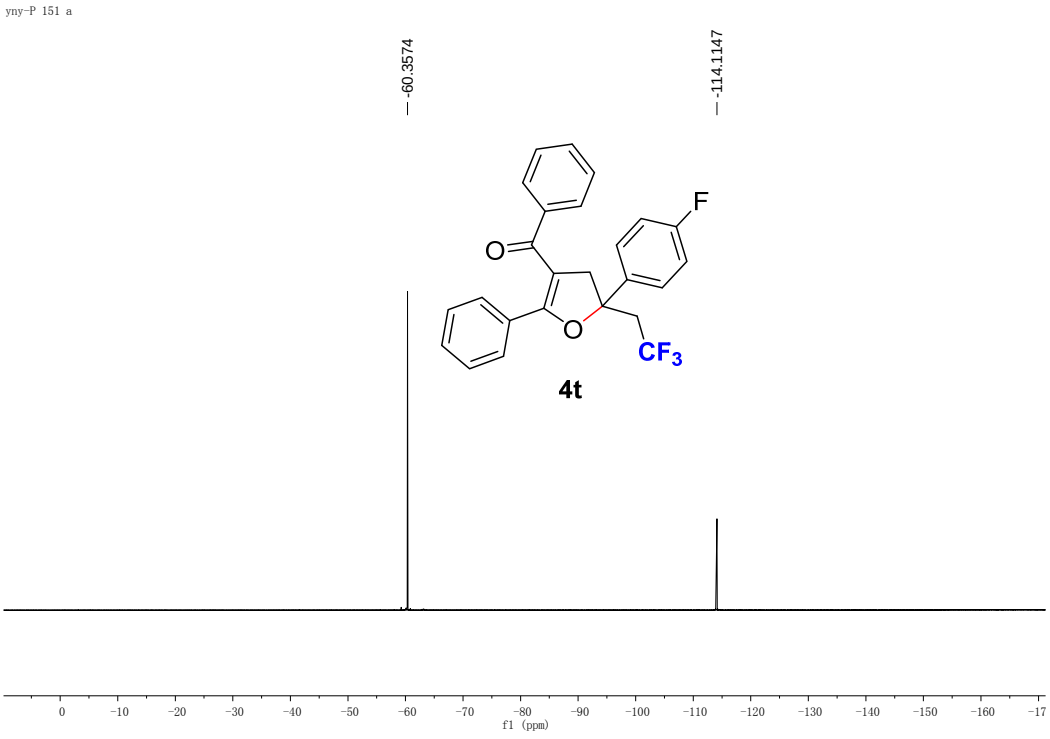
yny-P 3Ph 12-21 re

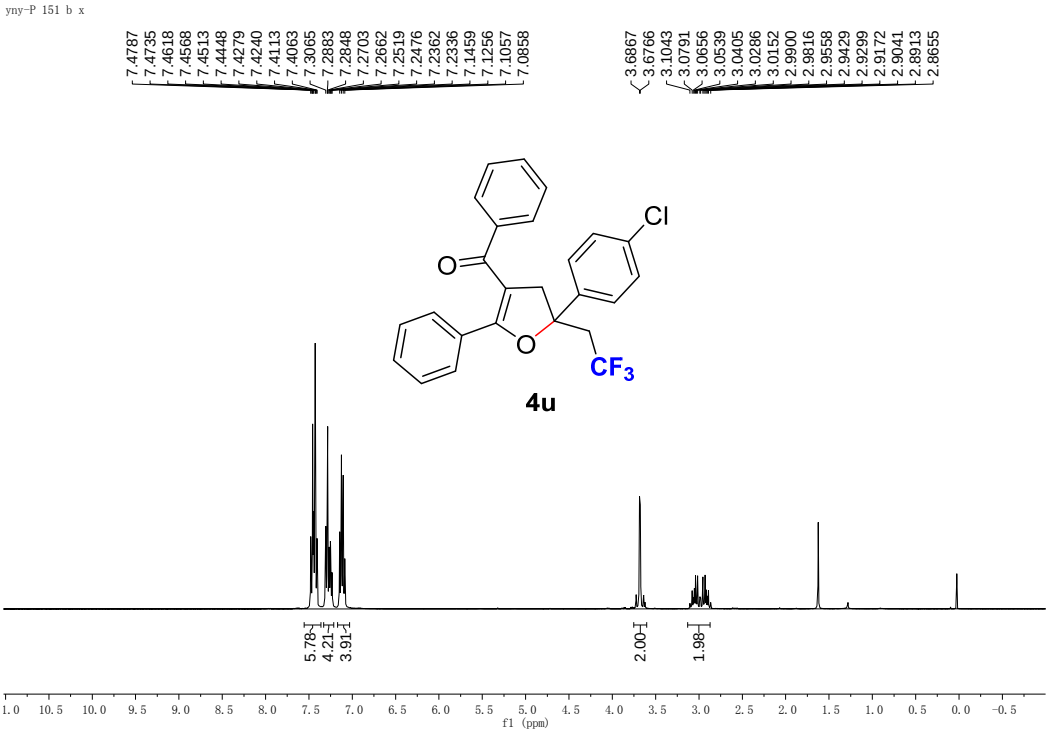


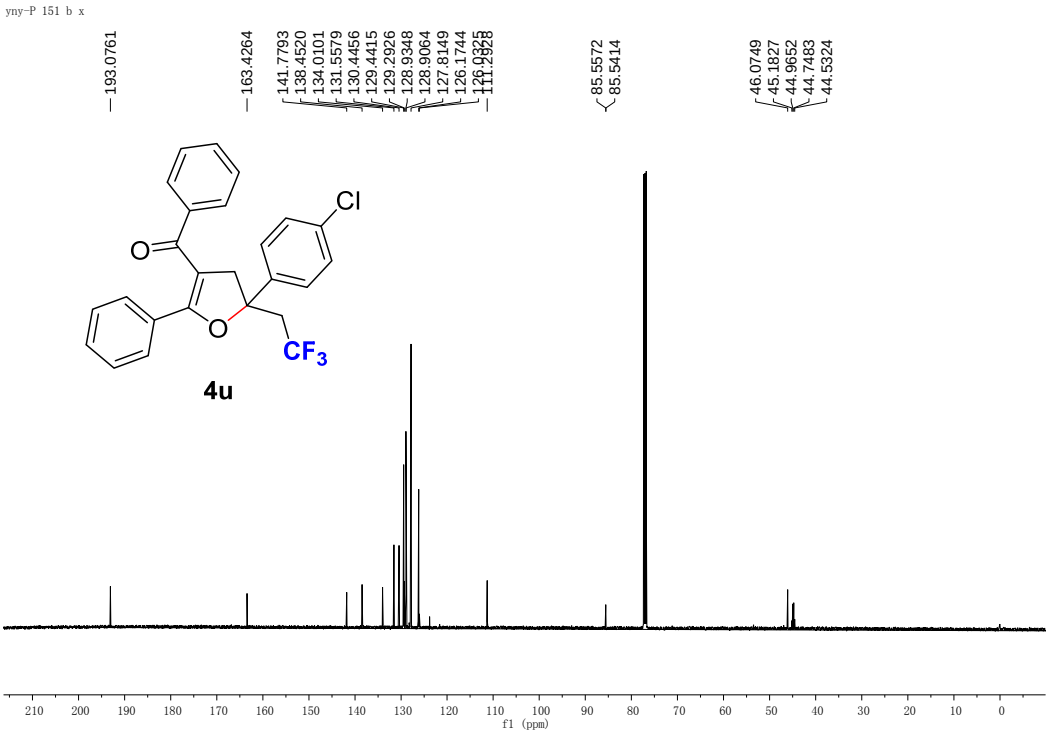
yny-P 151 a



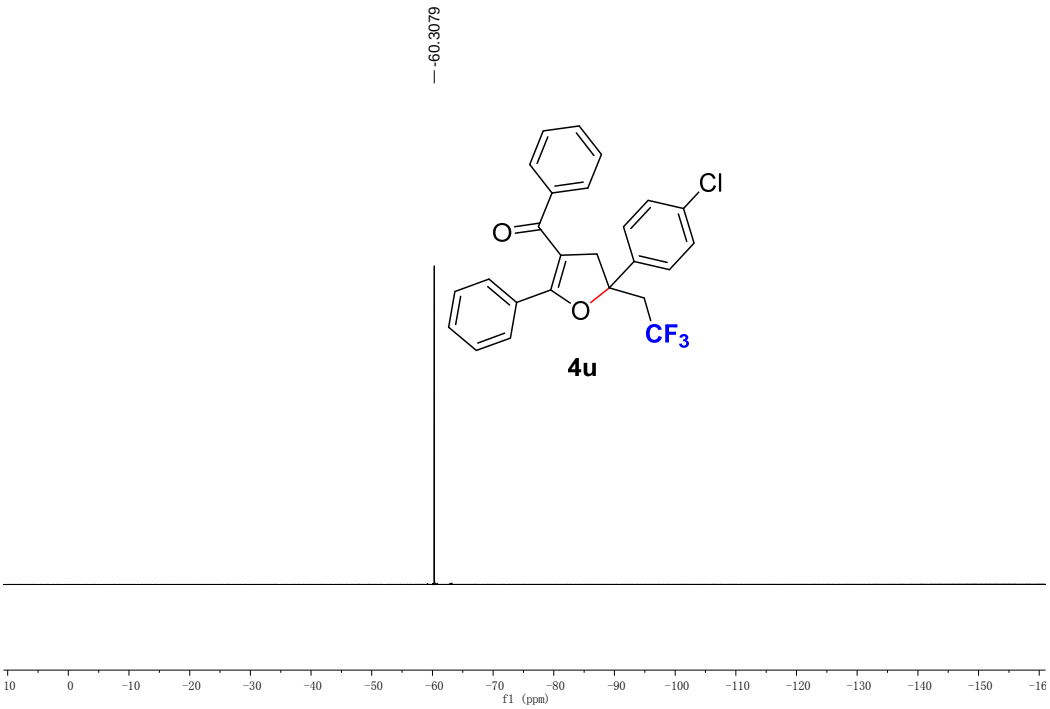

yny-P 151 a
193.0924
163.5680
163.4251
161.1104
139.0874
139.0555
138.5214
131.5162
130.3959
129.4285
129.3818
129.1271
128.9015
127.7995
