Supporting Information

Catalytic Mutual Multicomponent Reaction: Facile Access to α-Trifluoromethylthiolated Ketones

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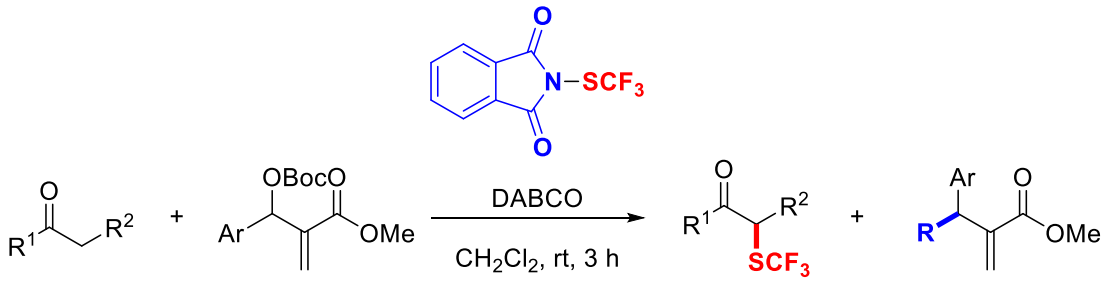
General Information

Unless Stated otherwise, the reactions and manipulations were performed under an atmosphere of argon by using standard Schlenk techniques and Drybox (Mikrouna, Supper 1220/750). Analytical thin layer chromatography (TLC) was performed on precoated silica gel 60GF254 plates. Flash column chromatography was performed using Tsingdao silica gel (60, particle size 0.040-0.063 mm). ^{1}H, ^{13}C and ^{19}F NMR spectra were recorded on a Bruker at 600 MHz, 125 MHz and 376 MHz. Chemical shift values are reported in ppm from tetramethylsilane as the internal standard (TMS: δ 7.26 for ^{1}H and δ 77.16 for ^{13}C). Data are reported asfollows: chemical shifts, integration, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, dd =doublet of doublets, dq = doublet of quartets, m = multiplet), and coupling constants (Hz). The enantiomeric excess values were determined by chiral HPLC with an Agilent 1200 LC instrument. High resolution mass spectroscopy (HRMS) analyses were performed at a Bruker Daltonics. Inc mass instrument (ESI). Commercial grade reagents and solvents were used without further purification except as indicated below. Toluene was distilled from sodium. Tetrahydrofuran was distilled from sodium and benzophenone. Dichloromethane was distilled from calcium hydride. Acetonitrile was distilled from both P_2O_5 and calcium hydride according to general method prior to use. N,N-Dimethylformamide and Dimethyl sulfoxide were distilled from calcium hydride. The chiral ligands was purchased from J&K Chemicals. The benzyl ketones (**1a-r**),[1] β-keto thioester **1s**,[2] 2-thio/2-furanacetophenones (**1t**, **1u**),[3] 2-acyl imidazoles (**1v**, **1w**),[4] monoarylated methyl ketone **1x**,[5] β-ketoesters (**5a-i**),[6a,6b] oxindoles,[6c] benzofuranones[6d] and MBH carbonates **2**[7] were prepared according to the reported procedure.

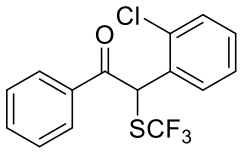
General Procedure for Diversity-Oriented Synthesis of α-Trifluoromethylthiolated Ketones and α-Methylene β-Amino Ester Libraries



1 **2** **3** **4**

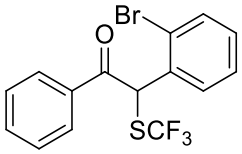
An oven-dried vial fitted with a stirrer bar was charged with acyclic ketones (0.1 mmol), MBH carbonates (0.11 mmol), *N*-SCF_3 phthalimide (0.11 mmol) and DABCO (0.2 equiv) in dry CH_2Cl_2 (1.0 mL) and the mixture was stirred at room temperature for 3 h. Concentration and purification by silica gel column chromatography gave the product **3** and **4**.

Analytic Data for Products



3a

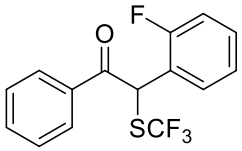
2-(2-chlorophenyl)-1-phenyl-2-(trifluoromethylthio)ethanone (3a). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.01 (d, *J* = 10.0 Hz, 2H), 7.60-7.53 (m, 1H), 7.49-7.40 (m, 4H), 7.28-7.21 (m, 2H), 6.66 (s, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 193.1, 134.4 134.2, 133.4, 133.1,130.43,130.42 (q, J_{CF} = 307.5 Hz), 130.4, 130.2, 129.09, 129.08, 128.1, 52.04; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -40.27 (s, 3F); **HRMS** (ESI) calcd for $C_{15}H_{10}ClF_3OSNa$ $[M+Na]^+$ 352.9991, found 352.9987.



3b

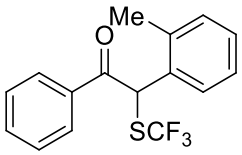
2-(2-bromophenyl)-1-phenyl-2-(trifluoromethylthio)ethanone (3b). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.02 (d, *J* = 10.0 Hz, 2H), 7.62 (d, *J* = 5.0 Hz, 1H), 7.59-7.55 (m, 1H), 7.49-7.42 (m, 3H), 7.31-7.25 (m, 1H), 7.18-7.14 (m, 1H), 6.63 (s, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 193.0,

134.5, 134.4, 133.9, 130.6, 130.5, 130.3 (q, J_{CF} = 306.0), 129.3, 129.1, 128.9, 124.2, 54.6; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -40.16 (s, 3F); **HRMS** (ESI) calcd for $C_{15}H_{10}BrF_3OSNa$ $[M+Na]^+$ 396.9486, found 396.9482.



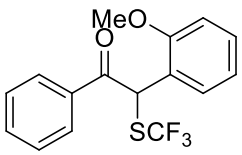
3c

2-(2-fluorophenyl)-1-phenyl-2-(trifluoromethylthio)ethanone (3c). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.01-7.94 (m, 2H), 7.60-7.53 (m, 1H), 7.49-7.39 (m, 3H), 7.32-7.25 (m, 1H), 7.16-7.06 (m, 2H), 6.53 (s, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 192.8, 159.4 (d, J_{CF} = 246.0 Hz), 134.4, 133.9, 131.0 (d, J_{CF} = 7.5 Hz), 130.6 (q, J_{CF} = 306.0), 129.9 (d, J_{CF} = 1.5 Hz), 129.1 (d, J_{CF} = 12.0 Hz), 125.4 (d, J_{CF} = 3.0 Hz), 123.2 (d, J_{CF} = 13.5 Hz), 48.4; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -40.48 (s, 3F), -117.85 (s, F); **HRMS** (ESI) calcd for $C_{15}H_{10}F_4OSNa$ $[M+Na]^+$ 337.0286, found 337.0282**.**



3d

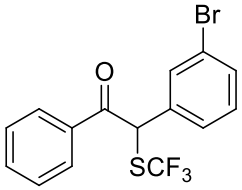
1-phenyl-2-*o*-tolyl-2-(trifluoromethylthio)ethanone (3d). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.86-7.80 (m, 2H), 7.56-7.49 (m, 1H), 7.45-7.37 (m, 2H), 7.28-7.18 (m, 3H), 7.17-7.10 (m, 1H), 6.23 (s, 1H), 2.58 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 193.5, 136.2, 135.0, 133.9, 132.1, 131.8, 130.4 (q, J_{CF} = 306.0 Hz), 129.3, 129.0, 128.82, 128.79, 127.3, 53.0, 19.5; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -40.76 (s, 3F); **HRMS** (ESI) calcd for $C_{16}H_{13}F_3OSNa$ $[M+Na]^+$ 333.0537, found 333.0533.



3e

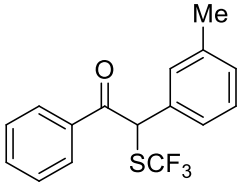
2-(2-methoxyphenyl)-1-phenyl-2-(trifluoromethylthio)ethanone (3e). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.02-7.94 (m, 2H), 7.56-7.48 (m, 1H), 7.43-7.36 (m, 2H), 7.35-7.30 (m, 1H), 7.29-7.24 (m, 1H), 6.95-6.88 (m, 2H), 6.68 (s, 1H), 3.97 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 193.8, 134.5, 133.9, 130.8 (q, J_{CF} = 304.5 Hz), 130.4, 129.4, 129.0, 128.8, 124.0, 121.7, 111.6, 56.1, 49.2; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -40.59 (s, 3F); **HRMS** (ESI) calcd for $C_{16}H_{13}F_3O_2SNa$ $[M+Na]^+$

349.0486, found 349.0483.



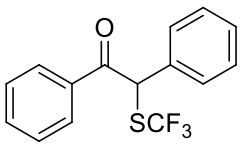
3f

2-(3-bromophenyl)-1-phenyl-2-(trifluoromethylthio)ethanone (3f). **^{1}H NMR** (600 MHz, $CDCl_3$) δ .96-7.91 (m, 2H), 7.63-7.55 (m, 2H), 7.50-7.36 (m, 4H), 7.25-7.19 (m, 1H), 6.06 (s, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 192.2, 137.7, 134.5, 134.1, 132.3, 131.5, 131.0, 130.5 (q, J_{CF} = 306.0 Hz), 129.3, 129.2, 127.4, 123.4, 55.5; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -39.97 (s, 3F); **HRMS** (ESI) calcd for $C_{15}H_{10}F_3OSNa$ $[M+Na]^+$ 396.9484, found 396.9484.



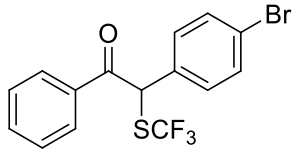
3g

1-phenyl-2-*m*-tolyl-2-(trifluoromethylthio)ethanone (3g). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.97-7.92 (m, 2H), 7.58-7.53 (m, 1H), 7.46-7.39 (m, 2H), 7.27-7.22 (m, 3H), 7.13-7.07 (m, 1H), 6.08 (s, 1H), 2.32 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 193.3, 139.5, 135.0, 134.5, 134.1, 130.7 (q, J_{CF} = 307.5 Hz), 130.0, 129.4, 129.3, 129.1, 129.0, 126.0, 56.3, 21.5; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -40.12 (s, 3F); **HRMS** (ESI) calcd for $C_{16}H_{13}F_3OSa$ $[M+Na]^+$ 333.0537, found 333.0533.



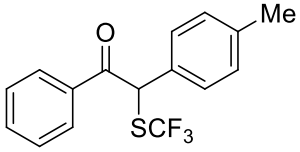
3h

1,2-diphenyl-2-(trifluoromethylthio)ethanone (3h). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.98-7.92 (m, 2H), 7.58-7.51 (m, 1H), 7.48-7.39 (m, 4H), 7.38-7.26 (m, 3H), 6.12 (s, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 193.23, 135.3, 134.4, 134.11, 130.7 (q, J_{CF} = 306.0 Hz), 129.6, 129.3, 129.05, 129.01, 128.7, 56.4; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -40.03 (s, 3F); **HRMS** (ESI) calcd for $C_{15}H_{11}F_3OSNa$ $[M+Na]^+$ 319.0380, found 319.0376.



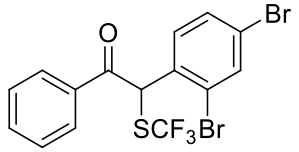
3i

2-(4-bromophenyl)-1-phenyl-2-(trifluoromethylthio)ethanone (3i). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.95-7.89 (m, 2H), 7.61-7.54 (m, 1H), 7.51-7.41 (m, 4H), 7.35-7.30 (m, 2H), 6.08 (s, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 192.9, 134.6, 134.4, 134.1, 132.8, 130.6 (q, J_{CF} = 306.0 Hz), 130.3, 129.2, 129.1, 123.4, 55.7; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -39.91 (s, 3F); **HRMS** (ESI) calcd for $C_{15}H_{10}BrF_3OS$ $[M+Na]^+$ 396.9486, found 396.9480.



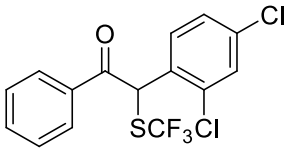
3j

1-phenyl-2-*p*-tolyl-2-(trifluoromethylthio)ethanone (3j). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.98-7.91 (m, 2H), 7.57-7.50 (m, 1H), 7.45-7.39 (m, 2H), 7.35-7.30 (m, 2H), 7.18-7.12 (m, 2H), 6.10 (s, 1H), 2.30 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 193.3, 139.1, 134.5, 134.0, 132.3, 132.2, 130.7 (q, J_{CF} = 306.0 Hz), 129.3, 129.0, 128.6, 56.3, 21.3; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -40.04 (s, 3F); **HRMS** (ESI) calcd for $C_{16}H_{13}F_3OSNa$ $[M+Na]^+$ 333.0537, found 333.0533.



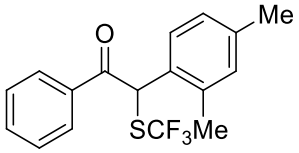
3k

2-(2,4-dibromophenyl)-1-phenyl-2-(trifluoromethylthio)ethanone (3k). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.04-7.97 (m, 2H), 7.77 (d, J = 2.9 Hz, 1H), 7.63-7.56 (m, 1H), 7.50-7.40 (m, 3H), 7.39-7.35 (m, 1H), 6.57 (s, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 192.7, 136.1, 134.6, 134.1, 133.9, 132.0, 131.6, 130.2 (q, J_{CF} = 306.0 Hz), 129.2, 129.1, 124.6, 123.8, 53.9; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -40.03 (s, 3F); **HRMS** (ESI) calcd for $C_{15}H_9Br_2F_3OSNa$ $[M+Na]^+$ 474.8591, found 474.8587.



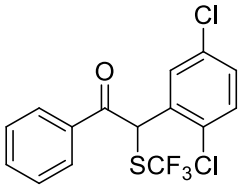
3l

2-(2,4-dichlorophenyl)-1-phenyl-2-(trifluoromethylthio)ethanone (3l). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.01-7.96 (m, 2H), 7.62-7.56 (m, 1H), 7.50-7.42 (m, 4H), 7.25-7.22 (m, 1H), 6.60 (s, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 192.8, 135.8, 134.6, 134.0, 134.0, 132.0, 131.2, 130.3 (q, J_{CF} = 306.0 Hz), 130.2, 129.2, 129.1, 128.6, 51.4; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -40.17 (s, 3F); **HRMS** (ESI) calcd for $C_{15}H_9Cl_2F_3OSNa$ $[M+Na]^+$ 386.9601, found 386.9597.



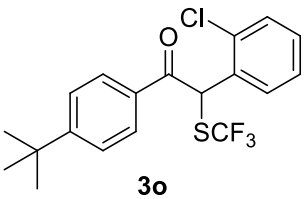
3m

2-(2,4-dimethylphenyl)-1-phenyl-2-(trifluoromethylthio)ethanone (3m). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.83 (d, J = 4.0 Hz, 2H), 7.52 (t, J = 4.0 Hz, 1H), 7.40 (t, J = 4.0 Hz, 2H), 7.12 (d, J = 4.0 Hz, 1H), 7.05 (s, 1H), 6.95 (d, J = 4.0 Hz, 1H),6.19 (s, 1H), 2.54 (s, 3H), 2.26 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 193.6, 139.3, 135.9, 135.1, 133.8, 132.6, 130.5 (q, J_{CF} = 307.5 Hz), 129.0, 128.8, 128.7, 128.6, 52.8, 21.2, 19.4; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -40.77 (s, 3F); **HRMS** (ESI) calcd for $C_{17}H_{15}F_3OSNa$ $[M+Na]^+$ 347.0693, found 347.0689.



3n

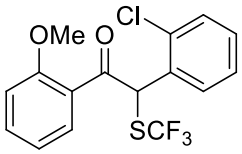
2-(2,5-dichlorophenyl)-1-phenyl-2-(trifluoromethylthio)ethanone (3n). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.01 (d, J = 6.0 Hz, 2H), 7.60 (t, J = 6.0 Hz, 1H), 7.52-7.45 (m, 3H), 7.36 (d, J = 6.0 Hz, 1H), 7.24-7.20 (m, 1H), 6.59 (s, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 192.6 135.1, 134.7, 134.0, 134.0, 131.5, 131.4, 130.6, 130.30 (q, J_{CF} = 306.0 Hz), 130.26, 129.2, 129.1, 51.5; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -40.21 (s, 3F); **HRMS** (ESI) calcd for $C_{15}H_9Cl_2F_3OSNa$ $[M+Na]^+$ 386.9601, found 386.9597.



3o

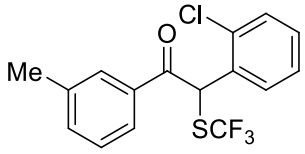
1-(4-*tert*-butylphenyl)-2-(2-chlorophenyl)-2-(trifluoromethylthio)ethanone (3o). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.98-7.93 (m, 2H), 7.52-7.40 (m, 4H), 7.27-7.20 (m, 2H), 6.65 (s, 1H); 1.30

(s, 9H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 192.5, 158.4, 133.4, 133.3, 131.6, 130.5 (q, J_{CF} = 306.0 Hz), 130.4, 130.29, 130.27, 129.12, 129.08, 126.1, 51.9, 35.4, 31.1; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -40.31 (s, 3F); **HRMS** (ESI) calcd for $C_{19}H_{19}ClF_3OS$ $[M+H]^+$ 387.0797, found 387.0794.



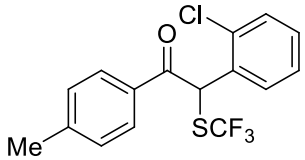
3p

2-(2-chlorophenyl)-1-(2-methoxyphenyl)-2-(trifluoromethylthio)ethanone (3p). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.60 (dd, J = 6.0, 8.0 Hz, 1H), 7.48-7.32 (m, 3H), 7.25-7.17 (m, 2H), 6.98-6.92 (m, 1H), 6.90 (d, J = 8.0 Hz, 1H), 6.83 (s, 1H), 3.88 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 195.1, 158.3, 134.6, 134.4, 133.0, 131.6, 130.50 (q, J_{CF} = 306.0 Hz), 130.50, 130.2, 130.0, 127.5, 126.0, 121.0, 111.5, 55.7, 55.1; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -40.59 (s, 3F); **HRMS** (ESI) calcd for $C_{16}H_{13}ClF_3O_2S$ $[M+H]^+$ 361.0277, found 361.0274.



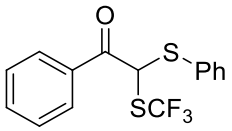
3q

2-(2-chlorophenyl)-1-*m*-tolyl-2-(trifluoromethylthio)ethanone (3q). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.83 (s, 1H), 7.80 (d, J = 6.0 Hz, 1H), 7.49-7.45 (m, 1H), 7.44-7.40 (m, 1H), 7.39-7.36 (m, 1H), 7.32 (t, J = 6.0 Hz, 1H), 7.25-7.21 (m, 2H), 6.65 (s, 1H), 2.38 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 193.3, 139.0, 135.2, 134.2, 133.33, 133.29, 130.4, 130.3, 130.2, 129.7, 128.9, 128.1, 126.2, 52.1, 21.4; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -40.26 (s, 3F); **HRMS** (ESI) calcd for $C_{16}H_{13}ClF_3OS$ $[M+H]^+$ 345.0328, found 345.0325.



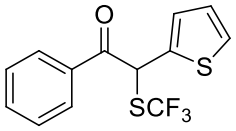
3r

2-(2-chlorophenyl)-1-*p*-tolyl-2-(trifluoromethylthio)ethanone (3r). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.95-7.87 (m, 2H), 7.50-7.44 (m, 1H), 7.43-7.38 (m, 1H), 7.27-7.20 (m, 4H), 6.63 (s, 1H), 2.37 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 192.67, 145.6, 133.4, 133.3, 131.7, 130.5 (q, J_{CF} = 306.0 Hz), 130.4, 130.3, 130.2, 129.8, 129.2, 128.1, 52.0, 21.9; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -40.26 (s, 3F); **HRMS** (ESI) calcd for $C_{16}H_{13}ClF_3OS$ $[M+H]^+$ 345.0328, found 345.0326..



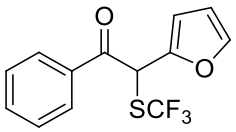
3s

1-phenyl-2-(phenylthio)-2-(trifluoromethylthio)ethanone (3s). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.01-7.94 (m, 2H), 7.68-7.60 (m, 1H), 7.54-7.47 (m, 2H), 7.42-7.36 (m, 3H), 7.35-7.30 (m, 2H), 6.03 (s, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 189.6, 135.9, 134.3, 133.6, 130.4, 130.2 (q, J_{CF} = 307.5 Hz), 129.4, 129.3, 129.1, 129.0, 57.3; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -39.96 (s, 3F); **HRMS** (ESI) calcd for $C_{15}H_{11}F_3OS_2Na$ $[M+Na]^+$ 351.0101, found 351.0098.



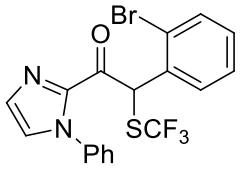
3t

1-phenyl-2-(thiophen-2-yl)-2-(trifluoromethylthio)ethanone (3t). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.02-7.95 (m, 2H), 7.59 (t, J = 8.0 Hz, 1H), 7.47 (t, J = 8.0 Hz, 2H), 7.33 (d, J = 4.0 Hz, 1H), 7.14 (d, J = 4.0 Hz, 1H), 6.97-6.93 (m, 1H), 6.41 (m, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 192.2, 136.9, 134.4 134.1, 130.3 (q, J_{CF} = 307.5 Hz), 129.3, 129.1, 128.6, 128.0, 127.6, 50.6; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -40.26 (s, 3F); **HRMS** (ESI) calcd for $C_{13}H_9F_3OS_2Na$ $[M+Na]^+$ 324.9945, found 324.9941.



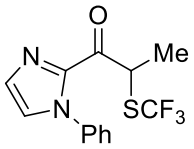
3u

2-(furan-2-yl)-1-phenyl-2-(trifluoromethylthio)ethanone (3u). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.98-7.92 (m, 2H), 7.63-7.55 (m, 1H), 7.50-7.43 (m, 2H), 7.42-7.40 (m, 1H), 6.44 (d, J = 4.0 Hz, 1H), 6.38-6.34 (m, 1H), 6.24 (s, 1H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 190.6, 147.4, 144.0, 134.4, 130.5 (q, J_{CF} = 307.5 Hz), 129.2, 129.1, 111.7, 110.8, 50.0; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -40.27 (s, 3F); **HRMS** (ESI) calcd for $C_{13}H_9F_3O_2SNa$ $[M+Na]^+$ 309.0173, found 309.0169.



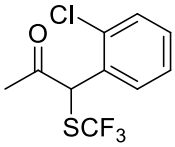
3v

2-(2-bromophenyl)-1-(1-phenyl-1*H*-imidazol-2-yl)-2-(trifluoromethylthio)ethanone (3v). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.62 (dd, *J* = 1.2, 8.0 Hz, 1H), 7.51 (dd, *J* = 1.2, 8.0 Hz, 1H), 7.49-7.44 (m, 3H), 7.33 (d, *J* = 1.2 Hz, 1H), 7.30-7.20 (m, 4H), 7.18-7.13 (m, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 183.1, 141.1, 137.8, 134.3, 133.8, 131.0, 130.5, 130.2, 130.2 (q, J_{CF} = 307.5 Hz), 129.3, 129.2, 129.5, 128.0, 125.8, 125.0, 52.9; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -40.45 (s, 3F); **HRMS** (ESI) calcd for $C_{18}H_{13}BrF_3N_2OS$ $[M+H]^+$ 440.9884, found 440.9880.



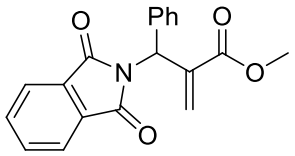
3w

1-(1-phenyl-1*H*-imidazol-2-yl)-2-(trifluoromethylthio)propan-1-one (3w). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.51-7.45 (m, 1H), 7.33 (d, *J* = 1.2 Hz, 1H), 7.30-7.25 (m, 3H), 5.39 (d, *J* = 8.0, 16.0 Hz, 1H), 1.69 (d, *J* = 8.0 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 187.1, 140.8, 137.9, 130.8 (q, J_{CF} = 306.0 Hz), 130.5, 129.3, 129.2, 128.3, 125.8, 44.8, 19.1; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -39.61 (s, 3F); **HRMS** (ESI) calcd for $C_{13}H_{12}F_3N_2OS$ $[M+H]^+$ 301.0622, found 301.0616.



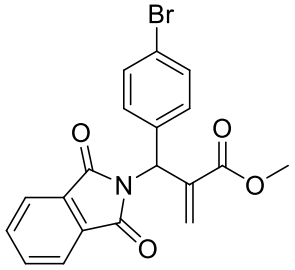
3x

1-(2-chlorophenyl)-1-(trifluoromethylthio)propan-2-one (3x). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.49-7.44 (m, 1H), 7.43-7.38 (m, 1H), 7.35-7.29 (m, 2H), 5.82 (s, 1H), 2.21 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 200.0, 133.9, 133.0, 130.5, 130.40 (q, J_{CF} = 306.0 Hz), 130.37, 130.2, 128.1, 56.7, 28.0; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -40.23 (s, 3F); **HRMS** (ESI) calcd for $C_{10}H_8F_3OSNa$ $[M+Na]^+$ 290.9834, found 290.9830.



4a

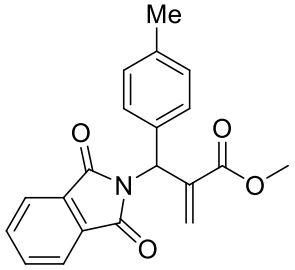
methyl 2-((1,3-dioxoisoindolin-2-yl)(phenyl)methyl)acrylate (4a). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.87-7.80 (m, 2H), 7.75-7.67 (m, 2H), 7.47-7.41 (m, 2H), 7.39-7.27 (m, 3H), 6.57 (d, *J* = 4.0 Hz, 1H), 6.41-6.38 (m, 1H), 5.63 (d, *J* = 1.2 Hz, 1H), 3.70 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 168.1, 166.2, 137.7, 137.1, 134.2, 131.9, 129.8, 128.8, 128.2, 123.5, 54.8, 52.3; **HRMS** (ESI) calcd for $C_{19}H_{16}NO_4$ $[M+H]^+$ 322.1079, found 322.1075.



4b

^{1}H NMR 400 MHz

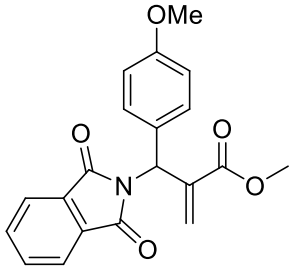
methyl 2-((4-bromophenyl)(1,3-dioxoisoindolin-2-yl)methyl)acrylate (4b). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.87-7.80 (m, 2H), 7.76-7.69 (m, 2H), 7.51-7.45 (m, 2H), 7.35-7.29 (m, 2H), 6.57 (d, *J* = 1.2 Hz, 1H), 6.41-6.38 (m, 1H), 5.64 (d, *J* = 1.2 Hz, 1H), 3.70 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 167.9, 166.0, 137.2, 136.2, 134.4, 132.0, 131.8, 130.6, 129.7, 123.7, 122.4, 54.2, 52.4; **HRMS** (ESI) calcd for $C_{19}H_{15}BrNO_4$ $[M+H]^+$ 400.0184, found 400.0180.



4c

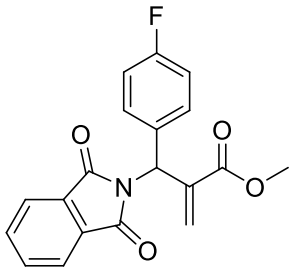
methyl 2-((1,3-dioxoisoindolin-2-yl)(p-tolyl)methyl)acrylate (4c). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.86-7.78 (m, 2H), 7.74-7.66 (m, 2H), 7.36-7.30 (m, 2H), 7.18-7.12 (m, 2H), 6.55 (d, *J* = 4.0 Hz,

1H), 6.38-6.33 (m, 1H), 5.64 (d, *J* = 1.2 Hz, 1H), 3.70 (s, 3H), 2.33 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 168.1, 166.3, 138.0, 137.8, 134.2, 132.0, 129.5, 129.5, 128.7, 123.5, 54.6, 52.3, 21.3; **HRMS** (ESI) calcd for $C_{20}H_{18}NO_4$ $[M+H]^+$ 336.1236, found 336.1231.



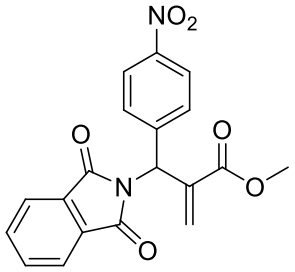
4d

methyl 2-((1,3-dioxoisoindolin-2-yl)(4-methoxyphenyl)methyl)acrylate (4d). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.86-7.79 (m, 2H), 7.74-7.66 (m, 2H), 7.41-7.35 (m, 2H), 6.90-6.84 (m, 2H), 6.54 (d, *J* = 4.0 Hz, 1H), 6.35-6.32 (m, 1H), 5.65 (d, *J* = 4.0 Hz, 1H), 3.79 (s, 3H), 3.69 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 168.1, 166.3, 159.5, 138.0, 134.2, 132.0, 130.2, 129.3, 129.2, 123.5, 114.1, 55.4, 54.4, 52.3; **HRMS** (ESI) calcd for $C_{20}H_{17}NO_5Na$ $[M+Na]^+$ 374.1004, found 374.0999.



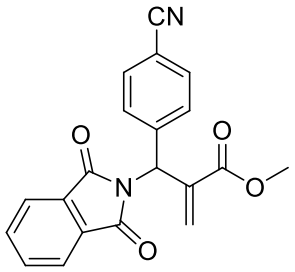
4e

methyl 2-((1,3-dioxoisoindolin-2-yl)(4-fluorophenyl)methyl)acrylate (4e). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.87-7.79 (m, 2H), 7.75-7.69 (m, 2H), 7.47-7.40 (m, 2H), 7.08-6.98 (m, 2H), 6.56 (d, *J* = 1.2 Hz, 1H), 6.40-6.36 (m, 1H), 5.63 (d, *J* = 1.2 Hz, 1H), 3.70 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 168.0 166.1, 162.6 (d, J_{CF} = 246.0 Hz), 137.6, 134.3, 132.9 (d, J_{CF} = 3.0 Hz), 131.9, 130.7 (d, J_{CF} = 9.0 Hz), 129.4, 123.6, 115.7 (d, J_{CF} = 22.5 Hz), 54.1, 52.4; **HRMS** (ESI) calcd for $C_{19}H_{15}FO_4$ $[M+H]^+$ 340.0985, found 340.0978.



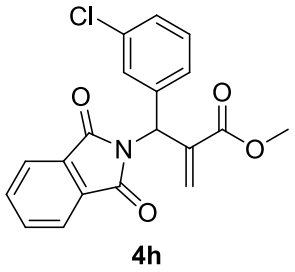
4f

methyl 2-((1,3-dioxoisoindolin-2-yl)(4-nitrophenyl)methyl)acrylate (4f). ^{1}**H NMR** (400 MHz, $CDCl_3$) δ 8.24-8.18 (m, 2H), 7.89-7.83 (m, 2H), 7.79-7.73 (m, 2H), 7.64-7.59 (m, 2H), 6.64 (d, *J* = 1.2 Hz, 1H), 6.55-6.50 (m, 1H), 5.68 (d, *J* = 4.0 Hz, 1H), 3.73 (s, 3H); ^{13}**C NMR** (150 MHz, $CDCl_3$) δ 167.8, 165.7, 147.8, 144.2, 136.5, 134.6, 134.5, 131.7, 130.0, 129.8, 124.0, 123.8, 123.7, 53.9, 52.6; **HRMS** (ESI) calcd for $C_{19}H_{14}N_2O_6$ $[M+H]^+$ 367.0930, found 367.0926.



4g

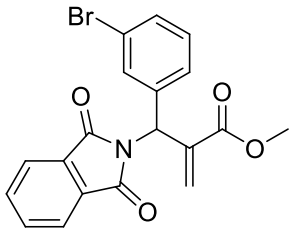
methyl 2-((4-cyanophenyl)(1,3-dioxoisoindolin-2-yl)methyl)acrylate (4g). ^{1}**H NMR** (400 MHz, $CDCl_3$) δ 7.89-7.83 (m, 2H), 7.78-7.72 (m, 2H), 7.68-7.63 (m, 2H), 7.58-7.53 (m, 2H), 6.62 (d, *J* = 1.2 Hz, 1H), 6.48-6.45 (m, 1H), 5.65 (d, *J* = 1.2 Hz, 1H), 3.72 (s, 3H); ^{13}**C NMR** (150 MHz, $CDCl_3$) δ 167.8, 165.8, 142.3, 136.6, 134.5, 132.6, 131.7, 130.0, 129.6, 123.8, 118.6, 112.3, 54.1, 52.5; **HRMS** (ESI) calcd for $C_{20}H_{15}N_2O_4$ $[M+H]^+$ 347.1032, found 347.1024.



4h

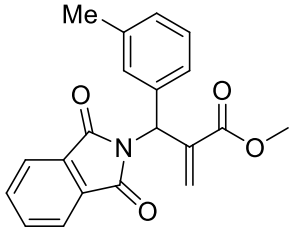
methyl 2-((3-chlorophenyl)(1,3-dioxoisoindolin-2-yl)methyl)acrylate (4h). ^{1}**H NMR** (600 MHz, $CDCl_3$) δ 7.88-7.81 (m, 2H), 7.76-7.70 (m, 2H), 7.43 (s, 1H), 7.36-7.26 (m, 3H),6.59 (s, 1H), 6.37 (s, 1H), 5.66 (s, 1H), 3.71 (s, 3H); ^{13}**C NMR** (150 MHz, $CDCl_3$) δ 167.9, 166.0, 139.1, 137.1,

134.7, 134.4, 131.9, 130.04, 130.0, 128.9, 128.6, 127.0, 123.7, 54.2, 52.4; **HRMS** (ESI) calcd for $C_{19}H_{15}ClNO_4$ $[M+H]^+$ 356.0690, found 356.0684.



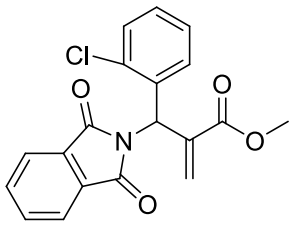
4i

methyl 2-((3-bromophenyl)(1,3-dioxoisoindolin-2-yl)methyl)acrylate (4i). ^{1}**H NMR** (600 MHz, $CDCl_3$) δ 7.88-7.82 (m, 2H), 7.76-7.71 (m, 2H), 7.58 (s, 1H), 7.46-7.42 (m, 1H),7.40-7.36 (m, 1H), 6.59 (s, 1H), 6.36 (s, 1H), 5.66 (d, *J* = 6.0 Hz, 1H), 3.71 (s, 3H); ^{13}**C NMR** (150 MHz, $CDCl_3$) δ 167.9, 166.0, 139.4, 137.1, 134.4, 131.83, 131.80, 131.5, 130.3, 130.0, 127.5, 123.7, 122.8, 54.1, 52.4; **HRMS** (ESI) calcd for $C_{19}H_{15}BrNO_4$ $[M+H]^+$ 400.0184, found 400.0179.



4j

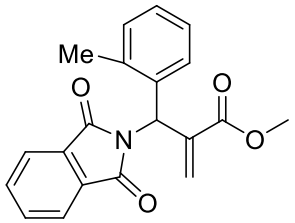
methyl 2-((1,3-dioxoisoindolin-2-yl)(*m*-tolyl)methyl)acrylate (4j). ^{1}**H NMR** (600 MHz, $CDCl_3$) δ 7.87-7.79 (m, 2H), 7.73-7.67 (m, 2H), 7.25-7.20 (m, 3H), 7.15-7.07 (m, 1H), 6.56 (d, *J* = 2.2 Hz, 1H), 6.35 (t, *J* = 2.3 Hz, 1H), 5.63 (d, *J* = 2.6 Hz, 1H), 3.70 (s, 3H), 2.33 (s, 3H); ^{13}**C NMR** (150 MHz, $CDCl_3$) δ 168.1, 166.2, 138.4, 137.7, 137.0, 134.1, 131.9, 129.7, 129.4, 129.0, 128.6, 125.79, 123.5, 54.7, 52.3, 21.5; **HRMS** (ESI) calcd for $C_{20}H_{17}NO_5Na$ $[M+Na]^+$ 374.1004, found 374.0999.



4k

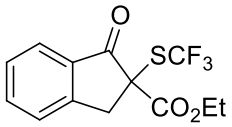
methyl 2-((2-chlorophenyl)(1,3-dioxoisoindolin-2-yl)methyl)acrylate (4k). ^{1}**H NMR** (400 MHz, $CDCl_3$) δ 7.87-7.81 (m, 2H), 7.76-7.70 (m, 2H), 7.54-7.48 (m, 1H), 7.42-7.35 (m, 1H), 7.29-7.23

(m, 2H), 6.76 (t, J = 1.2 Hz, 1H), 6.59 (d, J = 1.3 Hz, 1H), 5.60 (d, J = 1.7 Hz, 1H), 3.71 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 167.9, 165.9, 136.4, 134.5, 134.3, 133.8, 131.8, 130.4, 129.9, 129.6, 129.0, 126.9, 123.7, 52.4, 52.1; **HRMS** (ESI) calcd for $C_{19}H_{15}ClNO_4$ $[M+H]^+$ 356.0690, found 356.0684.



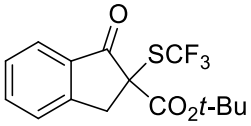
4l

methyl 2-((1,3-dioxoisoindolin-2-yl)(*o*-tolyl)methyl)acrylate (4l). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.86-7.79 (m, 2H), 7.74-7.67 (m, 2H), 48-7.40 (m, 1H), 7.24-7.12 (m, 3H), 6.58-6.48 (m, 2H), 5.52 (d, J = 1.2 Hz, 1H), 3.70 (s, 3H), 2.38 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 168.2, 166.2, 137.1, 136.2, 135.3, 134.2, 131.8, 130.7, 129.0, 128.6, 128.2, 126.3, 123.5, 52.3, 51.8, 19.4; **HRMS** (ESI) calcd for $C_{20}H_{18}NO_4$ $[M+H]^+$ 336.1236, found 336.1230.



6a

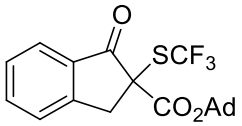
ethyl 1-oxo-2-(trifluoromethylthio)-2,3-dihydro-1*H*-indene-2-carboxylate (6a). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.83 (d, J = 12.0 Hz, 1H), 7.71 (t, J = 6.0 Hz, 1H), 7.53 (d, J = 6.0 Hz, 1H), 7.46 (t, J = 6.0 Hz, 1H), 4.31-4.21 (m, 2H), 4.19 (d, J = 18.0 Hz, 1H), 3.67 (d, J = 18.0 Hz, 1H), 1.26 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 195.1, 166.9, 151.9, 36.6, 133.04, 129.99 (q, J_{CF} = 307.5 Hz), 128.6, 126.4, 125.8, 63.8, 63.6, 40.5, 13.9; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -37.09 (s, 3F); **HRMS** (ESI) calcd for $C_{13}H_{12}F_3O_3S$ $[M+H]^+$ 305.0459, found 305.0455.



6b

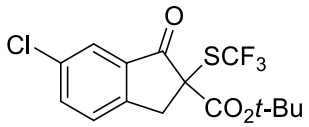
***tert*-butyl 1-oxo-2-(trifluoromethylthio)-2,3-dihydro-1*H*-indene-2-carboxylate (6b)**. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.83 (d, J = 6.0 Hz, 1H), 7.69 (t, J = 6.0 Hz, 1H), 7.51 (d, J = 6.0 Hz, 1H),

7.45 (t, J = 6.0 Hz, 1H), 4.09 (d, J = 18.0 Hz, 1H), 3.64 (d, J = 18.0 Hz, 1H), 1.42 (s, 9H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 195.7, 165.8, 151.9, 136.4, 133.3, 130.1 (q, J_{CF} = 306.0 Hz), 128.5, 126.3, 125.7, 85.0, 64.4, 40.6, 27.7; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -36.92 (s, 3F); **HRMS** (ESI) calcd for $C_{15}H_{15}F_3O_3SNa$ $[M+Na]^+$ 355.0592, found 355.0587.



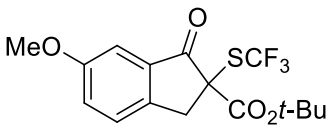
6c

adamantan-1-yl-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate (3d). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.83 (d, J = 6.0 Hz, 1H), 7.68 (t, J = 12.0 Hz, 1H), 7.50 (d, J = 12.0 Hz, 1H), 7.44 (t, J = 12.0 Hz, 1H), 4.08 (d, J = 18.0 Hz, 2H), 3.64 (d, J = 18.0 Hz, 1H), 2.14 (s, 3H), 2.04 (s, 6H), 1.62 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 195.8, 165.4, 151.9, 136.3, 133.4, 128.4, 126.2, 130.1 (q, J_{CF} = 307.5 Hz), 125.6, 85.0, 64.5, 40.9, 40.6, 36.0, 31.0; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -36.85 (s, 3F); **HRMS** (ESI) calcd for $C_{21}H_{21}F_3O_3SNa$ $[M+Na]^+$ 433.1061, found 433.1058.



6d

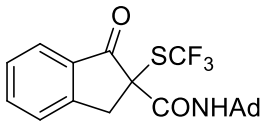
***tert*-butyl 6-chloro-1-oxo-2-(trifluoromethylthio)-2,3-dihydro-1*H*-indene-2-carboxylate (6d)**. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.79 (s, 1H), 7.65 (d, J = 6.0 Hz, 1H), 7.46 (d, J = 6.0 Hz, 1H), 4.04 (d, J = 18.0 Hz, 2H), 3.60 (d, J = 18.0 Hz, 1H), 1.42 (s, 9H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 194.6, 165.3, 149.9, 136.4, 134.9, 134.8, 129.9 (q, J_{CF} = 307.5 Hz), 127.5, 125.3, 85.4, 64.7, 40.1, 27.7; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -36.86 (s, 3F); **HRMS** (ESI) calcd for $C_{15}H_{14}ClF_3OSNa$ $[M+Na]^+$ 389.0202, found 389.0198.



6e

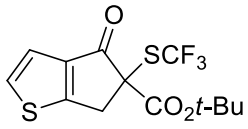
***tert*-butyl 6-methoxy-1-oxo-2-(trifluoromethylthio)-2,3-dihydro-1*H*-indene-2-carboxylate (6e)**.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.39 (d, J = 6.0 Hz, 1H), 7.29-7.25 (m, 1H), 7.24-7.21 (m, 1H), 3.98 (d, J = 12.0 Hz, 2H), 3.85 (s, 3H), 3.56 (d, J = 18.0 Hz, 1H), 1.42 (s, 9H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 195.7, 165.8, 160.1, 144.8, 134.6, 130.0 (q, J_{CF} = 307.5 Hz), 127.0, 126.0, 160.5, 85.0, 65.0, 55.8, 40.0, 27.7; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -36.96 (s, 3F); **HRMS** (ESI) calcd for $C_{16}H_{17}F_3O_4SNa$ $[M+Na]^+$ 385.0697, Found 385.0695.



6f

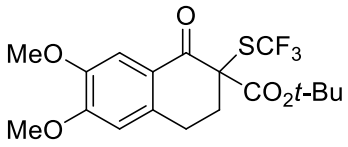
adamantan-1-yl-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxamide (6f). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.77 (d, J = 12.0 Hz, 1H), 7.69 (t, J = 6.0 Hz, 1H), 7.52 (d, J = 6.0 Hz, 1H), 7.42 (t, J = 6.0 Hz, 1H), 6.73 (s, 1H), 4.50 (d, J = 18.0 Hz, 1H), 3.48 (d, J = 18.0 Hz, 1H), 2.07 (s, 3H), 1.98 (d, J = 6.0 Hz, 6H), 1.66 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 198.6, 162.8, 153.5, 136.9, 132.7, 129.8 (q, J_{CF} = 309.0 Hz), 128.3, 126.5, 125.5, 63.1, 53.0, 41.0, 38.8, 36.4, 29.5; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -37.29 (s, 3F); **HRMS** (ESI) calcd for $C_{21}H_{23}F_3NO_2S$ $[M+H]^+$ 410.1402, found 410.1395.



6g

***tert*-butyl**

4-oxo-5-(trifluoromethylthio)-5,6-dihydro-4*H*-cyclopenta[*b*]thiophene-5-carboxylate (6g). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.41 (d, J = 5.2 Hz, 1H), 7.20 (t, J = 6.0 Hz, 1H), 4.16 (d, J = 18.0 Hz, 1H), 3.70 (d, J = 18.0 Hz, 1H), 1.45 (s, 9H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 186.8, 168.5, 165.3, 141.8, 132.2, 130.0 (q, J_{CF} = 307.5 Hz), 120.5, 85.3, 69.5, 38.9, 27.7; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -37.28 (s, 3F); **HRMS** (ESI) calcd for $C_{13}H_{13}F_3O_3S_2Na$ $[M+Na]^+$ 361.0156, found 361.0151.

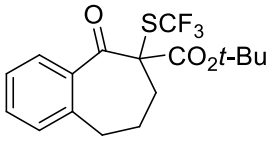


6h

***tert*-butyl**

6,7-dimethoxy-1-oxo-2-(trifluoromethylthio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate

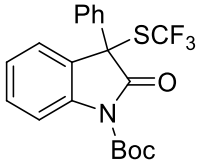
(6h). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.46 (s, 1H), 6.64 (s, 1H), 3.94 (s, 3H), 3.91 (s, 3H), 3.22-3.14 (m, 1H), 3.06-2.94 (m, 2H), 2.55-2.47 (m, 1H), 1.41 (s, 9H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 196.5, 188.4, 166.2, 154.6, 148.6, 137.7, 130.2 (q, J_{CF} = 306.0 Hz), 123.9, 110.0, 109.4, 84.2, 65.1, 56.3, 56.2, 33.2, 27.7, 26.4; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -35.66 (s, 3F); **HRMS** (ESI) calcd for $C_{18}H_{21}F_3O_5SNa$ $[M+Na]^+$ 429.0959, found 429.0957.



6i

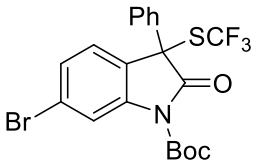
***tert*-butyl**

5-oxo-6-(trifluoromethylthio)-6,7,8,9-tetrahydro-5*H*-benzo[7]annulene-6-carboxylate (6i). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.51 (d, *J* = 6.0 Hz, 1H), 7.41-7.36 (m, 1H), 7.31-7.26 (m, 1H), 7.18 (d, *J* = 6.0 Hz, 1H), 3.15-3.05 (m, 2H), 2.97-2.89 (m, 1H), .45-2.35 (m, 1H), 2.25-2.15 (m, 1H), 1.97-1.88 (m, 1H), 1.12 (s, 9H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 197.8, 166.6, 140.7, 137.6, 131.8, 130.6, 130.4 (q, J_{CF} = 306.0 Hz), 130.0, 126.3, 83.9, 70.2, 36.3, 33.6, 27.1, 25.7; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -36.46 (s, 3F); **HRMS** (ESI) calcd for $C_{17}H_{19}F_3O_3SNa$ $[M+Na]^+$ 383.0905, found 383.0901.



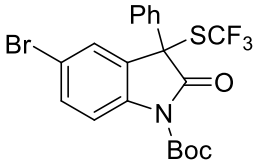
6j

***tert*-butyl 2-oxo-3-phenyl-3-(trifluoromethylthio)indoline-1-carboxylate (6j)**. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.97 (d, *J* = 12.0 Hz, 1H), 7.57 (d, *J* = 6.0 Hz, 1H), 7.54-7.49 (m, 2H), 7.46 (d, *J* = 12.0 Hz, 1H), 7.40-4.30 (m, 4H), 1.62 (s, 9H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 172.5, 149.1, 139.4, 134.2, 130.5, 129.5, 129.3, 127.8, 129.1, 128.7 (q, J_{CF} = 309.0 Hz), 126.2, 125.0, 115.8, 85.2, 59.7, 28.1; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -38.76 (s, 3F); **HRMS** (ESI) calcd for $C_{20}H_{18}F_3NO_3SNa$ $[M+Na]^+$ 432.0857, found 432.0853.



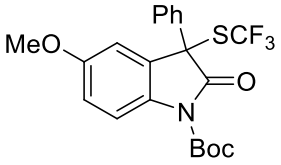
6k

***tert*-butyl 6-bromo-2-oxo-3-phenyl-3-(trifluoromethylthio)indoline-1-carboxylate (6k)**. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.15 (s, 1H), 7.43-7.38 (m, 3H), 7.37-7.33 (m, 1H), 7.31-7.27 (m, 3H), 1.54 (s, 9H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.9, 148.8, 140.3, 133.6, 129.8, 129.4, 128.6 (q, J_{CF} = 309.0 Hz), 128.2, 128.1, 127.7, 125.2, 124.4, 119.4, 85.8, 59.3, 28.1; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -38.66 (s, 3F); **HRMS** (ESI) calcd for $C_{20}H_{17}BrF_3NO_3SNa$ $[M+Na]^+$ 509.9962, found 509.9964.



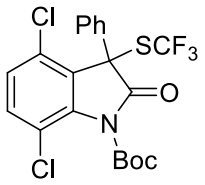
6l

***tert*-butyl 5-bromo-2-oxo-3-phenyl-3-(trifluoromethylthio)indoline-1-carboxylate (6l)**. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.89 (d, J = 6.0 Hz, 1H), 7.68 (d, J = 2.0 Hz, 1H); 7.58 (dd, J = 2.1, 8.8 Hz, 1H), 7.51-7.47 (m, 1H), 7.42-7.37 (m, 1H), 1.61 (s, 9H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.7, 148.9, 138.4, 133.6, 129.8, 129.5, 128.6 (q, J_{CF} = 309.0 Hz), 128.5, 127.7, 117.9, 117.6, 85.6, 59.3, 28.1; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -38.65 (s, 3F); **HRMS** (ESI) calcd for $C_{20}H_{17}BrF_3NO_3SNa$ $[M+Na]^+$ 509.9962, found 509.9960.



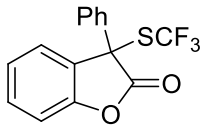
6m

***tert*-butyl 5-methoxy-2-oxo-3-phenyl-3-(trifluoromethylthio)indoline-1-carboxylate (6m)**. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.90 (d, J = 6.0 Hz, 1H), 7.55-7.49 (m, 2H), 7.39-7.33 (m, 3H), 7.10 (d, J = 2.0 Hz, 1H), 6.99 (dd, J = 2.1, 8.8 Hz, 1H), 3.85 (s, 3H), 1.61 (s, 9H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 172.5, 157.2, 149.1, 134.2, 132.7, 129.5, 129.3, 128.7 (q, J_{CF} = 309.0 Hz), 127.8, 127.5, 116.9, 115.9, 112.5, 85.0, 60.0, 55.9, 28.1; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -38.72 (s, 3F); **HRMS** (ESI) calcd for $C_{21}H_{20}F_3NO_4SNa$ $[M+Na]^+$ 462.0963, found 462.0959.



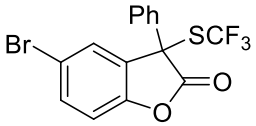
6n

***tert*-butyl 4,7-dichloro-2-oxo-3-phenyl-3-(trifluoromethylthio)indoline-1-carboxylate (6n)**. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.43 (d, J = 6.0 Hz, 1H), 7.40-7.33 (m, 5H), 7.22 (d, J = 12.0 Hz, 1H), 1.59 (s, 9H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 172.1, 147.1, 138.5, 133.1, 131.9, 131.0, 129.8, 129.4, 128.8 (q, J_{CF} = 309.0 Hz), 127.2, 127.0, 126.2, 117.8, 86.7, 60.3, 27.6; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -39.19 (s, 3F); **HRMS** (ESI) calcd for $C_{20}H_{16}Cl_2F_3NO_3SNa$ $[M+Na]^+$ 500.0078, found 500.0072.



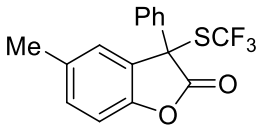
6o

3-phenyl-3-(trifluoromethylthio)benzofuran-2(3*H*)-one (6o). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.63-7.57 (m, 3H), 7.50-7.44 (m, 1H), 7.43-7.37 (m, 3H), 7.34 (t, J = 6.0 Hz, 1H), 7.21 (d, J = 12.0 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.9, 152.6, 132.9, 131.3, 129.9, 129.5, 128.4 (q, J_{CF} = 309.0 Hz), 127.6, 127.2, 125.8, 125.1, 111.8, 57.5; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -39.20 (s, 3F); **HRMS** (ESI) calcd for $C_{15}H_9F_3O_2SNa$ $[M+Na]^+$ 333.0173, found 333.0171.



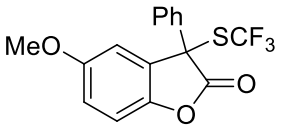
6p

5-bromo-3-phenyl-3-(trifluoromethylthio)benzofuran-2(3*H*)-one (6p). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.73 (d, J = 6.0 Hz, 1H), 7.62-7.54 (m, 3H), 7.46-7.40 (m, 3H), 7.12 (d, J = 6.0 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 173.1, 151.4, 134.4, 132.3, 130.2, 130.0, 129.7, 128.3 (q, J_{CF} = 309.0 Hz), 128.0, 127.4, 117.6, 113.5, 57.3; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -39.02 (s, 3F); **HRMS** (ESI) calcd for $C_{15}H_8BrF_3O_2SNa$ $[M+Na]^+$ 410.9278, found 410.9274.



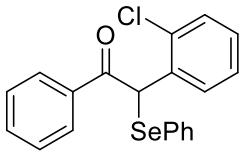
6q

5-methyl-3-phenyl-3-(trifluoromethylthio)benzofuran-2(3*H*)-one (6q). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.63-7.56 (m, 2H), 7.44-7.36 (m, 4H), 7.25 (d, *J* = 12.0 Hz, 1H), 7.09 (d, *J* = 6.0 Hz, 1H), 2.44 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 174.2, 150.5, 134.9, 133.1, 131.8, 130.0, 129.5, 128.4 (q, J_{CF} = 309.0 Hz), 127.6, 127.3, 125.6, 111.4, 57.7, 21.4; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -39.16 (s, 3F); **HRMS** (ESI) calcd for $C_{16}H_{11}F_3O_2SNa$ $[M+Na]^+$ 347.0330, found 347.0326.



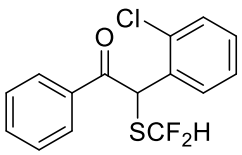
6r

5-methoxy-3-phenyl-3-(trifluoromethylthio)benzofuran-2(3*H*)-one (6r). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.62-7.56 (m, 2H), 7.48 (d, *J* = 12.0 Hz, 1H), 7.42-7.36 (m, 3H), 6.87 (dd, *J* = 6.0, 12.0 Hz, 1H), 6.76 (d, *J* = 6.0 Hz, 1H), 3.87 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 174.3, 162.2, 153.7, 133.4, 129.8, 129.5, 128.5 (q, J_{CF} = 309.0 Hz), 127.8, 127.6, 116.9, 111.4, 97.8, 57.6, 55.9; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -39.16 (s, 3F); **HRMS** (ESI) calcd for $C_{16}H_{11}F_3O_3SNa$ $[M+Na]^+$ 363.0279, found 363.0275.



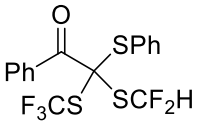
7

2-(2-chlorophenyl)-1-phenyl-2-(phenylselanyl)ethanone (7). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.96-7.90 (m, 2H), 7.63 (dd, *J* = 6.0, 12.0 Hz, 1H), 7.54-7.48 (m, 1H), 7.43-7.35 (m, 4H), 7.33-7.26 (m, 2H), 7.25-7.12 (m, 4H) 6.47 (s, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 195.0, 136.4, 135.7, 135.4, 133.5, 133.3, 131.5, 129.5, 129.0, 129.0, 129.0, 128.9, 128.8, 128.2, 127.5, 43.2; **HRMS** (ESI) calcd for $C_{20}H_{16}ClOSe$ $[M+H]^+$ 387.0055, found 387.0049.



8

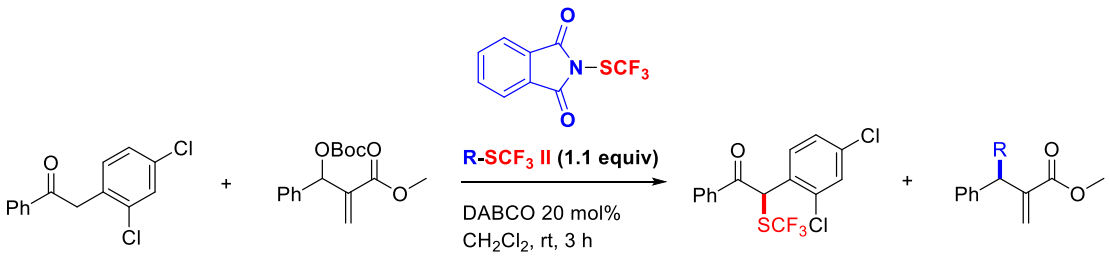
2-(2-chlorophenyl)-2-(difluoromethylthio)-1-phenylethanone (8). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.99 (d, *J* = 8.0 Hz, 2H), 7.56 (t, *J* = 4.0 Hz, 1H), 7.50-7.40 (m, 4H), 7.29-7.20 (m, 2H), 6.84 (t, *J* = 56.0 Hz, 1H), 6.57 (s, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 193.6, 134.6, 134.1, 133.8, 133.2, 130.5, 130.3, 130.1, 129.9 (t, J_{CF} = 273.0 Hz), 129.0, 128.1, 49.5; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -91.76 (dd, J = 60.2, 248.2 Hz, 1F), -94.82 (dd, *J* = 60.2, 248.2 Hz, 1F); **HRMS** (ESI) calcd for $C_{15}H_{11}F_2OSNa$ $(M+Na)^+$ 335.0085, found 335.0081.



9

2-(difluoromethylthio)-1-phenyl-2-(phenylthio)-2-(trifluoromethylthio)ethanone (9). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 6.0 Hz, 2H), 7.62 (t, *J* = 12.0 Hz, 1H), 7.48 (t, *J* = 12.0 Hz, 2H), 7.42 (t, *J* = 12.0 Hz, 1H), 7.37-7.33 (m, 2H), 7.29 (t, *J* = 12.0 Hz, 2H), 7.27 (t, *J* = 56.0 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 189.3, 137.1, 134.0, 132.9, 131.5, 131.1, 129.5, 128.4, 128.2 (q, J_{CF} = 306.0 Hz), 122.1 (t, J_{CF} = 270.0 Hz); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -36.82 (s, 3F), -93.96 (dd, *J* = 37.6, 173.0 Hz, 1F), -94.82 (dd, *J* = 37.6, 173.0 Hz, 1F); **HRMS** (ESI) calcd for $C_{16}H_{11}F_5OS_3Na$ $(M+Na)^+$ 432.9790, found 432.9786.

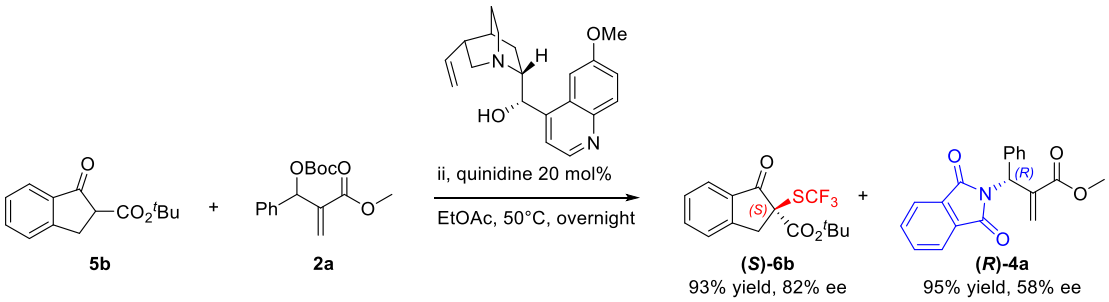
Scale-up Experiment



1 mmol **2a** **3i** 88% yield **4a** 92% yield

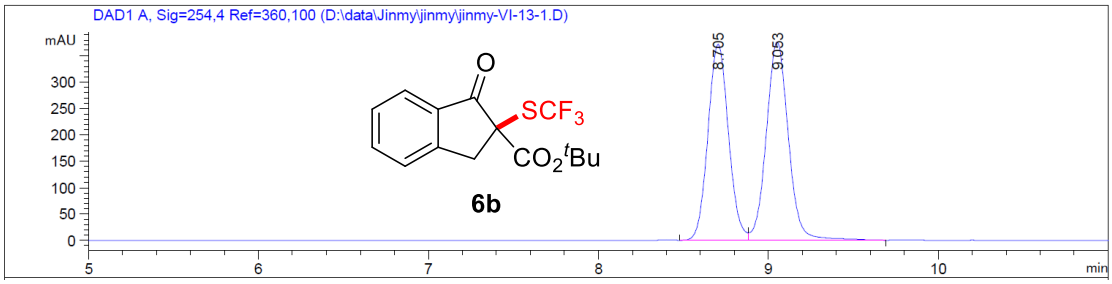
An oven-dried vial fitted with a stirrer bar was charged with acyclic ketones **1i** (1.0 mmol), MBH carbonates **2a** (1.1 mmol), *N*-SCF_3 phthalimide **II** (1.1 mmol) and DABCO (0.2 equiv) in dry CH_2Cl_2 (10.0 mL) and the mixture was stirred at room temperature for 3 h. Concentration and purification by silica gel column chromatography gave the product **3i** in 88% yield and **4a** in 92% yield .

General Procedure for a Double Asymmetric Cascade Reaction Catalyzed by Quinidine.



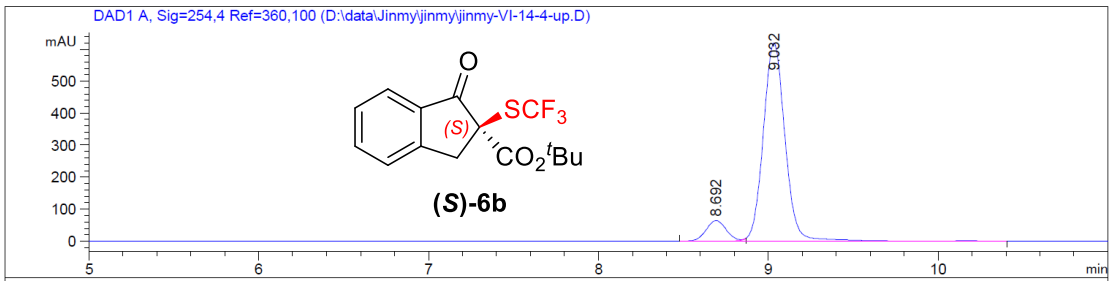
An oven-dried vial fitted with a stirrer bar was charged with acyclic ketones (0.1 mmol), MBH carbonates (0.11 mmol), *N*-SCF_3 phthalimide (0.11 mmol) and quinidine (0.2 equiv) in dry EtOAc (1.0 mL) and the mixture was stirred at 50 ºC for 12 h. Concentration and purification by silica gel column chromatography gave the product **(*S*)-6b** and (***R***)-**4a**.

HPLC: **(*S*)-6b** AD-H, 2-PrOH: *n*-hexane = 1:99, 25 °C, flow rate: 0.5 mL/min, λ = 254 nm, t_R = 8.69 min (minor) and t_R = 9.03 min (major).



