Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Palladium-catalyzed direct approach to α-CF_3 aryl ketones from arylboronic acids

Bo Jiang, [† a] Xiaofei Zhang[† b] and Chunhao Yang* [b]

[a]Nano Science and Technology Institute, University of Science and Technology of China, 215123 Suzhou, China.

[b]State Key Laboratory of Drug Research, Shanghai Institute of Materia Medica, Chinese Academy of Sciences, 555 Zuchongzhi Road, Shanghai 201203, China.

Supporting Information

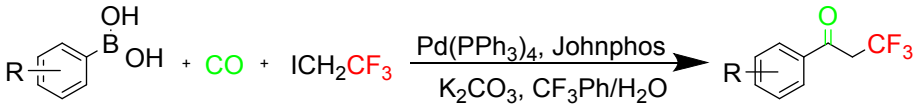
Lists of Contents

Experimental Section

General Experimental Information

Unless otherwise noted, all solvents and other reagents are commercially available and used without further purification. All reagents were weighed and handled in air at room temperature. NMR spectra were recorded on Brucker Avance 300 NMR spectrometer， Brucker Avance III 400 NMR spectrometer or Brucker Avance III 500 NMR spectrometer. Chemical shifts were reported in parts per million (ppm, δ). Proton coupling patterns are described as singlet (s), doublet (d), triplet (t), quartet (q) and multipet (m). Tetramethylsilane (TMS) was used as internal standard (^{1}H NMR: TMS at 0.00 ppm; $CHCl_3$ at 7.26 ppm; ^{13}C NMR: $CDCl_3$ at 77.16 ppm, DMSO at 39.50 ppm). Low and high-resolution mass spectra (LRMS and HRMS) were recorded on a Finnigan/MAT-95 (EI), Finnigan LCQ/DECA or Micromass Ultra Q-TOF (ESI) spectrometer. Melting points were measured by Büchi 510 melting point apparatus without further corrected.

General experimental procedure of α-CF_3 aryl ketones



1 **2**

To a 25 mL of two-neck bottle were added boronic acid (0.5mmol, 1.0 equiv), $Pd(PPh_3)_4$ (5 mol%), 2-(di-*tert*-butylphosphino)biphenyl (10 mol%), K_2CO_3 (0.5mmol, 1.0 equiv) with a condenser under a CO balloon. The mixture was then evacuated and backfilled with CO (5 times). And then 1,1,1-trifluoro-2-iodoethane (1.6 mmol, 3.2 equiv), and Trifluorotoluene (3 mL) , H_2O (1 mL) were added subsequently. The bottle was put into a preheated oil bath (70 °C). After stirring for 12 h, the reaction mixture was cooled to room temperature. Then, the reaction mixture was extracted with EtOAc/ H_2O, and the organic phase was washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated. The residue was subjected to silica gel column chromatography to give product (PE:EA=200:1~50:1).

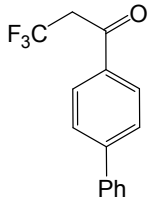
Experimental procedure of 2a in gram scale

To a 100 mL of two-neck bottle were added [1,1'-biphenyl]-4-ylboronic acid (1 g), $Pd(PPh_3)_4$ (290 mg), 2-(di-*tert*-butylphosphino)biphenyl (150 mg) and K_2CO_3 (700 mg). Then, the reaction was conducted with a condenser under a balloon of CO. The mixture was then evacuated and backfilled with CO (5 times). And then 1,1,1-trifluoro-

2-iodoethane (1.5 mL), and Trifluorotoluene (15 mL) , H_2O (5 mL) were added subsequently. The bottle was put into a preheated oil bath (70 ^oC). After stirring for 12 h, the reaction mixture was cooled to room temperature. Then, the reaction mixture was extracted with EtOAc/ H_2O, and the organic phase was washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated. The residue was subjected to silica gel column chromatography to give product **2a** (760 mg, 77%). (PE:EA=200:1).

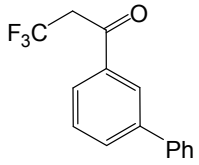
Characterization data

1-(Biphenyl-4-yl)-3,3,3-trifluoropropan-1-one (**2a**) (Lit.[1])



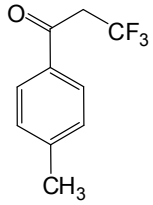
White solid (79%). M.P. 118-120 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.05 – 7.97 (m, 2H), 7.77 – 7.68 (m, 2H), 7.67 – 7.59 (m, 2H), 7.53 – 7.38 (m, 3H), 3.83 (q, *J* = 10.0 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 189.41, 147.05, 139.56, 134.63, 129.19, 129.14, 128.72, 127.67, 127.44, 124.08 (q, *J* = 278.67 Hz), 42.29 (q, *J* = 28.2 Hz). ^{19}F NMR (471 MHz, $CDCl_3$) δ -61.92 (t, *J* = 10.0 Hz). Q-TOF (ESI) m/z $[M-H]^-$ calculated for $C_{15}H_{10}F_3O$, 263.0689; found, 263.0685.

1-(Biphenyl-3-yl)-3,3,3-trifluoropropan-1-one (**2b**) (Lit.[2])



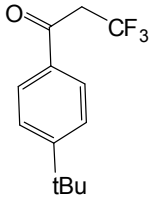
Colorless oil (68%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.14 (s, 1H), 7.87 (dd, *J* = 13.6, 7.8 Hz, 2H), 7.65 – 7.53 (m, 3H), 7.51 – 7.38 (m, *J* = 22.7, 7.1 Hz, 3H), 3.85 (q, *J* = 10.0 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 189.82, 142.35, 139.86, 136.47, 132.97, 129.53, 129.17, 128.23, 127.33, 127.25, 127.16, δ 124.14 (q, *J* = 277.0 Hz), 42.41 (q, *J* = 28.3 Hz). ^{19}F NMR (471 MHz, $CDCl_3$) δ -61.93 (t, *J* = 10.0 Hz). Q-TOF (ESI) m/z $[M-H]^-$ calculated for $C_{15}H_{10}F_3O$, 263.0689; found, 263.0687.

3,3,3-Trifluoro-1-p-tolylpropan-1-one (**2c**) (Lit.[1])



Colorless oil (50%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.84 (d, *J* = 8.2 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 3.77 (q, *J* = 10.0 Hz, 2H), 2.44 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 189.45, 145.45, 133.56, 129.76, 128.66, δ 124.21 (q, *J* = 277.0 Hz), 42.15 (q, *J* = 28.1 Hz), 21.86. ^{19}F NMR (471 MHz, $CDCl_3$) δ -62.00 (t, *J* = 10.0 Hz). HRMS (EI) m/z $[M]^+$ calculated for $C_{10}H_9OF_3$, 202.0600; found, 202.0601.

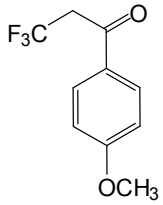
1-(4-Tert-butylphenyl)-3,3,3-trifluoropropan-1-one (**2d**) (Lit.[4])



Colorless oil (55%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.88 (dd, *J* = 8.7, 2.0 Hz, 2H), 7.52 (dd, *J* = 8.6, 1.9 Hz, 2H), 3.77 (q, *J* = 10.1 Hz, 2H), 1.35 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 189.45, 158.35, 133.46, 128.54,

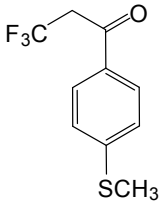
126.05, 124.22 (q, J = 277.2 Hz), 42.16 (q, J = 28.2 Hz), 35.41, 31.15. ^{19}F NMR (471 MHz, $CDCl_3$) δ -61.97 (t, J = 10.0 Hz). HRMS (EI) m/z $[M]^+$ calculated for $C_{13}H_{15}OF_3$, 244.1070; found, 244.1070.

3,3,3-Trifluoro-1-(4-methoxyphenyl)propan-1-one (**2e**) (Lit.[1])



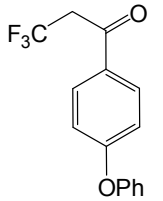
White solid (66%). M.P. 47-48 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.92 (d, J = 8.9 Hz, 2H), 6.97 (d, J = 8.9 Hz, 2H), 3.89 (s, 3H), 3.75 (q, J = 10.1 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 188.26, 164.50, 130.97, 129.10, 124.26 (q, J = 277.0 Hz), 114.25, 55.73, 41.98 (q, J = 28.0 Hz). ^{19}F NMR (471 MHz, $CDCl_3$) δ -61.95 (t, J = 10.1 Hz). HRMS (EI) m/z $[M]^+$ calculated for $C_{10}H_9O_2F_3$, 218.0549; found, 218.0550.

3,3,3-Trifluoro-1-(4-(methylthio)phenyl)propan-1-one (**2f**)



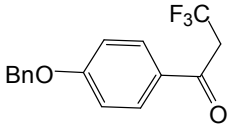
White solid (48%). M.P. 98-100 °C.^{1}H NMR (300 MHz, $CDCl_3$) δ 7.84 (dd, J = 8.8, 2.0 Hz, 2H), 7.28 (dd, J = 6.9, 5.1 Hz, 2H), 3.75 (q, J = 10.0 Hz, 2H), 2.54 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 188.73, 147.94, 132.18, 128.90, 125.18, 124.16 (q, J = 277.0 Hz), 42.09 (q, J = 28.2 Hz), 14.78. ^{19}F NMR (471 MHz, $CDCl_3$) δ -61.93 (t, J = 10.0 Hz). Q-TOF (ESI) m/z $[M+H]^+$ calculated for $C_{10}H_{10}F_3OS$, 235.0399; found, 235.0392.

3,3,3-Trifluoro-1-(4-phenoxyphenyl)propan-1-one (**2g**) (Lit.[2])



White solid (78%). M.P. 55-57 °C. ^{1}H NMR (300 MHz, DMSO) δ 8.02 (d, J = 8.9 Hz, 2H), 7.51 – 7.46 (m, 2H), 7.33 – 7.21 (m, 1H), 7.20 – 7.11 (m, 2H), 7.07 (d, J = 8.9 Hz, 2H), 4.36 (q, J = 10.9 Hz, 2H). ^{13}C NMR (125 MHz, DMSO) δ 189.48, 161.95, 154.72, 130.97, 130.42, 130.36, 125.00 (q, J = 276.2 Hz), 124.94, 120.09, 117.09, 41.33 (q, J = 26.5 Hz). ^{19}F NMR (471 MHz, DMSO) δ -60.88 (t, J = 10.8 Hz). HRMS (EI) m/z $[M]^+$ calculated for $C_{15}H_{11}O_2F_3$, 280.0706; found, 280.0704.

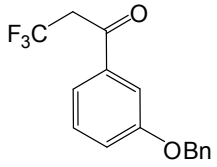
1-(4-(Benzyloxy)phenyl)-3,3,3-trifluoropropan-1-one (**2h**) (Lit.[3])



White solid (61%). M.P. 118-119 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.94 – 7.88 (m, 2H), 7.45 – 7.38 (m, 4H), 7.38 – 7.33 (m, 1H),

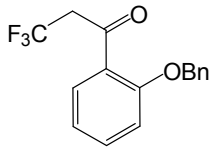
7.06 – 7.02 (m, 2H), 5.15 (s, 2H), 3.73 (q, J = 10.1 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 188.26, 163.62, 135.96, 130.99, 129.29, 128.90, 128.46, 127.63, 124.29 (q, J = 278.14 Hz), 115.13, 115.09, 70.44, 42.00 (q, J = 28.1 Hz). ^{19}F NMR (471 MHz, $CDCl_3$) δ -61.92 (t, J = 10.1 Hz). HRMS (EI) m/z $[M]^+$ calculated for $C_{16}H_{13}F_3O_2$, 294.0862; found, 294.0868.

1-(3-(Benzyloxy)phenyl)-3,3,3-trifluoropropan-1-one (**2i**)



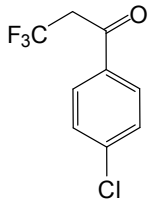
White solid (56%). M.P. 55-57 °C. ^{1}H NMR (300 MHz, DMSO) δ 7.63 – 7.53 (m, 2H), 7.53 – 7.27 (m, 7H), 5.17 (s, 2H), 4.40 (q, J = 10.9 Hz, 2H). ^{13}C NMR (125 MHz, DMSO) δ 190.90, 158.54, 137.03, 136.64, 130.05, 128.46, 127.94, 127.75, 125.00 (q, J = 276.2 Hz), 120.94, 120.74, 113.94, 69.51, δ 41.69 (q, J = 26.5 Hz). ^{19}F NMR (471 MHz, DMSO) δ -61.00 (t, J = 10.8 Hz). Q-TOF (ESI) m/z $[M-H]^-$ calculated for $C_{16}H_{12}F_3O_2$, 293.0795; found, 293.0793.

1-(2-(Benzyloxy)phenyl)-3,3,3-trifluoropropan-1-one (**2j**)



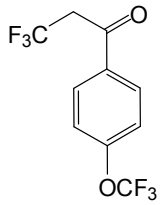
White solid (40%). M.P. 40-41 °C.^{1}H NMR (300 MHz, DMSO) δ 7.71 (dd, J = 7.7, 1.5 Hz, 1H), 7.66 – 7.48 (m, 3H), 7.37 (ddd, J = 29.0, 14.5, 7.6 Hz,4H), 7.09 (t, J = 7.5 Hz, 1H), 5.28 (s, 2H), 4.18 (q, J = 10.9 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 191.26, 158.23, 135.66, 134.98, 131.17, 129.05, 128.80, 127.88, 126.11 (q, J = 275.61 Hz), 121.46, 113.04, 71.21, 47.15 (q, J = 27.5 Hz). ^{19}F NMR (471 MHz, DMSO) δ -61.34 (t, J = 10.9 Hz). Q-TOF (ESI) m/z $[M-H]^-$ calculated for $C_{16}H_{12}F_3O_2$, 293.0795; found, 293.0793.

1-(2-(Benzyloxy)phenyl)-3,3,3-trifluoropropan-1-one (**2k**) (Lit.[1])



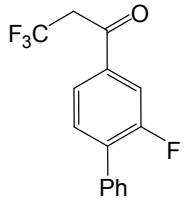
White solid (58%). M.P. 53-54 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.88 (d, J = 8.6 Hz, 2H), 7.49 (d, J = 8.7 Hz, 2H), 3.78 (q, J = 9.9 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 188.66, 141.05, 134.25, 129.91, 129.47, 123.96 (q, J = 277.1 Hz), 42.31 (q, J = 28.4 Hz). ^{19}F NMR (471 MHz, $CDCl_3$) δ -61.99 (t, J = 9.9 Hz). HRMS (EI) m/z $[M]^+$ calculated for $C_9H_6OClF_3$, 222.0054; found, 222.0057.

3,3,3-Trifluoro-1-(4-(trifluoromethoxy)phenyl)propan-1-one (**2l**)



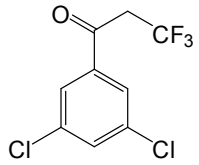
Colorless solid (45%). M.P. 42-43 °C.[1]H NMR (300 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.9 Hz, 2H), 7.34 (d, *J* = 8.1 Hz, 2H), 3.80 (q, *J* = 9.9 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 188.32, 153.58, 134.08, 130.67, δ 123.93 (q, *J* = 277.0 Hz), 120.73, δ 120.39 (q, *J* = 259.3 Hz), δ 42.39 (q, *J* = 28.6 Hz). ^{19}F NMR (471 MHz, $CDCl_3$) δ -57.62 (s, 3F), -61.99 (t, *J* = 9.8 Hz, 3F). HRMS (EI) m/z $[M]^+$ calculated for $C_{10}H_6O_2F_6$, 272.0267; found, 272.0258.

3,3,3-Trifluoro-1-(2-fluorobiphenyl-4-yl)propan-1-one (**2m**)



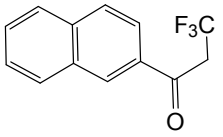
White solid (70%). M.P. 129-130 °C. ^1H NMR (300 MHz, $CDCl_3$) δ 7.82 – 7.67 (m, 2H), 7.66 – 7.54 (m, 3H), 7.54 – 7.41 (m, 3H), 3.81 (q, *J* = 9.9 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 188.33, 159.95 (d, *J* = 250.9 Hz), 136.49 (d, *J* = 6.4 Hz), 135.23 (d, *J* = 13.7 Hz), 134.39, 131.44 (d, *J* = 3.4 Hz), 129.17, 129.14, 128.99, 128.86, 124.54 (d, *J* = 3.4 Hz), 123.96 (q, *J* = 277.1 Hz), 116.24 (d, *J* = 24.6 Hz), 42.43 (q, *J* = 28.5 Hz). ^{19}F NMR (471 MHz, $CDCl_3$) δ -61.95 (t, *J* = 9.9 Hz, 3F), -115.62 – -115.73 (m, 1F). HRMS (EI) m/z $[M]^+$ calculated for $C_{15}H_{10}OF_4$, 282.0662; found, 282.0666.

1-(3,5-Dichlorophenyl)-3,3,3-trifluoropropan-1-one (**2n**)



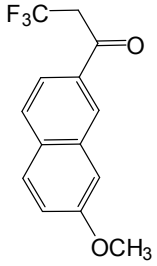
Colorless solid (33%). M.P. 40 °C. ^1H NMR (300 MHz, $CDCl_3$) δ 7.79 (d, *J* = 1.8 Hz, 1H), 7.63 (t, *J* = 1.8 Hz, 1H), 3.77 (q, *J* = 9.7 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 187.51, 138.19, 136.31, 134.03, 126.90, 123.68 (q, *J* = 277.2 Hz), 42.51 (q, *J* = 28.9 Hz). ^{19}F NMR (565 MHz, $CDCl_3$) δ -62.03 (t, *J* = 9.7 Hz). HRMS (EI) m/z $[M]^+$ calculated for $C_9H_5OCl_2F_3$, 255.9664; found, 255.9673.

3,3,3-Trifluoro-1-(naphthalen-2-yl)propan-1-one (**2o**) (Lit.[1])



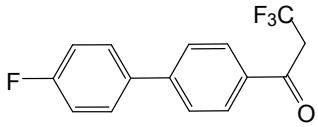
White solid (67%). M.P. 85-87 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.42 (s, 1H), 8.03 – 7.89 (m, 4H), 7.71 – 7.54 (m, 2H), 3.94 (q, *J* = 10.0 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 189.75, 136.13, 133.36, 132.49, 130.72, 129.86, 129.36, 129.11, 128.03, 127.42, 124.22 (q, *J* = 275.97 Hz), 123.64, 42.34 (q, *J* = 28.4 Hz). ^{19}F NMR (471 MHz, $CDCl_3$) δ -61.89 (t, *J* = 9.9 Hz). HRMS (EI) m/z $[M]^+$ calculated for $C_{13}H_9OF_3$, 238.0600; found, 238.0606.

3,3,3-Trifluoro-1-(7-methoxynaphthalen-2-yl)propan-1-one (**2p**) (Lit.[4])



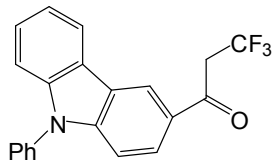
White solid (67%). M.P. 96-97 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.34 (s, 1H), 7.98 (dd, *J* = 8.7, 1.8 Hz, 1H), 7.86 (d, *J* = 9.0 Hz, 1H), 7.79 (d, *J* = 8.7 Hz, 1H), 7.23 (dd, *J* = 9.0, 2.5 Hz, 1H), 7.16 (d, *J* = 2.3 Hz, 1H), 3.96 (s, 3H), 3.90 (q, *J* = 20.2, 10.1 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 189.40, 160.49, 137.96, 131.45, 130.56, 127.79, 127.71, 124.44, 124.30 (q, *J* = 275.89 Hz), 120.33, 105.97, 55.63, 42.16 (q, *J* = 28.1 Hz). ^{19}F NMR (471 MHz, $CDCl_3$) δ -61.87 (t, *J* = 10.0 Hz). Q-TOF (ESI) m/z $[M+H]^+$ calculated for $C_{14}H_{12}F_3O_2$, 269.0784; found, 263.0778.

3,3,3-Trifluoro-1-(4'-fluorobiphenyl-4-yl)propan-1-one (**2q)**



White solid (61%). M.P. 110-111 °C. ^{1}H NMR (500 MHz, DMSO) δ 8.11 – 8.05 (m, 2H), 7.90 – 7.80 (m, 4H), 7.38 – 7.32 (m, 2H), 4.44 (q, *J* = 10.9 Hz, 2H). ^{19}F NMR (471 MHz, DMSO) δ -60.90 (t, *J* = 10.8 Hz, 3F), δ -113.67 – -113.78 (m, 1F). ^{13}C NMR (125 MHz, DMSO) δ 190.63, δ 162.51 (d, *J* = 246.1 Hz), 144.22, 135.07 (d, *J* = 3.0 Hz), 134.42, 129.24, 129.17, 129.05, 126.88, 125.05 (q, *J* = 276.3 Hz), 116.04, 115.87, 41.60 (q, *J* = 26.6 Hz). ^{19}F NMR (471 MHz, DMSO) δ -60.90 (t, *J* = 10.8 Hz, 3F), δ -113.67 – -113.78 (m, 1F). HRMS (EI) m/z $[M]^+$ calculated for $C_{15}H_{10}OF_4$, 282.0662; found, 282.0660.

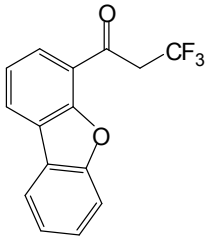
3,3,3-Trifluoro-1-(9-phenyl-9H-carbazol-3-yl)propan-1-one (**2r**)



White solid (60%). M.P. 112-113 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.75 (d, *J* = 1.4 Hz, 1H), 8.25 – 8.15 (m, 1H), 8.01 (dd, *J* = 8.8, 1.8 Hz, 1H), 7.71 – 7.59 (m, 2H), 7.59 – 7.43 (m, 4H), 7.43 – 7.32 (m, 3H), 3.93 (q, *J* = 10.1 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 189.06, 144.24, 142.05, 136.76, 130.29, 128.50, 128.47, 127.25, 126.76, 125.55,

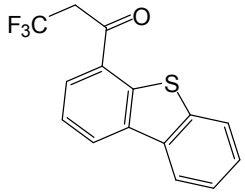
124.46 (q, J = 276.7 Hz), 123.52, 123.36, 122.16, 121.38, 120.75, 110.59, 109.98, δ 42.26 (q, J = 27.9 Hz). ^{19}F NMR (471 MHz, $CDCl_3$) δ -61.77 (t, J = 10.1 Hz). HRMS (EI) m/z $[M]^+$ calculated for $C_{21}H_{14}ONF_3$, 353.1022; found, 353.1023.

1-(Dibenzo[b,d]furan-4-yl)-3,3,3-trifluoropropan-1-one (**2s**)



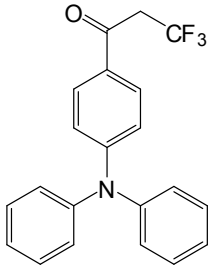
White solid (73%). M.P. 110-111 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.20 (dd, J = 7.6, 1.3 Hz, 1H), 8.11 (dd, J = 7.8, 1.3 Hz, 1H), 8.04 – 7.94 (m, 1H), 7.68 (d, J = 8.3 Hz, 1H), 7.62 – 7.51 (m, 1H), 7.51 – 7.38 (m, 2H), 4.26 (q, J = 10.0 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 187.23, 155.54, 154.00, 127.82, 127.42, 126.18, 125.64, 123.39, δ 123.29 (q, J = 277.19 Hz), 122.75, 122.53, 120.70, 120.45, 111.52, δ 45.88 (q, J = 27.9 Hz). ^{19}F NMR (471 MHz, $CDCl_3$) δ -62.32 (t, J = 10.0 Hz). HRMS (EI) m/z $[M]^+$ calculated for $C_{15}H_9O_2F_3$, 278.0549; found, 278.0555.

1-(Dibenzo[b,d]thiophen-4-yl)-3,3,3-trifluoropropan-1-one (**2t**) (Lit.[5])



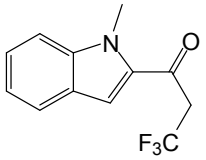
White solid (60%). M.P. 147-148 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.44 (d, J = 7.5 Hz, 1H), 8.29 – 8.13 (m, 1H), 8.09 – 7.89 (m, 2H), 7.62 (t, J = 7.7 Hz, 1H), 7.58 – 7.47 (m, 2H), 3.99 (q, J = 9.9 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 189.10, 142.17, 140.26, 137.91, 133.61, 129.78, 128.76, 127.70, 127.19, 124.95, 124.34, 124.14 (q, J = 27.0 Hz), 123.04, 121.64, 42.15 (q, J = 28.6 Hz). ^{19}F NMR (471 MHz, $CDCl_3$) δ -61.74 (t, J = 9.9 Hz). Q-TOF (ESI) m/z $[M-H]^-$ calculated for $C_{15}H_8F_3OS$, 293.0253; found, 293.0255.

1-(4-(Diphenylamino)phenyl)-3,3,3-trifluoropropan-1-one (**2u**)



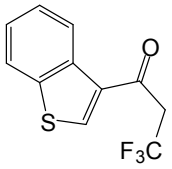
White solid (60%). M.P. 125-127 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.75 (d, J = 9.0 Hz, 2H), 7.35 (dd, J = 11.9, 4.0 Hz, 4H), 7.24 – 7.10 (m, 6H), 6.97 (d, J = 9.0 Hz, 2H), 3.69 (q, J = 10.2 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 187.70, 153.19, 146.14, 130.32, 129.90, 128.03, 126.49, 125.37, δ 124.36 (q, J = 276.06 Hz), δ 41.82 (q, J = 27.8 Hz). ^{19}F NMR (471 MHz, $CDCl_3$) δ -61.86 (t, J = 10.1 Hz). HRMS (EI) m/z $[M]^+$ calculated for $C_{21}H_{16}ONF_3$, 355.1179; found, 355.1172.

3,3,3-Trifluoro-1-(1-methyl-1H-indol-2-yl)propan-1-one (**2v**)



White solid (66%). M.P. 108-109 ^{o}C.^{1}H NMR (300 MHz, $CDCl_3$) δ 8.24 (d, *J* = 1.2 Hz, 1H), 7.87 (dd, *J* = 8.7, 1.5 Hz, 1H), 7.37 (d, *J* = 8.8 Hz, 1H), 7.15 (d, *J* = 3.2 Hz, 1H), 6.63 (d, *J* = 3.2 Hz, 1H), 3.86 (q, *J* = 10.2 Hz, 2H), 3.84 (s, 3H), ^{13}C NMR (125 MHz, $CDCl_3$) δ 189.69, 139.72, 131.05, 128.27, 128.14, δ 124.50 (q, *J* = 276.9 Hz), 123.58, 121.97, 109.67, 103.44, 42.10 (q, *J* = 27.7 Hz), 33.22. ^{19}F NMR (471 MHz, $CDCl_3$) δ -61.87 (t, *J* = 10.1 Hz). Q-TOF (ESI) m/z $[M+H]^+$ calculated for $C_{12}H_{11}F_3NO$, 242.0787; found, 242.0790.