126.5848
126.5034
126.3594
123.5904
120.8221
115.7633
115.5478
111.3490
85.6356
46.0944
45.4273
45.1552
44.8840
44.6146
O
O
F
CF3
4t
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


yny-P 151 a
-60.3574
-114.1147
O
O
F
CF3
4t
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -17
f1 (ppm)

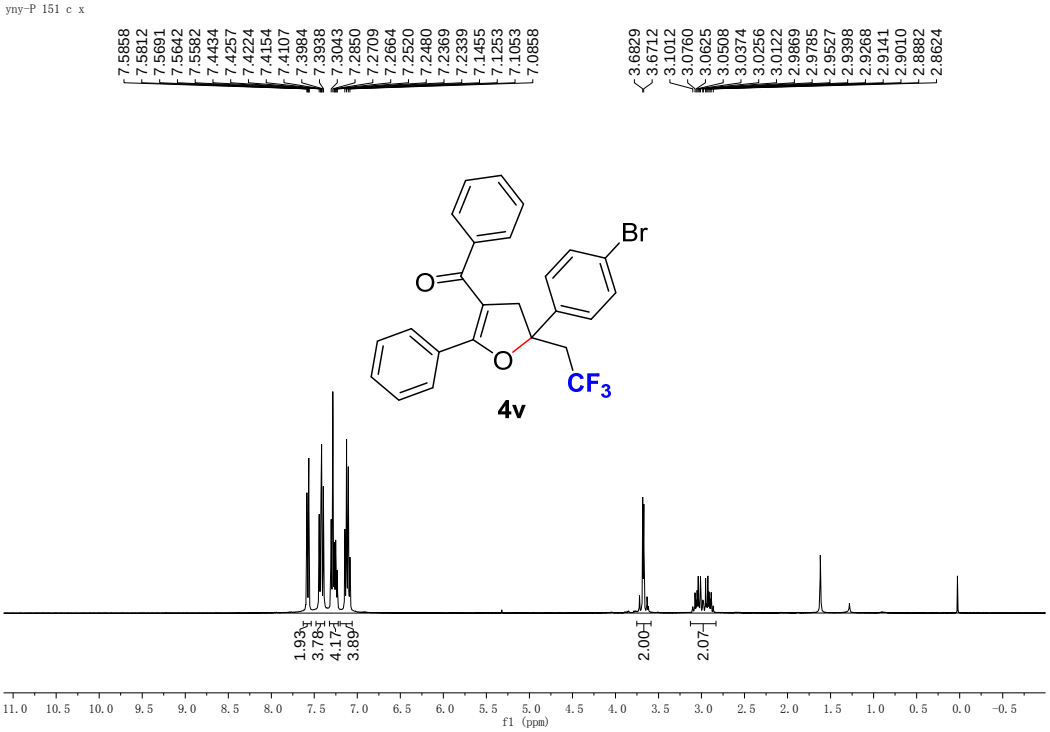

yny-P 151 b x
7.4787
7.4735
7.4618
7.4568
7.4513
7.4448
7.4279
7.4240
7.4113
7.4063
7.3065
7.2883
7.2848
7.2703
7.2662
7.2519
7.2476
7.2362
7.2336
7.1459
7.1256
7.1057
7.0858
3.6867
3.6766
3.1043
3.0791
3.0656
3.0539
3.0405
3.0286
3.0152
2.9900
2.9816
2.9558
2.9429
2.9299
2.9172
2.9041
2.8913
2.8655
Cl
O
O
CF3
4u
5.78
4.21
3.91
2.00
1.98
f1 (ppm)

