Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information for

Switchable Hydroxysulfonyloxylation and Defluorination-Decarboxylation Sulfonylation of *gem*-Difluoroalkenes with Sodium Sulfinate *via* Aerobic Oxidation

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1. General considerations

Unless otherwise noted, commercial reagents were purchased from Adamas, Alfa, Aladdin, TCI, *J&K* or Macklin and used without further purification. All reactions were carried out using oven-dried glassware and all reactions proceeded without special care. Column chromatography was performed on 200-300 mesh silica gel (Huanghai, China).

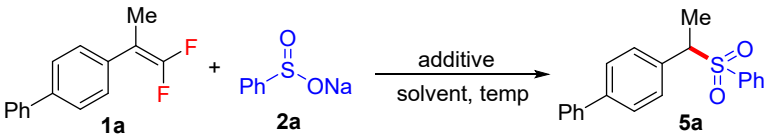
^{1}H, ^{19}F and $^{13}C\{^{1}H\}$ NMR spectra were recorded on an Bruker Ascend 400 MHz spectrometer at ambient temperature. ^{1}H NMR spectra are referred to the TMS signal (δ = 0 ppm) and ^{13}C NMR spectra are referred to the residual solvent signal (δ = 77.16 ppm). Data for ^{1}H NMR are reported as follows: chemical shifts (δ ppm), multiplicities (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad), coupling constants (Hz), integration.

The data of HRMS was carried out on a waters G2-XS high-resolution mass spectrometer (HR-ESI-MS) or Thermo Fisher Scientific LTQ FTICR-MS. Melting point were recorded using a SGW X-4 Melting Point Apparatus.

gem-Difluoroalkene substrates **1** are known and their spectral data are in accordance with the reported in the literature.[1-6]

2. Condition optimization for synthesis of 5a

Table S1. Optimization of reaction condition for synthesis of 5a[a]



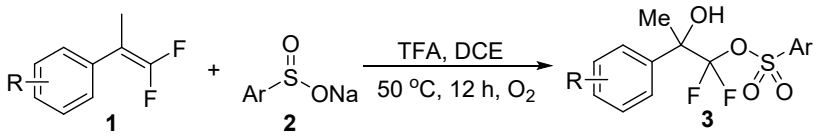
entry	additive	solvent	temp	yield
1	--	THF	60	trace
2	CsF	THF	60	n. d.
3	pyridine·HF	THF	60	trace
4	TBAF	THF	60	15
5	$BF_3·OEt_2$	THF	60	n. d.
6	KF	THF	60	42
7	$Et_3N·3HF$	THF	60	54
8	$Et_3N·3HF$	1,4-dioxane	60	23
6	$Et_3N·3HF$	DMF	60	trace
7	$Et_3N·3HF$	CH_2Cl_2	60	n. d.
8	$Et_3N·3HF$	DCE	60	n. d.
9 [b]	$Et_3N·3HF$	THF	60	56
10 [b,c]	**$Et_3N·3HF$**	**THF**	**60**	**58**
11 [b,c]	$Et_3N·3HF$	THF	40	45
12 [b,c]	$Et_3N·3HF$	THF	80	26
13 [b,c,d]	$Et_3N·3HF$	THF	60	trace

[a] Reaction condition: **1a** (0.2 mmol), **2a** (0.4 mmol, 2.0 equiv), additive (0.2 mmol, 2.0 equiv), solvent (2 mL), O_2 atmosphere, 12 h. Isolated yields. [b] $Et_3N·3HF$ (3.0 equiv). [c] **2a** (3.0 equiv). [d] N_2 atmosphere.

3. Experimental procedures and characterization data

Synthesis of product 3 according to the following procedure:

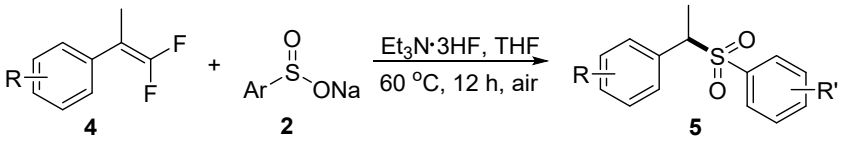
As exemplified for **3a**:



A pressure tube was charged with 4-(1,1-difluoroprop-1-en-2-yl)-1,1'-biphenyl **1a** (46.1 mg，0.2 mmol), sodium sulfinate **2a** (0.734 mg, 0.4 mmol) and DCE (2 mL). TFA (22.8 mg, 0.2 mmol) was added and the mixtures were heated with a heating mantle at 50 °C under O_2 atmosphere for 12 h. After cooling to room temperature, the solvent was volatilized and the crude product was purified by flash column chromatography on silica gel (eluent: PE/EA = 6/1, v/v), and the target compound **3a** was obtained.

Synthesis of product 5 according to the following procedure:

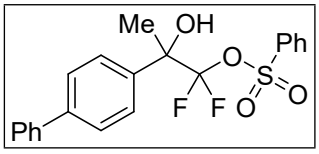
As exemplified for **5a**:



A pressure tube was charged with 4-(1,1-difluoroprop-1-en-2-yl)-1,1'-biphenyl **1a** (46.1 mg，0.2 mmol), sodium sulfinate **2a** (98.3 mg, 0.6 mmol) and THF (2 mL). $Et_3N{\cdot}3HF$ (96.7 mg, 0.6 mmol) was added and the mixtures were heated with a heating mantle at 60 °C under O_2 atmosphere for 12 h. After cooling to room temperature, the solvent was volatilized and the crude product was purified by preparative TLC (eluent: PE/EA = 6/1, v/v), and the target compound **5a** was obtained. In some cases, twice purifications are needed.

2.2 Characterization data

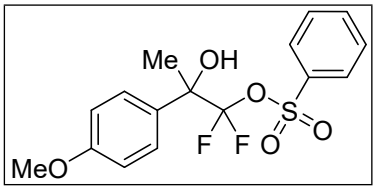
2-([1,1'-Biphenyl]-4-yl)-1,1-difluoro-2-hydroxypropyl benzenesulfonate (3a)



Flash column chromatography on silica gel (eluent: PE/EA = 6/1, v/v) to afford **3a**. Yellow solid (63.0 mg, 78%), mp 98.8-99.0 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 – 7.74 (m, 2H), 7.59 – 7.55 (m, 3H), 7.47 (d, *J* = 14.5 Hz, 6H), 7.43 (d, *J* = 4.4 Hz, 1H), 7.41 – 7.37 (m, 2H), 2.26 (s, 1H), 1.73 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.28, 140.44, 137.30, 136.82, 134.49, 129.22, 128.99, 128.00, 127.71, 127.17,

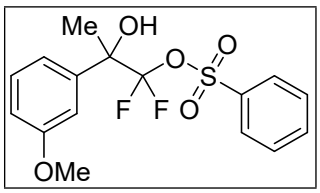
126.84, 126.81, 123.39 (t, J = 285.0 Hz), 76.07 (t, J = 27.0 Hz), 23.67. ^{19}F NMR (377 MHz, $CDCl_3$) δ -82.31, -82.42. HR-DART-MS (m/z): calcd for $C_{21}H_{22}NF_2O_4S$ $[M + NH_4]^+$: 422.1232, found: 422.1231.

1,1-Difluoro-2-hydroxy-2-(4-methoxyphenyl)propyl benzenesulfonate (3b)



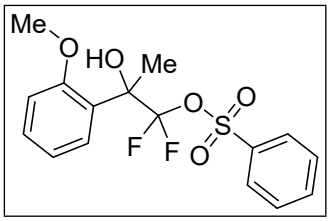
Flash column chromatography on silica gel (eluent: PE/EA = 6/1, v/v) to afford **3b**. Light yellow oil (45.1 mg, 63%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, J = 8.0 Hz, 2H), 7.67 – 7.61 (m, 1H), 7.47 (t, J = 7.8 Hz, 2H), 7.35 (d, J = 8.6 Hz, 2H), 6.80 (d, J = 8.7 Hz, 2H), 3.80 (s, 3H), 2.38 (s, 1H), 1.68 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.40, 139.95, 136.84, 134.51, 129.25, 129.19, 128.03, 123.38 (t, J = 285.0 Hz), 118.60, 113.88, 112.33, 76.08 (t, J = 27.0 Hz), 55.35, 23.81. ^{19}F NMR (377 MHz, $CDCl_3$) δ -82.56, -82.69. HR-GC-MS (m/z): calcd for $C_{16}H_{16}F_2O_5S$ [M]: 358.0687, found: 358.0690.

1,1-Difluoro-2-hydroxy-2-(3-methoxyphenyl)propyl benzenesulfonate (3c)



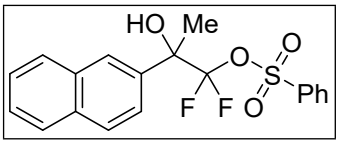
Flash column chromatography on silica gel (eluent: PE/EA = 6/1, v/v) to afford **3c**. Yellow oil (46.5 mg, 65%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 – 7.76 (m, 2H), 7.66 – 7.60 (m, 1H), 7.46 (t, J = 7.8 Hz, 2H), 7.23 – 7.16 (m, 1H), 7.00 (dd, J = 7.4, 1.9 Hz, 2H), 6.85 – 6.81 (m, 1H), 3.75 (s, 3H), 1.68 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.40, 139.95, 136.84, 134.51, 129.25, 129.19, 128.03, 123.38 (t, J = 285.0 Hz), 118.60, 113.88, 112.33, 76.08 (t, J = 27.0 Hz), 55.35, 23.81. ^{19}F NMR (377 MHz, $CDCl_3$) δ -82.12, -82.18. HR-GC-MS (m/z): calcd for $C_{16}H_{16}F_2O_5S$ [M]: 358.0687, found: 358.0687.

1,1-Difluoro-2-hydroxy-2-(2-methoxyphenyl)propyl benzenesulfonate (3d)



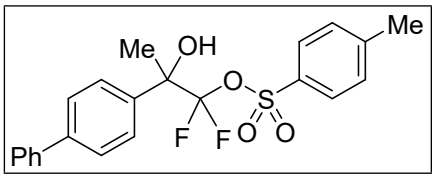
Flash column chromatography on silica gel (eluent: PE/EA = 6/1, v/v) to afford **3d**. Colorless oil (42.9 mg, 60%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 – 7.73 (m, 2H), 7.62 (t, J = 7.5 Hz, 1H), 7.45 (t, J = 7.9 Hz, 2H), 7.33 – 7.28 (m, 1H), 7.23 (dd, J = 7.9, 1.5 Hz, 1H), 6.97 (td, J = 7.6, 1.1 Hz, 1H), 6.88 (d, J = 8.3 Hz, 1H), 6.08 (s, 1H), 3.81 (s, 3H), 1.67 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 58.20, 137.28, 134.24, 130.28, 129.90, 129.15, 127.93, 125.83, 123.90 (t, J = 285.0 Hz), 121.60, 112.66, 77.96 (t, J = 27.0 Hz), 56.41, 22.47. ^{19}F NMR (377 MHz, $CDCl_3$) δ -82.18, -83.88. HR-DART-MS (m/z): calcd for $C_{16}H_{17}F_2O_5S$ $[M + H]^+$: 359.0759, found: 359.0761.

1,1-Difluoro-2-hydroxy-2-(naphthalen-2-yl)propyl benzenesulfonate (3e)



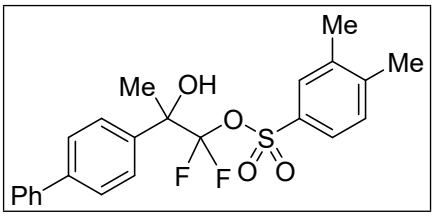
Flash column chromatography on silica gel (eluent: PE/EA = 6/1, v/v) to afford **3e**. Yellow oil (52.9 mg, 70%).^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.81 – 7.77 (m, 1H), 7.76 – 7.73 (m, 1H), 7.69 (d, *J* = 8.7 Hz, 1H), 7.62 (d, *J* = 7.7 Hz, 2H), 7.53 – 7.46 (m, 3H), 7.41 (t, *J* = 7.5 Hz, 1H), 7.18 (t, 2H), 2.53 (s, 1H), 1.78 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.50, 135.71, 134.32, 133.02, 132.74, 128.97, 128.87, 128.54, 127.81, 127.49, 126.69, 126.33, 126.26, 125.91, 123.85, 123.42 (t, *J* = 285.0 Hz), 120.57, 76.26 (t, *J* = 27.0 Hz), 23.67. ^{19}F NMR (377 MHz, $CDCl_3$) δ -82.09, -82.21. HR-GC-MS (m/z): calcd for $C_{19}H_{16}F_2O_4S$ [M]: 378.0737, found: 378.0739.

2-([1,1'-Biphenyl]-4-yl)-1,1-difluoro-2-hydroxypropyl 4-methylbenzenesulfonate (3f)



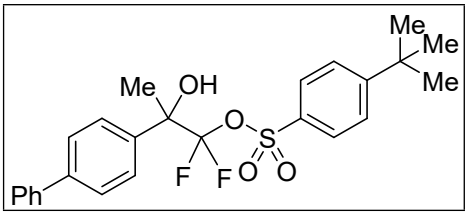
Flash column chromatography on silica gel (eluent: PE/EA = 6/1, v/v) to afford **3f**. Yellow solid (60.3 mg, 72%), mp 88.8-89.9 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.1 Hz, 2H), 7.59 – 7.55 (m, 2H), 7.49 (s, 4H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.39 – 7.34 (m, 1H), 7.20 (d, *J* = 8.1 Hz, 2H), 2.56 (s, 1H), 2.34 (s, 3H), 1.73 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.82, 141.21, 140.44, 137.34, 133.80, 129.84, 128.98, 128.11, 127.71, 127.15, 126.84, 126.74, 123.32 (t, *J* = 285.0 Hz), 76.10 (t, *J* = 27.0 Hz), 23.73, 21.76. ^{19}F NMR (377 MHz, $CDCl_3$) δ -82.47, -82.57. HR-GC-MS (m/z): calcd for $C_{22}H_{20}F_2O_4S$ [M]: 418.1050, found: 418.1055.

2-([1,1'-Biphenyl]-4-yl)-1,1-difluoro-2-hydroxypropyl 3,4-dimethylbenzenesulfonate (3g)



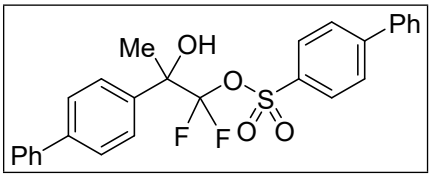
Flash column chromatography on silica gel (eluent: PE/EA = 6/1, v/v) to afford **3g**. Light yellow oil (58.7 mg, 68%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.53 (m, 4H), 7.51 (s, 4H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.36 (t, *J* = 7.2 Hz, 1H), 7.16 (d, *J* = 7.9 Hz, 1H), 2.62 (s, 1H), 2.24 (s, 3H), 2.20 (s, 3H), 1.73 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.59, 141.11, 140.38, 138.15, 137.41, 133.87, 130.30, 128.96, 128.71, 127.69, 127.12, 126.86, 126.67, 125.63, 123.33 (t, *J* = 285.0 Hz), 76.09 (t, *J* = 27.0 Hz), 23.78, 20.17, 19.86. ^{19}F NMR (377 MHz, $CDCl_3$) δ -82.41, -82.53. HR-GC-MS (m/z): calcd for $C_{23}H_{22}F_2O_4S$ [M]: 432.1207, found: 432.1214.

2-([1,1'-Biphenyl]-4-yl)-1,1-difluoro-2-hydroxypropyl 4-(tert-butyl)benzenesulfonate (3h)



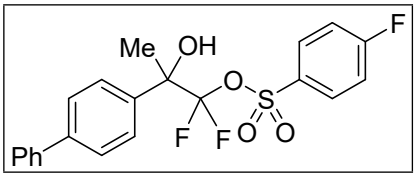
Flash column chromatography on silica gel (eluent: PE/EA = 6/1, v/v) to afford **3h**. Colorless oil (59.8 mg, 65%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.4 Hz, 2H), 7.58 (dd, *J* = 8.2, 1.4 Hz, 2H), 7.51 (s, 4H), 7.47 – 7.38 (m, 5H), 2.50 (s, 1H), 1.75 (s, 3H), 1.24 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.71, 141.24, 140.41, 137.37, 133.71, 129.00, 127.92, 127.74, 127.17, 126.85, 126.77, 126.23, 123.34 (t, *J* = 285.0 Hz), 76.14 (t, *J* = 27.0 Hz), 35.40, 30.99, 23.79. ^{19}F NMR (377 MHz, $CDCl_3$) δ -82.51, -82.57. HR-GC-MS (m/z): calcd for $C_{25}H_{26}F_2O_4S$ [M]: 460.1520, found: 460.1527.

2-([1,1'-Biphenyl]-4-yl)-1,1-difluoro-2-hydroxypropyl [1,1'-biphenyl]-4-sulfonate (3i)



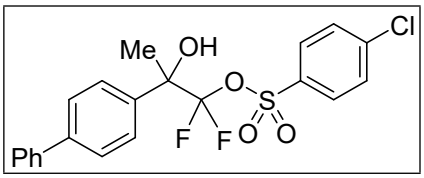
Flash column chromatography on silica gel (eluent: PE/EA = 6/1, v/v) to afford **3i**. Yellow solid (64.3 mg, 67%), mp 188.4-188.9 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.3 Hz, 2H), 7.56 (d, *J* = 8.5 Hz, 2H), 7.52 – 7.47 (m, 6H), 7.45 – 7.35 (m, 8H), 2.56 (s, 1H), 1.76 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.33, 141.25, 140.30, 138.75, 137.31, 135.09, 129.24, 129.01, 128.97, 128.53, 127.72, 127.64, 127.44, 127.16, 126.84, 126.72, 123.30 (t, *J* = 285.0 Hz), 76.12 (t, *J* = 27.0 Hz), 23.63. ^{19}F NMR (377 MHz, $CDCl_3$) δ -82.48, -82.53. HR-GC-MS (m/z): calcd for $C_{27}H_{22}F_2O_4S$ [M]: 480.1207, found: 480.1212.

2-([1,1'-Biphenyl]-4-yl)-1,1-difluoro-2-hydroxypropyl 4-fluorobenzenesulfonate (3j)



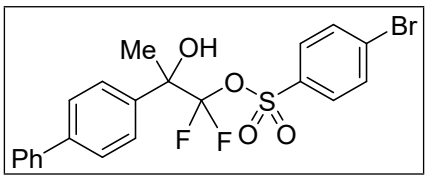
Flash column chromatography on silica gel (eluent: PE/EA = 6/1, v/v) to afford **3j**. Yellow oil (48.9 mg, 58%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 – 7.75 (m, 2H), 7.59 – 7.56 (m, 2H), 7.53 – 7.44 (m, 6H), 7.40 – 7.35 (m, 1H), 7.08 (t, *J* = 8.5 Hz, 2H), 2.49 (s, 1H), 1.75 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 166.12 (d, *J* = 258.0 Hz), 141.44, 140.31, 137.16, 132.74 (d, *J* = 3.3 Hz), 131.05 (d, *J* = 9.8 Hz), 129.05, 128.99, 127.81, 127.17, 126.83, 123.36 (t, *J* = 285.0 Hz), 116.64 (d, *J* = 23.0 Hz), 76.06 (t, *J* = 27.0 Hz), 23.67. ^{19}F NMR (377 MHz, $CDCl_3$) δ -82.51, -82.62, -101.38. HR-GC-MS (m/z): calcd for $C_{21}H_{17}F_3O_4S$ [M]: 422.0800, found: 422.0787.

2-([1,1'-Biphenyl]-4-yl)-1,1-difluoro-2-hydroxypropyl 4-chlorobenzenesulfonate (3k)



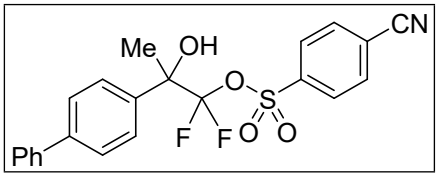
Flash column chromatography on silica gel (eluent: PE/EA = 6/1, v/v) to afford **3k**. Yellow solid (56.1 mg, 64%), mp 79.0-80.9 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.4 Hz, 2H), 7.60 – 7.57 (m, 2H), 7.51 – 7.44 (m, 6H), 7.40 – 7.35 (m, 3H), 2.47 (s, 1H), 1.75 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.48, 141.32, 140.29, 137.12, 135.21, 129.57, 129.45, 129.05, 127.82, 127.21, 126.83, 126.52, 123.39 (t, *J* = 285.0 Hz), 76.07 (t, *J* = 27.0 Hz), 23.66. ^{19}F NMR (377 MHz, $CDCl_3$) δ -82.38, -82.45. HR-GC-MS (m/z): calcd for $C_{21}H_{17}ClF_2O_4S$ [M]: 438.0504, found: 438.0503.

2-([1,1'-Biphenyl]-4-yl)-1,1-difluoro-2-hydroxypropyl 4-bromobenzenesulfonate (3l)



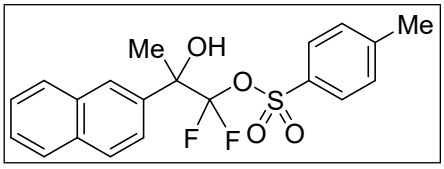
Flash column chromatography on silica gel (eluent: PE/EA = 6/1, v/v) to afford **3l**. Light yellow oil (58.8 mg, 61%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 – 7.56 (m, 4H), 7.55 – 7.44 (m, 8H), 7.38 (t, *J* = 7.4 Hz, 1H), 1.75 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.44, 140.26, 137.11, 135.72, 132.55, 129.92, 129.42, 129.04, 127.81, 127.22, 126.83, 126.80, 123.38 (t, *J* = 285.0 Hz), 76.03 (t, *J* = 27.0 Hz), 23.61. ^{19}F NMR (377 MHz, $CDCl_3$) δ -82.36, -82.43. HR-GC-MS (m/z): calcd for $C_{21}H_{17}BrF_2O_4S$ [M]: 481.9999, found: 482.0003.

2-([1,1'-Biphenyl]-4-yl)-1,1-difluoro-2-hydroxypropyl 4-cyanobenzenesulfonate (3m)



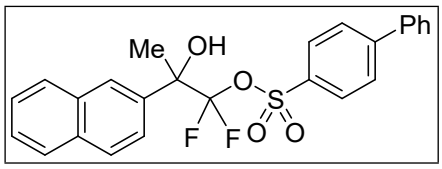
Flash column chromatography on silica gel (eluent: PE/EA = 6/1, v/v) to afford **3m**. White solid (48.1 mg, 56%), mp 141.9-142.7 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.2 Hz, 2H), 7.65 (d, *J* = 8.3 Hz, 2H), 7.59 (d, *J* = 7.4 Hz, 2H), 7.54 – 7.46 (m, 6H), 7.40 (t, *J* = 7.4 Hz, 1H), 2.56 (s, 1H), 1.77 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 141.55, 140.78, 139.99, 136.94, 132.89, 129.20, 128.54, 128.01, 127.08, 126.90, 126.78, 123.54 (t, *J* = 285.0 Hz), 118.03, 116.81, 75.96 (t, *J* = 27.0 Hz), 23.48. ^{19}F NMR (377 MHz, $CDCl_3$) δ -82.03, -82.20. HR-GC-MS (m/z): calcd for $C_{22}H_{17}F_2NO_4S$ [M]: 429.0846, found: 429.0850.

1,1-Difluoro-2-hydroxy-2-(naphthalen-2-yl)propyl 4-methylbenzenesulfonate (3n)



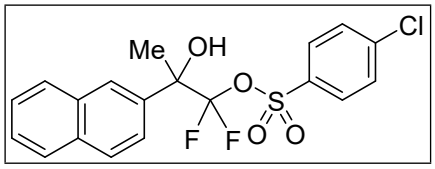
Flash column chromatography on silica gel (eluent: PE/EA = 6/1, v/v) to afford **3n**. Colorless oil (52.7 mg, 67%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 1.8 Hz, 1H), 7.82 – 7.78 (m, 1H), 7.76 – 7.68 (m, 2H), 7.54 – 7.45 (m, 5H), 6.94 (d, *J* = 8.1 Hz, 2H), 2.78 (s, 1H), 2.26 (s, 3H), 1.79 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.65, 135.75, 133.42, 133.03, 132.76, 129.58, 128.52, 127.88, 127.74, 127.46, 126.63, 126.28, 125.90, 123.91, 123.28 (t, *J* = 284.0 Hz), 76.29 (t, *J* = 27.0 Hz), 23.70, 21.69. ^{19}F NMR (377 MHz, $CDCl_3$) δ -82.24, -82.34. HRMS-ESI (m/z): calcd for $C_{20}H_{19}F_2O_4S$ $[M + H]^+$: 393.0972, found: 393.0972.

1,1-Difluoro-2-hydroxy-2-(naphthalen-2-yl)propyl [1,1'-biphenyl]-4-sulfonate (3o)



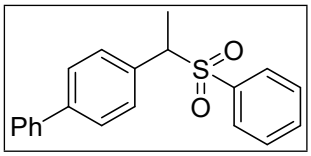
Flash column chromatography on silica gel (eluent: PE/EA = 6/1, v/v) to afford **3o**. Colorless oil (54.5 mg, 60%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 1.8 Hz, 1H), 7.78 – 7.72 (m, 2H), 7.70 (d, *J* = 8.8 Hz, 1H), 7.65 (d, *J* = 8.3 Hz, 2H), 7.55 – 7.51 (m, 1H), 7.49 – 7.40 (m, 7H), 7.34 (d, J = 8.4 Hz, 2H), 2.77 (s, 1H), 1.82 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.19, 138.70, 135.74, 134.88, 133.00, 132.77, 129.13, 128.96, 128.49, 128.37, 127.78, 127.44, 127.09, 126.66, 126.39, 125.93, 123.90, 123.38 (t, *J* = 285.0 Hz), 76.31 (t, *J* = 27.0 Hz), 23.72. ^{19}F NMR (377 MHz, $CDCl_3$) δ -82.06, -82.24. HR-GC-MS (m/z): calcd for $C_{25}H_{20}FO_2S$ [M]: 454.1050, found: 454.1058.