Signal 1: DAD1 A, Sig=254,4 Ref=360,100

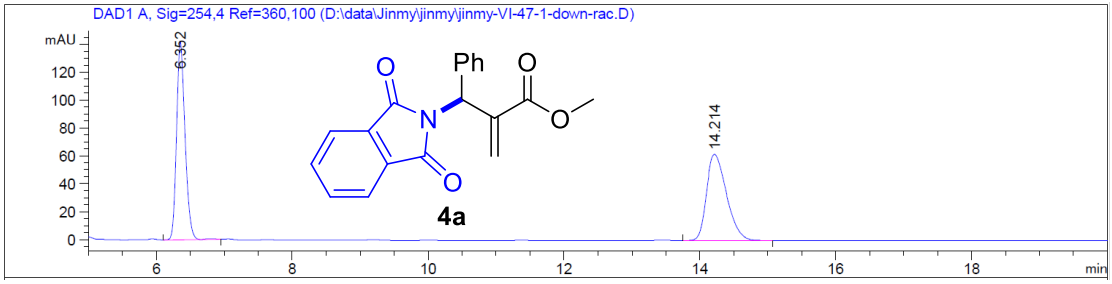
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.705	BV	0.1298	3118.67529	371.95346	47.9030
2	9.053	VB	0.1392	3391.72266	376.17200	52.0970
Totals :				6510.39795	748.12546	



Signal 1: DAD1 A, Sig=254,4 Ref=360,100

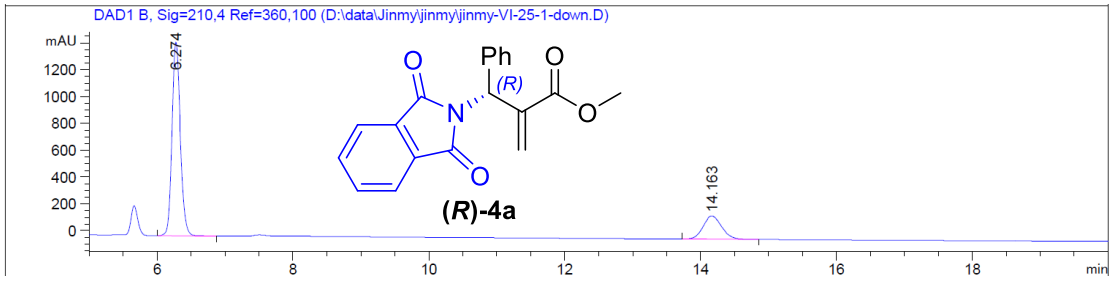
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.692	BV E	0.1274	526.33350	64.34969	8.6974
2	9.032	VV R	0.1377	5525.26123	620.07062	91.3026
Totals :				6051.59473	684.42030	

HPLC: **(*R*)-4a** OD-H, 2-PrOH: *n*-hexane = 30:70, 25 ºC, flow rate: 1.0 mL/min, λ = 210 nm, t_R = 6.27 min (major) and t_R = 14.16 min (minor).



Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.352	BV R	0.1370	1258.40991	142.48625	49.9691
2	14.214	BB	0.3159	1259.96753	61.79457	50.0309
Totals :				2518.37744	204.28082	



Signal 2: DAD1 B, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.274	BB	0.1314	1.23205e4	1445.95996	79.1008
2	14.163	BB	0.2936	3255.20313	172.92360	20.8992
Totals :				1.55757e4	1618.88356	

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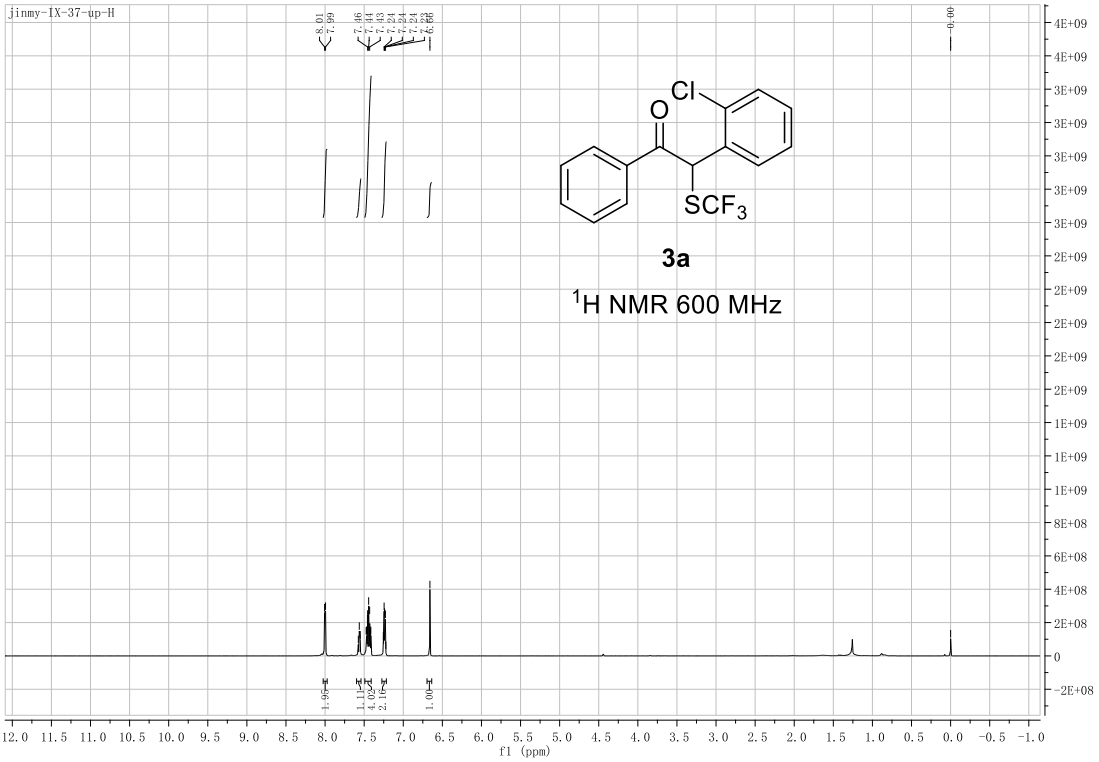
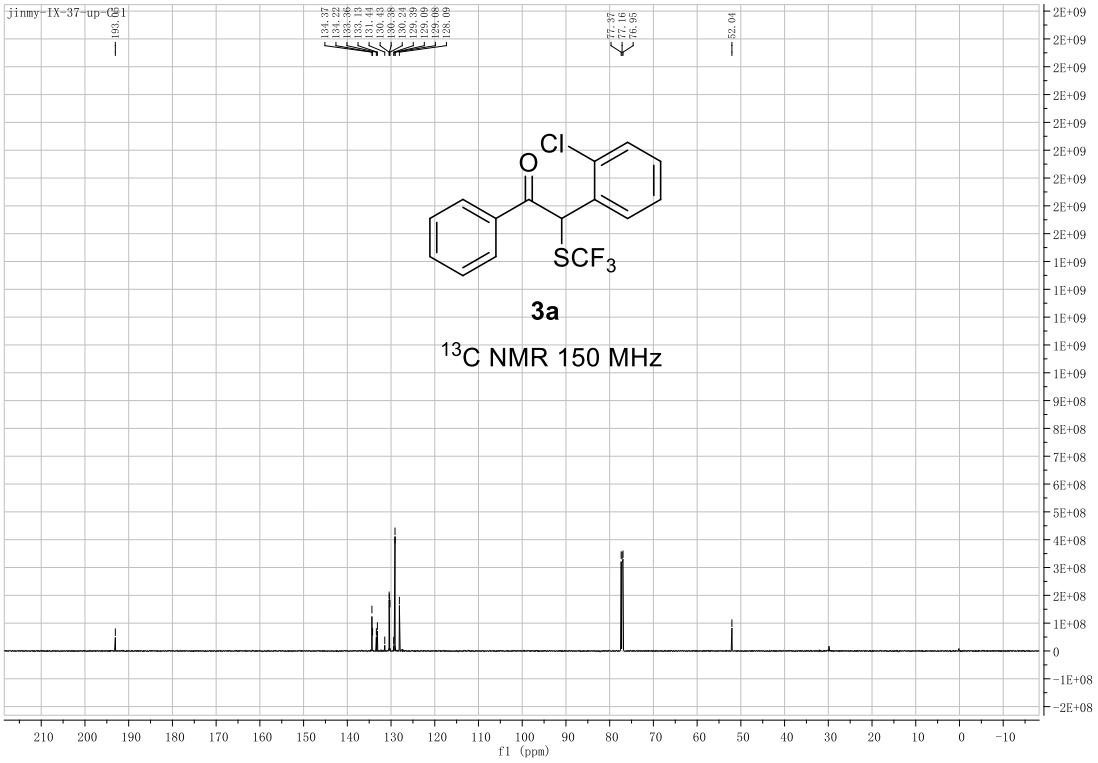
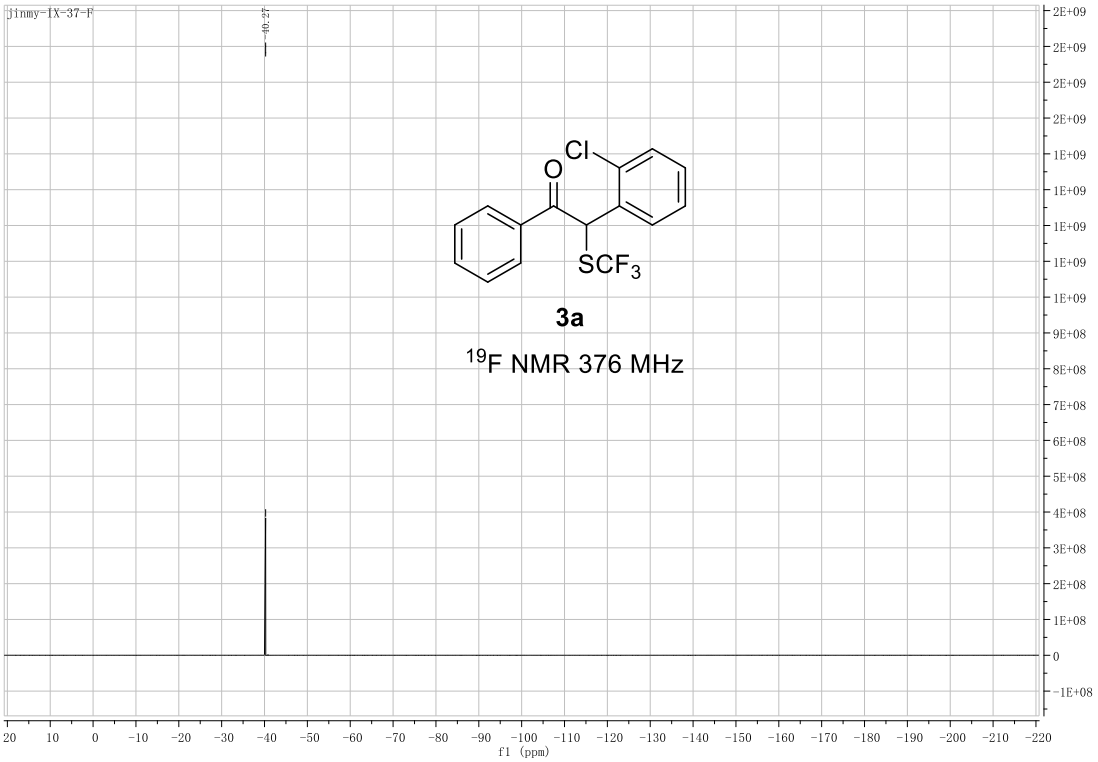
^{1}H NMR, ^{13}C NMR and ^{19}F NMR



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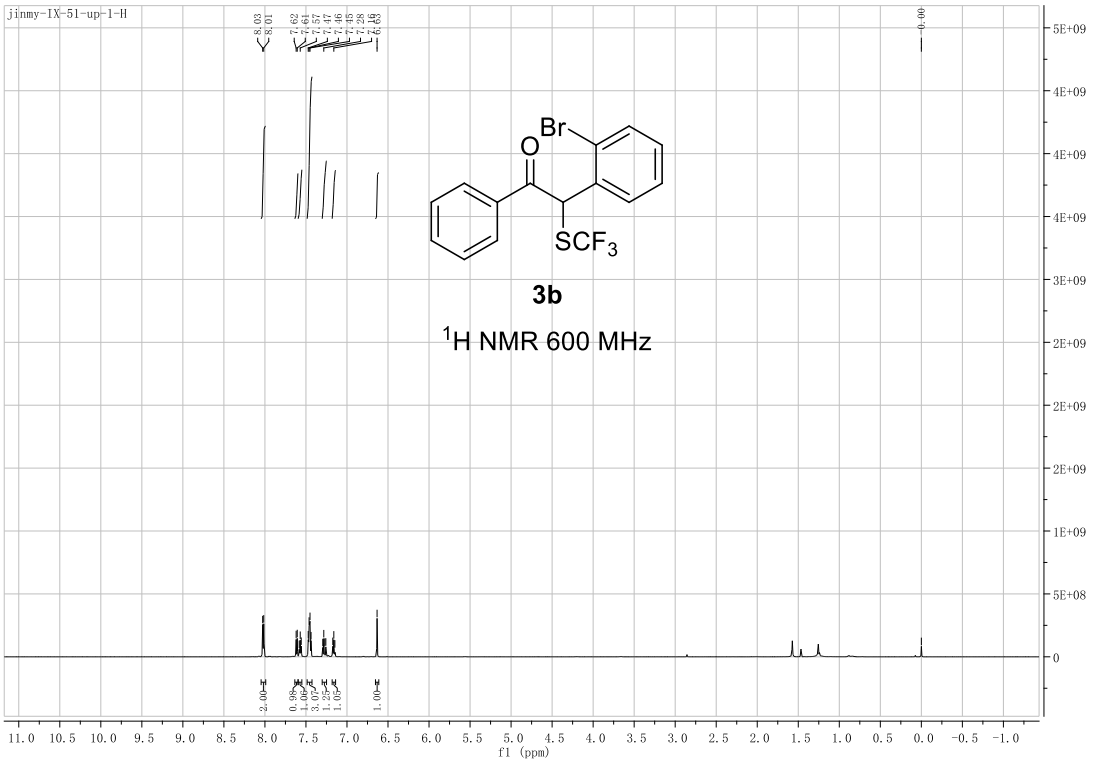
Cl
O
SCF3
3a
19F NMR 376 MHz
f1 (ppm)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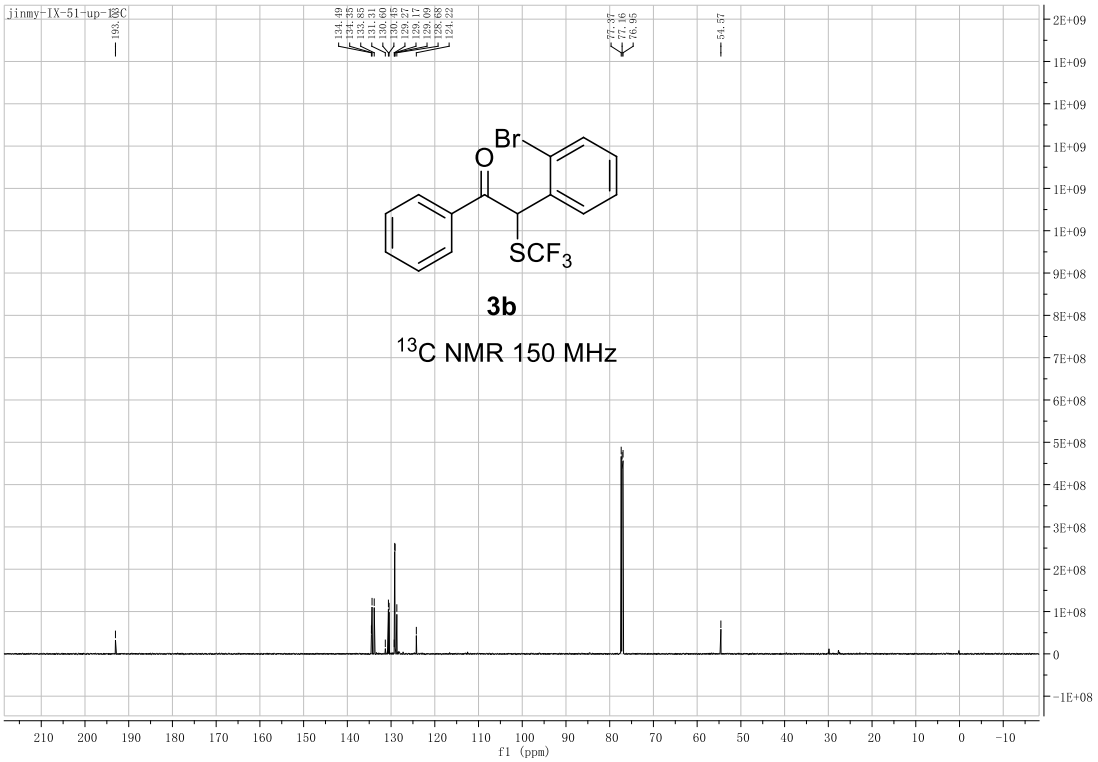
8.01
7.62
7.61
7.57
7.47
7.46
7.45
7.28
7.26
0.00
Br
O
SCF3
3b
1H NMR 600 MHz
2.00
0.98
1.00
3.07
2.04
1.05
1.00
f1 (ppm)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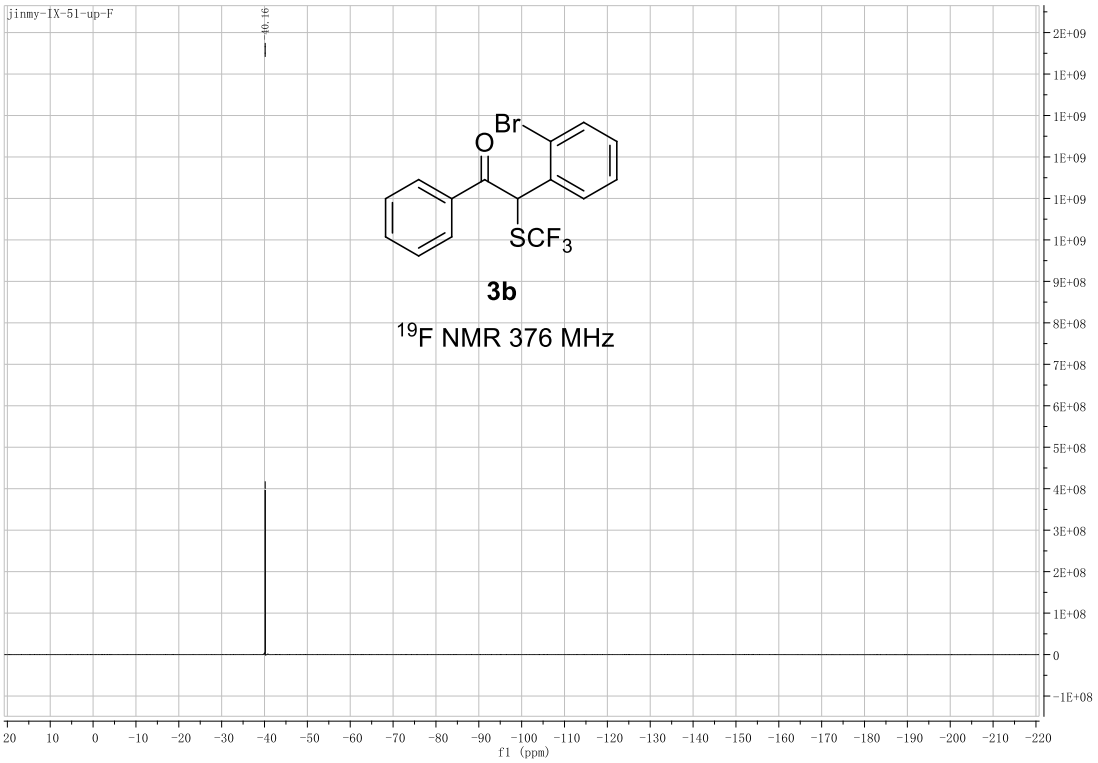
193.18
134.49
134.35
133.85
131.31
130.60
130.45
129.27
129.17
129.09
128.88
124.22
77.37
77.16
76.95
54.57
Br
O
SCF3
3b
13C NMR 150 MHz
f1 (ppm)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O
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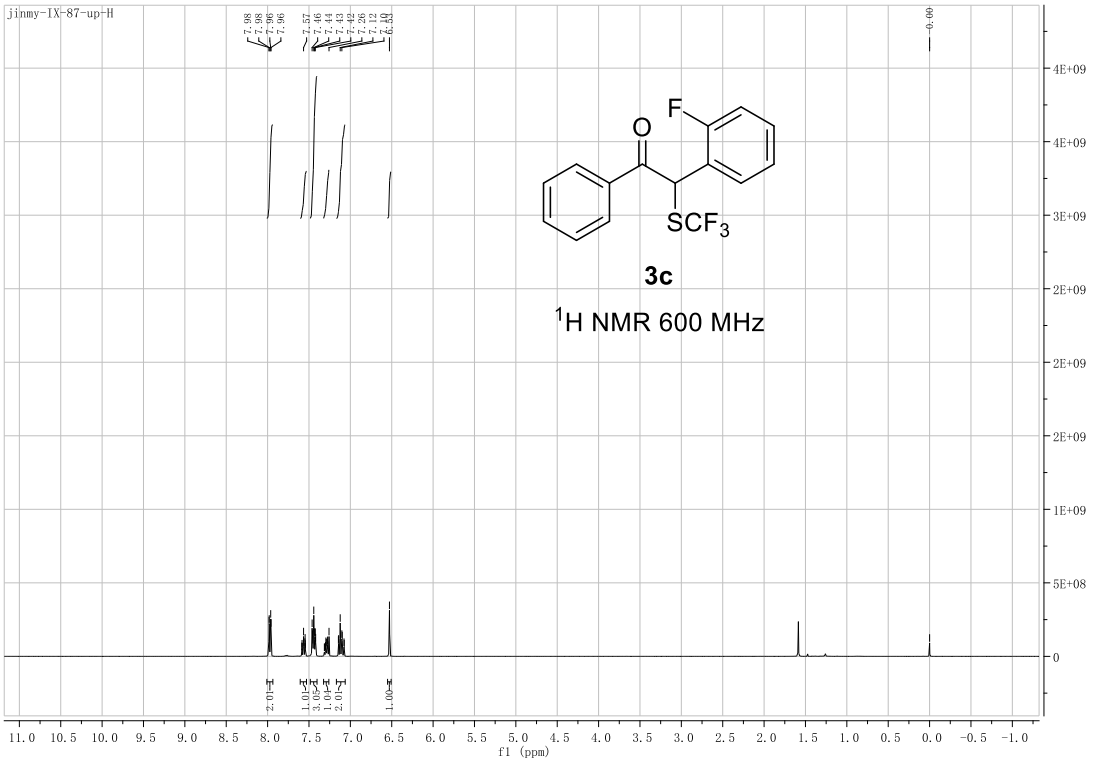
3b
19F NMR 376 MHz
f1 (ppm)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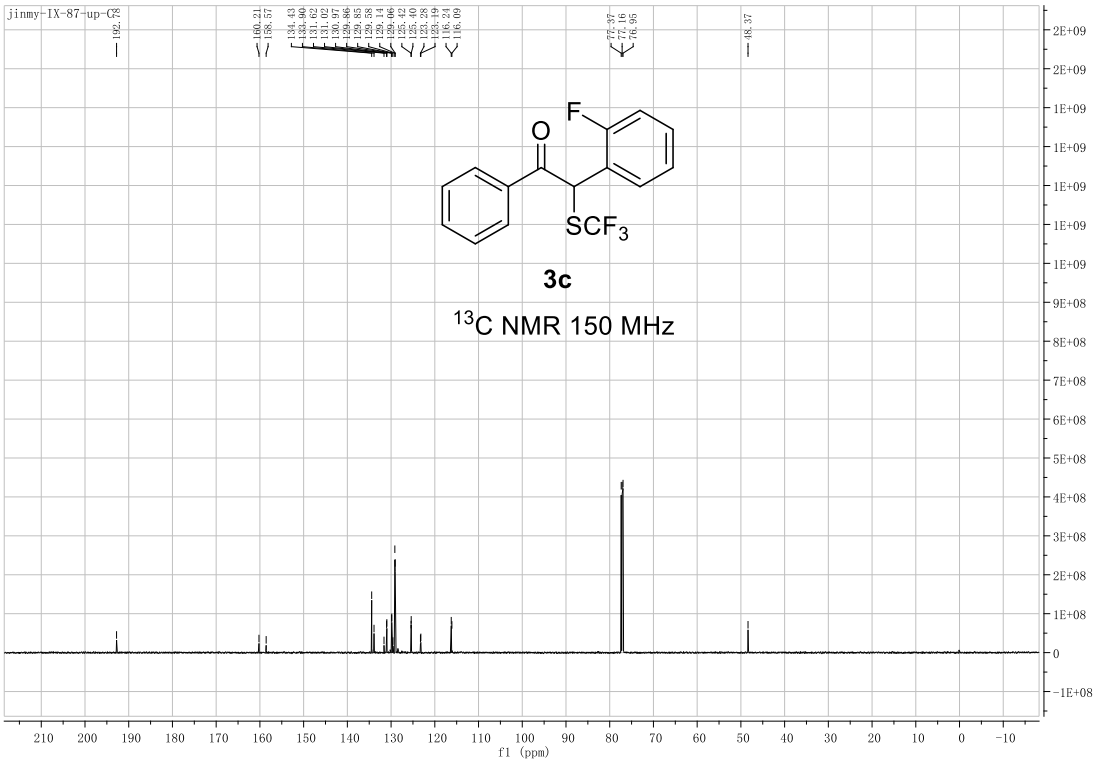
F
O
SCF3
3c
1H NMR 600 MHz
f1 (ppm)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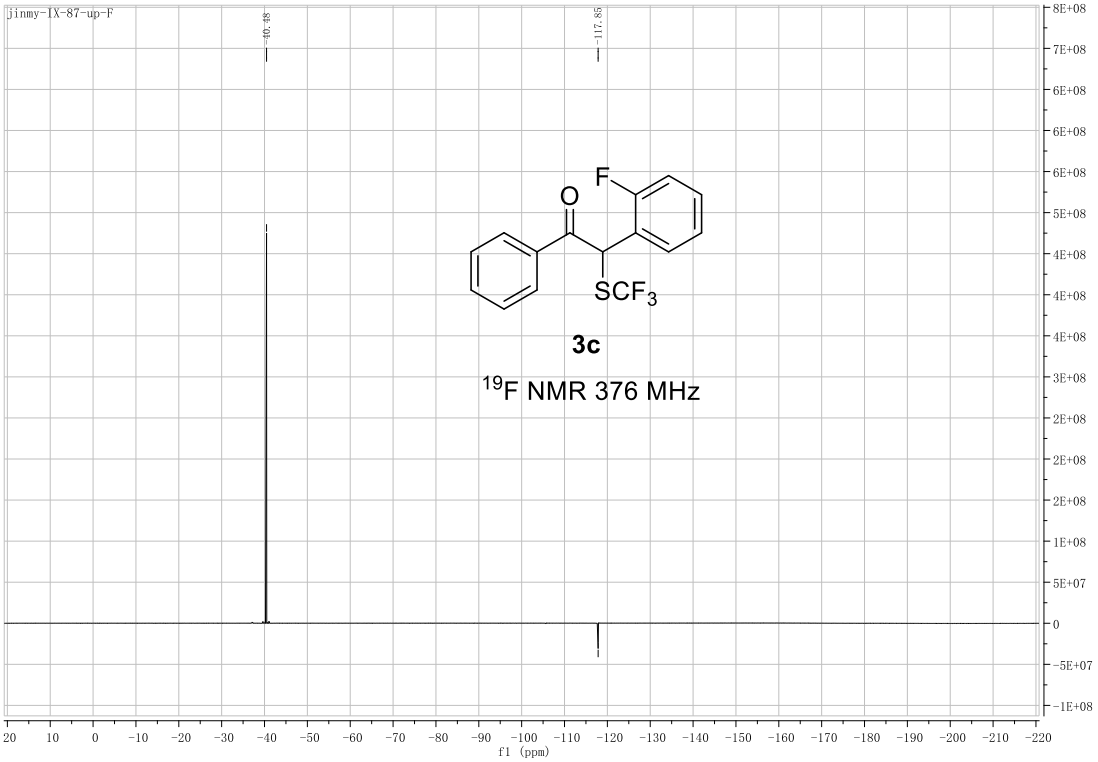
F
O
SCF3
3c
13C NMR 150 MHz
f1 (ppm)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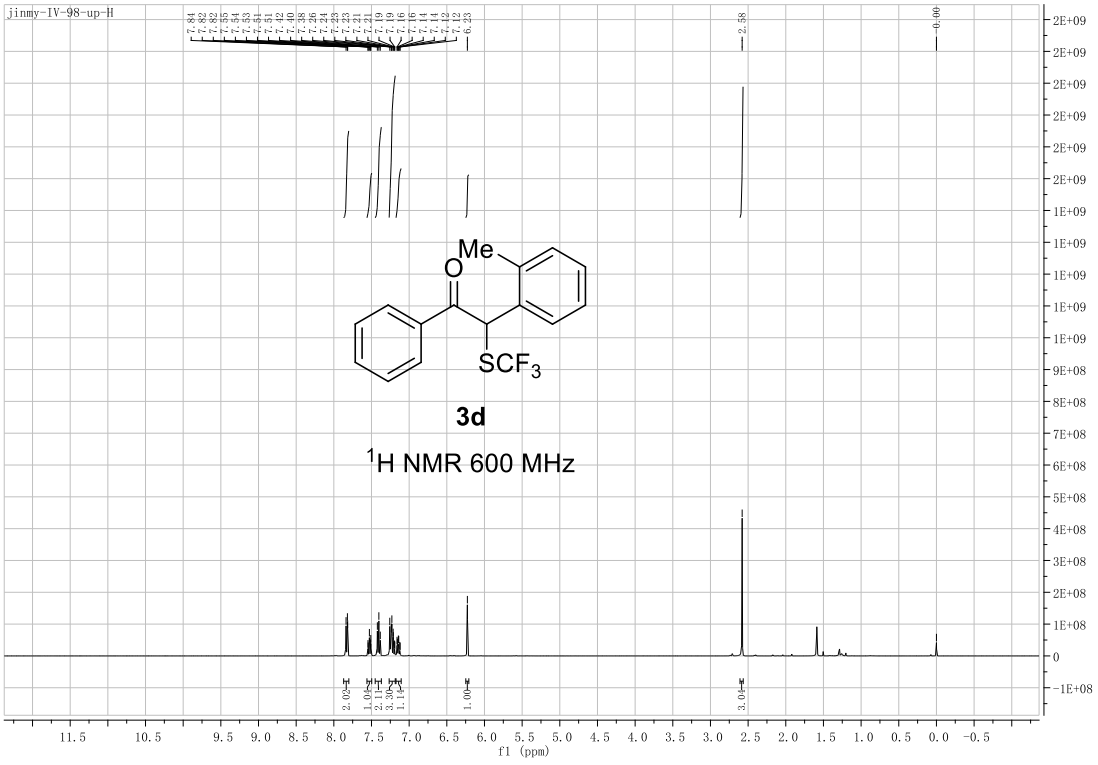
F
O
SCF3
3c
19F NMR 376 MHz
f1 (ppm)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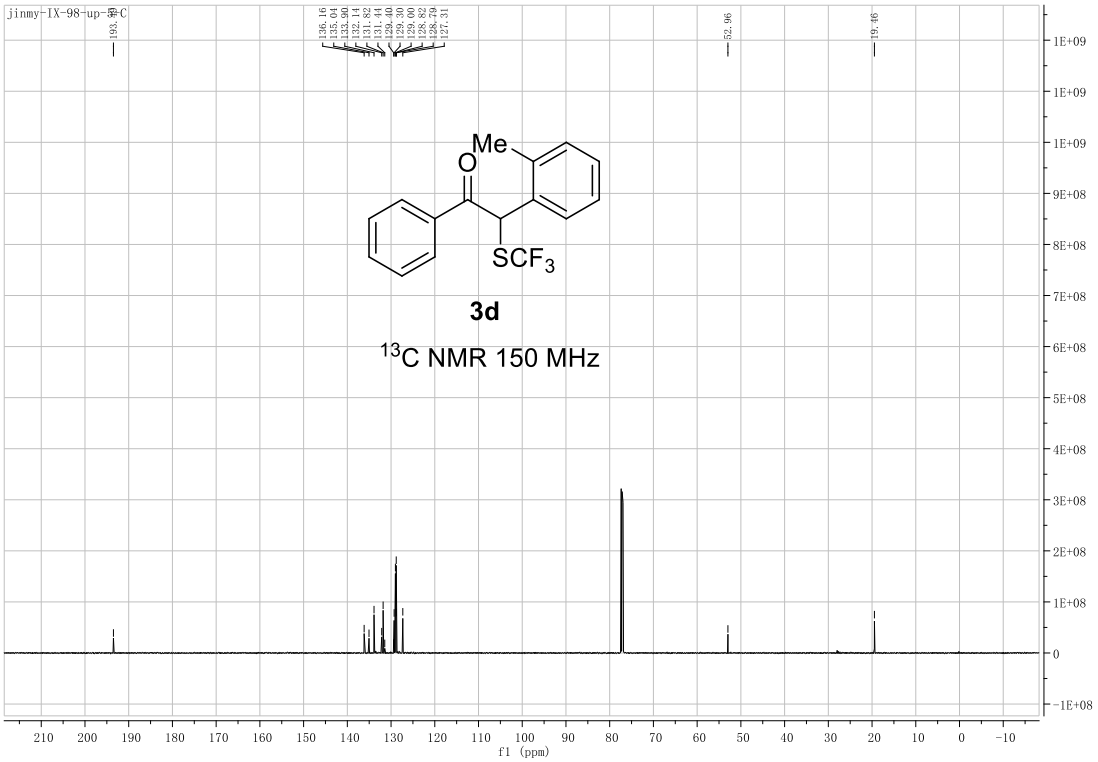
0.00
Me
O
SCF3
3d
1H NMR 600 MHz
f1 (ppm)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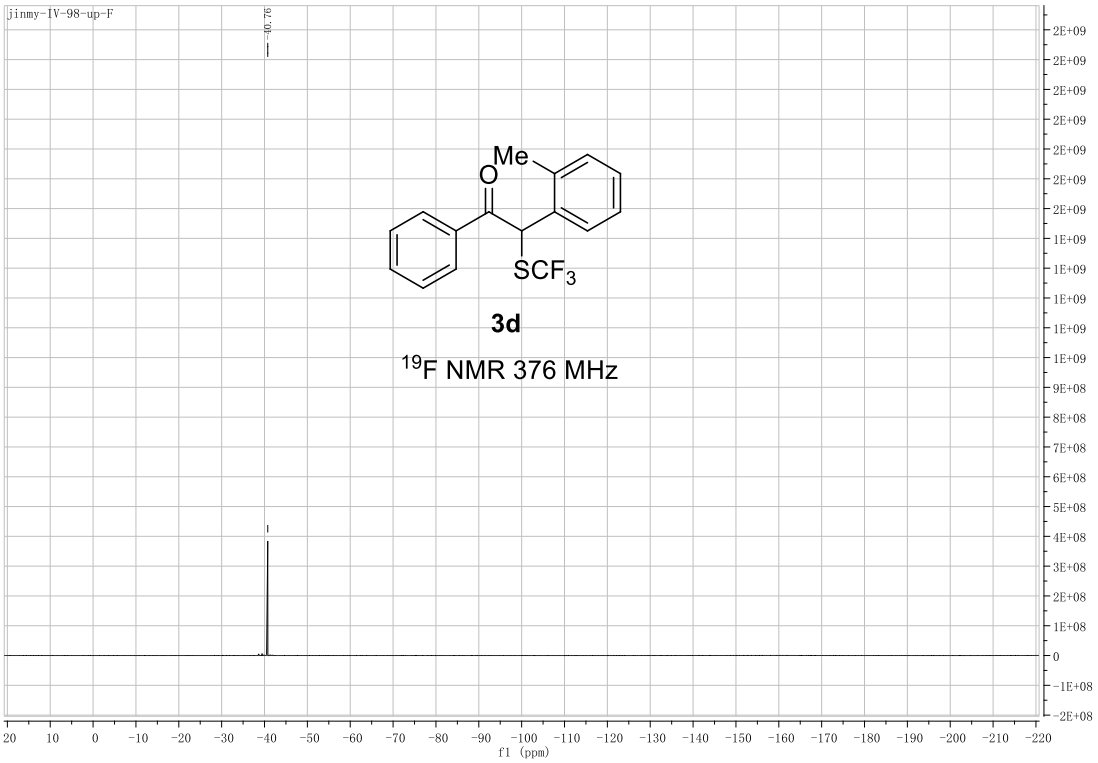
193.49
136.16
135.04
133.90
132.41
131.82
131.44
129.40
129.30
128.60
128.82
128.79
127.31
52.96
19.46
Me
O
SCF3
3d
13C NMR 150 MHz
f1 (ppm)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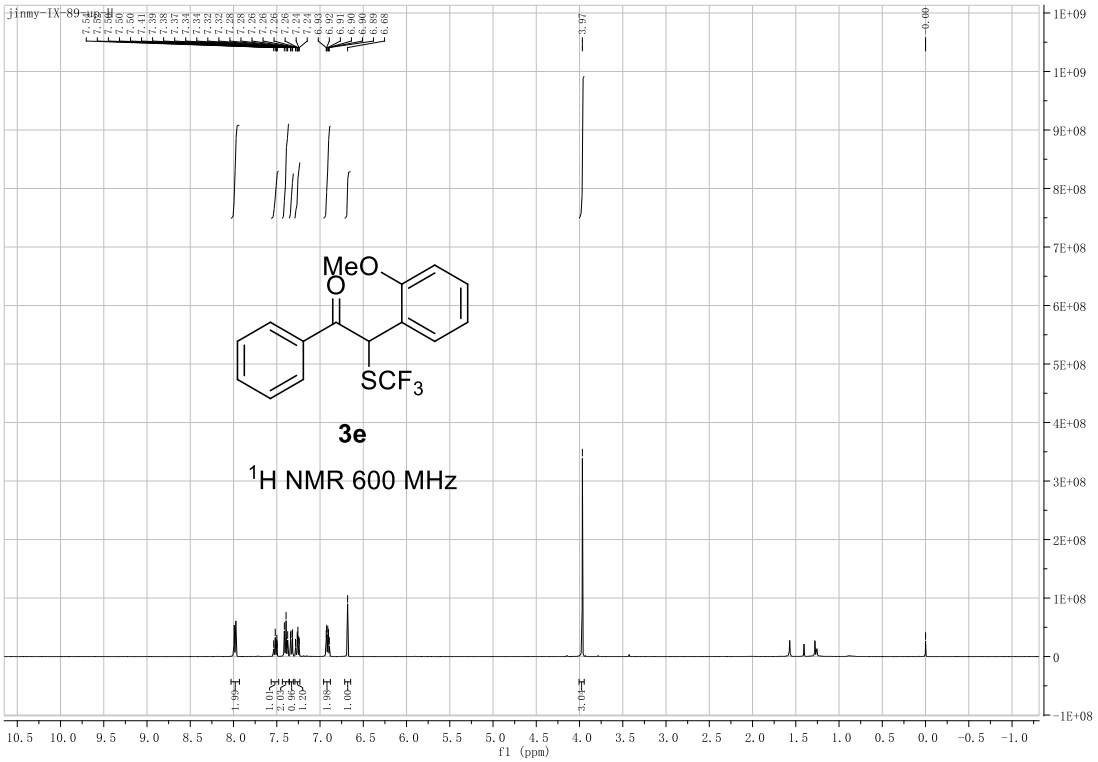
Me
O
SCF3
3d
19F NMR 376 MHz
f1 (ppm)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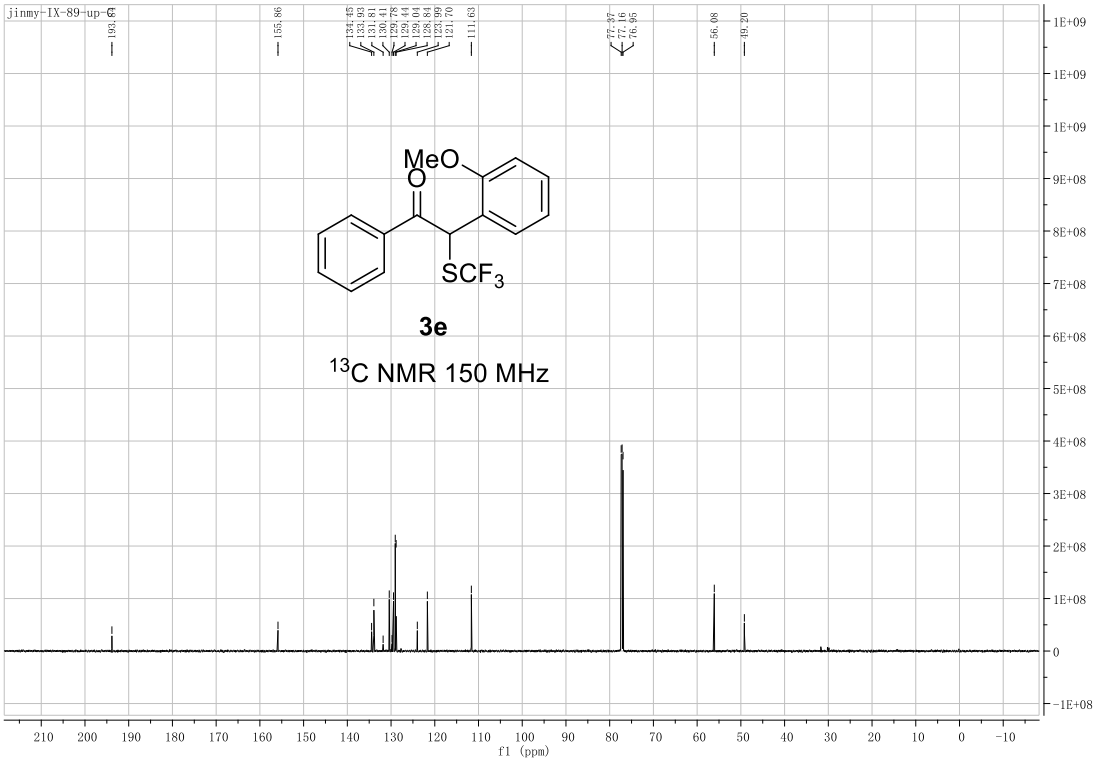
MeO
O
SCF3
3e
1H NMR 600 MHz
f1 (ppm)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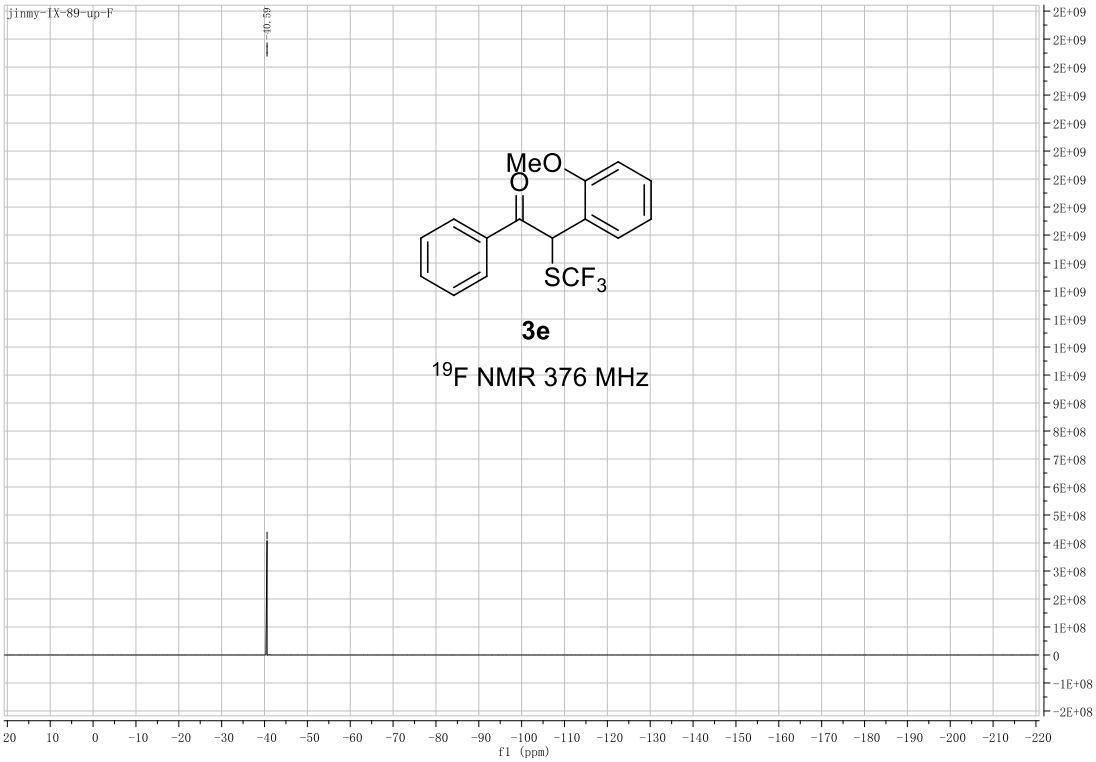
MeO
O
SCF3
3e
13C NMR 150 MHz
f1 (ppm)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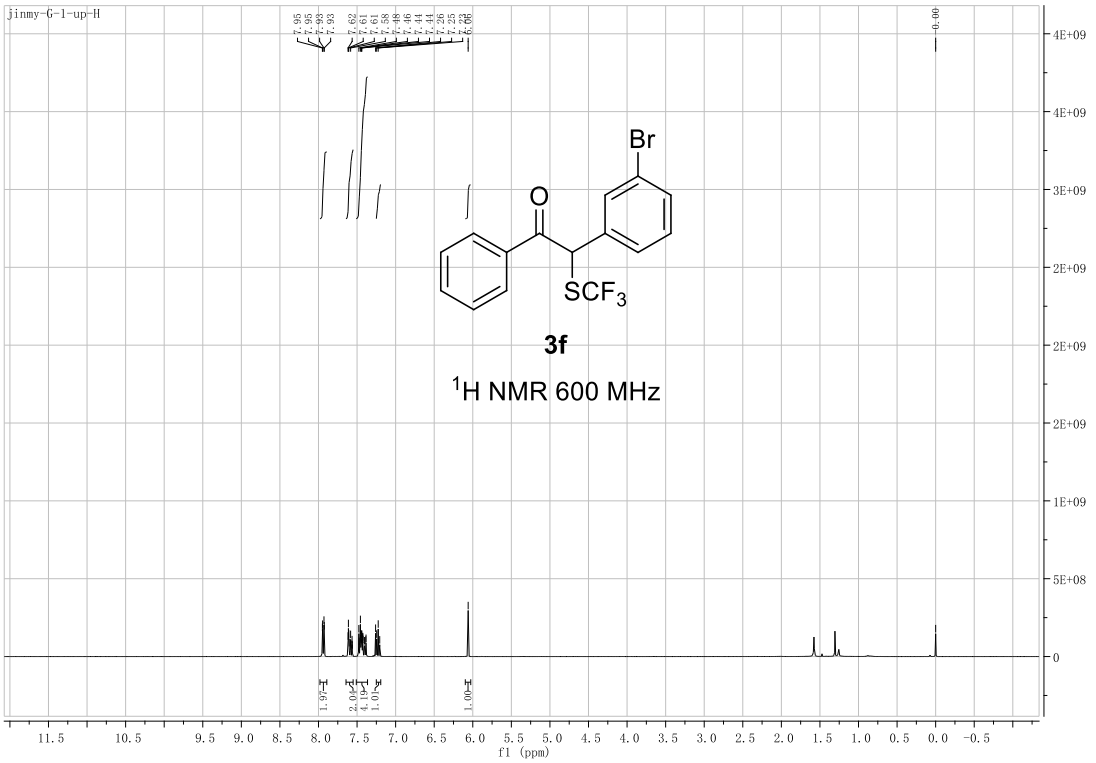
MeO
O
SCF3
3e
19F NMR 376 MHz
f1 (ppm)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7.95
7.93
7.93
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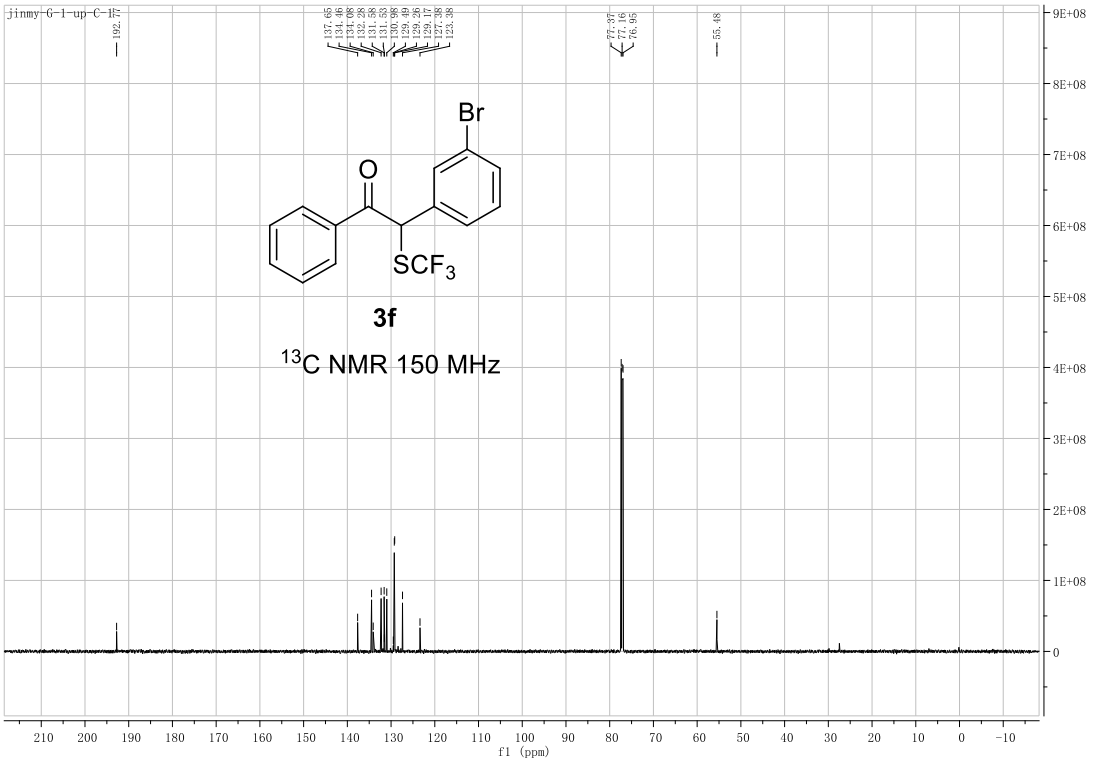
7.61
7.58
7.48
7.46
7.44
7.26
7.25
7.23
6.00
0.00
Br
O
SCF3
3f
1H NMR 600 MHz
1.97
2.04
4.19
1.01
1.00
f1 (ppm)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134.46
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132.28
131.58
131.53
130.98
129.49
129.26
129.17
127.38
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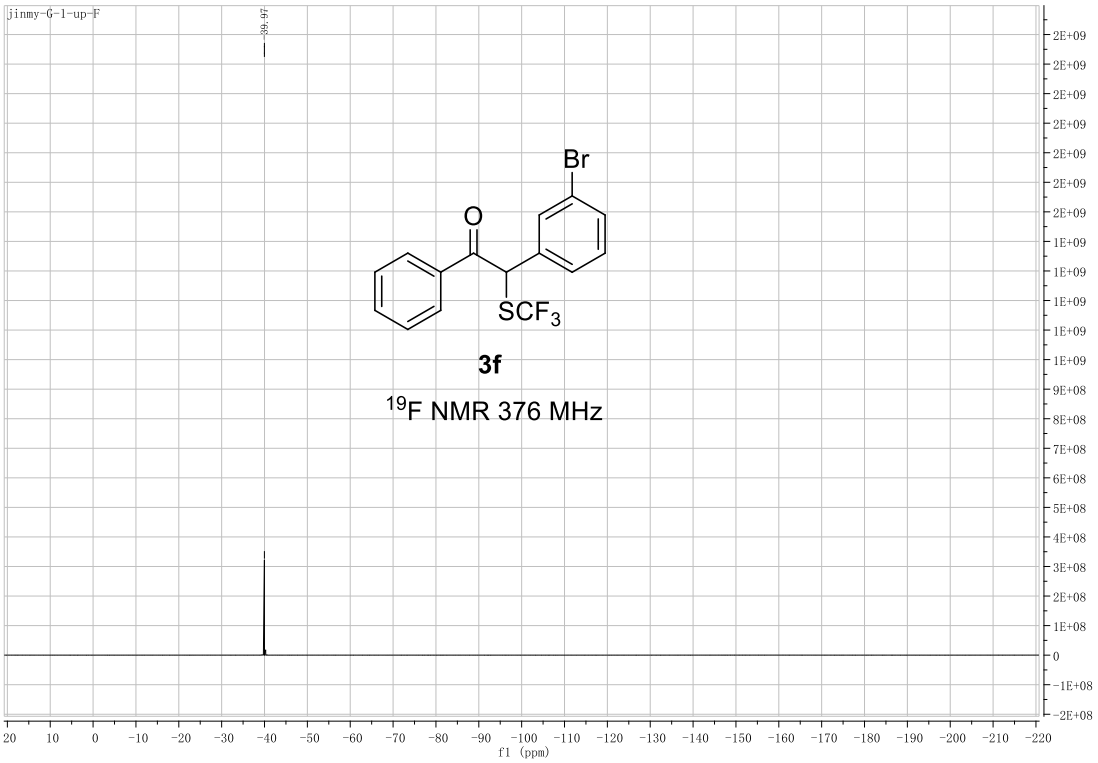
77.37
77.16
76.95
55.48
Br
O
SCF3
3f
13C NMR 150 MHz
f1 (ppm)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O
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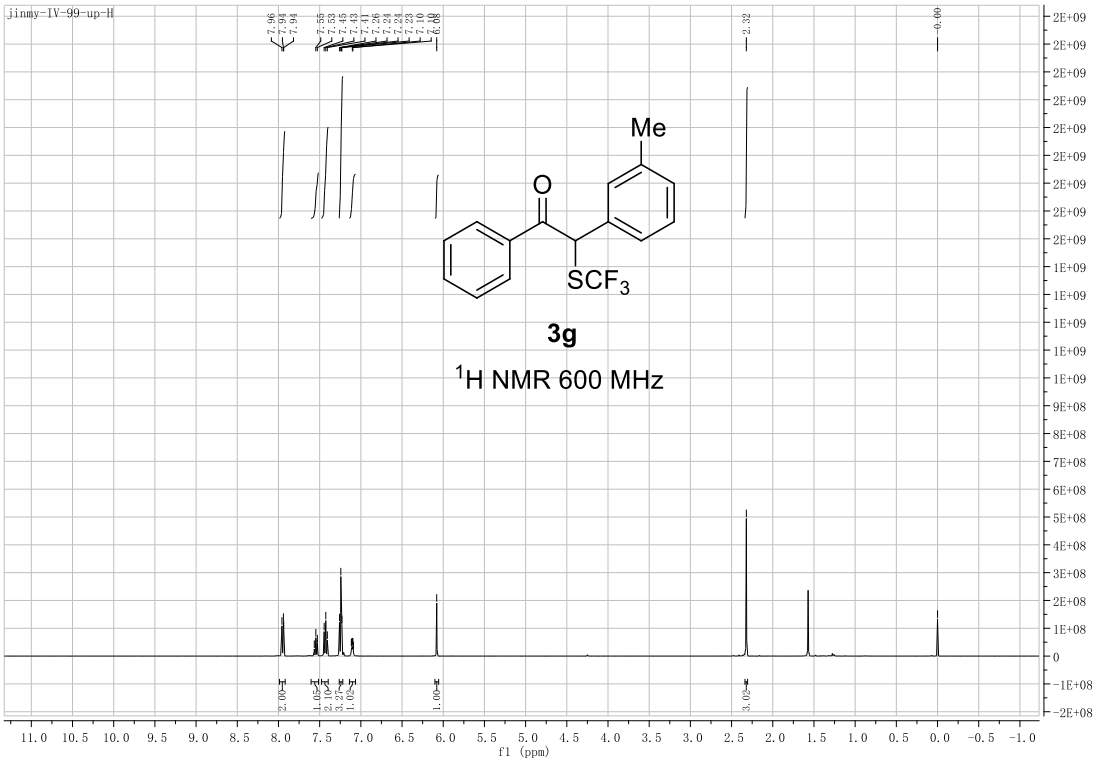
3f
19F NMR 376 MHz
f1 (ppm)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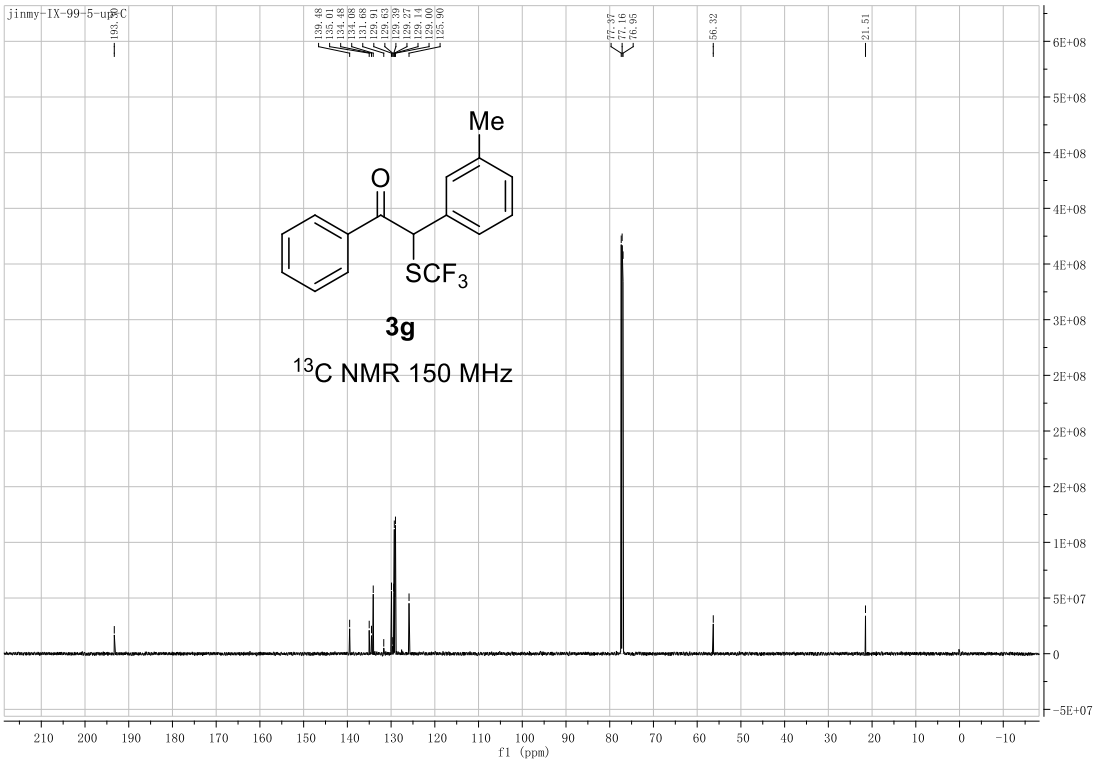
Me
O
SCF3
3g
1H NMR 600 MHz
f1 (ppm)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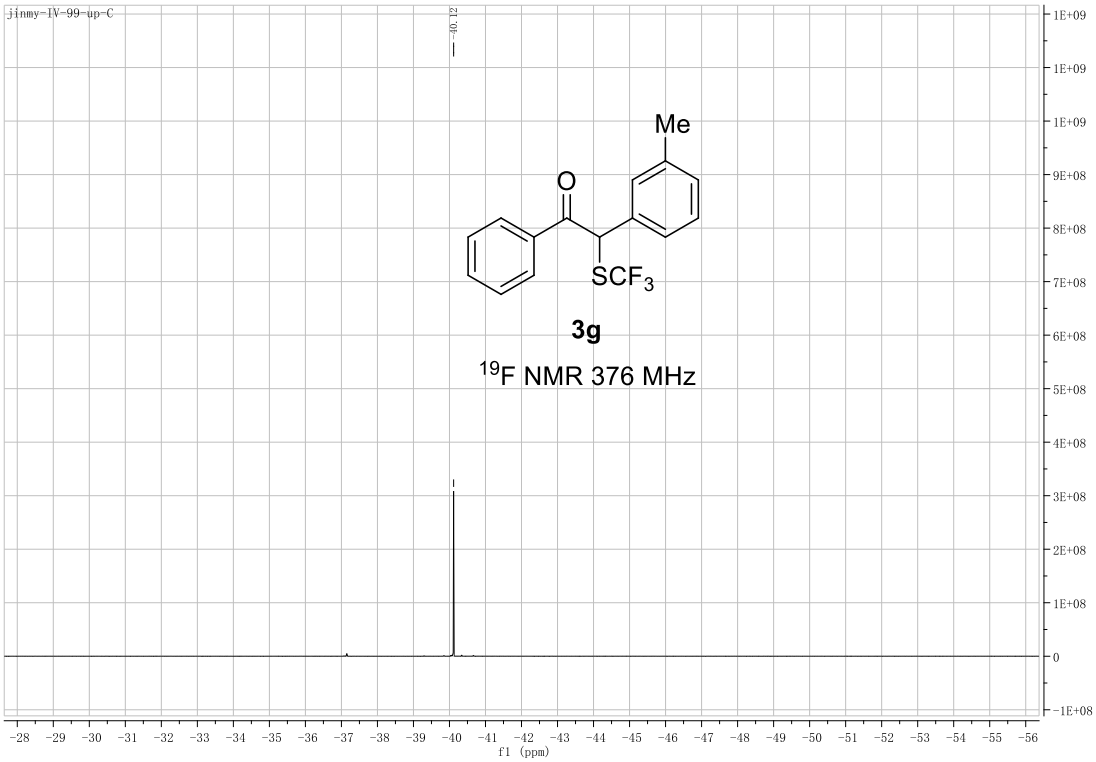
Me
O
SCF3
3g
13C NMR 150 MHz
f1 (ppm)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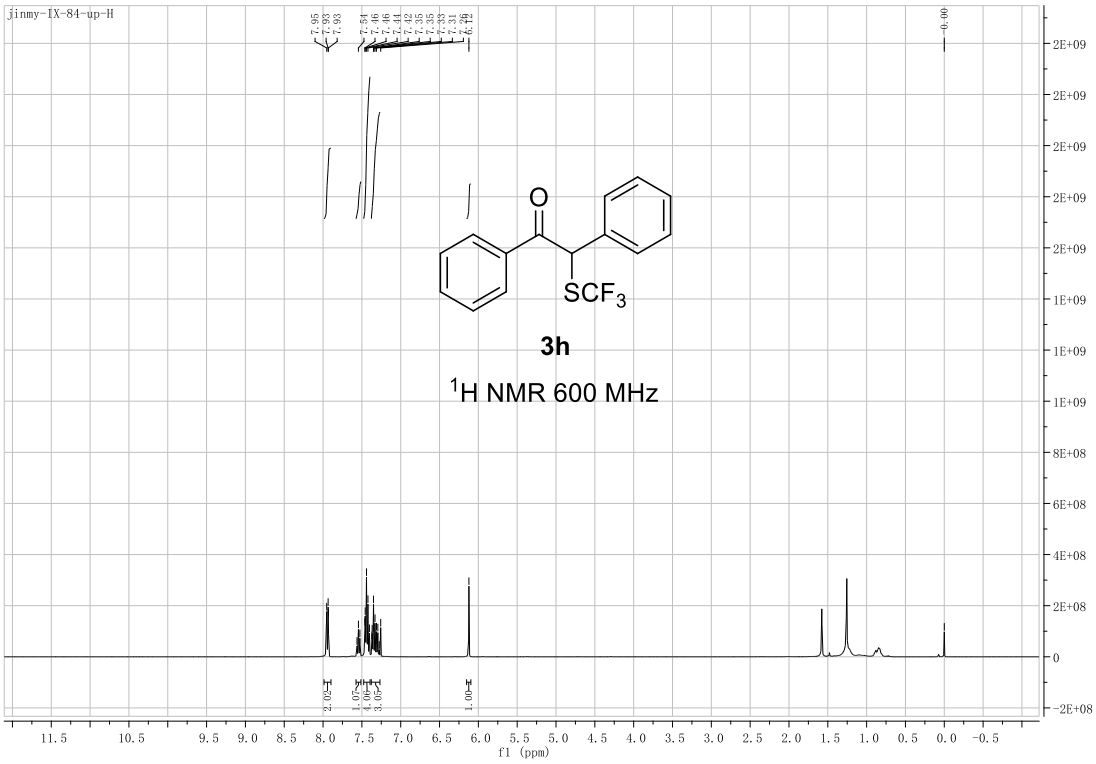
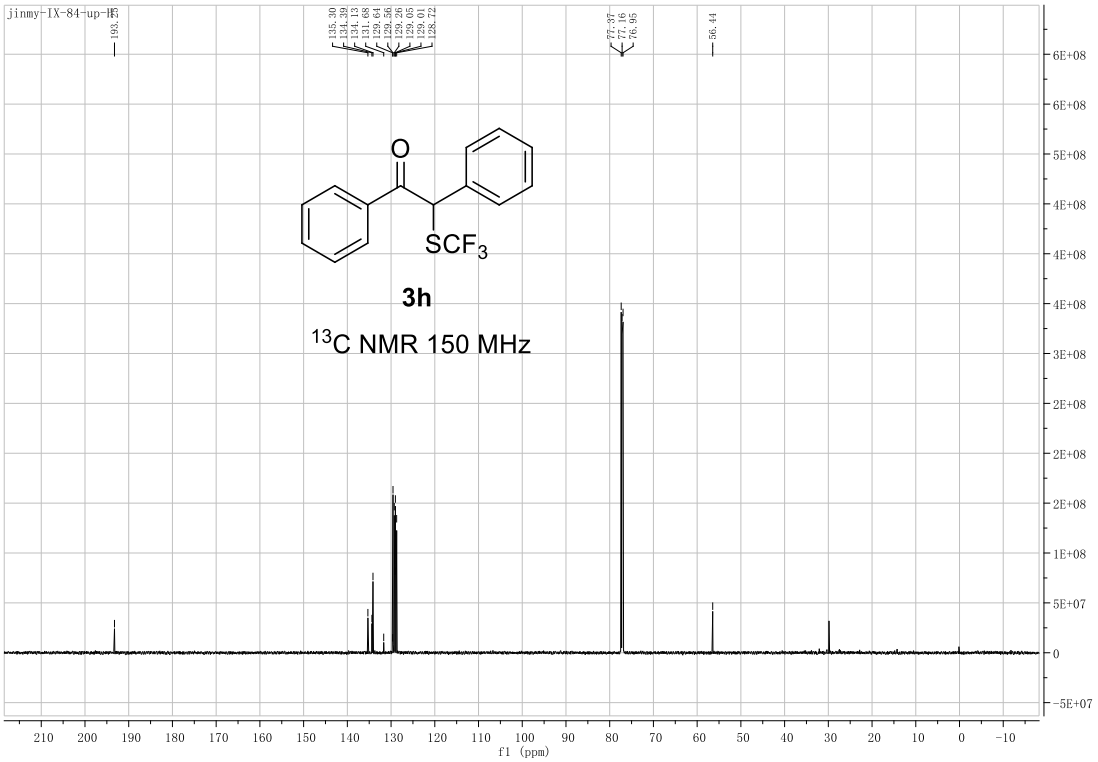
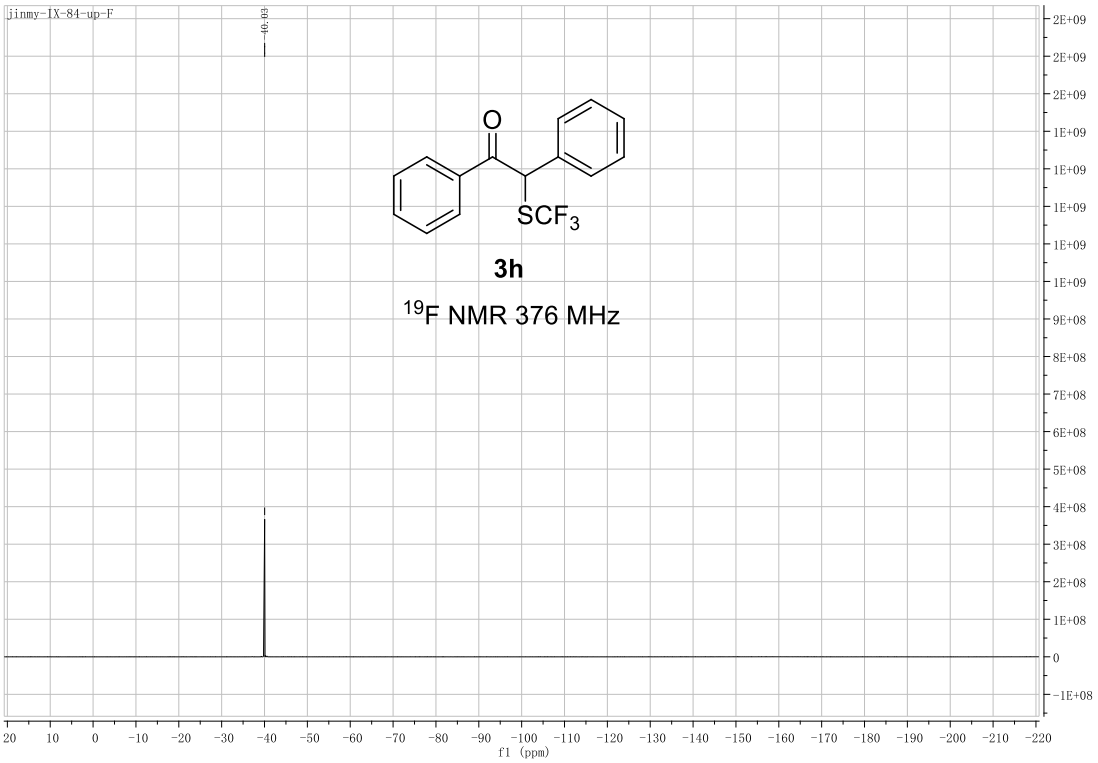
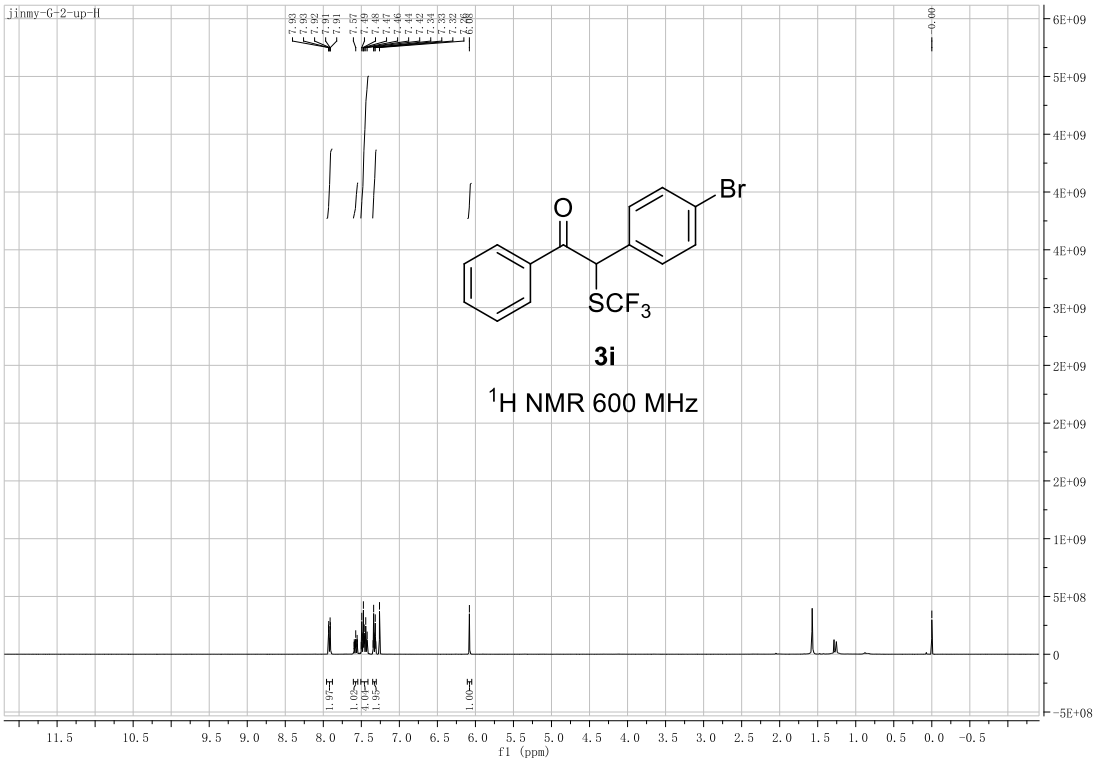
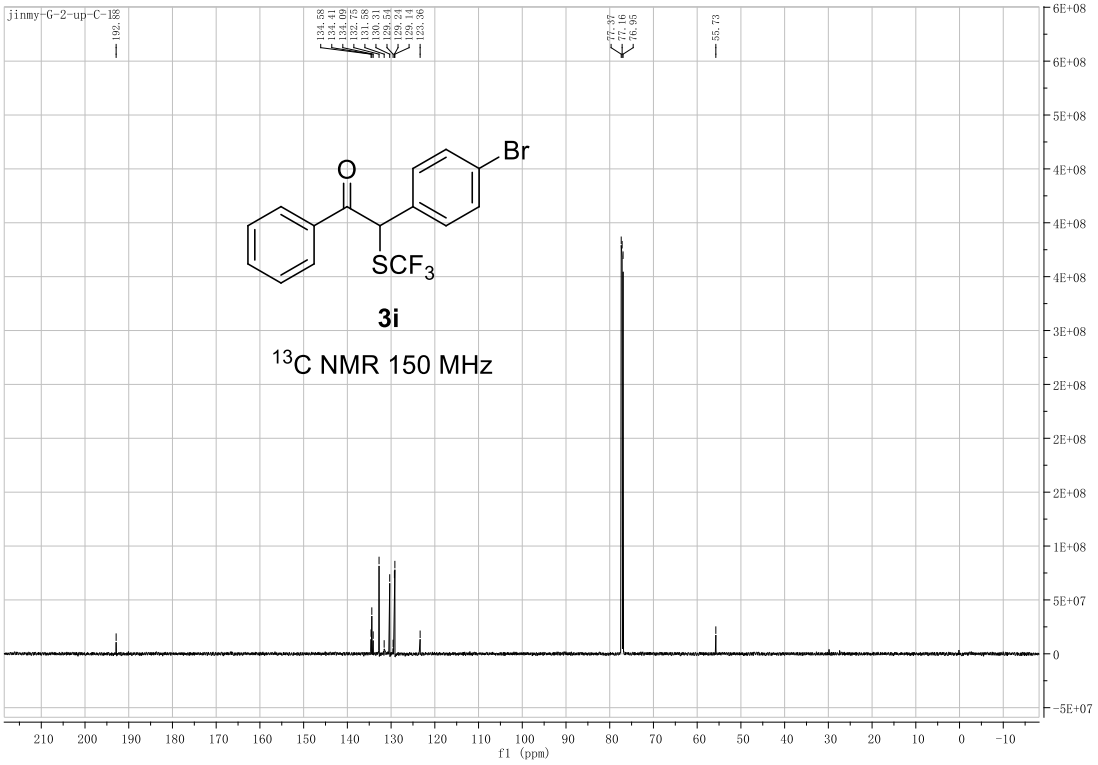
SCF3
3g
19F NMR 376 MHz
f1 (ppm)