1-(Benzo[b]thiophen-3-yl)-3,3,3-trifluoropropan-1-one (**2w**) (Lit.[5])



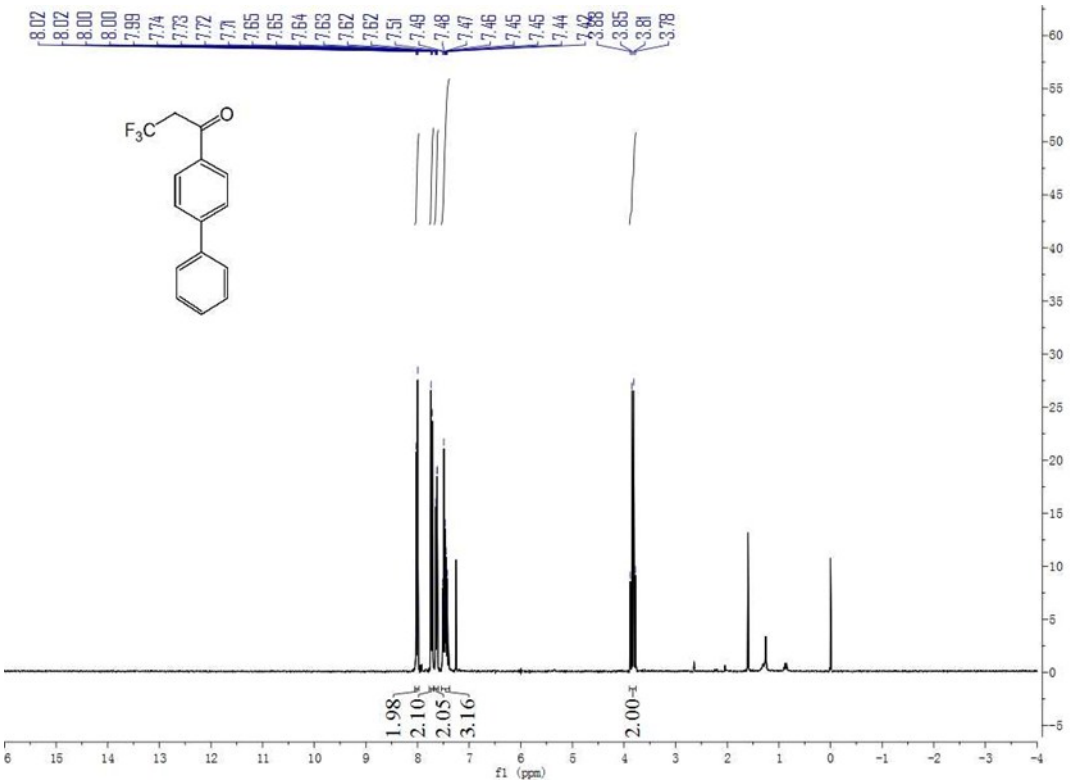
White solid (50%). M.P. 110-111 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.77 (dd, *J* = 8.7, 0.7 Hz, 1H), 8.29 (s, 1H), 7.92 – 7.83 (m, 1H), 7.59 – 7.40 (m, 2H), 3.81 (q, *J* = 10.1 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 184.32, 139.84, 138.86, 136.30, 134.50, 126.48, 126.16, 125.78, 124.02 (q, *J* = 277.3 Hz), 122.44, 43.93 (q, *J* = 28.2 Hz). ^{19}F NMR (471 MHz, $CDCl_3$) δ -61.80 (t, *J* = 10.1 Hz). HRMS (EI) m/z $[M]^+$ calculated for $C_{11}H_7OF_3S$, 244.0164; found, 244.0157.

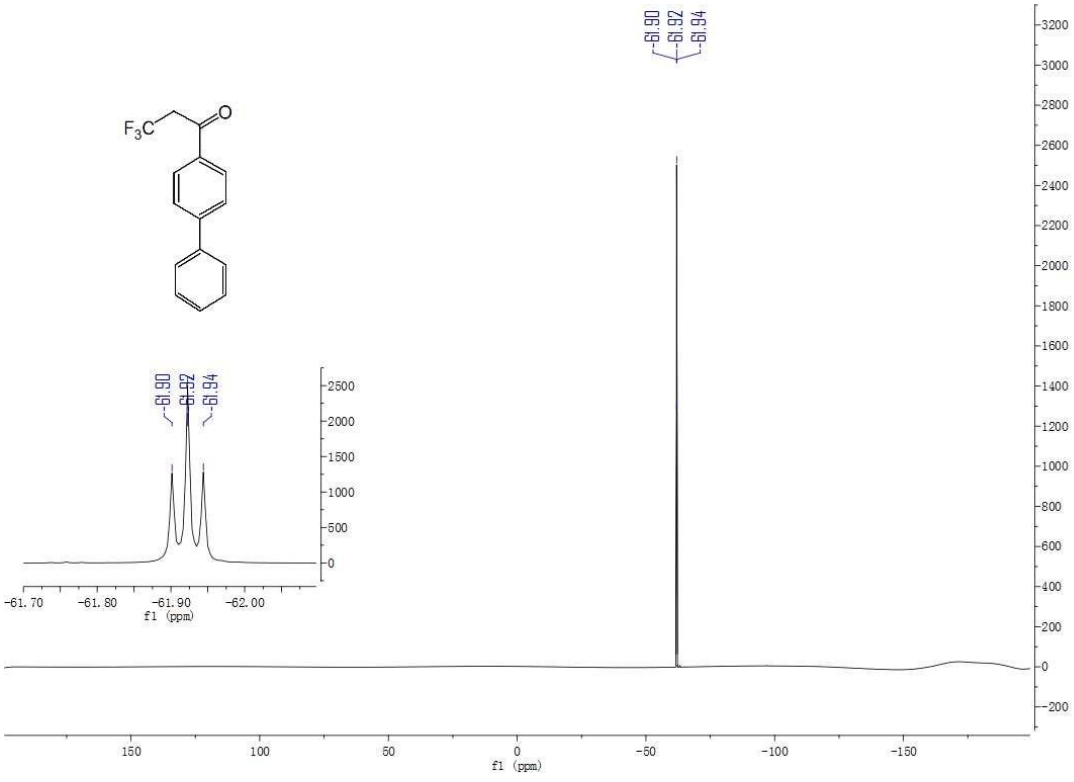
References

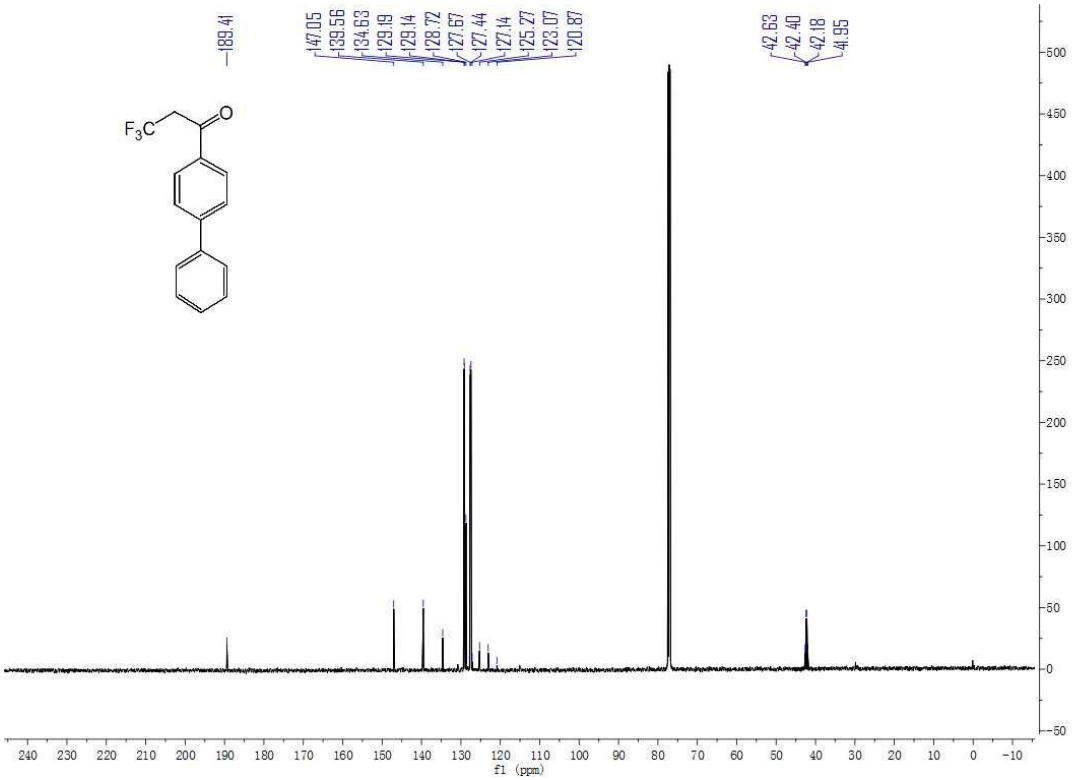
1. N. Petr, L. Anton. Et al. *J. Am. Chem. Soc.*, 2012, 134, 16167−16170.
2. Q.-Q. Lu, C. Liu. Et al. *Chem. Commun.*, 2014, 50, 14101—14104.
3. K. R. Chung., C. Kun., Et al. *Bioorganic & Medicinal Chemistry Letters.* 1995, 5, 133-138.
4. A. Maji, A. Hazra, and D. Maiti. *Org. Lett.* 2014, 16, 4524−4527.
5. A. Deb, S. Manna., *Angew. Chem. Int. Ed.* 2013, 52, 9747 –9750.

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

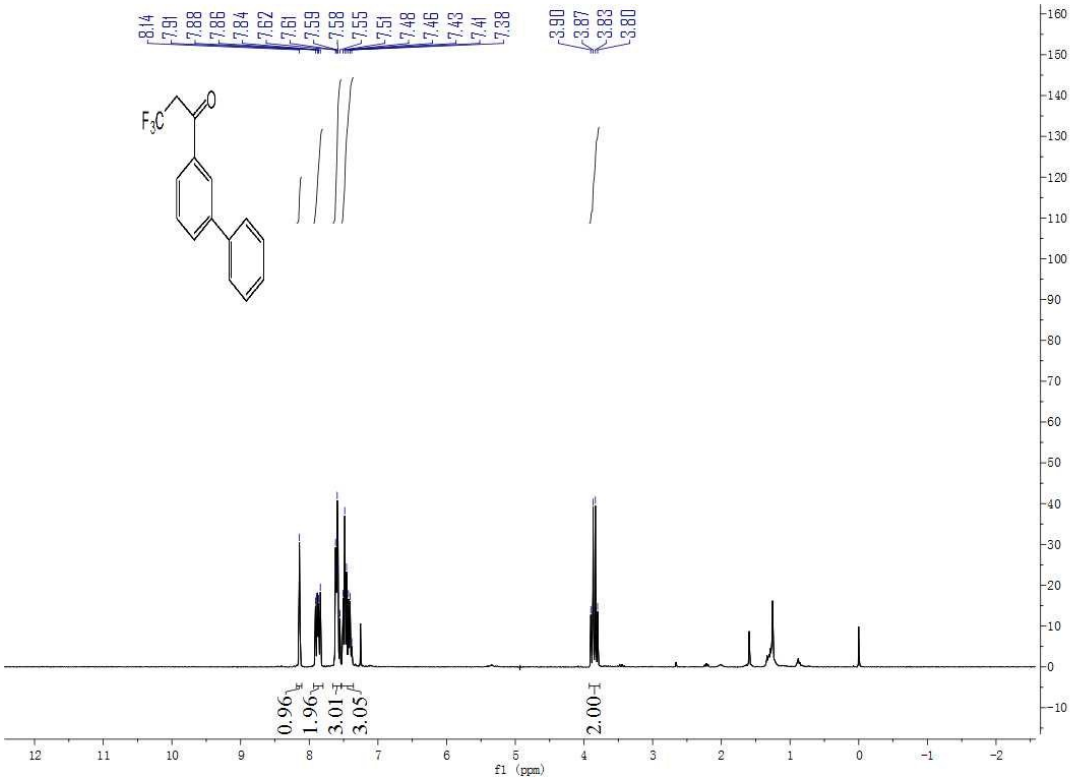
1-(Biphenyl-4-yl)-3,3,3-trifluoropropan-1-one (**2a**)

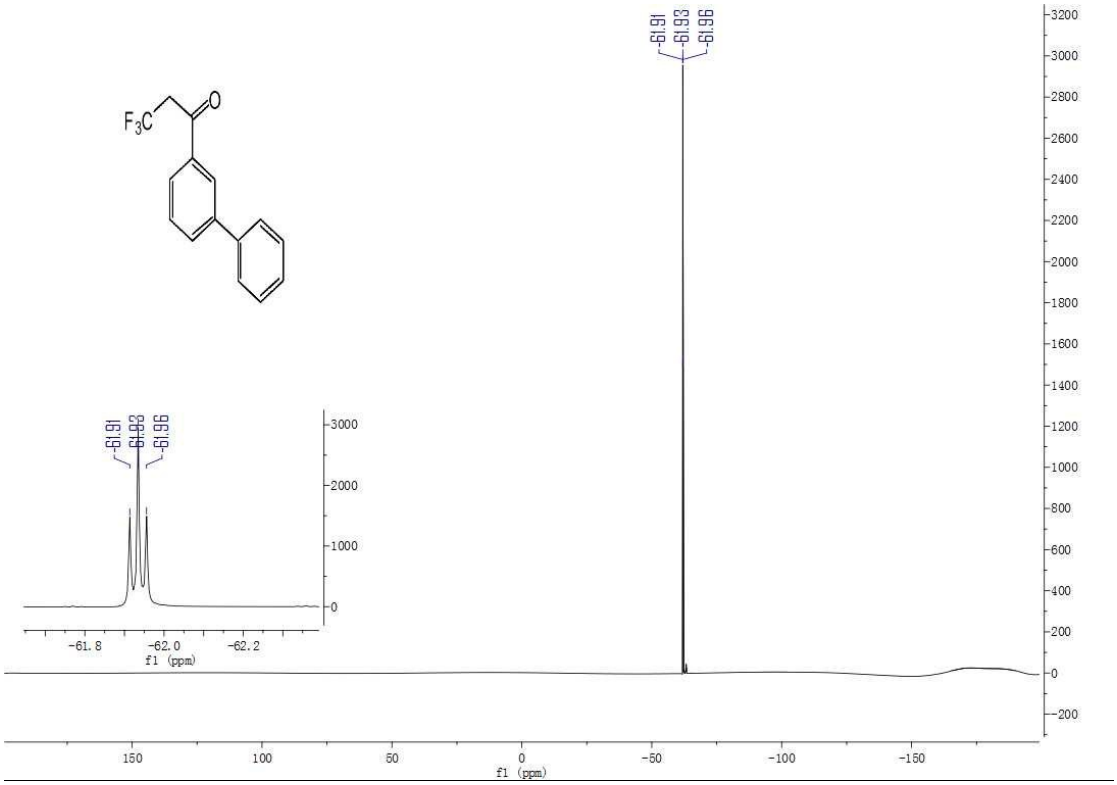

8.02
8.02
8.00
8.00
7.99
7.74
7.73
7.72
7.71
7.65
7.65
7.64
7.63
7.62
7.62
7.51
7.49
7.48
7.47
7.46
7.45
7.45
7.44
3.85
3.81
3.78
F3C
O
1.98
2.10
2.05
3.16
2.00
f1 (ppm)

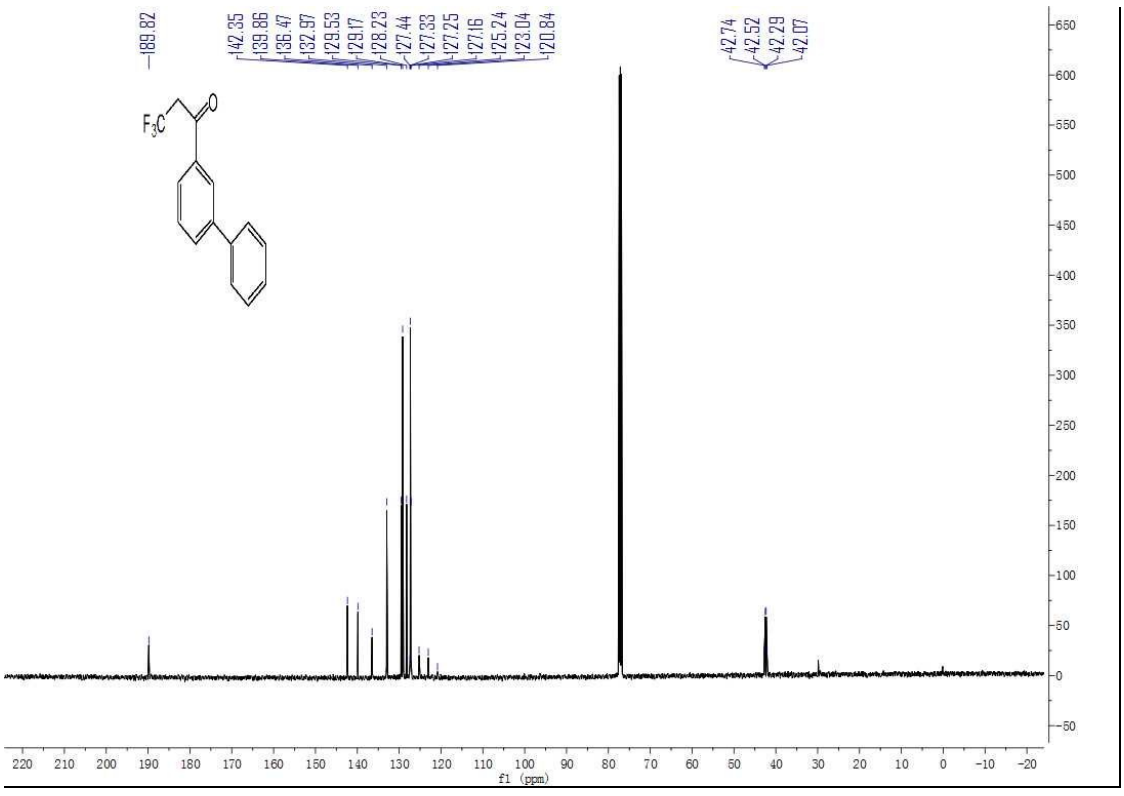

-61.90
-61.92
-61.94
F3C
O
-61.90
-61.92
-61.94
-61.70
-61.80
-61.90
-62.00
f1 (ppm)
f1 (ppm)



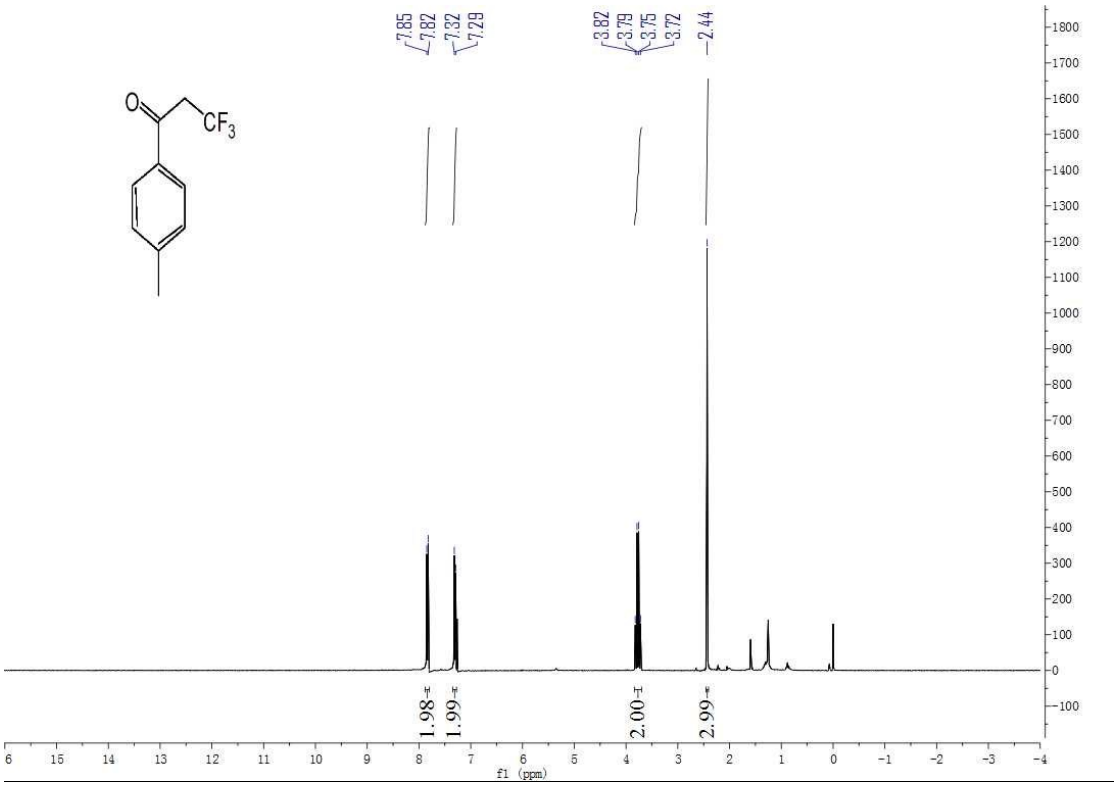
1-(Biphenyl-3-yl)-3,3,3-trifluoropropan-1-one (**2b**)

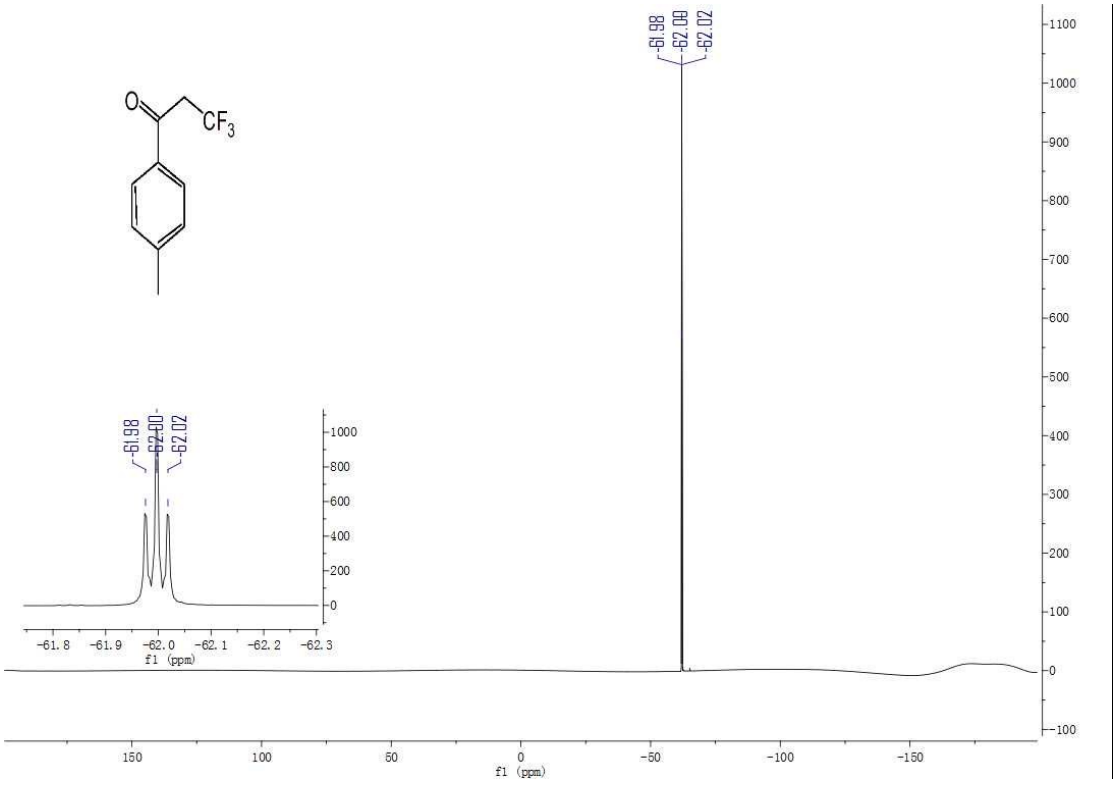


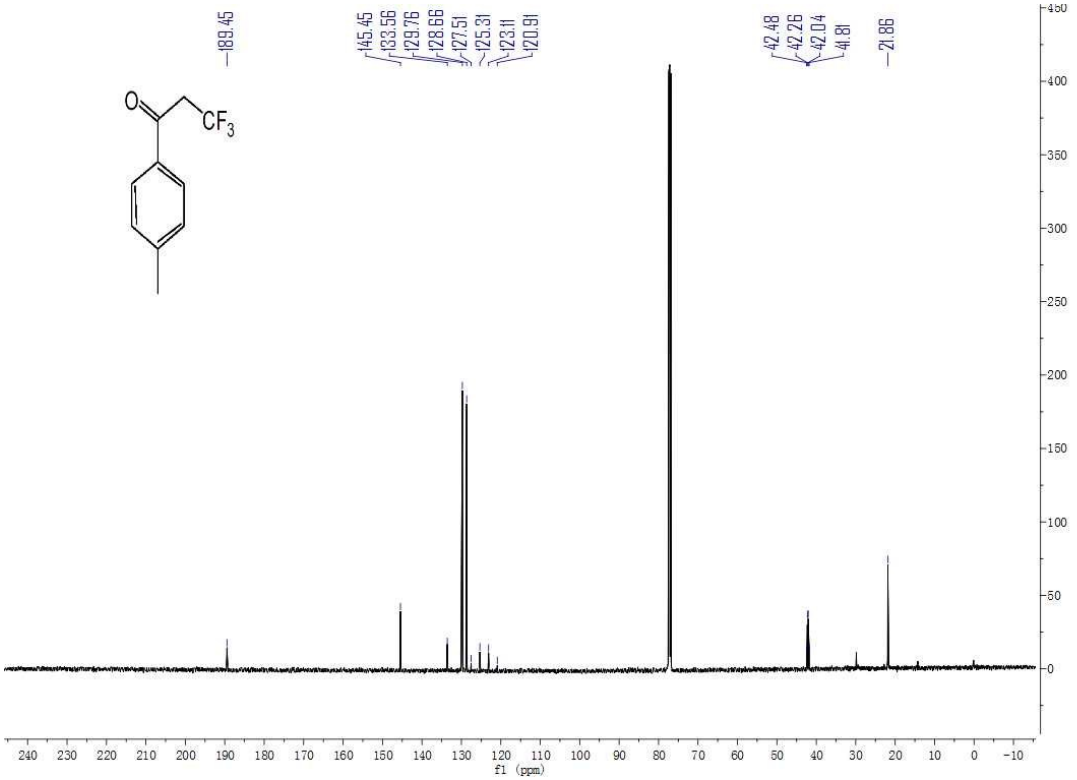

F3C
O
-61.91
-61.93
-61.96
f1 (ppm)


F3C
O
189.82
142.35
139.86
136.47
132.97
129.53
129.17
128.23
127.44
127.33
127.25
127.16
125.24
123.04
120.84
42.74
42.52
42.29
42.07
f1 (ppm)