1,1-Difluoro-2-hydroxy-2-(naphthalen-2-yl)propyl 4-chlorobenzenesulfonate (3p)



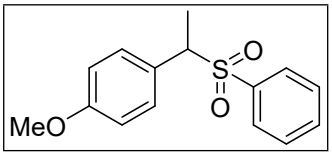
Flash column chromatography on silica gel (eluent: PE/EA = 6/1, v/v) to afford **3p**. Light yellow oil (52.7 mg, 64%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 – 7.81 (m, 2H), 7.79 – 7.74 (m, 1H), 7.71 (d, *J* = 8.7 Hz, 1H), 7.53 (td, *J* = 6.6, 6.0, 3.5 Hz, 2H), 7.48 (t, *J* = 8.7 Hz, 3H), 7.06 (d, *J* = 8.5 Hz, 2H), 2.65 (s, 1H), 1.82 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.13, 135.51, 134.80, 133.06, 132.72, 129.28, 129.20, 128.43, 127.84, 127.53, 126.89, 126.60, 125.90, 123.77, 123.35 (t, *J* = 285.0 Hz), 76.27 (t, *J* = 27.0 Hz), 23.60. ^{19}F NMR (377 MHz, $CDCl_3$) δ -82.08, -82.16. HR-GC-MS (m/z): calcd for $C_{19}H_{15}ClF_2O_4S$ [M]: 412.0348, found: 412.0349.

4-(1-(Phenylsulfonyl)ethyl)-1,1'-biphenyl (5a)



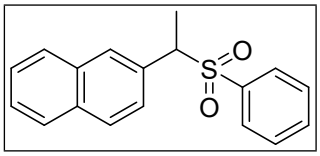
Purified by preparative TLC (eluent: PE/EA = 6/1, v/v) to afford **5a**. Yellow solid (37.3 mg, 58%), mp 167.4-168.3 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (dd, *J* = 15.4, 7.7 Hz, 5H), 7.49 (d, *J* = 8.0 Hz, 2H), 7.43 (dt, *J* = 10.4, 7.6 Hz, 4H), 7.36 (t, *J* = 7.3 Hz, 1H), 7.21 (d, *J* = 8.0 Hz, 2H), 4.29 (q, *J* = 7.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.73, 140.35, 136.97, 133.70, 132.68, 129.94, 129.35, 128.97, 128.81, 127.76, 127.17, 127.14, 65.90, 14.21. HR-DART-MS (m/z): calcd for $C_{20}H_{19}O_2S$ $[M + H]^+$: 323.1100, found: 323.1099.

1-Methoxy-4-(1-(phenylsulfonyl)ethyl)benzene (5b)



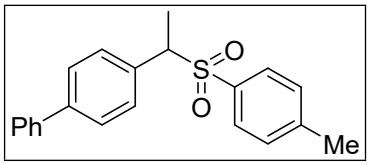
Purified by preparative TLC (eluent: PE/EA = 6/1, v/v) to afford **5b**. Yellow solid (22.1 mg, 40%), mp 92.4-93.5 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 7.7 Hz, 3H), 7.45 – 7.39 (m, 2H), 7.08 – 7.03 (m, 2H), 6.80 – 6.74 (m, 2H), 4.20 (q, *J* = 7.2 Hz, 1H), 3.79 (s, 3H), 1.73 (d, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 137.0, 133.6, 130.7, 129.3, 128.7, 125.6, 113.9, 65.5, 55.4, 14.2. HR-DART-MS (m/z): calcd for $C_{15}H20NO_3S$ $[M + NH_4]^+$: 294.1158, found: 294.1158.

2-(1-(Phenylsulfonyl)ethyl)naphthalene (5c)



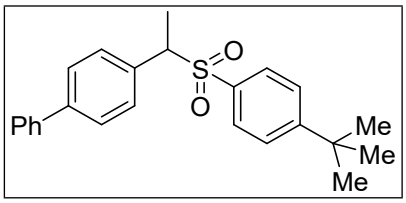
Purified by preparative TLC (eluent: PE/EA = 6/1, v/v) to afford **5c**. Yellow solid (18.9 mg, 32%), mp 137.8-138.9 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 – 7.79 (m, 1H), 7.75 – 7.68 (m, 2H), 7.58 – 7.50 (m, 4H), 7.50 – 7.44 (m, 2H), 7.35 (t, *J* = 7.7 Hz, 2H), 7.30 – 7.27 (m, 1H), 4.41 (q, *J* = 7.2 Hz, 1H), 1.86 (d, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.9, 133.7, 133.3, 133.0, 131.3, 129.3, 129.2, 128.8, 128.2, 128.2, 127.7, 126.8, 126.7, 126.5, 66.3, 14.4. HR-DART-MS (m/z): calcd for $C_{18}H_{20}NO_2S$ $[M +NH_4]^+$: 314.1209, found: 314.1209.

4-(1-Tosylethyl)-1,1'-biphenyl (5d)



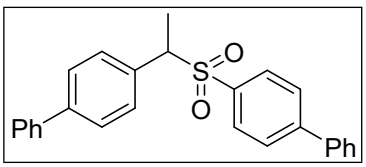
Purified by preparative TLC (eluent: PE/EA = 6/1, v/v) to afford **5d**. Yellow solid (24.9 mg, 37%), mp 180.3-182.4 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.0 Hz, 2H), 7.51 – 7.42 (m, 6H), 7.39 – 7.35 (m, 1H), 7.22 (t, *J* = 7.4 Hz, 4H), 4.27 (q, *J* = 7.2 Hz, 1H), 2.40 (s, 3H), 1.82 – 1.74 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.7, 141.7, 140.4, 134.0, 132.9, 130.0, 129.5, 129.4, 129.0, 127.7, 127.2, 127.1, 65.9, 21.8, 14.3. HR-GC-MS (m/z): calcd for $C_{21}H_{20}O_2S$ [M]: 336.1184, found: 336.1186.

4-(1-((4-(Tert-butyl)phenyl)sulfonyl)ethyl)-1,1'-biphenyl (5e)



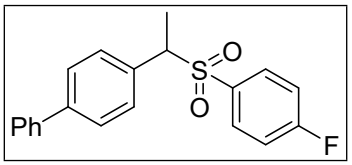
Purified by preparative TLC (eluent: PE/EA = 6/1, v/v) to afford **5e**. Light yellow oil (30.3 mg, 40%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.52 (m, 4H), 7.51 – 7.47 (m, 2H), 7.47 – 7.41 (m, 4H), 7.39 – 7.33 (m, 1H), 7.24 (d, *J* = 8.2 Hz, 2H), 4.27 (q, *J* = 7.1 Hz, 1H), 1.78 (d, *J* = 7.1 Hz, 3H), 1.32 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.7, 141.7, 140.5, 134.0, 132.8, 130.0, 129.2, 129.0, 127.7, 127.2, 127.1, 125.8, 65.9, 35.4, 31.2, 14.4. HR-DART-MS (m/z): calcd for $C_{24}H_{30}NO_2S$ $[M + NH_4]^+$: 396.1992, found: 396.1992.

4-((1-([1,1'-Biphenyl]-4-yl)ethyl)sulfonyl)-1,1'-biphenyl (5f)



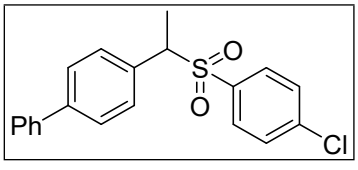
Purified by preparative TLC (eluent: PE/EA = 6/1, v/v) to afford **5f**. Yellow solid (28.7 mg, 36%), mp 258.9-259.7 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 – 7.61 (m, 4H), 7.58 (dd, *J* = 7.9, 6.0 Hz, 4H), 7.53 – 7.49 (m, 3H), 7.48 – 7.41 (m, 5H), 7.36 (t, *J* = 7.3 Hz, 1H), 7.28 (s, 1H), 4.33 (q, *J* = 7.2 Hz, 1H), 1.83 (d, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.6, 141.8, 140.4, 139.2, 135.5, 132.7, 130.0, 129.9, 129.2, 129.0, 128.8, 127.8, 127.5, 127.4, 127.2, 66.0, 14.4. HR-DART-MS (m/z): calcd for $C_{26}H_{26}NO_2S$ $[M + NH_4]^+$: 416.1679, found: 416.1677.

4-(1-((4-Fluorophenyl)sulfonyl)ethyl)-1,1'-biphenyl (5g)



Purified by preparative TLC (eluent: PE/EA = 6/1, v/v) to afford **5g**. Yellow solid (31.3 mg, 46%), mp 152.4-153.5 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 – 7.55 (m, 4H), 7.52 – 7.48 (m, 2H), 7.48 – 7.42 (m, 2H), 7.39 – 7.34 (m, 1H), 7.21 (d, *J* = 7.9 Hz, 2H), 7.11 – 7.05 (m, 2H), 4.28 (q, *J* = 7.1 Hz, 1H), 1.81 (d, *J* = 6.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.2, 164.6, 141.9, 140.2, 132.9 (d, J = 3.2 Hz), 132.6, 132.2 (d, J = 9.6 Hz), 130.9, 129.0, 127.8, 127.2 (d, *J* = 4.1 Hz), 116.1 (d, *J* = 22.5 Hz), 66.1, 14.1. HR-DART-MS (m/z): calcd for $C_{20}H_{21}NFO_2S$ $[M + NH_4]^+$: 358.1272, found: 358.1271.

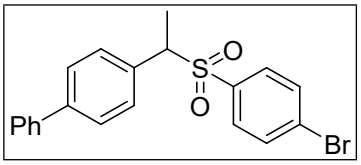
4-(1-((4-Bromophenyl)sulfonyl)ethyl)-1,1'-biphenyl (5h)



Purified by preparative TLC (eluent: PE/EA = 6/1, v/v) to afford **5h**. Yellow solid (38.5 mg, 54%), mp 144.1-145.6 ℃. ^{1}H NMR (400 MHz,

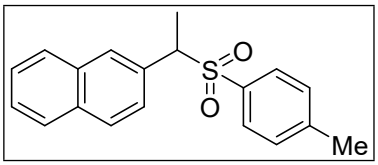
$CDCl_3$) δ 7.61 – 7.55 (m, 4H), 7.50 (dd, *J* = 8.3, 2.0 Hz, 2H), 7.48 – 7.42 (m, 2H), 7.39 – 7.34 (m, 1H), 7.21 (dd, *J* = 8.3, 2.0 Hz, 2H), 7.11 – 7.05 (m, 2H), 4.28 (q, *J* = 7.3 Hz, 1H), 1.81 (d, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.2, 164.6, 141.9, 140.2, 132.6, 132.2, 132.1, 129.9, 129.0, 127.9, 127.2, 116.1, 66.1, 29.9, 14.1. HR-DART-MS (m/z): calcd for $C_{20}H_{18}ClO_2S$ $[M + H]^+$: 357.0716, found: 357.0724.

2-(1-Tosylethyl)naphthalene (5i)



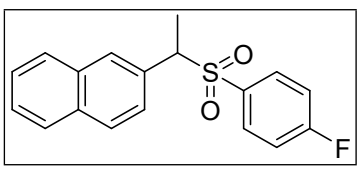
Purified by preparative TLC (eluent: PE/EA = 6/1, v/v) to afford **5i**. Yellow solid (42.1 mg, 53%), mp 136.4-137.6 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (t, *J* = 8.2 Hz, 4H), 7.51 (d, *J* = 8.0 Hz, 2H), 7.48 – 7.41 (m, 4H), 7.38 (d, *J* = 7.3 Hz, 1H), 7.22 (d, *J* = 7.9 Hz, 2H), 4.28 (q, *J* = 7.2 Hz, 1H), 1.80 (d, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.9, 140.2, 136.0, 132.4, 132.1, 130.9, 129.9, 129.2, 129.0, 127.9, 127.3, 127.2, 66.0, 14.1. HR-DART-MS (m/z): calcd for $C_{20}H_{21}NBrO_2S$ $[M + NH_4]^+$: 418.0471, found: 418.0470.

2-(1-([1,1'-Biphenyl]-4-ylsulfonyl)ethyl)naphthalene (5j)



Purified by preparative TLC (eluent: PE/EA = 6/1, v/v) to afford **5j**. White powder (15.5 mg, 25%), mp 149.9-150.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 – 7.79 (m, 1H), 7.73 (dd, *J* = 8.8, 6.0 Hz, 2H), 7.58 (d, *J* = 1.8 Hz, 1H), 7.50 – 7.46 (m, 2H), 7.43 (d, *J* = 8.2 Hz, 2H), 7.29 (dd, *J* = 8.5, 1.9 Hz, 1H), 7.15 (d, *J* = 8.0 Hz, 2H), 4.39 (q, *J* = 7.2 Hz, 1H), 2.37 (s, 3H), 1.84 (d, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.6, 134.0, 133.3, 133.0, 131.5, 129.4, 129.4, 129.1, 128.2, 128.1, 127.7, 126.8, 126.7, 126.4, 66.3, 21.7, 14.5. HR-GC-MS MALDI (m/z): calcd for $C_{19}H_{18}O_2S$ [M]: 310.1028, found: 310.1029.

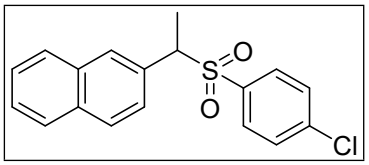
2-(1-((4-Fluorophenyl)sulfonyl)ethyl)naphthalene (5k)



Purified by preparative TLC (eluent: PE/EA = 6/1, v/v) to afford **5k**. Colorless oil (15.7 mg, 25%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 – 7.80 (m, 1H), 7.73 (t, *J* = 8.8 Hz, 2H), 7.56 (d, *J* = 1.8 Hz, 1H), 7.55 – 7.45 (m, 4H), 7.27 (d, *J* = 1.9 Hz, 1H), 7.01 (t, *J* = 8.6 Hz, 2H), 4.40 (q, *J* = 7.2 Hz, 1H), 1.88 (d, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.1, 164.6, 133.4, 133.0, 132.2, 132.1, 131.2,

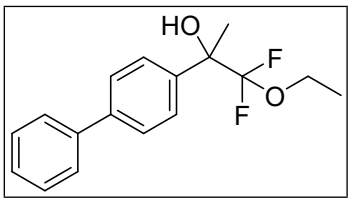
129.1, 128.3, 128.2, 127.8, 126.9, 126.6 (d, J = 3.4 Hz), 116.1 (d, J = 22.6 Hz), 66.5, 14.3. HR-GC-MS (m/z): calcd for $C_{18}H_{15}F_2O_4S$ [M]: 314.0777, found: 314.0780.

2-(1-((4-Chlorophenyl)sulfonyl)ethyl)naphthalene (5l)



Purified by preparative TLC (eluent: PE/EA = 6/1, v/v) to afford **5l**. Colorless oil (17.1 mg, 26%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 – 7.80 (m, 1H), 7.74 (t, J = 7.8 Hz, 2H), 7.58 (d, J = 1.7 Hz, 1H), 7.50 (td, J = 6.9, 6.1, 3.7 Hz, 2H), 7.45 (d, J = 8.4 Hz, 2H), 7.32 (d, J = 8.3 Hz, 2H), 7.28 (d, J = 1.8 Hz, 1H), 4.40 (q, J = 7.1 Hz, 1H), 1.87 (d, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.5, 135.4, 133.4, 133.0, 131.0, 130.8, 129.2, 129.1, 128.4, 128.2, 127.8, 126.9, 126.7, 126.6, 66.5, 14.3. HR-GC-MS (m/z): calcd for $C_{18}H_{15}ClO_2S$ [M]: 330.0481, found: 330.0482.

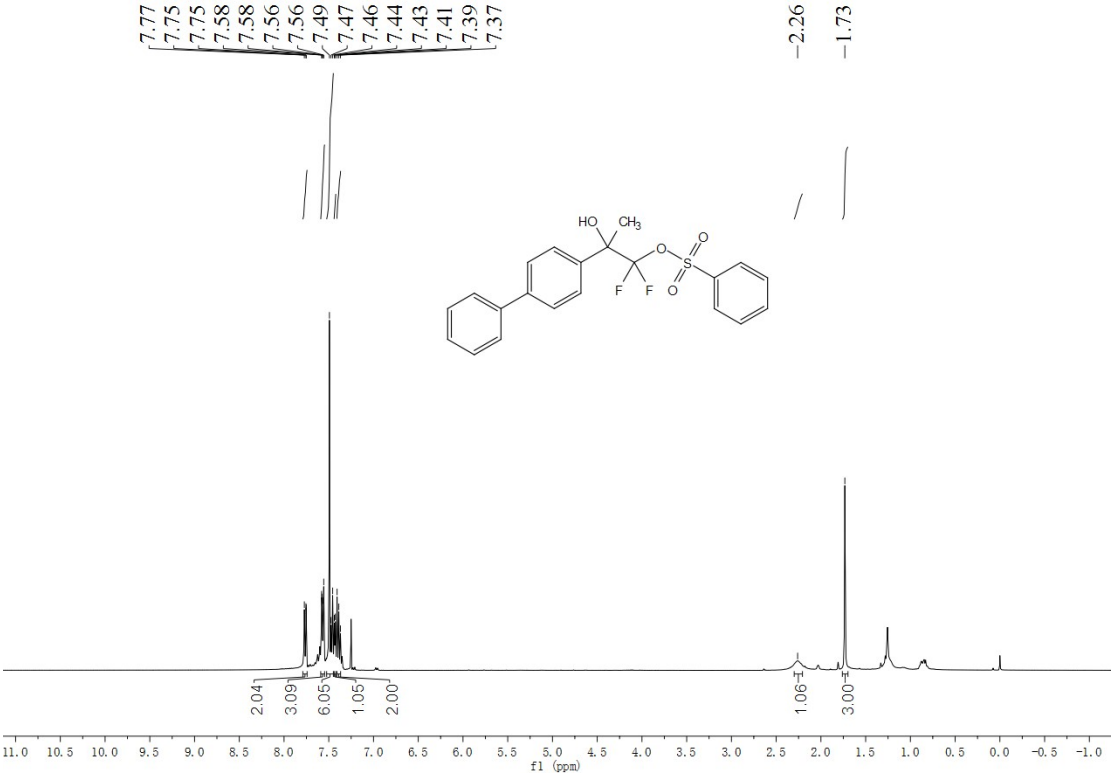
2-([1,1'-Biphenyl]-4-yl)-1-ethoxy-1,1-difluoropropan-2-ol (6)

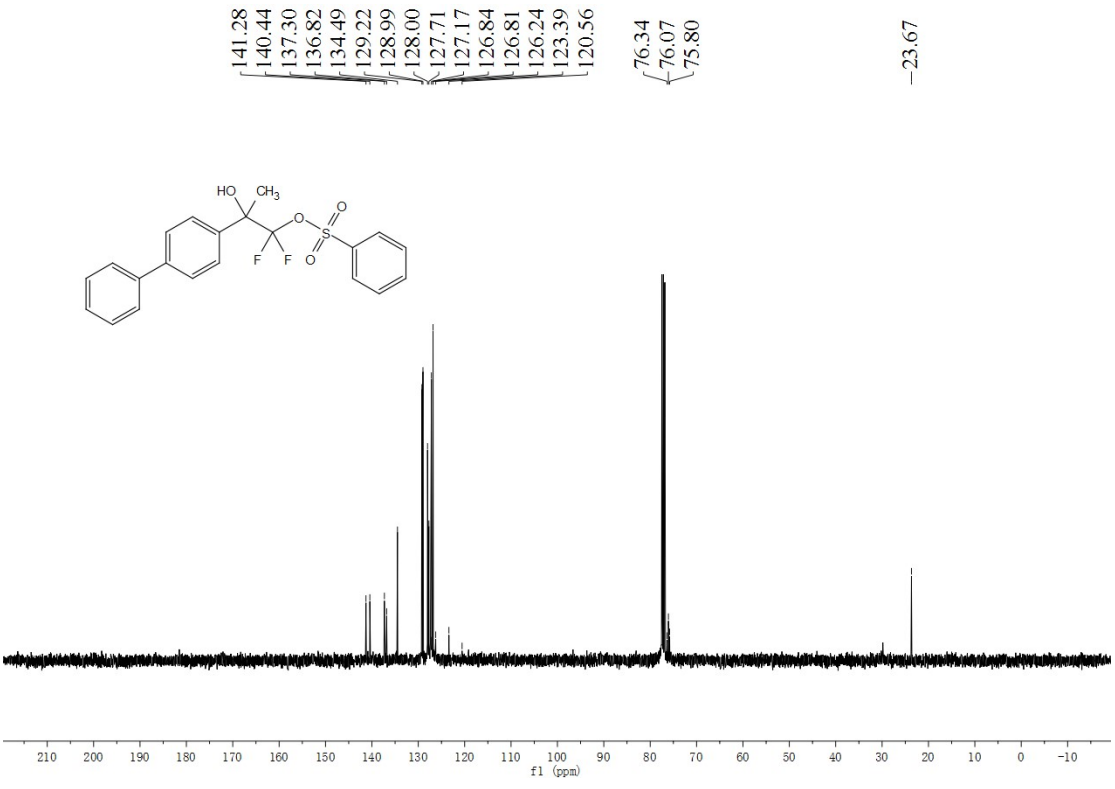


Flash column chromatography on silica gel (eluent: PE/EA = 6/1, v/v) to afford **6**. Colorless oil (36.2 mg, 62%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.56 (m, 7H), 7.44 (t, J = 7.6 Hz, 2H), 7.35 (t, J = 7.3 Hz, 1H), 4.25 (q, J = 13.6, 7.0 Hz, 2H), 3.85 (s, 1H), 1.82 (s, 3H), 1.29 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.75, 141.97, 140.73, 128.90, 127.51, 127.22, 127.15, 125.79, 123.20 (t, J = 285.0 Hz), 75.68 (t, J = 27.0 Hz), 62.66, 26.88, 14.20. ^{19}F NMR (377 MHz, $CDCl_3$) δ -86.08, -86.46. HRMS-ESI (m/z): calcd for $C_{17}H_{19}F_2O_2$ $[M+H]^+$: 293.1353, found: 293.1352.