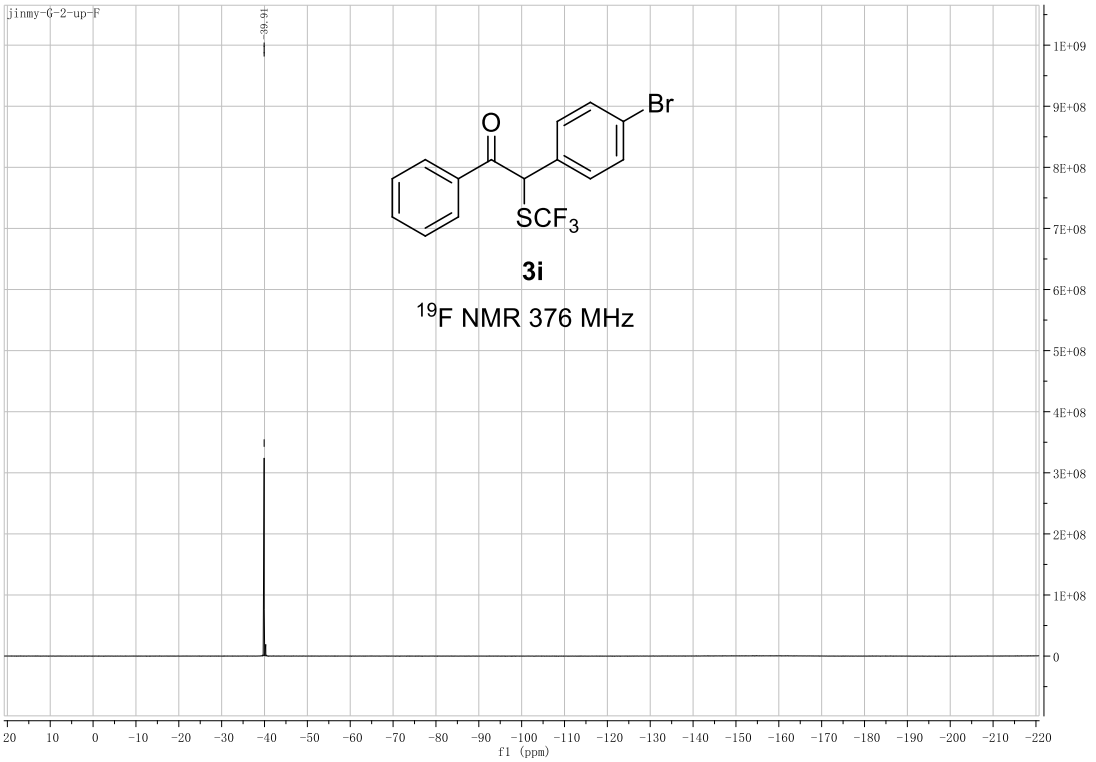

jinmy-IX-84-up-H
7.95
7.93
7.54
7.46
7.46
7.44
7.42
7.35
7.33
7.31
6.12
0.00
O
SCF3
3h
1H NMR 600 MHz
2.02
1.07
4.08
3.05
1.00
f1 (ppm)

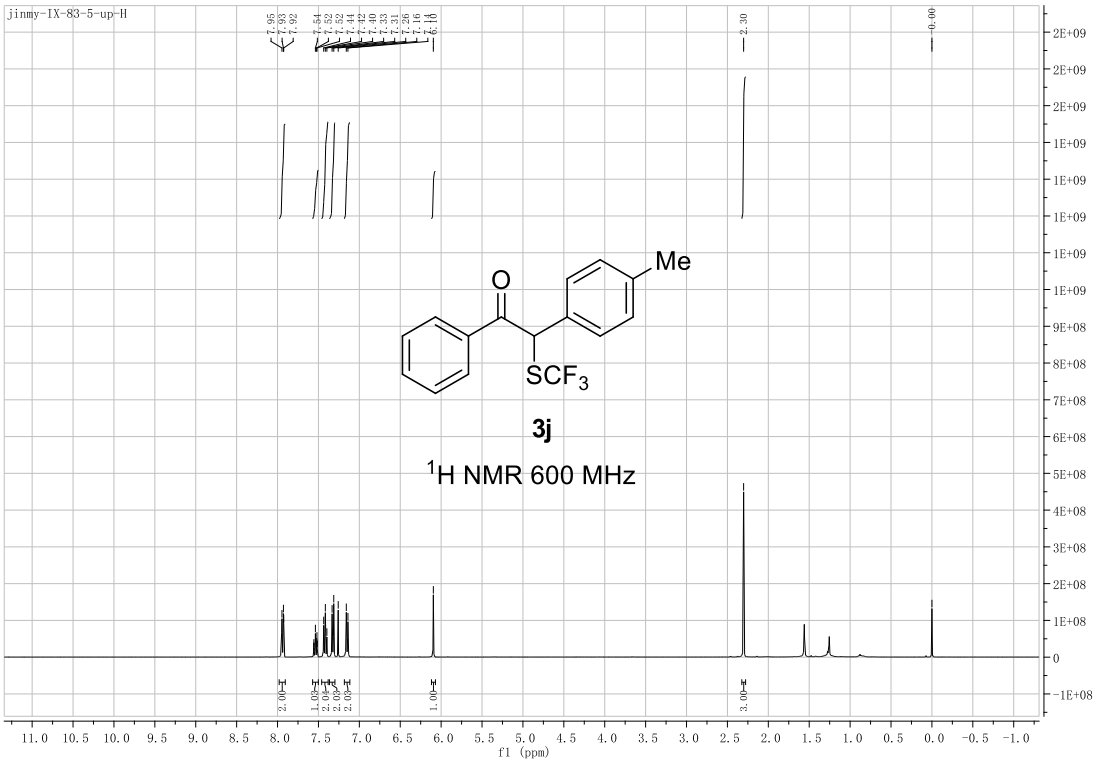

jinmy-IX-84-up-H
193.51
135.30
134.13
131.68
129.64
129.56
129.26
129.05
129.01
128.72
77.37
77.16
76.95
56.44
O
SCF3
3h
13C NMR 150 MHz
f1 (ppm)

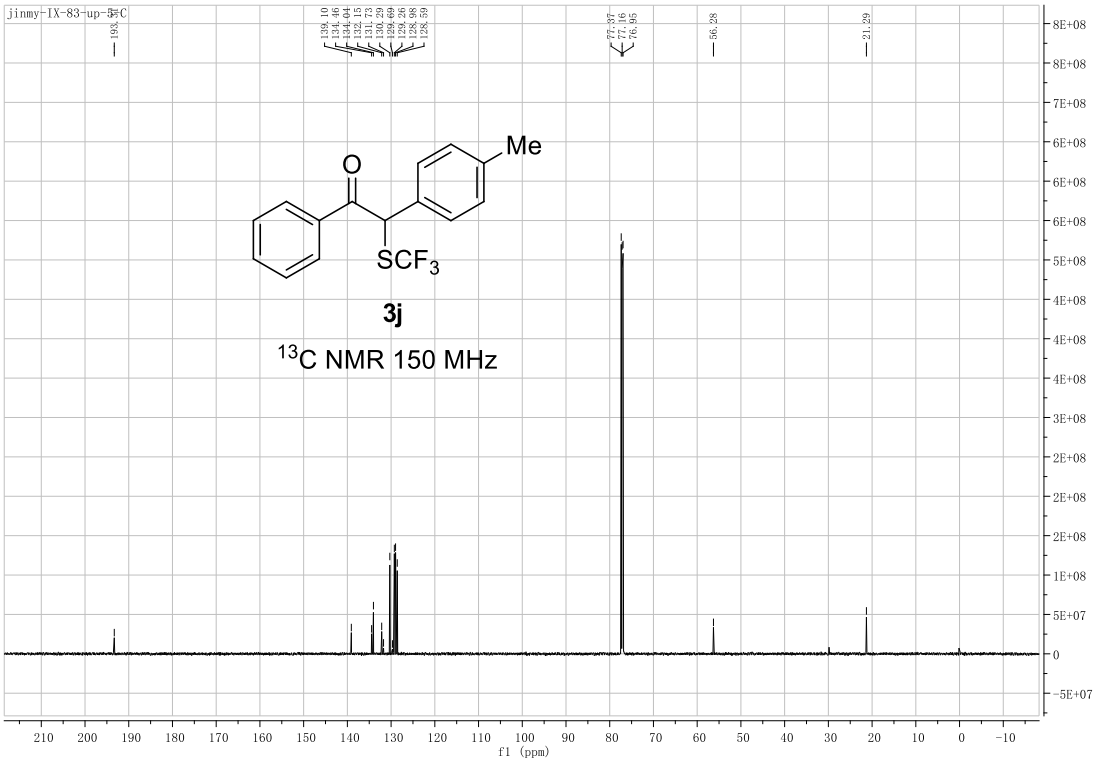

jinmy-IX-84-up-F
-40.03
O
SCF3
3h
19F NMR 376 MHz
f1 (ppm)

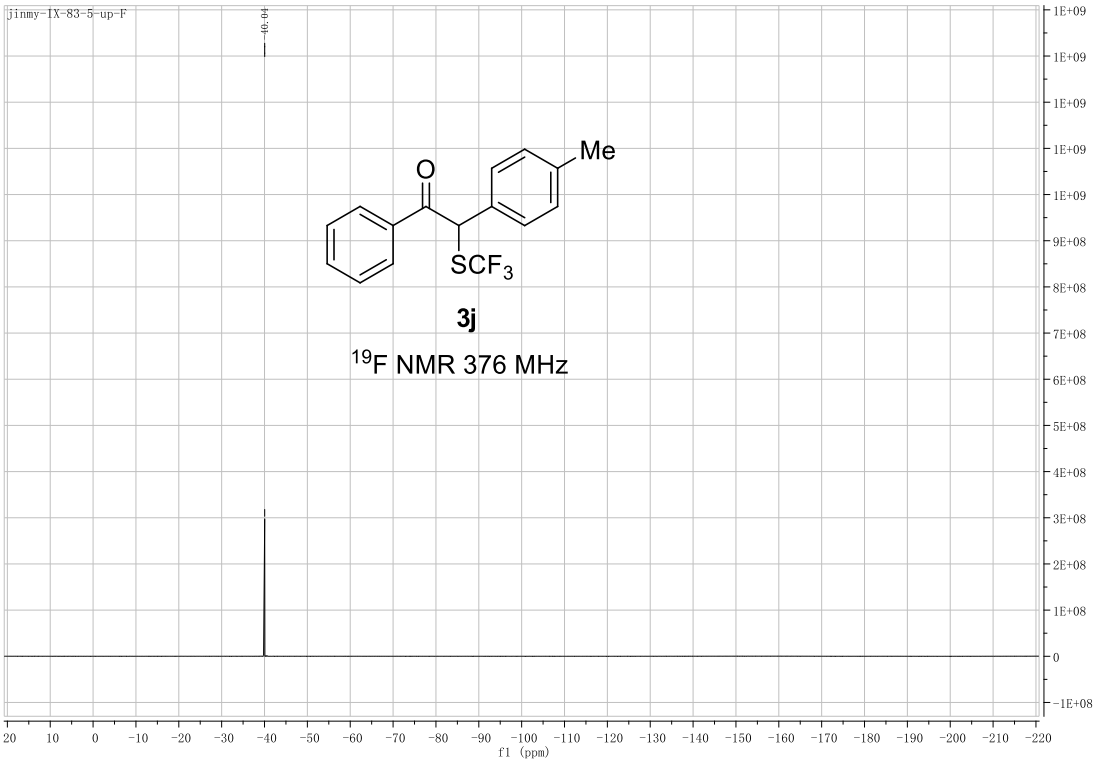

jinmy-G-2-up-H
Br
O
SCF3
3i
1H NMR 600 MHz
f1 (ppm)

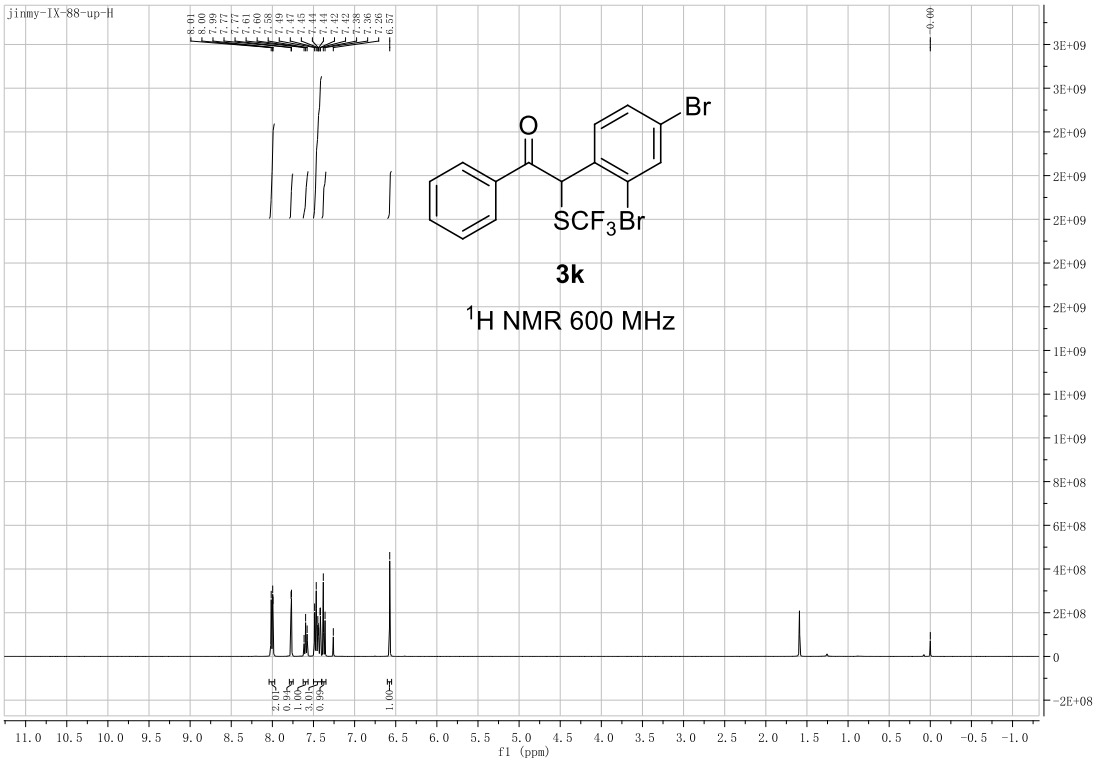

jinmy-G-2-up-C-1
Br
O
SCF3
3i
13C NMR 150 MHz
f1 (ppm)

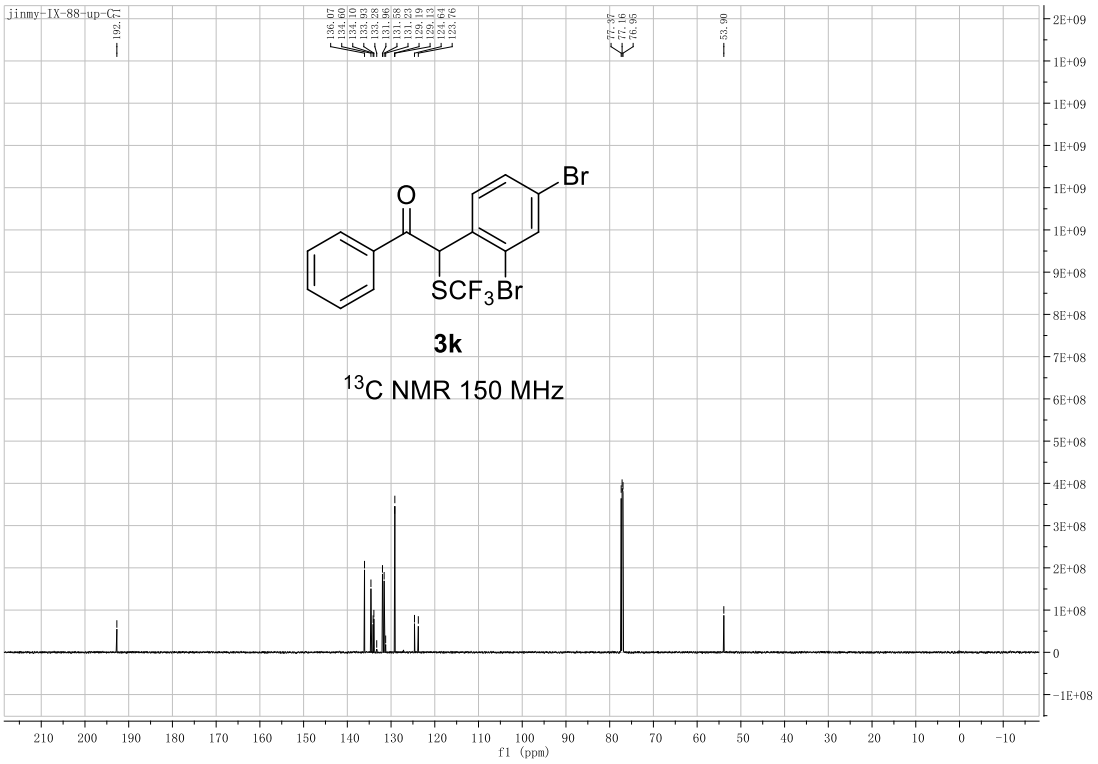

jinmy-G-2-up-F
-39.91
Br
O
SCF3
3i
19F NMR 376 MHz
f1 (ppm)

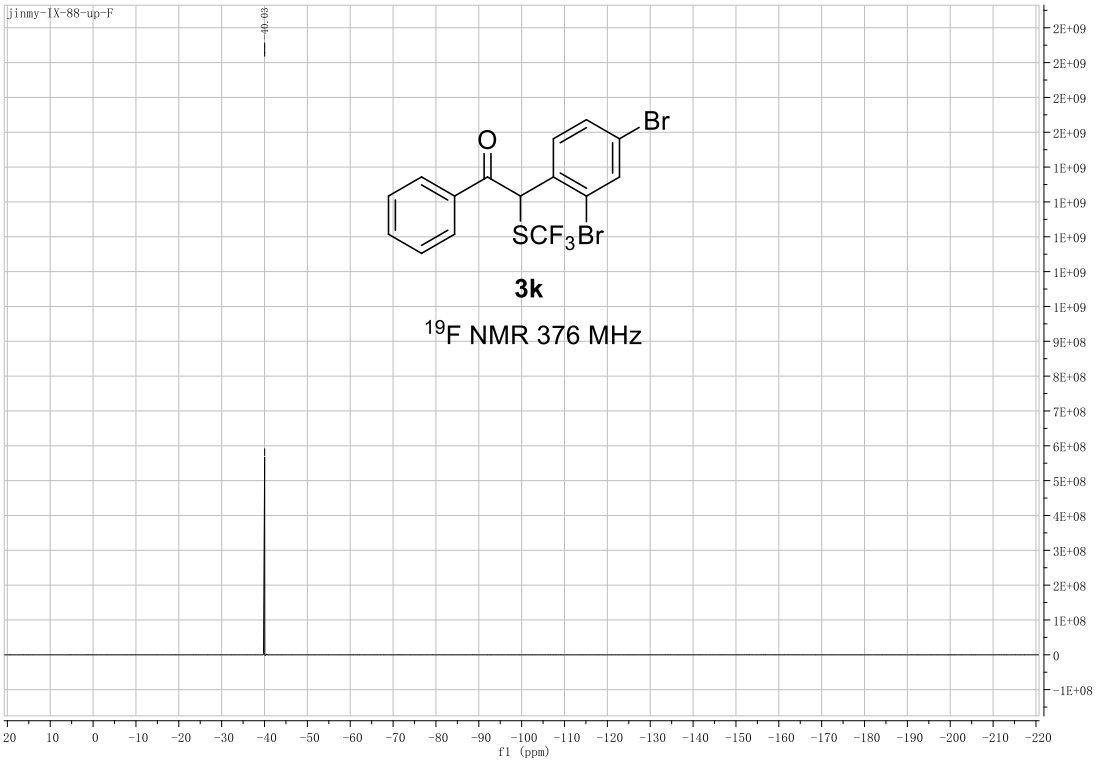

jinmy-IX-83-5-up-H
7.95
7.93
7.92
7.84
7.82
7.82
7.44
7.42
7.40
7.33
7.31
7.26
7.16
6.14
2.30
0.00
Me
O
SCF3
3j
1H NMR 600 MHz
2.00
1.02
2.04
2.02
2.03
1.00
3.00
f1 (ppm)

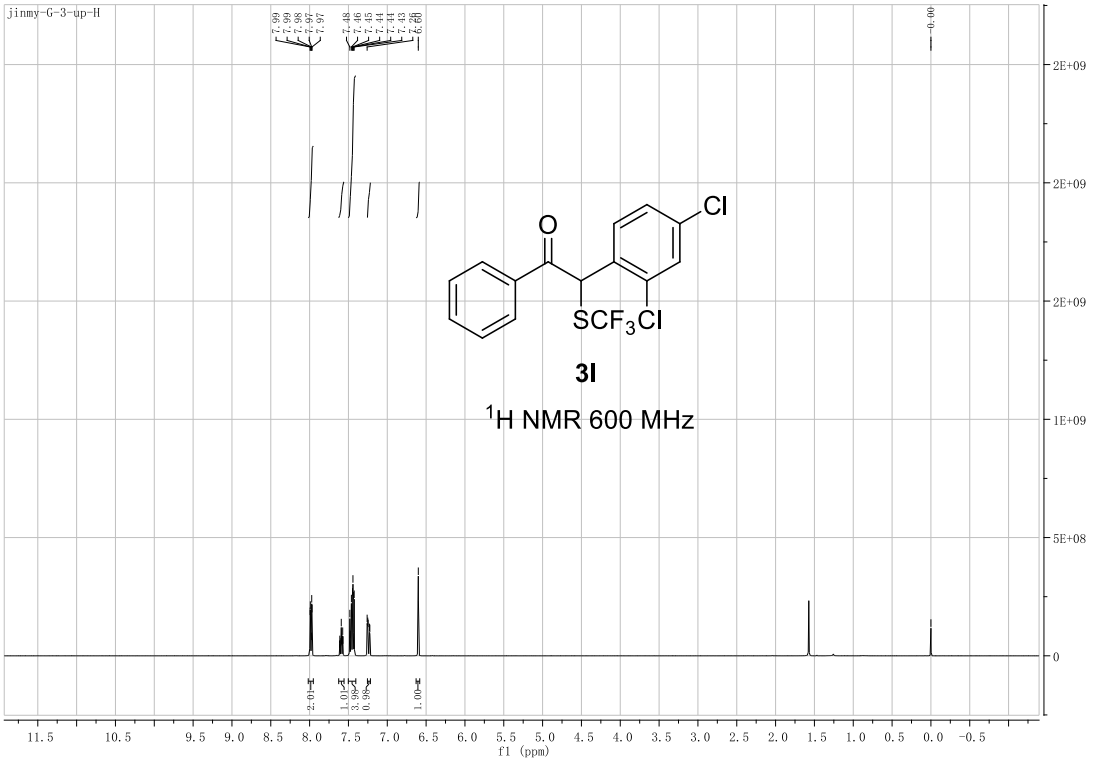

jinmy-IX-83-up-13C
193.37
139.10
134.46
134.04
132.15
131.73
130.29
129.69
129.26
128.98
128.69
77.37
77.16
76.95
56.28
21.29
Me
O
SCF3
3j
13C NMR 150 MHz
f1 (ppm)

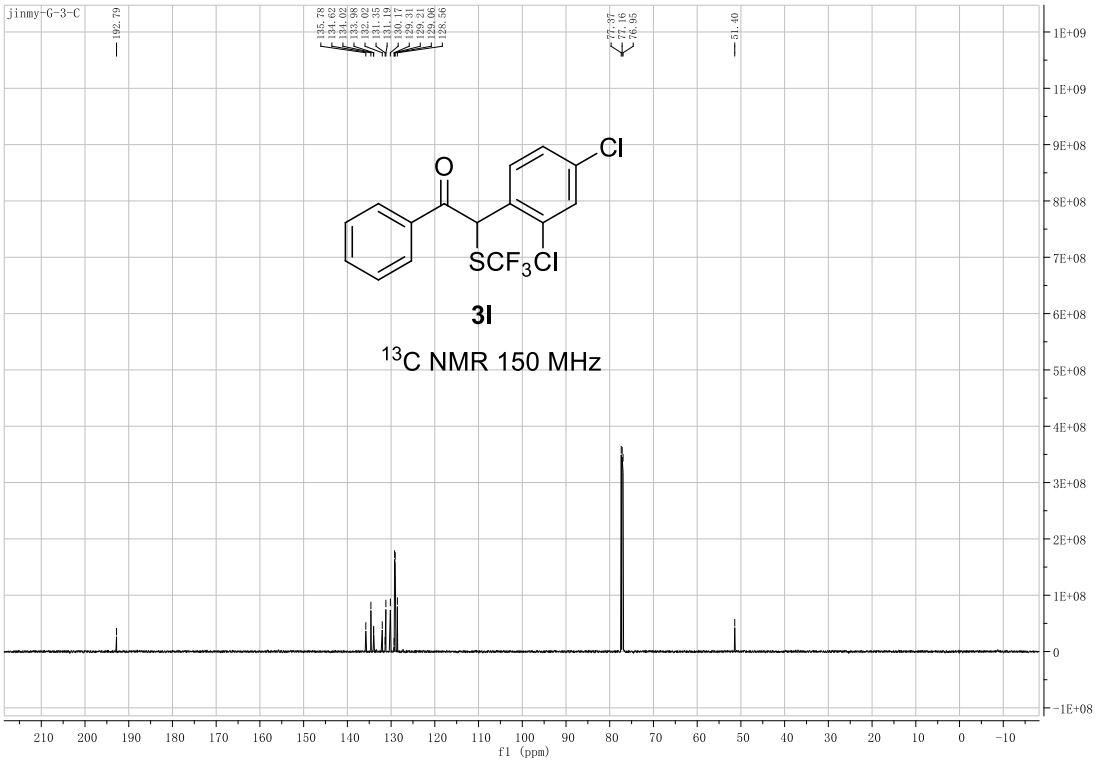

jinmy-IX-83-5-up-F
-40.04
Me
O
SCF3
3j
19F NMR 376 MHz
f1 (ppm)

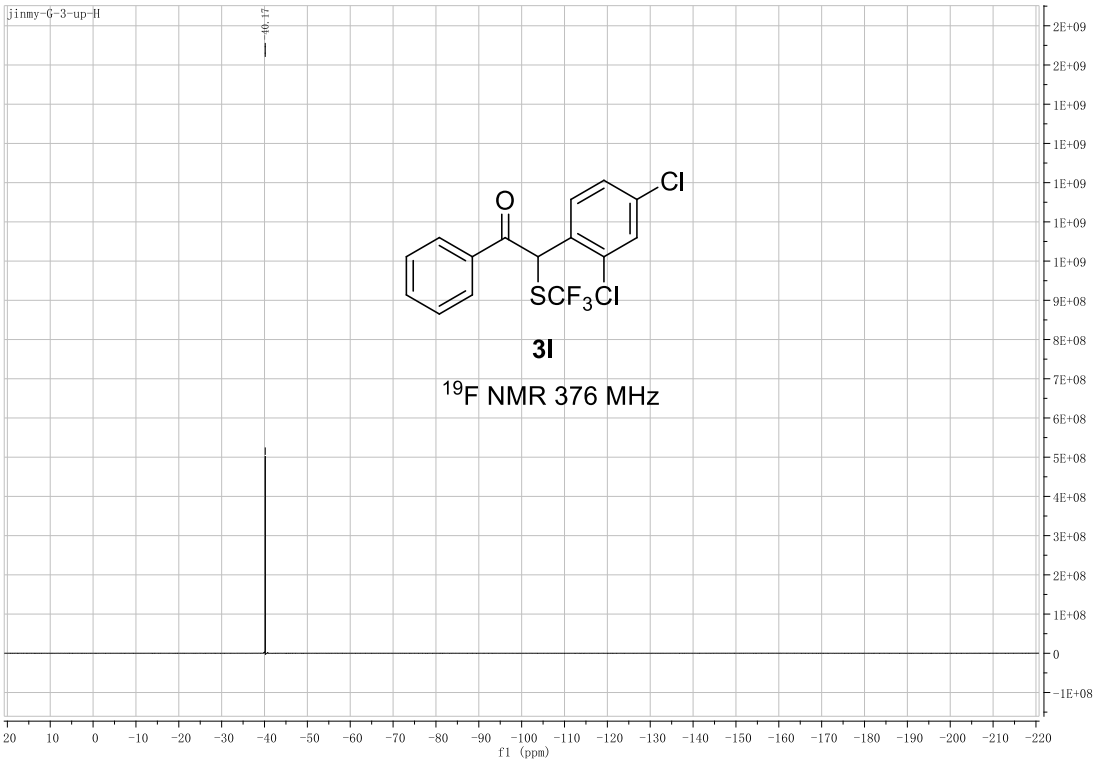

jinmy-IX-88-up-H
Br
O
SCF3Br
3k
1H NMR 600 MHz
f1 (ppm)

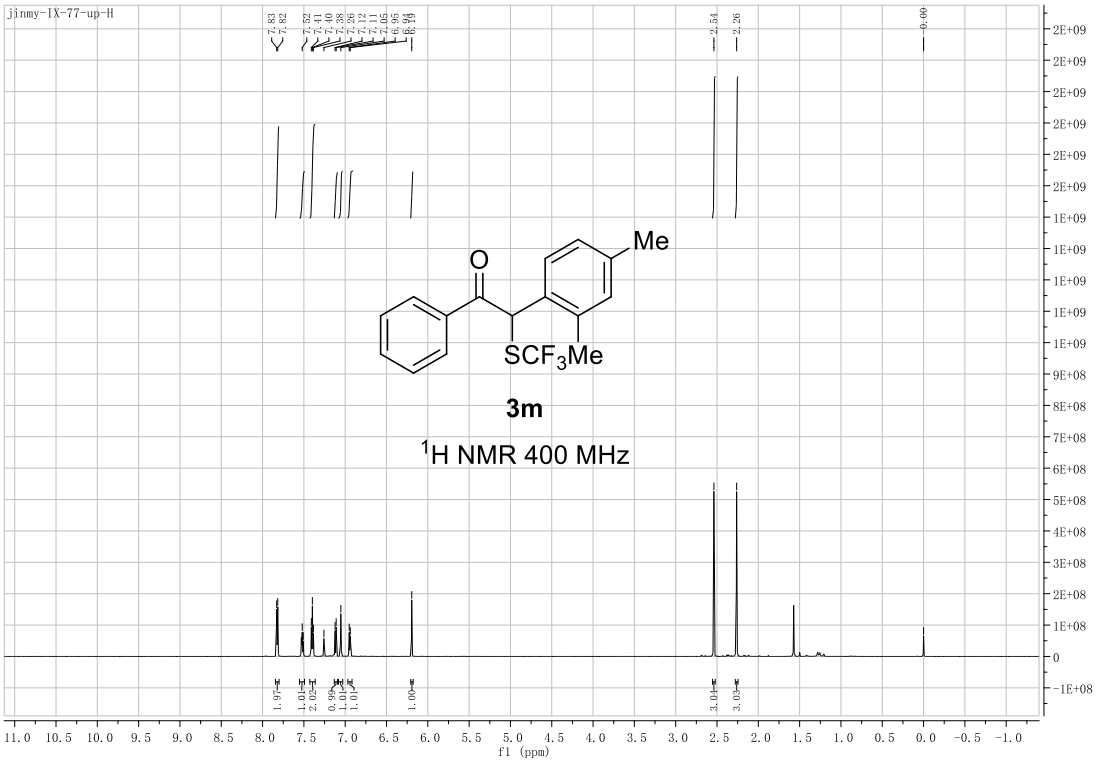

jinmy-IX-88-up-C1
Br
O
SCF3Br
3k
13C NMR 150 MHz
f1 (ppm)

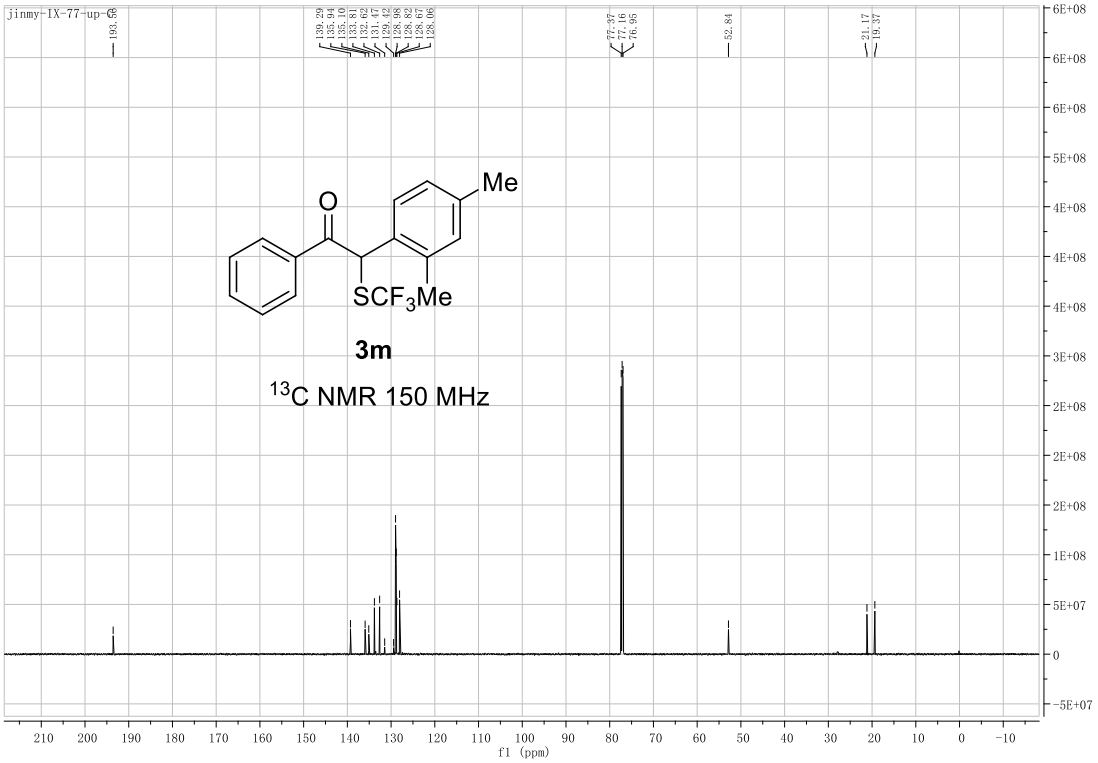

jinmy-IX-88-up-F
-40.03
Br
O
SCF3Br
3k
19F NMR 376 MHz
f1 (ppm)

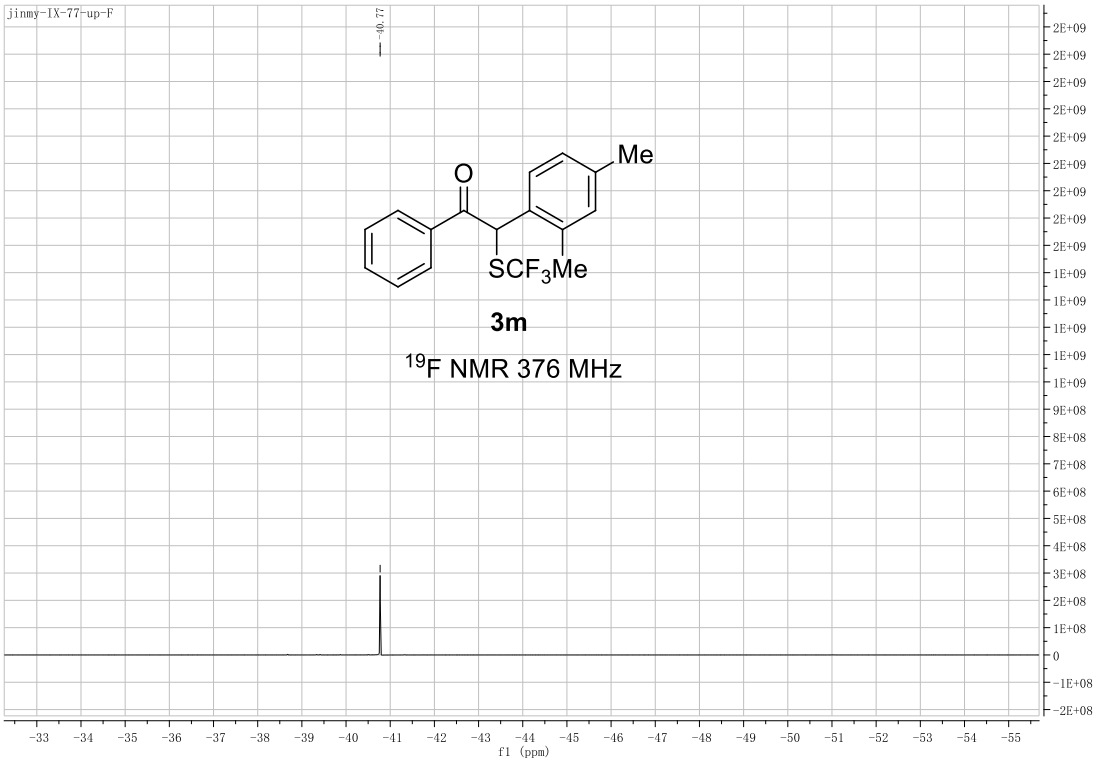

jinmy-G-3-up-H
7.99
7.98
7.97
7.48
7.46
7.45
7.44
7.43
6.68
0.00
Cl
O
SCF3Cl
3l
1H NMR 600 MHz
2.01
1.02
0.98
1.00
f1 (ppm)

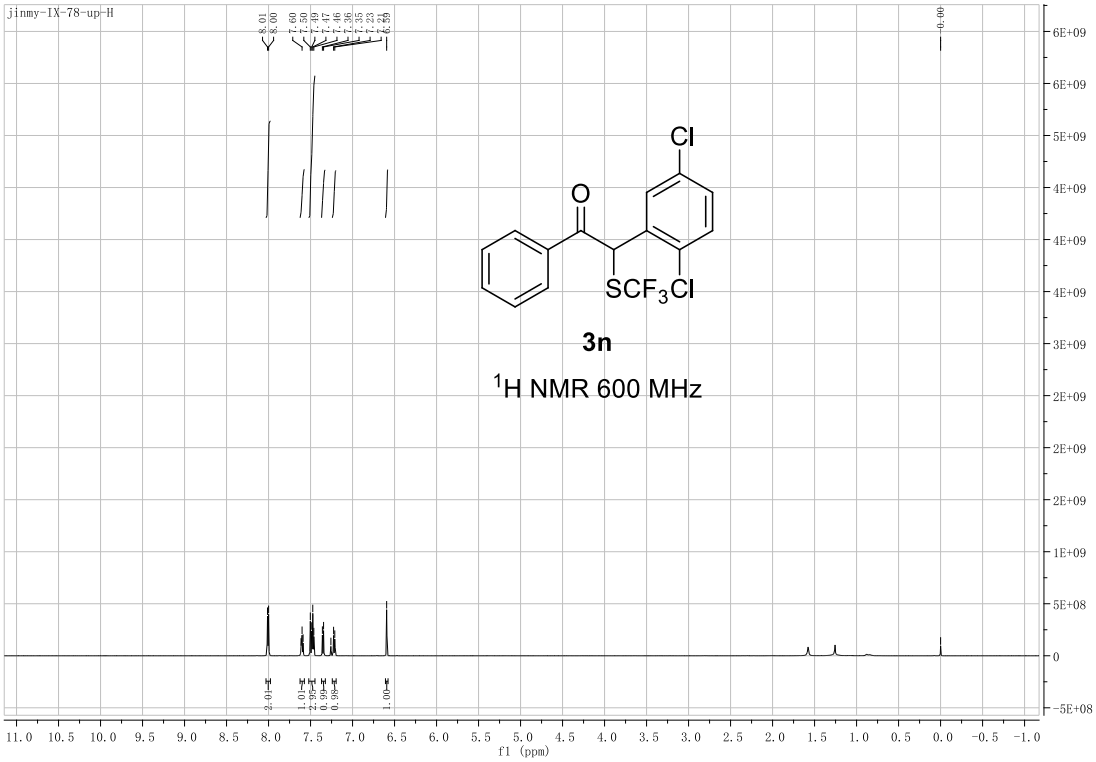

jinmy-G-3-C
192.79
135.78
134.62
133.02
133.08
132.02
131.35
131.19
130.17
129.31
129.21
129.06
128.96
77.37
77.16
76.95
51.40
Cl
O
SCF3Cl
3l
13C NMR 150 MHz
f1 (ppm)

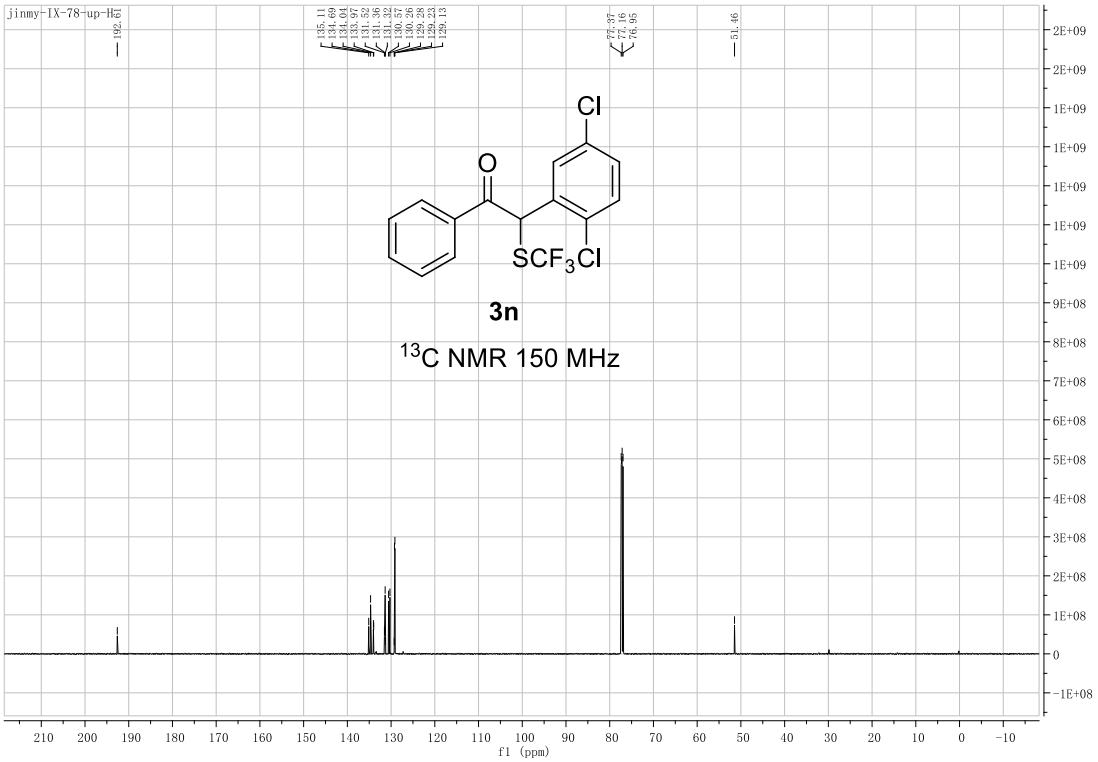

jinmy-G-3-up-H
-40.17
Cl
O
SCF3Cl
3l
19F NMR 376 MHz
f1 (ppm)

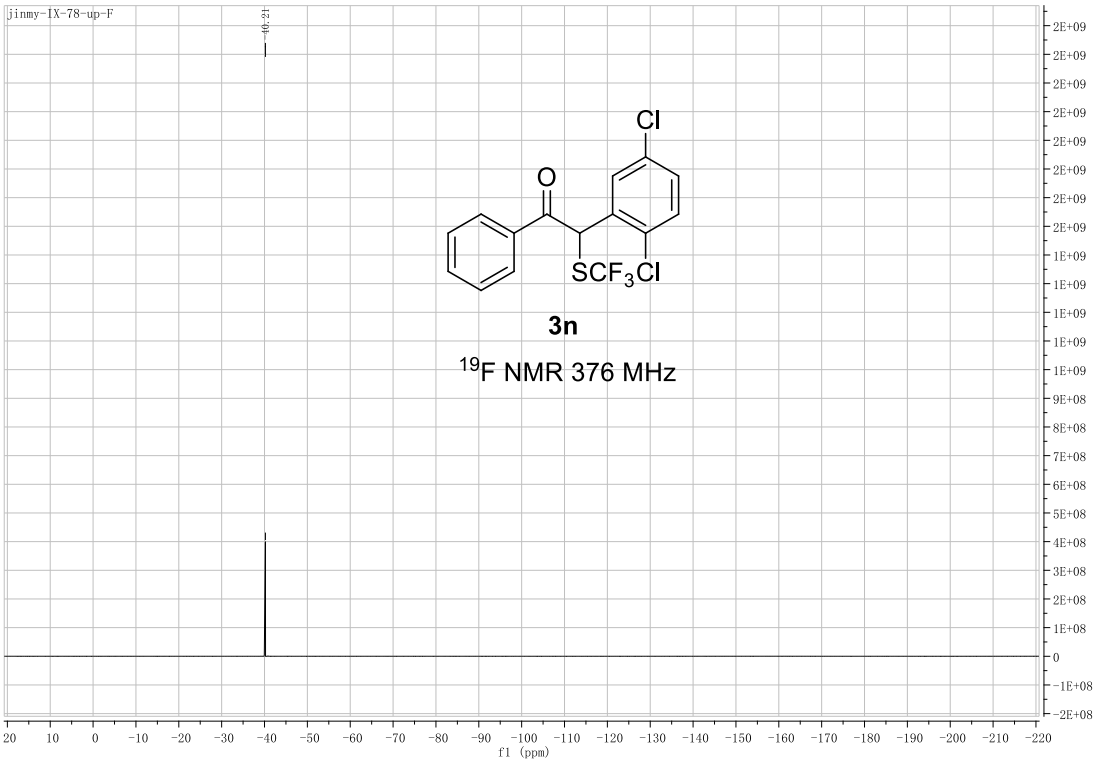

jinmy-IX-77-up-H
Me
O
SCF3Me
3m
1H NMR 400 MHz
f1 (ppm)

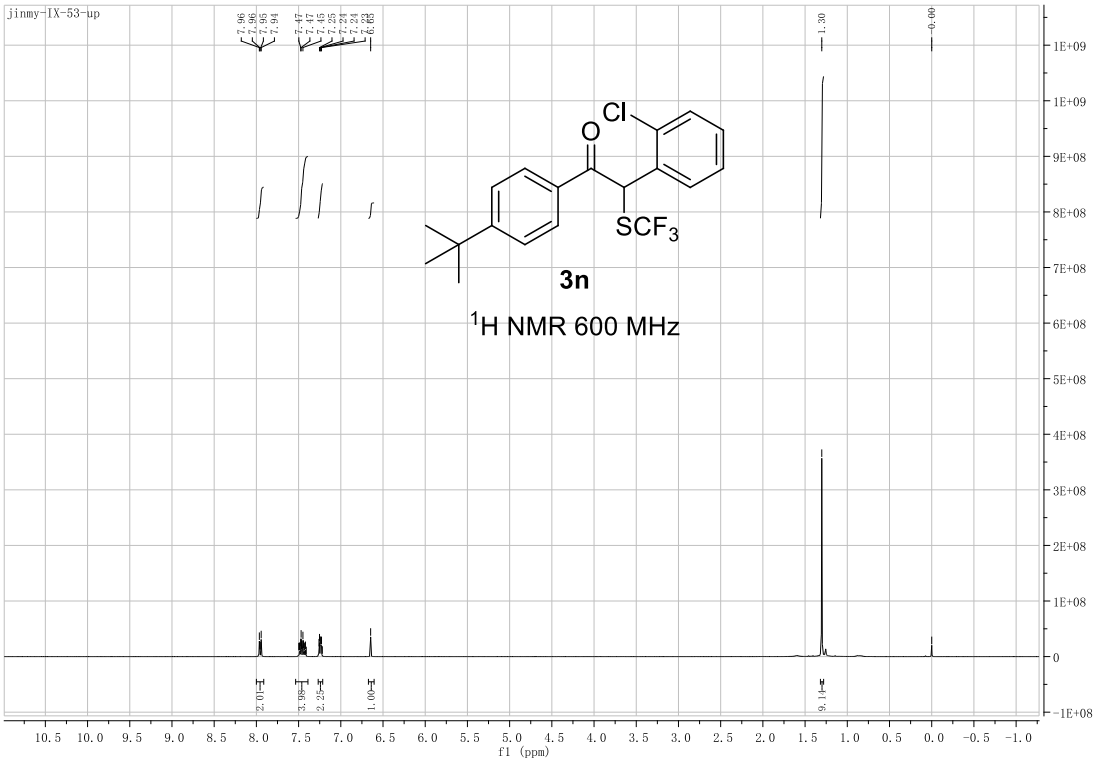

jinmy-IX-77-up-C
Me
O
SCF3Me
3m
13C NMR 150 MHz
f1 (ppm)

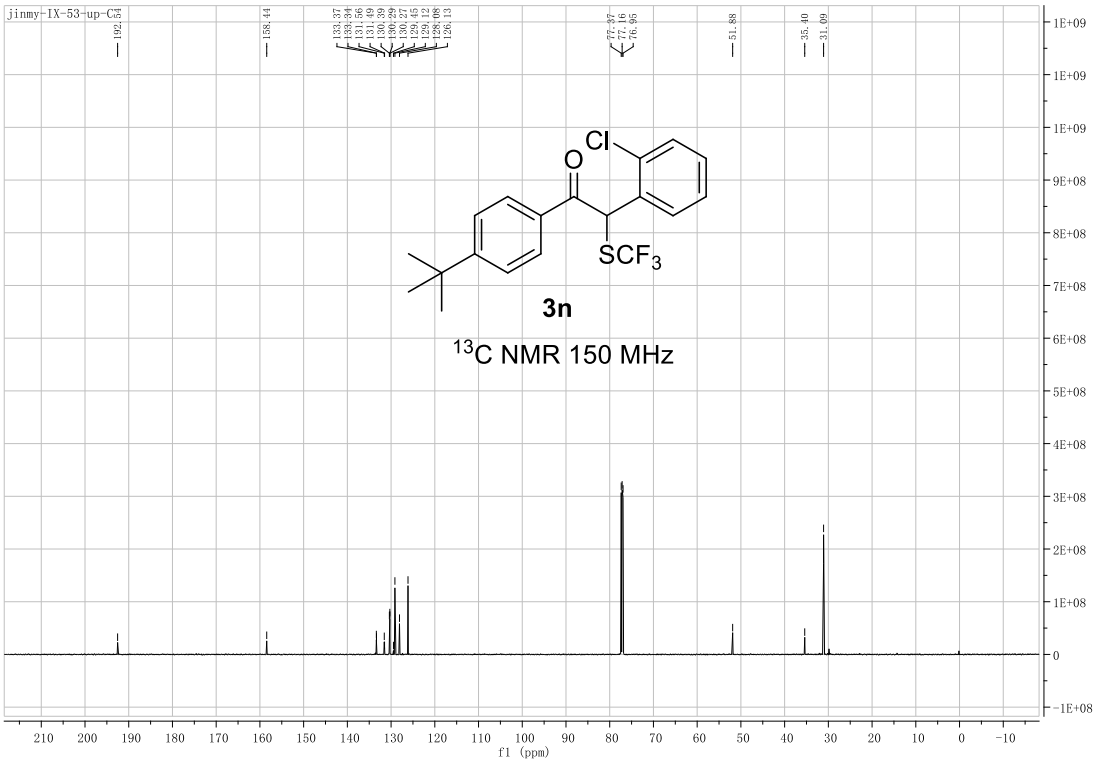

jinmy-IX-77-up-F
-40.77
O
Me
SCF3Me
3m
19F NMR 376 MHz
f1 (ppm)

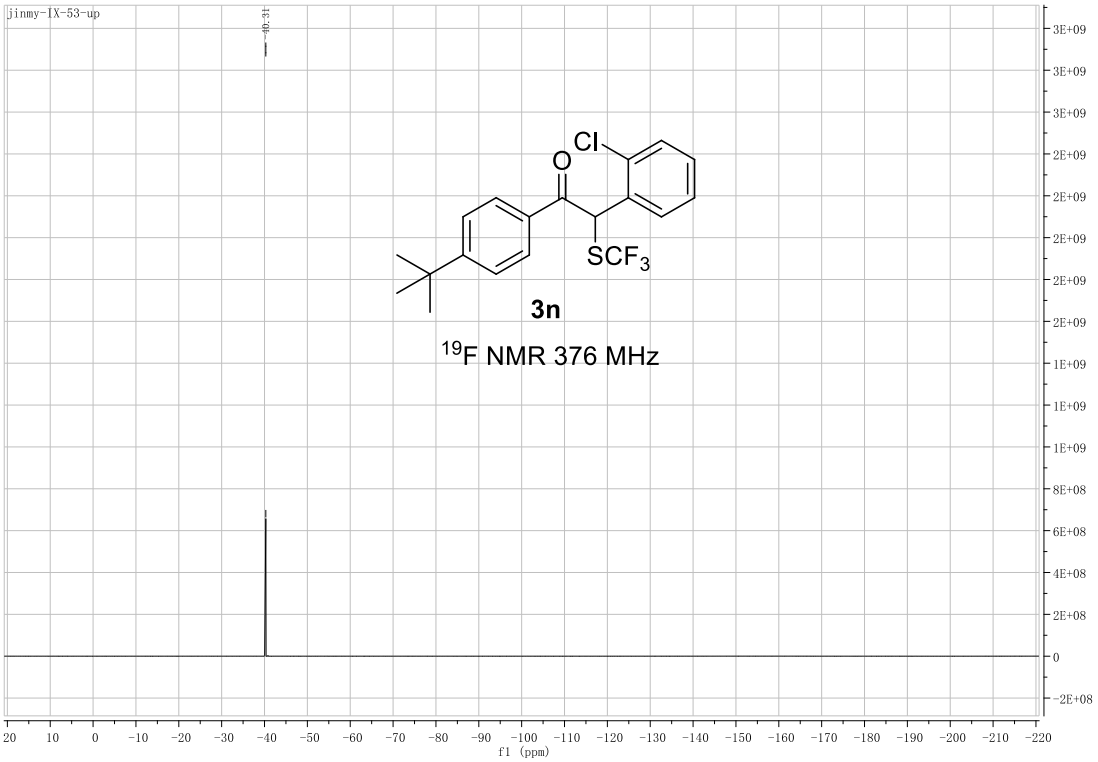

jinmy-IX-78-up-H
8.01
8.00
7.60
7.50
7.49
7.47
7.46
7.36
7.35
7.23
7.22
6.59
0.00
Cl
O
SCF3Cl
3n
1H NMR 600 MHz
2.01
1.01
1.28
0.99
0.98
1.00
f1 (ppm)

