Electronic Supplementary Material (ESI) for ChemComm.

Copper-mediated *ortho* C-H sulfonylation of benzoic acid derivatives with sodium sulfinates

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Supporting Information

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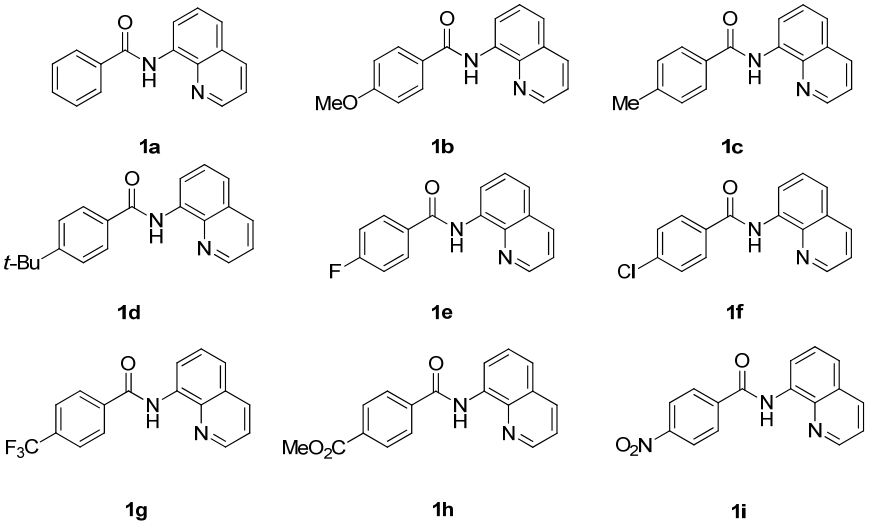
1. General information

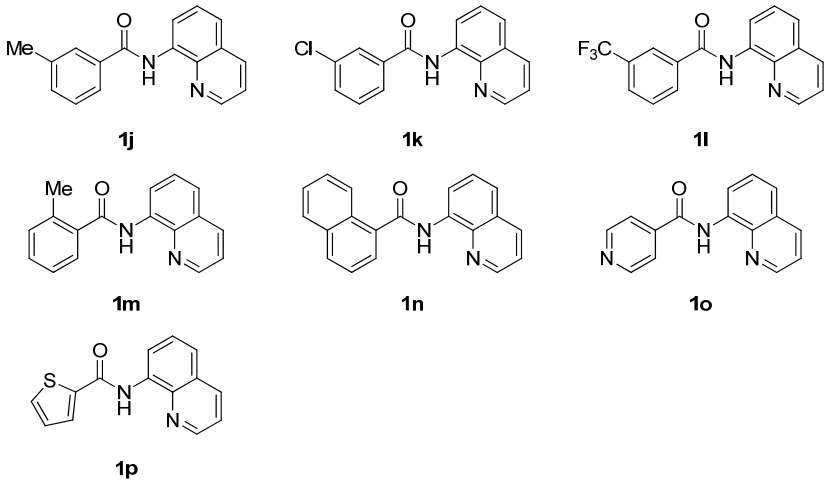
^{1}H NMR and ^{13}C NMR were recorded in $CDCl_3$ or DMSO-d_6 at room temperature on the Varian INOVA-400 spectrometer (400 MHz ^{1}H) or Bruker spectrometer (400 MHz ^{1}H). The chemical-shifts scale is based on internal TMS. The peak patterns are indicated as follows: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; qui, quintet; sxt, sextet. The coupling constants, *J* are reported in Hertz (Hz). Mass spectroscopy data were collected on an HRMS-EI instrument.

Unless otherwise noted, all reagents were obtained from commercial suppliers and used without further purification. Anhydrous $Cu(OAc)_2$ was purchased from Alfa Aesar. All solvents were purified and dried according to standard methods prior to use. Products were purified by flash column chromatography on 200-300 mesh silica gel, SiO_2.

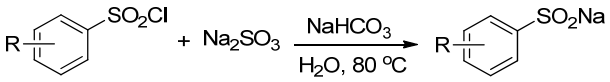
2. Typical procedure for the preparation of benzamides

All benzamides **1** were synthesized from the corresponding benzoic acids or benzoyl chlorides and 8-aminoquinoline. The deuterated amides were synthesized according to a literature method, spectral properties are consistent with literature values.[1] The following amides were synthesized according to literature procedures.[2]





3. Typical procedure for the preparation of sodium sulfinates



Sulfinic acid sodium salts **2a**, **2b** and **2k** were purchased from Alfa-Aesar and were used as received without further purification. 4-Methoxybenzenesulfinic acid sodium salt **2c** was prepared by heating 5.0 g of sodium sulfite, 4.12 g of 4-methoxybenzenesulphonyl chloride, and 3.36 g of sodium bicarbonate in 20 mL of water at 80 ^{o}C for 8 h. After cooling to room temperature, water was removed under vacuum. Recrystallization of the residure in ethanol afforded the product as a white solid in 67% (2.68 g) yield. Similarly, other sodium arenesulfinates **2d**-**2j** were prepared from their corresponding sulphonyl chlorides.[3]

4. Cu(II)-mediated sulfonylation of sp^2 C-H bonds

4.1 Optimization of reaction conditions

Scheme S1 Ineffective directing groups

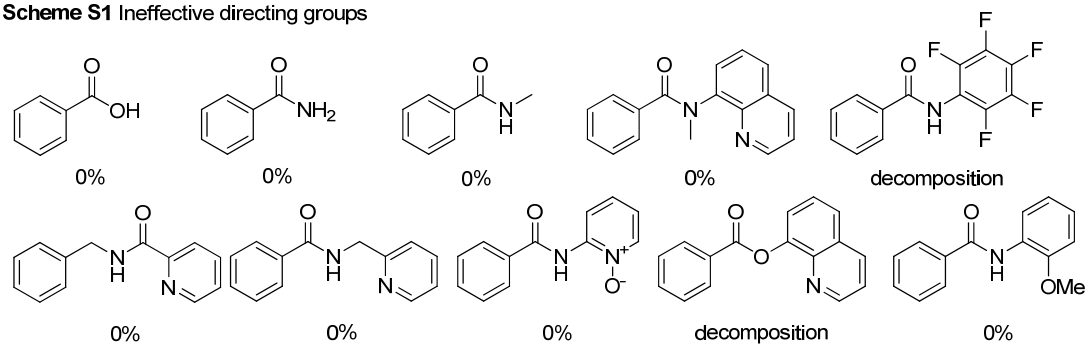
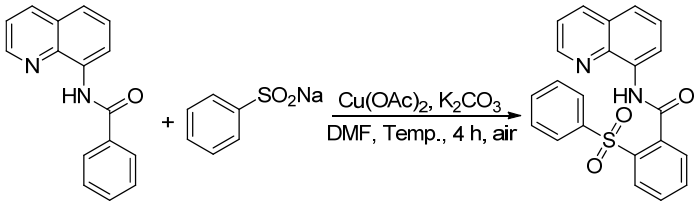


Table S1 Screening of temperation[a]

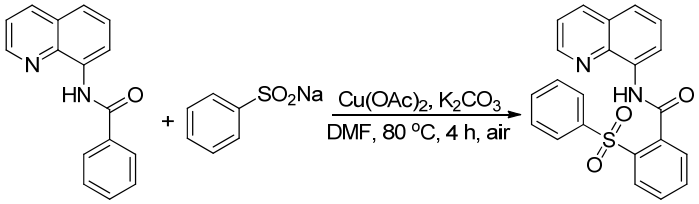


1a **2a** **3a**

Entry	Temp. (°C)	Yield[b] (%)
1	r.t.	trace
2	50	31
3	70	65
4	80	76
5	90	74

[a] Reaction condition: amide **1a** (0.3 mmol), **2a** (0.6 mmol), $Cu(OAc)_2$ (0.3 mmol), K_2CO_3 (0.6 mmol), DMF (1 mL) under air for 4 h. [b] Isolated yield.

Table S2 Screening of amount of $Cu(OAc)_2$[a]



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

Entry	$Cu(OAc)_2$	Yield[b] (%)
1	0	0
2	0.1 eq	8
3	0.2 eq	14
4	0.5 eq	55
5	1.0 eq	76
6	1.5 eq	68

[a] Reaction condition: amide **1a** (0.3 mmol), **2a** (0.6 mmol), K_2CO_3 (0.6 mmol), DMF (1 mL) under air for 4 h. [b] Isolated yield.

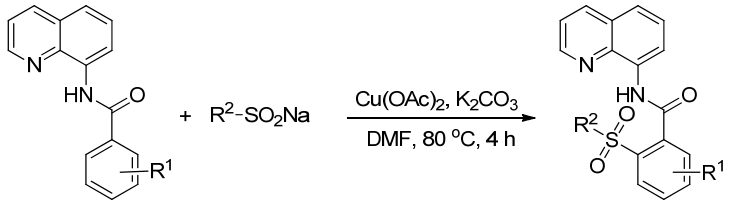
Table S3 Screening of oxidants[a]

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

Entry	Oxidant	Yield[b] (%)	SM[b] (%)
1	Ag_2CO_3	26	35
2	AgOAc	22	30
3	Select F	8	67
4	NFSI	0	52
5	$K_2S_2O_8$	trace	0
6	NMO	34	40

[a] Reaction condition: amide **1a** (0.3 mmol), **2a** (0.6 mmol), $Cu(OAc)_2$ (0.06 mmol), K_2CO_3 (0.6 mmol), oxidant (0.3 mmol), DMF (1 mL) under air for 4 h. [b] Isolated yield.

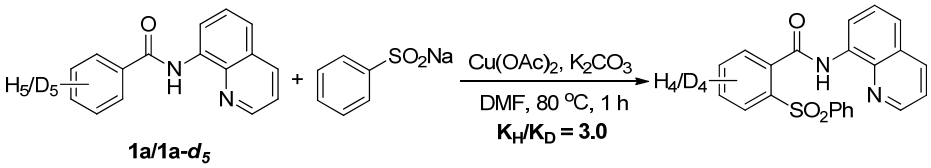
4.2 General procedure for copper-mediated C-H sulfonylation of benzoic acid derivatives.



1 **2** **3**

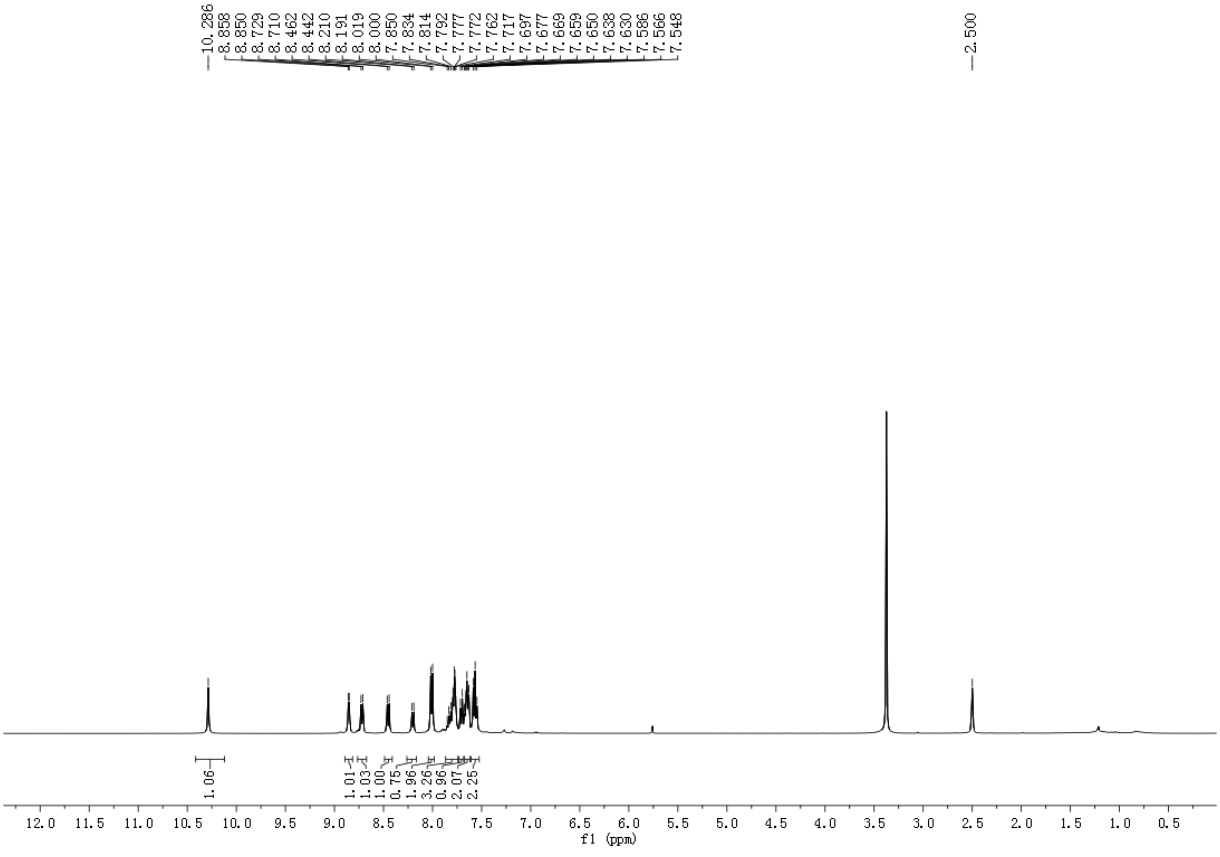
Benzamide **1** (0.3 mmol), anhydrous $Cu(OAc)_2$ (55 mg, 0.3 mmol), K_2CO_3 (83 mg, 0.6 mmol), sulfinic acid sodium salt **2** (0.6 mmol) and anhydrous DMF (1 mL) were added to a 25-mL Schlenk flask equipped with a high-vacuum PTFE valve-to-glass seal. Then the flask was sealed under air and stirred at 80 °C for 4 h. After the completion of the reaction, the solvent was evaporated under reduced pressure and the residue was then quenched with 1 M HCl aqueous solution (10 mL). The mixture was extracted with ethyl acetate, and the combined organic layer was dried over sodium sulfate. Concentration in vacuo followed by silica gel column purification with petroleum ether/ethyl acetate elutent gave the desired product **3**.

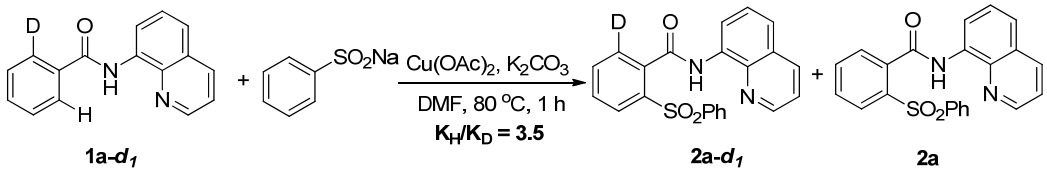
4.3 Deuterium-labeling experiments.



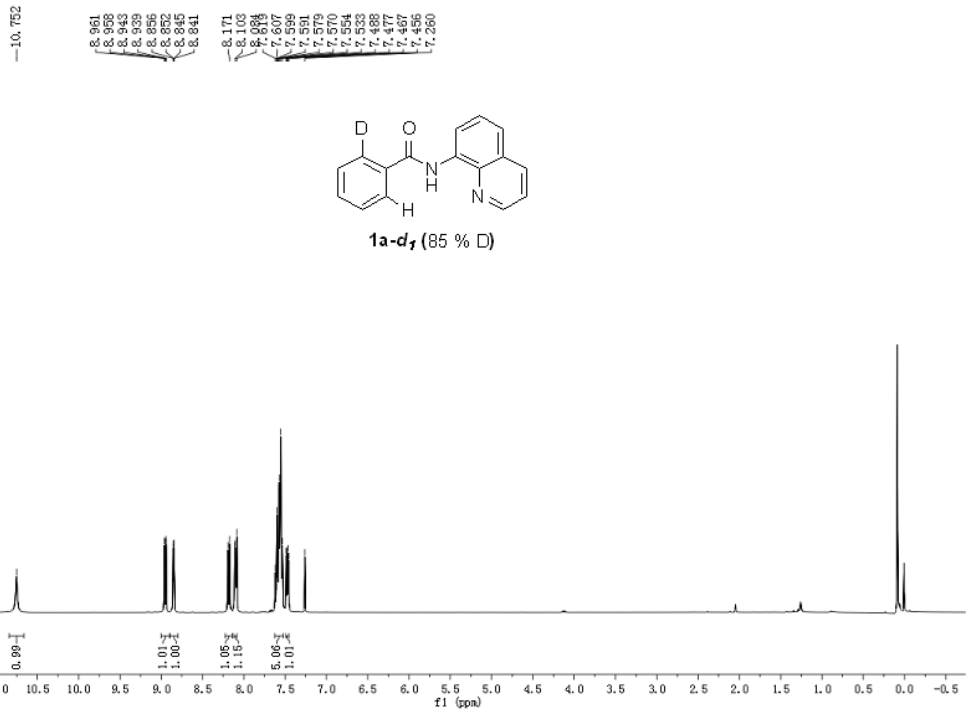
1a/1a-*d*$_5$

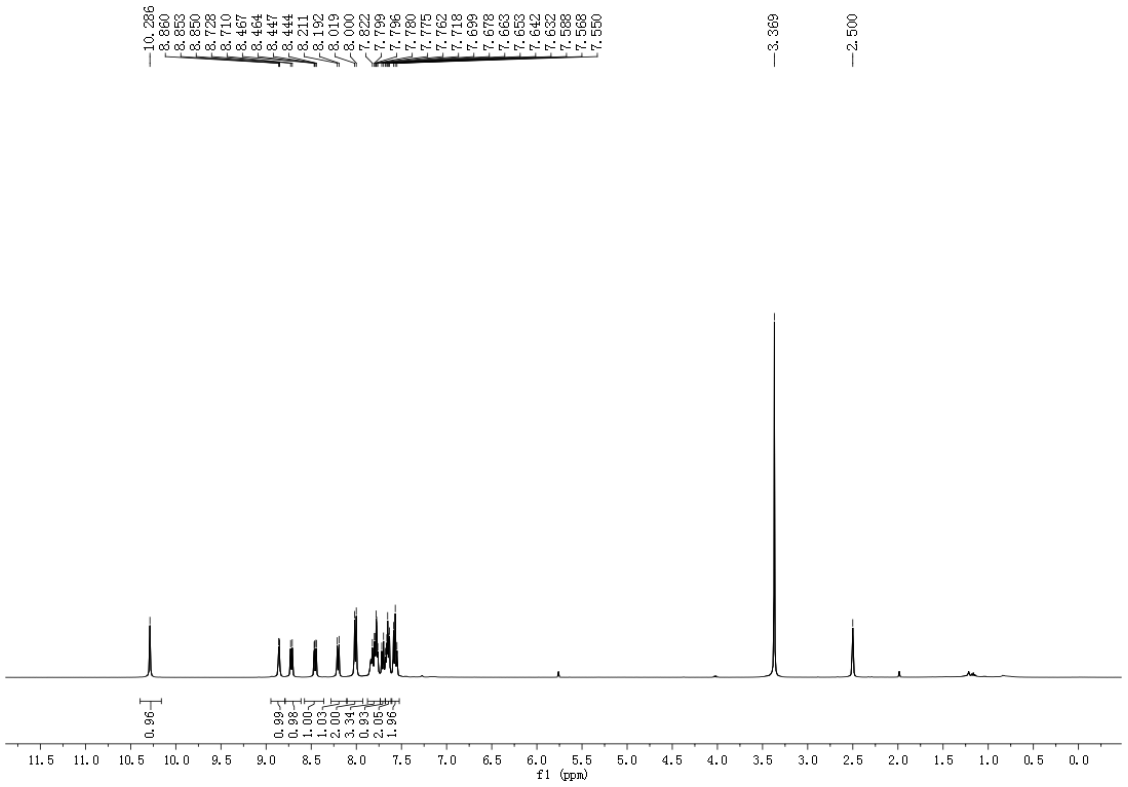
Intermolecular competition KIE Following general procedure: **1a** (74 mg, 0.3 mmol), **1a-*d*$_5$** (76 mg, 0.3 mmol), $Cu(OAc)_2$ (109 mg, 0.6 mmol), K_2CO_3 (166 mg, 1.2 mmol), sodium benzenesulfinate (197 mg, 1.2 mmol) and anhydrous DMF (2 mL) were added to a 25-mL Schlenk flask equipped with a high-vacuum PTFE valve-to-glass seal. Then the flask was sealed under air and stirred at 80 °C for 1 h. The product was separated by column chromatography to give the desired product less than 40 % yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.29 (s, 1H), 8.85 (d, J = 3.2 Hz, 1H), 8.72 (d, J = 7.5 Hz, 1H), 8.45 (d, J = 8.0 Hz, 1H), 8.20 (d, J = 7.7 Hz, 0.75H), 8.01 (d, J = 7.6 Hz, 2H), 7.87-7.74 (m, 3.26H), 7.71 (d, J = 7.8 Hz, 1H), 7.67-7.62 (m, 2H), 7.57 (t, J = 7.5 Hz, 2.25H). The KIE value was calculated as k_H/k_D = 3.0.



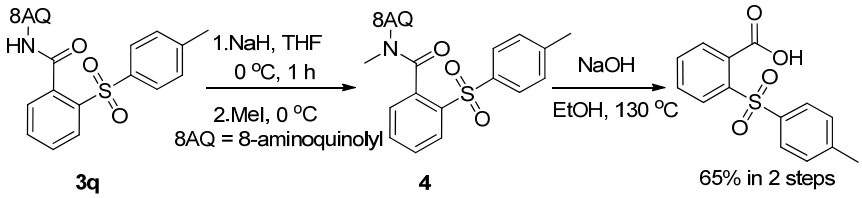


Intramolecular competition KIE Following general procedure: **1a-*d*$_1$** (75 mg, 0.3 mmol), $Cu(OAc)_2$ (55 mg, 0.3 mmol), K_2CO_3 (83 mg, 0.6 mmol), sodium benzenesulfinate (98 mg, 0.6 mmol) and anhydrous DMF (1 mL) were added to a 25-mL Schlenk flask equipped with a high-vacuum PTFE valve-to-glass seal. Then the flask was sealed under air and stirred at 80 °C for 1 h. The product was separated by column chromatography to give the desired product less than 40 % yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.29 (s, 1H), 8.95-8.79 (m, 1H), 8.72 (d, J = 7.4 Hz, 1H), 8.46 (dd, J = 8.3, 1.2 Hz, 1H), 8.20 (d, J = 7.8 Hz, 1H), 8.01 (d, J = 7.5 Hz, 2H), 7.88-7.73 (m, 3.34H), 7.71 (d, J = 7.8 Hz, 1H), 7.68-7.61 (m, 2H), 7.57 (t, J = 7.6 Hz, 2H). The KIE value was calculated as k_H/k_D = 3.5.





4.4 Removal of directing group.

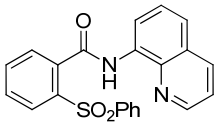


2-Tosylbenzoic acid: *N*-(quinolin-8-yl)-2-tosylbenzamide **3q** (402 mg, 1 mmol) was dissolved in anhydrous THF (10 mL) and the resulting solution was cooled to 0°C. To this solution, NaH (80 mg, 2 mmol) was added in portions over 10 min. The resulting solution was allowed to stir for 1 h. MeI (710 mg, 5 mmol) was added dropwise over 5 min, and reaction mixture was stirred for additional 1 hours at 0 °C and stirred overnight at rt. After the reaction was quenched by addition water, the mixture was extracted with Et_2O, and the organic layer was dried by anhydrous Na_2SO_4. After remove the solvent, the residue was purified by column chromatography (eluent: ethyl acetate/petrol ether =1/1) to give intermediate **4** as yellow solid (341 mg, 82%). Intermediate **4** (208 mg, 0.5 mmol) and NaOH (307 mg, 7.5 mmol) were dissolved in EtOH (5 ml). The resulting mixture was stirred at 130 ^{0}C for 24 hours. After that, reaction mixture was diluted with EtOAc (100 mL) and 1N HCl (30

mL) was added. Organic layer was washed with 1N HCl (5 x 20 mL), dried over anhydrous Na_2SO_4, filtered and the solvent was evaporated under vacuum affording pure product as a yellow solid (80%). ^{1}H NMR (400 MHz, DMSO-d_6): δ 13.62 (br, 1H), 8.13 (d, J = 7.4 Hz, 1H), 7.86 (d, J = 8.2 Hz, 2H), 7.78-7.69 (m, 2H), 7.65-7.58 (m, 1H), 7.41 (d, J = 8.1 Hz, 2H), 2.37 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 168.93, 144.76, 138.72, 138.30, 134.96, 134.38, 131.24, 130.23, 130.21, 129.05, 128.34, 21.56. HRMS (EI, m/z): calcd for $C_{14}H_{12}O_4S^+$ [M^+]: 276.0446; Found: 276.0451.

