Supporting Information

Visible light induced hydrogen atom transfer trifluoromethylthiolation of aldehydes with bismuth catalyst

Jun Dong,[a] Zhuang Tang,[a] Luqian Zou,[a] Yongyun Zhou*[b] and Jingchao Chen*[a,b]

a. Key Laboratory of Chemistry in Ethnic Medicinal Resources, Yunnan Minzu University, Yuehua Street, Kunming, 650504, China. Email: zhouyongyundf@163.com (Y. Y. Zhou), chenjingchao84@163.com (J. C. Chen).

b. Yunnan Key Laboratory of Chiral Functional Substance Research and Application, Yunnan Minzu University, Yuehua Street, Kunming 650504, China.

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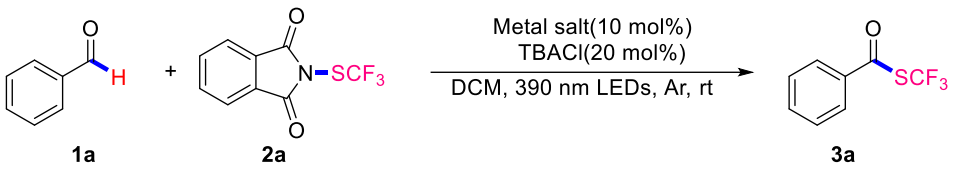
1. General information

Unless stated otherwise, all reactions were carried out under argon. ^{1}H NMR spectra were recorded using a Bruker 400 MHz instrument with tetramethylsilane (TMS) as an internal standard. ^{13}C NMR spectra were obtained at 101 MHz and referenced to the internal solvent signals. ^{19}F NMR spectra were obtained at 376 MHz. High resolution mass spectra (HRMS) were performed on a VG Autospec-3000 spectrometer. Flash column chromatography was carried out using 200-300 mesh silica gel at increased pressure with petroleum ether and ethyl acetate as eluents. Commercially available reagents were used without further purification unless indicated otherwise, all solvents were dried, super dry dichloromethane (DCM) (water ≤ 50 ppm) was purchased Energy Chemical Ltd, the following chemical reagent was purchased from Energy Chemical Ltd and Leyan Ltd: $BiCl_3$, TBACl and benzaldehyde. The light source was 30 W purple LED (390 nm, 1 W*30, 30-50 cd/m^2, made in Everlight Electronics., Ltd.); borosilicate glass Schlenk tube was used as the irradiation vessel; the distance from the light source to the irradiation vessel was 2-3 cm and no filter was used.

2. Reaction Optimizations

Table S1: Screening of Metal salts optimization

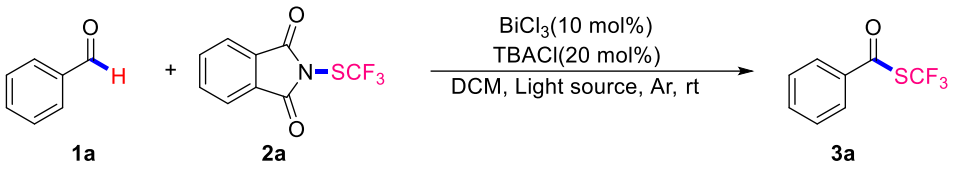


1a 2a 3a

Entry	Metal salt	Yield (%)
1	$FeCl_3$	58
2	$BiCl_3$	84
3	$CeCl_3$	47
4	BiOCl	0
5	BiF_3	0
6	$BiBr_3$	0

Reaction conditions: **1a** (21.4 mg, 0.20 mmol, 1.0 equiv.), **2a** (99.2 mg, 0.40 mmol, 2.0 equiv.), metal salt (0.02 mmol), TBACl (11.2 mg, 0.04 mmol), and DCM (2.0 mL, 0.1 M) under Ar and stirred at rt for 10 h under 30 W 390 nm LEDs irradiation. Yield of the isolated product after column chromatography.

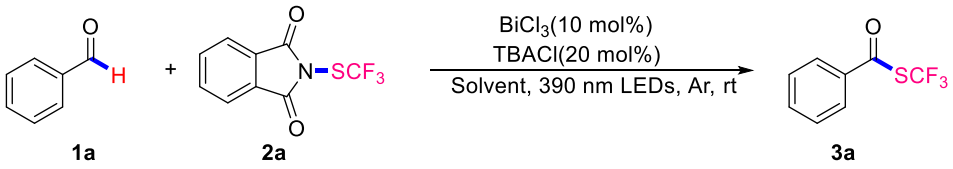
Table S2: Screening of wavelength of LEDs



Entry	Light source	Yield (%)
1	dark	0
2	365 nm	26
3	390 nm	84
4	450 nm	0

Reaction conditions: **1a** (21.4 mg, 0.20 mmol, 1.0 equiv.), **2a** (99.2 mg, 0.40 mmol, 2.0 equiv.), $BiCl_3$ (6.4mg, 0.02 mmol), TBACl (11.2 mg, 0.04 mmol), and DCM (2.0 mL, 0.1 M) under Ar and stirred at rt for 10 h under 30 W different Light source irradiation. Yield of the isolated product after column chromatography.

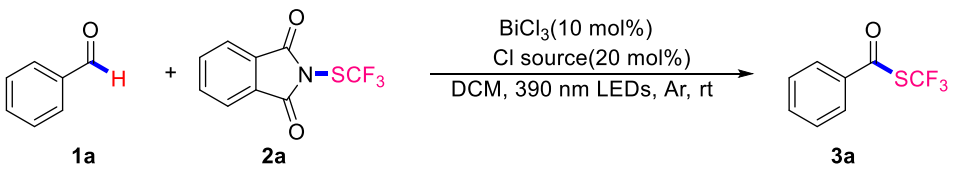
Table S3: Screening of solvents



Entry	Solvent	Yield (%)
1	DCM	84
2	MeCN	60
3	DCE	66
4	Tol	38
5	DMF	0
6	THF	0
7	TFE	0

Reaction conditions: **1a** (21.4 mg, 0.20 mmol, 1.0 equiv.), **2a** (99.2 mg, 0.40 mmol, 2.0 equiv.), $BiCl_3$ (6.4mg, 0.02 mmol), TBACl (11.2 mg, 0.04 mmol), and Solvent (2.0 mL, 0.1 M) under Ar and stirred at rt for 10 h under 30 W 390 nm LEDs irradiation. Yield of the isolated product after column chromatography.

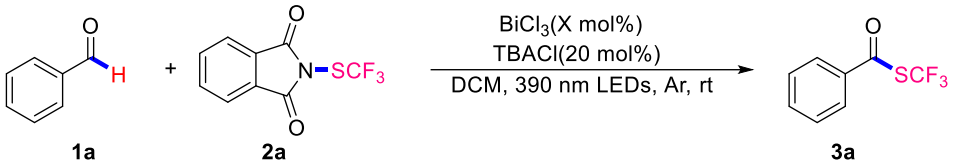
Table S4: Screening of "Cl" source



Entry	"Cl" Source	Yield (%)
1	TBACl	84
2	NaCl	<5
3	LiCl	<5
4	$MgCl_2$	<5

Reaction conditions: **1a** (21.4 mg, 0.20 mmol, 1.0 equiv.), **2a** (99.2 mg, 0.40 mmol, 2.0 equiv.), $BiCl_3$ (6.4mg, 0.02 mmol), "Cl" Source (0.04 mmol), and DCM (2.0 mL, 0.1 M) under Ar and stirred at rt for 10 h under 30 W 390 nm LEDs irradiation. Yield of the isolated product after column chromatography.

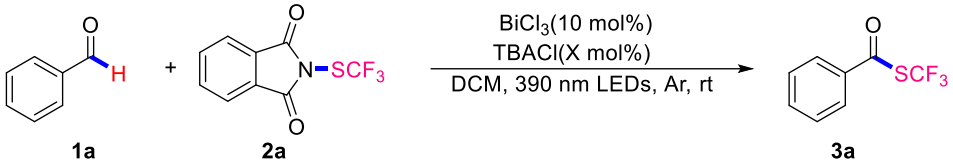
Table S5: Screening of the amount of bismuth catalyst



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

Entry	Amount of iron catalyst	Yield (%)
1	0 mol%	0
2	5 mol%	61
3	10 mol%	84
4	20 mol%	51

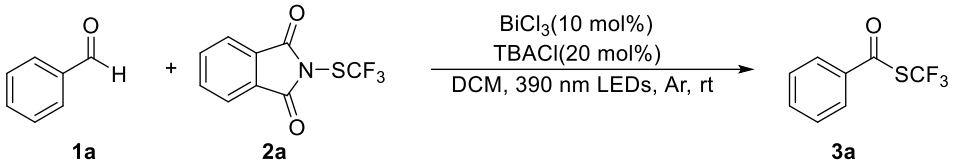
Table S6: Screening of the amount of TBACl



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

Entry	Amount of TBACl	Yield (%)
1	0 mol%	0
2	5 mol%	44
3	10 mol%	68
4	20 mol%	84
5	30 mol%	77

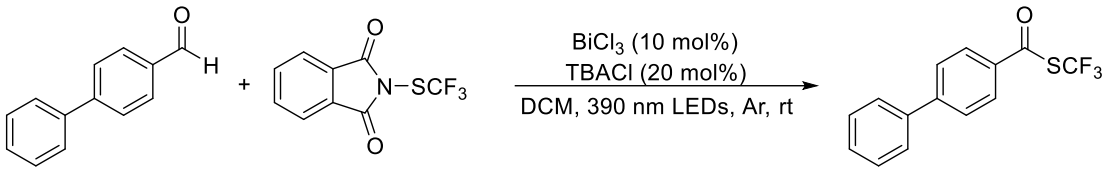
3. Standard Reaction Conditions



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

To an oven dried Schlenk-tube, benzaldehyde (21.4 mg, 0.20 mmol, 1.0 equiv.), N-(trifluoromethylthio)phthalimide (99.2 mg, 0.40 mmol, 2.0 equiv.), $BiCl_3$ (6.4 mg, 0.02 mmol), TBACl (11.2 mg, 0.04 mmol) and DCM (2 mL) were added under argon atmosphere. The reaction mixture was stirred under the irradiation of 30 W Purple LED (390 nm) at room temperature. After completion of the reaction, the reaction mixture was concentrated by vacuum, purified by silica gel chromatography, and eluted by petroleum ether to obtain products.

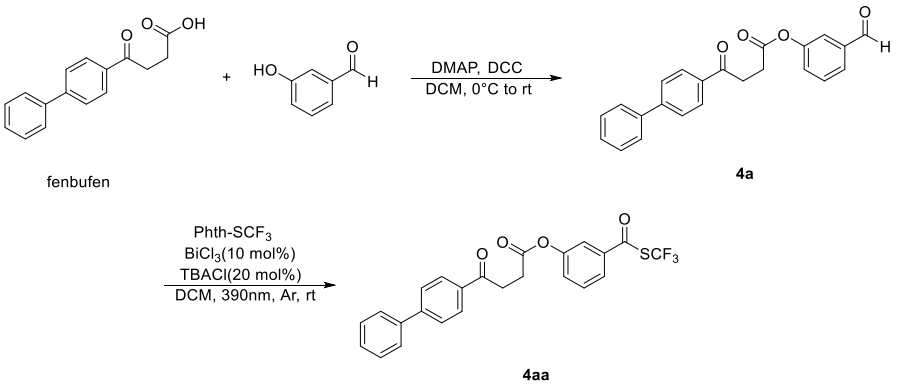
4. Gram-scale Reaction



1q, 5.5 mmol **2a**, 2.0 equiv **3q**, 66 %, 1.02 g

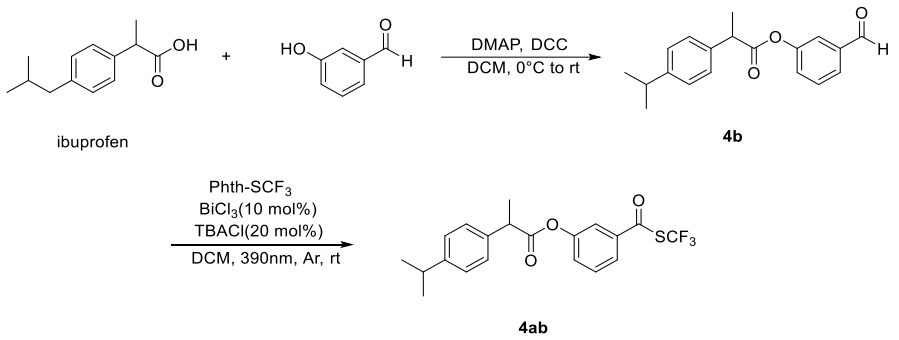
An oven-dried 100 mL three-neck Schlenk flask with magnetic stirring bar was charged with 4-biphenylcarboxaldehyde (1.002 g, 5.5 mmol, 1.0 equiv.), the N-(trifluoromethylthio)phthalimide (2.719 g, 11 mmol, 2 equiv.), $BiCl_3$ (176.0 mg, 0.55 mmol), TBACl (308.0 mg, 1.1 mmol) and DCM (30 mL).The reaction mixture was degassed by bubbling with Ar. The mixture was then stirred rapidly and irradiated with 30 W 390 nm LEDs at room temperature for 30 h. The reaction mixture was concentrated in vacuo to remove the DCM. Purified by silica gel chromatography, and eluted by petroleum ether to obtain products (1.024 g, 66%).

5. Derivatives of drug and natural product



Aldehyde **4a** was synthesized according to literature report.[1] 3-hydroxybenzaldehyde (5.0 mmol, 610.6 mg) and fenbufen (5.0 mmol, 1.271 g) and dry DCM (50 mL) were added sequentially to a dry round-bottom flask at room temperature. The reaction was cooled to 0 ℃ and a catalytic amount of 4-dimethylaminopyridine (DMAP, 0.75 mmol, 0.15 equiv.) and dicyclohexylcarbodiimide (DCC, 7.5 mmol, 1.5 equiv.) were added. The natural return to room temperature and further stirred for 8 hours. Upon completion, the product extracted with DCM (3 × 20 mL). The combined organic phases was washed with brine (20 mL), dried with Na_2SO_4, then filtered and concentrated in vacuo. The crude product was purified by flash column chromatography. The residue was purified by chromatography (PE: EA = 8: 1 v/v) to give **4a** with 72% yield.

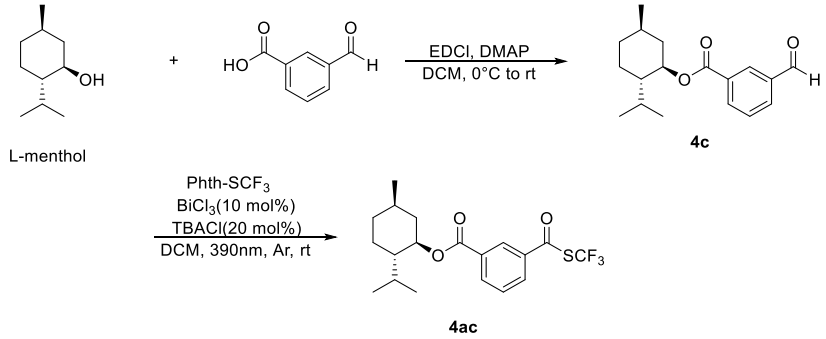
Under argon, to an oven dried Schlenk-tube, **4a** (71.7 mg, 0.20 mmol, 1.0 equiv.), N-(trifluoromethylthio)phthalimide (99.2 mg, 0.40 mmol, 2.0 equiv.), $BiCl_3$ (6.4mg, 0.02 mmol), TBACl (11.2 mg, 0.04 mmol) and DCM (2 mL) were added under argon atmosphere. The reaction mixture was stirred under the irradiation of 30 W purple LED (390 nm) at room temperature. After completion of the reaction, the solvent was evaporated under vacuum and the residue was purified by flash chromatography eluting with PE: EA (10:1 v/v) on a silica gel to afford the **4aa** as a yellow solid in 48% yield.[1]



Aldehyde **4b** was synthesized according to literature report.[1] 3-hydroxybenzaldehyde (5.0 mmol, 610.6 mg) and ibuprifen (5.0 mmol, 1.031 g) and dry DCM (50 mL) were added sequentially to a dry round-bottom flask at room temperature. The reaction was cooled to 0 ℃ and a catalytic amount of 4-dimethylaminopyridine (DMAP, 0.75 mmol, 0.15 equiv.) and dicyclohexylcarbodiimide (DCC, 7.5 mmol, 1.5 equiv.) were added. The natural return to room temperature and further stirred for 8 hours. Upon completion, the product extracted with DCM (3 × 20 mL). The combined organic phases was washed with brine (20 mL), dried with Na_2SO_4, then filtered and concentrated in vacuo. The crude product was purified by flash column chromatography. The residue was purified by chromatography (PE: EA = 20: 1 v/v) to give **4b** with 78% yield.

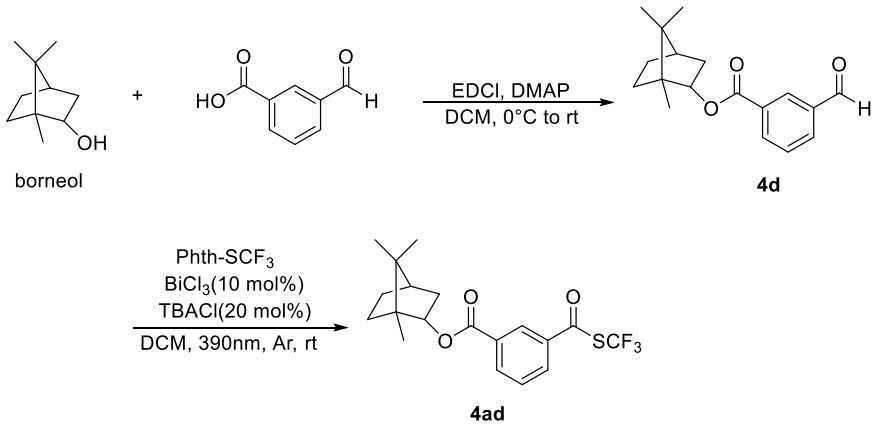
Under argon, to an oven dried Schlenk-tube, **4b** (59.3 mg, 0.20 mmol, 1.0 equiv.), N-(trifluoromethylthio)phthalimide (99.2 mg, 0.40 mmol, 2.0 equiv.), $BiCl_3$ (6.4mg, 0.02 mmol), TBACl (11.2 mg, 0.04 mmol) and DCM (2 mL) were added under argon atmosphere. The reaction mixture was stirred under the irradiation of 30 W purple LED (390 nm) at room temperature. After completion of the reaction, the solvent was

evaporated under vacuum and the residue was purified by flash chromatography eluting with PE: EA (40:1 v/v) on a silica gel to afford the **4ab** as a yellow solid in 45% yield.[1]



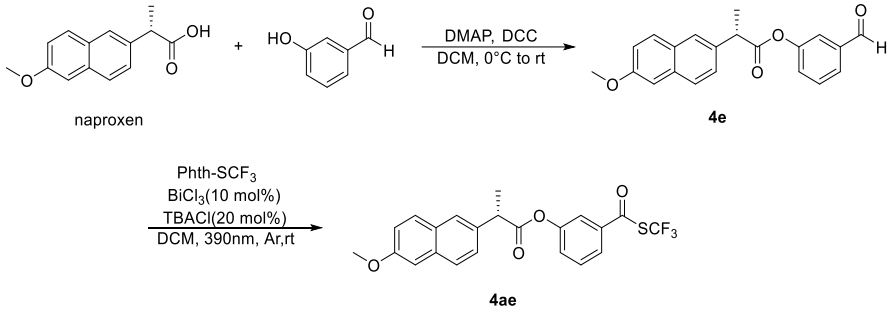
Aldehyde **4c** was synthesized according to literature report.[3] 3-carboxybenzaldehyde (5.0 mmol, 750.6 mg) and L-menthol (5.0 mmol, 781.4 mg) and dry DCM (50 mL) were added sequentially to a dry round-bottom flask at room temperature. The reaction was cooled to 0 ℃ and a catalytic amount of 4-dimethylaminopyridine (DMAP, 0.25 mmol, 0.05 equiv.) and EDCl (5.5 mmol, 1.1 equiv.) were added. The natural return to room temperature and further stirred for 14 hours. Upon completion, the product extracted with DCM (3 × 20 mL). The combined organic phases was washed with brine (20 mL), dried with Na_2SO_4, then filtered and concentrated in vacuo. The crude product was purified by flash column chromatography. The residue was purified by chromatography (PE: EA = 40: 1 v/v) to give **4c** with 66% yield.

Under argon, to an oven dried Schlenk-tube, **4c** (57.7 mg, 0.20 mmol, 1.0 equiv.), N-(trifluoromethylthio)phthalimide (99.2 mg, 0.40 mmol, 2.0 equiv.), $BiCl_3$ (6.4mg, 0.02 mmol), TBACl (11.2 mg, 0.04 mmol) and DCM (2 mL) were added under argon atmosphere. The reaction mixture was stirred under the irradiation of 30 W purple LED (390 nm) at room temperature. After completion of the reaction, the solvent was evaporated under vacuum and the residue was purified by flash chromatography eluting with PE: EA (50:1 v/v) on a silica gel to afford the **4ac** as a yellow solid in 51% yield.[3]



Aldehyde **4d** was synthesized according to literature report.[5] 3-carboxybenzaldehyde (5.0 mmol, 750.6 mg) and borneol (5.0 mmol, 771.3 mg) and dry DCM (50 mL) were added sequentially to a dry round-bottom flask at room temperature. The reaction was cooled to 0 ℃ and a catalytic amount of 4-dimethylaminopyridine (DMAP, 0.25 mmol, 0.05 equiv.) and EDCl (5.5 mmol, 1.1 equiv.) were added. The natural return to room temperature and further stirred for 14 hours. Upon completion, the product extracted with DCM (3 × 20 mL). The combined organic phases was washed with brine (20 mL), dried with Na_2SO_4, then filtered and concentrated in vacuo. The crude product was purified by flash column chromatography. The residue was purified by chromatography (PE: EA = 40: 1 v/v) to give **4d** with 70% yield.

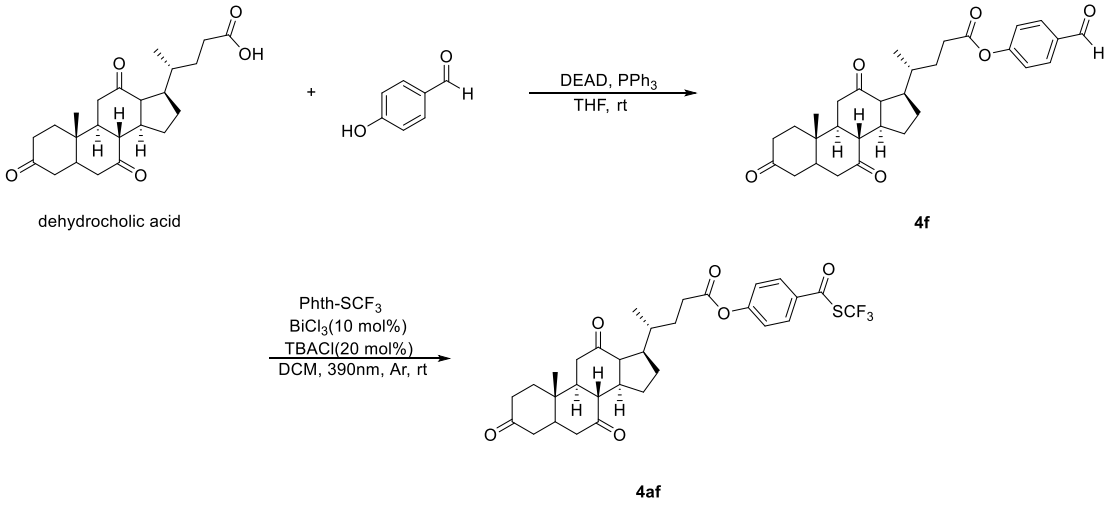
Under argon, to an oven dried Schlenk-tube, **4d** (57.3 mg, 0.20 mmol, 1.0 equiv.), N-(trifluoromethylthio)phthalimide (99.2 mg, 0.40 mmol, 2.0 equiv.), $BiCl_3$ (6.4mg, 0.02 mmol), TBACl (11.2 mg, 0.04 mmol) and DCM (2 mL) were added under argon atmosphere. The reaction mixture was stirred under the irradiation of 30 W purple LED (390 nm) at room temperature. After completion of the reaction, the solvent was evaporated under vacuum and the residue was purified by flash chromatography eluting with PE: EA (50:1 v/v) on a silica gel to afford the **4ad** as a yellow solid in 53% yield.[5]



Aldehyde **4e** was synthesized according to literature report.[6] 3-hydroxybenzaldehyde (5.0 mmol, 610.6 mg) and naproxen (5.0 mmol, 1.152 g) and dry DCM (50 mL) were added sequentially to a dry round-bottom flask at room temperature. The reaction was cooled to 0 ℃ and a catalytic amount of 4-dimethylaminopyridine (DMAP, 0.75 mmol, 0.15 equiv.) and dicyclohexylcarbodiimide (DCC, 7.5 mmol, 1.5 equiv.) were added. The natural return to room temperature and further stirred for 8 hours. Upon completion, the product extracted with DCM (3 × 20 mL). The combined organic phases was washed with brine (20 mL), dried with Na_2SO_4, then filtered and concentrated in vacuo. The crude product was purified by flash column chromatography. The residue was purified by chromatography (PE: EA = 10: 1 v/v) to give **4d** with 82% yield.

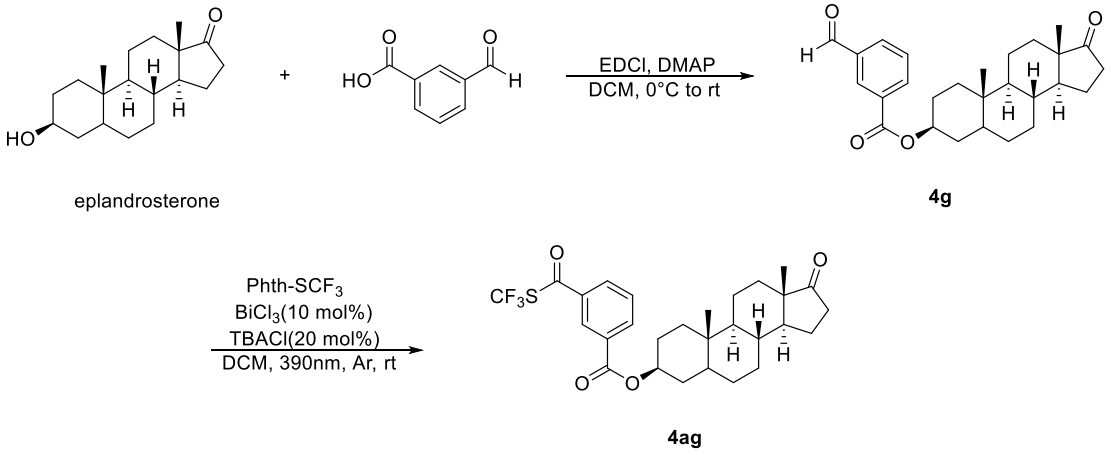
Under argon, to an oven dried Schlenk-tube, **4e** (66.9 mg, 0.20 mmol, 1.0 equiv.), N-(trifluoromethylthio)phthalimide (99.2 mg, 0.40 mmol, 2.0 equiv.), $BiCl_3$ (6.4mg, 0.02 mmol), TBACl (11.2 mg, 0.04 mmol) and DCM (2 mL) were added under argon atmosphere. The reaction mixture was stirred under the irradiation of 30 W purple LED (390 nm) at room temperature. After completion of the reaction, the solvent was

evaporated under vacuum and the residue was purified by flash chromatography eluting with PE: EA (20:1 v/v) on a silica gel to afford the **4ae** as a yellow solid in 45% yield.[6]



4f were synthesized according to literature report, to a solution of DEAD (diethylazodicarboxylate) (5.00 mmol, 1.00 equiv.) in THF (31 mL) was added 4-hydroxybenzaldehyde (5.00 mmol, 1.00 equiv.), dehydrocholic acid (5.00 mmol, 1.00 equiv.), and triphenylphosphine (5.00 mmol, 1.00 equiv.). The reaction mixture was stirred for 30 hours at room temperature. The reaction mixture was concentrated in vacuo and the residue was purified by chromatography on silica gel to afford the desired product **4f**.[2] The yield was 82%.

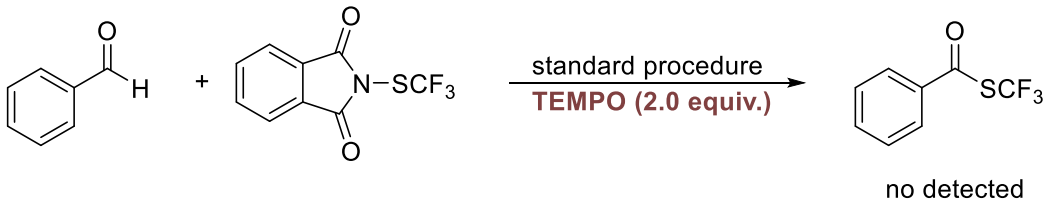
Under argon, to an oven dried Schlenk-tube, **4f** (98.6 mg, 0.20 mmol, 1.0 equiv.), N-(trifluoromethylthio)phthalimide (99.2 mg, 0.40 mmol, 2.0 equiv.), $BiCl_3$ (6.4mg, 0.02 mmol), TBACl (11.2 mg, 0.04 mmol) and DCM (2 mL) were added under argon atmosphere. The reaction mixture was stirred under the irradiation of 30 W purple LED (390 nm) at room temperature. After completion of the reaction, the solvent was evaporated under vacuum and the residue was purified by flash chromatography eluting with PE: EA (2:1 v/v) on a silica gel to afford the **4af** as a yellow solid in 45% yield.[2]



Aldehyde **4g** was synthesized according to literature report.[2] 3-carboxybenzaldehyde (5.0 mmol, 750.6 mg) and eplandrosterone (5.0 mmol, 1.453 g) and dry DCM (50 mL) were added sequentially to a dry round-bottom flask at room temperature. The reaction was cooled to 0 ℃ and a catalytic amount of 4-dimethylaminopyridine (DMAP, 0.25 mmol, 0.05 equiv.) and EDCl (5.5 mmol, 1.1 equiv.) were added. The natural return to room temperature and further stirred for 14 hours. Upon completion, the product extracted with DCM (3 × 20 mL). The combined organic phases was washed with brine (20 mL), dried with Na_2SO_4, then filtered and concentrated in vacuo. The crude product was purified by flash column chromatography. The residue was purified by chromatography (PE: EA = 2: 1 v/v) to give **4g** with 52% yield.

Under argon, to an oven dried Schlenk-tube, **4g** (84.6 mg, 0.20 mmol, 1.0 equiv.), N-(trifluoromethylthio)phthalimide (99.2 mg, 0.40 mmol, 2.0 equiv.), $BiCl_3$ (6.4mg, 0.02 mmol), TBACl (11.2 mg, 0.04 mmol) and DCM (2 mL) were added under argon atmosphere. The reaction mixture was stirred under the irradiation of 30 W purple LED (390 nm) at room temperature. After completion of the reaction, the solvent was evaporated under vacuum and the residue was purified by flash chromatography eluting with PE: EA (3:1 v/v) on a silica gel to afford the **4ag** as a yellow solid in 42% yield.[2]

6. Mechanistic Studies



To an oven dried Schlenk-tube, Benzaldehyde (21.4 mg, 0.20 mmol, 1.0 equiv.), N-(trifluoromethylthio)phthalimide (99.2 mg, 0.40 mmol, 2.0 equiv.), $BiCl_3$ (6.4mg, 0.02 mmol), TBACl (11.2 mg, 0.04 mmol), TEMPO (62.6 mg, 0.4 mmol, 2.0 equiv.) and DCM (2 mL). were added under argon atmosphere. The mixture was then stirred rapidly and irradiated with 30 W 390 nm LEDs (approximately 2 cm away from the light source) at room temperature for 10 h. The reaction was suppressed.

To an oven dried Schlenk-tube, Benzaldehyde (21.4 mg, 0.20 mmol, 1.0 equiv.), N-(trifluoromethylthio)phthalimide (99.2 mg, 0.40 mmol, 2.0 equiv.), $BiCl_3$ (6.4mg, 0.02 mmol), TBACl (11.2 mg, 0.04 mmol), 1,1'-(1,2-ethenediyl) dibenzene (0.12 mL,

0.4 mmol, 2.0 equiv.) and DCM (2 mL). were added under argon atmosphere. The mixture was then stirred rapidly and irradiated with 30 W 390 nm LEDs (approximately 2 cm away from the light source) at room temperature for 10 h. The reaction was suppressed. The radical trapping product can be observed by GC-MS.

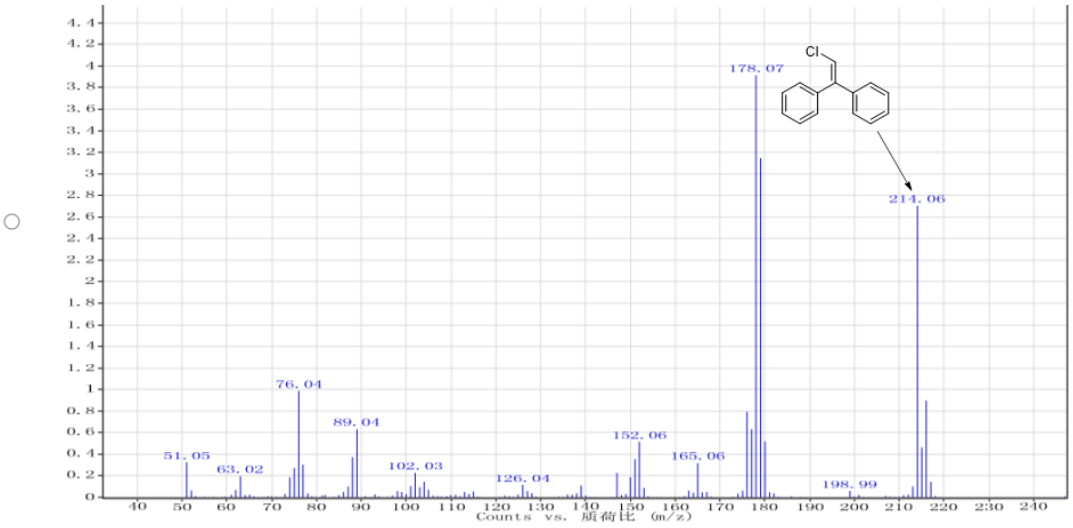
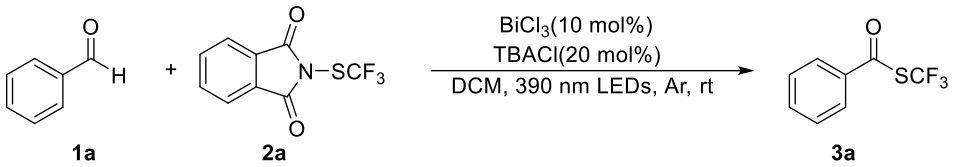


Figure S1 GC-MS analysis of radical trapping adducts

7. Light/Dark experiment



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

To an oven dried Schlenk-tube, benzaldehyde (21.4 mg, 0.20 mmol, 1.0 equiv.), N-(trifluoromethylthio)phthalimide (99.2 mg, 0.40 mmol, 2.0 equiv.), $BiCl_3$ (6.4 mg, 0.02 mmol), TBACl (11.2 mg, 0.04 mmol) and DCM (2 mL) were added under argon atmosphere. The reaction mixture was stirred under the irradiation of 30 W Purple LED (390 nm) at room temperature. The reaction tube was wrapped in tin foil and a 20 μL sample of the reaction mixture was taken with a syringe and measured by GC. After being stirred for 2 hours in dark, a 20 μL sample of the reaction mixture was taken with a syringe and measured by GC. The reaction mixture was then irradiated with a 30 W Purple LED (390 nm) lamp and stirred for 2 hours. This process was repeated four times.

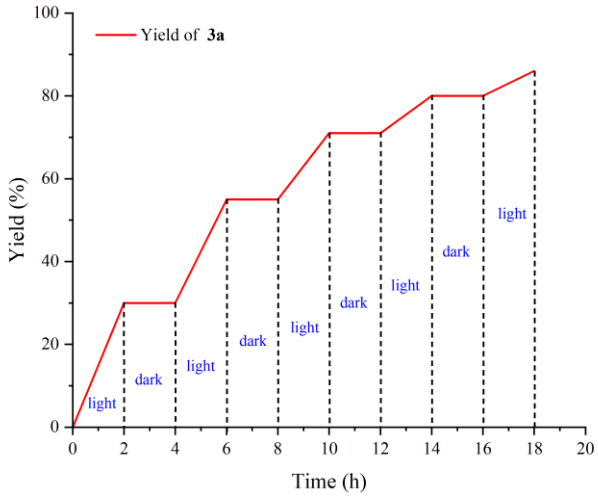


Figure S2 light on-off experiments

8. Measurement of Quantum Yields

The photon flux of purple LEDs was determined by standard ferrioxalate actinometry.

0.15 mol/L solution of ferrioxalate was prepared by dissolving potassium ferrioxalate hydrate (328 mg, 0.750 mmol) in 5.0 mL of 0.20 mol/L aqueous sulfuric acid.

0.15 mol/L buffered solution of 1,10-phenanthroline was prepared by dissolving 1,10-phenanthroline (54.1 mg, 0.3 mmol) and sodium acetate (1.23 g, 15.0 mmol) in 20 mL of 0.20 mol/L aqueous sulfuric acid. The actinometry measurements were done as follows: To a reaction tube equipped with a stir bar was added 0.50 mL of the ferrioxalate solution. The reaction tube was sealed and placed 2 cm away from a 10 W purple LEDs. After irradiation for 30 seconds, 1.5 mL of the aqueous sulfuric acid and 2.0 mL of the buffered solution was added to the reaction tube. The solution was then allowed to rest for 1 hour to allow the resultant ferrous ions to react completely with 1,10-phenanthroline. 50 μL of the resulting solution was taken as an aliquot and diluted with 3.0 mL of 0.20 mol/L aqueous sulfuric acid. The absorbance of the resulting solution in a cuvette (l = 1.0 cm) at 510 nm was measured by UV-Vis spectrometer. A non-irradiated sample was also prepared and the absorbance at 510 nm was measured.

The amount of ferrous ion formed was calculated as follows:

$$mol\,Fe^{2+} = \frac{V \times \Delta A}{l \times \varepsilon}$$

where V is the total volume (0.024 L) of the solution that was analyzed, ΔA is the difference in absorbance at 510 nm between the irradiated and non-irradiated samples,

l is the path length (1.00 cm), and ε is the molar absorptivity at 510 nm (11,100 L/(mol•cm)).

The photon flux was calculated as follows:

$$photo\ flux\ =\ \frac{mol\ Fe^{2+}}{\Phi \times t \times f}$$

where Φ is the quantum yield for the ferrioxalate actinometer, *t* is the irradiation time, and *f* is the fraction of light absorbed at 390 nm (0.2106).

The fraction of light absorbed was determined by the following equation:

$$f\ =\ 1.0000 - 10^{-A}$$

where *A* is the measured absorbance (0.1027) of the 0.15 mol/L solution of potassium ferrioxalate at 390 nm.

The photo flux is 1.66 x 10^{-7} Einstein/s.

Determination of quantum yield:

In an oven-dried reaction tube containing a magnetic stirring bar was charged with a sample of $BiCl_3$(0.02 mmol) in DCM (2 mL) followed by the addition of benzaldehyde **1a** (0.2 mmol), **2a** (0.4 mmol) and TBACl (0.04 mmol). The reaction mixture was stirred under the irradiation of 10 W LED at room temperature and placed 2 cm away from 10 W purple LEDs. After 3 hours of irradiation, the molar number of the product **3a** was determined by ^{19}F NMR spectroscopy with (trifluoromethoxy-benzene) as the internal standard. The yield of **3a** was 16% (0.032 mmol).

