Supporting Information for

Copper(II)-Catalyzed Direct Sulfonylation of C(sp^2)–H bonds with Sodium Sulfinates

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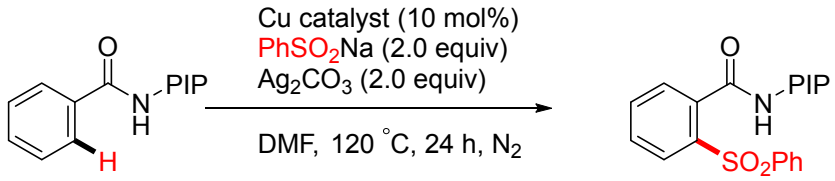
General information: NMR spectra were recorded on Bruker Avanced 400 MHz (for ^{1}H NMR) and 100 MHz (for ^{13}C NMR) using TMS as internal standard. Chemical shifts are given relative to the residual solvents of $CDCl_3$ (7.26 ppm for ^{1}H NMR, 77.0 ppm for ^{13}C NMR). HRMS for new compounds were recorded on Mass Spectrometry Facilities, Zhejiang University. Solvents were used after purification directed by *Purification of Laboratory Chemicals, 6th Ed*. $Cu(OAc)_2$ (Adamas) was purchased and used without any further purification. Ag_2CO_3 (Adamas) and $PhSO_2Na$ (Annaiji) were purchased and used after removing the residual water in vacuum. (*p*-Me)$PhSO_2Na$ (Alfa Aesar), (*p*-Cl)$PhSO_2Na$ (Alfa Aesar) and (*p*-Br)$PhSO_2Na$ (Alfa Aesar) were purchased from the above mentioned company and used without any further purification. Other sodium sulfinates involved were prepared according to the literature.[1] Other chemical reagents were commercially available and directly used without any further purification. The substrates benzamides were synthesized from the corresponding carboxylic acids and PIP–NH_2 (2-pyridinyl isopropyl amine) according to the literature.[2]

Optimization of reaction conditions

Table S1. Optimization of Cu catalyst[a]



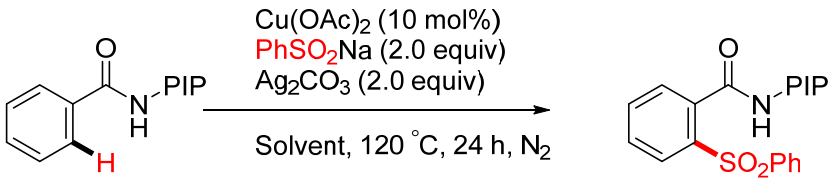
1 **1a**

entry	Cu catalyst (10 mol%)	yield[b]
1	CuI	/
2	CuBr	trace
3	CuTc	trace
4	$Cu_2(OH)_2CO_3$	/
5	CuOAc	trace
6	**$Cu(OAc)_2$**	**15%**
7	$CuBr_2$	/
8	CuCl	/
9	CuCN	/
10	$CuBr{\cdot}Me_2S$	trace

[a]Reaction conditions: **1** (0.1 mmol), $PhSO_2Na$ (0.2 mmol), Cu catalyst (10 mol%), Ag_2CO_3 (0.2 mmol) in DMF (1.0 mL) as the solvent at 120 °C for 24 hours under N_2.

[b]Yields determined by ^1H NMR using CH_2Br_2 as the internal standard.

Table S2. Optimization of solvent[a]

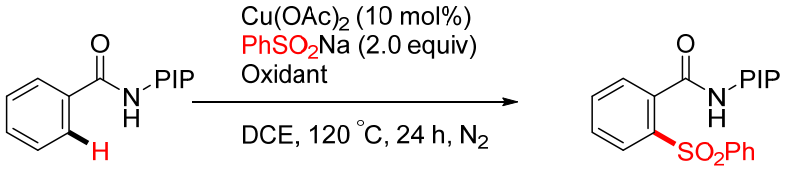


1 **1a**

entry	solvent	yield[b]
1	DMF	15%
2	NMP	trace
3	DMSO	trace
4	Toluene	12%
5	**DCE**	**73%(72%)[c]**
6	Dioxane	15%
7	t-AmyOH	/
8	t-BuOH	/
9	DMAc	/
10	DME	/

[a]Reaction conditions: **1** (0.1 mmol), $PhSO_2Na$ (0.2 mmol), $Cu(OAc)_2$ (10 mol%), Ag_2CO_3 (0.2 mmol) in the solvent (1.0 mL) at 120 ℃ for 24 hours under N_2. [b]Yields determined by ^1H NMR using CH_2Br_2 as the internal standard. [c]Isolated yield in the parentheses.

Table S3. Optimization of oxidant[a]

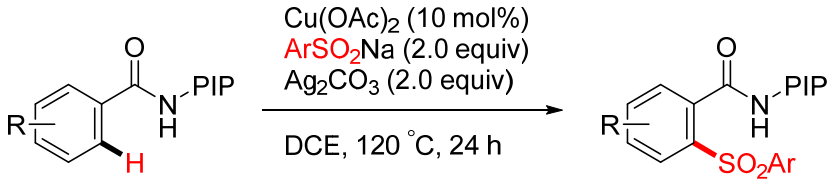


1 **1a**

entry	oxidant	yield[b]
1	**Ag_2CO_3 (2 equiv)**	**73%(72%)[c]**
2	O_2 (1 atm)	trace
3	air (1 atm)	trace
4[d]	air (1 atm)	trace
5	AgOAc (2 equiv)	/
6	$PhI(OAc)_2$ (2 equiv)	/
7	NMO (2 equiv)	/
7[e]	Ag_2CO_3 (2 equiv)	32%
8[f]	Ag_2CO_3 (2 equiv)	27%
9	O_2 or air	/
10[g]	Ag_2CO_3 (2 equiv)	/

[a]Reaction conditions: **1** (0.1 mmol), $PhSO_2Na$ (0.2 mmol), $Cu(OAc)_2$ (10 mol%), Oxidant (0.2 mmol) in DCE (1.0 mL) at 120 °C for 24 hours under N_2. [b]Yield determined by ^1H NMR using CH_2Br_2 as the internal standard. [c]Isolated yield in parentheses. [d]$Cu(OAc)_2$ (0.1 mmol, 1.0 equiv) was used. [e]Under air. [f]Under O_2. [g]No $Cu(OAc)_2$.

General procedures for the sulfonylation of benzamides

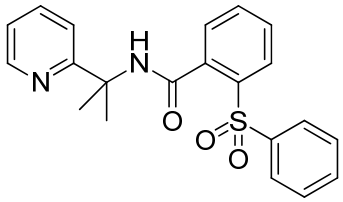


1 **1a**

As the phenylsulfonylation of **1** for example: To a 30 mL Schlenk flask were added **1** (48 mg, 0.2 mmol), $Cu(OAc)_2$ (3.6 mg, 0.02 mmol), $PhSO_2Na$ (66 mg, 0.4 mmol, 2.0 equiv), Ag_2CO_3 (111 mg, 0.4 mmol, 2.0 equiv) and DCE (2.0 mL). The flask was then

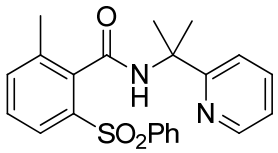
charged with N_2 via twice N_2-vacuum exchanges, and the mixture was stirred at 120 ℃ for 24 hours. After being allowed to cool to room temperature, the reaction was diluted with DCM (10 mL) and treated with $NH_3 \cdot H_2O$ (1.0 mL). Then, the mixture was stirred at room temperature for 10 minutes and was filtered through a pad of Celite, which was washed with copious DCM. Evaporation of the organic solvent and purification by silica gel column chromatography (petroleum ether: EtOAc= 1:1) gave the desired product **1a** as a white foam (55 mg) in 72% yield.

2-(phenylsulfonyl)-*N*-(2-(pyridin-2-yl)propan-2-yl)benzamide (1a)



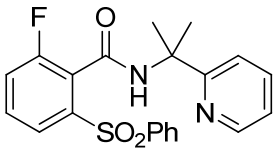
1a was obtained as white foam (55 mg) in 72% isolated yield from **1**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 4.4 Hz, 1H), 8.18 (s, 1H), 8.11–8.08 (m, 3H), 7.74 (t, *J* = 7.6 Hz, 1H), 7.63 – 7.58 (m, 1H), 7.56 – 7.45 (m, 6H), 7.18 (dd, *J* = 6.8, 5.2 Hz, 1H), 1.94 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.84, 164.15, 147.55, 141.57, 138.37, 138.30, 137.15, 133.44, 133.14, 130.06, 129.70, 128.96, 128.89, 128.28, 121.91, 119.49, 57.50, 27.22. HRMS (EI-TOF) calcd for $C_{21}H_{20}N_2O_3S$ (M^+): 380.1195, found: 380.1194.

2-methyl-6-(phenylsulfonyl)-*N*-(2-(pyridin-2-yl)propan-2-yl)benzamide (2a)



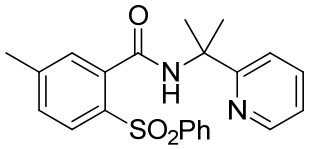
2a was obtained as white solid (43 mg) in 55% isolated yield from **2**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (d, *J* = 4.4 Hz, 1H), 8.26 (s, 1H), 8.03 (d, *J* = 7.6 Hz, 2H), 7.92 (d, *J* = 6.8 Hz, 1H), 7.74 (t, *J* = 7.2 Hz, 1H), 7.55 – 7.33 (m, 6H), 7.23 – 7.11 (m, 1H), 2.42 (s, 3H), 1.99 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.95, 164.13, 147.38, 141.90, 137.94, 137.43, 137.22, 137.18, 135.58, 133.03, 128.91, 128.08, 127.36, 121.93, 119.55, 57.49, 27.01, 19.22. HRMS (EI-TOF) calcd for $C_{22}H_{22}N_2O_3S$ (M^+): 394.1351, found: 394.1352.

2-fluoro-6-(phenylsulfonyl)-*N*-(2-(pyridin-2-yl)propan-2-yl)benzamide (3a)



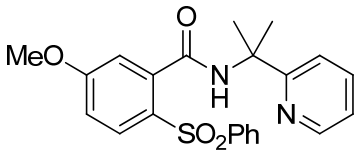
3a was obtained as colorless oil (41 mg) in 52% isolated yield from **3**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 4.8 Hz, 1H), 8.30 (s, 1H), 8.07 (d, *J* = 7.2 Hz, 2H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.74 (td, *J* = 8.0, 1.6 Hz, 1H), 7.57 – 7.46 (m, 5H), 7.33 (t, *J* = 8.4 Hz, 1H), 7.19 (dd, *J* = 6.8, 5.2 Hz, 1H), 1.97 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.91, 161.11, 159.46, 147.45, 141.10, 140.35, 137.18, 133.46, 130.64, 129.04, 128.37, 126.33, 125.66, 121.92, 121.15, 119.51, 57.92, 27.20. ^{19}F NMR (376 MHz, $CDCl_3$) δ -113.48. HRMS (EI-TOF) calcd for $C_{21}H_{19}FN_2O_3S$ (M^+): 398.1100, found: 398.1095.

5-methyl-2-(phenylsulfonyl)-*N*-(2-(pyridin-2-yl)propan-2-yl)benzamide (4a)



4a was obtained as white solid (55 mg) in 70% isolated yield from **4**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 4.0 Hz, 1H), 8.11 (s, 1H), 8.05 (d, *J* = 7.2 Hz, 2H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.74 (dt, *J* = 7.6, 1.2 Hz, 1H), 7.56 – 7.39 (m, 4H), 7.34 – 7.26 (m, 2H), 7.22 – 7.13 (m, 1H), 2.41 (s, 3H), 1.94 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.01, 164.20, 147.57, 144.59, 141.88, 138.28, 137.14, 135.27, 132.97, 130.27, 130.12, 129.54, 128.86, 128.09, 121.90, 119.52, 57.48, 27.21, 21.39. HRMS (EI-TOF) calcd for $C_{22}H_{22}N_2O_3S$ (M^+): 394.1351, found: 394.1350.

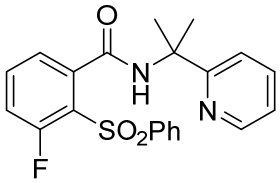
5-methoxy-2-(phenylsulfonyl)-*N*-(2-(pyridin-2-yl)propan-2-yl)benzamide (5a)



5a was obtained as colorless oil (48 mg) in 58% isolated yield from **5**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 4.4 Hz, 1H), 8.17 (s, 1H), 8.03 (d, *J* = 7.6 Hz, 3H), 7.73 (dt, *J* = 8.0, 1.6 Hz, 1H), 7.52 – 7.43 (m, 4H), 7.19 (dd, *J* = 6.8, 5.2 Hz, 1H), 7.05 – 6.91 (m, 2H), 3.87 (s, 3H), 1.93 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.52, 164.12, 163.25, 147.55, 142.25, 140.39, 137.14, 132.81, 132.42, 129.75, 128.82,

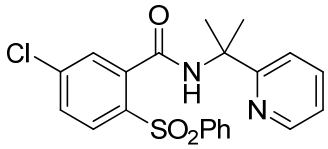
127.90, 121.91, 119.48, 114.55, 57.49, 55.86, 27.18. HRMS (EI-TOF) calcd for $C_{22}H_{22}N_2O_4S$ (M^+): 410.1300, found: 410.1303.

3-fluoro-2-(phenylsulfonyl)-*N*-(2-(pyridin-2-yl)propan-2-yl)benzamide (6a)



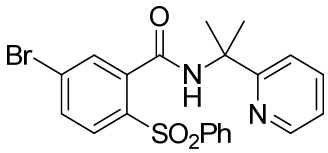
6a was obtained as white-off solid (60 mg) in 75% isolated yield from **6**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (d, *J* = 4.0 Hz, 1H), 8.32 (s, 1H), 8.23 (d, *J* = 8.0 Hz, 2H), 7.75 (td, *J* = 8.0, 1.6 Hz, 1H), 7.63 – 7.43 (m, 5H), 7.31 (d, *J* = 7.6 Hz, 1H), 7.20 (dd, *J* = 6.8, 5.2 Hz, 1H), 7.13 (td, *J* = 8.8, 0.8 Hz, 1H), 1.97 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.03, 166.02, 164.10, 159.83, 147.45, 140.80, 137.27, 135.48, 133.69, 129.01, 128.58, 128.57, 126.78, 124.59, 122.01, 119.53, 117.87, 57.49, 27.16. ^{19}F NMR (376 MHz, $CDCl_3$) δ -104.15. HRMS (EI-TOF) calcd for $C_{21}H_{19}FN_2O_3S$ (M^+): 398.1100, found: 398.1102.

5-chloro-2-(phenylsulfonyl)-*N*-(2-(pyridin-2-yl)propan-2-yl)benzamide (7a)



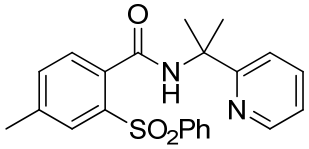
7a was obtained as white-off solid (63 mg) in 76% isolated yield from **7**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (d, *J* = 4.4 Hz, 1H), 8.30 (s, 1H), 8.06 – 8.02 (m, 3H), 7.74 (dt, *J* = 8.0, 1.2 Hz, 1H), 7.59 – 7.38 (m, 6H), 7.20 (dd, *J* = 7.2, 5.6 Hz, 1H), 1.94 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.38, 163.84, 147.52, 141.20, 139.97, 139.71, 137.27, 136.83, 133.38, 131.61, 129.83, 129.06, 129.00, 128.28, 122.03, 119.45, 57.59, 27.14. HRMS (EI-TOF) calcd for $C_{21}H_{19}ClN_2O_3S$ (M^+): 414.0805, found: 414.0805.

5-bromo-2-(phenylsulfonyl)-*N*-(2-(pyridin-2-yl)propan-2-yl)benzamide (8a)



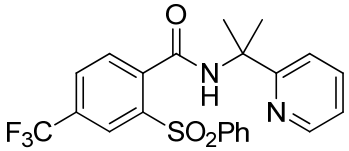
8a was obtained as white solid (63 mg) in 69% isolated yield from **8**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (d, *J* = 4.4 Hz, 1H), 8.30 (s, 1H), 8.05 (d, *J* = 7.2 Hz, 2H), 7.95 (d, *J* = 8.4 Hz, 1H), 7.75 (td, *J* = 8.0, 1.6 Hz, 1H), 7.67 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.64 (d, *J* = 2.0 Hz, 1H), 7.58 – 7.51 (m, 1H), 7.50 – 7.46 (m, 3H), 7.22 – 7.18 (m, 1H), 1.94 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.26, 163.83, 147.52, 141.14, 139.68, 137.36, 137.27, 133.40, 132.86, 131.92, 131.60, 129.01, 128.46, 128.29, 122.04, 119.46, 57.60, 27.14. HRMS (EI-TOF) calcd for $C_{21}H_{19}BrN_2O_3S$ (M^+): 458.0300, found: 458.0298.

4-methyl-2-(phenylsulfonyl)-*N*-(2-(pyridin-2-yl)propan-2-yl)benzamide (9a)



9a was obtained as white-off solid (57 mg) in 73% isolated yield from **9**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (d, *J* = 4.0 Hz, 1H), 8.16 – 8.01 (m, 3H), 7.90 (s, 1H), 7.73 (t, *J* = 7.6 Hz, 1H), 7.56 – 7.44 (m, 4H), 7.43– 7.38 (dd, *J* = 11.6, 7.6 Hz, 2H), 7.18 (t, *J* = 7.6 Hz, 1H), 2.43 (s, 3H), 1.92 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.03, 164.22, 147.56, 141.69, 140.17, 138.02, 137.11, 135.76, 134.03, 133.06, 130.29, 128.95, 128.87, 128.23, 121.87, 119.50, 57.44, 27.22, 21.23. HRMS (EI-TOF) calcd for $C_{22}H_{22}N_2O_3S$ (M^+): 394.1351, found: 394.1348.

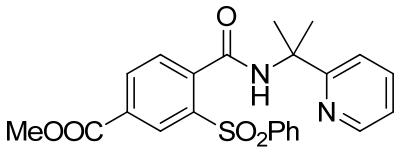
2-(phenylsulfonyl)-*N*-(2-(pyridin-2-yl)propan-2-yl)-4-(trifluoromethyl)benzamide (10a)



10a was obtained as colorless oil (66 mg) in 74% isolated yield from **10**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (d, *J* = 4.8 Hz, 2H), 8.37 (s, 1H), 8.09 (d, *J* = 7.6 Hz, 2H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.75 (t, *J* = 7.2 Hz, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.57 (t, *J* = 7.2 Hz, 1H), 7.50 (dd, *J* = 12.4, 7.6 Hz, 3H), 7.19 (dd, *J* = 6.8, 5.2 Hz, 1H), 1.95 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.59, 163.75, 147.45, 141.34, 140.68, 139.69, 137.33, 133.68, 132.06, 130.22, 129.77, 129.11, 128.52, 127.21, 122.91, 122.08,

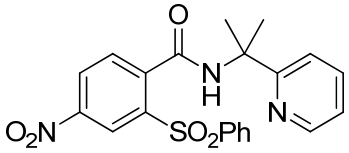
119.46, 57.63, 27.16. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.82. HRMS (EI-TOF) calcd for $C_{22}H_{19}F_3N_2O_3S$ (M^+): 448.1068, found: 448.1071.

Methyl 3-(phenylsulfonyl)-4-((2-(pyridin-2-yl)propan-2-yl)carbamoyl)benzoate (11a)



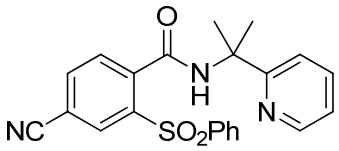
11a was obtained as colorless oil (67 mg) in 76% isolated yield from **11**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73 (s, 1H), 8.43 (d, *J* = 4.8 Hz, 1H), 8.32 (s, 1H), 8.23 (d, *J* = 8.0 Hz, 1H), 8.09 (d, *J* = 7.6 Hz, 2H), 7.74 (t, *J* = 8.0 Hz, 1H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.66 – 7.47 (m, 4H), 7.19 (dd, *J* = 6.8, 5.6 Hz, 1H), 3.96 (s, 3H), 1.95 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.09, 164.96, 163.86, 147.50, 141.78, 141.02, 139.09, 137.27, 134.34, 133.45, 131.64, 131.29, 129.28, 129.01, 128.46, 122.03, 119.47, 57.62, 52.74, 27.19. HRMS (EI-TOF) calcd for $C_{23}H_{22}N_2O_5S$ (M^+): 438.1249, found: 438.1249.

4-nitro-2-(phenylsulfonyl)-*N*-(2-(pyridin-2-yl)propan-2-yl)benzamide (12a)



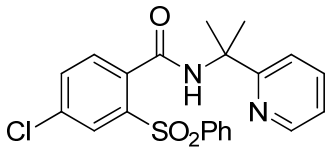
12a was obtained as colorless oil (64 mg) in 75% isolated yield from **12**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.92 (d, *J* = 2.0 Hz, 1H), 8.52 (s, 1H), 8.42 (dd, *J* = 8.4, 2.4 Hz, 2H), 8.11 (d, *J* = 7.6 Hz, 2H), 7.77 (dt, *J* = 7.6, 1.6 Hz, 1H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.63 – 7.56 (m, 1H), 7.55 – 7.51 (m, 2H), 7.49 (d, *J* = 8.0 Hz, 1H), 7.21 (dd, *J* = 7.6, 5.2 Hz, 1H), 1.96 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.96, 163.54, 147.99, 147.42, 143.18, 140.78, 140.16, 137.44, 133.99, 130.39, 129.24, 128.72, 127.98, 125.49, 122.19, 119.46, 57.75, 27.15. HRMS (EI-TOF) calcd for $C_{21}H_{19}N_3O_5S$ (M^+): 425.1045, found: 425.1048.

4-cyano-2-(phenylsulfonyl)-*N*-(2-(pyridin-2-yl)propan-2-yl)benzamide (13a)



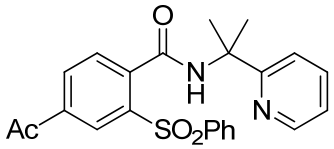
13a was obtained as yellowish oil (35 mg) in 43% isolated yield from **13**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (s, 1H), 8.44 (d, *J* = 4.4 Hz, 1H), 8.39 (d, *J* = 1.2 Hz, 1H), 8.08 (d, *J* = 7.2 Hz, 2H), 7.87 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.76 (td, *J* = 7.6, 1.6 Hz, 1H), 7.61 (dd, *J* = 16.4, 7.6 Hz, 2H), 7.53 (t, *J* = 7.6 Hz, 2H), 7.48 (d, *J* = 8.4 Hz, 1H), 7.22 (dd, *J* = 6.8, 5.2 Hz, 1H), 1.95 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.12, 163.59, 147.43, 141.65, 140.32, 140.27, 137.41, 136.50, 133.93, 133.83, 129.88, 129.21, 128.64, 122.16, 119.45, 116.72, 114.13, 57.70, 27.13. HRMS (EI-TOF) calcd for $C_{22}H_{19}N_3O_3S$ (M^+): 405.1147, found: 405.1152.

4-chloro-2-(phenylsulfonyl)-*N*-(2-(pyridin-2-yl)propan-2-yl)benzamide (14a)



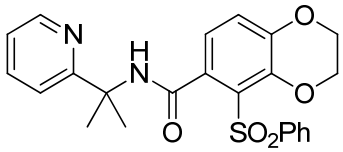
14a was obtained as white solid (51 mg) in 62% isolated yield from **14**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (d, *J* = 3.2 Hz, 1H), 8.28 (s, 1H), 8.13 – 7.99 (m, 3H), 7.78 – 7.67 (m, 1H), 7.58 – 7.39 (m, 6H), 7.24 – 7.11 (m, 1H), 1.92 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.90, 163.92, 147.50, 140.89, 140.09, 137.24, 136.62, 135.71, 133.53, 133.43, 130.32, 129.95, 129.04, 128.47, 122.00, 119.47, 57.54, 27.17. HRMS (EI-TOF) calcd for $C_{21}H_{19}ClN_2O_3S$ (M^+): 414.0805, found: 414.0808.

4-acetyl-2-(phenylsulfonyl)-*N*-(2-(pyridin-2-yl)propan-2-yl)benzamide (15a)



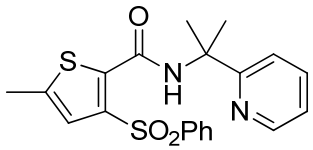
15a was obtained as white solid (33 mg) in 39% isolated yield from **15**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (s, 1H), 8.44 (d, *J* = 4.4 Hz, 1H), 8.35 (s, 1H), 8.16 (d, *J* = 7.6 Hz, 1H), 8.10 (d, *J* = 7.2 Hz, 2H), 7.75 (dt, *J* = 7.6, 1.6 Hz, 1H), 7.63 (d, *J* = 7.6 Hz, 1H), 7.56 (t, *J* = 7.2 Hz, 1H), 7.50 (t, *J* = 7.6 Hz, 4H), 7.20 (dd, *J* = 6.8, 4.8 Hz, 2H), 2.66 (s, 3H), 1.95 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.73, 166.00, 163.84, 147.48, 141.78, 140.99, 139.27, 137.92, 137.28, 133.49, 132.85, 129.94, 129.55, 129.04, 128.42, 122.04, 119.47, 57.62, 27.19, 26.73. HRMS (EI-TOF) calcd for $C_{23}H_{22}N_2O_4S$ (M^+): 422.1300, found: 422.1304.

5-(phenylsulfonyl)-*N*-(2-(pyridin-2-yl)propan-2-yl)-2,3-dihydrobenzo[*b*][1,4]dioxine-6-carboxamide (16a)



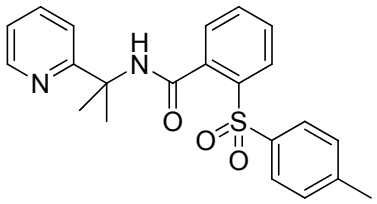
16a was obtained as colorless oil (50 mg) in 57% isolated yield from **16**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 4.4 Hz, 1H), 8.18 (d, *J* = 8.0 Hz, 2H), 8.09 (s, 1H), 7.71 (t, *J* = 7.6 Hz, 1H), 7.57 – 7.40 (m, 4H), 7.21 – 7.08 (m, 1H), 7.02 (d, *J* = 8.4 Hz, 1H), 6.97 (d, *J* = 8.4 Hz, 1H), 4.19 (d, *J* = 5.2 Hz, 4H), 1.93 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.19, 164.43, 147.48, 144.49, 142.49, 141.41, 137.13, 133.16, 133.07, 128.63, 128.54, 126.33, 122.04, 121.86, 121.05, 119.56, 64.25, 63.73, 57.31, 27.19. HRMS (EI-TOF) calcd for $C_{23}H_{22}N_2O_5S$ (M^+): 438.1249, found: 438.1245.

5-methyl-3-(phenylsulfonyl)-*N*-(2-(pyridin-2-yl)propan-2-yl)thiophene-2-carboxamide (17a)



17a was obtained as colorless oil (45 mg) in 56% isolated yield from **17**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.20 (s, 1H), 8.56 (d, *J* = 4.0 Hz, 1H), 8.10 – 7.94 (m, 2H), 7.66 – 7.60 (m, 2H), 7.53 (t, *J* = 7.6 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 1H), 7.18 (s, 1H), 7.15 (dd, *J* = 6.8, 5.2 Hz, 1H), 2.44 (s, 3H), 1.81 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.97, 158.59, 148.47, 143.12, 142.85, 141.22, 136.59, 136.40, 133.70, 129.32, 128.09, 127.44, 121.74, 119.25, 58.26, 27.60, 15.27. HRMS (EI-TOF) calcd for $C_{20}H_{20}N_2O_3S$ (M^+): 400.0915, found: 400.0915.