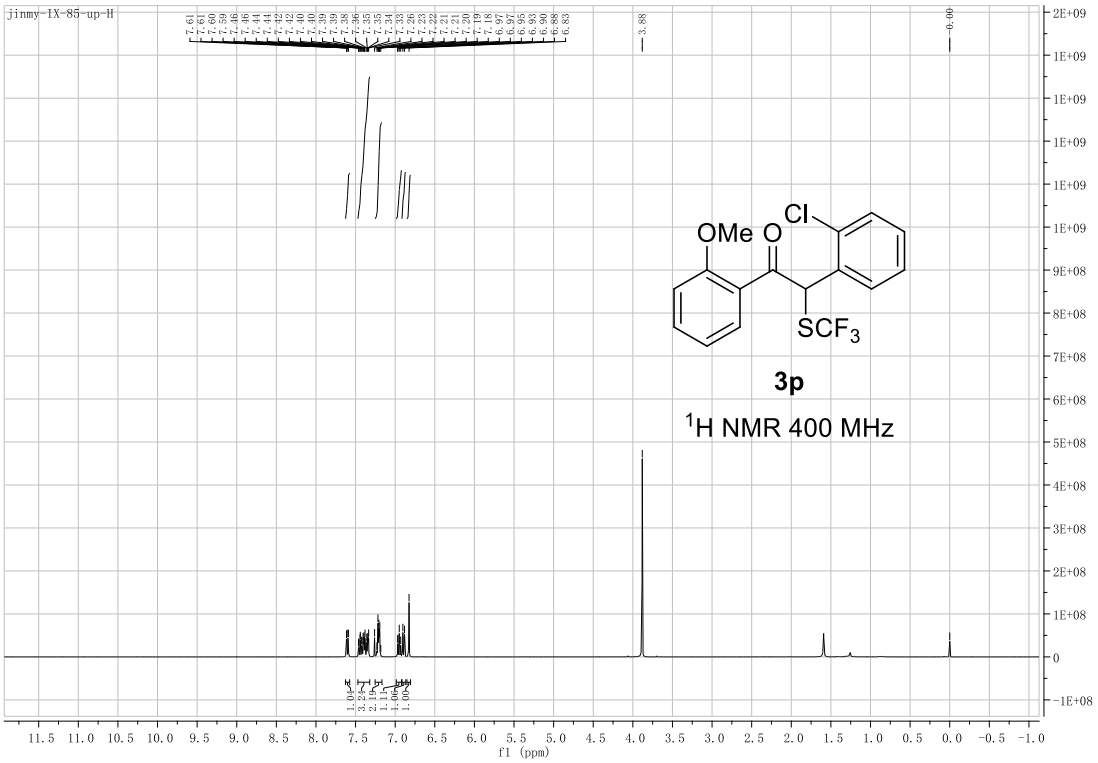

jinmy-IX-78-up-Hc
192.61
135.11
134.69
133.04
132.57
131.52
131.36
131.32
130.57
130.36
129.28
129.23
129.13
77.37
77.16
76.95
51.46
Cl
O
SCF3Cl
3n
13C NMR 150 MHz
f1 (ppm)

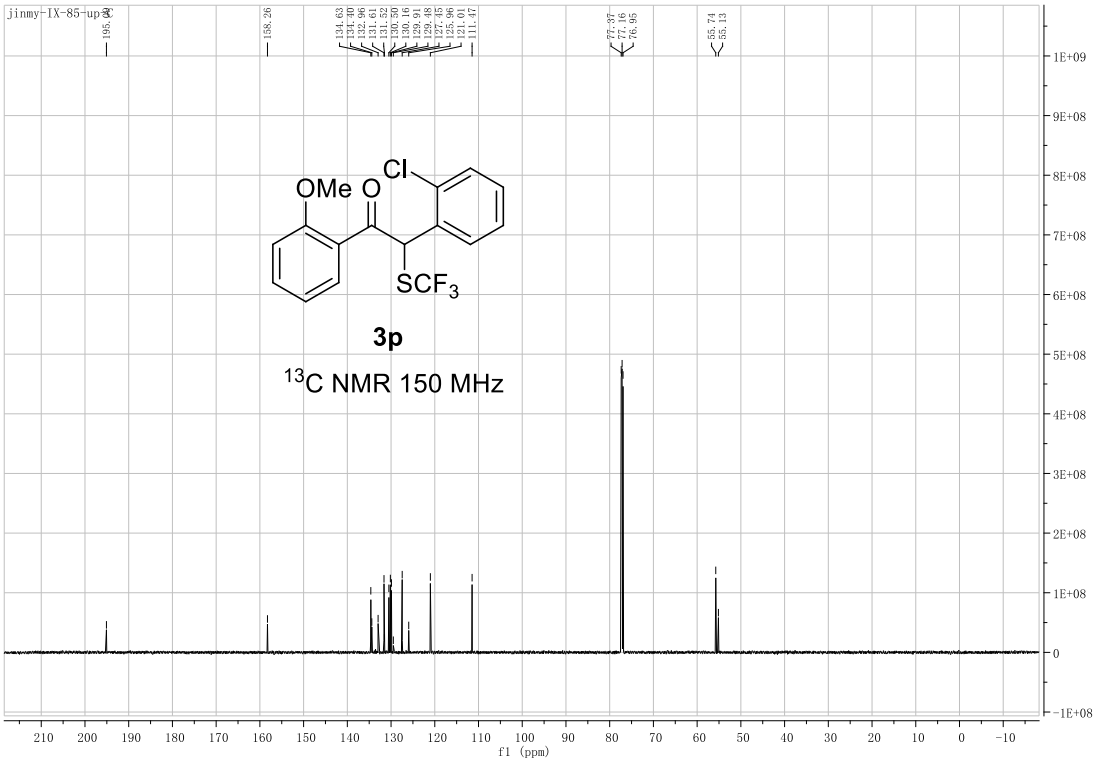

jinmy-IX-78-up-F
-40.21
Cl
O
SCF3Cl
3n
19F NMR 376 MHz
f1 (ppm)

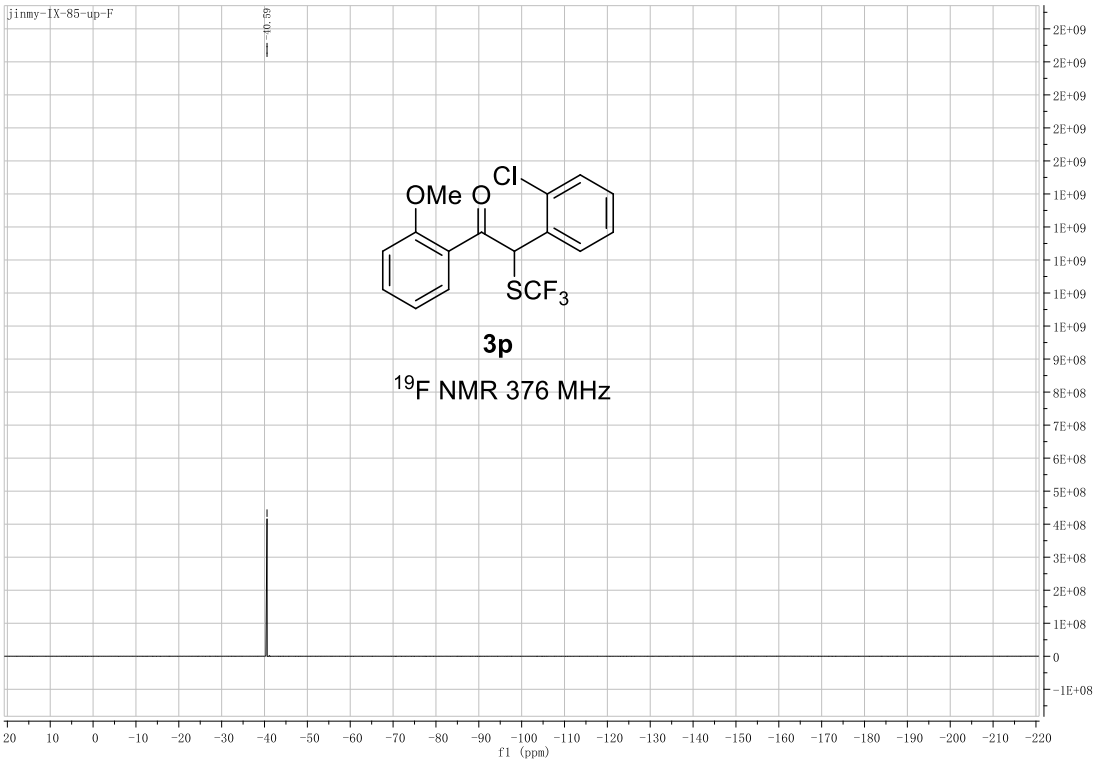

jinmy-IX-53-up
Cl
O
SCF3
3n
1H NMR 600 MHz
f1 (ppm)

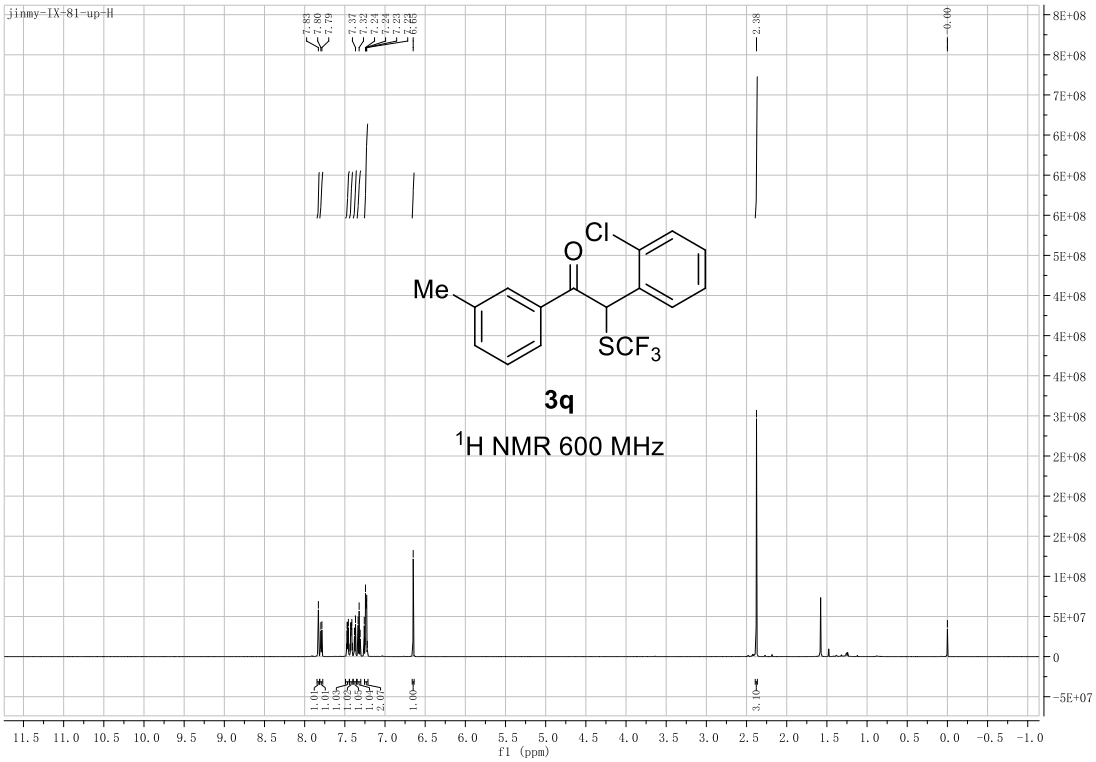

jinmy-IX-53-up-C13
Cl
O
SCF3
3n
13C NMR 150 MHz
f1 (ppm)

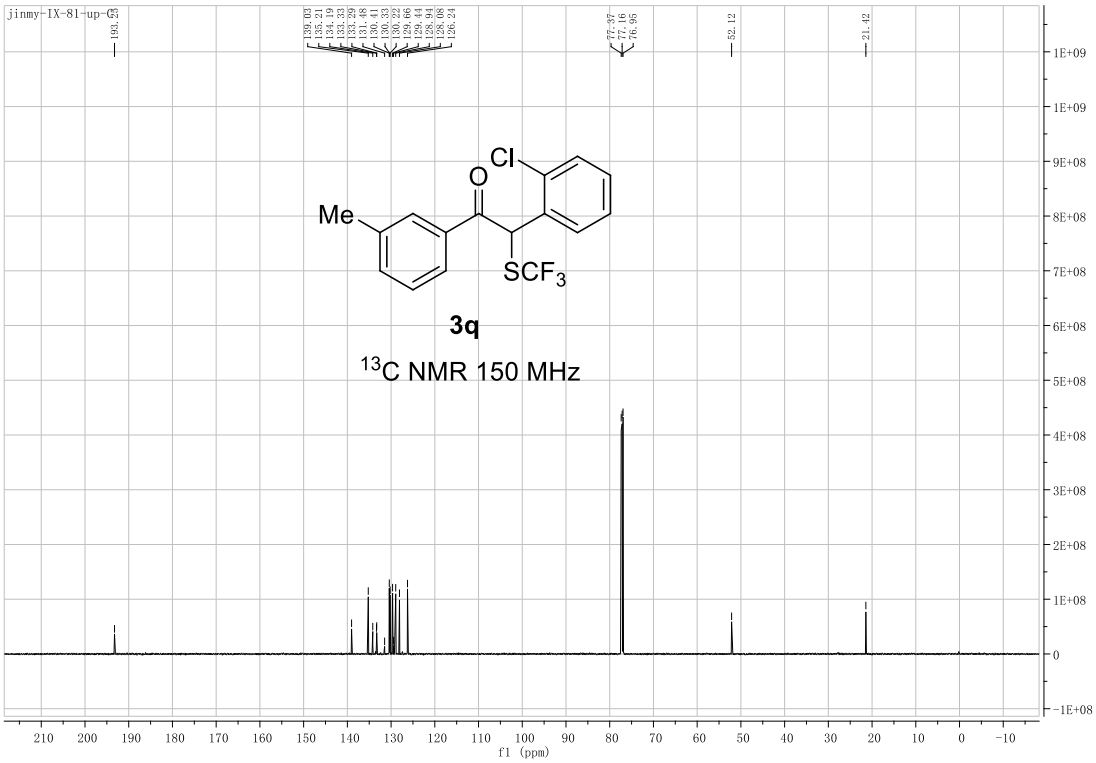

jinmy-IX-53-up
-40.31
Cl
O
SCF3
3n
19F NMR 376 MHz
f1 (ppm)

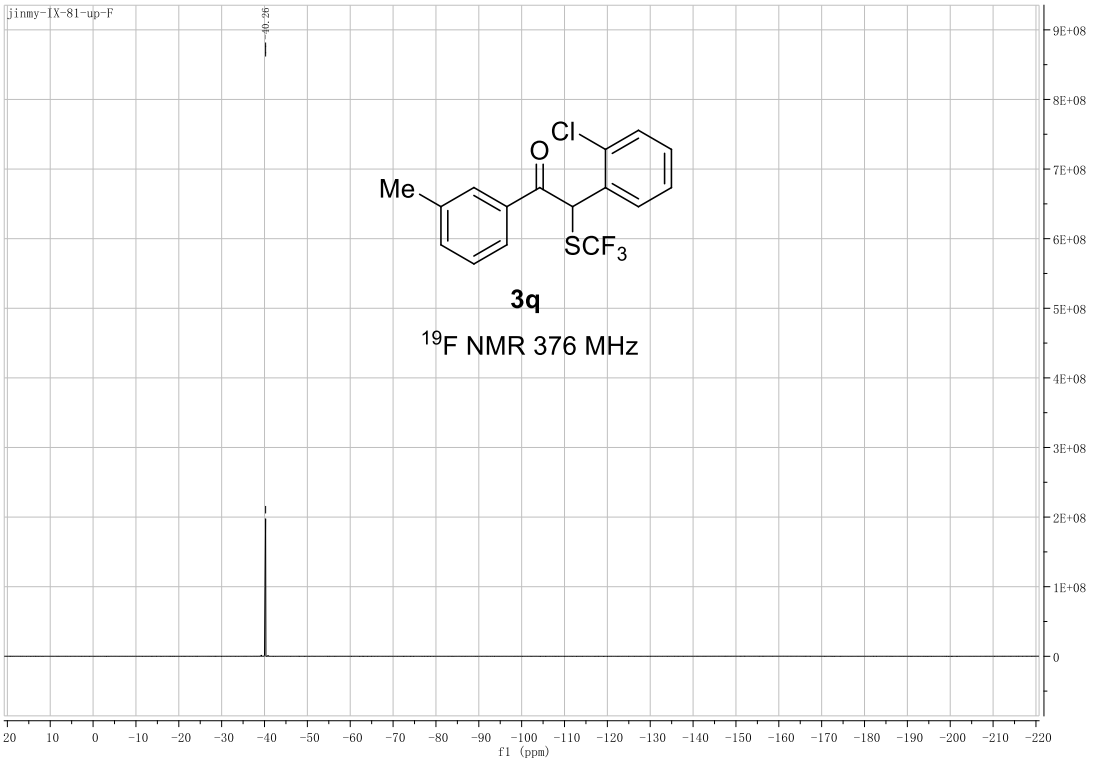

jinmy-IX-85-up-H
3.88
0.00
OMe
O
Cl
SCF3
3p
1H NMR 400 MHz
f1 (ppm)

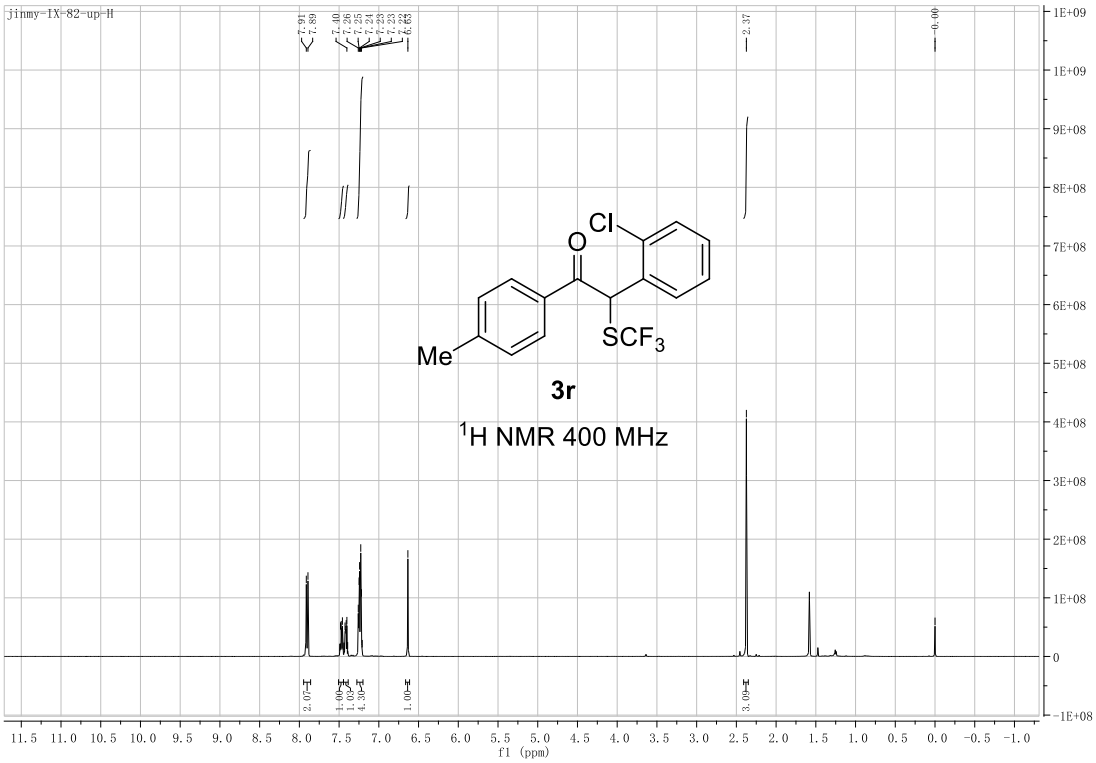

jinmy-IX-85-up-C
195.04
158.26
134.63
134.30
132.96
131.61
131.32
130.59
130.16
129.91
129.48
127.45
125.96
121.01
111.47
77.37
77.16
76.95
55.74
55.13
OMe O
Cl
SCF3
3p
13C NMR 150 MHz
f1 (ppm)

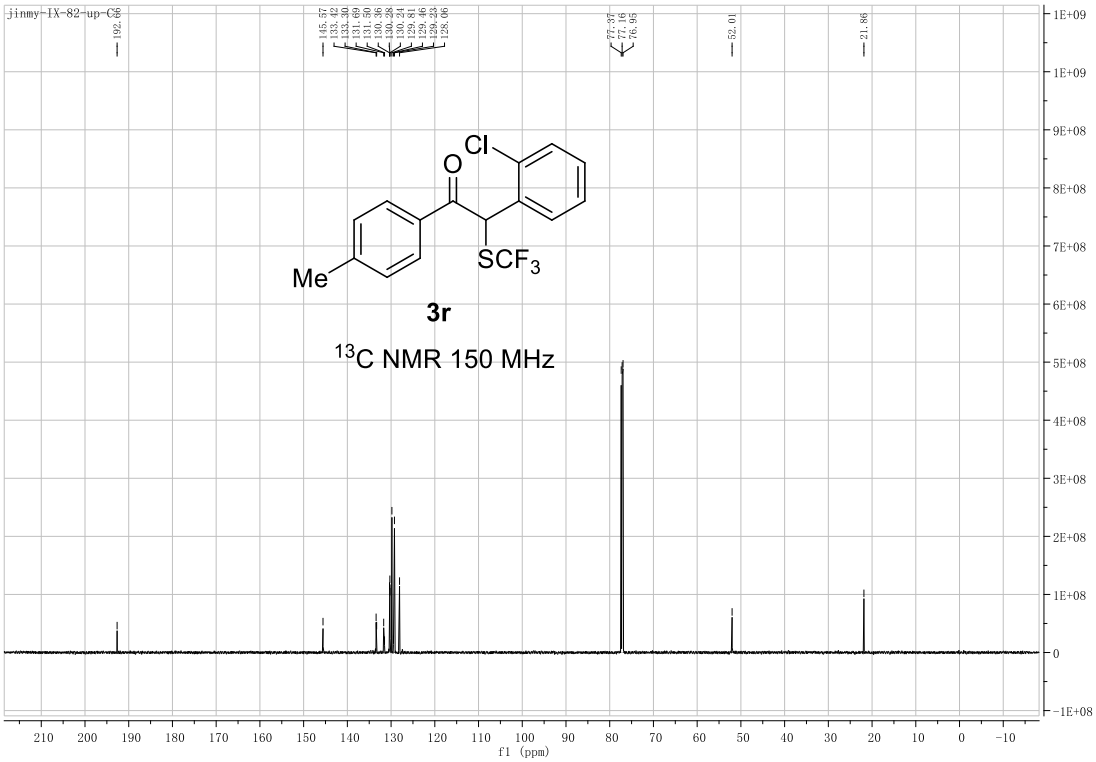

jinmy-IX-85-up-F
-40.59
OMe O
Cl
SCF3
3p
19F NMR 376 MHz
f1 (ppm)

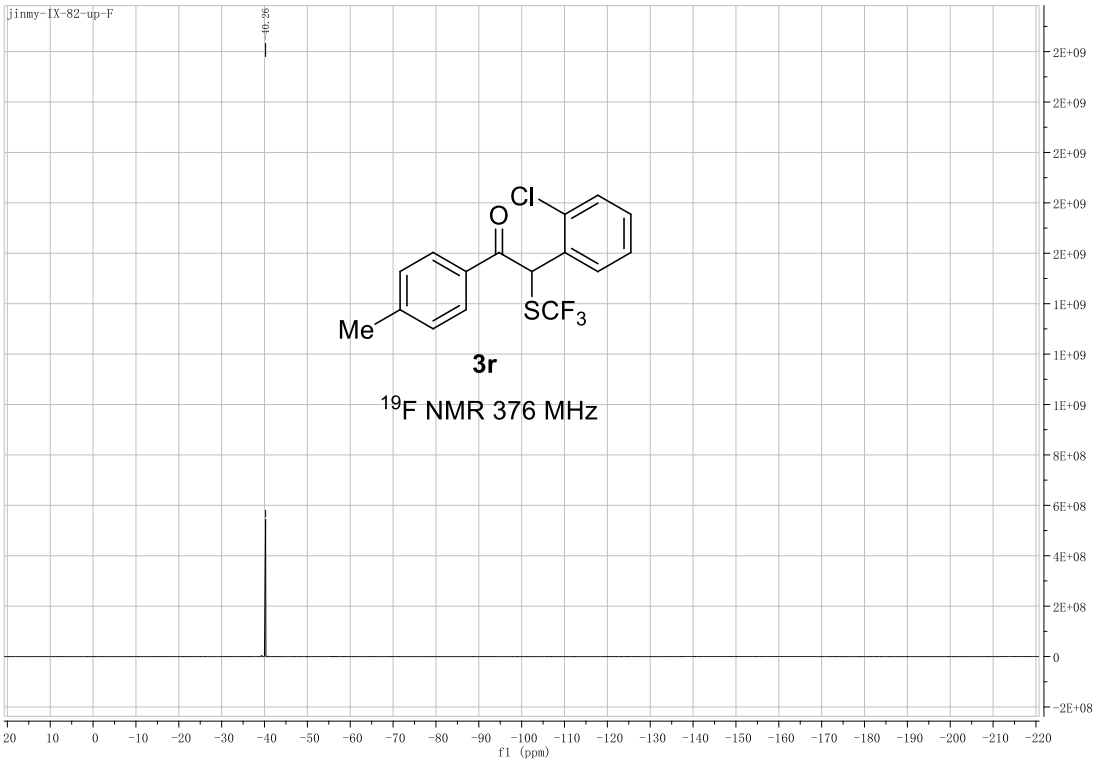

jinmy-IX-81-up-H
Cl
O
Me
SCF3
3q
1H NMR 600 MHz
f1 (ppm)

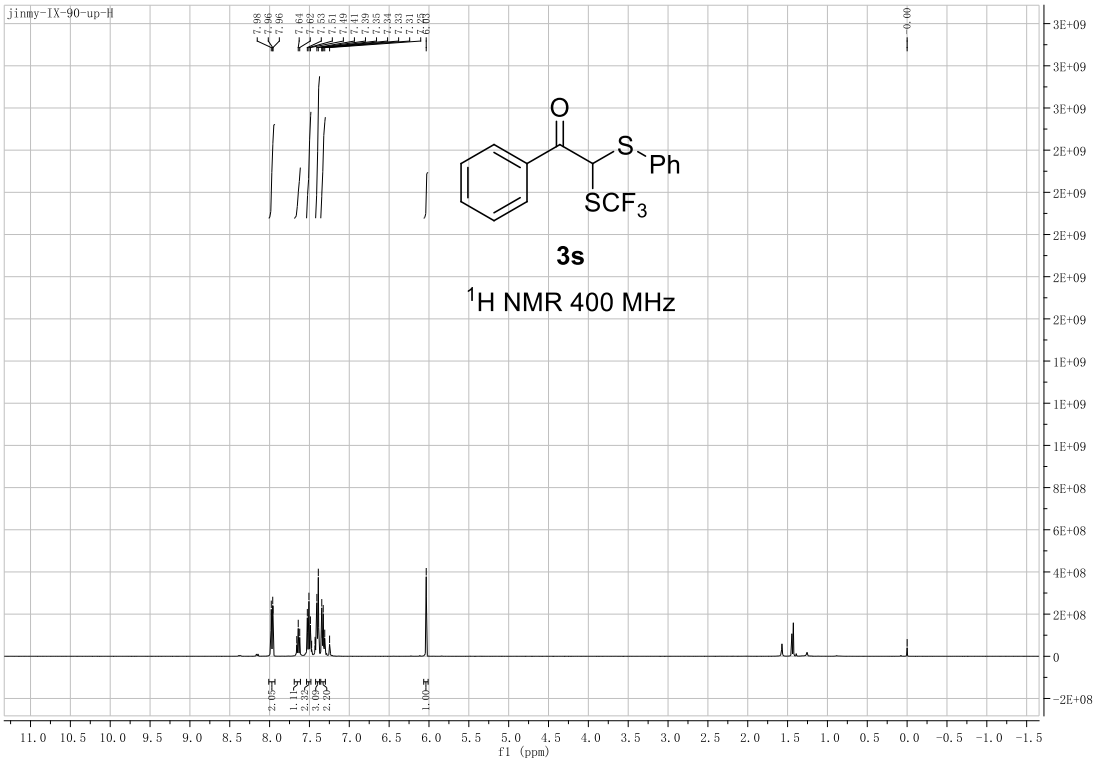

jinmy-IX-81-up-C
Cl
O
Me
SCF3
3q
13C NMR 150 MHz
f1 (ppm)

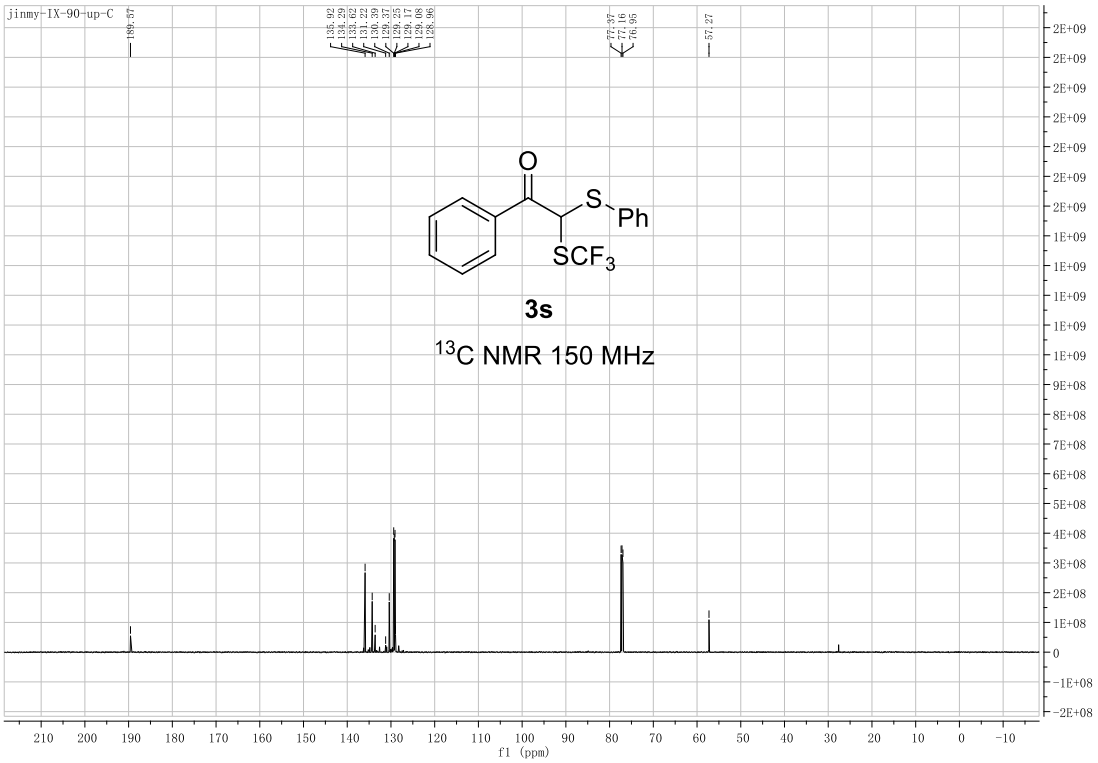

jinmy-IX-81-up-F
-40.296
Cl
O
Me
SCF3
3q
19F NMR 376 MHz
f1 (ppm)

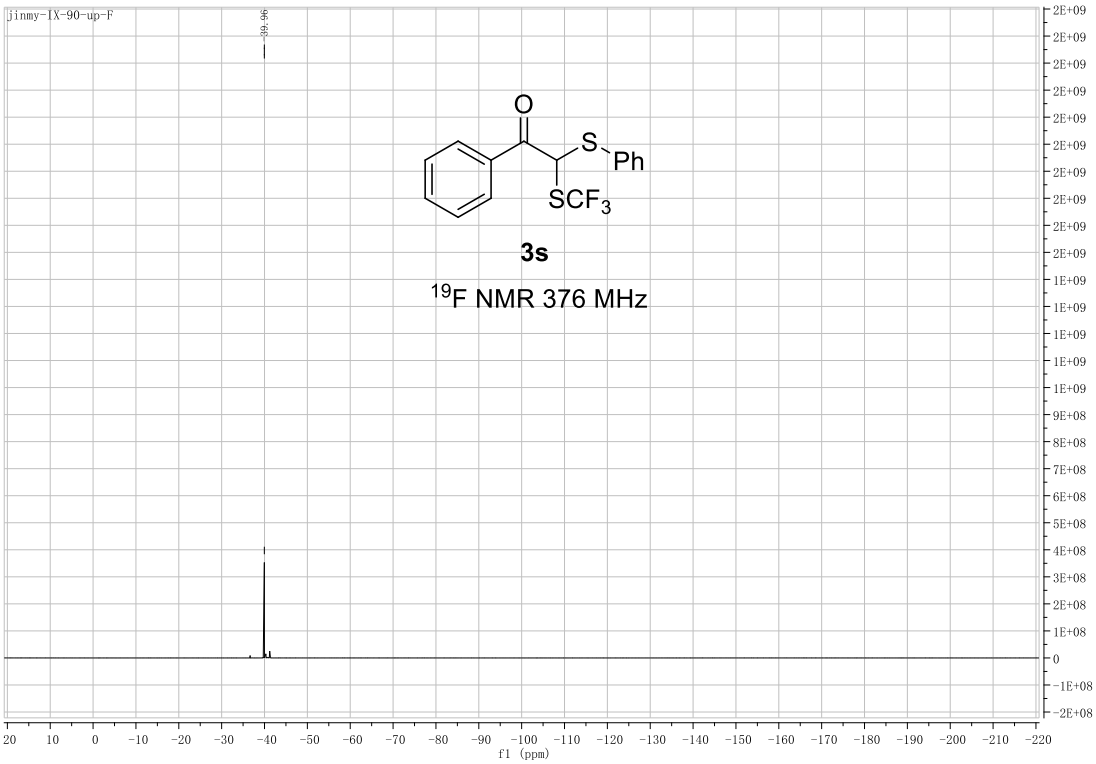

jinmy-IX-82-up-H
7.91
7.89
7.40
7.26
7.25
7.24
7.23
7.23
7.22
7.20
2.37
-0.00
Cl
O
Me
SCF3
3r
1H NMR 400 MHz
2.07
1.00
1.02
4.30
1.00
3.00
f1 (ppm)

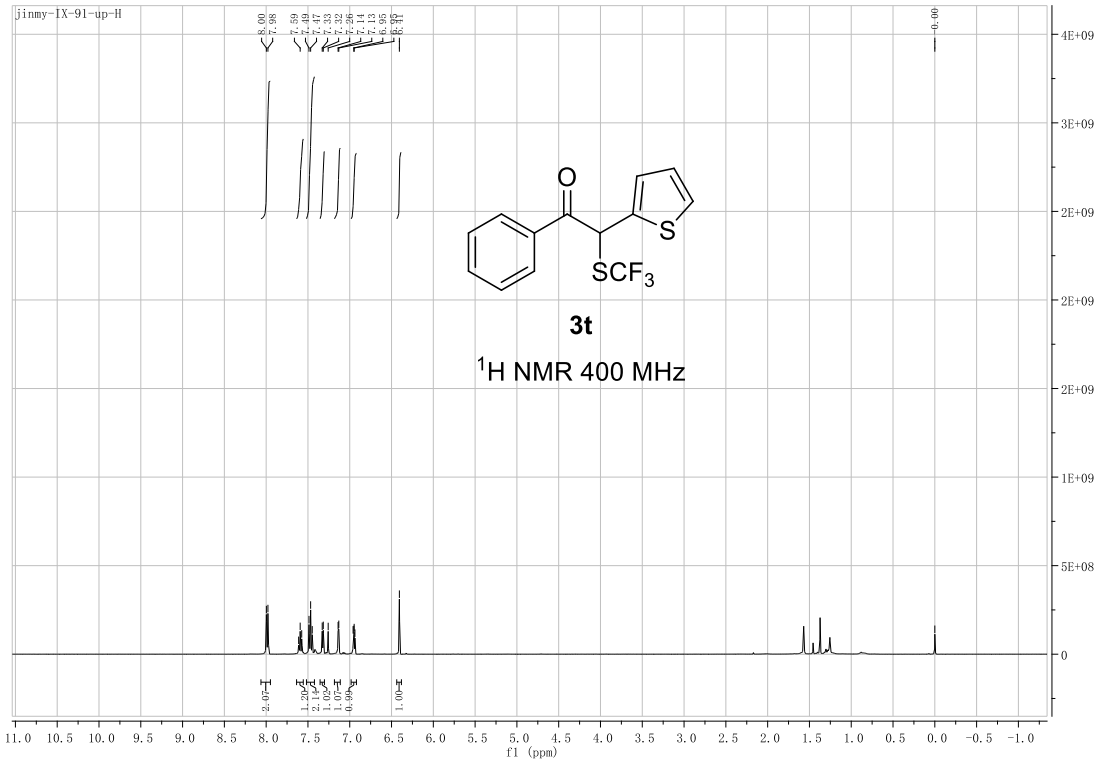

jinmy-IX-82-up-C
192.66
145.57
133.42
133.30
131.69
131.58
130.36
130.28
130.24
129.41
129.46
129.23
128.06
77.37
77.16
76.95
52.01
21.86
Cl
O
SCF3
Me
3r
13C NMR 150 MHz
f1 (ppm)

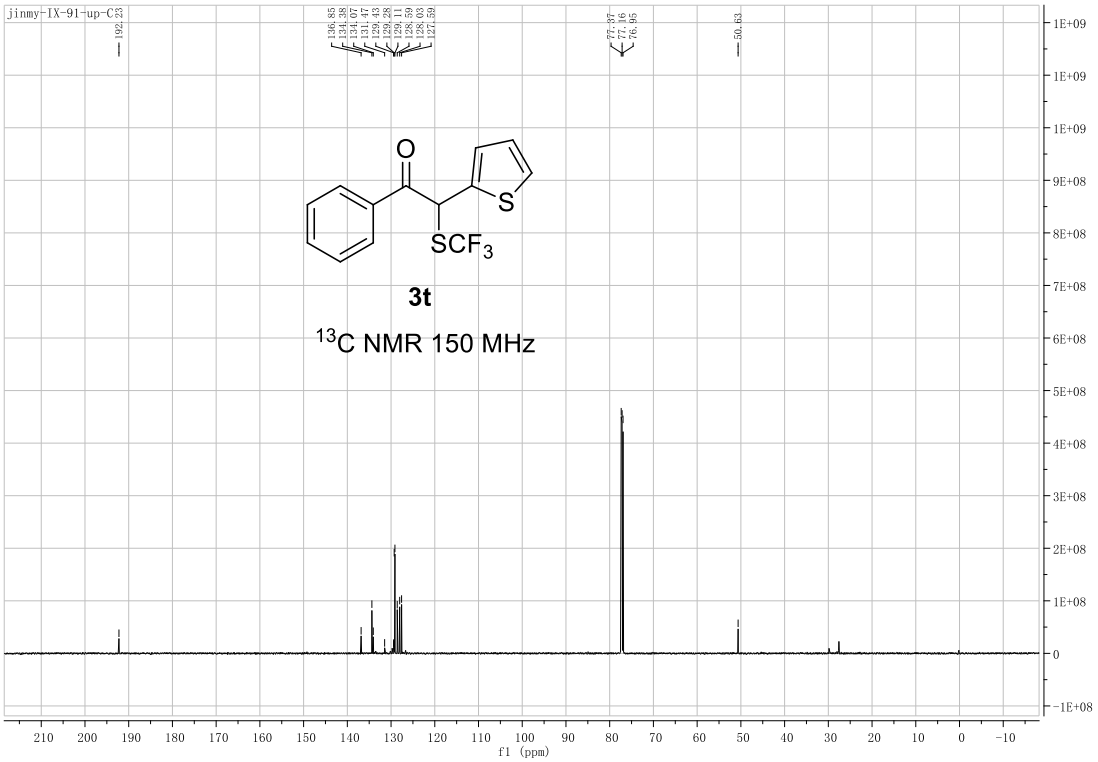

jinmy-IX-82-up-F
-40.26
Cl
O
SCF3
Me
3r
19F NMR 376 MHz
f1 (ppm)

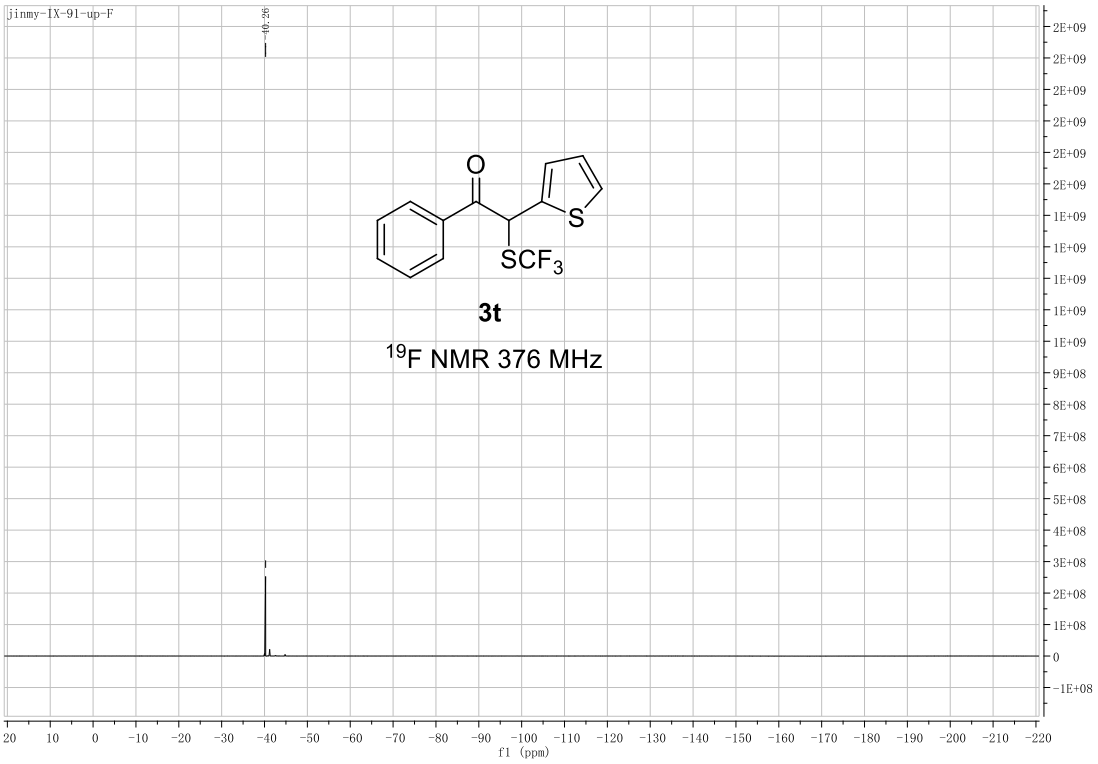

jinmy-IX-90-up-H
O
S
Ph
SCF3
3s
1H NMR 400 MHz
f1 (ppm)

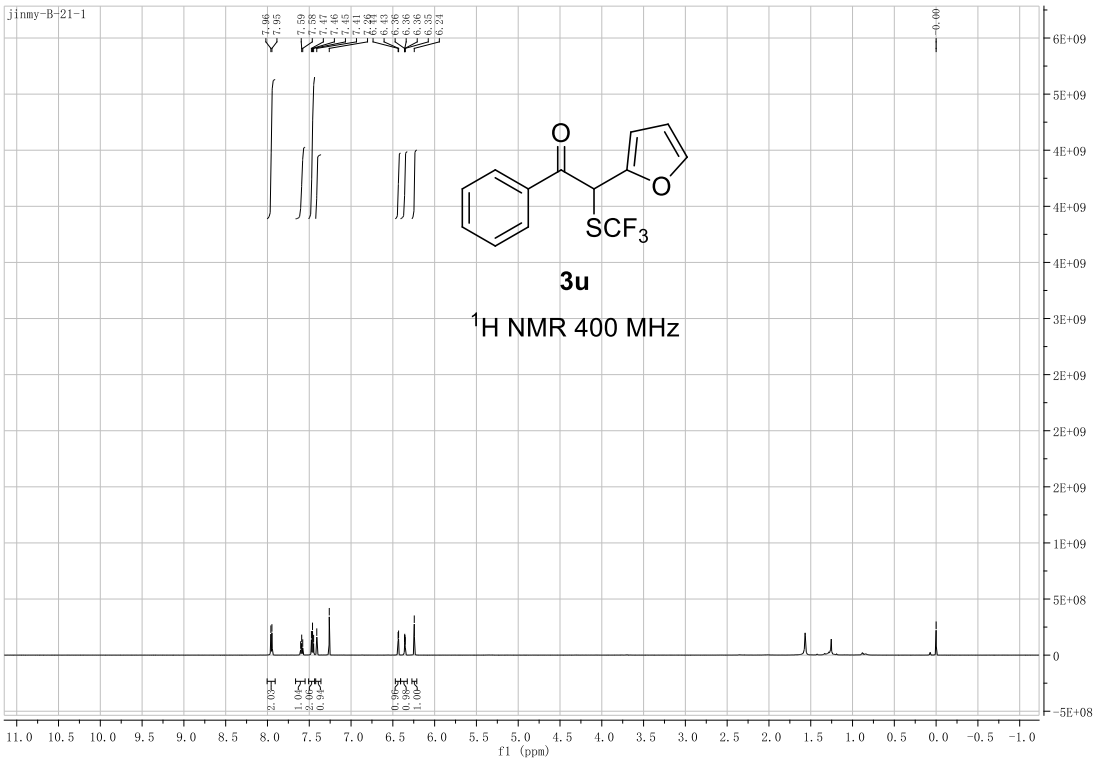

jinmy-IX-90-up-C
O
S
Ph
SCF3
3s
13C NMR 150 MHz
f1 (ppm)

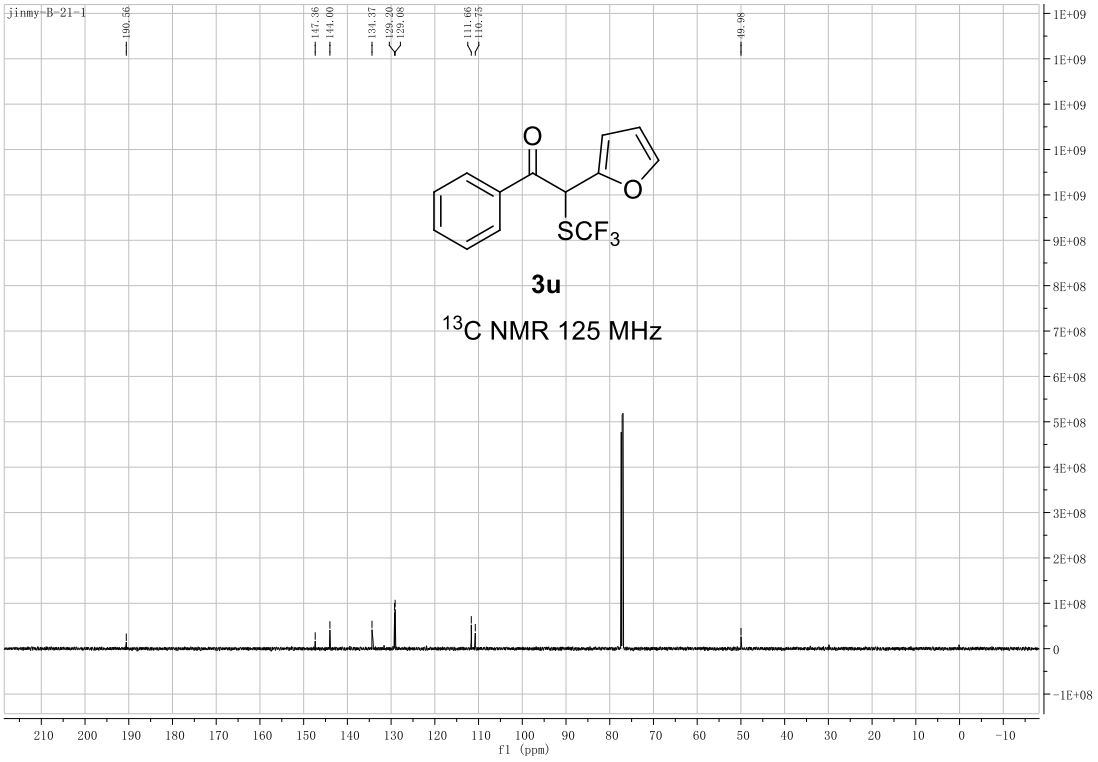

jinmy-IX-90-up-F
-39.96
O
S
Ph
SCF3
3s
19F NMR 376 MHz
f1 (ppm)

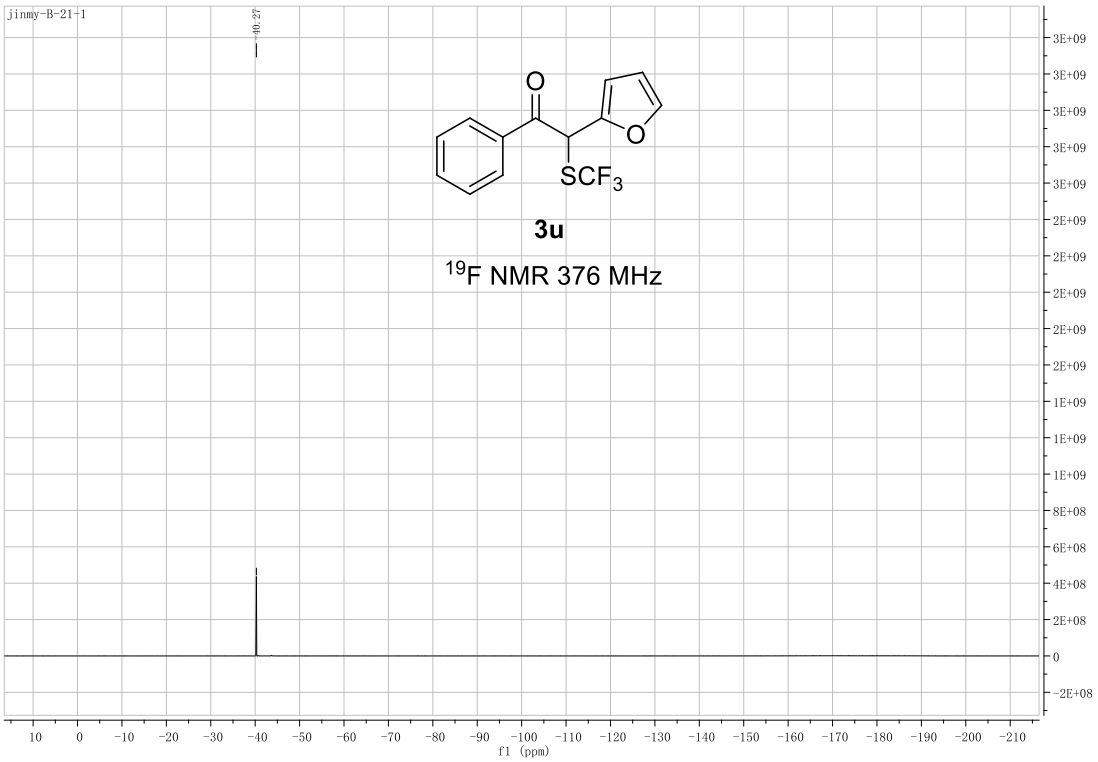

jinmy-IX-91-up-H
8.00
7.98
7.59
7.49
7.47
7.33
7.32
7.18
7.14
7.13
6.95
6.93
0.00
O
S
SCF3
3t
1H NMR 400 MHz
2.07
2.20
2.14
1.02
1.07
0.88
1.00
f1 (ppm)

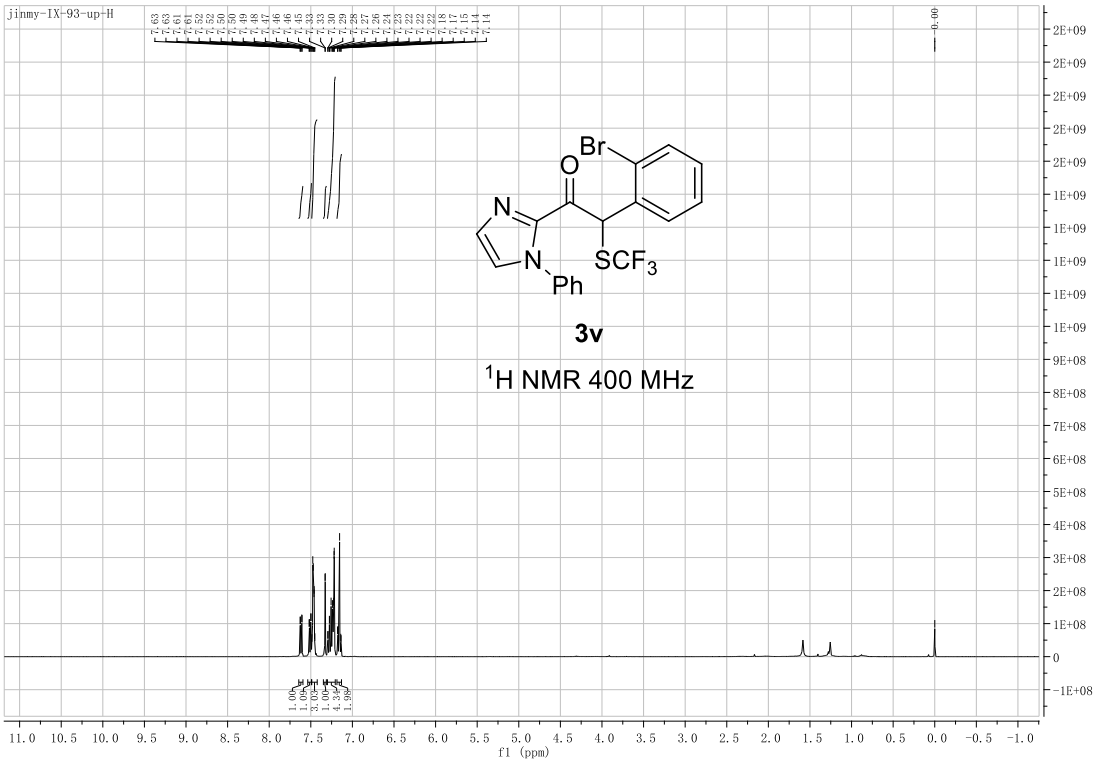

jinmy-IX-91-up-C.23
192.23
136.85
134.38
134.07
131.47
129.43
129.28
128.11
128.08
128.03
127.59
77.37
77.16
76.95
50.63
O
S
SCF3
3t
13C NMR 150 MHz
f1 (ppm)

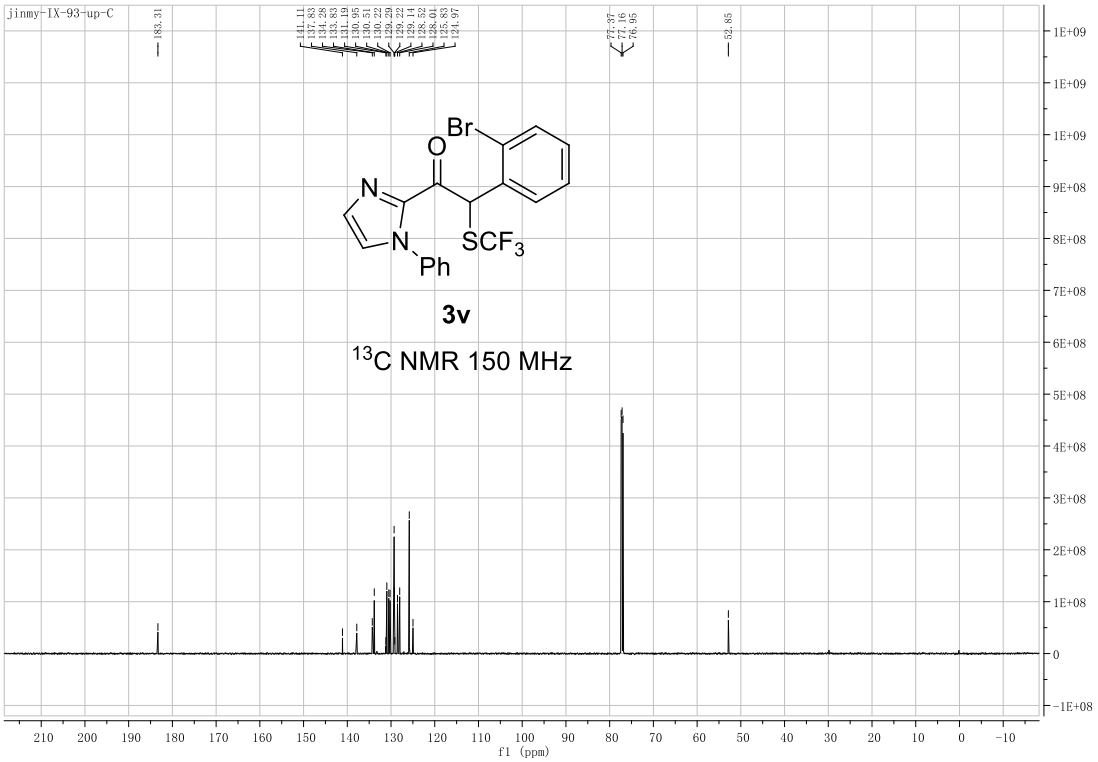

jinmy-IX-91-up-F
-40.26
O
S
SCF3
3t
19F NMR 376 MHz
f1 (ppm)

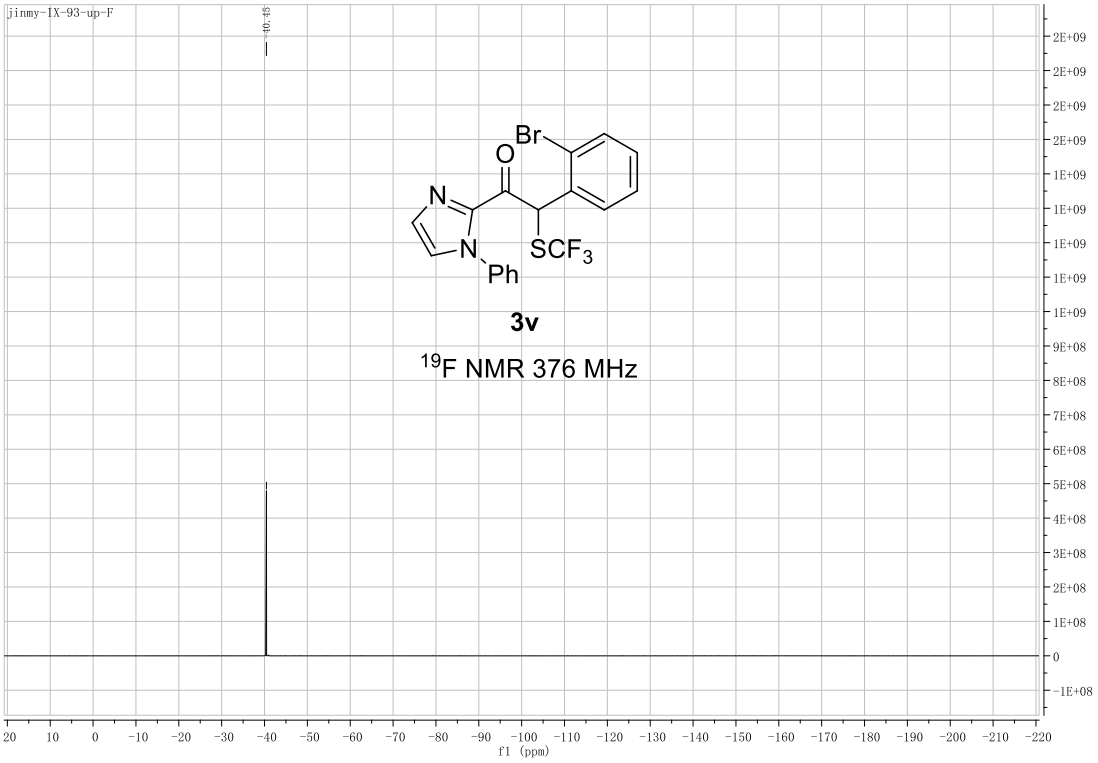

jinmy-B-21-1
O
O
SCF3
3u
1H NMR 400 MHz
f1 (ppm)

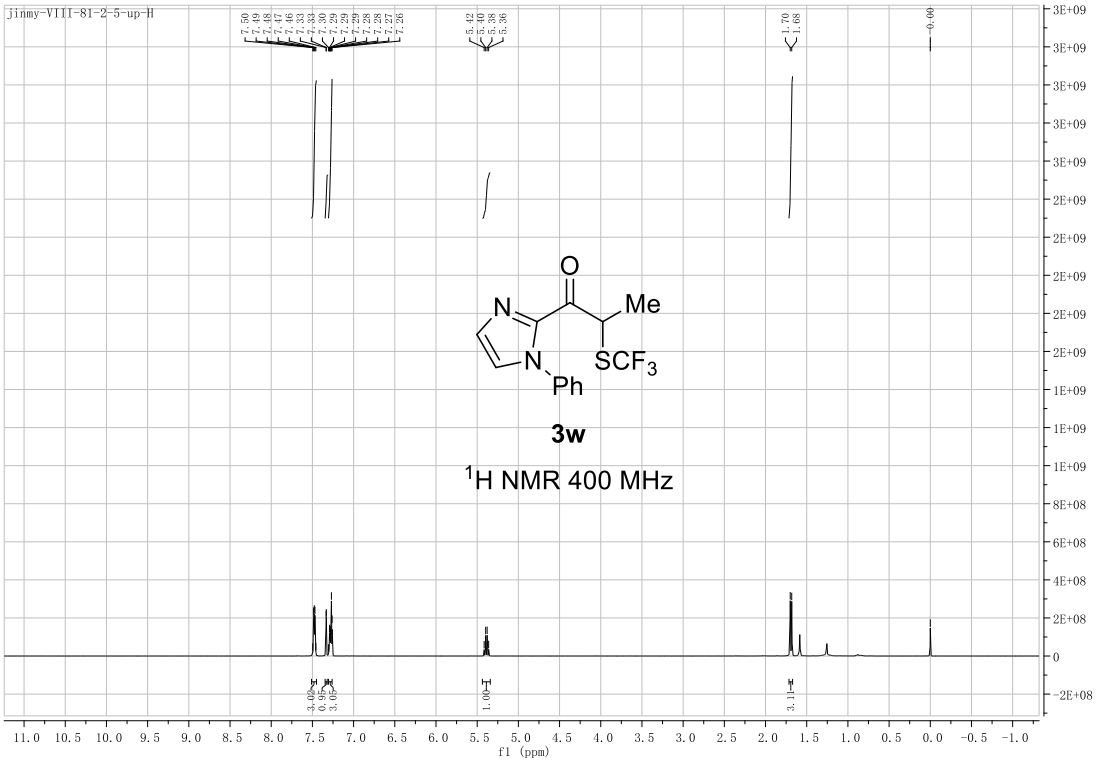

jinmy-B-21-1
O
O
SCF3
3u
13C NMR 125 MHz
f1 (ppm)

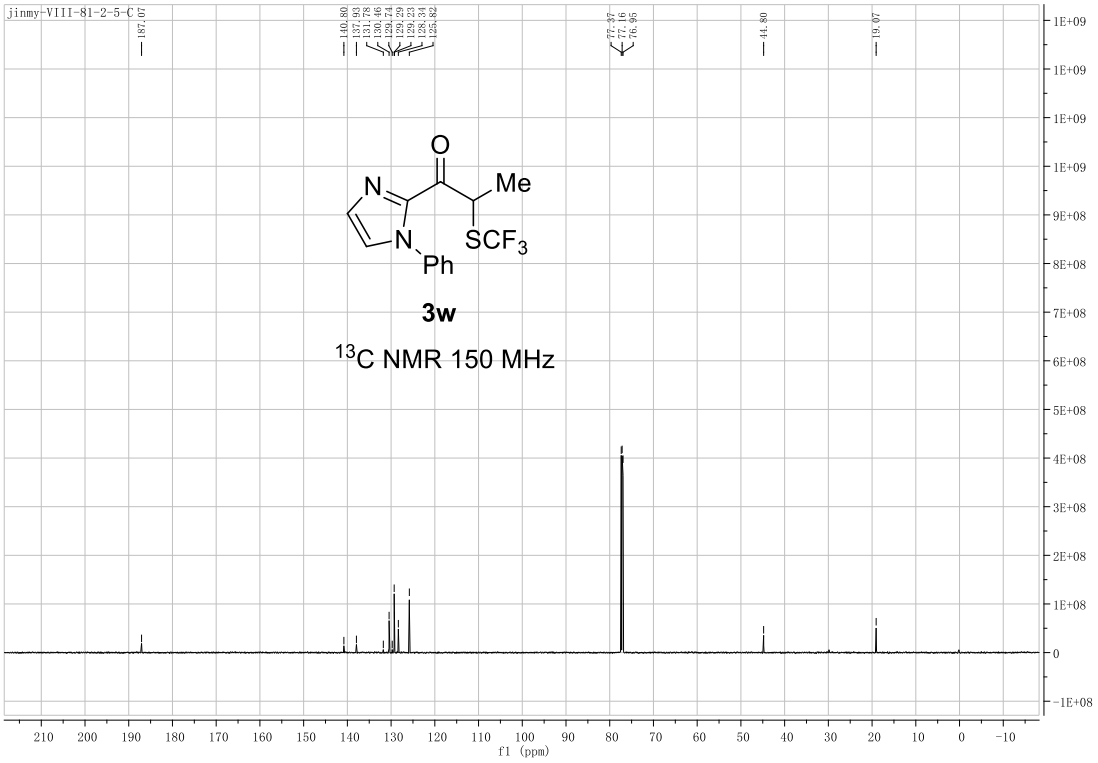

jinmy-B-21+1
-40.27
O
O
SCF3
3u
19F NMR 376 MHz
f1 (ppm)