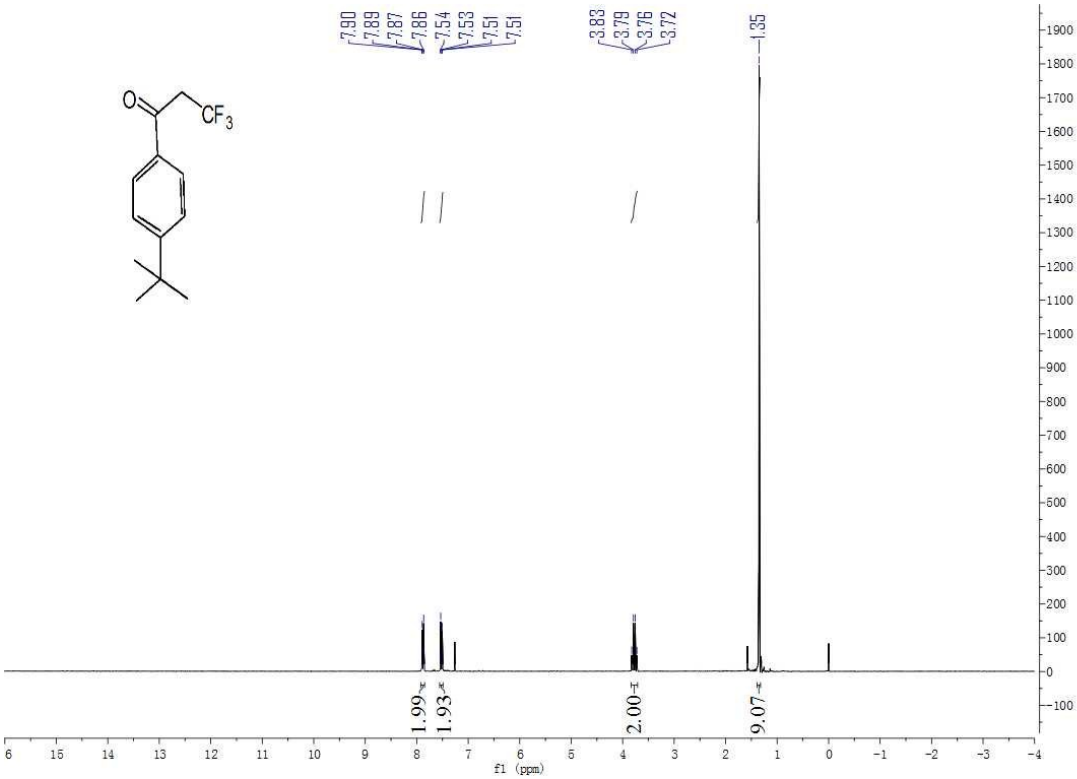
3,3,3-Trifluoro-1-p-tolylpropan-1-one (**2c**)

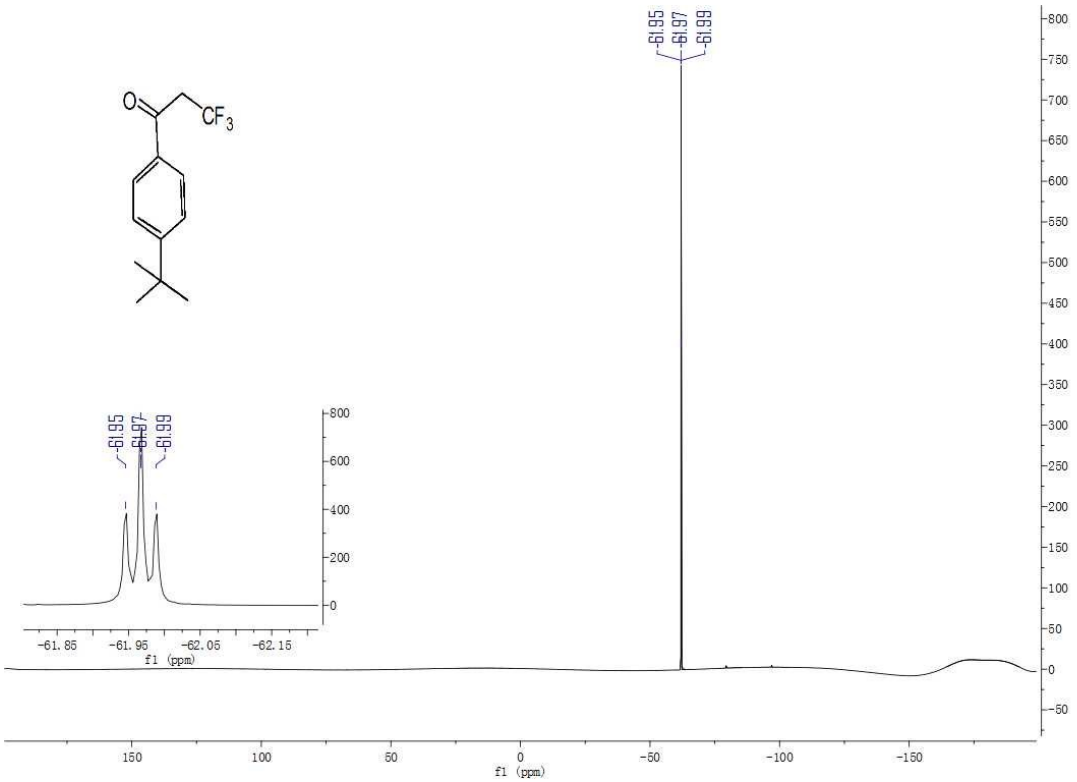


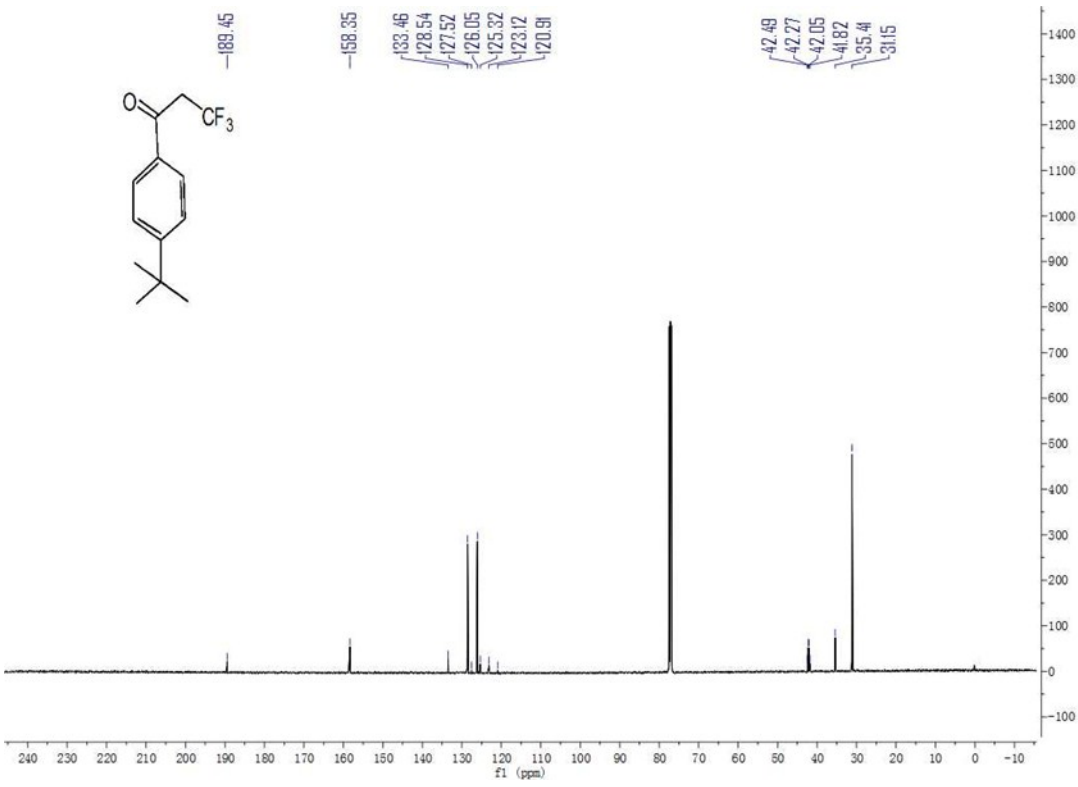




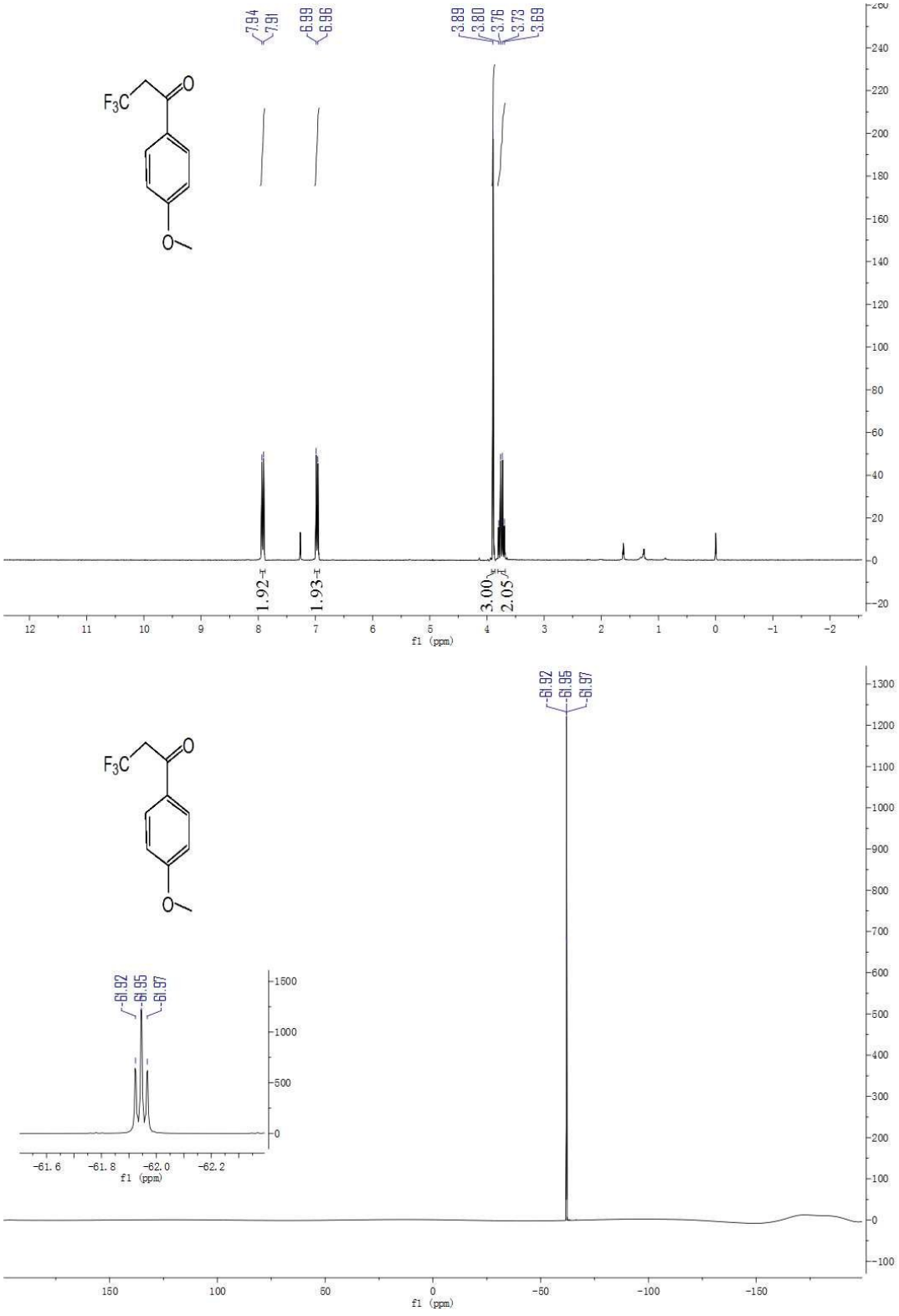
1-(4-Tert-butylphenyl)-3,3,3-trifluoropropan-1-one (**2d**)

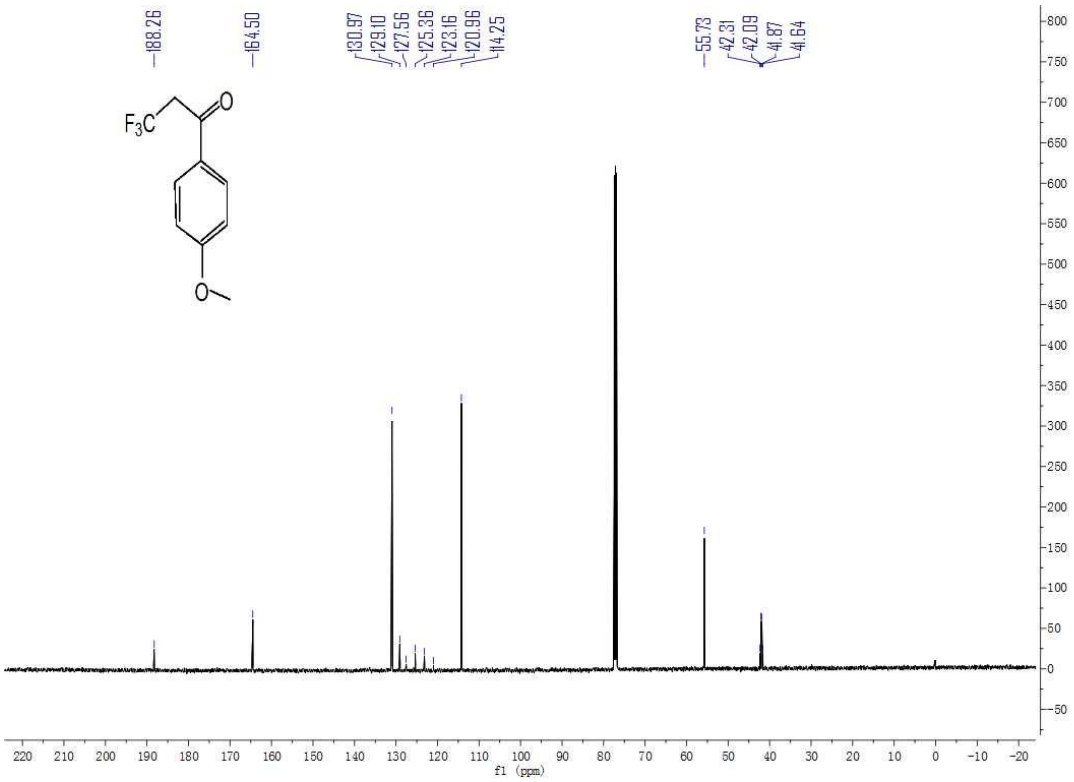



O
CF3
-61.95
-61.97
-61.99
f1 (ppm)

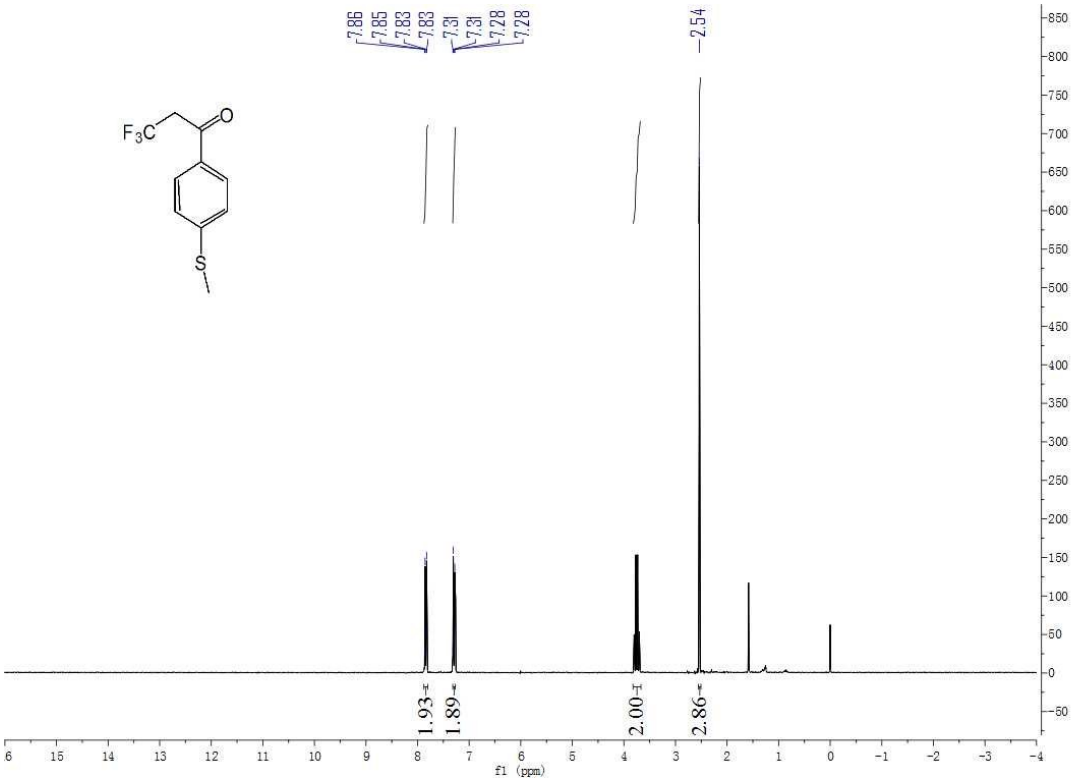

O
CF3
189.45
158.35
133.46
128.54
127.52
126.05
125.32
123.12
120.91
42.49
42.27
42.05
41.82
35.44
31.15
f1 (ppm)

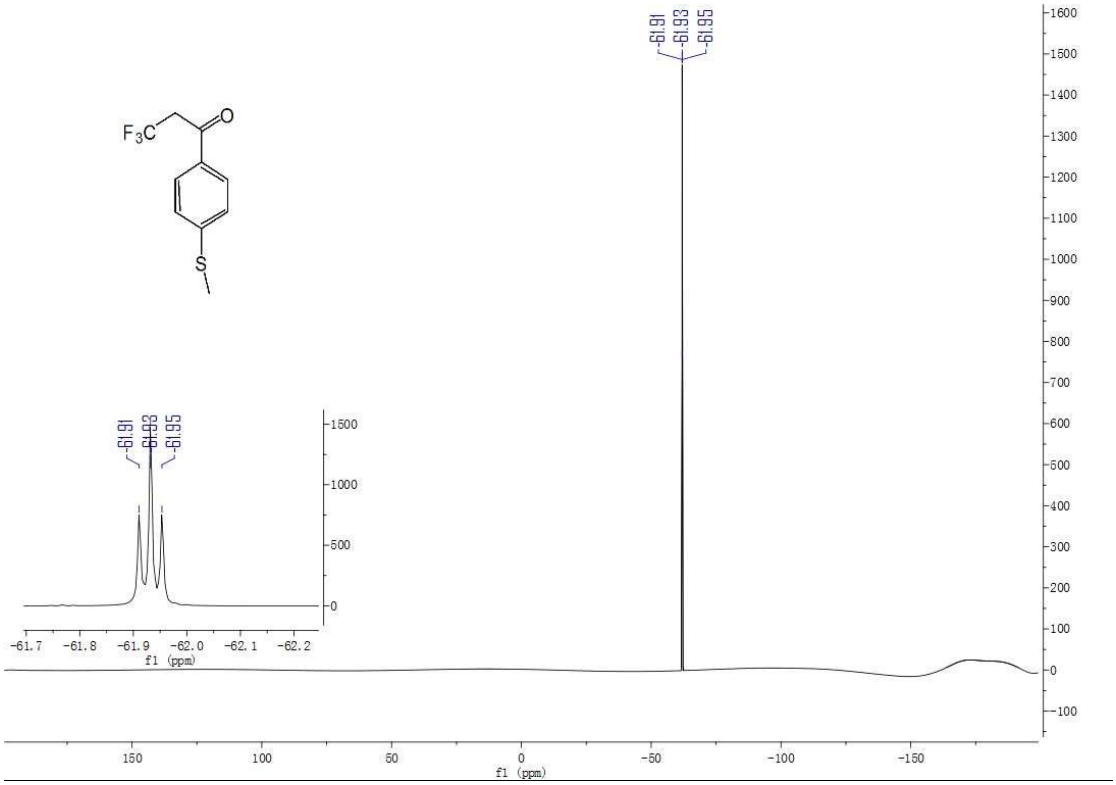
3,3,3-Trifluoro-1-(4-methoxyphenyl)propan-1-one (**2e**)

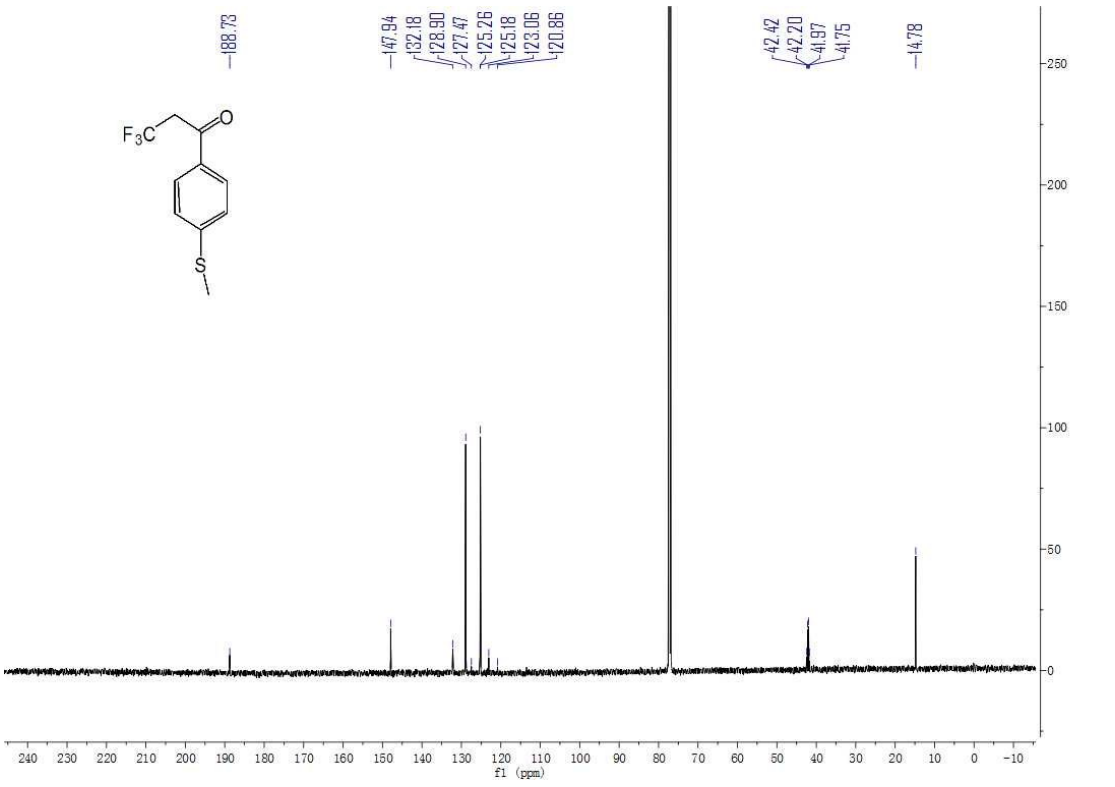




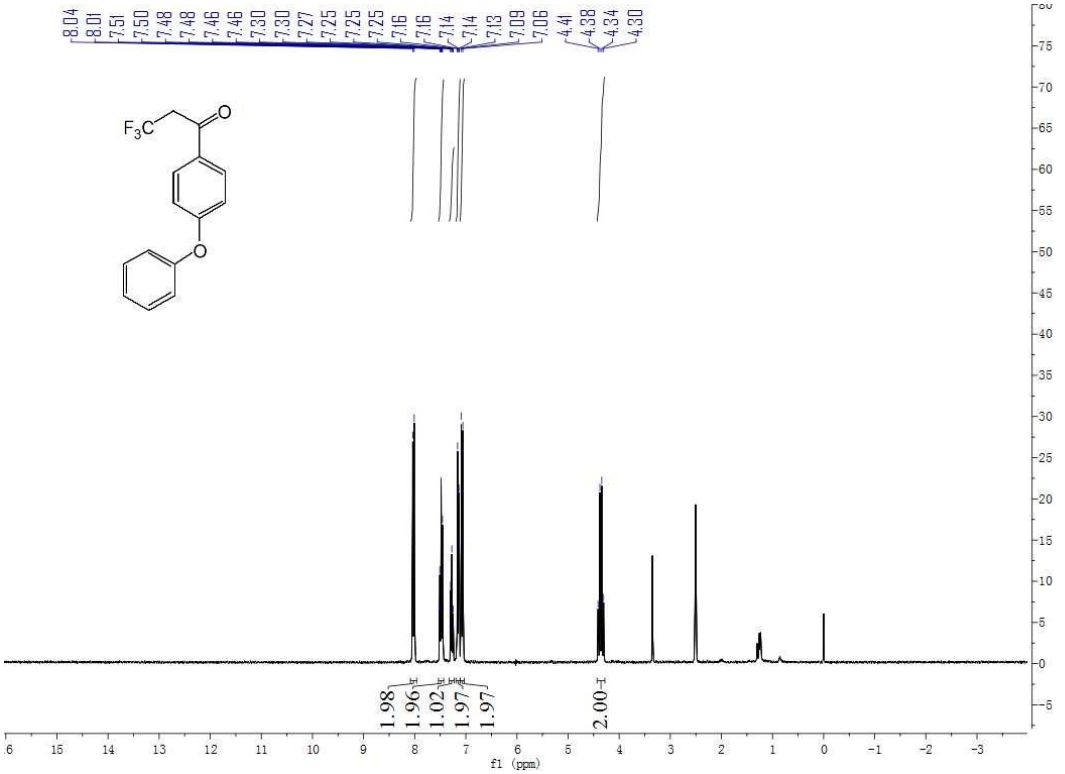
3,3,3-Trifluoro-1-(4-(methylthio)phenyl)propan-1-one (**2f**)