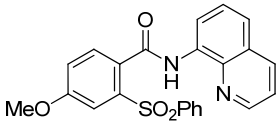
5 Characterization data of products.

2-(Phenylsulfonyl)-*N*-(quinolin-8-yl)benzamide (3a)



Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/petrol ether =1/2) as a yellow solid in 76% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.28 (s, 1H), 8.85 (dd, J = 4.1, 1.4 Hz, 1H), 8.72 (d, J = 7.2 Hz, 1H), 8.45 (dd, J = 8.3, 1.4 Hz, 1H), 8.20 (d, J = 7.9 Hz, 1H), 8.01 (d, J = 7.4 Hz, 2H), 7.87-7.74 (m, 4H), 7.71 (d, J = 7.8 Hz, 1H), 7.68-7.62 (m, 2H), 7.57 (t, J = 7.6 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 166.04, 149.59, 141.53, 138.63, 138.16, 137.20, 137.14, 134.73, 134.66, 134.17, 131.29, 130.39, 129.82, 129.28, 128.33, 128.29, 127.50, 123.22, 122.77, 117.73. HRMS (EI, m/z): calcd for $C_{22}H_{16}N_2O_3S^+$ [M^+]: 388.0863; Found: 388.0876.

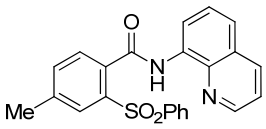
4-Methoxy-2-(phenylsulfonyl)-*N*-(quinolin-8-yl)benzamide (3b)



Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/petrol ether =1/1) as a yellow solid in 74% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.13 (s, 1H), 8.85 (dd, J = 4.1, 1.5 Hz, 1H), 8.68 (d, J = 7.4 Hz, 1H), 8.45 (dd, J = 8.3, 1.5 Hz, 1H), 8.01 (d, J = 7.4 Hz, 2H), 7.79-7.63 (m, 6H), 7.55 (t, J = 7.7 Hz, 2H), 7.38 (dd, J = 8.4, 2.4 Hz, 1H), 3.92 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 165.71, 160.74, 149.56, 141.34, 139.74, 138.48,

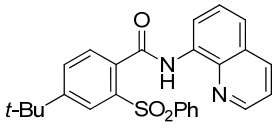
137.15, 134.66, 134.16, 131.10, 129.73, 129.64, 128.39, 128.29, 127.50, 123.03, 122.77, 119.59, 117.34, 115.59, 56.59. HRMS (EI, m/z): calcd for $C_{23}H_{18}N_2O_4S^+$ [M^+]: 418.0982; Found: 418.0986.

4-Methyl-2-(phenylsulfonyl)-*N*-(quinolin-8-yl)benzamide (3c)



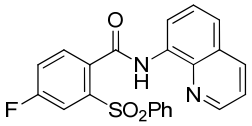
Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/petrol ether =1/2) as a yellow solid in 71% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.17 (s, 1H), 8.84 (d, J = 2.9 Hz, 1H), 8.71 (d, J = 7.4 Hz, 1H), 8.53-8.37 (m, 1H), 8.08-7.98 (m, 3H), 7.77 (d, J = 7.8 Hz, 1H), 7.73-7.60 (m, 5H), 7.56 (t, J = 7.6 Hz, 2H), 2.46 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 166.06, 149.57, 141.62, 141.58, 138.50, 138.06, 137.13, 135.10, 134.63, 134.07, 130.45, 129.82, 129.75, 129.17, 128.26, 128.13, 127.50, 123.08, 122.76, 117.45, 21.18. HRMS (EI, m/z): calcd for $C_{23}H_{18}N_2O_3S^+$ [M^+]: 402.1032; Found: 402.1033.

4-(*tert*-Butyl)-2-(phenylsulfonyl)-*N*-(quinolin-8-yl)benzamide (3d)



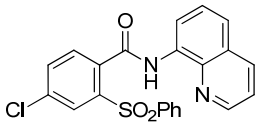
Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/petrol ether =1/2) as a yellow solid in 75% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.22 (s, 1H), 8.82 (dd, J = 4.2, 1.5 Hz, 1H), 8.73 (d, J = 7.0 Hz, 1H), 8.42 (dd, J = 8.3, 1.5 Hz, 1H), 8.14 (d, J = 1.8 Hz, 1H), 8.07-8.01 (m, 2H), 7.84 (dd, J = 8.0, 1.8 Hz, 1H), 7.77-7.65 (m, 3H), 7.64-7.59 (m, 2H), 7.55 (t, J = 7.5 Hz, 2H), 1.32 (s, 9H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 165.96, 154.22, 149.48, 141.57, 138.49, 138.07, 137.09, 134.74, 134.63, 134.07, 131.68, 129.76, 129.28, 128.33, 128.27, 127.48, 126.54, 123.07, 122.72, 117.41, 35.37, 31.10. HRMS (EI, m/z): calcd for $C_{26}H_{24}N_2O_3S^+$ [M^+]: 444.1500; Found: 444.1502.

4-Fluoro-2-(phenylsulfonyl)-*N*-(quinolin-8-yl)benzamide (3e)



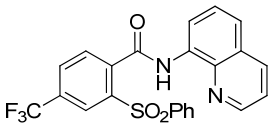
Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/petrol ether =1/2) as a yellow solid in 62% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.40 (s, 1H), 8.86 (dd, J = 4.0, 1.2 Hz, 1H), 8.72 (d, J = 7.3 Hz, 1H), 8.44 (dd, J = 8.3, 1.3 Hz, 1H), 8.13-8.03 (m, 3H), 7.85 (dd, J = 8.4, 5.2 Hz, 1H), 7.78 (d, J = 7.5 Hz, 1H), 7.71-7.62 (m, 4H), 7.58 (t, J = 7.6 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 165.33, 162.48 (d, $J_{C\text{-}F}$ = 250.1 Hz), 149.55, 140.91, 140.54 (d, $J_{C\text{-}F}$ = 6.5 Hz), 138.73, 137.11, 134.71, 134.44, 133.95, 132.50 (d, $J_{C\text{-}F}$ = 8.0 Hz), 129.84, 128.62, 128.34, 127.46, 123.31, 122.73, 121.70 (d, $J_{C\text{-}F}$ = 21.3 Hz), 117.97, 117.43 (d, $J_{C\text{-}F}$ = 24.7 Hz). ^{19}F NMR (377 MHz, DMSO-d_6): δ -108.03. HRMS (EI, m/z): calcd for $C_{22}H_{15}FN_2O_3S^+$ [M^+]: 406.0781; Found: 406.0782.

4-Chloro-2-(phenylsulfonyl)-*N*-(quinolin-8-yl)benzamide (3f)



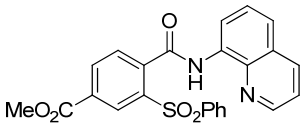
Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/petrol ether =1/2) as a yellow solid in 68% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.48 (s, 1H), 8.86 (dd, J = 4.0, 1.2 Hz, 1H), 8.72 (d, J = 7.3 Hz, 1H), 8.44 (dd, J = 8.3, 1.3 Hz, 1H), 8.22 (d, J = 1.9 Hz, 1H), 8.08 (d, J = 7.5 Hz, 2H), 7.87 (dd, J = 8.2, 1.9 Hz, 1H), 7.78 (dd, J = 8.3, 2.5 Hz, 2H), 7.72-7.62 (m, 3H), 7.58 (t, J = 7.6 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 165.31, 149.54, 140.90, 140.12, 138.79, 137.10, 136.00, 135.51, 134.71, 134.48, 131.33, 129.87, 129.68, 128.65, 128.57, 128.36, 127.45, 123.40, 122.72, 118.17. HRMS (EI, m/z): calcd for $C_{22}H_{15}ClN_2O_3S^+$ [M^+]: 422.0484; Found: 422.0486.

2-(Phenylsulfonyl)-*N*-(quinolin-8-yl)-4-(trifluoromethyl)benzamide (3g)



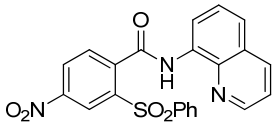
Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/petrol ether =1/2) as a yellow solid in 59% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.72 (s, 1H), 8.87 (d, J = 3.0 Hz, 1H), 8.74 (d, J = 7.5 Hz, 1H), 8.51-8.39 (m, 2H), 8.20 (d, J = 7.9 Hz, 1H), 8.10 (d, J = 7.7 Hz, 2H), 7.98 (d, J = 7.9 Hz, 1H), 7.79 (d, J = 8.0 Hz, 1H), 7.74-7.63 (m, 3H), 7.59 (t, J = 7.6 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 165.29, 149.59, 140.91, 140.75, 139.52, 139.01, 137.08, 134.81, 134.62, 131.51 (q, $J_{C\text{-}F}$ = 3.4 Hz), 131.36, 131.05, 129.96, 128.73, 128.43, 127.45, 126.78 (q, $J_{C\text{-}F}$ = 3.4 Hz), 123.58, 123.55 (q, $J_{C\text{-}F}$ = 271.8 Hz), 122.74, 118.50. ^{19}F NMR (377 MHz, DMSO-d_6): δ -61.36. HRMS (EI, m/z): calcd for $C_{23}H_{15}F_3N_2O_3S^+$ [M^+]: 456.0743; Found: 456.0750.

Methyl 3-(phenylsulfonyl)-4-(quinolin-8-ylcarbamoyl)benzoate (3h)



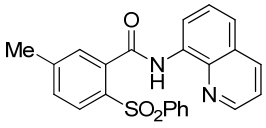
Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/petrol ether =1/1) as a yellow solid in 57% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.60 (s, 1H), 8.92-8.81 (m, 1H), 8.71 (d, J = 7.5 Hz, 1H), 8.59 (d, J = 1.2 Hz, 1H), 8.45 (dd, J = 8.3, 1.1 Hz, 1H), 8.30 (dd, J = 7.9, 1.2 Hz, 1H), 8.03 (d, J = 7.6 Hz, 2H), 7.91 (d, J = 7.9 Hz, 1H), 7.79 (d, J = 8.0 Hz, 1H), 7.73-7.62 (m, 3H), 7.59 (t, J = 7.6 Hz, 2H), 3.94 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 165.51, 164.94, 149.63, 140.99, 140.90, 138.93, 138.85, 137.10, 134.94, 134.69, 134.48, 131.98, 130.43, 130.37, 129.98, 128.41, 127.46, 123.56, 122.76, 118.40, 53.43 (one signal was overlapped by other ones). HRMS (EI, m/z): calcd for $C_{24}H_{18}N_2O_5S^+$ [M^+]: 446.0932; Found: 446.0935.

4-Nitro-2-(phenylsulfonyl)-*N*-(quinolin-8-yl)benzamide (3i)



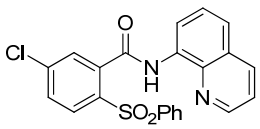
Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/petrol ether =1/1) as a yellow solid in 50% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.81 (s, 1H), 8.95-8.85 (m, 1H), 8.74 (d, J = 7.5 Hz, 1H), 8.56-8.39 (m, 4H), 8.06 (d, J = 7.6 Hz, 2H), 7.81 (d, J = 8.1 Hz, 1H), 7.71 (t, J = 8.0 Hz, 2H), 7.64 (dt, J = 15.6, 5.8 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 164.49, 150.49, 149.60, 143.32, 140.47, 139.07, 138.64, 137.10, 134.86, 134.81, 132.22, 130.04, 128.71, 128.43, 127.43, 125.68, 124.65, 123.62, 122.73, 118.68. HRMS (EI, m/z): calcd for $C_{22}H_{15}N_3O_5S^+$ [M^+]: 433.0734; Found: 433.0730.

5-Methyl-2-(phenylsulfonyl)-*N*-(quinolin-8-yl)benzamide (3j)



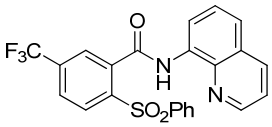
Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/petrol ether =1/2) as a yellow solid in 72% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.20 (s, 1H), 8.85 (d, J = 2.9 Hz, 1H), 8.72 (d, J = 7.4 Hz, 1H), 8.45 (dd, J = 8.2, 1.1 Hz, 1H), 8.07 (d, J = 8.0 Hz, 1H), 7.98 (d, J = 7.5 Hz, 2H), 7.78 (d, J = 7.8 Hz, 1H), 7.70 (d, J = 7.8 Hz, 1H), 7.68-7.53 (m, 6H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 166.05, 149.58, 145.63, 141.83, 138.52, 137.15, 135.28, 134.63, 133.99, 131.64, 130.42, 129.76, 129.58, 128.30, 128.10, 127.51, 123.14, 122.78, 117.54, 21.32 (one signal was overlapped by other ones). HRMS (EI, m/z): calcd for $C_{23}H_{18}N_2O_3S^+$ [M^+]: 402.1032; Found: 402.1035.

5-Chloro-2-(phenylsulfonyl)-*N*-(quinolin-8-yl)benzamide (3k)



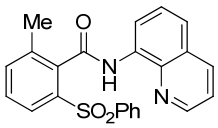
Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/petrol ether =1/2) as a yellow solid in 70% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.57 (s, 1H), 8.92-8.84 (m, 1H), 8.72 (d, J = 7.5 Hz, 1H), 8.44 (dd, J = 8.3, 1.1 Hz, 1H), 8.18 (d, J = 8.6 Hz, 1H), 8.02 (d, J = 7.6 Hz, 2H), 7.88 (d, J = 1.9 Hz, 1H), 7.84-7.76 (m, 2H), 7.67 (ddd, J = 12.0, 9.8, 6.1 Hz, 3H), 7.58 (t, J = 7.6 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 164.79, 149.55, 141.28, 139.38, 138.92, 138.90, 137.06, 136.97, 134.77, 134.30, 132.27, 131.00, 129.85, 129.33, 128.36, 128.34, 127.42, 123.42, 122.70, 118.30. HRMS (EI, m/z): calcd for $C_{22}H_{15}ClN_2O_3S^+$ [M^+]: 422.0484; Found: 422.0482.

2-(Phenylsulfonyl)-*N*-(quinolin-8-yl)-5-(trifluoromethyl)benzamide (3l)



Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/petrol ether =1/2) as a yellow solid in 62% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.77 (s, 1H), 8.89 (d, J = 3.3 Hz, 1H), 8.78 (d, J = 7.6 Hz, 1H), 8.44 (d, J = 8.1 Hz, 1H), 8.39 (d, J = 8.3 Hz, 1H), 8.15 (s, 1H), 8.11 (d, J = 8.5 Hz, 1H), 8.07 (d, J = 7.8 Hz, 2H), 7.79 (d, J = 8.0 Hz, 1H), 7.73-7.58 (m, 5H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 165.07, 149.53, 141.90, 140.76, 139.04, 138.26, 137.04, 134.94, 134.58, 133.85 (q, $J_{C\text{-}F}$ = 32.5 Hz), 131.45, 129.94, 128.61, 128.41, 127.87 (q, $J_{C\text{-}F}$ = 3.4 Hz), 127.41, 126.74 (q, $J_{C\text{-}F}$ = 3.6 Hz), 123.51 (q, $J_{C\text{-}F}$ = 271.7 Hz), 123.48, 122.66, 118.56. ^{19}F NMR (377 MHz, DMSO-d_6): δ -61.76. HRMS (EI, m/z): calcd for $C_{23}H_{15}F_3N_2O_3S^+$ [M^+]: 456.0743; Found: 456.0747.

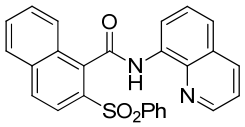
2-Methyl-6-(phenylsulfonyl)-*N*-(quinolin-8-yl)benzamide (3m)



Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/petrol ether =1/2) as a yellow solid in 65% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ

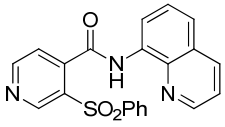
10.33 (s, 1H), 8.84 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.78 (dd, *J* = 7.5, 1.2 Hz, 1H), 8.43 (dd, *J* = 8.3, 1.6 Hz, 1H), 8.04-7.92 (m, 3H), 7.77 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.70 (t, *J* = 7.9 Hz, 1H), 7.66-7.59 (m, 4H), 7.53 (t, *J* = 7.6 Hz, 2H), 2.38 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 165.70, 149.54, 141.81, 138.88, 137.94, 137.24, 137.05, 136.65, 136.26, 134.67, 134.07, 130.34, 129.84, 128.39, 128.09, 127.60, 127.51, 123.20, 122.67, 118.12, 19.21. HRMS (EI, m/z): calcd for $C_{23}H_{18}N_2O_3S^+$ [M^+]: 402.1032; Found: 402.1036.

2-(Phenylsulfonyl)-*N*-(quinolin-8-yl)-1-naphthamide (3n)



Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/petrol ether =1/2) as a yellow solid in 72% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.78 (s, 1H), 8.90 (dd, *J* = 7.5, 1.2 Hz, 1H), 8.83 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.46 (dd, *J* = 8.3, 1.6 Hz, 1H), 8.25 (d, *J* = 8.9 Hz, 1H), 8.15-8.03 (m, 5H), 7.83 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.76 (t, *J* = 7.9 Hz, 2H), 7.72-7.56 (m, 5H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 165.51, 149.62, 141.67, 139.18, 137.08, 136.40, 135.19, 134.92, 134.36, 134.31, 131.05, 129.98, 129.24, 128.83, 128.49, 128.20, 127.55, 126.86, 124.31, 123.57, 122.69, 118.82 (two signals were overlapped by other ones). HRMS (EI, m/z): calcd for $C_{26}H_{18}N_2O_3S^+$ [M^+]: 438.1036; Found: 438.1039.

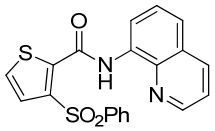
3-(Phenylsulfonyl)-*N*-(quinolin-8-yl)isonicotinamide (3o)



Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/petrol ether =1/1) as a yellow solid in 47% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.85 (s, 1H), 9.33 (s, 1H), 8.97 (d, *J* = 4.9 Hz, 1H), 8.89 (dd, *J* = 4.0, 1.3 Hz, 1H), 8.74 (d, *J* = 7.4 Hz, 1H), 8.44 (dd, *J* = 8.2, 1.2 Hz, 1H), 8.10 (d, *J* = 7.5 Hz, 2H), 7.79 (dd, *J* = 9.8, 6.6 Hz, 2H), 7.74-7.67 (m, 2H), 7.70-7.59 (m, 3H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 164.57, 155.28, 150.53, 149.62, 144.06, 141.12, 139.07, 137.07, 134.74, 134.59, 133.94, 129.97, 128.55, 128.45, 127.42,

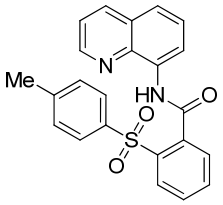
123.72, 123.34, 122.74, 118.73. HRMS (EI, m/z): calcd for $C_{21}H_{15}N_3O_3S^+$ [M^+]: 389.0831; Found: 389.0833.

3-(Phenylsulfonyl)-*N*-(quinolin-8-yl)thiophene-2-carboxamide (3p)



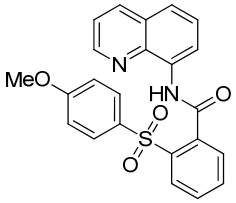
Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/petrol ether =1/2) as a yellow solid in 42% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.93 (s, 1H), 8.95 (dd, J = 4.1, 1.4 Hz, 1H), 8.62 (d, J = 7.6 Hz, 1H), 8.47 (dd, J = 8.3, 1.3 Hz, 1H), 8.13-8.04 (m, 2H), 7.97 (d, J = 5.3 Hz, 1H), 7.81 (d, J = 8.2 Hz, 1H), 7.73-7.59 (m, 6H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 158.75, 149.81, 142.70, 141.20, 138.86, 138.84, 137.18, 134.59, 134.18, 130.48, 130.12, 129.02, 128.39, 128.01, 127.42, 123.95, 122.92, 118.37. HRMS (EI, m/z): calcd for $C_{20}H_{14}N_2O_3S_2^+$ [M^+]: 394.0446; Found: 394.0448.

***N*-(quinolin-8-yl)-2-tosylbenzamide (3q)**



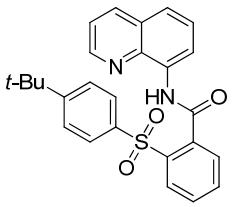
Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/petrol ether =1/2) as a yellow solid in 80% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.18 (s, 1H), 8.84 (d, J = 3.0 Hz, 1H), 8.72 (d, J = 7.4 Hz, 1H), 8.50-8.39 (m, 1H), 8.18 (d, J = 7.8 Hz, 1H), 7.86 (d, J = 8.2 Hz, 2H), 7.83-7.72 (m, 4H), 7.70 (t, J = 7.9 Hz, 1H), 7.64 (dd, J = 8.3, 4.2 Hz, 1H), 7.32 (d, J = 8.1 Hz, 2H), 2.29 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 165.95, 149.53, 144.79, 138.55, 138.51, 138.49, 137.12, 137.03, 134.63, 134.54, 131.22, 130.24, 130.15, 129.22, 128.32, 127.50, 123.14, 122.74, 117.56, 21.47 (one signal was overlapped by other ones). HRMS (EI, m/z): calcd for $C_{23}H_{18}N_2O_3S^+$ [M^+]: 402.1032; Found: 402.1034.

2-((4-Methoxyphenyl)sulfonyl)-*N*-(quinolin-8-yl)benzamide (3r)



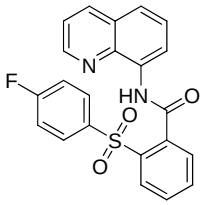
Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/petrol ether =1/1) as a yellow solid in 75% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.17 (s, 1H), 8.84 (dd, J = 4.0, 1.2 Hz, 1H), 8.72 (d, J = 7.3 Hz, 1H), 8.45 (dd, J = 8.3, 1.3 Hz, 1H), 8.21-8.10 (m, 1H), 7.91 (d, J = 8.9 Hz, 2H), 7.84-7.73 (m, 4H), 7.70 (t, J = 7.9 Hz, 1H), 7.64 (dd, J = 8.3, 4.2 Hz, 1H), 7.03 (d, J = 8.9 Hz, 2H), 3.76 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 166.06, 163.65, 149.55, 138.98, 138.52, 137.14, 136.84, 134.65, 134.36, 132.78, 131.22, 130.73, 129.95, 129.18, 128.31, 127.51, 123.15, 122.78, 117.54, 115.01, 56.21. HRMS (EI, m/z): calcd for $C_{23}H_{18}N_2O_4S^+$ [M^+]: 418.0982; Found: 418.0985.

2-((4-(*tert*-Butyl)phenyl)sulfonyl)-*N*-(quinolin-8-yl)benzamide (3s)



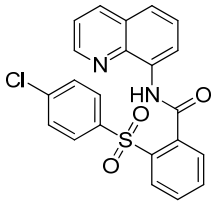
Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/petrol ether =1/2) as a yellow solid in 72% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.22 (s, 1H), 8.84 (dd, J = 4.1, 1.4 Hz, 1H), 8.74 (d, J = 7.0 Hz, 1H), 8.44 (dd, J = 8.3, 1.4 Hz, 1H), 8.25-8.17 (m, 1H), 7.93 (d, J = 8.5 Hz, 2H), 7.83-7.73 (m, 4H), 7.70 (t, J = 7.9 Hz, 1H), 7.63 (dd, J = 8.3, 4.2 Hz, 1H), 7.54 (d, J = 8.6 Hz, 2H), 1.20 (s, 9H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 166.00, 157.32, 149.52, 138.54, 138.53, 137.13, 137.05, 134.65, 134.55, 131.26, 130.20, 129.16, 128.32, 127.49, 126.66, 123.15, 122.75, 117.60, 35.36, 31.09 (two signals were overlapped by other ones). HRMS (EI, m/z): calcd for $C_{26}H_{24}N_2O_3S^+$ [M^+]: 444.1500; Found: 444.1508.