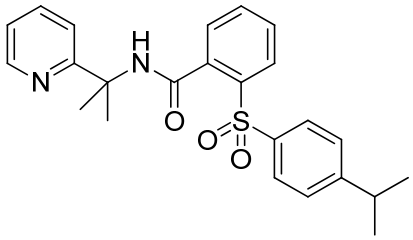
***N*-(2-(pyridin-2-yl)propan-2-yl)-2-tosylbenzamide (1b)**



1b was obtained as white foam (58 mg) in 74% isolated yield from **1**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 4.0 Hz, 1H), 8.14 (s, 1H), 8.09 (d, *J* = 8.0 Hz, 1H), 7.94 (d, *J* = 8.0 Hz, 2H), 7.74 (t, *J* = 7.2 Hz, 1H), 7.63 – 7.56 (m, 1H), 7.55 – 7.50 (m, 3H),

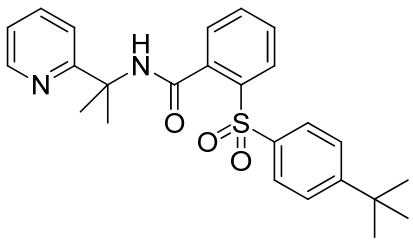
7.26 (d, *J* = 7.6 Hz, 2H), 7.19 (dd, *J* = 6.8, 5.2 Hz, 1H), 2.37 (s, 3H), 1.94 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.87, 164.19, 147.56, 144.03, 138.64, 138.58, 138.21, 137.12, 133.24, 129.88, 129.63, 129.54, 128.95, 128.35, 121.88, 119.50, 57.50, 27.23, 21.61. HRMS (EI-TOF) calcd for $C_{22}H_{22}N_2O_3S$ (M^+): 394.1351, found: 394.1346.

2-((4-isopropylphenyl)sulfonyl)-*N*-(2-(pyridin-2-yl)propan-2-yl)benzamide (1c)



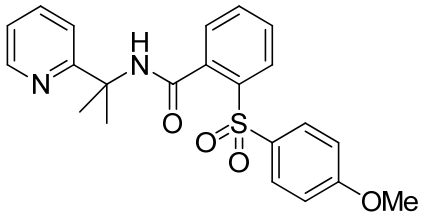
1c was obtained as white-off solid (54 mg) in 64% isolated yield from **1**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 4.4 Hz, 1H), 8.14 (s, 1H), 8.08 (d, *J* = 7.6 Hz, 1H), 7.99 (d, *J* = 8.0 Hz, 2H), 7.74 (t, *J* = 7.6 Hz, 1H), 7.60 – 7.56 (m, 1H), 7.55 – 7.50 (m, 3H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.20 – 7.17 (m, 1H), 2.92 (hept, *J* = 6.8 Hz, 1H), 1.95 (s, 6H), 1.22 (d, *J* = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.97, 164.21, 154.64, 147.57, 138.82, 138.71, 138.22, 137.11, 133.21, 129.95, 129.66, 128.95, 128.49, 127.07, 121.88, 119.50, 57.52, 34.20, 27.23, 23.57. HRMS (EI-TOF) calcd for $C_{24}H_{26}N_2O_3S$ (M^+): 422.1664, found: 422.1667.

2-((4-(tert-butyl)phenyl)sulfonyl)-*N*-(2-(pyridin-2-yl)propan-2-yl)benzamide (1d)



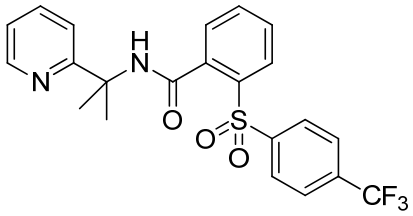
1d was obtained as white solid (61 mg) in 70% isolated yield from **1**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 4.0 Hz, 1H), 8.14 (s, 1H), 8.09 (d, *J* = 7.6 Hz, 1H), 8.00 (d, *J* = 8.4 Hz, 2H), 7.74 (dt, *J* = 7.6, 1.6 Hz, 1H), 7.62 – 7.55 (m, 2H), 7.51 (d, *J* = 8.0 Hz, 2H), 7.49 (d, *J* = 8.8 Hz, 2H), 7.18 (dd, *J* = 6.8, 5.2 Hz, 1H), 1.95 (s, 6H), 1.29 (s, 9H).^{13}C NMR (100 MHz, $CDCl_3$) δ 166.99, 164.22, 156.89, 147.58, 138.72, 138.47, 138.22, 137.11, 133.21, 129.97, 129.67, 128.95, 128.20, 125.98, 121.88, 119.50, 57.53, 35.14, 31.03, 27.23. HRMS (EI-TOF) calcd for $C_{25}H_{28}N_2O_3S$ (M^+): 436.1821, found: 436.1822.

2-((4-methoxyphenyl)sulfonyl)-*N*-(2-(pyridin-2-yl)propan-2-yl)benzamide (1e)



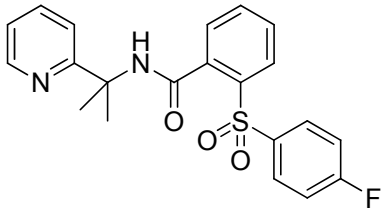
1e was obtained as white solid (50 mg) in 62% isolated yield from **1**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 4.4 Hz, 1H), 8.13 (s, 1H), 8.06 (d, *J* = 8.0 Hz, 1H), 8.01 (d, *J* = 8.8 Hz, 2H), 7.73 (dt, *J* = 8.0, 1.6 Hz, 1H), 7.59 – 7.55 (m, 1H), 7.54 – 7.42 (m, 3H), 7.18 (dd, *J* = 6.8, 5.2 Hz, 1H), 6.94 (d, *J* = 8.8 Hz, 2H), 3.81 (s, 3H), 1.95 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.04, 164.19, 163.33, 147.57, 139.07, 138.01, 137.12, 133.09, 133.05, 130.68, 129.71, 129.65, 128.91, 121.89, 119.50, 114.13, 57.50, 55.54, 27.25. HRMS (EI-TOF) calcd for $C_{22}H_{22}N_2O_4S$ (M^+): 410.1300, found: 410.1303.

***N*-(2-(pyridin-2-yl)propan-2-yl)-2-((4-(trifluoromethyl)phenyl)sulfonyl)benzamid e (1f)**



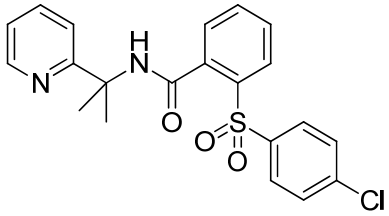
1f was obtained as light-yellow solid (50 mg) in 56% isolated yield from **1**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (d, *J* = 4.4 Hz, 1H), 8.29 (s, 1H), 8.20 (d, *J* = 8.4 Hz, 2H), 8.16 (d, *J* = 8.0 Hz, 1H), 7.79 – 7.27 (m, 3H), 7.65 (t, *J* = 7.2 Hz, 1H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.55 (d, *J* = 7.6 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.20 (dd, *J* = 6.8, 5.2 Hz, 1H), 1.94 (s, 6H).^{13}C NMR (100 MHz, $CDCl_3$) δ 166.75, 163.97, 147.51, 145.22, 138.72, 137.47, 137.24, 134.04, 130.37, 129.92, 128.94, 128.91, 125.99, 122.02, 119.49, 57.49, 27.18. ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.20. HRMS (EI-TOF) calcd for $C_{22}H_{19}F_3N_2O_3S$ (M^+): 448.1068, found: 448.1064.

2-((4-fluorophenyl)sulfonyl)-*N*-(2-(pyridin-2-yl)propan-2-yl)benzamide (1g)



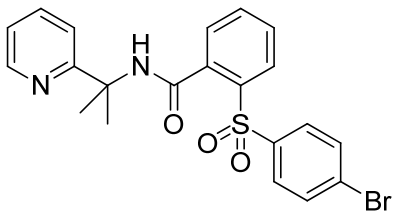
1g was obtained as colorless oil (60 mg) in 76% isolated yield from **1**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 4.4 Hz, 1H), 8.22 (s, 1H), 8.12 – 8.09 (m, 3H), 7.74 (t, *J* = 7.6 Hz, 1H), 7.63 – 7.59 (m, 1H), 7.60 – 7.49 (m, 3H), 7.20 – 7.12 (m, 3H), 1.94 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.93, 165.44, 164.06, 147.54, 138.32, 137.66, 137.18, 133.57, 131.32, 129.89, 128.90, 121.96, 119.48, 116.23, 116.00, 57.49, 27.21. ^{19}F NMR (376 MHz, $CDCl_3$) δ -104.58. HRMS (EI-TOF) calcd for $C_{22}H_{19}FN_2O_3S$ (M^+): 398.1100, found: 398.1096.

2-((4-chlorophenyl)sulfonyl)-*N*-(2-(pyridin-2-yl)propan-2-yl)benzamide (1h)



1h was obtained as white solid (60 mg) in 72% isolated yield from **1**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (d, *J* = 4.2 Hz, 1H), 8.23 (s, 1H), 8.10 (d, *J* = 7.6 Hz, 1H), 8.01 (d, *J* = 8.4 Hz, 2H), 7.74 (t, *J* = 7.2 Hz, 1H), 7.67 – 7.59 (m, 1H), 7.58 – 7.47 (m, 3H), 7.43 (d, *J* = 8.4 Hz, 2H), 7.23 – 7.12 (m, 1H), 1.93 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.82, 164.02, 147.53, 140.15, 139.76, 138.44, 137.99, 137.20, 133.70, 130.09, 129.88, 129.82, 129.16, 128.92, 121.97, 119.48, 57.49, 27.21. HRMS (EI-TOF) calcd for $C_{21}H_{19}ClN_2O_3S$ (M^+): 414.0805, found: 414.0810.

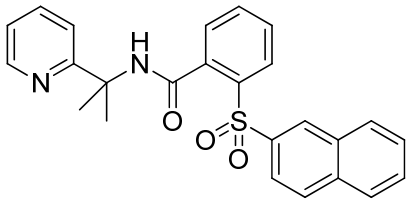
2-((4-bromophenyl)sulfonyl)-*N*-(2-(pyridin-2-yl)propan-2-yl)benzamide (1i)



1i was obtained as light-yellow solid (72 mg) in 78% isolated yield from **1**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (d, *J* = 4.4 Hz, 1H), 8.23 (s, 1H), 8.11 (d, *J* = 8.0 Hz, 1H),

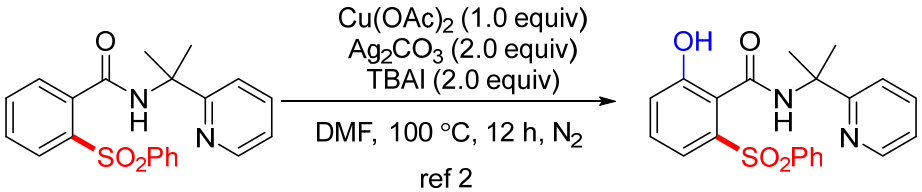
7.93 (d, J = 8.4 Hz, 2H), 7.74 (dt, J = 8.0, 1.2 Hz, 1H), 7.65 – 7.47 (m, 6H), 7.19 (dd, J = 6.8, 5.2 Hz, 1H), 1.93 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.82, 164.01, 147.53, 140.66, 138.45, 137.93, 137.21, 133.73, 132.16, 130.11, 129.95, 129.84, 128.93, 128.44, 121.99, 119.49, 57.48, 27.20. HRMS (EI-TOF) calcd for $C_{21}H_{19}BrN_2O_3S$ (M^+): 458.0300, found: 458.0299.

2-(naphthalen-2-ylsulfonyl)-*N*-(2-(pyridin-2-yl)propan-2-yl)benzamide (1j)



1j was obtained as white solid (69 mg) in 80% isolated yield from **1**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (s, 1H), 8.36 (d, J = 4.4 Hz, 1H), 8.24 – 8.11 (m, 2H), 8.05 (d, J = 8.8 Hz, 1H), 7.93 – 7.88 (m, 2H), 7.83 (d, J = 8.0 Hz, 1H), 7.72 (t, J = 7.6 Hz, 1H), 7.61– 7.49 (m, 6H), 7.15 ((dd, J = 6.4, 5.6 Hz, 1H), 1.96 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.79, 164.10, 147.49, 138.47, 138.41, 138.19, 137.13, 135.14, 133.47, 132.11, 130.10, 129.82, 129.71, 129.60, 129.19, 129.09, 128.94, 127.88, 127.25, 123.20, 121.89, 119.48, 57.52, 27.26. HRMS (EI-TOF) calcd for $C_{25}H_{22}N_2O_3S$ (M^+): 430.1351, found: 430.1349.

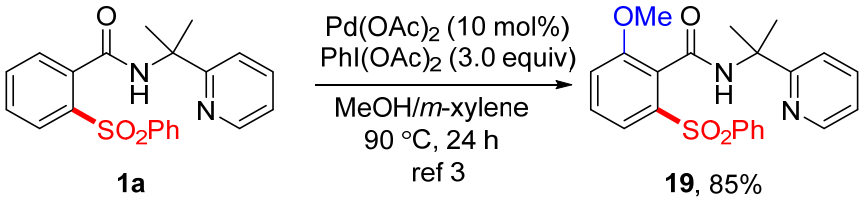
Diverse transformations[2, 3, 4]



1a **18**, 81%

To a 30 mL Schlenk flask were added **1a** (76 mg, 0.2 mmol), $Cu(OAc)_2$ (36 mg, 0.2 mmol, 1.0 equiv), TBAI (148 mg, 0.4 mmol, 2.0 equiv), Ag_2CO_3 (111 mg, 0.4 mmol, 2.0 equiv) and DCE (2.0 mL). The flask was then charged with N_2 via twice N_2-vacuum exchanges, and the mixture was stirred at 100 ℃ for 12 hours. After being allowed to cool to room temperature, the reaction was diluted with EtOAc (20 mL). The resulting mixture was filtered through a pad of Celite. The filtrate was then transferred to a seperatory funnel and washed with water (10 mL×3). The organic phase was dried over anhydrous $MgSO_4$. Evaporation of the organic solvent and

purification by silica gel column chromatography (petroleum ether: EtOAc= 3:2) gave the desired product **18** as colorless oil (64 mg) in 81% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.38 (s, br, 1H), 8.43 (d, *J* = 4.4 Hz, 1H), 8.12 – 7.88 (m, 2H), 7.78 (t, *J* = 7.6 Hz, 1H), 7.51 – 7.39 (m, 5H), 7.34 (t, *J* = 8.0 Hz, 1H), 7.21 (dd, *J* = 6.8, 5.2 Hz, 1H), 7.12 (d, *J* = 8.0 Hz, 1H), 6.64 – 6.48 (m, 1H), 1.84 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.35, 163.52, 156.46, 147.20, 141.54, 138.97, 138.52, 133.06, 130.74, 128.85, 128.29, 122.89, 122.83, 122.25, 120.71, 120.32, 58.28, 29.02. HRMS (EI-TOF) calcd for $C_{21}H_{20}N_2O_4S$ (M^+): 396.1144, found: 396.1146.

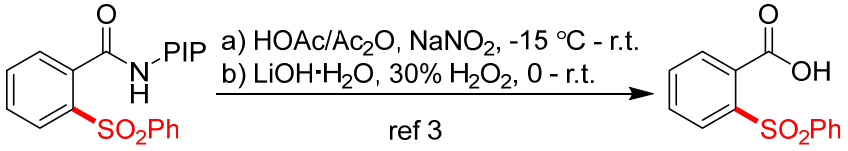


1a **19**, 85%

To a 30 mL Schlenk flask were added **1a** (76 mg, 0.2 mmol), $Pd(OAc)_2$ (4.5 mg, 10 mol%), $PhI(OAc)_2$ (193 mg, 0.6 mmol, 3.0 equiv) and *m*-xylene/MeOH (2.0 mL, 1:1; *v:v*). The flask was then charged with N_2 via twice N_2-vacuum exchanges, and the mixture was stirred at 90 ℃ for 24 hours. After being allowed to cool to room temperature, the reaction was diluted with EtOAc (20 mL). The resulting mixture was then transferred to a 50 mL vial. Evaporation of the organic solvent and purification by silica gel column chromatography (petroleum ether: EtOAc= 1:1) gave the desired product **19** as colorless oil (70 mg) in 85% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 4.0 Hz, 1H), 8.05 (d, *J* = 7.2 Hz, 2H), 7.80 (s, 1H), 7.71 (t, *J* = 8.0 Hz, 1H), 7.64 (d, *J* = 8.0 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.48 (t, *J* = 7.2 Hz, 1H), 7.44 – 7.41 (m, 3H), 7.16 (t, *J* = 6.0 Hz, 1H), 7.11 (d, *J* = 8.4 Hz, 1H), 3.82 (s, 3H), 1.94 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.49, 163.66, 157.30, 147.54, 141.67, 139.23, 136.91, 133.09, 130.19, 128.90, 128.20, 127.50, 121.70, 121.42, 119.71, 116.24, 57.87, 56.47, 27.36. HRMS (EI-TOF) calcd for $C_{22}H_{22}N_2O_4S$ (M^+): 410.1300, found: 410.1296.

1a **20**, 76%

To a 30 mL Schlenk flask were added **1a** (76 mg, 0.2 mmol), $Cu(OAc)_2 \cdot H_2O$ (40 mg, 0.2 mmol, 1.0 equiv), S_8 (102 mg, 0.4 mmol, 2.0 equiv), TBAI (74 mg, 0.2 mmol, 1.0 equiv), Ag_2O (116 mg, 0.5 mmol, 2.5 equiv) and DCM (2.0 mL). The flask was then sealed with Teflon-lined cap and stirred at 90 °C for 18 h. After being allowed to cool to room temperature, the reaction was diluted with EtOAc (20 mL). The resulting mixture was filtered through a pad of Celite. Evaporation of the organic solvent and purification by silica gel column chromatography (petroleum ether: EtOAc= 1:1) gave the desired product **20** as white-off solid (62 mg) in 76% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (d, J = 4.4 Hz, 1H), 8.27 (dd, J = 6.0, 2.8 Hz, 1H), 7.81 (d, J = 8.0 Hz, 2H), 7.70 – 7.65 (m, 2H), 7.49 (dt, J = 7.8, 1.2 Hz, 1H), 7.39 (t, J = 7.8 Hz, 1H), 7.23 (d, J = 8.8 Hz, 2H), 7.14 (d, J = 8.0 Hz, 1H), 7.04 (dd, J = 6.8, 5.2 Hz, 1H), 1.89 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.67, 160.97, 148.77, 143.21, 141.07, 140.07, 136.30, 132.63, 130.61, 128.62, 128.05, 127.55, 125.81, 122.19, 121.74, 119.72, 63.64, 27.31. HRMS (EI-TOF) calcd for $C_{21}H_{18}N_2O_3S_2$ (M^+): 410.0759, found: 410.0757.



1a **21**, 83%

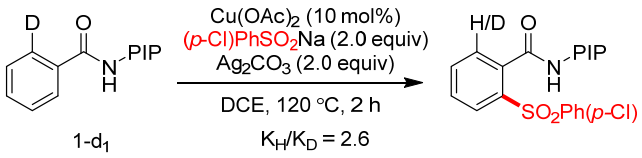
Nitrosylation step: A solution of **1a** (76 mg, 0.2 mmol, 1.0 equiv) in a mixture of acetic acid (0.27 mL) and acetic anhydride (1.35 mL) was cooled to -15 °C and granular sodium nitrite (303 mg, 4.4 mmol, 22.0 equiv) was added slowly in three portions. After being stirred for 2 hours at -15 °C, the mixture was allowed to be warmed naturally to room temperature and stirred overnight followed by being poured into ice-water mixture (Caution! the nitrosoamide is unstable and the subsequent work-up should be carried out below 10 °C). The nitrosoamide was extracted with

ice-cold ether, and the organic phase was sequentially washed with ice water, an aqueous solution of sodium carbonate (5%) and ice water, and then dried over anhydrous $MgSO_4$. Evaporation of the solvent under reduced pressure in an ice-water bath to give the residue.

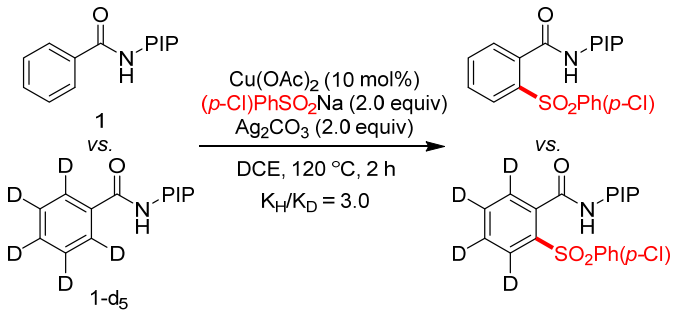
Hydrolysis step: The residue was dissolved with THF-H_2O mixture (3 mL:1 mL) and stirred at -15 ℃. Then lithium hydroxide monohydrate (84 mg, 2.0 mmol, 10.0 equiv) followed by 30% H_2O_2 (0.50 mL) was added. The mixture was stirred at -15 ℃ for 2 hours and at 0 ℃ for another 2 hours, and then quenched with saturated aqueous solution of Na_2SO_3. The mixture was basified with 1*N* NaOH (aq.) and washed with EtOAc (20 mL). The aqueous phase was acidified with 1*N* HCl (aq.) and extracted with EtOAc (20 mL) three times. The combined organic phase was washed with brine and dried over anhydrous $MgSO_4$ and concentrated *in vacuo*. The residue was purified by column chromatography (petroleum ether/EtOAc/HOAc = 1:1:0.01) to afford **21** as pale oil (43 mg, 83%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (dd, *J* = 4.8, 2.4 Hz, 1H), 7.99 (d, *J* = 7.2 Hz, 2H), 7.74 (dd, *J* = 5.2, 2.4 Hz, 1H), 7.67 (dd, *J* = 4.8, 2.4 Hz, 2H), 7.59 – 7.55 (m, 1H), 7.50 (d, *J* = 7.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.96, 141.23, 139.42, 133.41, 133.30, 132.33, 131.47, 130.37, 129.82, 128.97, 128.03. HRMS (ESI): calcd for $C_{13}H_{11}O_4S$ $[M+H]^+$ 263.0373, found: 263.0372.

Intra- and intermolecular KIE experiments

a) Intramoleculcar KIE experiment

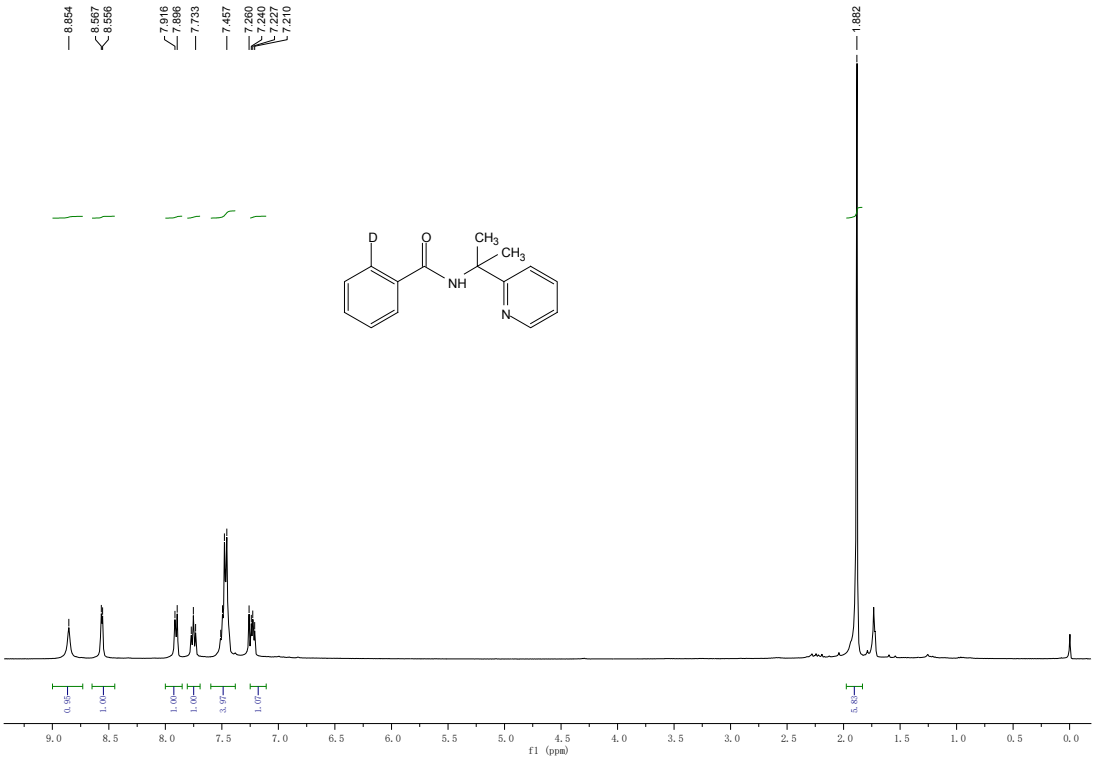


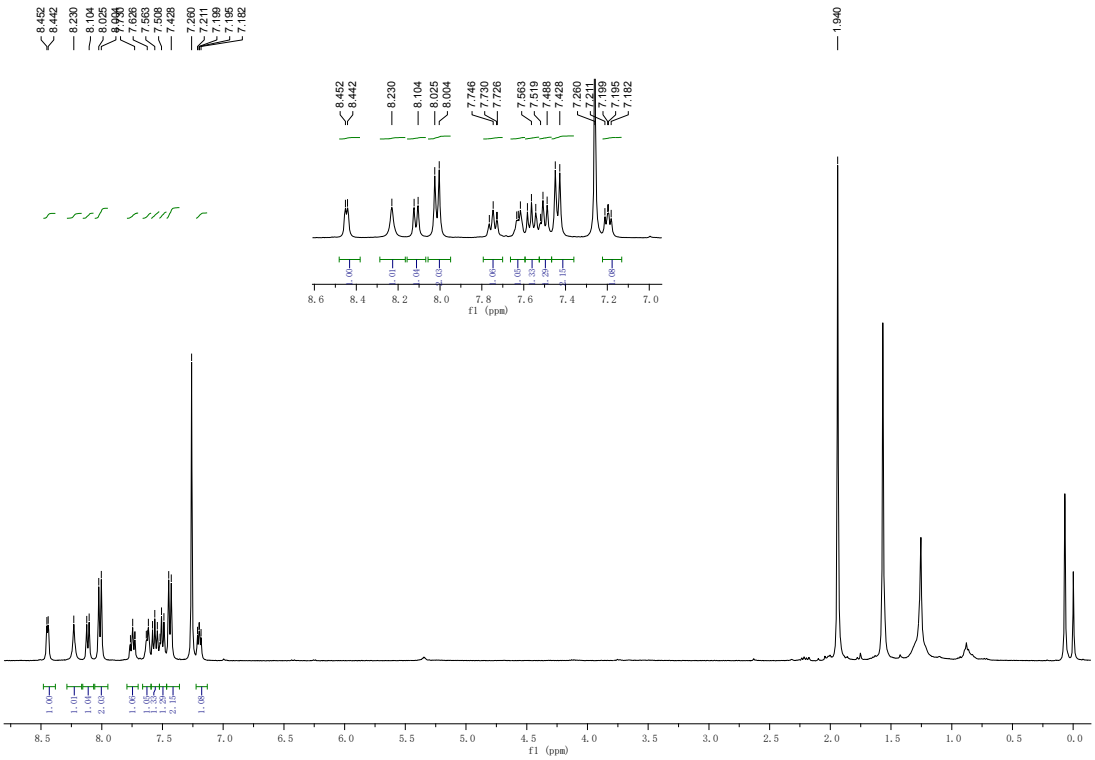
b) Intermoleculcar KIE experiment



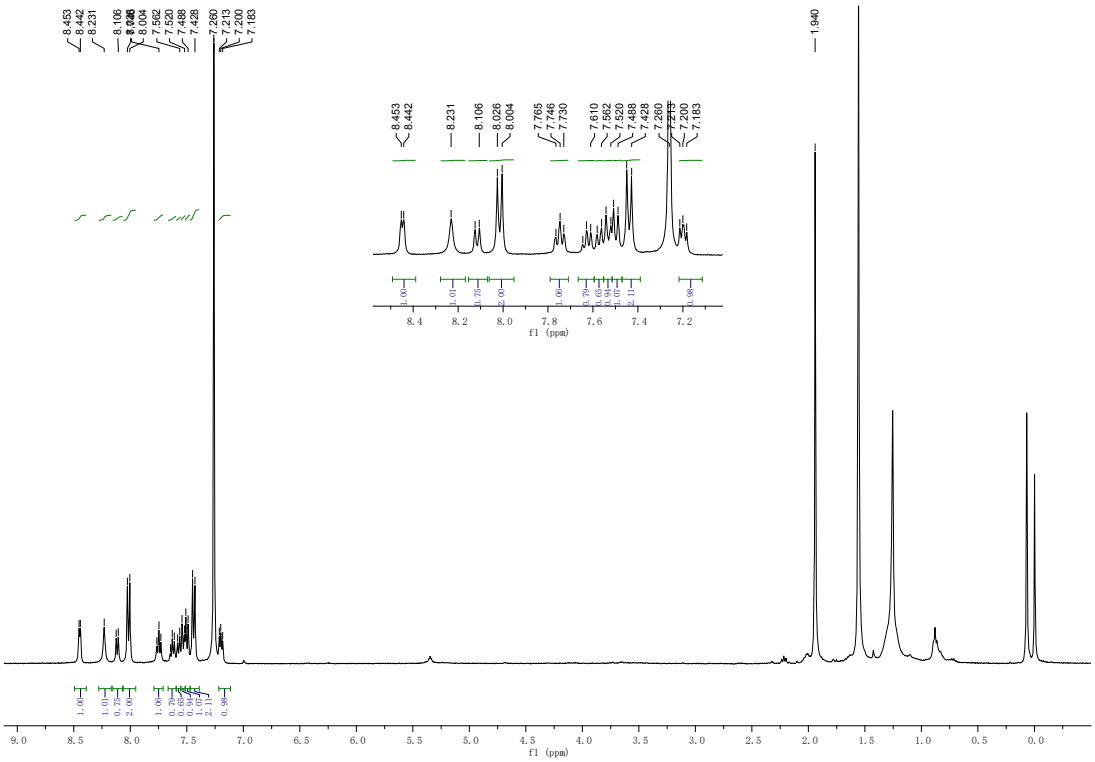
Intramolecular KIE experiment: To a 30 mL Schlenk flask were added **1-d$_1$** (48.2