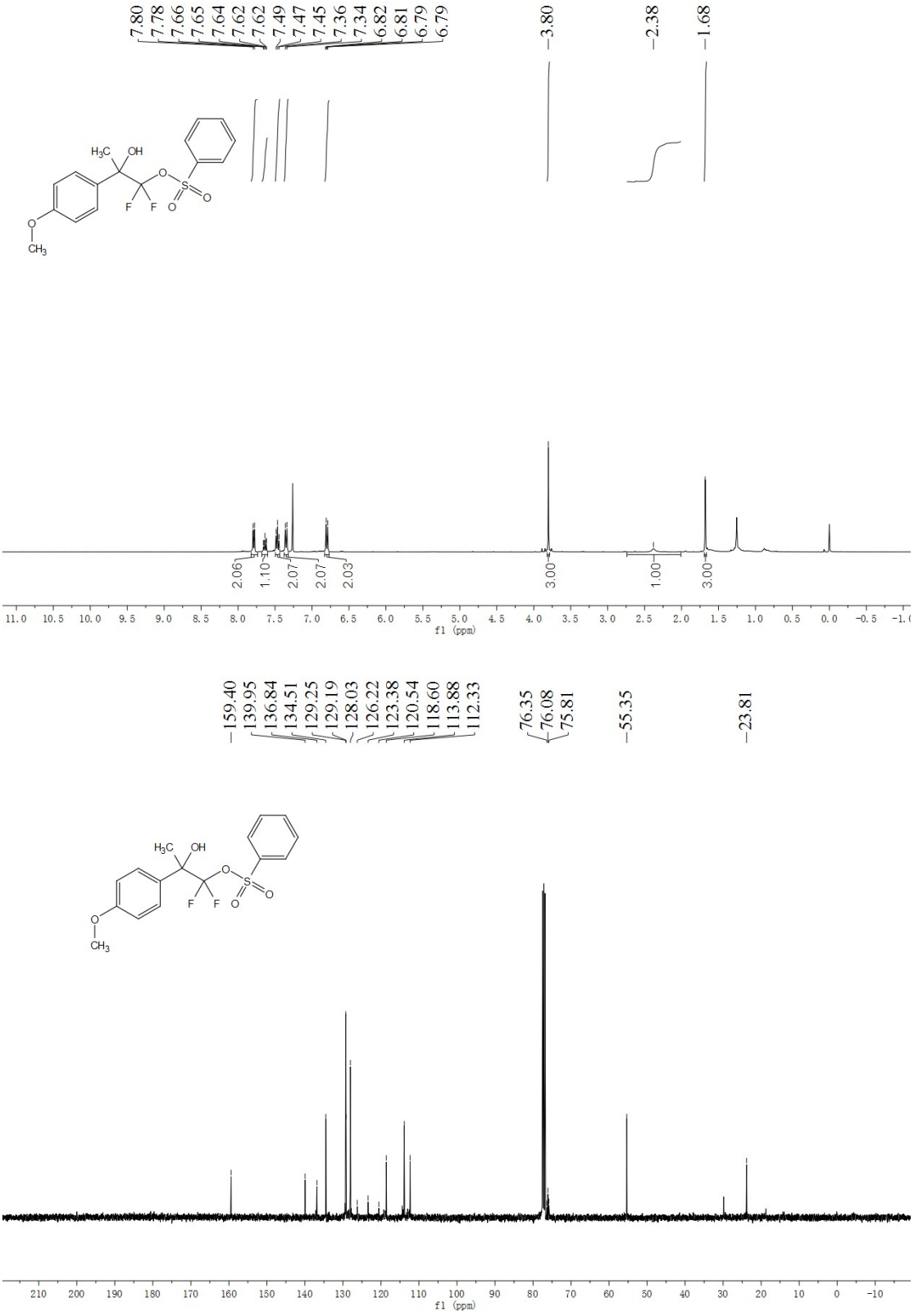
4. NMR spectra for new compounds

^{1}H NMR and ^{13}C NMR spectrum of compound **3a**

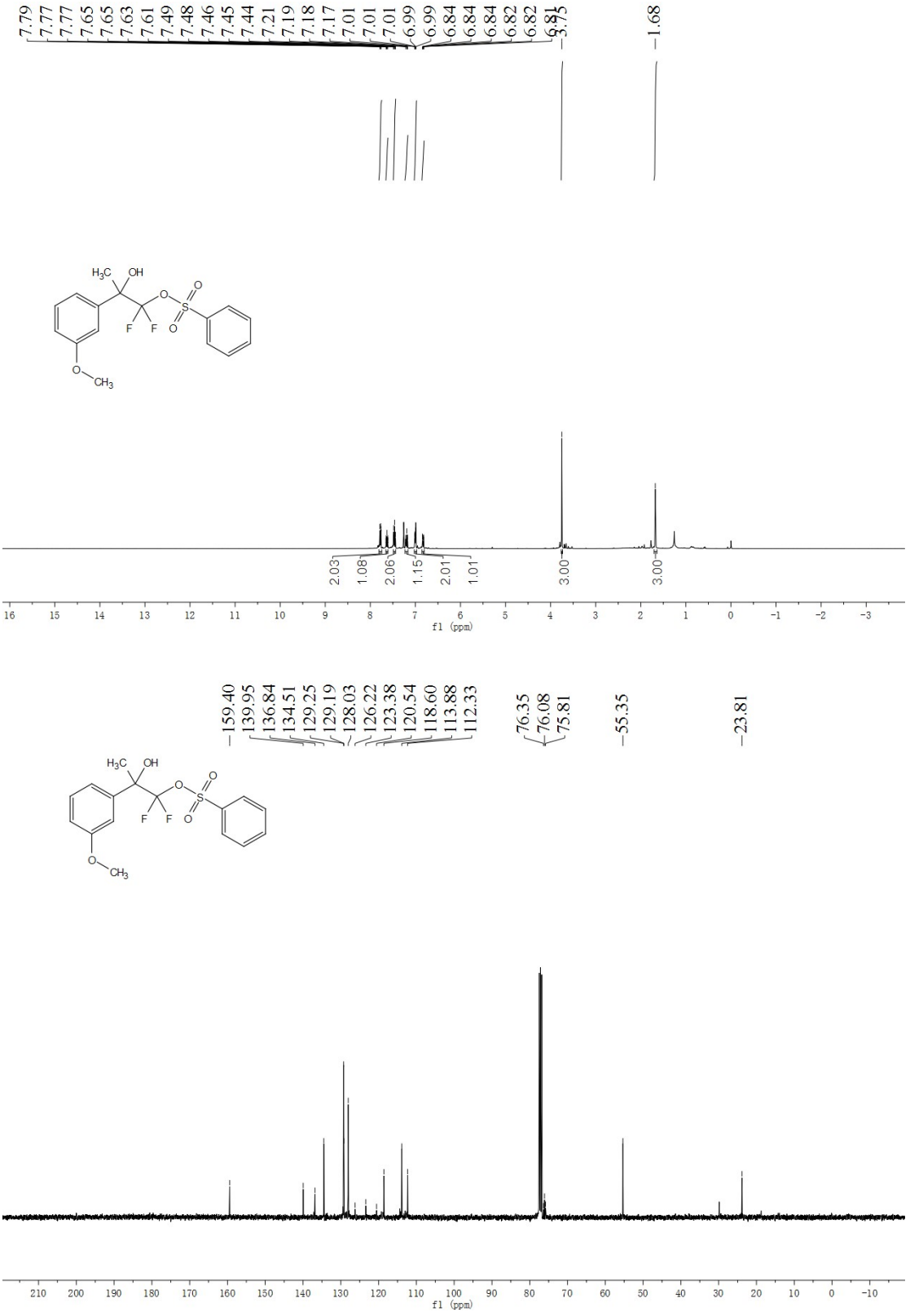




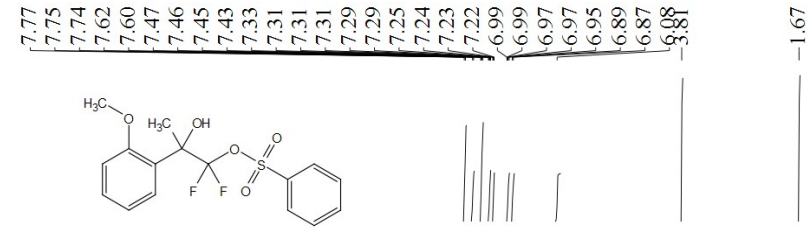
^{1}H NMR and ^{13}C NMR spectrum of compound **3b**

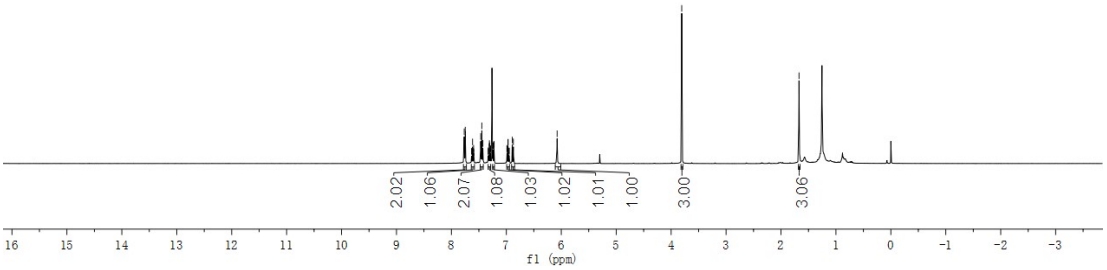


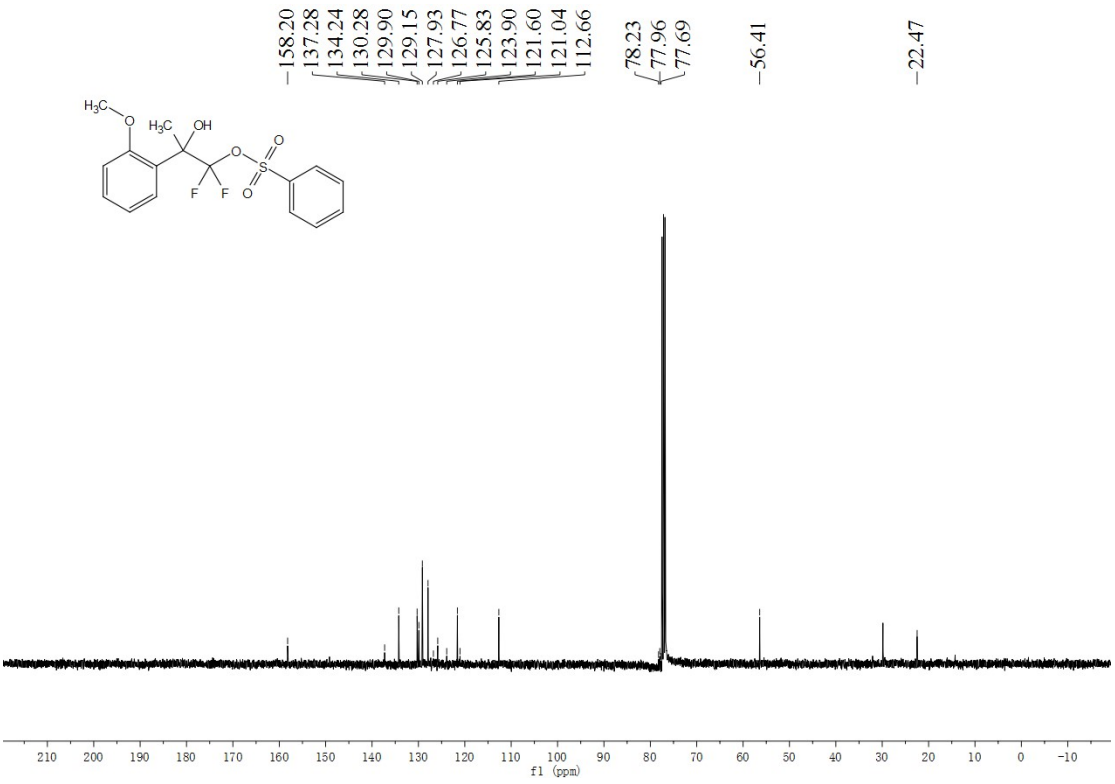
^{1}H NMR and ^{13}C NMR spectrum of compound **3c**



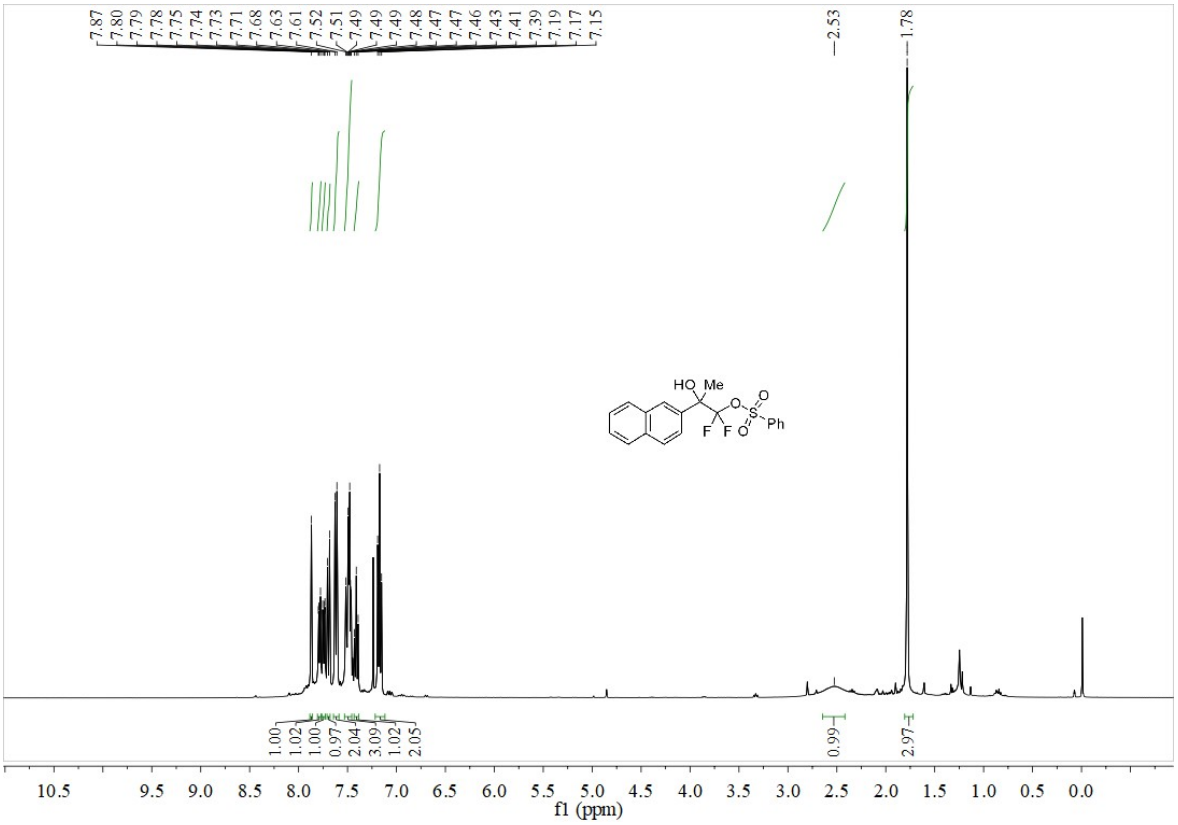
^{1}H NMR and ^{13}C NMR spectrum of compound **3d**

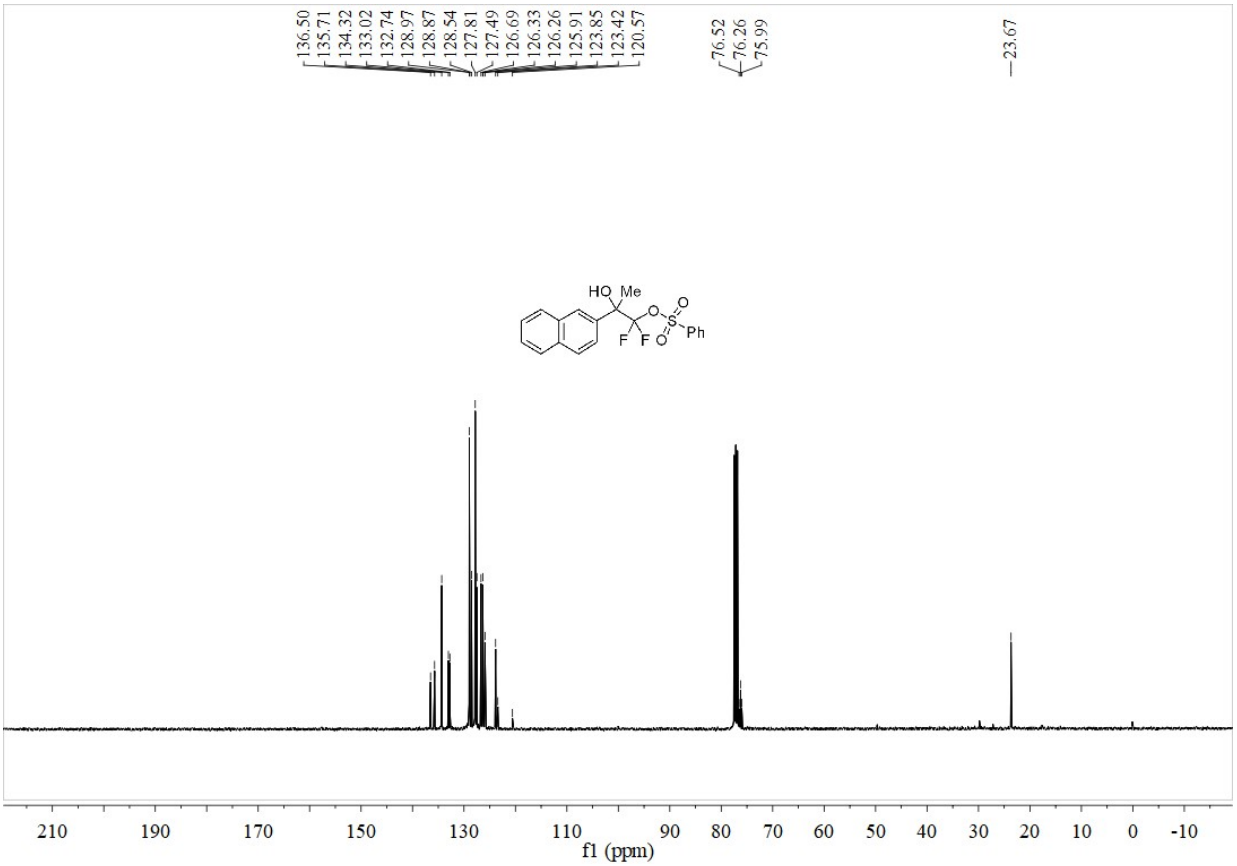




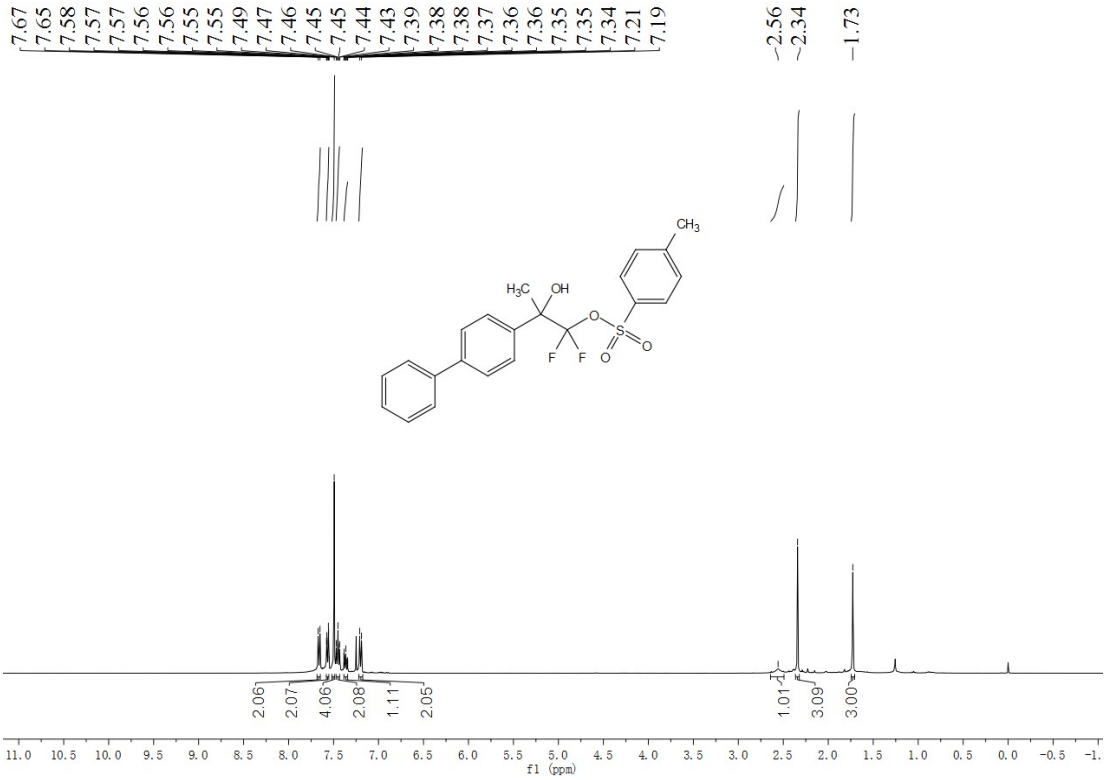


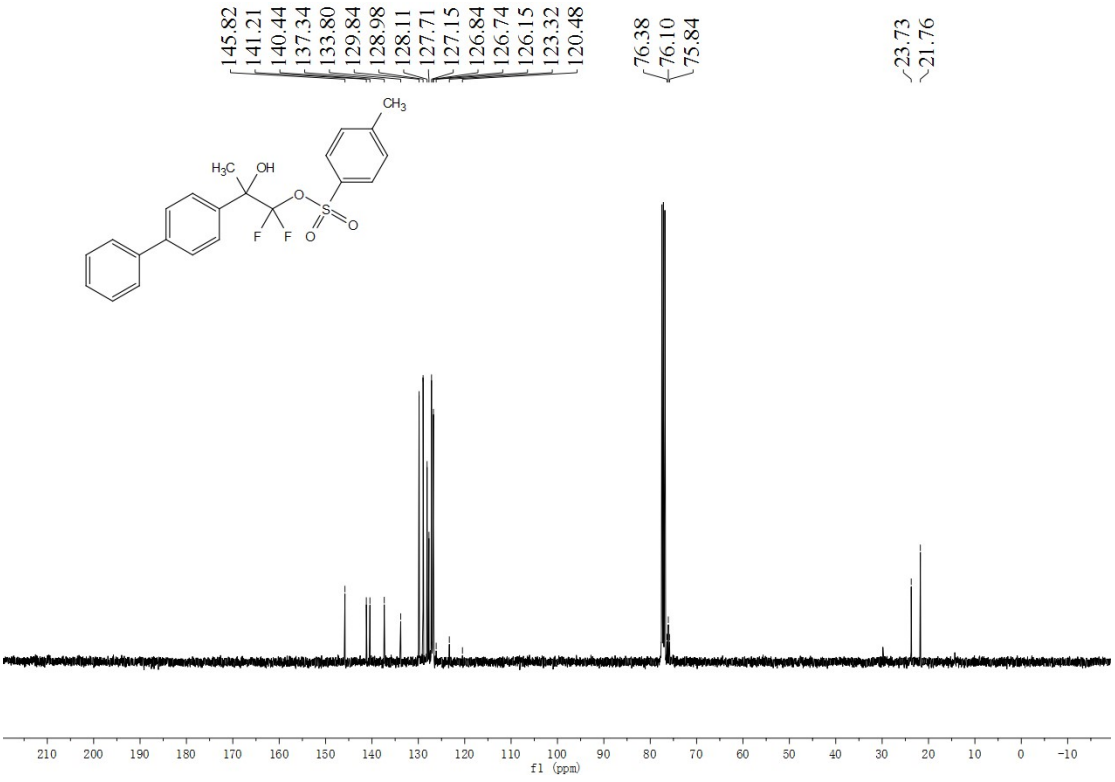
^{1}H NMR and ^{13}C NMR spectrum of compound **3e**



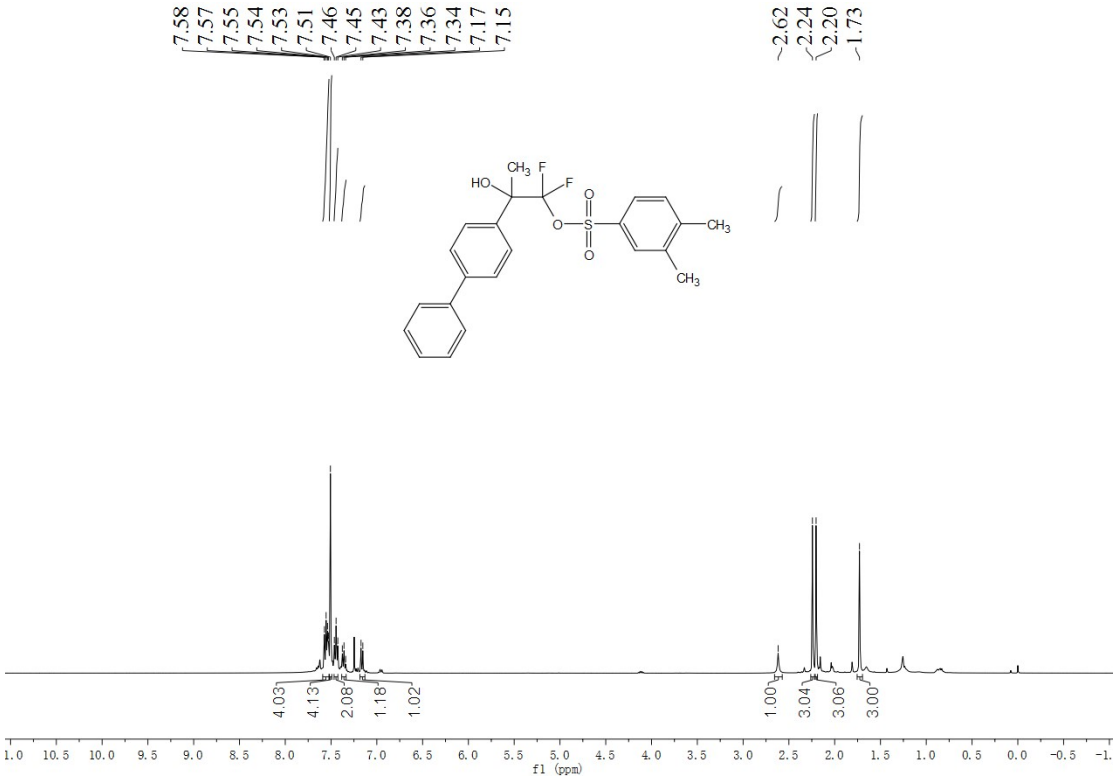


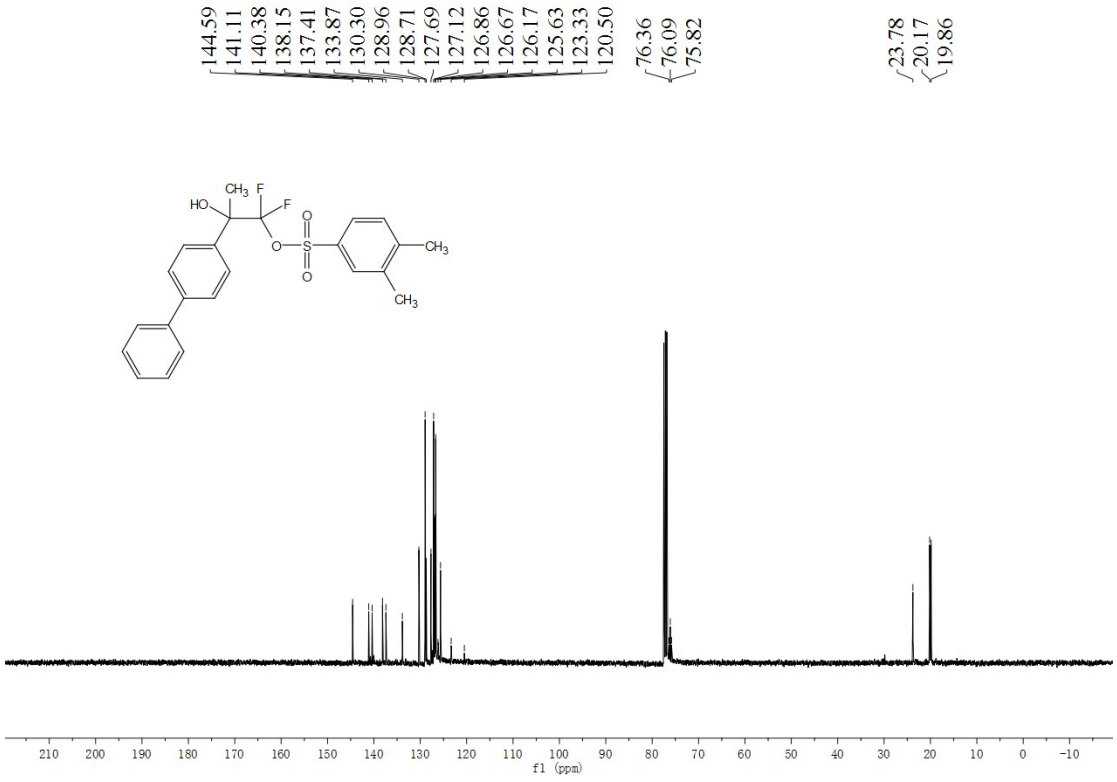
^{1}H NMR and ^{13}C NMR spectrum of compound **3f**