2-((4-Fluorophenyl)sulfonyl)-*N*-(quinolin-8-yl)benzamide (3t)



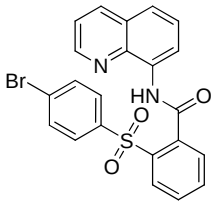
Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/petrol ether =1/2) as a yellow solid in 68% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.30 (s, 1H), 8.86 (d, J = 2.8 Hz, 1H), 8.71 (d, J = 7.4 Hz, 1H), 8.45 (d, J = 8.2 Hz, 1H), 8.22 (d, J = 7.7 Hz, 1H), 8.15-8.02 (m, 2H), 7.87-7.75 (m, 4H), 7.69 (t, J = 7.9 Hz, 1H), 7.64 (dd, J = 8.2, 4.2 Hz, 1H), 7.41 (t, J = 8.6 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 166.08, 165.38 (d, $J_{C\text{-}F}$ = 251.8 Hz), 149.60, 138.66, 138.06, 137.86 (d, $J_{C\text{-}F}$ = 2.6 Hz), 137.15 (d, $J_{C\text{-}F}$ = 4.1 Hz), 134.83, 134.63, 131.67, 131.57, 131.32, 130.37, 129.29, 128.34, 127.47, 123.29, 122.77, 117.82, 117.06 (d, $J_{C\text{-}F}$ = 22.8 Hz). ^{19}F NMR (377 MHz, DMSO-d_6): δ -104.66. HRMS (EI, m/z): calcd for $C_{22}H_{15}FN_2O_3S^+$ [M^+]: 406.0781; Found: 406.0782.

2-((4-Chlorophenyl)sulfonyl)-*N*-(quinolin-8-yl)benzamide (3u)



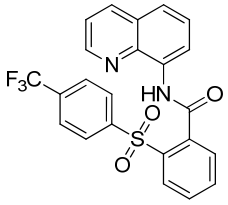
Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/petrol ether =1/2) as a yellow solid in 72% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.28 (s, 1H), 8.85 (dd, J = 4.1, 1.4 Hz, 1H), 8.70 (d, J = 7.5 Hz, 1H), 8.45 (dd, J = 8.3, 1.5 Hz, 1H), 8.23 (d, J = 7.7 Hz, 1H), 8.00 (d, J = 8.6 Hz, 2H), 7.87-7.76 (m, 4H), 7.69 (t, J = 7.9 Hz, 1H), 7.66-7.60 (m, 3H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 165.95, 149.59, 140.37, 139.28, 138.63, 137.71, 137.27, 137.12, 134.97, 134.59, 131.35, 130.45, 130.23, 129.96, 129.33, 128.33, 127.45, 123.30, 122.76, 117.81. HRMS (EI, m/z): calcd for $C_{22}H_{15}ClN_2O_3S^+$ [M^+]: 422.0484; Found: 422.0490.

2-((4-Bromophenyl)sulfonyl)-*N*-(quinolin-8-yl)benzamide (3v)



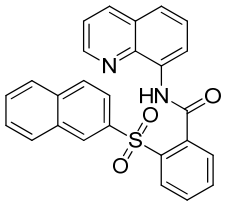
Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/petrol ether =1/2) as a yellow solid in 65% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.28 (s, 1H), 8.84 (d, J = 2.3 Hz, 1H), 8.70 (d, J = 7.5 Hz, 1H), 8.44 (d, J = 8.2 Hz, 1H), 8.23 (d, J = 7.6 Hz, 1H), 7.92 (d, J = 7.8 Hz, 2H), 7.86-7.74 (m, 6H), 7.69 (t, J = 7.9 Hz, 1H), 7.63 (dd, J = 7.5, 4.1 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 165.93, 149.57, 140.79, 138.61, 137.66, 137.27, 137.10, 134.96, 134.58, 132.89, 131.34, 130.45, 130.24, 129.33, 128.40, 128.32, 127.44, 123.29, 122.75, 117.78. HRMS (EI, m/z): calcd for $C_{22}H_{15}BrN_2O_3S^+$ [M^+]: 465.9986; Found: 465.9983.

_N_-(Quinolin-8-yl)-2-((4-(trifluoromethyl)phenyl)sulfonyl)benzamide (3w)



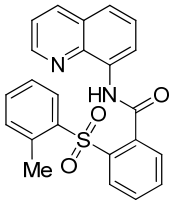
Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/petrol ether =1/2) as a yellow solid in 54% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.34 (s, 1H), 8.83 (d, J = 3.0 Hz, 1H), 8.69 (d, J = 7.5 Hz, 1H), 8.44 (d, J = 8.2 Hz, 1H), 8.29 (d, J = 7.9 Hz, 1H), 8.20 (d, J = 8.2 Hz, 2H), 7.94 (d, J = 8.3 Hz, 2H), 7.90-7.77 (m, 4H), 7.69 (t, J = 7.9 Hz, 1H), 7.63 (dd, J = 8.3, 4.2 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 165.87, 149.55, 145.46, 138.68, 137.51, 137.08 (d, $J_{C\text{-}F}$ = 5.3 Hz), 135.27, 134.55, 133.74, 133.42, 131.42, 130.73, 129.41, 129.21, 128.33, 127.41, 126.96 (d, $J_{C\text{-}F}$ = 3.8 Hz), 123.74 (q, $J_{C\text{-}F}$ = 271.5 Hz), 123.36, 122.73, 117.92. ^{19}F NMR (377 MHz, DMSO-d_6): δ -61.78. HRMS (EI, m/z): calcd for $C_{23}H_{15}F_3N_2O_3S^+$ [M^+]: 456.0743; Found: 456.0750.

2-(Naphthalen-2-ylsulfonyl)-_N_-(quinolin-8-yl)benzamide (3x)



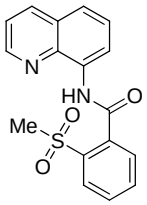
Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/petrol ether =1/2) as a yellow solid in 70% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.11 (s, 1H), 8.72 (d, J = 7.4 Hz, 1H), 8.62 (d, J = 3.2 Hz, 1H), 8.57 (s, 1H), 8.43-8.37 (m, 1H), 8.33-8.27 (m, 1H), 8.06 (d, J = 8.7 Hz, 1H), 7.99-7.93 (m, 2H), 7.89-7.74 (m, 5H), 7.71-7.62 (m, 2H), 7.58-7.52 (m, 2H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 165.74, 149.34, 138.39, 138.30, 137.99, 137.25, 136.99, 135.05, 134.78, 134.51, 131.98, 131.29, 130.38, 129.99, 129.81, 129.75, 129.67, 129.40, 128.25, 128.22, 128.11, 127.46, 123.17, 123.07, 122.67, 117.55. HRMS (EI, m/z): calcd for $C_{26}H_{18}N_2O_3S^+$ [M^+]: 438.1034; Found: 438.1039.

_N_-(quinolin-8-yl)-2-(_o_-tolylsulfonyl)benzamide (3y)



Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/petrol ether =1/2) as a yellow solid in 52% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.12 (s, 1H), 8.82 (dd, J = 4.1, 1.3 Hz, 1H), 8.54 (d, J = 7.5 Hz, 1H), 8.43 (dd, J = 8.3, 1.3 Hz, 1H), 8.18-8.09 (m, 1H), 7.88-7.73 (m, 5H), 7.67-7.60 (m, 2H), 7.42 (t, J = 7.5 Hz, 1H), 7.28 (d, J = 7.5 Hz, 1H), 7.18 (t, J = 7.6 Hz, 1H), 2.34 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 164.99, 149.54, 138.87, 138.39, 137.73, 137.45, 137.13, 136.94, 134.72, 134.35, 134.24, 133.04, 131.15, 129.83, 129.75, 129.64, 128.23, 127.43, 126.73, 123.15, 122.78, 117.22, 20.04. HRMS (EI, m/z): calcd for $C_{23}H_{18}N_2O_3S^+$ [M^+]: 402.1032; Found: 402.1038.

2-(Methylsulfonyl)-_N_-(quinolin-8-yl)benzamide (3z)



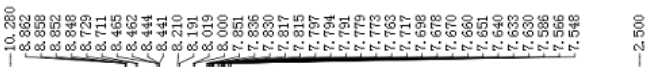
Following the general procedure the title compound was isolated by flash chromatography (eluent: ethyl acetate/petrol ether =1/2) as a yellow solid in 46% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.42 (s, 1H), 8.89 (dd, J = 4.2, 1.5 Hz, 1H), 8.68 (d, J = 6.9 Hz, 1H), 8.45 (dd, J = 8.3, 1.5 Hz, 1H), 8.07 (d, J = 7.8 Hz, 1H), 7.90 (d, J = 3.9 Hz, 2H), 7.85-7.75 (m, 2H), 7.72-7.61 (m, 2H), 3.44 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 166.56, 149.69, 138.79, 138.48, 137.40, 137.16, 134.67, 134.55, 131.20, 130.00, 129.01, 128.35, 127.42, 123.41, 122.80, 118.01, 45.57. HRMS (EI, m/z): calcd for $C_{17}H_{14}N_2O_3S^+$ [M^+]: 326.0722; Found: 326.0726.

References

1. A. M. Suess, M. Z. Ertem, C. J. Cramer, S. S. Stahl, *J. Am. Chem. Soc.,* 2013, **135**, 9797.

2. (*a*) L. D. Tran, I. Popov, O. Daugulis, *J. Am. Chem. Soc.,* 2012, **134**, 18237; (*b*) T. Truong, K. Klimovica, O. Daugulis, *J. Am. Chem. Soc.,* 2013, **135**, 9342; (*c*) L. D. Tran, J. Roane, O. Daugulis, *Angew. Chem., Int. Ed.,* 2013, **52**, 6043; (*d*) J. Roane, O. Daugulis, *Org. Lett.,* 2013, **15**, 5842; (*e*) M. Nishino, K. Hirano, T. Satoh, M. Miura, *Angew. Chem., Int. Ed.,* 2013, **52**, 4457.

3. L. Liu, Y. Chi, K. Jen, *J. Org. Chem.,* 1980, **45**, 406.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8.711
8.465
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8.441
8.210
8.191
8.019
8.000
7.851
7.836
7.830
7.817
7.815
7.797
7.794
7.791
7.779
7.773
7.763
7.717
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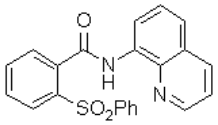
7.630
7.586
7.566
7.548
2.500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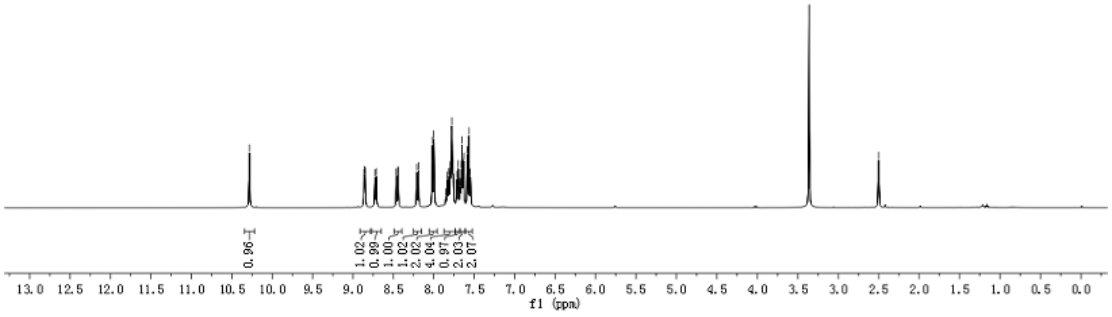
N
H
N
SO2Ph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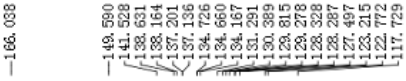
1.02
0.99
1.00
1.02
2.02
4.04
0.97
2.03
2.07
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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129.278
128.328
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127.497
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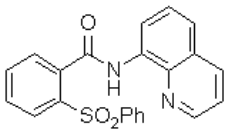
40.209
40.000
39.791
39.583
39.374


O
N
H
N
SO2Ph

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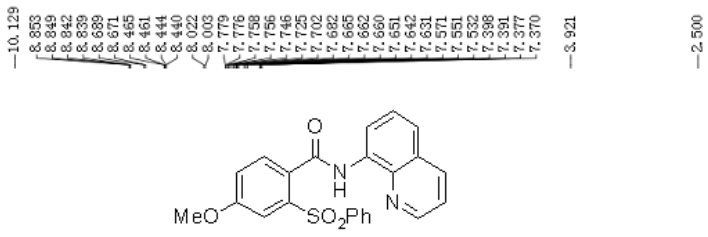
f1 (ppm)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7.758
7.756
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7.571
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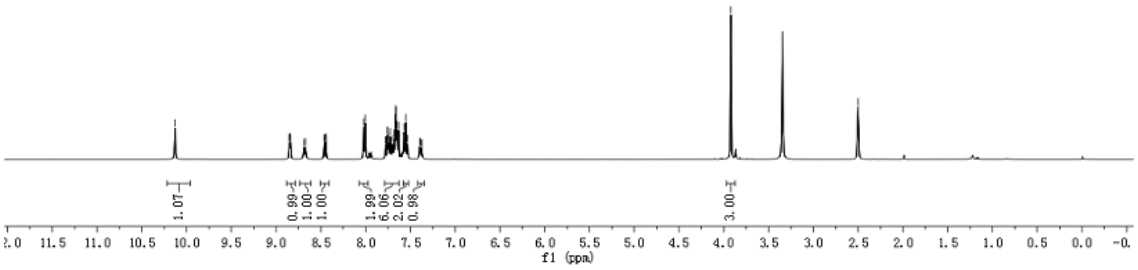
N
H
O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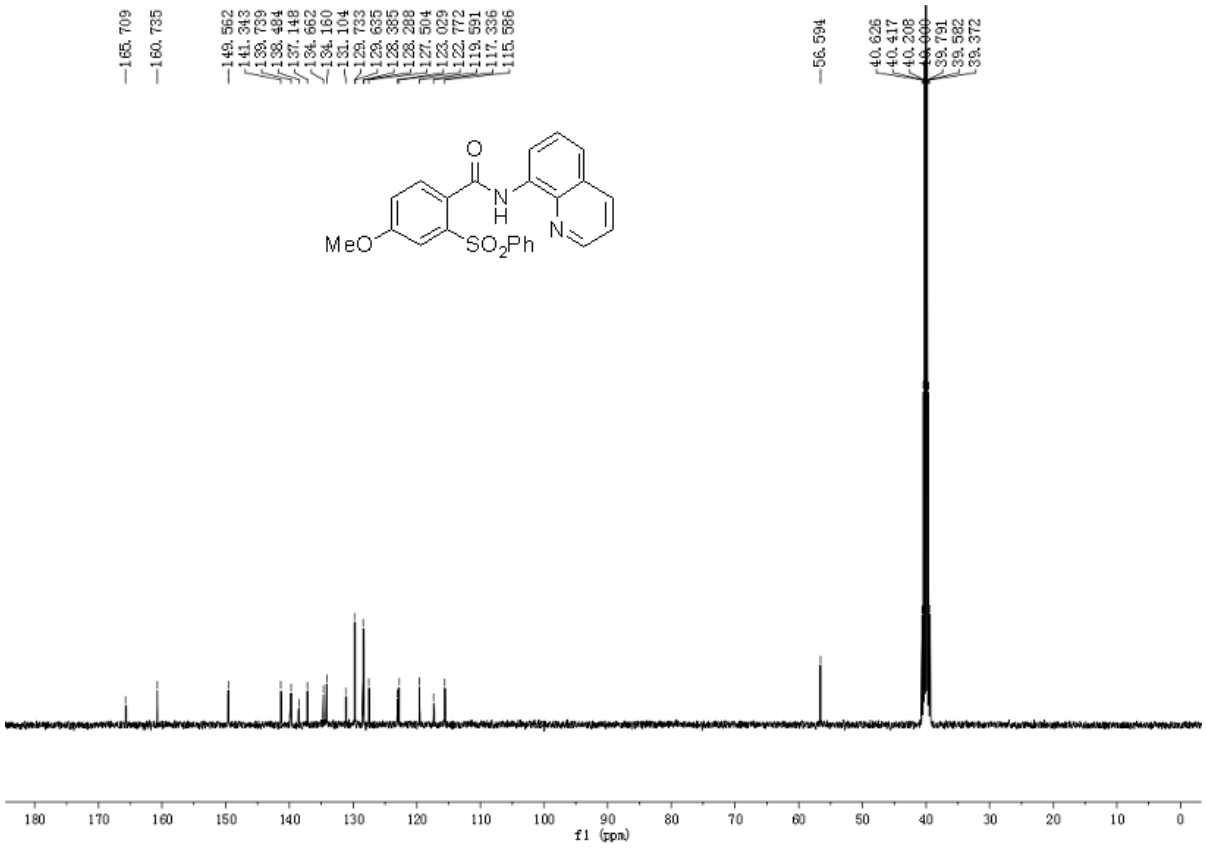
f1 (ppm)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128.288
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122.772
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MeO
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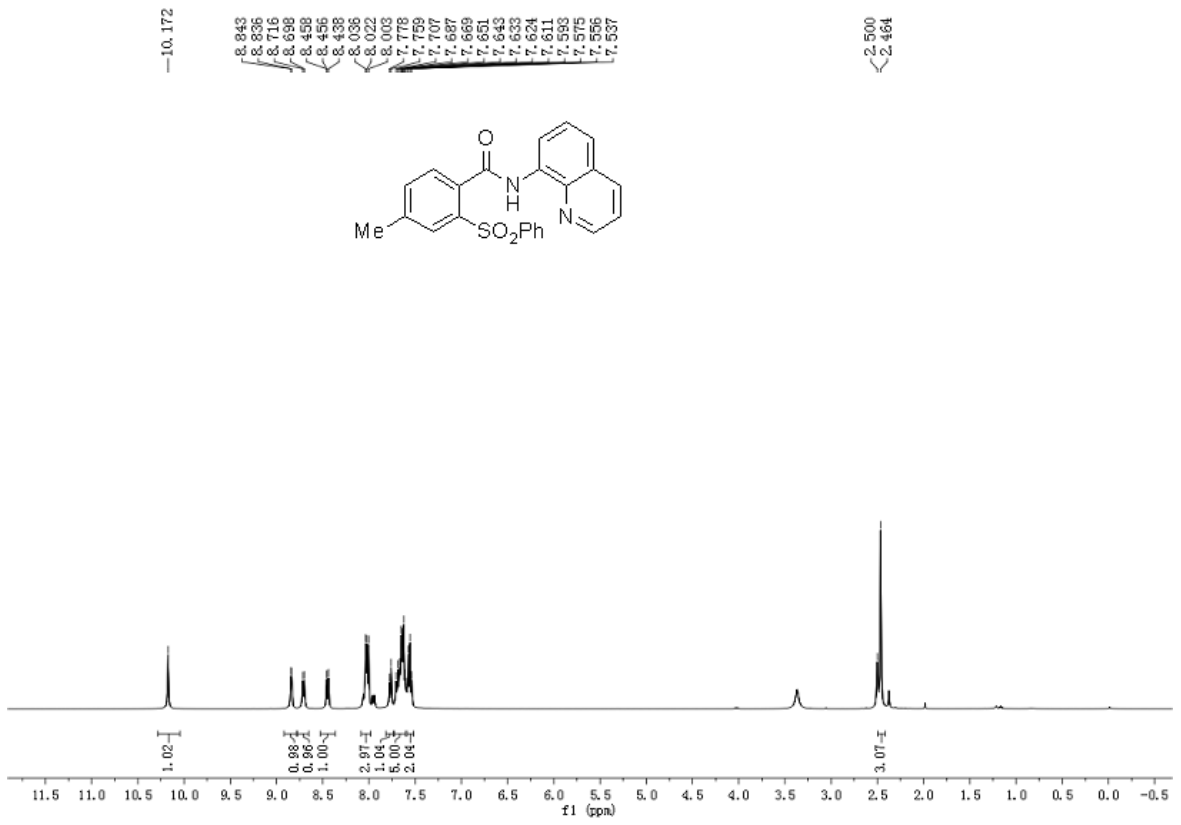
N
H
O
f1 (ppm)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7.611
7.593
7.575
7.556
7.537
2.500
2.464
O
N
H
N
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SO2Ph
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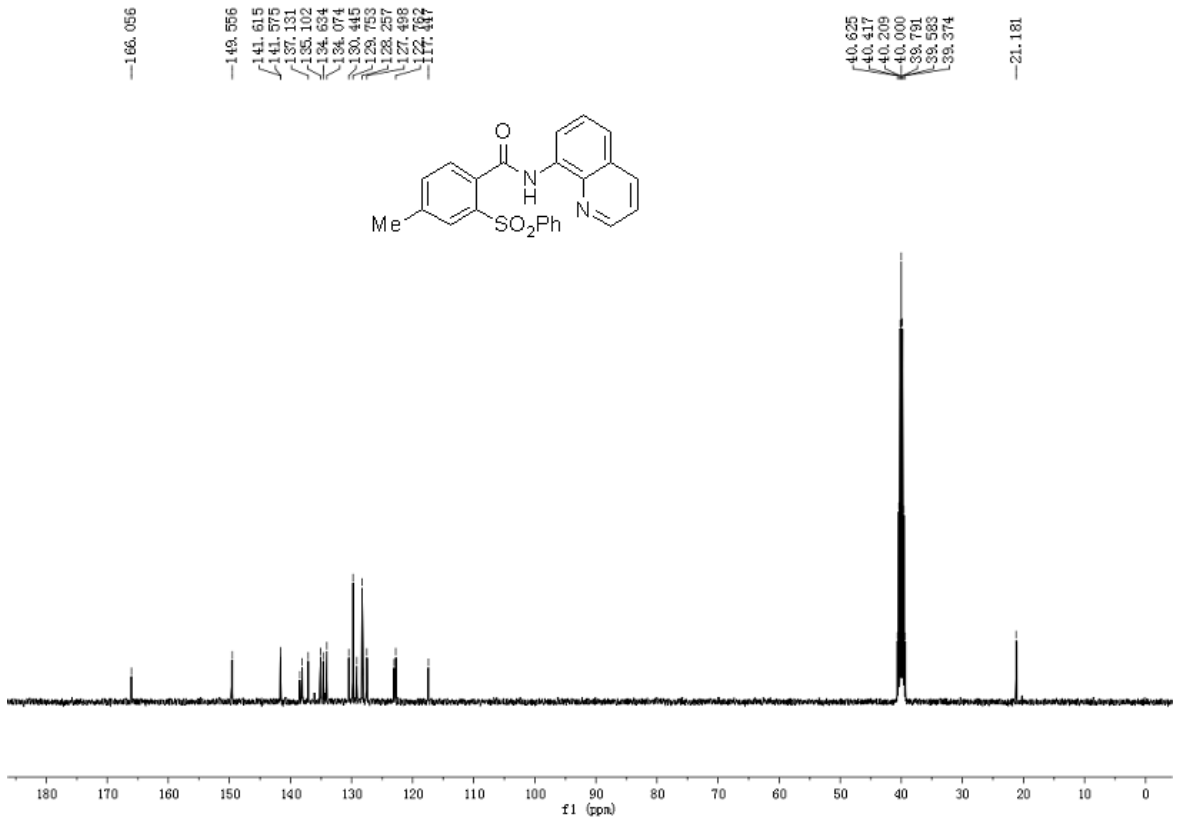
5.00
2.04
3.07
f1 (ppm)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122.762
117.447
40.625
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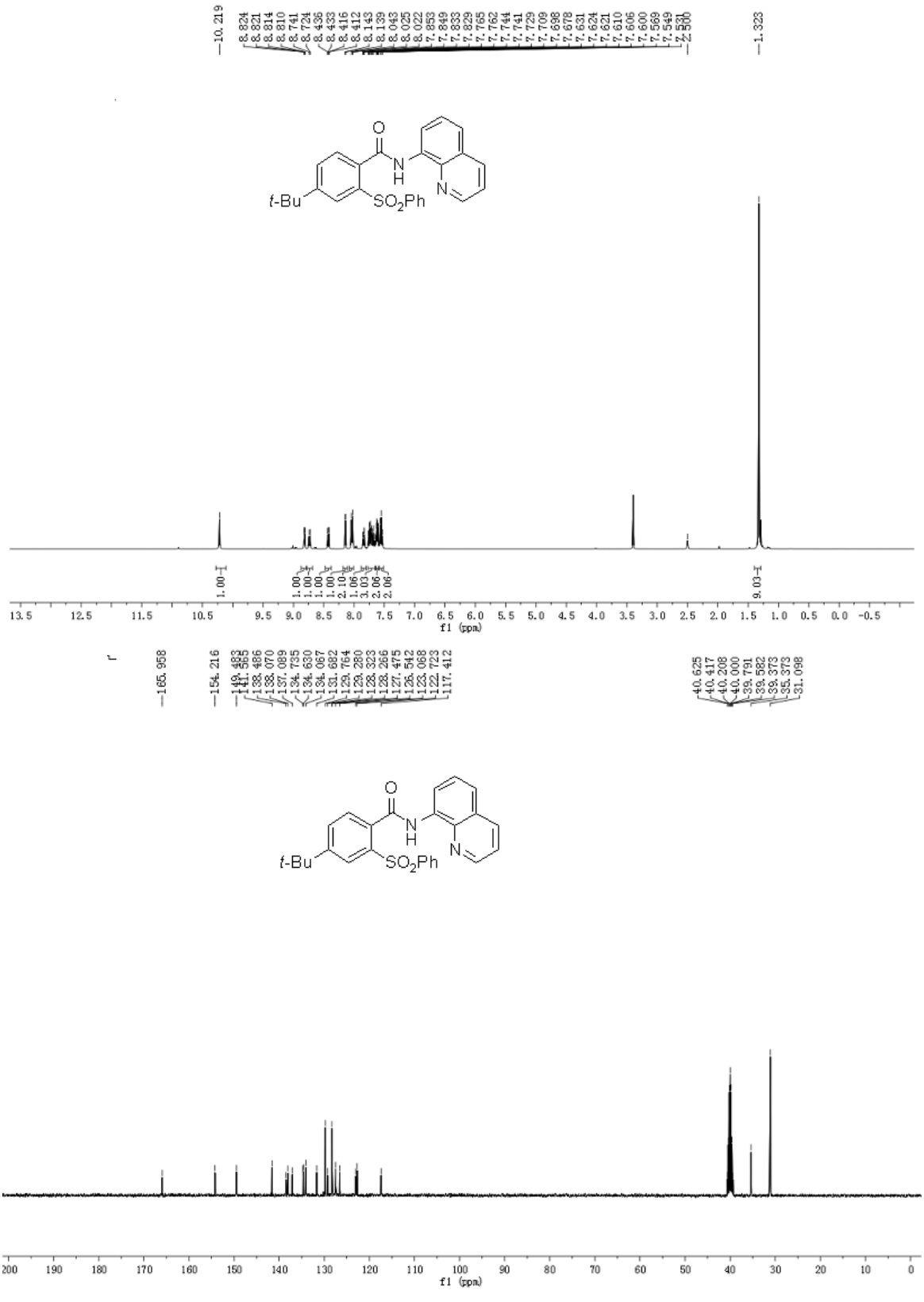
N
H
N
Me
SO2Ph
f1 (ppm)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7.531
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SO2Ph
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2.06
9.03
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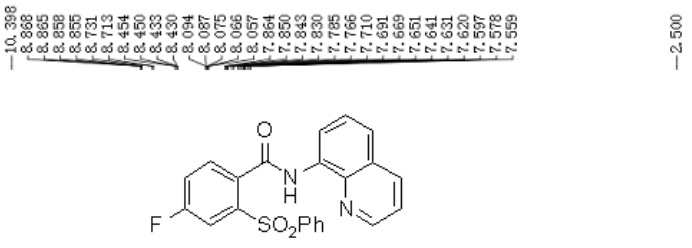
t-Bu
SO2Ph
f1 (ppm)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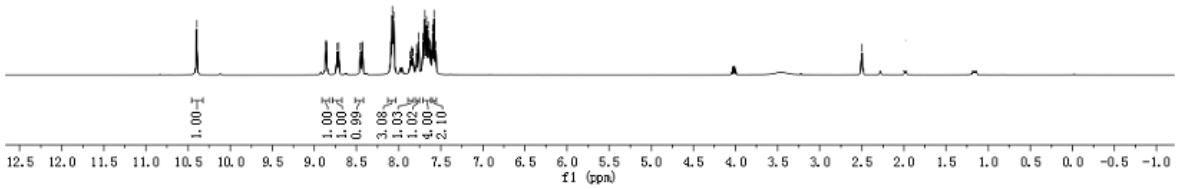
H
F
SO2Ph
N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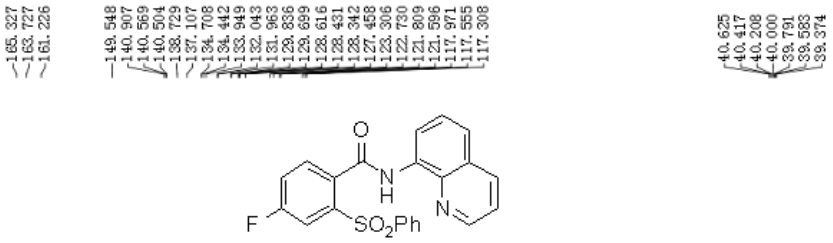
f1 (ppm)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129.699
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128.431
128.342
127.458
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122.730
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40.000
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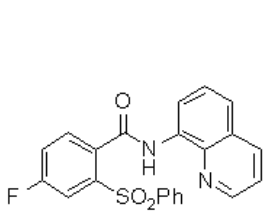
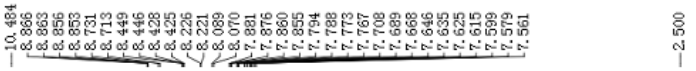
f1 (ppm)