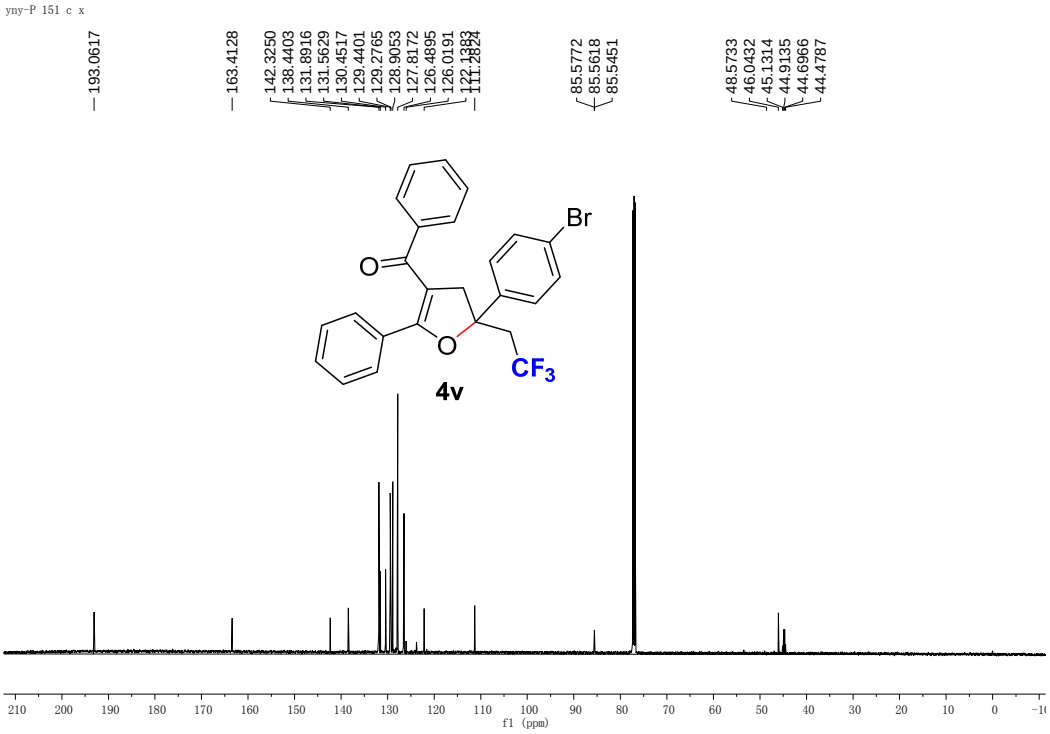

yny-P 151 b x
193.0761
163.4264
141.7793
138.4520
134.0101
131.5579
130.4456
129.4415
129.2926
128.9348
128.9064
127.8149
126.1744
85.5572
85.5414
46.0749
45.1827
44.9652
44.7483
44.5324
Cl
O
O
CF3
4u
f1 (ppm)