mg, 0.2 mmol), $Cu(OAc)_2$ (3.6 mg, 0.02 mmol), (*p*-Cl)$PhSO_2Na$ (80 mg, 0.4 mmol, 2.0 equiv), Ag_2CO_3 (111 mg, 0.4 mmol, 2.0 equiv) and DCE (2.0 mL). The flask was then charged with N_2 via twice N_2-vacuum exchanges, and the mixture was stirred at 120 ℃ for 2 hours. After being allowed to cool to room temperature, the reaction was diluted with DCM (10 mL) and treated with $NH_3 \cdot H_2O$ (1.0 mL). Then, the mixture was stirred at room temperature for 10 minutes and was filtered through a pad of Celite, which was washed with copious DCM. Evaporation of the organic solvent and purification by flash chromatography (petroleum ether: EtOAc= 1:1) gave the desired product in 6% yield. The KIE value was calculated K_H/K_D = 2.6.





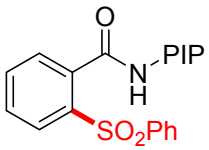
Intermolecular KIE experiment: To a 30 mL Schlenk flask were added **1-d_5** (24.5 mg, 0.1 mmol), **1** (24 mg, 0.1 mmol), $Cu(OAc)_2$ (3.6 mg, 0.02 mmol), (*p*-Cl)$PhSO_2Na$ (80 mg, 0.4 mmol, 2.0 equiv), Ag_2CO_3 (111 mg, 0.4 mmol, 2.0 equiv) and DCE (2.0 mL). The flask was then charged with N_2 via twice N_2-vacuum exchanges, and the mixture was stirred at 120 ℃ for 2 hours. After being allowed to cool to room temperature, the reaction was diluted with DCM (10 mL) and treated with $NH_3 \cdot H_2O$ (1.0 mL). Then, the mixture was stirred at room temperature for 10 minutes and was filtered through a pad of Celite, which was washed with copious DCM. Evaporation of the organic solvent and purification by flash chromatography (petroleum ether: EtOAc= 1:1) gave the desired product in 6% yield. The KIE value was calculated K_H/K_D = 3.0.



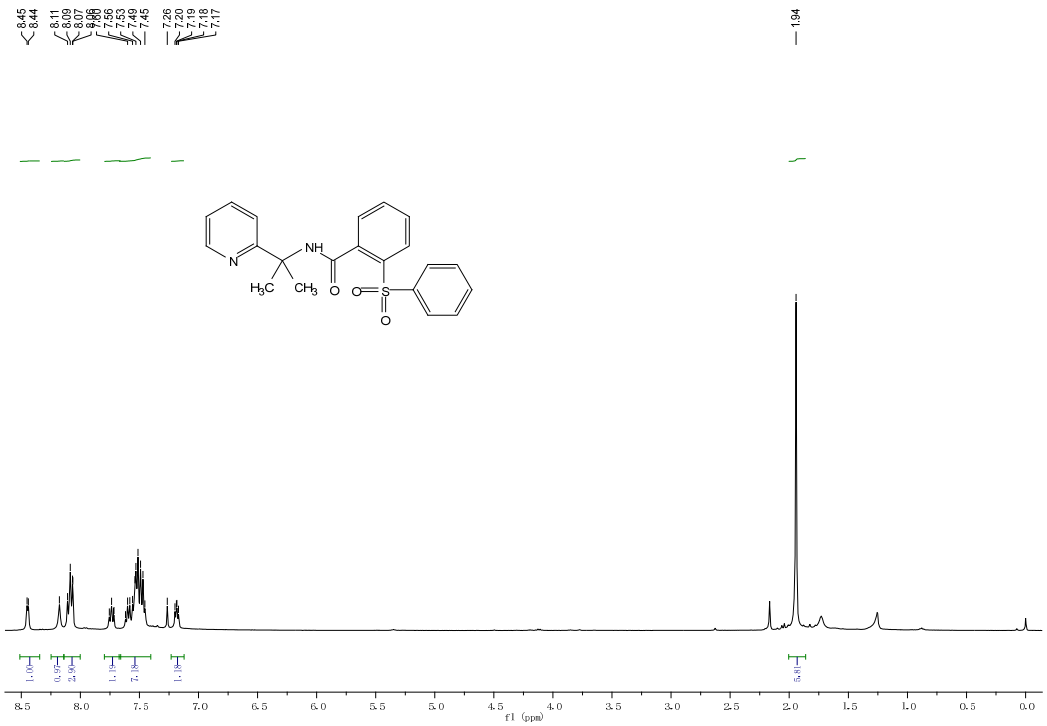
References

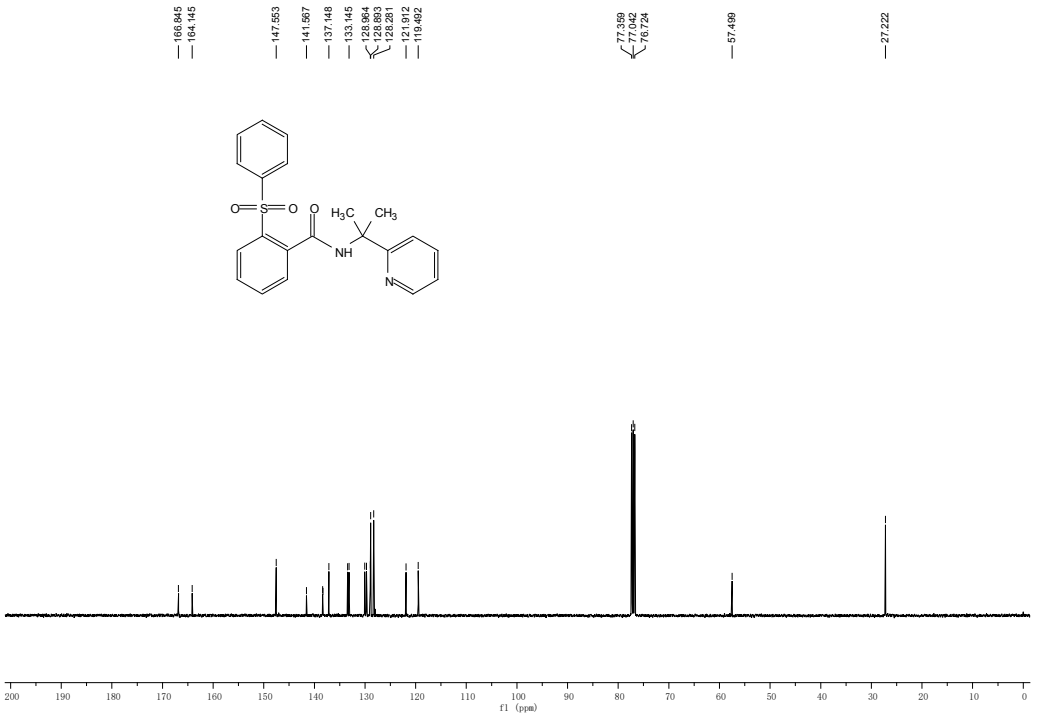
1. Zhou, X.; Luo, J.; Liu, J.; Peng, S.; Deng, G.-J. *Org. Lett.* **2011**, *13,* 1432.
2. Li, X.; Liu, Y.-H.; Gu, W.-J.; Li, B.; Chen, F.-J.; Shi, B.-F. *Org. Lett.* **2014**, *16,* 3904.
3. Chen, F.-J.; Liao, G.; Li, X.; Wu, J.; Shi, B.-F. *Org. Lett.* **2014**, 16, 5644.
4. Chen, F.-J.; Zhao, S.; Hu, F.; Chen, K.; Zhang, Q.; Zhang, S.-Q.; Shi, B.-F. *Chem. Sci.* **2013**, 4, 4187.

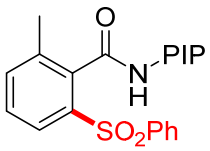
NMR spectra



1a



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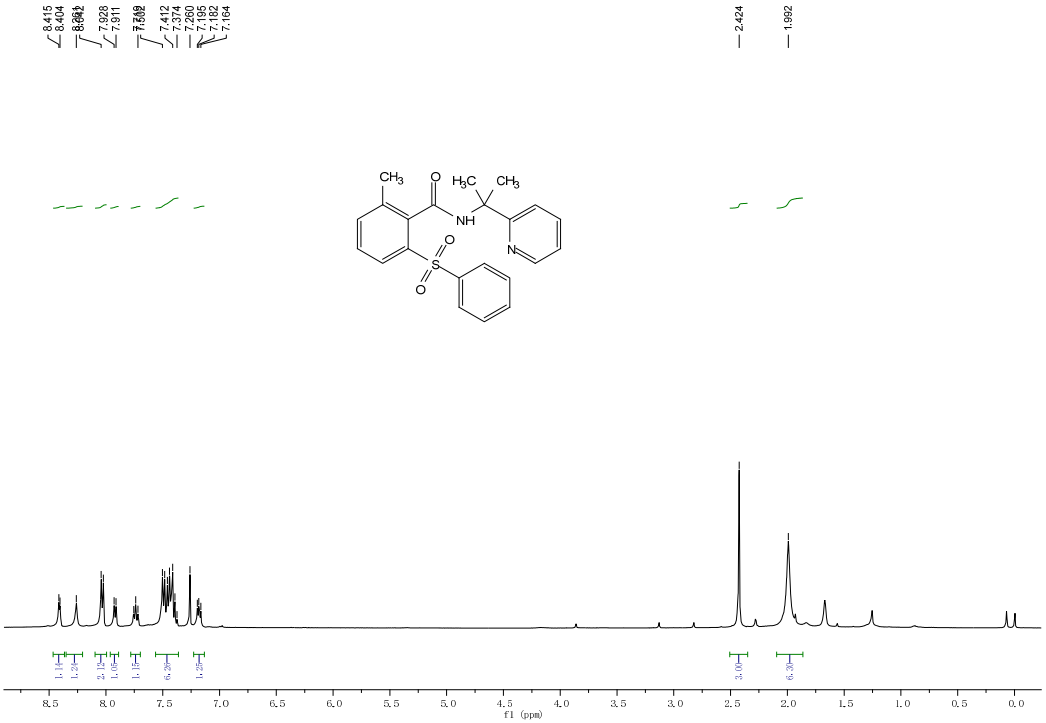
H
PIP
SO2Ph

2a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O
H3C
CH3
NH
N
S
O
O
1.14
1.24
2.12
1.08
1.18
6.28
1.28
3.00
6.38
8.5
8.0
7.5
7.0
6.5
6.0
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2.5
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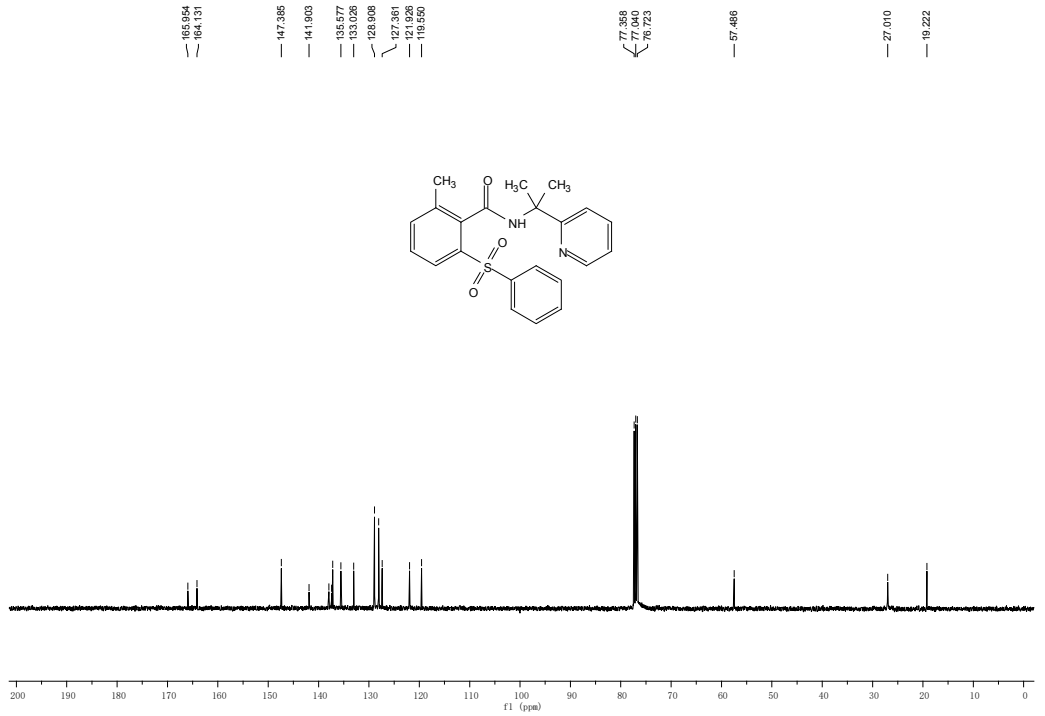
f1 (ppm)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27.010
19.222
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H3C
CH3
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N
S
O
O
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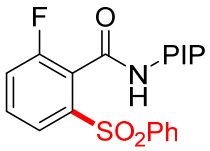
f1 (ppm)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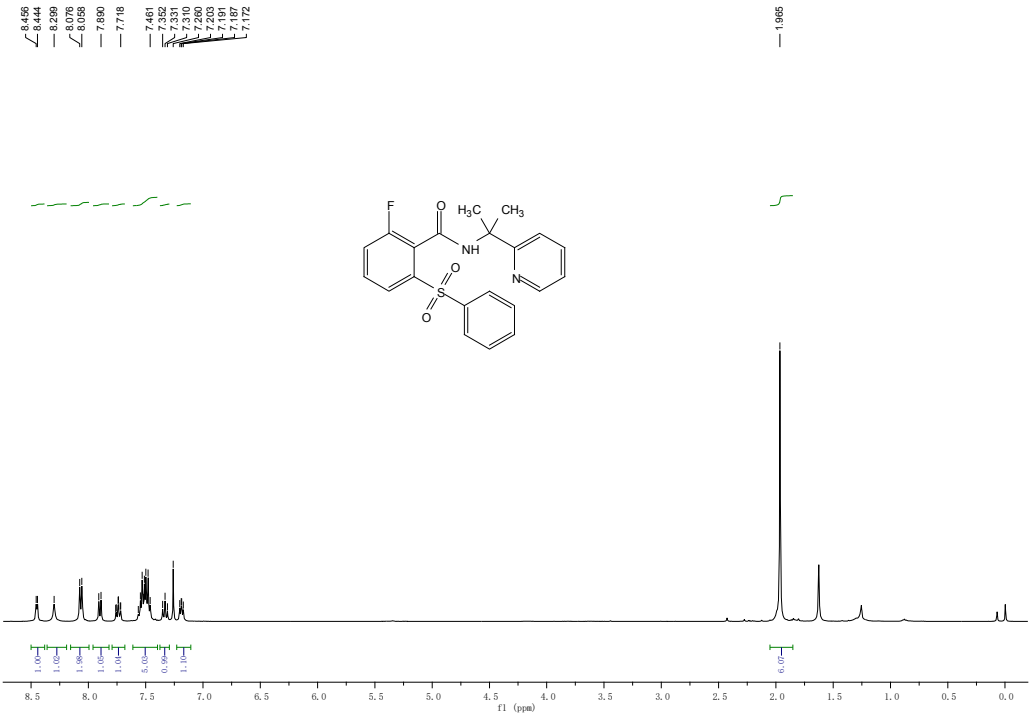
PIP
N
H
SO2Ph

3a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7.187
7.172
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O
H3C
CH3
NH
N
S
O
O
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1.07
1.04
5.03
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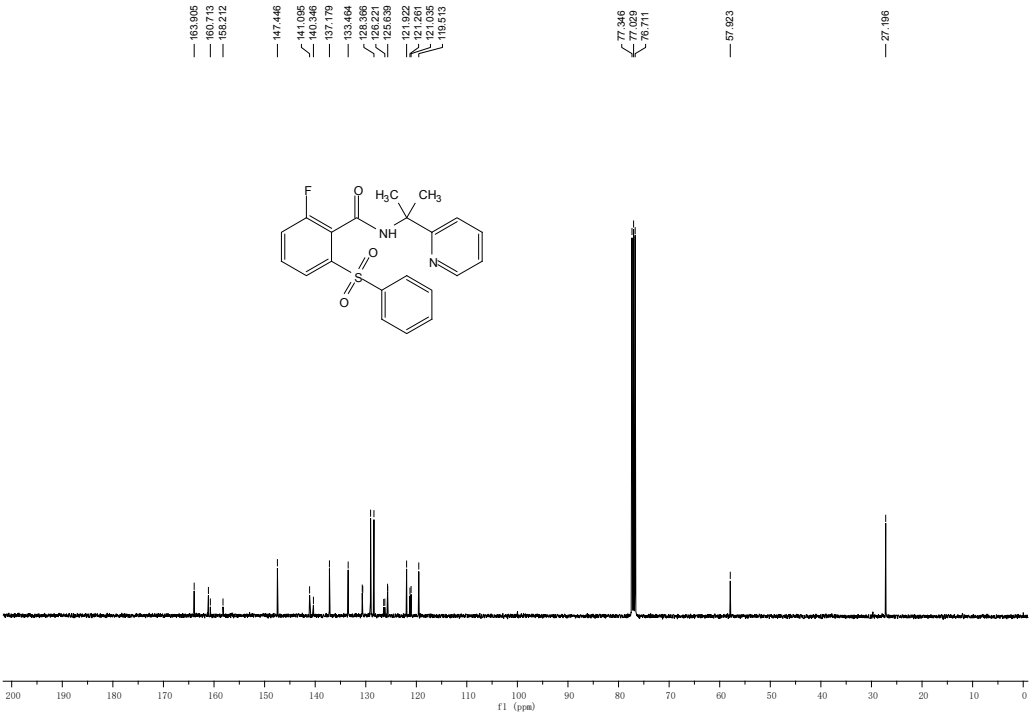
f1 (ppm)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77.029
76.711
57.923
27.196
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CH3
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N
S
O
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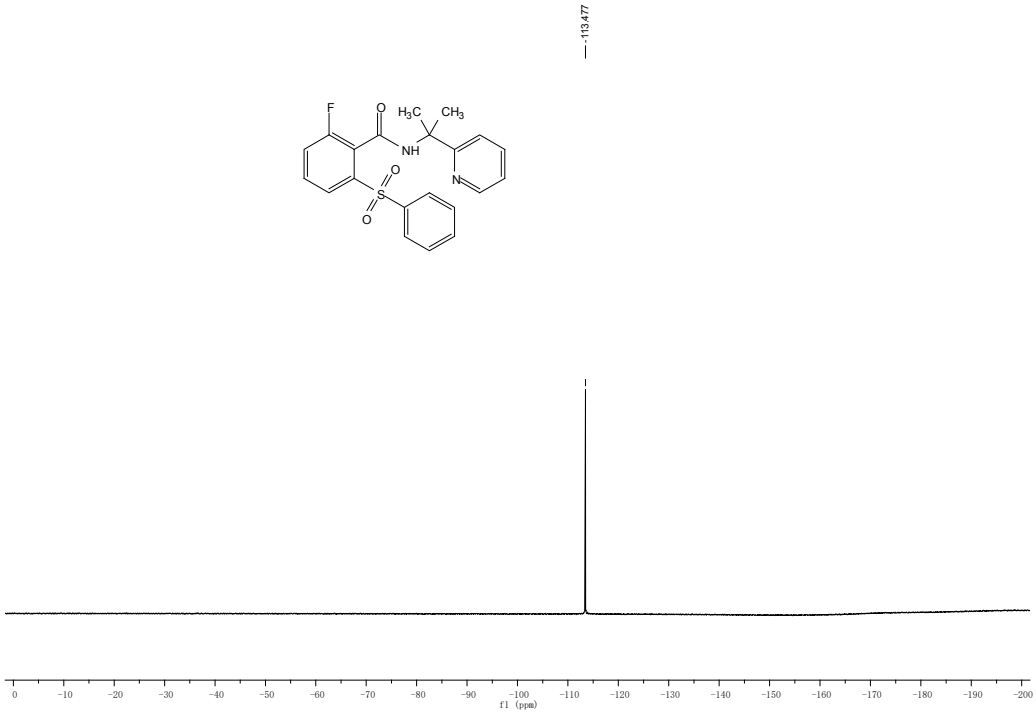
f1 (ppm)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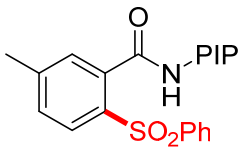
f1 (ppm)