O
N
H
F
SO2Ph
N

-108.034
20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190
f1 (ppm)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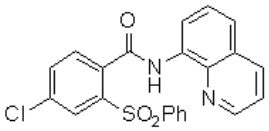
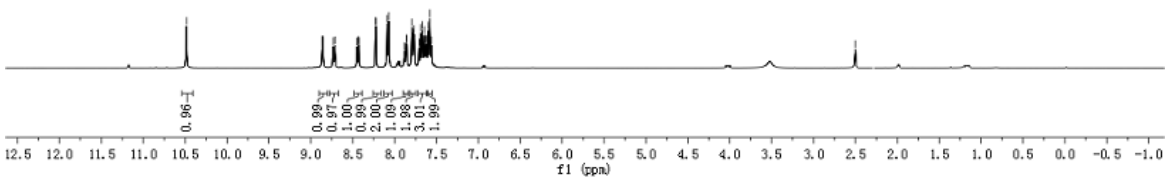
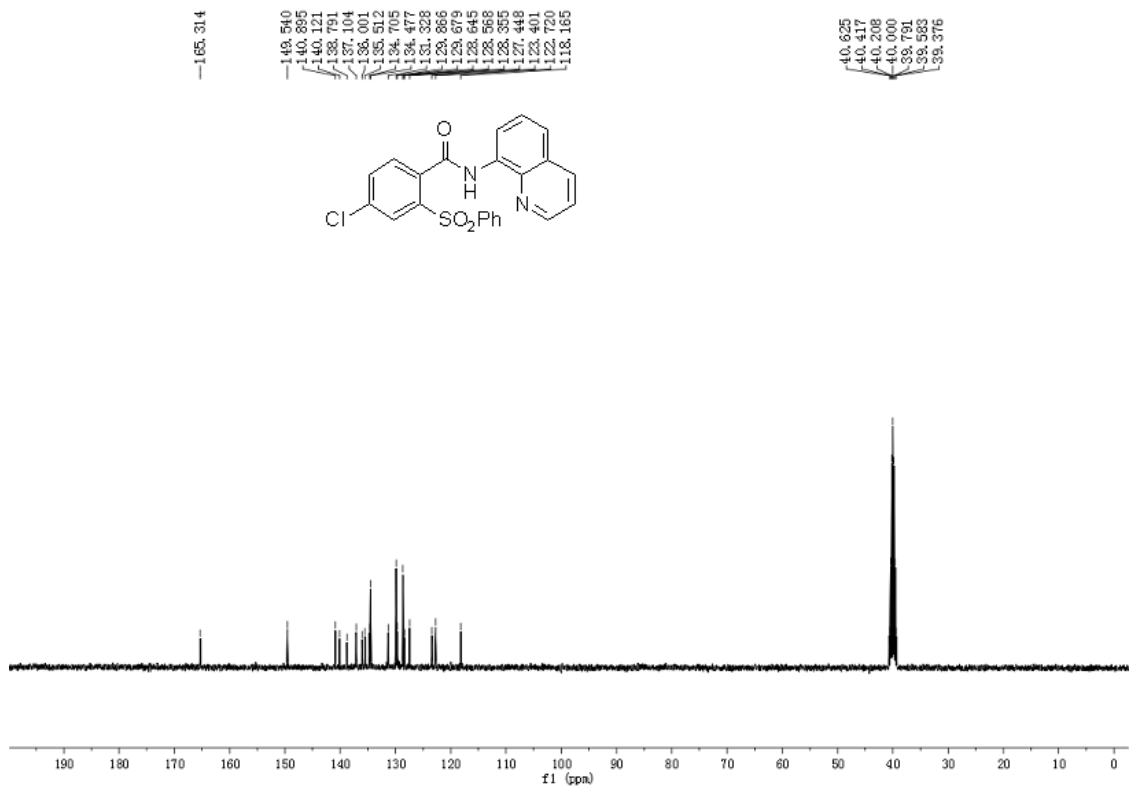
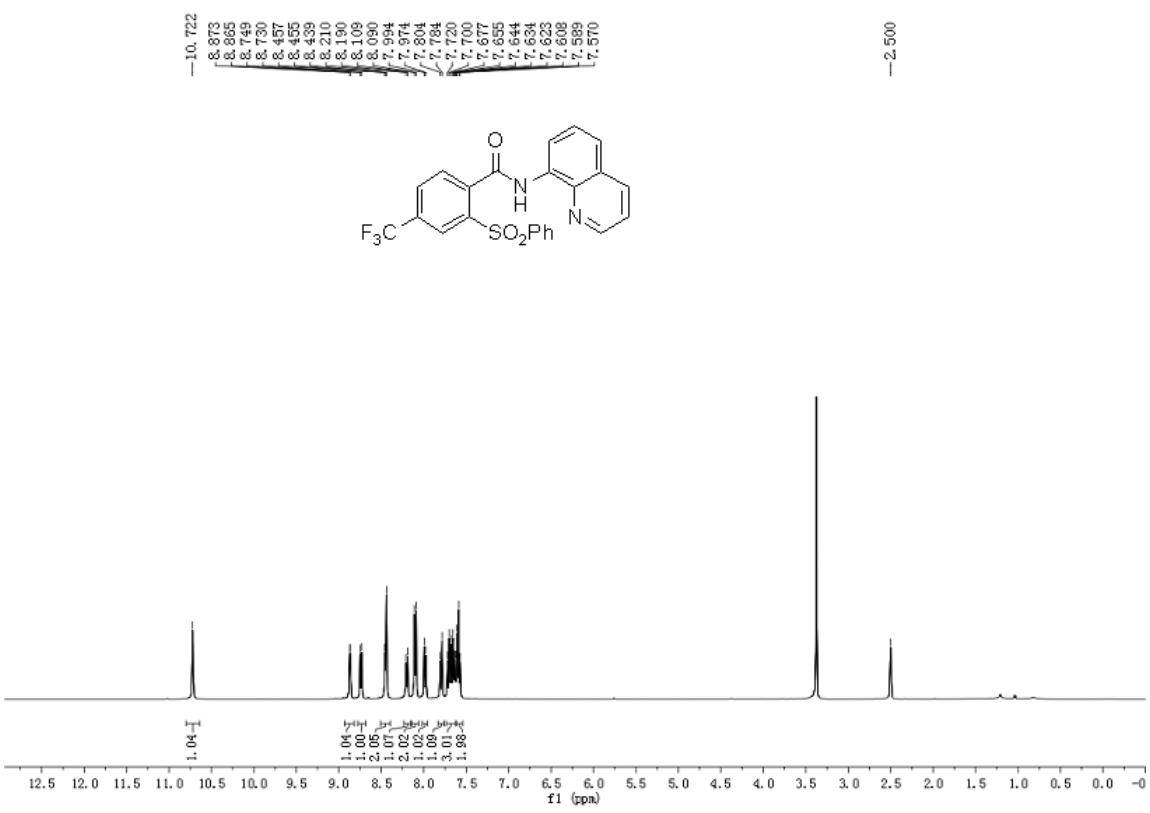
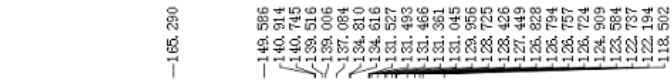
8.863
8.856
8.853
8.731
8.713
8.449
8.446
8.428
8.425
8.226
8.221
8.089
8.070
7.881
7.876
7.860
7.855
7.794
7.788
7.773
7.767
7.708
7.689
7.668
7.646
7.635
7.625
7.615
7.599
7.579
7.561
2.500

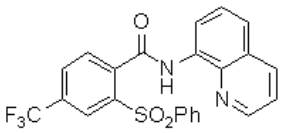

O
N
H
Cl
SO2Ph
N

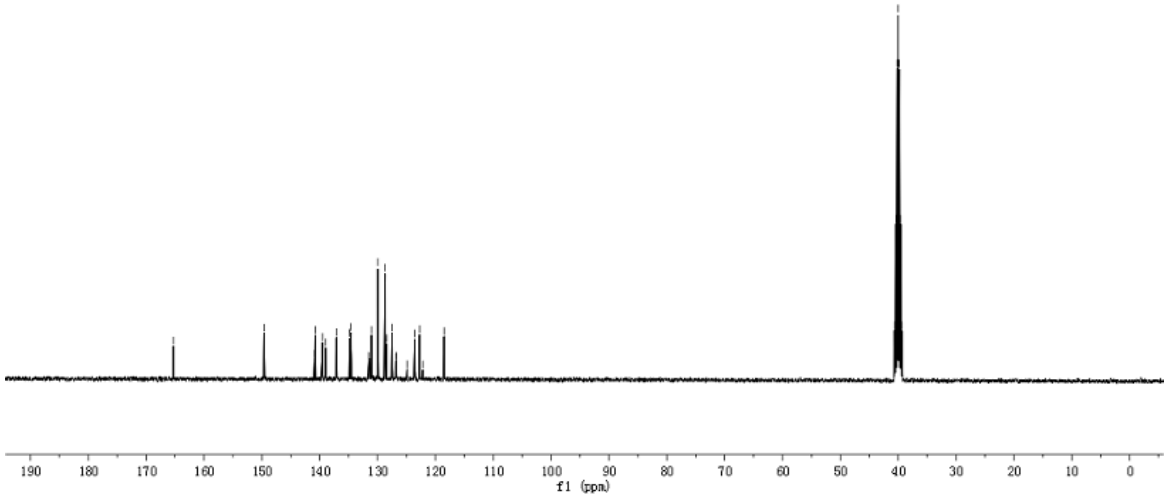

0.96
0.99
0.97
1.00
0.99
2.00
1.09
1.98
3.01
1.99
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


165.314
149.540
140.895
140.121
138.791
137.104
136.001
135.512
134.705
134.477
131.328
129.866
129.679
128.645
128.568
128.355
127.448
123.401
122.720
118.165
40.625
40.417
40.208
40.000
39.791
39.583
39.376
O
N
H
Cl
SO2Ph
N
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

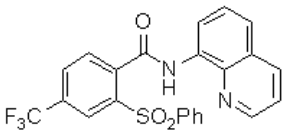

10.722
8.873
8.865
8.749
8.730
8.457
8.455
8.439
8.210
8.190
8.109
8.090
7.994
7.974
7.804
7.784
7.720
7.700
7.677
7.655
7.644
7.634
7.623
7.608
7.589
7.570
2.500
O
N
H
F3C
SO2Ph
N
1.04
1.04
1.00
2.05
1.07
2.02
1.02
1.08
3.01
1.98
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)

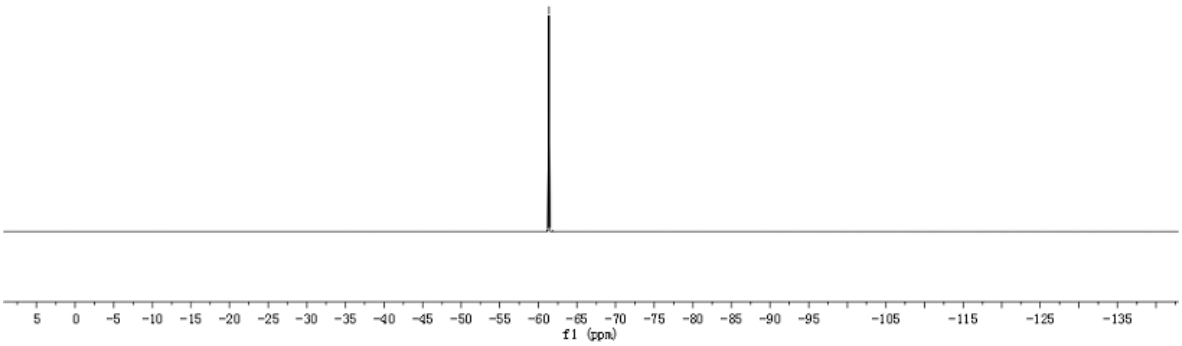

165.290
149.586
140.914
140.745
139.516
139.006
137.084
134.810
134.616
131.527
131.493
131.466
131.361
131.045
129.956
128.725
128.426
127.449
126.828
126.794
126.757
126.724
124.909
123.584
122.737
122.194
118.502
40.626
40.418
40.209
40.000
39.792
39.583
39.374

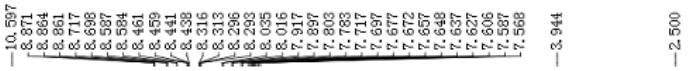

O
N
H
N
F3C
SO2Ph

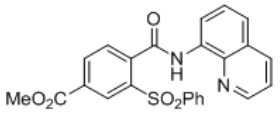

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

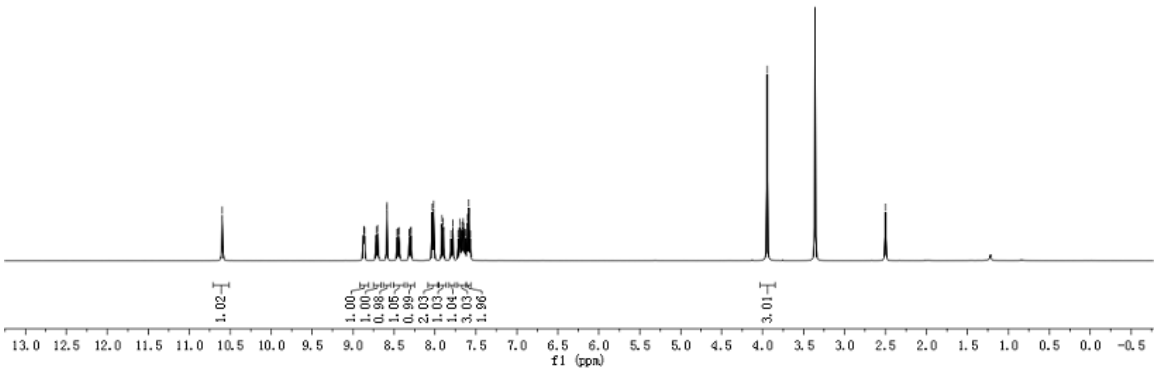

-61.359

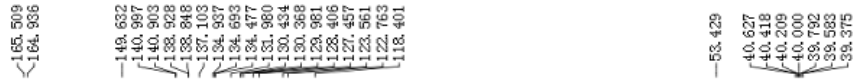

O
N
H
N
F3C
SO2Ph

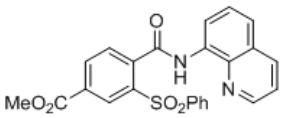

5
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-105
-115
-125
-135
f1 (ppm)


10.597
8.871
8.864
8.861
8.717
8.698
8.597
8.584
8.461
8.459
8.441
8.438
8.316
8.313
8.296
8.293
8.035
8.016
7.917
7.897
7.803
7.783
7.717
7.697
7.677
7.672
7.657
7.648
7.637
7.627
7.606
7.587
7.568
3.944
2.500

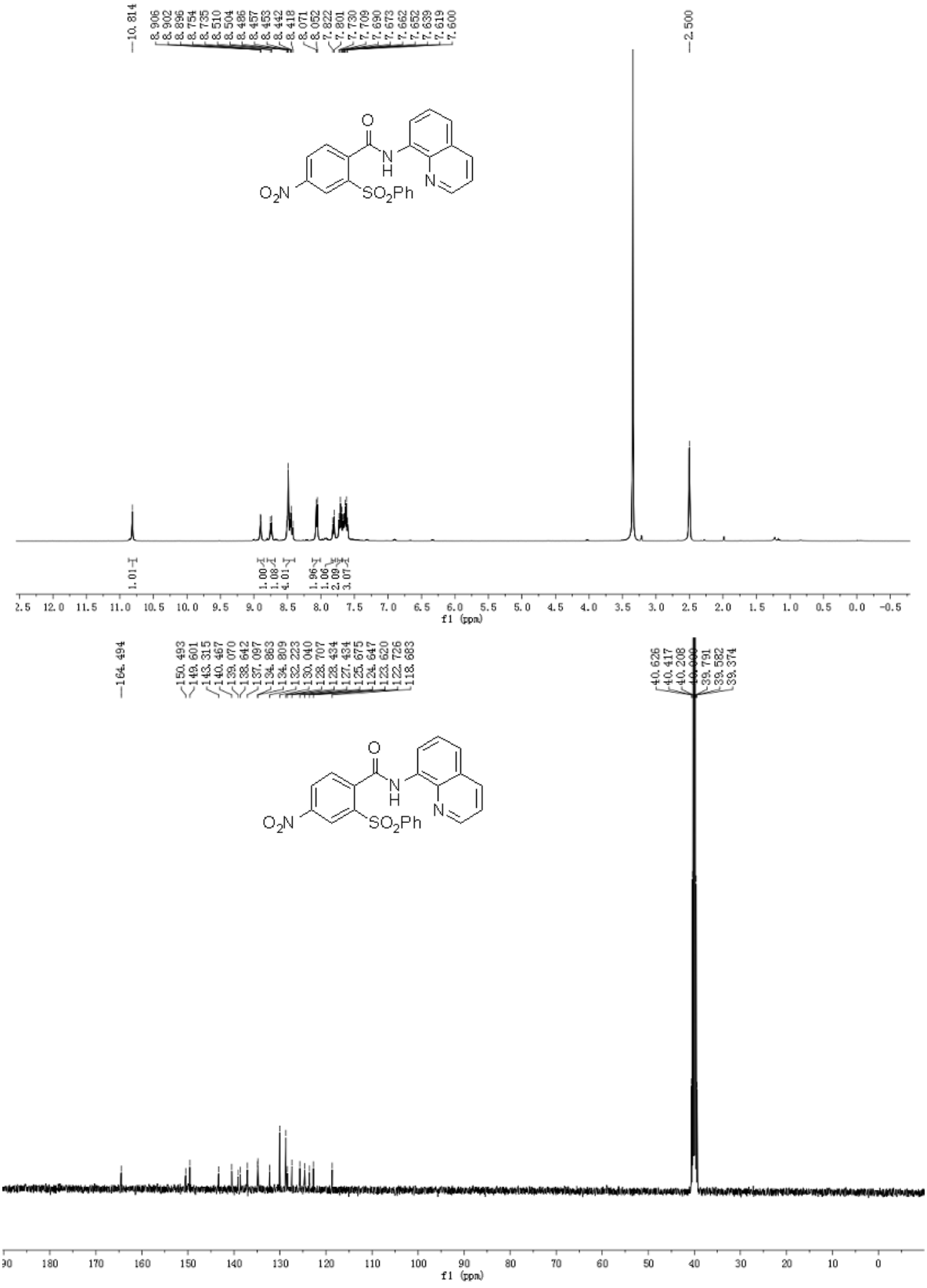

O
N
H
N
MeO2C
SO2Ph

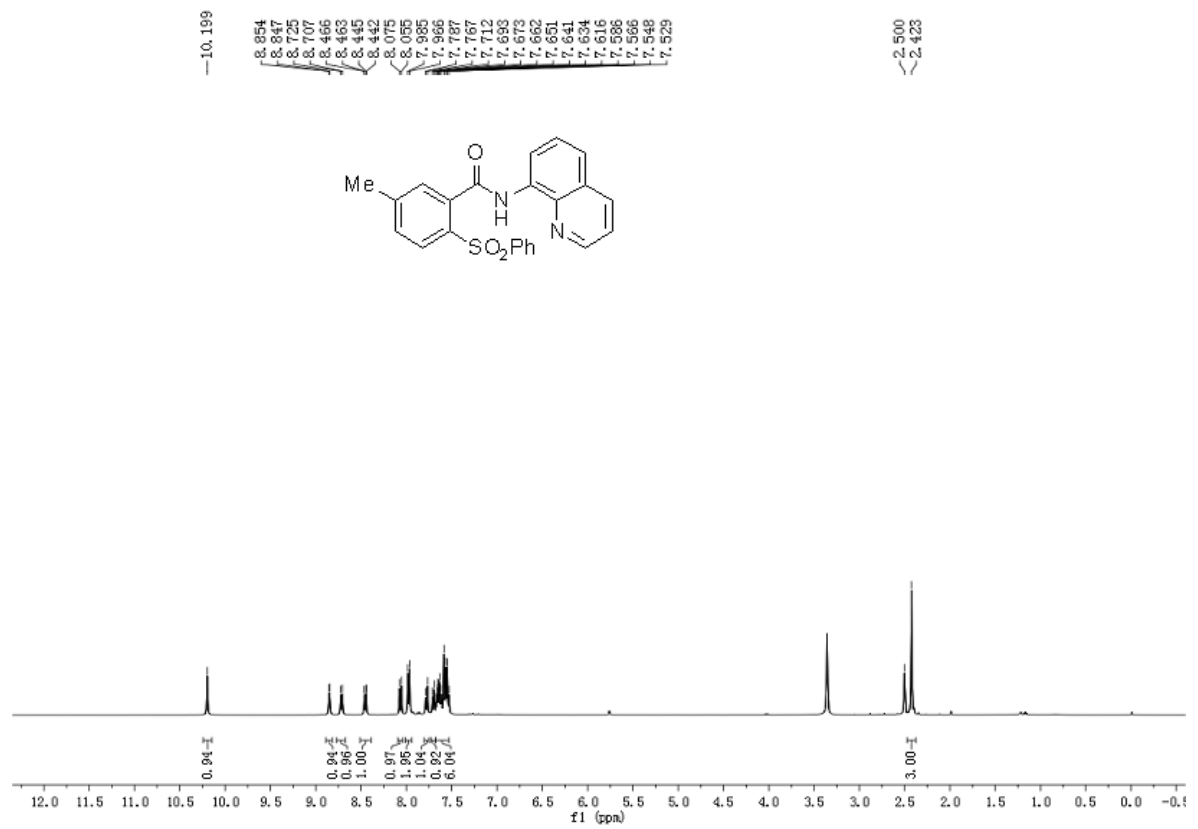

1.02
1.00
1.00
0.98
1.05
0.99
2.03
1.03
1.04
3.03
1.96
3.01
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