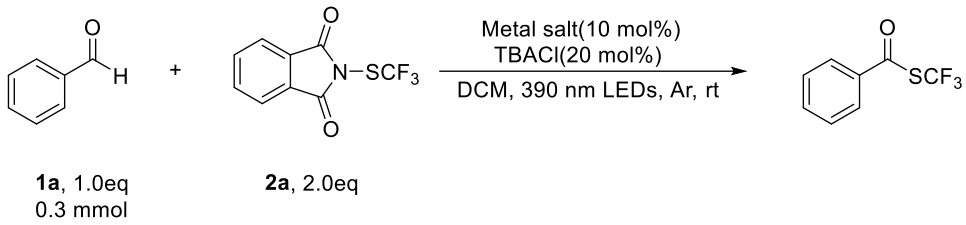
The quantum yield was calculated as follows:

$$\Phi\ =\ \frac{mol\ product}{photon\ flux \times t \times f}$$

Where flux is the photon flux determined by ferrioxalate actinometry (1.66 x 10^{-7} Einstein/s), *t* is the time, and *f* is the fraction of light absorbed by the irradiated reaction system at 390 nm, and the absorbance of the irradiated reaction system at 390 nm was 0.019. The fraction of light absorbed at 390 nm was calculated: $f = 1.0000 - 10^{-A} = 1.0000 - 10^{-0.019} = 0.0428$.

The quantum yield was calculated: Φ = 0.22

9. Kinetics of the Reaction



1a, 1.0eq
0.3 mmol

2a, 2.0eq

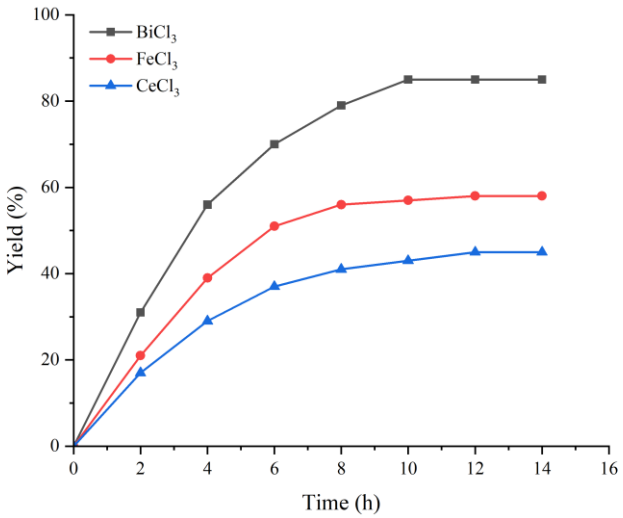


Figure S3 Kinetics spectra of 1a (0.30 mmol) + 2a (0.60 mmol) + Metal salt (10 mol %) + TBACl (20 mol %) in DCM (3mL) under 30 W 390 nm LED irradiation (100% intensity).

10. UV Spectroscopic Studies

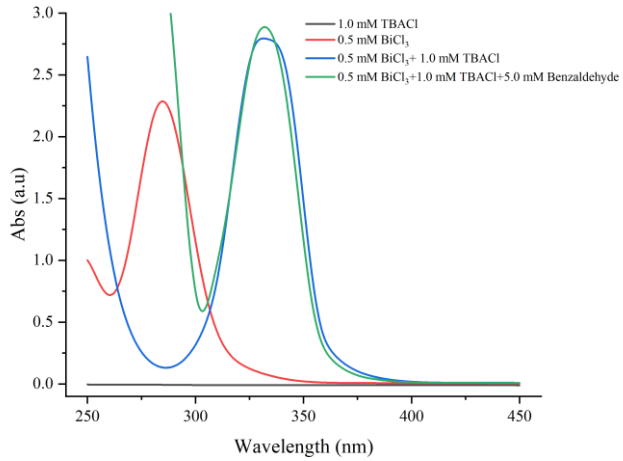
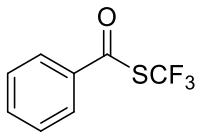
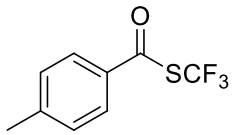


Figure S4 UV-Vis spectroscopic study of reaction mixture

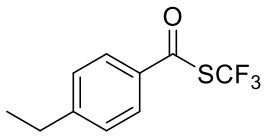
11. Characterization data of products



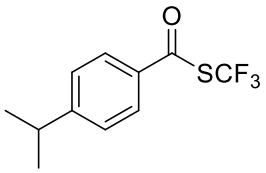
***S*-(trifluoromethyl) benzothioate(3a)**[2]
34.6 mg, 84% yield; Colorless liquid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.86 – 7.82 (m, 2H), 7.66 (t, *J* = 7.5 Hz, 1H), 7.50 (t, *J* = 7.9 Hz, 2H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 183.4, 135.3 (q, *J* = 2.9 Hz), 129.4, 128.3 (q, *J* = 309.5 Hz), 127.8.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.80.



***S*-(trifluoromethyl) 4-methylbenzothioate(3b)**[2]
35.2 mg, 80% yield; Colorless liquid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.75 (d, *J* = 8.3 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 2.44 (s, 3H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 183.0, 146.6, 132.8 (q, *J* = 2.6 Hz), 130.1, 128.3 (q, *J* = 309.3 Hz), 128.0, 22.0.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.59.



***S*-(trifluoromethyl) 4-ethylbenzothioate(3c)**[1]
37.4 mg, 80% yield; Colorless liquid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.78 (d, *J* = 8.4 Hz, 2H), 7.33 (d, *J* = 8.3 Hz, 2H), 2.73 (q, *J* = 7.6 Hz, 2H), 1.27 (t, *J* = 7.6 Hz, 3H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 183.0, 152.7, 133.0 (q, *J* = 2.7 Hz), 129.0, 128.4 (q, *J* = 309.3 Hz), 128.1, 29.3, 15.2.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.58.



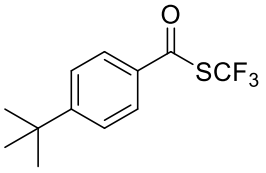
***S*-(trifluoromethyl) 4-isopropylbenzothioate(3d)**[1]

36.2 mg, 73% yield; Colorless liquid

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.79 (d, *J* = 8.5 Hz, 2H), 7.36 (d, *J* = 8.2 Hz, 2H), 3.06 – 2.91 (m, 1H), 1.27 (d, *J* = 6.9 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 183.0, 157.3, 133.1 (q, *J* = 3.0 Hz), 128.4 (q, *J* = 309.0 Hz), 128.2, 127.5, 34.6, 23.8.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.58.



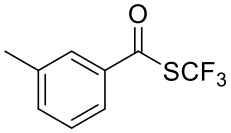
***S*-(trifluoromethyl) 4-(tert-butyl)benzothioate(3e)**[2]

47.6 mg, 91% yield; Colorless liquid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.80 (d, *J* = 8.6 Hz, 2H), 7.52 (d, *J* = 8.6 Hz, 2H), 1.35 (s, 9H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 183.0, 159.5, 132.7 (q, *J* = 2.8 Hz), 128.4 (q, *J* = 309.4 Hz), 127.9, 126.4, 35.6, 31.2.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.57.



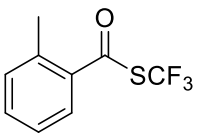
***S*-(trifluoromethyl) 3-methylbenzothioate(3f)**[1]

33. 8mg, 77% yield; Colorless liquid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.69 – 7.63 (m, 2H), 7.48 (d, *J* = 7.6 Hz, 1H), 7.43 – 7.35 (m, 1H), 2.43 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 183.6, 139.5, 136.1, 135.3 (q, *J* = 2.8 Hz), 129.3, 128.3 (q, *J* = 309.4 Hz), 128.2, 125.1, 21.5.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.70.



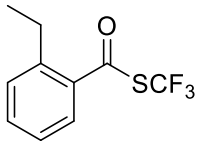
***S*-(trifluoromethyl) 2-methylbenzothioate(3g)**[2]

29. 4mg, 67% yield; Colorless liquid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.73 – 7.68 (m, 1H), 7.49 (t, *J* = 7.5 Hz, 1H), 7.31 (t, *J* = 6.5 Hz, 2H), 2.54 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 184.6, 139.0, 134.7 (q, *J* = 2.6 Hz), 133.8, 132.6, 129.0, 128.2 (q, *J* = 309.8 Hz), 126.5, 21.1.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -40.42.



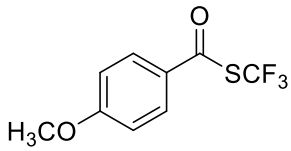
***S*-(trifluoromethyl) 2-ethylbenzothioate(3h)**[2]

30. 4mg, 65% yield; Colorless liquid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.67 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.52 (td, J = 7.6, 1.3 Hz, 1H), 7.37 – 7.28 (m, 2H), 2.87 (q, *J* = 7.5 Hz, 2H), 1.26 – 1.21 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 184.9, 144.8, 134.8 (q, *J* = 2.5 Hz), 133.7, 131.0, 128.8, 128.1 (q, *J* = 309.9 Hz), 126.6, 27.0, 15.9.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -40.61.



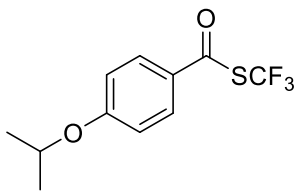
***S*-(trifluoromethyl) 4-methoxybenzothioate(3i)**[2]

38.2 mg, 81% yield; White solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.76 (d, *J* = 9.0 Hz, 2H), 6.89 (d, *J* = 9.0 Hz, 2H), 3.82 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 181.7, 165.3, 130.3, 128.4 (q, *J* = 309.1 Hz), 128.1 (q, *J* = 2.8 Hz), 114.6, 56.0.

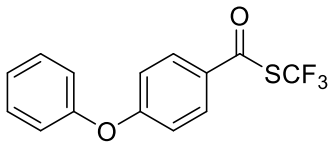
^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.43.



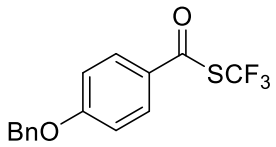
***S*-(trifluoromethyl) 4-isopropoxybenzothioate(3j)**

44.8 mg, 85% yield; Colorless liquid.

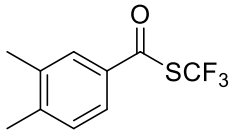
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.80 (d, *J* = 8.9 Hz, 2H), 6.93 (d, *J* = 9.0 Hz, 2H), 4.66 (hept, *J* = 6.0 Hz, 1H), 1.38 (d, *J* = 6.1 Hz, 6H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 181.6, 163.9, 130.4, 128.5 (q, *J* = 309.0 Hz), 127.5 (q, *J* = 2.8 Hz), 115.8, 70.8, 22.0.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.41.
TOFMS-ESI^{+} (m/z) $[M+H]^{+}$ calcd for $C_{11}H_{11}F_3O_2S$ 265.0505, found 265.0507.



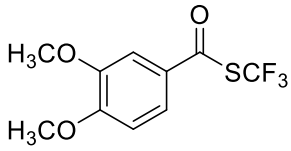
***S*-(trifluoromethyl) 4-phenoxybenzothioate(3k)[1]**
48.8 mg, 82% yield; Colorless liquid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.90 – 7.77 (m, 2H), 7.49 – 7.35 (m, 2H), 7.29 – 7.23 (m, 1H), 7.12 – 7.05 (m, 2H), 7.06 – 6.96 (m, 2H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 181.8, 164.0, 155.0, 130.5, 130.3, 129.5 (q, *J* = 2.9 Hz), 128.3 (q, *J* = 309.4 Hz), 125.5, 120.7, 117.7.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.46.



***S*-(trifluoromethyl) 4-(benzyloxy)benzothioate(3l)[1]**
38.6 mg, 62% yield; White solid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.82 (d, *J* = 8.9 Hz, 2H), 7.45 – 7.33 (m, 5H), 7.03 (d, *J* = 8.9 Hz, 2H), 5.15 (s, 2H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 181.7, 164.4, 135.8, 130.3, 129.0, 128.7, 128.4 (q, *J* = 309.2 Hz), 128.2 (q, *J* = 2.2 Hz), 127.7, 115.5, 70.6.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.41.



***S*-(trifluoromethyl) 3,4-dimethylbenzothioate(3m)[1]**
39. 7mg, 85% yield; Colorless liquid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.63 – 7.54 (m, 2H), 7.24 (d, *J* = 8.0 Hz, 1H), 2.33 (d, *J* = 5.6 Hz, 6H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 183.1, 145.4, 138.1, 133.1 (q, *J* = 2.7 Hz), 130.6, 128.4 (q, *J* = 309.2 Hz), 128.8, 125.6, 20.4, 20.0.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.62.



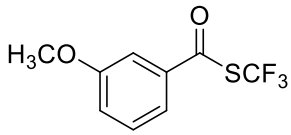
***S*-(trifluoromethyl) 3,4-dimethoxybenzothioate(3n)**[1]

43.6 mg, 82% yield; White solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.51 (dd, *J* = 8.5, 2.2 Hz, 1H), 7.37 (d, *J* = 2.2 Hz, 1H), 6.92 (d, *J* = 8.5 Hz, 1H), 3.97 (s, 3H), 3.94 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 182.0, 155.1, 149.6, 128.4 (q, *J* = 309.2 Hz), 128.1 (q, *J* = 2.7 Hz), 122.9, 110.6, 109.6, 56.5, 56.3.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.49.



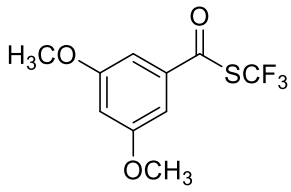
***S*-(trifluoromethyl) 3-methoxybenzothioate(3o)**[1]

34. 4mg, 73% yield; Colorless liquid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.46 – 7.38 (m, 2H), 7.39 – 7.34 (m, 1H), 7.20 (ddd, *J* = 7.5, 2.6, 1.7 Hz, 1H), 3.86 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 183.4, 160.4, 136.6 (q, *J* = 2.6 Hz), 130.4, 128.1 (q, *J* = 309.7 Hz), 121.7, 120.4, 112.0, 55.8.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.77.



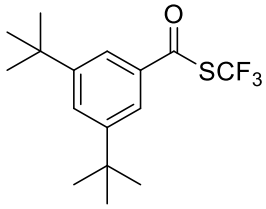
***S*-(trifluoromethyl) 3,5-dimethoxybenzothioate(3p)**[1]

24.4 mg, 46% yield; White solid.

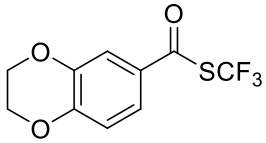
^{1}H NMR (400 MHz, Chloroform-*d*) δ 6.97 (d, *J* = 2.2 Hz, 2H), 6.72 (t, *J* = 2.2 Hz, 1H), 3.84 (s, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 183.5, 161.4, 137.1 (q, *J* = 2.3, 1.8 Hz), 128.2 (d, *J* = 309.6 Hz), 107.4, 105.5, 56.0.

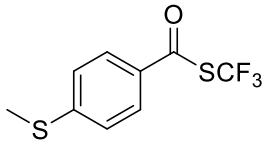
^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.88.



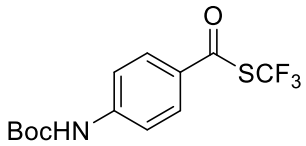
***S*-(trifluoromethyl) 3,5-di-*tert*-butylbenzothioate(3q)**[1]
40.7 mg, 64% yield; White solid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.73 (t, *J* = 1.8 Hz, 1H), 7.68 (d, *J* = 1.8 Hz, 2H), 1.35 (s, 18H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 184.2, 152.5, 135.1 (q, *J* = 2.5 Hz), 129.7, 128.4 (q, *J* = 309.6 Hz), 122.1, 35.3, 31.5.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.74.



***S*-(trifluoromethyl) 2,3-dihydrobenzo[*b*][1,4]dioxine-6-carbothioate(3r)**[1]
40.1 mg, 76% yield; White solid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.42 – 7.35 (m, 2H), 6.94 (d, *J* = 8.8 Hz, 1H), 4.38 – 4.31 (m, 2H), 4.33 – 4.26 (m, 2H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 181.7, 149.9, 144.0, 129.9, 128.7 (q, *J* = 2.7 Hz), 126.8, 122.1, 118.1, 117.3, 65.0, 64.3.
^{13}C NMR (101 MHz, Chloroform-*d*) δ 181.7, 150.0, 144.0, 128.7 (q, *J* = 2.7 Hz), 128.4 (q, *J* = 309.3 Hz), 122.1, 118.1, 117.3, 65.0, 64.3.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.56.



***S*-(trifluoromethyl) 4-(methylthio)benzothioate(3s)**[3]
35.7 mg, 71% yield; White solid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.75 (d, *J* = 8.6 Hz, 2H), 7.28 (d, *J* = 8.6 Hz, 2H), 2.53 (s, 3H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 182.3, 149.4, 131.3 (q, *J* = 2.8 Hz), 128.4 (q, *J* = 309.7 Hz), 128.2, 125.4, 14.8.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.43.



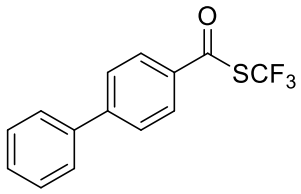
***S*-(trifluoromethyl)4-((*tert*-butoxycarbonyl)amino)benzothioate(3t)**[3]

46.2 mg, 72% yield; White solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.80 (d, *J* = 8.8 Hz, 2H), 7.50 (d, *J* = 8.8 Hz, 2H), 6.82 (s, 1H), 1.53 (s, 9H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 181.9, 152.6, 145.0, 129.6, 129.5 (q, *J* = 2.5 Hz), 128.4 (q, *J* = 309.4 Hz), 117.9, 82.1, 28.4.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.42.



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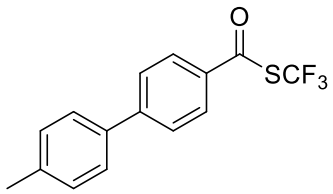
***S*-(trifluoromethyl) [1,1'-biphenyl]-4-carbothioate(3u)**[1]

41.7 mg, 74% yield; White solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83 (d, *J* = 8.5 Hz, 2H), 7.63 (d, *J* = 8.5 Hz, 2H), 7.53 (d, *J* = 7.2 Hz, 2H), 7.45 – 7.30 (m, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 183.0, 148.1, 139.3, 133.9 (q, *J* = 2.8 Hz), 129.3, 129.0, 128.5, 128.3 (q, *J* = 309.5 Hz), 127.9, 127.5.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.49.



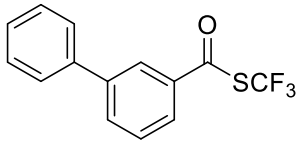
***S*-(trifluoromethyl) 4'-methyl-[1,1'-biphenyl]-4-carbothioate(3v)**[4]

31.3 mg, 53% yield; White solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83 (d, *J* = 8.5 Hz, 2H), 7.62 (d, *J* = 8.5 Hz, 2H), 7.44 (d, *J* = 8.1 Hz, 2H), 7.21 (d, *J* = 7.9 Hz, 2H), 2.34 (s, 3H).

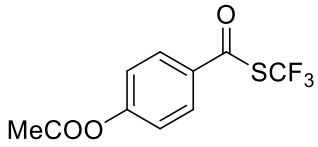
^{13}C NMR (101 MHz, Chloroform-*d*) δ 182.9, 148.1, 139.2, 136.4, 133.7 (q, *J* = 2.6 Hz), 130.1, 128.5, 128.3 (q, *J* = 309.5 Hz), 127.7, 127.4, 21.4.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.50.

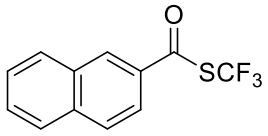


***S*-(trifluoromethyl) [1,1'-biphenyl]-3-carbothioate(3w)**[1]

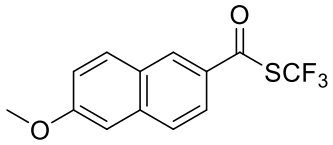
47.3 mg, 84% yield; White solid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.05 (s, 1H), 7.88 (d, *J* = 7.8 Hz, 1H), 7.82 (d, *J* = 7.9 Hz, 1H), 7.59 (d, *J* = 7.9 Hz, 3H), 7.48 (t, *J* = 7.5 Hz, 2H), 7.41 (t, *J* = 7.3 Hz, 1H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 183.6, 142.8, 139.4, 135.9 (q, *J* = 2.7 Hz), 133.8, 129.9, 129.3, 128.5, 128.2 (q, *J* = 309.7 Hz), 127.4, 126.5, 126.4.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.60.



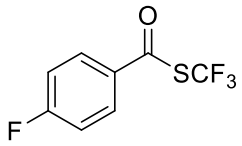
4-(((trifluoromethyl)thio)carbonyl)phenyl acetate(3x)
21.6 mg, 41% yield; Yellow liquid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.90 (d, *J* = 8.9 Hz, 2H), 7.26 (d, *J* = 8.8 Hz, 2H), 2.34 (s, 3H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 182.3, 168.7, 156.0, 132.7 (q, *J* = 2.7 Hz), 129.6, 128.1 (q, *J* = 309.5 Hz), 122.7, 21.4.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.57.
TOFMS-ESI^{+} (m/z) $[M+H]^{+}$ calcd for $C_{10}H_7F_3O_3S$ 265.0141, found 265.0141.



***S*-(trifluoromethyl) naphthalene-2-carbothioate(3y)**[2]
24.5 mg, 48% yield; White solid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.40 (s, 1H), 8.02 – 7.83 (m, 4H), 7.71 – 7.57 (m, 2H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 183.4, 136.6, 132.7 (q, *J* = 2.7 Hz), 132.5, 130.1, 130.0, 129.8, 129.5, 128.3 (q, *J* = 309.6 Hz), 128.2, 127.8, 122.8.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.51.



***S*-(trifluoromethyl) 6-methoxynaphthalene-2-carbothioate(3z)**[1]
29.1 mg, 51% yield; White solid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.32 (s, 1H), 7.90 – 7.76 (m, 3H), 7.29 – 7.21 (m, 1H), 7.16 (d, *J* = 2.5 Hz, 1H), 3.96 (s, 3H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 183.0, 160.9, 138.6, 131.6, 130.6 (q, *J* = 2.5 Hz), 130.0, 128.8 (q, *J* = 309.7 Hz), 128.0, 127.8, 123.6, 120.8, 106.1, 55.8.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.42.



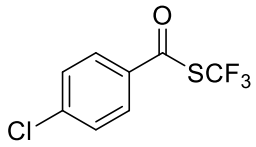
***S*-(trifluoromethyl) 4-fluorobenzothioate(3aa)**[2]

29.1 mg, 65% yield; Yellow liquid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 – 7.77 (m, 2H), 7.13 (t, *J* = 8.5 Hz, 2H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 182.04, 167.00 (d, *J* = 258.5 Hz), 131.67 (q, *J* = 2.9 Hz), 130.63 (d, *J* = 9.7 Hz), 128.06 (q, *J* = 309.7 Hz), 116.81 (d, *J* = 22.4 Hz).

^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.54, -100.96.



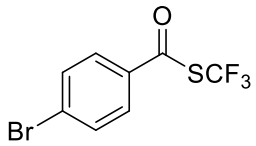
***S*-(trifluoromethyl) 4-chlorobenzothioate(3ab)**[2]

22.0 mg, 46% yield; White solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.74 (d, *J* = 8.7 Hz, 2H), 7.43 (d, *J* = 8.7 Hz, 2H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 182.4, 142.0, 133.7 (q, *J* = 2.8 Hz), 129.8, 129.2, 128.0 (q, *J* = 309.8 Hz).

^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.53.



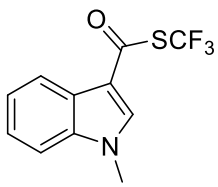
***S*-(trifluoromethyl) 4-bromobenzothioate(3ac)**[2]

21.6 mg, 38% yield; White solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.72 (d, *J* = 8.7 Hz, 1H), 7.66 (d, *J* = 8.7 Hz, 1H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 182.6, 134.1 (q, *J* = 2.9 Hz), 130.7, 129.2, 127.7 (d, *J* = 309.9 Hz).

^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.53.

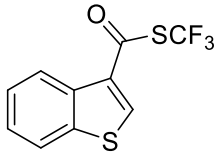


***S*-(trifluoromethyl) 1-methyl-1H-indole-3-carbothioate(3ad)**[2]

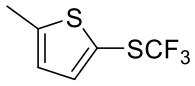
44.0 mg, 85% yield; White solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.17 – 8.12 (m, 1H), 7.69 (s, 1H), 7.37 – 7.29 (m, 3H), 3.83 (s, 3H).

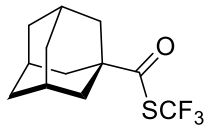
^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.9, 137.7, 136.0, 128.8(q, *J* = 308.9 Hz), 125.5, 124.5, 123.7, 121.9, 114.3 (q, *J* = 3.2 Hz), 110.4, 34.1.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -38.22.



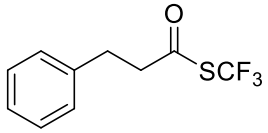
S-(trifluoromethyl) benzo[b]thiophene-3-carbothioate(3ae)[2]
23.5 mg, 45% yield; White solid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.51 (d, *J* = 8.1 Hz, 1H), 8.36 (s, 1H), 7.89 (d, *J* = 7.8 Hz, 1H), 7.61 – 7.43 (m, 2H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 176.3, 139.9, 138.4, 135.3, 132.9 (q, *J* = 2.9 Hz), 128.1 (q, *J* = 309.7 Hz), 126.8, 126.6, 124.9, 122.7.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.13.



2-methyl-5-((trifluoromethyl)thio)thiophene(3af)[1]
21.6 mg, 48% yield; Colorless liquid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.58 (d, *J* = 3.9 Hz, 1H), 6.85 (dd, *J* = 3.9, 1.0 Hz, 1H), 2.57 (s, 3H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.1, 152.7, 137.1 (q, *J* = 3.5 Hz), 134.1, 128.1 (q, *J* = 309.6 Hz), 127.4, 16.4.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -38.84.

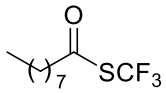


S-(trifluoromethyl) adamantane-1-carbothioate(3ag)[2]
35.9 mg, 68% yield; White solid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 2.09 (s, 3H), 1.91 (d, *J* = 2.6 Hz, 6H), 1.73 (q, *J* = 12.4 Hz, 6H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 197.5, 128.7 (q, *J* = 309.3 Hz), 50.3 (q, *J* = 2.5 Hz), 38.8, 36.3, 28.1.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.92.

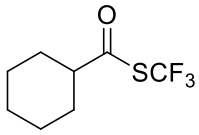


S-(trifluoromethyl) 3-phenylpropanethioate(3ah)[4]

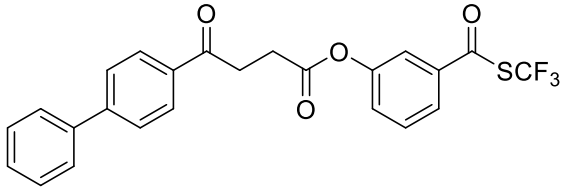
21.5 mg, 46% yield; Colorless liquid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.33 – 7.28 (m, 2H), 7.25 – 7.21 (m, 1H), 7.20 – 7.17 (m, 2H), 3.04 – 2.98 (m, 2H), 2.97 – 2.91 (m, 2H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 189.8, 139.0, 129.0, 128.9, 128.5, 127.8(q, *J* = 310.1 Hz), 127.0, 46.3 (q, *J* = 2.7 Hz), 30.7.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -40.13.



S-(trifluoromethyl) decanethioate(3ai)[4]
38. 4mg, 75% yield; Colorless liquid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 2.61 (t, *J* = 7.4 Hz, 2H), 1.69 (p, *J* = 7.4 Hz, 2H), 1.38 – 1.21 (m, 12H), 0.88 (t, *J* = 6.9 Hz, 3H).
13C NMR (101 MHz, Chloroform-*d*) δ 190.6, 128.0 (q, *J* = 309.9 Hz), 44.9 (q, *J* = 2.7 Hz), 32.0, 29.5, 29.4, 29.3, 28.9, 24.9, 22.9, 14.3.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -40.24.

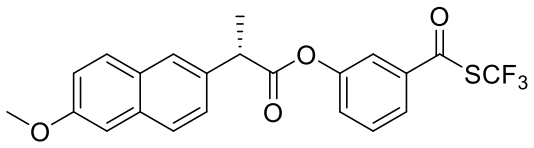


S-(trifluoromethyl) cyclohexanecarbothioate(3aj)[2]
30. 5mg, 72% yield; Colorless liquid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 2.49 (tt, *J* = 11.2, 3.6 Hz, 1H), 2.01 – 1.92 (m, 2H), 1.87 – 1.76 (m, 2H), 1.73 – 1.63 (m, 1H), 1.54 – 1.42 (m, 2H), 1.38 – 1.18 (m, 3H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.0, 128.2 (q, *J* = 309.7 Hz), 53.4 (q, *J* = 2.4 Hz), 28.0, 25.5, 25.3.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -40.09.

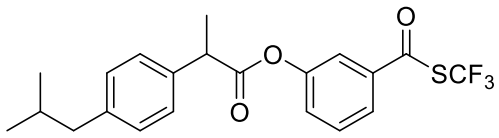


3-(((trifluoromethyl)thio)carbonyl)phenyl-4-([1,1'-biphenyl]-4-yl)-4-oxobutanoate(4aa)[1]
43.9 mg, 48% yield; Yellow solid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.12 – 8.05 (m, 1H), 7.66 – 7.61 (m, 2H), 7.54 (t, *J* = 7.9 Hz, 1H), 7.48 (ddt, *J* = 7.5, 6.1, 1.3 Hz, 2H), 7.44 – 7.37 (m, 1H), 3.48 (t, *J* = 6.4 Hz, 1H), 3.06 (t, *J* = 6.4 Hz, 1H).

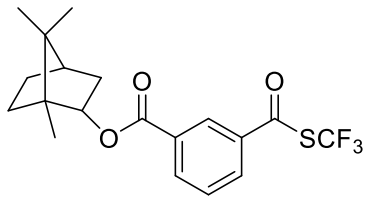
^{13}C NMR (101 MHz, Chloroform-*d*) δ 197.5, 182.7, 171.4, 151.4, 146.4, 140.0, 136.6 (q, *J* = 2.7 Hz), 130.5, 129.2, 128.9, 128.8, 128.6, 128.0 (q, *J* = 309.7 Hz), 127.6, 127.5, 125.2, 124.6, 121.0, 33.6, 28.7.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.63.



3-(((trifluoromethyl)thio)carbonyl)phenyl-(*S*)-2-(6-methoxynaphthalen-2-yl)propanoate(4ab)
39.0 mg, 45% yield; White solid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.80 – 7.71 (m, 3H), 7.68 (ddd, *J* = 7.8, 1.8, 1.0 Hz, 1H), 7.53 – 7.42 (m, 3H), 7.29 (ddd, *J* = 8.2, 2.3, 1.0 Hz, 1H), 7.21 – 7.12 (m, 2H), 4.12 (q, *J* = 7.1 Hz, 1H), 3.93 (s, 3H), 1.71 (d, *J* = 7.1 Hz, 3H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 182.7, 173.0, 158.1, 151.5, 136.5 (q, *J* = 2.5 Hz), 134.7, 134.1, 130.4, 129.5, 129.2, 128.5, 127.8, 127.7(q, *J* = 309.2 Hz), 126.4, 126.1, 125.1, 120.9, 119.5, 105.8, 55.6, 45.7, 18.6.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.66.
TOFMS-ESI^{+} (m/z) $[M+H]^{+}$ calcd for $C_{22}H_{17}F_3O_4S$ 435.0872, found 435.0878.

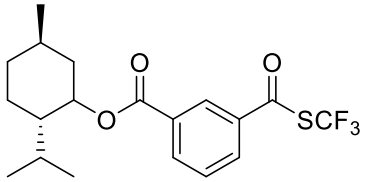


3-(((trifluoromethyl)thio)carbonyl)phenyl-2-(4-isobutylphenyl)propanoate(4ac)[1]
36. 9mg, 45% yield; Colorless liquid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.71 – 7.65 (m, 1H), 7.51 – 7.45 (m, 2H), 7.33 – 7.27 (m, 3H), 7.16 (d, *J* = 8.1 Hz, 2H), 3.96 (q, *J* = 7.1 Hz, 1H), 2.48 (d, *J* = 7.2 Hz, 2H), 1.87 (dp, *J* = 13.7, 6.8 Hz, 1H), 1.62 (d, *J* = 7.2 Hz, 3H), 0.91 (d, *J* = 6.6 Hz, 6H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 182.7, 173.0, 151.6, 141.4, 136.9, 136.5 (q, *J* = 2.7 Hz), 130.4, 129.9, 128.5, 127.4, 126.5, 125.1, 124.9 (d, *J* = 309.6 Hz), 120.9, 45.4, 45.2, 30.4, 22.6, 18.6.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.66.

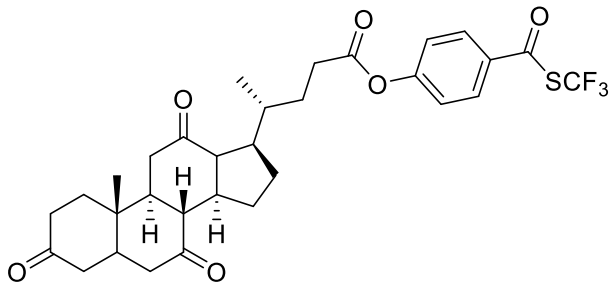


(2*S*)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl-3-(((trifluoromethyl)thio)carbonyl) benzoate(4ad)
40. 9mg, 53% yield; Colorless liquid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.51 (t, *J* = 1.6 Hz, 1H), 8.34 (dt, *J* = 7.8, 1.4 Hz, 1H), 8.05 (dt, *J* = 7.9, 1.6 Hz, 1H), 7.63 (t, *J* = 7.8 Hz, 1H), 5.16 (ddd, *J* = 10.0, 3.5, 2.2 Hz, 1H), 2.56 – 2.44 (m, 1H), 2.10 (ddd, *J* = 13.4, 9.4, 4.4 Hz, 1H), 1.84 (tq, *J* = 12.1, 4.2 Hz, 1H), 1.77 (t, *J* = 4.5 Hz, 1H), 1.52 – 1.39 (m, 1H), 1.33 (ddd, *J* = 12.2, 9.5, 4.5 Hz, 1H), 1.13 (dd, *J* = 13.9, 3.5 Hz, 1H), 0.98 (s, 3H), 0.93 (d, *J* = 2.1 Hz, 6H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 183.1, 165.4, 135.8, 135.6 (q, *J* = 2.0 Hz), 132.4, 131.5, 129.7, 129.5, 128.8, 128.1 (q, *J* = 309.9 Hz), 81.8, 49.4, 48.2, 45.2, 37.1, 28.3, 27.6, 20.0, 19.1, 13.8.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.5
TOFMS-ESI^{+} (m/z) $[M+H]^{+}$ calcd for $C_{19}H_{21}F_3O_3S$ 387.1236, found 387.1221.

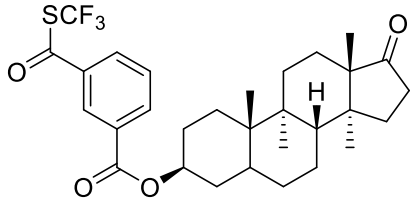


(2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl-3-(((trifluoromethyl)thio)carbonyl)benzoate(4ae)[3]
39. 5mg, 51% yield; Colorless liquid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.49 (t, *J* = 1.6 Hz, 1H), 8.33 (dt, *J* = 7.8, 1.4 Hz, 1H), 8.03 (ddd, *J* = 7.8, 1.8, 1.2 Hz, 1H), 7.62 (t, *J* = 7.8 Hz, 1H), 4.98 (td, *J* = 10.9, 4.4 Hz, 1H), 2.19 – 2.05 (m, 1H), 1.92 (ddq, *J* = 11.2, 7.0, 4.2, 3.5 Hz, 1H), 1.83 – 1.68 (m, 2H), 1.62 – 1.52(m, 3H), 1.21 – 1.05 (m, 2H), 0.94 (dd, *J* = 6.7, 5.6 Hz, 6H), 0.81 (d, *J* = 7.0 Hz, 3H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 183.1, 164.7, 135.9, 135.6 (q, *J* = 2.7 Hz), 132.4, 131.5, 129.7, 128.9,128.0 (q, *J* = 310.3 Hz), 76.1, 47.4, 41.1, 34.4, 31.7, 26.8, 23.8, 22.2, 21.0, 16.7.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.57.



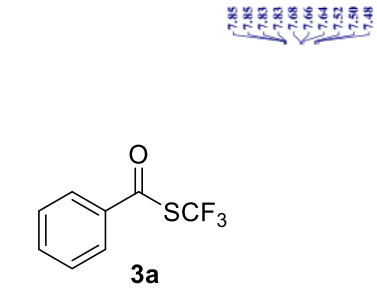
4-(((trifluoromethyl)thio)carbonyl)phenyl-(4*R*)-4-((8*S*,9*S*,10*S*,14*R*,17*R*)-10-methyl-3,7,12-trioxohexadecahydro-1*H*-cyclopenta[*a*]phenanthren-17-yl)pentanoate(4af)[2]
53.2 mg, 45% yield; White solid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.90 (d, *J* = 8.7 Hz, 2H), 7.26 (d, *J* = 7.7 Hz, 2H), 2.96 – 2.80 (m, 3H), 2.72 – 2.65 (m, 1H), 2.60 – 2.51 (m, 1H), 2.39 – 2.13 (m,

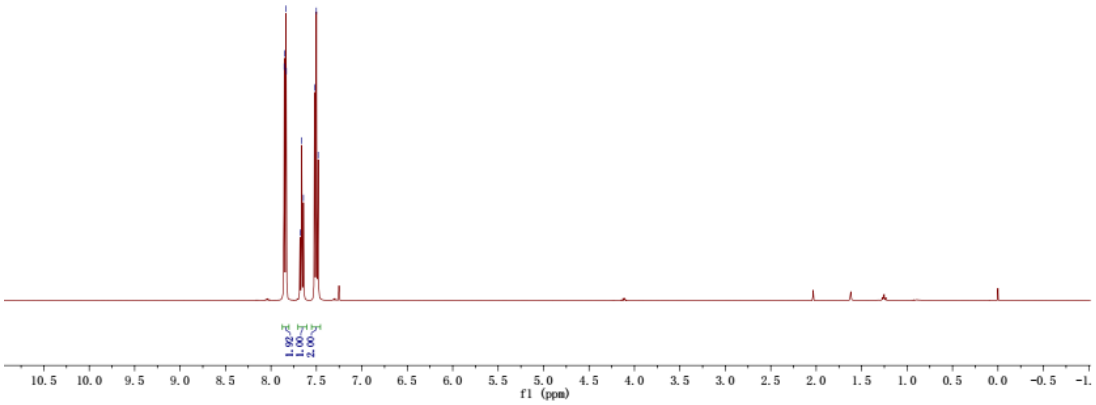
8H), 2.10 – 1.94 (m, 5H), 1.87 (td, *J* = 11.4, 7.1 Hz, 1H), 1.69 – 1.49 (m, 3H), 1.41 (s, 3H), 1.10 (s, 3H), 0.92 (d, *J* = 6.6 Hz, 3H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 212.2, 209.3, 208.9, 182.3, 171.9, 156.1, 133.3 (d, *J* = 3.7 Hz), 132.6 (q, *J* = 2.8 Hz), 129.5, 128.1 (q, *J* = 309.8 Hz), 122.7, 122.6, 57.1, 52.0, 49.2, 47.0, 45.7, 45.2, 43.0, 38.8, 36.7, 36.2, 35.7, 35.4, 31.7, 30.4, 27.9, 25.3, 22.1, 18.9, 12.1.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.55.