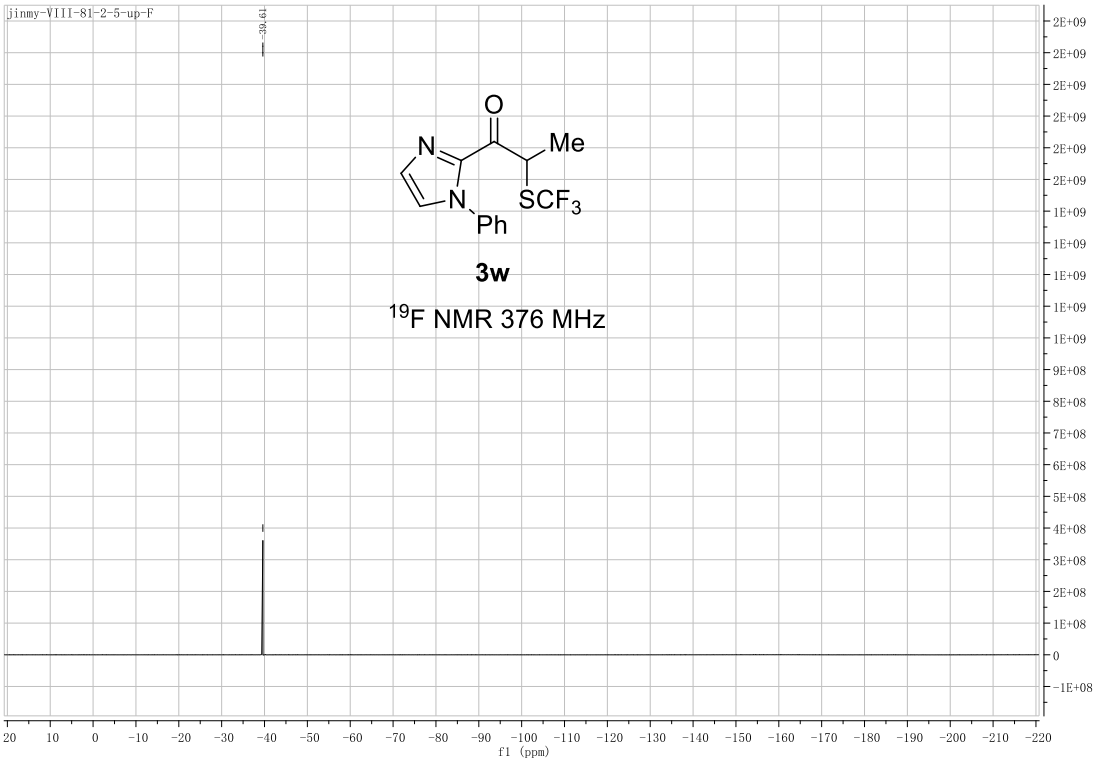

jinmy-IX-93-up+H
-0.00
Br
O
N
N
Ph
SCF3
3v
1H NMR 400 MHz
f1 (ppm)

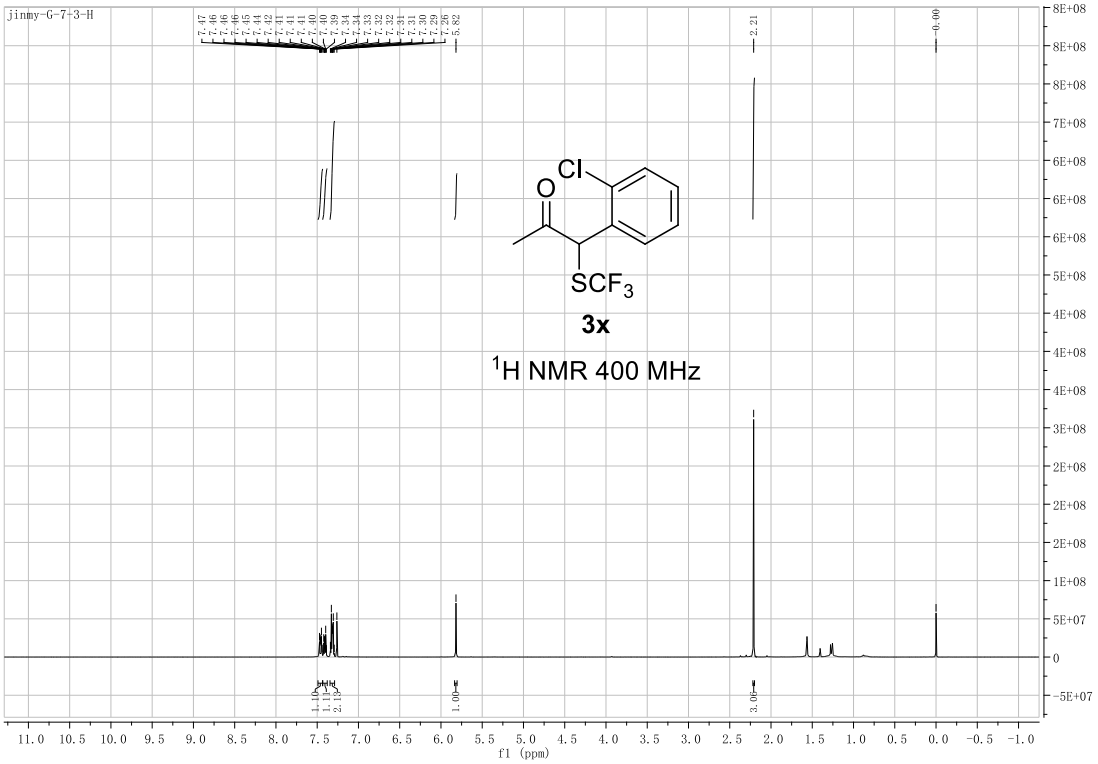

jinmy-IX-93-up-C
183.31
141.11
137.83
134.28
133.83
131.19
130.95
130.53
130.22
129.29
129.22
129.11
128.52
128.01
125.83
121.97
77.37
77.16
76.95
62.85
Br
O
N
N
Ph
SCF3
3v
13C NMR 150 MHz
f1 (ppm)

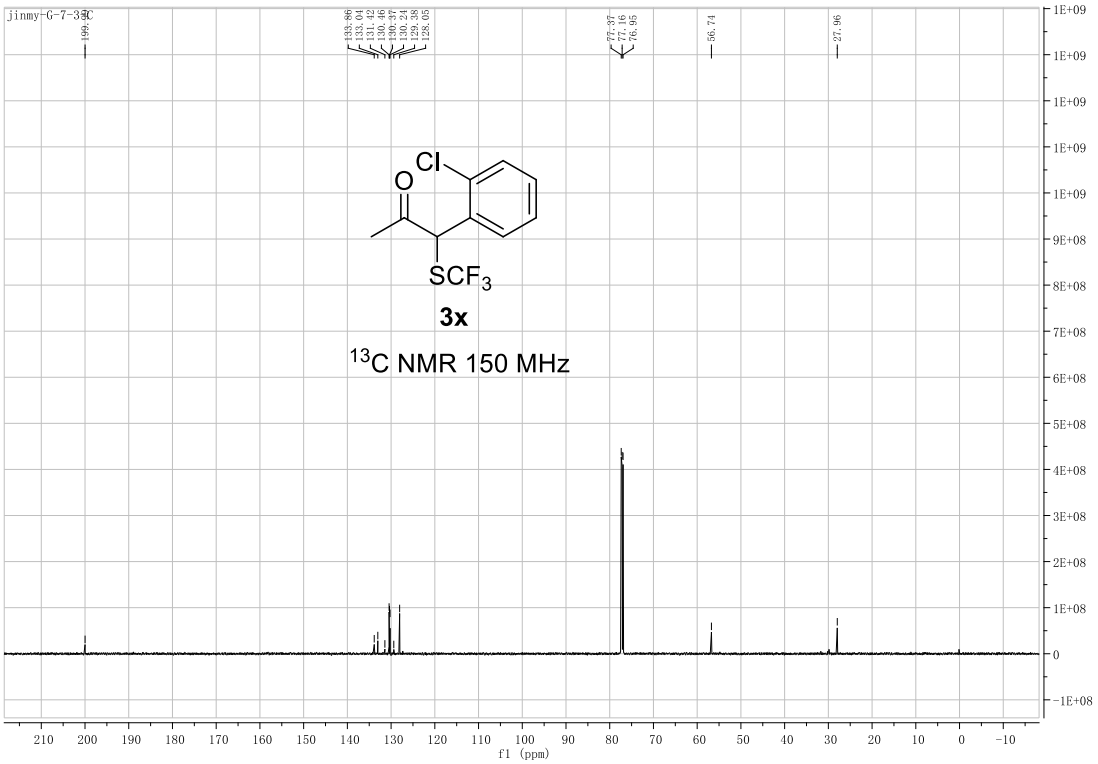

jinmy-IX-93-up-F
-40.45
Br
O
N
N
Ph
SCF3
3v
19F NMR 376 MHz
f1 (ppm)

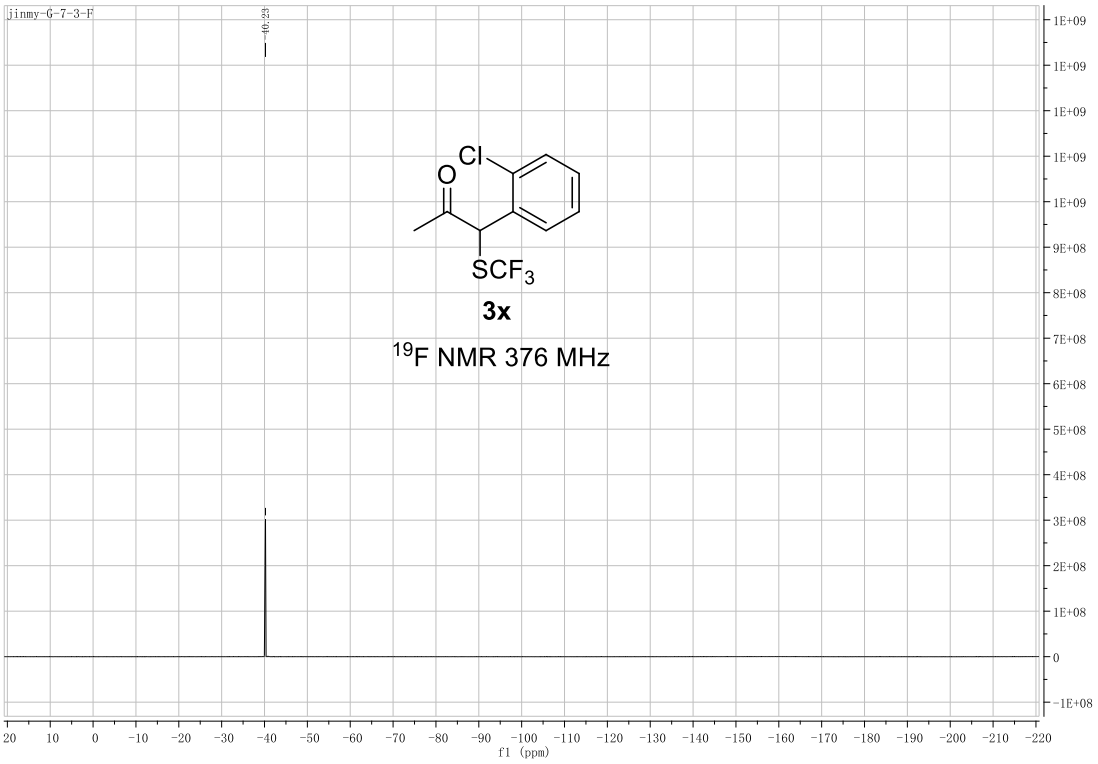

jinmy-VIII-81-2-5-up-H
O
N
Me
N
SCF3
Ph
3w
1H NMR 400 MHz
f1 (ppm)

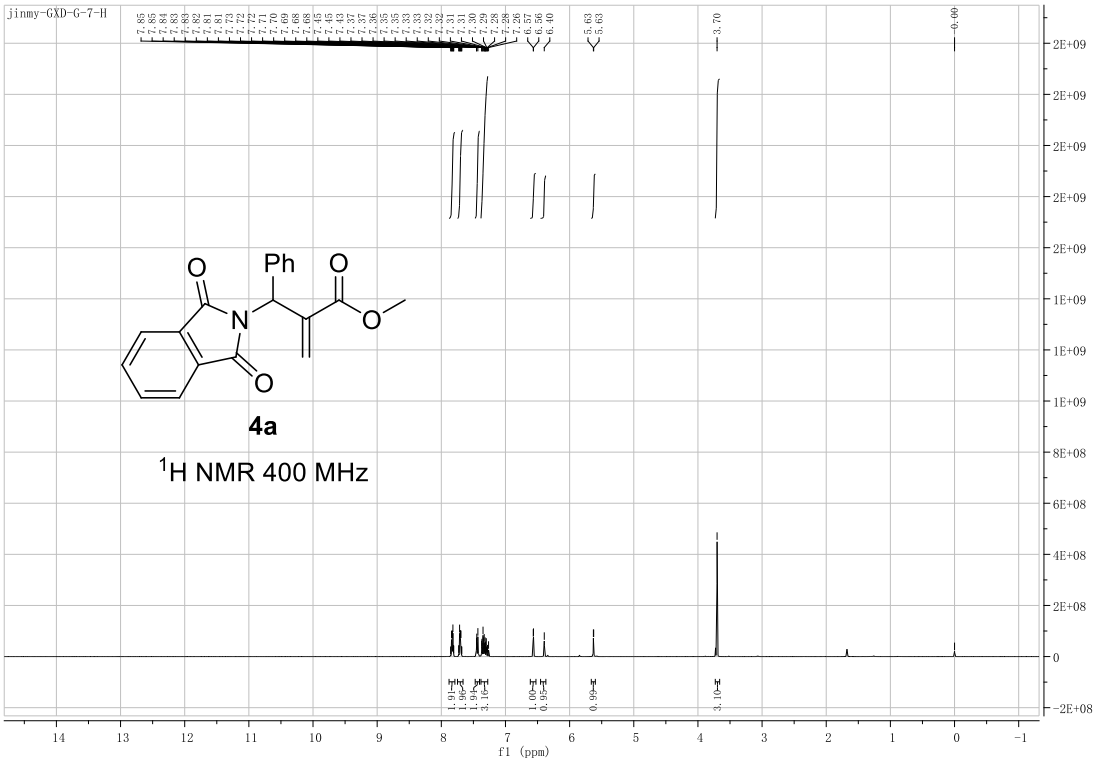

jinmy-VIII-81-2-5-C
O
N
Me
N
SCF3
Ph
3w
13C NMR 150 MHz
f1 (ppm)

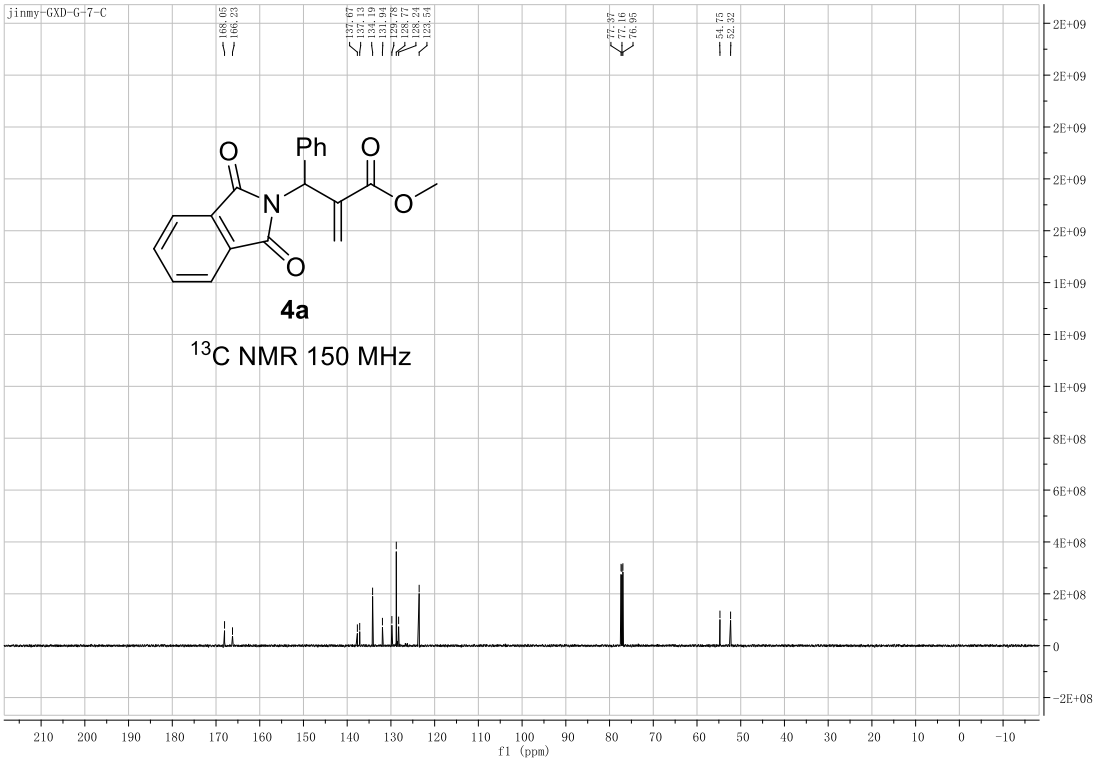

jinmy-VIII-81-2-5-up-F
-39.61
O
N
Me
N
SCF3
Ph
3w
19F NMR 376 MHz
f1 (ppm)

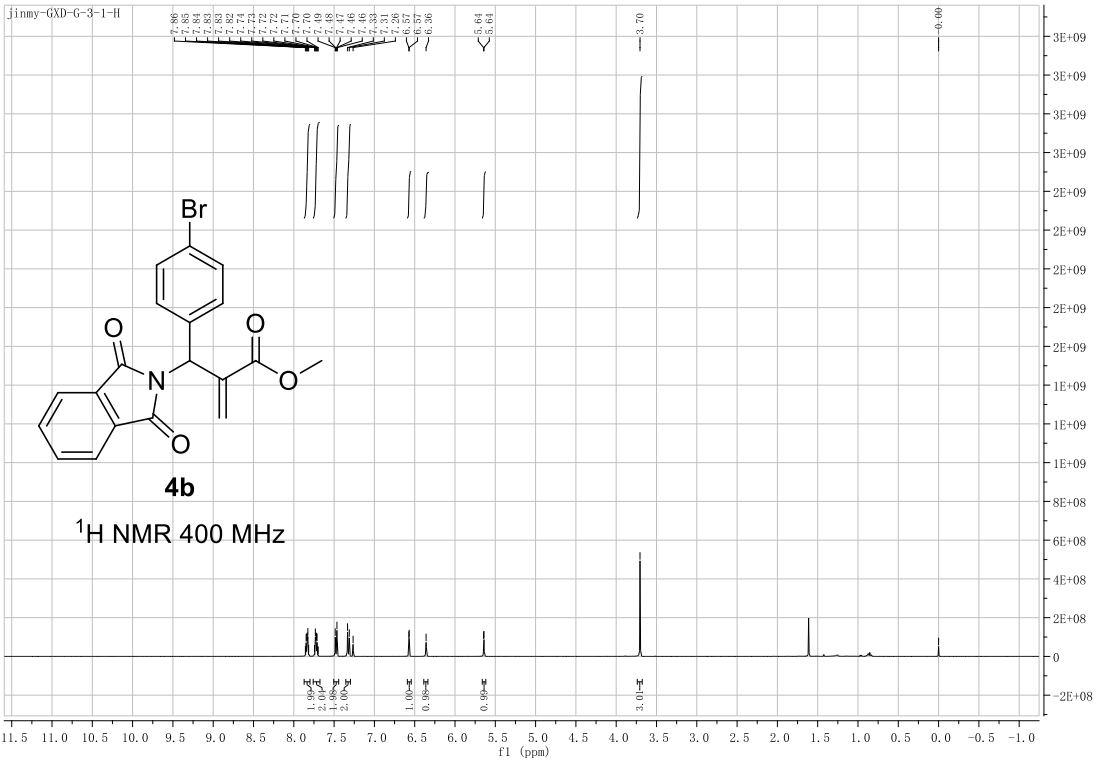

jinmy-G-7-3-H
7.47
7.46
7.46
7.45
7.44
7.42
7.41
7.41
7.40
7.40
7.39
7.34
7.34
7.33
7.32
7.31
7.31
7.30
7.29
7.26
5.82
2.21
0.00
Cl
O
SCF3
3x
1H NMR 400 MHz
1.00
3.07
f1 (ppm)

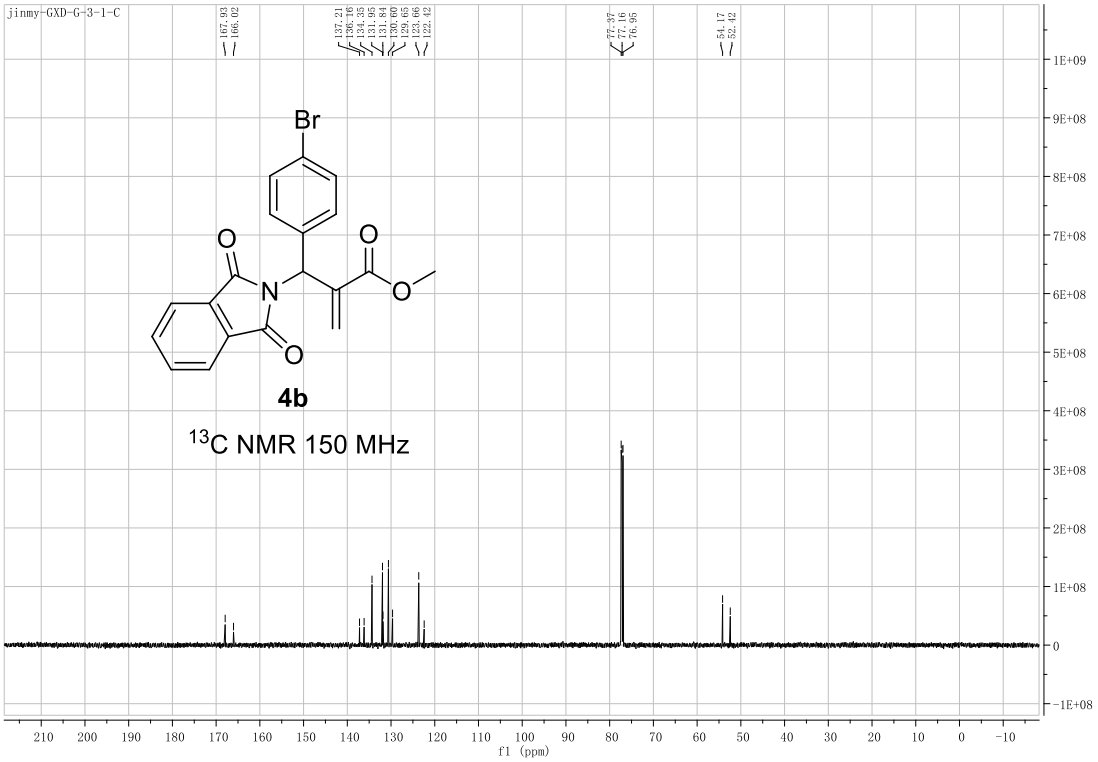

jinmy-G-7-3-C
199.42
133.86
133.04
131.42
131.16
130.37
130.24
129.38
128.05
77.37
77.16
76.95
56.74
27.96
Cl
O
SCF3
3x
13C NMR 150 MHz
f1 (ppm)

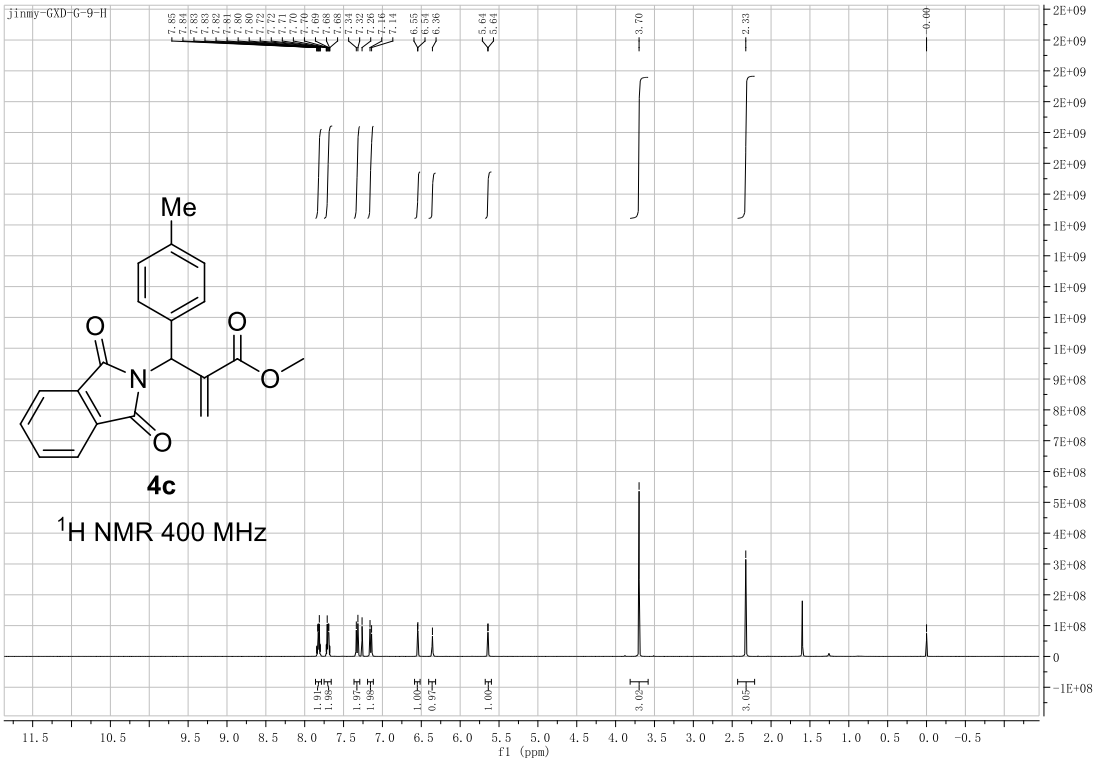

jinmy-G-7-3-F
-40.23
Cl
O
SCF3
3x
19F NMR 376 MHz
f1 (ppm)

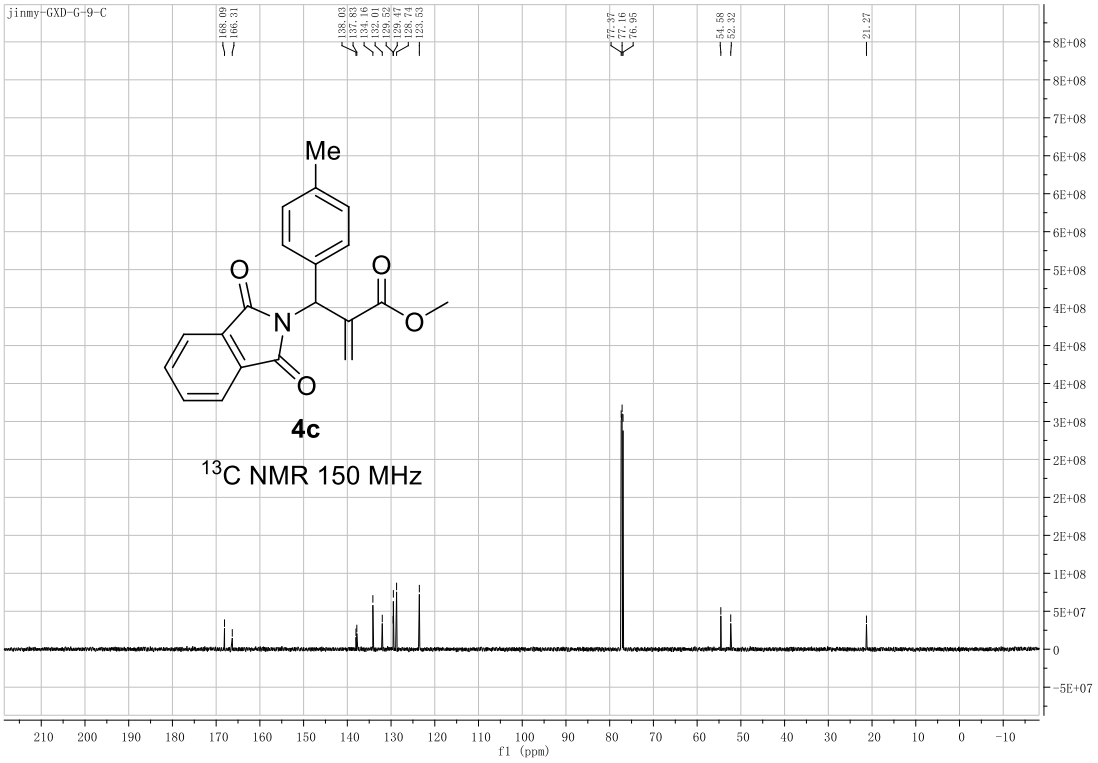

jinmy-GXD-G-7-H
Ph
O
N
O
O
O
4a
1H NMR 400 MHz
f1 (ppm)

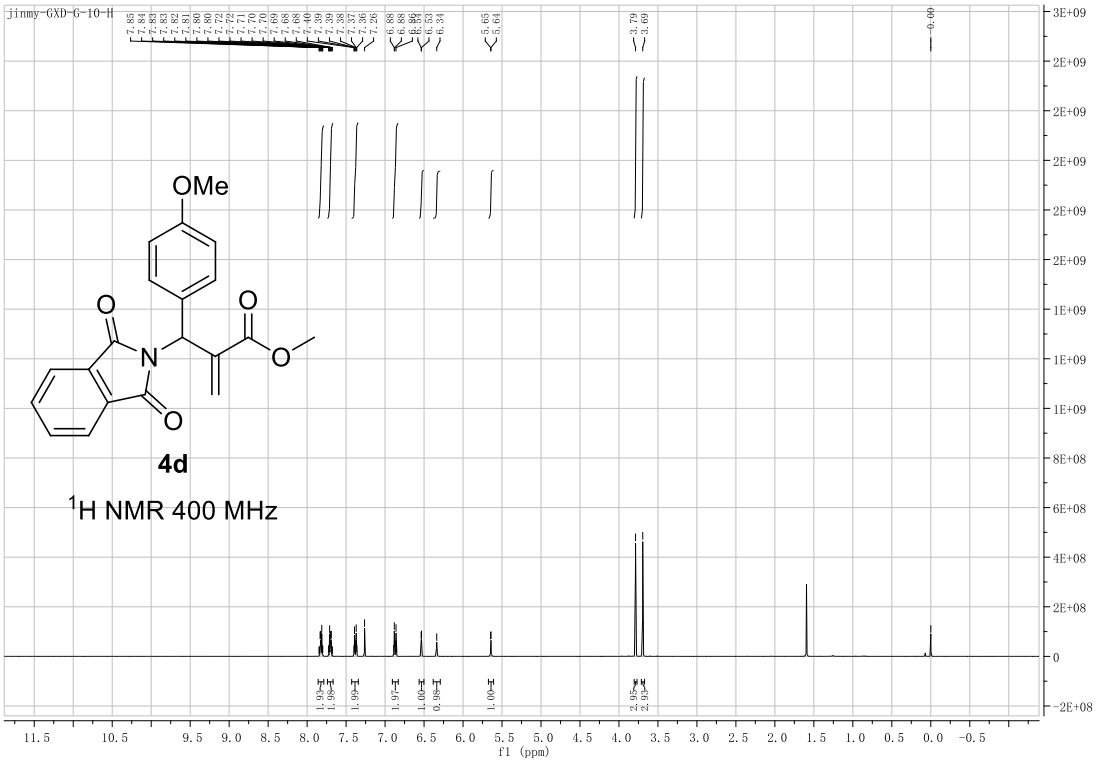

jinmy-GXD-G-7-C
Ph
O
N
O
O
O
4a
13C NMR 150 MHz
f1 (ppm)

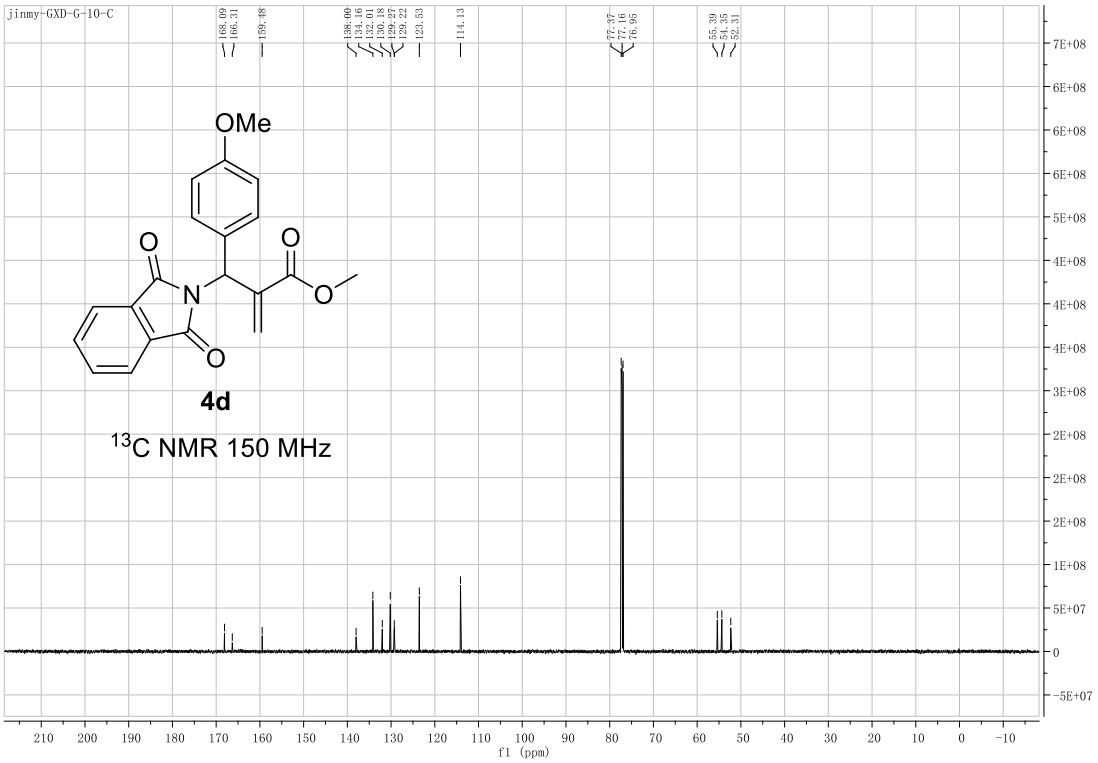

jinmy-GXD-G-3-1-H
Br
O
O
N
O
O
4b
1H NMR 400 MHz
f1 (ppm)

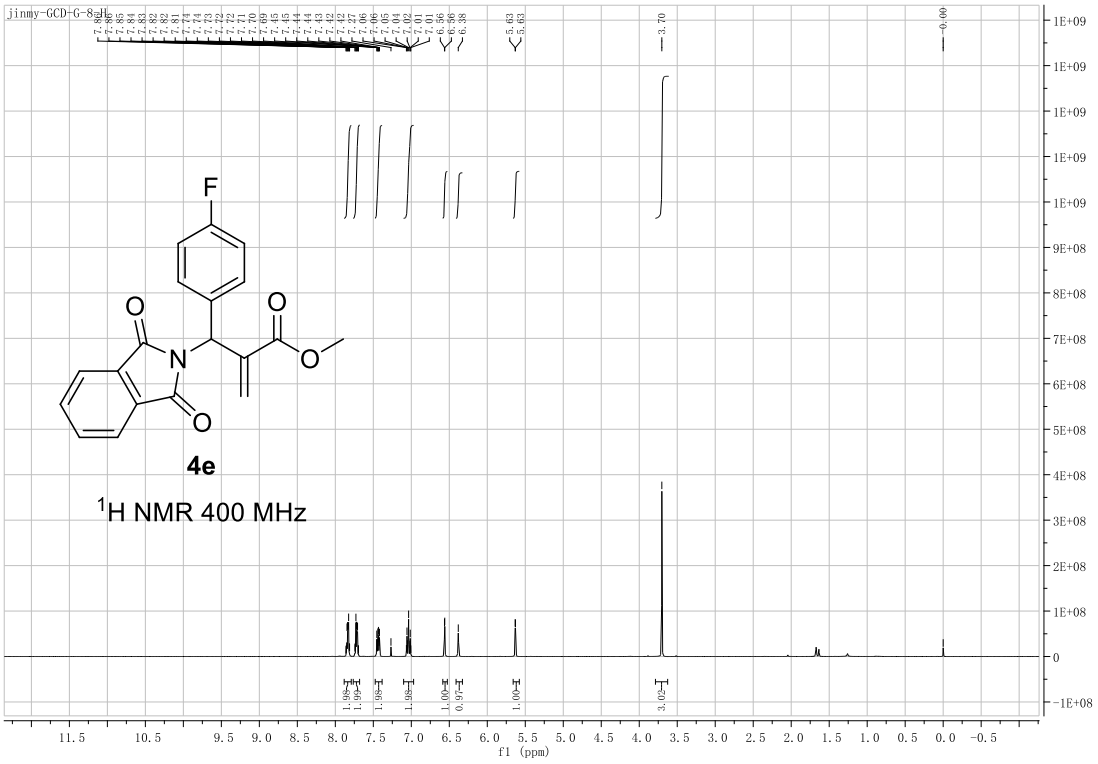

jinmy-GXD-G-3-1-C
Br
O
O
N
O
O
4b
13C NMR 150 MHz
f1 (ppm)

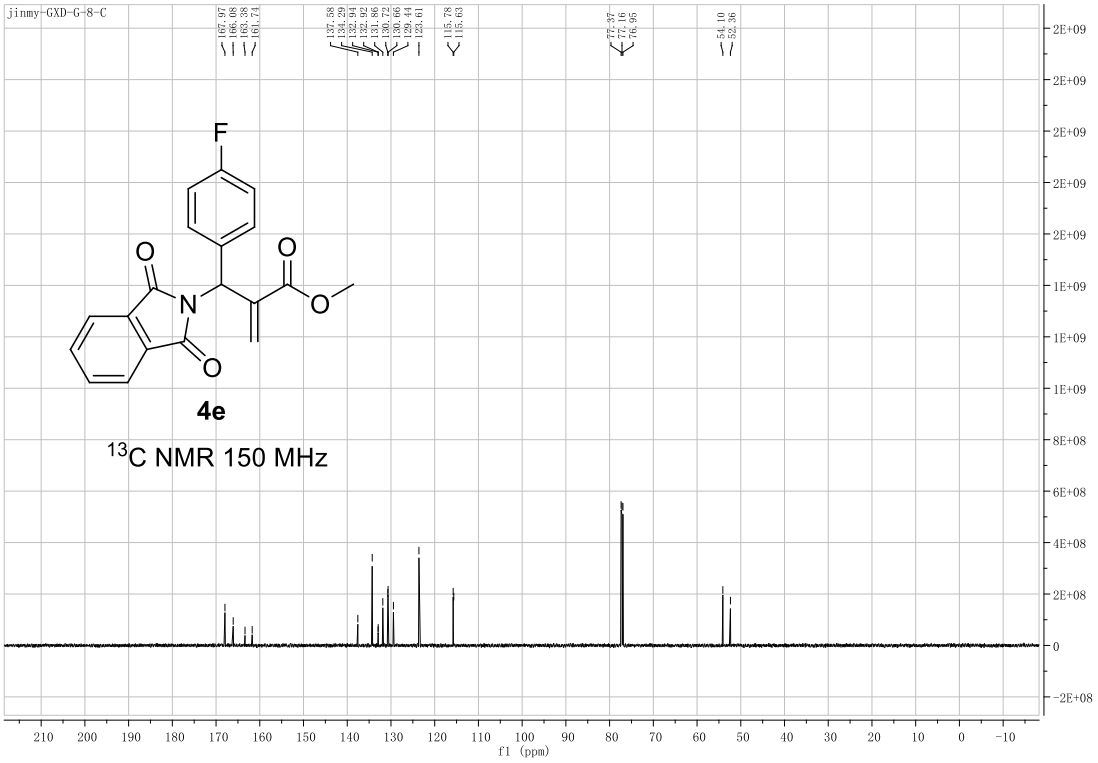

jinmy-GXD-G-9-H
Me
O
O
N
O
O
4c
1H NMR 400 MHz
f1 (ppm)

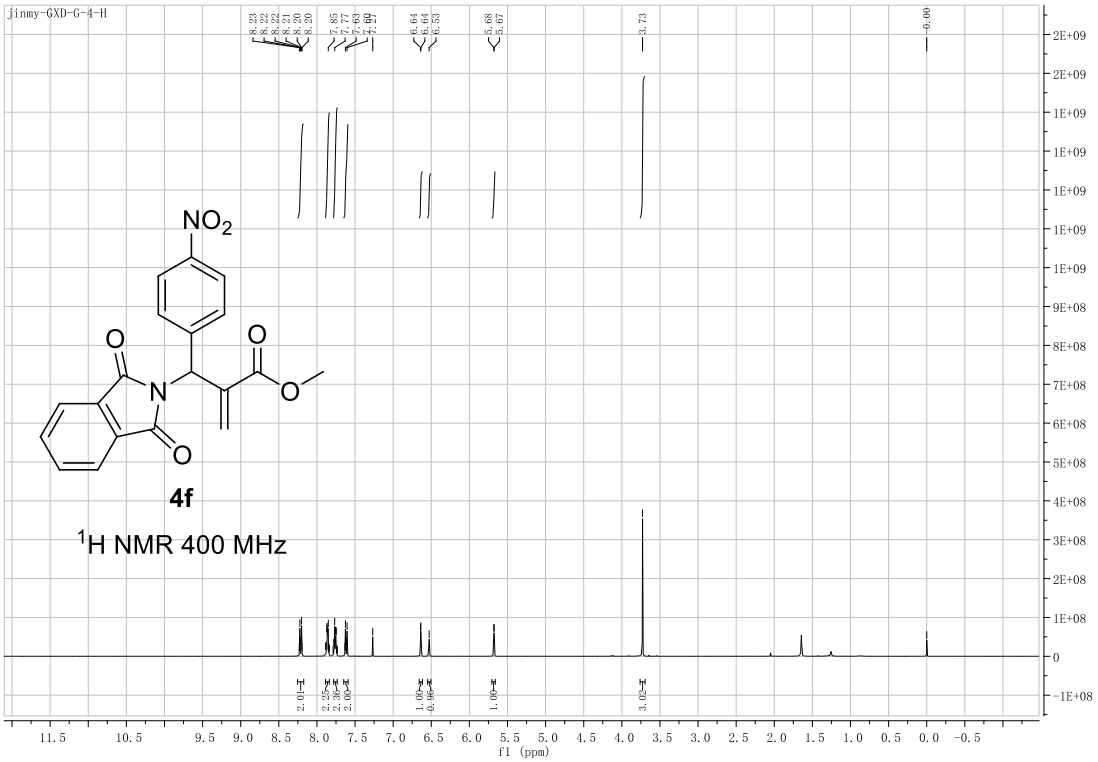

jinmy-GXD-G-9-C
Me
O
O
N
O
O
4c
13C NMR 150 MHz
f1 (ppm)

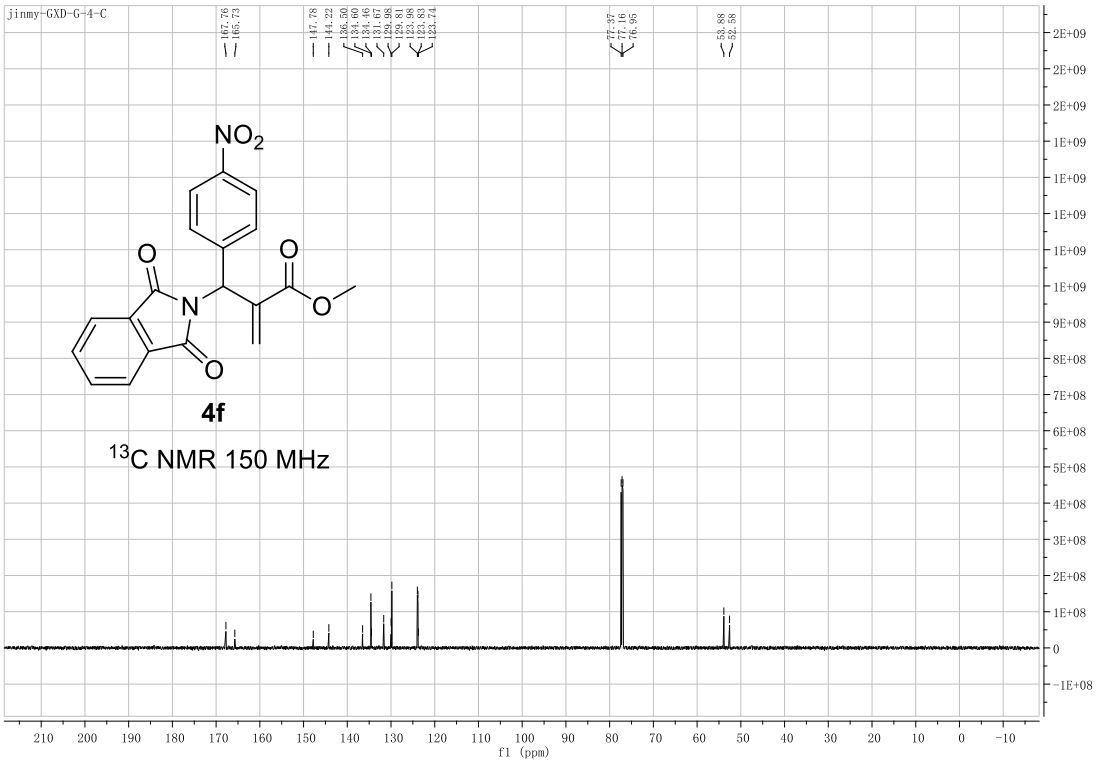

jinmy-GXD-G-10-H
OMe
O
O
N
O
O
4d
1H NMR 400 MHz
f1 (ppm)

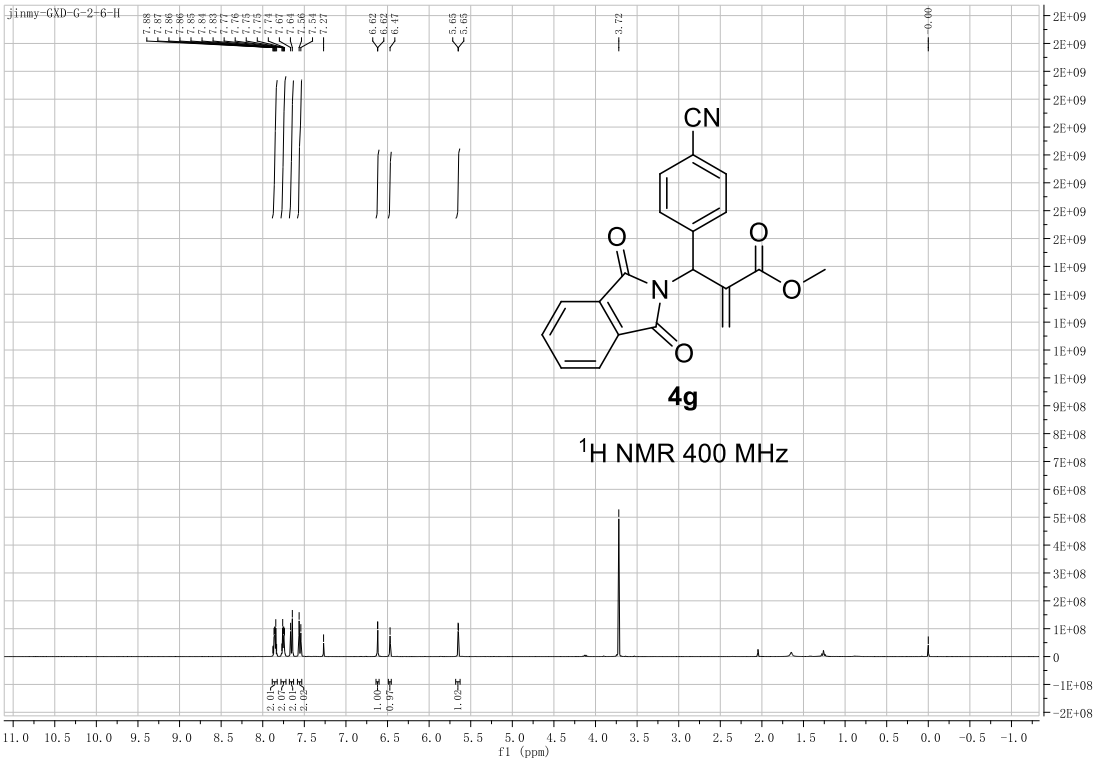

jinmy-GXD-G-10-C
OMe
O
O
N
O
O
4d
13C NMR 150 MHz
f1 (ppm)

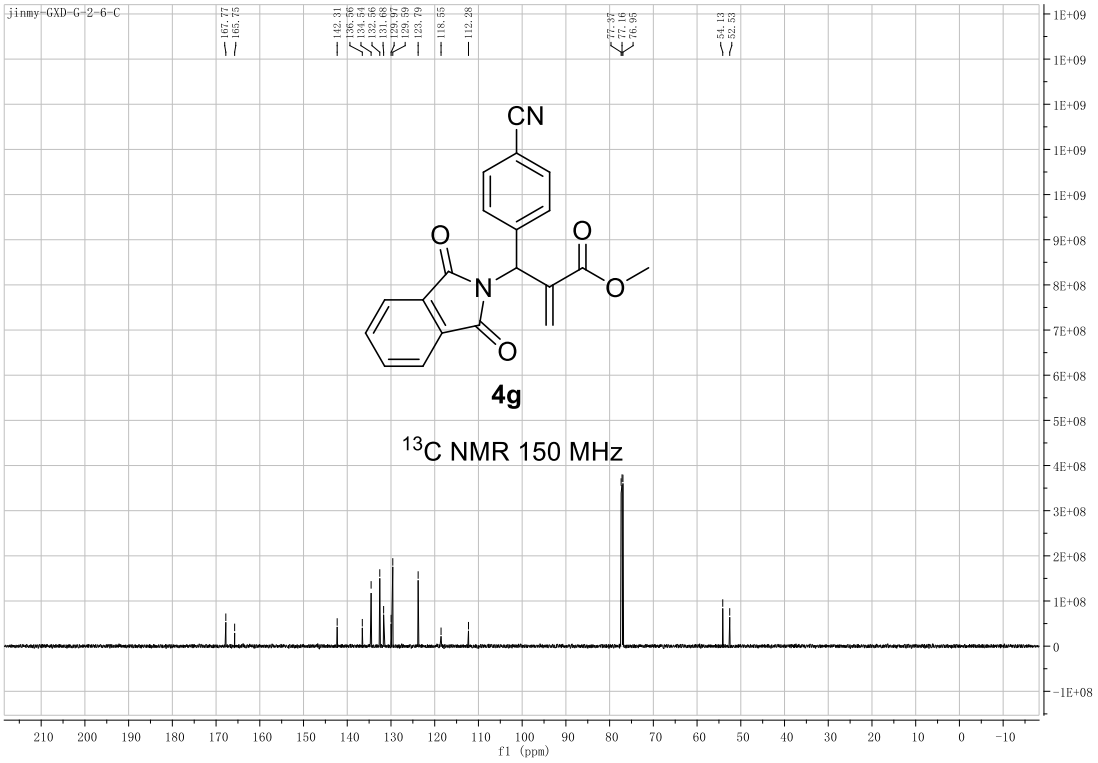

jinmy-GCD+G-8-H
F
O
O
N
O
O
4e
1H NMR 400 MHz
f1 (ppm)

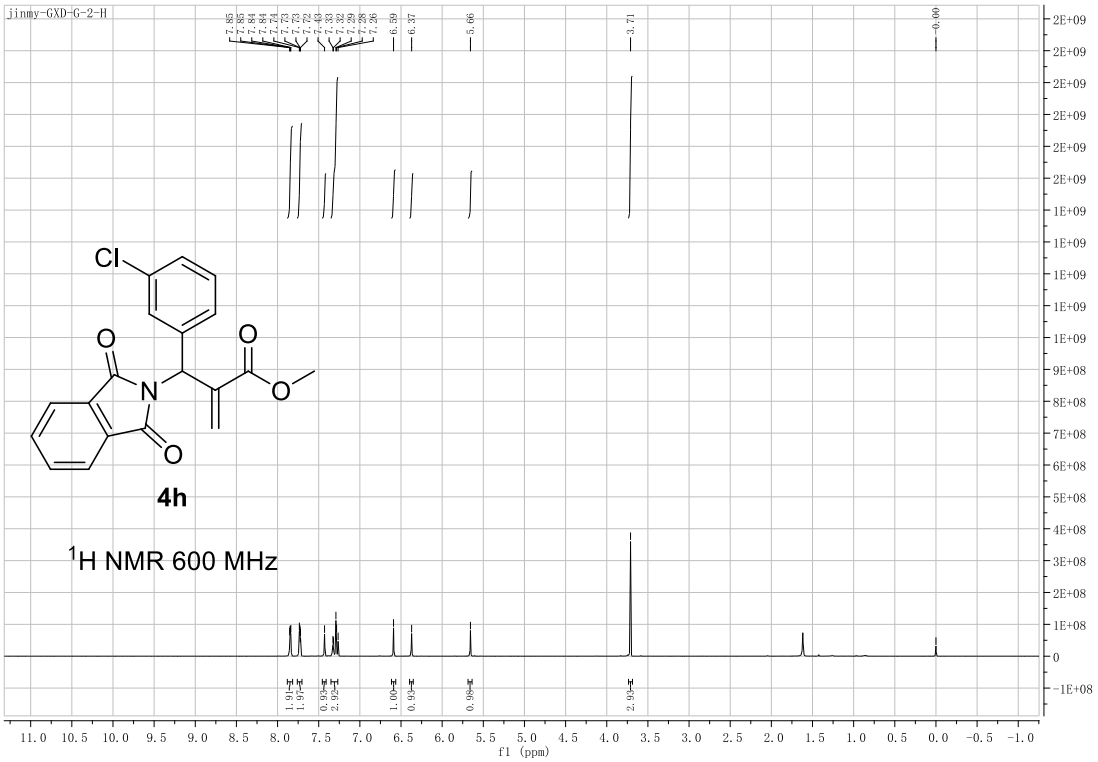

jinmy-GXD-G-8-C
F
O
O
N
O
O
4e
13C NMR 150 MHz
f1 (ppm)

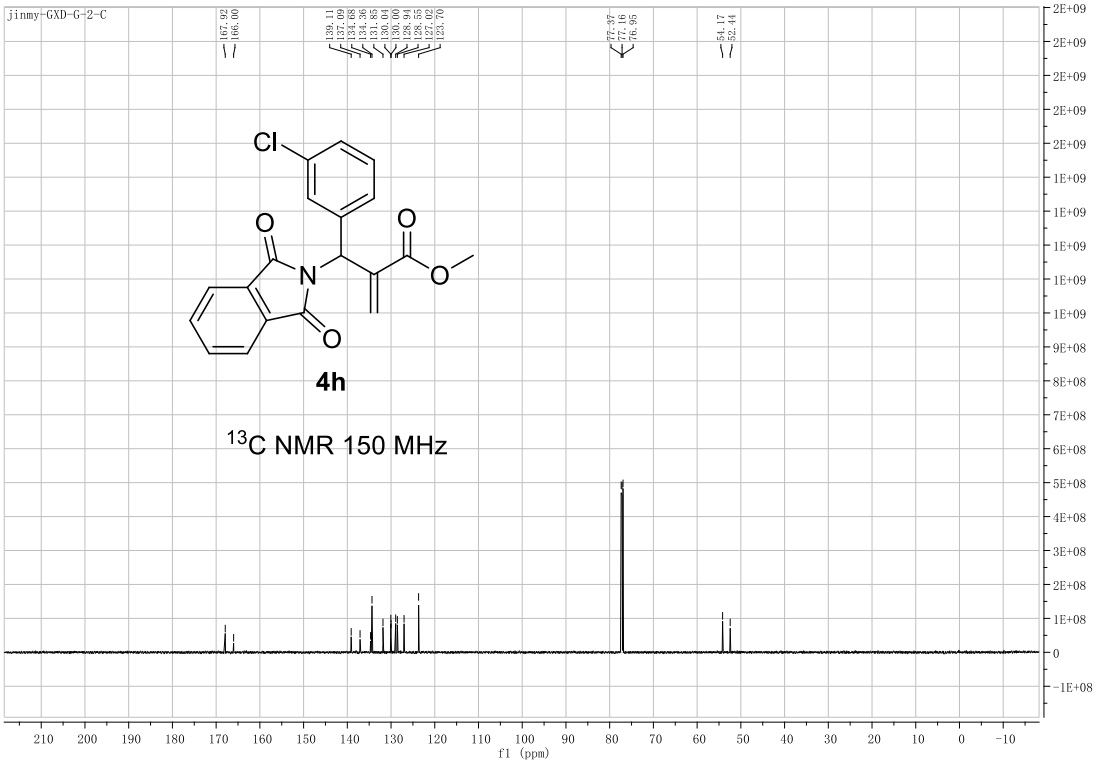

jinmy-GXD-G-4-H
NO2
O
O
N
O
O
4f
1H NMR 400 MHz
f1 (ppm)

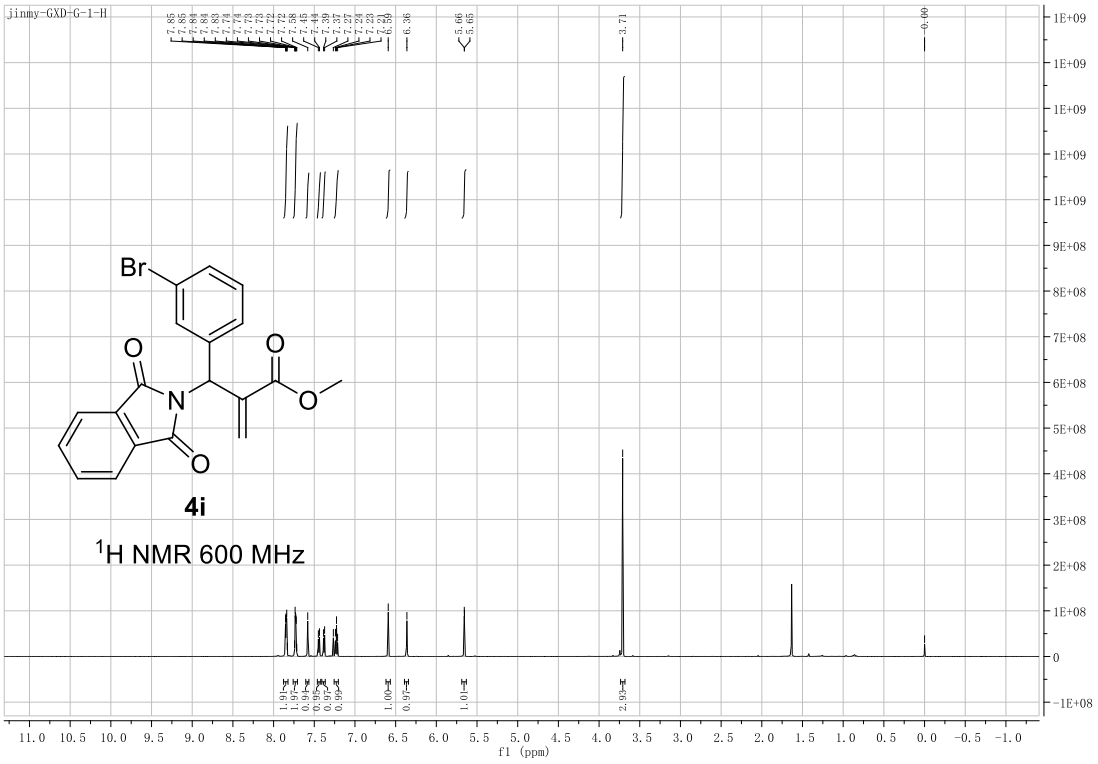

jinmy-GXD-G-4-C
NO2
O
O
N
O
O
4f
13C NMR 150 MHz
f1 (ppm)

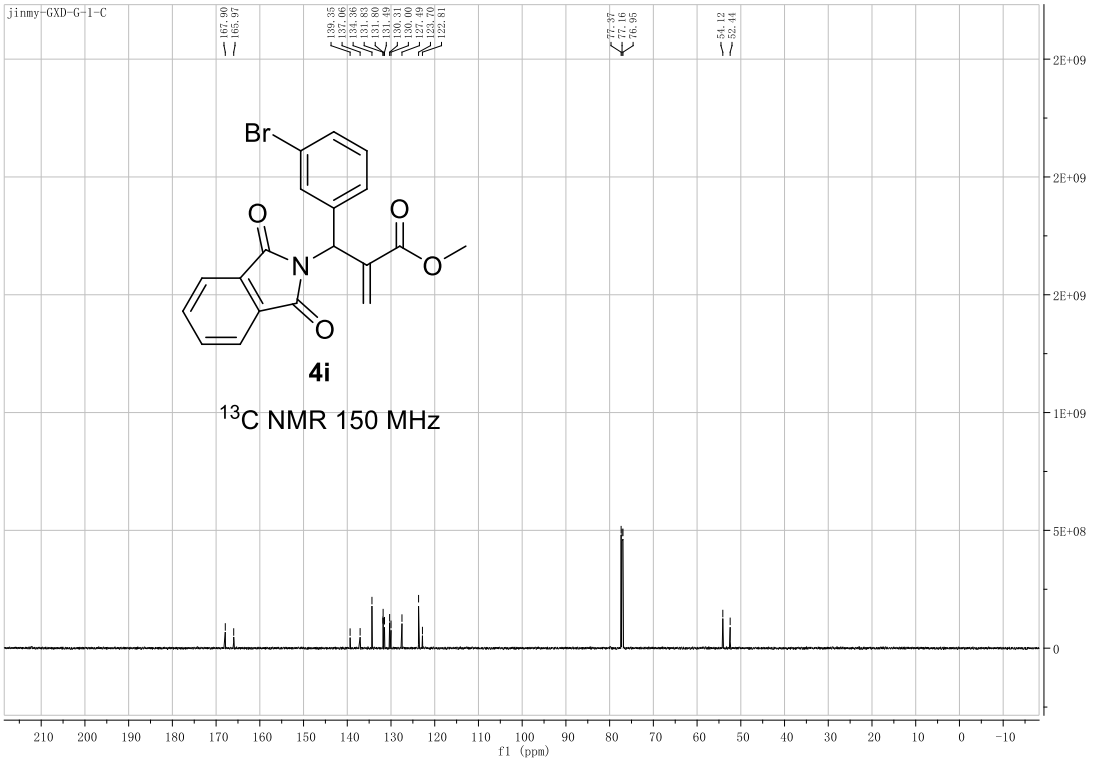

jinmy-GXD-G-2-6-H
CN
O
O
N
O
O
4g
1H NMR 400 MHz
f1 (ppm)

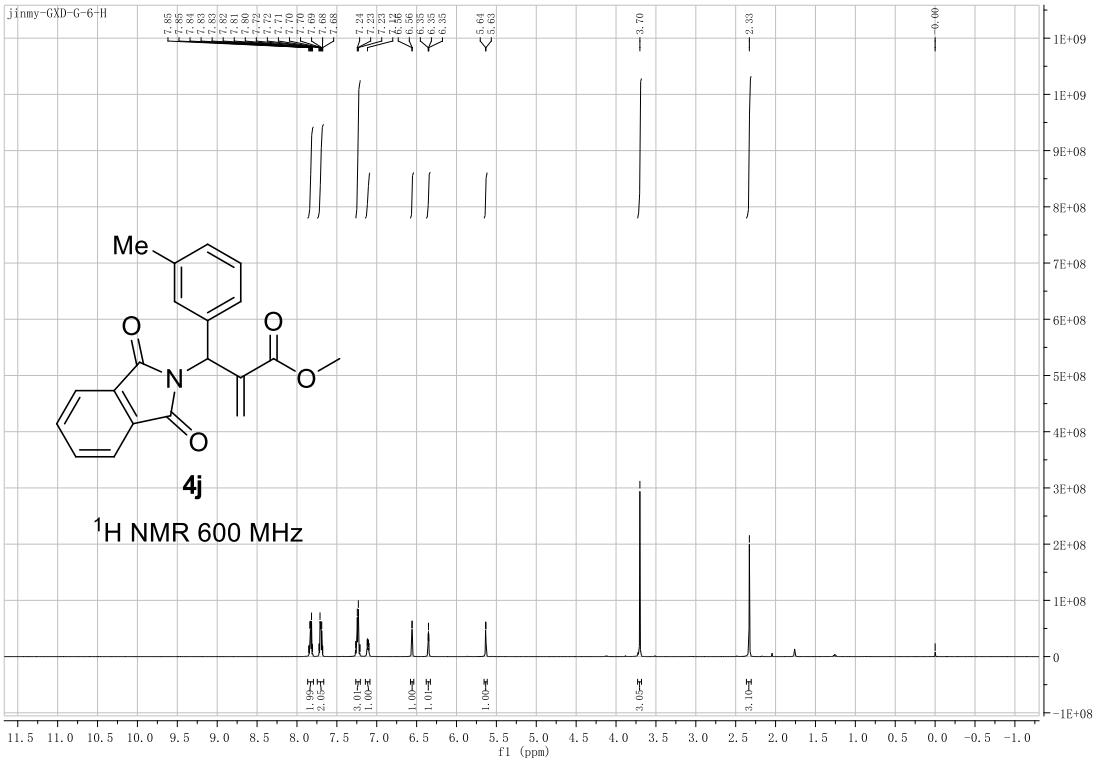

jinmy-GXD-G-2-6-C
CN
O
O
N
O
O
4g
13C NMR 150 MHz
f1 (ppm)