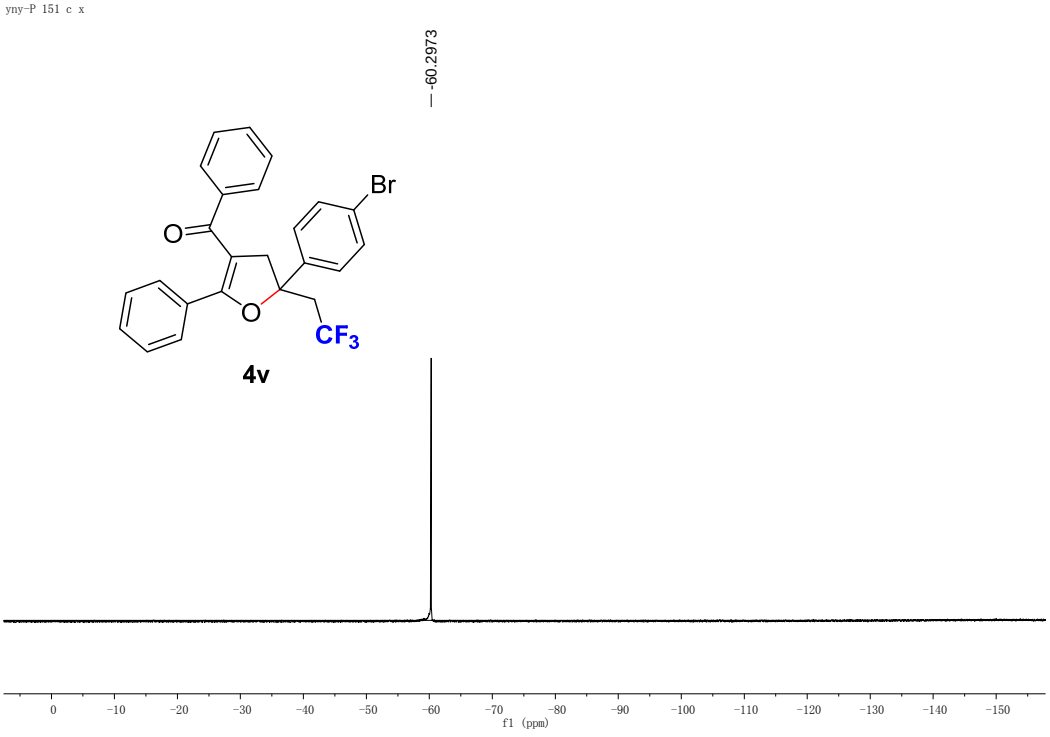
yny-P 151 b x



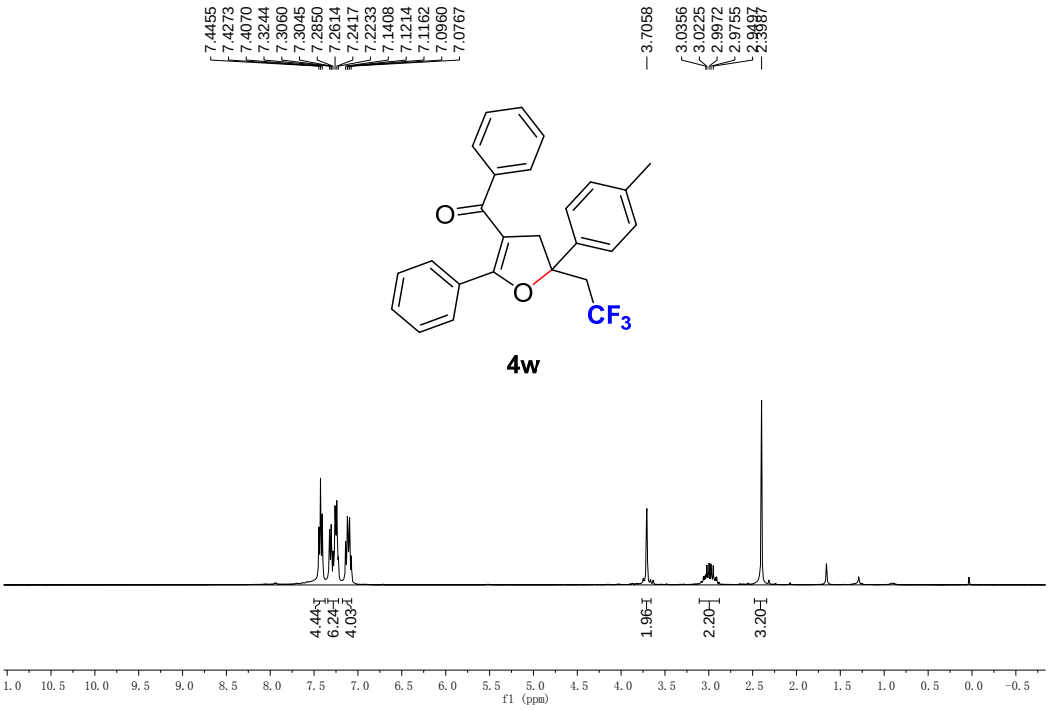
yny-P 151 c x



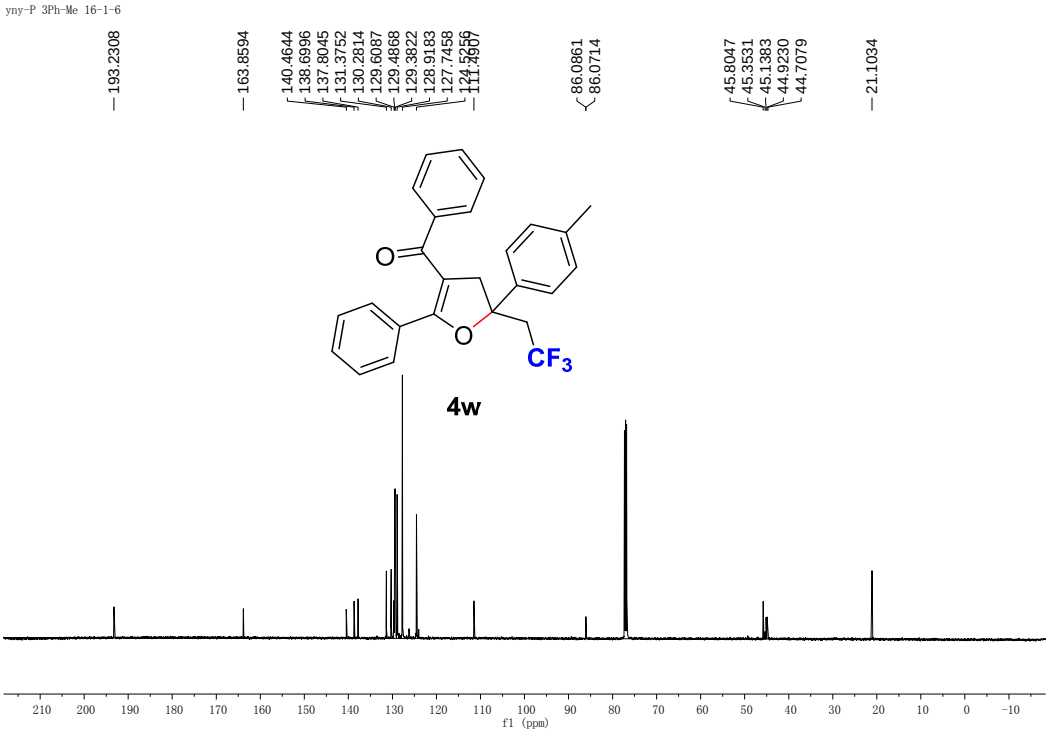

yny-P 151 c x
193.0617
163.4128
142.3250
138.4403
131.8916
131.5629
130.4517
129.4401
129.2765
128.9053
127.8172
126.4895
126.0191
122.1383
111.2824
85.5772
85.5618
85.5451
48.5733
46.0432
45.1314
44.9135
44.6966
44.4787
Br
O
O
CF3
4v
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


yny-P 151 c x
-60.2973
Br
O
O
CF3
4v
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150
f1 (ppm)