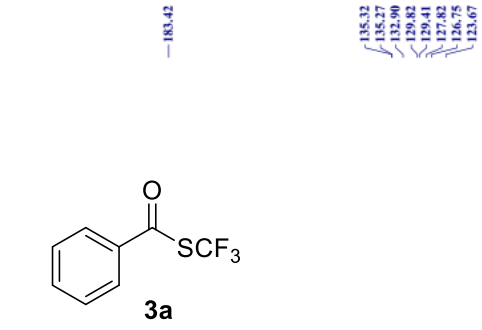


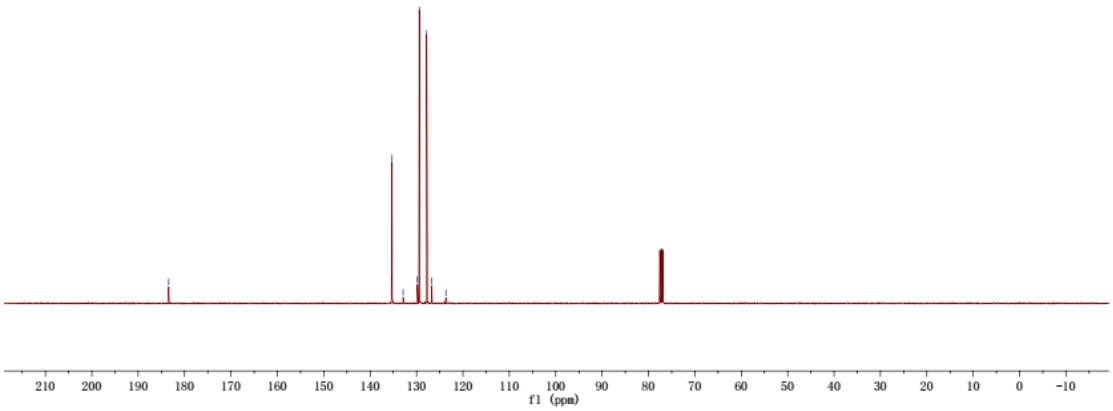
(3*S*,8*R*,9*S*,10*S*,13*S*,14*S*)-9,10,13,14-tetramethyl-17-oxohexadecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl-3-(((trifluoromethyl)thio)carbonyl)benzoate(4ag)[2]
43.8 mg, 42% yield; White solid.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.48 (s, 1H), 8.33 (d, *J* = 7.8 Hz, 1H), 8.03 (d, *J* = 7.9 Hz, 1H), 7.61 (t, *J* = 7.8 Hz, 1H), 4.99 (tt, *J* = 11.1, 4.9 Hz, 1H), 2.45 (dd, *J* = 19.2, 8.7 Hz, 1H), 2.14 – 2.03 (m, 1H), 2.01 – 1.90 (m, 2H), 1.87 – 1.75 (m, 4H), 1.74 – 1.45 (m, 8H), 1.41 – 1.20 (m, 8H), 1.08 (dtd, *J* = 37.5, 12.5, 12.1, 4.1 Hz, 2H), 0.90 (d, *J* = 17.6 Hz, 6H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 183.1, 164.7, 135.9, 135.5 (q, *J* = 2.8 Hz), 132.3, 131.5, 129.6, 128.8, 128.0 (q, *J* = 309.9 Hz), 75.3, 54.5, 51.6, 48.0, 44.9, 36.9, 36.1, 35.9, 35.2, 34.2, 31.7, 31.0, 28.5, 27.7, 22.0, 20.7, 14.0, 12.5.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -39.57.

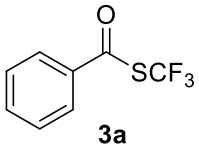
12. NMR spectra










O
SCF3

3a

-39.80
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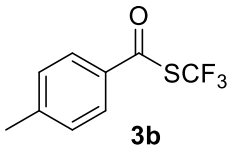
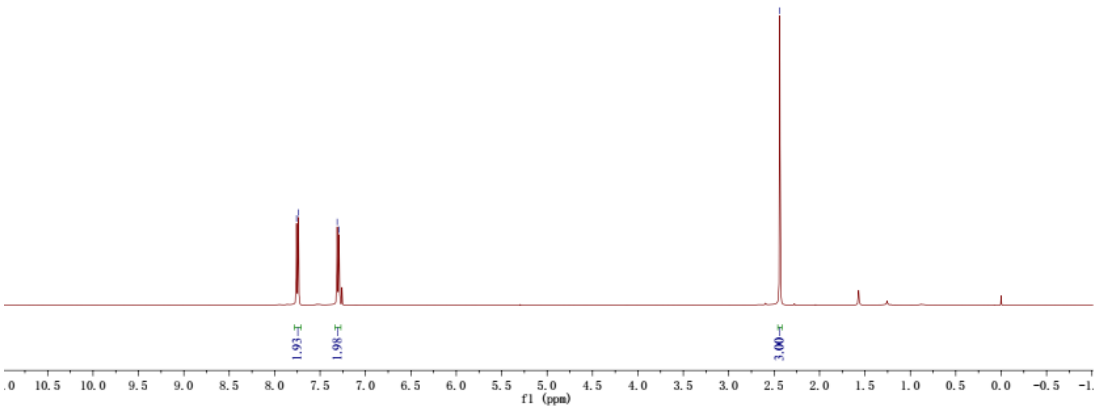
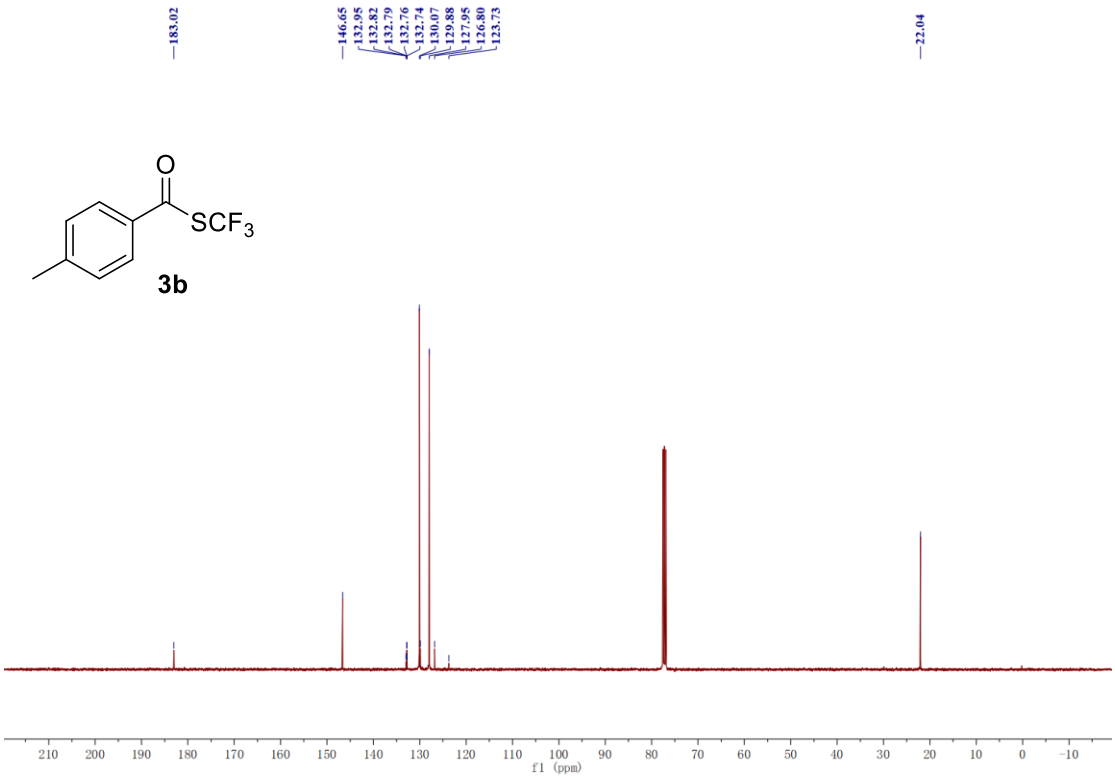
f1 (ppm)

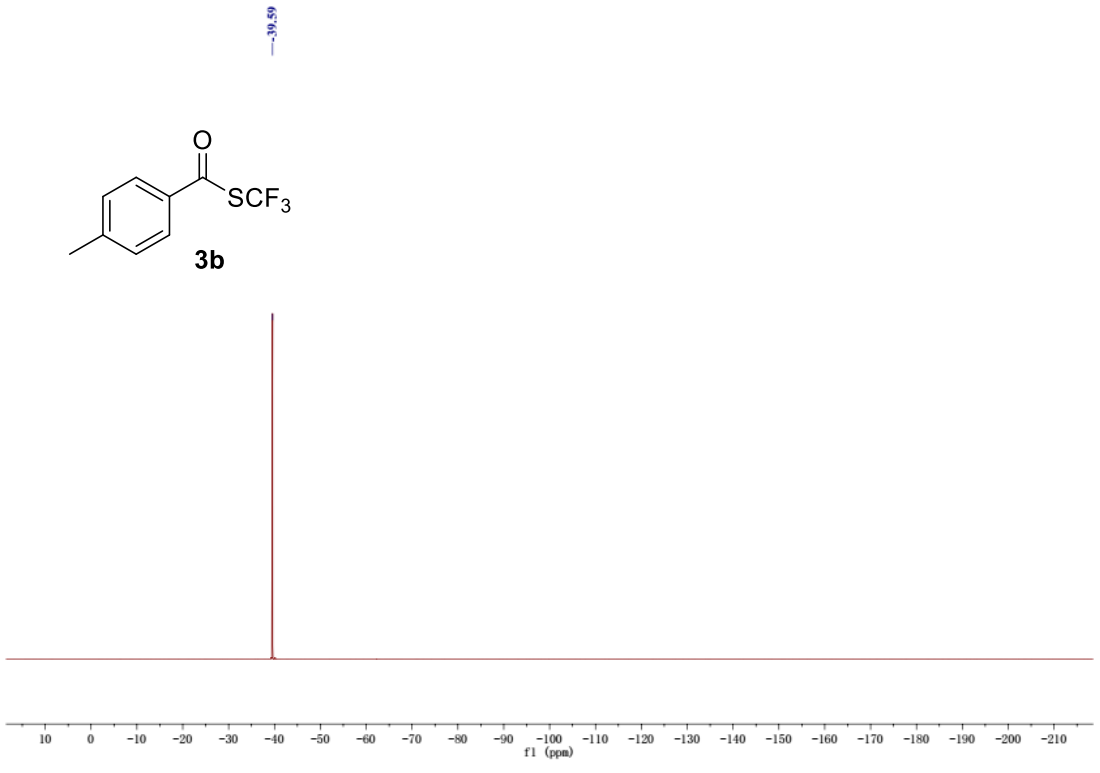
7.76
7.74
7.31
7.29
2.44

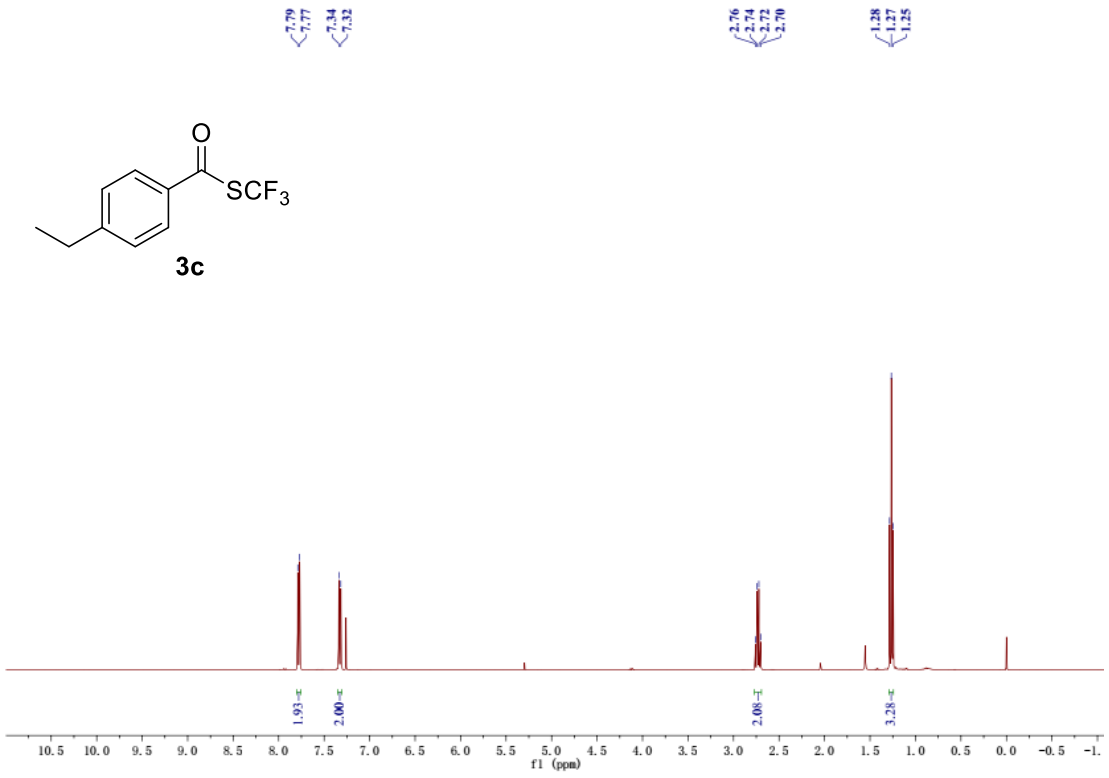

O
SCF3

3b

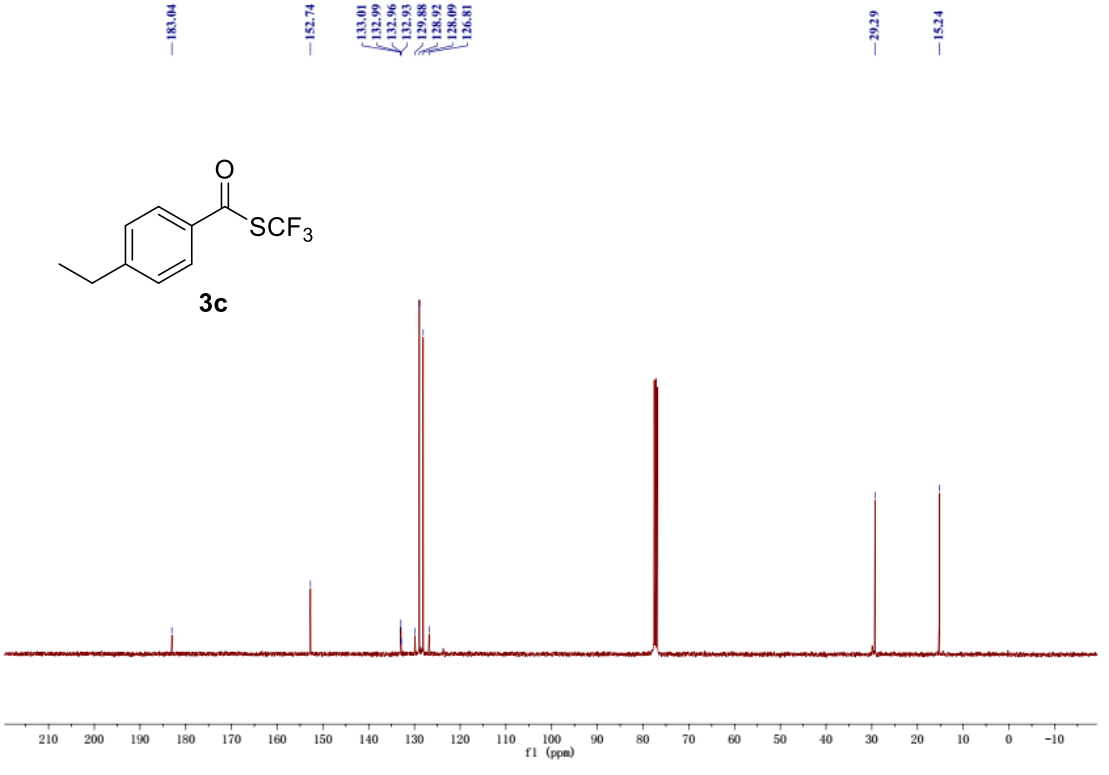

1.93
1.98
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


183.02
146.65
132.95
132.82
132.79
132.76
132.74
130.07
129.88
127.95
126.80
123.73
22.04
O
SCF3
3b
f1 (ppm)


-39.59
O
SCF3
3b
f1 (ppm)


7.79
7.77
7.34
7.32
2.76
2.74
2.72
2.70
1.28
1.27
1.25
O
SCF3
1.93
2.00
2.08
3.28
f1 (ppm)

3c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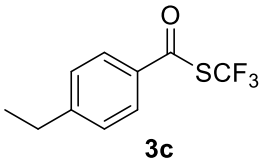
152.74
133.01
132.99
132.96
132.93
129.88
128.92
128.09
126.81
29.39
15.24
O
SCF3
f1 (ppm)

3c


O
SCF3

3c

-39.58
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f1 (ppm)
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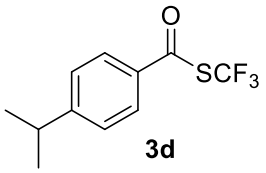
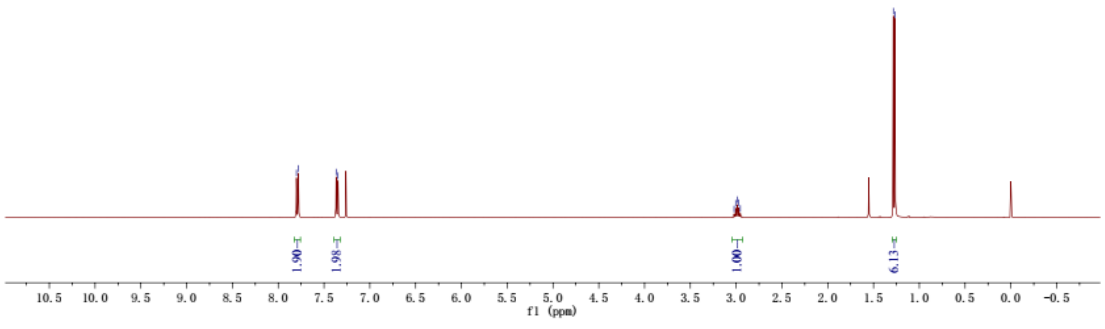
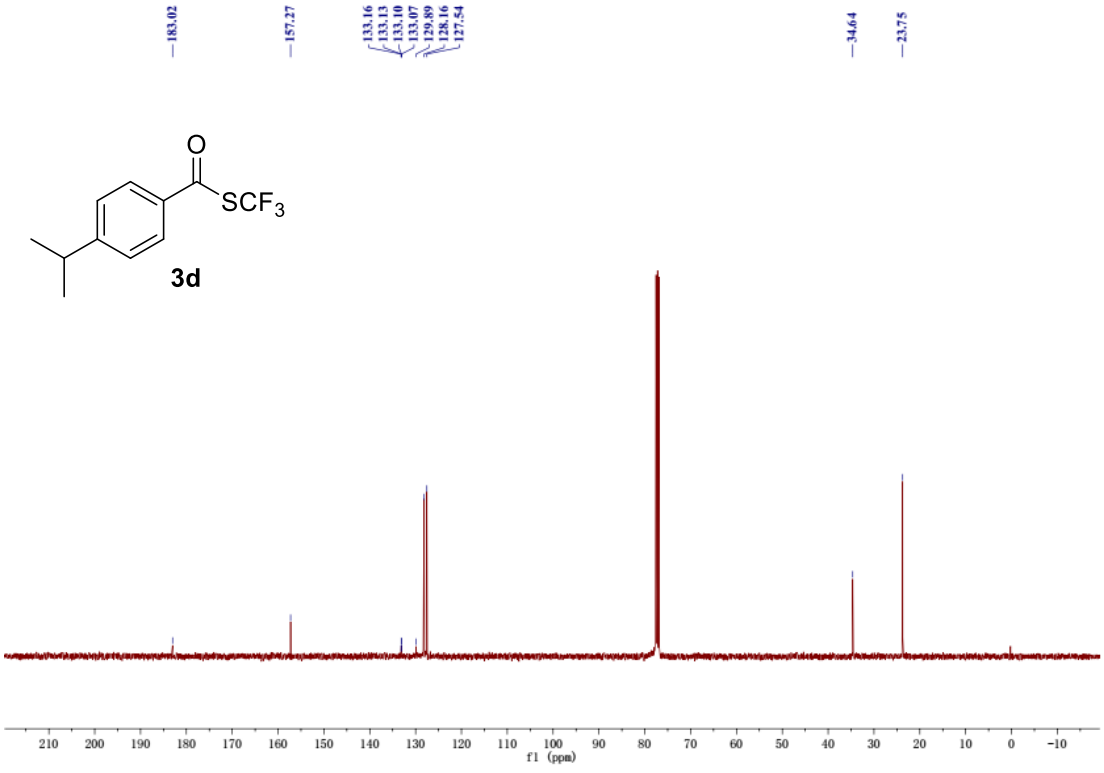
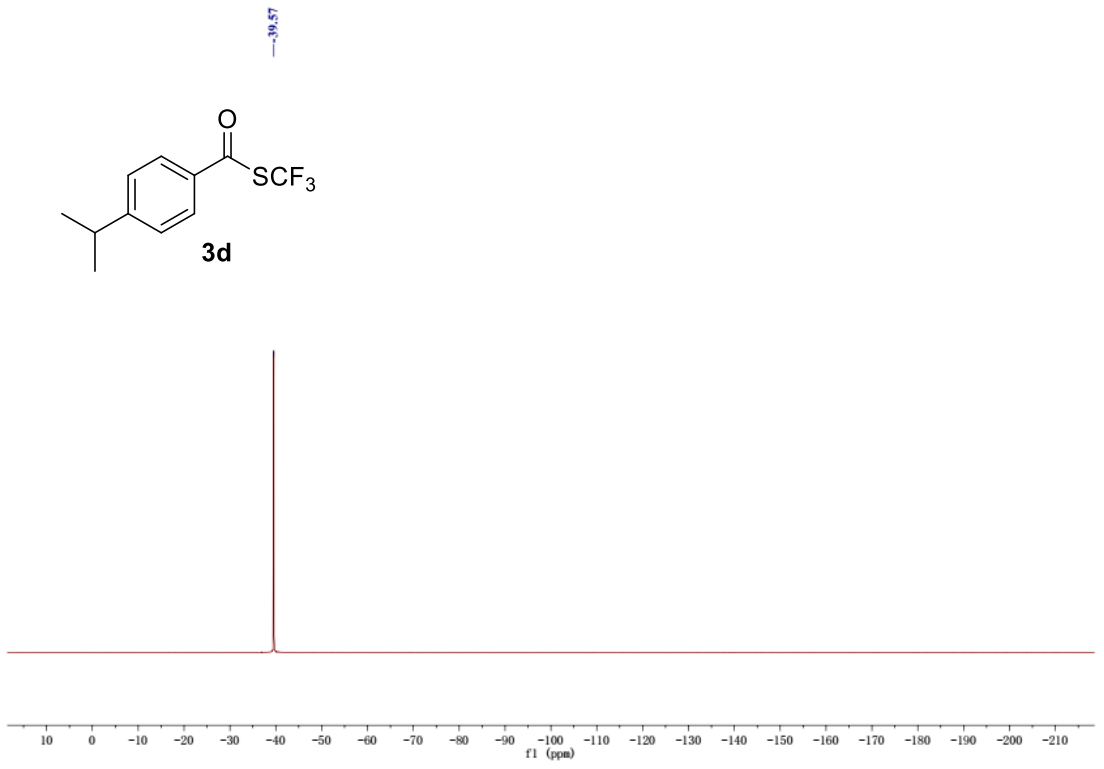
7.78
7.37
7.35
3.02
3.01
2.99
2.97
2.95
1.28
1.27

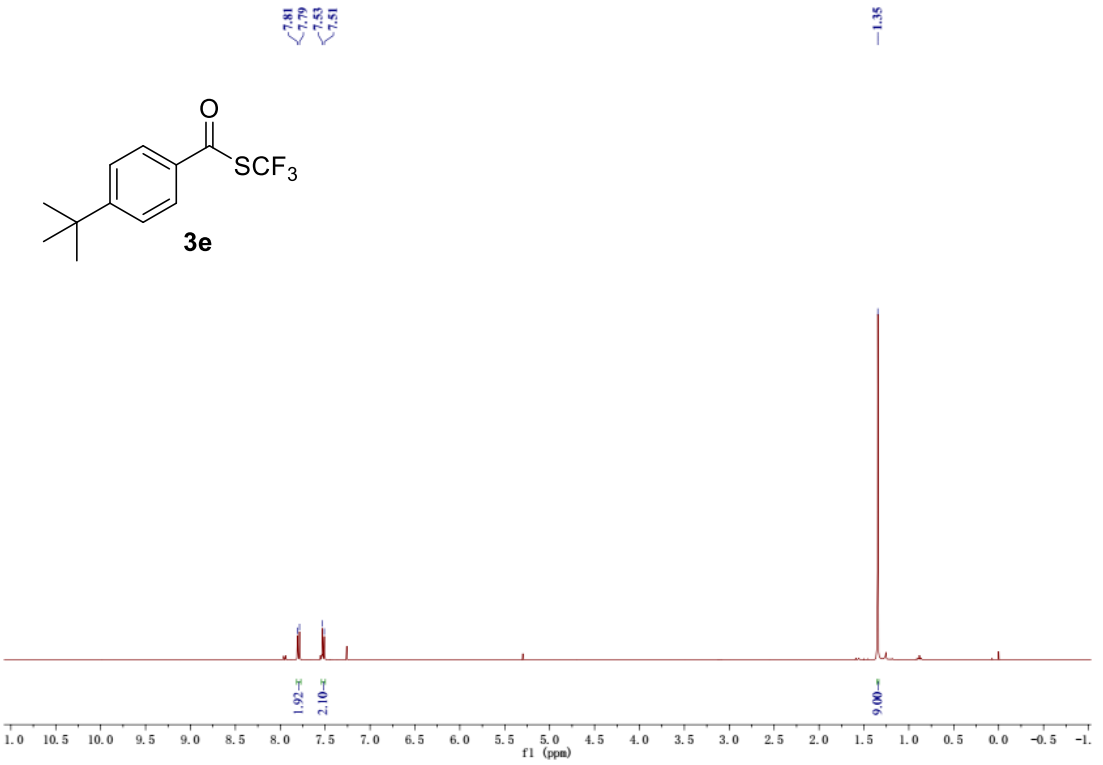

O
SCF3

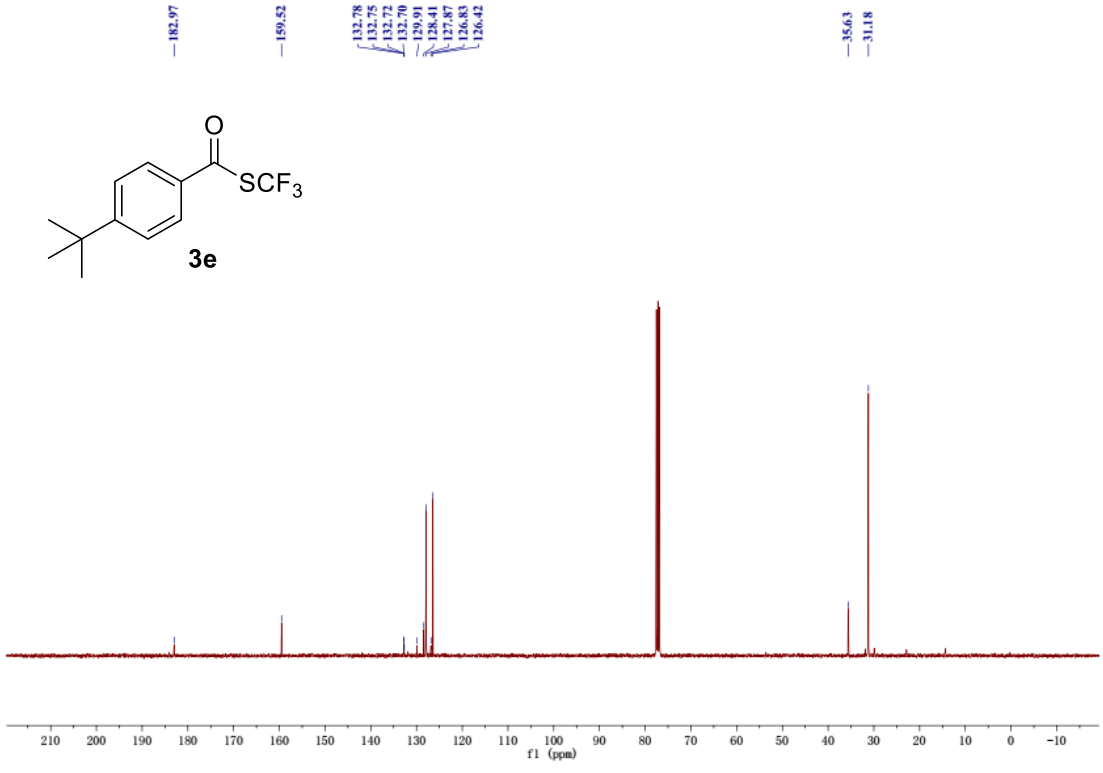
3d

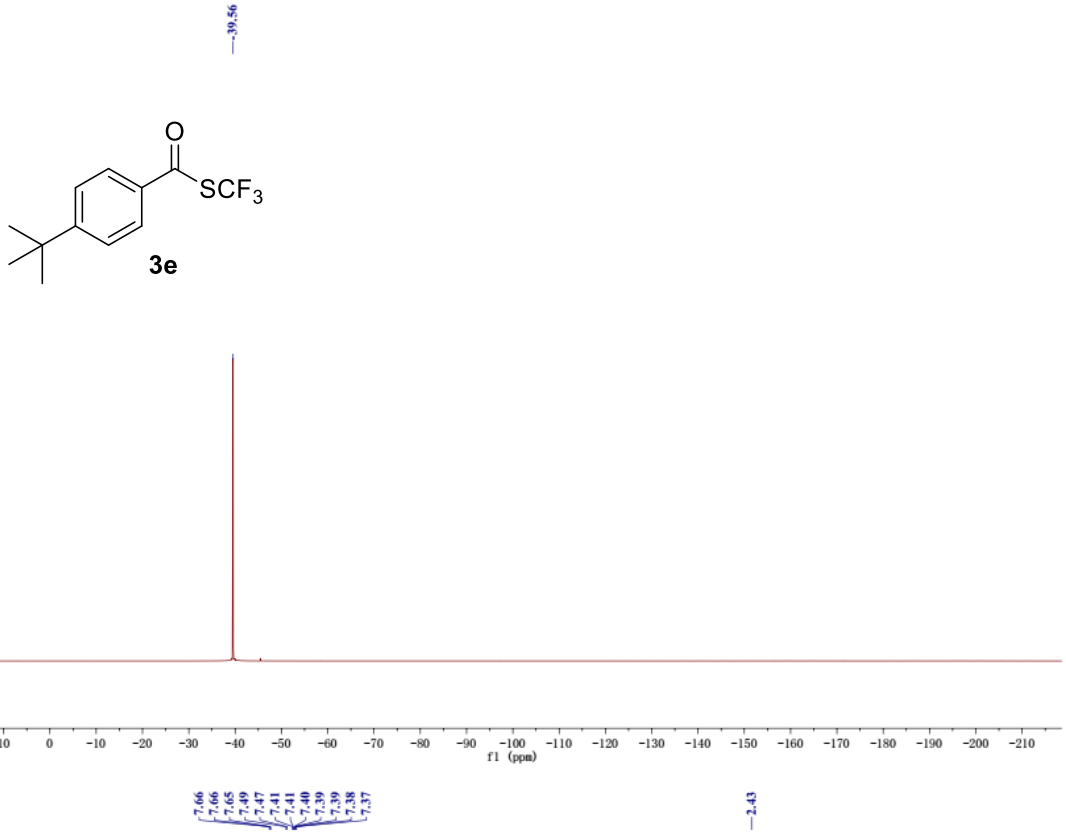

1.90
1.98
1.00
6.13
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


183.02
157.27
133.16
133.13
133.10
133.07
129.89
128.16
127.54
34.64
23.75
O
SCF3
3d
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)


-39.57
O
SCF3
3d
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)


7.81
7.79
7.53
7.51
1.35
O
SCF3
3e
1.92
2.10
9.00
f1 (ppm)


182.97
159.52
132.78
132.75
132.72
132.70
129.91
128.41
127.87
126.83
126.42
35.63
31.18
O
SCF3
3e
f1 (ppm)


-39.56
O
SCF3
3e
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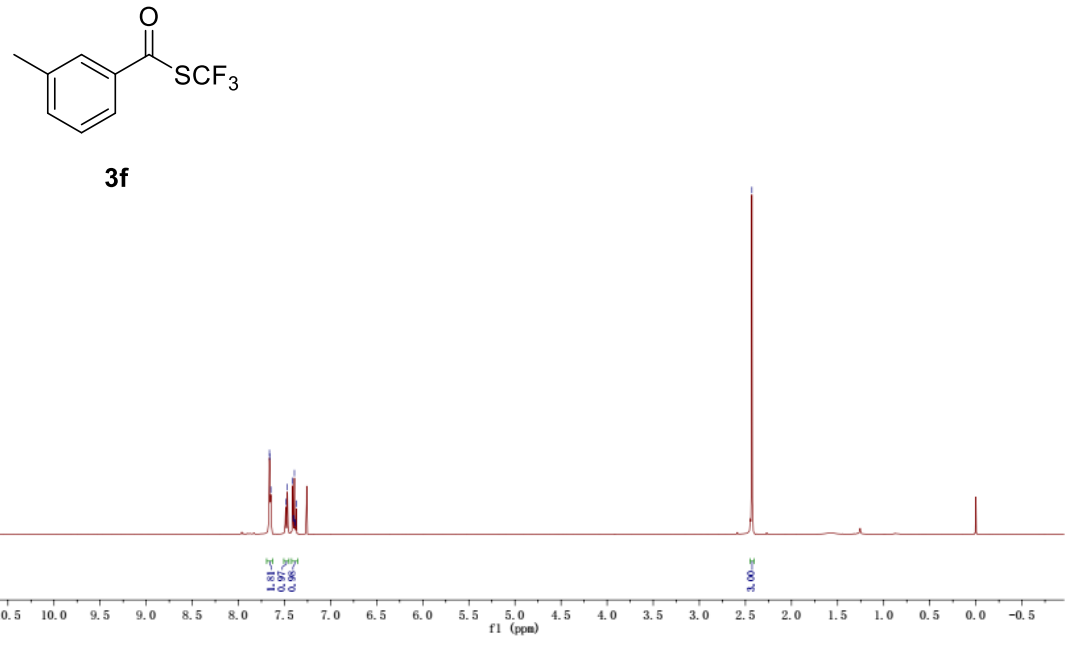
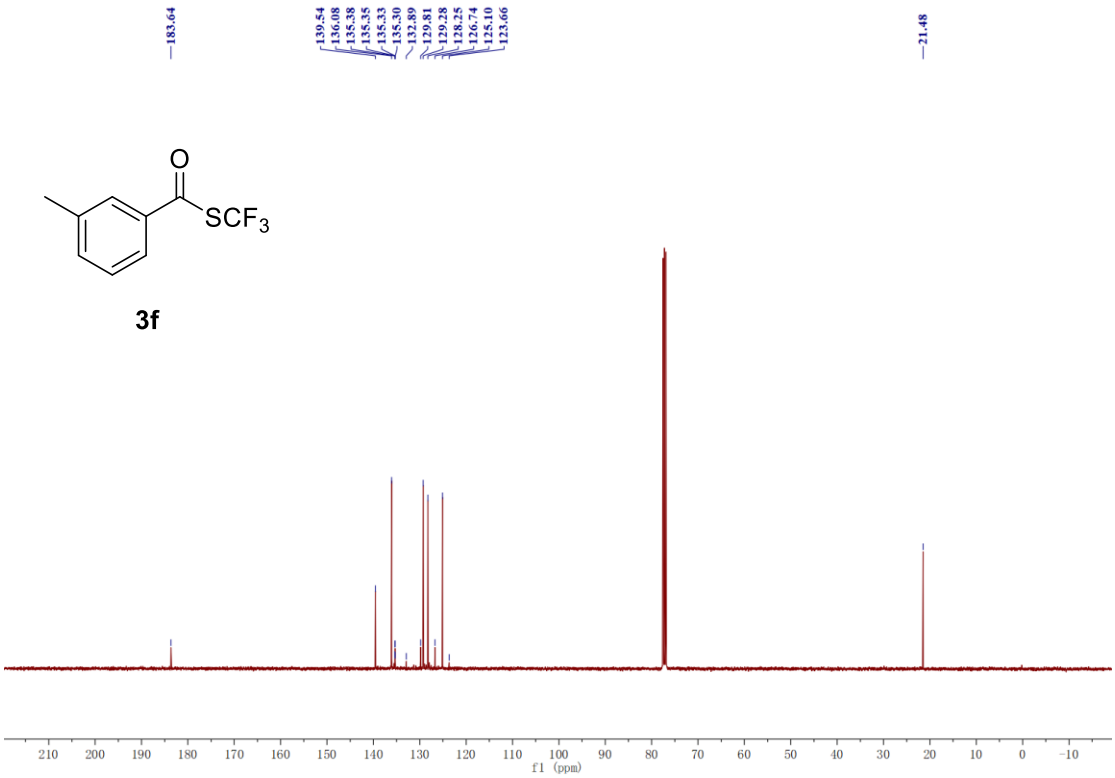
f1 (ppm)
7.66
7.66
7.65
7.49
7.47
7.41
7.41
7.40
7.39
7.39
7.38
7.37
2.43


O
SCF3
3f
1.81
0.97
0.98
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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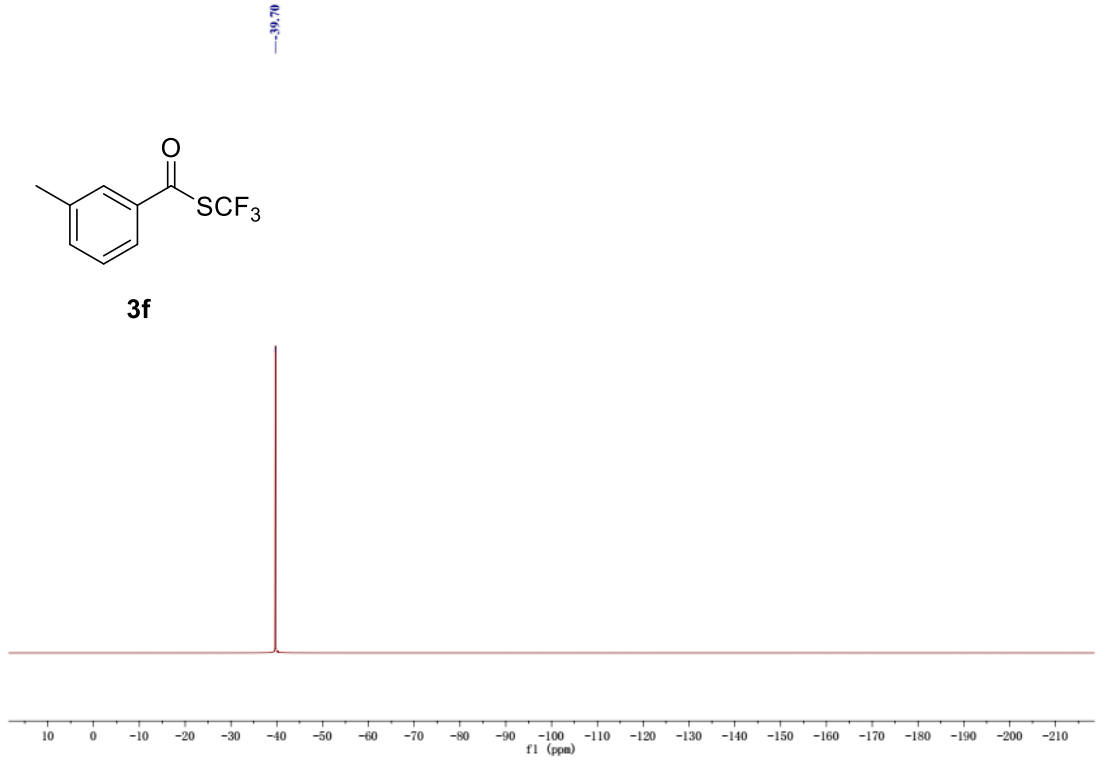
136.08
135.38
135.35
135.33
135.30
132.89
129.81
129.28
128.25
126.74
125.10
123.66
21.48
O
SCF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

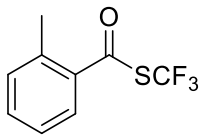
3f


-39.70
O
SCF3
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)