O
N
H
PIP
SO2Ph

4a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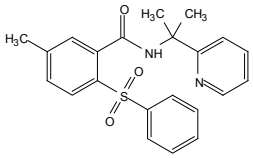
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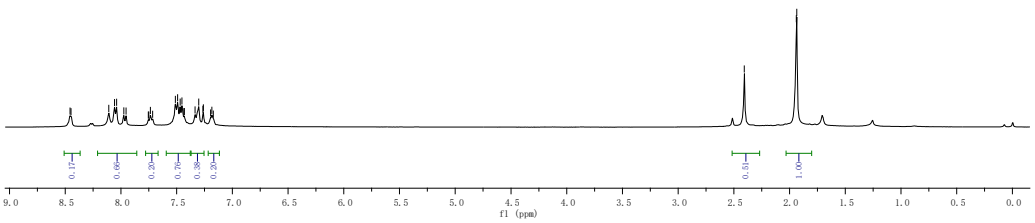
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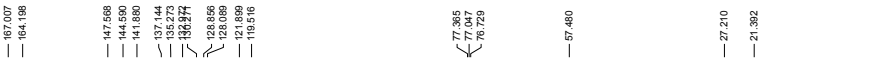
f1 (ppm)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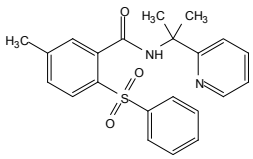
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S
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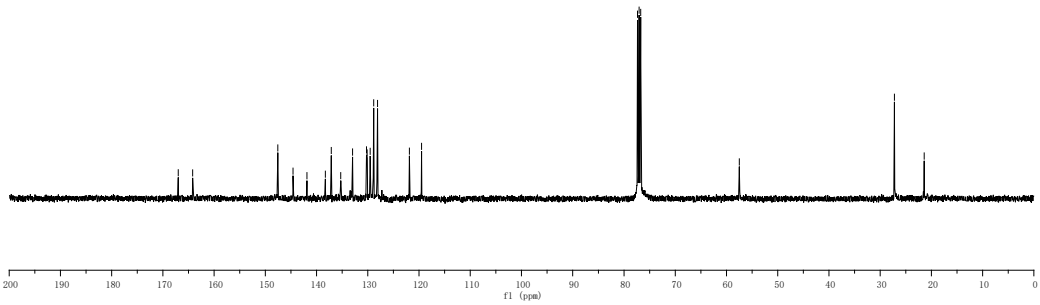
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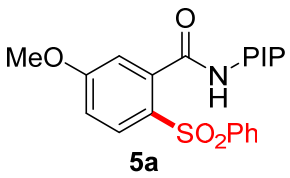
f1 (ppm)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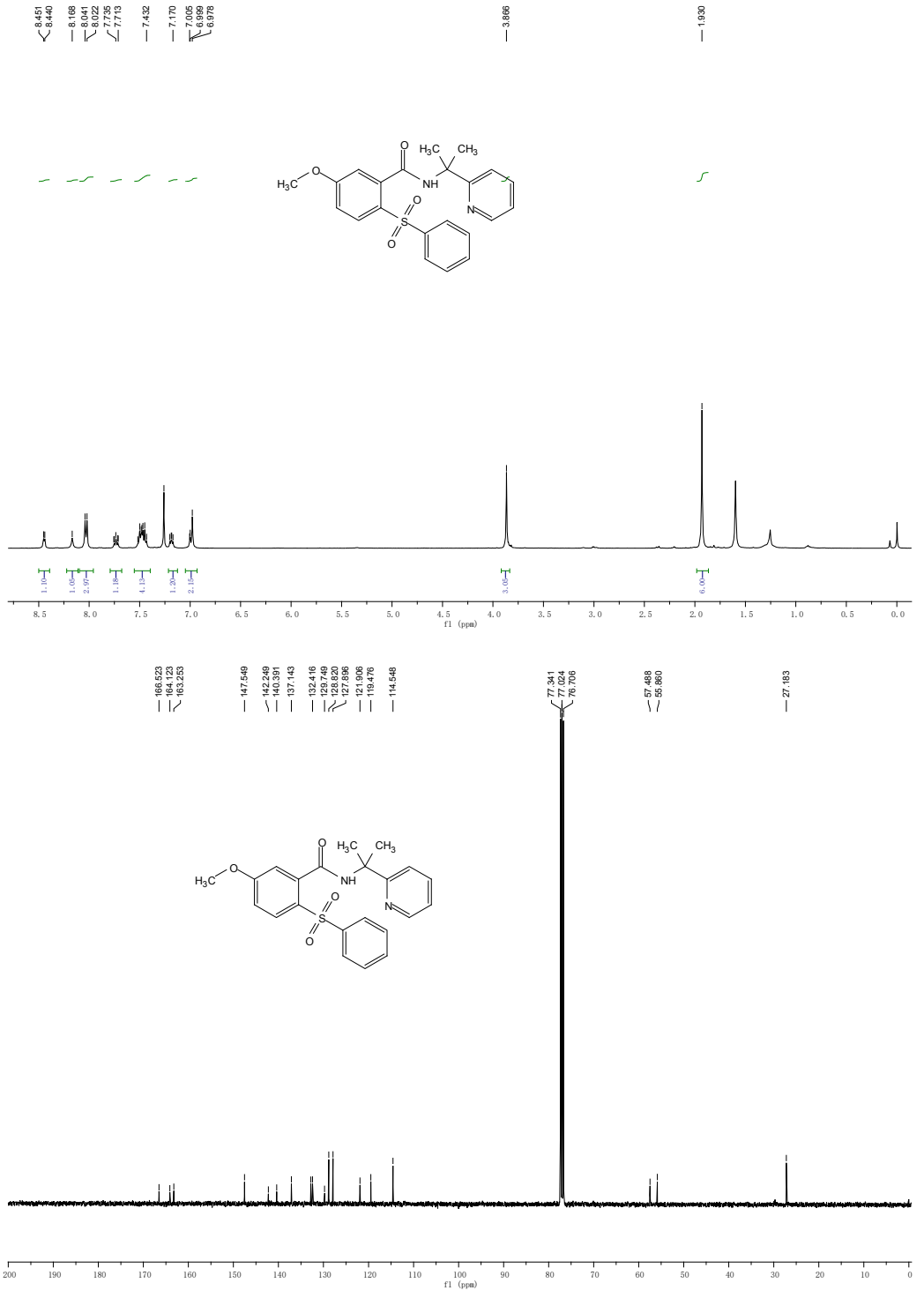
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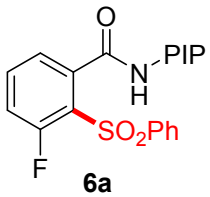
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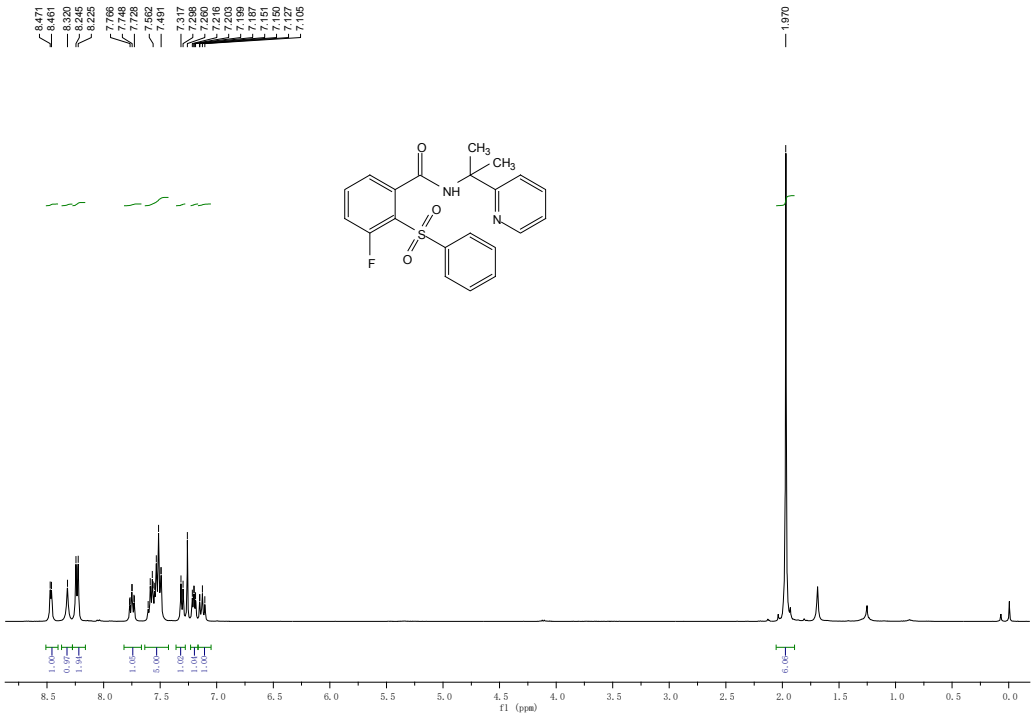
SO2Ph
F

6a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O
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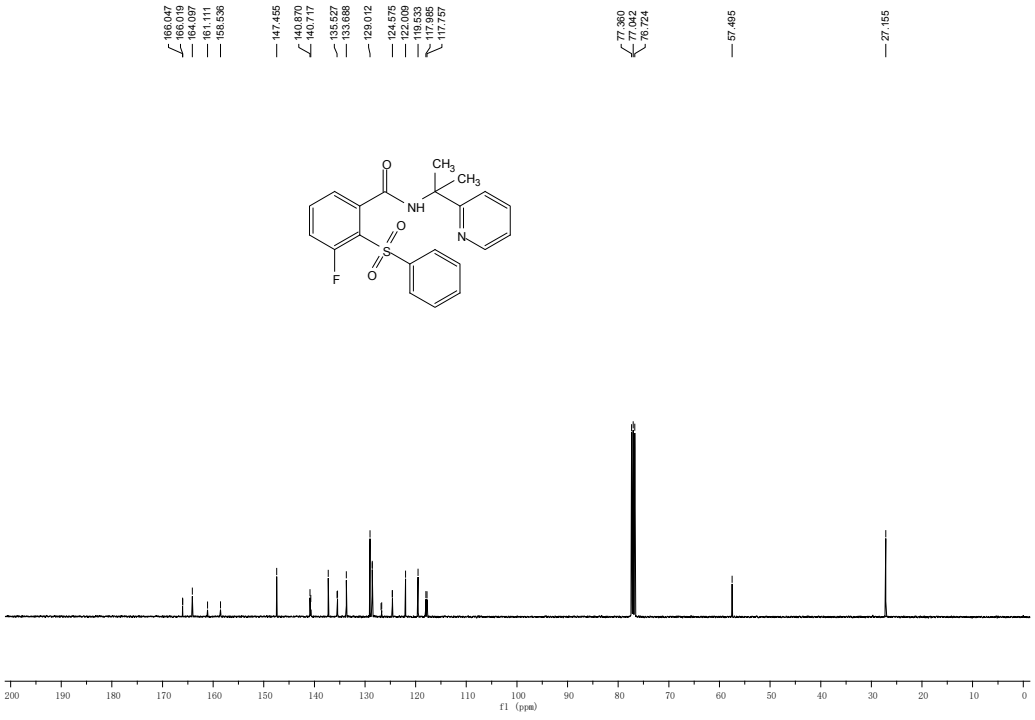
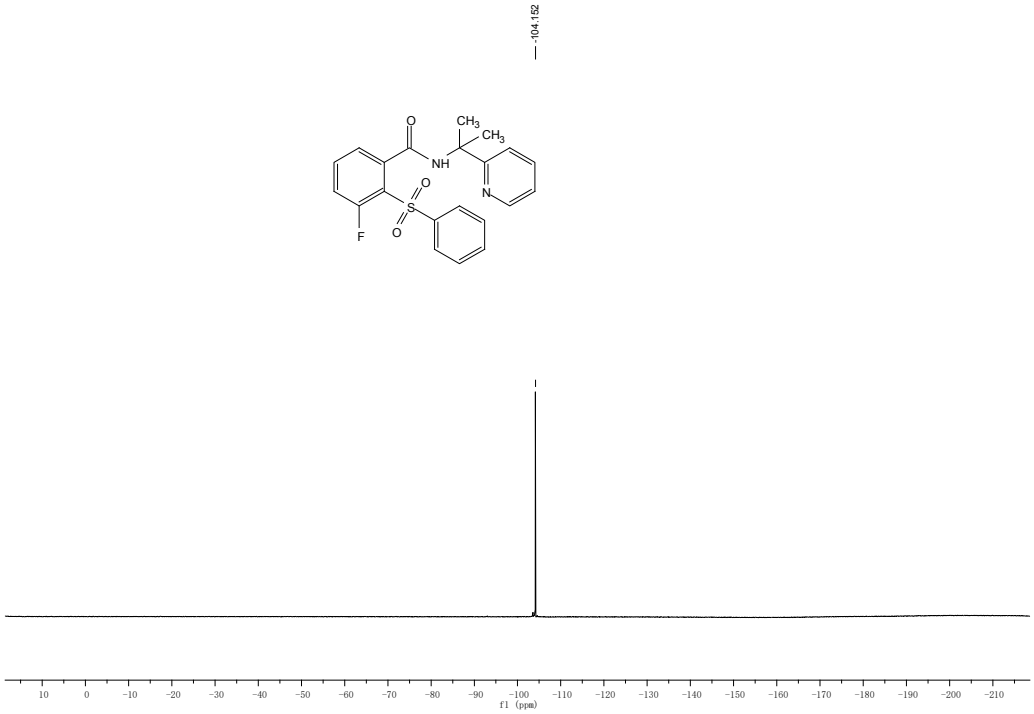
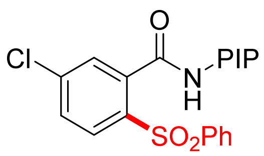
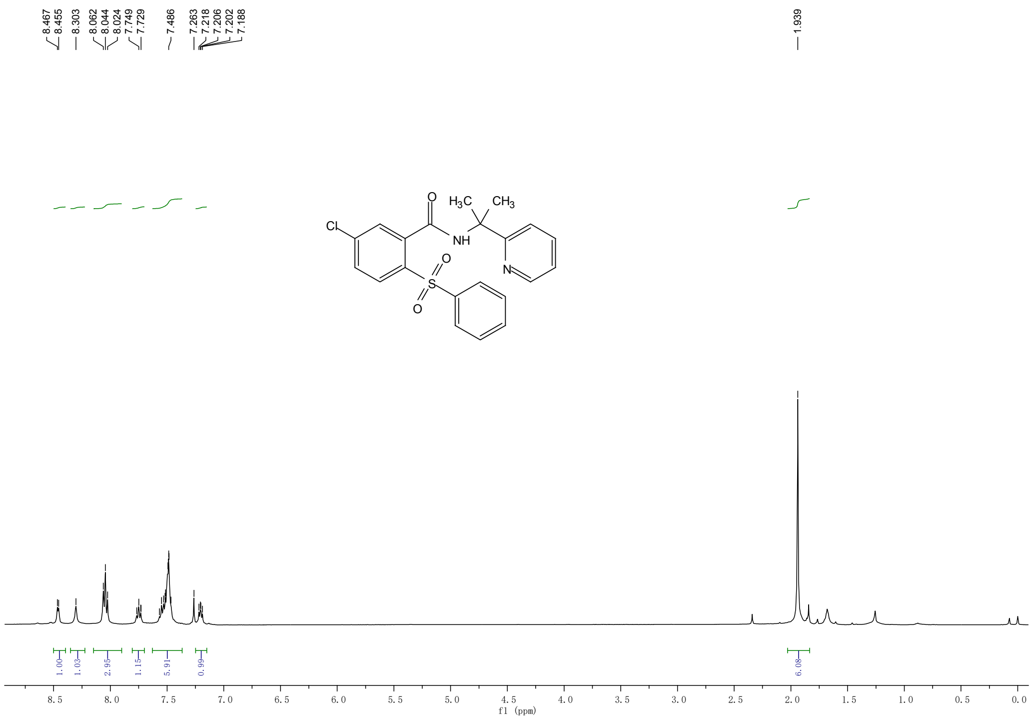
O
S
O
F
f1 (ppm)

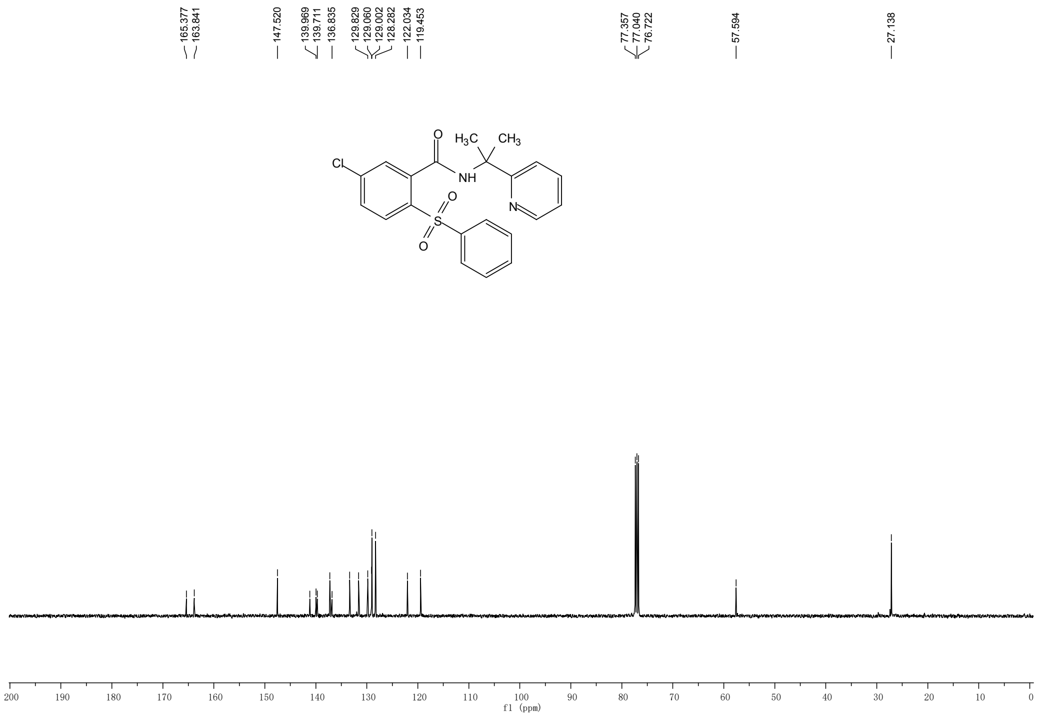

166.047
166.019
164.097
161.111
158.536
147.455
140.870
140.717
135.527
133.688
129.012
124.575
122.009
119.533
117.985
117.757
77.360
77.042
76.724
57.495
27.155
O
CH3
CH3
NH
N
O
S
O
F
f1 (ppm)

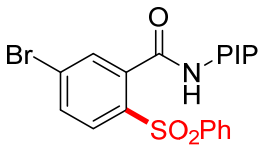

-104.152
O
CH3
CH3
NH
N
O
S
O
F
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


Cl
O
N
H
PIP
SO2Ph

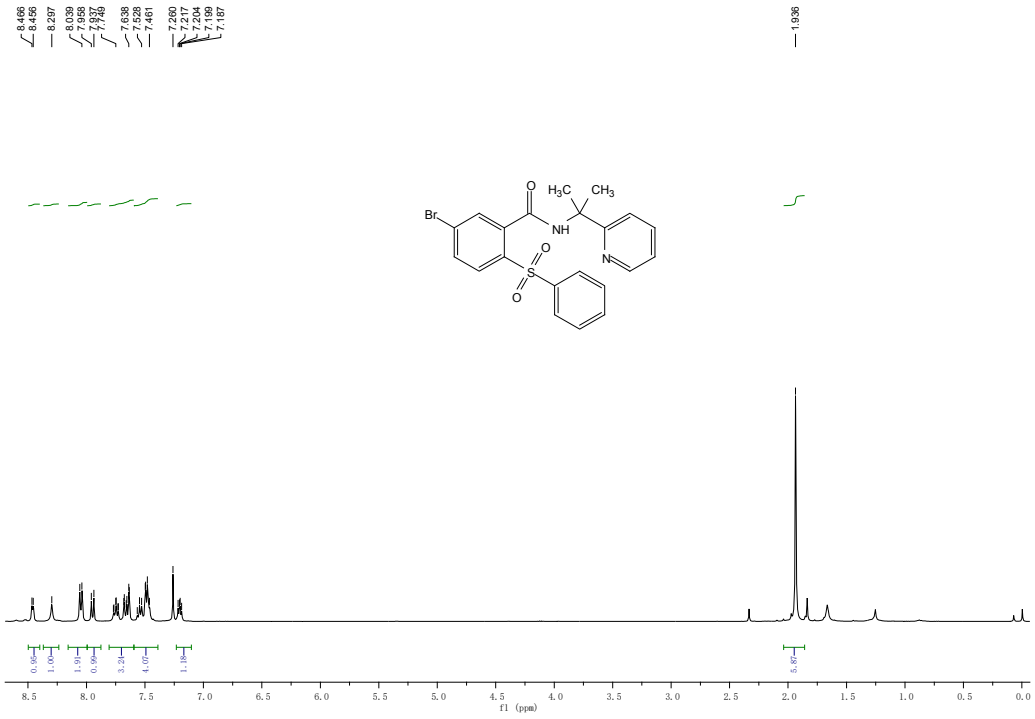
7a

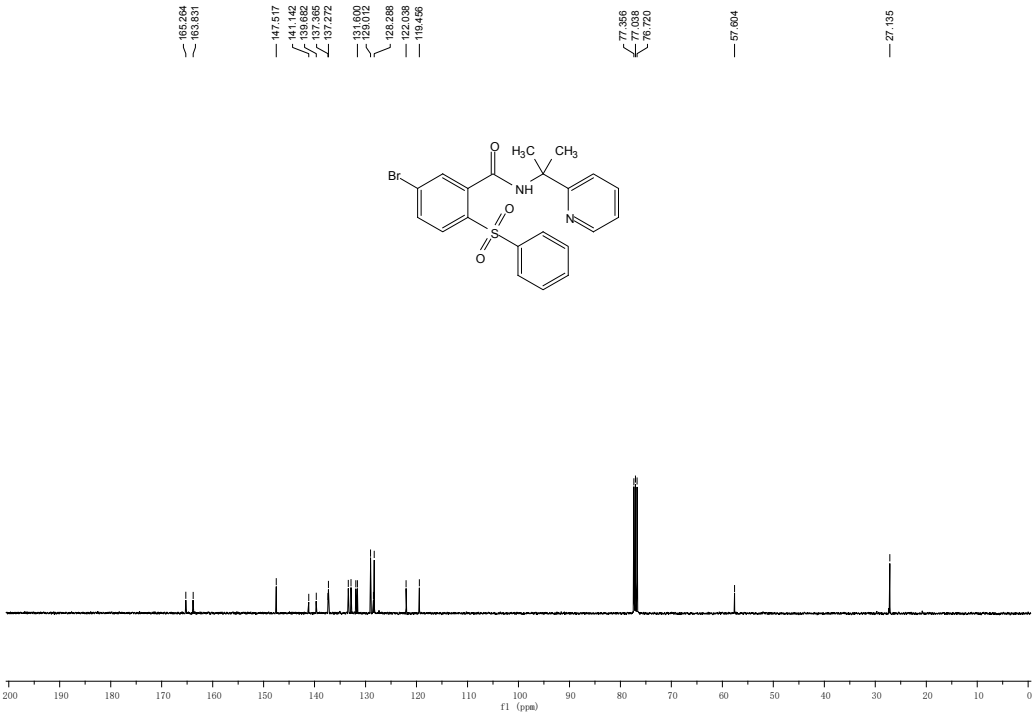

8.467
8.455
8.303
8.062
8.044
8.024
7.749
7.729
7.486
7.263
7.218
7.206
7.202
7.188
1.939
1.00
1.03
2.95
1.15
5.91
0.99
6.08
f1 (ppm)

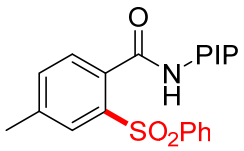

165.377
163.841
147.520
139.969
139.711
136.835
129.829
129.060
129.002
128.282
122.034
119.453
77.357
77.040
76.722
57.594
27.138
f1 (ppm)


O
Br
N
PIP
H
SO2Ph

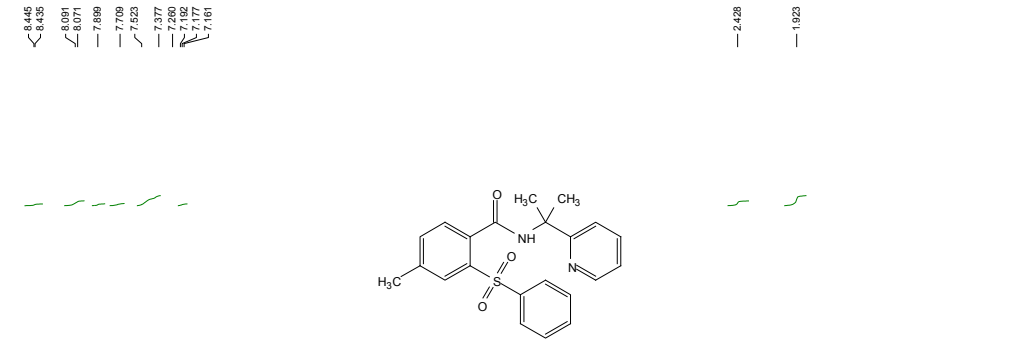
8a

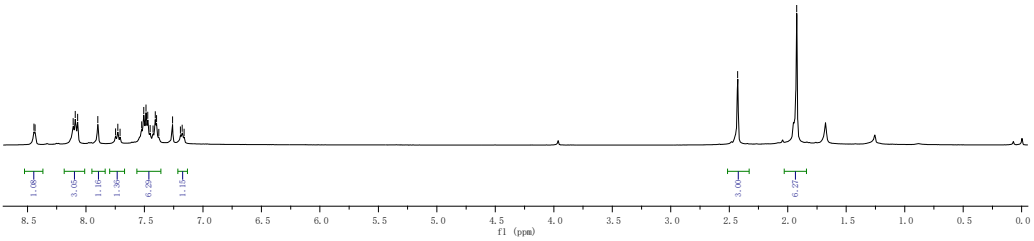

8.466
8.456
8.297
8.039
7.958
7.937
7.749
7.638
7.528
7.461
7.200
7.177
7.204
7.199
7.187
1.936
O
H3C
CH3
Br
NH
N
O
S
O
0.98
1.00
1.91
0.99
3.24
4.00
1.18
5.87
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

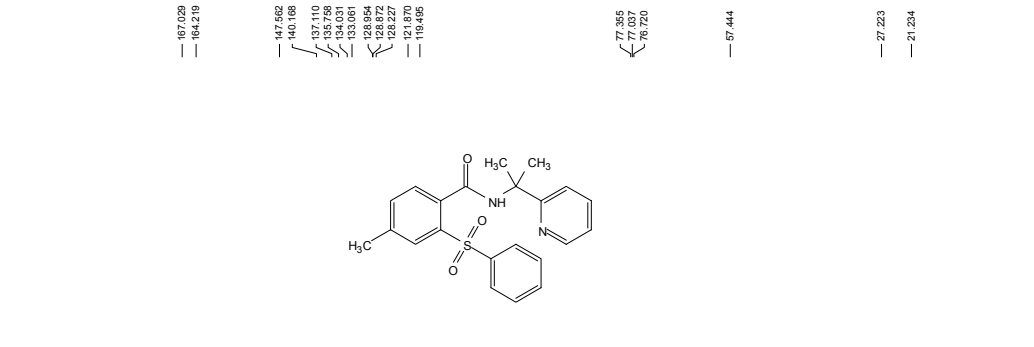

165.264
163.831
147.517
141.142
139.682
137.365
137.272
131.600
129.012
128.288
122.038
119.456
77.366
77.058
76.720
57.604
27.135
O
H3C
CH3
Br
NH
N
O
S
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

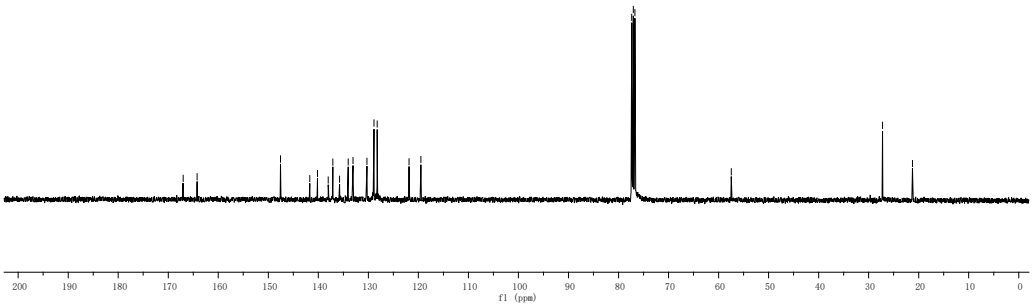

O
N
H
PIP
SO2Ph

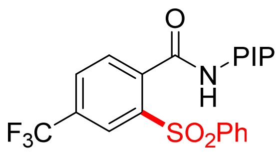
9a


8.445
8.435
8.091
8.071
7.899
7.709
7.523
7.377
7.260
7.192
7.177
7.161
2.428
1.923
O
H3C
CH3
NH
N
H3C
S
O
O

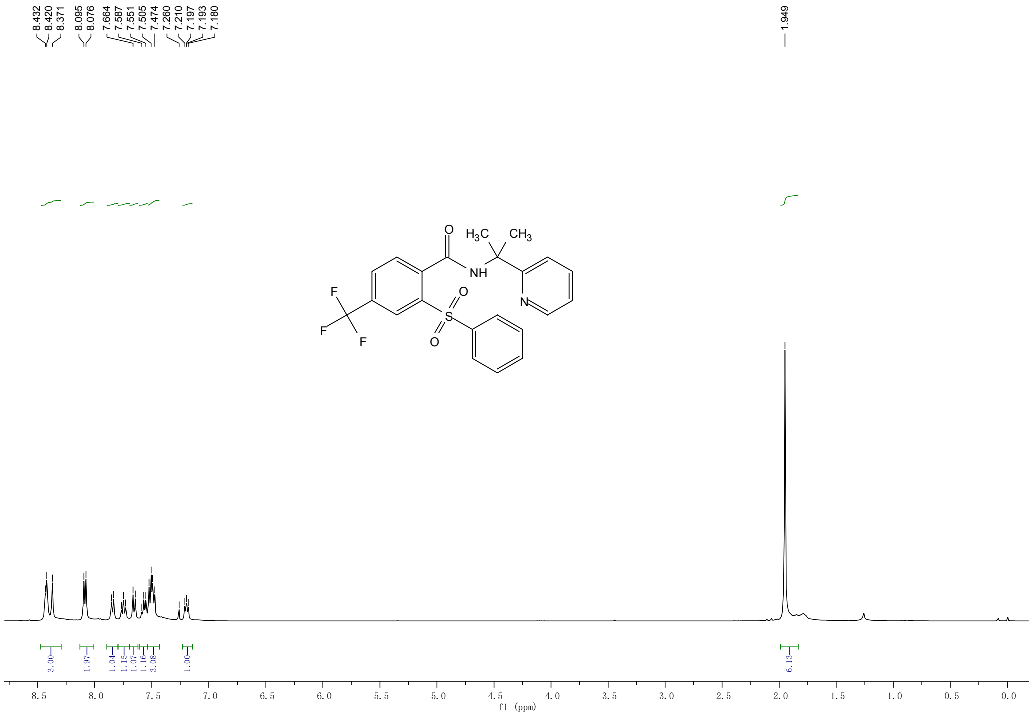

1.08
3.05
1.10
1.38
6.29
1.10
3.00
6.27
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