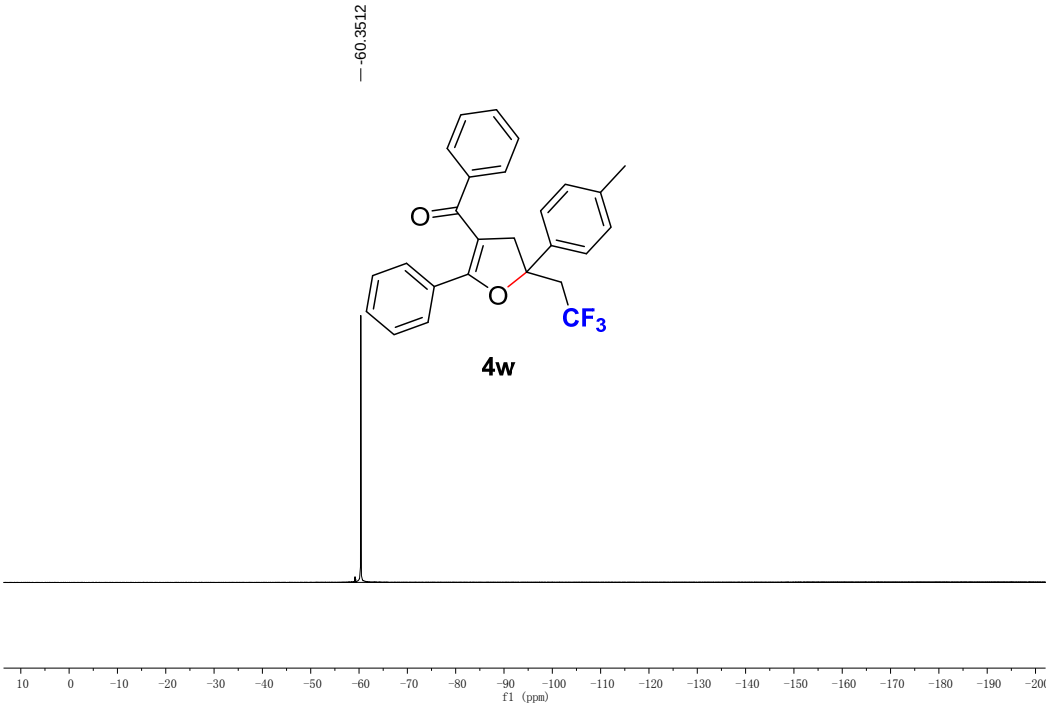
yny-P 3Ph-Me 16-1-6



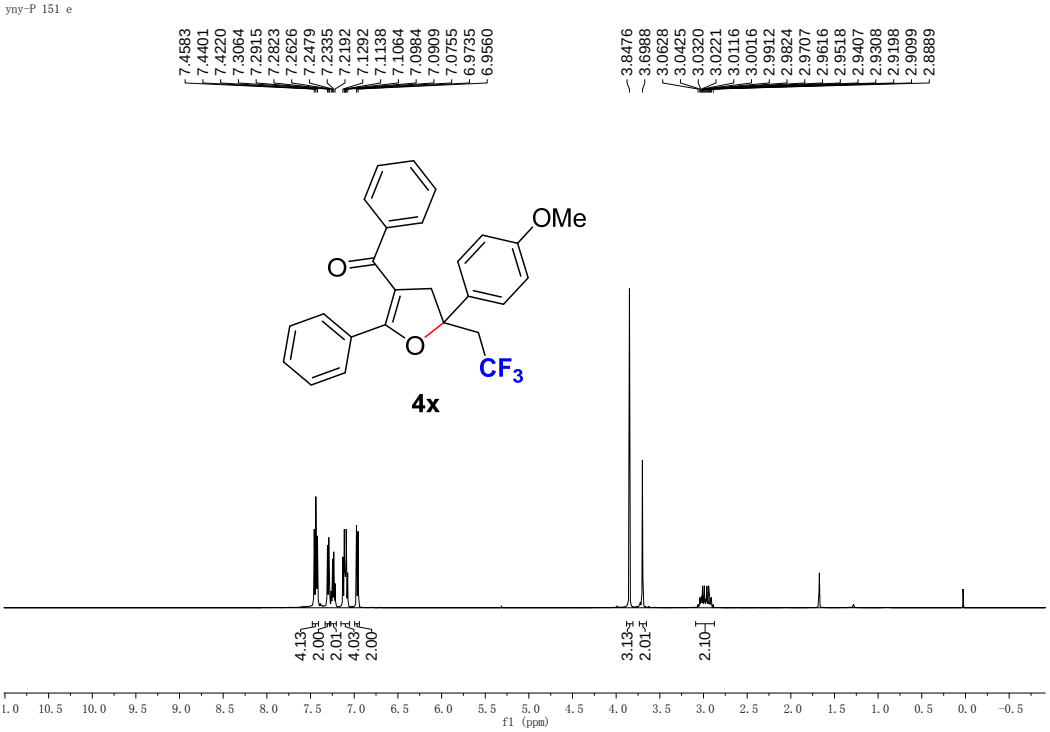
yny-P 3Ph-Me 16-1-6

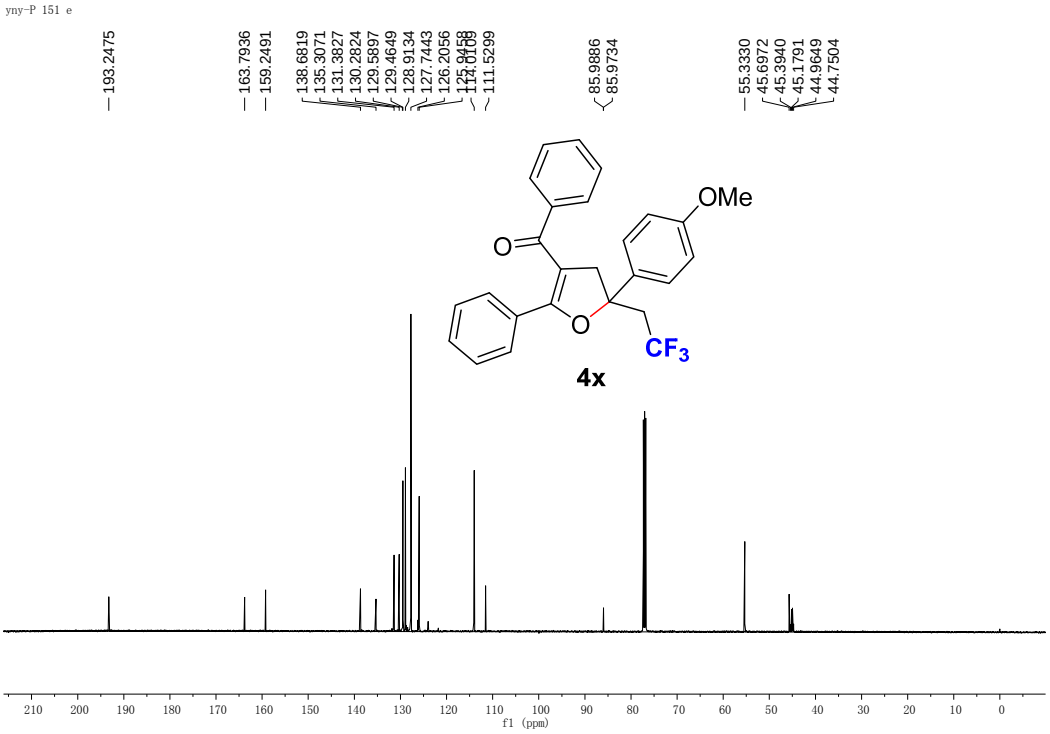


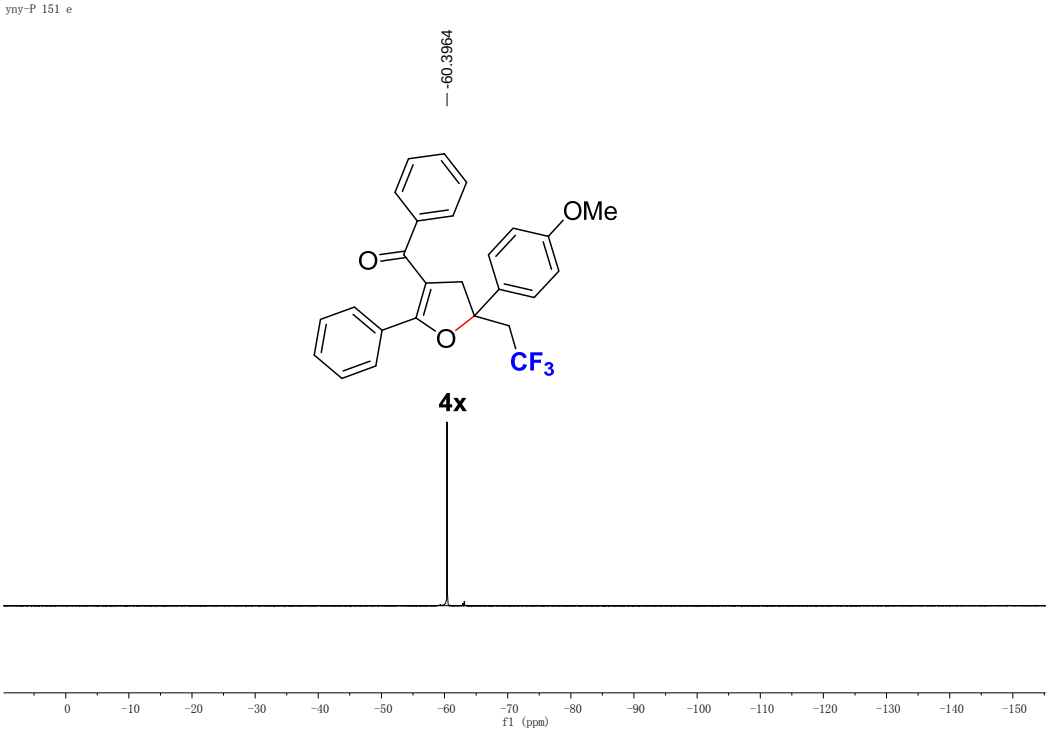
yny-P 3Ph-Me 16-1-6

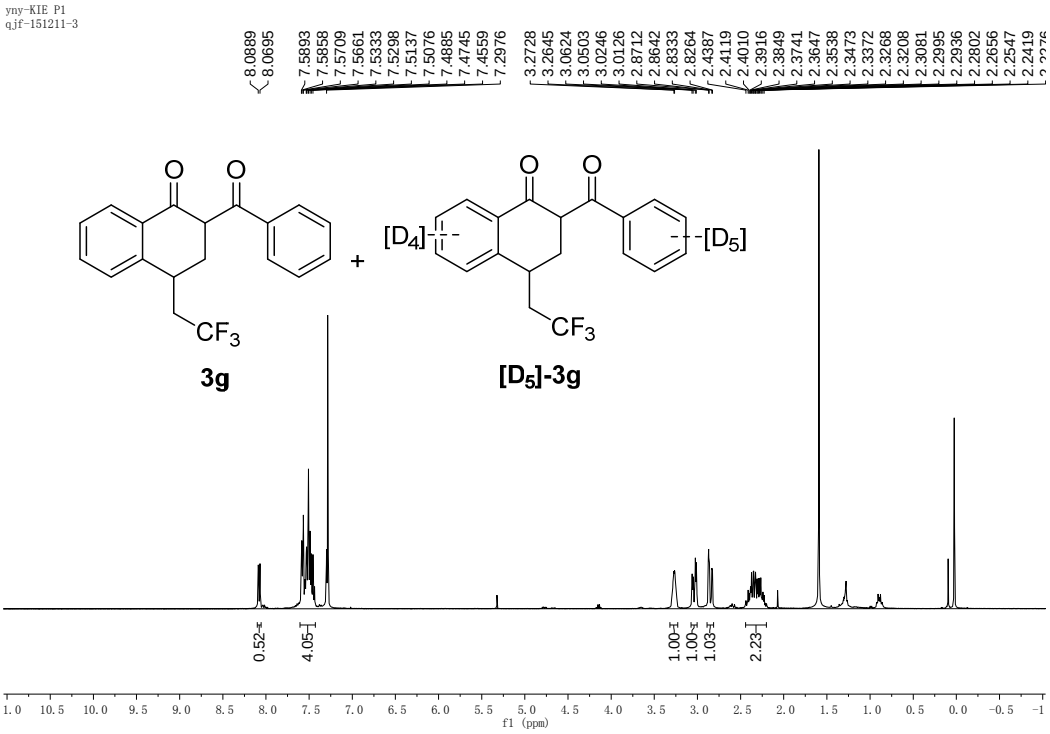


yny-P 151 e




yny-P 151 e
193.2475
163.7936
159.2491
138.6819
135.3071
131.3827
130.2824
129.5897
129.4649
128.9134
127.7443
126.2056
125.9458
114.0108
111.5299
85.9886
85.9734