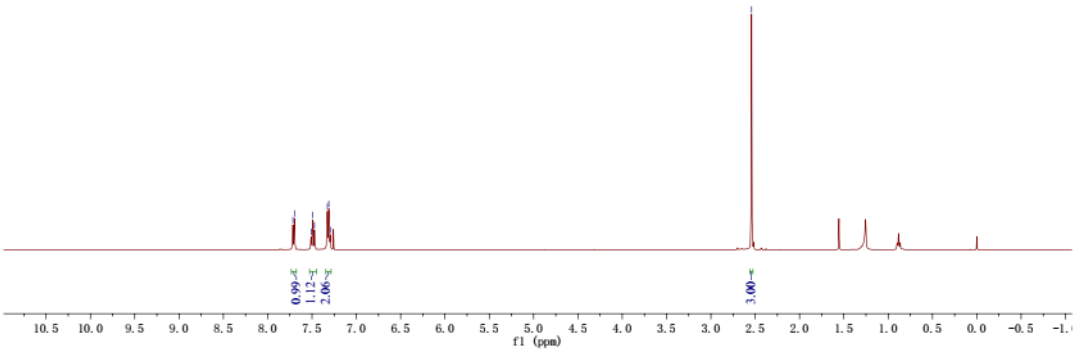
3f


7.72
7.70
7.51
7.49
7.47
7.33
7.31
7.29


2.54


O
SCF3

3g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1.12
2.06
3.00
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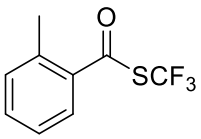
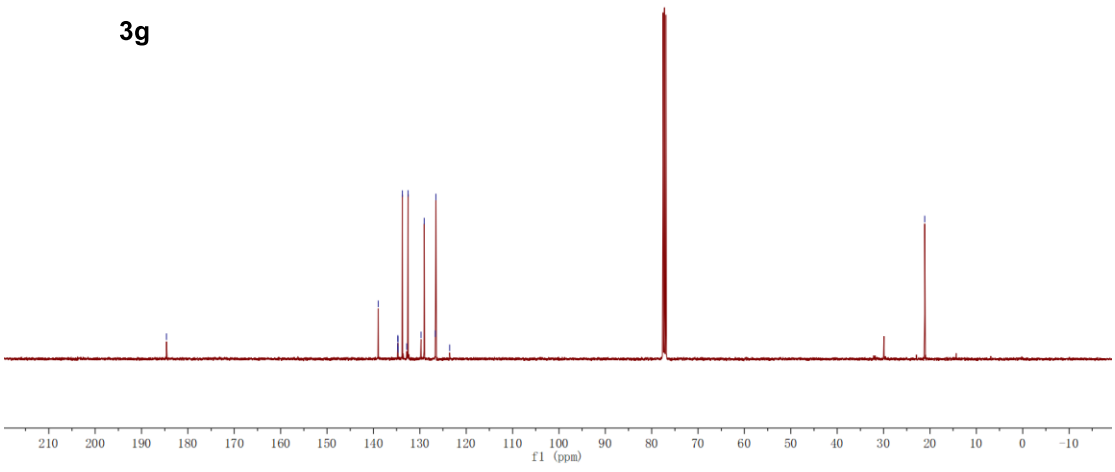
f1 (ppm)

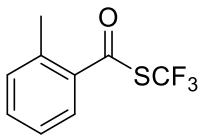

184.62
138.96
134.77
134.74
134.71
134.69
133.75
132.81
132.56
129.73
129.04
126.65
126.50
123.57

21.12


O
SCF3

3g


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)


O
SCF3

3g

-40.42
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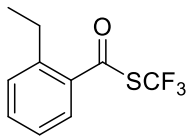
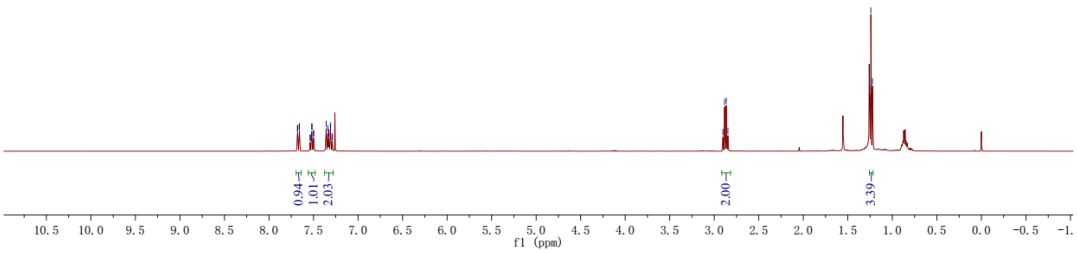
f1 (ppm)
7.68 7.68 7.66 7.66 7.54 7.54 7.52 7.52 7.50 7.50 7.36 7.34 7.33 7.33 7.31 7.31 7.29 7.29
2.90 2.88 2.86 2.85
1.25 1.24 1.22


O
SCF3

3h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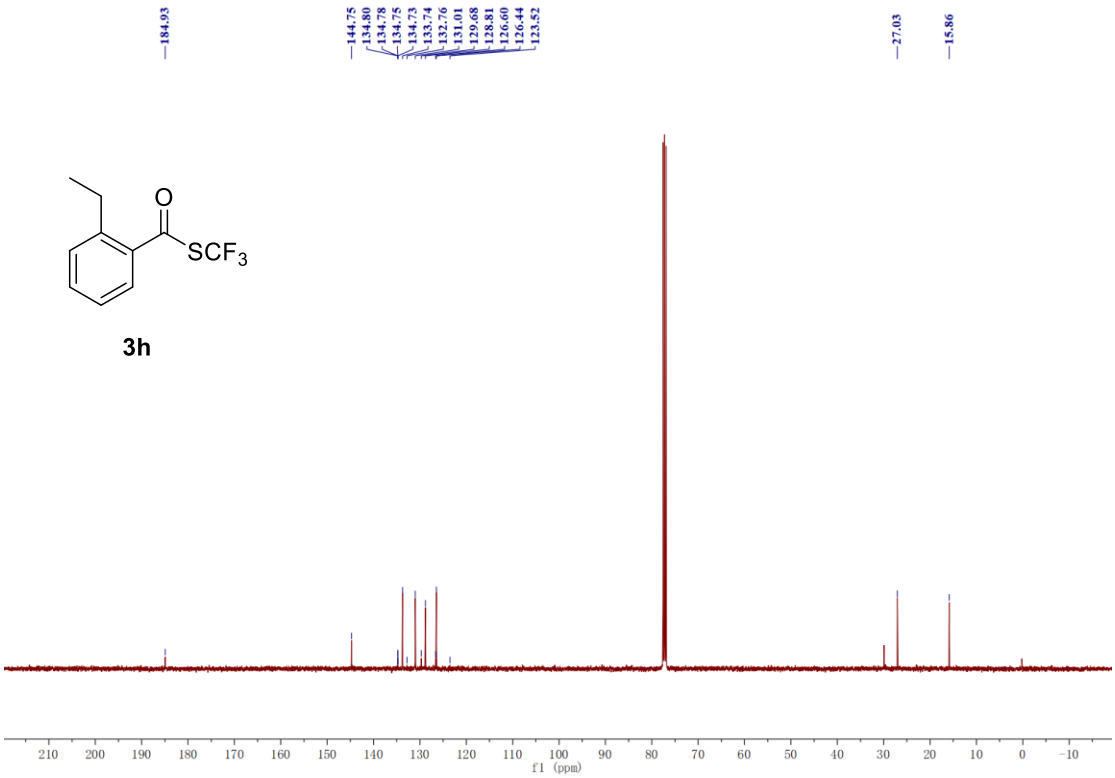
1.01
2.03
2.00
3.39
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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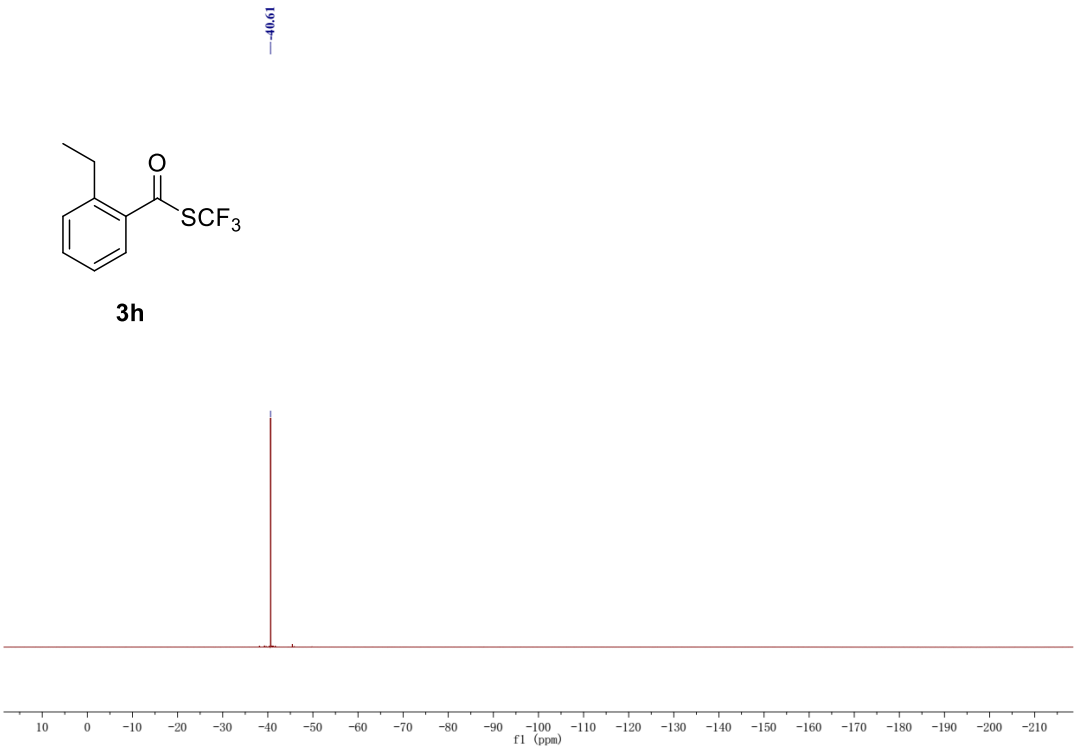
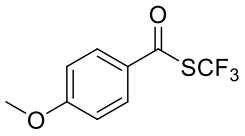
144.75
134.80
134.78
134.75
134.73
133.74
132.76
131.01
129.68
128.81
126.60
126.44
123.52
27.03
15.86
O
SCF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

3h

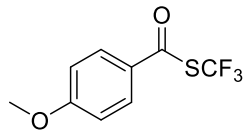

40.61
O
SCF3
10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)

3h


O
SCF3
O

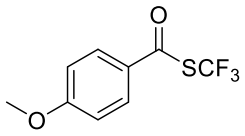
3i

7.77
7.74
6.91
6.88
3.82
2.05
2.12
3.00
f1 (ppm)


O
SCF3
O

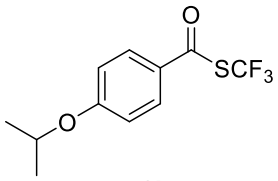
3i

181.71
165.29
130.31
129.96
128.11
128.08
128.05
128.03
126.88
114.64
55.92
f1 (ppm)

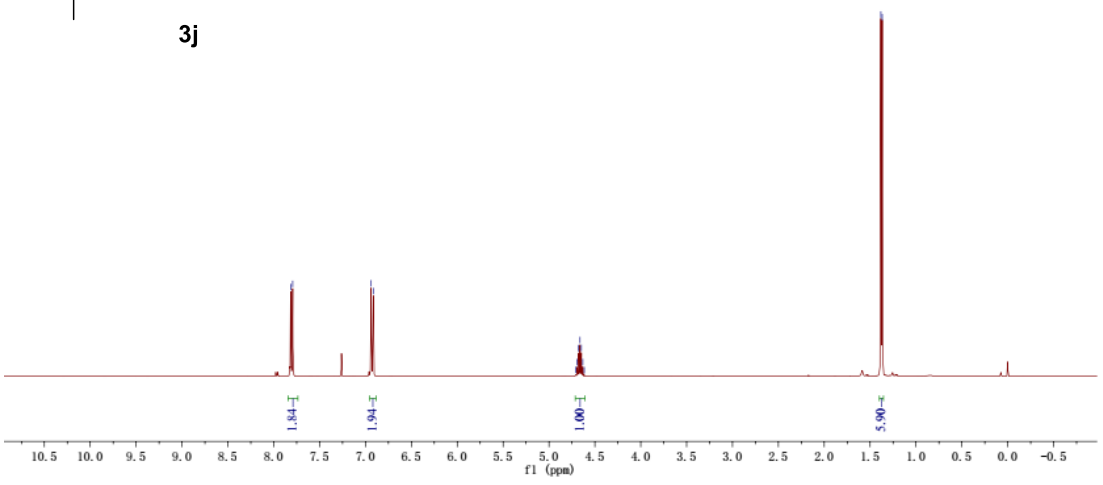

O
SCF3
O

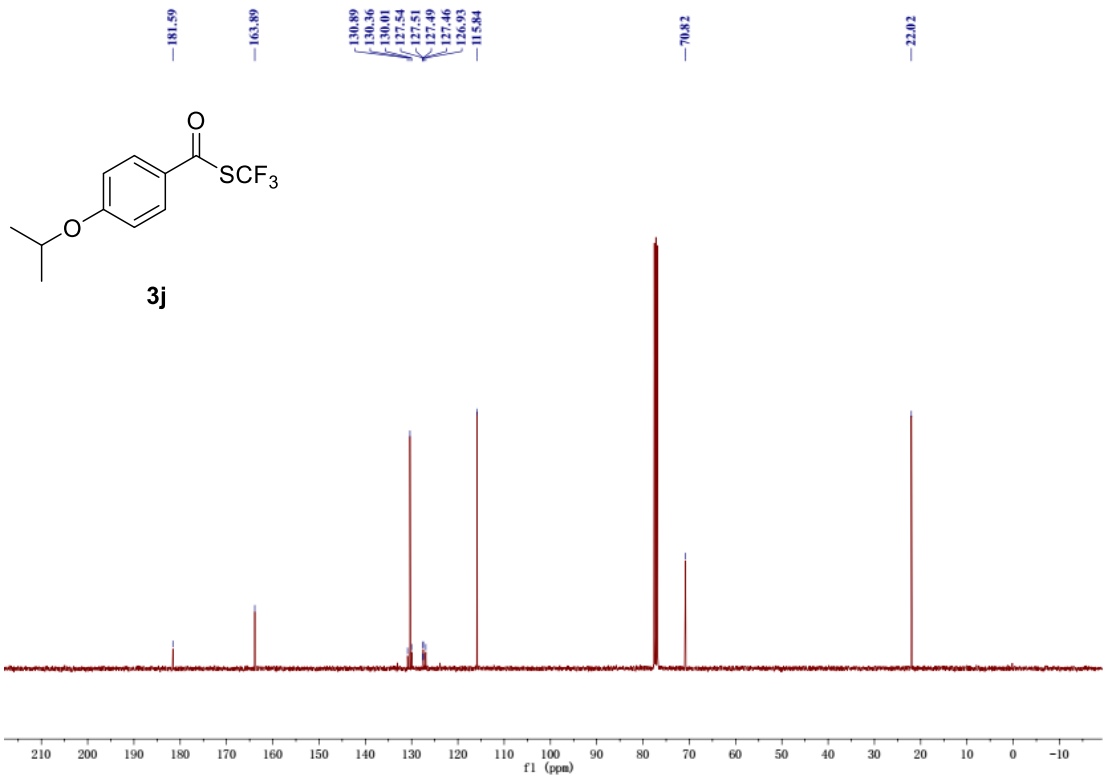
3i

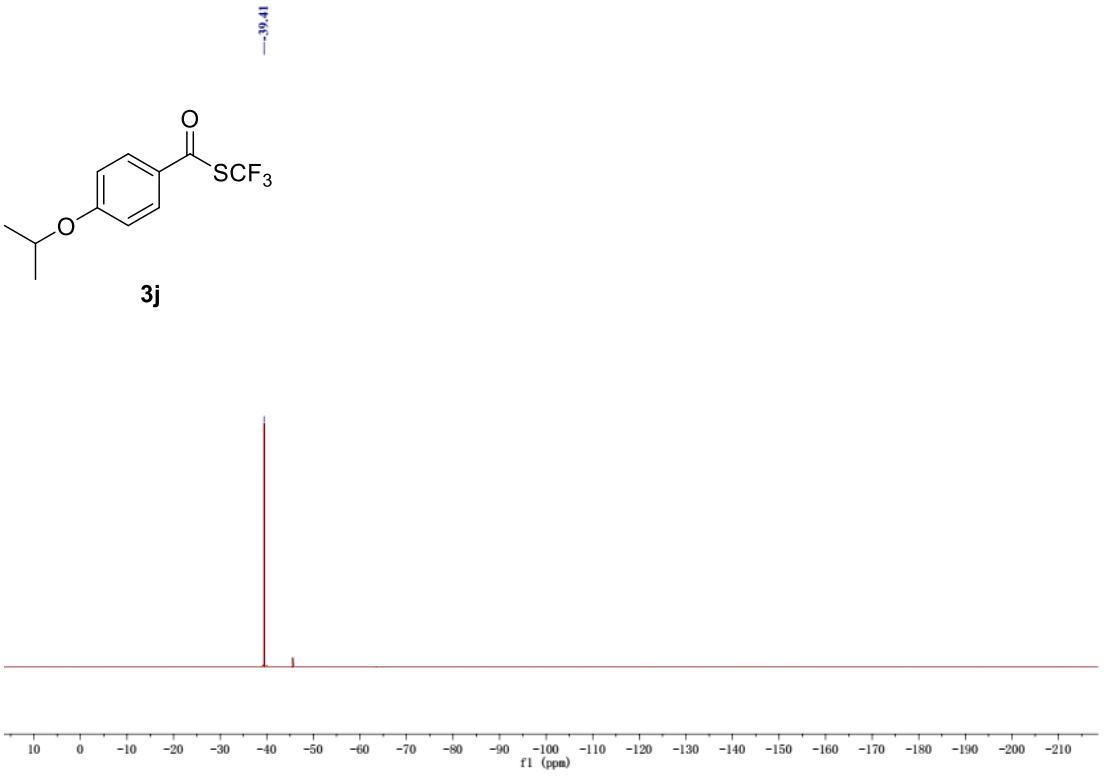
-39.43
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)
7.82
7.79
6.94
6.92
4.71
4.69
4.68
4.66
4.65
4.63
4.62
1.38
1.37


O
SCF3
O

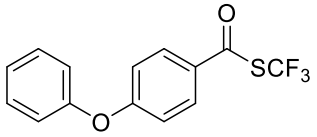
3j


1.84
1.94
1.00
5.90
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)

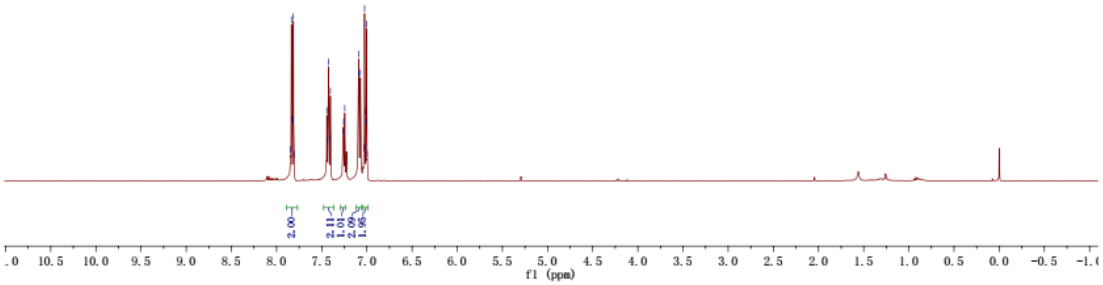

181.59
163.89
130.89
130.36
130.01
127.54
127.51
127.49
127.46
126.93
115.84
70.82
22.02
O
SCF3
O
3j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-39.41
O
SCF3
O
3j
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)

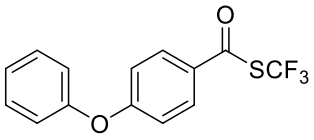

7.84
7.84
7.83
7.82
7.81
7.81
7.44
7.44
7.42
7.41
7.40
7.26
7.24
7.09
7.09
7.07
7.03
7.02
7.01
7.00
7.00


O
SCF3
O

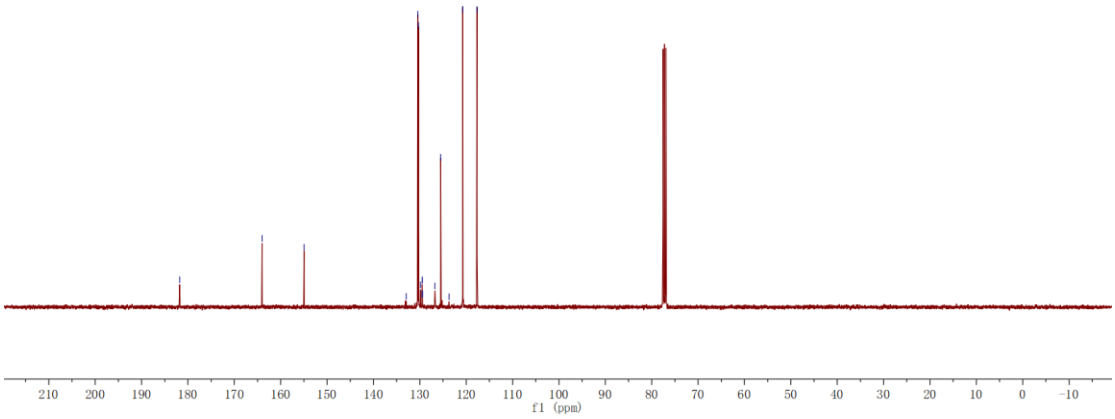
3k

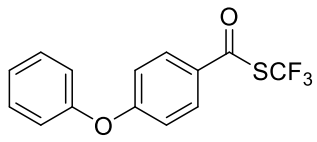

2.00
2.11
1.01
2.09
1.85
f1 (ppm)


181.80
164.04
154.96
132.93
130.46
130.29
129.86
129.52
129.49
129.46
129.43
126.78
125.49
123.70
120.74
117.67


O
SCF3
O

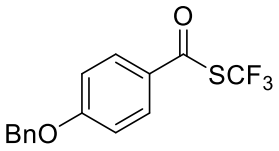
3k


f1 (ppm)

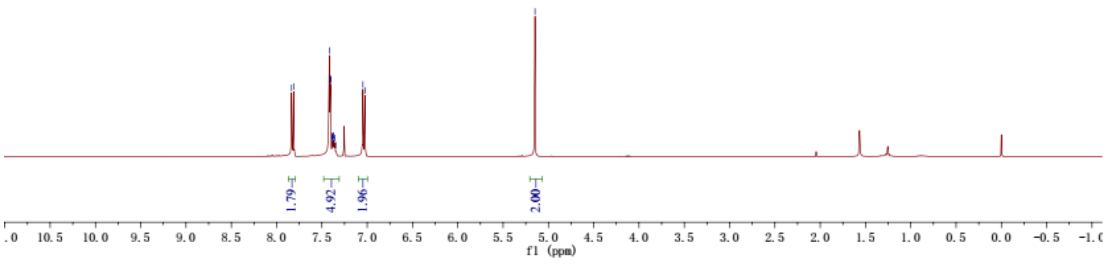

O
SCF3
O

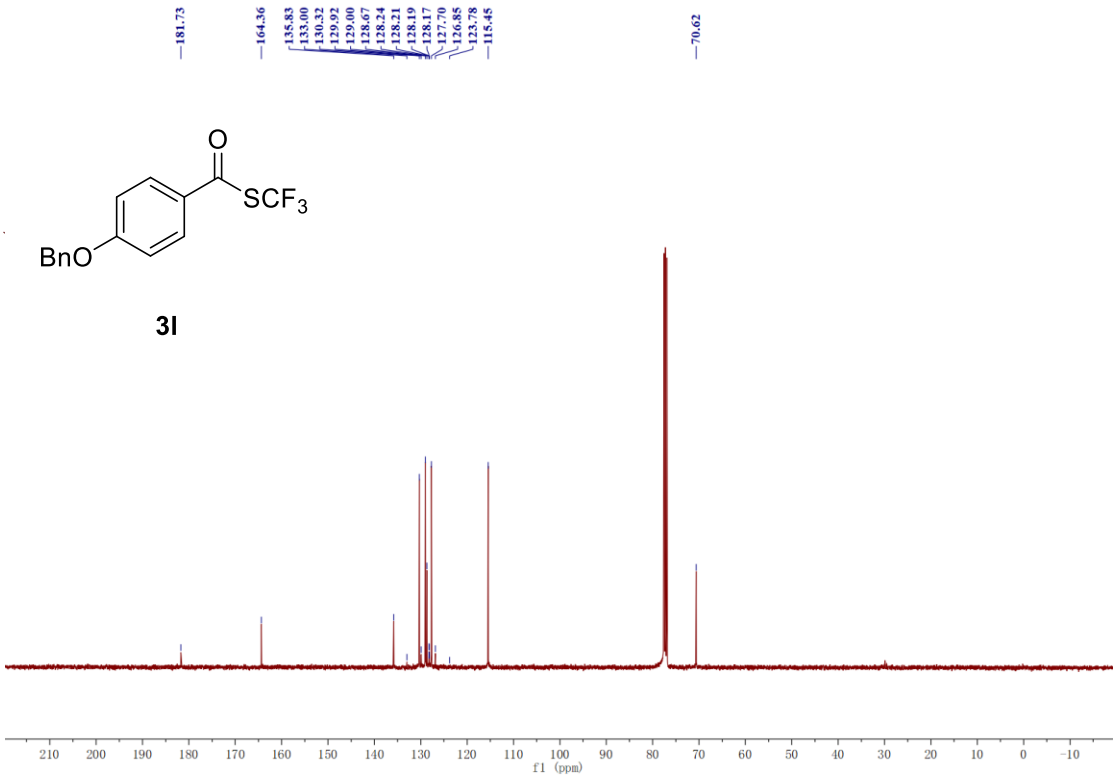
3k

-39.46
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)
7.83
7.81
7.42
7.41
7.41
7.40
7.39
7.39
7.38
7.38
7.37
7.37
7.36
7.35
7.05
7.02
5.15

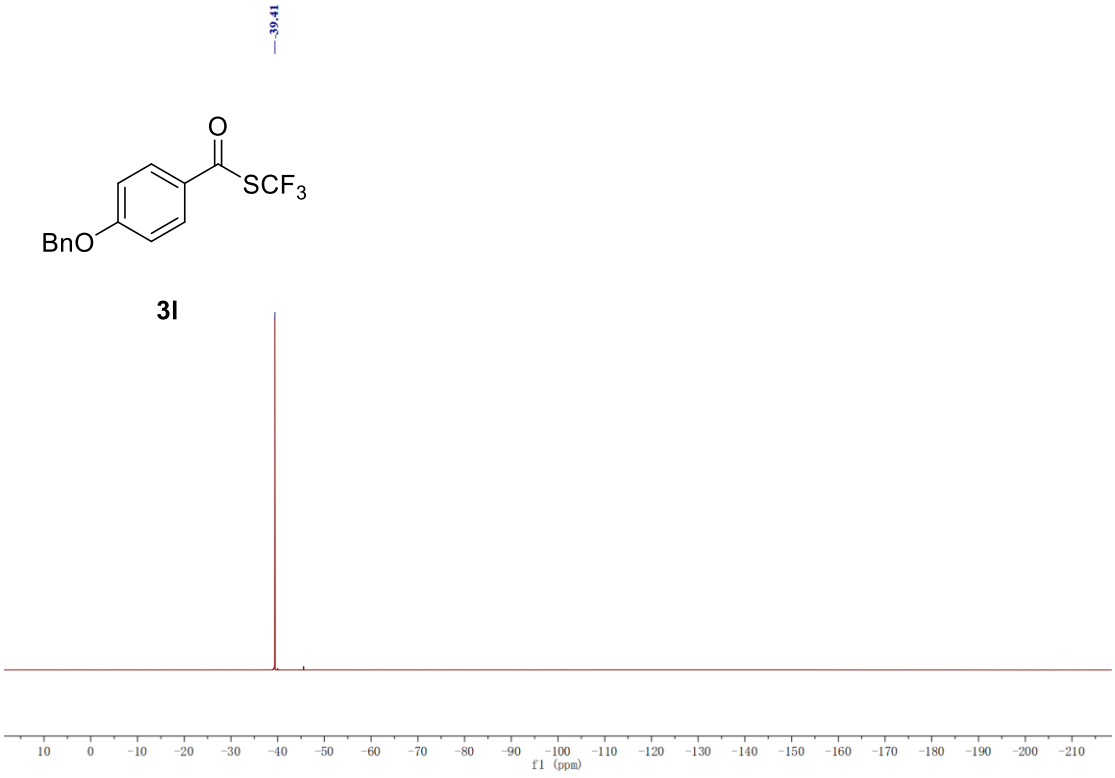

O
SCF3
BnO

3l

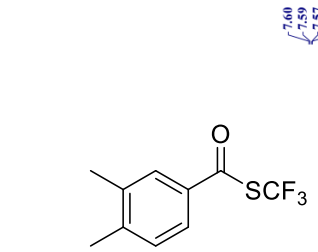

1.79
4.92
1.96
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


181.73
164.36
135.83
133.00
130.32
129.92
129.00
128.67
128.24
128.21
128.19
128.17
127.70
126.85
123.78
115.45
70.62
O
SCF3
BnO
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)

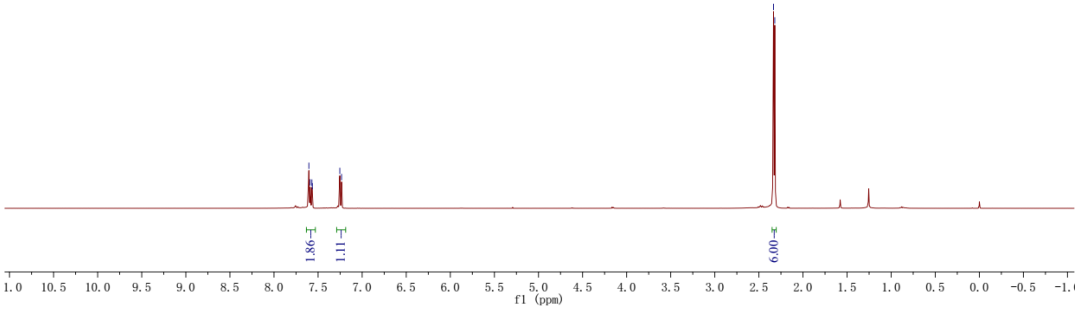
3l

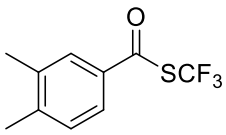

39.41
O
SCF3
BnO
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

3l


O
SCF3

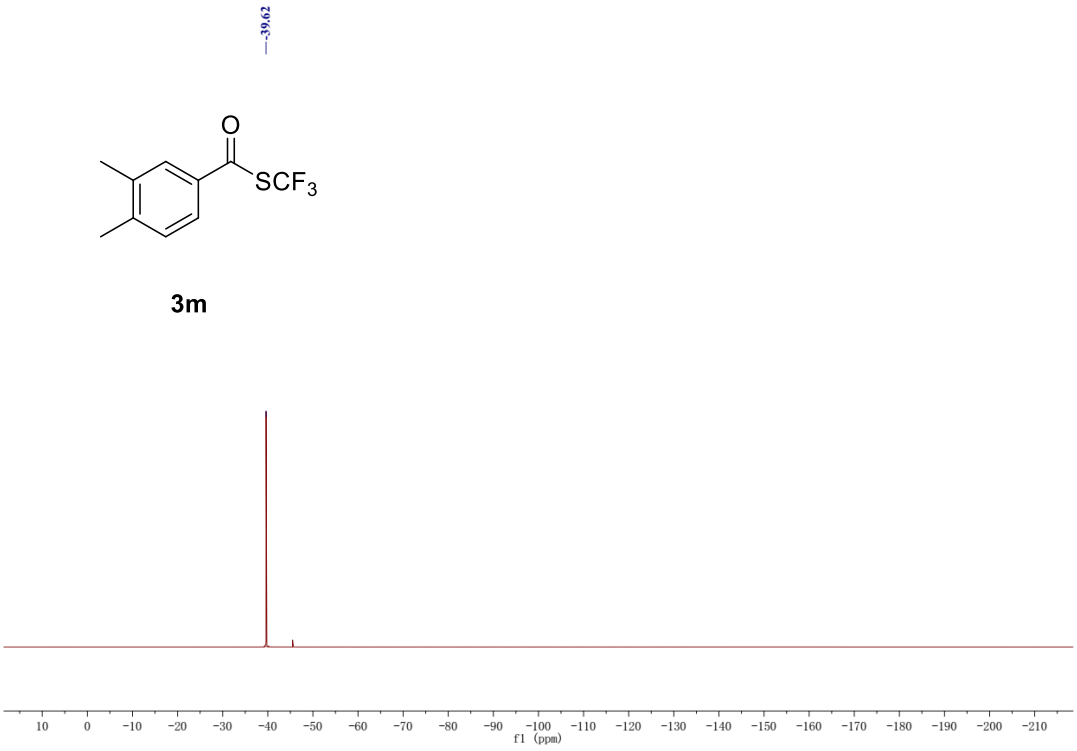
3m


7.60
7.59
7.57
7.57
7.25
7.23
2.33
2.32
1.86
1.11
6.00
f1 (ppm)

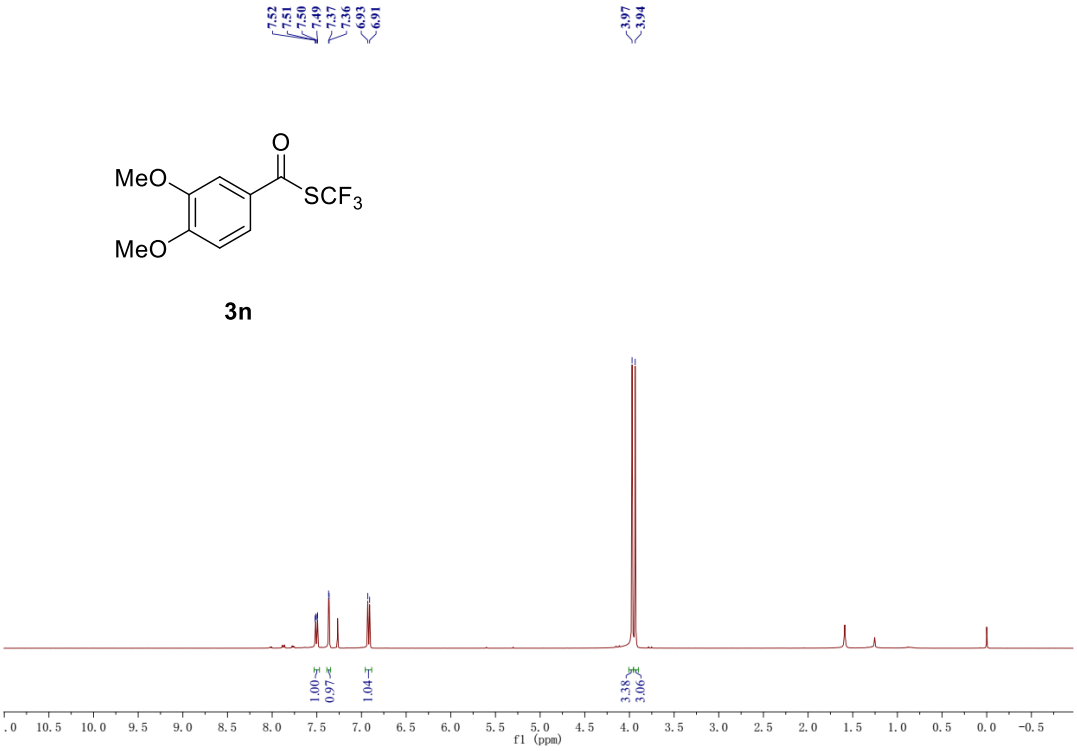

O
SCF3

3m

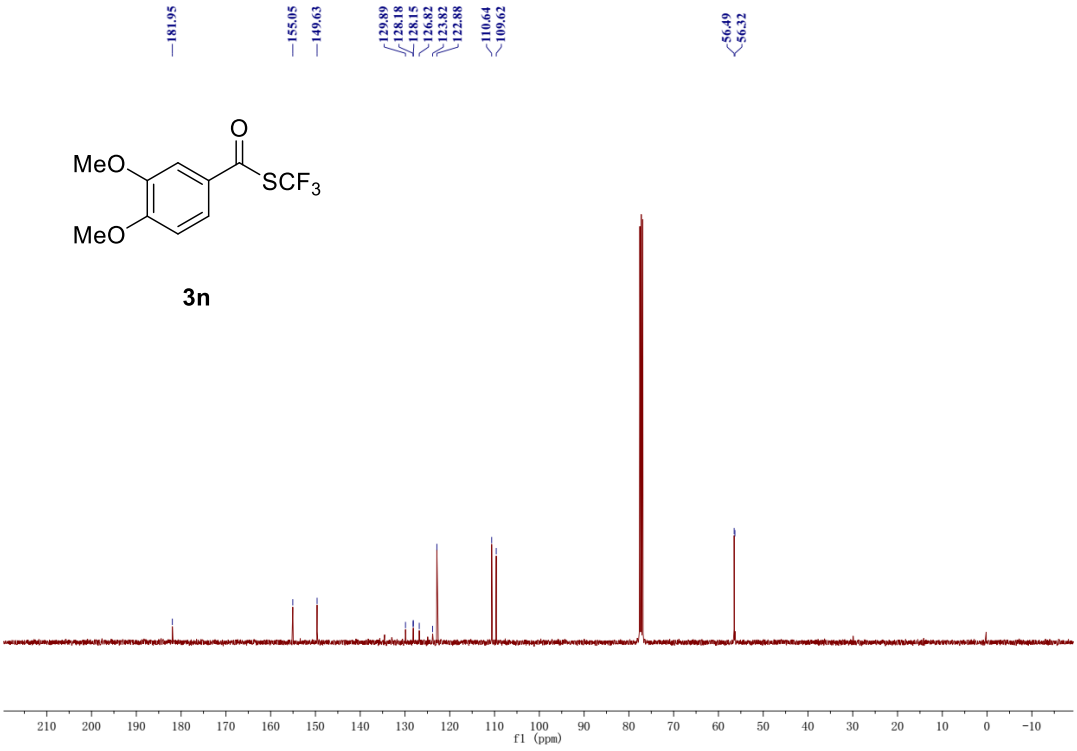
183.14
145.39
138.08
133.16
133.13
133.10
133.08
133.00
130.55
129.93
128.78
126.85
126.12
125.57
20.44
19.96
f1 (ppm)


-39.62
O
SCF3
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)

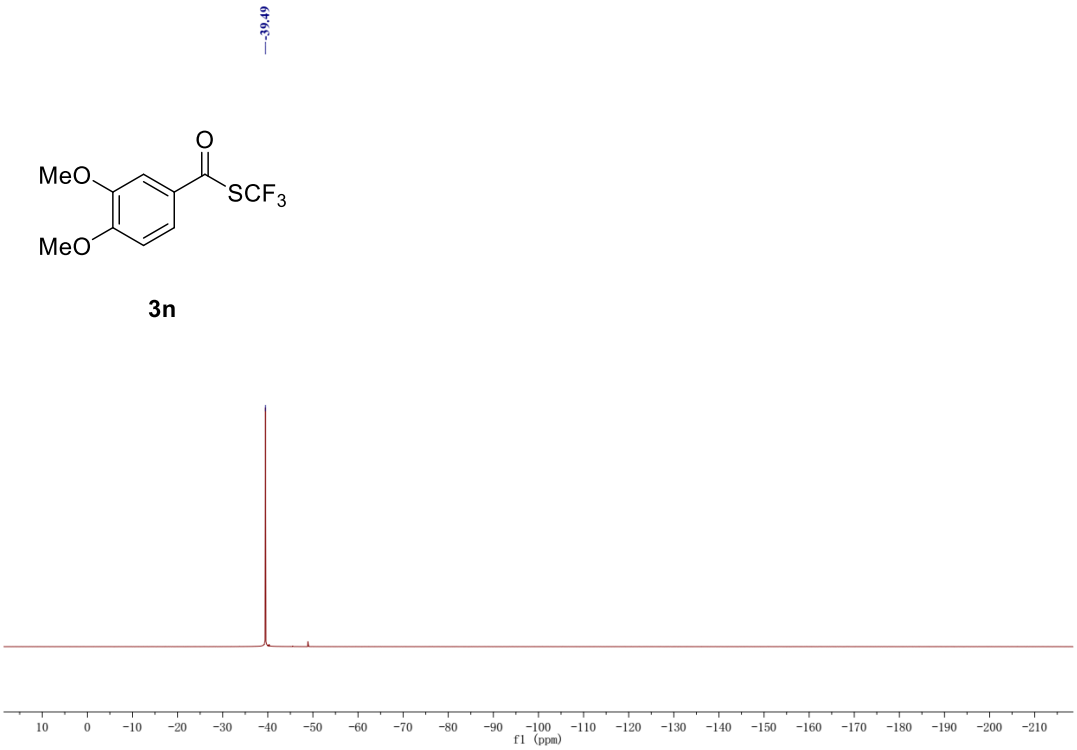
3m


7.52
7.51
7.50
7.49
7.37
7.36
6.93
6.91
3.97
3.94
O
MeO
MeO
SCF3
1.00
0.97
1.04
3.38
3.06
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)