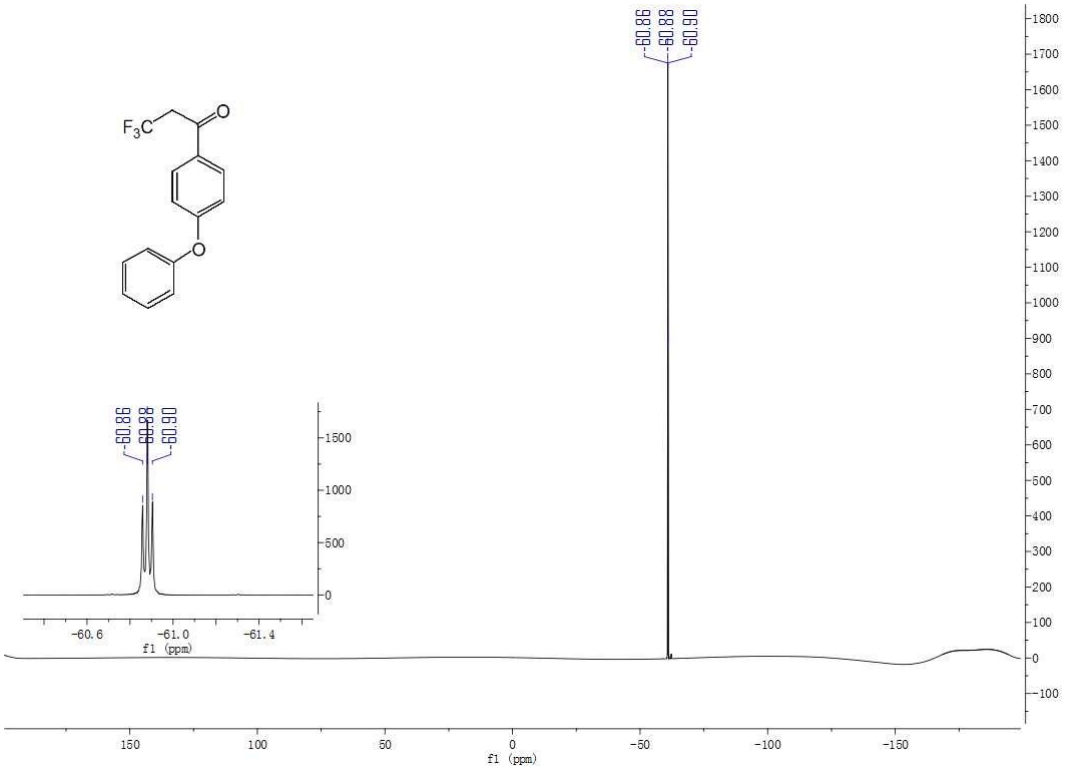


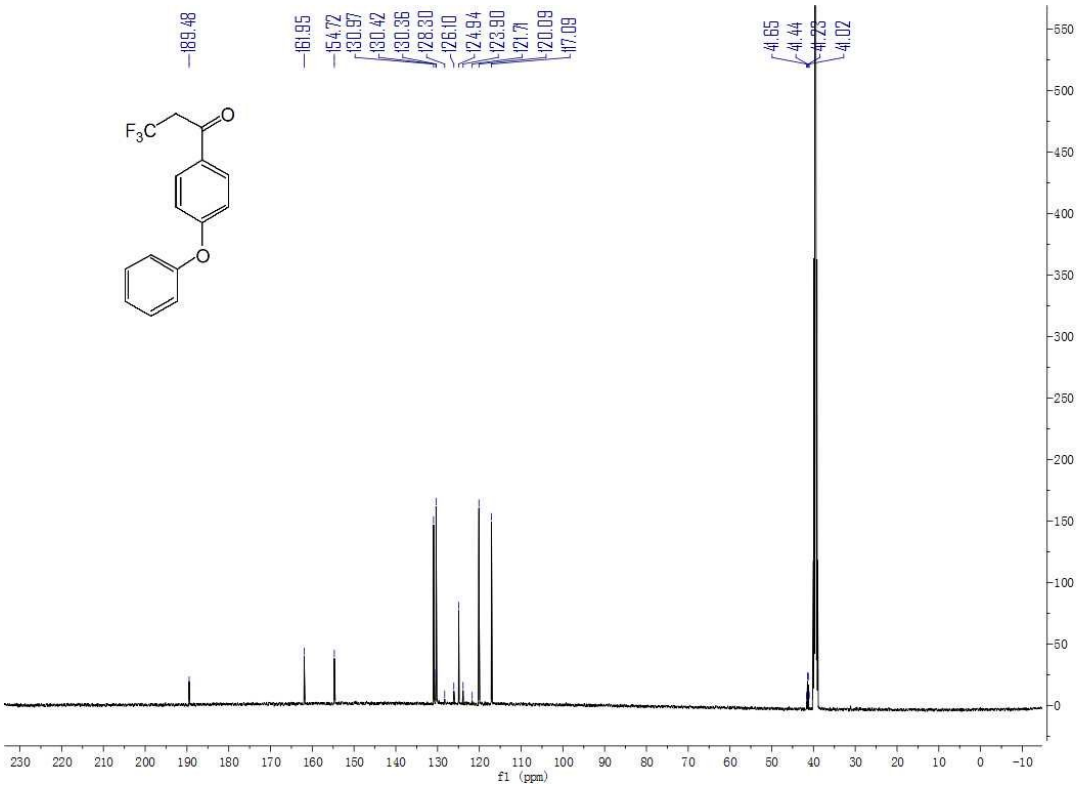

-61.91
-61.93
-61.95
F3C
O
S
f1 (ppm)


188.73
147.94
132.18
128.90
127.47
125.26
125.18
123.06
120.86
42.42
42.20
41.97
41.75
14.78
F3C
O
S
f1 (ppm)

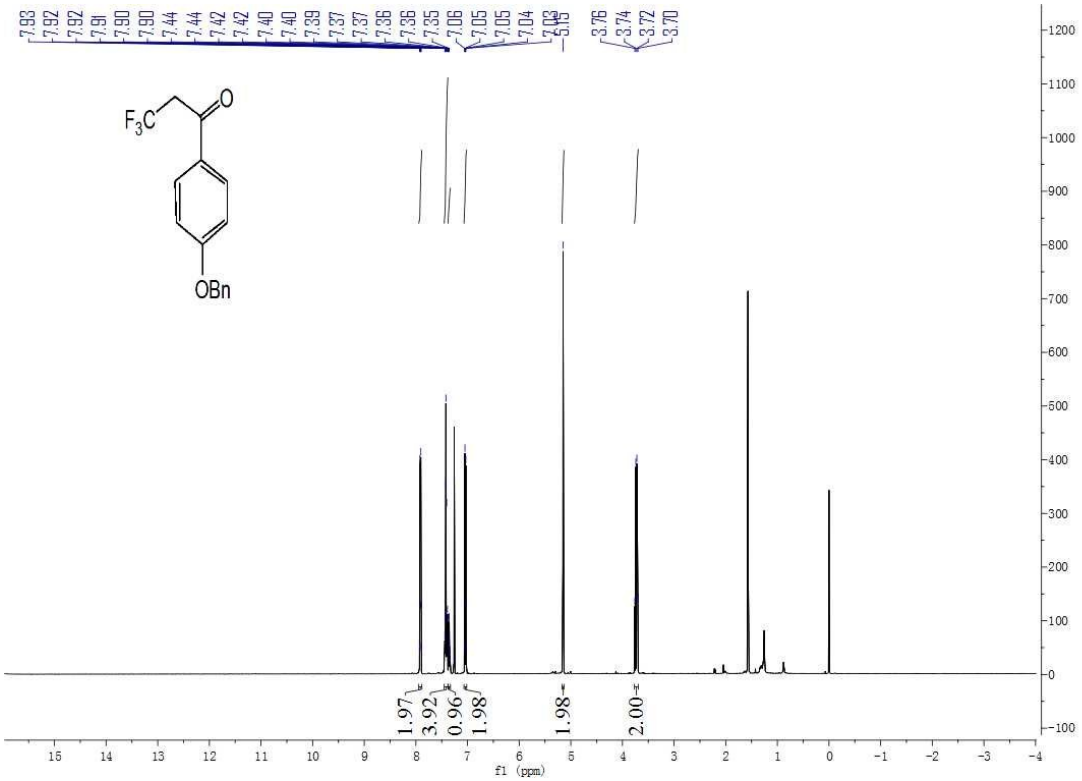
3,3,3-Trifluoro-1-(4-phenoxyphenyl)propan-1-one (**2g**)

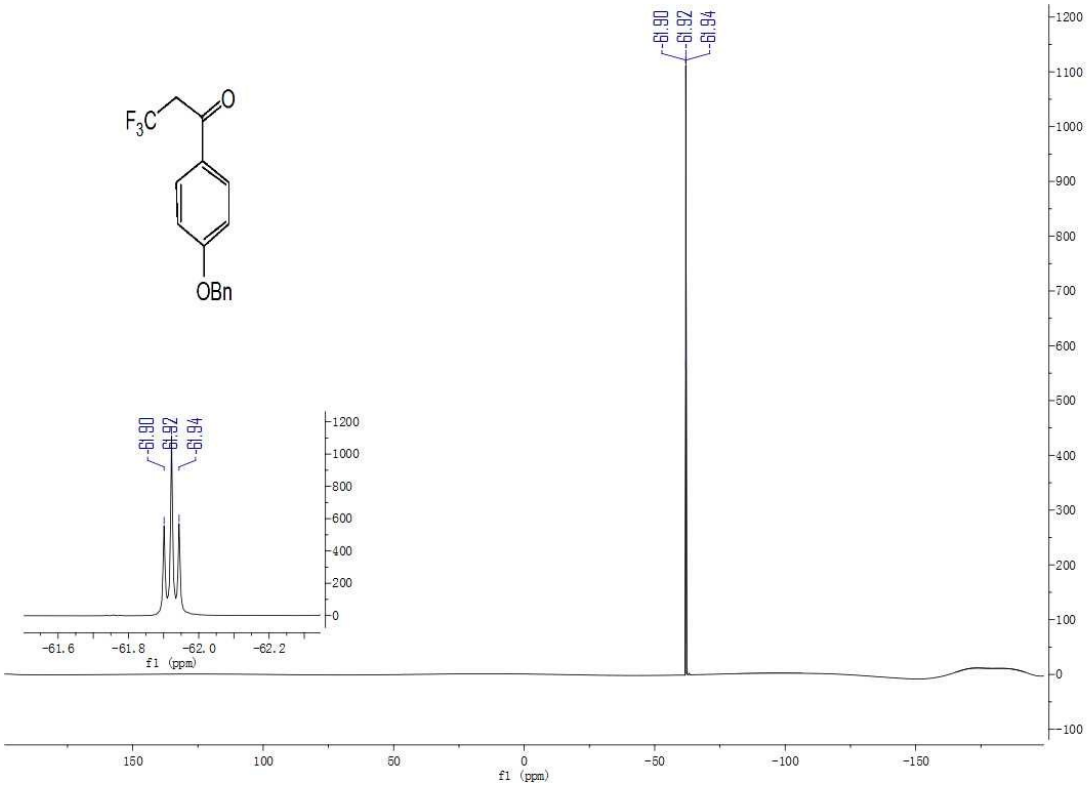


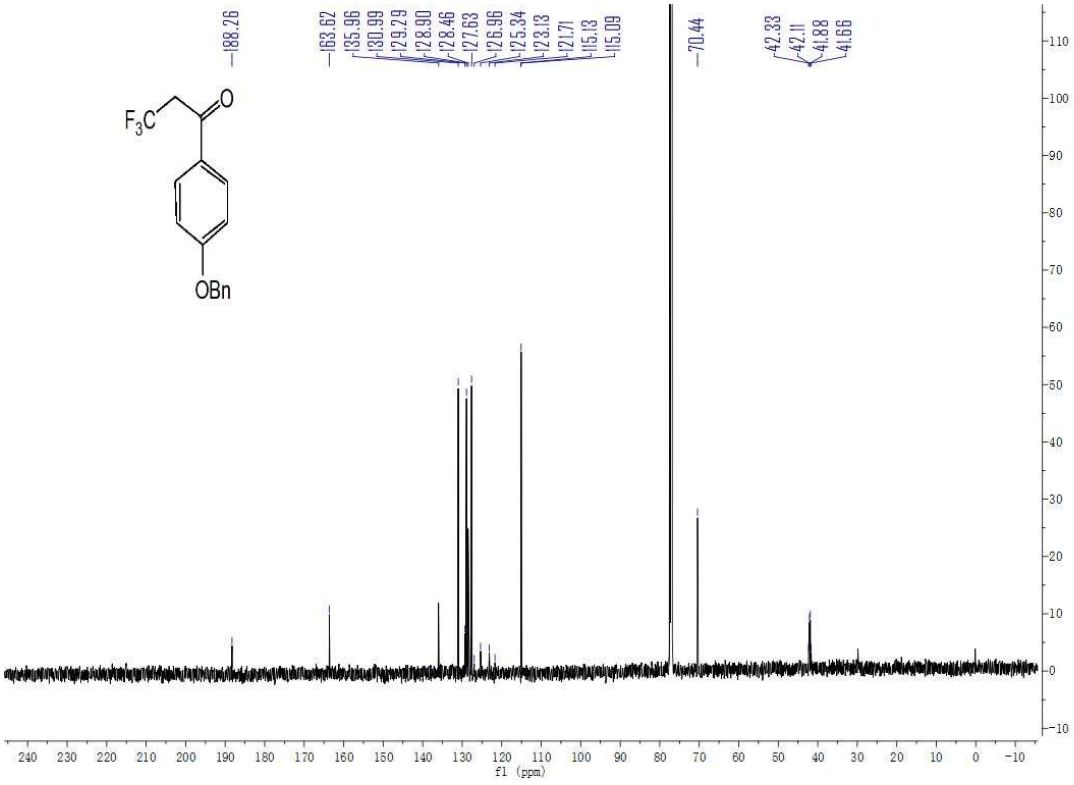




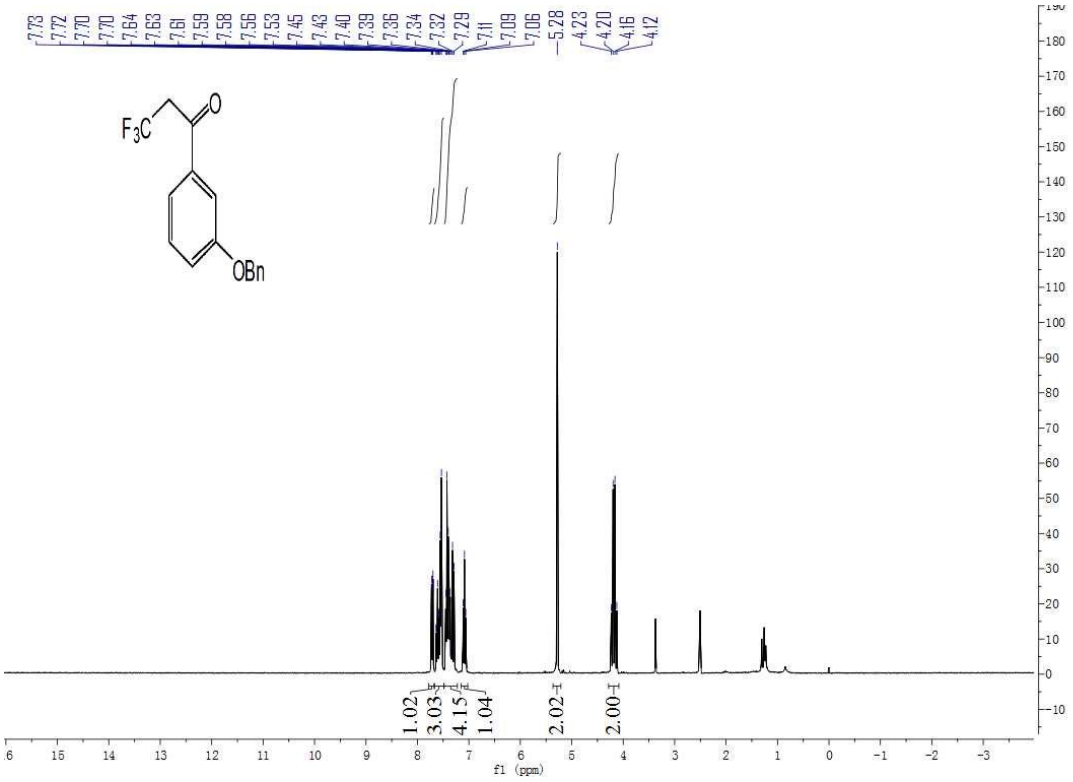
1-(4-(Benzyloxy)phenyl)-3,3,3-trifluoropropan-1-one (**2h**)

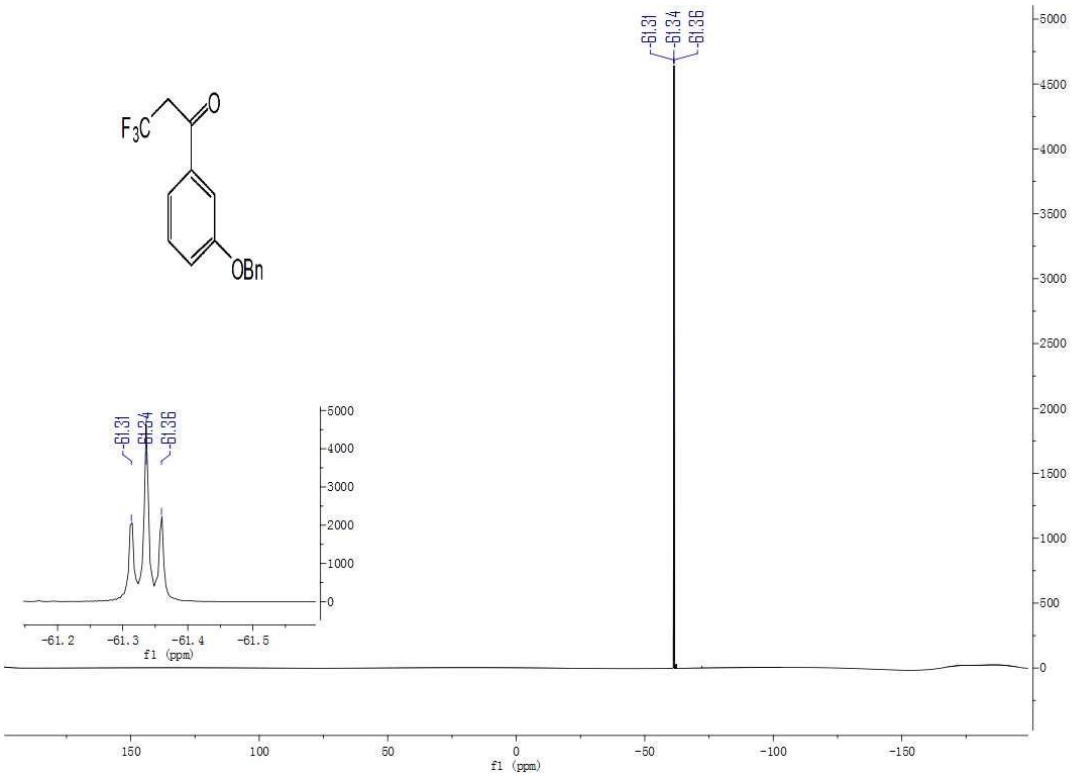


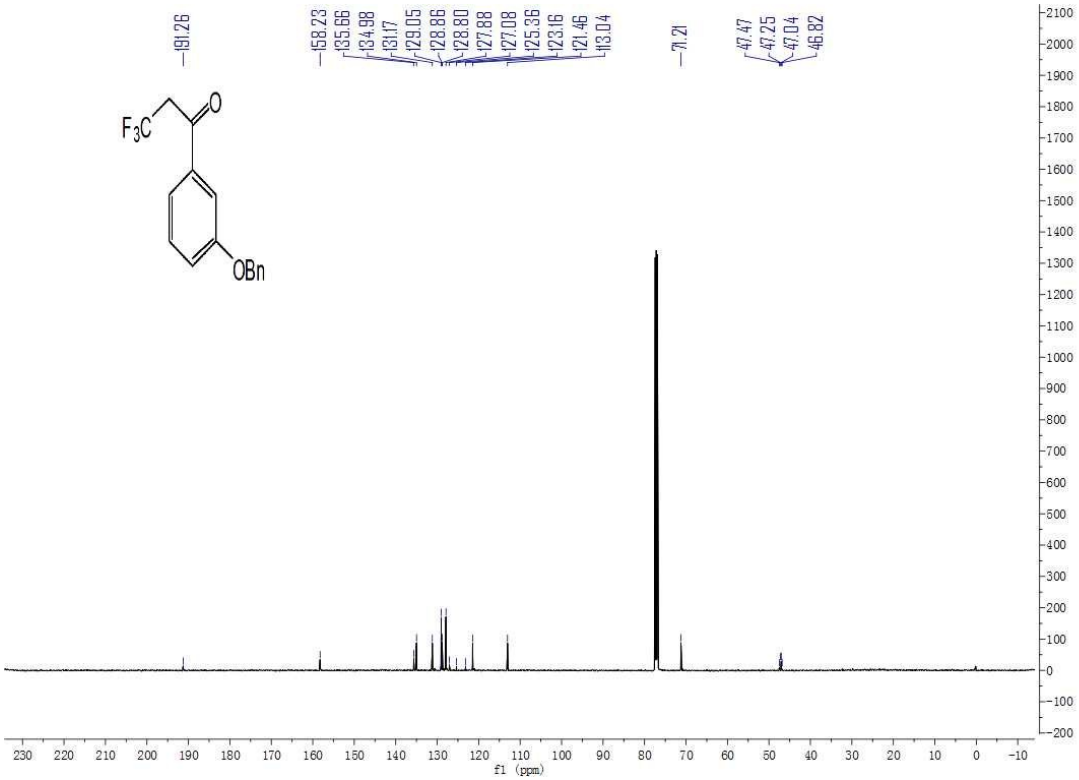

F3C
O
OBn
-61.90
-61.92
-61.94
f1 (ppm)


F3C
O
OBn
188.26
163.62
135.96
130.99
129.29
128.90
128.46
127.63
126.96
125.34
123.13
121.71
115.13
115.09
70.44
42.33
42.11
41.88
41.66
f1 (ppm)

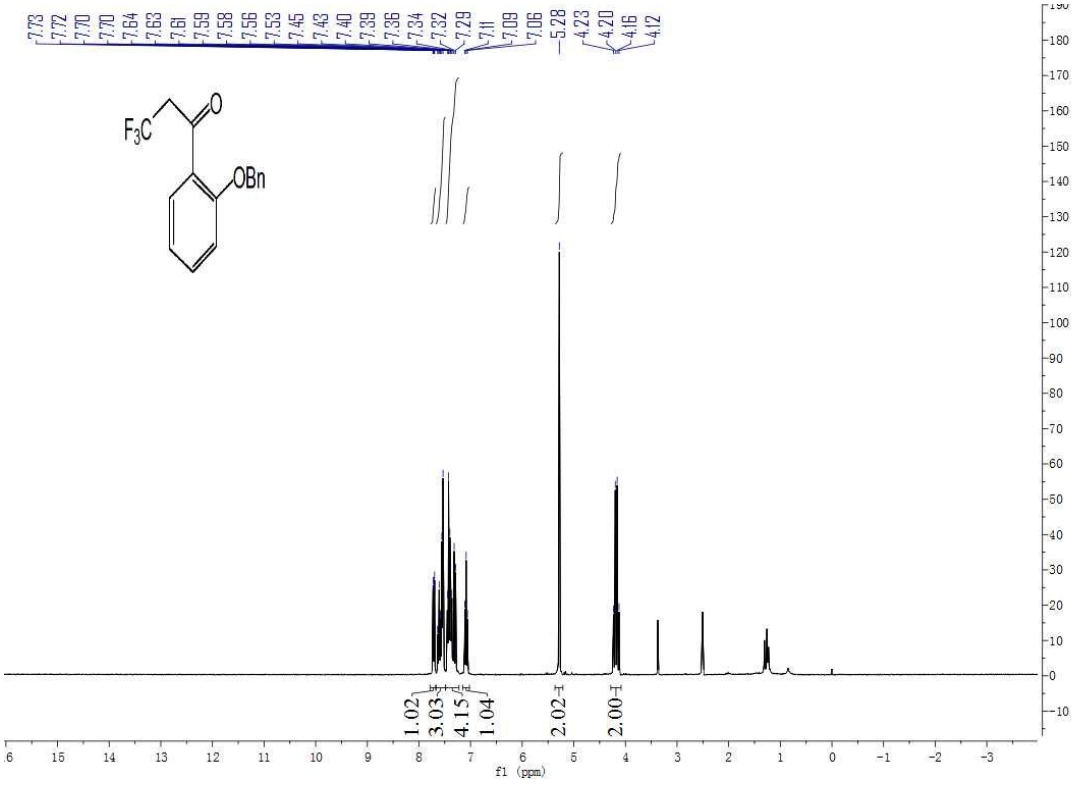
1-(3-(Benzyloxy)phenyl)-3,3,3-trifluoropropan-1-one (**2i**)