167.029
164.219
147.562
140.168
137.110
135.758
134.031
133.061
128.954
128.572
128.227
121.870
119.485
77.355
77.037
76.720
57.444
27.223
21.234
O
H3C
CH3
NH
N
H3C
S
O
O


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


PIP
SO2Ph
F3C

10a


8.432
8.420
8.371
8.095
8.076
7.664
7.587
7.551
7.505
7.474
7.260
7.210
7.197
7.193
7.180
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1.97
1.04
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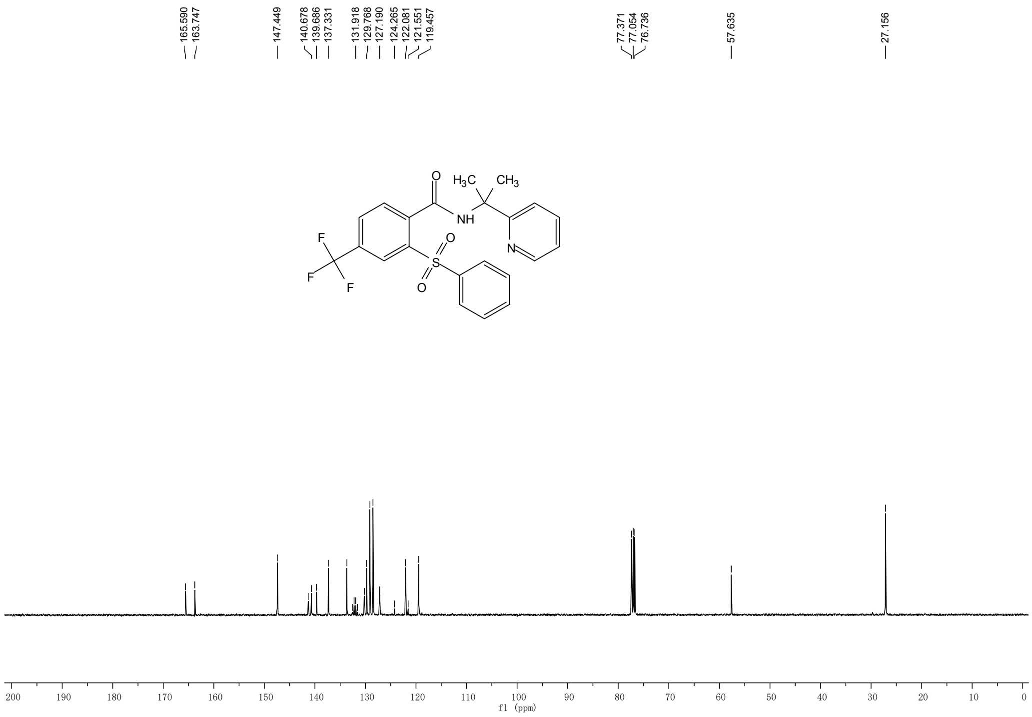
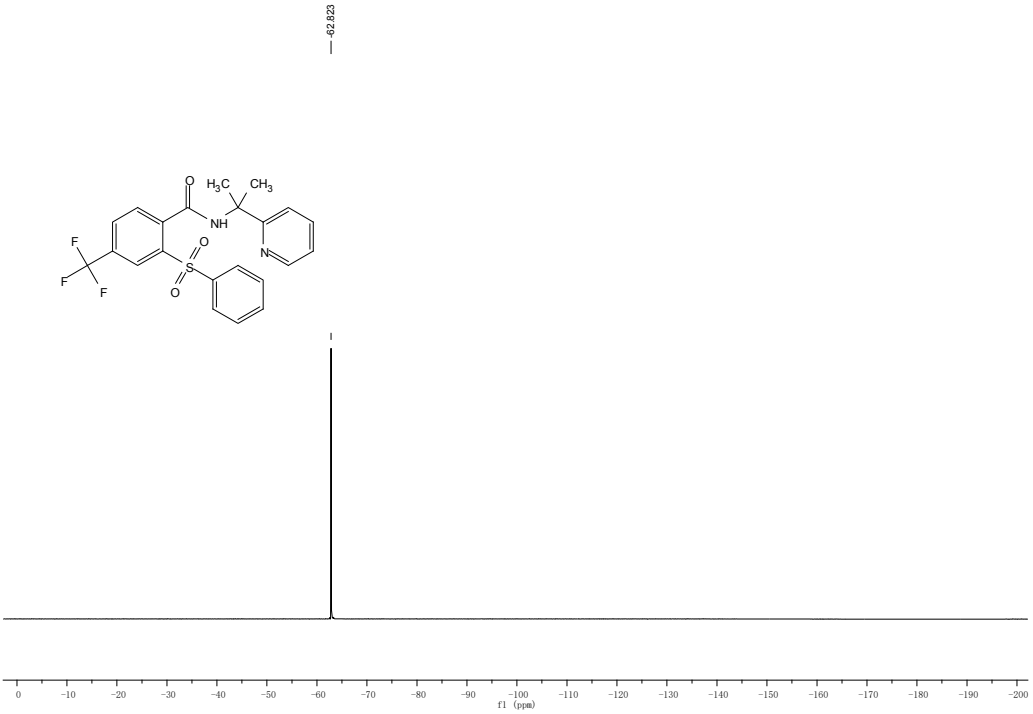
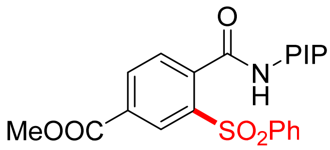
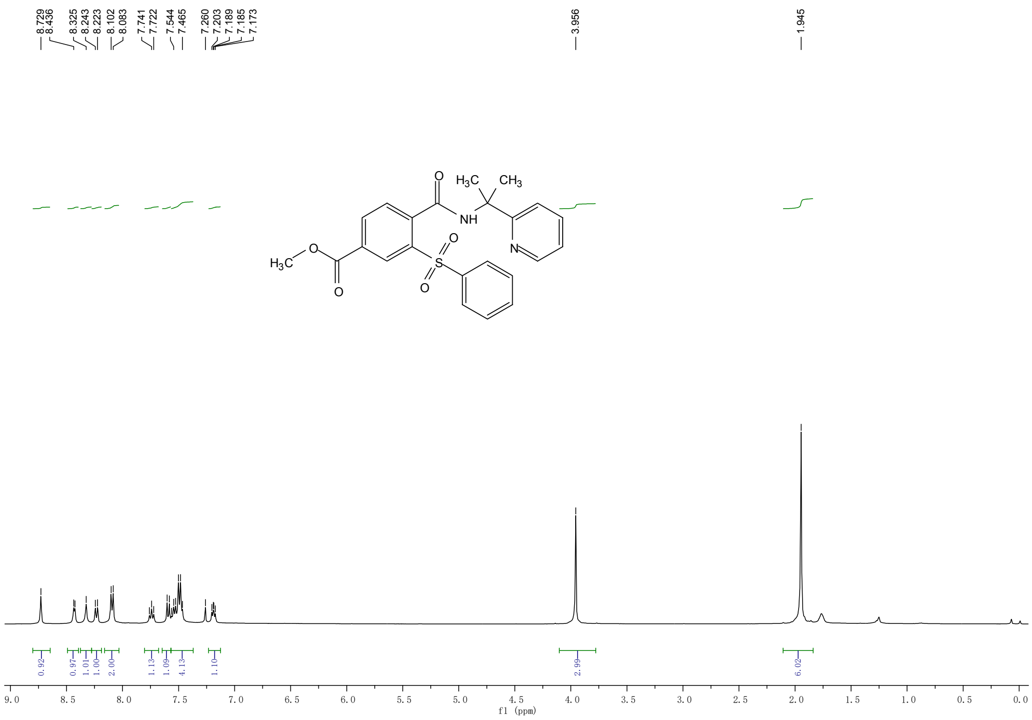
1.07
1.16
3.08
1.00
6.13
f1 (ppm)


165.590
163.747
147.449
140.678
139.686
137.331
131.918
129.768
127.190
124.285
122.081
121.551
119.457
77.371
77.054
76.736
57.635
27.156
f1 (ppm)


-62.823
O
H3C
CH3
NH
N
F
F
F
O
S
O
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)


MeOOC
N
H
PIP
O
SO2Ph

11a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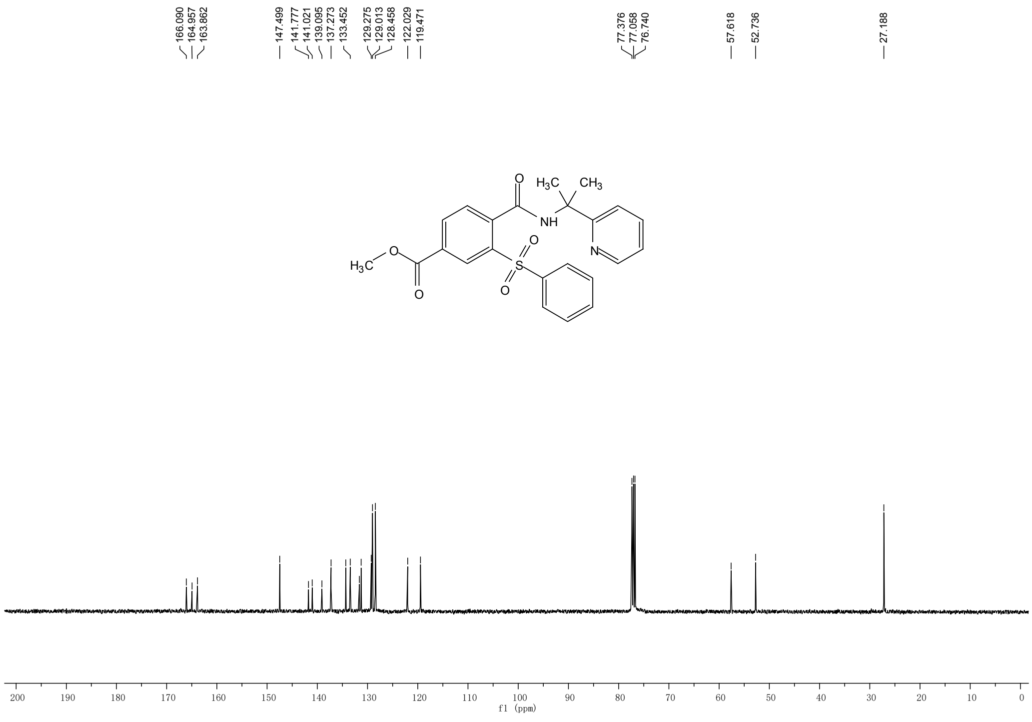
8.436
8.325
8.243
8.223
8.102
8.083
7.741
7.722
7.544
7.465
7.260
7.203
7.189
7.185
7.173
3.956
1.945
0.92
0.97
1.01
1.00
2.00
1.13
1.09
4.13
1.10
2.99
6.02
f1 (ppm)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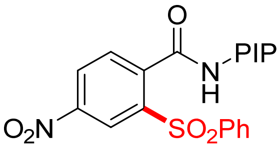
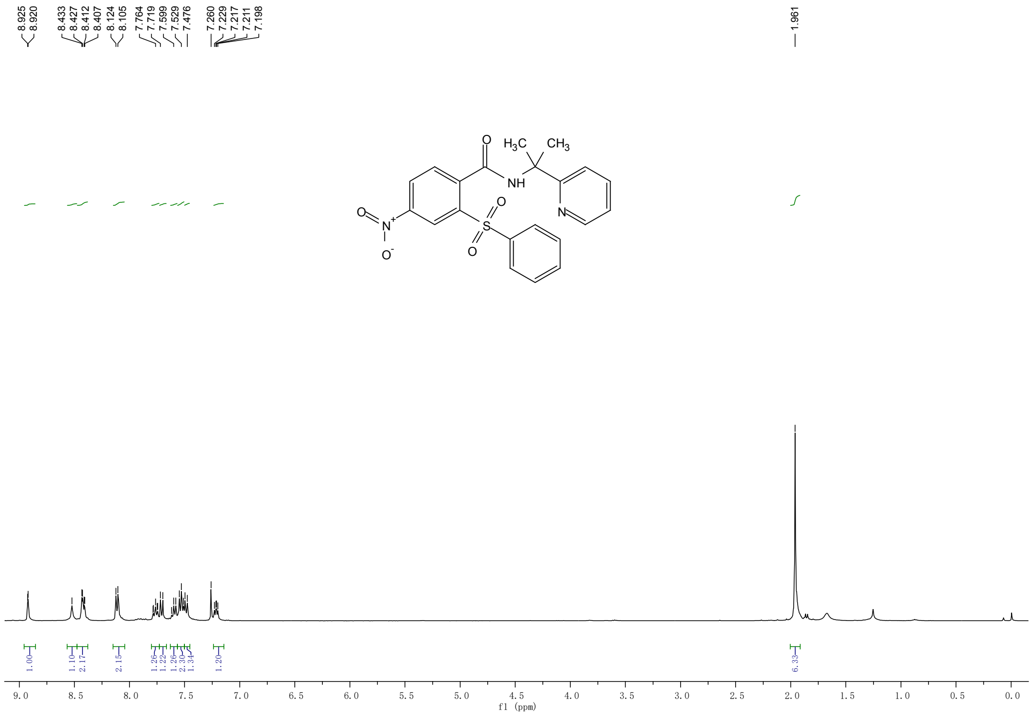
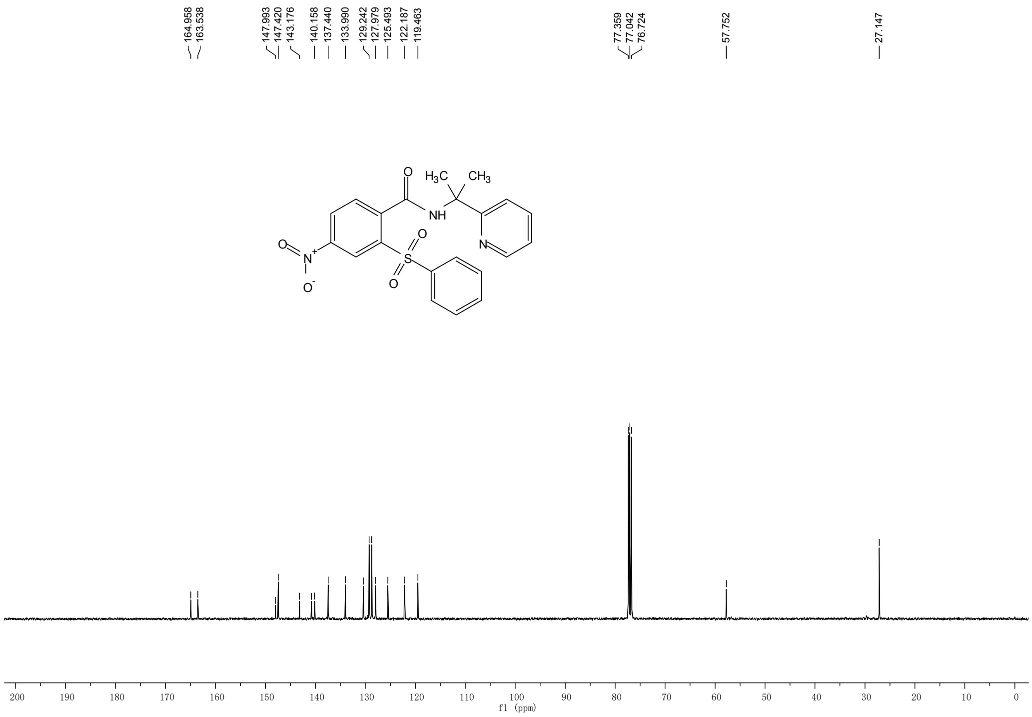
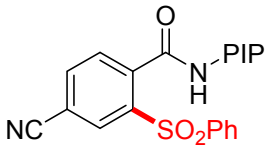
164.957
163.862
147.499
141.777
141.021
139.095
137.273
133.452
129.275
129.013
128.458
122.029
119.471
77.376
77.058
76.740
57.618
52.736
27.188
f1 (ppm)


O
N
H
PIP
O_2N
SO_2Ph

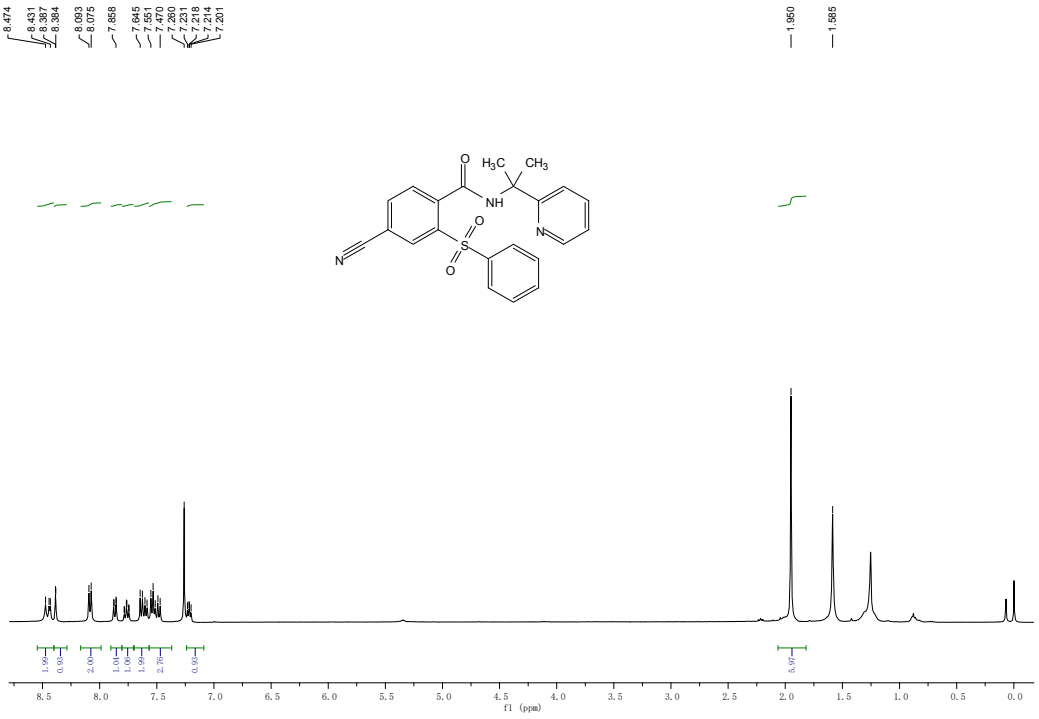
12a


8.925
8.920
8.433
8.427
8.412
8.407
8.124
8.105
7.764
7.719
7.599
7.529
7.476
7.260
7.229
7.217
7.211
7.198
1.961
1.00
1.10
2.17
2.15
1.26
1.22
1.26
2.30
1.34
1.20
6.33
f1 (ppm)


164.958
163.538
147.993
147.420
143.176
140.158
137.440
133.990
129.242
127.979
125.493
122.187
119.463
77.359
77.042
76.724
57.752
27.147
f1 (ppm)


O
N
PIP
H
NC
SO2Ph

13a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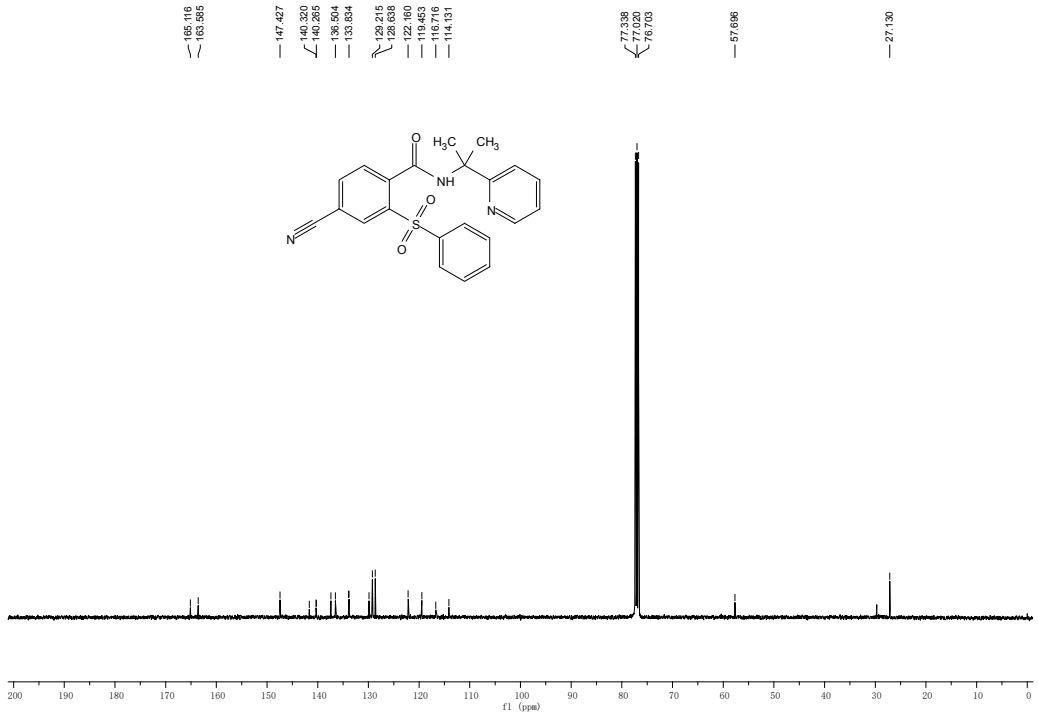
8.387
8.384
8.093
8.075
7.858
7.645
7.551
7.470
7.260
7.231
7.218
7.214
7.201
1.950
1.585
O
H3C
CH3
NH
N
O
S
O
N
1.99
0.99
2.08
1.04
1.06
1.99
2.78
0.98
5.97
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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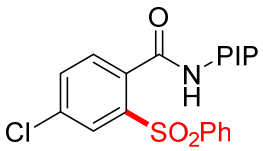
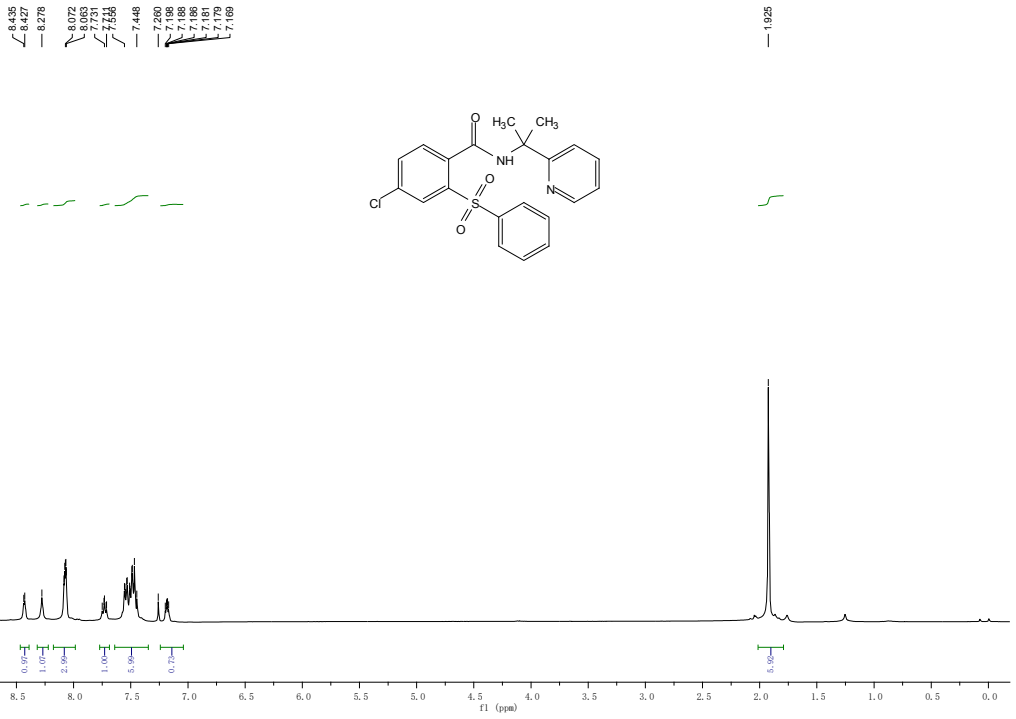
140.320
140.265
136.504
133.834
129.215
128.638
122.160
119.453
116.716
114.131
77.338
77.020
76.703
57.696
27.130
O
H3C
CH3
NH
N
O
S
O
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