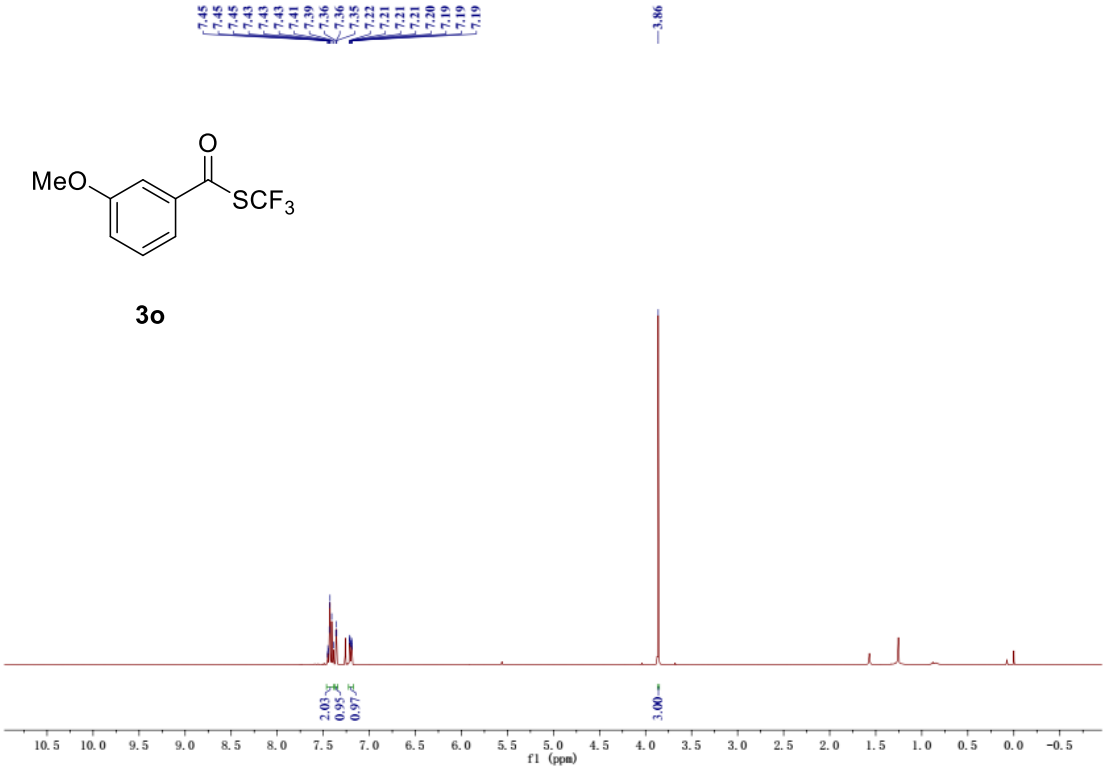
3n


181.95
155.05
149.63
129.89
128.18
128.15
126.82
123.82
122.88
110.64
109.62
56.49
56.32
MeO
MeO
O
SCF3
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)

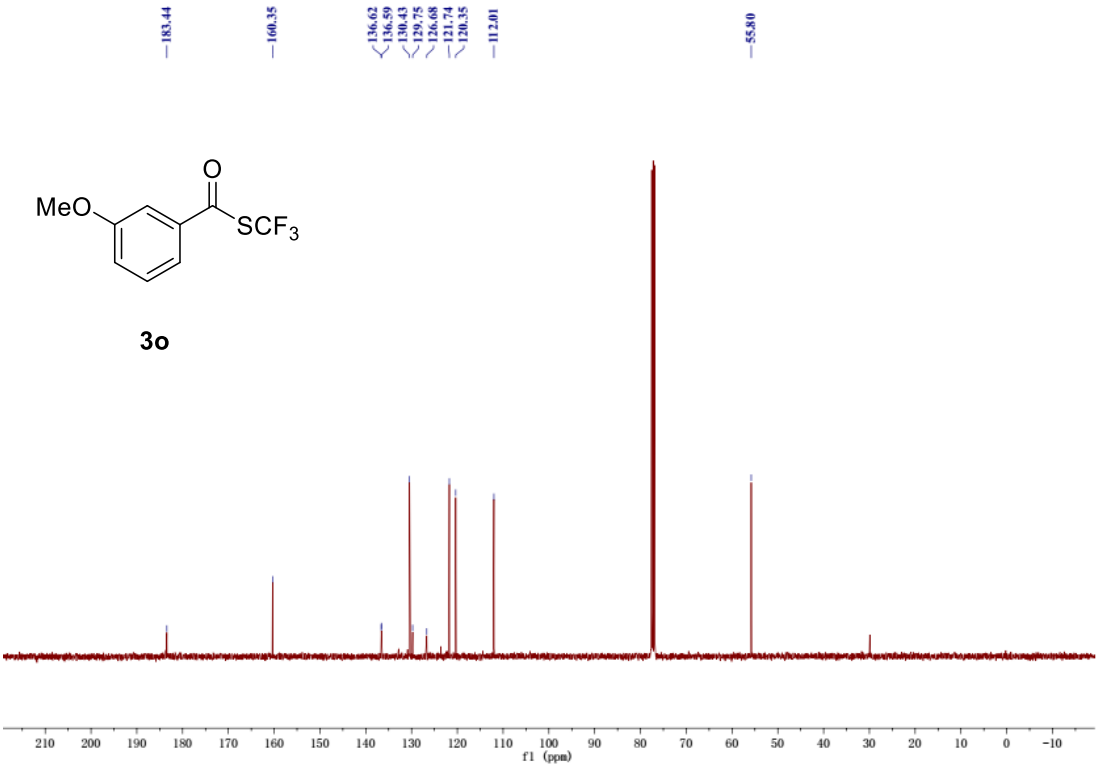
3n


−39.49
MeO
MeO
O
SCF3
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)

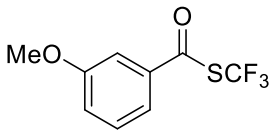
3n


7.45
7.45
7.45
7.43
7.43
7.43
7.41
7.39
7.36
7.36
7.35
7.22
7.21
7.21
7.21
7.20
7.19
7.19
7.19
3.86
MeO
O
SCF3
2.03
0.95
0.97
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

3o

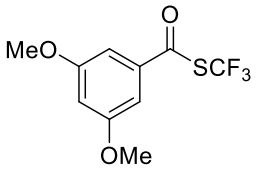

183.44
160.35
136.62
136.59
130.43
129.75
126.68
121.74
120.35
112.01
55.80
MeO
O
SCF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3o


MeO
O
SCF3

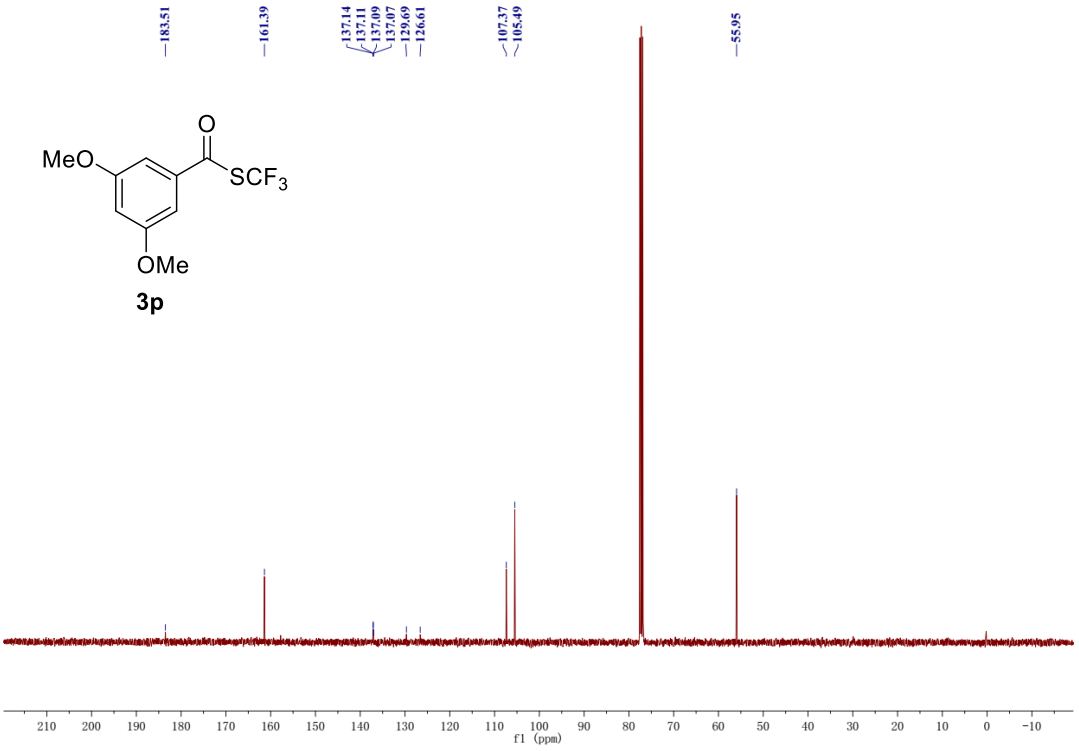
3o

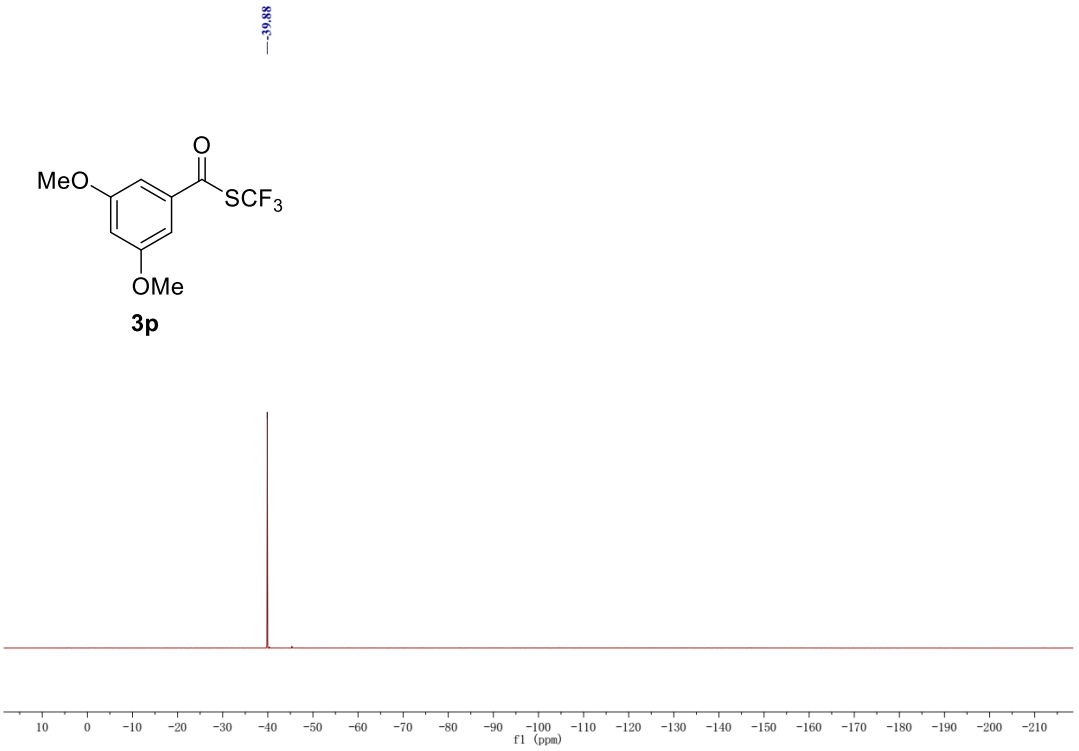
-39.77
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

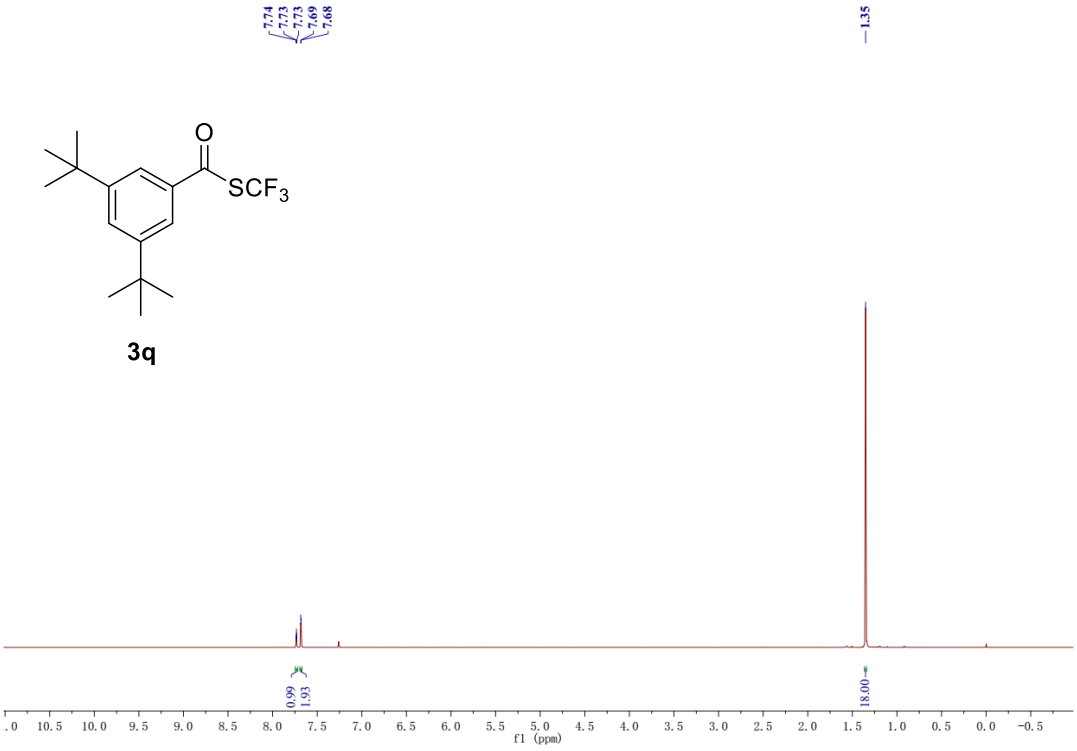

MeO
O
SCF3
OMe

3p

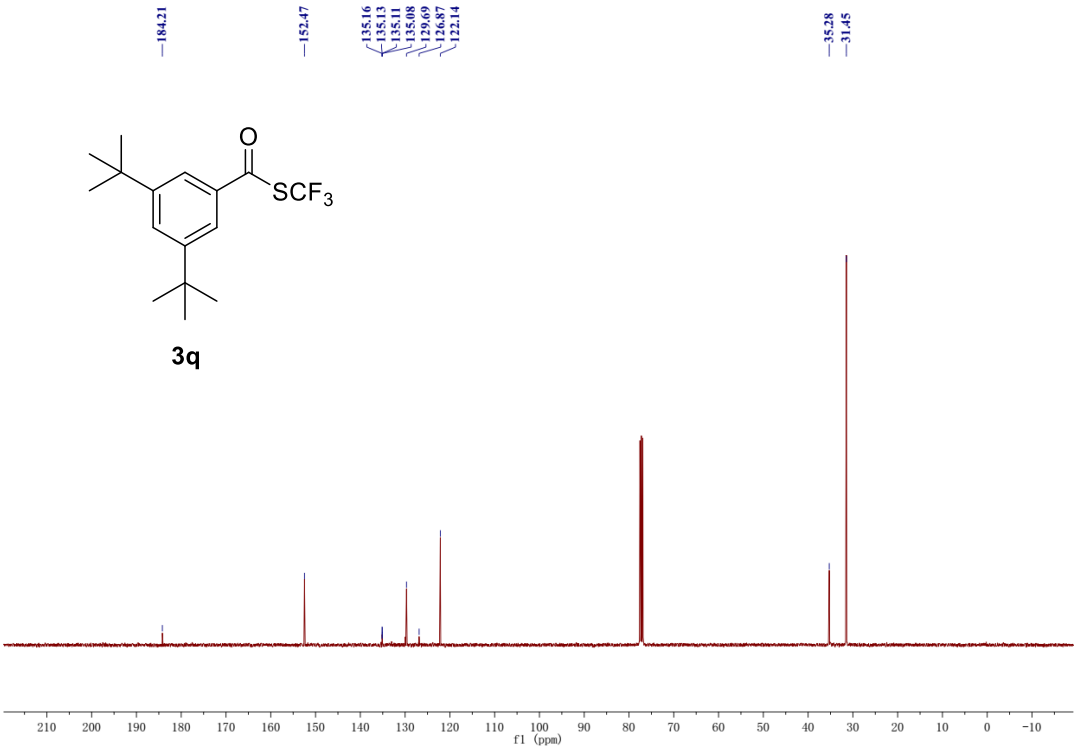
6.98
6.97
6.73
6.72
6.72
3.84
1.84
0.93
6.00
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)


183.51
161.39
137.14
137.11
137.09
137.07
129.69
126.61
107.37
105.49
55.95
MeO
O
SCF3
OMe
3p
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)

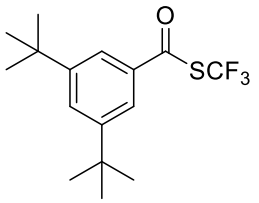

39.88
MeO
O
SCF3
OMe
3p
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


7.74
7.73
7.73
7.69
7.68
1.35
O
SCF3
0.99
1.93
18.00
f1 (ppm)

3q


184.21
152.47
135.16
135.13
135.11
135.08
129.69
126.87
122.14
35.28
31.45
O
SCF3
f1 (ppm)

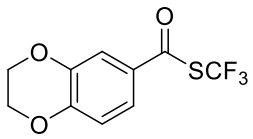
3q


O
SCF3

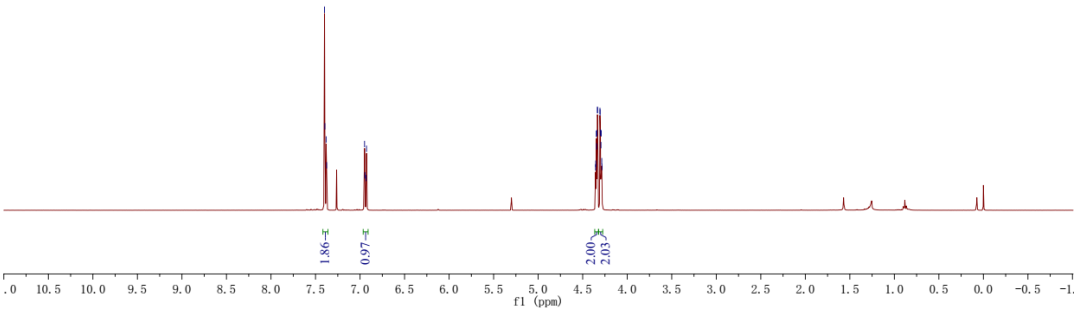
3q

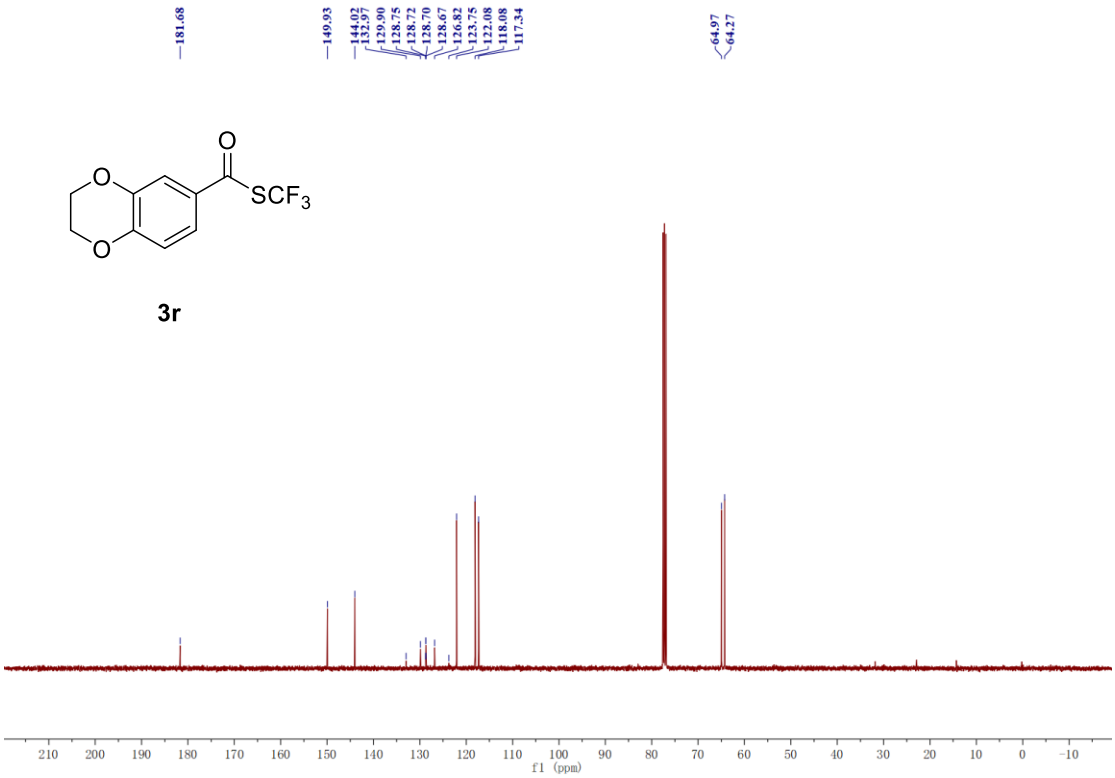
-39.74
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

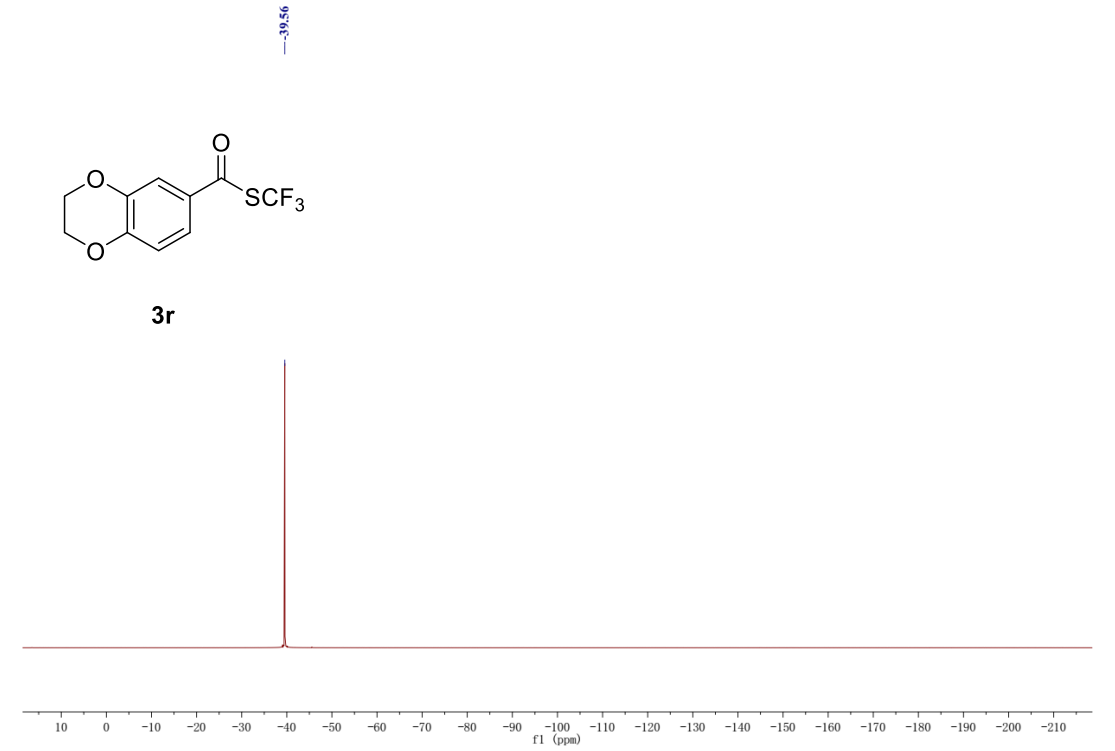

7.40
7.40
7.38
7.38
6.95
6.95
6.93
6.93
4.36
4.35
4.35
4.34
4.34
4.33
4.33
4.31
4.30
4.30
4.29
4.29
4.29
4.28

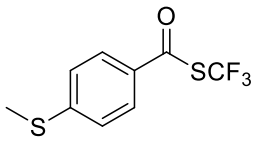

O
O
O
SCF3

3r


1.86
0.97
2.00
2.03
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)


181.68
149.93
144.02
132.97
129.90
128.75
128.72
128.70
128.67
126.82
123.75
122.08
118.08
117.34
64.97
64.27
O
O
O
SCF3
3r
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)

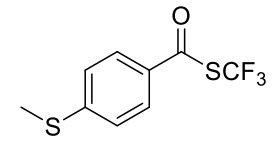

-39.56
O
O
O
SCF3
3r
10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)


O
SCF3
S

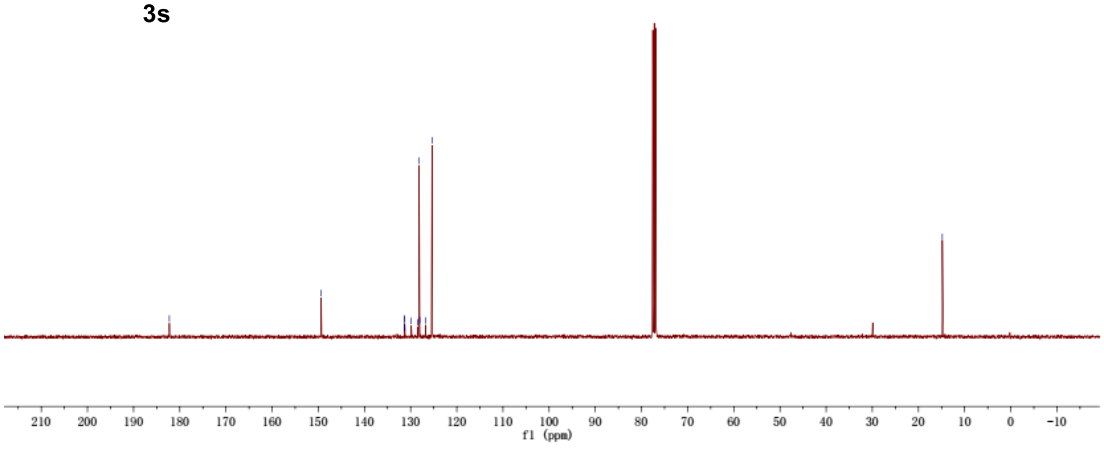
3s

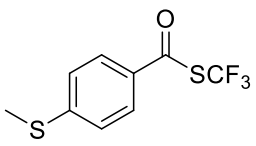
7.76
7.74
7.29
7.27
2.53
1.94
1.93
3.00
f1 (ppm)


182.26
149.36
131.33
131.30
131.27
131.25
129.85
128.47
128.15
128.03
126.78
125.36
14.83


O
SCF3
S

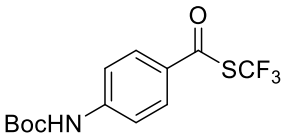
3s


f1 (ppm)

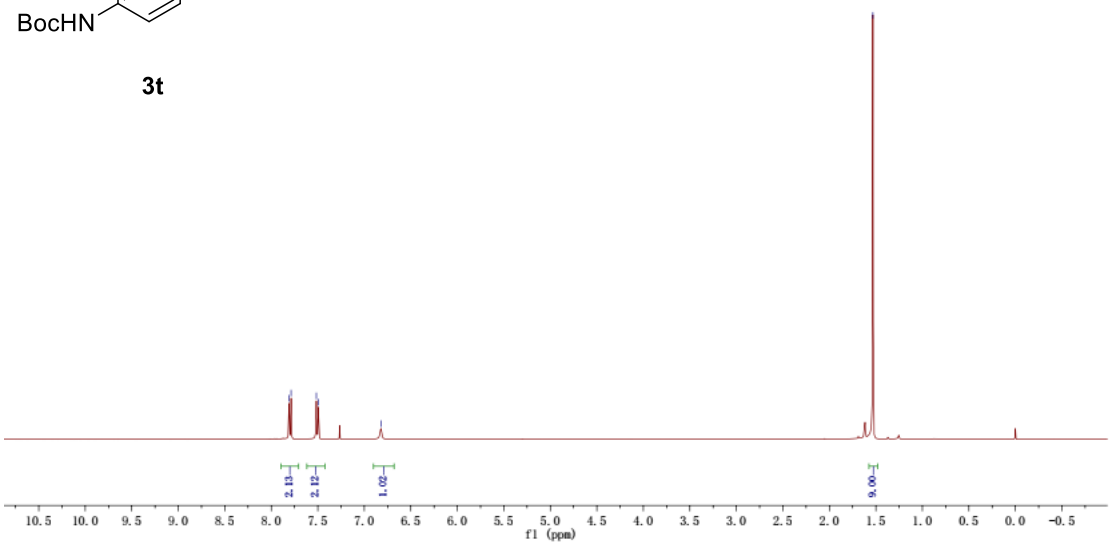

O
SCF3
S

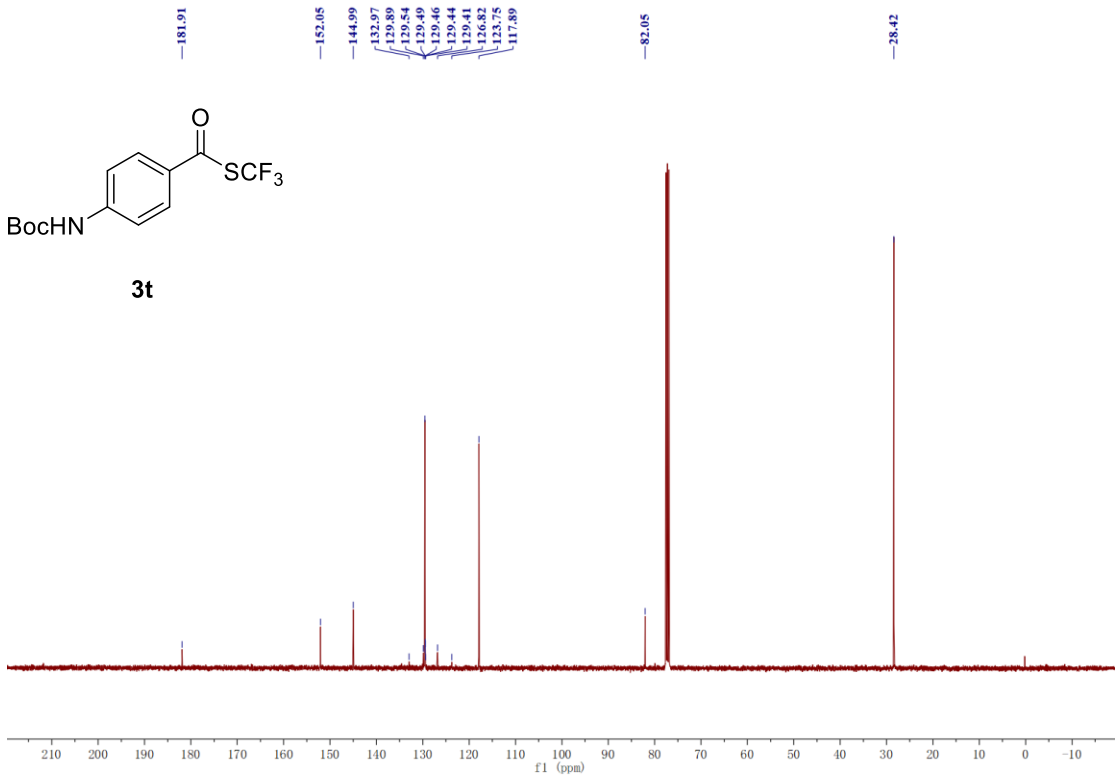
3s

-39.43
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)
7.81
7.79
7.52
7.49
6.82
1.53

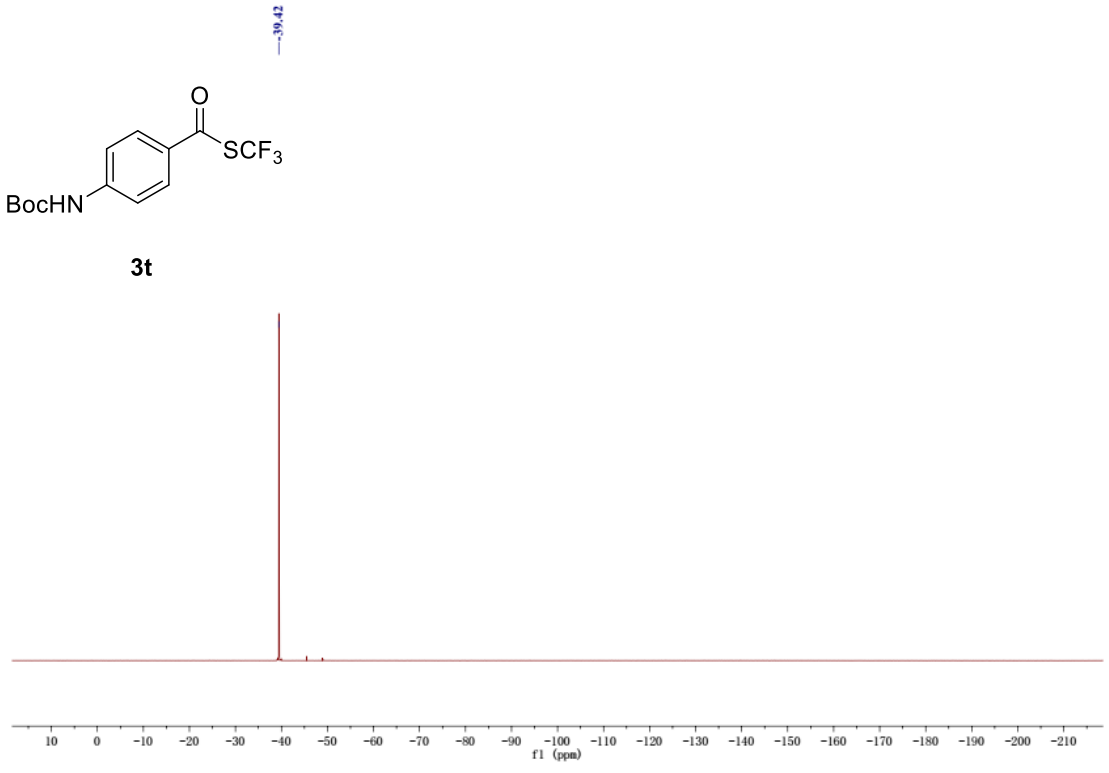

O
SCF3
BocHN

3t


2.13
2.12
1.02
9.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

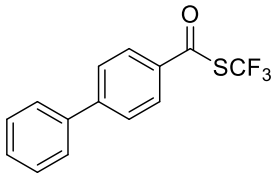

181.91
152.05
144.99
132.97
129.89
129.54
129.49
129.46
129.44
129.41
126.82
123.75
117.89
82.05
28.42
O
SCF3
BocHN
f1 (ppm)

3t

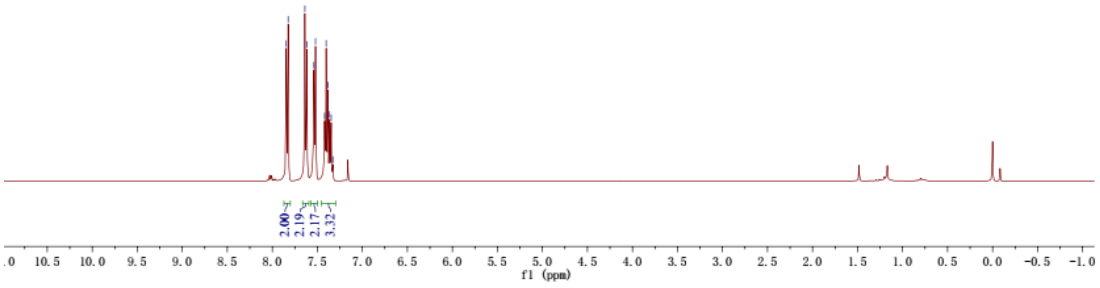

-39.42
O
SCF3
BocHN
f1 (ppm)

3t

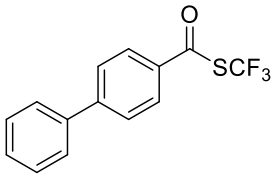

7.85
7.82
7.64
7.62
7.54
7.52
7.42
7.40
7.38
7.36
7.35
7.33


O
SCF3

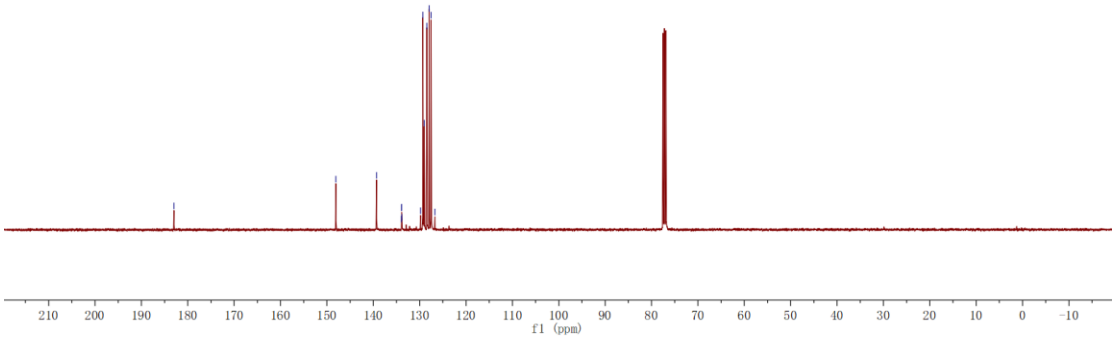
3u

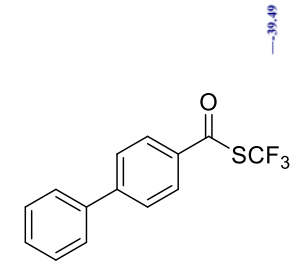

2.00
2.19
2.17
3.32
f1 (ppm)


182.98
148.07
139.31
133.93
133.90
133.87
133.84
129.82
129.32
129.01
128.45
127.94
127.51
126.74


O
SCF3

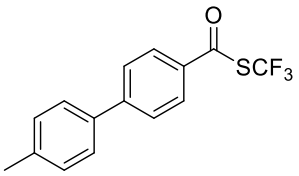
3u


f1 (ppm)