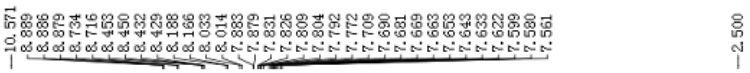

165.509
164.936
149.632
140.997
140.903
138.928
138.848
137.103
134.937
134.693
134.477
131.980
130.434
130.368
129.981
128.406
127.457
123.561
122.763
118.401
53.429
40.627
40.418
40.209
40.000
39.792
39.583
39.375


O
N
H
N
MeO2C
SO2Ph

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


10.814
8.906
8.902
8.896
8.754
8.735
8.510
8.504
8.486
8.457
8.453
8.442
8.418
8.071
8.052
7.822
7.801
7.730
7.709
7.690
7.673
7.662
7.652
7.639
7.619
7.600
2.500
1.01
1.00
1.08
4.01
1.96
1.06
2.09
3.07
f1 (ppm)
164.494
150.493
149.601
143.315
140.467
139.070
138.642
137.097
134.863
134.809
132.223
130.040
128.707
128.434
127.434
125.675
124.647
123.620
122.726
118.683
40.626
40.417
40.208
39.791
39.582
39.374
f1 (ppm)


10.199
8.854
8.847
8.725
8.707
8.466
8.463
8.445
8.442
8.075
8.055
7.985
7.966
7.787
7.767
7.712
7.693
7.673
7.662
7.651
7.641
7.634
7.616
7.588
7.566
7.548
7.529
2.500
2.423
Me
O
N
H
N
SO2Ph
0.94
0.94
0.96
1.00
0.97
1.95
1.04
0.92
6.04
3.00
f1 (ppm)
166.052
149.578
145.632
141.828
138.522
137.148
135.276
134.627
133.995
131.639
130.422
129.756
129.579
128.304
128.101
127.512
123.138
122.777
117.538
40.626
40.417
40.209
40.000
39.791
39.583
39.374
21.324
Me
O
N
H
N
SO2Ph
f1 (ppm)


10.571
8.889
8.886
8.879
8.734
8.716
8.453
8.450
8.432
8.429
8.188
8.166
8.033
8.014
7.883
7.879
7.831
7.826
7.809
7.804
7.792
7.772
7.709
7.690
7.681
7.669
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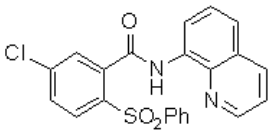
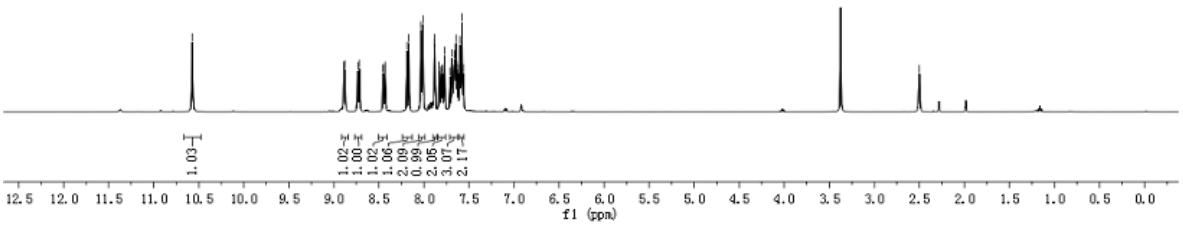
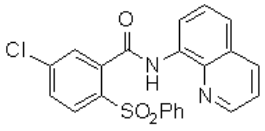
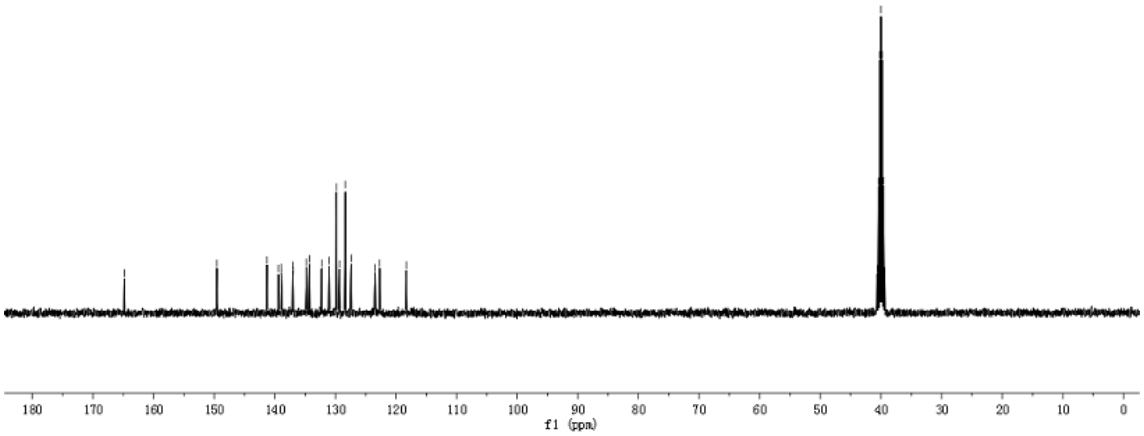
7.633
7.622
7.599
7.580
7.561
2.500


O
Cl
N
H
N
SO2Ph

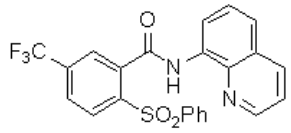

1.03
1.02
1.00
1.02
1.06
2.09
0.99
2.05
3.07
2.17
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

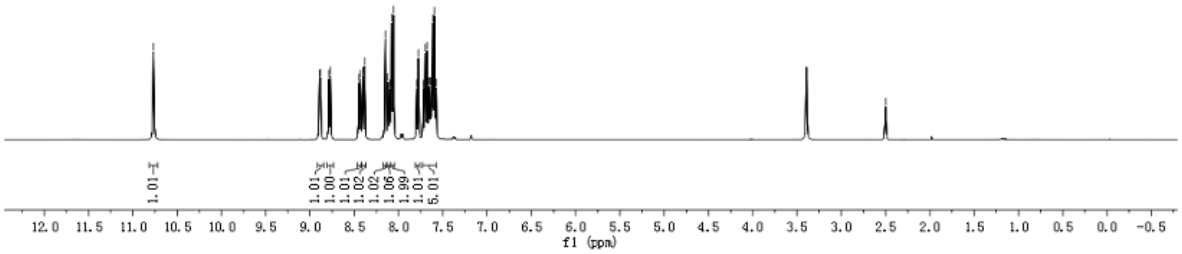

164.785
149.549
141.284
139.384
138.924
138.902
137.056
136.971
134.773
134.302
132.267
131.003
129.851
129.327
128.359
128.344
127.419
123.417
122.700
118.304
40.625
40.417
40.208
40.000
39.791
39.583
39.371

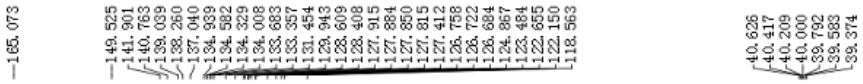

O
Cl
N
H
N
SO2Ph

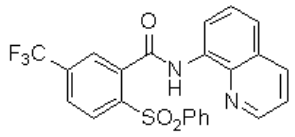

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

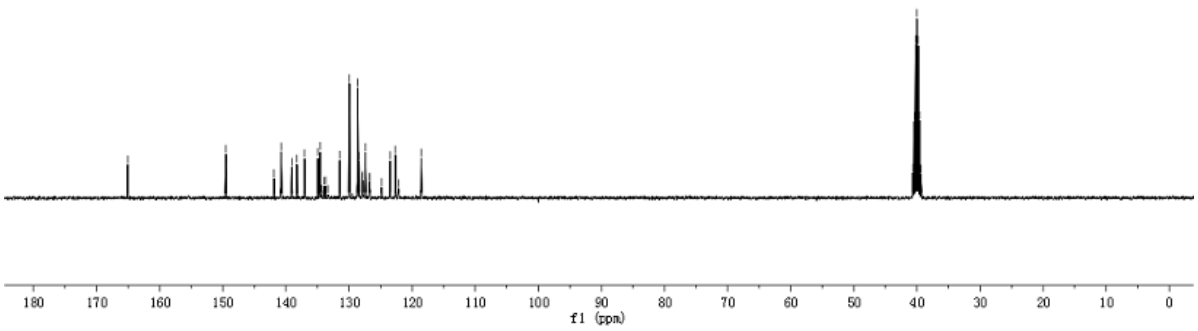

10.767
8.891
8.883
8.787
8.768
8.447
8.427
8.403
8.382
8.148
8.120
8.099
8.077
8.058
7.795
7.775
7.719
7.699
7.678
7.658
7.647
7.636
7.626
7.614
7.593
7.575
2.500

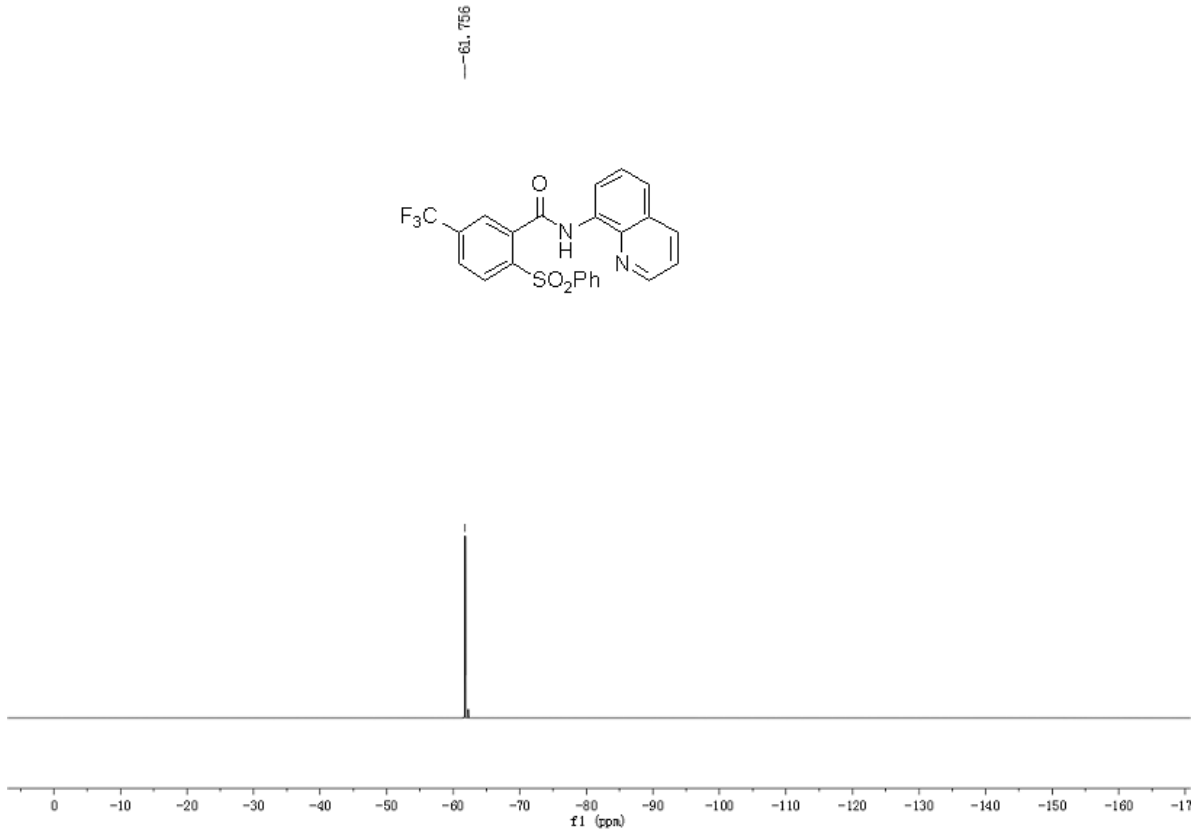

O
F3C
N
H
N
SO2Ph

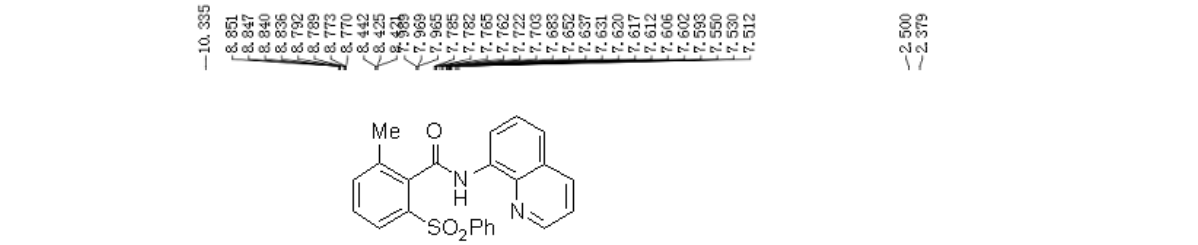

1.01
1.00
1.01
1.02
1.06
1.99
1.01
6.01
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


165.073
149.525
141.901
140.763
139.039
138.260
137.040
134.939
134.582
134.329
134.008
133.683
133.357
131.454
129.943
128.609
128.408
127.915
127.884
127.850
127.815
127.412
126.758
126.722
126.684
124.867
123.484
122.655
122.150
118.563
40.626
40.417
40.209
40.000
39.792
39.583
39.374


O
F3C
N
H
N
SO2Ph


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


-61.756
F3C
O
N
H
N
SO2Ph
f1 (ppm)


10.335
8.851
8.847
8.840
8.836
8.792
8.789
8.773
8.770
8.442
8.425
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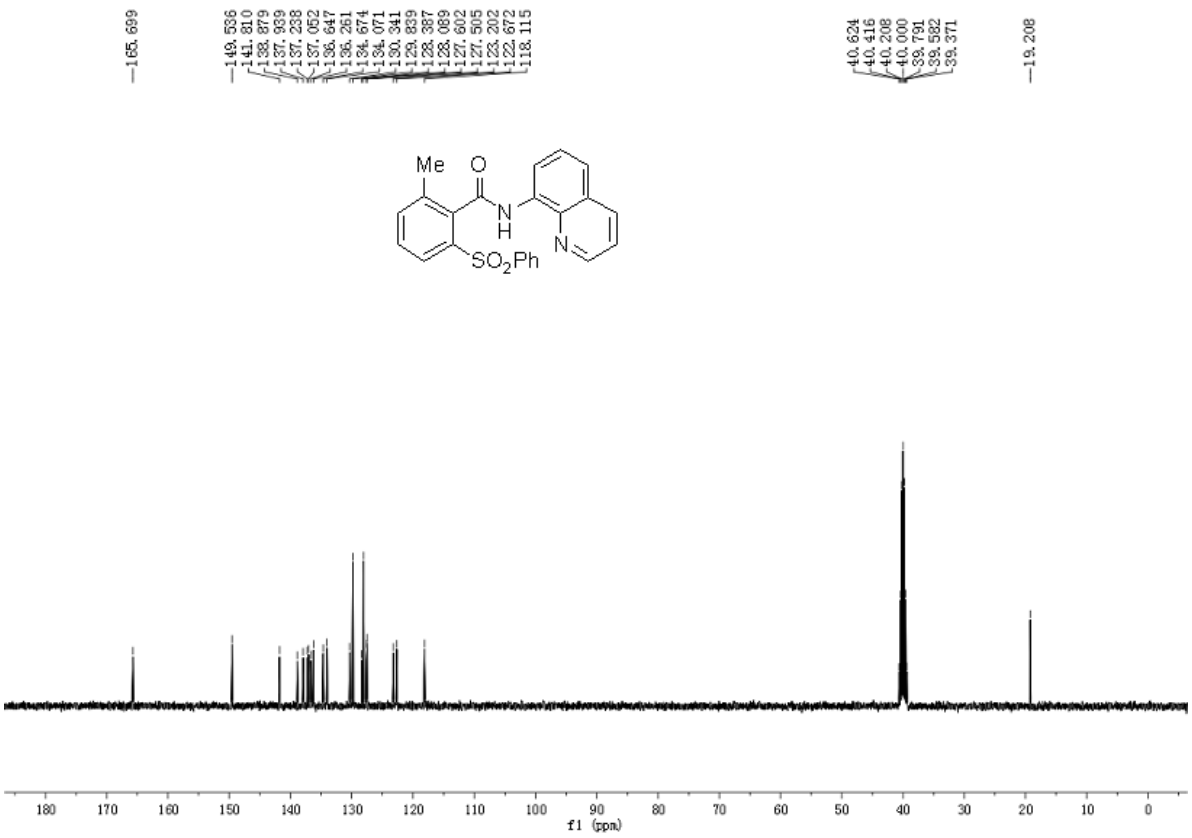
7.965
7.785
7.782
7.765
7.762
7.722
7.703
7.683
7.652
7.637
7.631
7.620
7.617
7.612
7.606
7.602
7.593
7.550
7.530
7.512
2.500
2.379