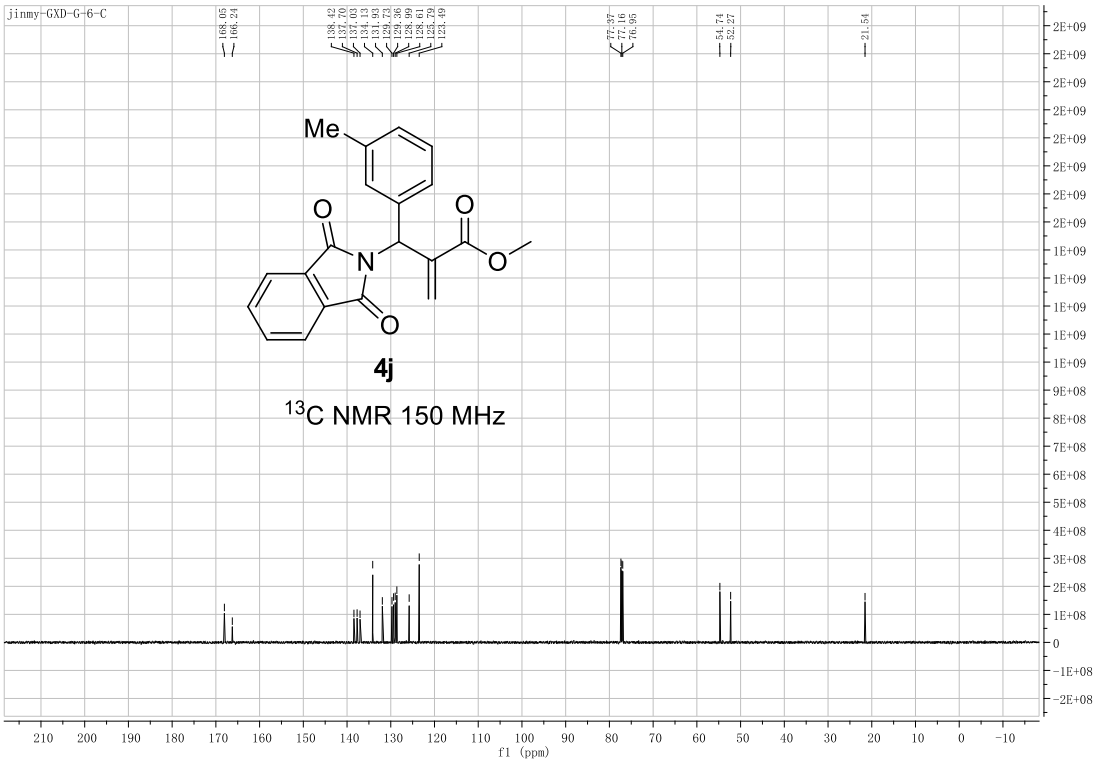

jinmy-GXD-G-2-H
Cl
O
O
N
O
O
4h
1H NMR 600 MHz
f1 (ppm)

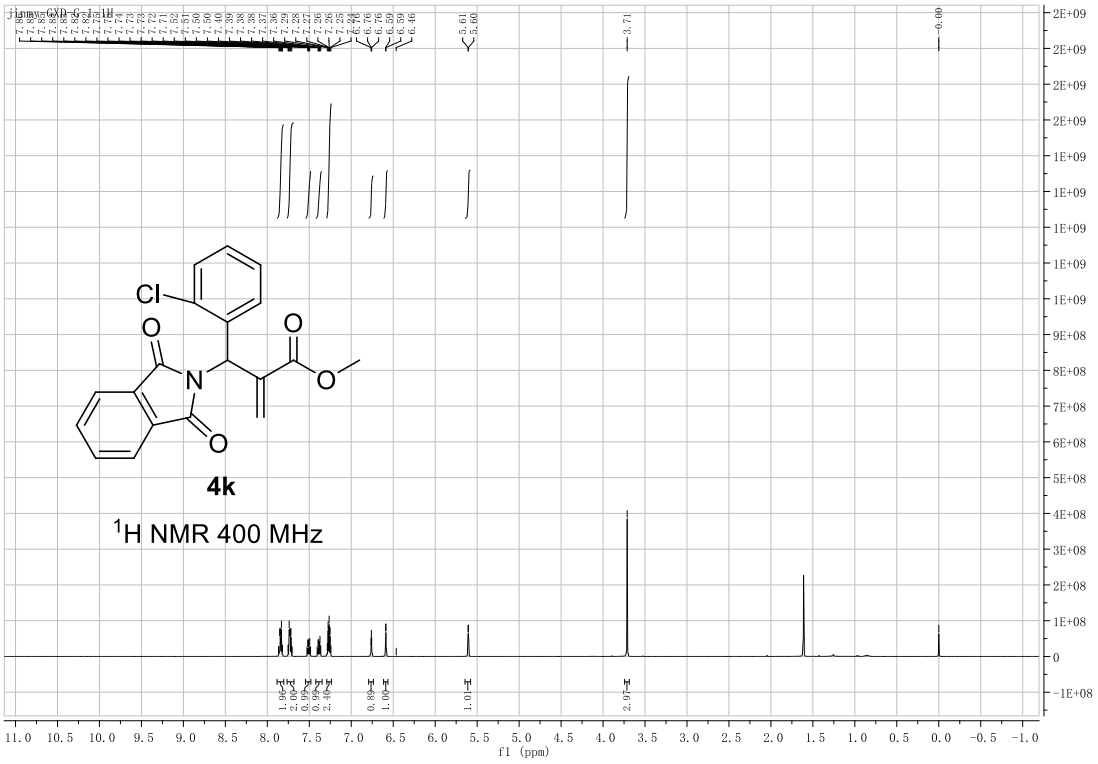

jinmy-GXD-G-2-C
Cl
O
O
N
O
O
4h
13C NMR 150 MHz
f1 (ppm)

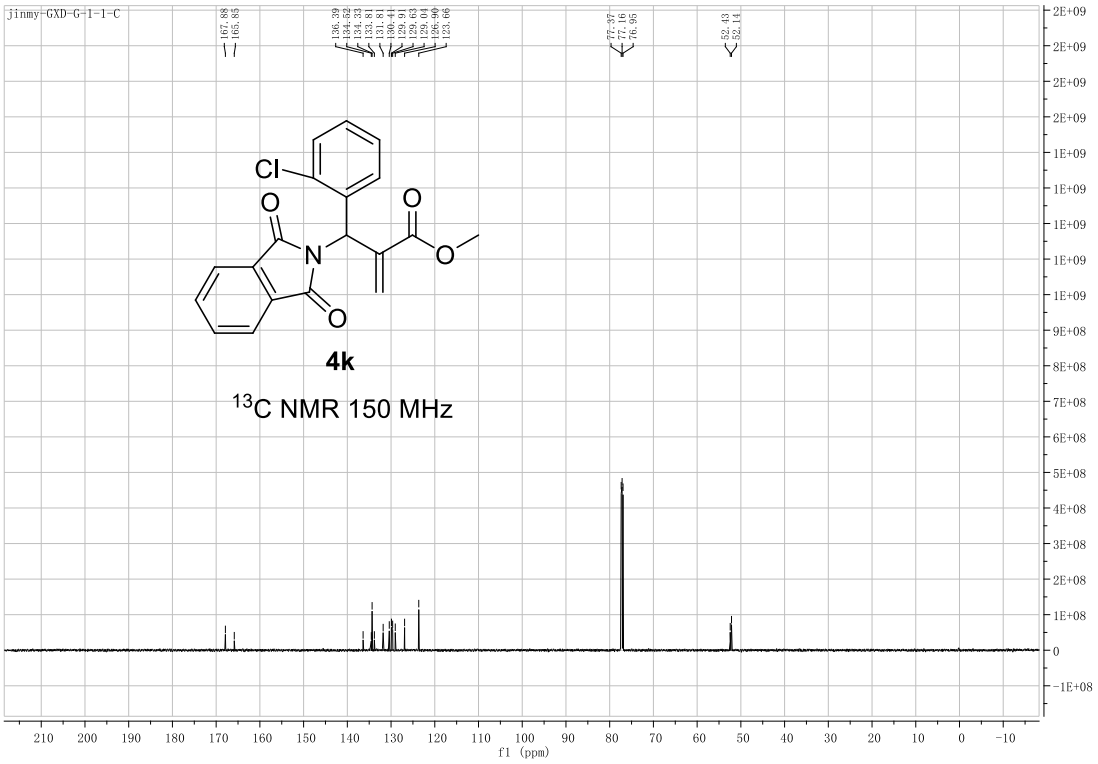

jinmy-GXD-G-1-H
Br
O
O
N
O
O
O
4i
1H NMR 600 MHz
f1 (ppm)

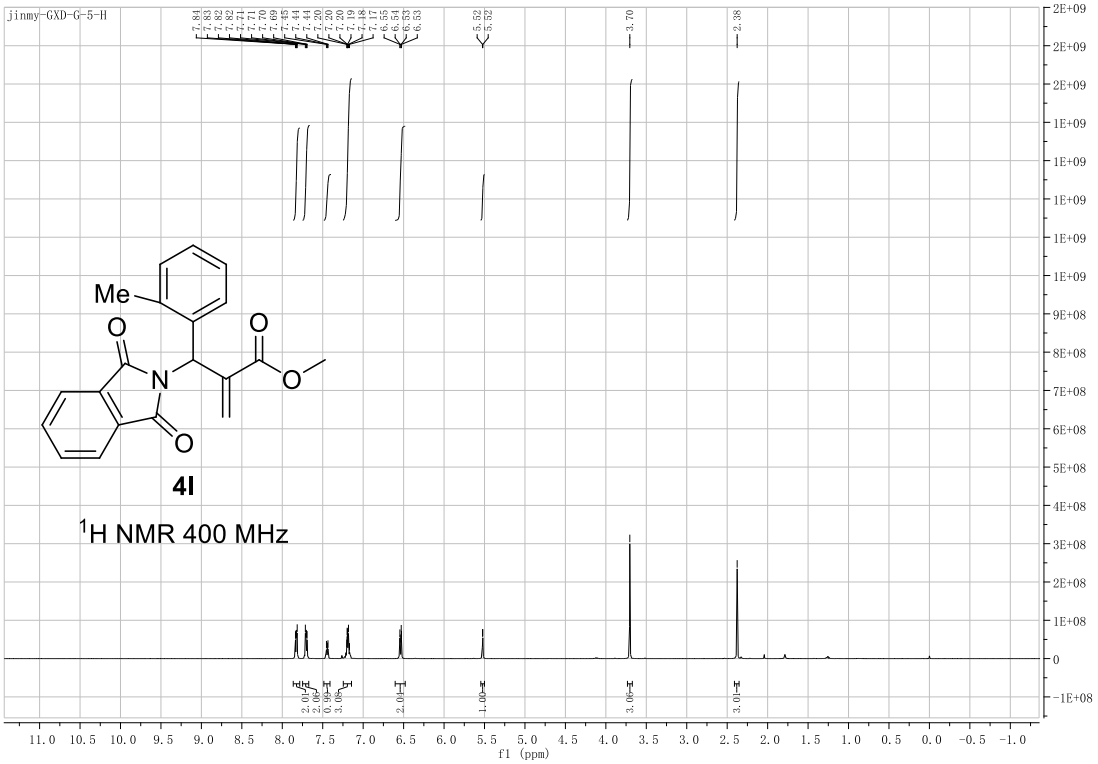

jinmy-GXD-G-1-C
Br
O
O
N
O
O
O
4i
13C NMR 150 MHz
f1 (ppm)

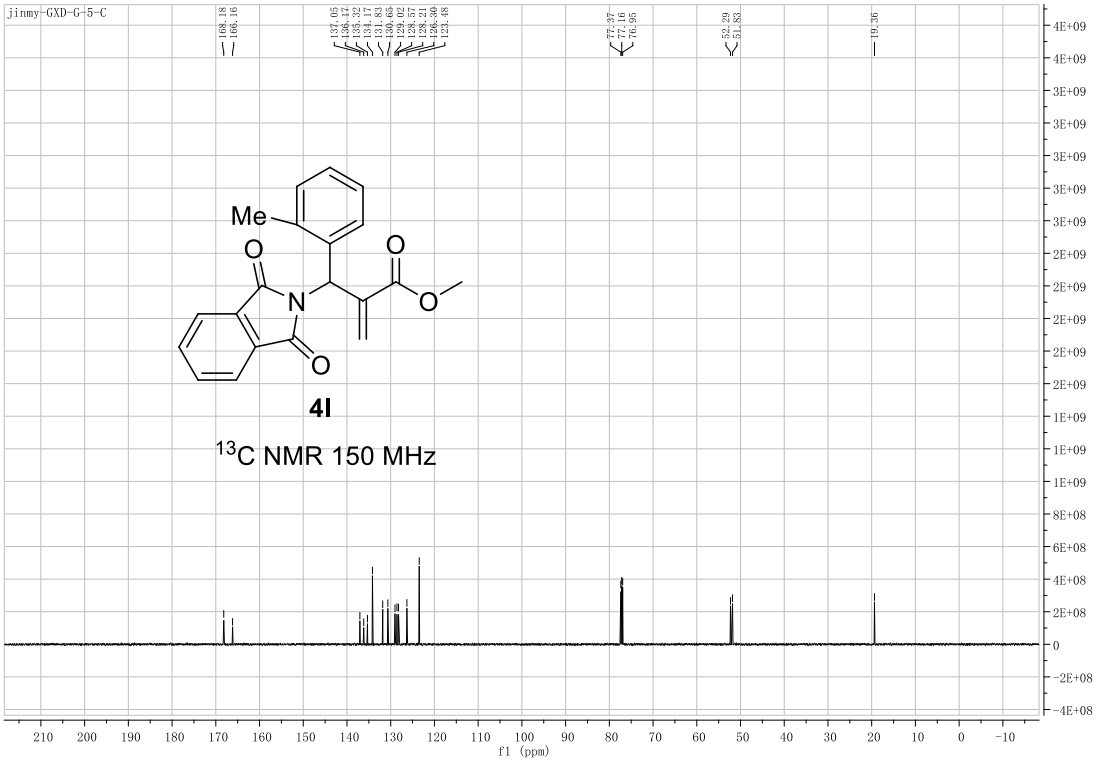

jinmy-GXD-G-6-H
Me
O
O
N
O
O
4j
1H NMR 600 MHz
f1 (ppm)

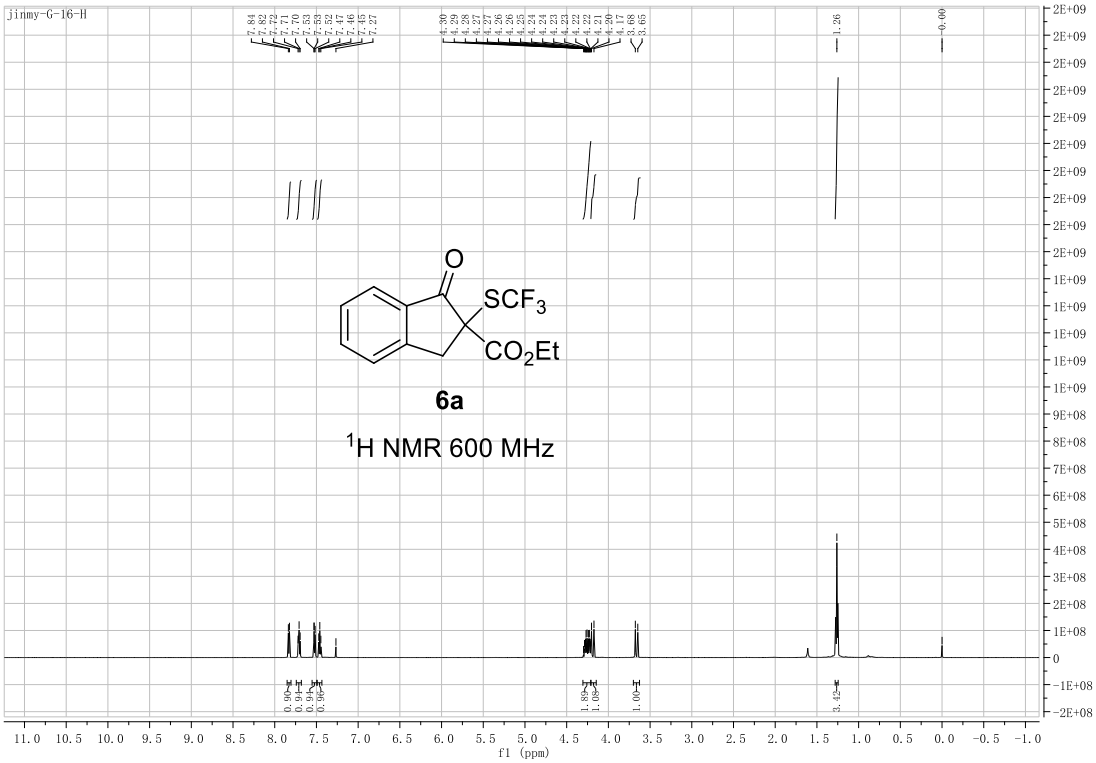

jinmy-GXD-G-6-C
Me
O
O
N
O
O
4j
13C NMR 150 MHz
f1 (ppm)

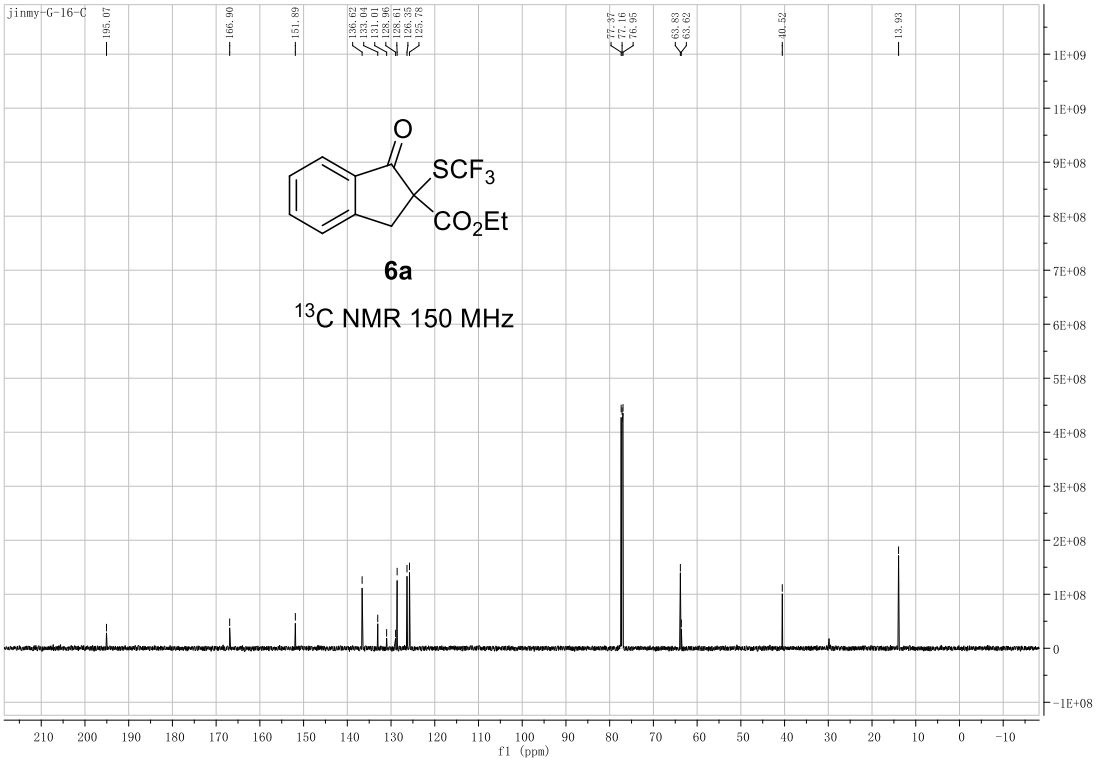

jinmy-GXD-G-1-1H
Cl
O
O
N
O
O
4k
1H NMR 400 MHz
f1 (ppm)

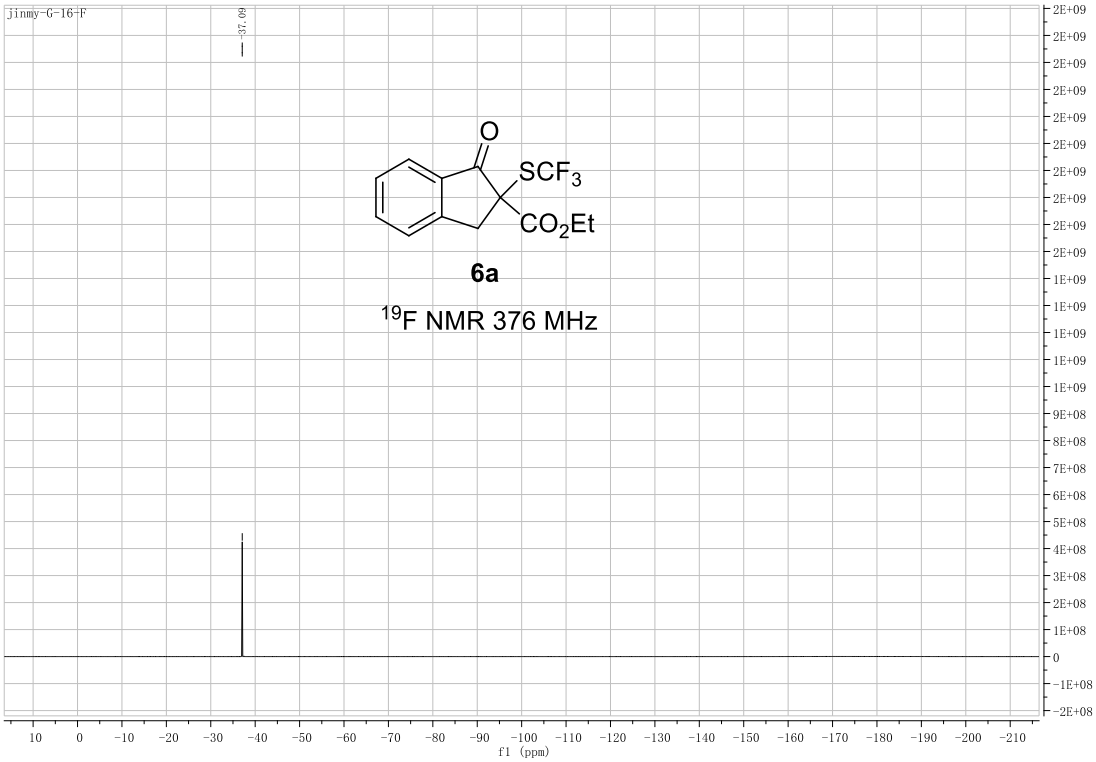

jinmy-GXD-G-1-1-C
Cl
O
O
N
O
O
4k
13C NMR 150 MHz
f1 (ppm)

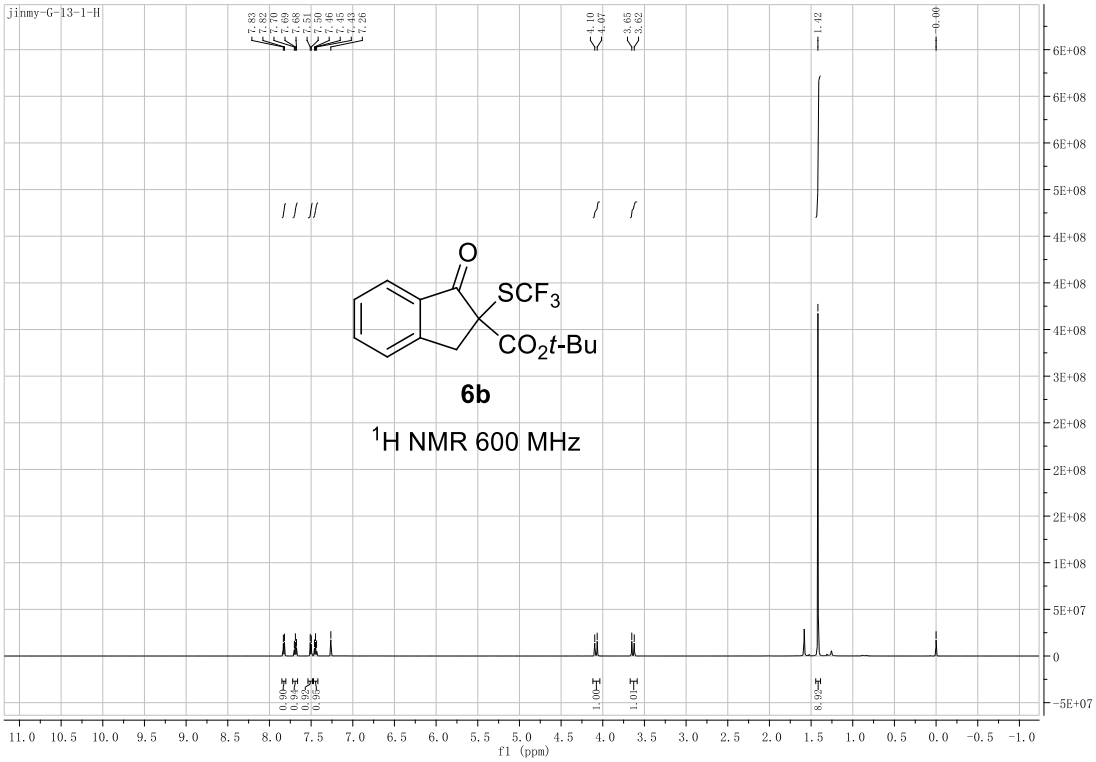

jinmy-GXD-G-5-H
Me
O
O
N
O
O
4l
1H NMR 400 MHz
f1 (ppm)

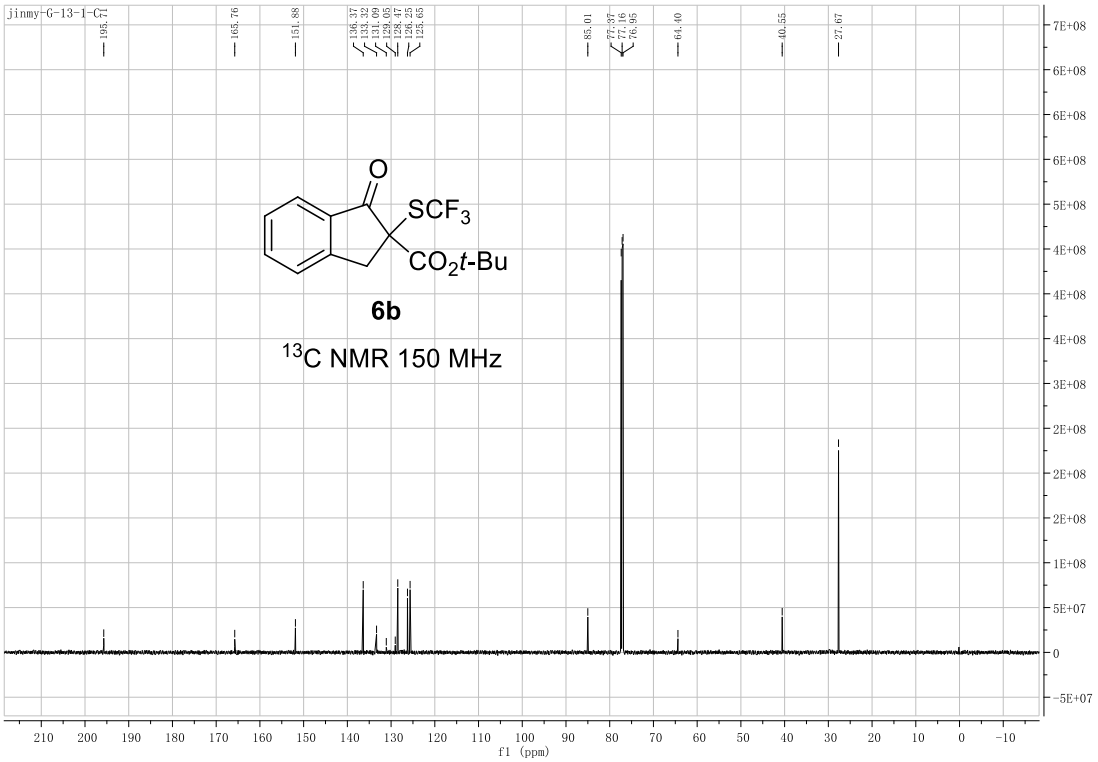

jinmy-GXD-G-5-C
Me
O
O
N
O
O
4l
13C NMR 150 MHz
f1 (ppm)

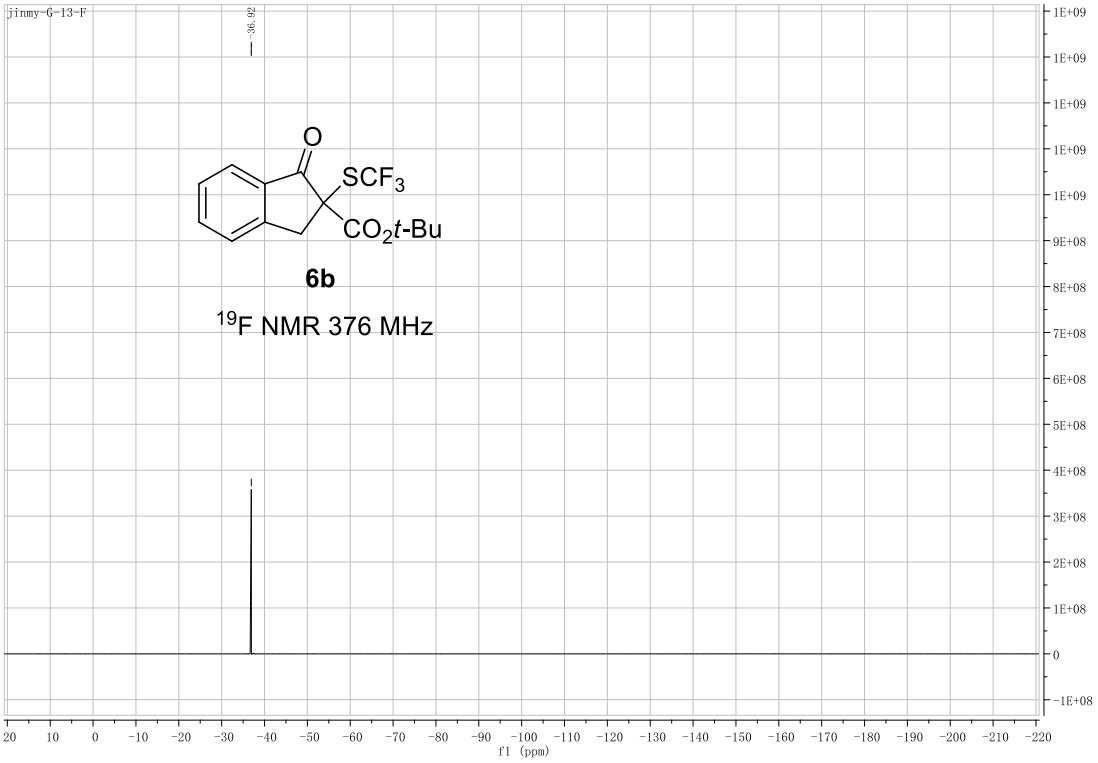

jinmy-G-16-H
O
SCF3
CO2Et
6a
1H NMR 600 MHz
f1 (ppm)

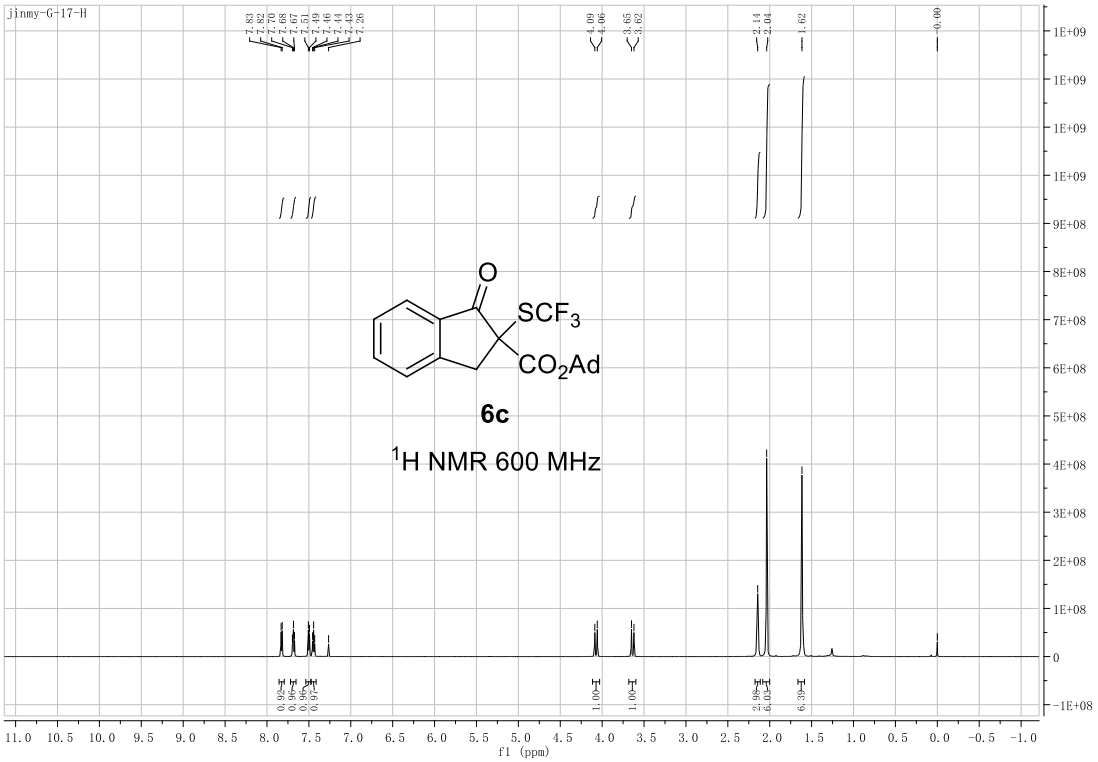

jinmy-G-16-C
O
SCF3
CO2Et
6a
13C NMR 150 MHz
f1 (ppm)

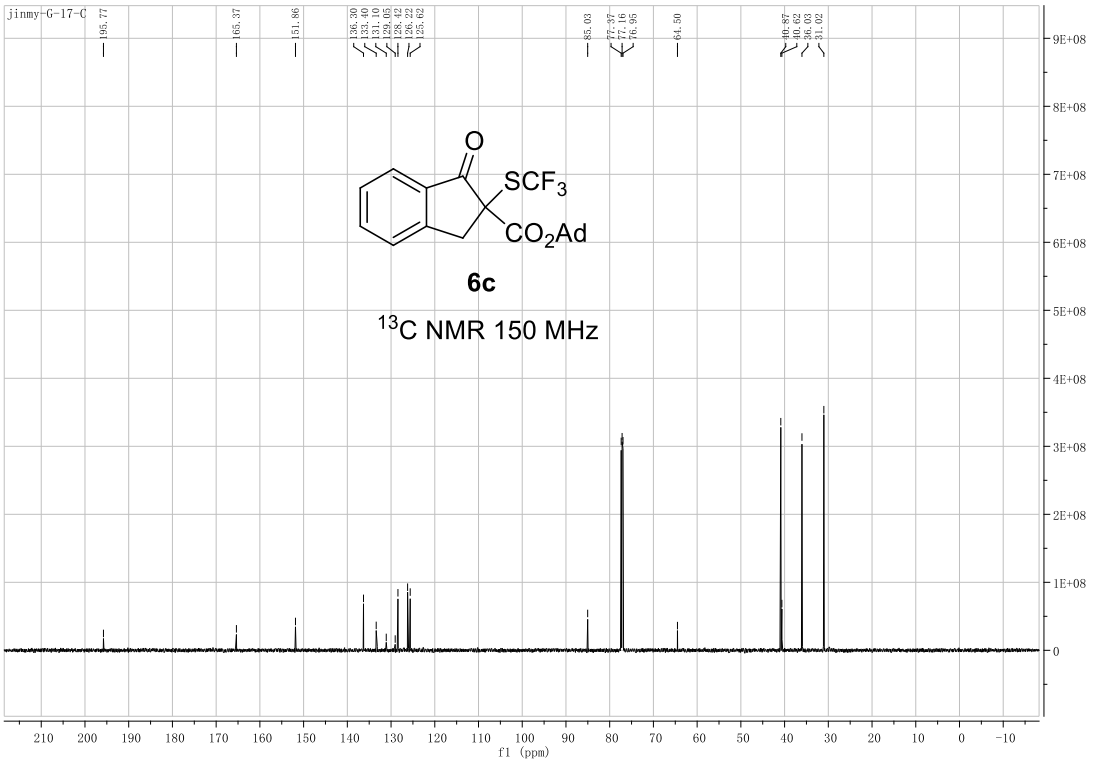

jinmy-G-16-F
-37.09
O
SCF3
CO2Et
6a
19F NMR 376 MHz
f1 (ppm)

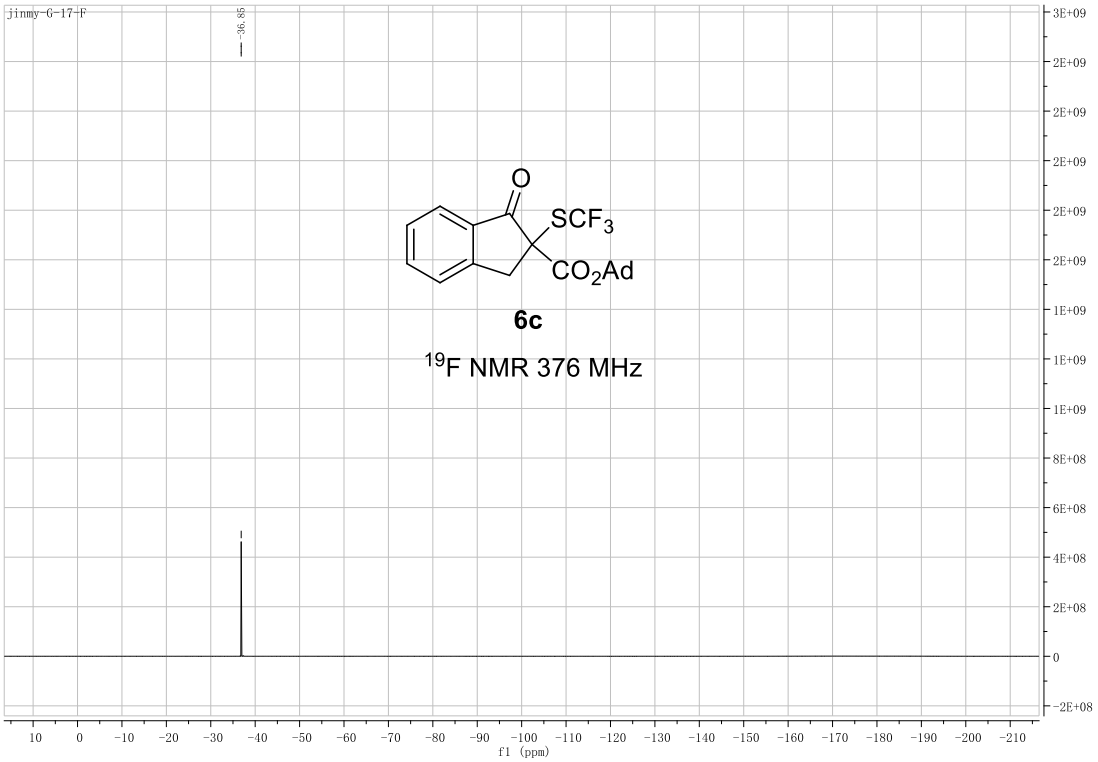

jinmy-G-13-1-H
7.83
7.82
7.70
7.68
7.51
7.50
7.46
7.45
7.43
7.26
4.10
4.07
3.65
3.62
1.42
0.00
O
SCF3
CO2t-Bu
6b
1H NMR 600 MHz
0.90
0.94
0.92
0.95
1.00
1.01
8.92
f1 (ppm)

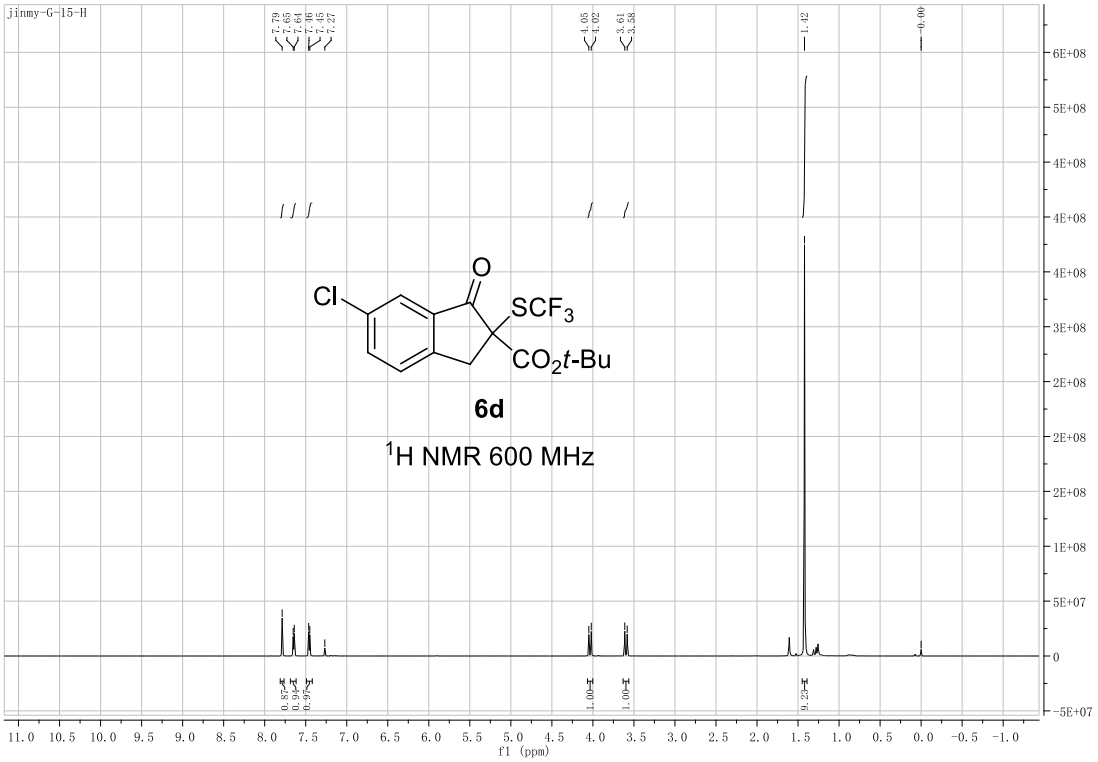

jinmy-G-13-1-C-f1
195.71
165.76
151.88
136.37
133.32
131.09
129.05
128.47
126.35
125.65
85.01
77.37
77.16
76.95
64.40
40.55
27.67
O
SCF3
CO2t-Bu
6b
13C NMR 150 MHz
f1 (ppm)

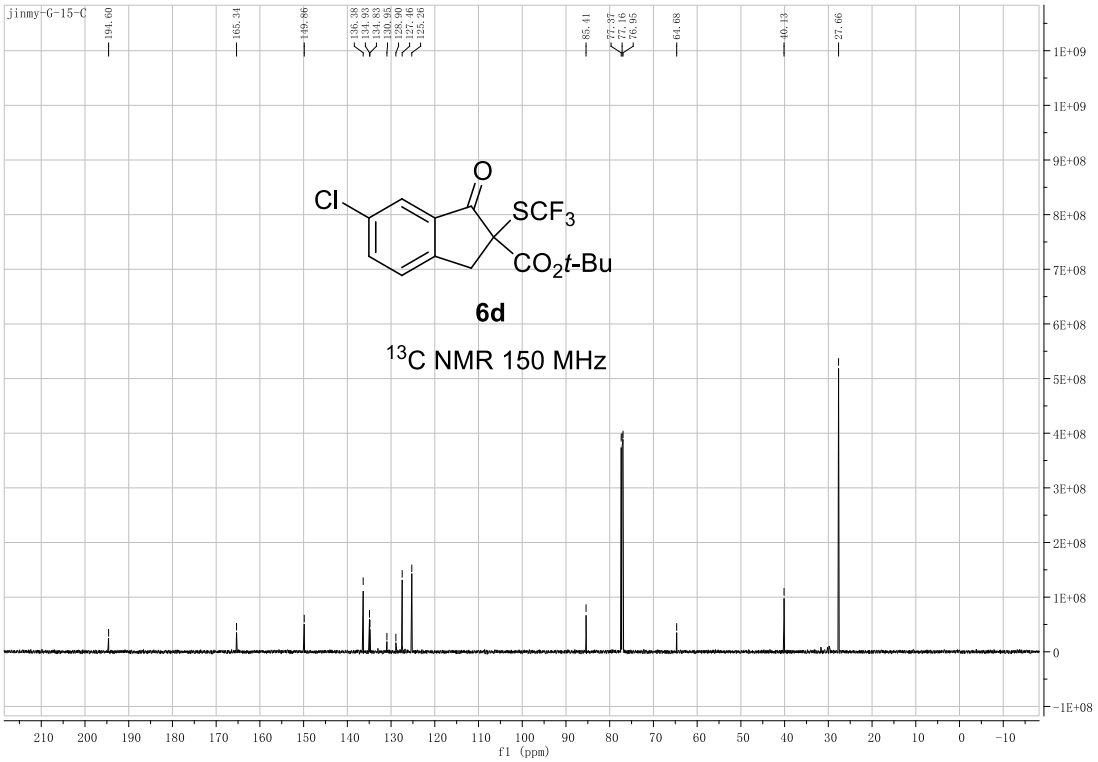

jinmy-G-13-F
-36.92
O
SCF3
CO2t-Bu
6b
19F NMR 376 MHz
f1 (ppm)

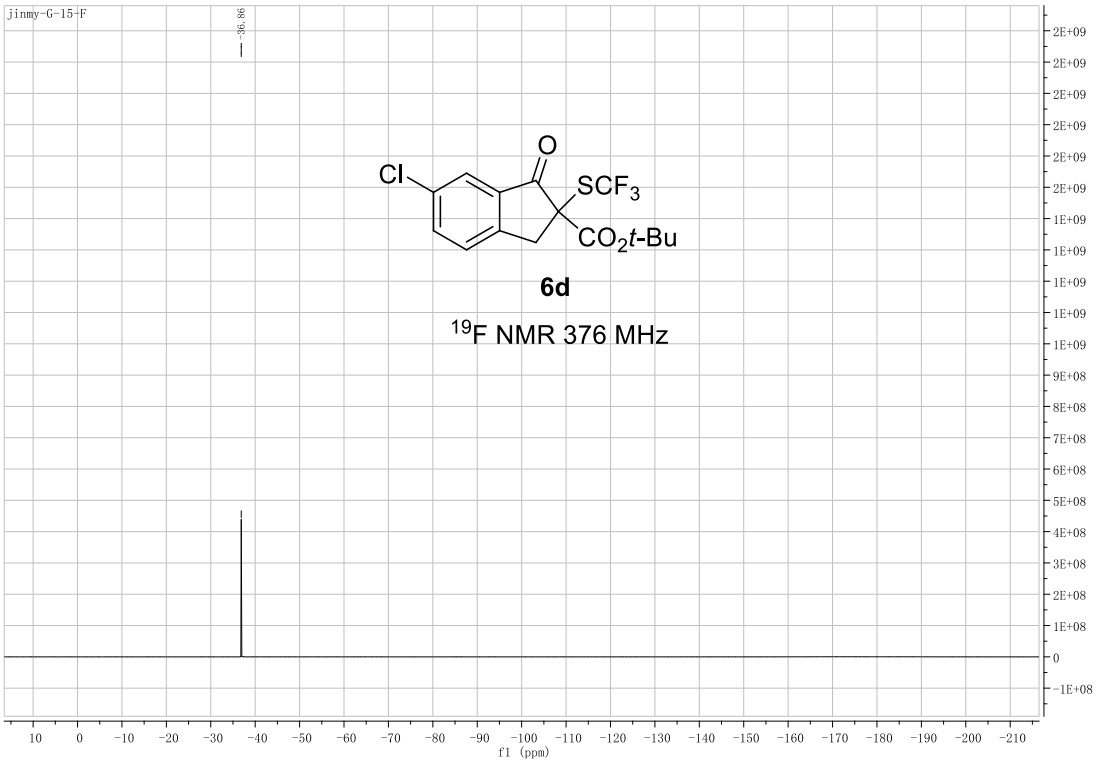

jinmy-G-17-H
O
SCF3
CO2Ad
6c
1H NMR 600 MHz
f1 (ppm)

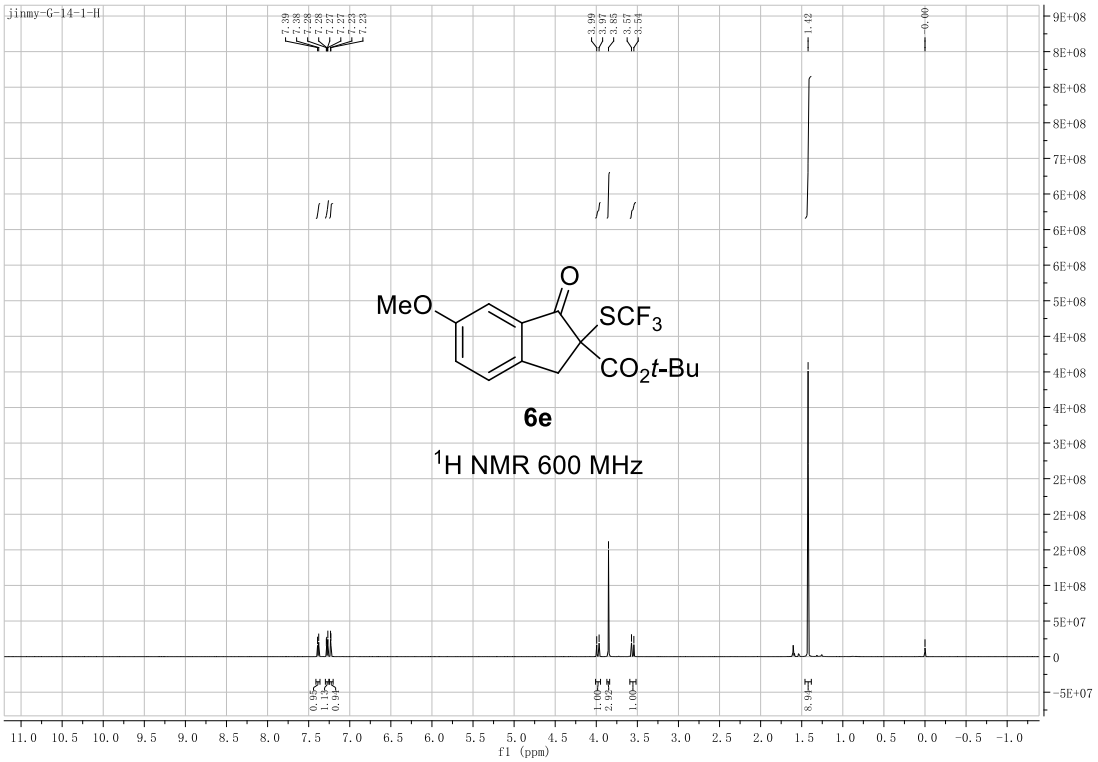

jinmy-G-17-C
O
SCF3
CO2Ad
6c
13C NMR 150 MHz
f1 (ppm)

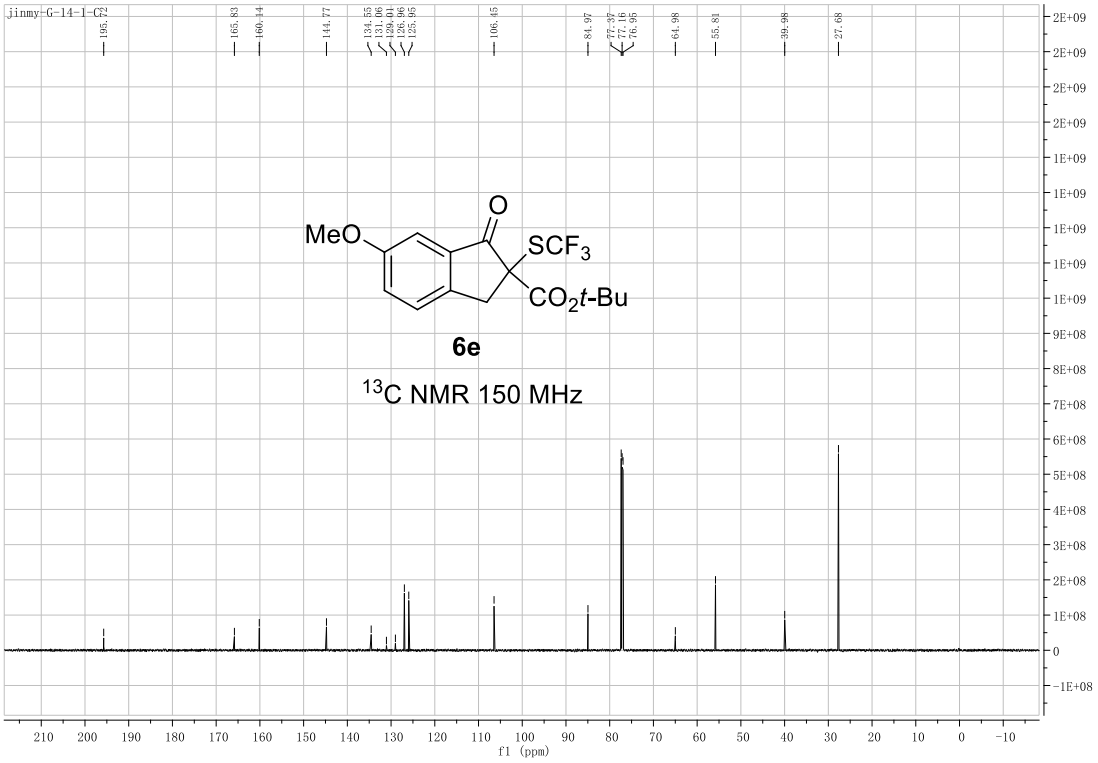

jinmy-G-17-F
-36.65
O
SCF3
CO2Ad
6c
19F NMR 376 MHz
f1 (ppm)

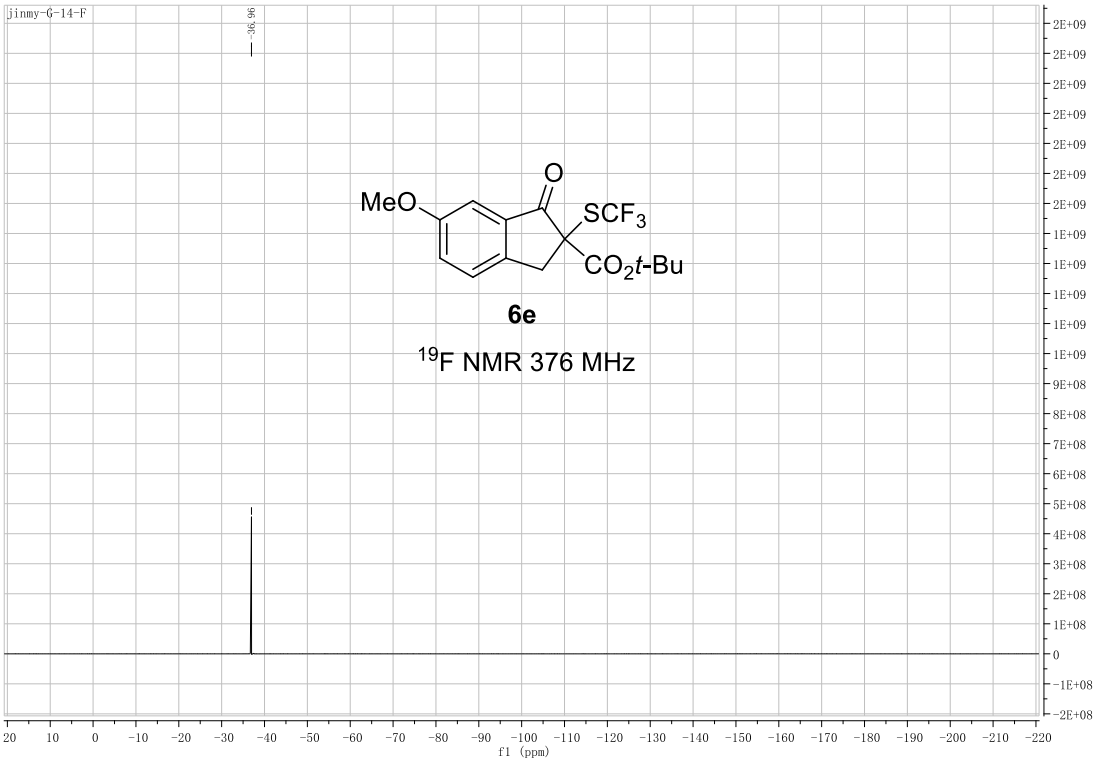

jinmy-G-15-H
7.79
7.65
7.46
7.45
7.27
4.05
4.02
3.61
3.58
1.42
0.00
O
Cl
SCF3
CO2t-Bu
6d
1H NMR 600 MHz
0.87H
0.94H
0.97H
1.00H
1.00H
9.22H
f1 (ppm)

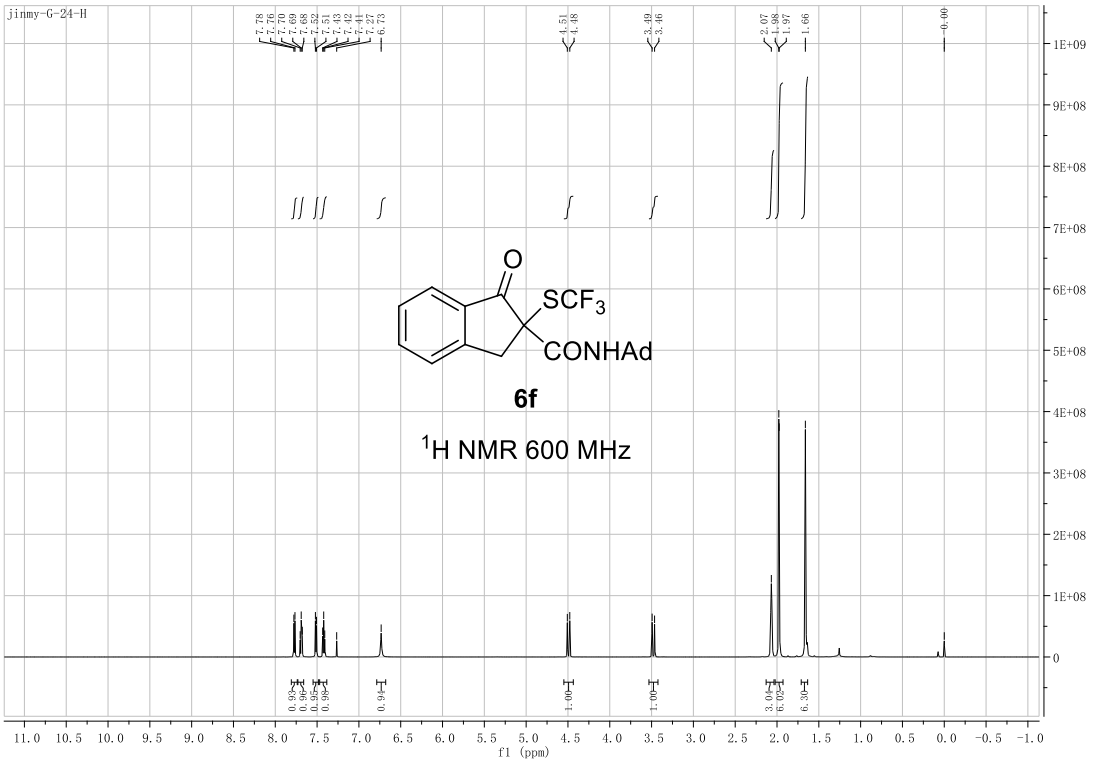

jinmy-G-15-C
194.60
165.34
149.86
136.38
134.93
134.83
130.95
128.90
127.46
125.26
85.41
77.37
77.16
76.95
64.68
40.13
27.66
Cl
O
SCF3
CO2t-Bu
6d
13C NMR 150 MHz
f1 (ppm)

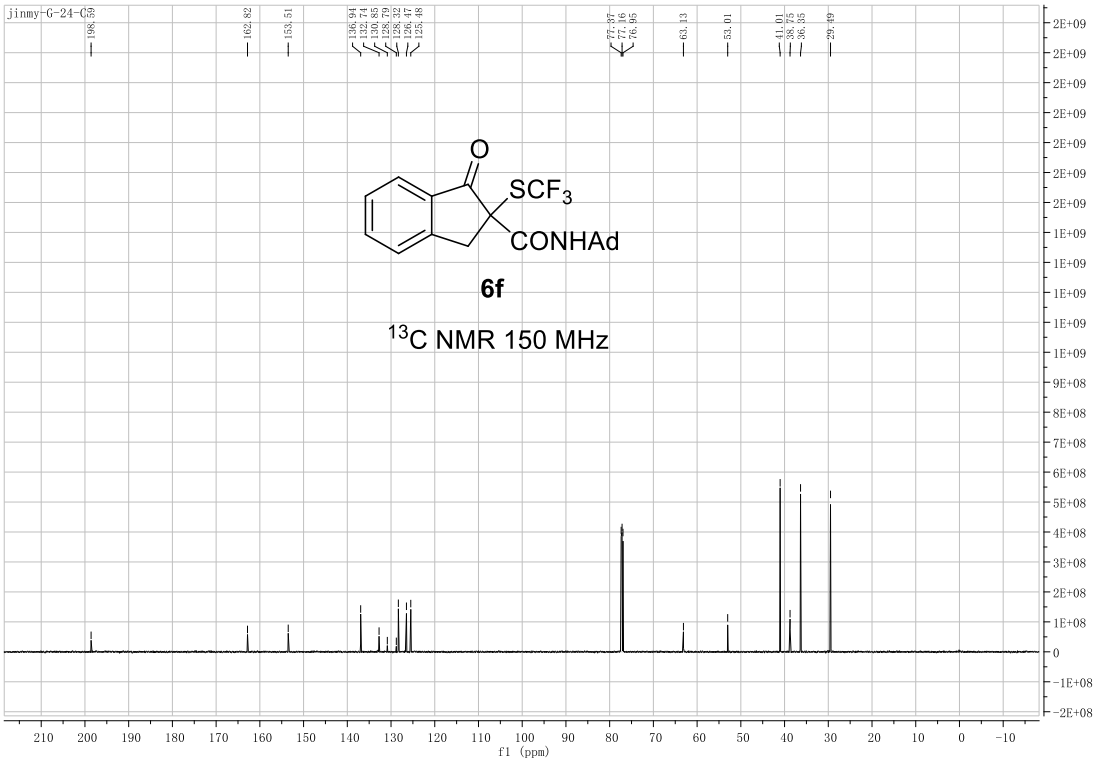

jinmy-G-15-F
-36.86
Cl
O
SCF3
CO2t-Bu
6d
19F NMR 376 MHz
f1 (ppm)