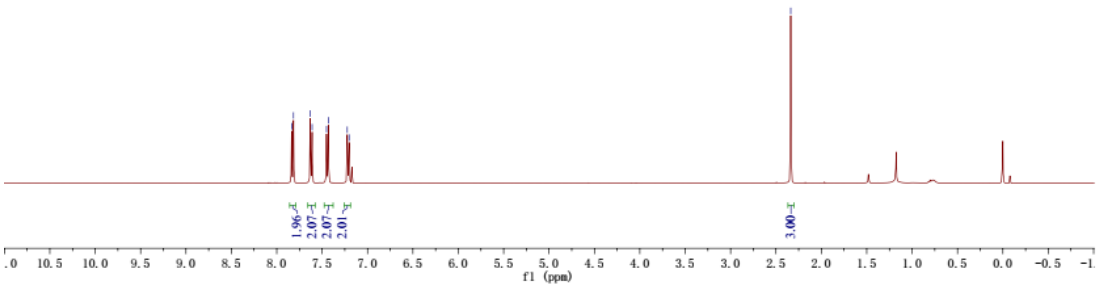

O
SCF3

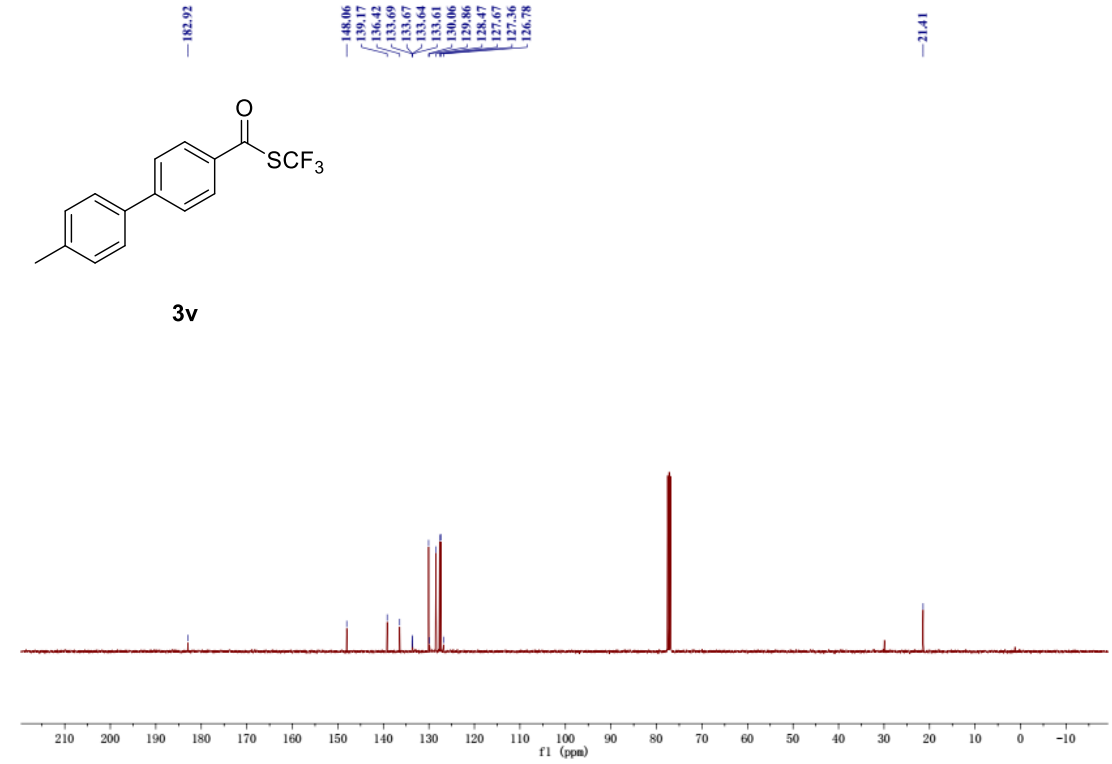
3u

-39.49
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)
7.84
7.82
7.63
7.61
7.45
7.43
7.22
7.20
2.34

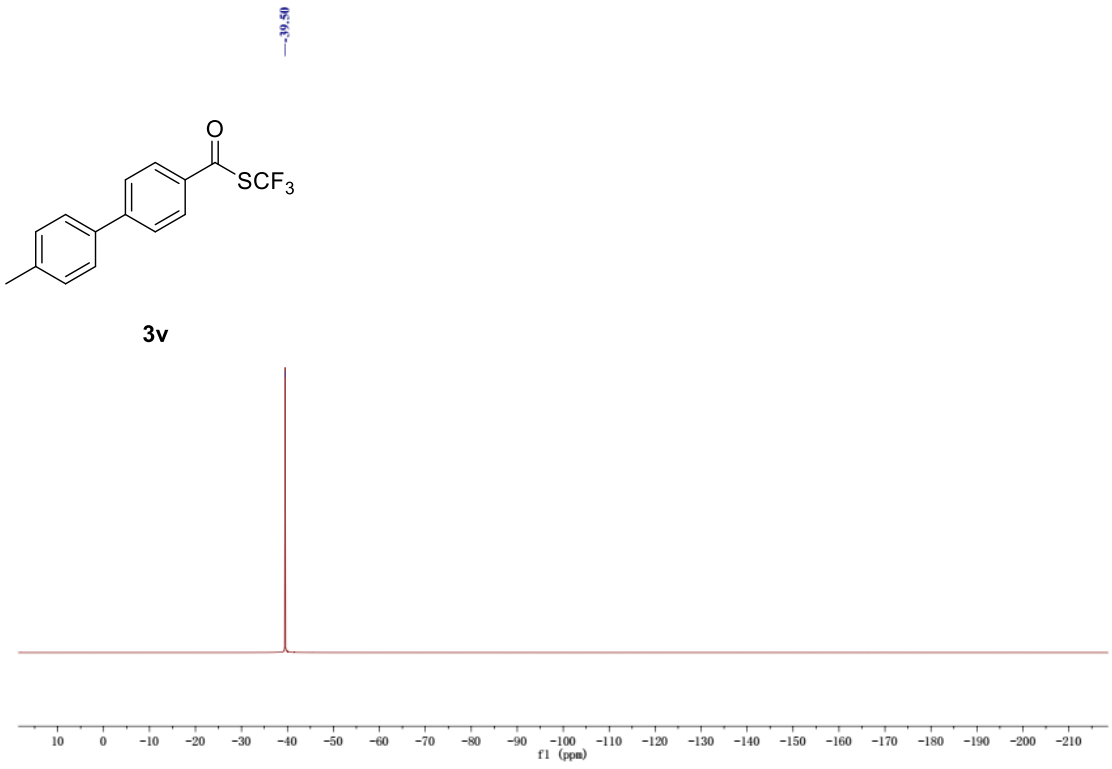

O
SCF3

3v


1.96
2.07
2.07
2.01
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

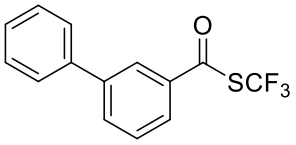

182.92
148.06
139.17
136.42
133.69
133.67
133.64
133.61
130.06
129.86
128.47
127.67
127.36
126.78
21.41
O
SCF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3v

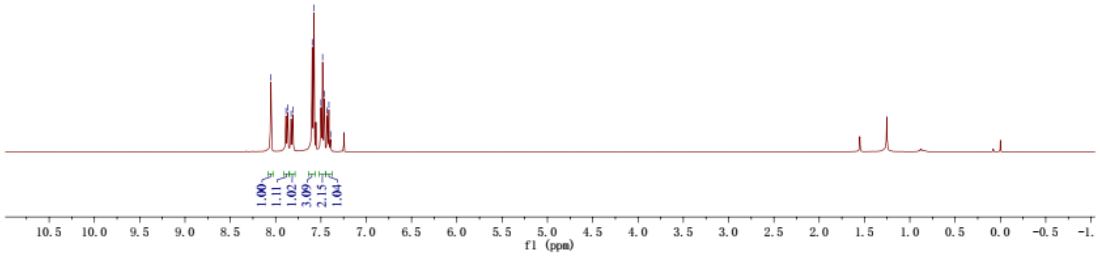

-39.50
O
SCF3
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

3v

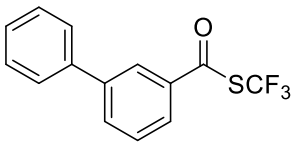

8.05
7.89
7.87
7.83
7.81
7.60
7.58
7.50
7.48
7.46
7.43
7.41
7.39


O
SCF3

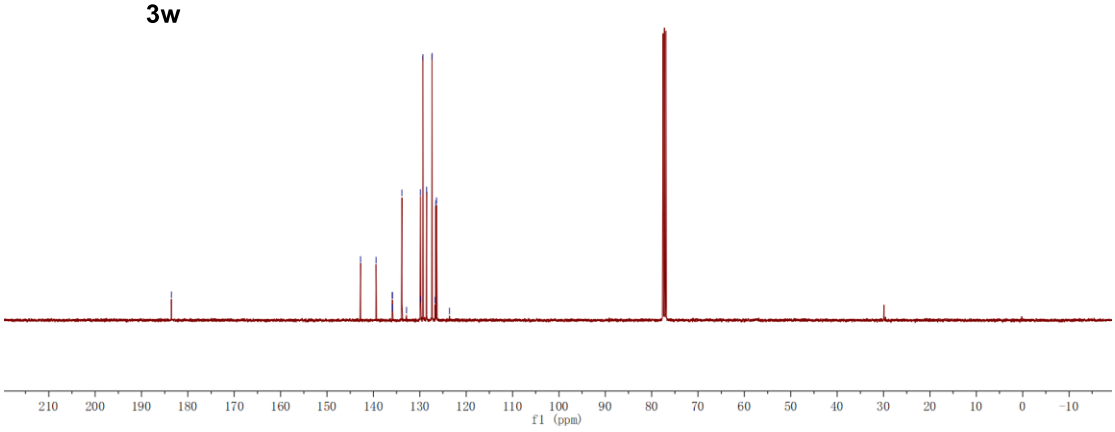
3w

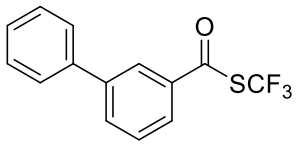

1.00
1.11
1.02
3.09
2.15
1.04
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.
f1 (ppm)


183.55
142.77
139.43
135.95
135.93
135.90
135.88
133.84
132.85
129.88
129.77
129.32
128.52
127.37
126.69
126.53
126.39
123.62


O
SCF3

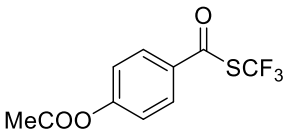
3w


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)

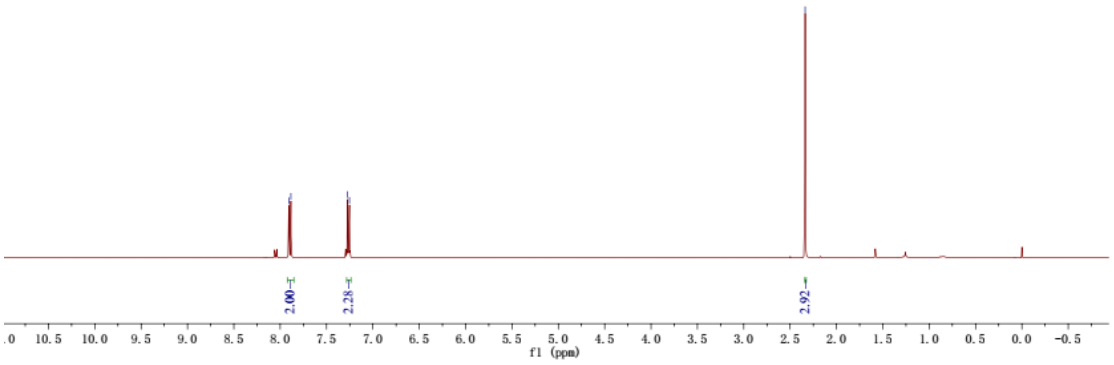

O
SCF3

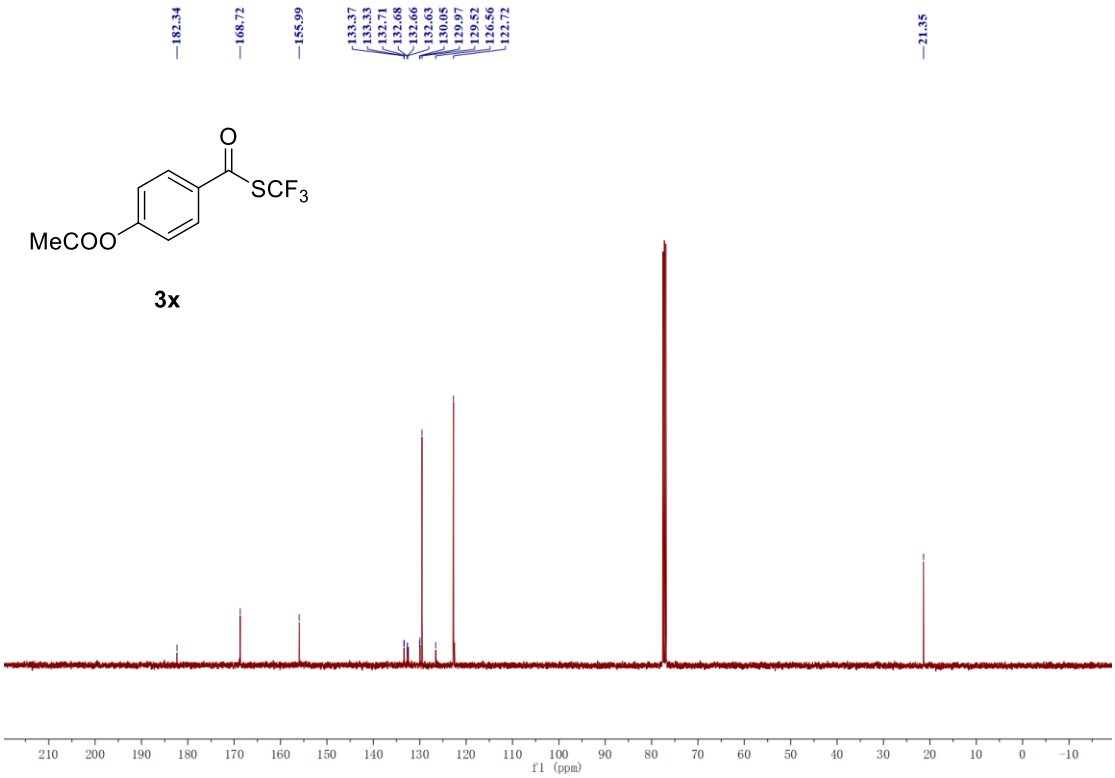
3w

-39.60
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)
7.91
7.88
7.28
7.25
2.34

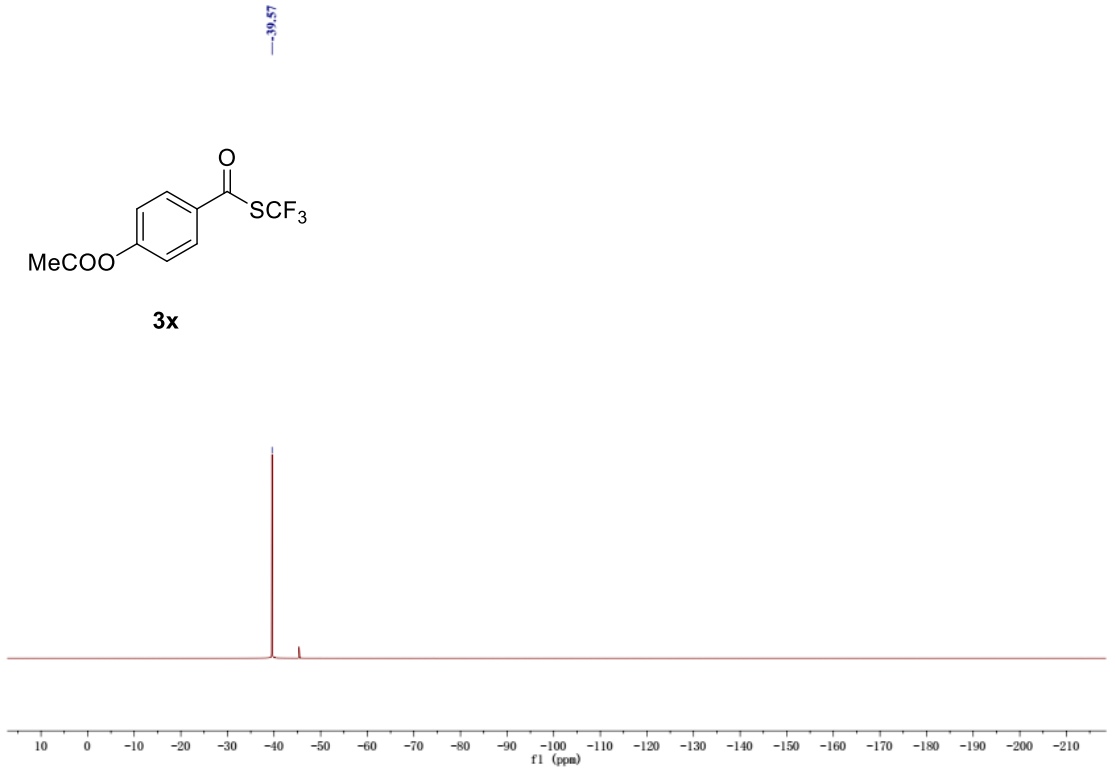

O
SCF3
MeCOO

3x


2.00
2.28
2.92
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)

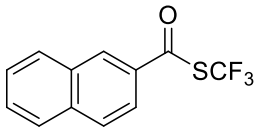

182.34
168.72
155.99
133.37
133.33
132.71
132.68
132.66
132.63
130.05
129.97
129.52
126.56
122.72
21.35
O
SCF3
MeCOO
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3x

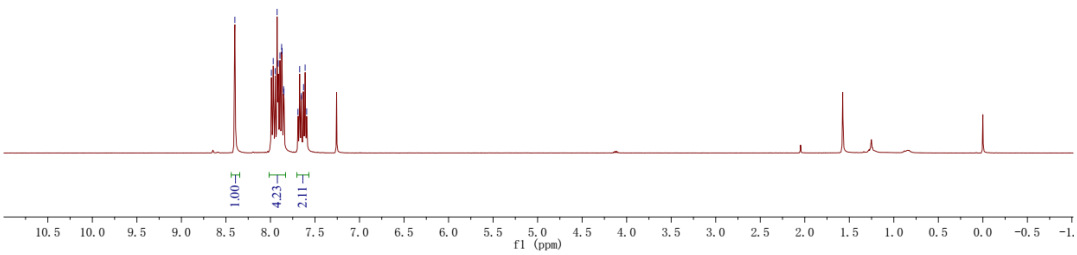

-39.57
O
SCF3
MeCOO
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

3x

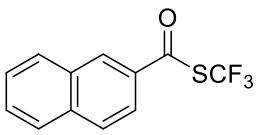

8.40
7.99
7.97
7.95
7.92
7.91
7.89
7.87
7.87
7.85
7.85
7.69
7.67
7.65
7.63
7.61
7.59


O
SCF3

3y

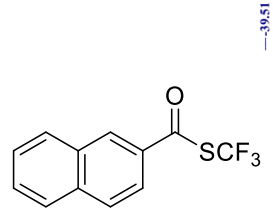

1.00
4.23
2.11
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)


183.39
136.59
132.94
132.69
132.66
132.64
132.61
132.48
130.09
129.95
129.87
129.80
129.51
128.19
127.78
126.79
123.71
122.80


O
SCF3

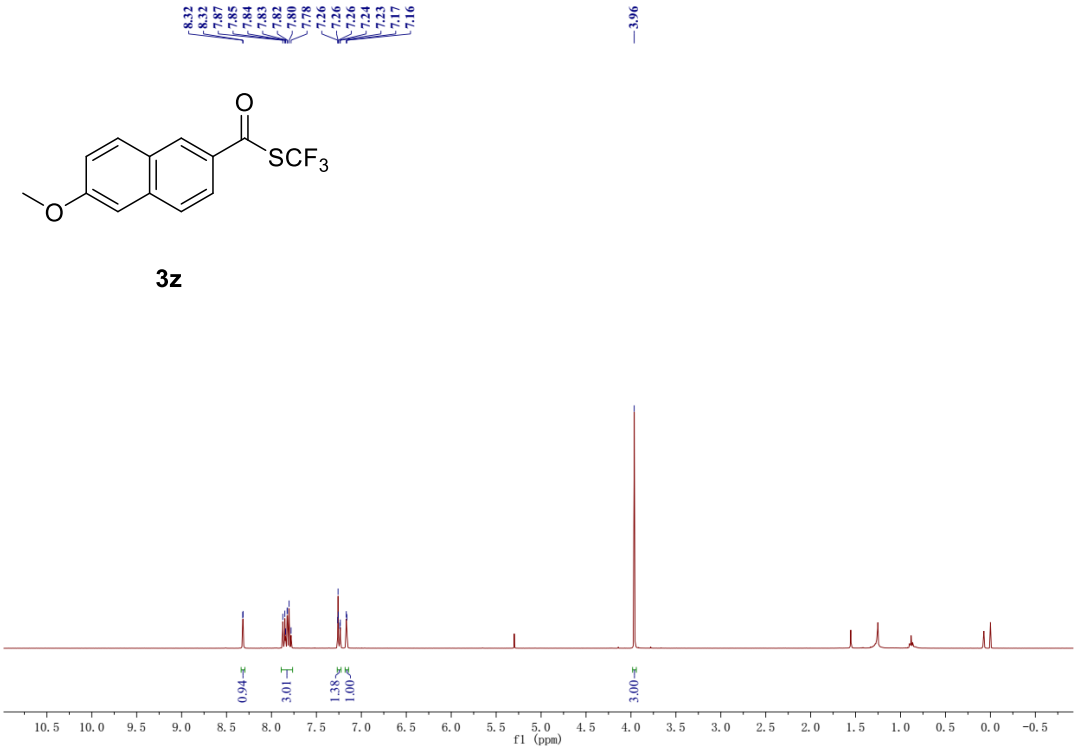
3y

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)

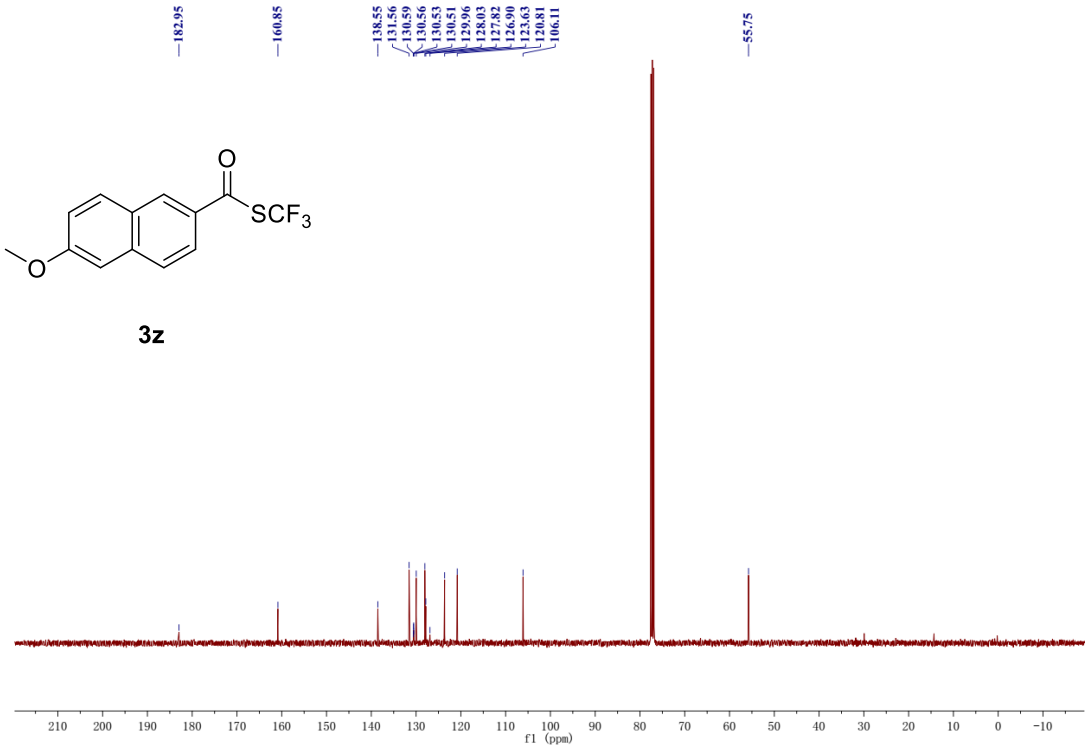

O
SCF3

3y

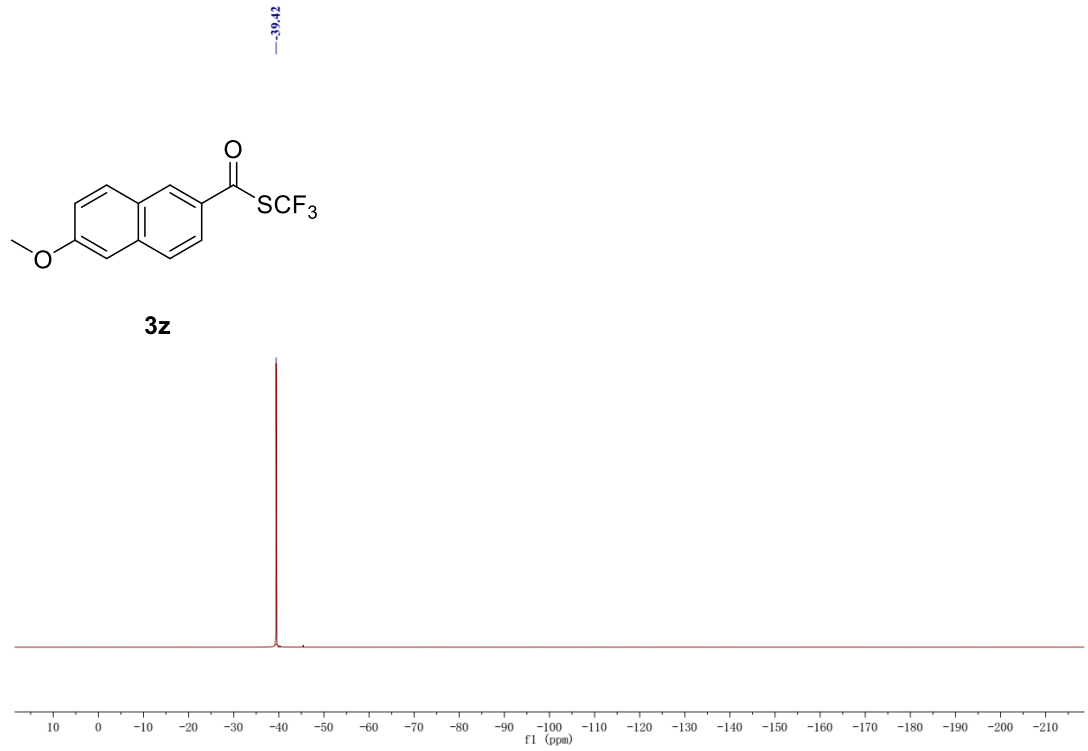
-39.51
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


8.32
8.32
7.87
7.85
7.84
7.83
7.82
7.80
7.78
7.26
7.26
7.26
7.24
7.23
7.17
7.16
3.96
O
SCF3
O
0.94
3.01
1.38
1.00
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

3z

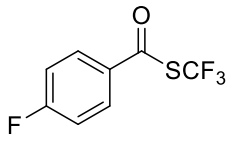

182.95
160.85
138.55
131.56
130.59
130.56
130.53
130.51
129.96
128.03
127.82
126.90
123.63
120.81
106.11
55.75
O
SCF3
O
f1 (ppm)

3z

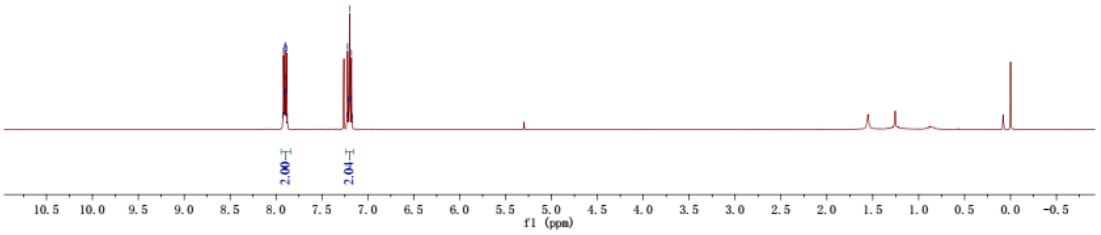

39.42
O
SCF3
O
f1 (ppm)

3z

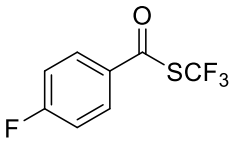

7.93
7.92
7.91
7.91
7.90
7.90
7.89
7.88
7.88
7.23
7.22
7.22
7.20
7.18
7.18
7.17


O
SCF3
F

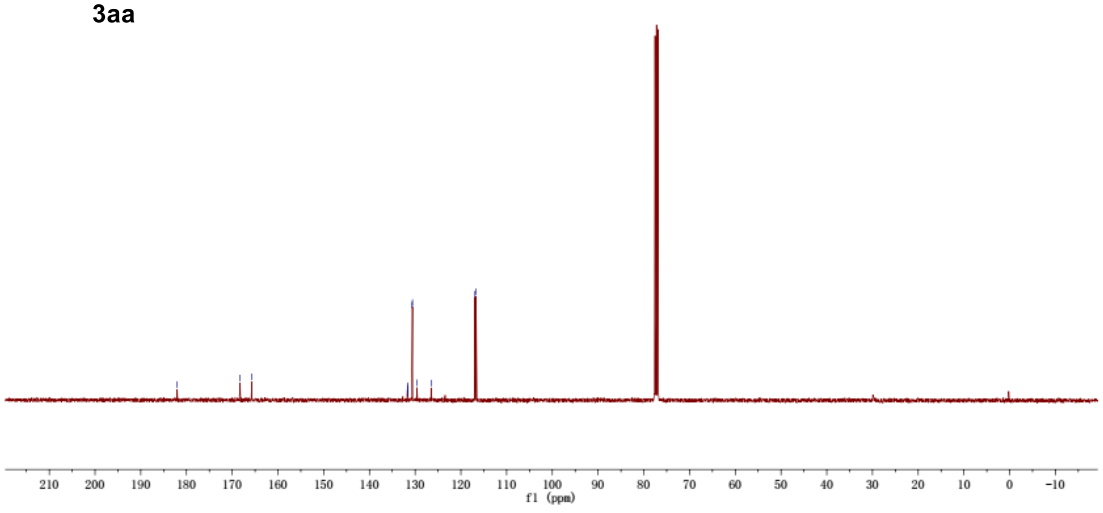
3aa

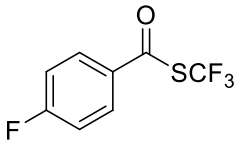

2.00
2.04
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


182.03
168.29
165.72
131.71
131.68
131.66
131.63
130.68
130.59
129.59
126.52
116.92
116.70


O
SCF3
F

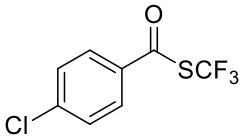
3aa


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)

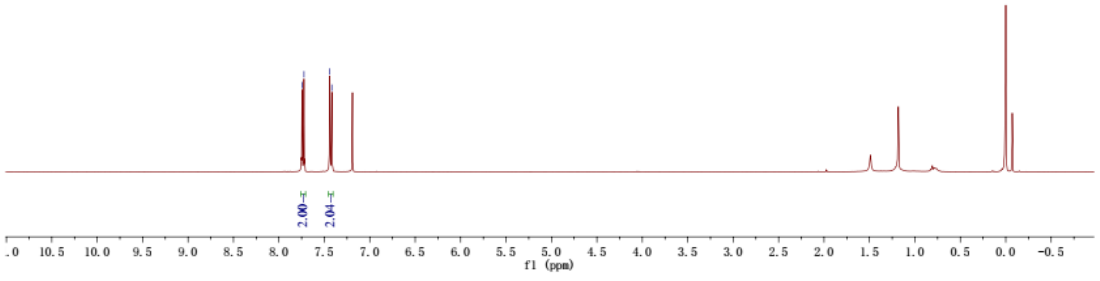

O
SCF3
F

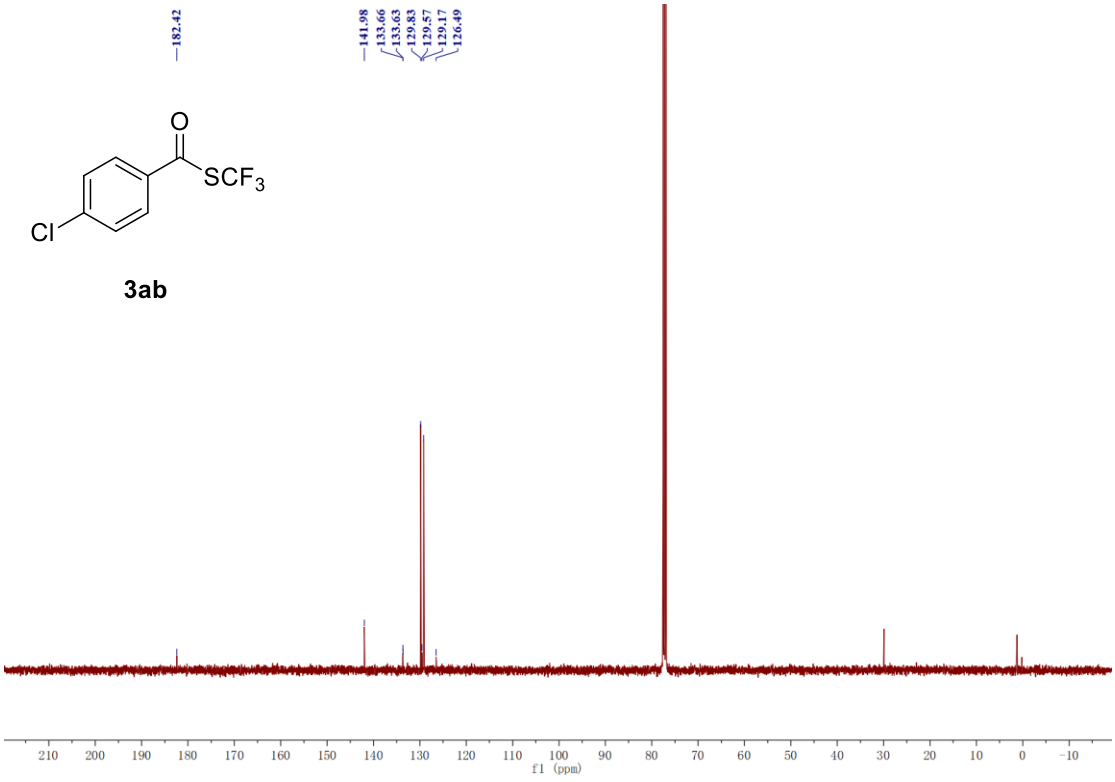
3aa

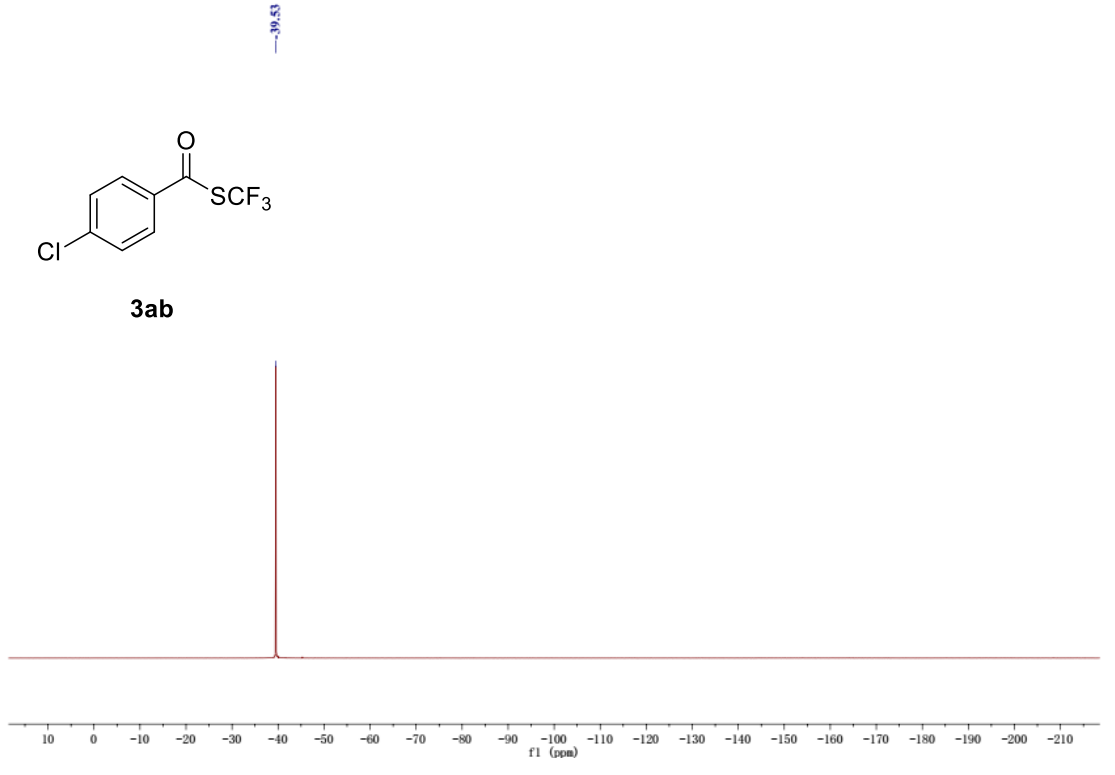
-39.54
-100.96
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)
7.75
7.72
7.44
7.42


O
SCF3
Cl

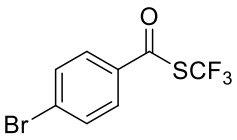
3ab


2.00
2.04
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)

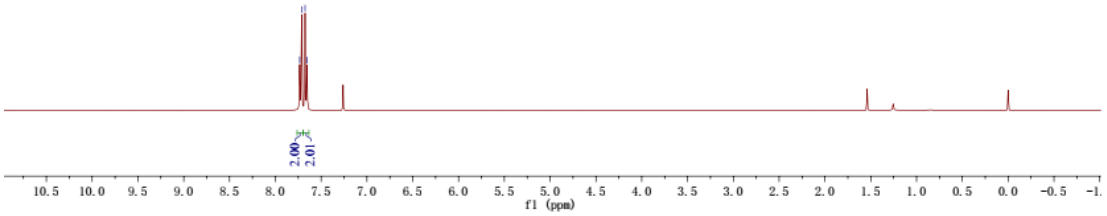

182.42
141.98
133.66
133.63
129.83
129.57
129.17
126.49
O
SCF3
Cl
3ab
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-39.53
O
SCF3
Cl
3ab
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)

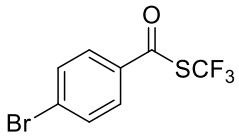

7.73
7.71
7.68
7.65


O
SCF3
Br

3ac

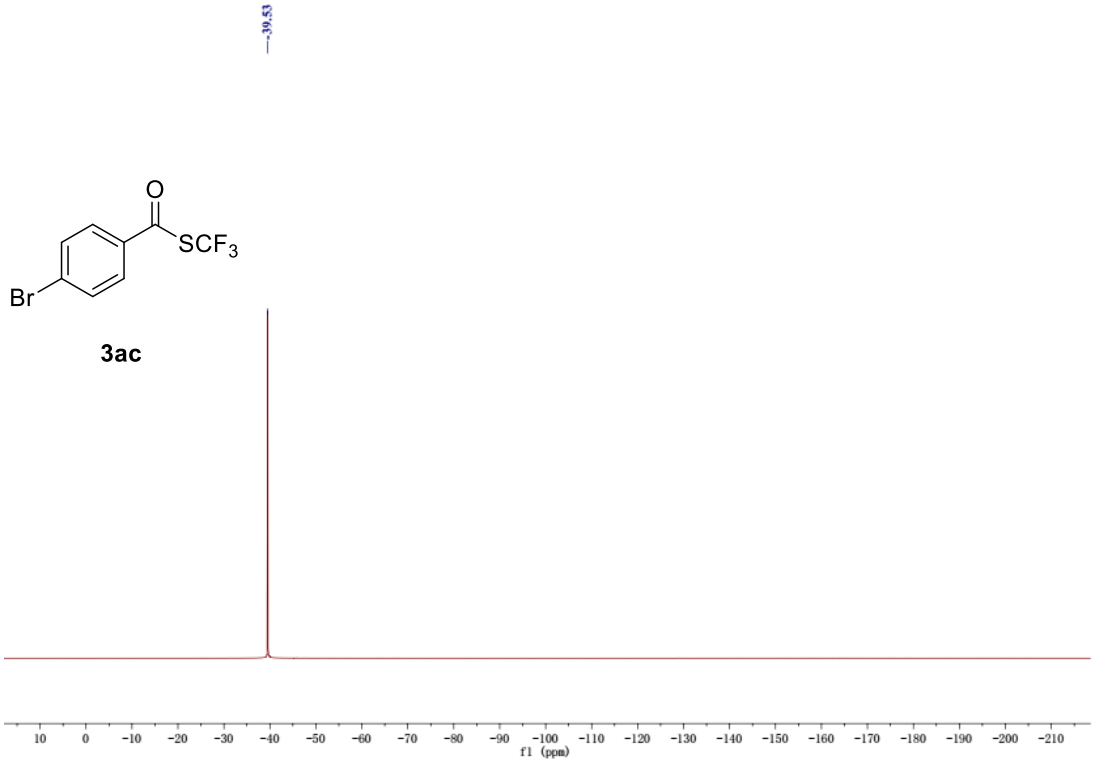

2.00
2.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.
f1 (ppm)