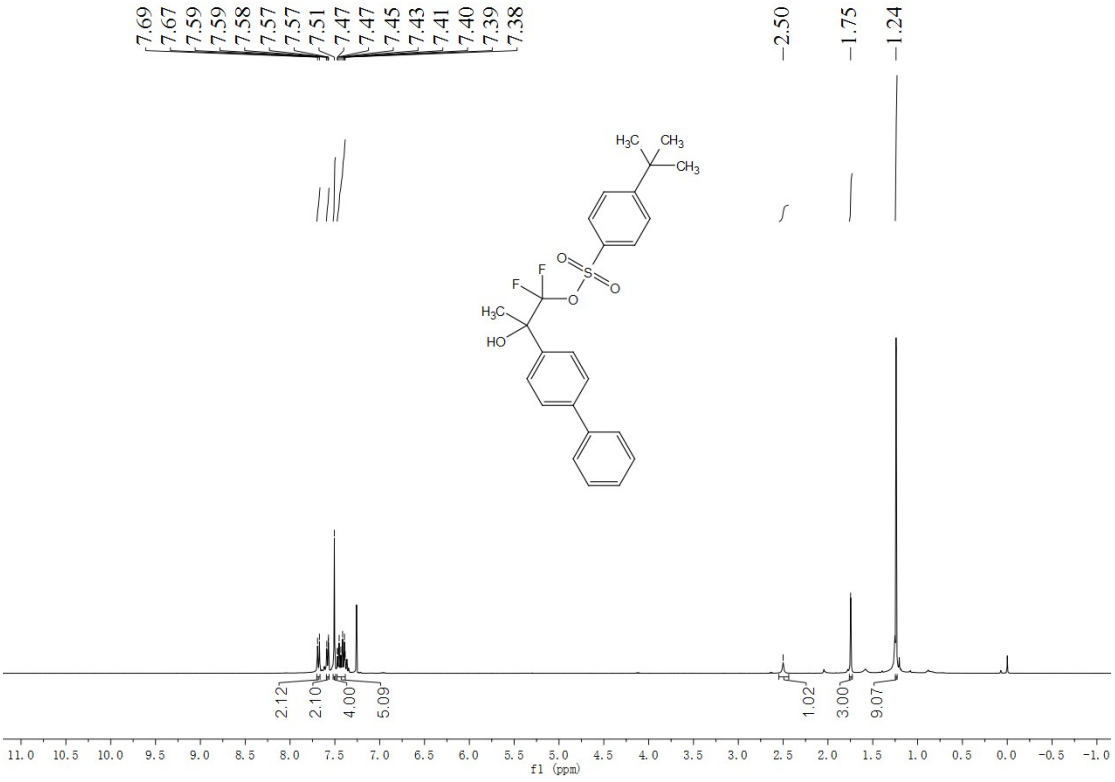


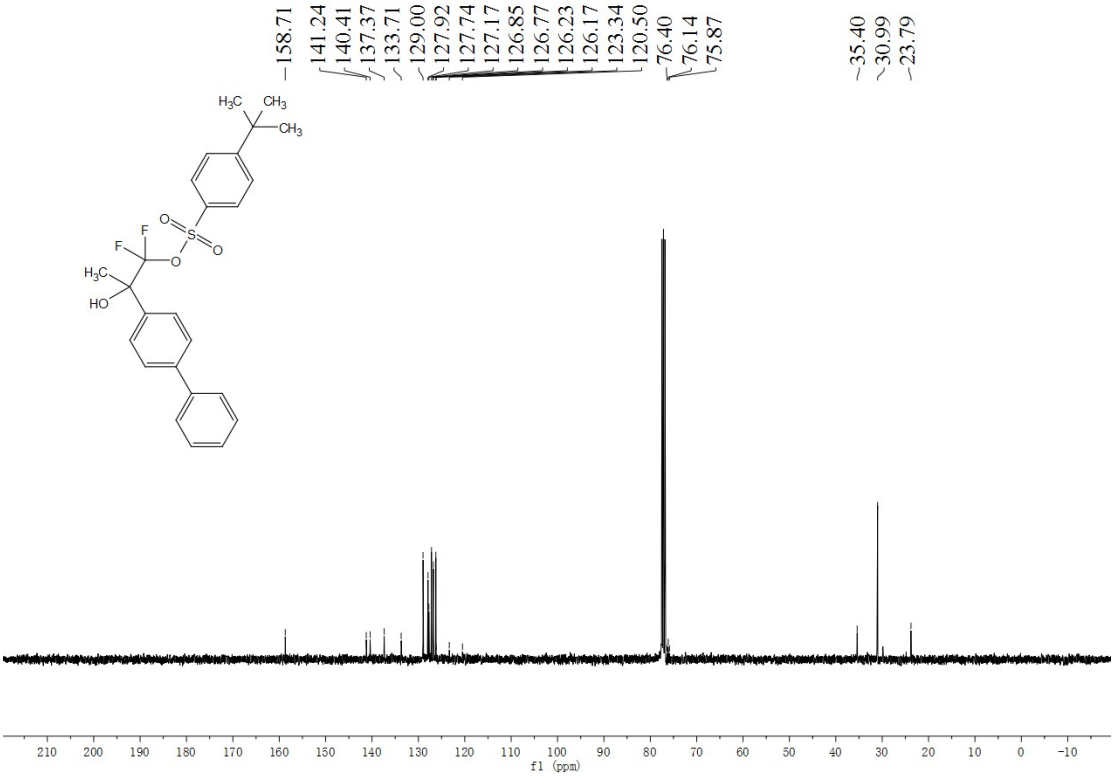
^{1}H NMR and ^{13}C NMR spectrum of compound **3g**



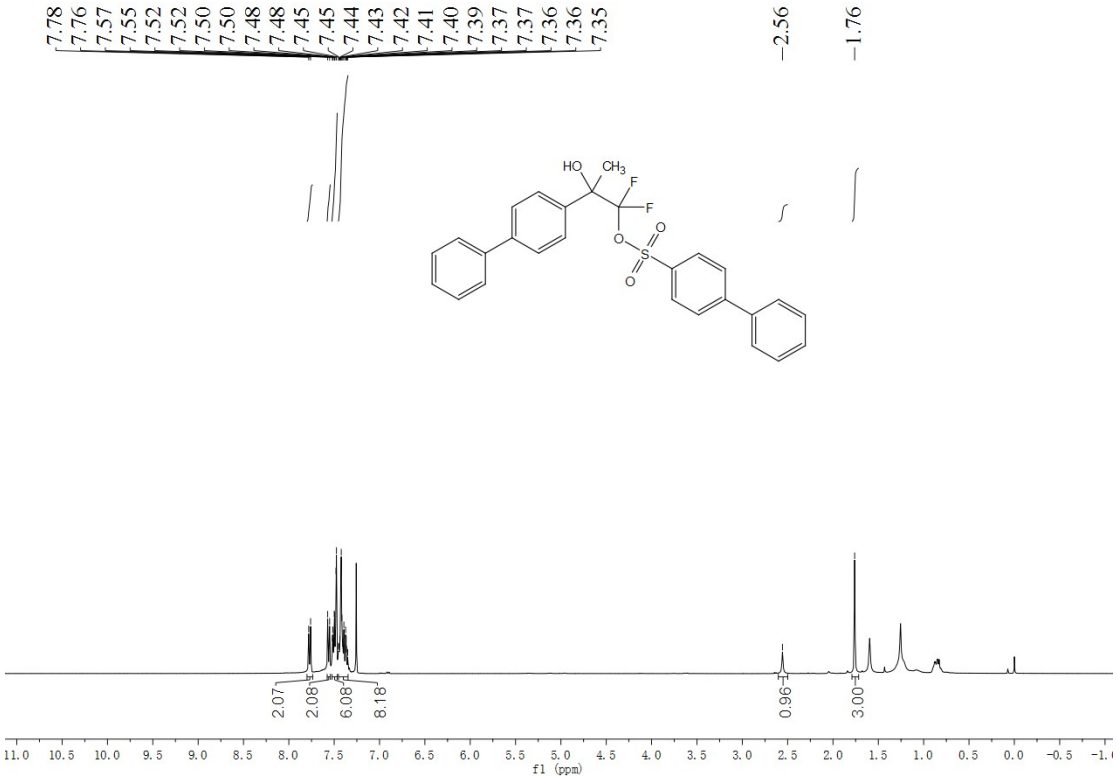


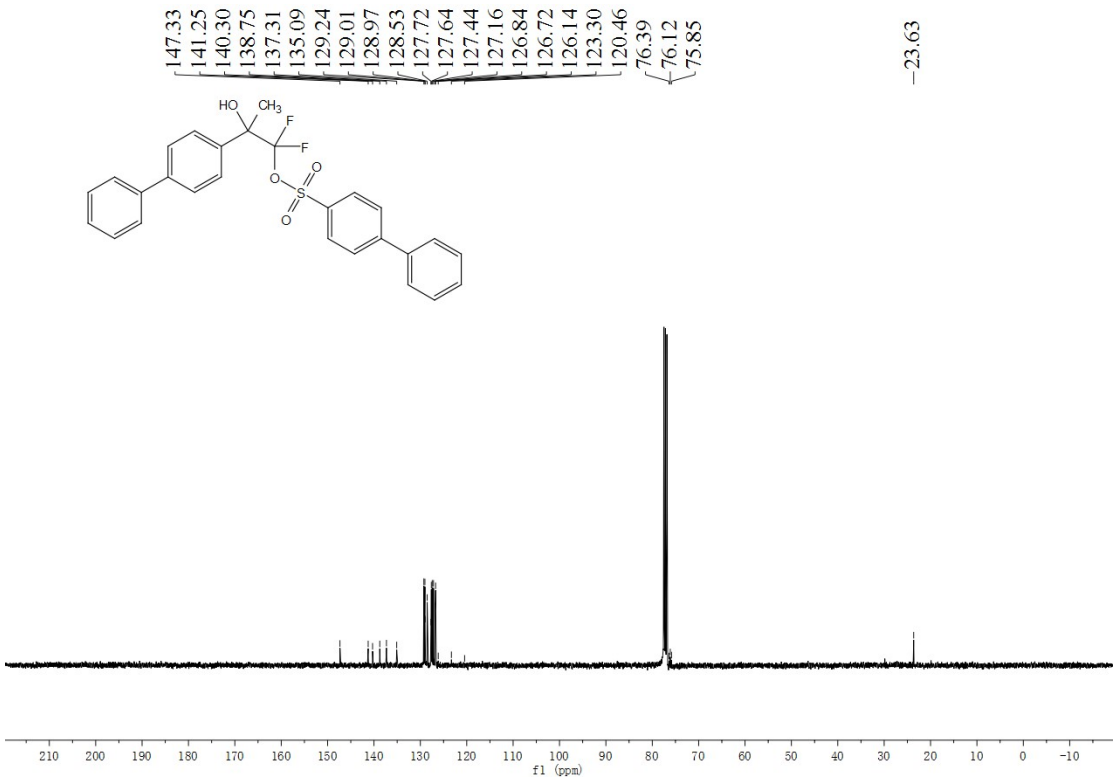
^{1}H NMR and ^{13}C NMR spectrum of compound **3h**



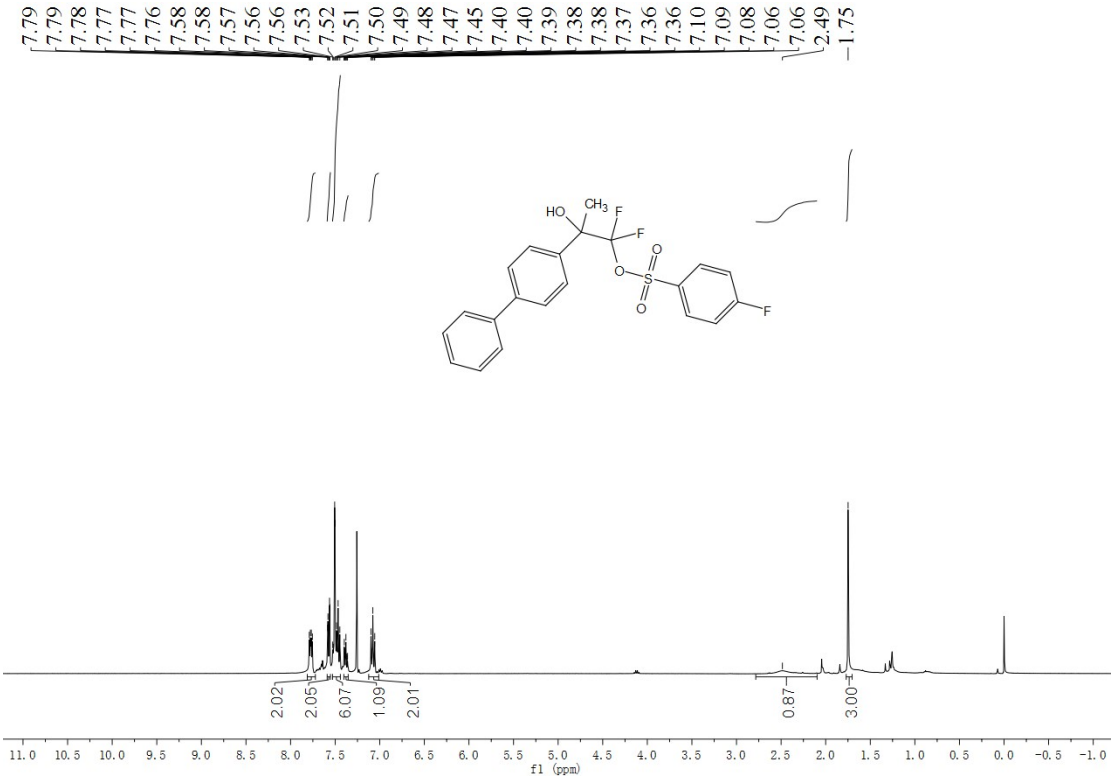


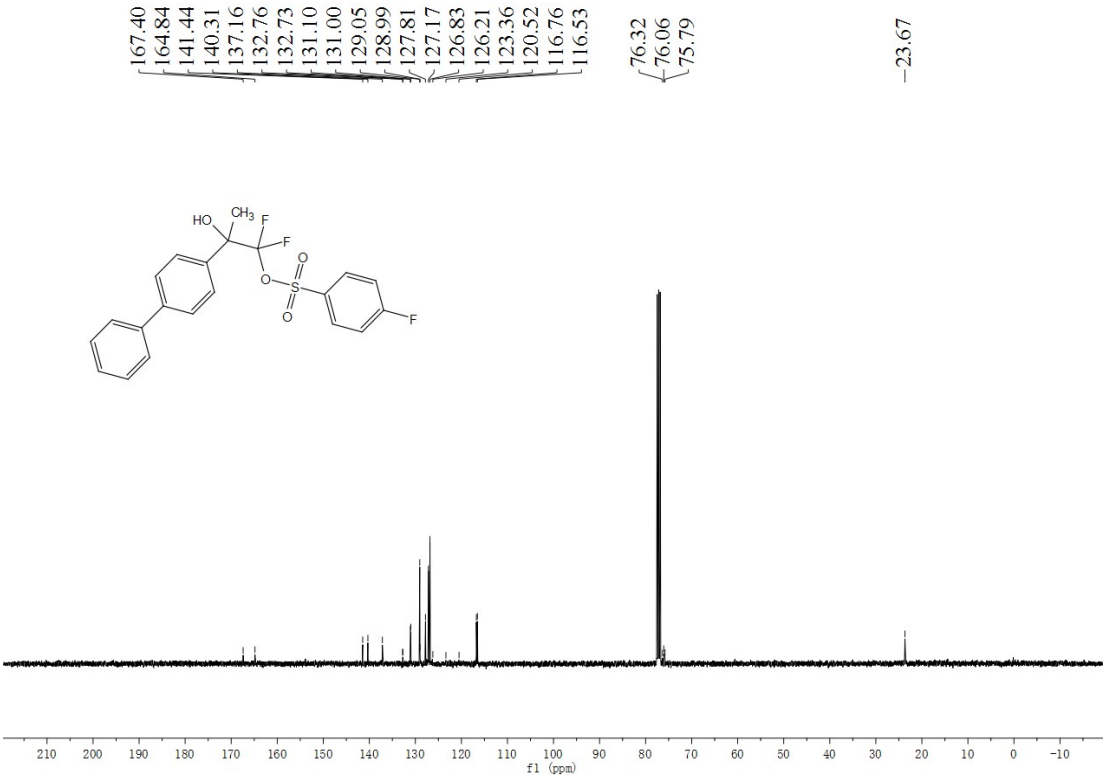
^{1}H NMR and ^{13}C NMR spectrum of compound **3i**



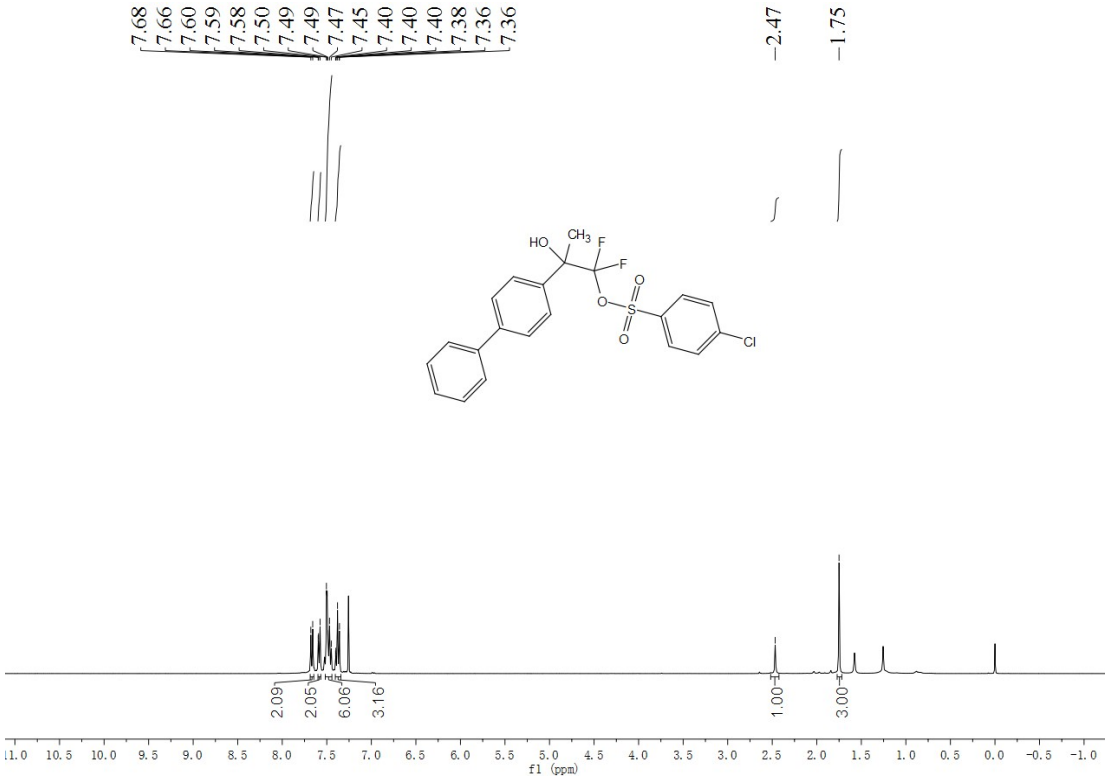


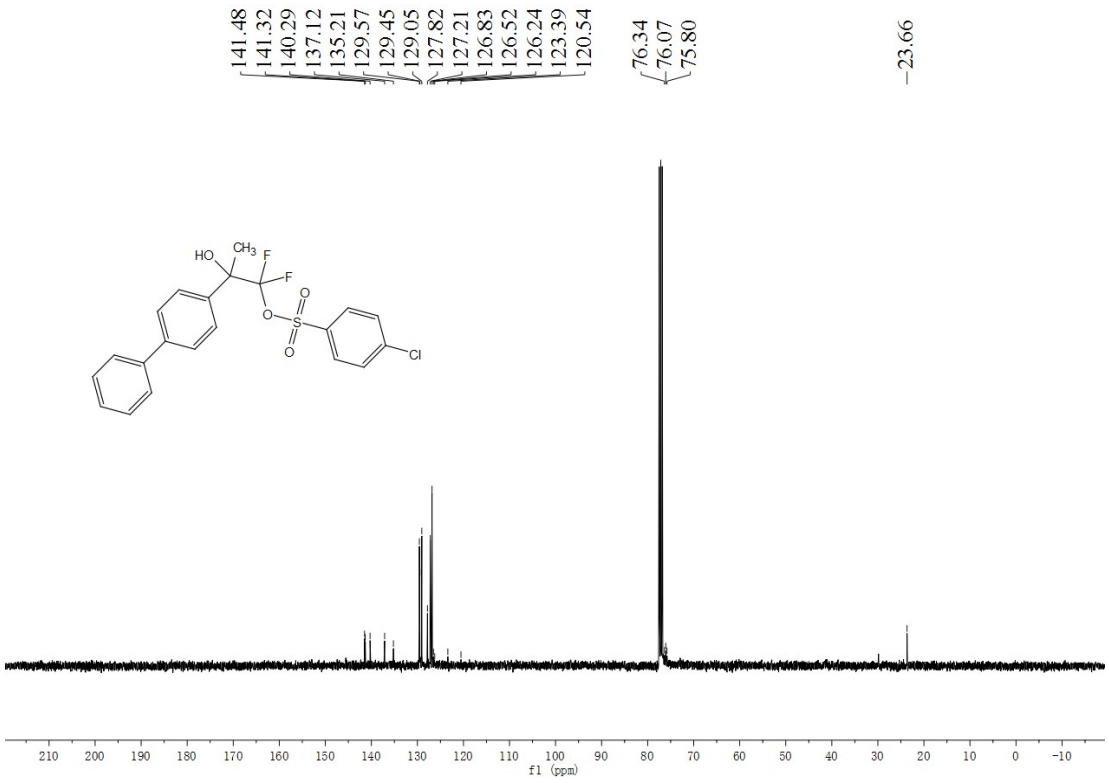
^{1}H NMR and ^{13}C NMR spectrum of compound **3j**



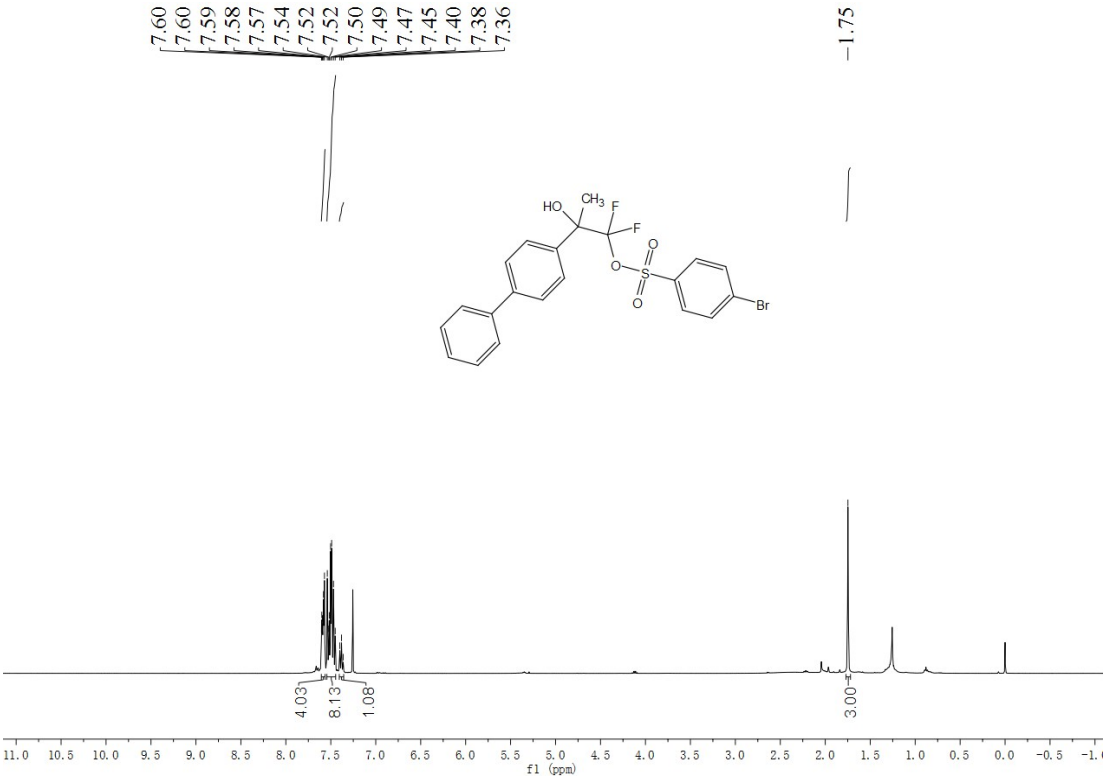


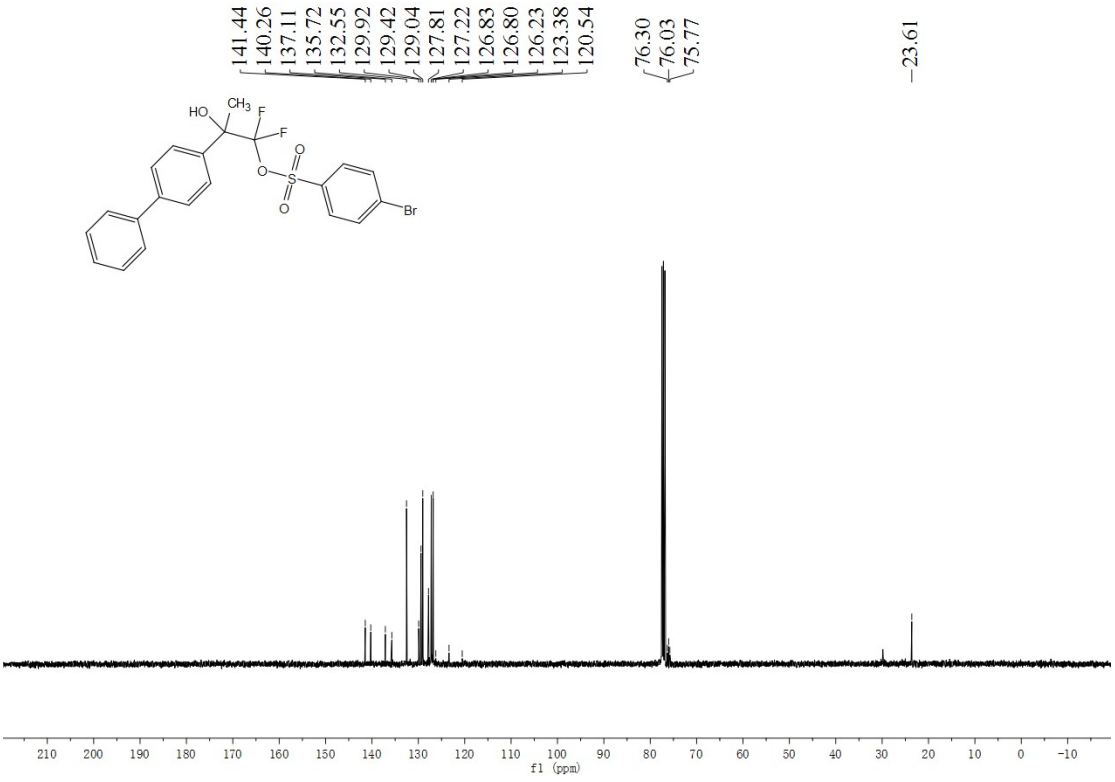
^{1}H NMR and ^{13}C NMR spectrum of compound **3k**