O
N
H
PIP
Cl
SO2Ph

14a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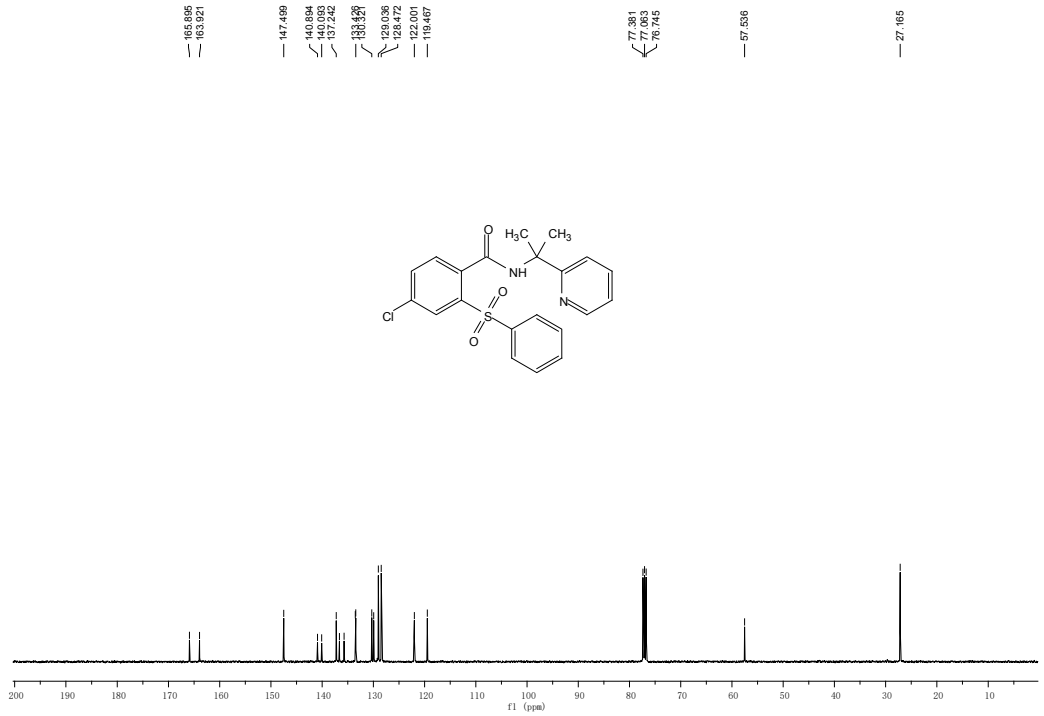
8.427
8.278
8.072
8.063
7.731
7.711
7.556
7.448
7.260
7.198
7.188
7.186
7.165
7.179
7.169
1.925
O
H3C
CH3
NH
N
Cl
S
O
O
0.95
1.00
2.98
1.00
5.98
0.72
5.98
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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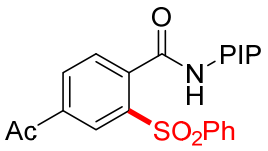
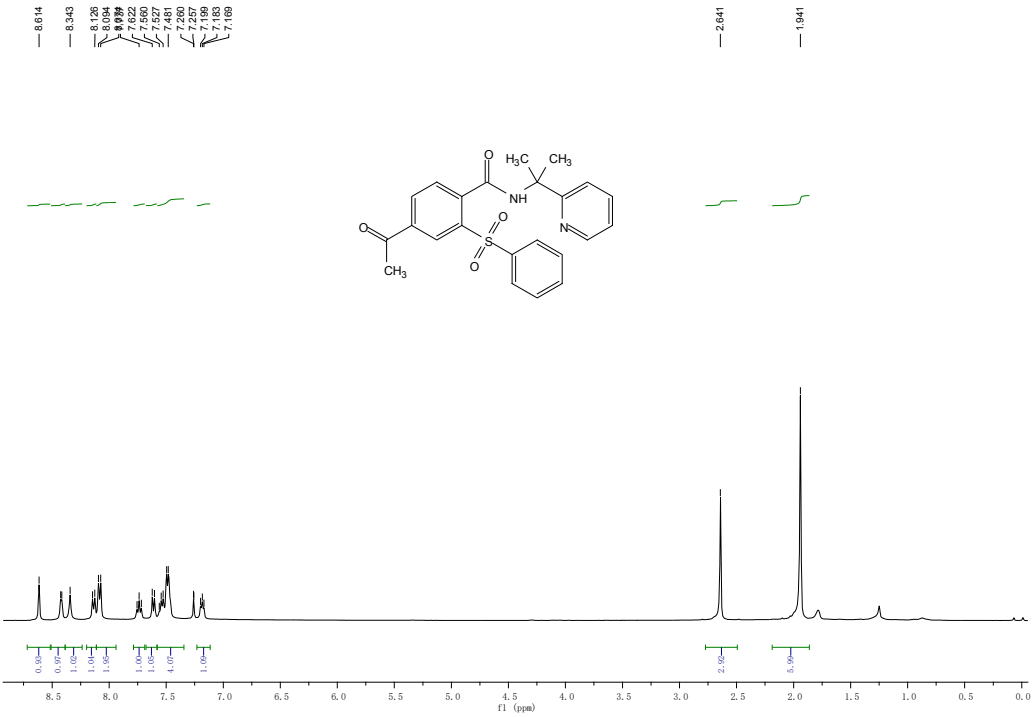
140.093
137.242
133.426
130.321
129.036
128.472
122.001
119.467
77.381
77.063
76.745
57.536
27.165
O
H3C
CH3
NH
N
Cl
S
O
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


O
N
H
PIP
Ac
SO2Ph

15a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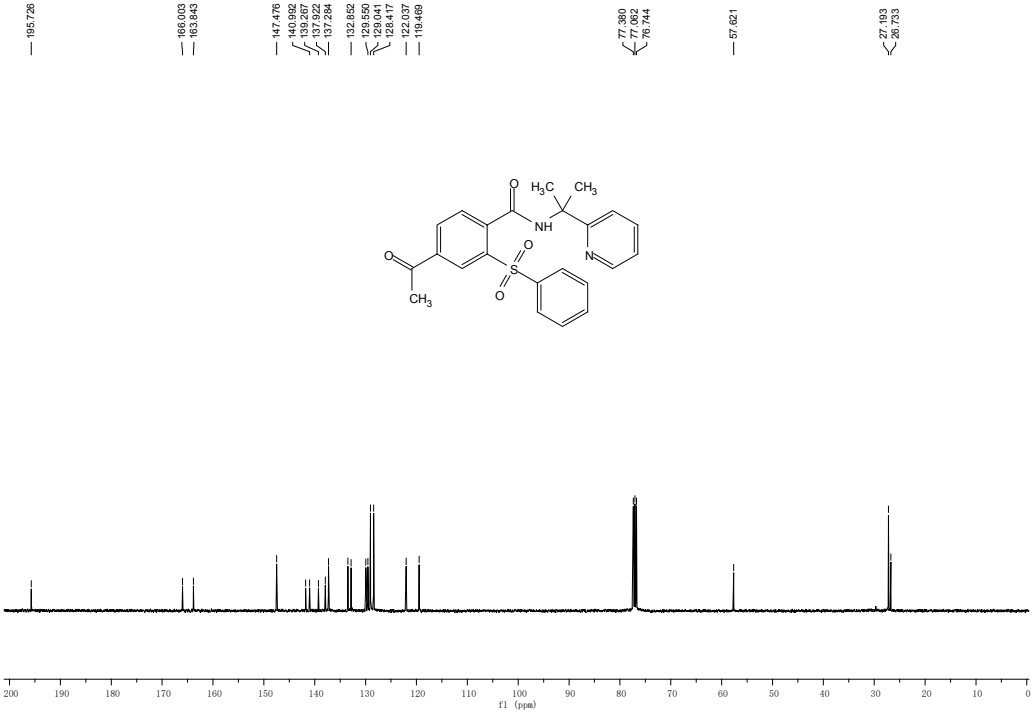
8.094
7.622
7.560
7.527
7.481
7.260
7.257
7.199
7.183
7.169
2.641
1.941
O
H3C
CH3
NH
N
O
S
O
O
CH3
0.98
0.98
1.01
1.04
1.95
1.01
1.01
4.07
1.00
2.90
5.99
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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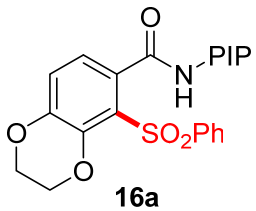
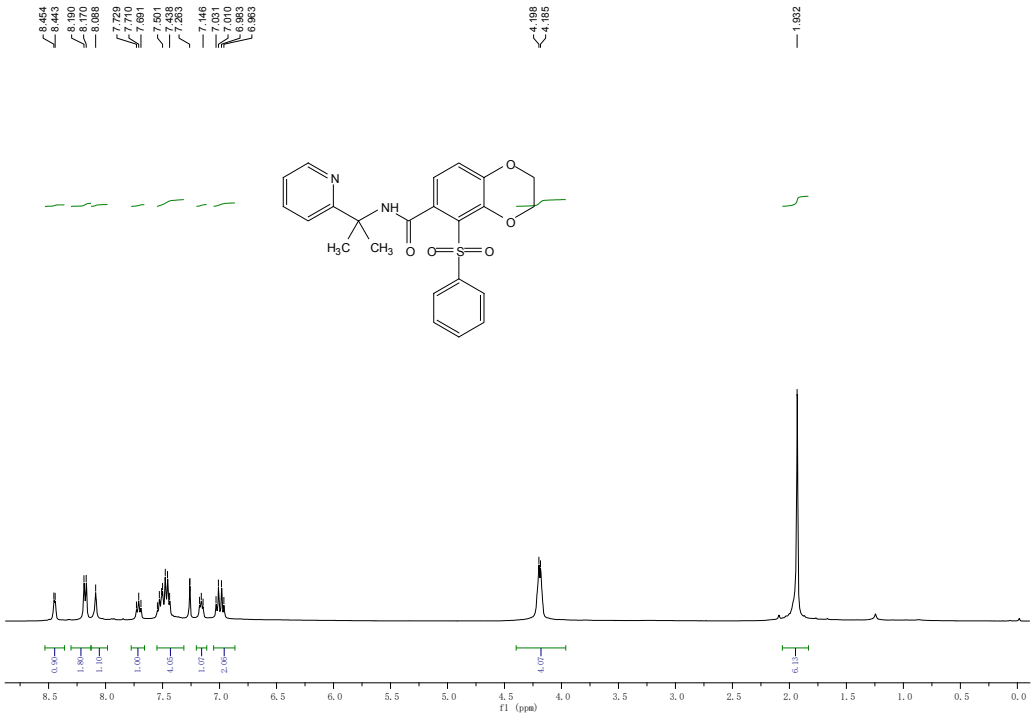
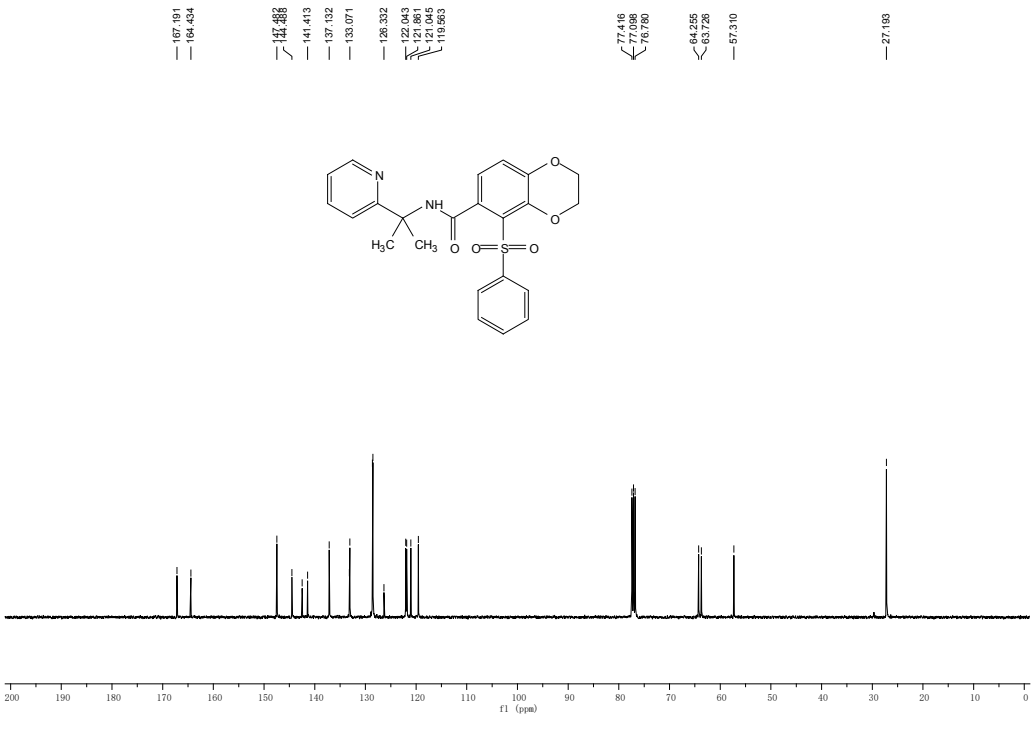
147.476
140.992
139.267
137.922
137.284
132.852
129.566
129.041
128.417
122.037
119.469
77.380
77.062
76.744
57.621
27.193
26.733
O
H3C
CH3
NH
N
O
S
O
O
CH3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


O
N
PIP
H
O
SO2Ph
O

16a


8.454
8.443
8.190
8.170
8.088
7.729
7.710
7.691
7.501
7.438
7.263
7.146
7.031
7.010
6.983
6.963
4.198
4.185
1.932
N
NH
H3C
CH3
O
O
S
O
O
O
0.96
1.88
1.10
1.00
4.08
1.07
2.06
4.07
6.10
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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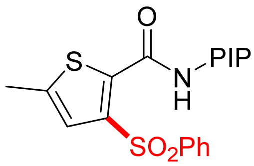
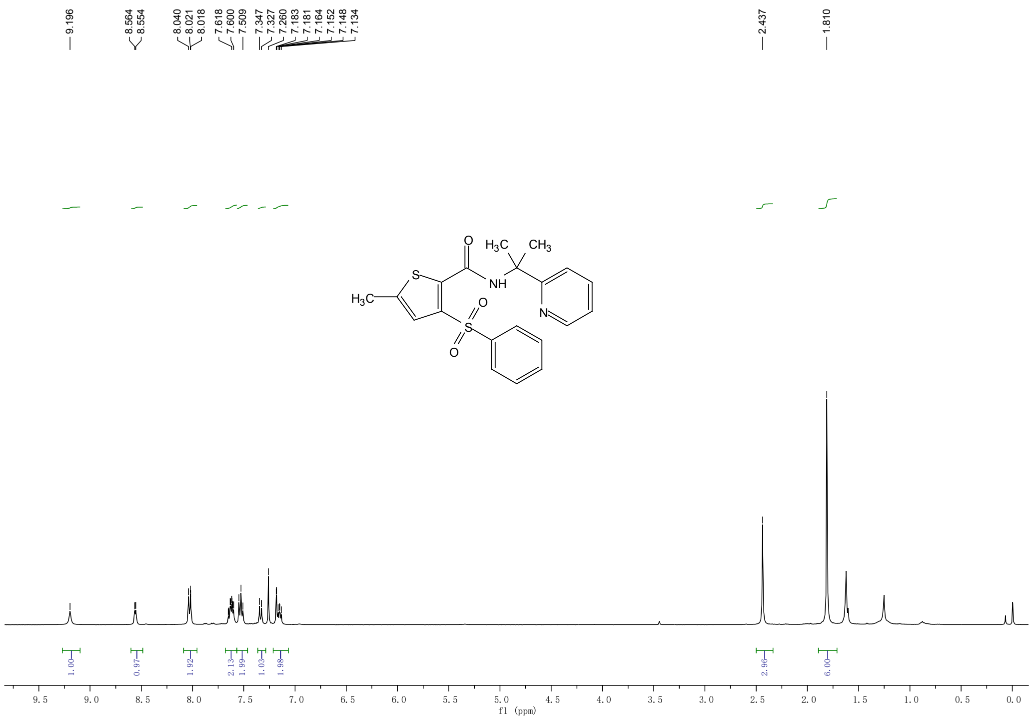
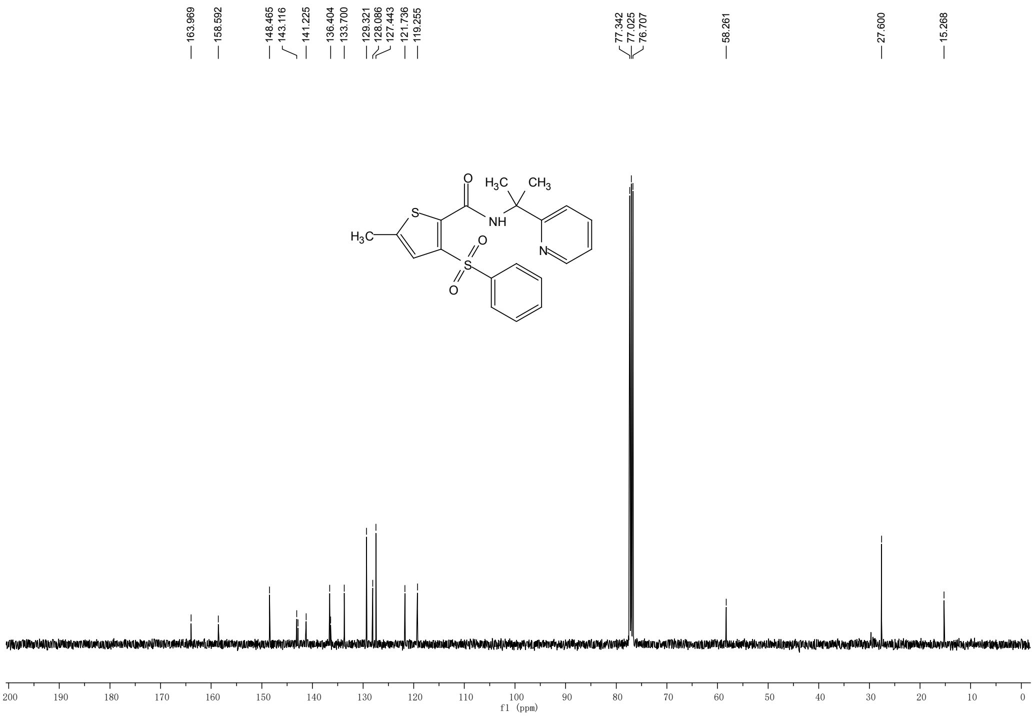
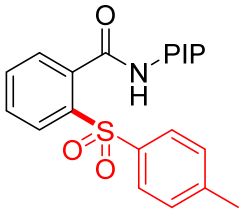
164.434
147.486
144.488
141.413
137.132
133.071
126.332
122.043
121.861
121.045
119.563
77.416
77.098
76.780
64.255
63.726
57.310
27.193
N
NH
H3C
CH3
O
O
S
O
O
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


O
S
N
PIP
H
SO2Ph

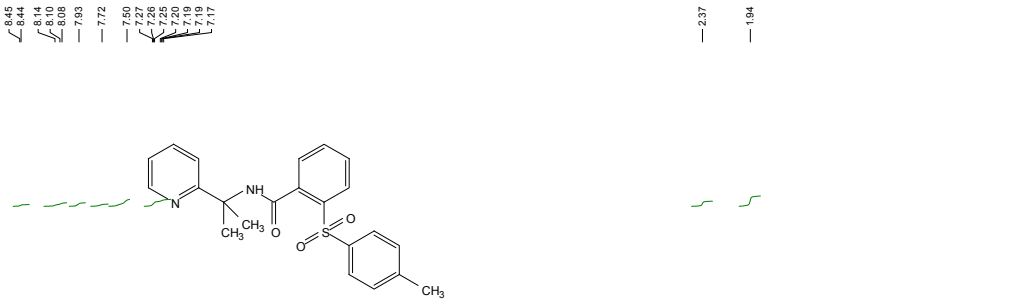
17a

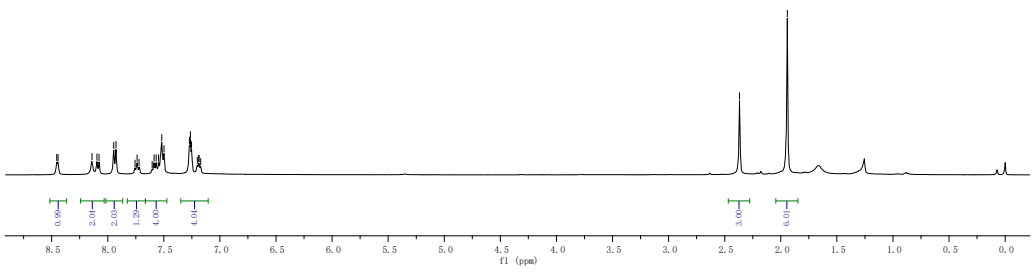

9.196
8.564
8.554
8.040
8.021
8.018
7.618
7.600
7.509
7.347
7.327
7.260
7.183
7.181
7.164
7.152
7.148
7.134
2.437
1.810
1.00
0.97
1.92
2.13
1.99
1.03
1.98
2.96
6.00
f1 (ppm)

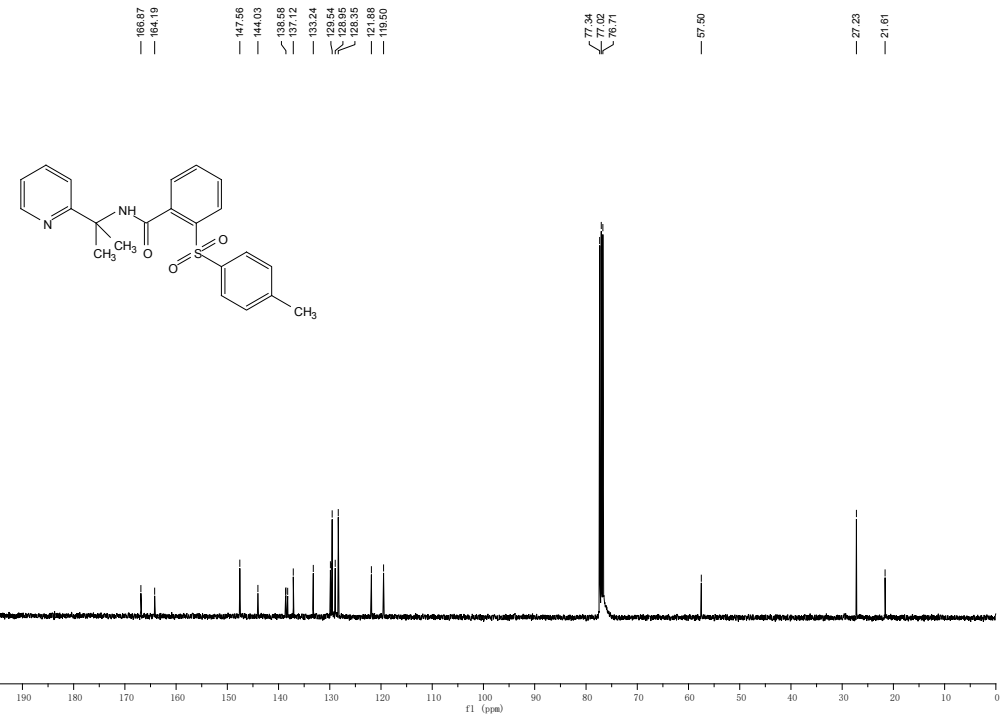

163.969
158.592
148.465
143.116
141.225
136.404
133.700
129.321
128.086
127.443
121.736
119.255
77.342
77.025
76.707
58.261
27.600
15.268
f1 (ppm)

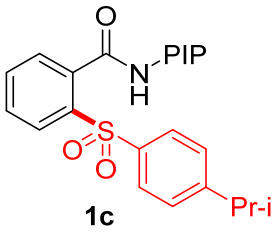

O
N
PIP
H
S
O
O

1b


8.45
8.44
8.14
8.10
8.08
7.93
7.72
7.50
7.27
7.26
7.25
7.20
7.19
7.19
7.17
2.37
1.94
NH
N
CH3
CH3
O
S
O
O
CH3

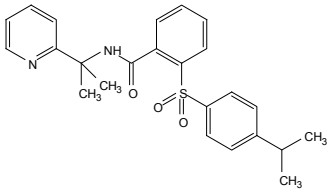

0.98
2.01
2.00
1.28
4.00
4.00
3.00
6.01
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

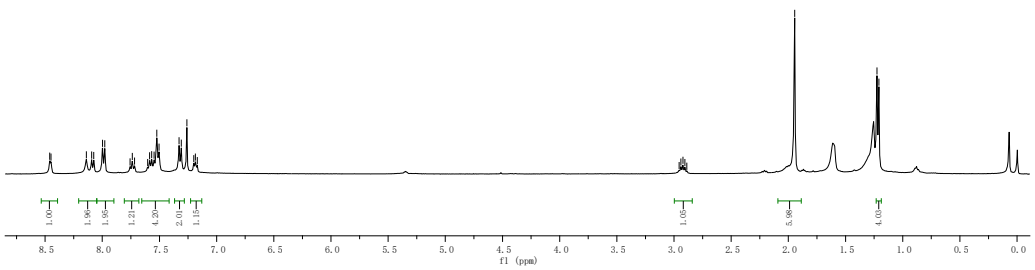

166.87
164.19
147.56
144.03
138.58
137.12
133.24
129.54
128.95
128.35
121.88
119.50
77.34
77.02
76.71
57.50
27.23
21.61
NH
N
CH3
CH3
O
O
S
O
CH3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

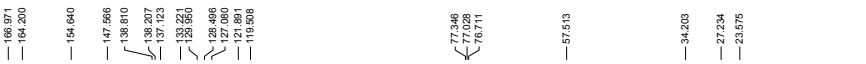

O
N
PIP
H
S
O
O
Pr-i

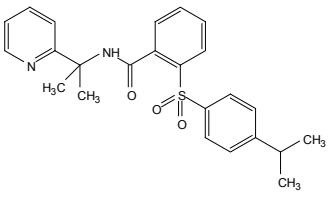
1c

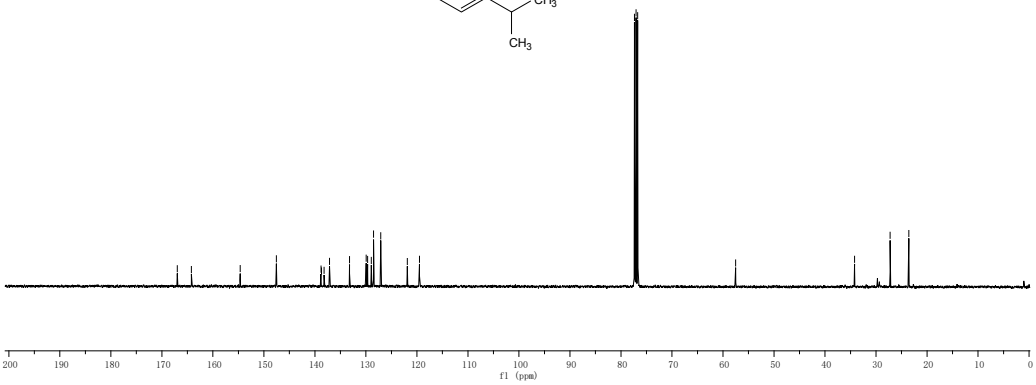

8.459
8.448
8.140
8.094
8.075
7.998
7.978
7.737
7.718
7.568
7.503
7.329
7.309
7.290
7.200
7.186
7.170
2.956
2.939
2.922
2.905
2.888
1.945
1.225
1.208

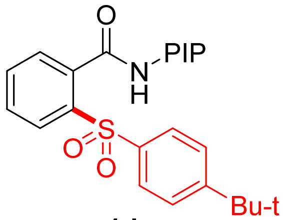

NH
N
CH3
CH3
O
O
S
O
CH3
CH3


1.00
1.98
1.98
1.21
4.20
2.00
1.10
1.00
5.98
4.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

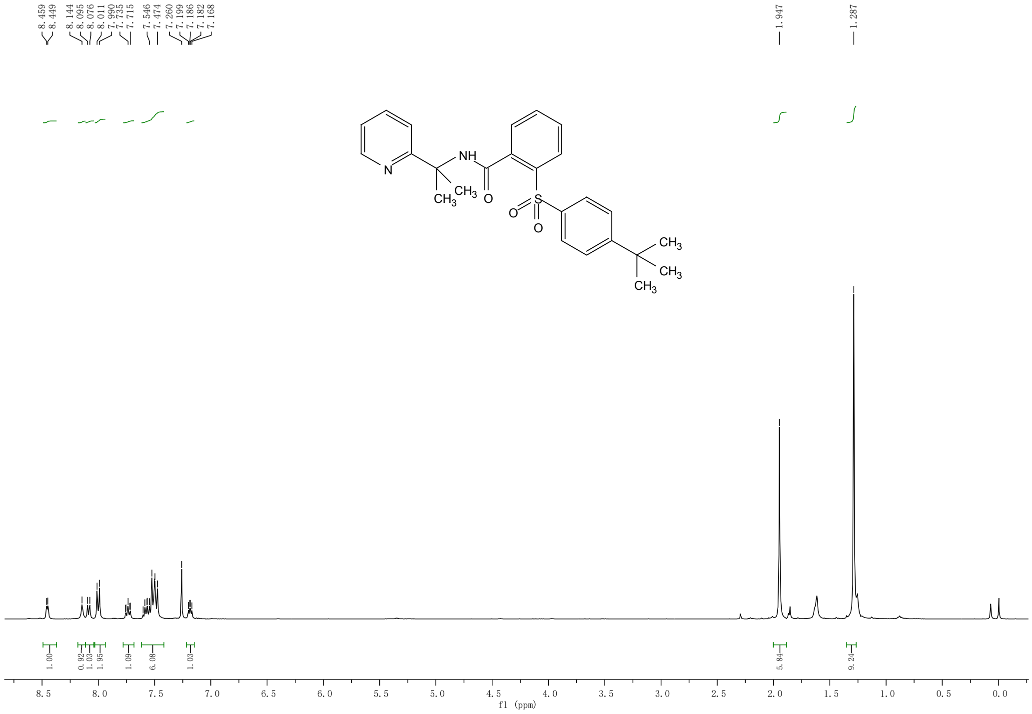

166.971
164.200
154.640
147.566
138.810
138.207
137.123
133.221
129.950
128.496
127.080
121.891
119.508
77.346
77.028
76.711
57.513
34.203
27.234
23.575