Me
O
N
H
N
SO2Ph
0.99
1.03
1.03
1.00
3.03
0.99
1.05
3.96
1.98
3.02
f1 (ppm)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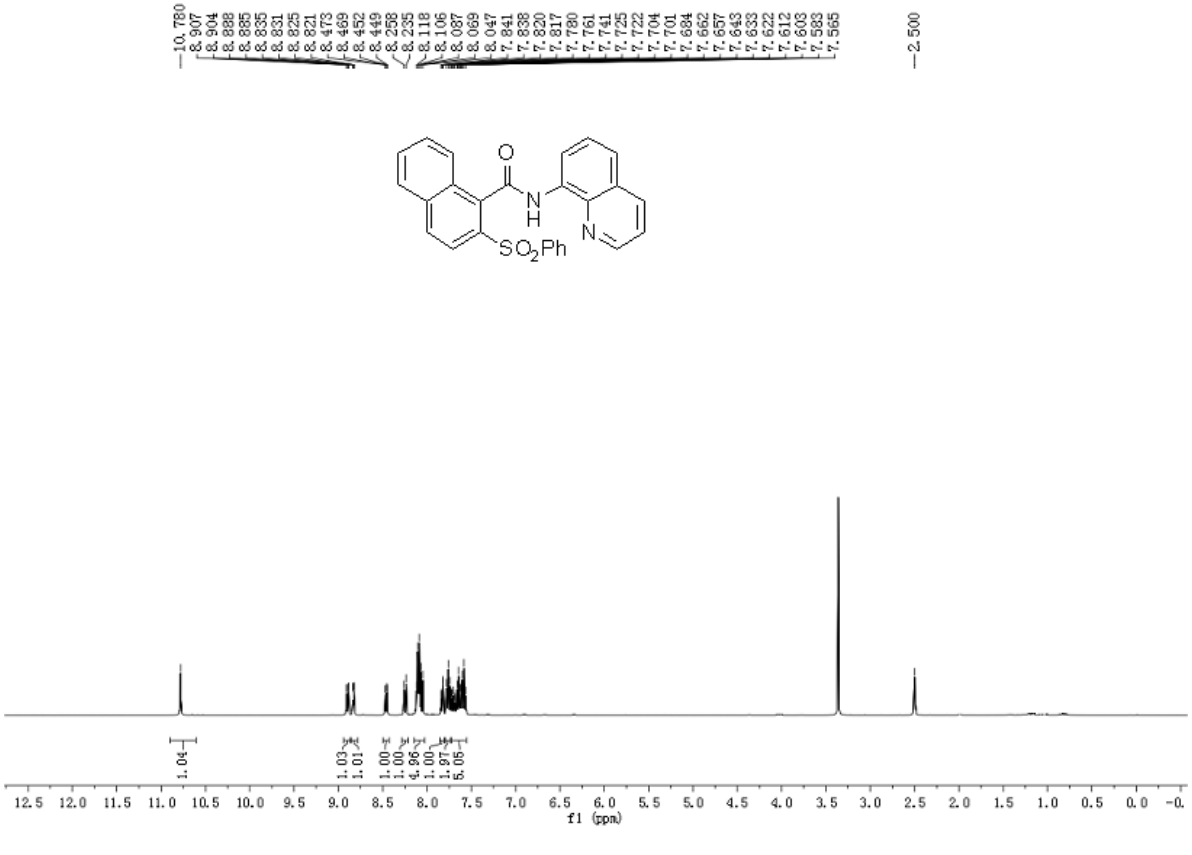
141.810
138.879
137.939
137.238
137.052
136.647
136.261
134.674
134.071
130.341
129.839
128.387
128.089
127.602
127.505
123.202
122.672
118.115
40.624
40.416
40.208
40.000
39.791
39.582
39.371
19.208
Me
O
N
H
N
SO2Ph
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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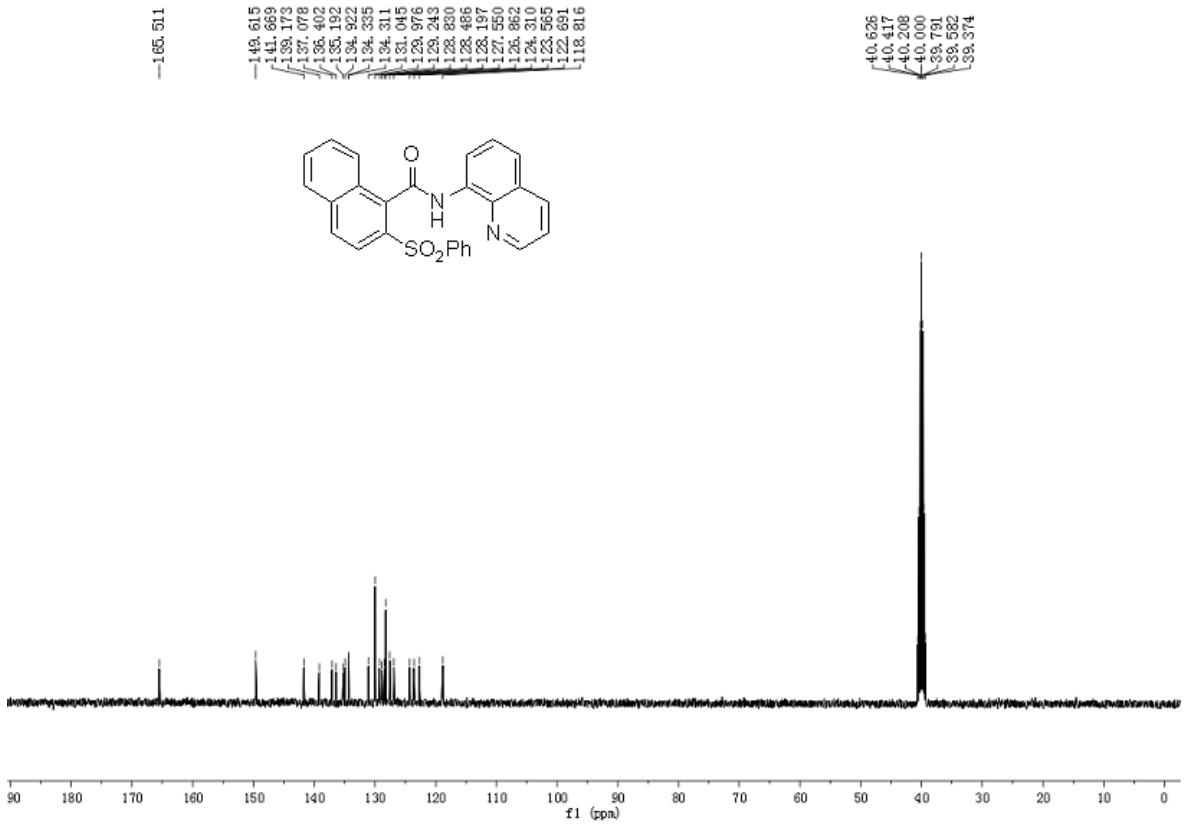
8.904
8.888
8.885
8.835
8.831
8.825
8.821
8.473
8.469
8.452
8.449
8.258
8.235
8.118
8.106
8.087
8.069
8.047
7.841
7.838
7.820
7.817
7.780
7.761
7.741
7.725
7.722
7.704
7.701
7.684
7.662
7.657
7.643
7.633
7.622
7.612
7.603
7.583
7.565
2.500
O
N
H
N
SO2Ph
1.04
1.03
1.01
1.00
1.00
4.96
1.00
1.97
6.05
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)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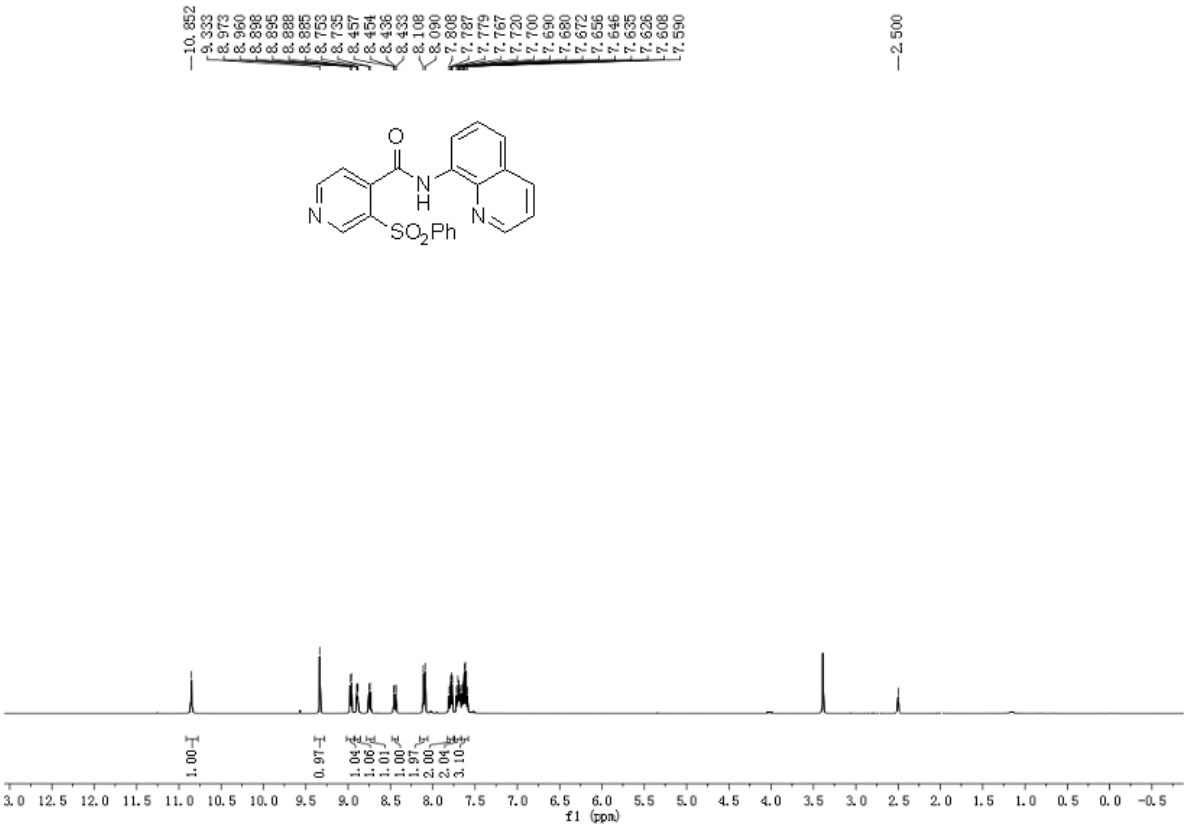
141.669
139.173
137.078
136.402
135.192
134.922
134.335
134.311
131.045
129.976
129.243
128.830
128.486
128.197
127.550
126.862
124.310
123.565
122.691
118.816
40.626
40.417
40.208
40.000
39.791
39.582
39.374
O
N
H
N
SO2Ph
90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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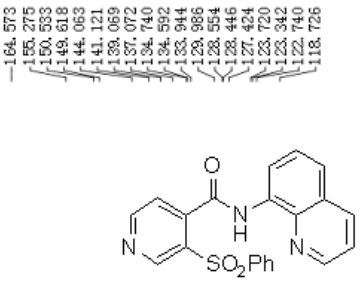
8.973
8.960
8.898
8.895
8.888
8.885
8.753
8.735
8.457
8.454
8.436
8.433
8.108
8.090
7.808
7.787
7.779
7.767
7.720
7.700
7.690
7.680
7.672
7.656
7.646
7.635
7.626
7.608
7.590
2.500
O
N
H
N
N
SO2Ph
1.00
0.97
1.04
1.06
1.01
1.00
1.97
2.00
2.04
3.10
3.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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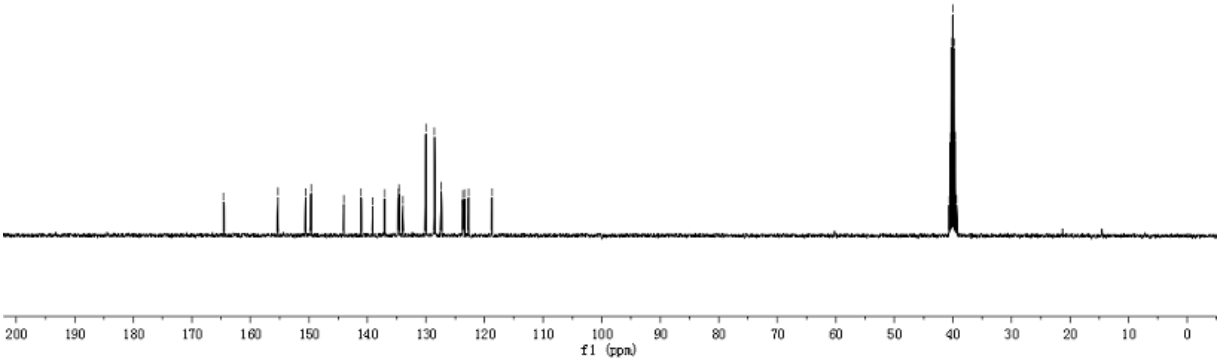
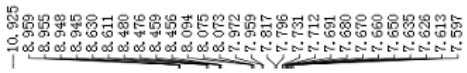
150.533
149.618
144.063
141.121
139.069
137.072
134.740
134.592
133.944
129.986
128.554
128.446
127.424
123.720
123.342
122.740
118.726
40.626
40.418
40.209
40.000
39.792
39.583
39.375
O
N
H
N
N
SO2Ph


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


10.925
8.959
8.955
8.948
8.945
8.630
8.611
8.480
8.476
8.459
8.456
8.094
8.075
8.073
7.972
7.959
7.817
7.796
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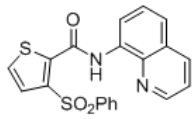
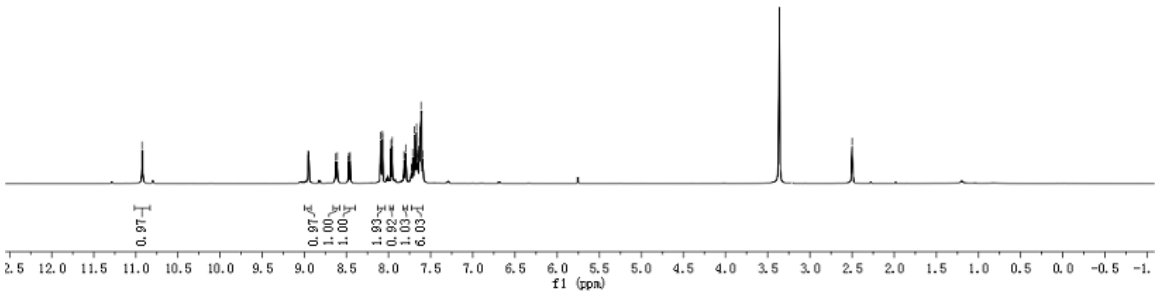
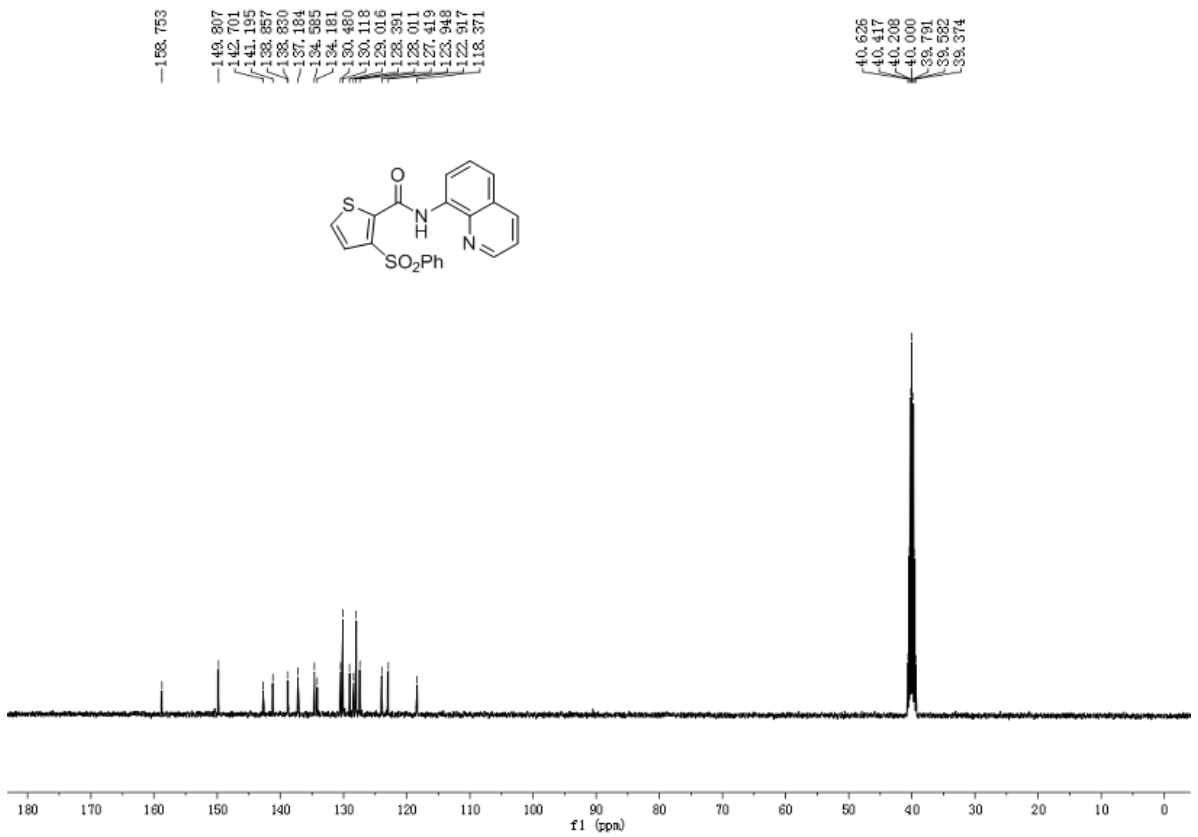
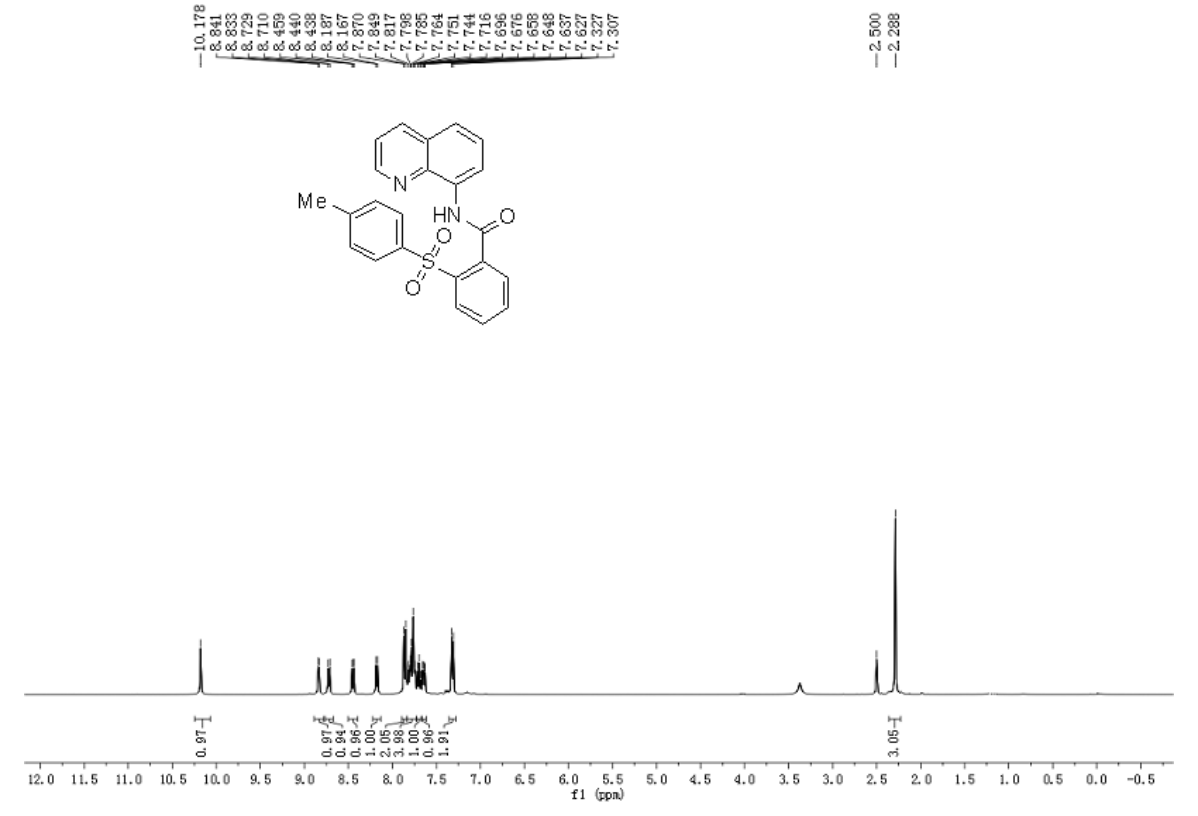
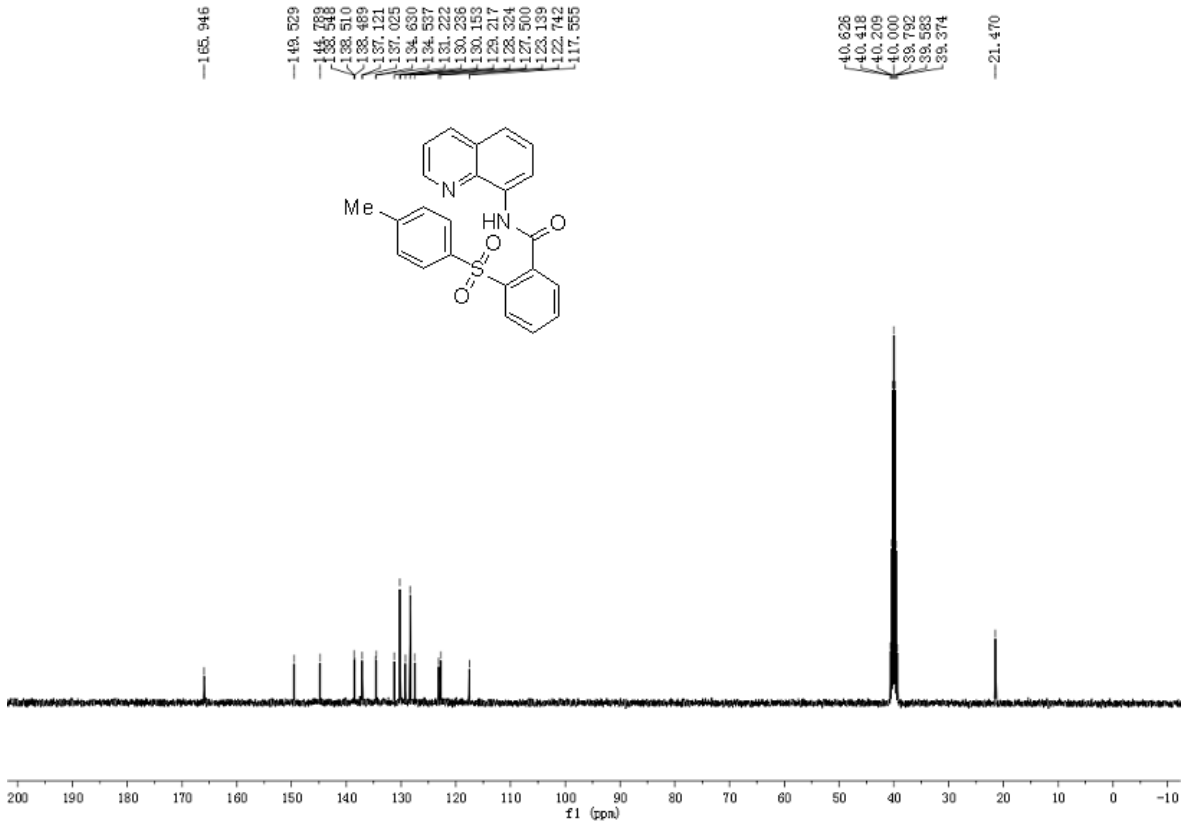
7.650
7.635
7.626
7.613
7.597
2.500


O
S
N
H
N
SO2Ph


0.97
0.97
1.00
1.00
1.93
0.92
1.03
6.03
f1 (ppm)


158.753
149.807
142.701
141.195
138.857
138.830
137.184
134.585
134.181
130.480
130.118
129.016
128.391
128.011
127.419
123.948
122.917
118.371
40.626
40.417
40.208
40.000
39.791
39.582
39.374
O
S
N
H
N
SO2Ph
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