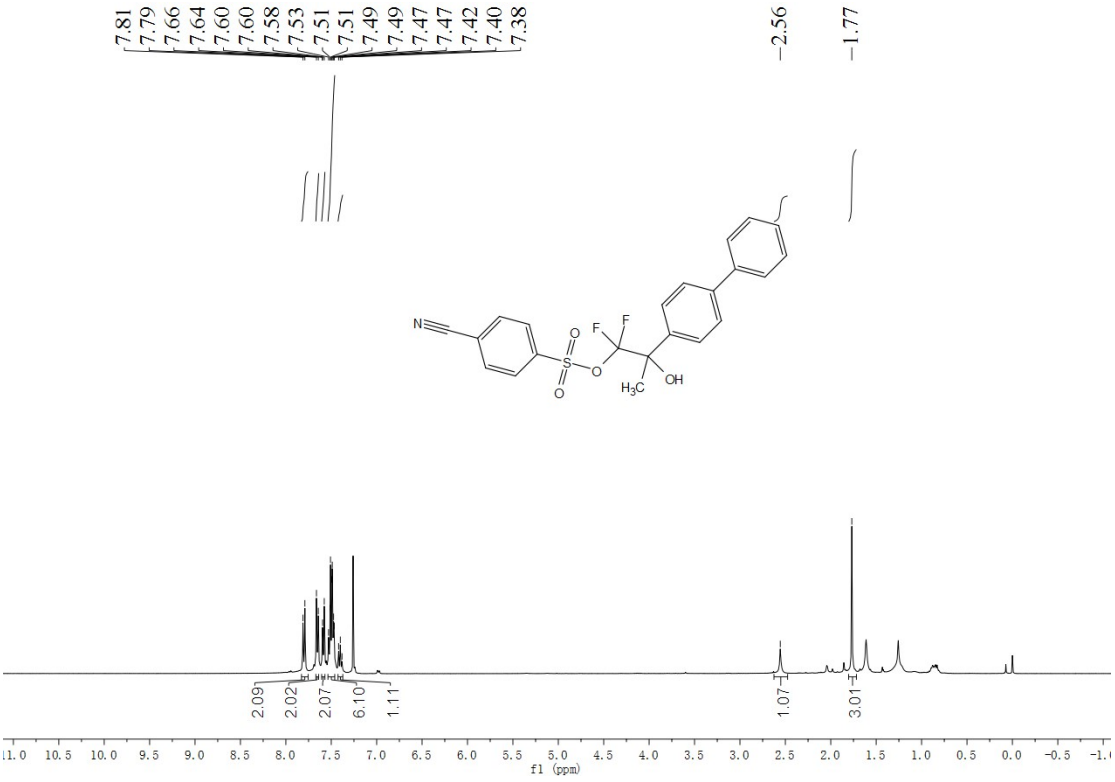


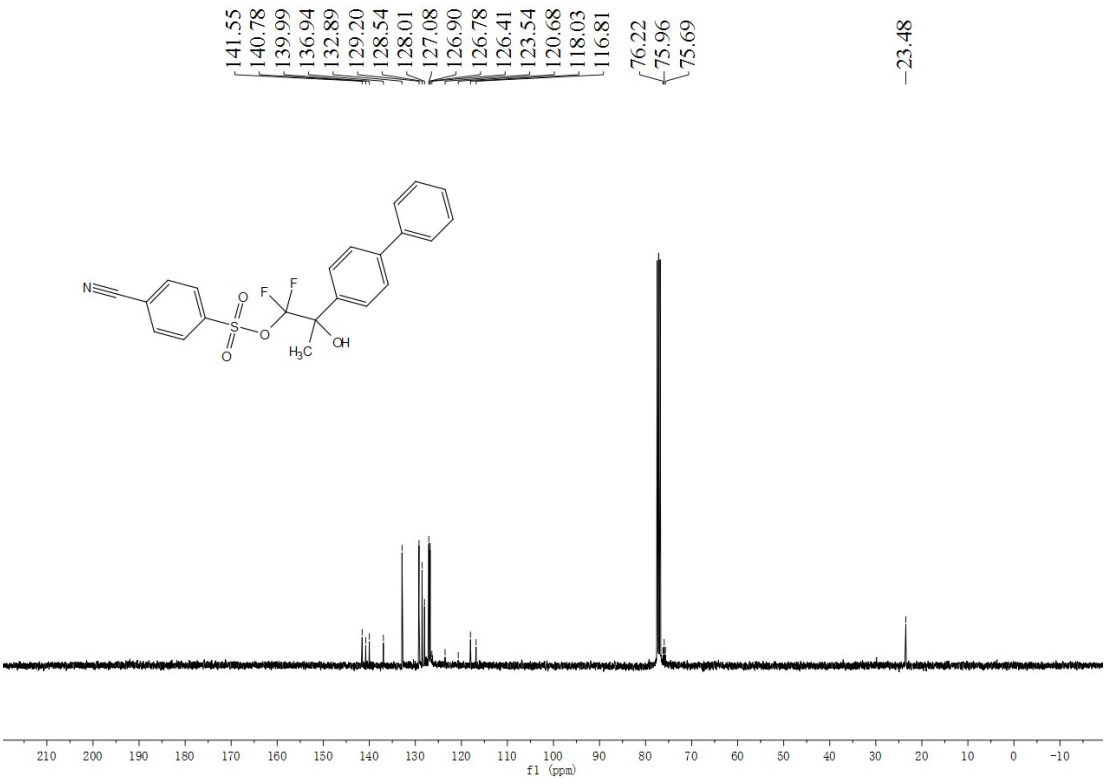
^{1}H NMR and ^{13}C NMR spectrum of compound **3l**



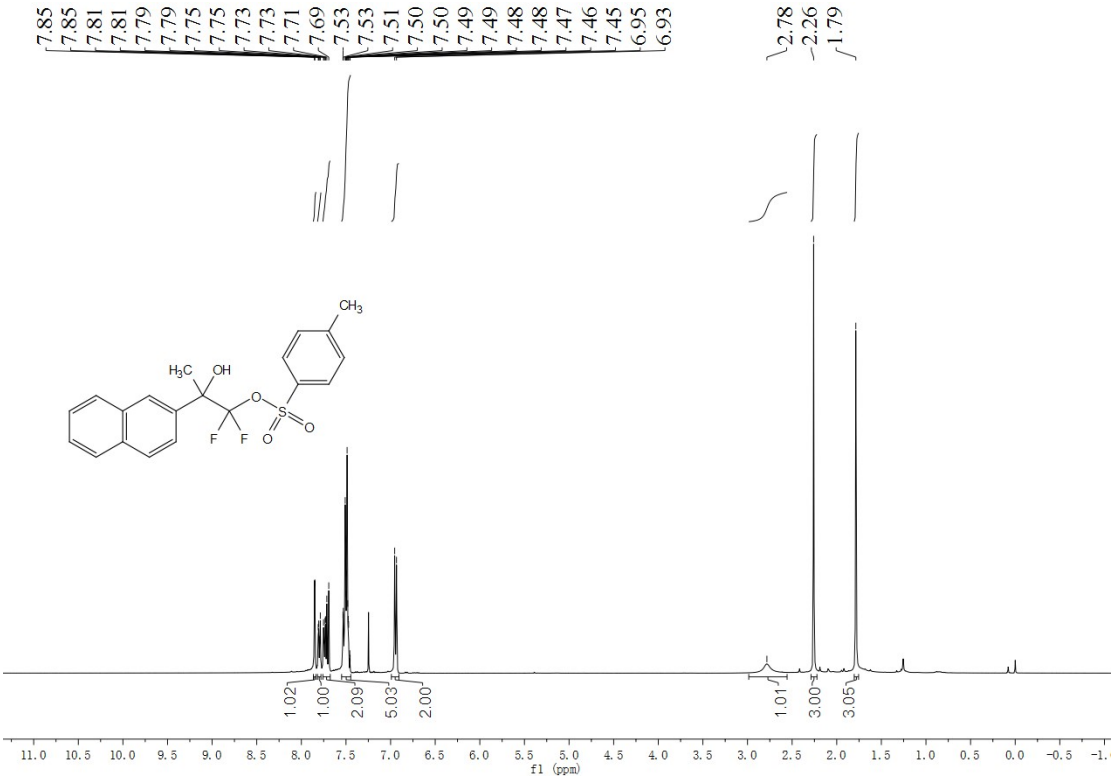


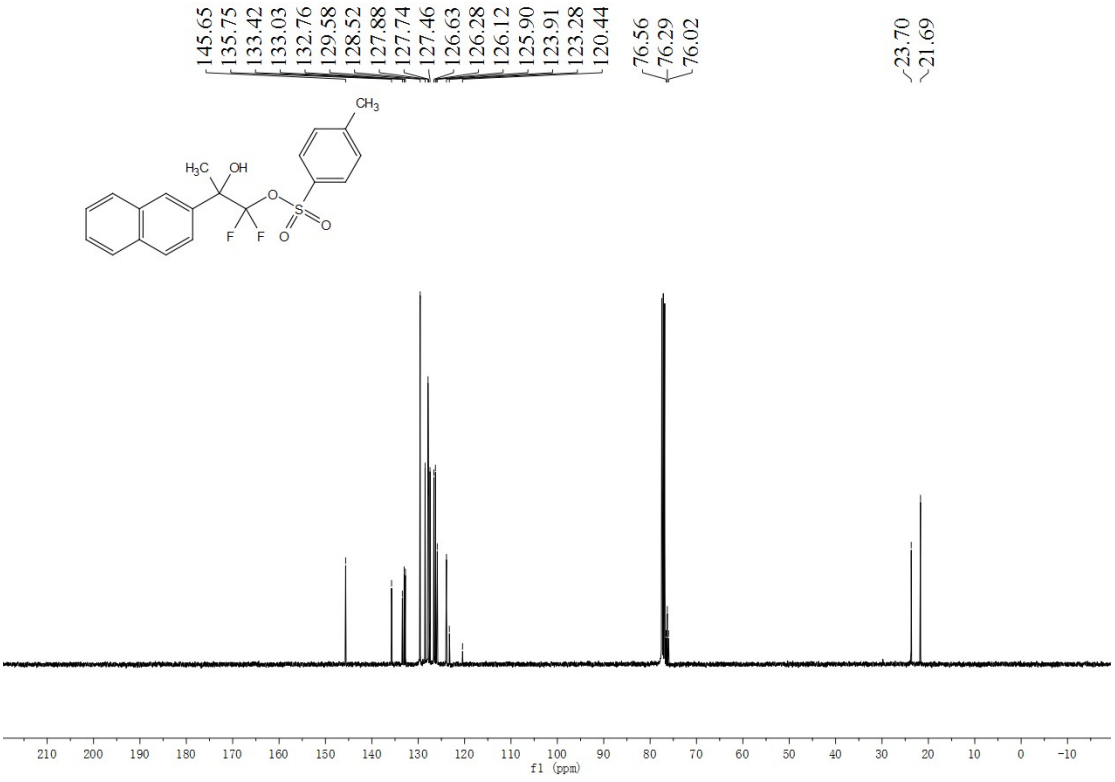
^{1}H NMR and ^{13}C NMR spectrum of compound **3m**



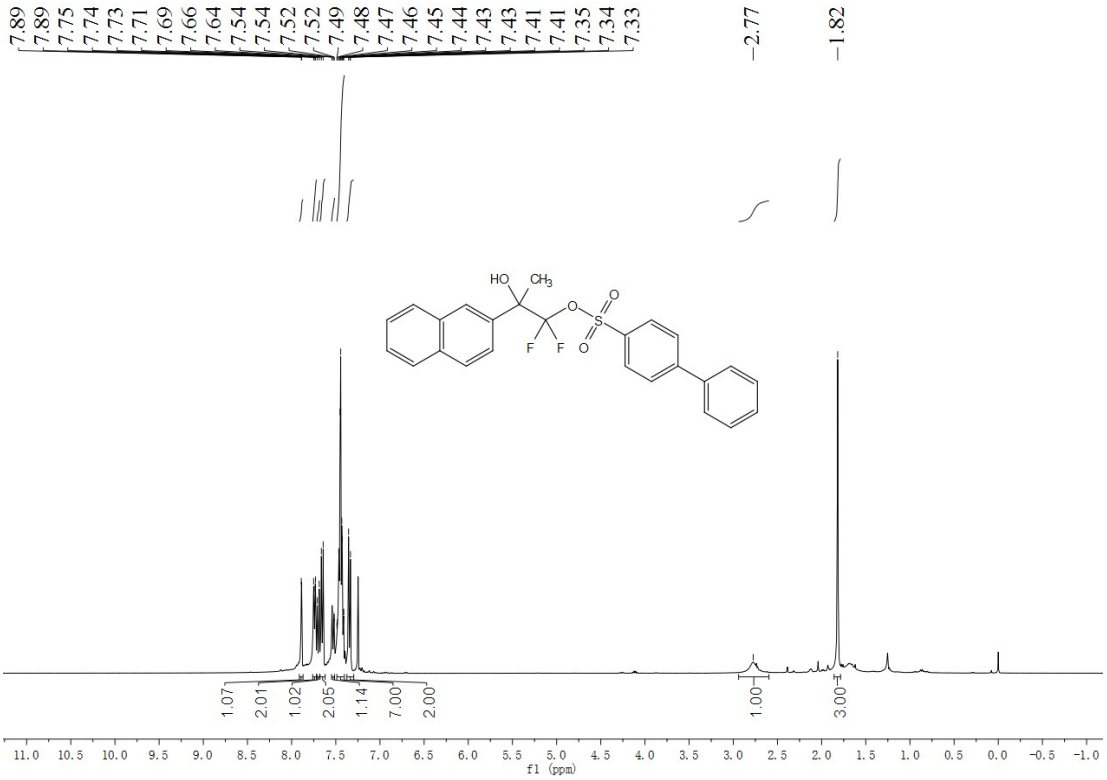


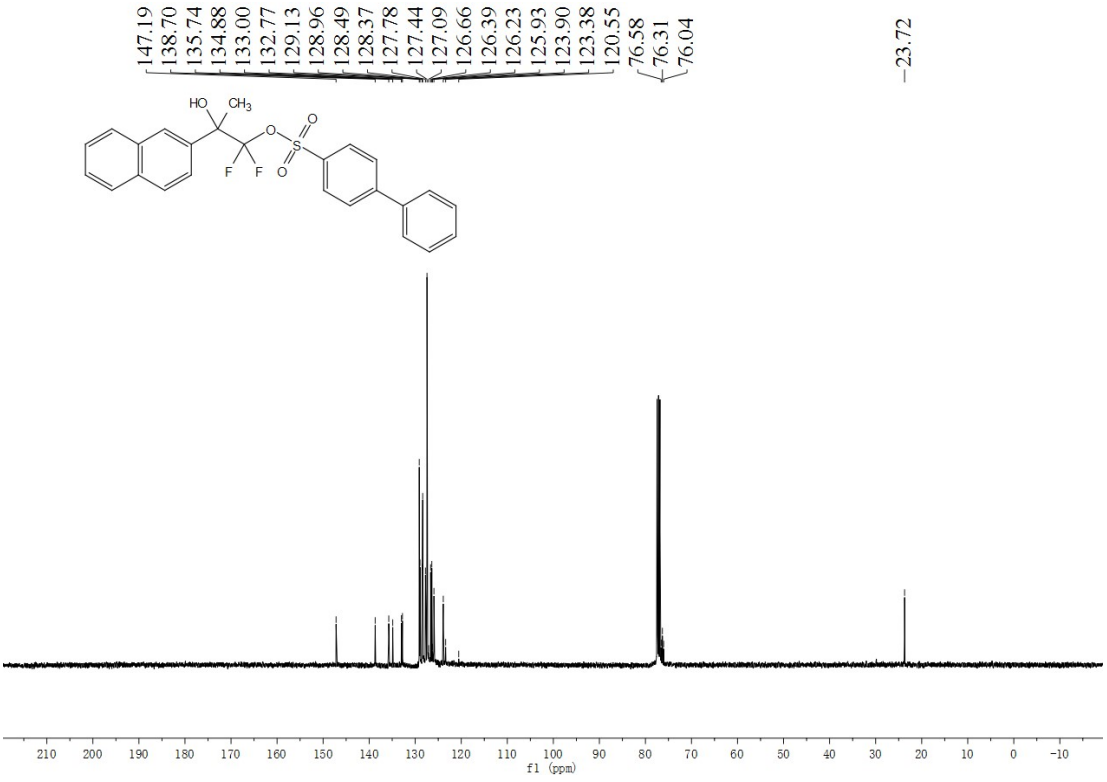
^{1}H NMR and ^{13}C NMR spectrum of compound **3n**



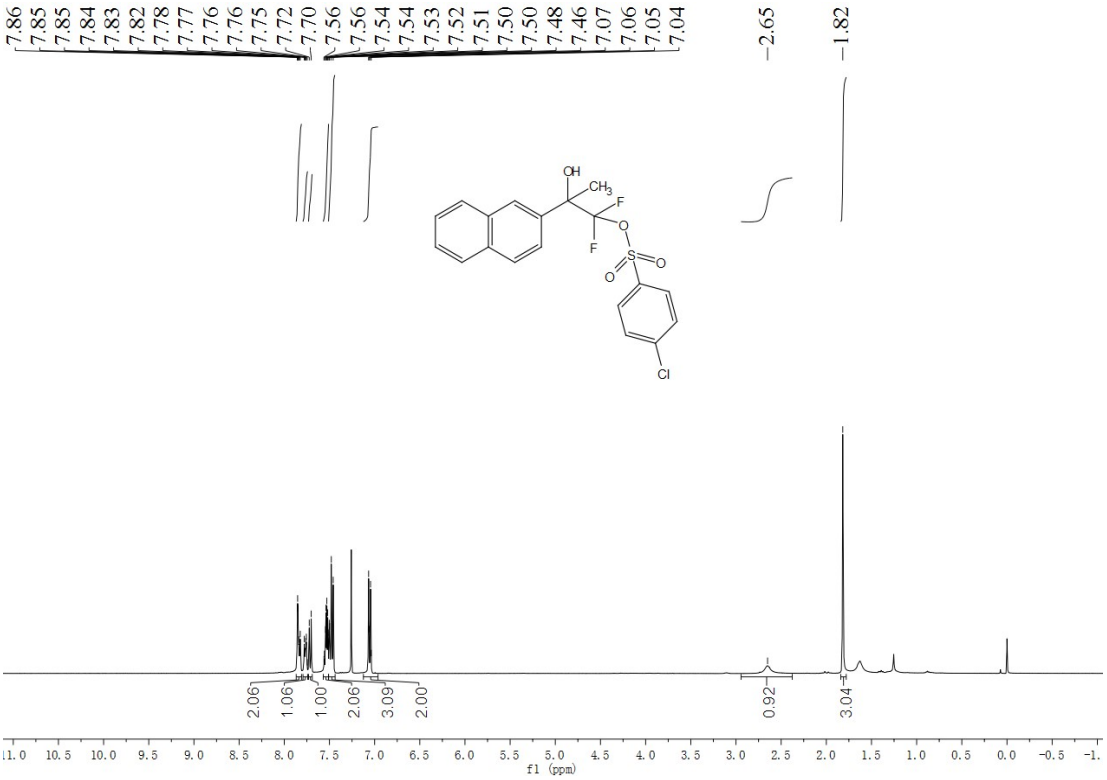


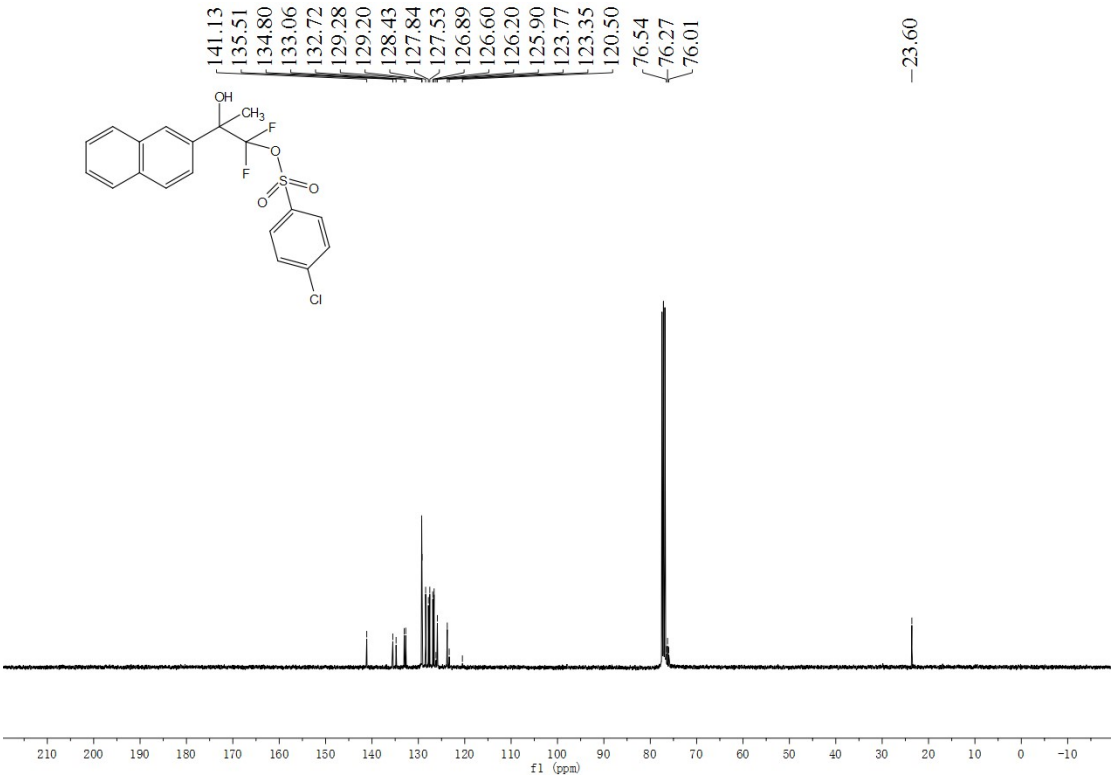
^{1}H NMR and ^{13}C NMR spectrum of compound **3o**