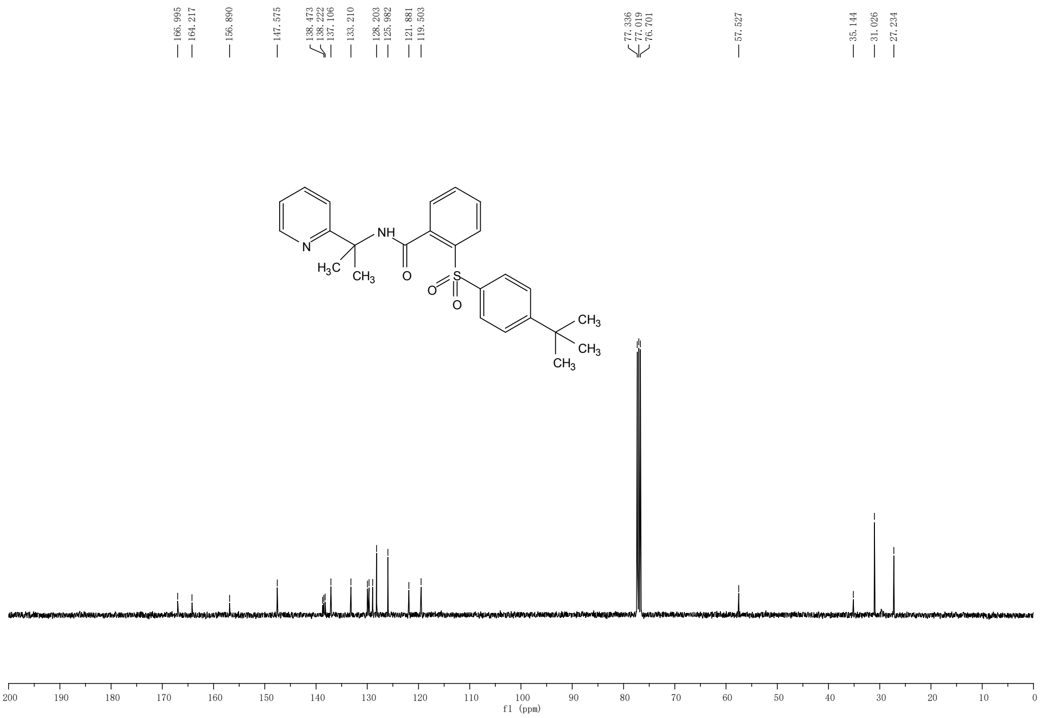

NH
N
H3C
CH3
O
O
S
O
CH3
CH3

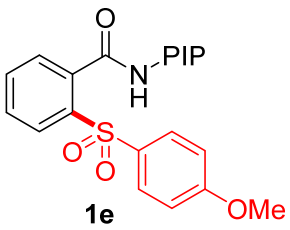

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


O
N
PIP
H
S
O
O
Bu-t

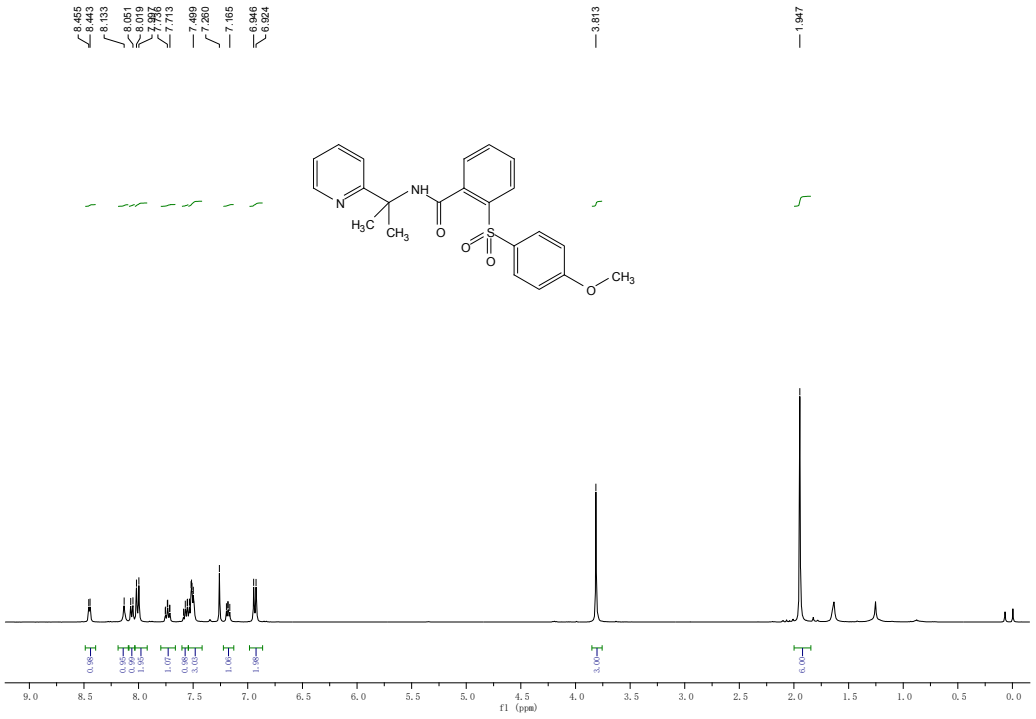
1d

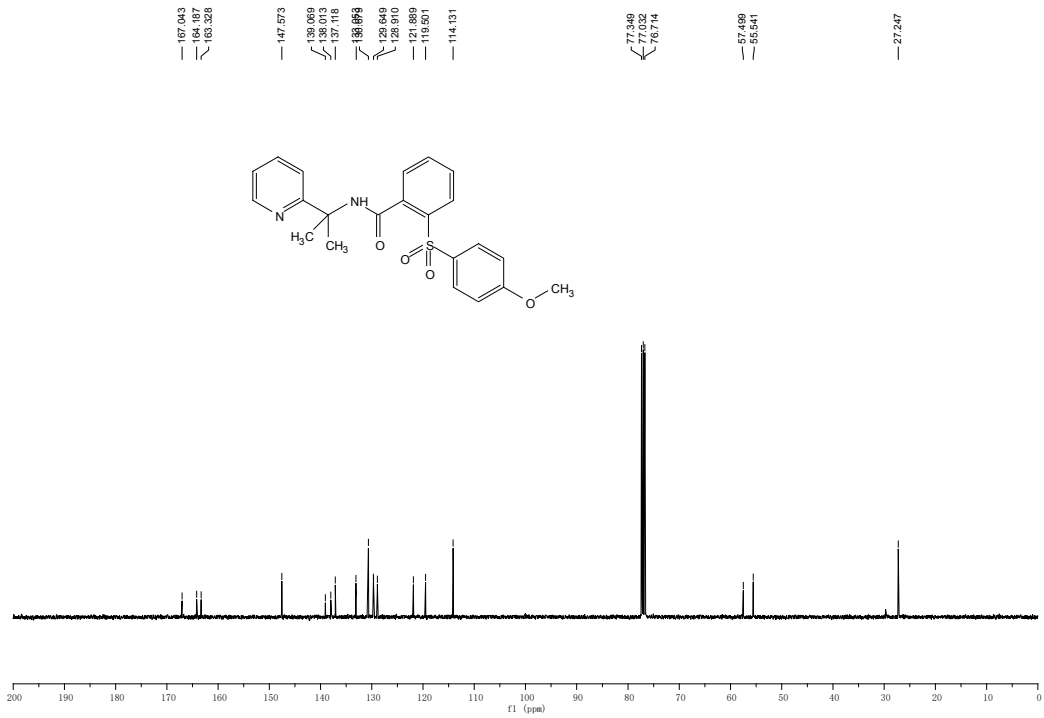

8.459
8.449
8.144
8.095
8.076
8.011
7.990
7.735
7.715
7.546
7.474
7.260
7.199
7.186
7.182
7.168
1.947
1.287
1.00
0.92
1.03
1.95
1.09
6.08
1.03
5.84
9.24
f1 (ppm)

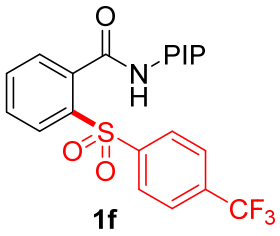

166.995
164.217
156.890
147.575
138.473
138.222
137.106
133.210
128.203
125.982
121.881
119.503
77.336
77.019
76.701
57.527
35.144
31.026
27.234
f1 (ppm)


O
N
PIP
H
S
O
O
OMe

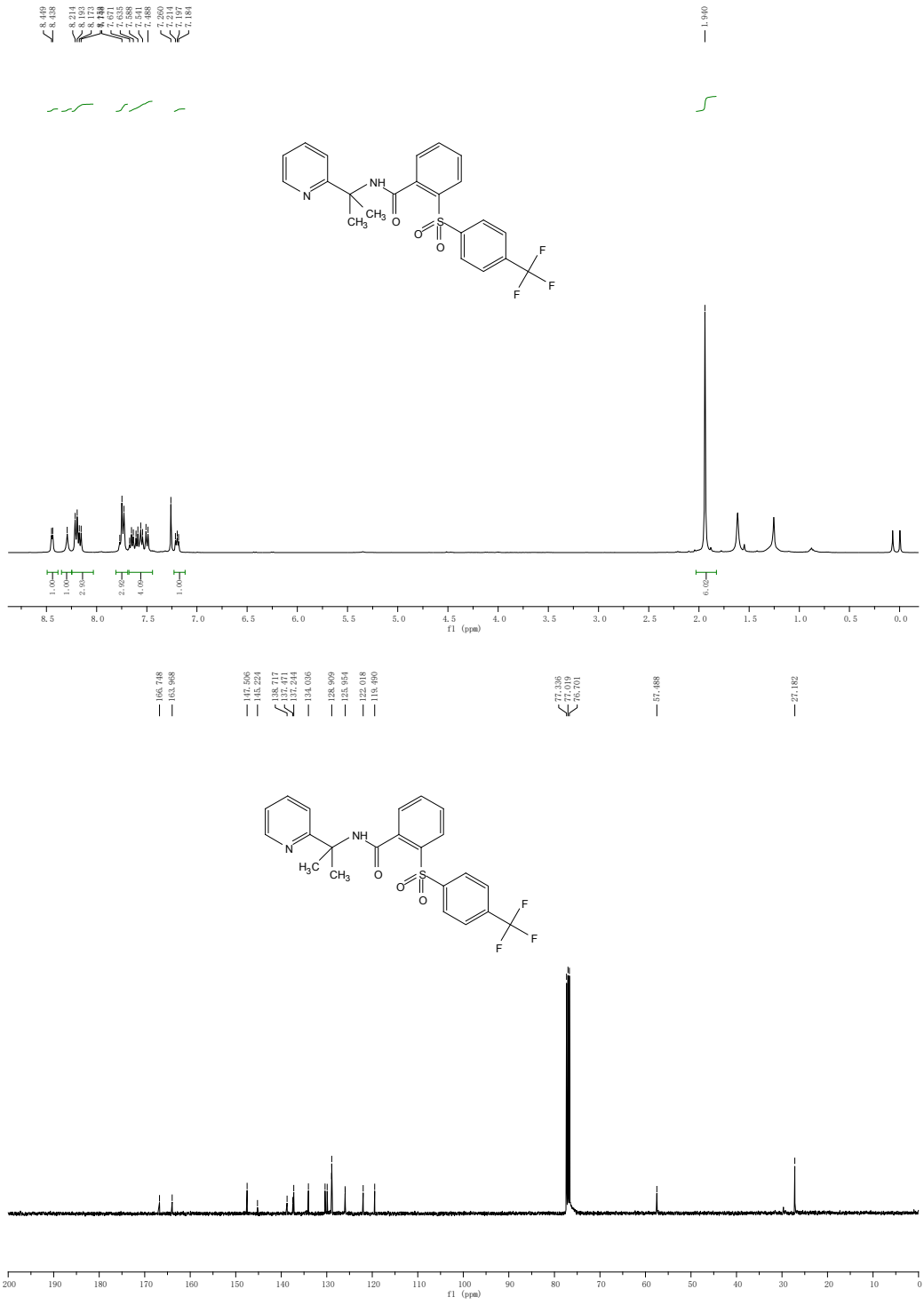
1e

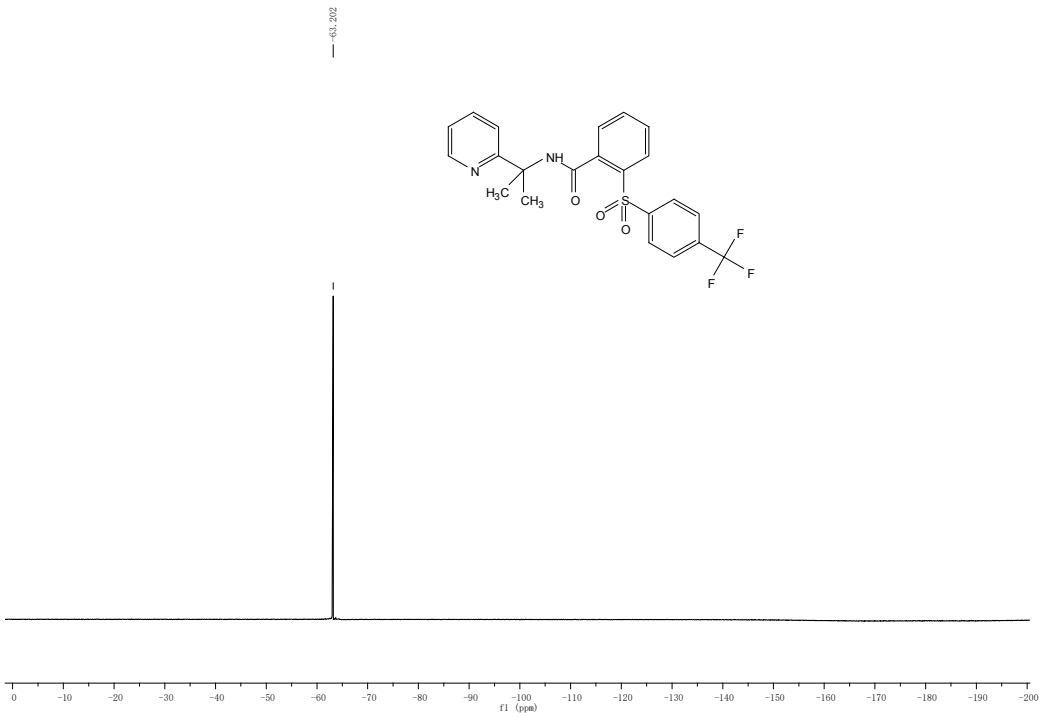

8.455
8.443
8.133
8.051
8.019
7.713
7.499
7.260
7.165
6.946
6.924
3.813
1.947
NH
N
H3C
CH3
O
S
O
O
CH3
f1 (ppm)

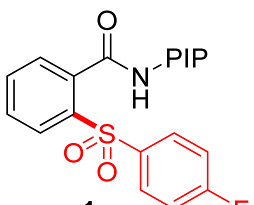

167.043
164.187
163.328
147.573
139.069
138.013
137.118
129.649
128.910
121.889
119.501
114.131
77.349
77.032
76.714
57.499
55.541
27.247
NH
N
H3C
CH3
O
S
O
O
CH3
f1 (ppm)


O
N
PIP
H
S
O
O
CF3

1f

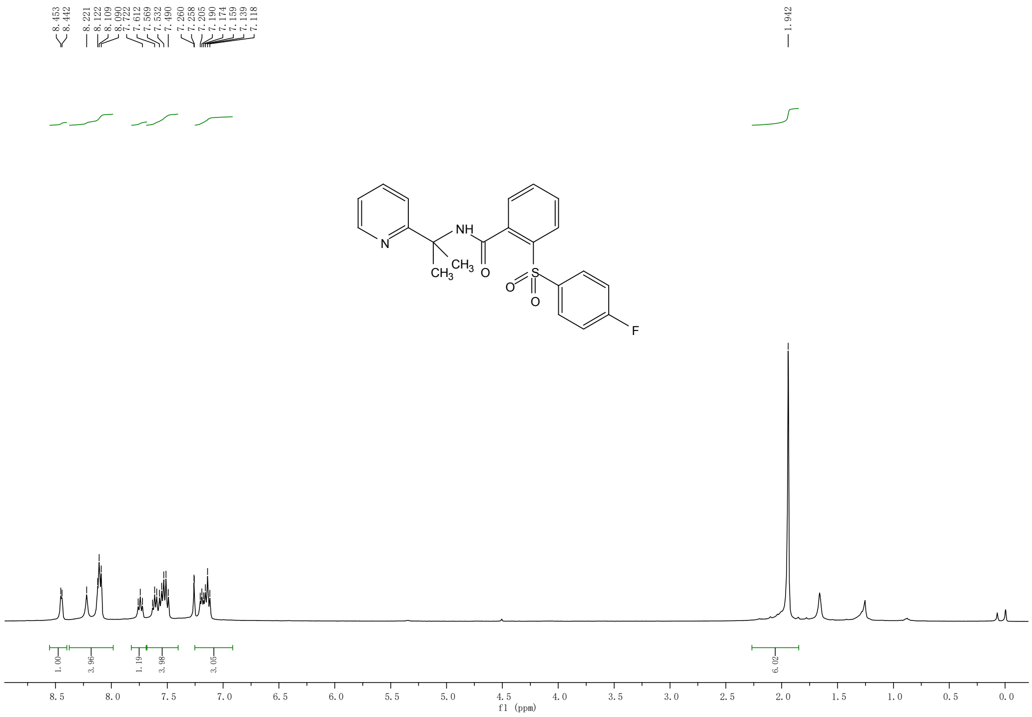

8.449
8.438
8.214
8.193
8.175
7.671
7.653
7.588
7.541
7.488
7.260
7.214
7.195
7.184
1.940
NH
N
CH3
CH3
O
S
O
O
F
F
F
1.00
1.00
2.35
2.02
4.09
1.00
6.02
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
166.748
163.968
147.506
145.224
138.717
137.471
137.244
134.036
128.909
125.954
122.018
119.490
77.336
77.019
76.701
57.488
27.182
NH
N
H3C
CH3
O
S
O
O
F
F
F
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-63.202
N
NH
O
S
O
O
F
F
F
H3C
CH3
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)

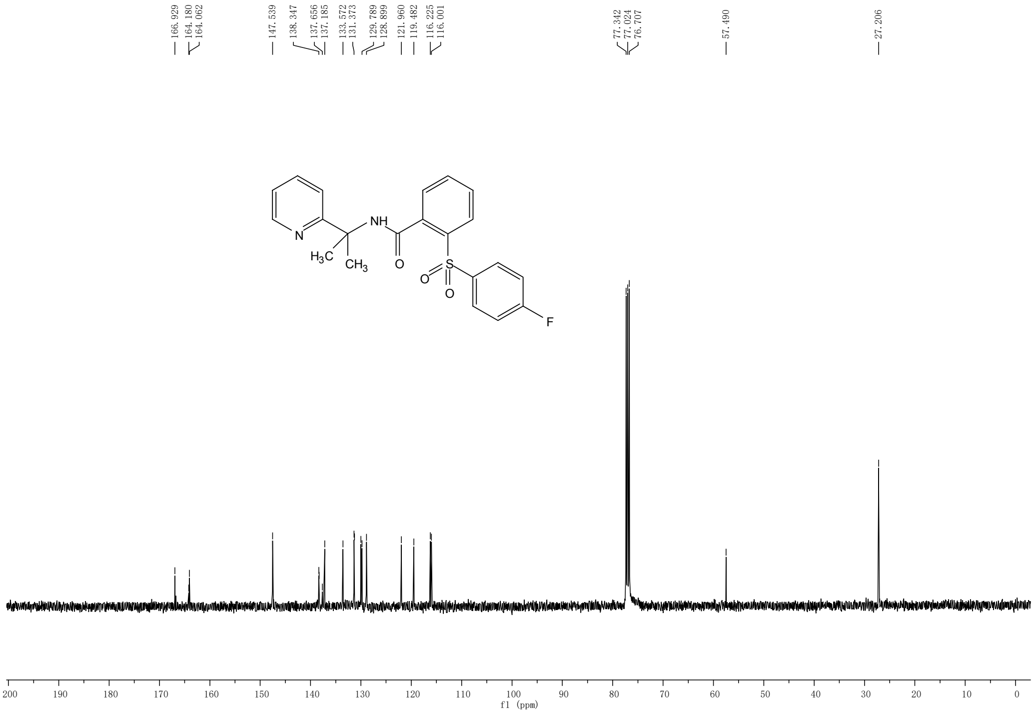


PIP
N
H
O
S
F

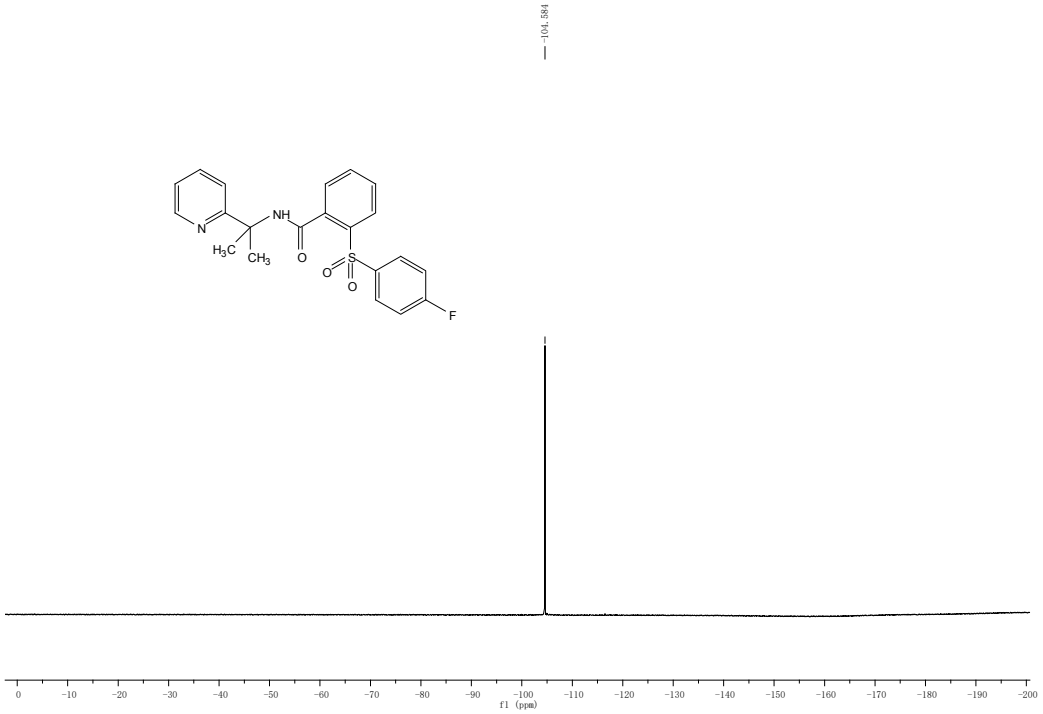
1g

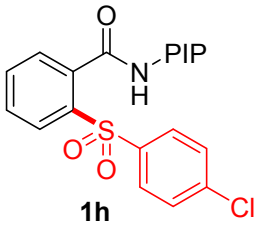


8.453
8.412
8.221
8.122
8.109
8.090
7.722
7.612
7.569
7.532
7.490
7.260
7.258
7.205
7.190
7.174
7.159
7.139
7.118
1.942
NH
N
CH3
CH3
O
S
O
O
F
1.00
3.96
1.19
3.98
3.05
6.02
f1 (ppm)

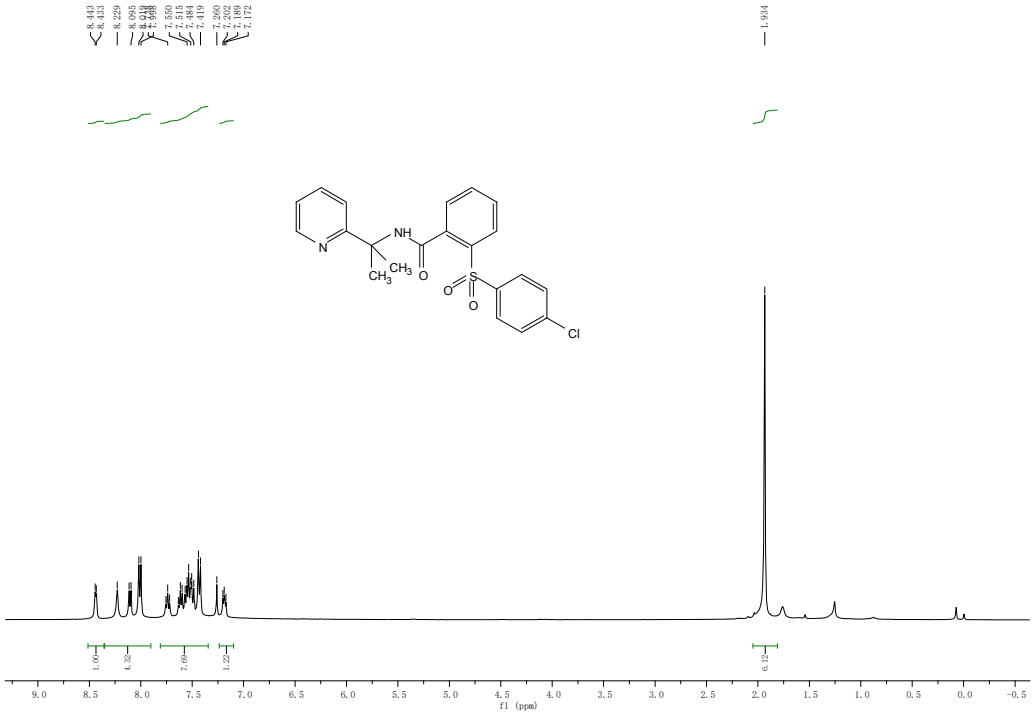


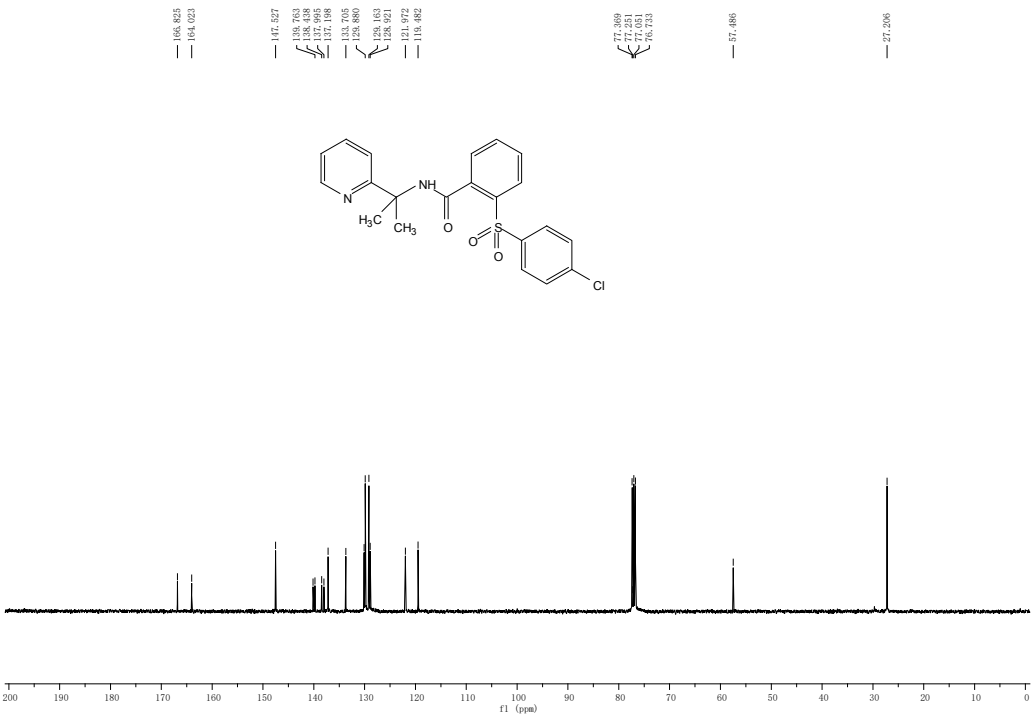
166.929
164.180
164.062
147.539
138.347
137.656
137.185
133.572
131.373
129.789
128.899
121.960
119.482
116.225
116.001
77.342
77.024
76.707
57.490
27.206
NH
N
H3C
CH3
O
S
O
O
F
f1 (ppm)