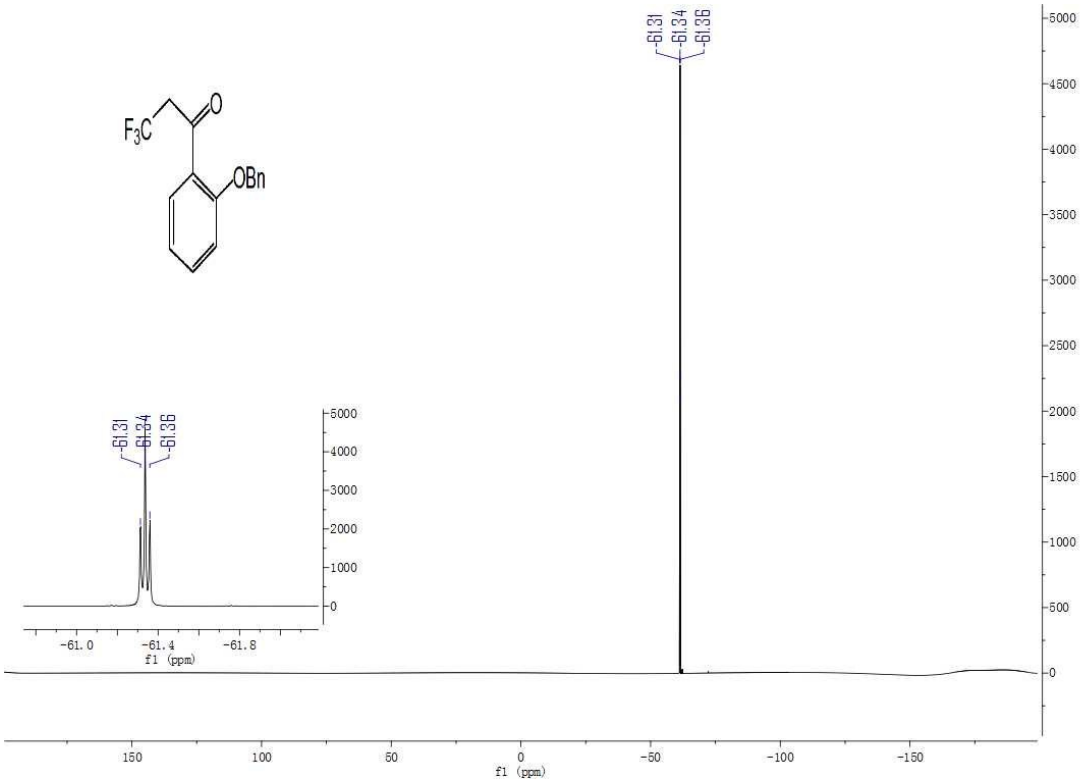


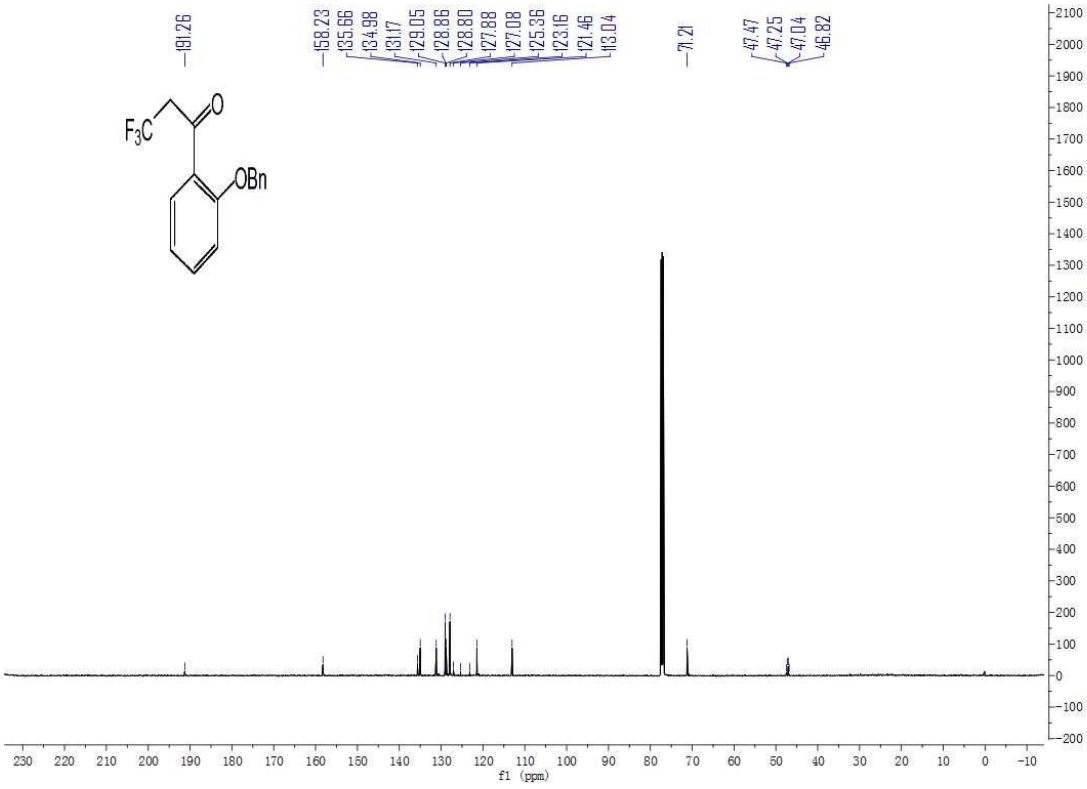




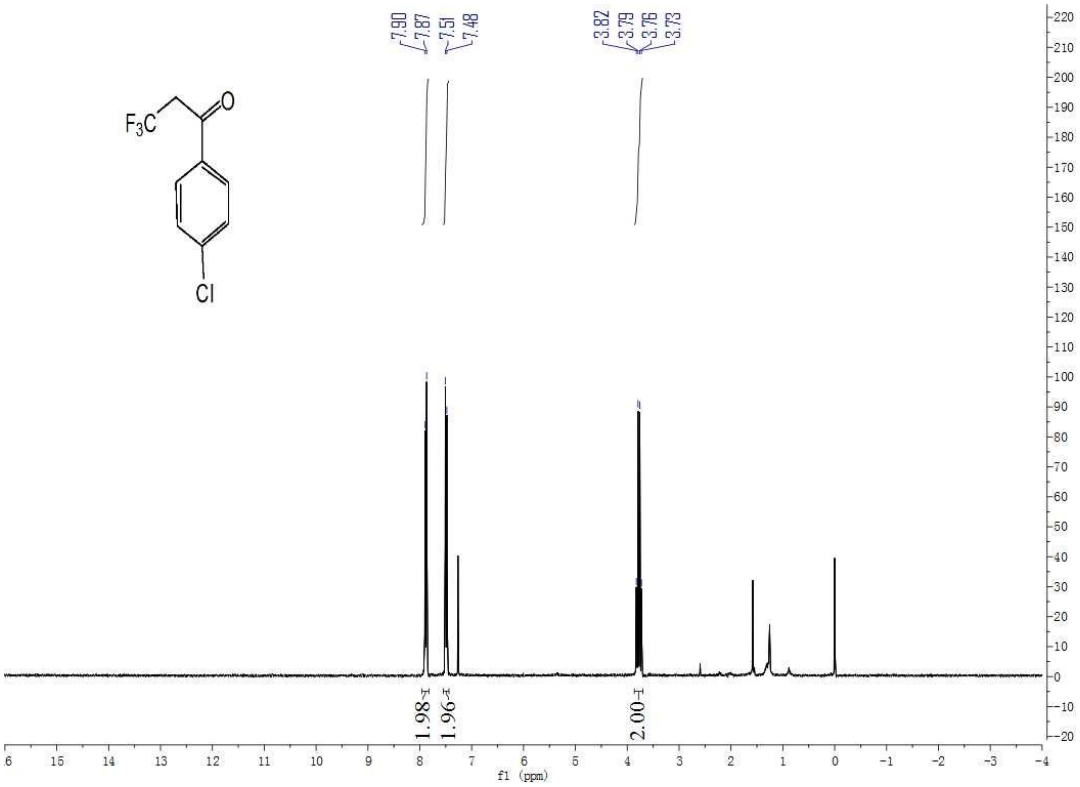
1-(2-(Benzyloxy)phenyl)-3,3,3-trifluoropropan-1-one (**2j**)

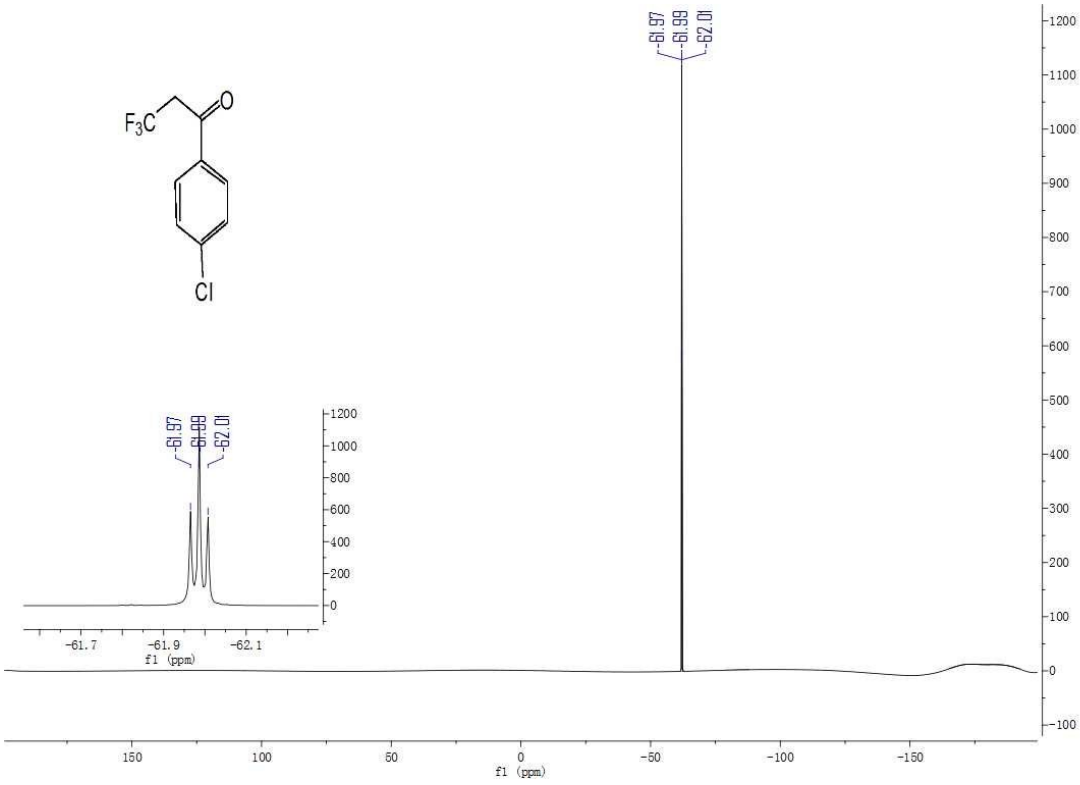


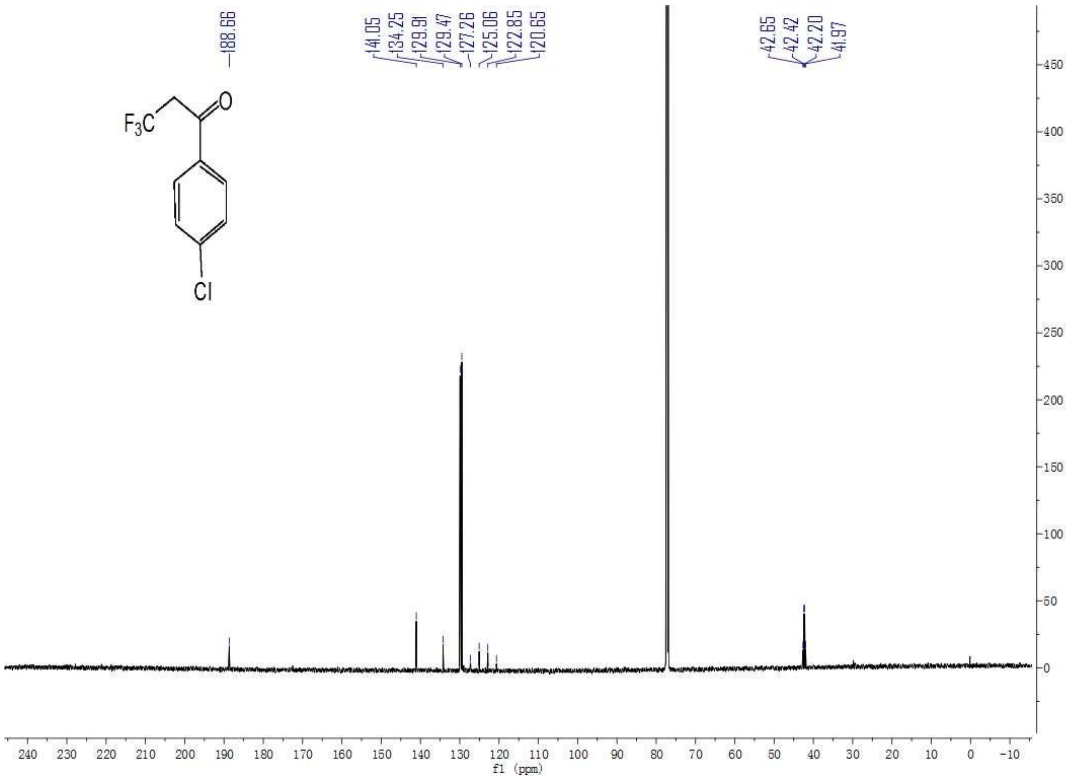

F3C
O
OBn
-61.31
-61.34
-61.36
f1 (ppm)


F3C
O
OBn
191.26
158.23
135.66
134.98
131.17
129.05
128.86
128.80
127.88
127.08
125.36
123.16
121.46
113.04
71.21
47.47
47.25
47.04
46.82
f1 (ppm)

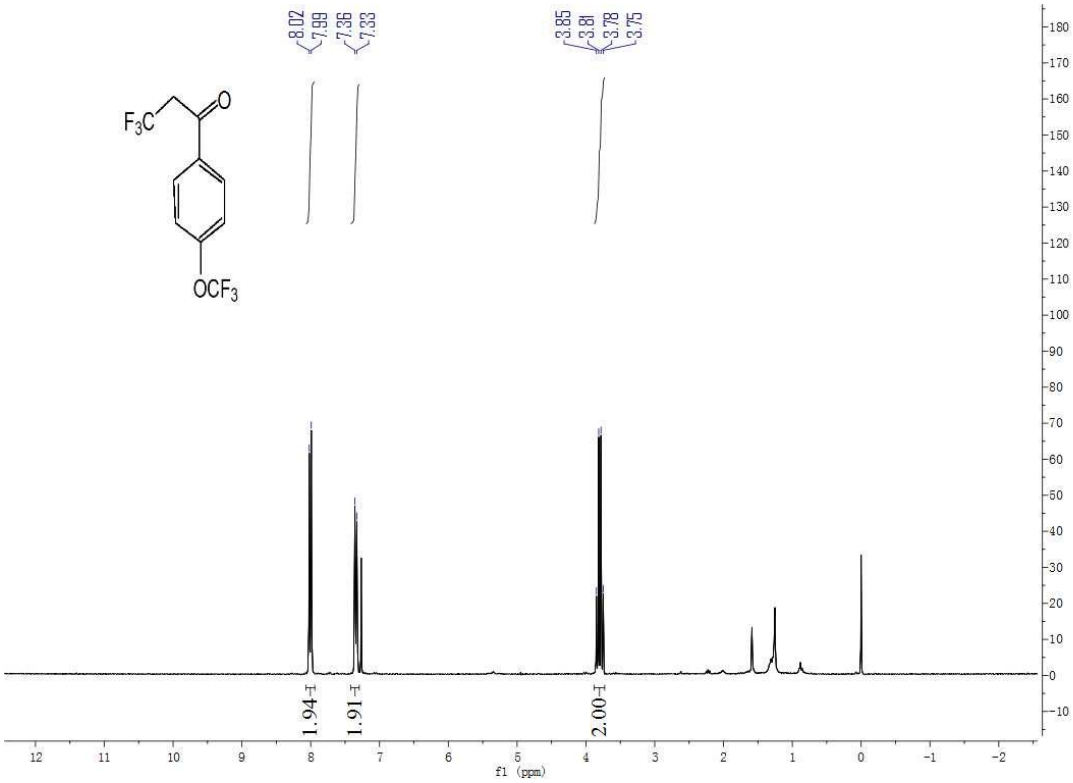
1-(2-(Benzyloxy)phenyl)-3,3,3-trifluoropropan-1-one (**2k**)

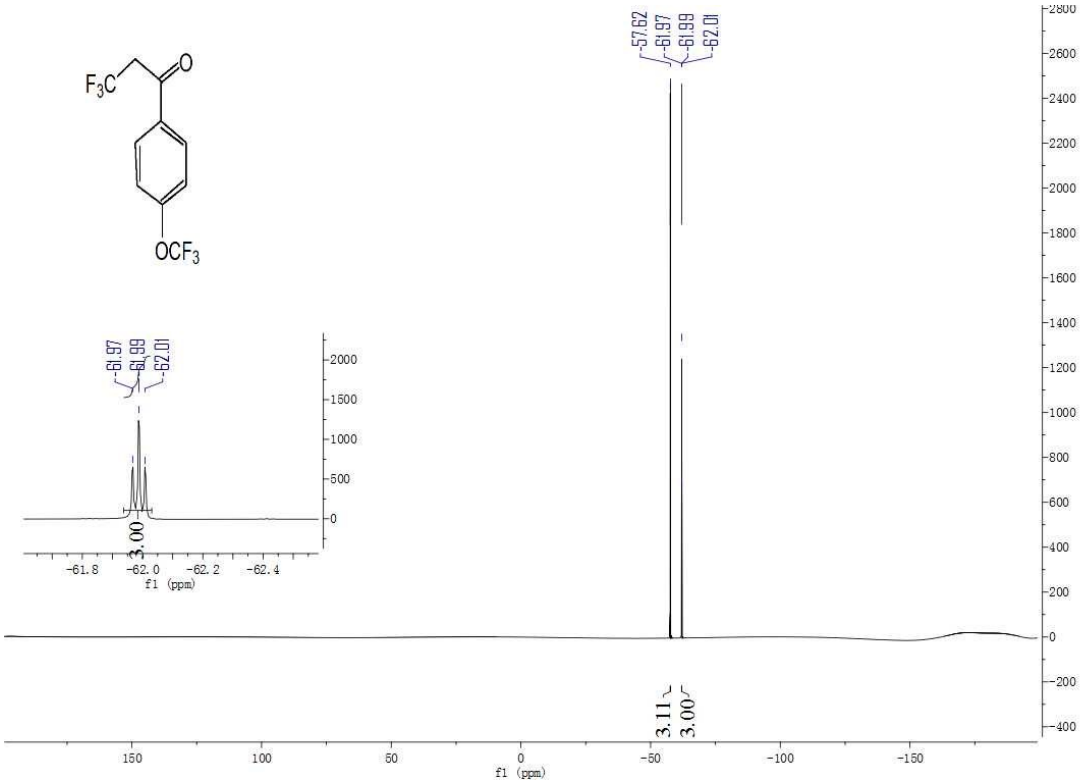


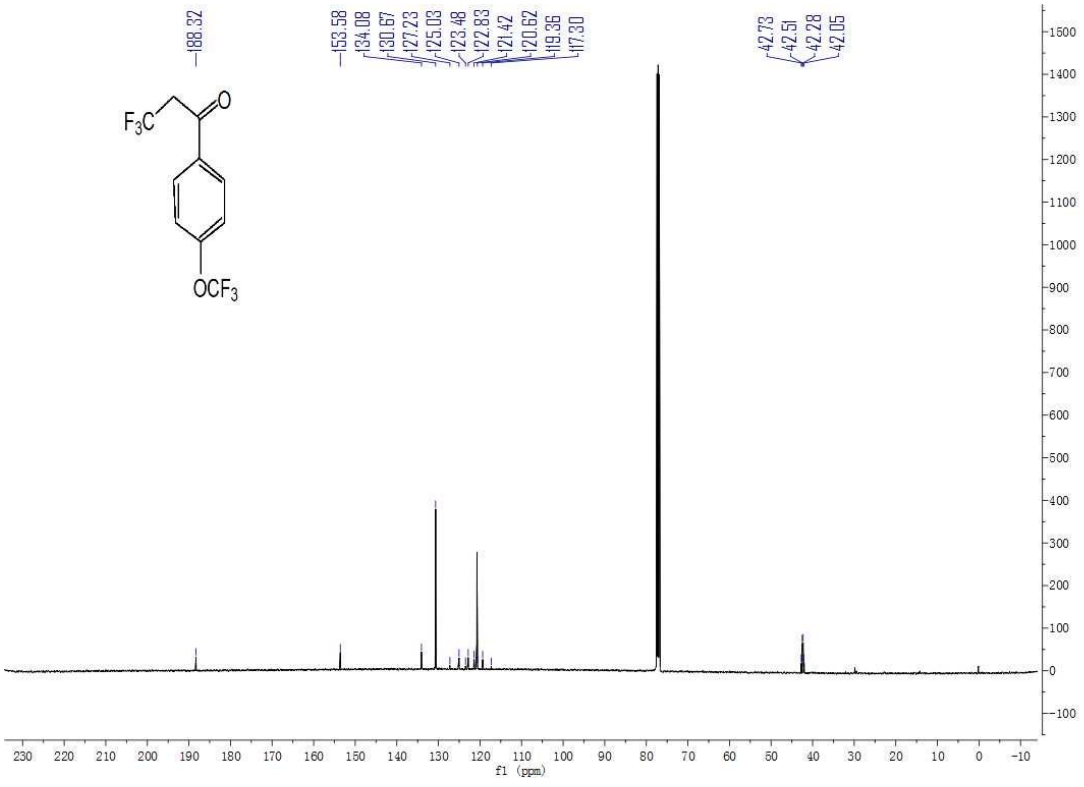




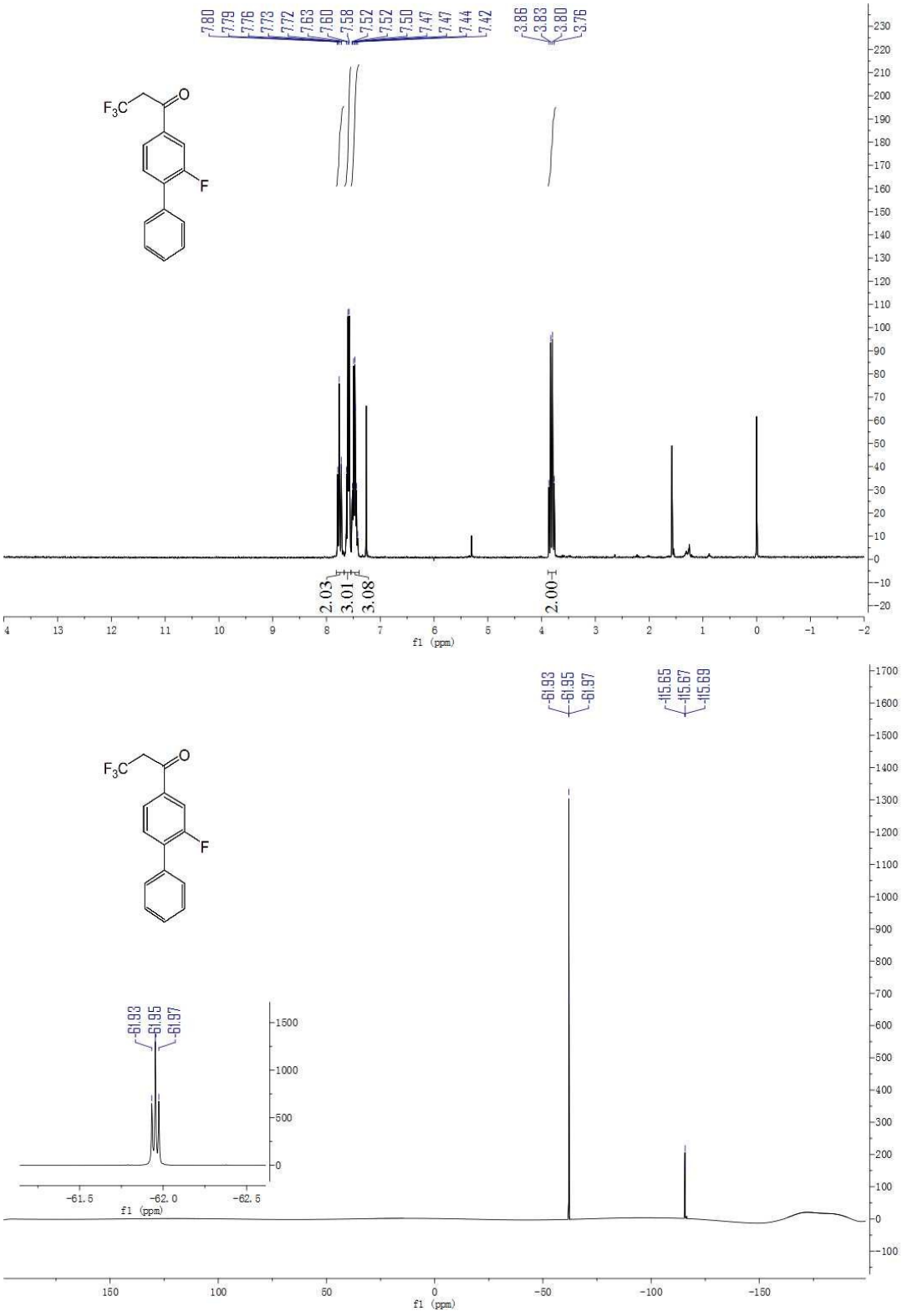
3,3,3-Trifluoro-1-(4-(trifluoromethoxy)phenyl)propan-1-one (**2l**)

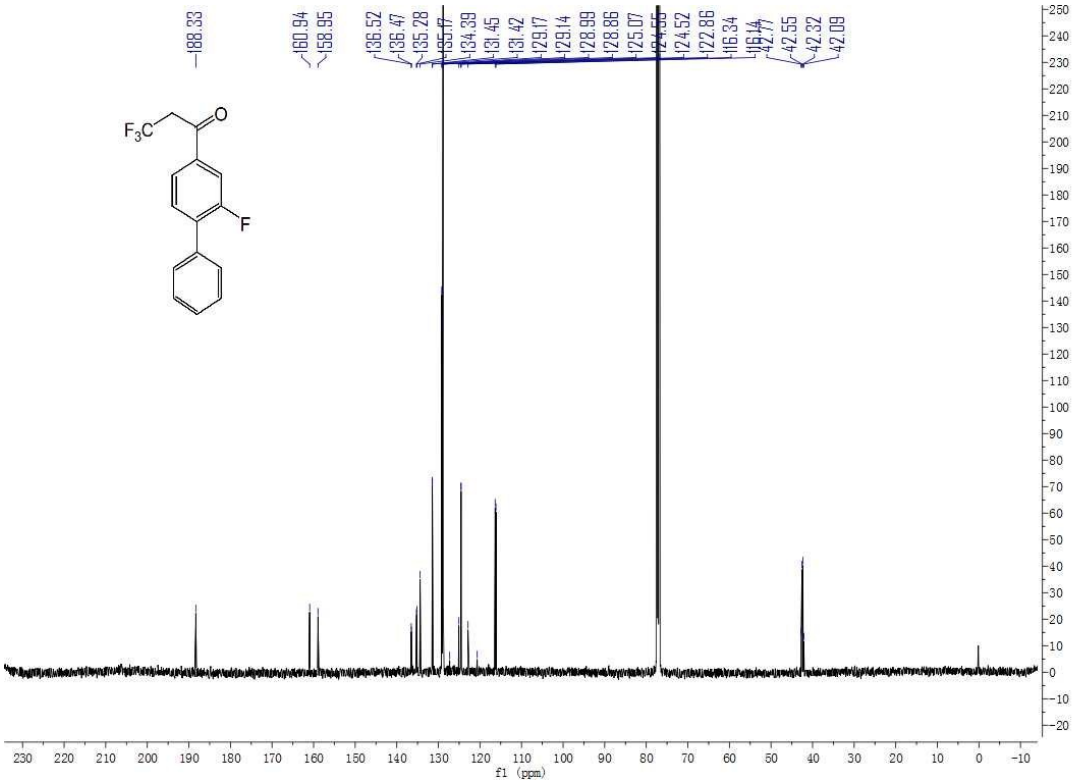



F3C
O
OCF3
-57.62
-61.97
-61.99
-62.01
3.11
3.00
f1 (ppm)