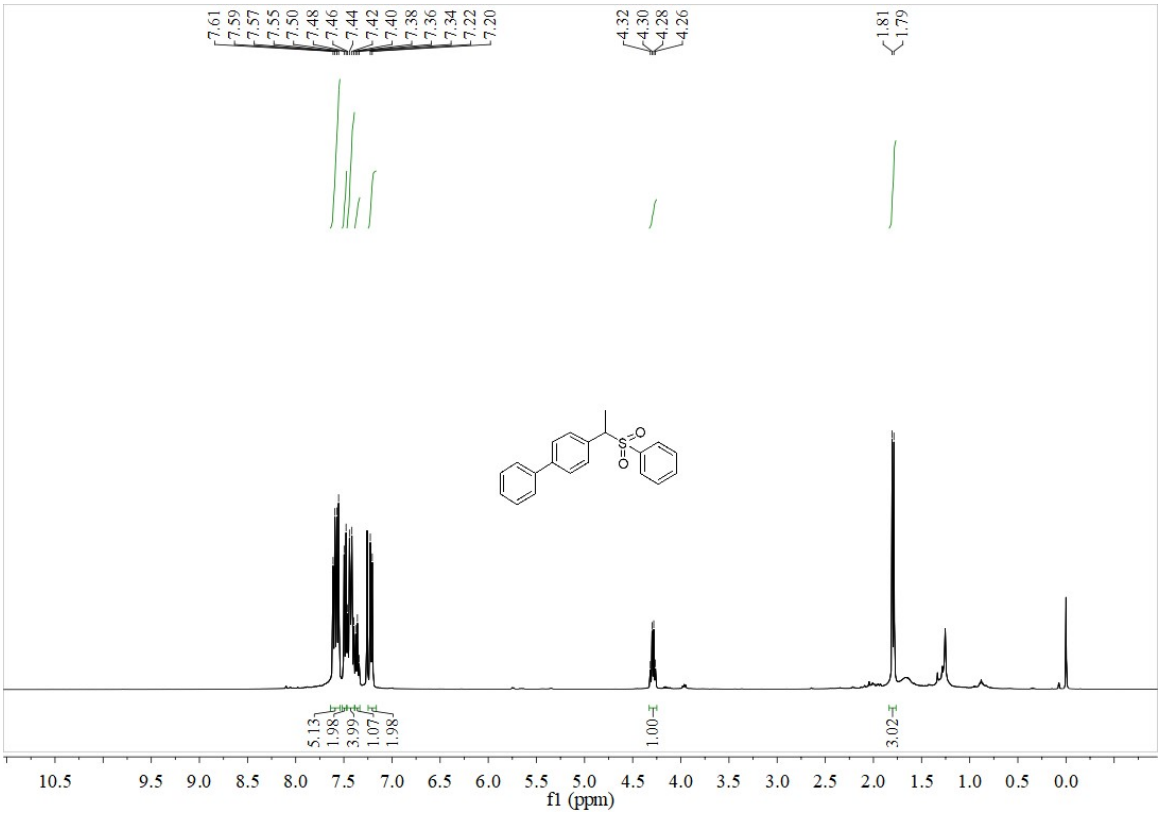


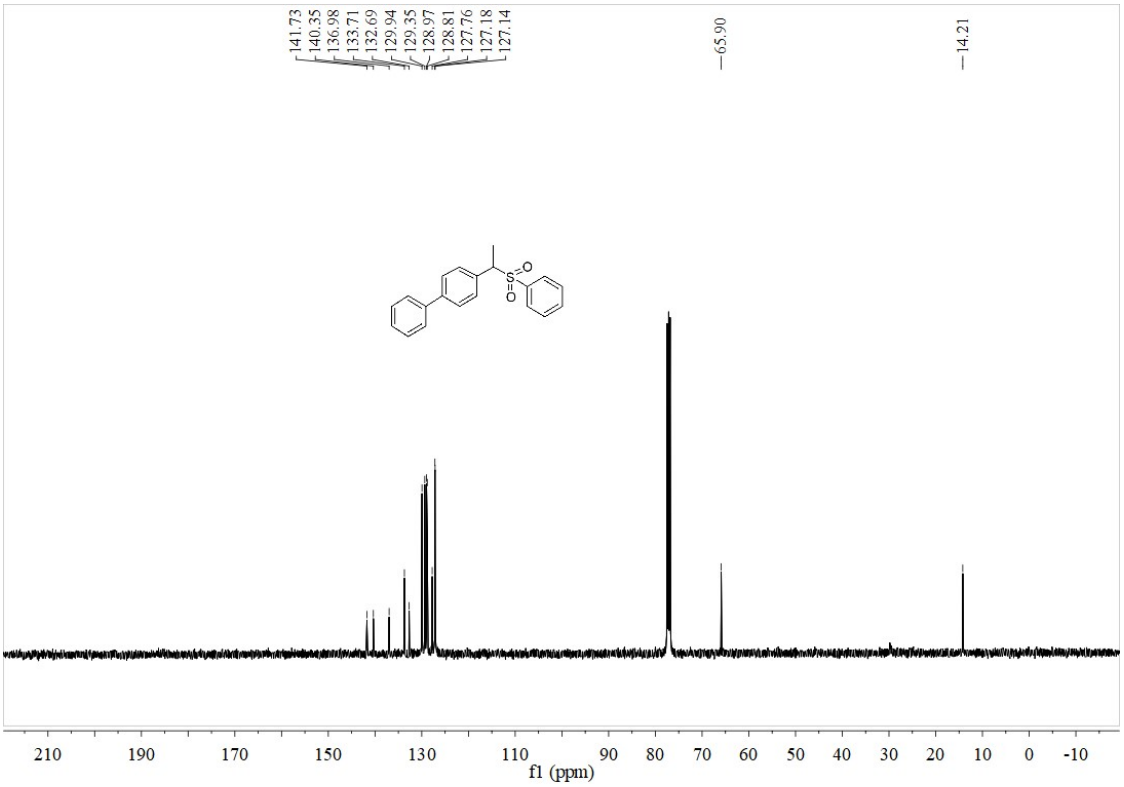
^{1}H NMR and ^{13}C NMR spectrum of compound **3p**



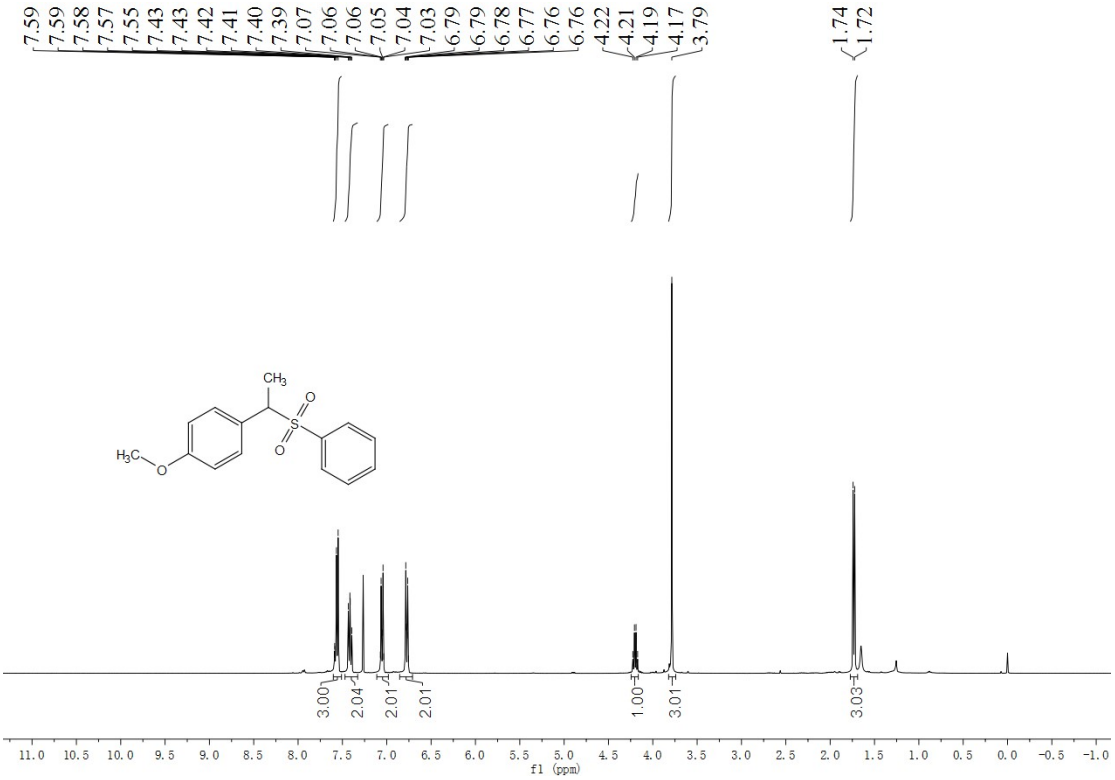


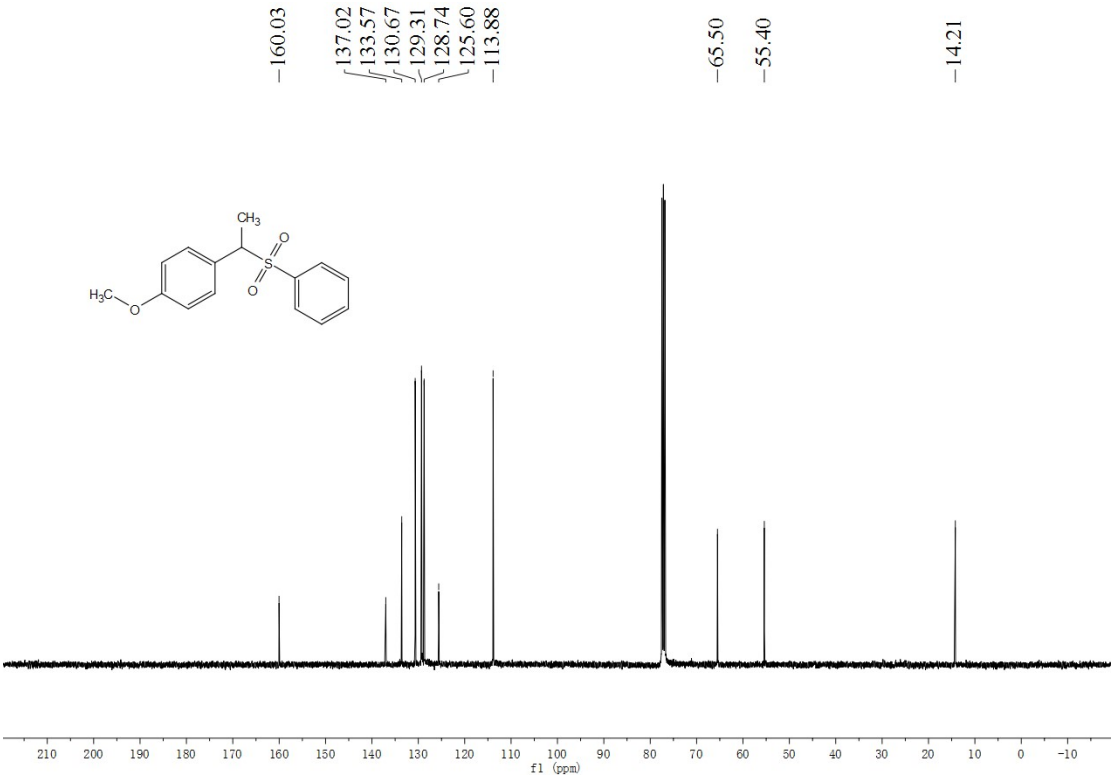
^{1}H NMR and ^{13}C NMR spectrum of compound **5a**



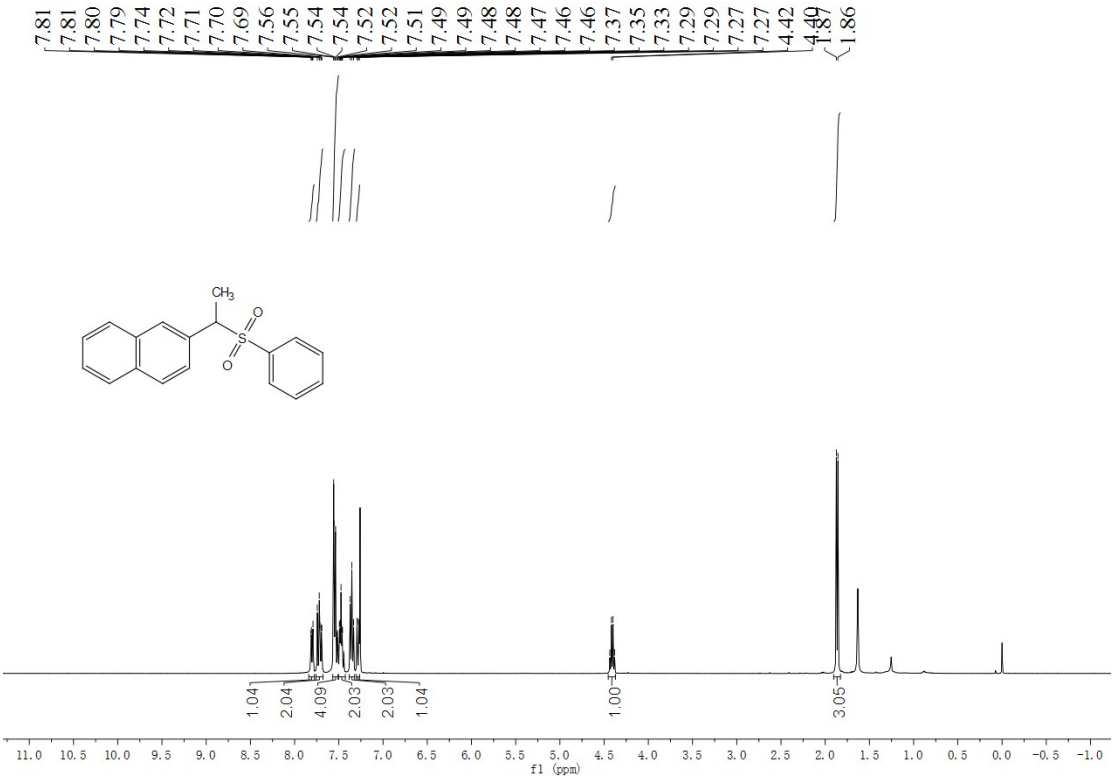


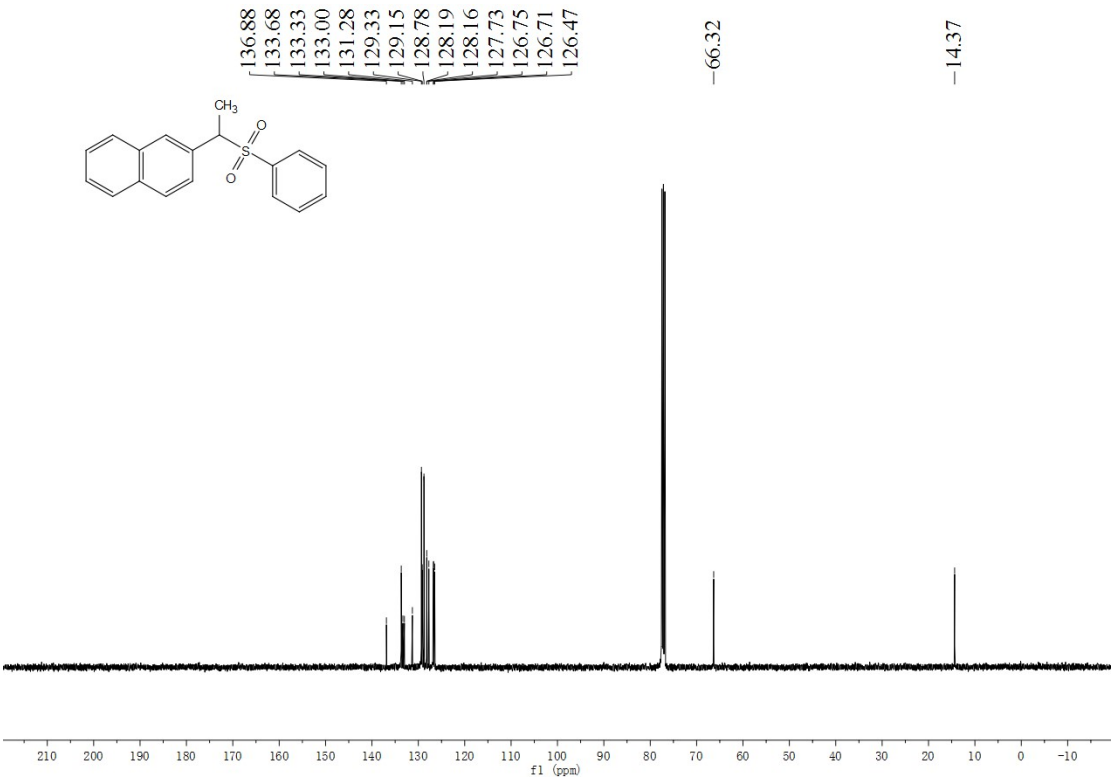
^{1}H NMR and ^{13}C NMR spectrum of compound **5b**



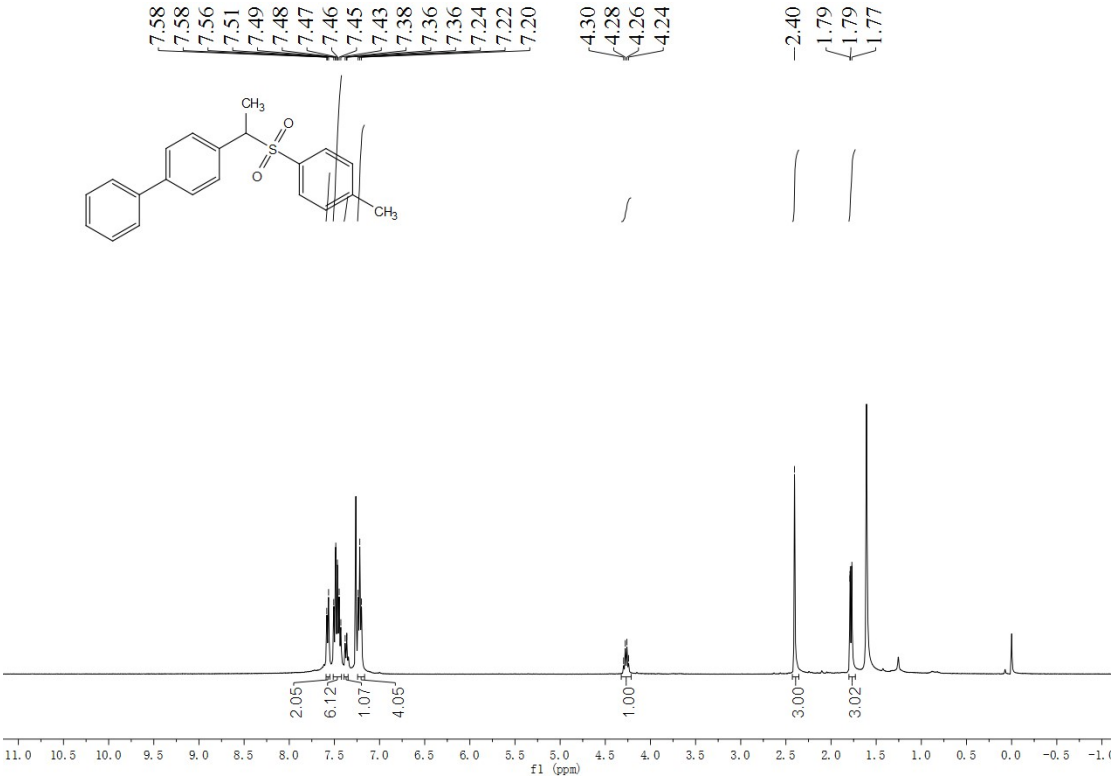


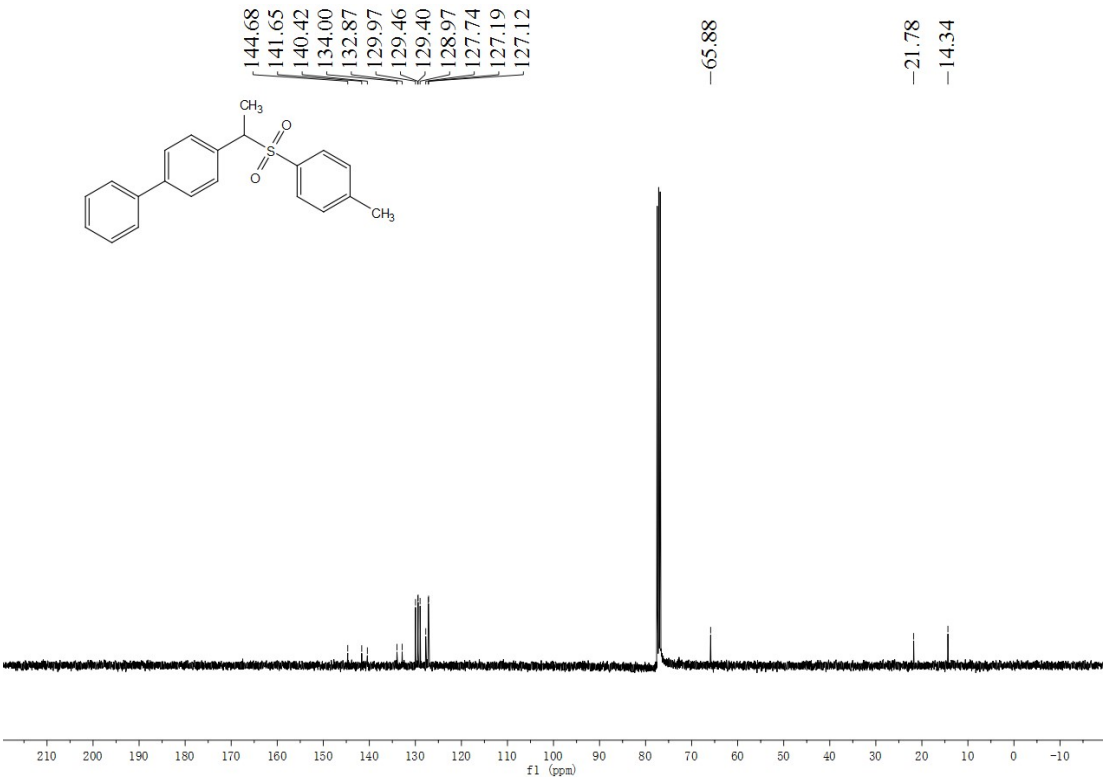
^{1}H NMR and ^{13}C NMR spectrum of compound **5c**



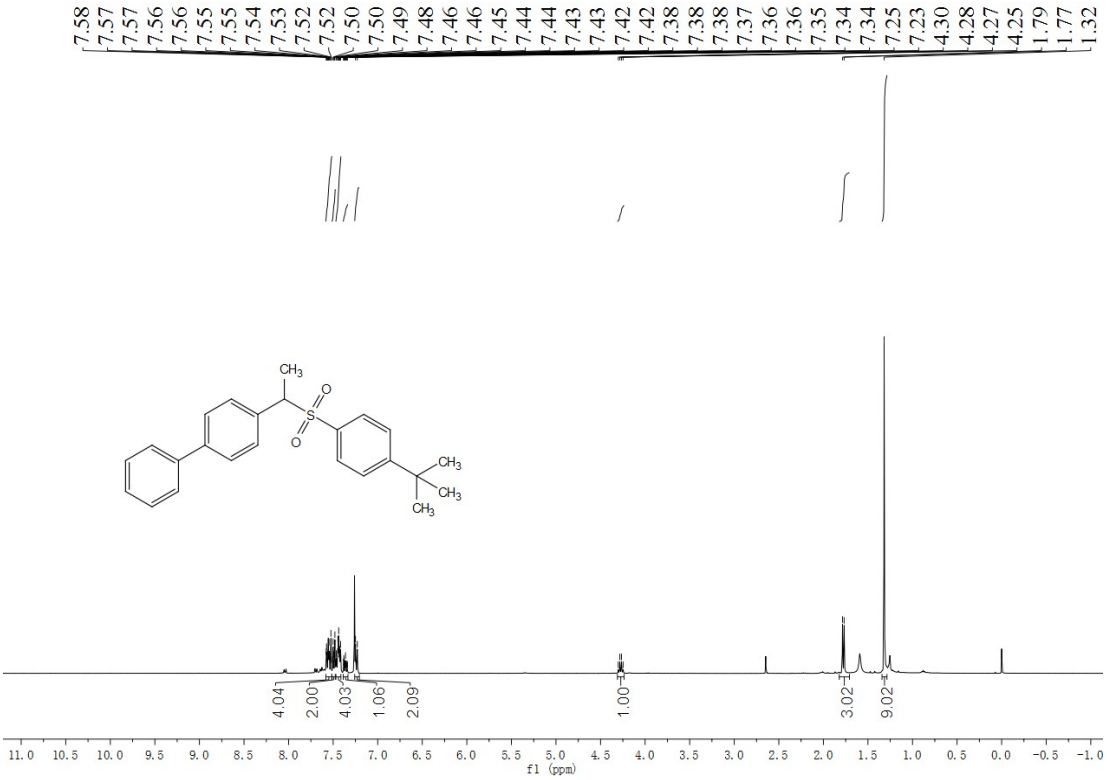


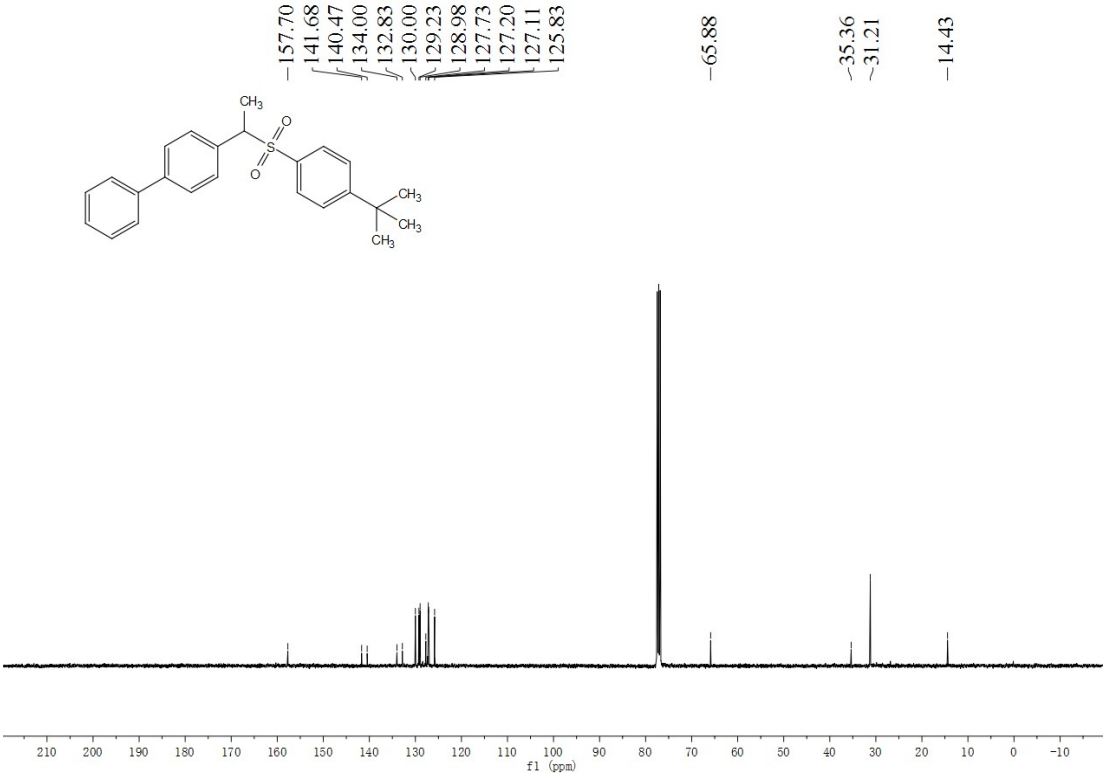
^{1}H NMR and ^{13}C NMR spectrum of compound **5d**