55.3330
45.6972
45.3940
45.1791
44.9649
44.7504
OMe
O
O
CF3
4x
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


yny-P 151 e
-60.3964
OMe
O
O
CF3
4x
0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150
f1 (ppm)


yny-KIE P1
qjf-151211-3
8.0889
8.0695
7.5893
7.5858
7.5709
7.5661
7.5333
7.5298
7.5137
7.5076
7.4885
7.4745
7.4559
7.2976
3.2728
3.2645
3.0624
3.0503
3.0246
3.0126
2.8712
2.8642
2.8333
2.8264
2.4387
2.4119
2.4010
2.3916
2.3849
2.3741
2.3647
2.3538
2.3473
2.3372
2.3268
2.3208
2.3081
2.2995
2.2936
2.2802
2.2656
2.2547
2.2419
O
O
CF3
3g
+
[D4]
[D5]
[D5]-3g
0.52
4.05
1.00
1.00
1.03
2.23
f1 (ppm)

Reference:

1. L. Li, M. Deng, S.-C. Zheng, Y.-P. Xiong, B. Tan and X.-Y. Liu, *Org. Lett.*, 2014, **16**, 504.
2. C. Hansch, A. Leo and R. W. Taft, *Chem. Rev.*, 1991, **91**, 165.
3. (a)C. Walling, E. R. Briggs, K. B. Wolfstirn and F. R. Mayo, *J. Am. Chem. Soc.*, 1948, **70**, 1537;