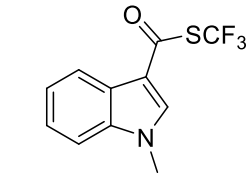

182.64
134.15
134.12
134.09
134.06
132.83
130.72
129.18
128.94
126.46


O
SCF3
Br

3ac

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)


-39.53
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)

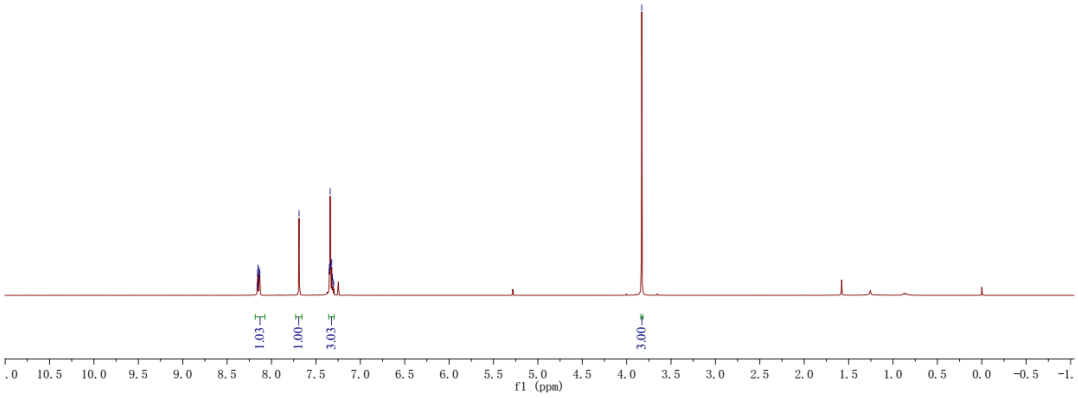

O
SCF3
Br

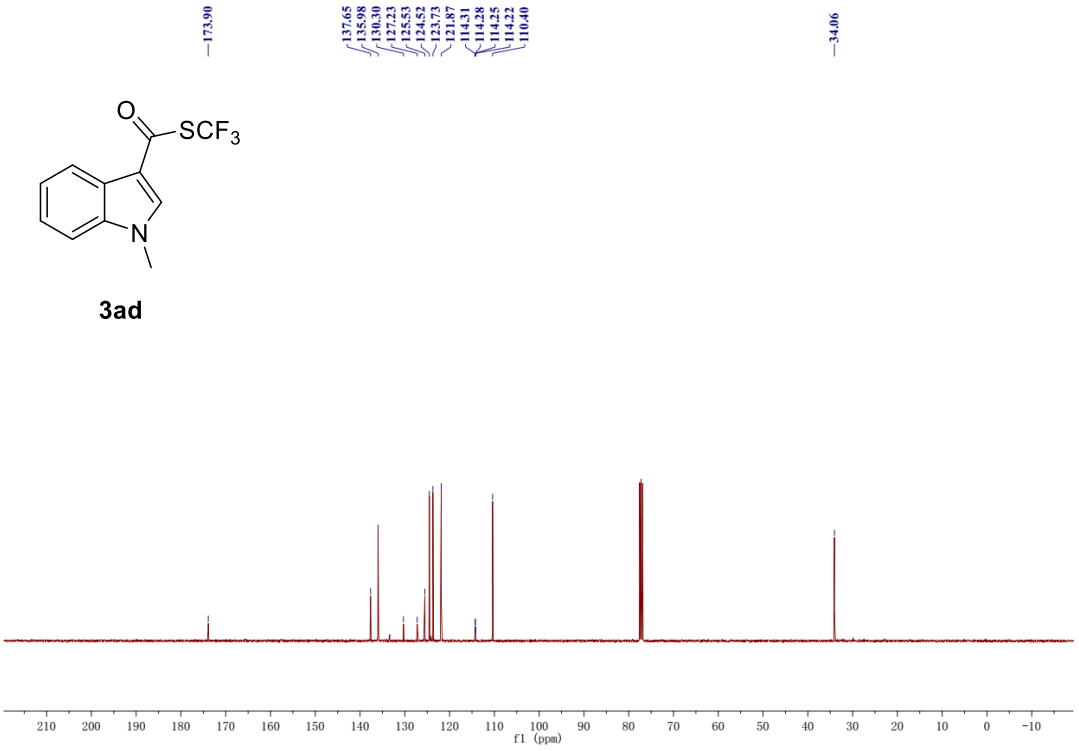
3ac


8.16
8.16
8.15
8.14
8.14
8.14
8.13
7.69
7.35
7.35
7.34
7.33
7.32
7.31
7.31
7.30
3.83

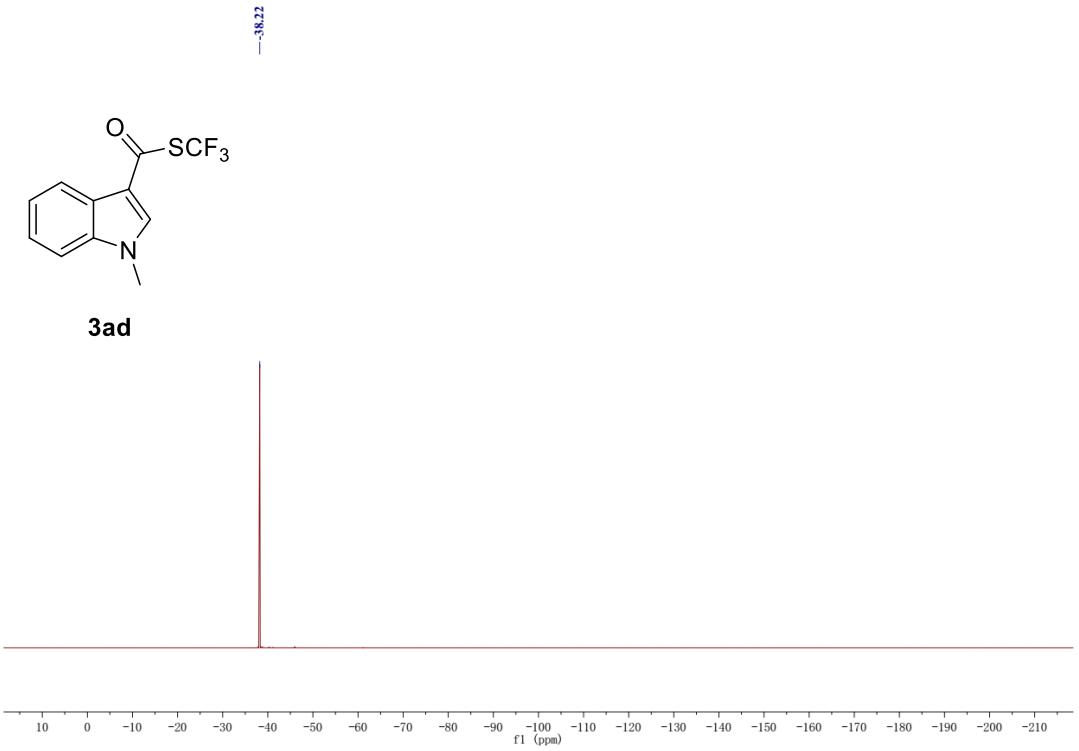
O
SCF3
N

3ad


1.03
1.00
3.03
3.00
f1 (ppm)

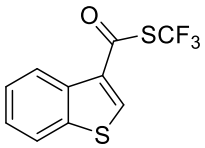

173.90
137.65
135.98
130.30
127.23
125.53
124.52
123.73
121.87
114.31
114.28
114.25
114.22
110.40
34.06
O
SCF3
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

3ad

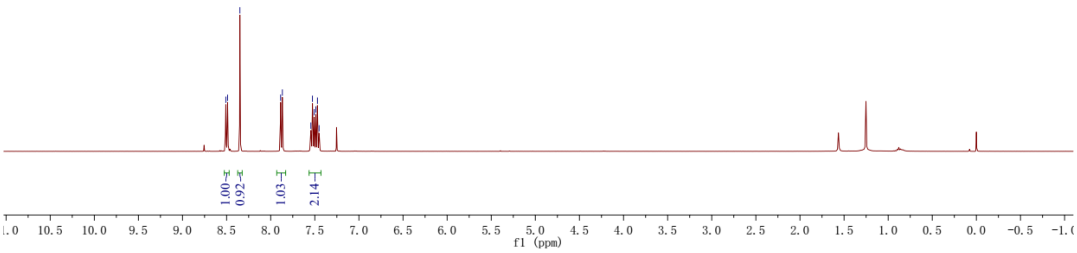

38.22
O
SCF3
N
10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)

3ad

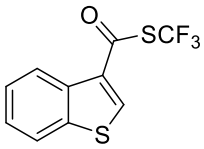

8.51
8.49
8.35
7.89
7.87
7.54
7.53
7.51
7.49
7.47
7.45


O
SCF3
S

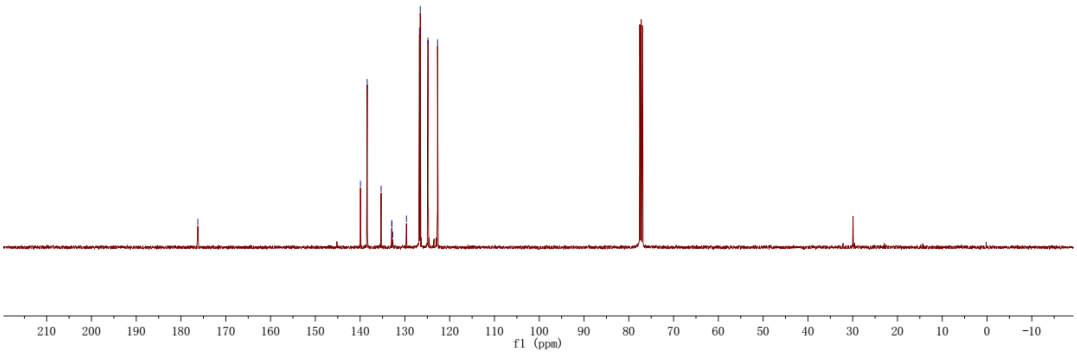
3ae

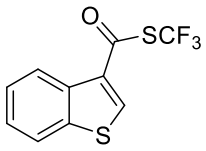

1.00
0.92
1.03
2.14
f1 (ppm)


176.25
139.93
138.41
135.31
132.94
132.91
132.73
129.66
126.75
126.58
124.85
122.71


O
SCF3
S

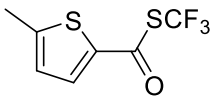
3ae


f1 (ppm)

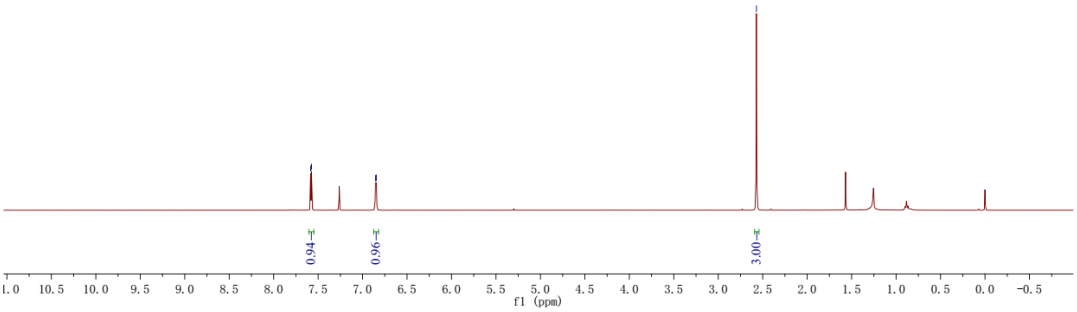

O
SCF3
S

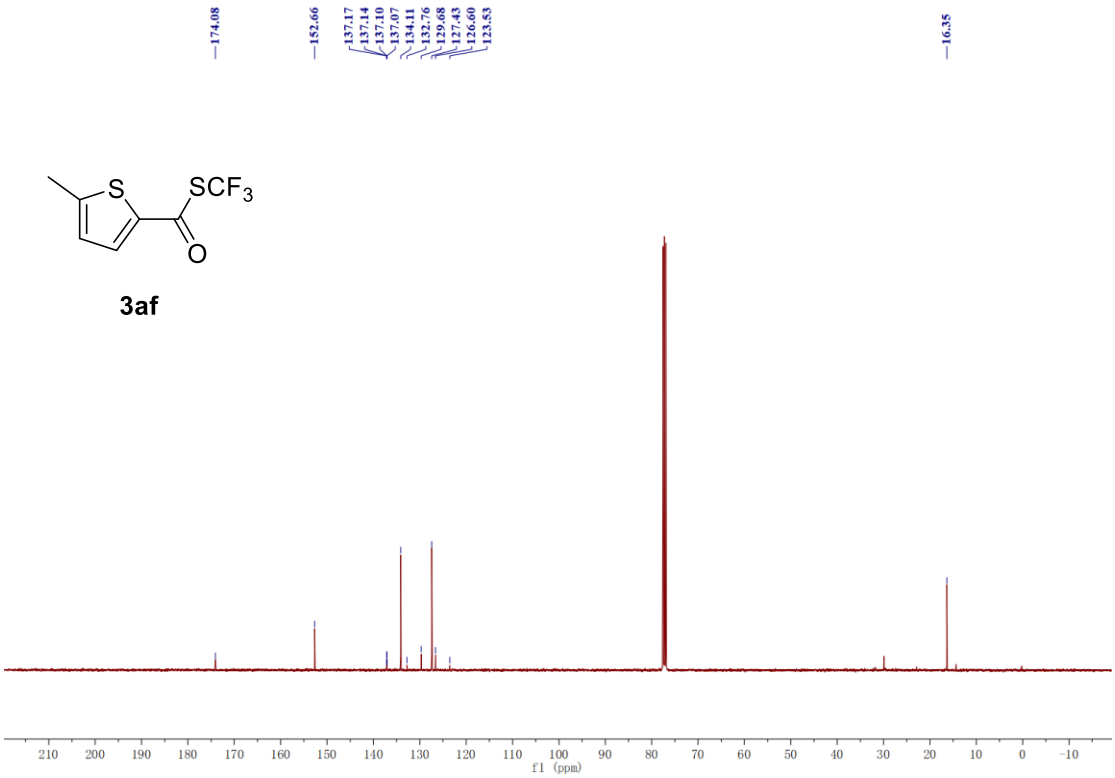
3ae

-39.13
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)
7.58
7.57
6.86
6.85
2.57

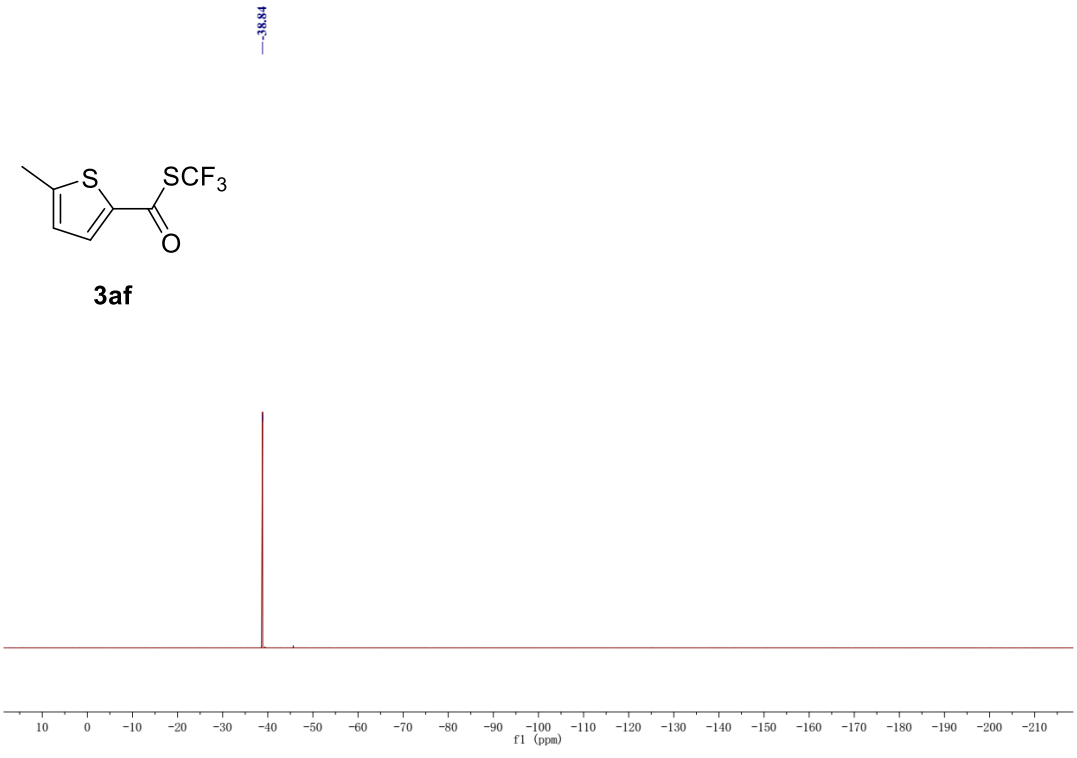

S
SCF3
O

3af

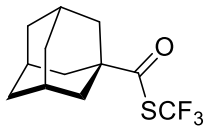

0.94
0.96
3.00
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


174.08
152.66
137.17
137.14
137.10
137.07
134.11
132.76
129.68
127.43
126.60
123.53
16.35
S
SCF3
O
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)

3af

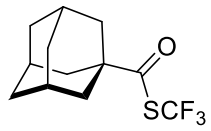

-38.84
S
SCF3
O
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

3af


O
SCF3

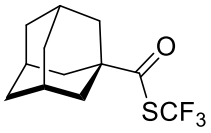
3ag

2.09
1.91
1.90
1.78
1.75
1.71
1.68
3.00
6.13
6.36
f1 (ppm)


O
SCF3

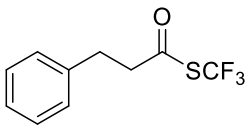
3ag

197.49
133.30
130.22
127.15
124.07
50.31
50.28
38.75
36.29
28.07
f1 (ppm)

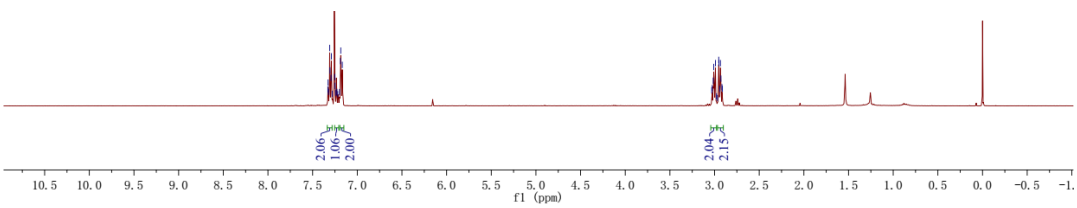

O
SCF3

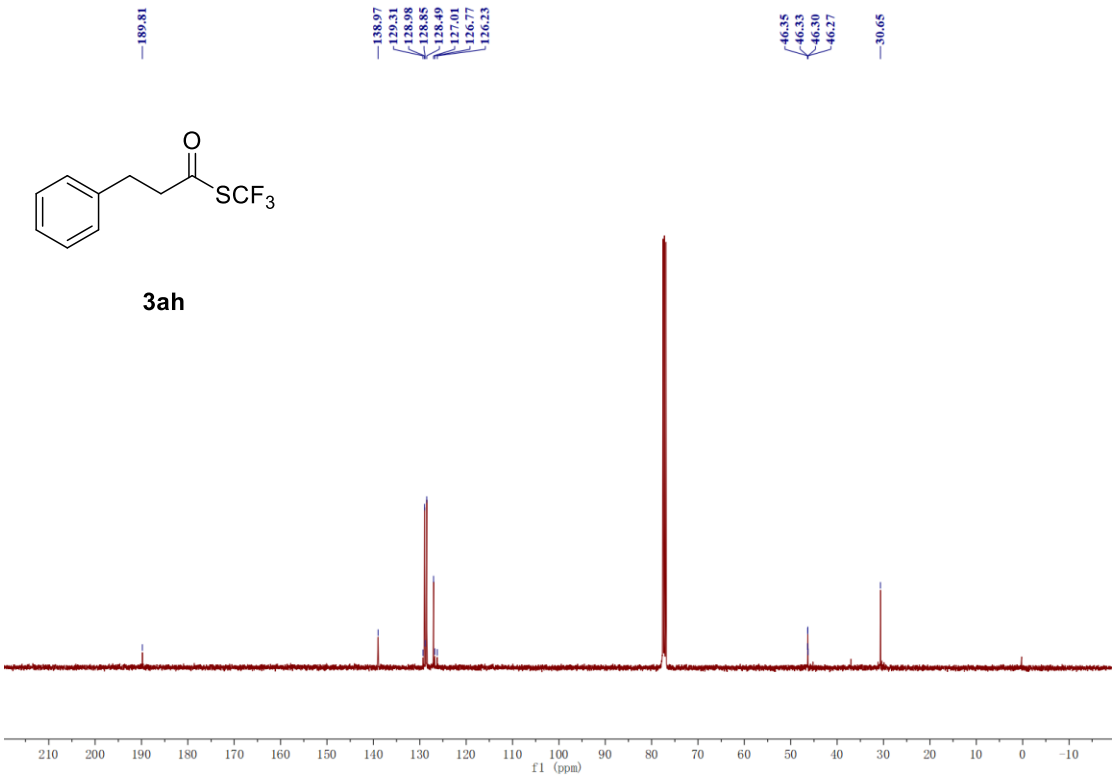
3ag

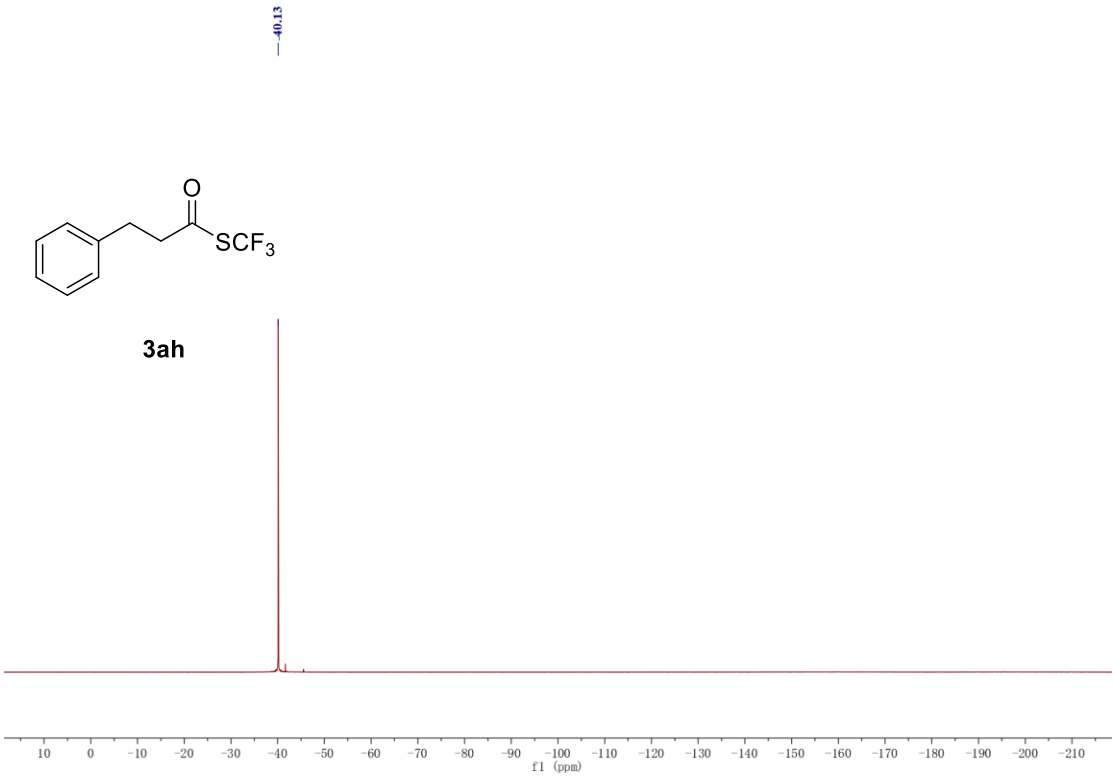
-39.92
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)
7.33 7.33 7.32 7.31 7.31 7.29 7.29 7.28 7.25 7.25 7.24 7.23 7.22 7.20 7.19 7.18 7.17
3.03 3.03 3.01 3.01 2.99 2.98 2.97 2.95 2.95 2.94 2.93 2.93 2.92 2.91

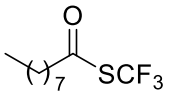

O
SCF3

3ah

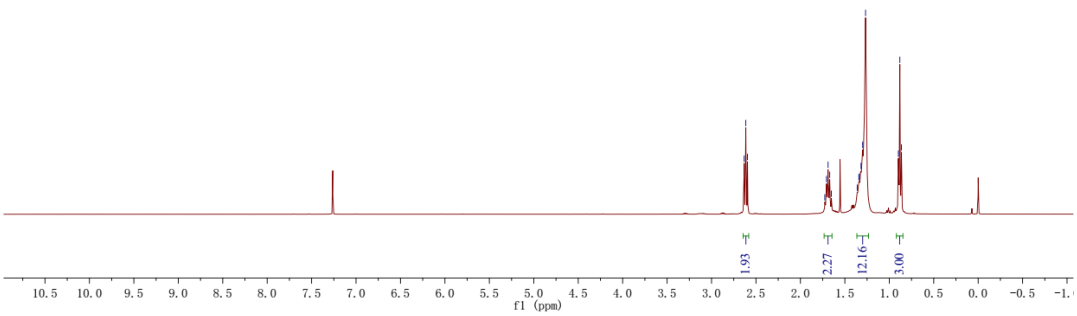

2.06
1.06
2.00
2.04
2.15
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

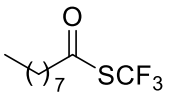

189.81
138.97
129.31
128.98
128.85
128.49
127.01
126.77
126.23
46.35
46.33
46.30
46.27
30.65
O
SCF3
3ah
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


40.13
O
SCF3
3ah
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)

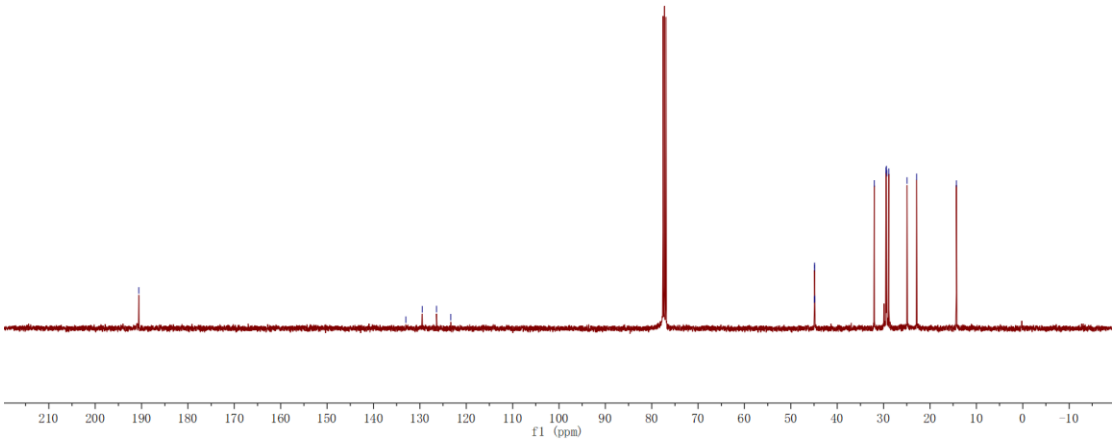


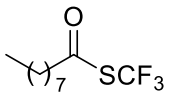
3ai





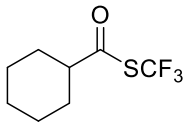
3ai



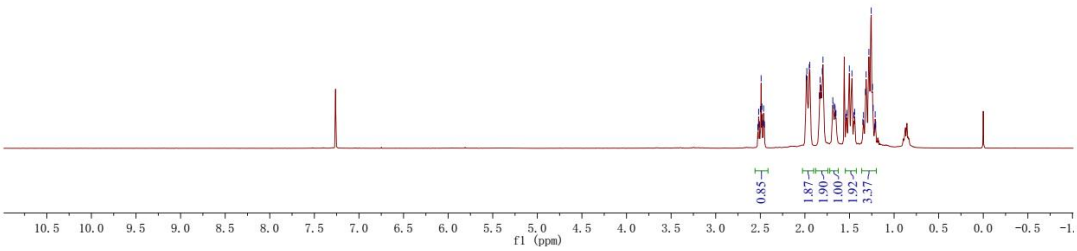

O
7
SCF3

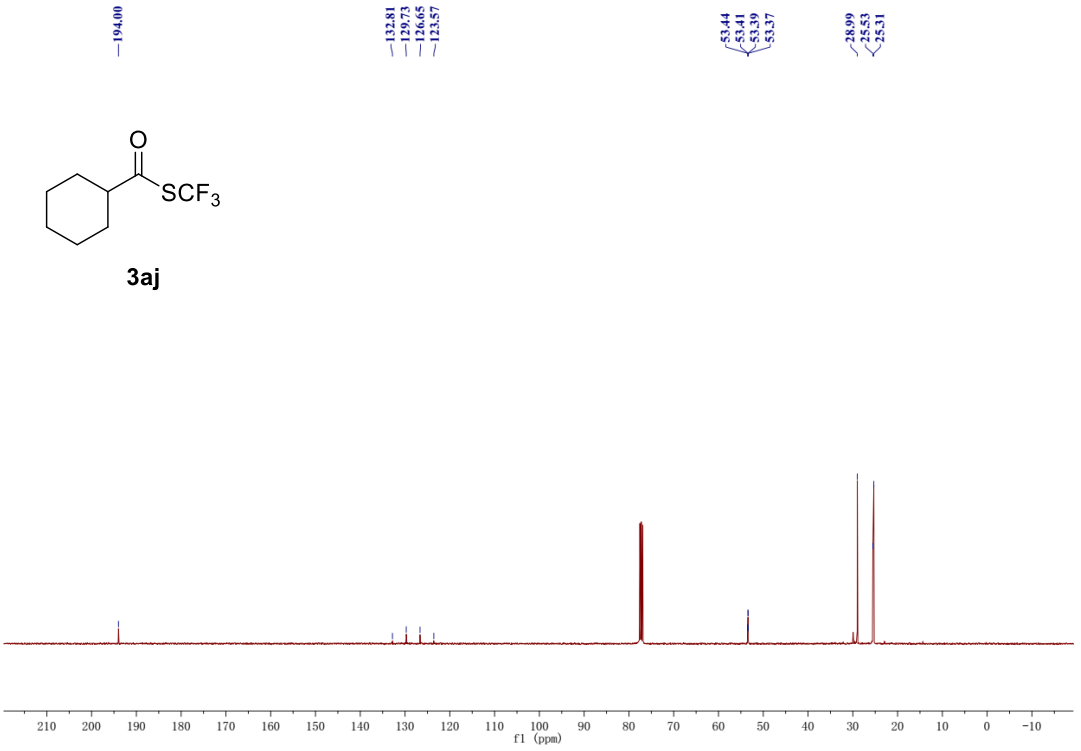
3ai

-40.24
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)
2.53 2.52 2.51 2.50 2.49 2.48 2.47 2.46 2.45 1.98 1.98 1.95 1.94 1.84 1.83 1.82 1.81 1.80 1.69 1.68 1.67 1.66 1.66 1.65 1.54 1.53 1.50 1.47 1.45 1.44 1.35 1.34 1.32 1.31 1.28 1.26 1.24 1.23 1.22 1.21 1.21

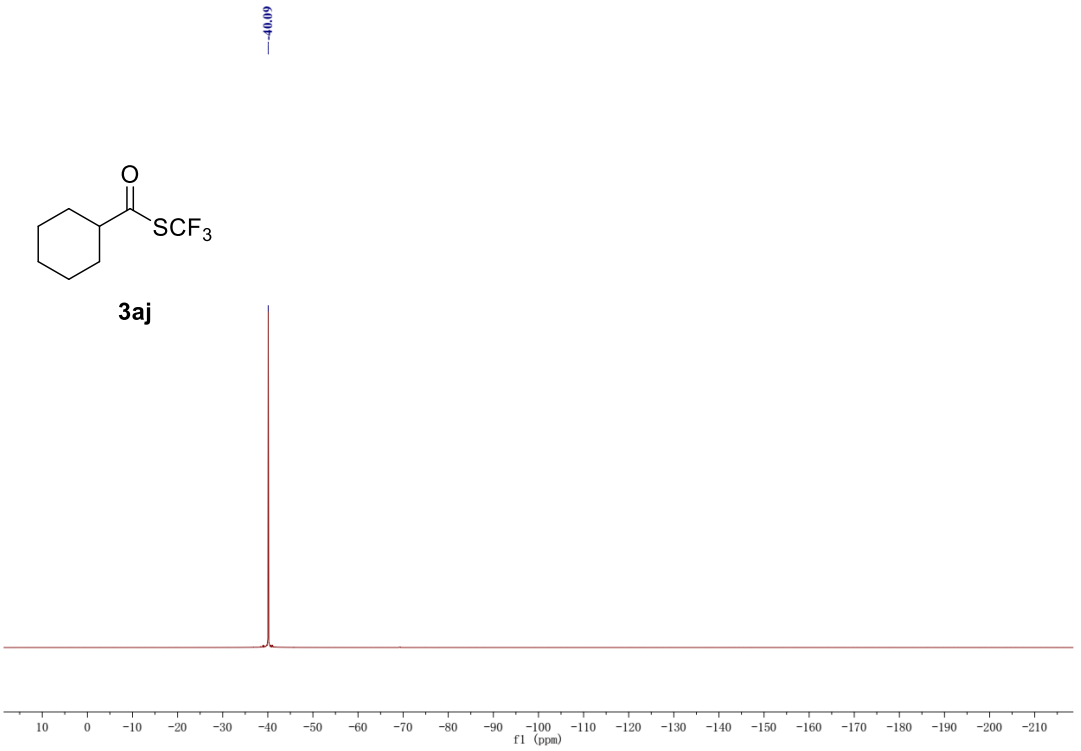

O
SCF3

3aj

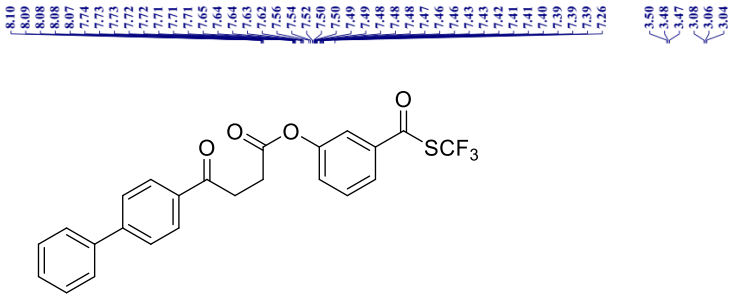

0.85
1.87
1.90
1.00
1.92
3.37
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


194.00
132.81
129.73
126.65
123.57
53.44
53.41
53.39
53.37
28.99
25.53
25.31
O
SCF3
f1 (ppm)

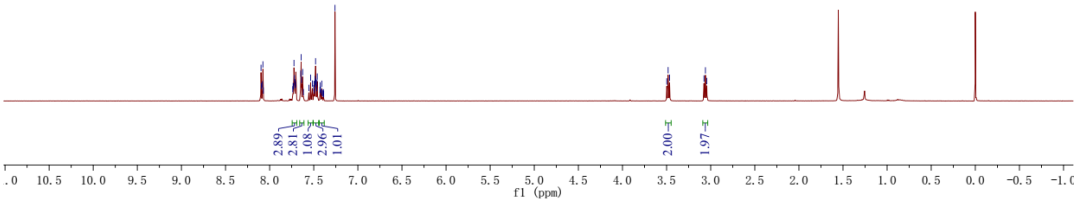
3aj

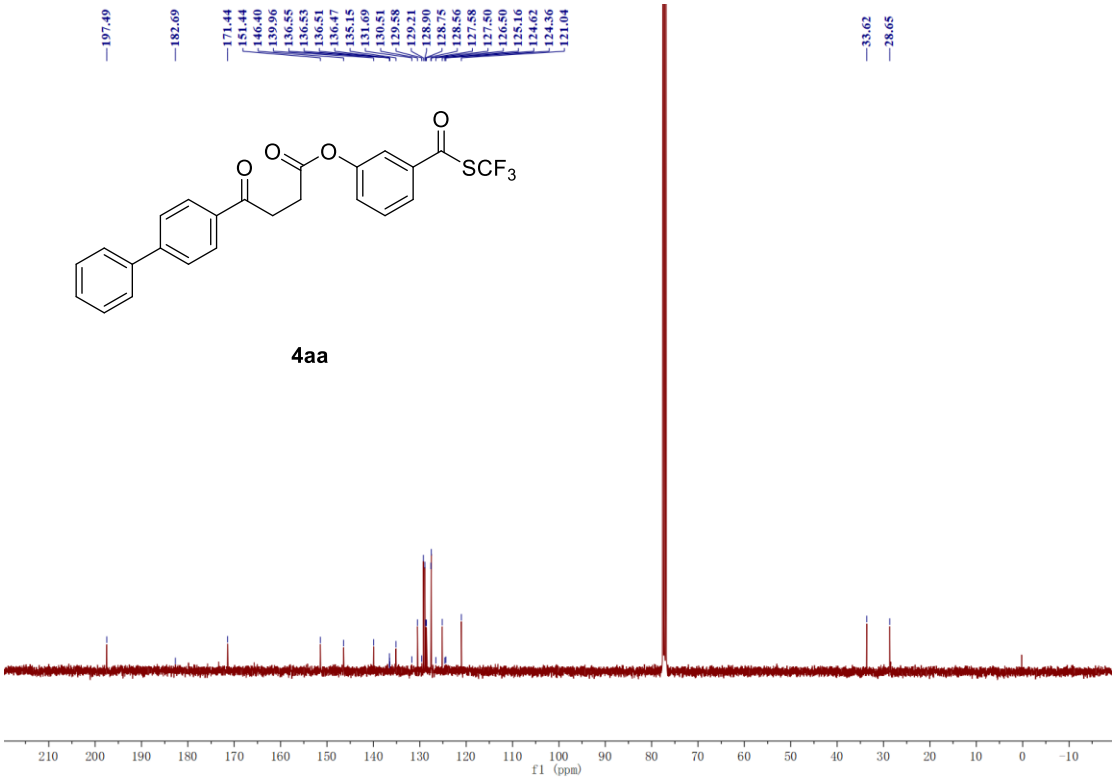

-40.09
O
SCF3
f1 (ppm)