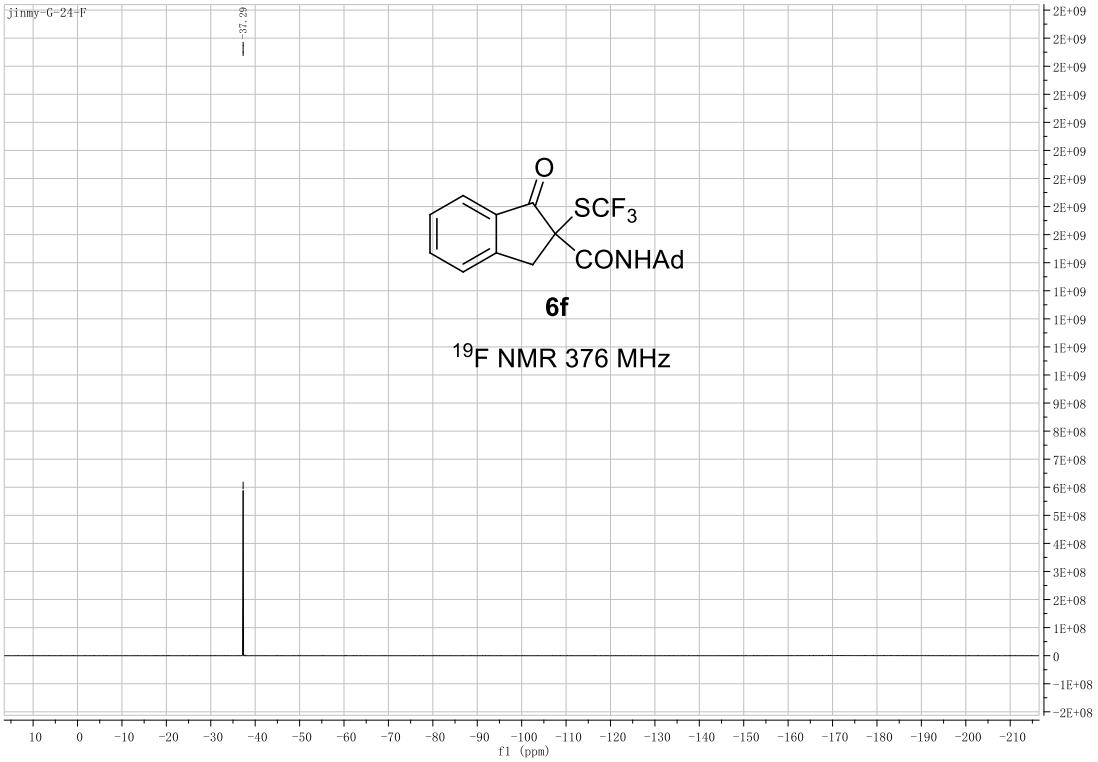

jinmy-G-14-1-H
MeO
O
SCF3
CO2t-Bu
6e
1H NMR 600 MHz
f1 (ppm)

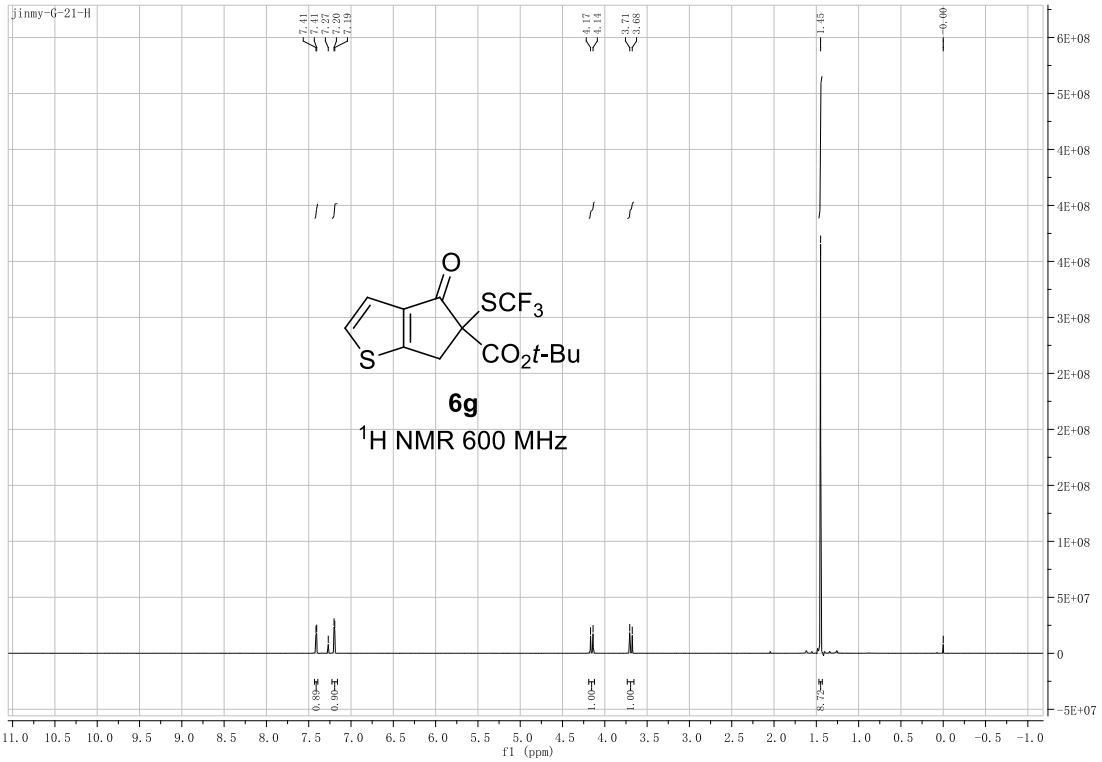

jinmy-G-14-1-C?2
MeO
O
SCF3
CO2t-Bu
6e
13C NMR 150 MHz
f1 (ppm)

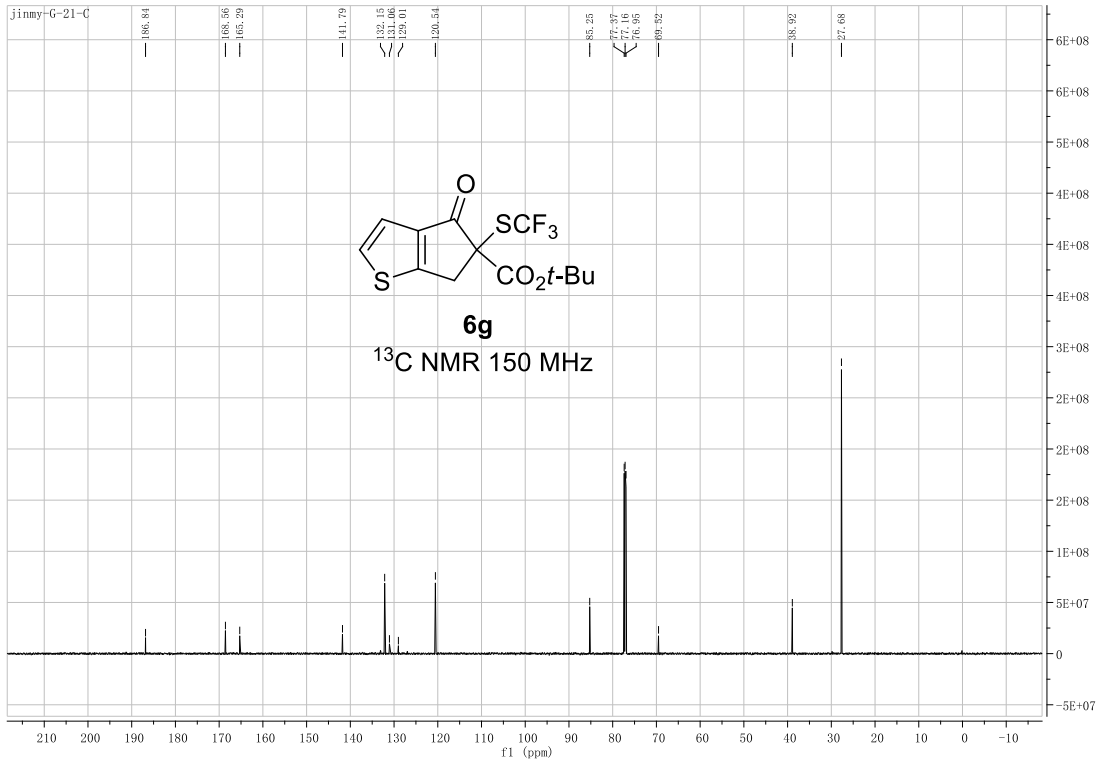

jinmy-G-14-F
-36.96
MeO
O
SCF3
CO2t-Bu
6e
19F NMR 376 MHz
f1 (ppm)

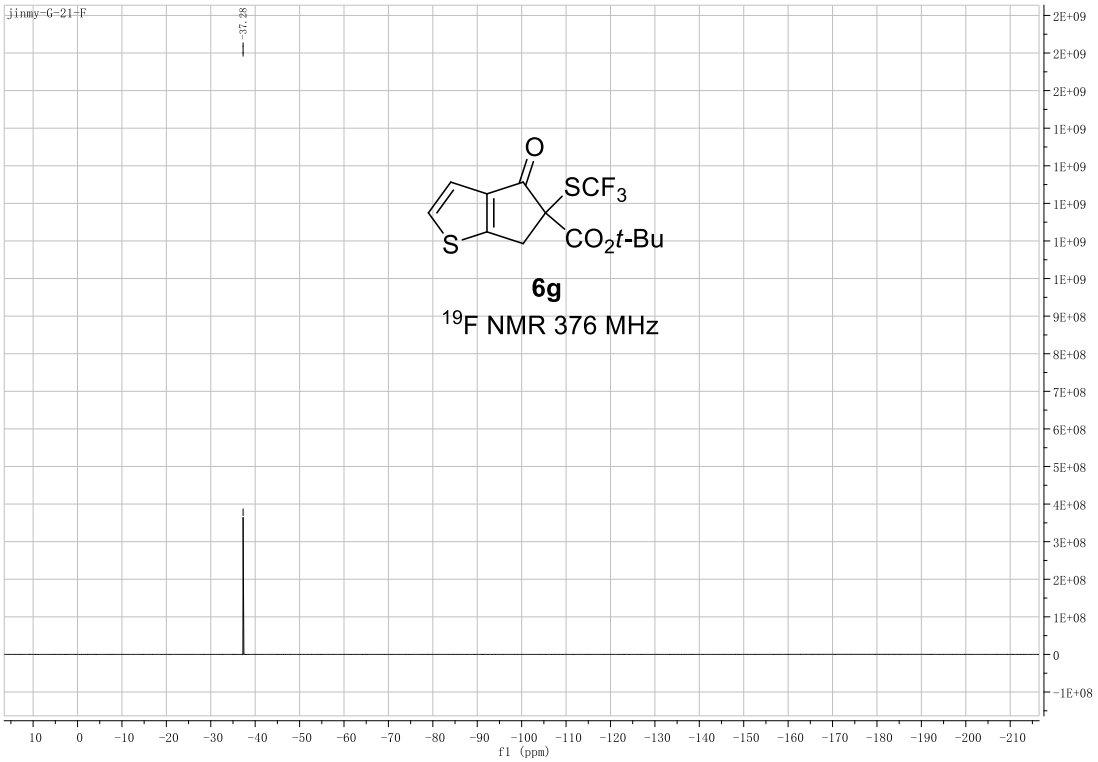

jinmy-G-24-H
7.78
7.76
7.70
7.69
7.68
7.52
7.51
7.43
7.42
7.41
7.27
6.73
4.51
4.48
3.49
3.46
2.07
1.98
1.97
1.66
0.00
O
SCF3
CONHAd
6f
1H NMR 600 MHz
0.98
0.99
0.95
0.98
0.94
1.00
1.00
3.04
6.02
6.30
f1 (ppm)

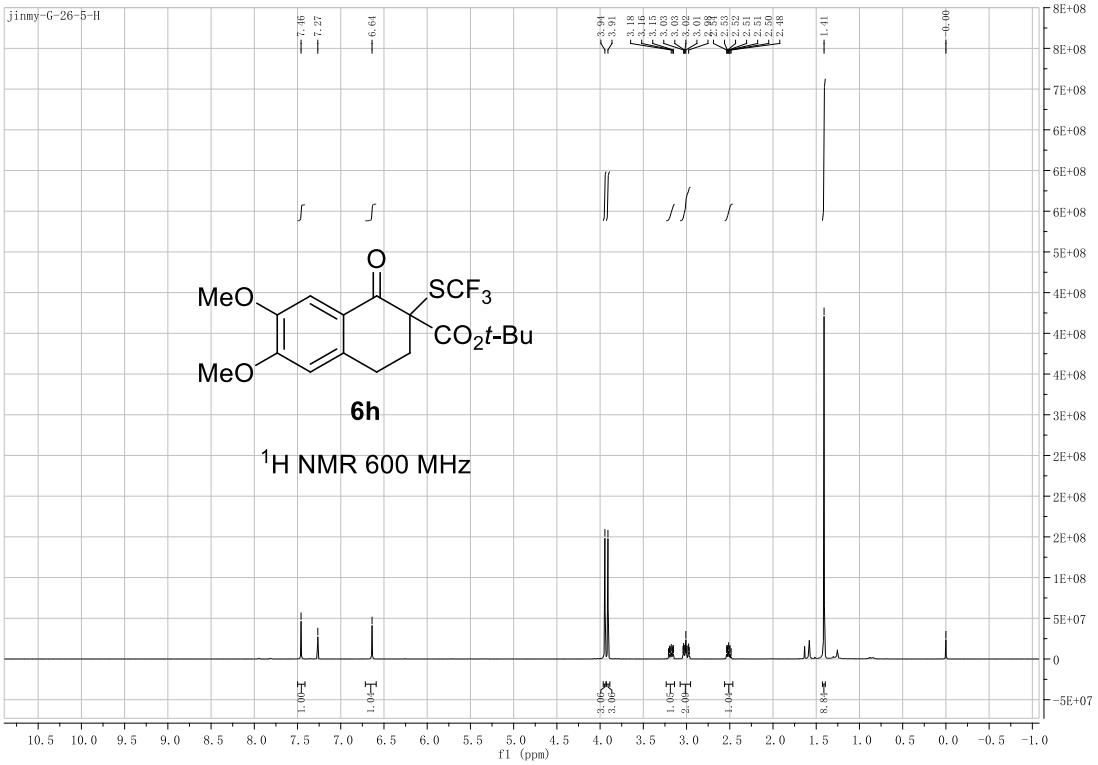

jinmy-G-24-C59
198.59
162.82
153.51
136.94
132.74
130.85
128.79
128.72
126.47
125.48
77.37
77.16
76.95
63.13
53.01
41.01
38.75
36.85
29.49
O
SCF3
CONHAd
6f
13C NMR 150 MHz
f1 (ppm)

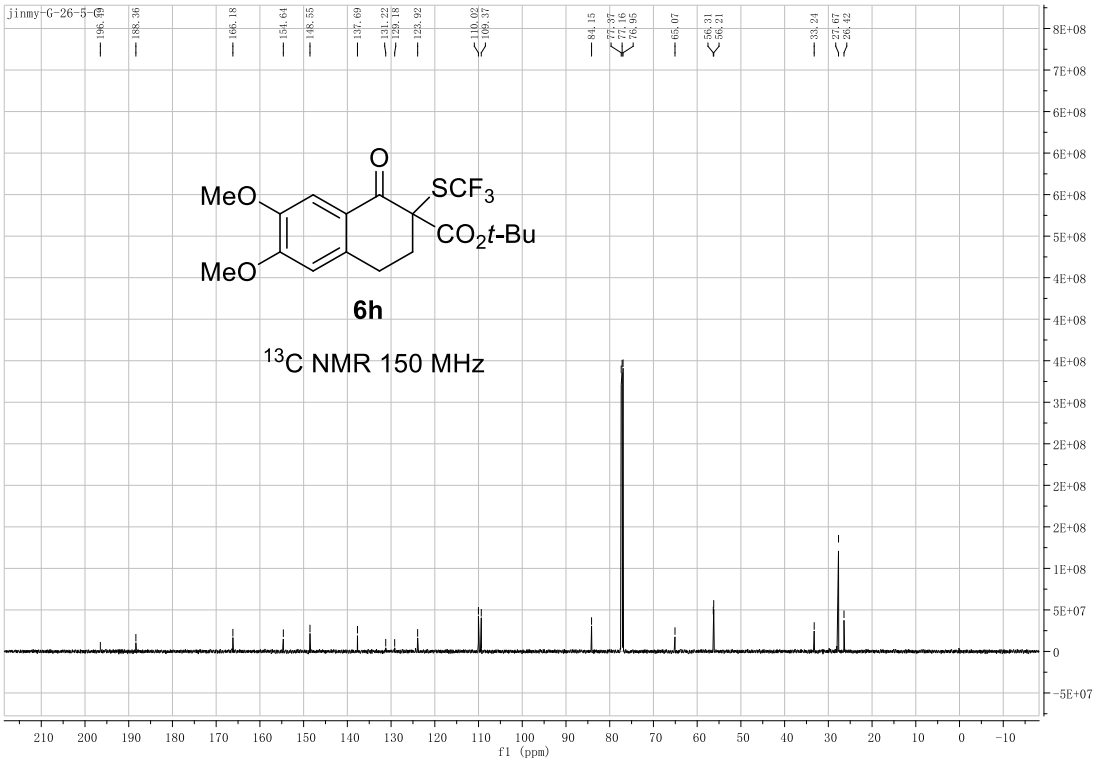

jinmy-G-24-F
-37.29
O
SCF3
CONHAd
6f
19F NMR 376 MHz
f1 (ppm)

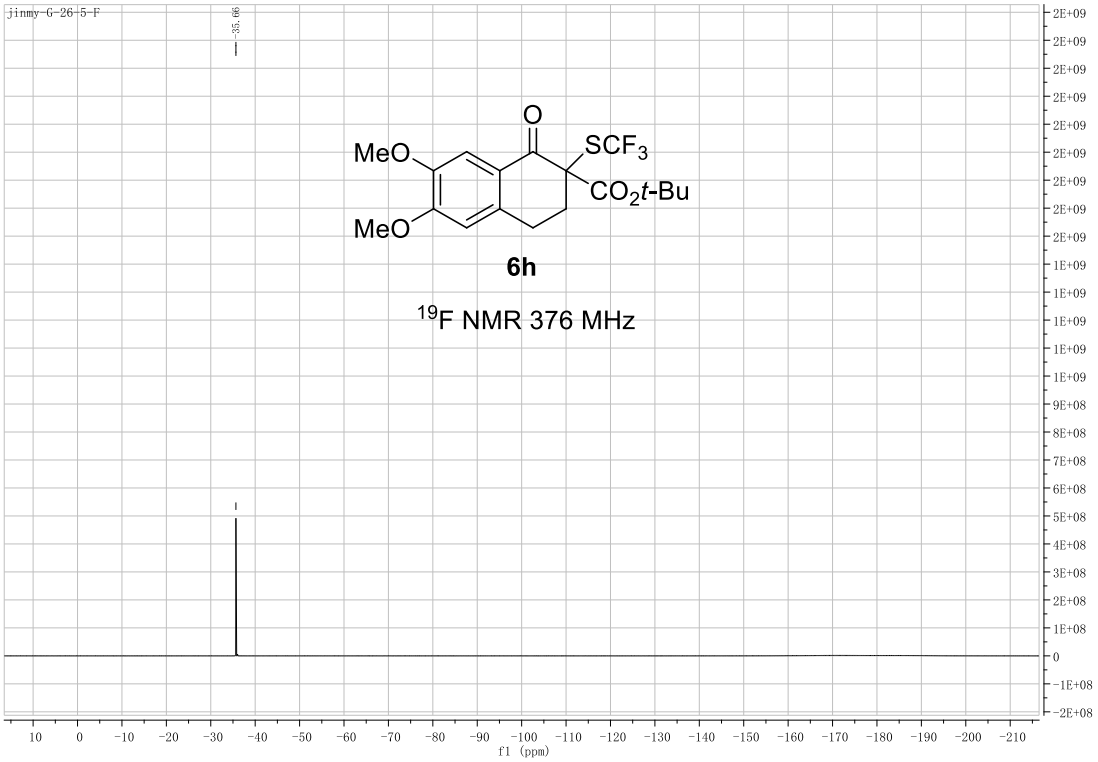

jinmy-G-21-H
7.41
7.41
7.27
7.20
7.19
4.17
4.14
3.71
3.68
1.45
0.00
O
SCF3
S
CO2t-Bu
6g
1H NMR 600 MHz
0.89
0.90
1.00
1.00
8.72
f1 (ppm)

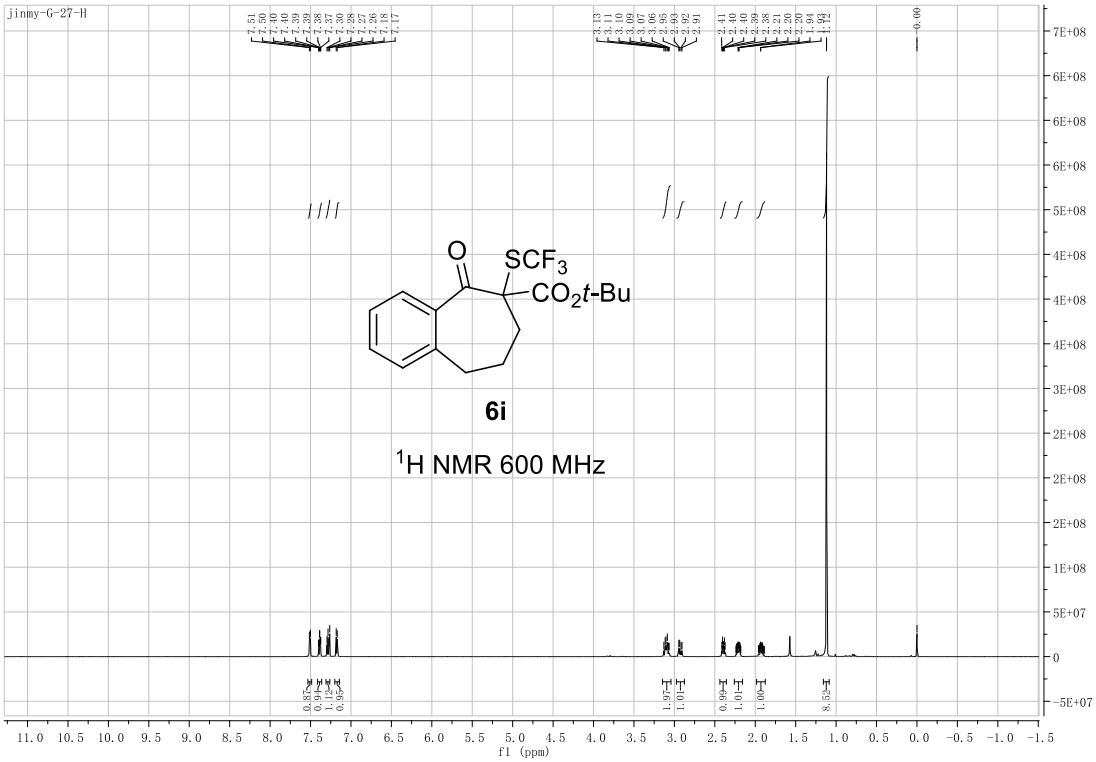

jinmy-G-21-C
186.84
168.56
165.29
141.79
132.15
131.06
129.01
120.54
85.25
77.37
77.16
76.95
69.82
38.92
27.68
O
SCF3
S
CO2t-Bu
6g
13C NMR 150 MHz
f1 (ppm)

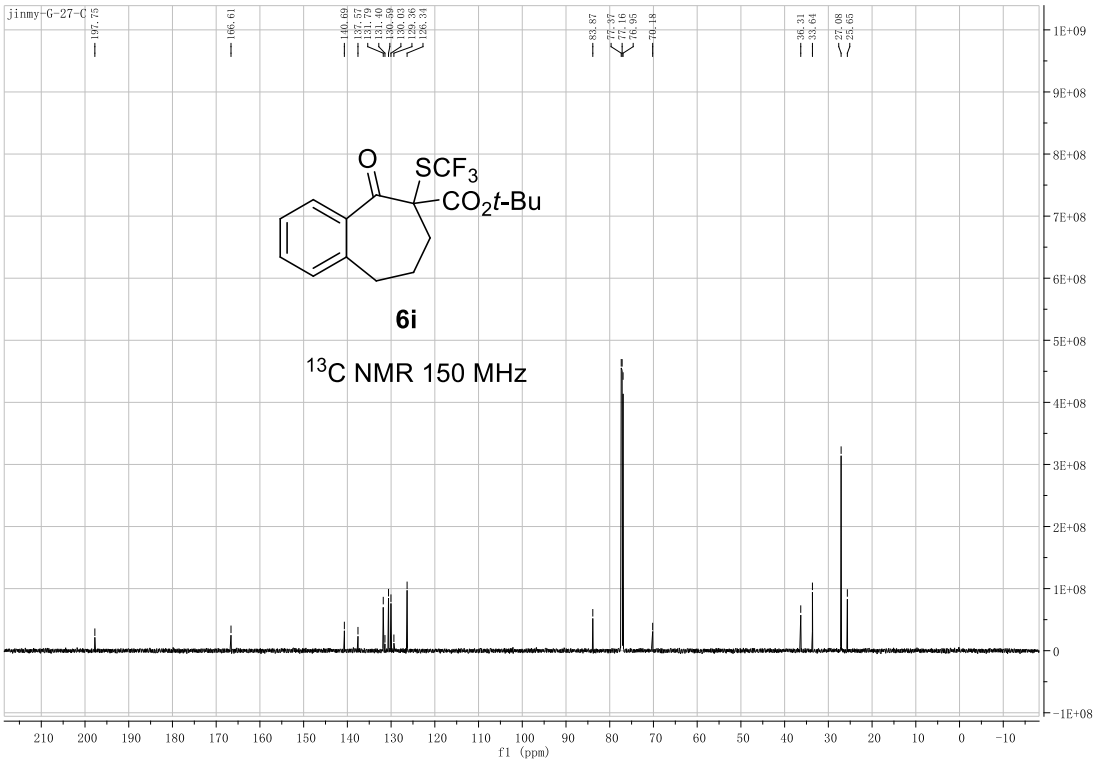

jinmy-G-21-F
-37.28
O
SCF3
CO2t-Bu
S
6g
19F NMR 376 MHz
f1 (ppm)

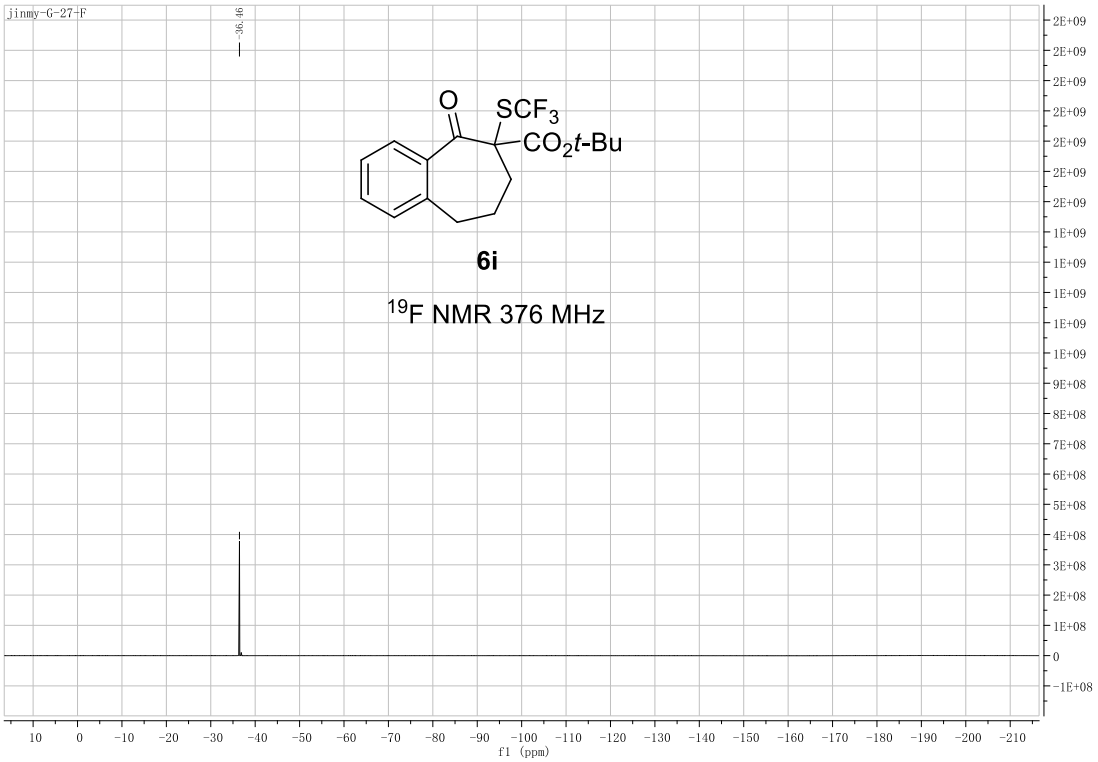

jinmy-G-26-5-H
7.46
7.27
6.64
3.94
3.91
3.18
3.16
3.15
3.03
3.02
3.01
2.53
2.52
2.51
2.50
2.48
1.41
0.00
O
MeO
MeO
SCF3
CO2t-Bu
6h
1H NMR 600 MHz
1.00
1.04
3.06
3.00
1.07
2.09
1.04
8.84
f1 (ppm)

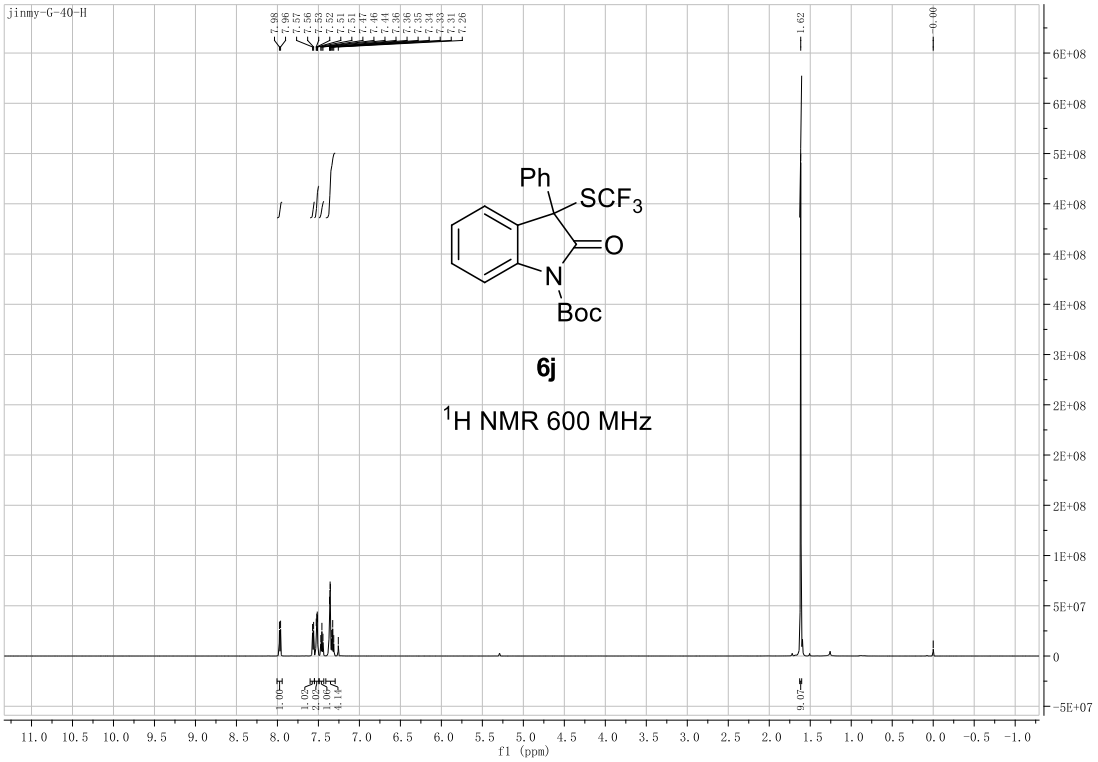

jinmy-G-26-5-F
196.49
188.36
166.18
154.64
148.55
137.69
131.22
129.18
123.92
110.02
109.37
84.15
77.37
77.16
76.95
65.07
56.31
56.21
33.24
27.67
26.42
MeO
MeO
O
SCF3
CO2t-Bu
6h
13C NMR 150 MHz
f1 (ppm)

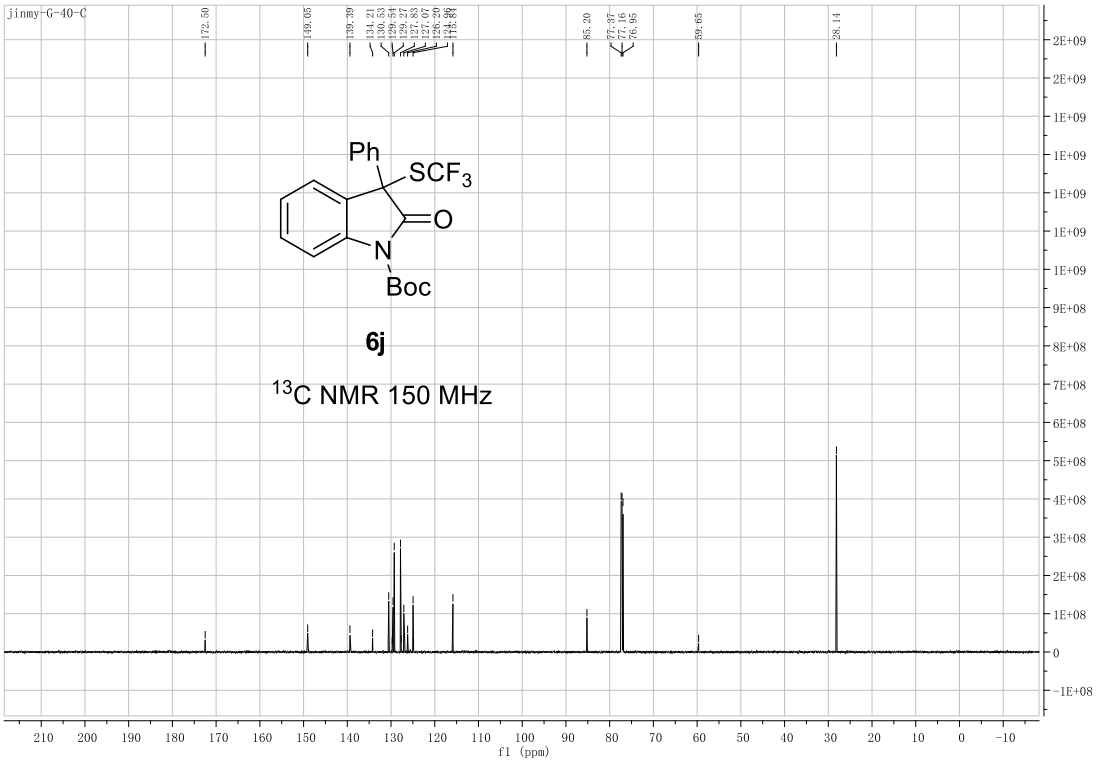

jinmy-G-26-5-F
-35.66
MeO
MeO
O
SCF3
CO2t-Bu
6h
19F NMR 376 MHz
f1 (ppm)

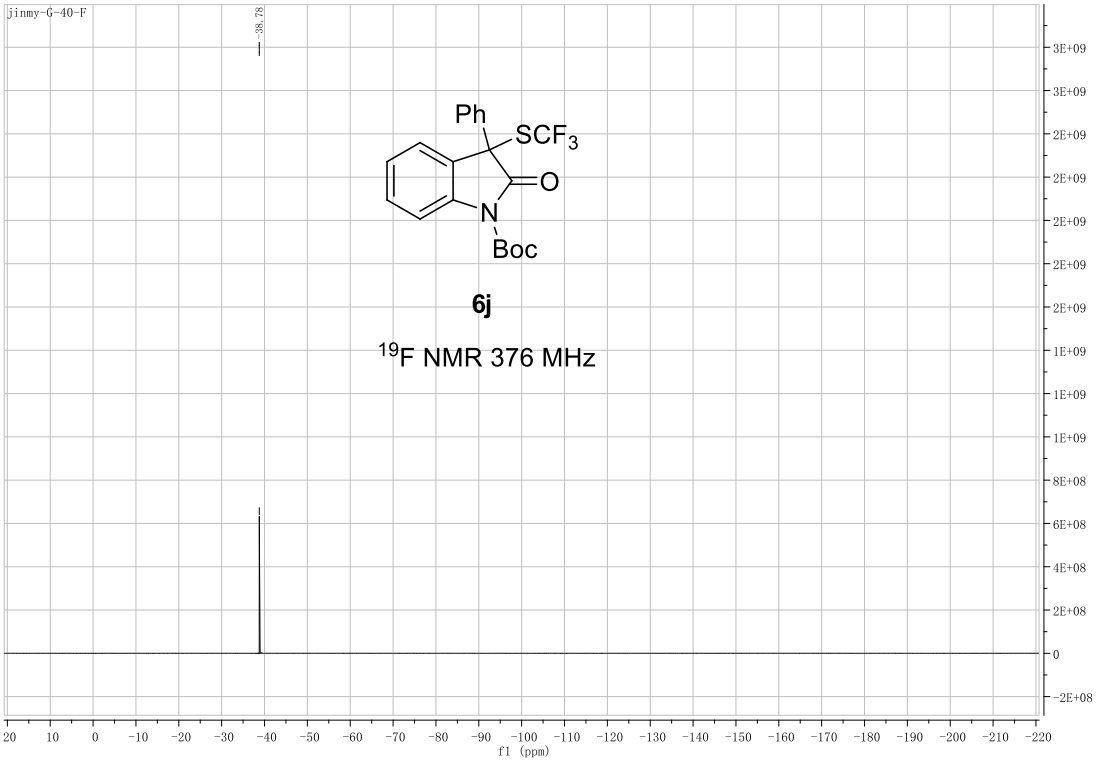

jinmy-G-27-H
O
SCF3
CO2t-Bu
6i
1H NMR 600 MHz
f1 (ppm)

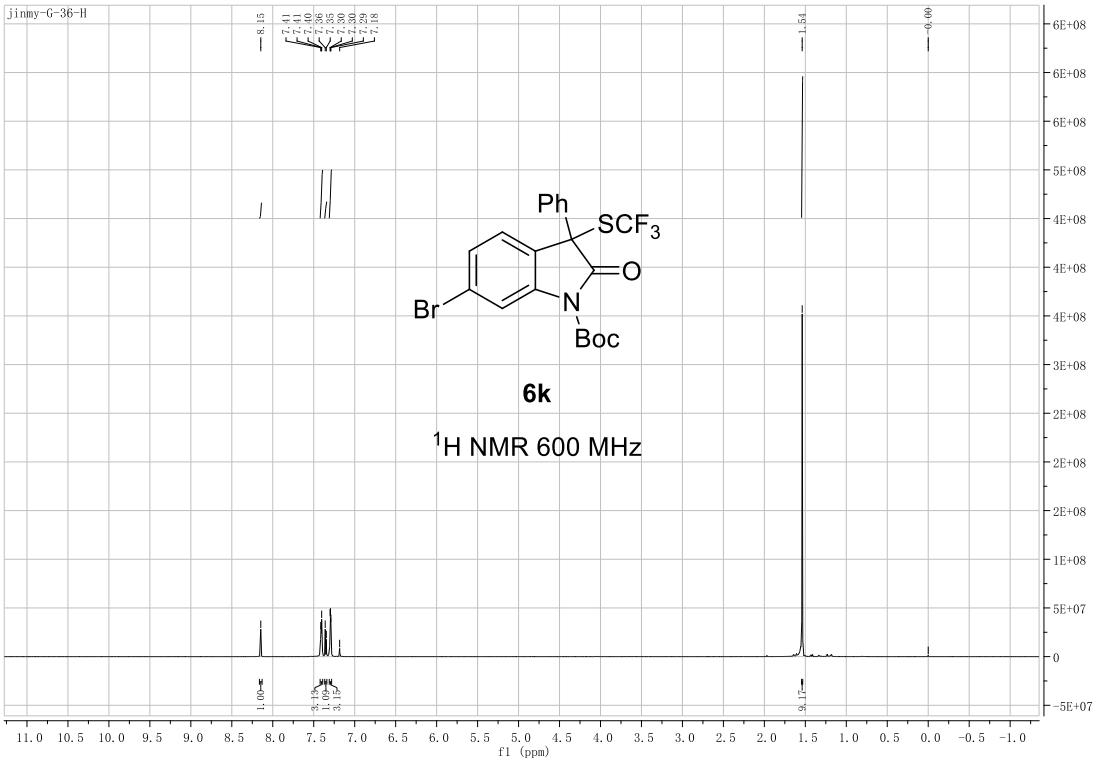

jinmy-G-27-C
O
SCF3
CO2t-Bu
6i
13C NMR 150 MHz
f1 (ppm)

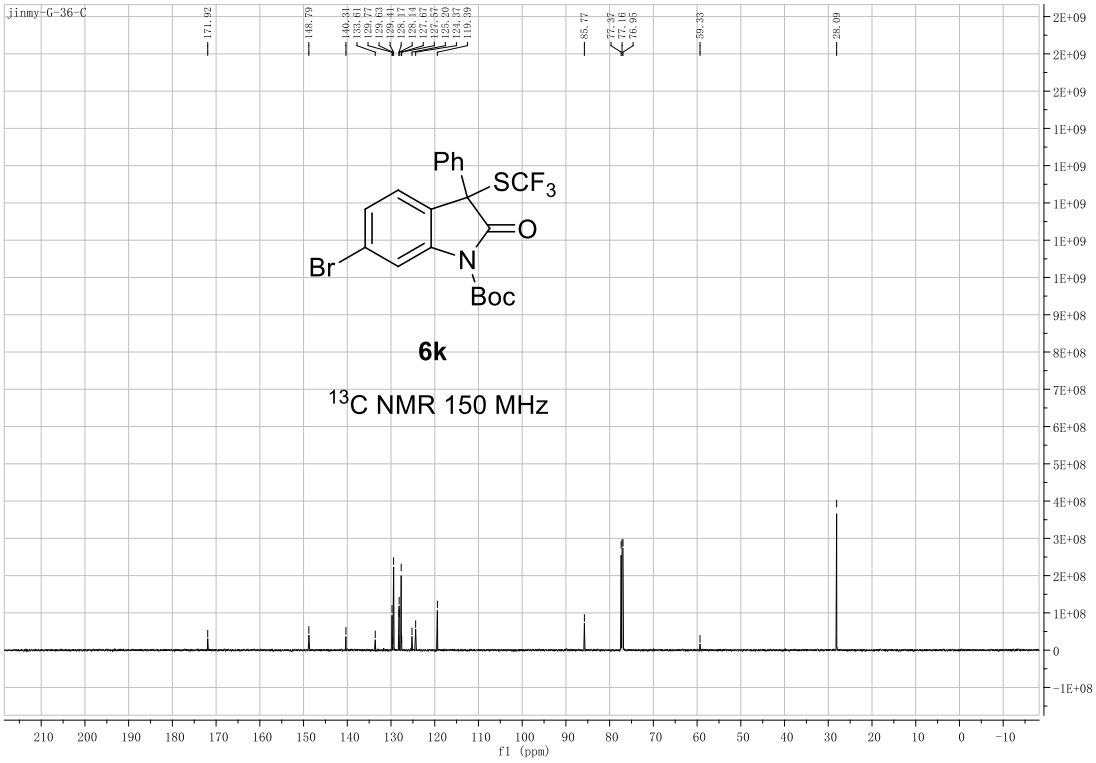

jinmy-G-27-F
-36.46
O
SCF3
CO2t-Bu
6i
19F NMR 376 MHz
f1 (ppm)

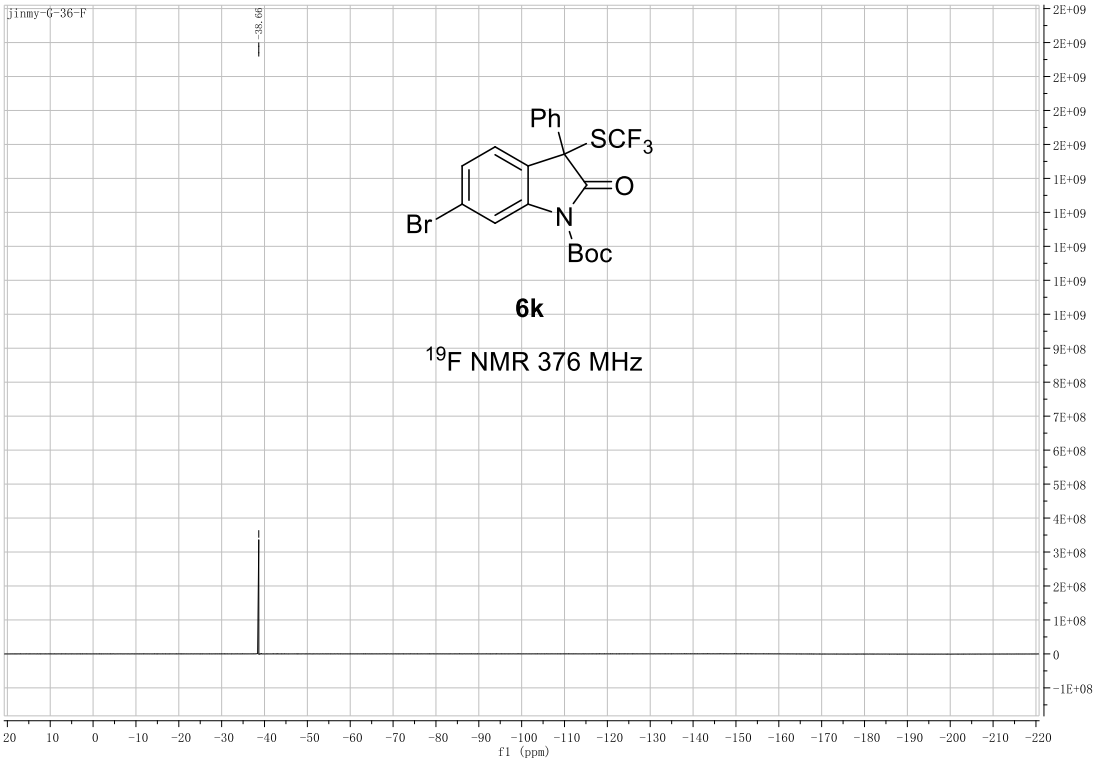

jinmy-G-40-H
7.98
7.96
7.57
7.56
7.53
7.52
7.51
7.47
7.46
7.44
7.36
7.35
7.34
7.33
7.31
7.26
1.62
0.00
Ph
SCF3
O
N
Boc
6j
1H NMR 600 MHz
1.00
1.02
2.02
4.14
9.07
f1 (ppm)

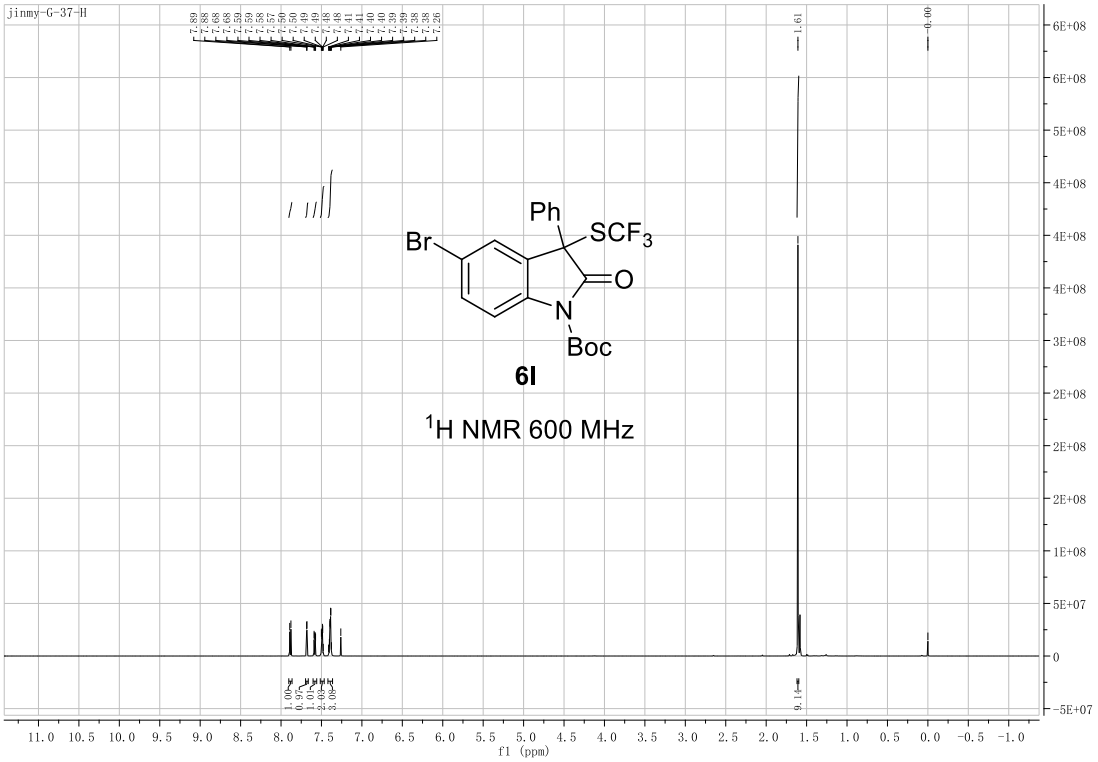

jinmy-G-40-C
172.50
149.05
139.39
134.21
130.53
129.94
129.27
127.83
127.57
126.70
124.80
113.84
85.20
77.37
77.16
76.95
59.65
28.14
Ph
SCF3
O
N
Boc
6j
13C NMR 150 MHz
f1 (ppm)


jinmy-G-40-F
-38.78
Ph
SCF3
O
N
Boc
6j
19F NMR 376 MHz
f1 (ppm)


jinmy-G-36-H
Ph
SCF3
O
Br
N
Boc
6k
1H NMR 600 MHz
f1 (ppm)


jinmy-G-36-C
Ph
SCF3
O
Br
N
Boc
6k
13C NMR 150 MHz
f1 (ppm)


jinmy-G-36-F
-38.66
Ph
SCF3
O
Br
N
Boc
6k
19F NMR 376 MHz
f1 (ppm)


jinmy-G-37-H
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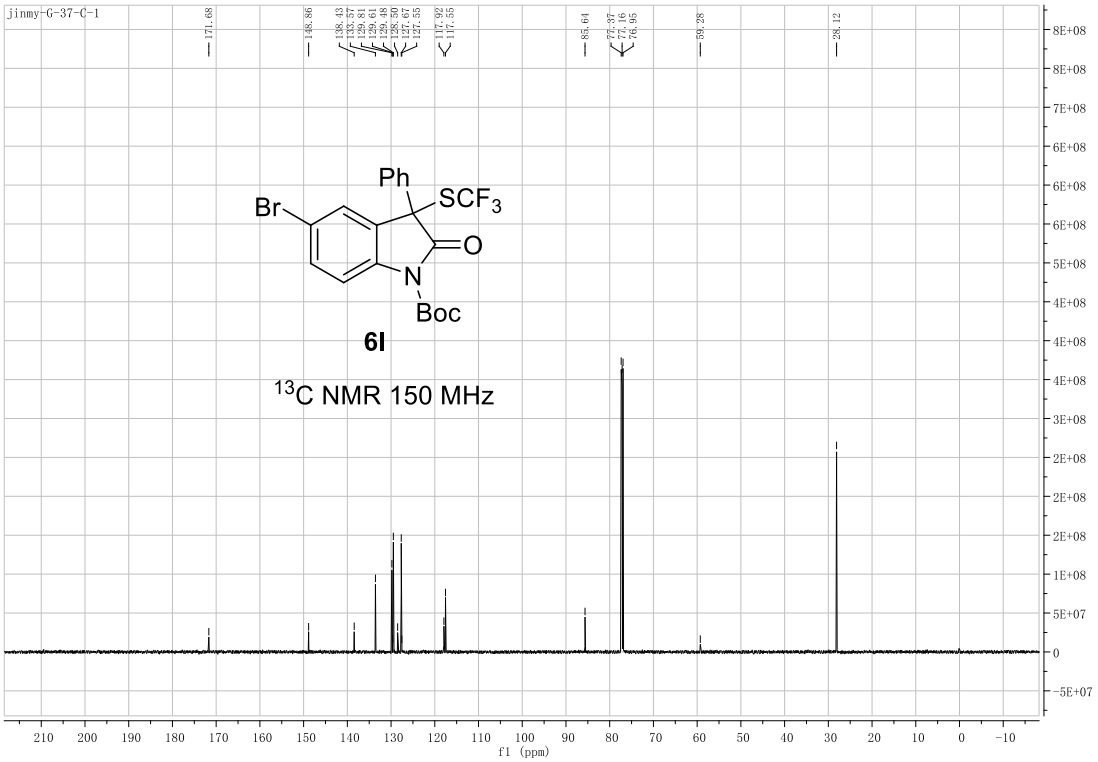
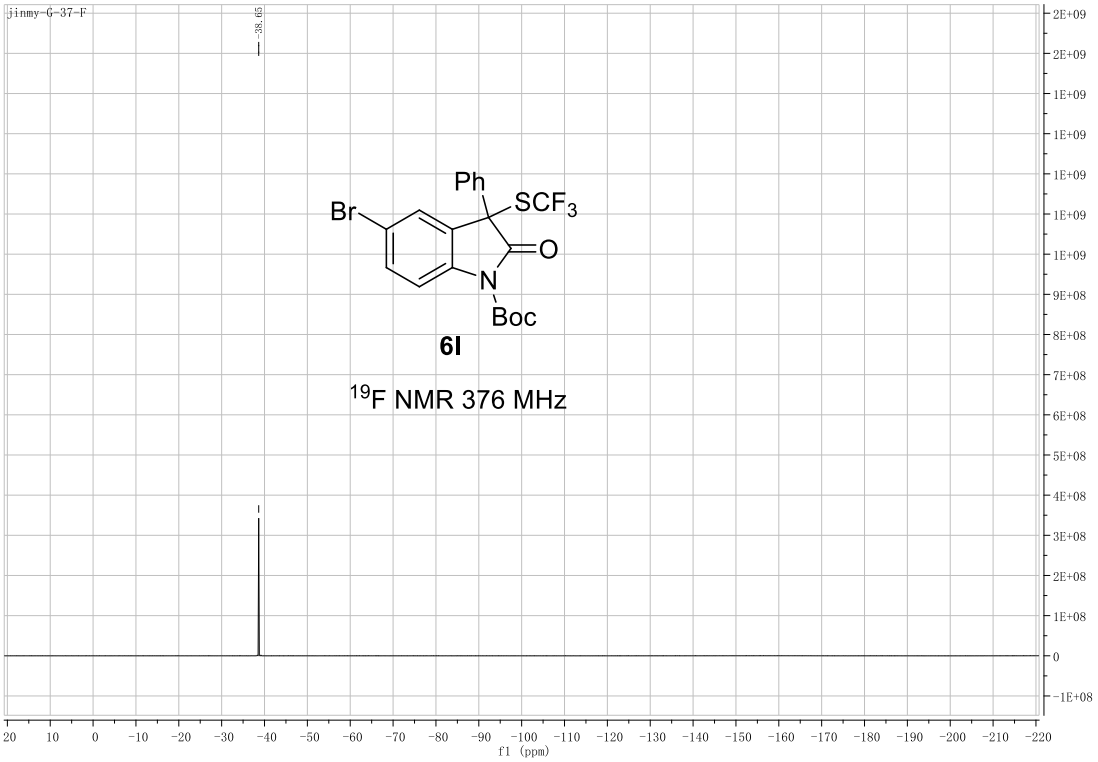
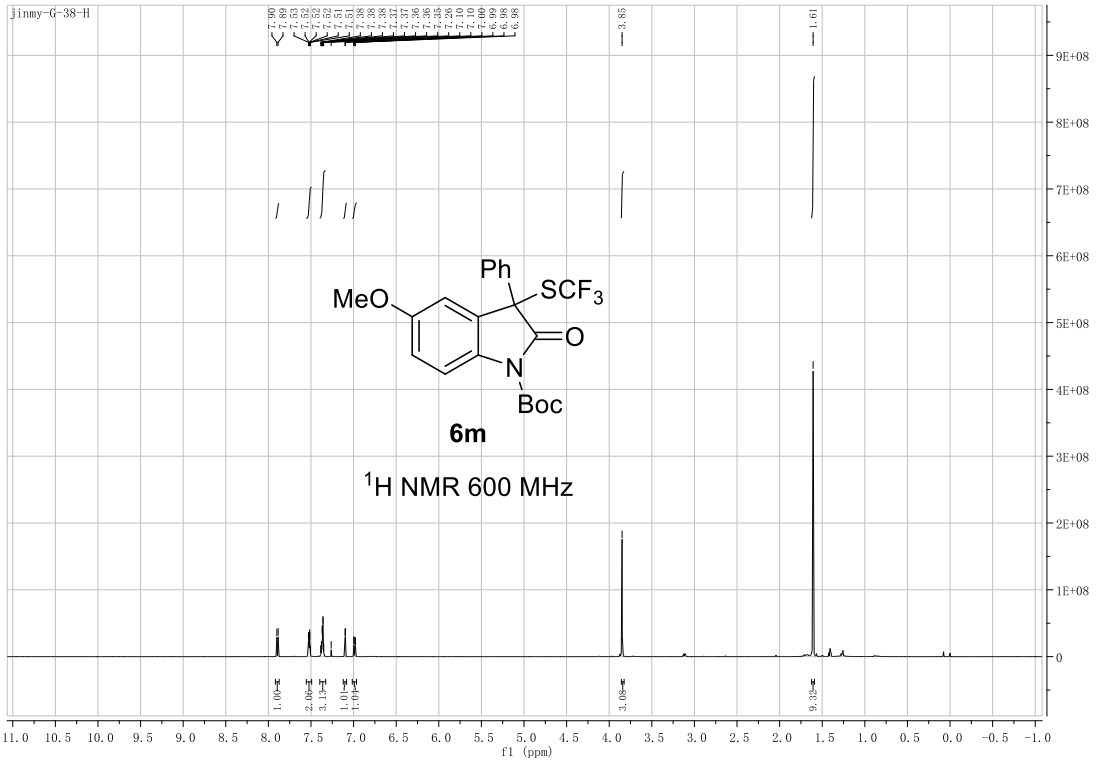
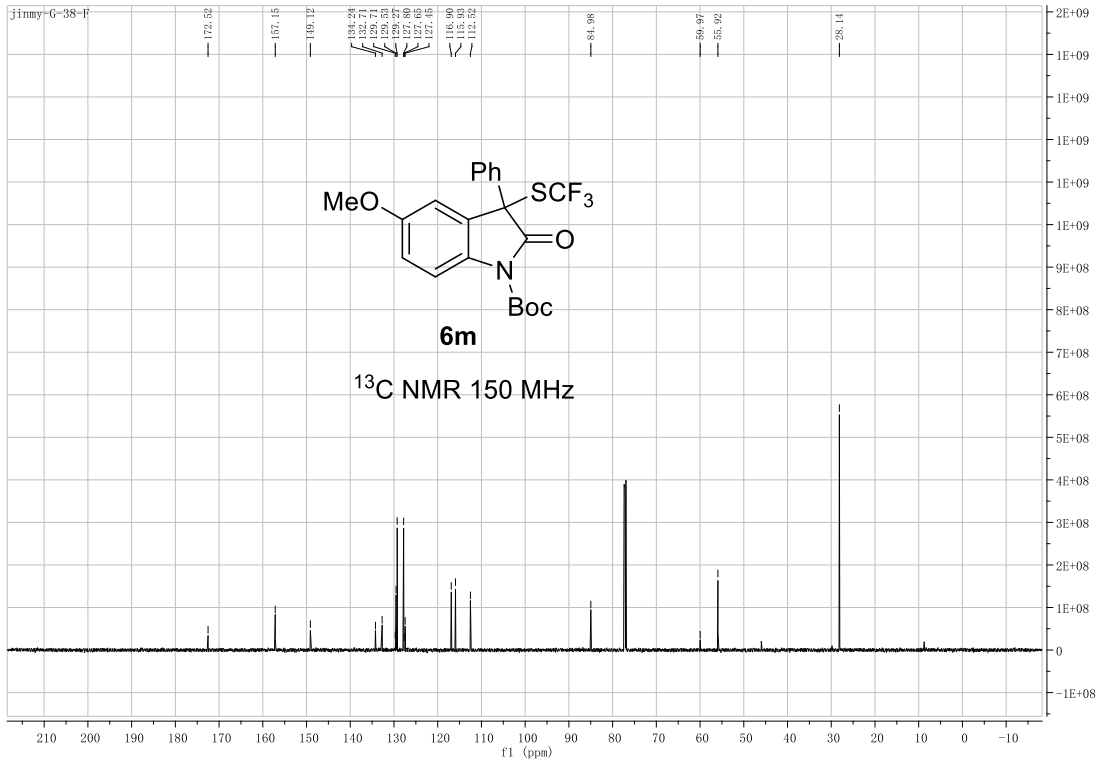
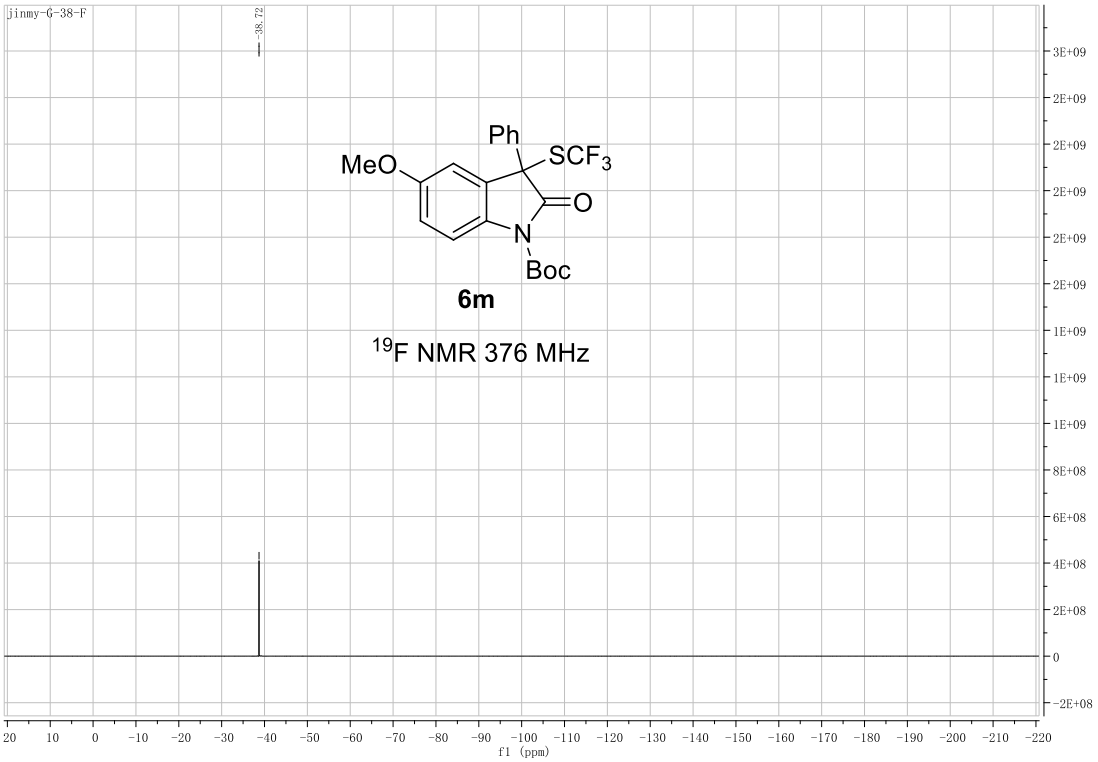
0.00
Ph
SCF3
Br
O
N
Boc
6l
1H NMR 600 MHz
f1 (ppm)

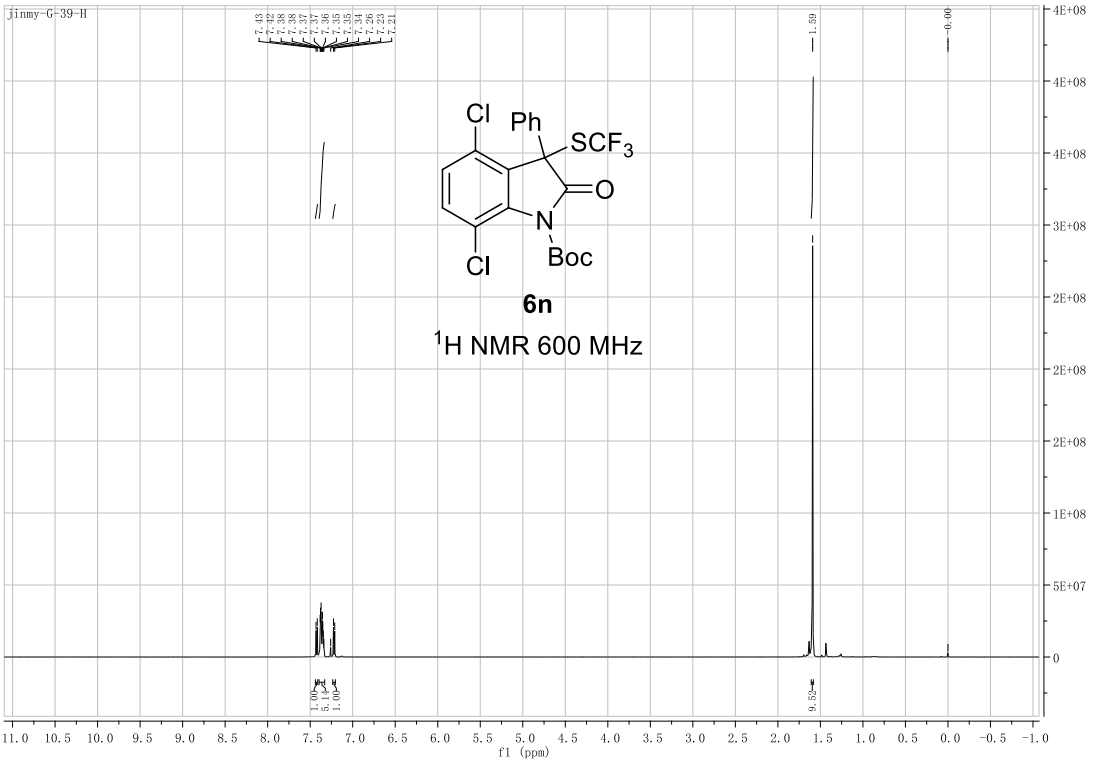

jinmy-G-37-C-1
171.68
148.86
138.43
133.57
129.61
129.48
128.30
127.67
127.55
117.92
117.55
83.64
77.37
77.16
76.95
59.28
28.12
Ph
SCF3
Br
O
N
Boc
6l
13C NMR 150 MHz
f1 (ppm)