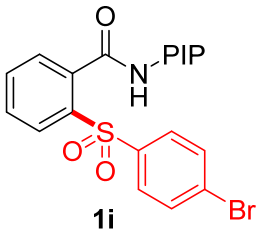

-104.584
N
NH
H3C
CH3
O
O
S
O
F
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)


O
N
PIP
H
S
O
O
Cl

1h

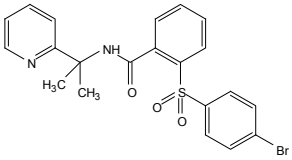

8.443
8.433
8.229
8.095
7.550
7.515
7.484
7.419
7.260
7.202
7.189
7.172
1.934
NH
N
CH3
CH3
O
S
O
O
Cl
1.00
4.32
7.60
1.22
6.12
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
f1 (ppm)

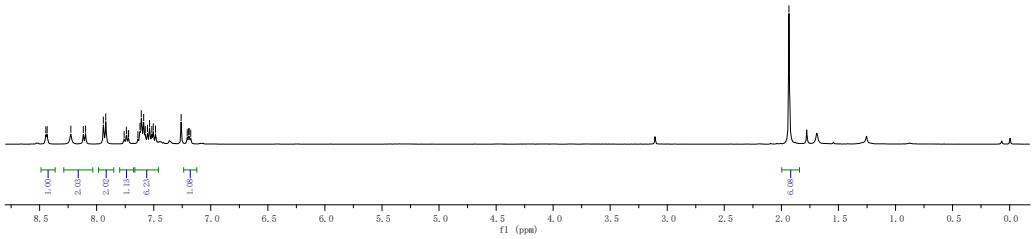

166.825
164.023
147.527
139.763
138.438
137.995
137.198
133.705
129.880
129.163
128.921
121.972
119.482
77.369
77.251
77.051
76.733
57.486
27.206
N
NH
H3C
CH3
O
O
S
O
O
Cl
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


O
N
PIP
H
S
O
O
Br

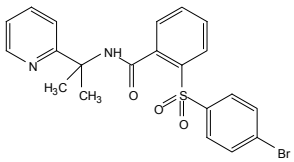
1i

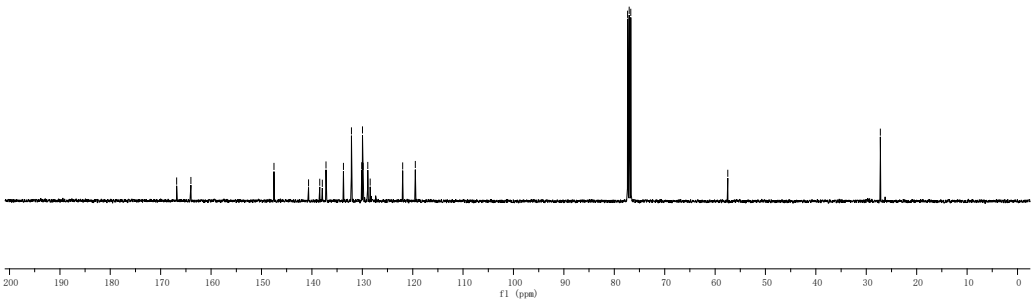

8.445
8.434
8.227
8.097
7.920
7.620
7.555
7.484
7.260
7.206
7.194
7.190
7.176
1.933

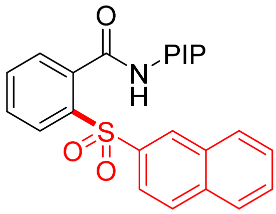

N
NH
H3C
CH3
O
O
S
O
Br


1.00
2.03
2.02
1.10
6.28
1.08
6.08
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

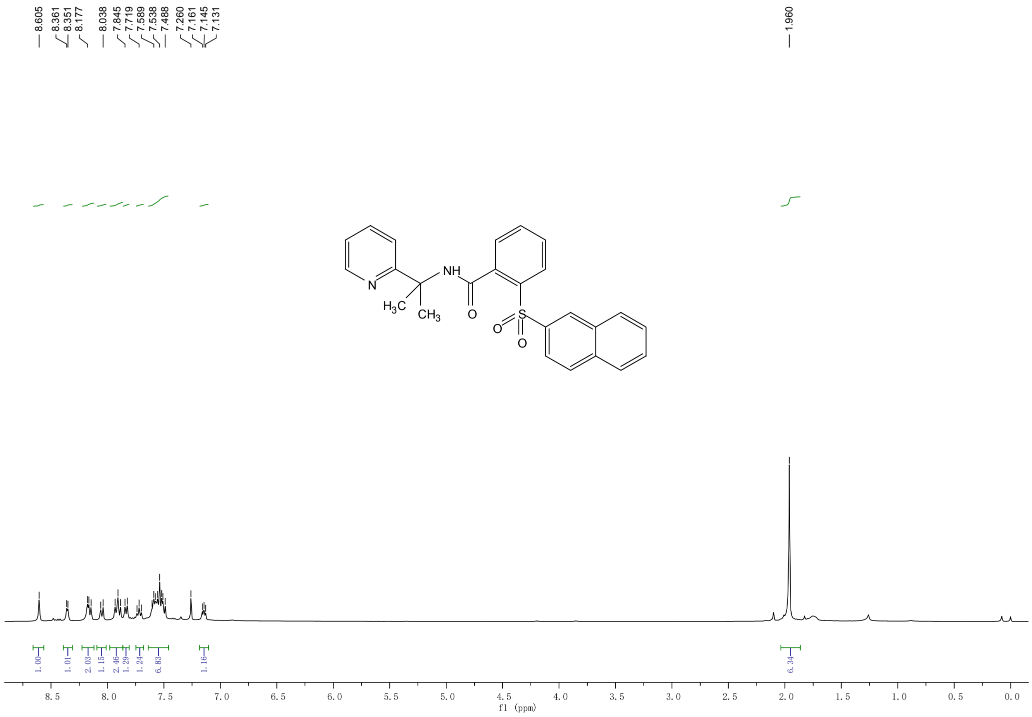

166.819
164.007
147.531
138.447
137.934
137.211
129.952
129.836
128.925
128.444
121.988
119.487
77.356
77.039
76.721
57.475
27.199


N
NH
H3C
CH3
O
O
S
O
Br

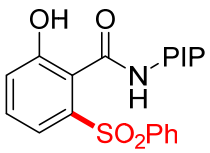

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


O
N
PIP
H
O
S
O

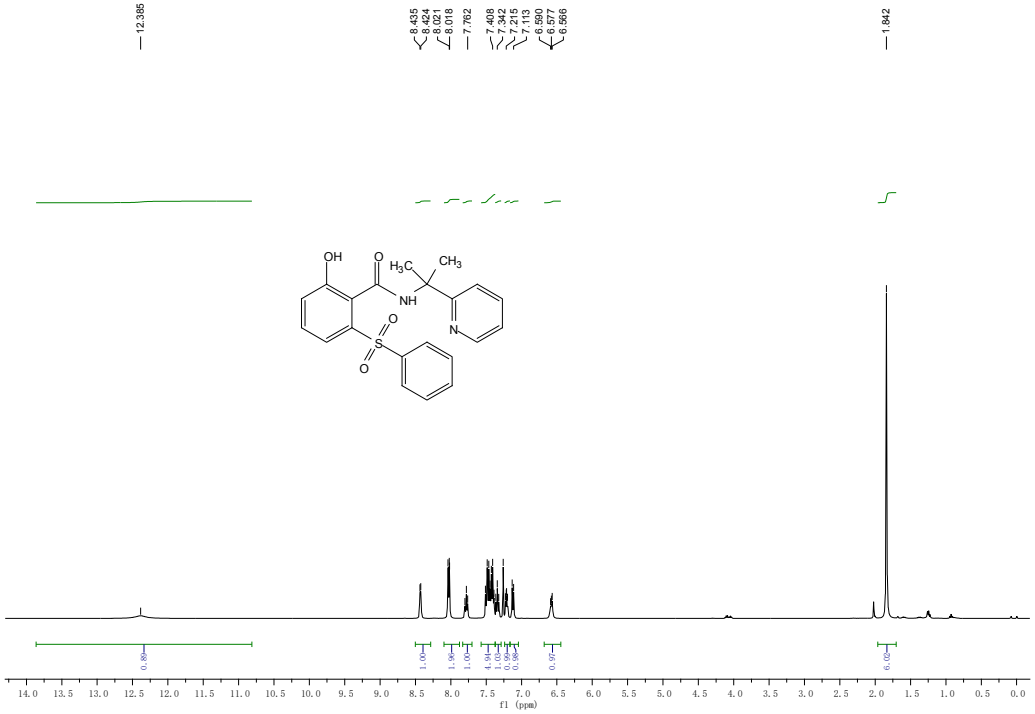
1j

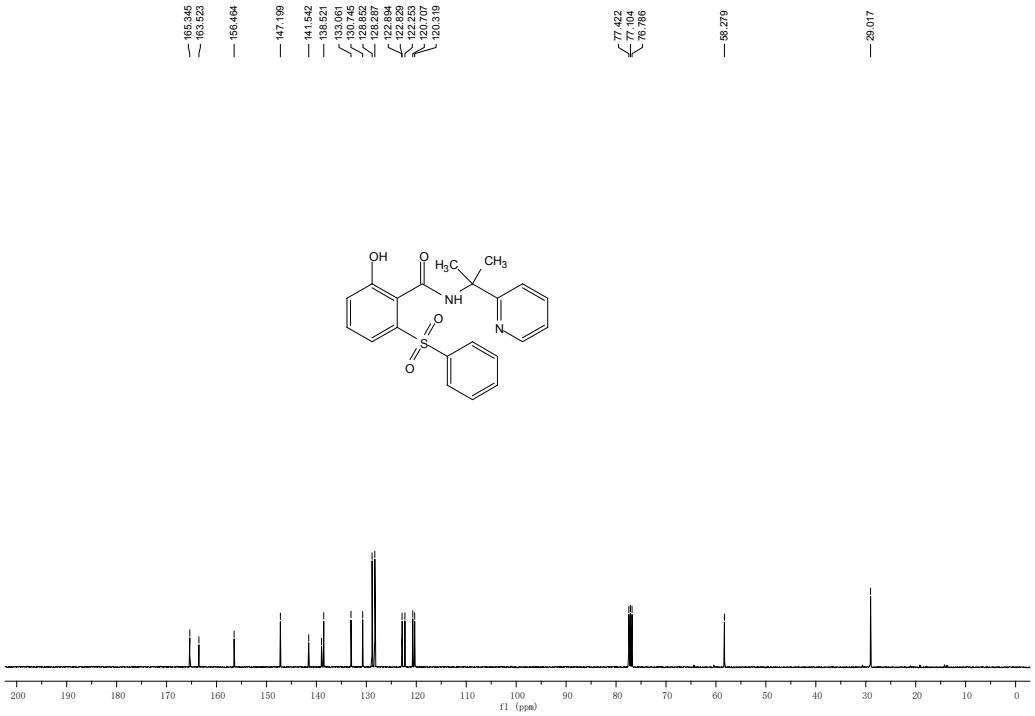

8.605
8.361
8.351
8.177
8.038
7.845
7.719
7.589
7.538
7.488
7.260
7.161
7.145
7.131
1.960
1.00
1.01
2.03
1.15
2.46
1.29
1.24
6.83
1.16
6.34
f1 (ppm)

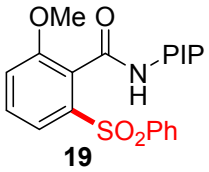

166.793
164.098
147.493
137.132
133.470
130.099
129.706
129.185
128.943
127.253
121.894
119.482
77.384
77.066
76.749
57.516
27.264
f1 (ppm)


OH
O
N
H
PIP
SO2Ph

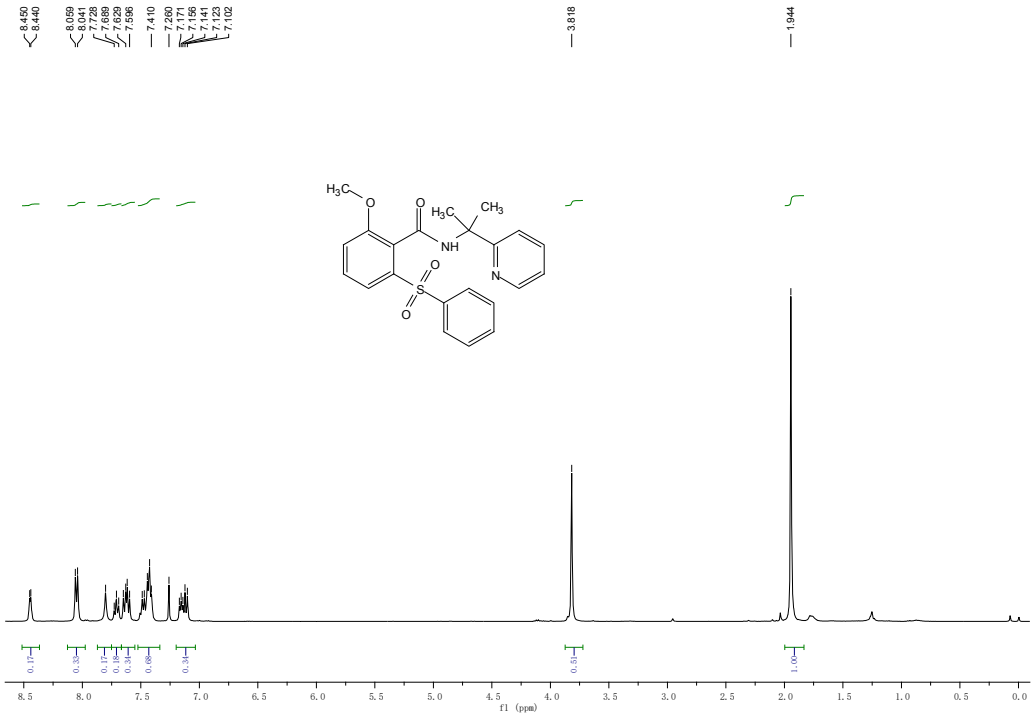
18

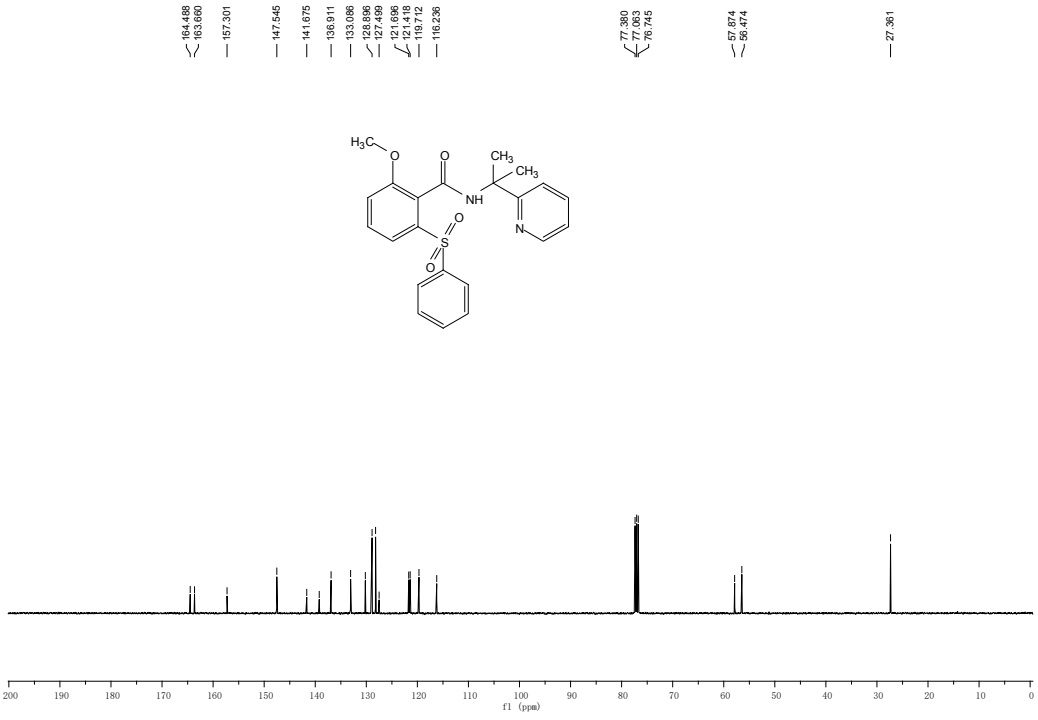

12.385
8.435
8.424
8.021
8.018
7.762
7.408
7.342
7.215
7.113
6.590
6.577
6.566
1.842
OH
O
H3C
CH3
NH
N
O
S
O
f1 (ppm)

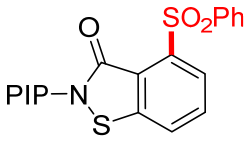

165.345
163.523
156.464
147.199
141.542
138.521
133.061
130.745
128.852
128.287
122.894
122.829
122.253
120.707
120.319
77.422
77.104
76.786
58.279
29.017
OH
O
H3C
CH3
NH
N
O
S
O
f1 (ppm)


OMe O
PIP
N
H
SO2Ph

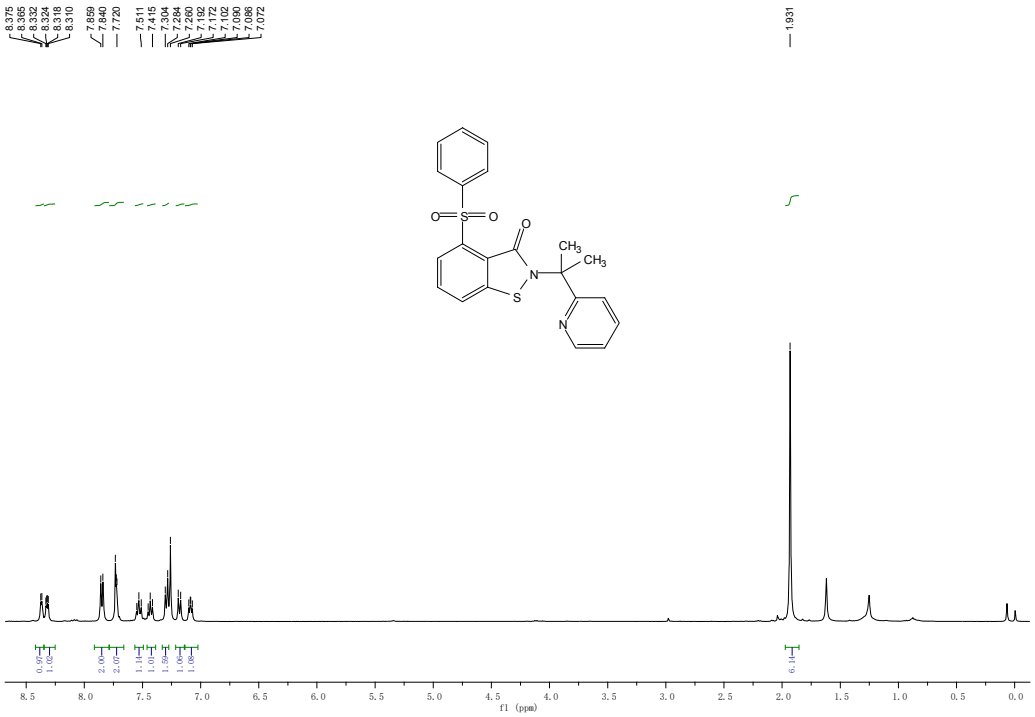
19

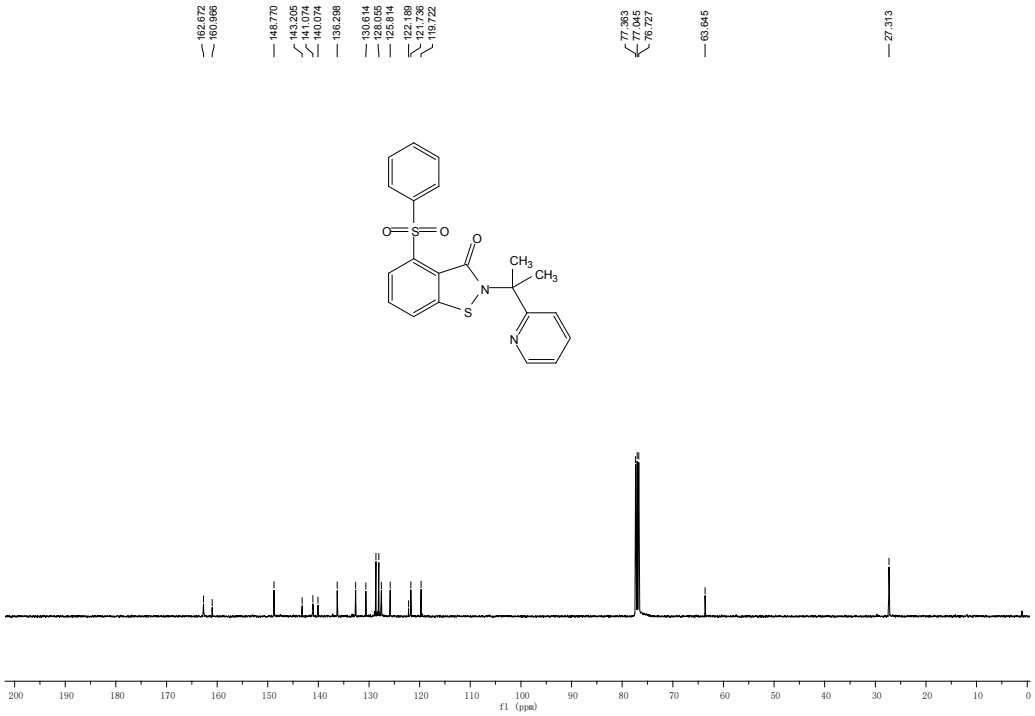

8.450
8.440
8.059
8.041
7.728
7.689
7.629
7.596
7.410
7.260
7.171
7.156
7.141
7.123
7.102
3.818
1.944
f1 (ppm)

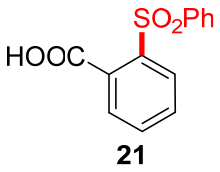

164.488
163.660
157.301
147.545
141.675
136.911
133.086
128.896
127.499
121.696
121.418
119.712
116.236
77.380
77.063
76.745
57.874
56.474
27.361
f1 (ppm)


SO2Ph
O
PIP–N
S

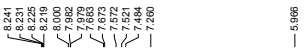
20

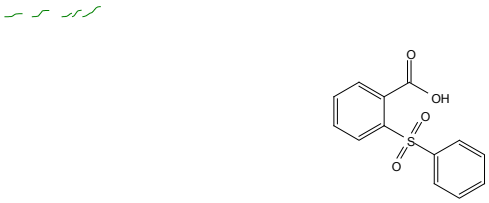

8.375
8.365
8.332
8.324
8.318
8.310
7.859
7.840
7.720
7.511
7.415
7.304
7.284
7.260
7.192
7.172
7.102
7.090
7.086
7.072
1.931
O=S=O
O
CH3
CH3
N
S
N
0.99
1.02
2.00
2.00
1.14
1.01
1.89
1.06
1.08
6.14
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

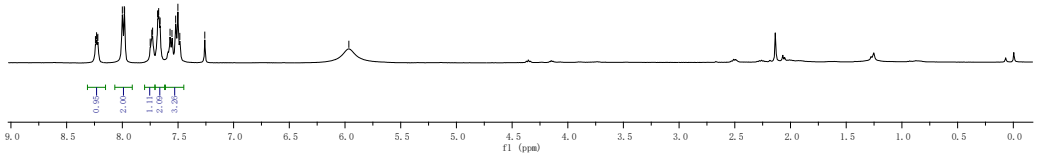

162.672
160.966
148.770
143.205
141.074
140.074
136.298
130.614
128.055
125.814
122.189
121.736
119.722
77.363
77.045
76.727
63.645
27.313
O=S=O
O
CH3
CH3
N
S
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


SO2Ph
HOOC

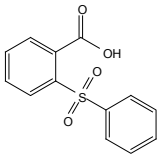
21

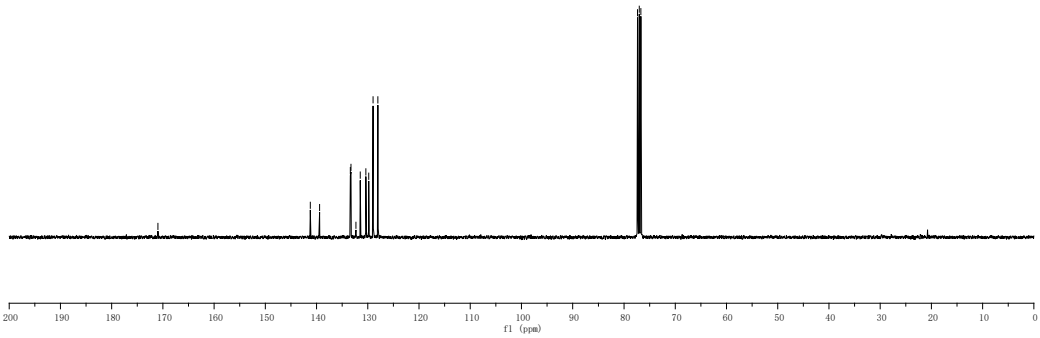

8.241
8.231
8.225
8.219
8.000
7.982
7.973
7.965
7.673
7.572
7.521
7.484
7.260
5.966




0.98
2.00
1.10
2.00
3.26
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


170.956
141.228
139.421
133.408
133.303
132.325
131.470
130.372
129.821
128.967
128.032
77.350
77.032
76.714




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