10.178
8.841
8.833
8.729
8.710
8.459
8.440
8.438
8.187
8.167
7.870
7.849
7.817
7.798
7.785
7.764
7.751
7.744
7.716
7.696
7.676
7.658
7.648
7.637
7.627
7.327
7.307
2.500
2.288
N
HN
O
Me
S
O
O
0.97
0.97
0.94
0.96
1.00
2.05
3.98
1.00
0.96
1.91
3.05
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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144.789
143.648
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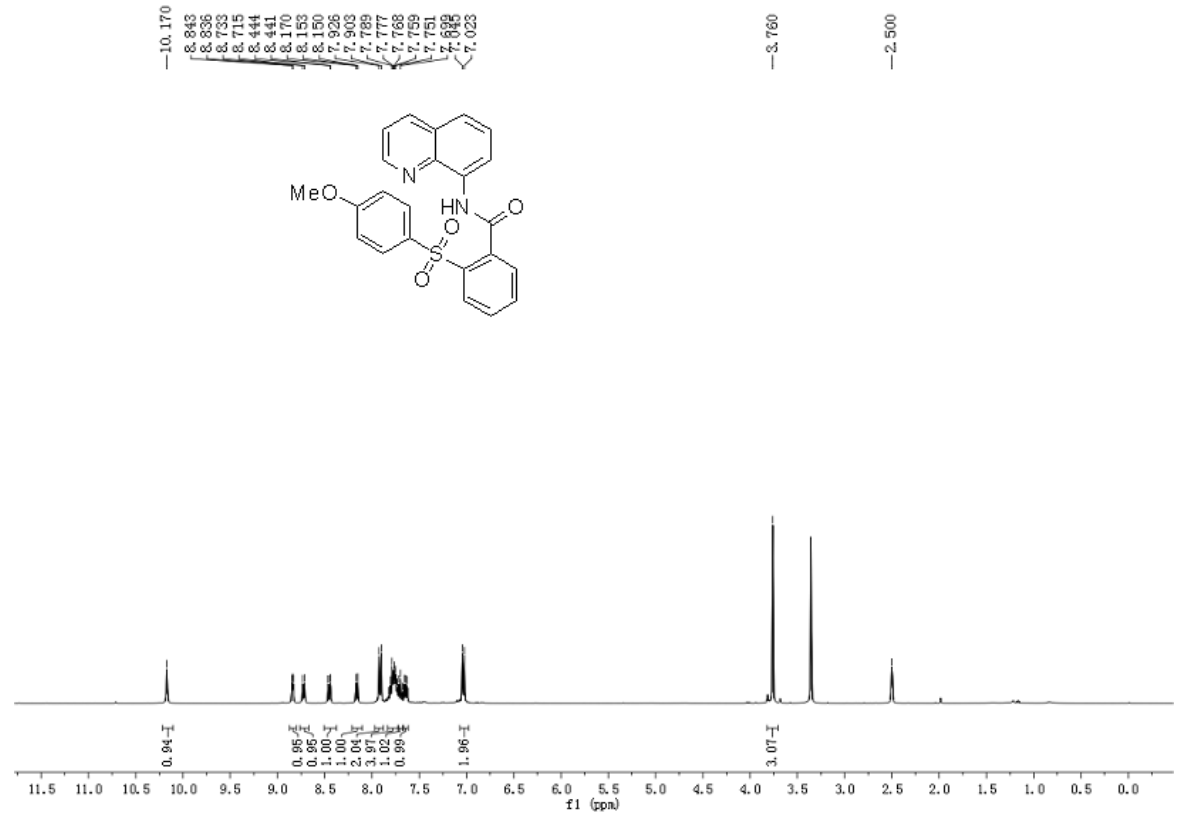
138.469
137.121
137.025
134.630
134.537
131.222
130.236
130.153
129.217
128.324
127.500
123.139
122.742
117.555
40.626
40.418
40.209
40.000
39.792
39.583
39.374
21.470
Me
HN
O
N
O
S
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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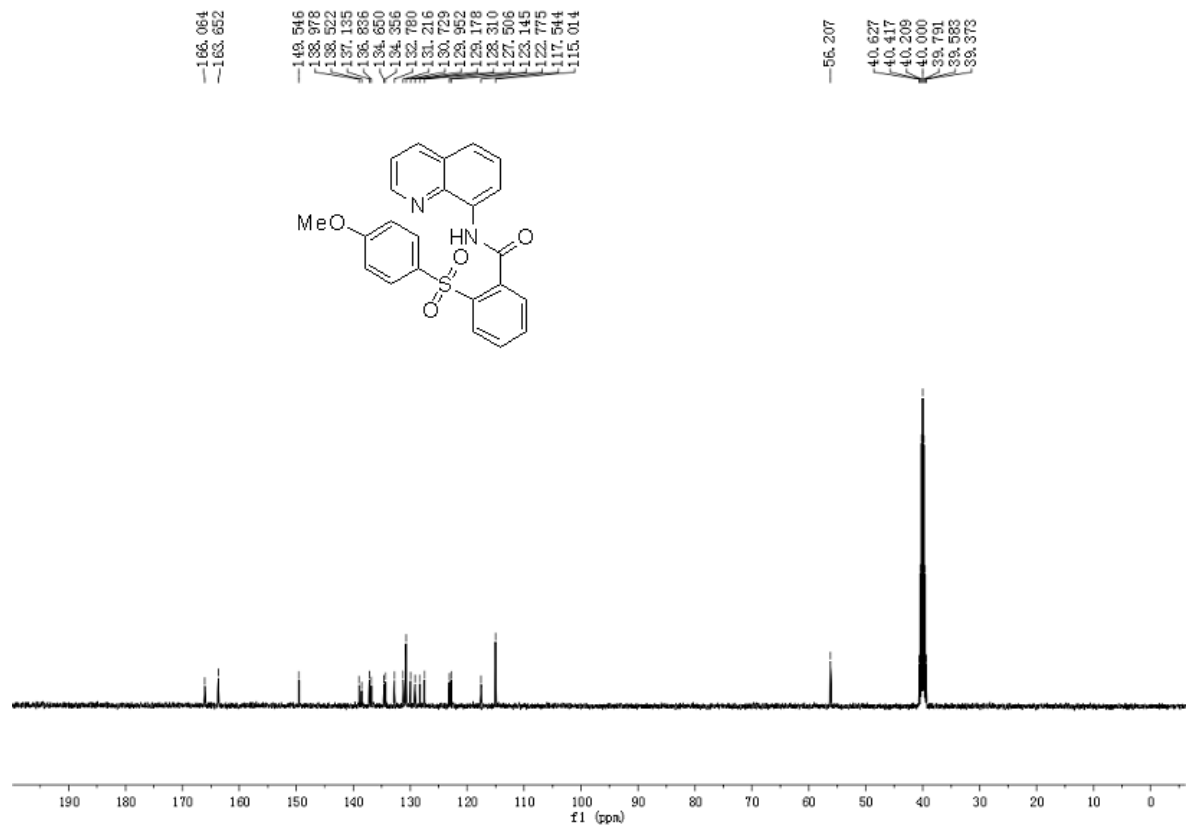
8.836
8.733
8.715
8.444
8.441
8.170
8.153
8.150
7.926
7.903
7.789
7.777
7.768
7.759
7.751
7.023
3.760
2.500
MeO
HN
O
N
O
S
O
0.94
0.95
0.95
1.00
2.04
3.97
1.02
0.99
1.96
3.07
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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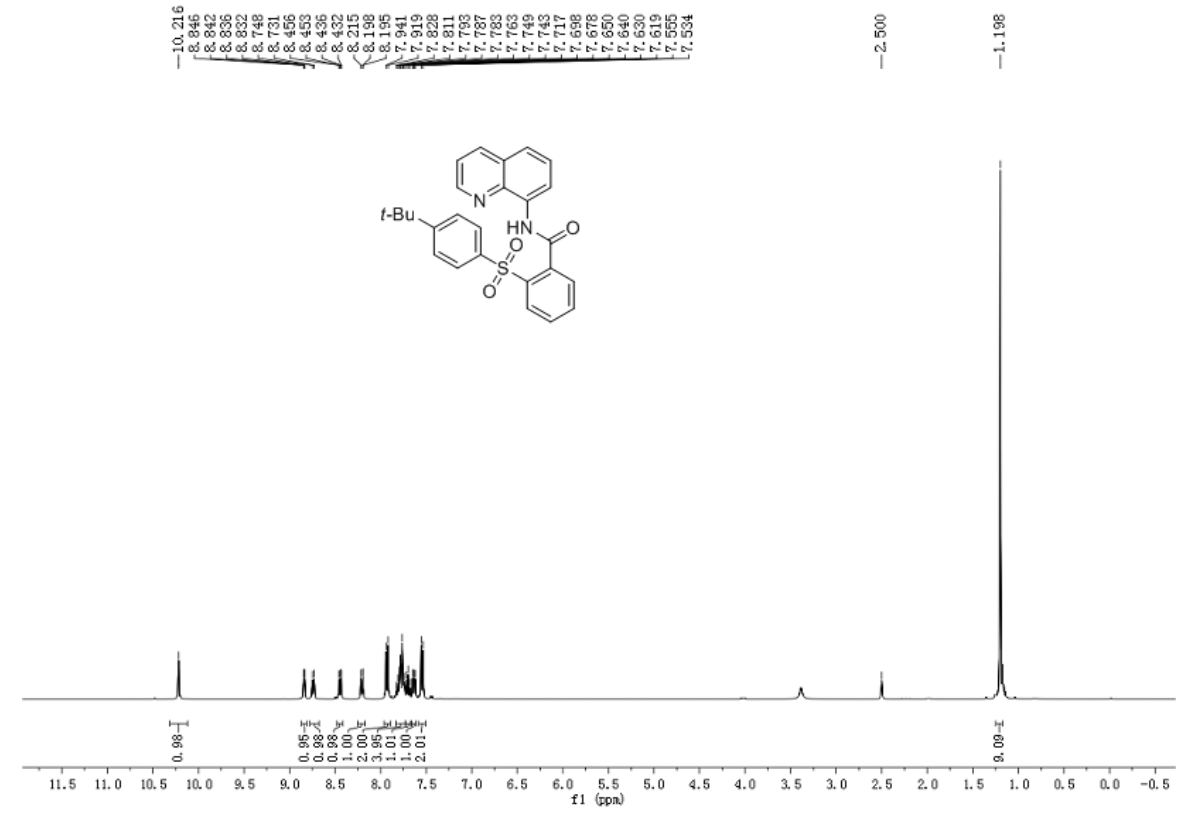
163.652
149.546
138.978
138.522
137.135
136.836
134.650
134.356
132.780
131.216
130.729
129.952
129.178
128.310
127.506
123.145
122.775
117.544
115.014
56.207
40.627
40.417
40.209
40.000
39.791
39.583
39.373
MeO
HN
O
N
S
O
O
f1 (ppm)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8.832
8.748
8.731
8.456
8.453
8.436
8.432
8.215
8.198
8.195
7.941
7.919
7.828
7.811
7.793
7.787
7.783
7.763
7.749
7.743
7.717
7.698
7.678
7.650
7.640
7.630
7.619
7.555
7.534
2.500
1.198
t-Bu
HN
O
N
S
O
O
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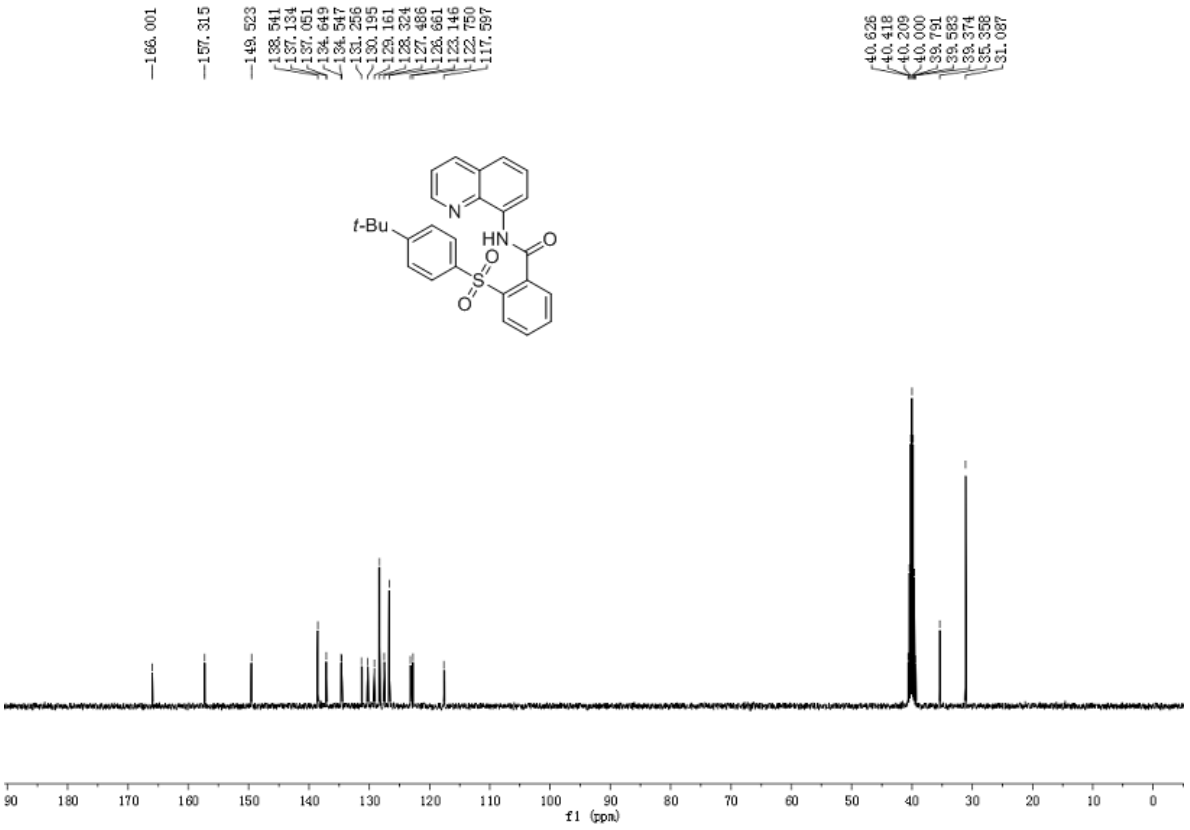
0.95
0.88
1.00
2.00
3.01
1.00
2.01
9.09
f1 (ppm)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149.523
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137.134
137.051
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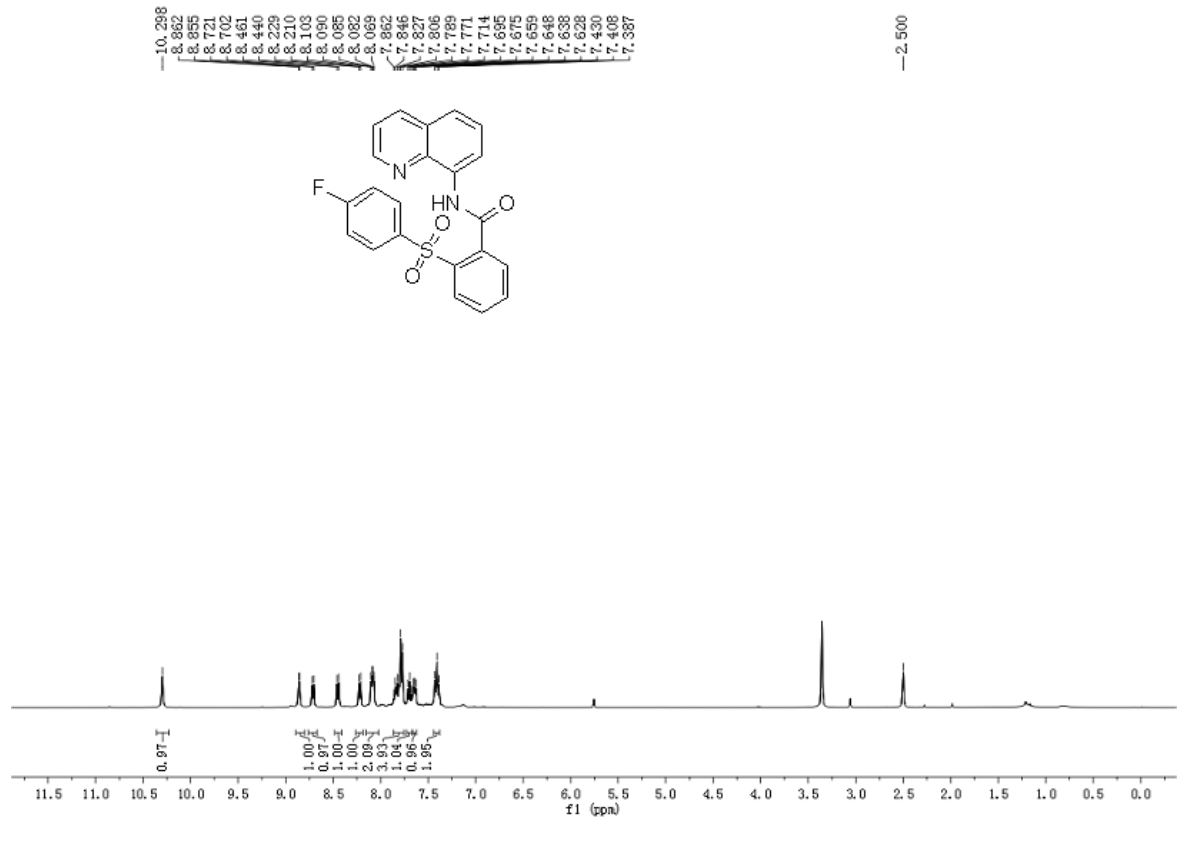
134.547
131.256
130.195
129.161
128.324
127.486
126.661
123.146
122.750
117.597
40.626
40.418
40.209
40.000
39.791
39.583
39.374
35.358
31.087
t-Bu
HN
O
S
O
O
N
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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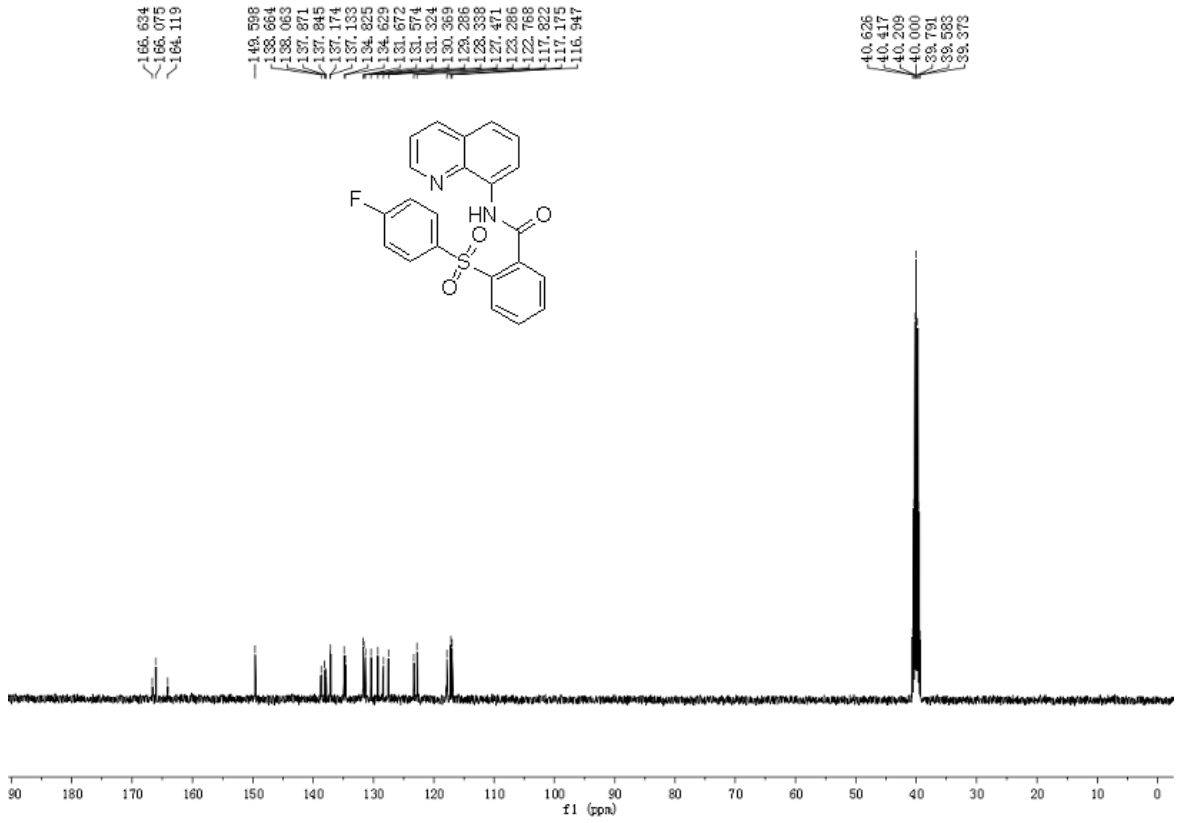
8.702
8.461
8.440
8.229
8.210
8.103
8.090
8.085
8.082
8.069
7.862
7.846
7.827
7.806
7.789
7.771
7.714
7.695
7.675
7.659
7.648
7.638
7.628
7.430
7.408
7.387
2.500
F
HN
O
S
O
O
N
0.97
1.00
0.97
1.00
1.00
2.09
3.93
1.04
0.96
1.95
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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137.845
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134.825
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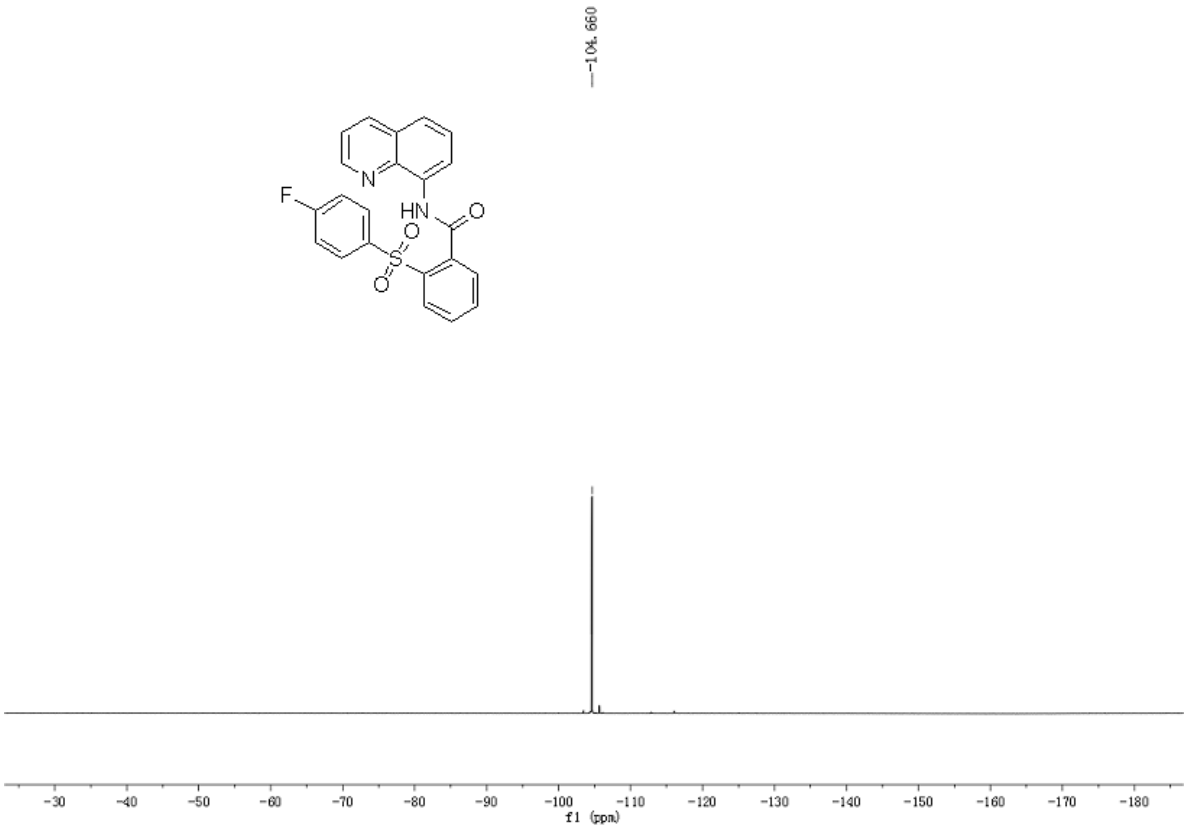
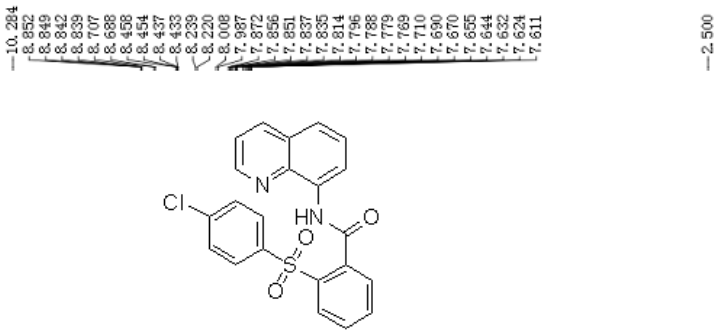
131.672
131.574
131.324
130.369
129.286
128.338
127.471
123.286
122.768
117.822
117.175
116.947
40.626
40.417
40.209
40.000
39.791
39.583
39.373
F
HN
O
O
O
S
N
90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-104.660
F
HN
O
O
O
S
N
-30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180
f1 (ppm)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8.707
8.688
8.458
8.454
8.437
8.433
8.239
8.220
8.008
7.987
7.872
7.856
7.851
7.837
7.835
7.814
7.796
7.788
7.779
7.769
7.710
7.690
7.670
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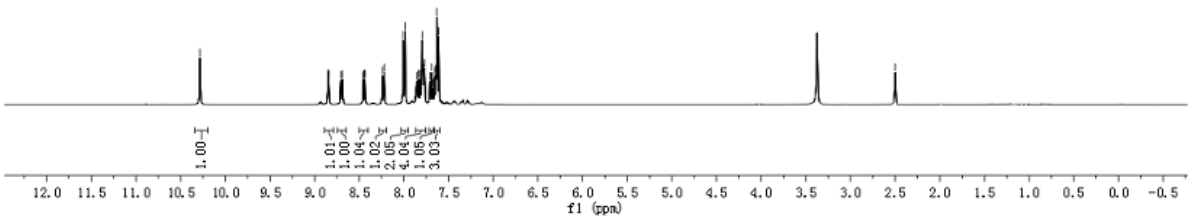
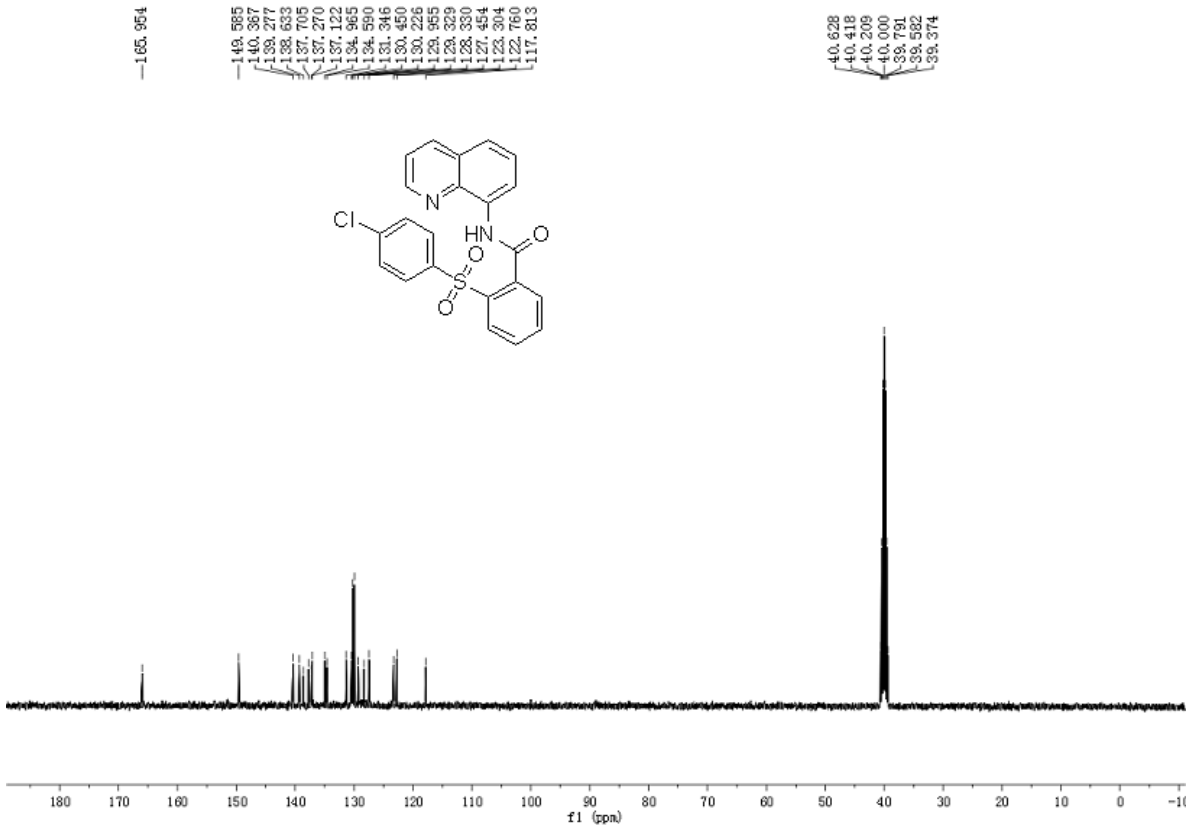
7.644
7.632
7.624
7.611
2.500
Cl
HN
O
O
O
S
N


1.00
1.01
1.00
1.04
1.02
2.05
4.04
1.05
3.03
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