3aj

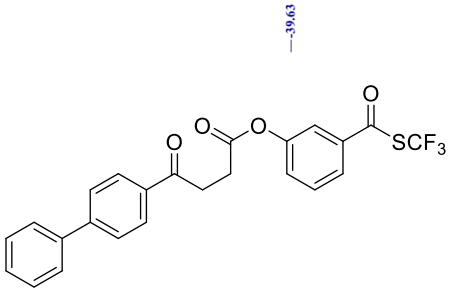


4aa

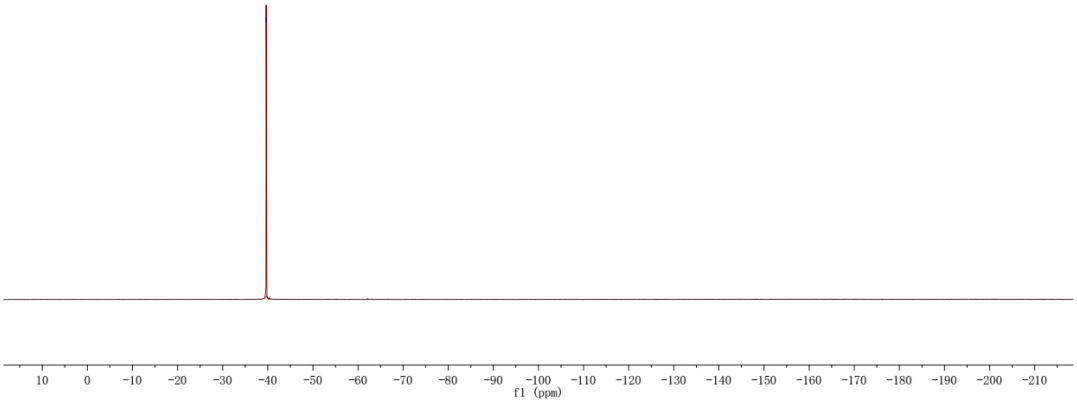




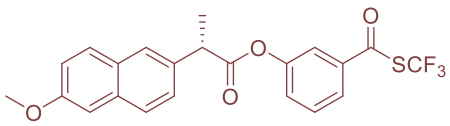
4aa


-39.63
O
O
O
O
SCF3

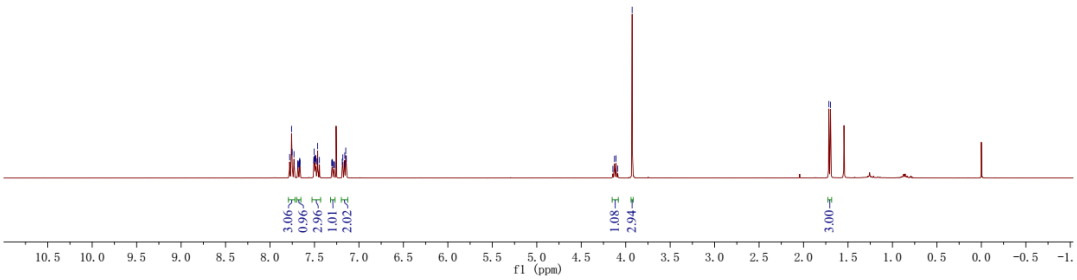
4aa

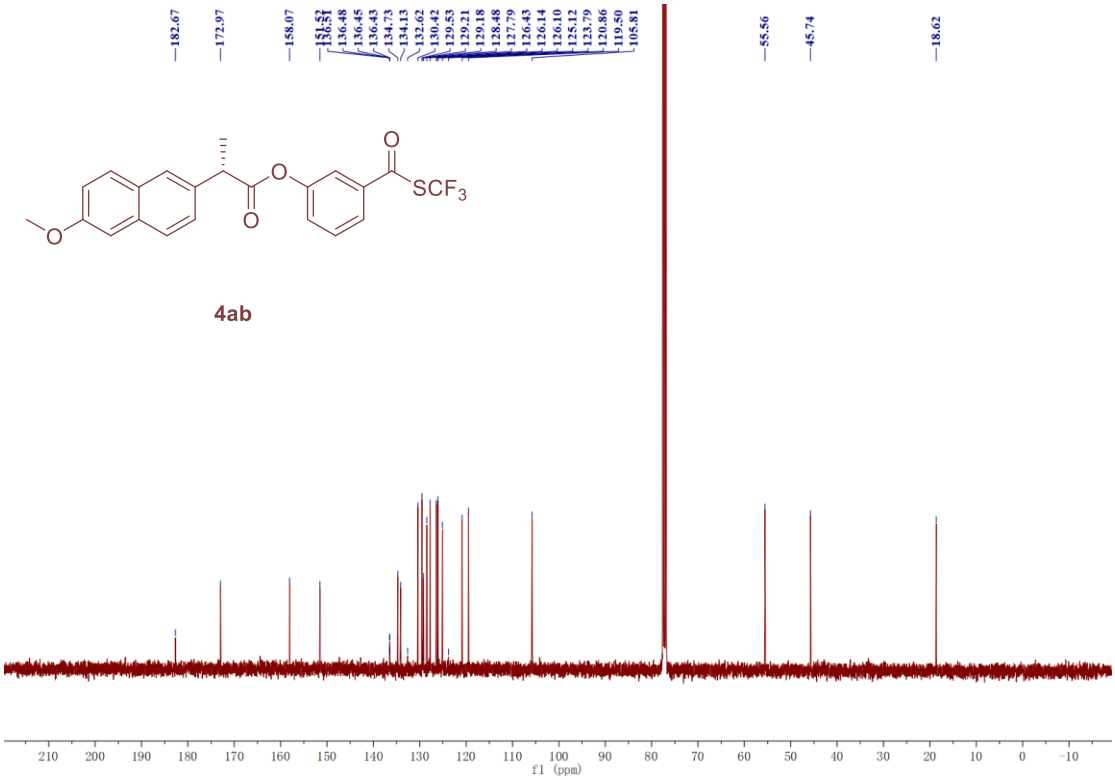

10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

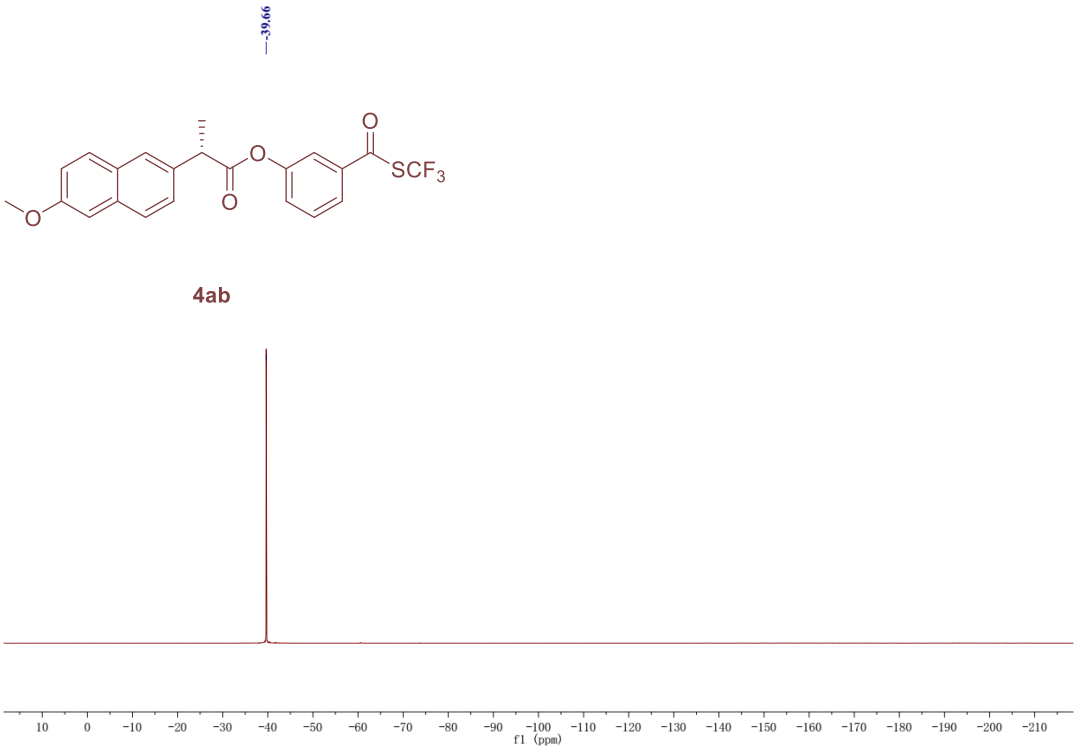

7.78 7.76 7.75 7.73 7.69 7.69 7.68 7.68 7.67 7.67 7.67 7.66 7.51 7.50 7.50 7.49 7.49 7.48 7.47 7.46 7.44 7.31 7.30 7.30 7.30 7.28 7.28 7.28 7.19 7.18 7.17 7.16 7.15 7.14
4.14 4.13 4.11 4.09 3.93
1.71 1.70


O
O
O
O
SCF3

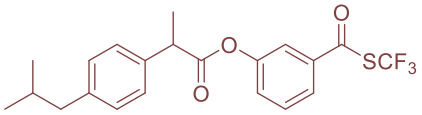
4ab


3.06 0.96 2.96 1.01 2.02
1.08 2.94
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

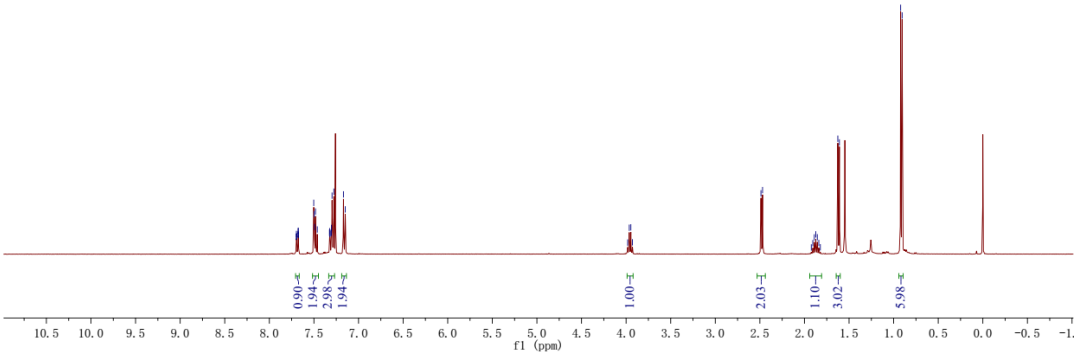

182.67
172.97
158.07
151.52
136.51
136.48
136.45
136.43
134.73
134.13
132.62
130.42
129.53
129.21
129.18
128.48
127.79
126.43
126.14
126.10
125.12
123.79
120.86
119.50
105.81
55.56
45.74
18.62
O
O
O
SCF3
O
4ab
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


-39.66
O
O
O
SCF3
O
4ab
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)

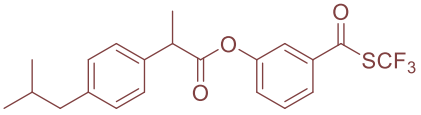

7.70
7.70
7.69
7.68
7.68
7.68
7.67
7.50
7.50
7.49
7.48
7.46
7.33
7.32
7.32
7.32
7.30
7.30
7.30
7.28
7.17
7.15
3.98
3.96
3.95
3.93
2.49
2.47
1.92
1.91
1.89
1.87
1.86
1.84
1.82
1.63
1.61
0.92
0.90


O
O
O
SCF3

4ac

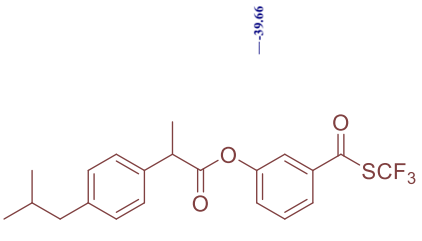

0.90
1.94
2.98
1.94
1.00
2.03
1.10
3.02
5.98
f1 (ppm)


182.70
173.02
151.56
141.36
136.87
136.51
136.48
136.45
136.43
130.40
129.88
128.52
127.52
127.38
126.47
125.08
123.39
122.08
120.88
45.42
45.24
30.41
22.60
18.62

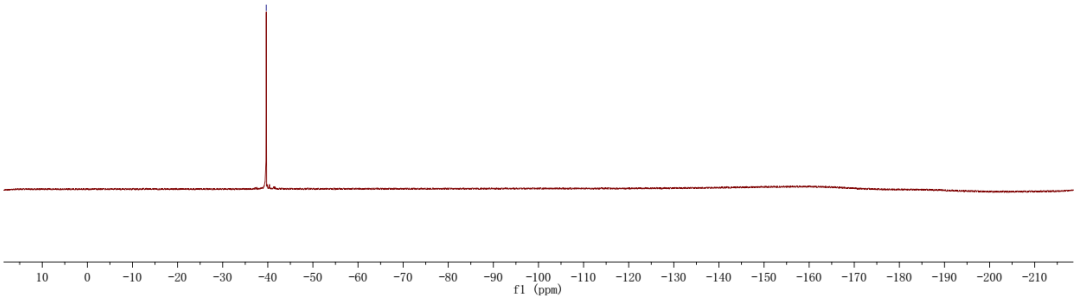

O
O
O
SCF3

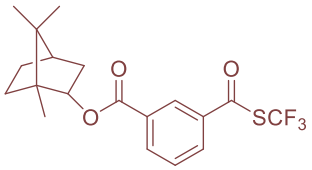
4ac

f1 (ppm)

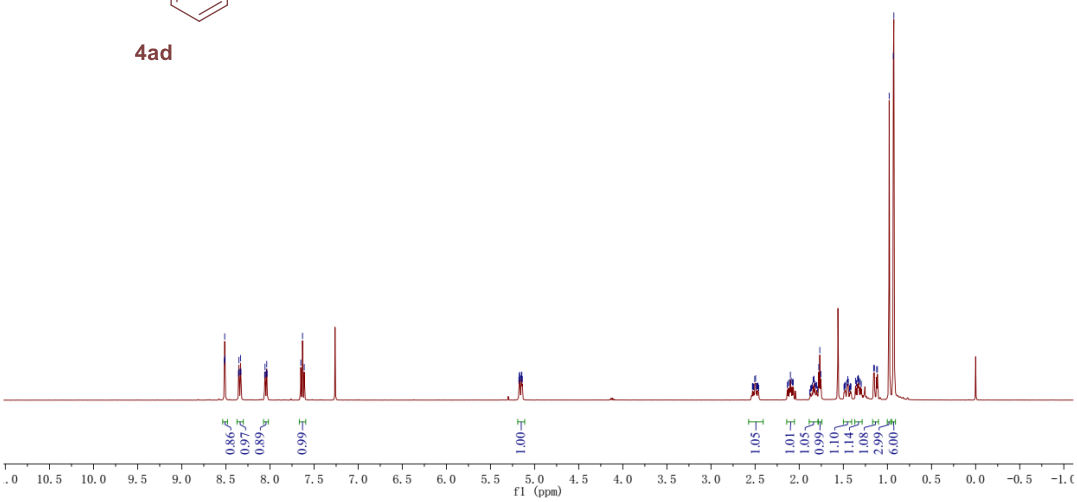

-39.66
O
O
O
SCF3

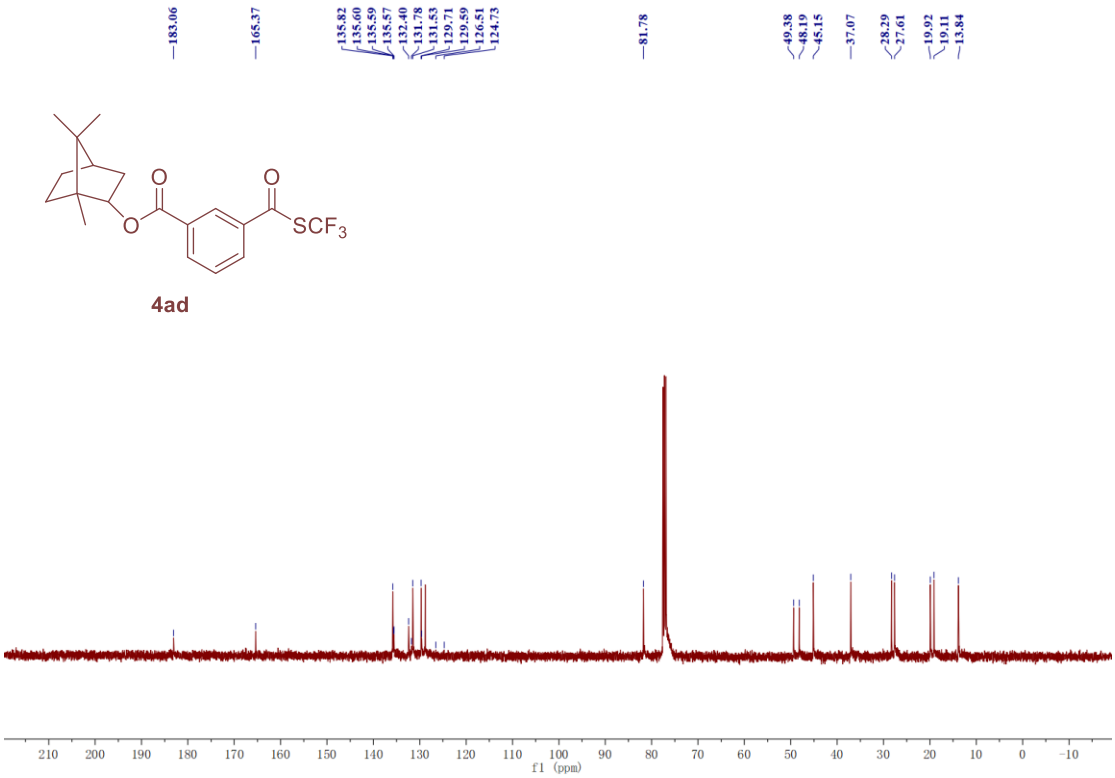
4ac

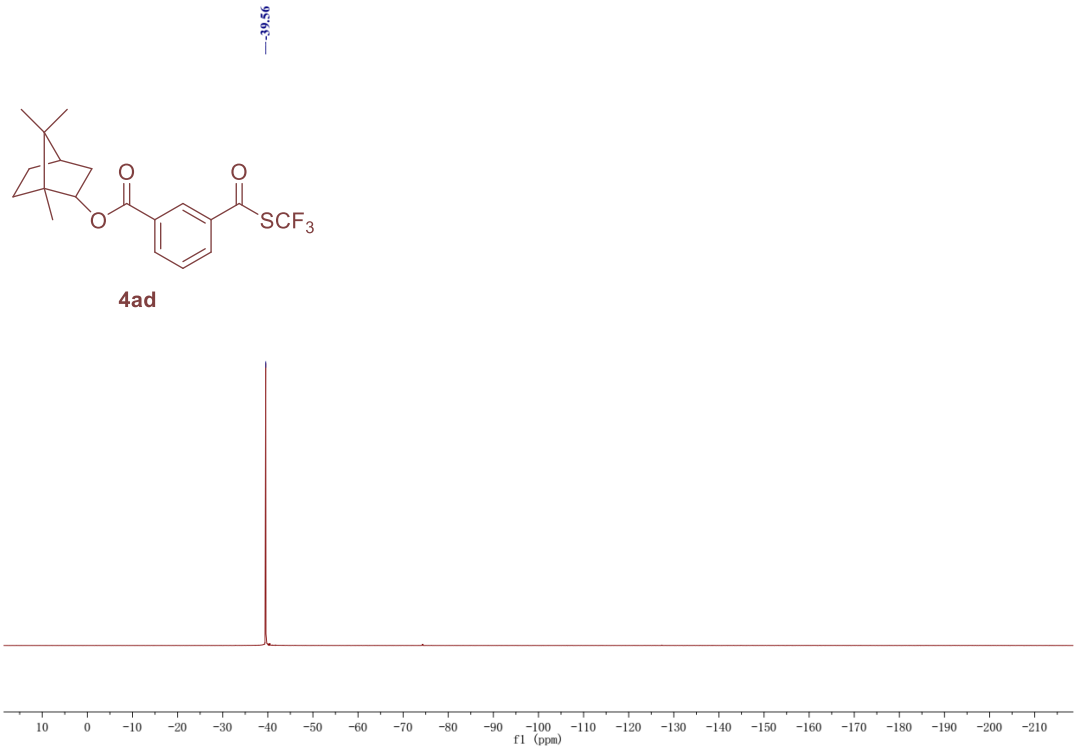

10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

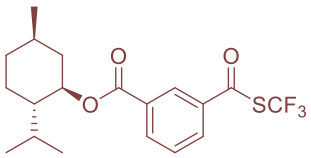

O
O
O
SCF3

4ad

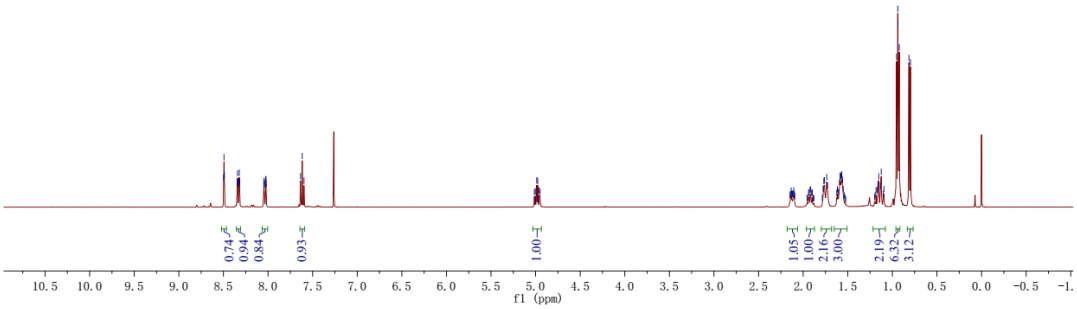

0.86
0.97
0.89
0.99
1.00
1.05
1.01
1.05
0.99
1.10
1.14
1.08
2.99
6.00
f1 (ppm)

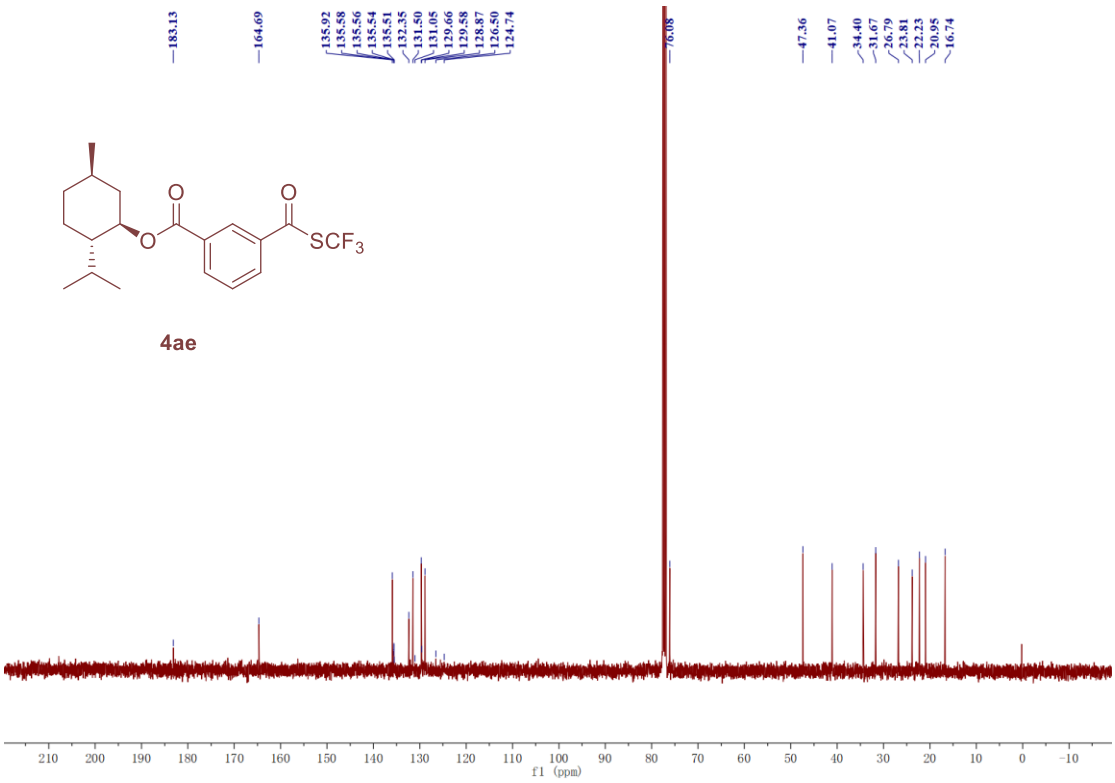

183.06
165.37
135.82
135.60
135.59
135.57
132.40
131.78
131.53
129.71
129.59
126.51
124.73
81.78
49.38
48.19
45.15
37.07
28.29
27.61
19.92
19.11
13.84
O
O
O
SCF3
4ad
f1 (ppm)


-39.56
O
O
O
SCF3
4ad
f1 (ppm)

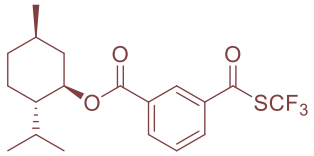


4ae



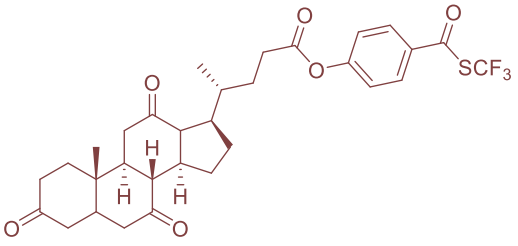


4ae

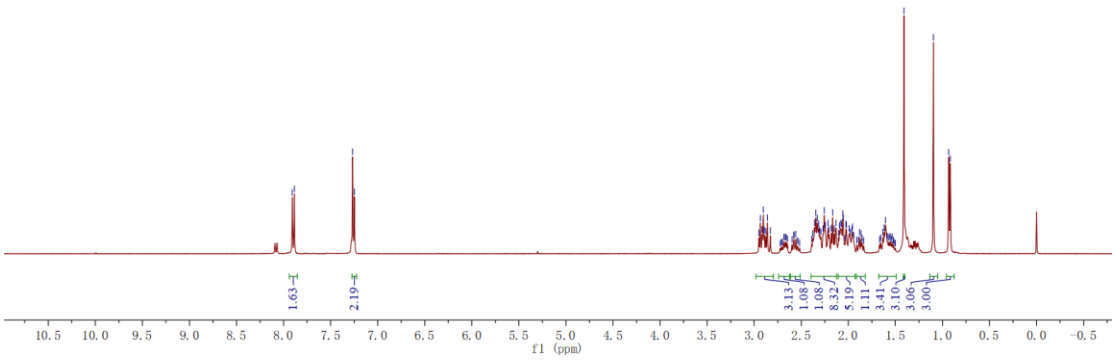

O
O
O
SCF3

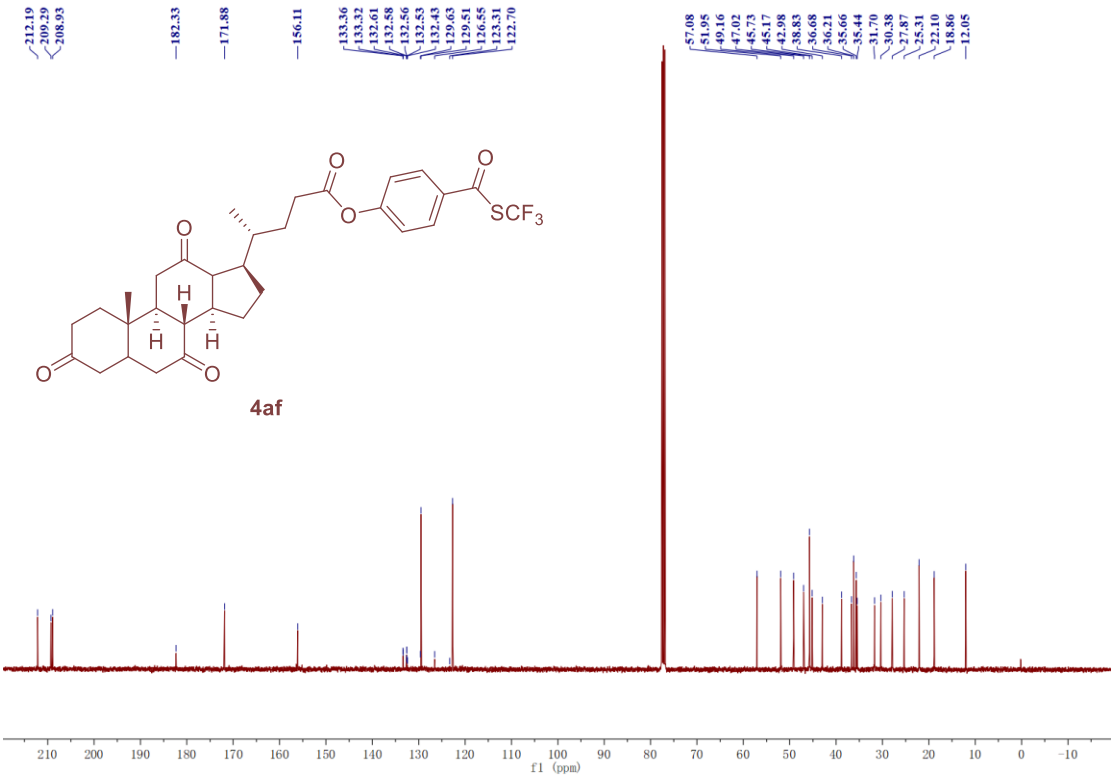
4ae

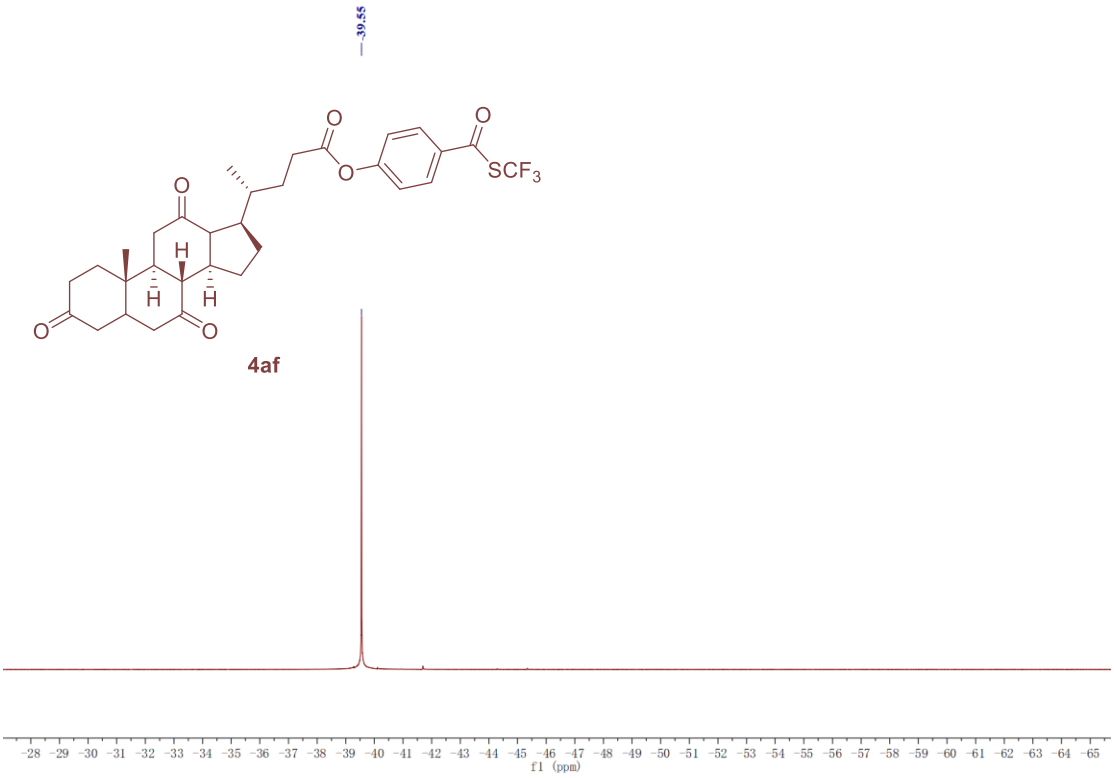
-39.57
10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)
7.91 7.89 7.27 7.25 2.95 2.93 2.92 2.90 2.89 2.88 2.86 2.83 2.68 2.67 2.66 2.65 2.60 2.58 2.58 2.56 2.39 2.38 2.36 2.35 2.33 2.32 2.30 2.29 2.27 2.26 2.24 2.22 2.20 2.18 2.17 2.15 2.13 2.10 2.09 2.08 2.07 2.06 2.05 2.04 2.03 2.02 1.99 1.98 1.96 1.96 1.94 1.91 1.89 1.88 1.86 1.85 1.84 1.67 1.65 1.63 1.62 1.60 1.58 1.57 1.56 1.55 1.53 1.52 1.41 1.10 0.93 0.92

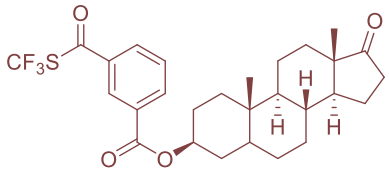

O
O
O
SCF3
O
H
H
H
O
O

4af

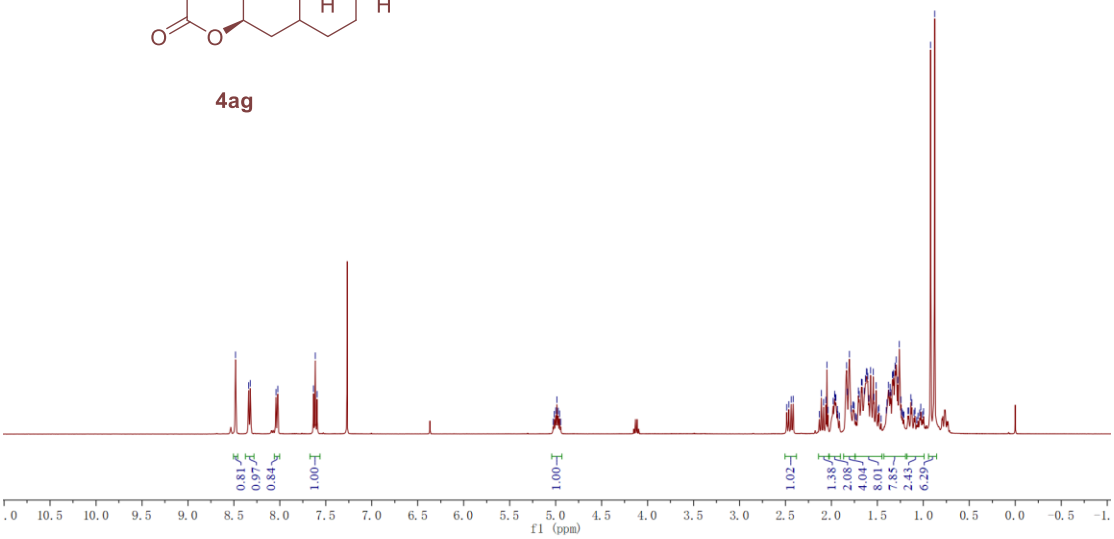

1.63
2.19
3.13
1.08
1.08
8.32
5.19
1.11
3.41
3.10
3.06
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5
f1 (ppm)

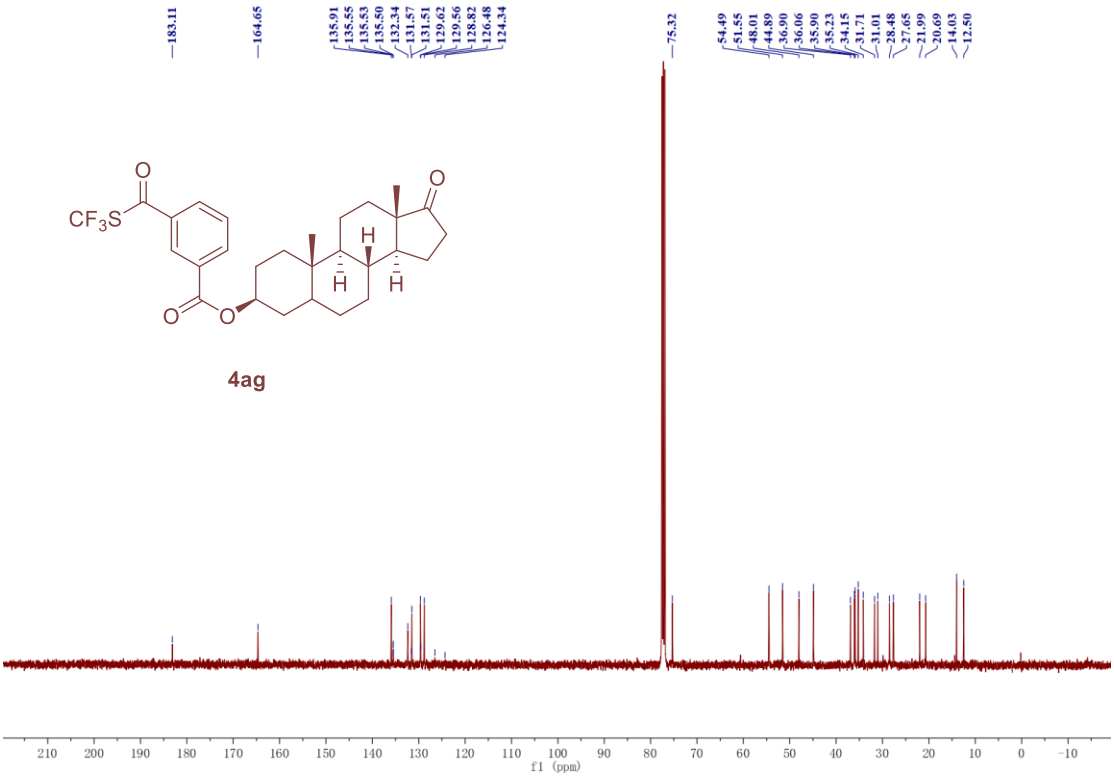

212.19
209.29
208.93
182.33
171.88
156.11
133.36
133.32
132.61
132.58
132.56
132.53
132.43
129.63
129.51
126.55
123.31
122.70
57.08
51.95
49.16
47.02
45.73
45.17
42.98
38.83
36.68
36.21
35.66
35.44
31.70
30.38
27.87
25.31
22.10
18.86
12.05
O
O
O
SCF3
H
H
H
O
O
4af
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


39.55
O
O
O
SCF3
H
H
H
O
O
4af
−28 −29 −30 −31 −32 −33 −34 −35 −36 −37 −38 −39 −40 −41 −42 −43 −44 −45 −46 −47 −48 −49 −50 −51 −52 −53 −54 −55 −56 −57 −58 −59 −60 −61 −62 −63 −64 −65
f1 (ppm)

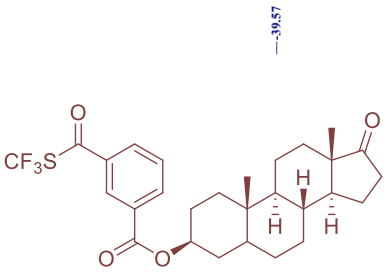


4ag

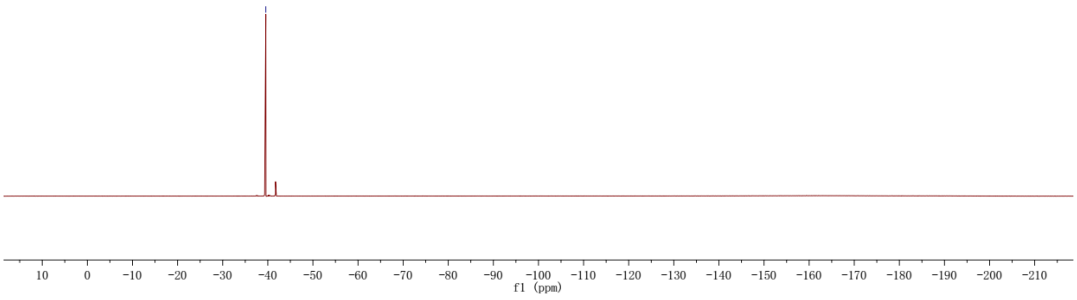




4ag


-39.57
O
CF3S
O
O
H
H
H
O

4ag


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)

13. Reference

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[3] Mao, R.; Bera, S.; Cheseaux, A.; Hu, X. Deoxygenative Trifluoromethylthi-olation of Carboxylic Acids. *Chem. Sci*. **2019**, *10* (41), 9555–9559.

[4] Ye, Z.; Lei, Z.; Ye, X.; Zhou, L.; Wang, Y.; Yuan, Z.; Gao, F.; Britton, R. Decatungstate Catalyzed Synthesis of Trifluoromethylthioesters from Aldehydes via a Radical Process. *J. Org. Chem.* **2022**, *87*, 765−775.

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