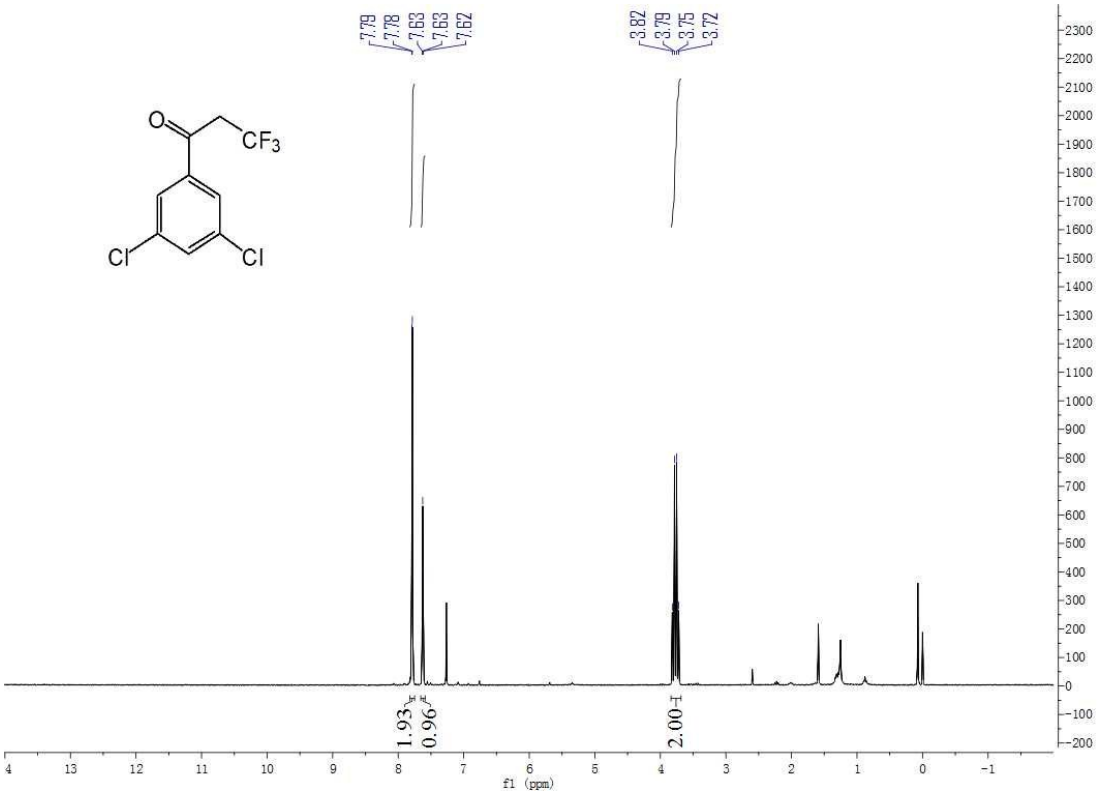

F3C
O
OCF3
188.32
153.58
134.08
130.67
127.23
125.03
123.48
122.83
121.42
120.62
119.36
117.30
42.73
42.51
42.28
42.05
f1 (ppm)

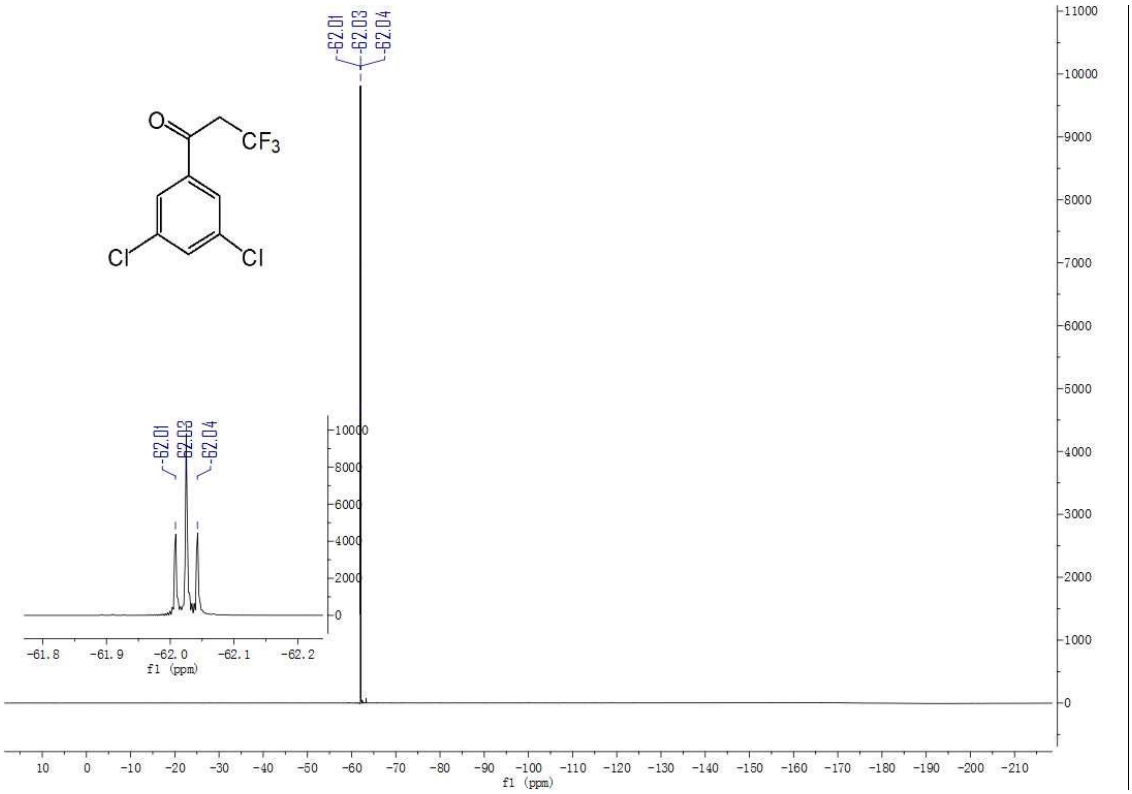
3,3,3-Trifluoro-1-(2-fluorobiphenyl-4-yl)propan-1-one (**2m**)

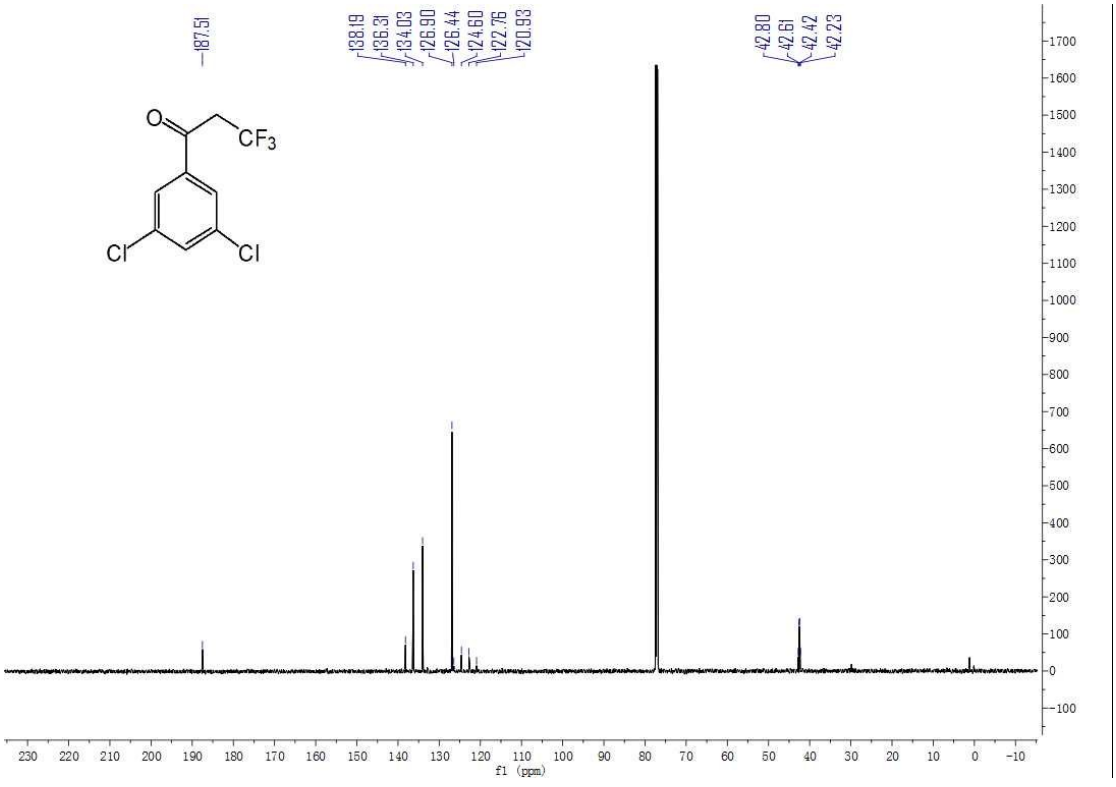




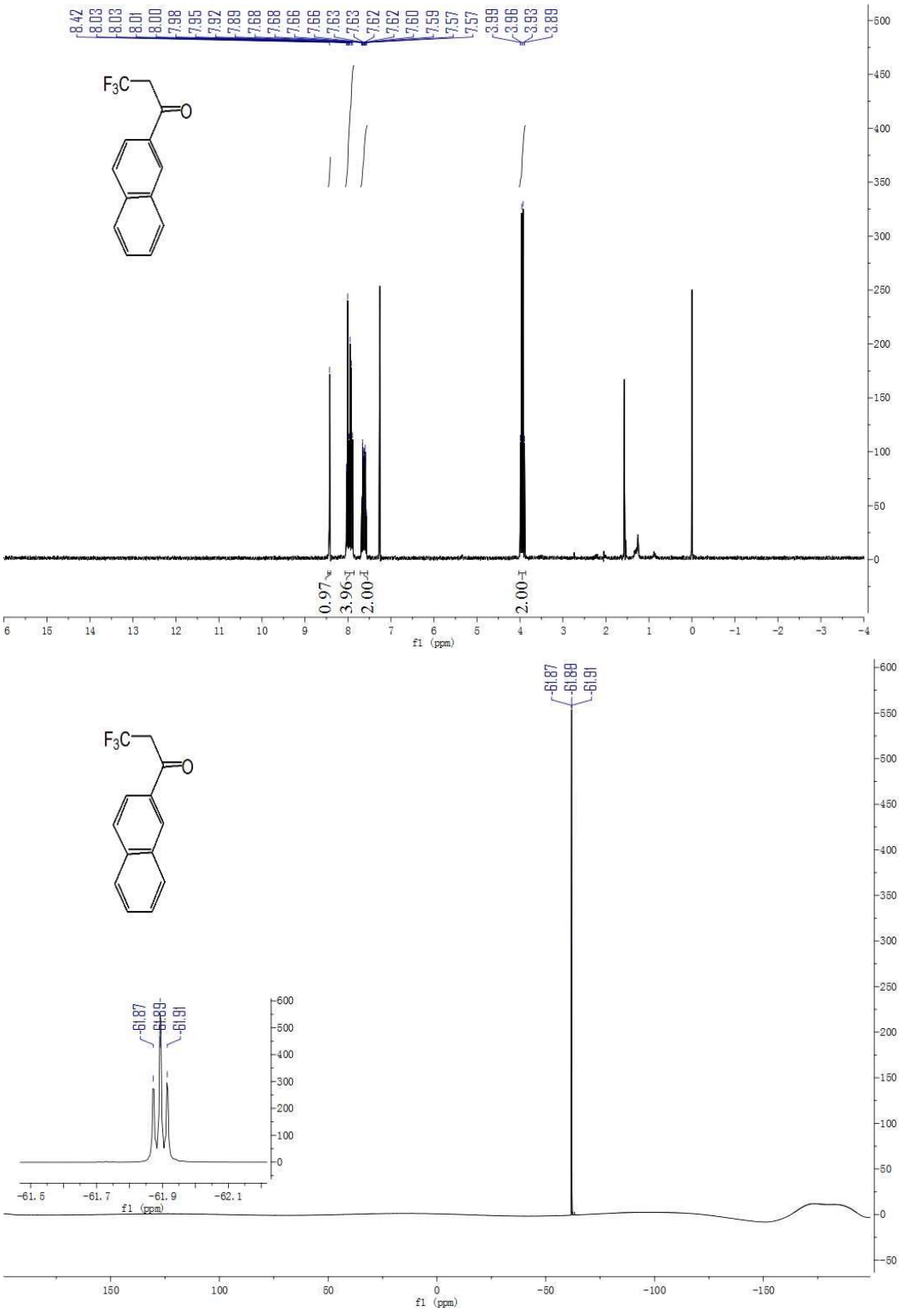
1-(3,5-Dichlorophenyl)-3,3,3-trifluoropropan-1-one (**2n**)

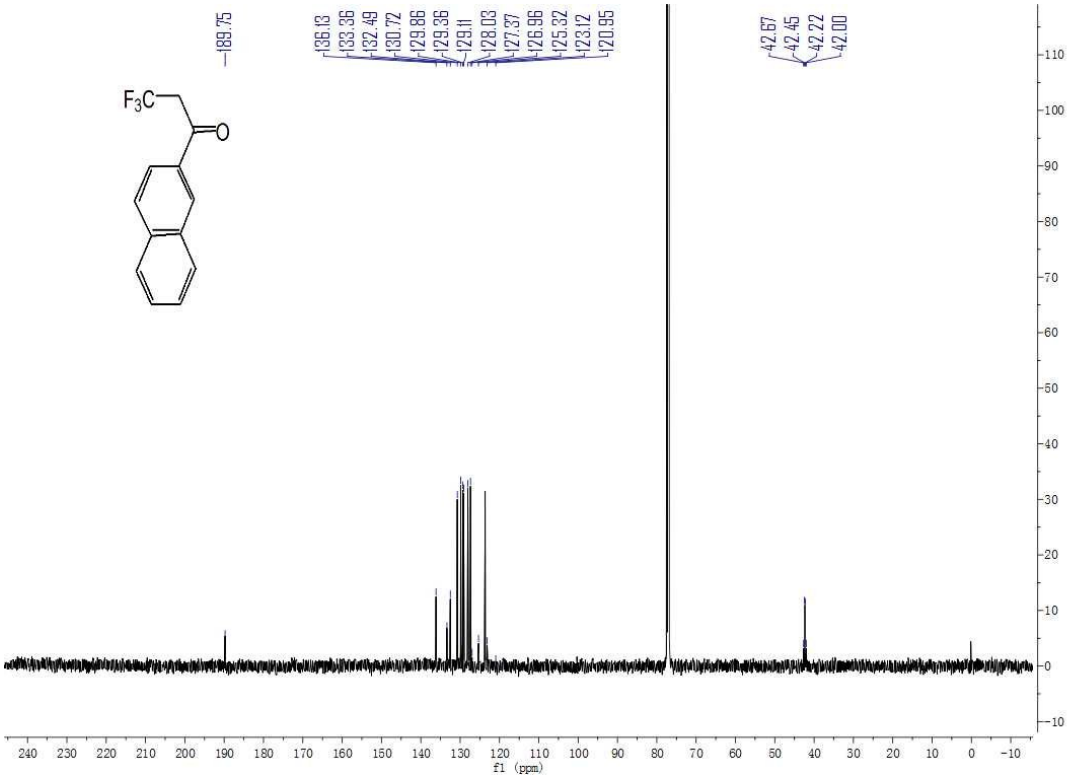



-62.01
-62.03
-62.04
O
CF3
Cl
Cl
f1 (ppm)

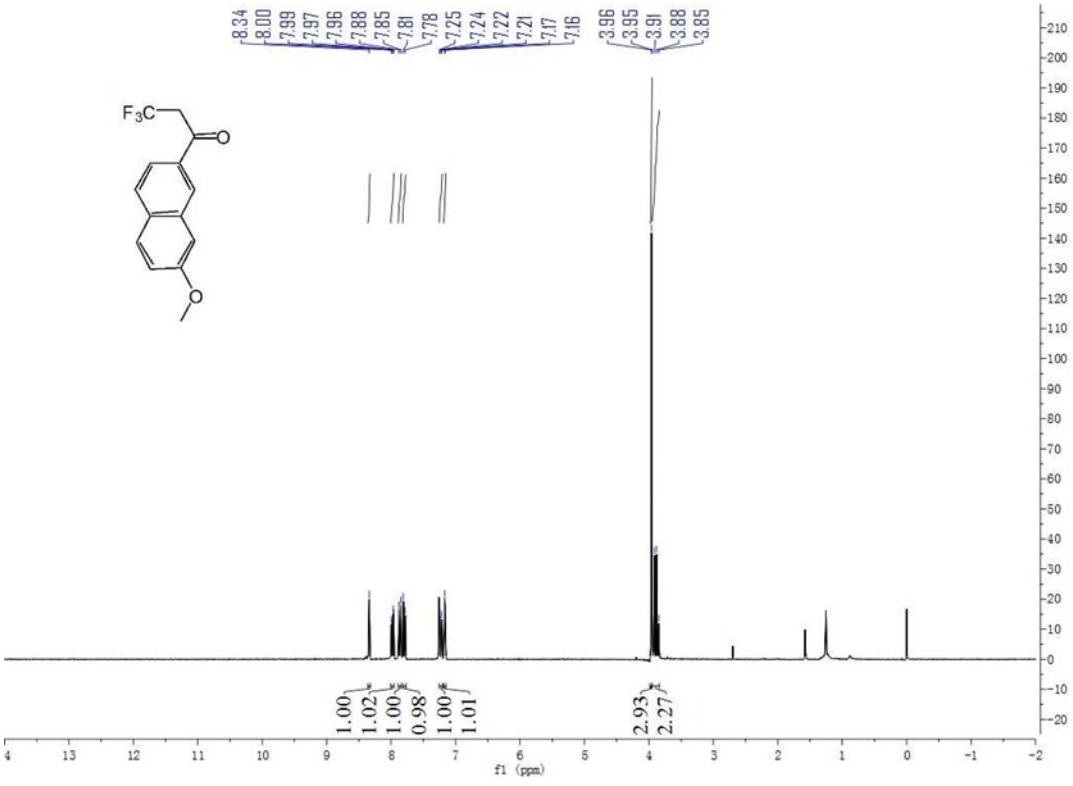

187.51
138.19
136.31
134.03
126.90
126.44
124.60
122.76
120.93
42.80
42.61
42.42
42.23
O
CF3
Cl
Cl
f1 (ppm)

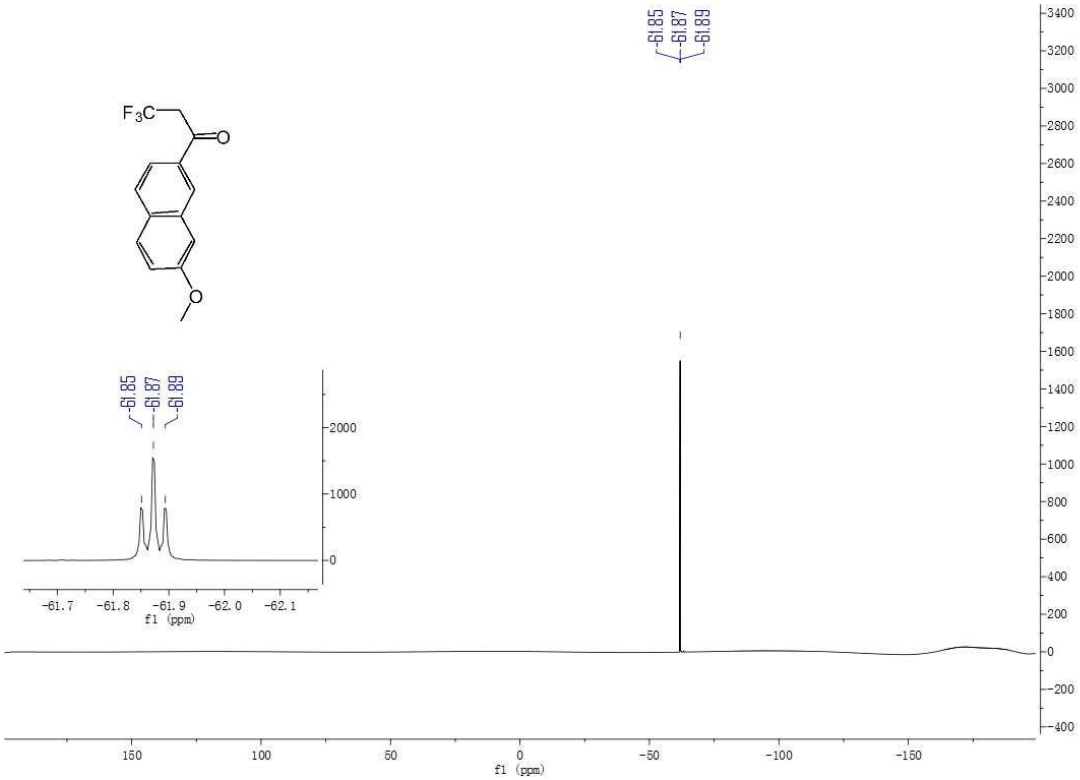
3,3,3-Tifluoro-1-(naphthalen-2-yl)propan-1-one (**2o**)

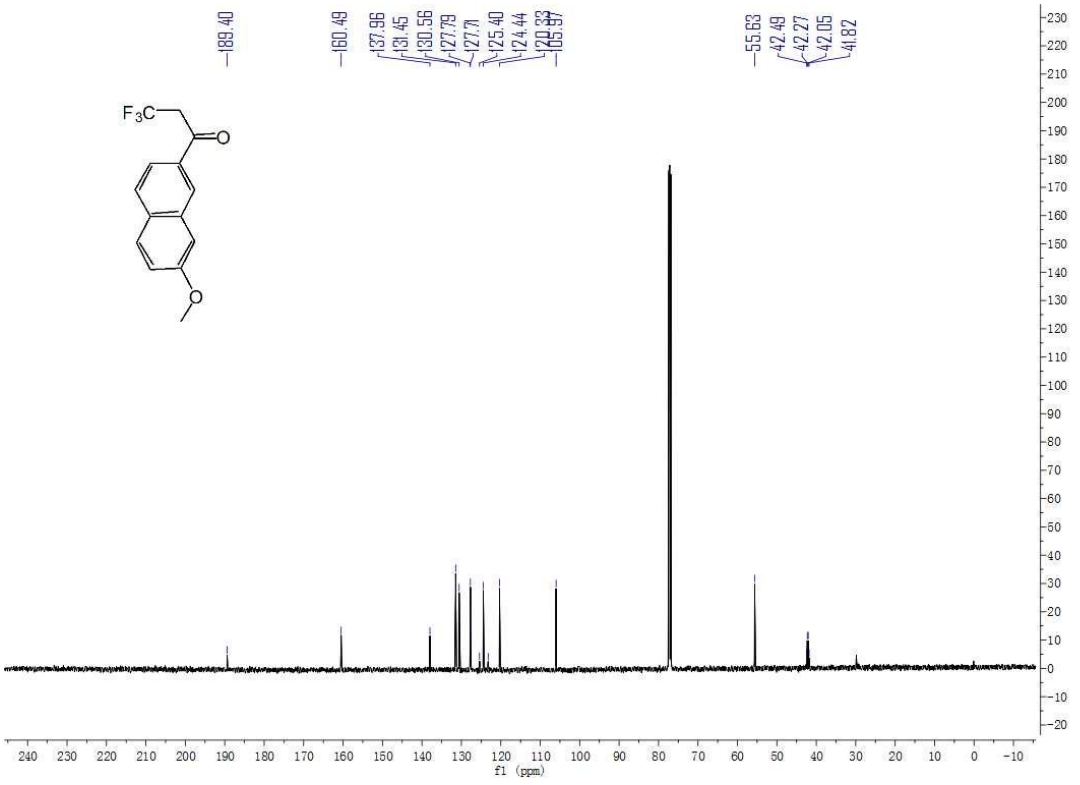




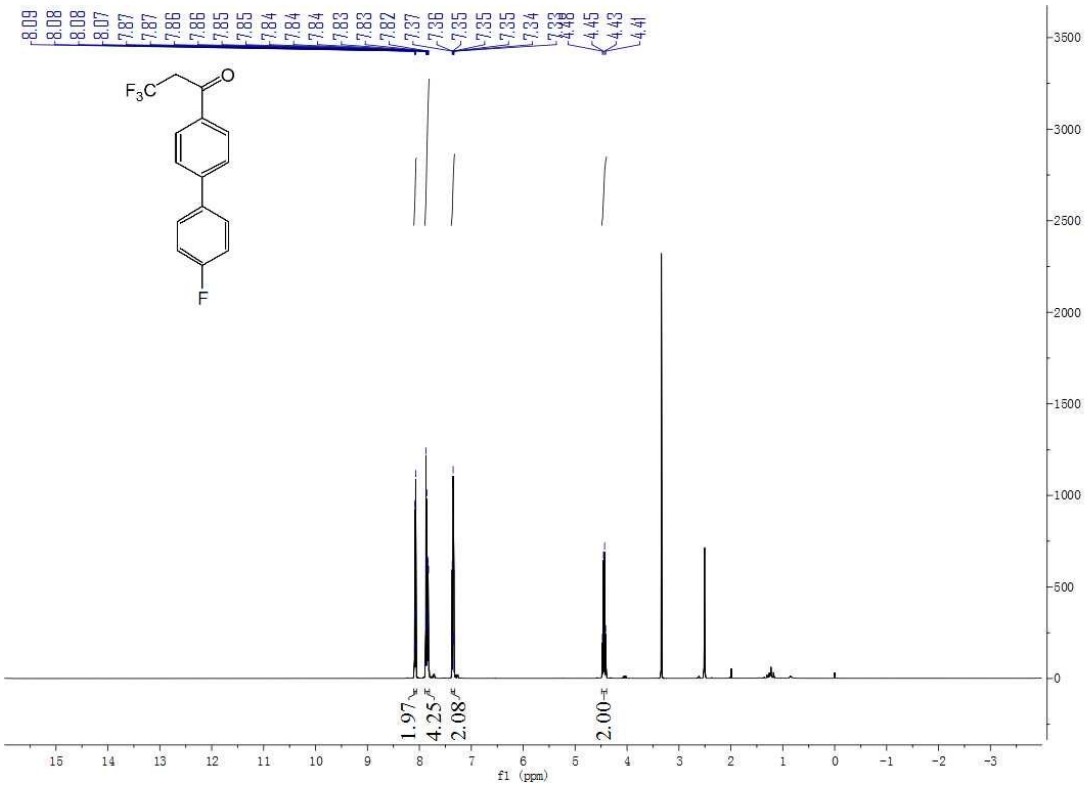
3,3,3-Trifluoro-1-(7-methoxynaphthalen-2-yl)propan-1-one (**2p**)