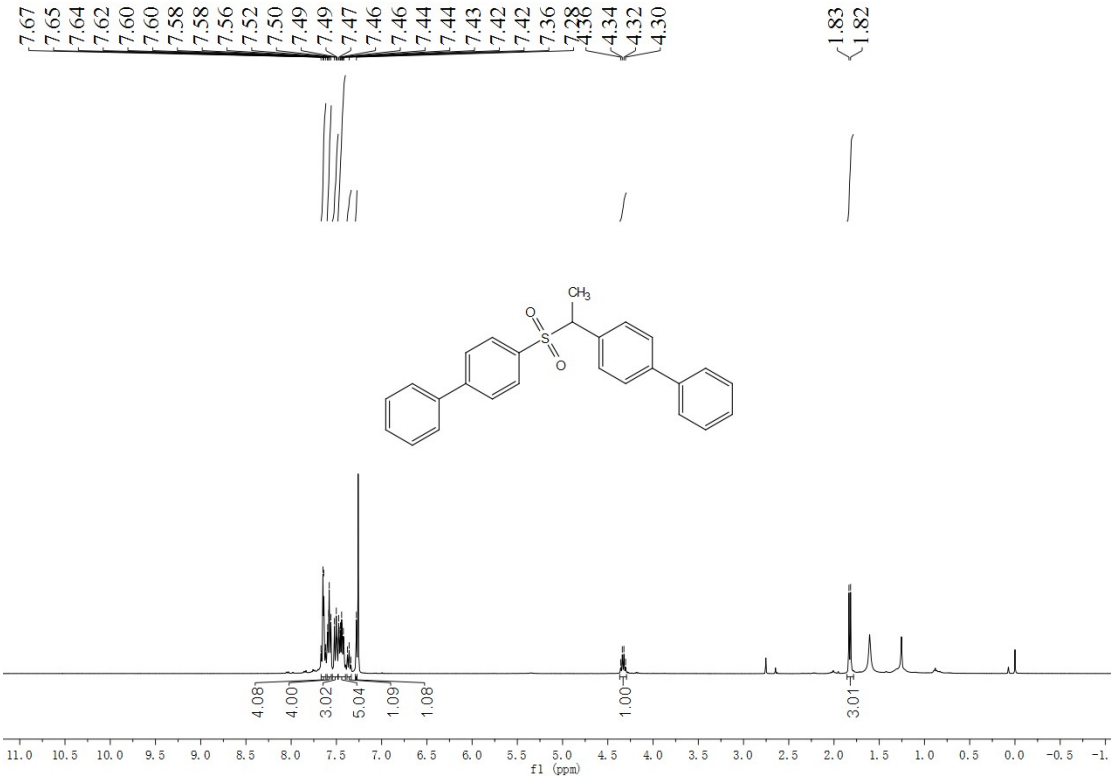


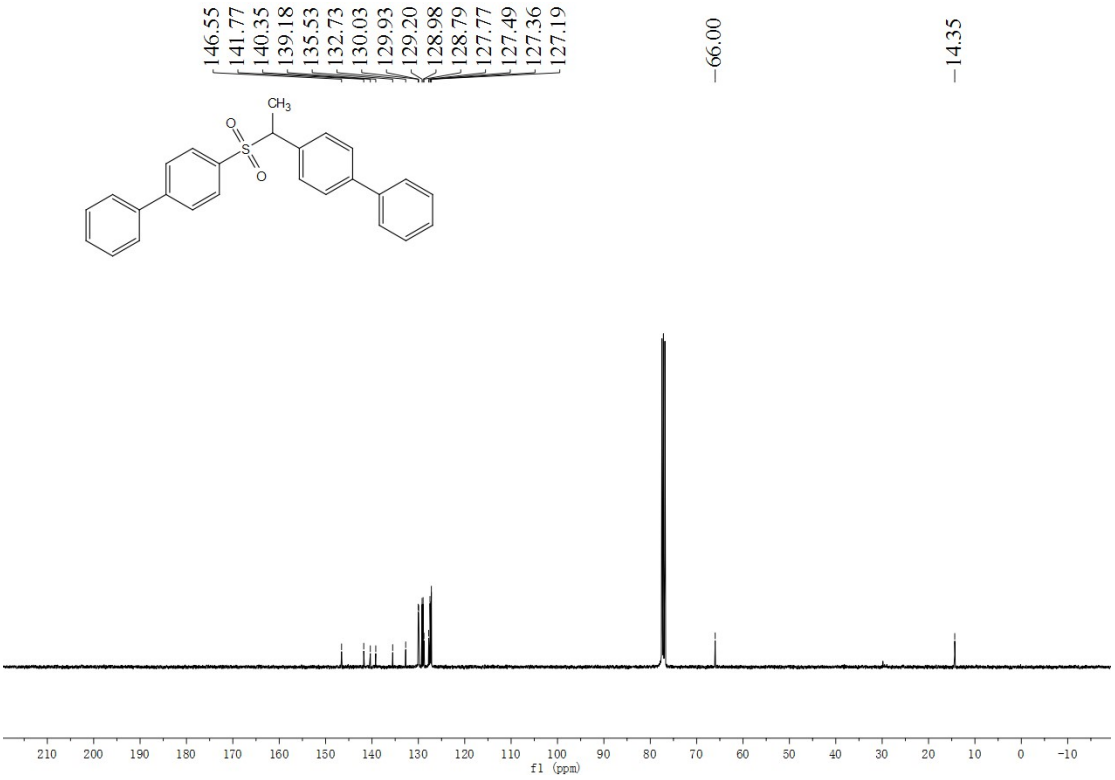
^{1}H NMR and ^{13}C NMR spectrum of compound **5e**



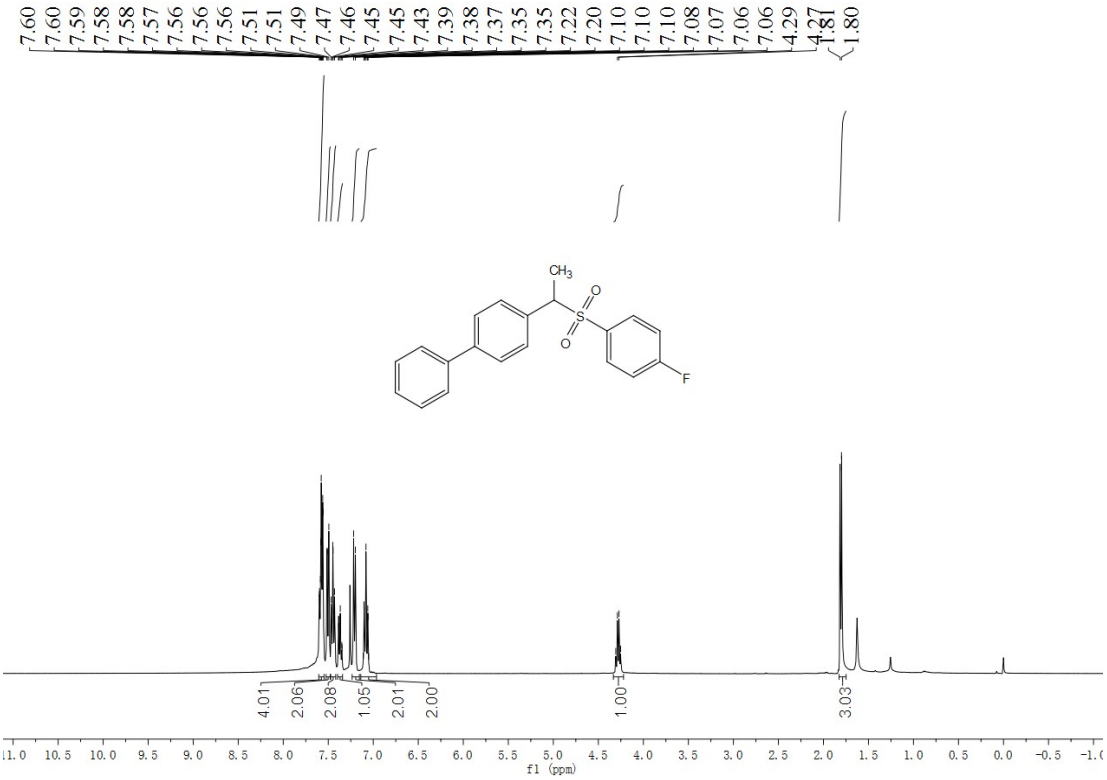


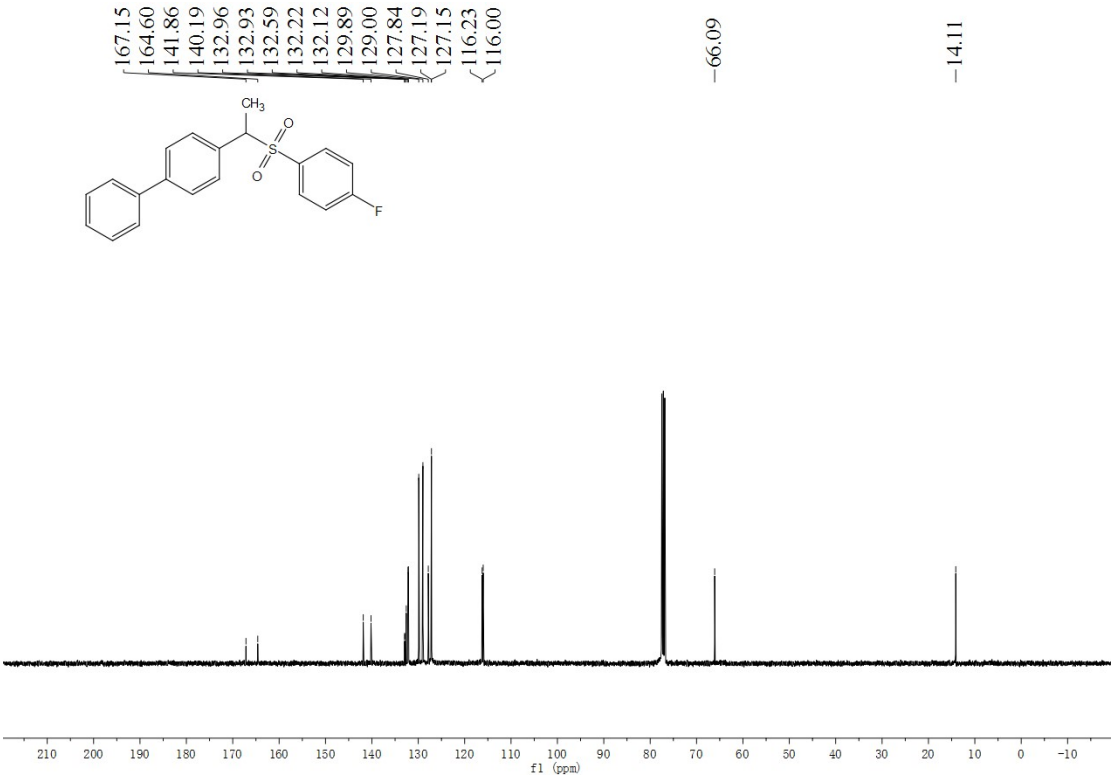
^{1}H NMR and ^{13}C NMR spectrum of compound **5f**



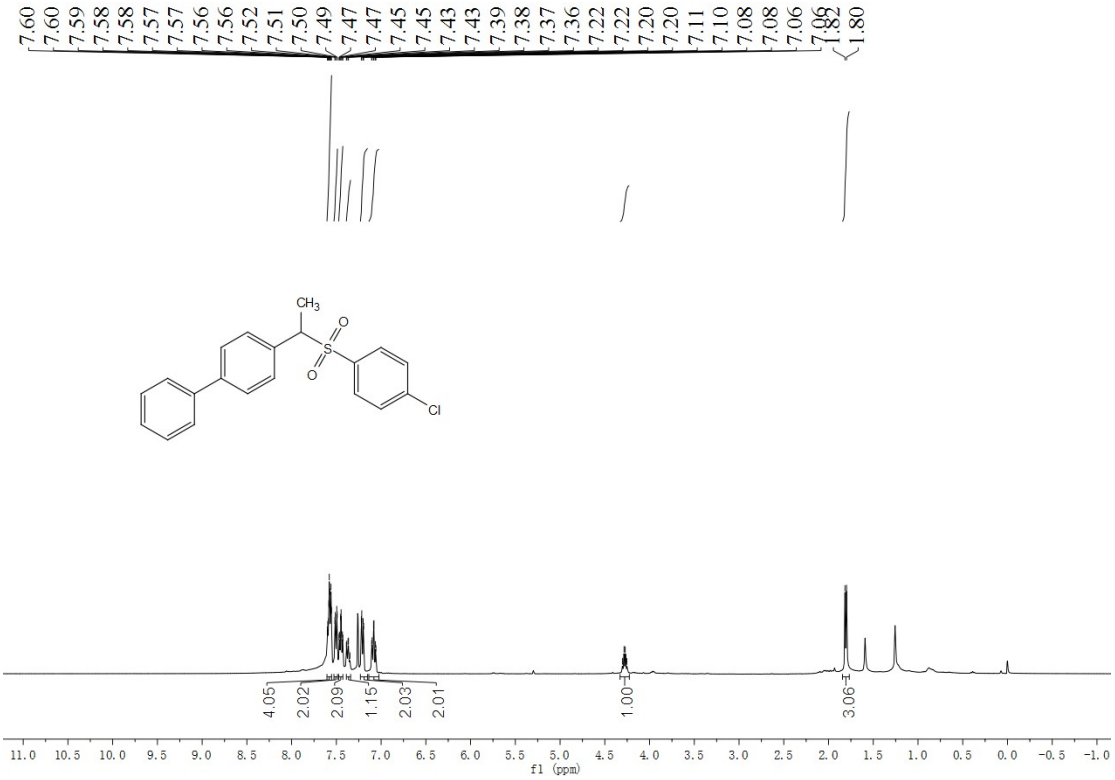


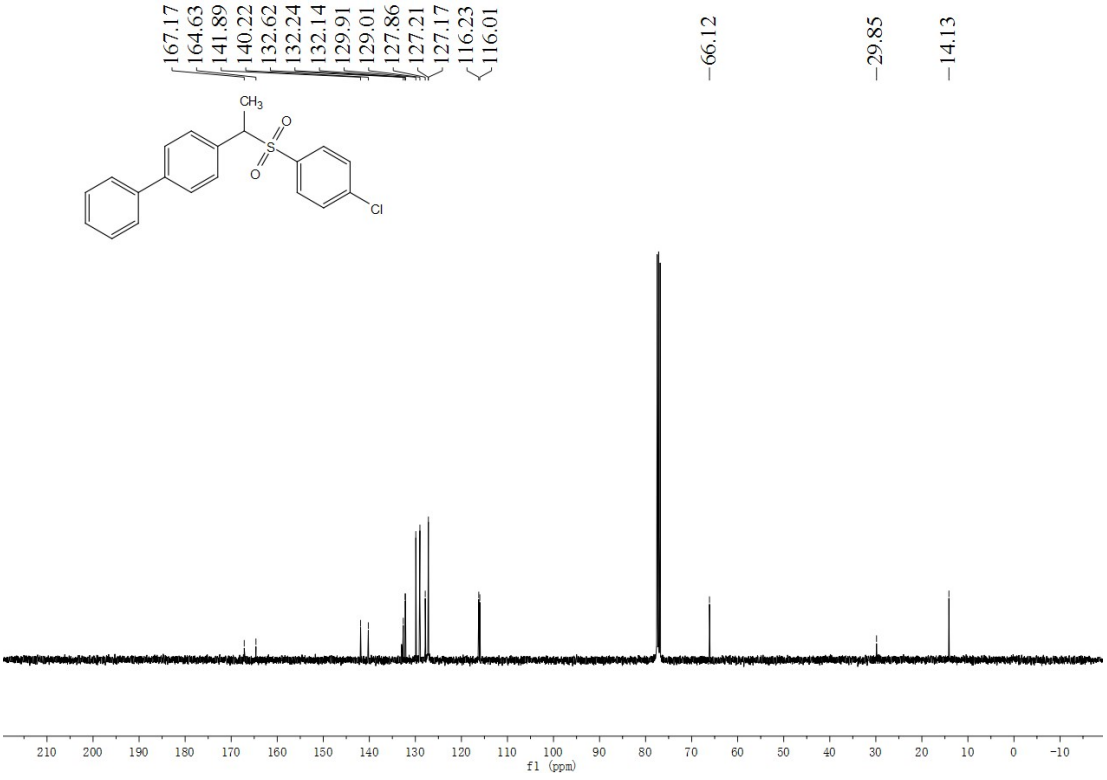
^{1}H NMR and ^{13}C NMR spectrum of compound **5g**



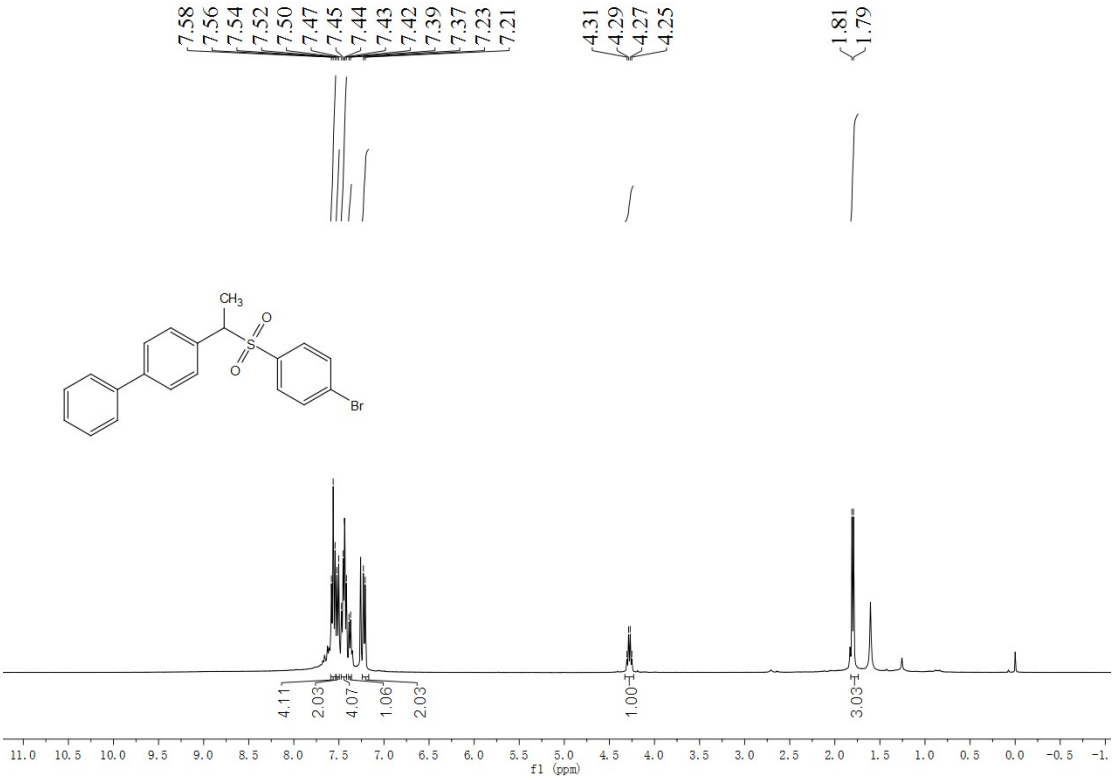


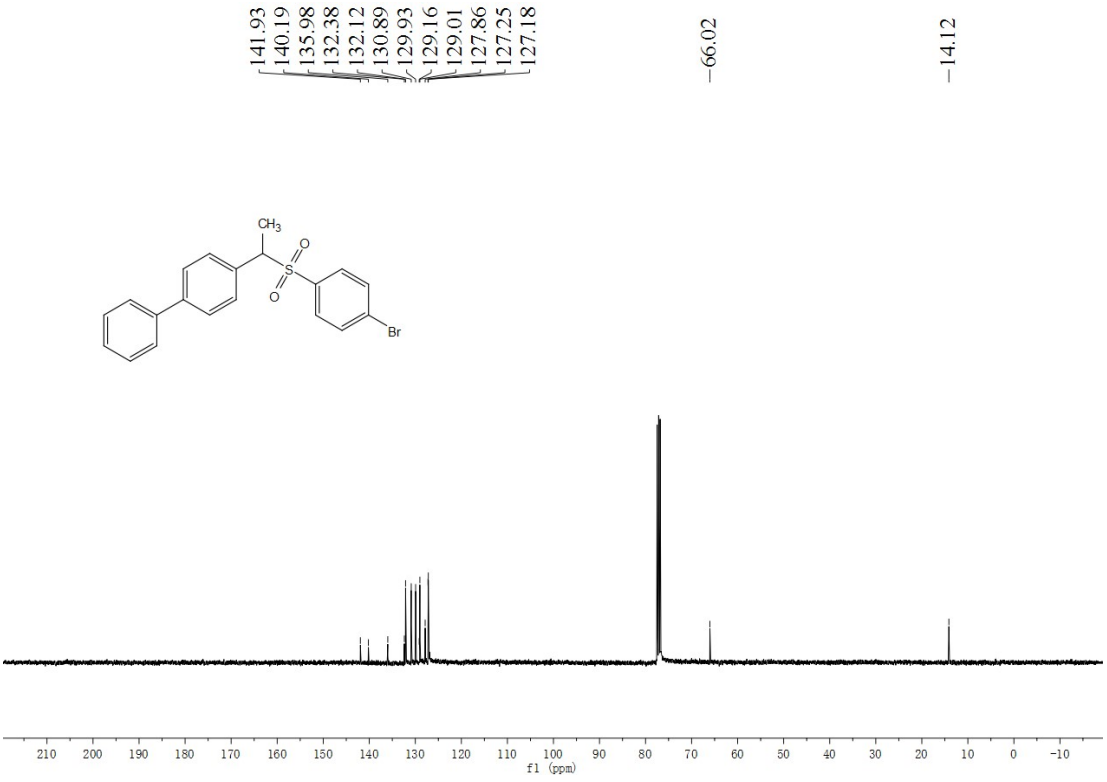
^{1}H NMR and ^{13}C NMR spectrum of compound **5h**



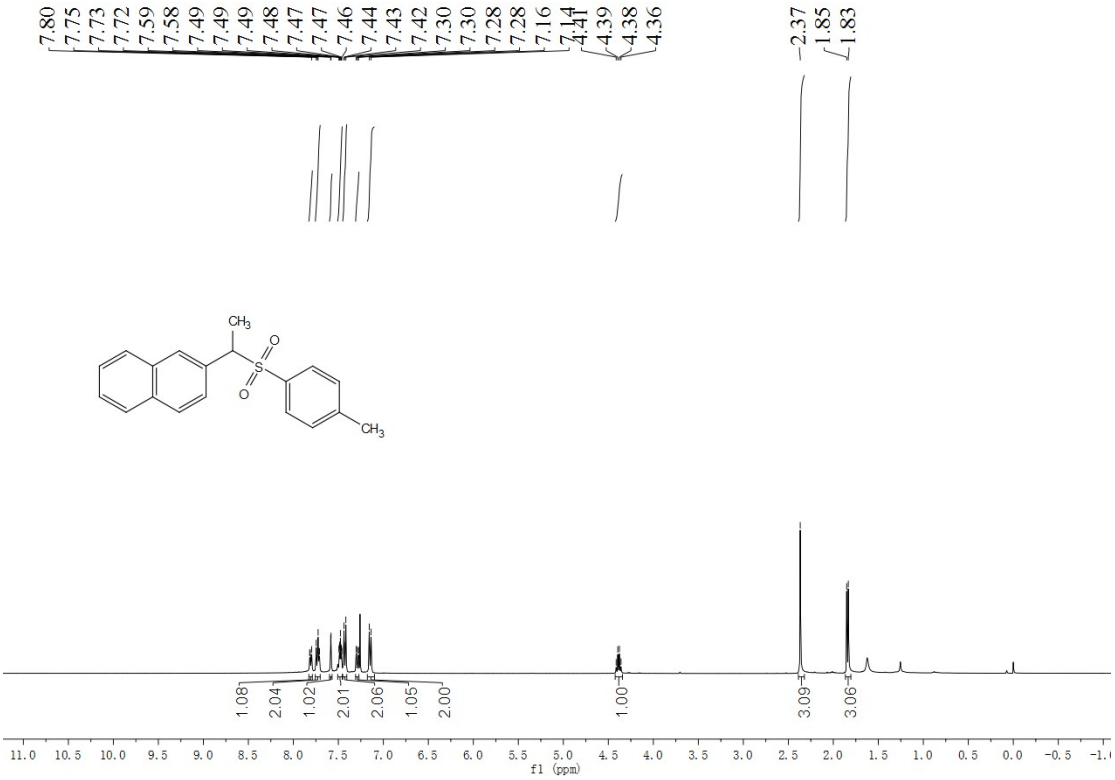


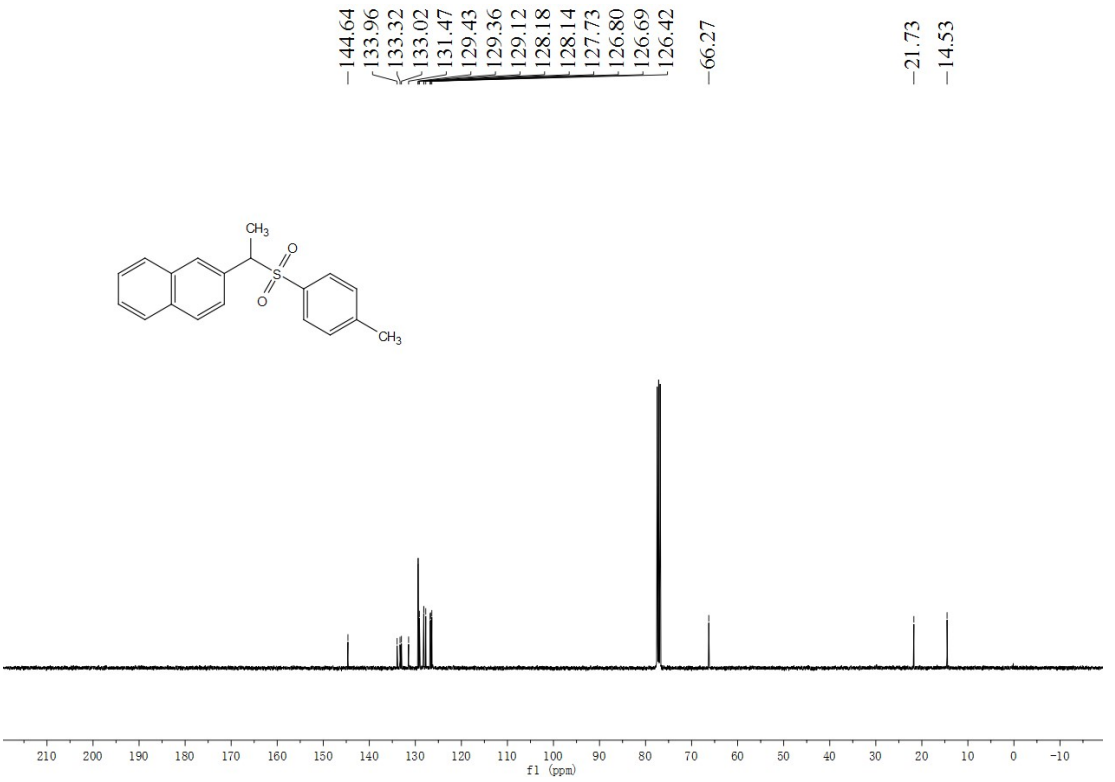
^{1}H NMR and ^{13}C NMR spectrum of compound **5i**