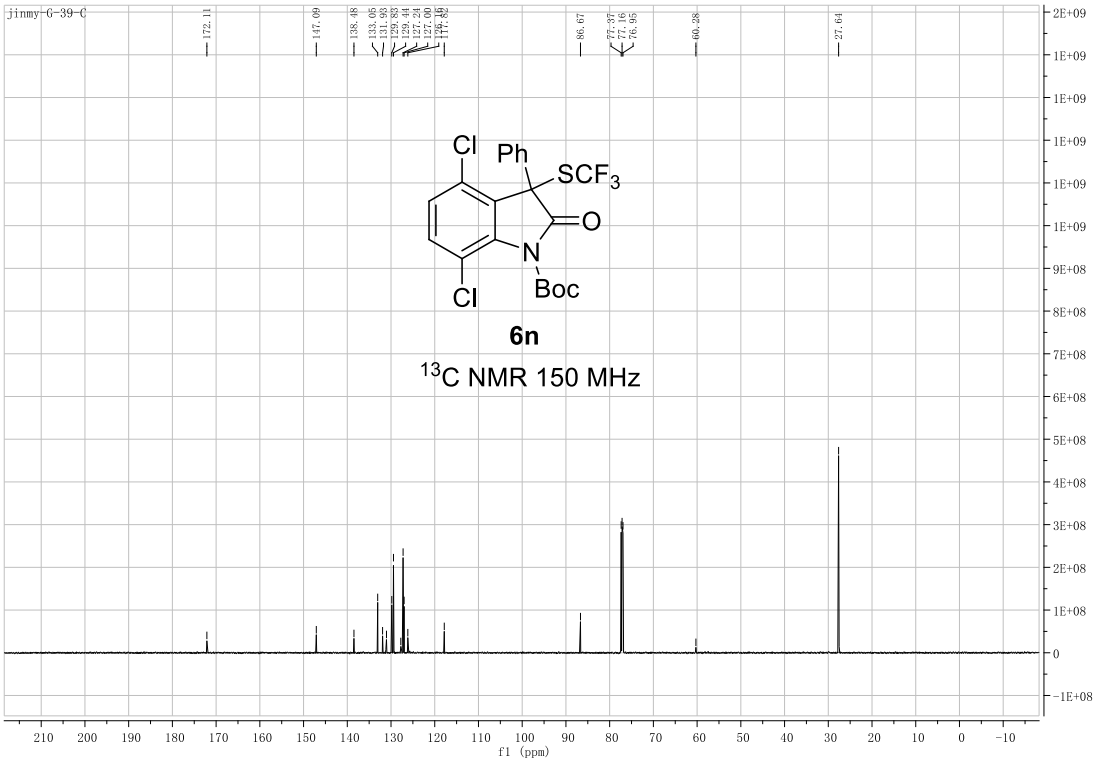

jinmy-G-37-F
-38.65
Ph
SCF3
Br
O
N
Boc
6l
19F NMR 376 MHz
f1 (ppm)

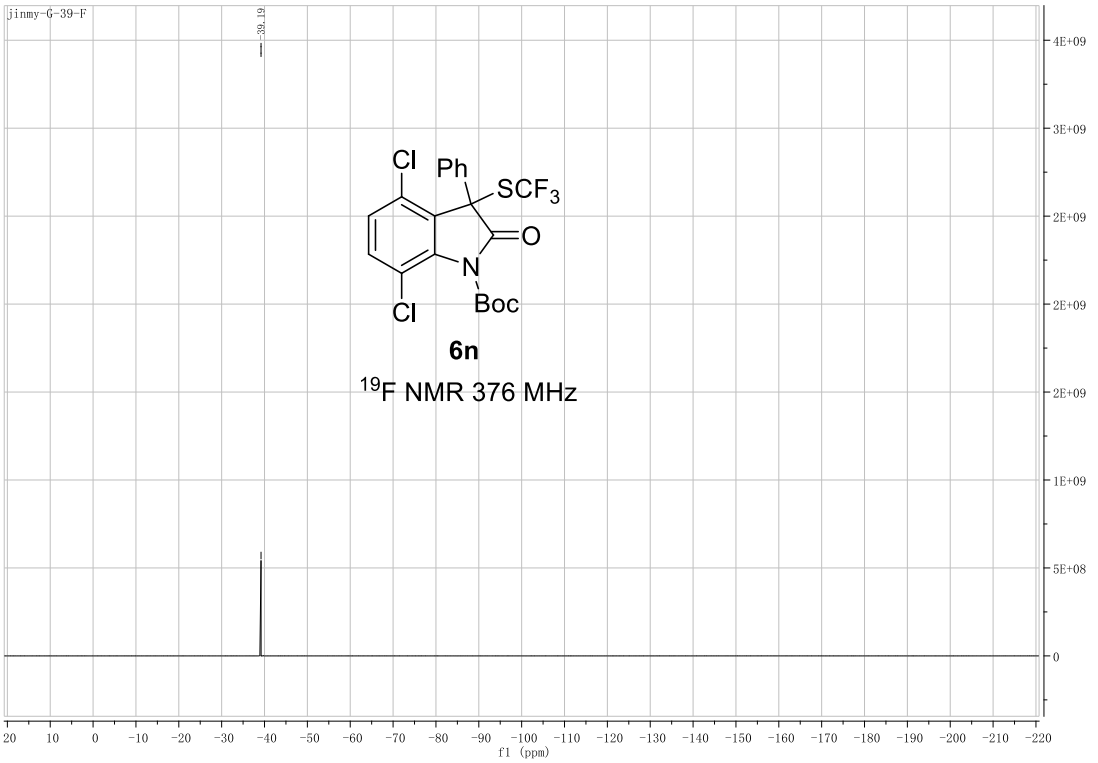

jinmy-G-38-H
7.90
7.89
7.53
7.52
7.52
7.52
7.51
7.51
7.38
7.38
7.38
7.37
7.37
7.36
7.36
7.35
7.26
7.10
7.10
7.09
6.99
6.98
6.98
3.85
1.61
Ph
SCF3
MeO
O
N
Boc
6m
1H NMR 600 MHz
1.00
2.06
3.13
1.01
1.04
3.08
9.32
f1 (ppm)

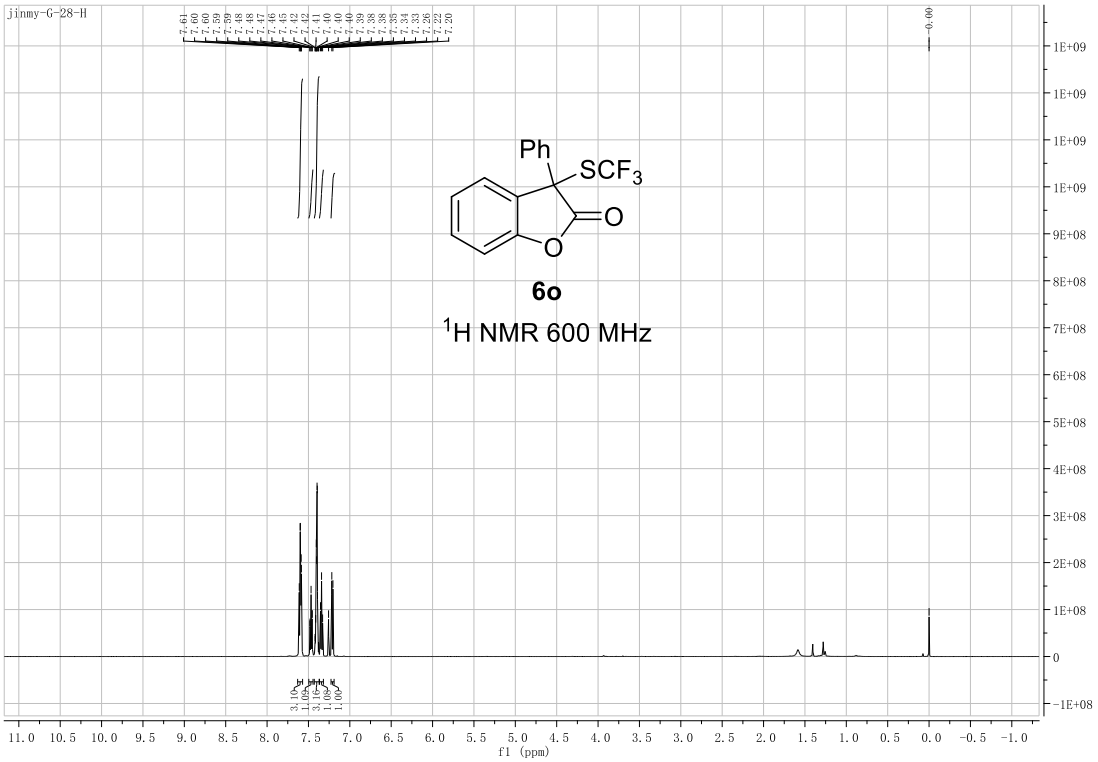

jinmy-G-38-F
172.52
157.15
149.12
134.24
132.71
129.71
129.53
129.27
127.80
127.65
127.45
116.90
115.93
112.52
84.98
69.97
55.92
28.14
Ph
SCF3
MeO
O
N
Boc
6m
13C NMR 150 MHz
f1 (ppm)

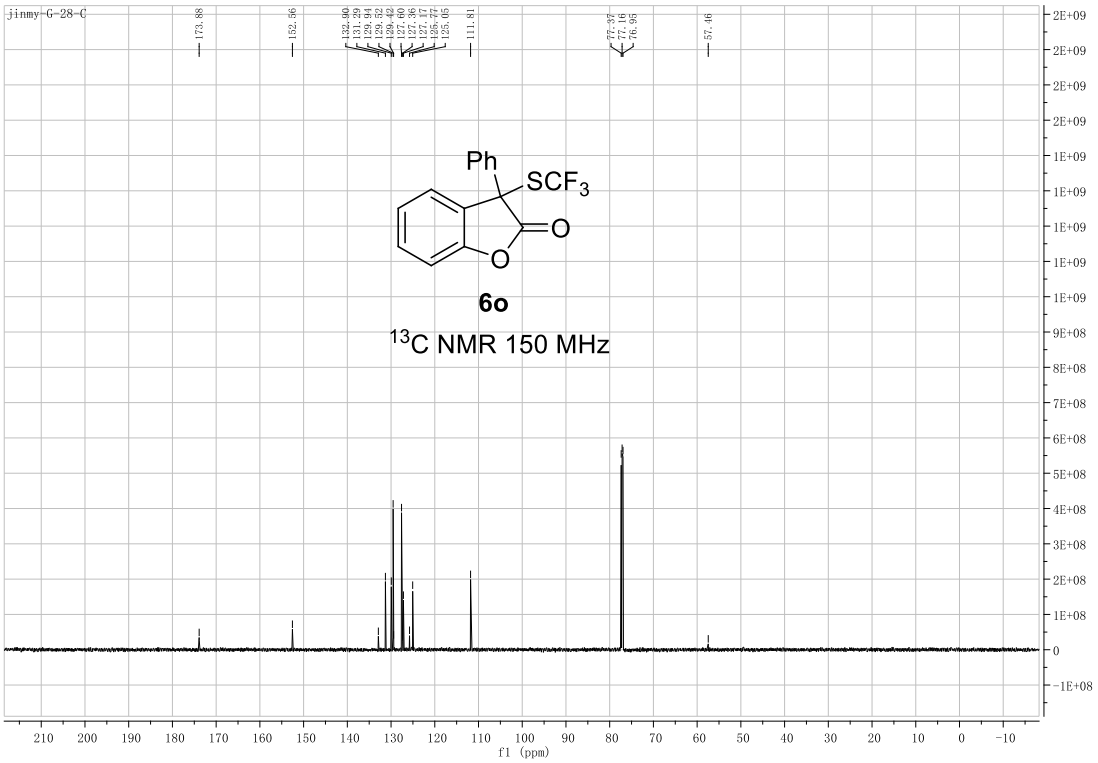

jinmy-G-38-F
-38.72
Ph
SCF3
MeO
O
N
Boc
6m
19F NMR 376 MHz
f1 (ppm)

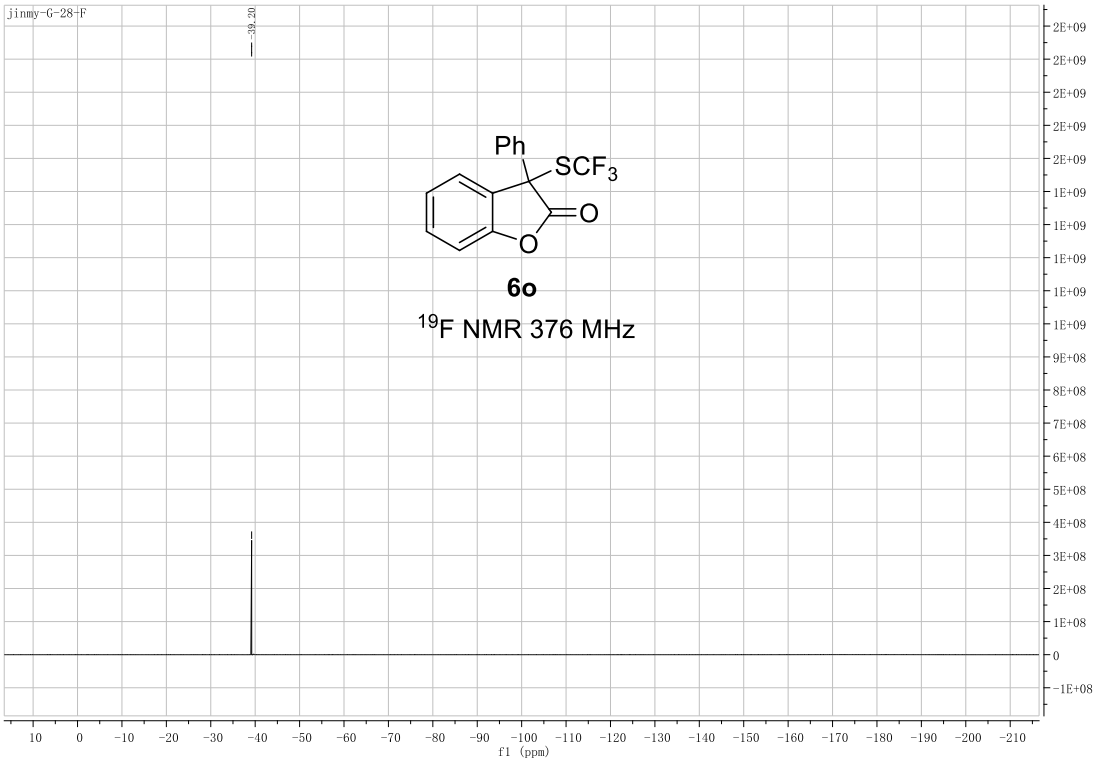

jinmy-G-39-H
7.43
7.42
7.38
7.37
7.37
7.36
7.35
7.34
7.26
7.25
7.21
1.59
0.00
Cl
Ph
SCF3
O
N
Boc
Cl
6n
1H NMR 600 MHz
1.00
1.02
1.00
9.62
f1 (ppm)

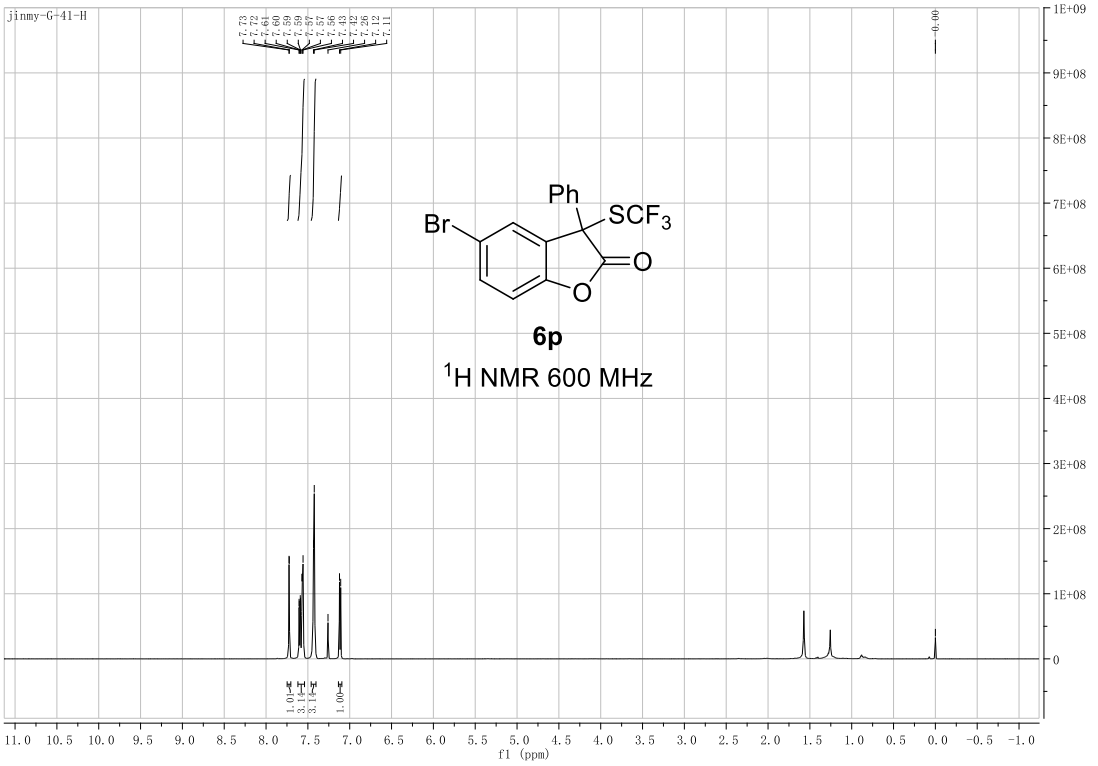

jinmy-G-39-C
172.11
147.09
138.48
133.05
131.85
129.44
127.24
127.00
86.67
77.37
77.16
76.95
60.28
27.64
Cl
Ph
SCF3
O
N
Boc
Cl
6n
13C NMR 150 MHz
f1 (ppm)

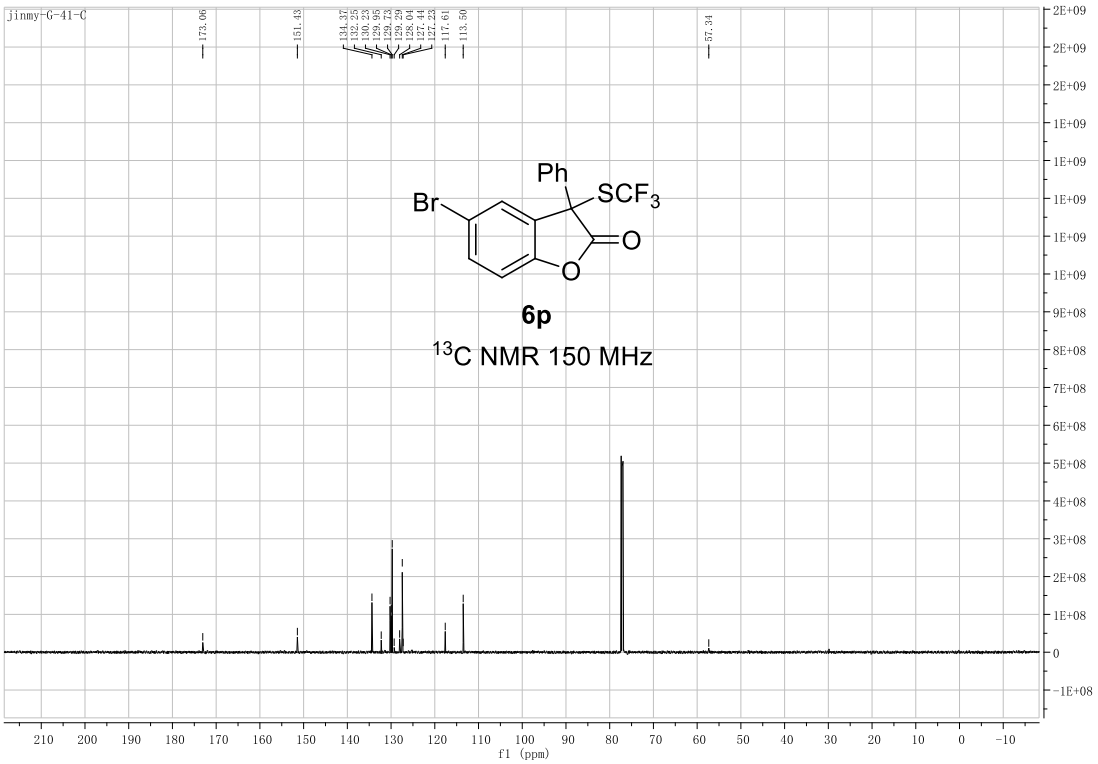

jinmy-G-39-F
-39.19
Cl
Ph
SCF3
O
N
Boc
Cl
6n
19F NMR 376 MHz
f1 (ppm)

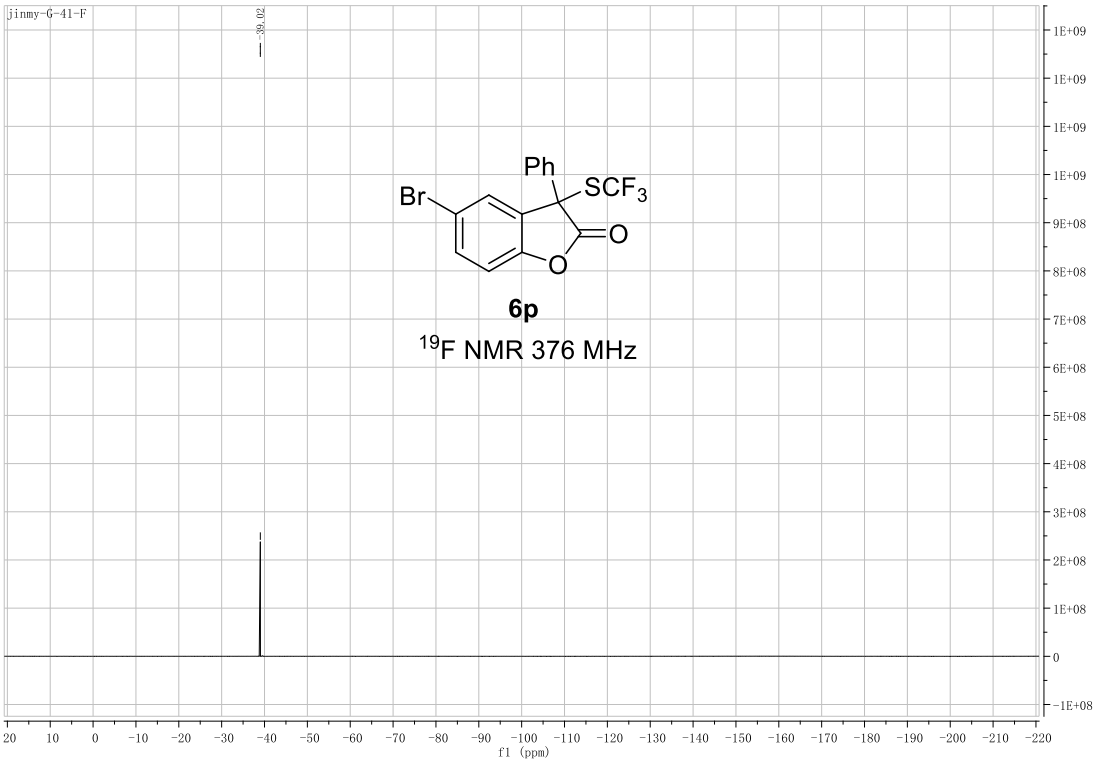

jinmy-G-28-H
Ph
SCF3
O
O
6o
1H NMR 600 MHz
f1 (ppm)

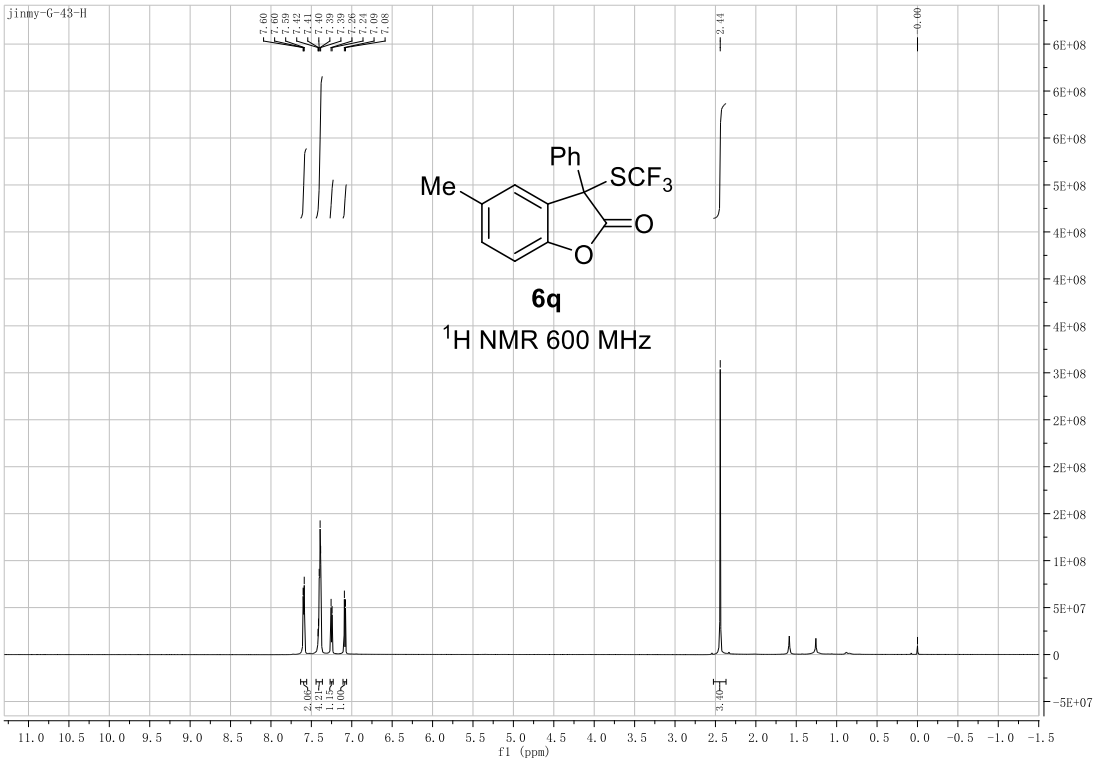

jinmy-G-28-C
Ph
SCF3
O
O
6o
13C NMR 150 MHz
f1 (ppm)

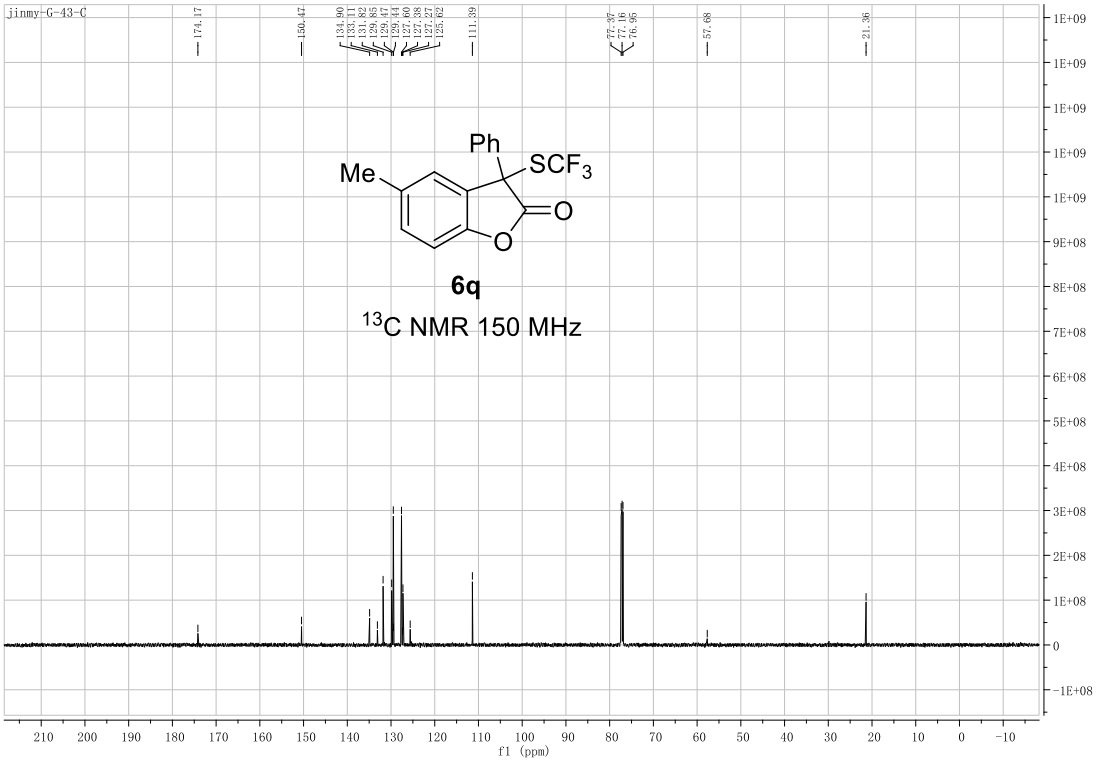

jinmy-G-28-F
-39.20
Ph
SCF3
O
O
6o
19F NMR 376 MHz
f1 (ppm)

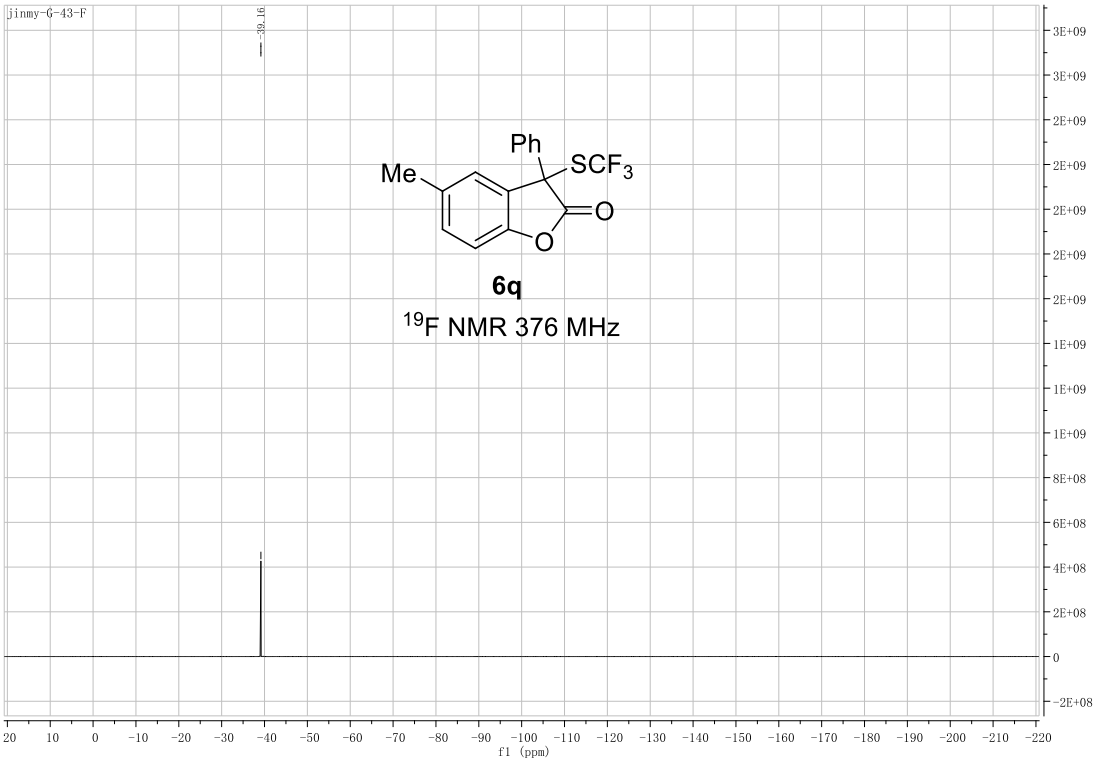

jinmy-G-41-H
7.73
7.72
7.61
7.60
7.59
7.58
7.57
7.56
7.43
7.42
7.26
7.12
7.11
0.00
Ph
SCF3
Br
O
O
6p
1H NMR 600 MHz
1.00
3.14
3.14
1.00
f1 (ppm)

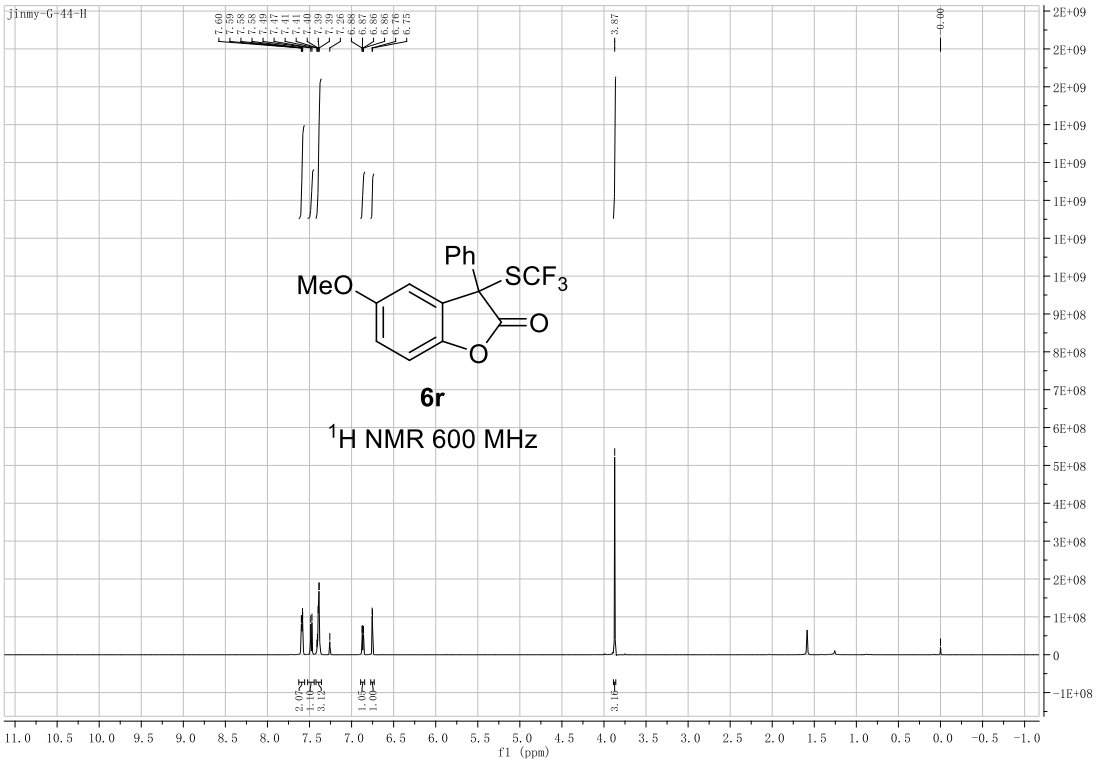

jinmy-G-41-C
173.06
151.43
134.37
132.55
130.23
129.95
129.73
129.29
128.84
127.44
127.23
117.61
113.50
57.34
Ph
SCF3
Br
O
O
6p
13C NMR 150 MHz
f1 (ppm)

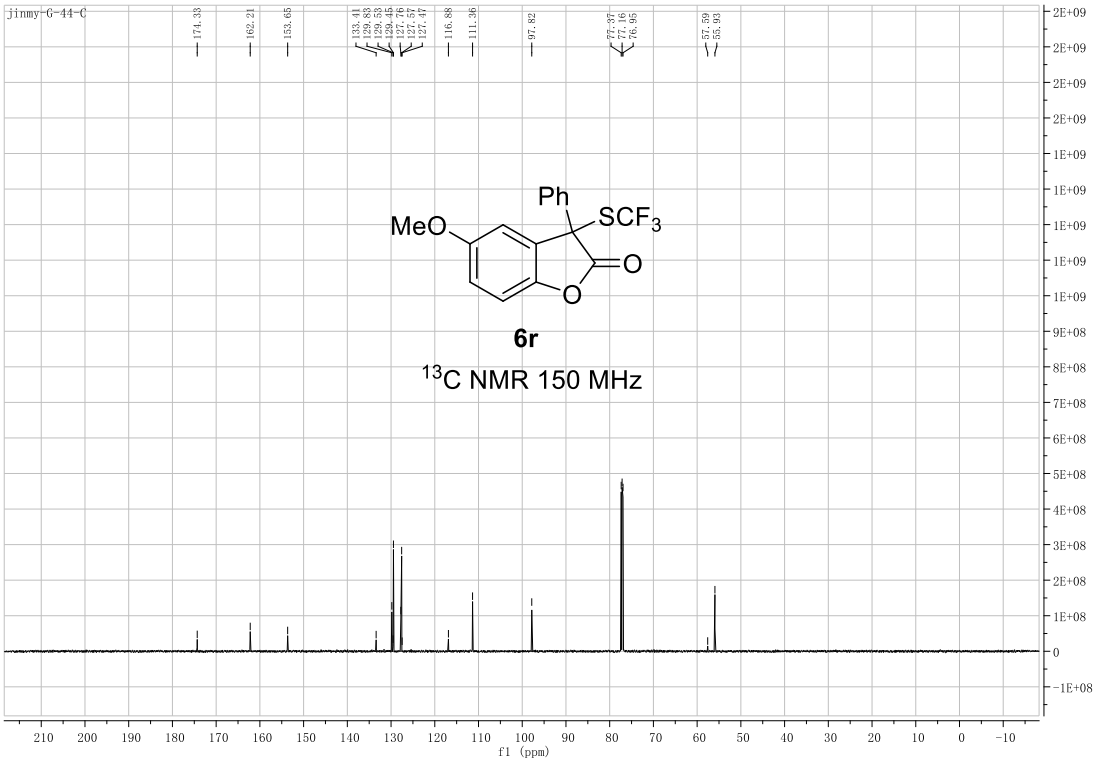

jinmy-G-41-F
-39.02
Ph
SCF3
Br
O
O
6p
19F NMR 376 MHz
f1 (ppm)

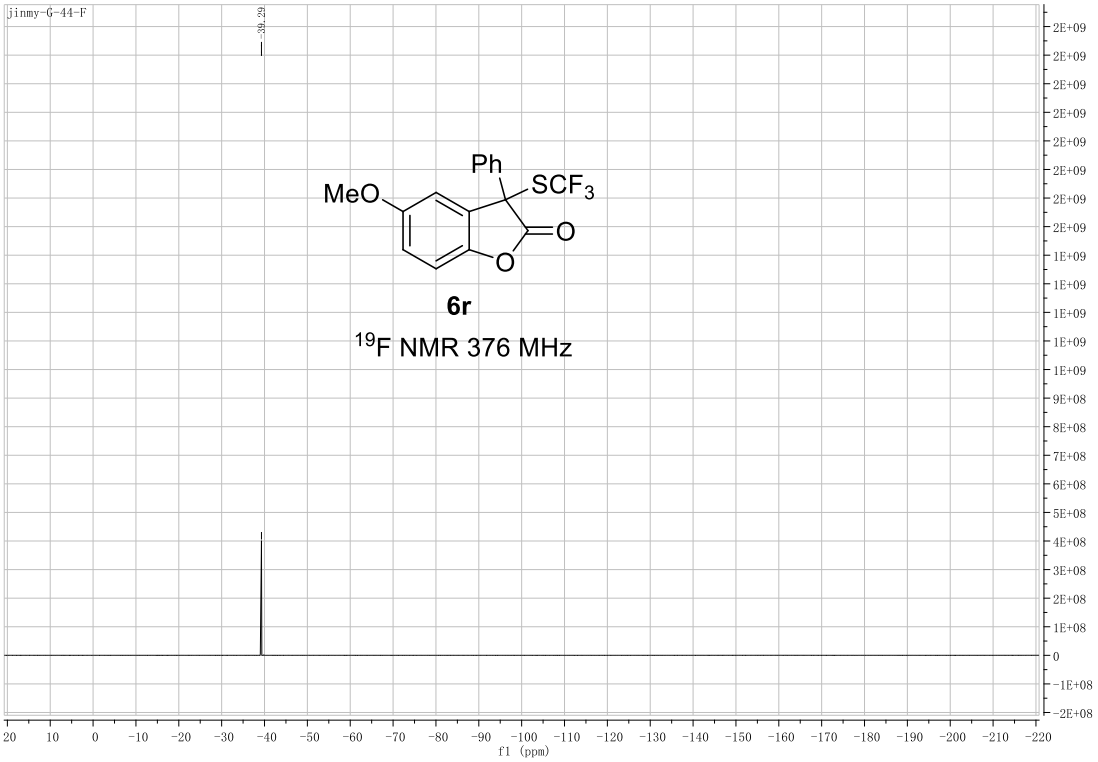

jinmy-G-43-H
Ph
SCF3
Me
O
O
6q
1H NMR 600 MHz
f1 (ppm)

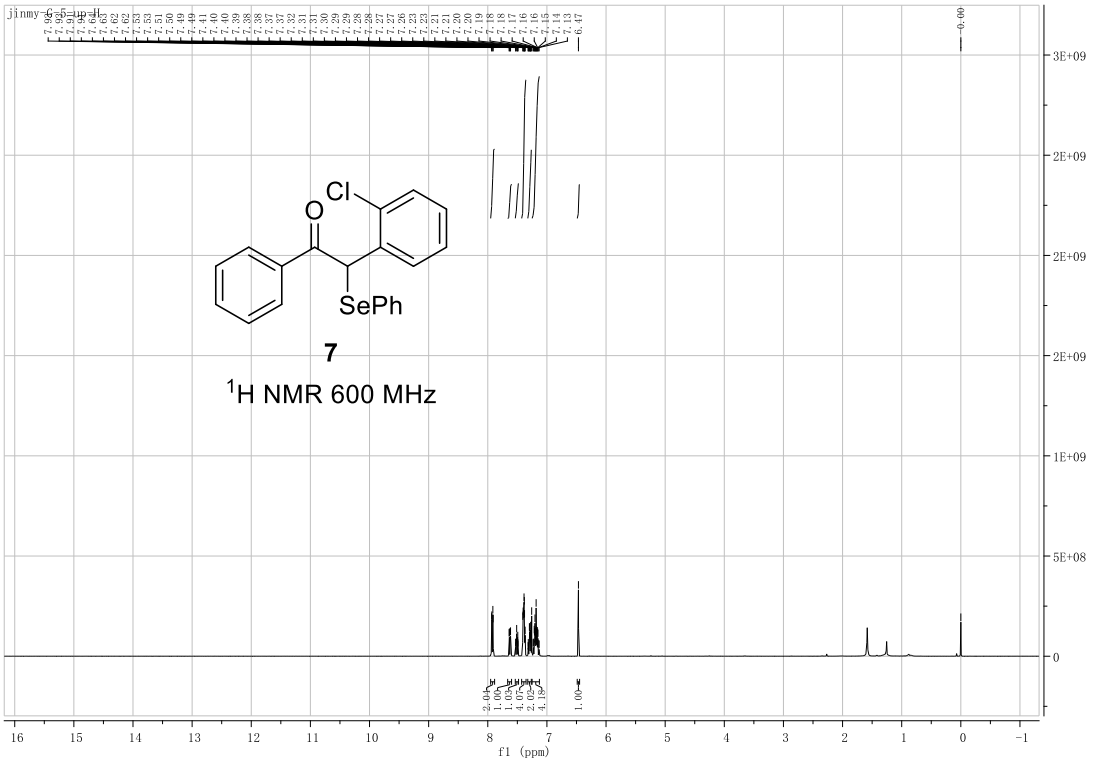

jinmy-G-43-C
Ph
SCF3
Me
O
O
6q
13C NMR 150 MHz
f1 (ppm)

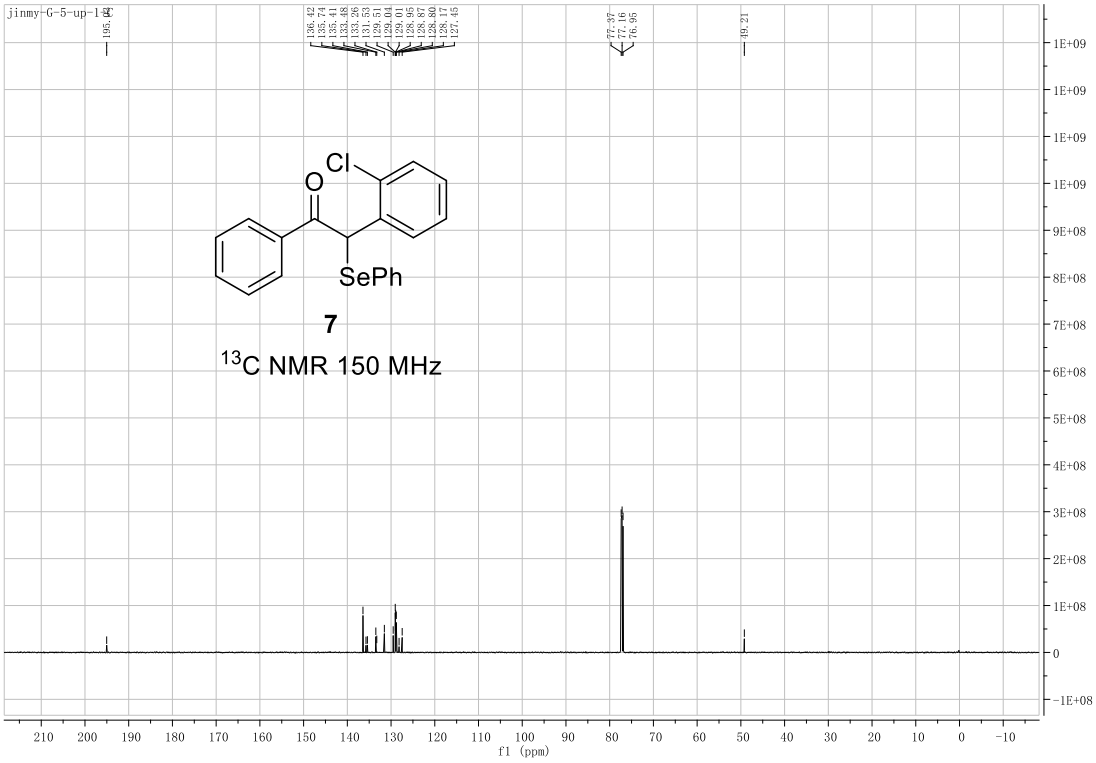

jinmy-G-43-F
-39.16
Ph
SCF3
Me
O
O
6q
19F NMR 376 MHz
f1 (ppm)

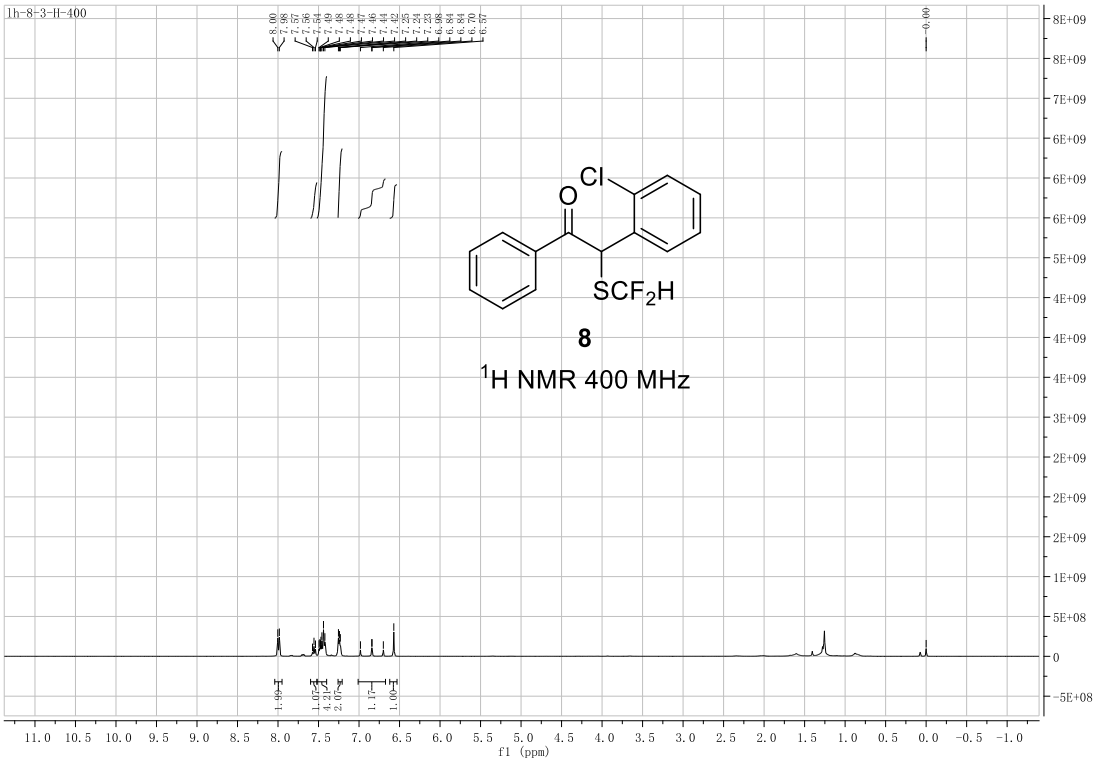

jinmy-G-44-H
7.60
7.59
7.58
7.58
7.49
7.47
7.41
7.40
7.39
7.38
6.88
6.87
6.86
6.86
6.76
6.75
3.87
0.00
Ph
SCF3
MeO
O
O
6r
1H NMR 600 MHz
2.07
2.04
3.12
1.07
1.00
3.16
f1 (ppm)

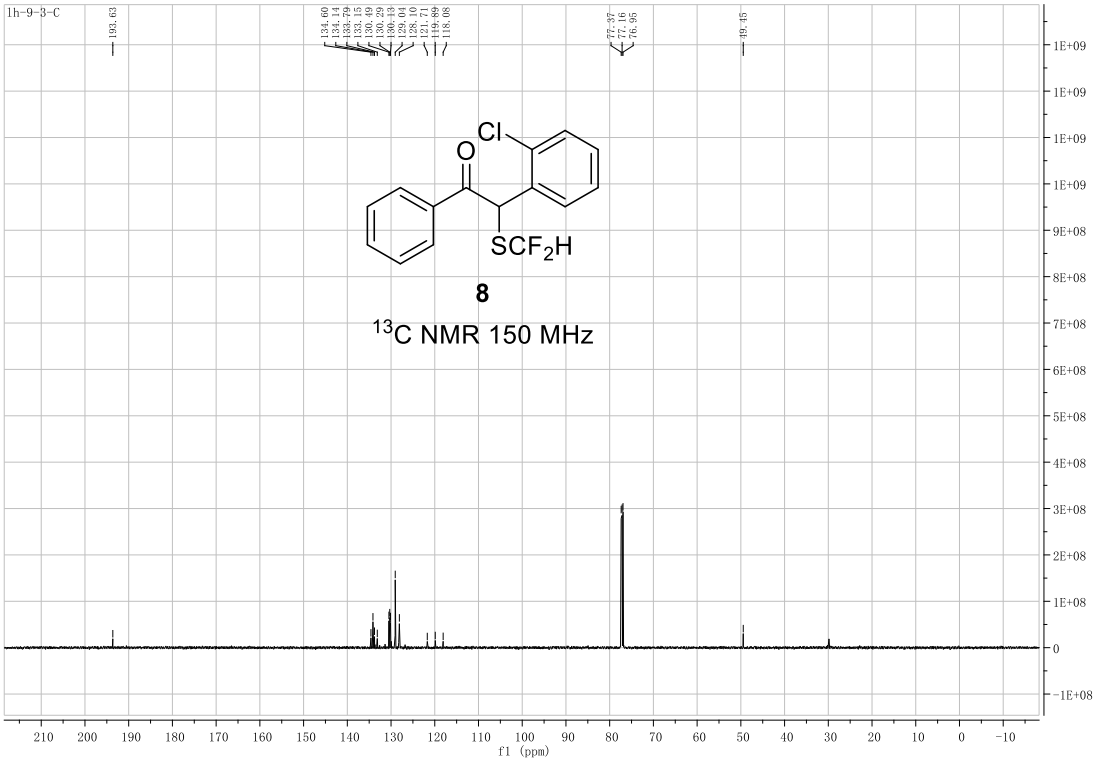

jinmy-G-44-C
174.33
162.21
153.65
133.41
129.88
129.53
129.45
127.76
127.57
127.47
116.88
111.36
97.82
77.37
77.16
76.95
57.69
55.93
Ph
MeO
SCF3
O
O
6r
13C NMR 150 MHz
f1 (ppm)

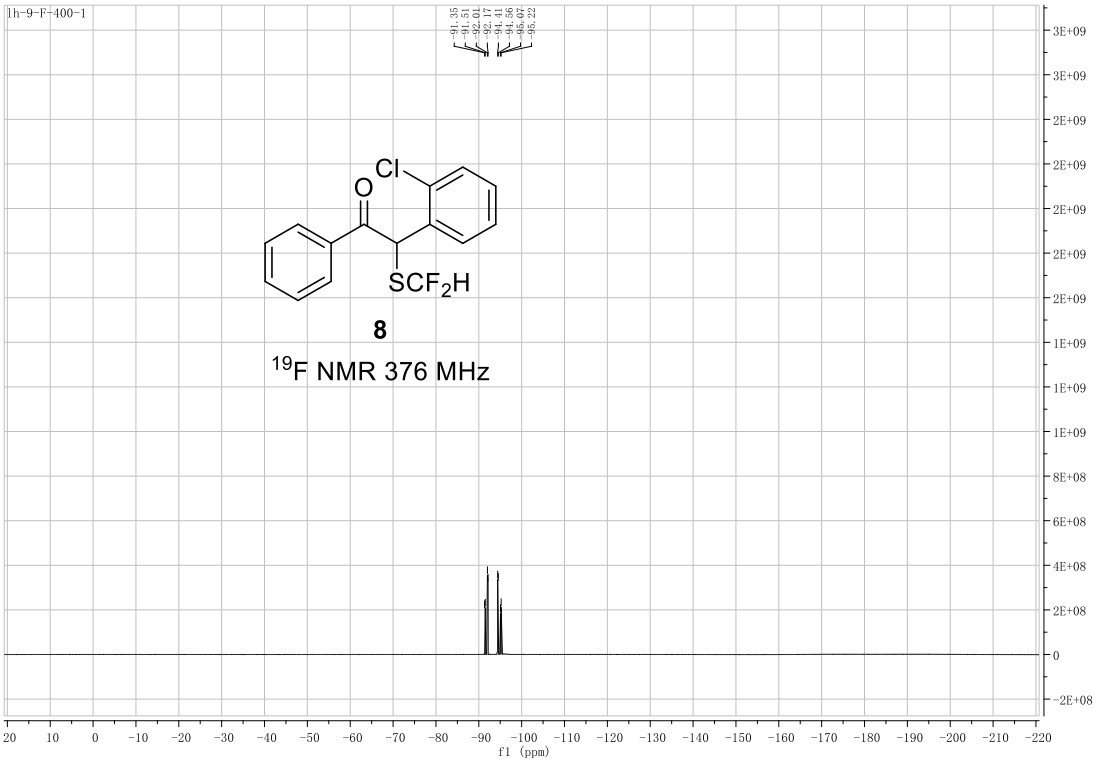

jinmy-G-44-F
-39.29
Ph
MeO
SCF3
O
O
6r
19F NMR 376 MHz
f1 (ppm)

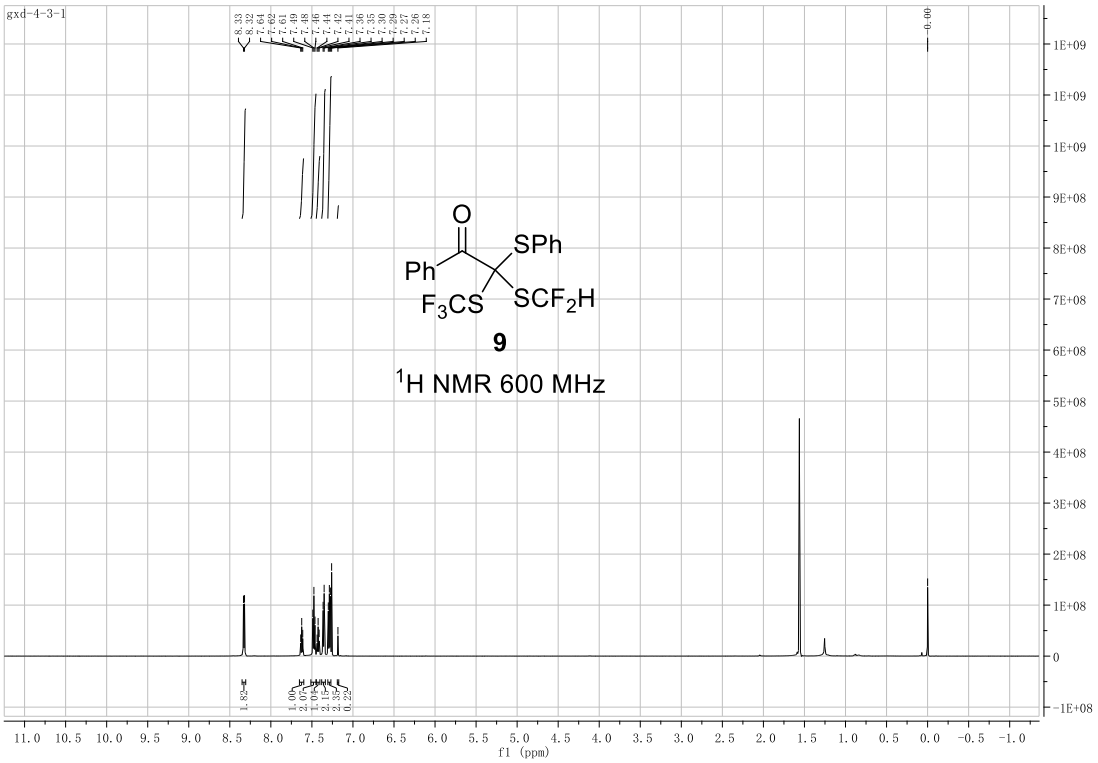

Cl
O
SePh
7
1H NMR 600 MHz
f1 (ppm)

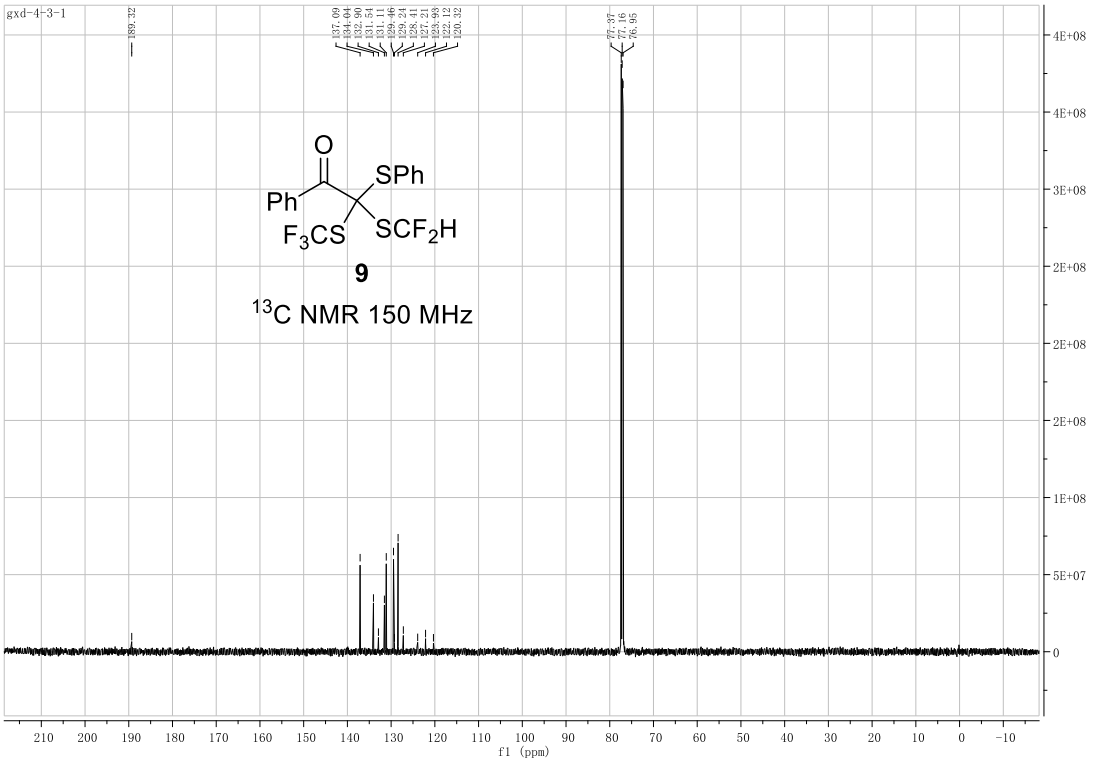

Cl
O
SePh
7
13C NMR 150 MHz
f1 (ppm)

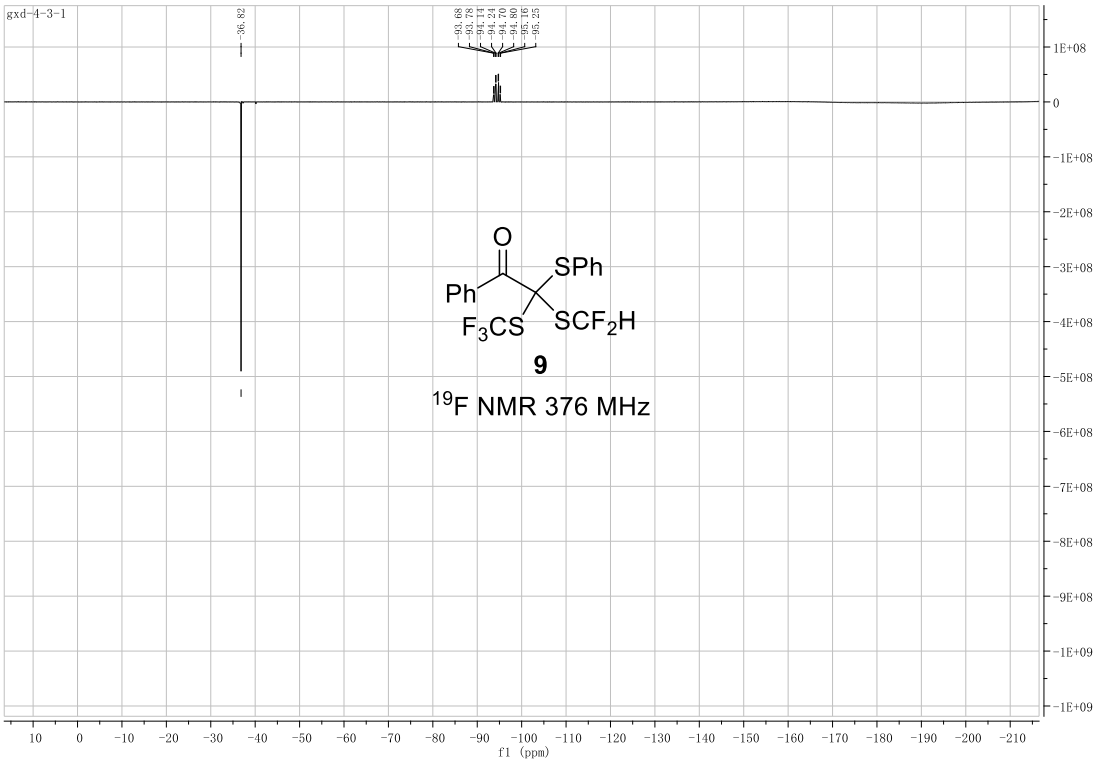

1h-8-3-H-400
Cl
O
SCF2H
8
1H NMR 400 MHz
f1 (ppm)


1h-9-3-C
Cl
O
SCF2H
8
13C NMR 150 MHz
f1 (ppm)


lh-9-F+400-1
Cl
O
SCF2H
8
19F NMR 376 MHz
f1 (ppm)


gxd-4-3-1
O
SPh
Ph
F3CS
SCF2H
9
1H NMR 600 MHz
f1 (ppm)


gxd-4-3-1
189.32
137.09
134.04
132.90
131.54
131.11
129.46
129.24
128.41
127.71
123.93
122.12
120.32
77.37
77.16
76.95
O
SPh
Ph
F3CS
SCF2H
9
13C NMR 150 MHz
f1 (ppm)


gxd-4-3-1
-36.82
-93.68
-93.78
-94.14
-94.24
-94.70
-94.80
-95.16
-95.25
O
SPh
Ph
F3CS
SCF2H
9
19F NMR 376 MHz
f1 (ppm)