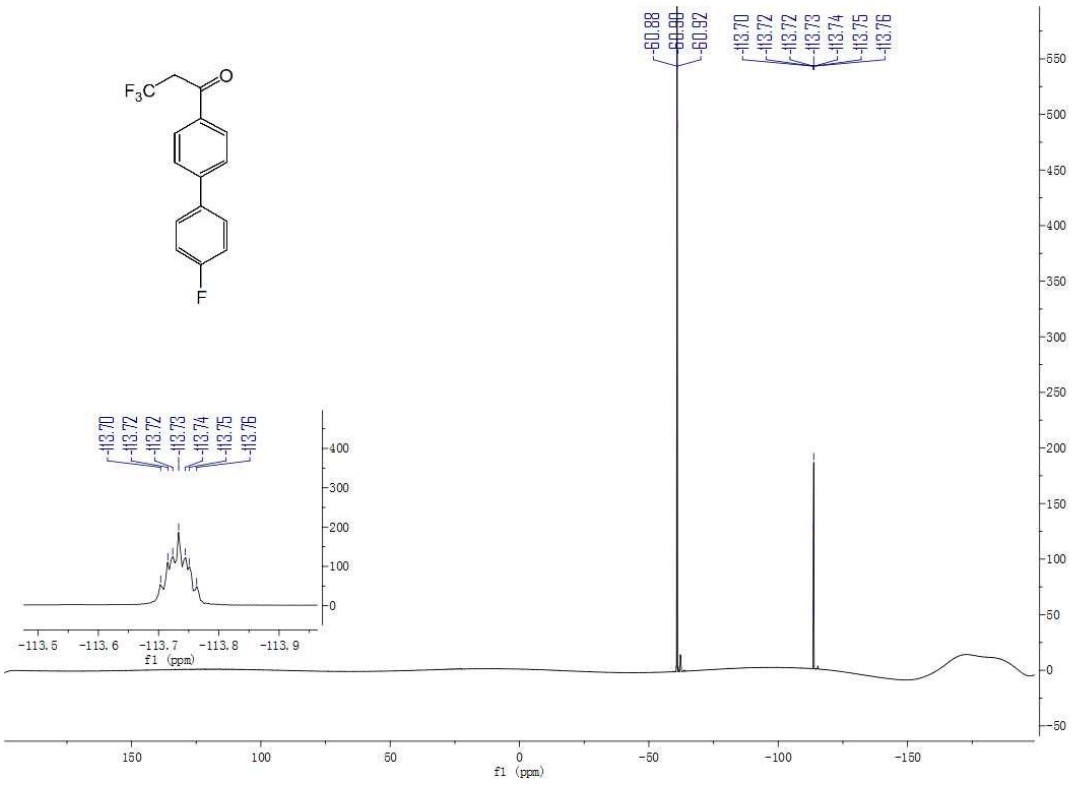


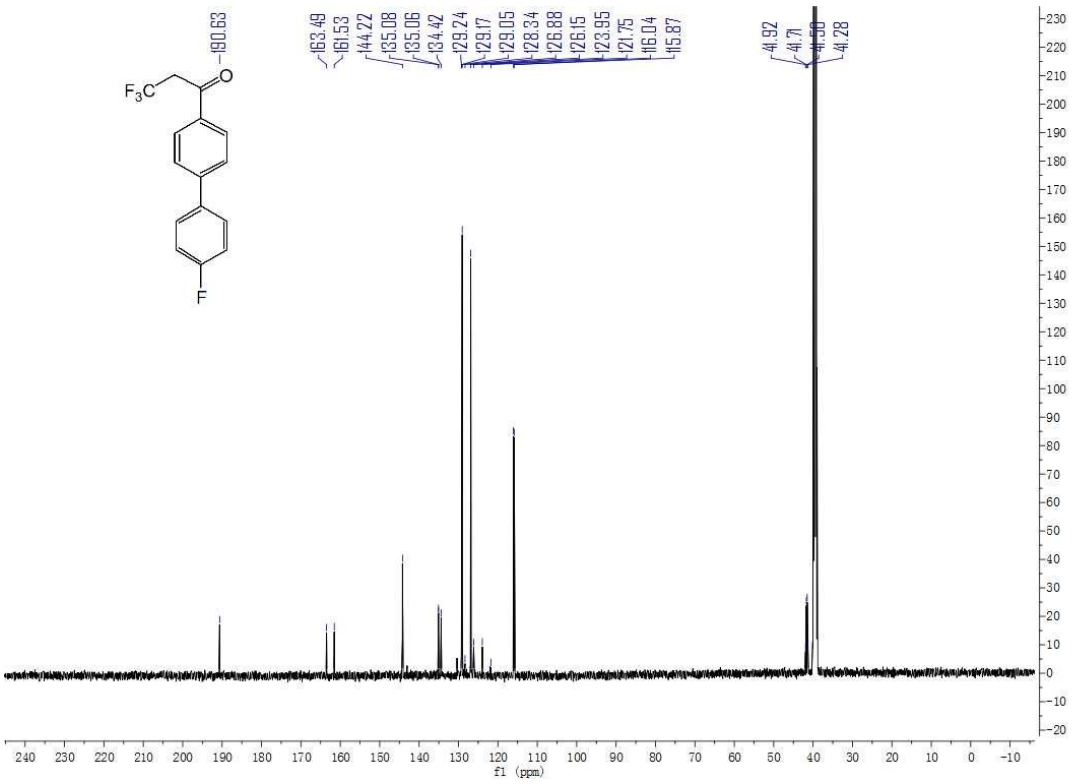

-61.85
-61.87
-61.89
F3C
O
O
f1 (ppm)


189.40
160.49
137.96
131.45
130.56
127.79
127.71
125.40
124.44
120.33
105.97
55.63
42.49
42.27
42.05
41.82
F3C
O
O
f1 (ppm)

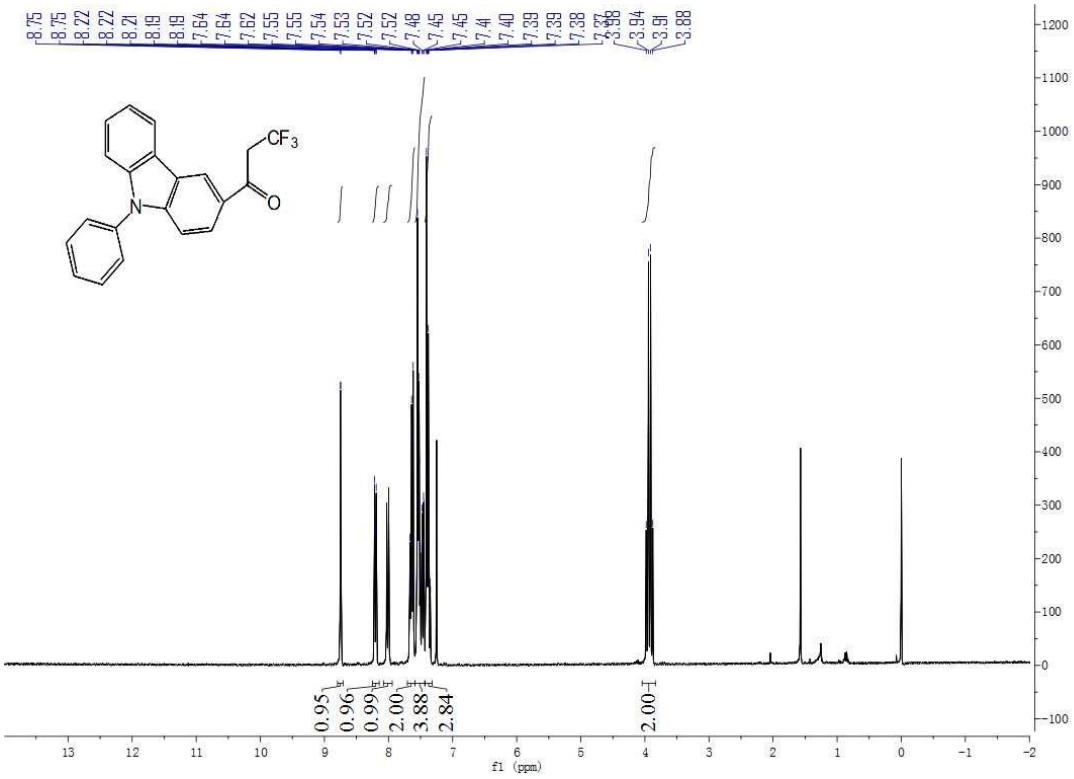
3,3,3-Trifluoro-1-(4'-fluorobiphenyl-4-yl)propan-1-one (**2q**)

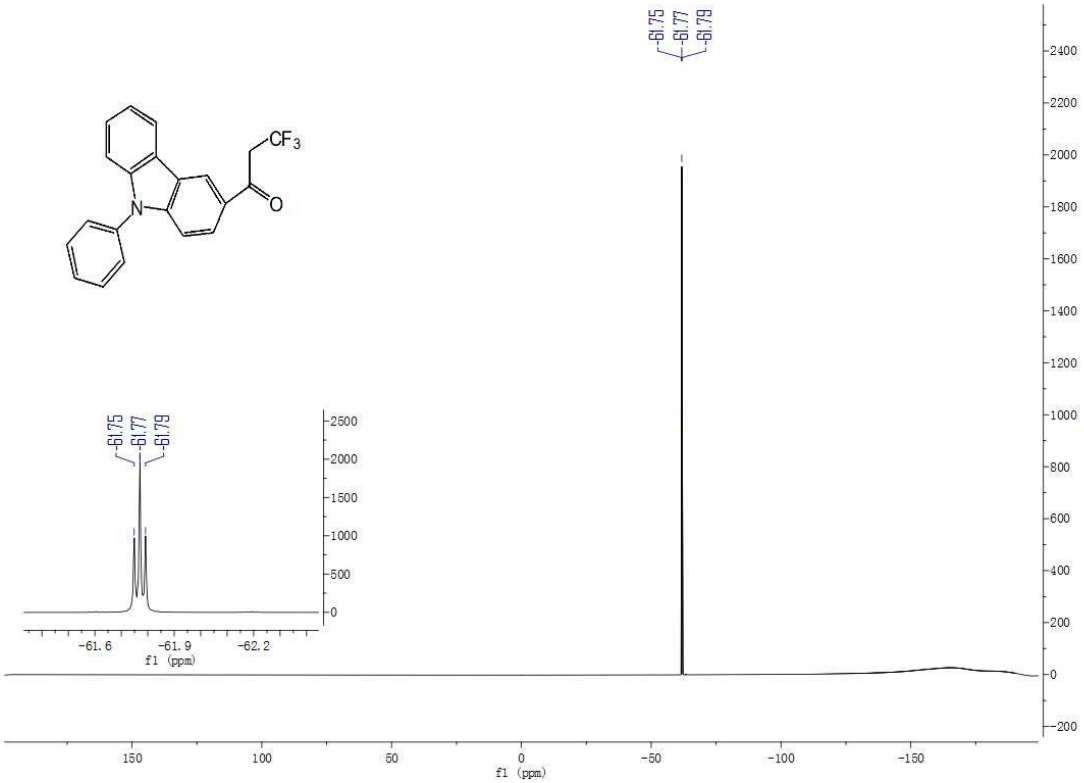


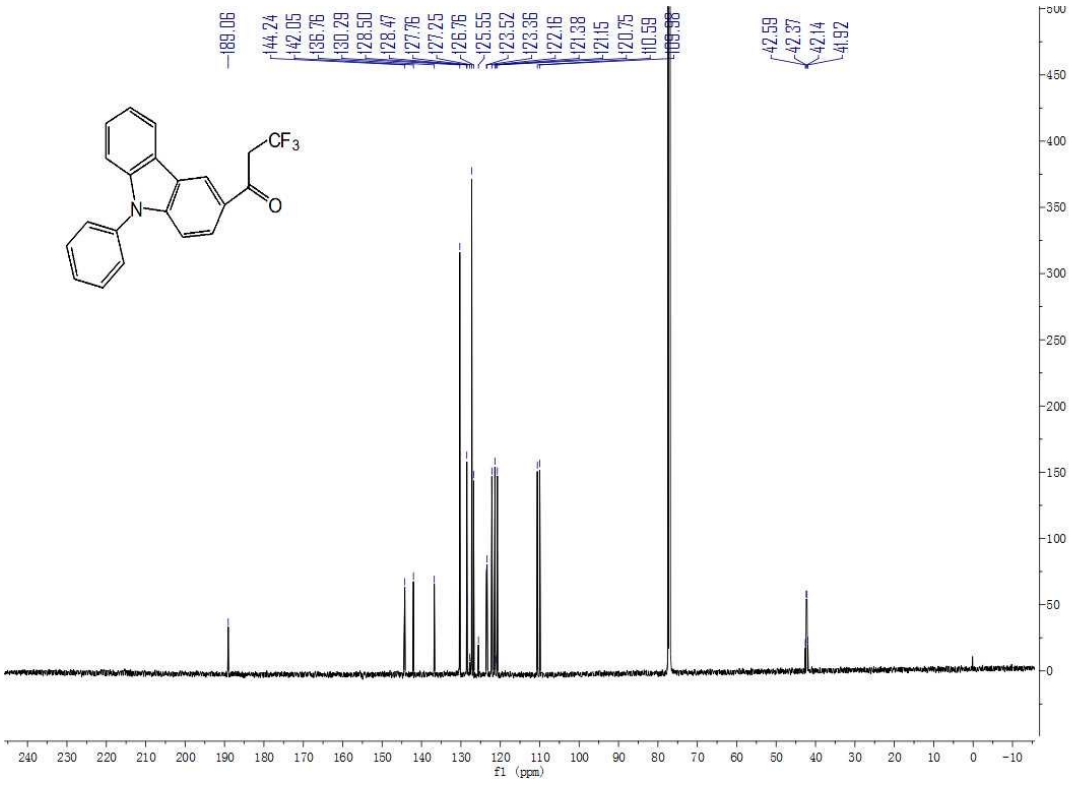




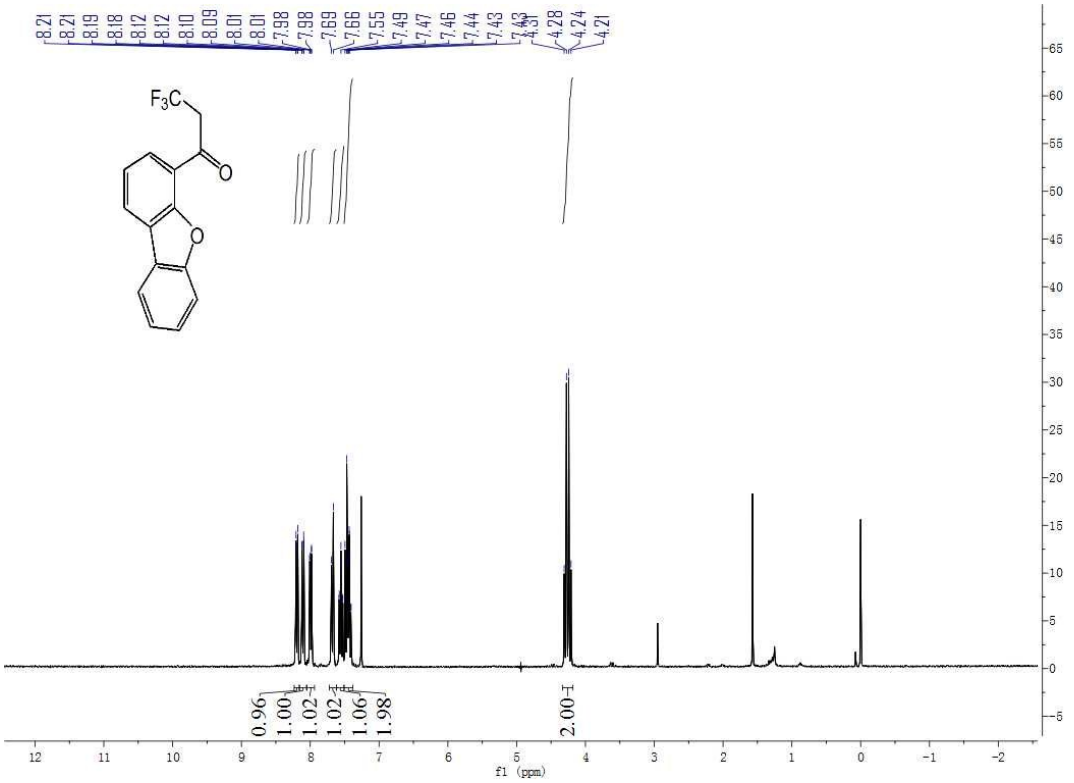
3,3,3-Trifluoro-1-(9-phenyl-9H-carbazol-3-yl)propan-1-one (**2r**)

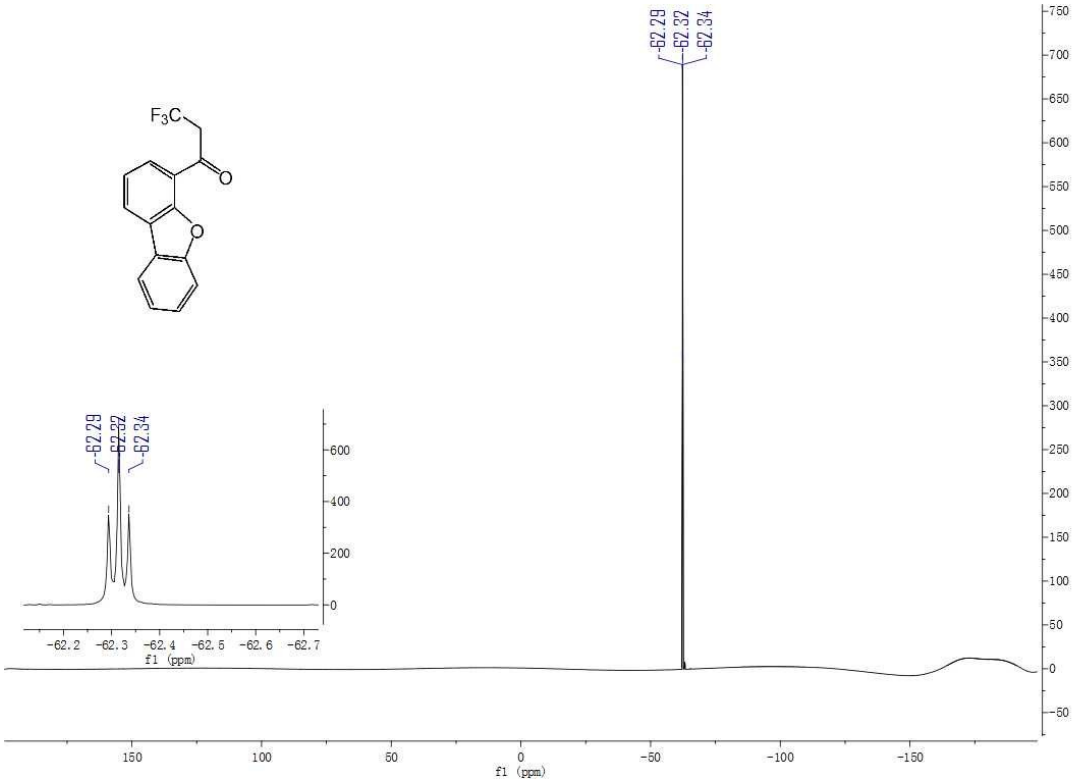


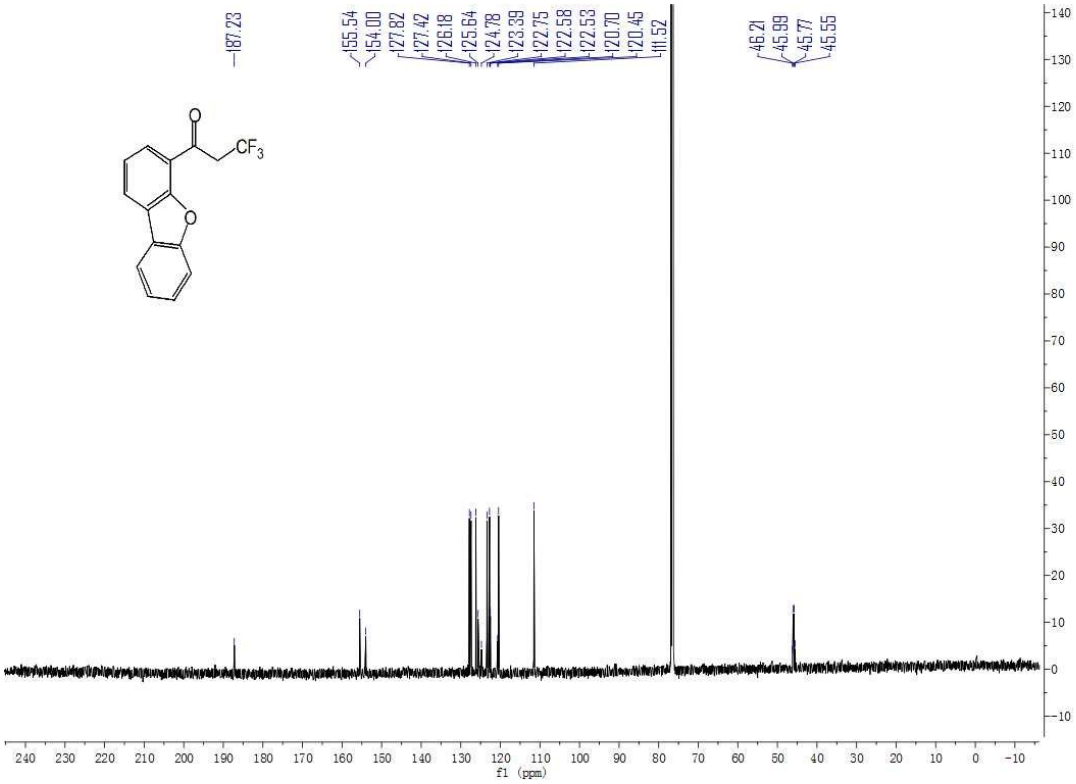

-61.75
-61.77
-61.79
CF3
O
N
f1 (ppm)


189.06
144.24
142.05
136.76
130.29
128.50
128.47
127.76
127.25
126.76
125.55
123.52
123.36
122.16
121.38
121.15
120.75
110.59
108.98
42.59
42.37
42.14
41.92
CF3
O
N
f1 (ppm)

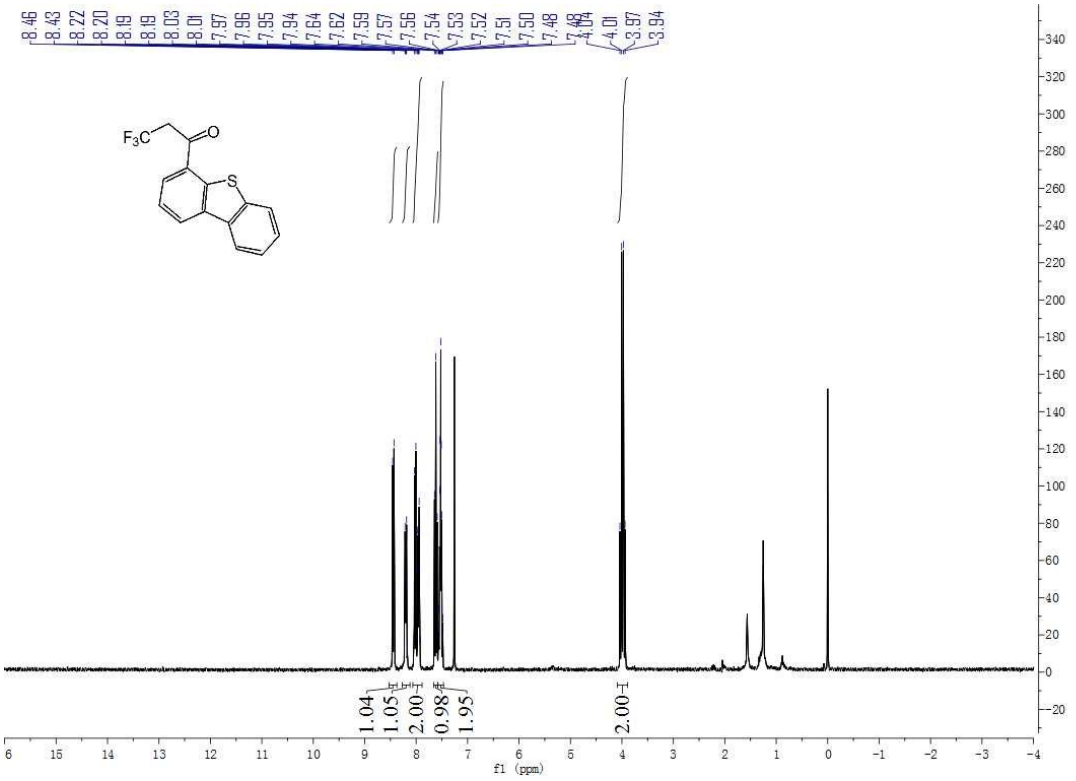
1-(Dibenzo[b,d]furan-4-yl)-3,3,3-trifluoropropan-1-one (**2s**)