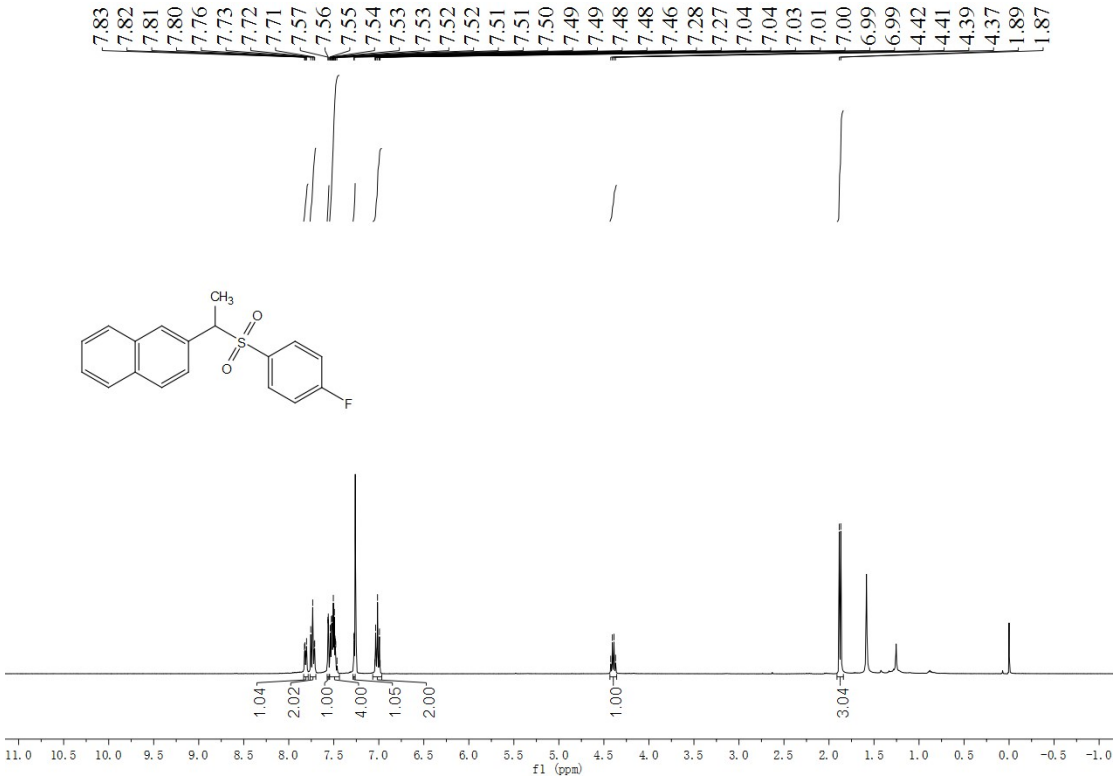


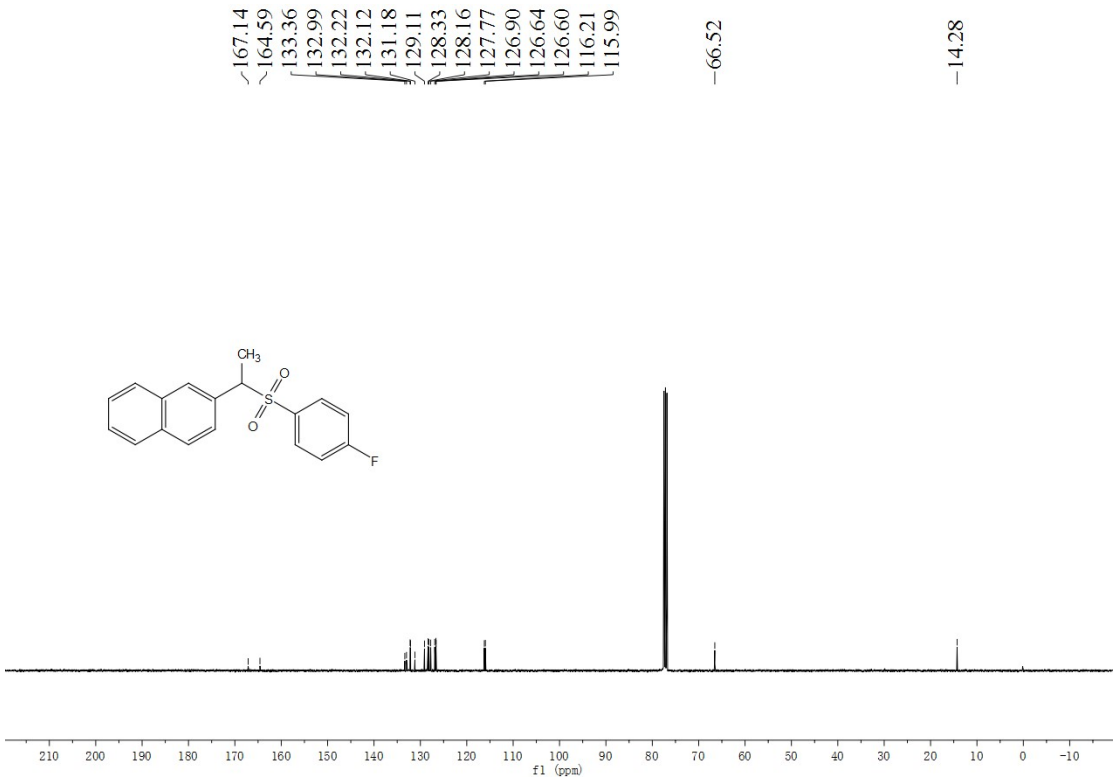
^{1}H NMR and ^{13}C NMR spectrum of compound **5j**



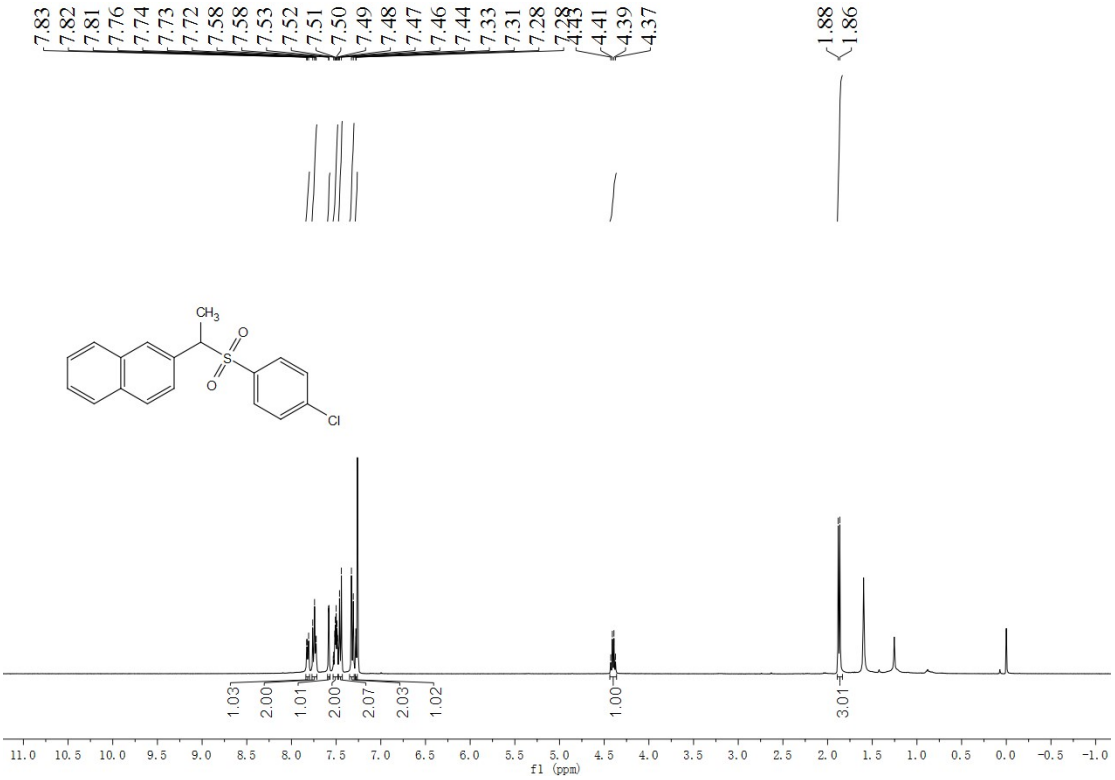


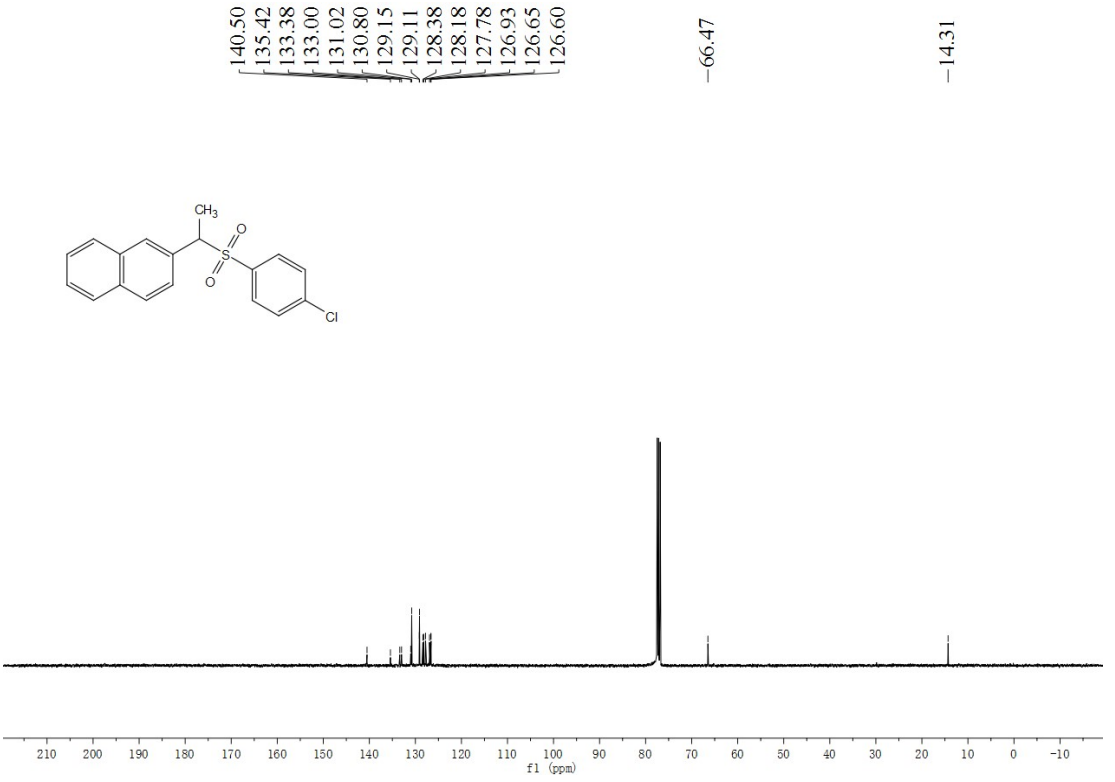
^{1}H NMR and ^{13}C NMR spectrum of compound **5k**



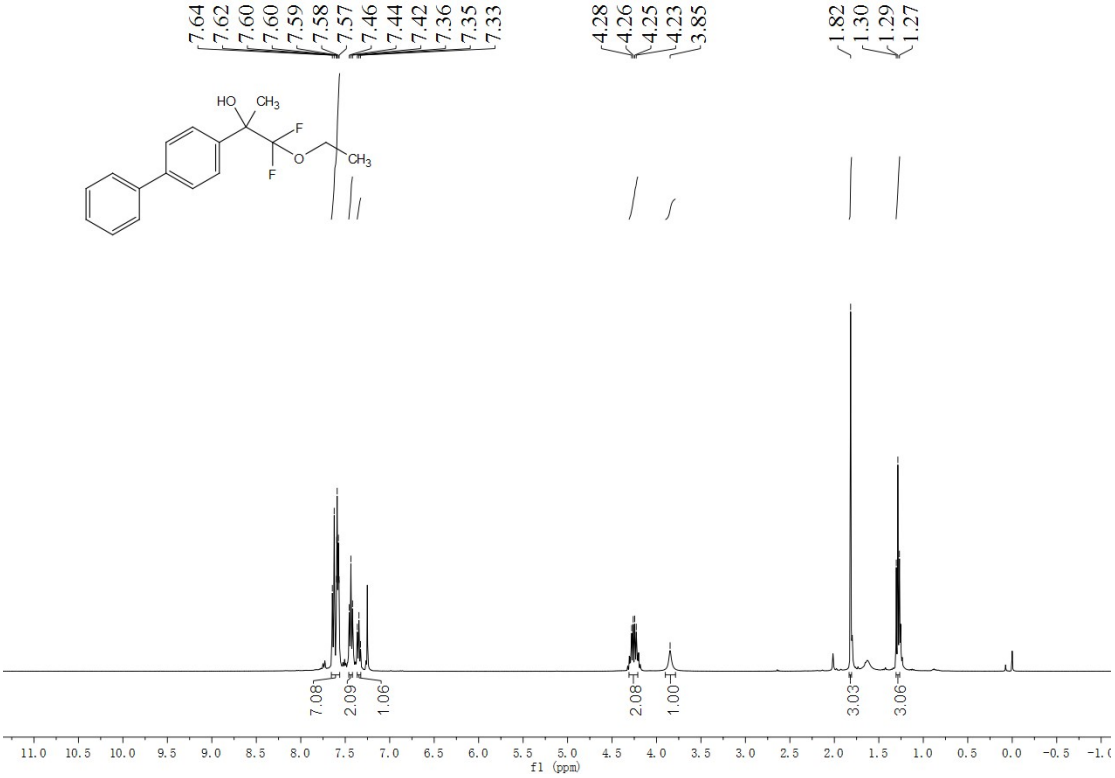


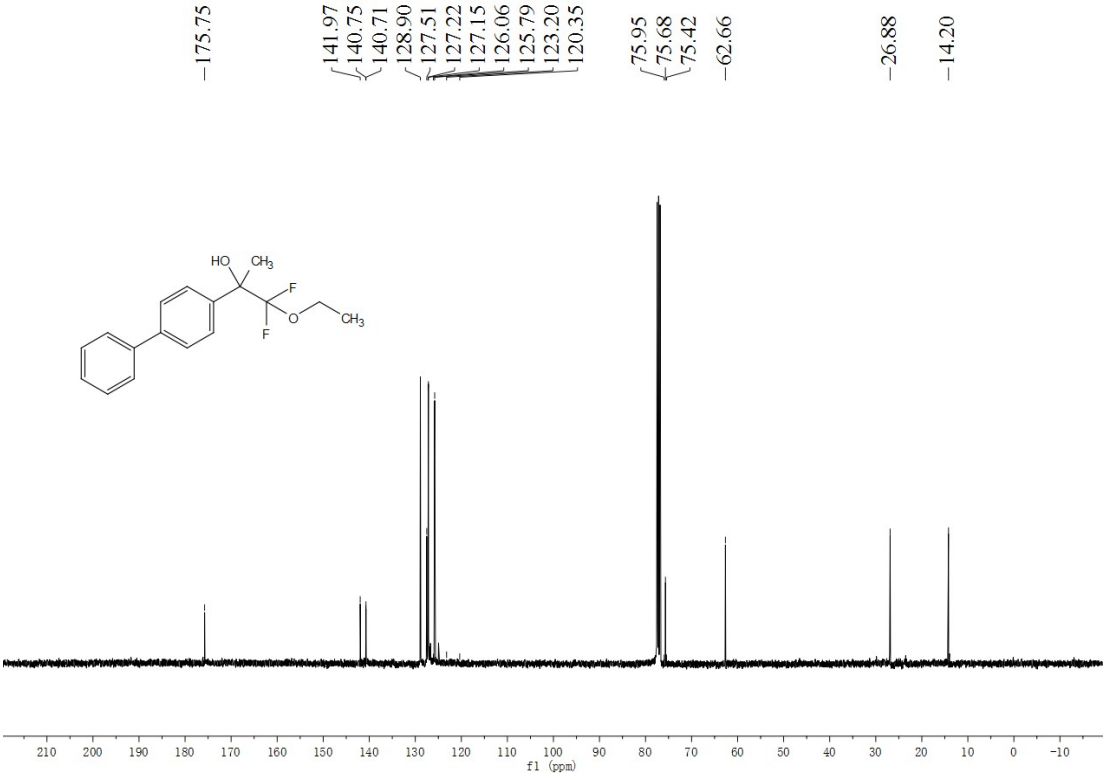
^{1}H NMR and ^{13}C NMR spectrum of compound **5l**





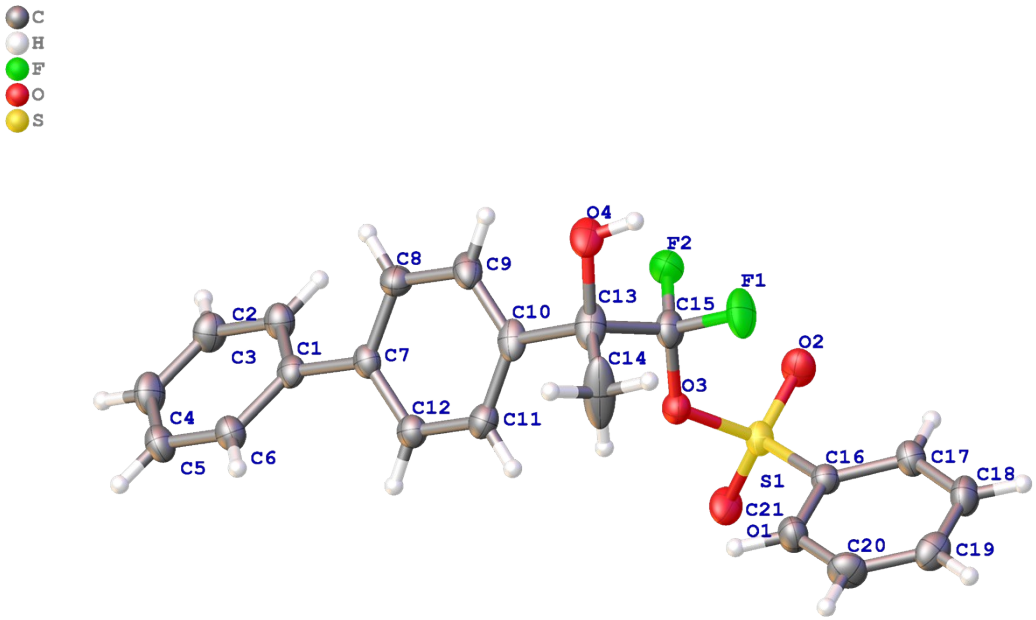
^{1}H NMR and ^{13}C NMR spectrum of compound **6**





5. X-ray crystallographic data

Figure S1 X-ray single crystal structure of **3a**



Single crystals of **3a** were grown by slow evaporation of its DCM/PE solution. Single-crystal X-ray diffraction data were collected with a 'multiwire proportional' diffractometer. The crystal was kept at 100 K during data collection. Using Olex2, the structure was solved with the olex2.solve structure solution program using Charge Flipping and refined with the olex2.refine refinement package using Least Squares minimization. Supplementary crystallographic data have been deposited at the Cambridge Crystallographic Data Center (CCDC 2094381).

Table S2 Crystal data and structure refinement for 3a.

Identification code	3a
Empirical formula	$C_{21}H_{18}F_2O_4S$
Formula weight	404.41
Temperature/K	149.99(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	6.0267(3)
b/Å	18.6496(7)
c/Å	16.3446(7)
α/°	90
β/°	96.788(4)
γ/°	90
Volume/Å^3	1824.18(14)
Z	4
ρ_{calc}g/cm^3	1.473
μ/mm^{-1}	1.991

Table S2 Crystal data and structure refinement for 3a.

F(000)	840.0
Crystal size/mm^3	0.13 × 0.1 × 0.08
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.22 to 133.146
Index ranges	-7 ≤ h ≤ 4, -21 ≤ k ≤ 22, -19 ≤ l ≤ 19
Reflections collected	6693
Independent reflections	3223 [R_{int} = 0.0893, R_{sigma} = 0.0929]
Data/restraints/parameters	3223/0/265
Goodness-of-fit on F^2	1.050
Final R indexes [I>=2σ (I)]	R_1 = 0.0597, wR_2 = 0.1395
Final R indexes [all data]	R_1 = 0.0789, wR_2 = 0.1566

Table S3 Bond Lengths for 3a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	O1	1.424(2)	C7	C8	1.394(4)
S1	O2	1.419(2)	C7	C12	1.392(5)
S1	O3	1.621(2)	C8	C9	1.389(5)
S1	C16	1.750(3)	C9	C10	1.381(5)
F1	C15	1.361(4)	C10	C11	1.397(5)
F2	C15	1.343(4)	C10	C13	1.528(5)
O3	C15	1.395(4)	C11	C12	1.391(5)
O4	C13	1.473(6)	C13	C14	1.505(6)
O5	C13	1.38(2)	C13	C15	1.536(5)
C1	C2	1.390(5)	C16	C17	1.387(4)
C1	C6	1.390(5)	C16	C21	1.380(5)
C1	C7	1.485(4)	C17	C18	1.381(5)
C2	C3	1.391(5)	C18	C19	1.382(5)
C3	C4	1.381(5)	C19	C20	1.384(5)
C4	C5	1.386(5)	C20	C21	1.386(5)
C5	C6	1.389(5)			

Table S4 Bond Angles for 3a.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	S1	O3	101.39(14)	C11	C12	C7	120.8(3)
O1	S1	C16	110.07(16)	O4	C13	C10	106.3(3)
O2	S1	O1	120.57(16)	O4	C13	C14	116.0(5)
O2	S1	O3	109.81(14)	O4	C13	C15	104.2(4)
O2	S1	C16	110.18(15)	O5	C13	C10	120.1(12)

Table S4 Bond Angles for 3a.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O3	S1	C16	103.10(14)	O5	C13	C14	81(2)
C15	O3	S1	123.4(2)	O5	C13	C15	121.5(12)
C2	C1	C6	118.2(3)	C10	C13	C15	109.1(3)
C2	C1	C7	120.8(3)	C14	C13	C10	112.2(4)
C6	C1	C7	120.9(3)	C14	C13	C15	108.6(3)
C1	C2	C3	120.9(3)	F1	C15	O3	109.7(3)
C4	C3	C2	120.4(3)	F1	C15	C13	111.0(3)
C3	C4	C5	119.1(3)	F2	C15	F1	105.4(3)
C4	C5	C6	120.5(3)	F2	C15	O3	110.1(3)
C5	C6	C1	120.8(3)	F2	C15	C13	110.3(3)
C8	C7	C1	120.4(3)	O3	C15	C13	110.3(3)
C12	C7	C1	121.4(3)	C17	C16	S1	118.7(3)
C12	C7	C8	118.2(3)	C21	C16	S1	119.8(3)
C9	C8	C7	120.9(3)	C21	C16	C17	121.4(3)
C10	C9	C8	121.0(3)	C18	C17	C16	119.2(3)
C9	C10	C11	118.5(3)	C17	C18	C19	119.8(3)
C9	C10	C13	119.4(3)	C18	C19	C20	120.7(3)
C11	C10	C13	122.1(3)	C19	C20	C21	119.9(3)
C12	C11	C10	120.6(3)	C16	C21	C20	118.9(3)

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