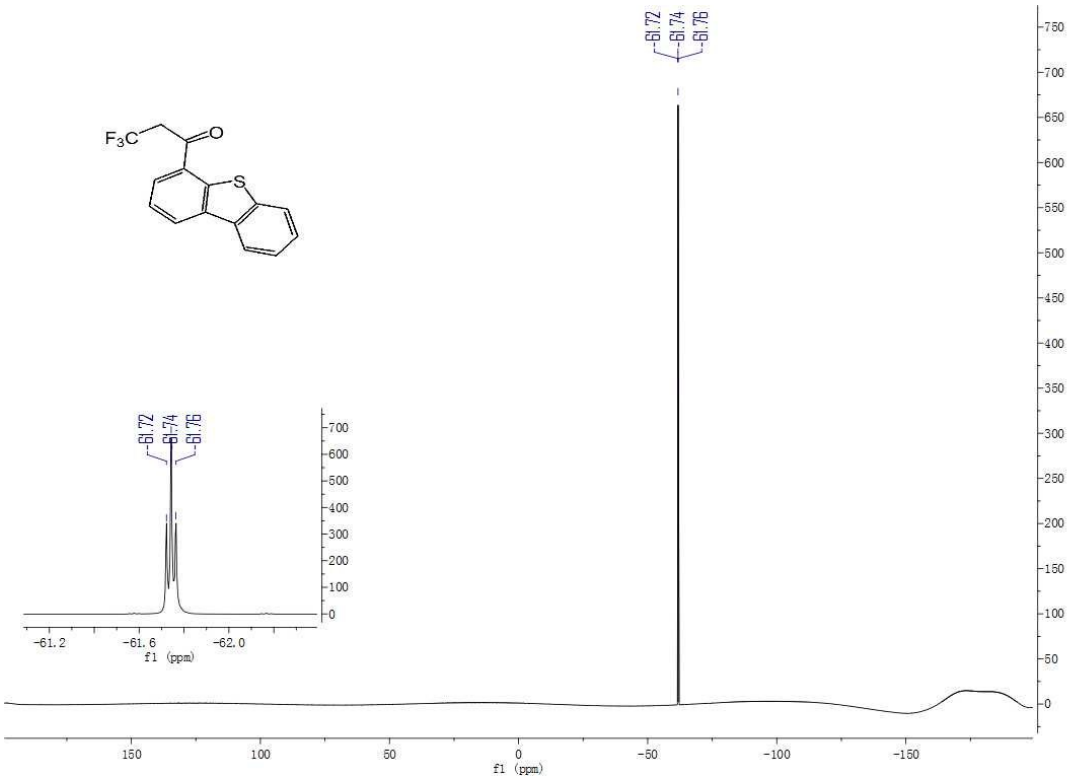


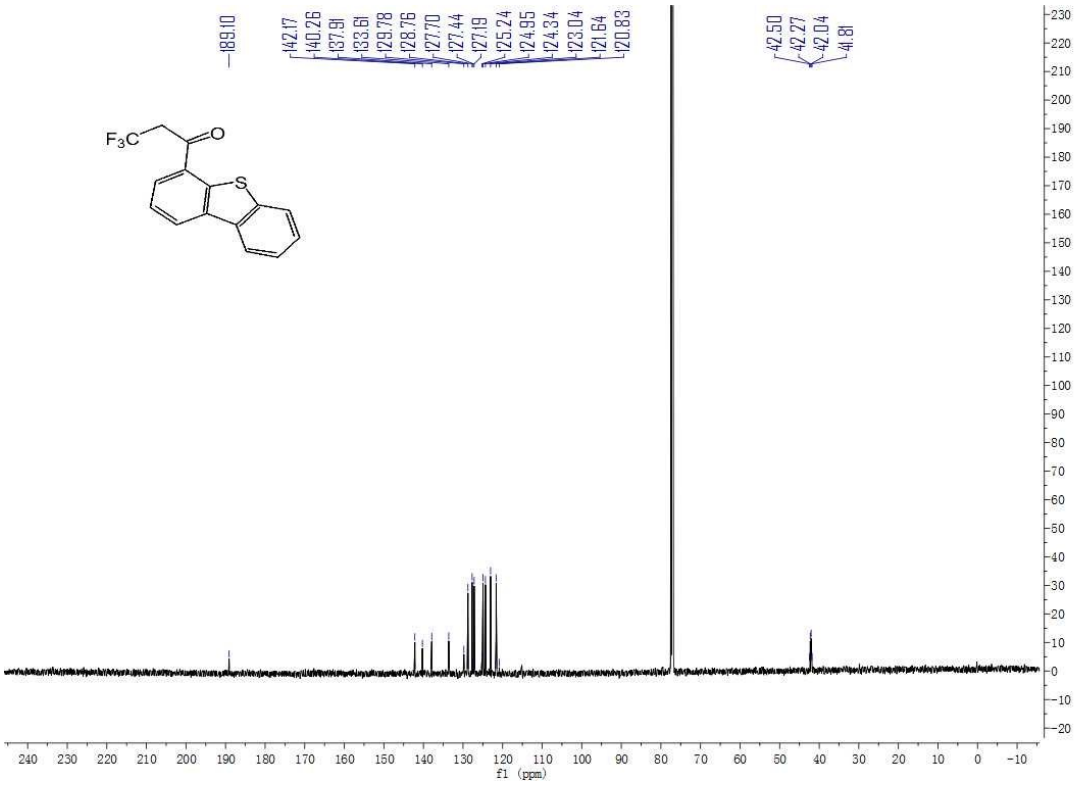




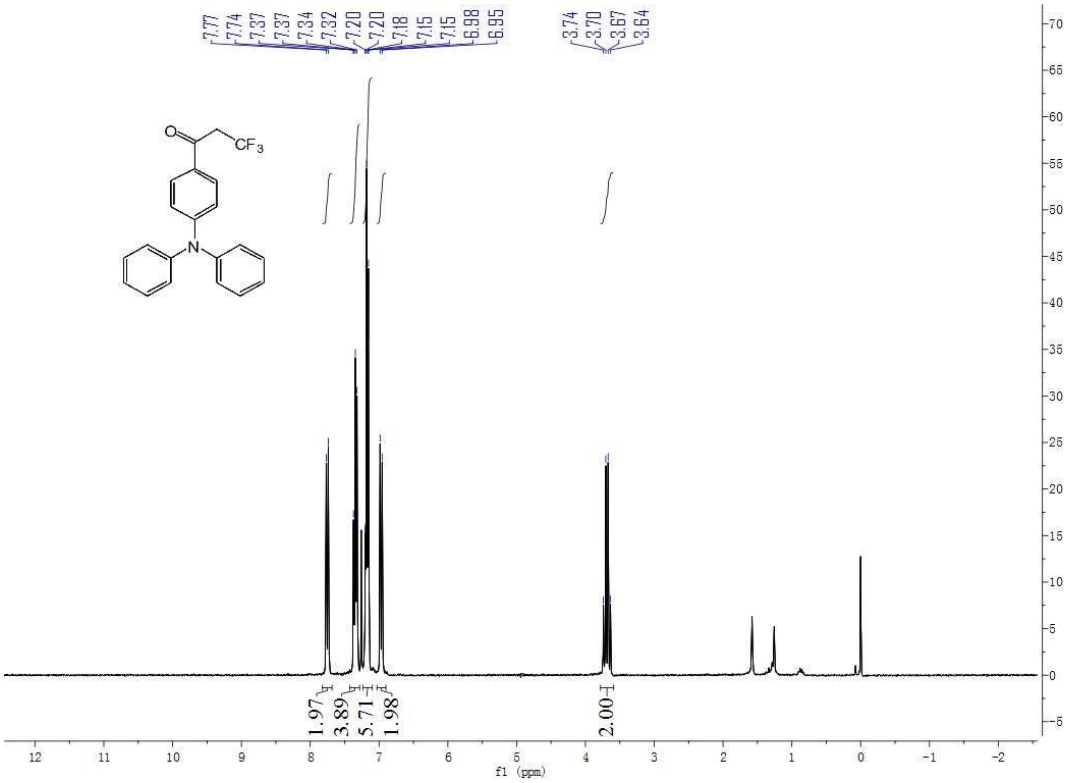
1-(Dibenzo[b,d]thiophen-4-yl)-3,3,3-trifluoropropan-1-one (**2t**)

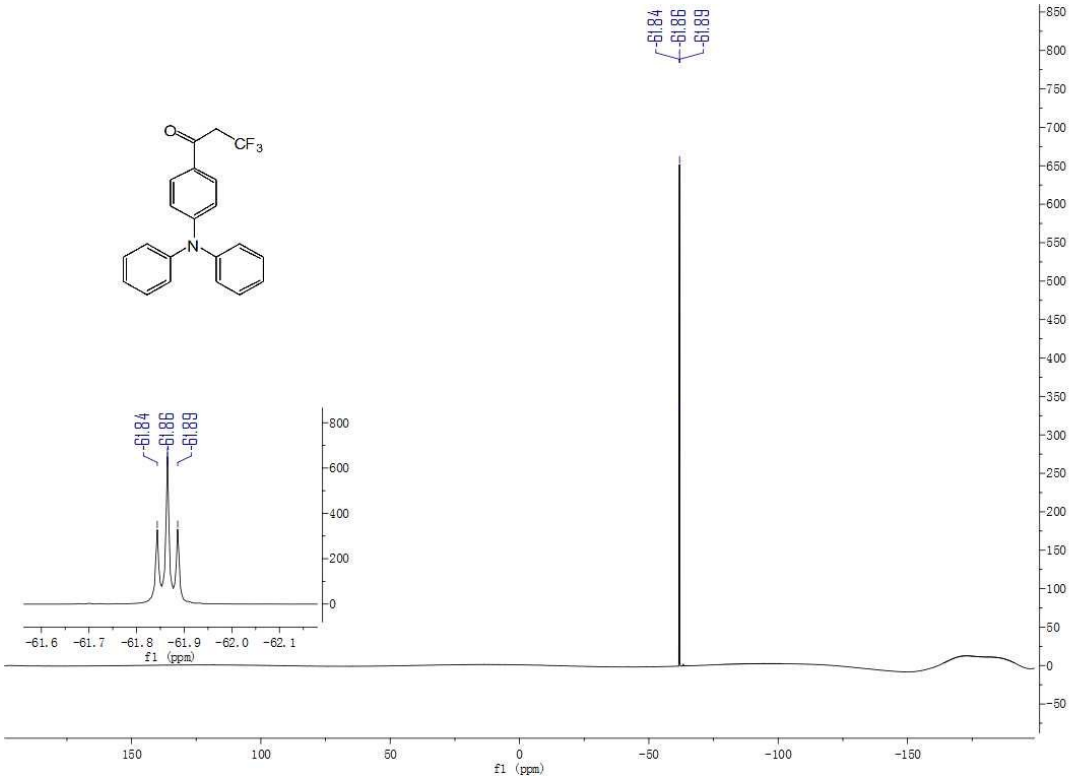


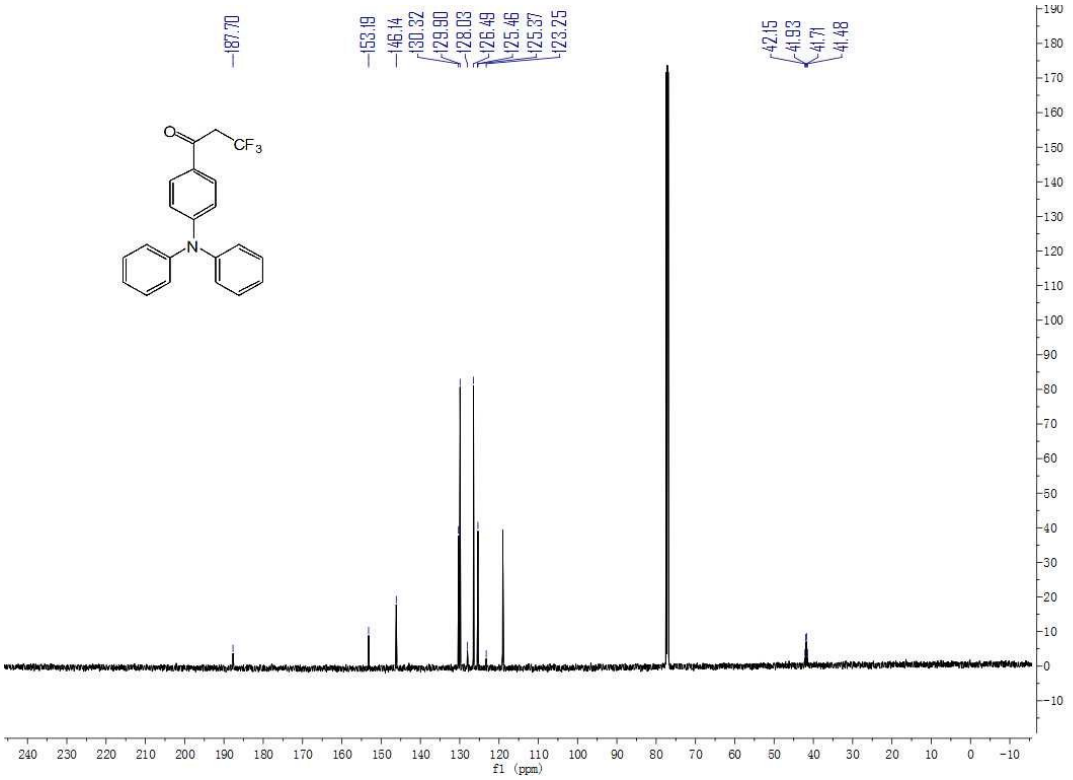

-61.72
-61.74
-61.76
F3C
O
S
f1 (ppm)


189.10
142.17
140.26
137.91
133.61
129.78
128.76
127.70
127.44
127.19
125.24
124.95
124.34
123.04
121.64
120.83
42.50
42.27
42.04
41.81
F3C
O
S
f1 (ppm)

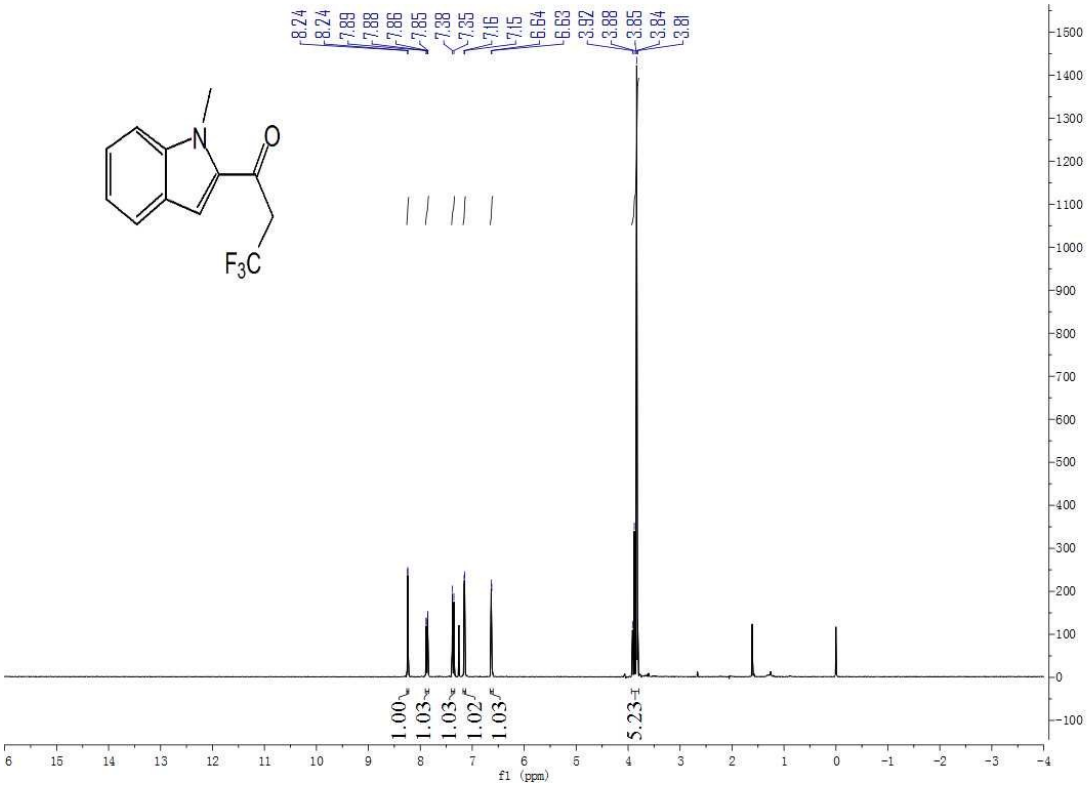
1-(4-(Diphenylamino)phenyl)-3,3,3-trifluoropropan-1-one (**2u**)

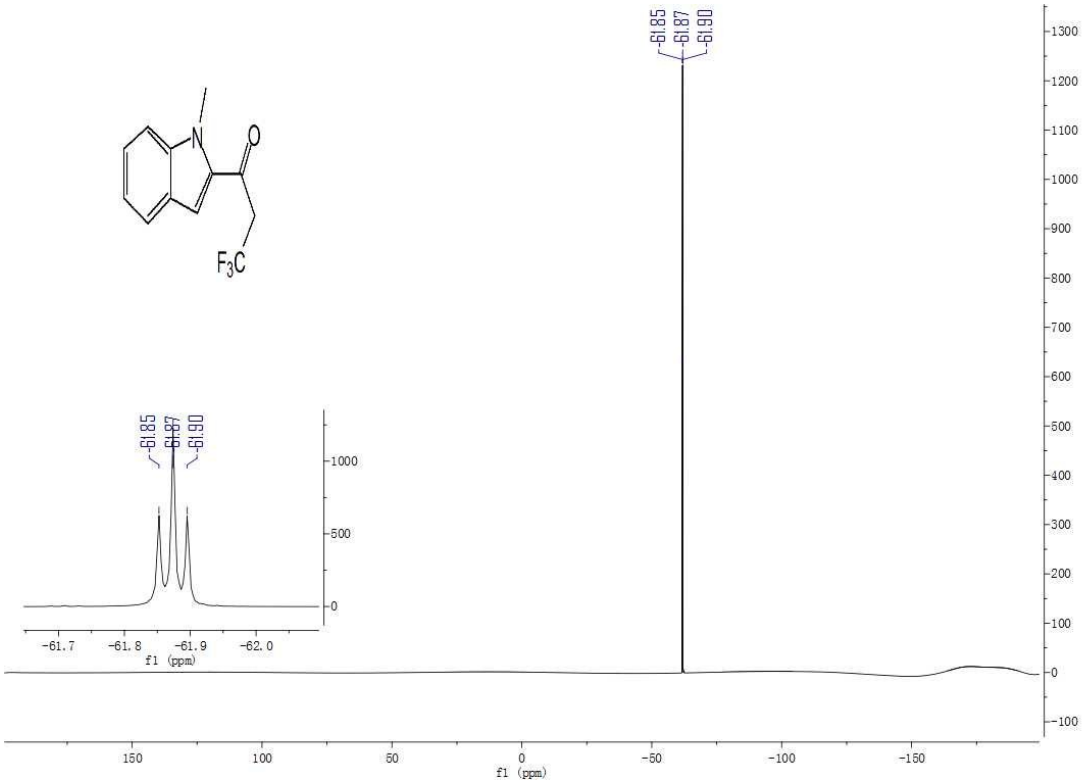


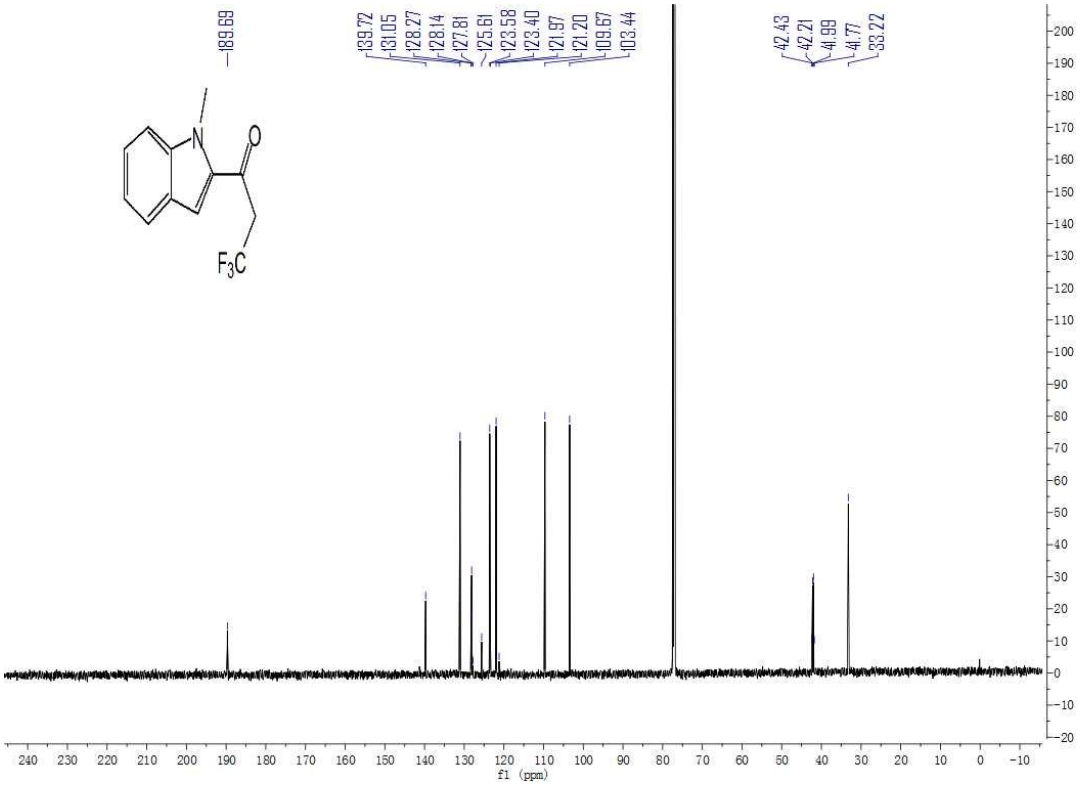




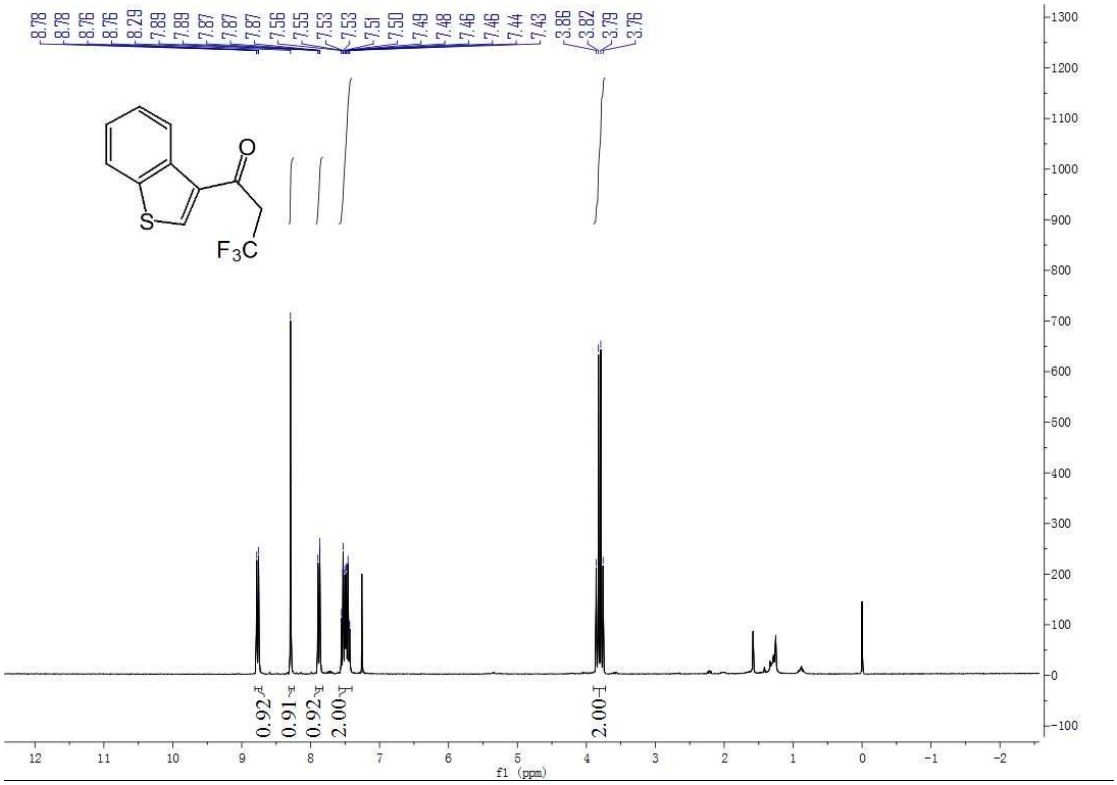
3,3,3-Trifluoro-1-(1-methyl-1H-indol-2-yl)propan-1-one (**2v**)

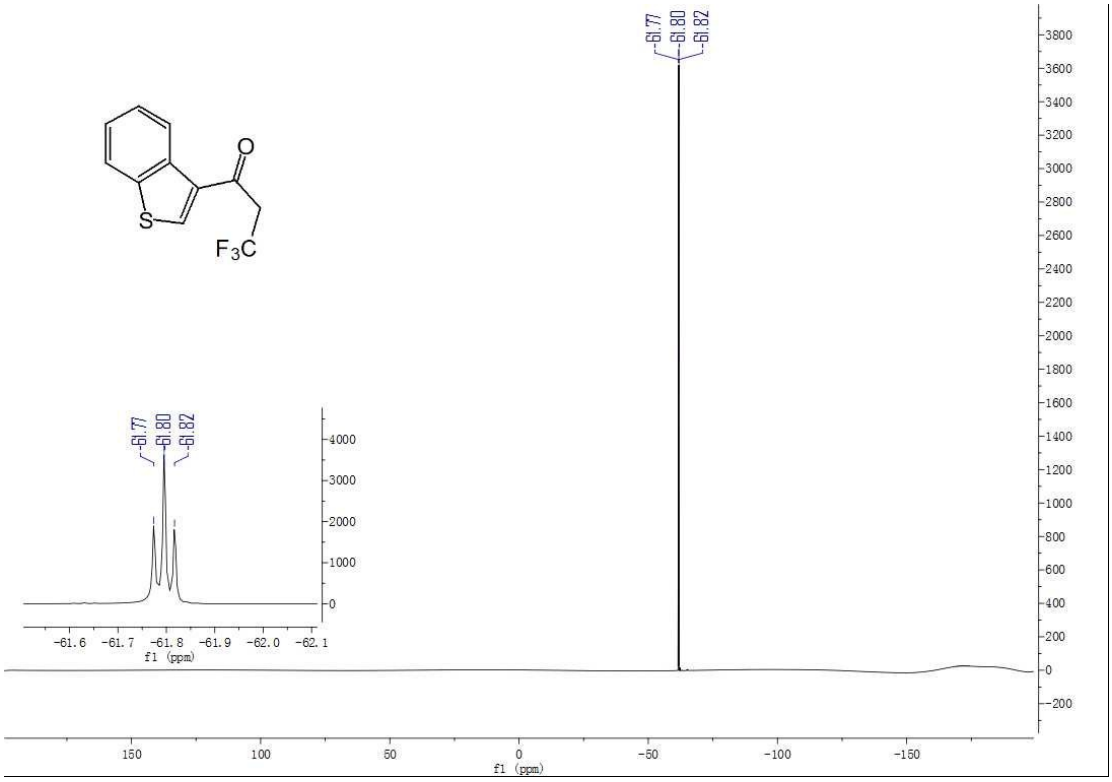


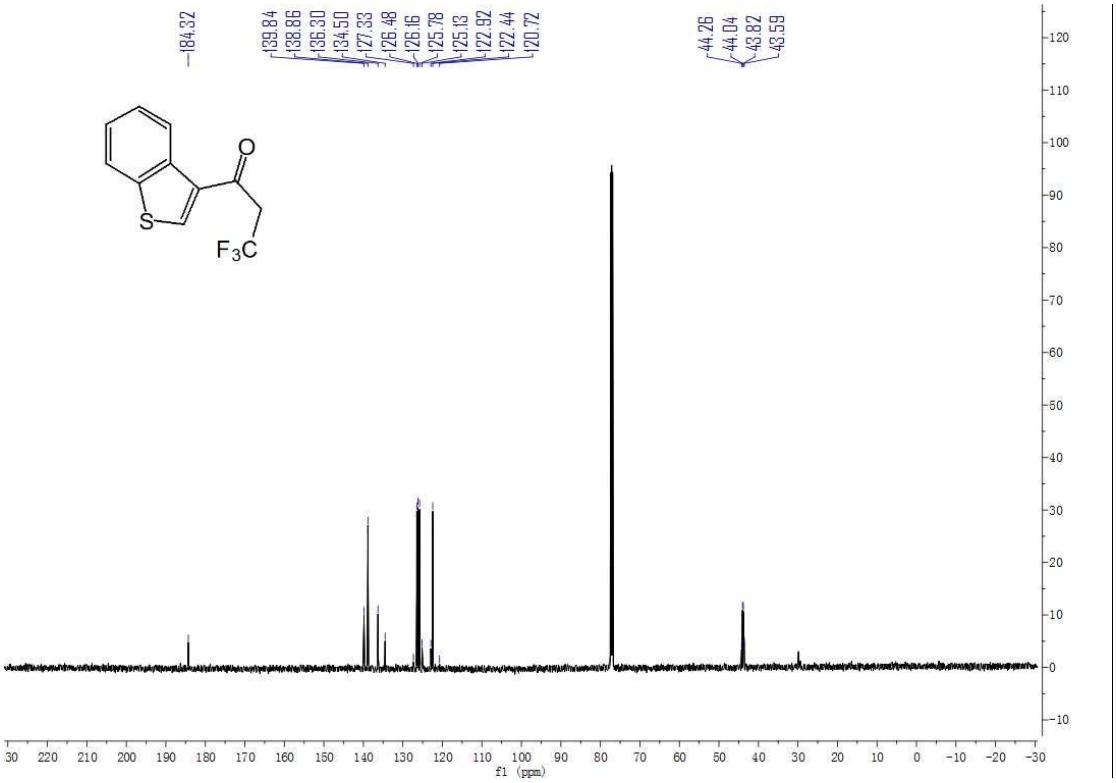

-61.85
-61.87
-61.90
F3C
f1 (ppm)


189.69
139.72
131.05
128.27
128.14
127.81
125.61
123.58
123.40
121.97
121.20
109.67
103.44
42.43
42.21
41.99
41.77
33.22
F3C
f1 (ppm)

1-(Benzo[b]thiophen-3-yl)-3,3,3-trifluoropropan-1-one (**2w**)






184.32
139.84
138.86
136.30
134.50
127.33
126.48
126.16
125.78
125.13
122.92
122.44
120.72
44.26
44.04
43.82
43.59
O
S
F3C
f1 (ppm)