165.954
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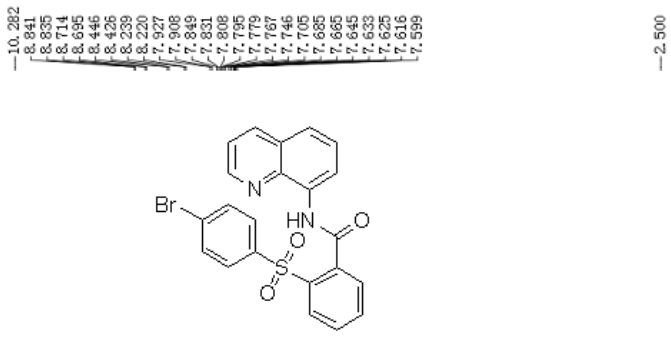
140.367
139.277
138.633
137.705
137.270
137.122
134.965
134.590
131.346
130.450
130.226
129.955
129.329
128.330
127.454
123.304
122.760
117.813
40.628
40.418
40.209
40.000
39.791
39.582
39.374
Cl
HN
O
O
O
S
N
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.841
8.835
8.714
8.695
8.446
8.426
8.239
8.220
7.927
7.908
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7.831
7.808
7.795
7.779
7.767
7.746
7.705
7.685
7.665
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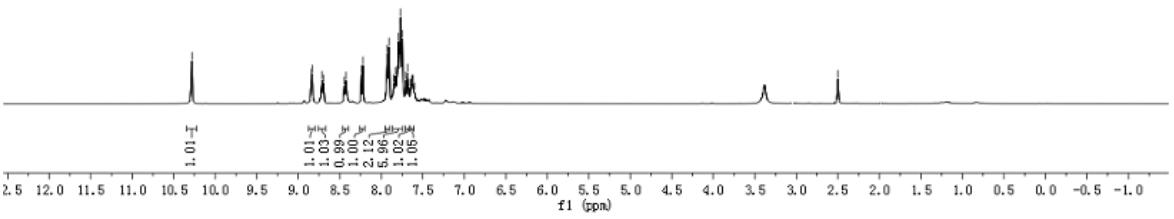
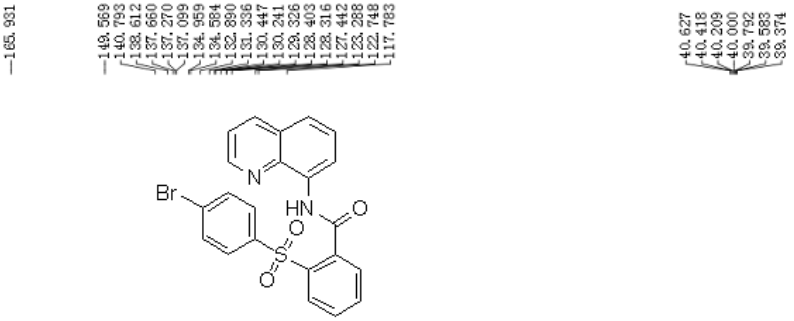
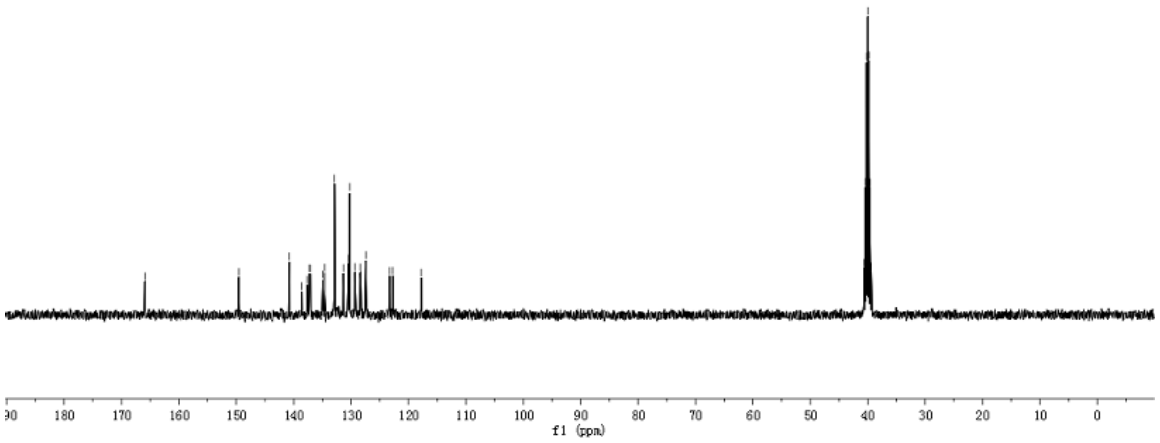
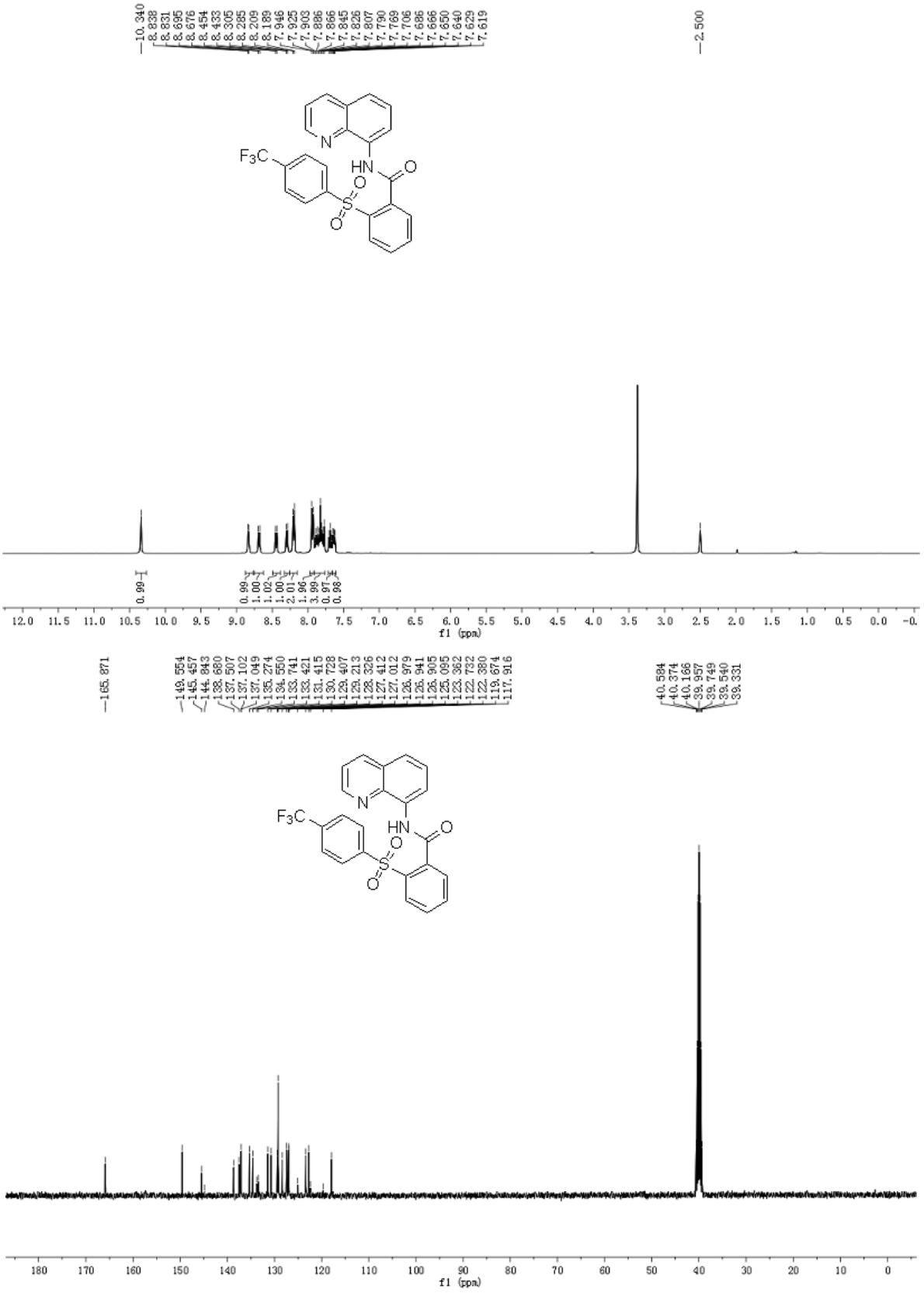
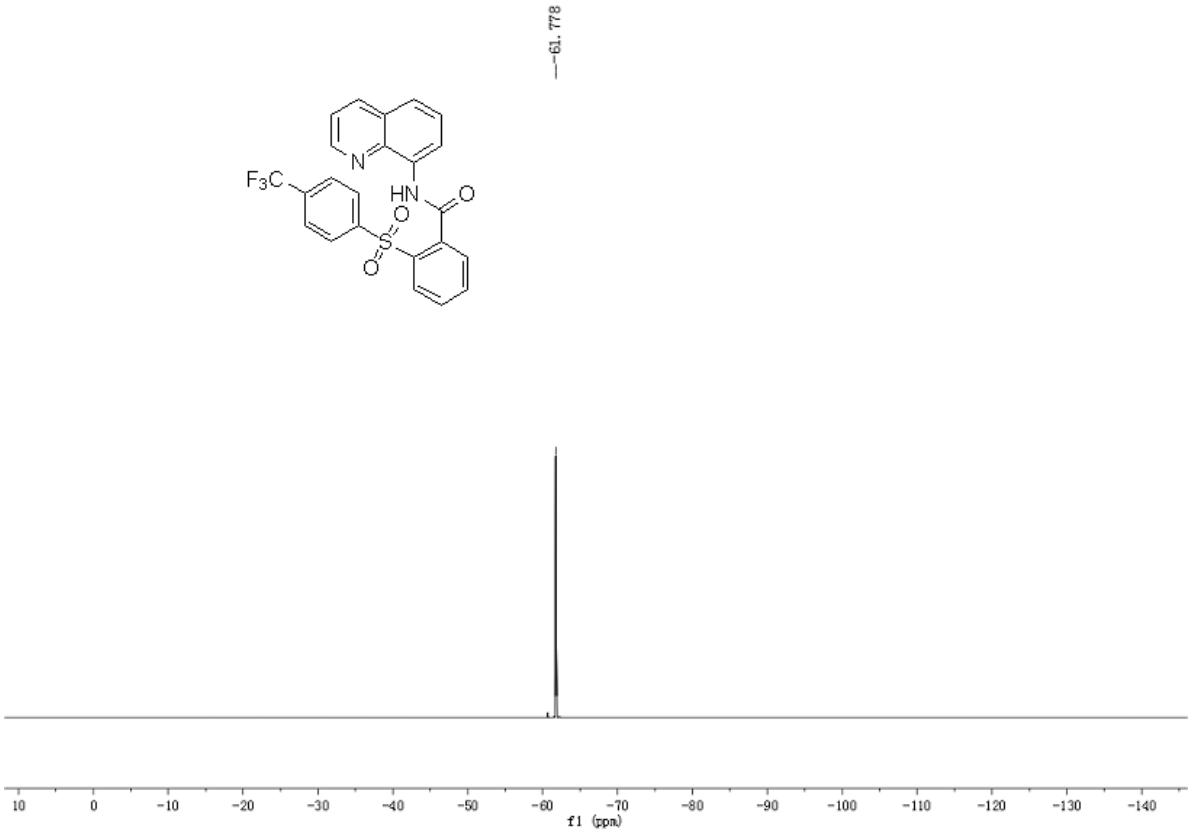
7.633
7.625
7.616
7.599
2.500
Br
HN
O
N
O
S
O

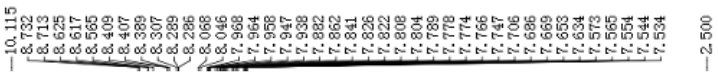

1.01
1.03
0.99
1.00
2.12
5.96
1.02
1.05
f1 (ppm)

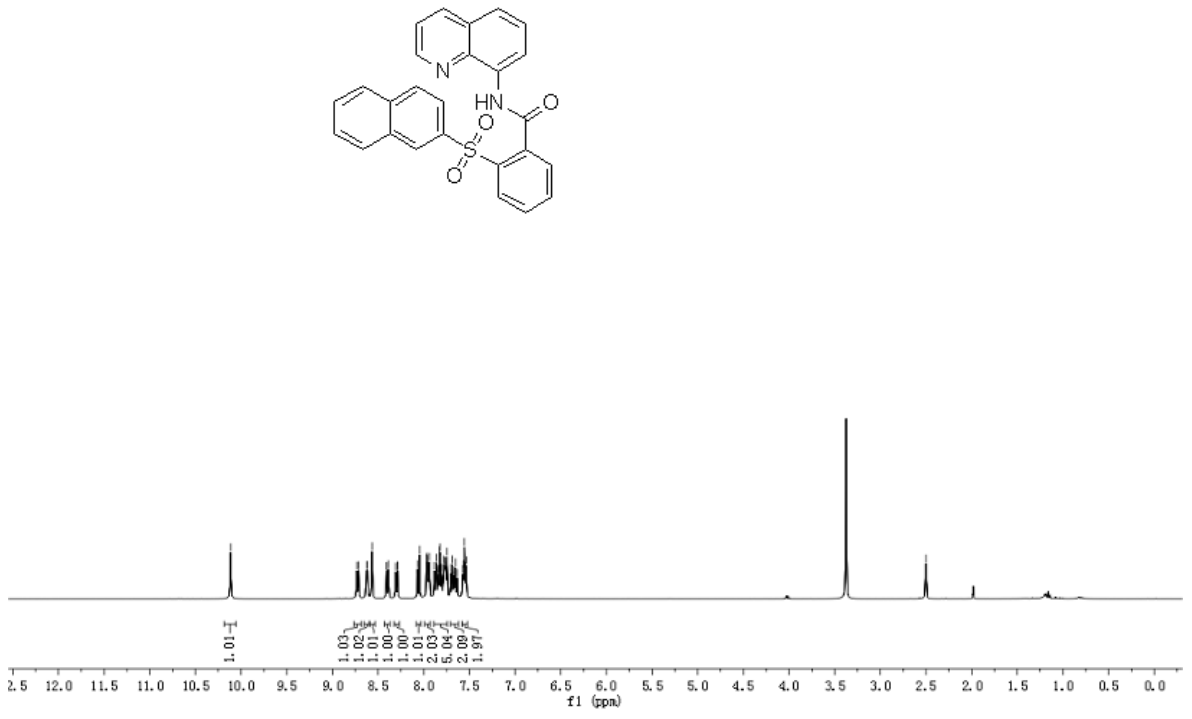

165.931
149.569
140.793
138.612
137.660
137.270
137.099
134.959
134.584
132.890
131.336
130.447
130.241
129.326
128.403
128.316
127.442
123.288
122.748
117.783
40.627
40.418
40.209
40.000
39.792
39.583
39.374
Br
HN
O
N
O
S
O

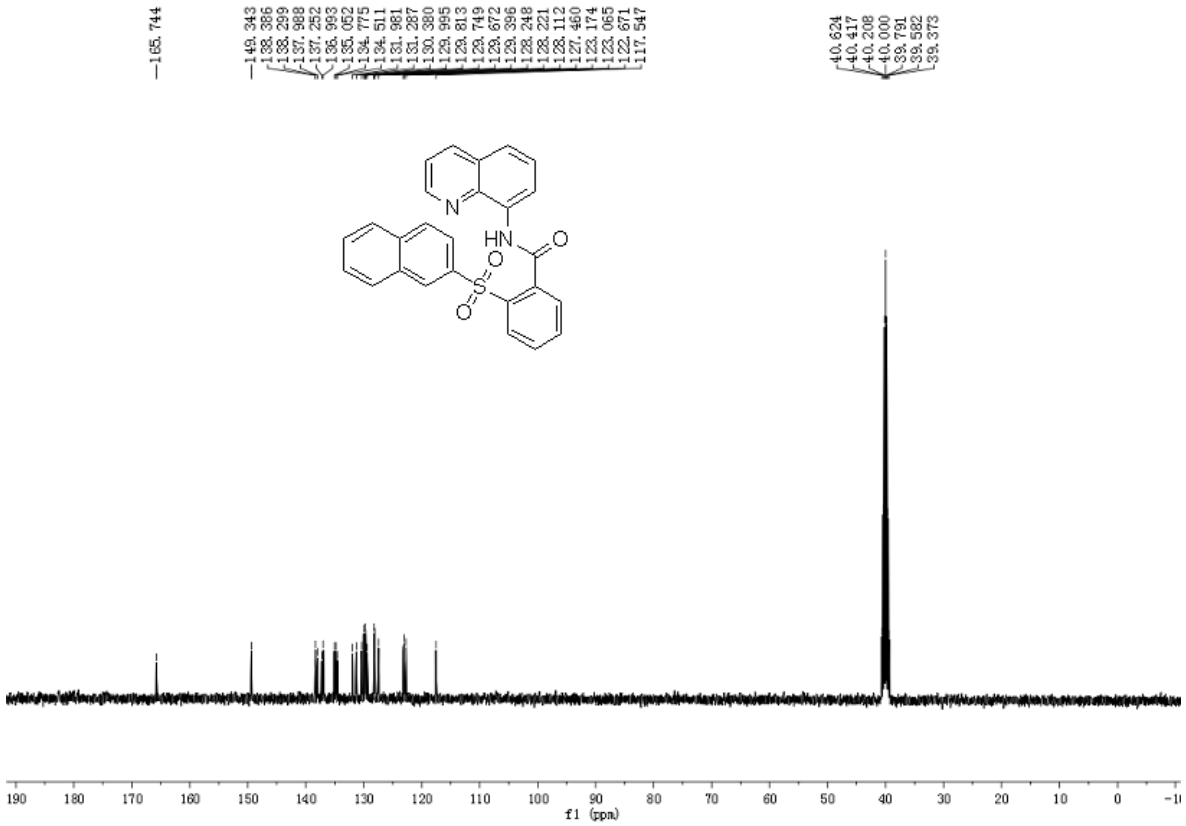

f1 (ppm)

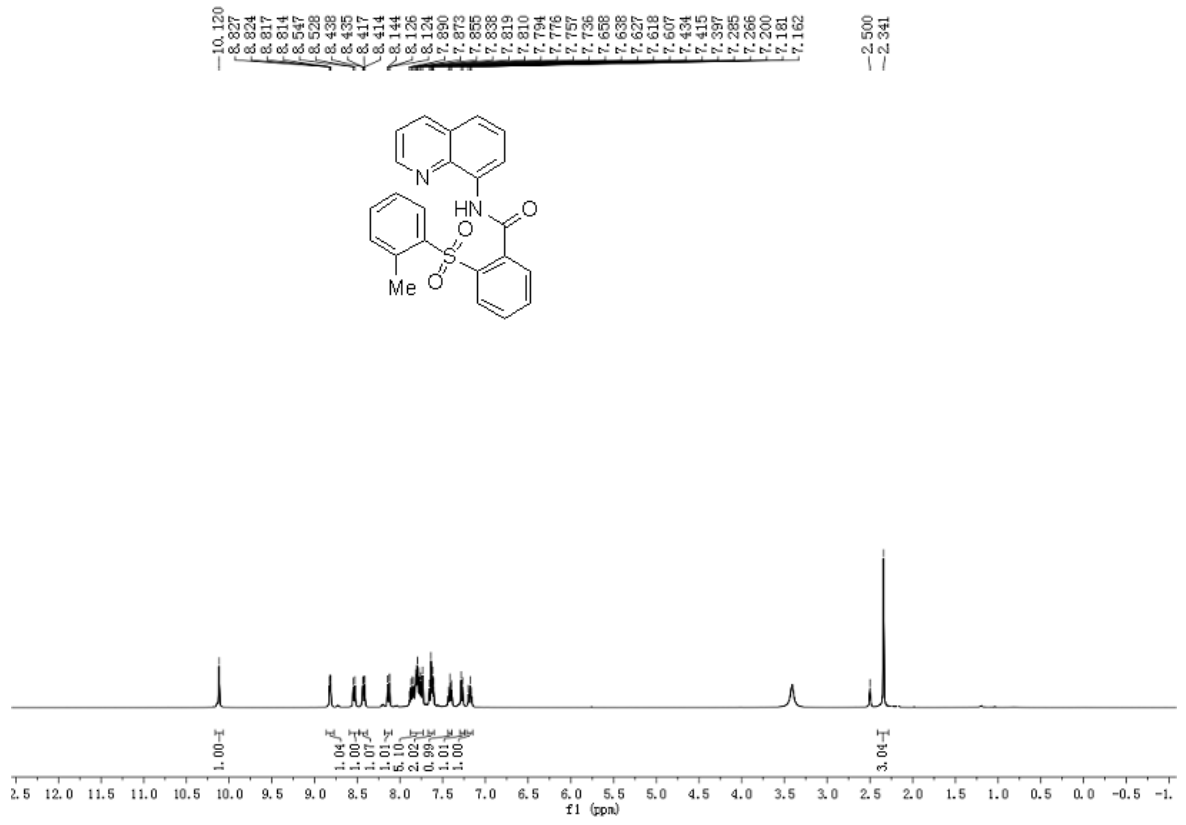

10.340
8.838
8.831
8.695
8.676
8.454
8.433
8.305
8.285
8.209
8.189
7.946
7.925
7.903
7.886
7.866
7.845
7.826
7.807
7.790
7.769
7.706
7.686
7.666
7.650
7.640
7.629
7.619
2.500
F3C
HN
O
N
S
0.99
1.00
1.02
1.00
2.01
1.96
3.99
0.97
0.98
f1 (ppm)
165.871
149.554
145.457
144.843
138.680
137.507
137.102
137.049
135.274
134.550
133.741
133.421
131.415
130.728
129.407
129.213
128.326
127.412
127.012
126.979
126.941
126.905
125.095
123.362
122.732
122.380
119.674
117.916
40.584
40.374
40.166
39.957
39.749
39.540
39.331
f1 (ppm)

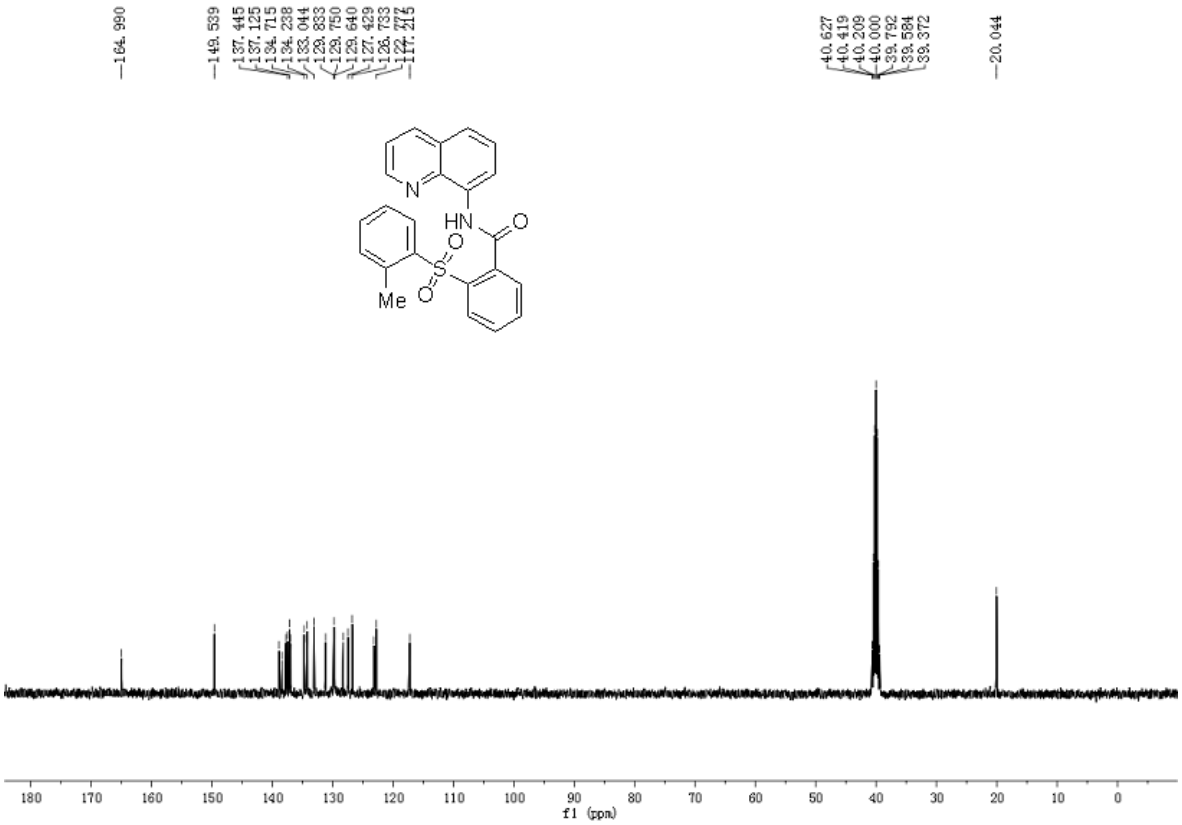

-61.778
F3C
HN
O
N
O=S=O
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140
f1 (ppm)

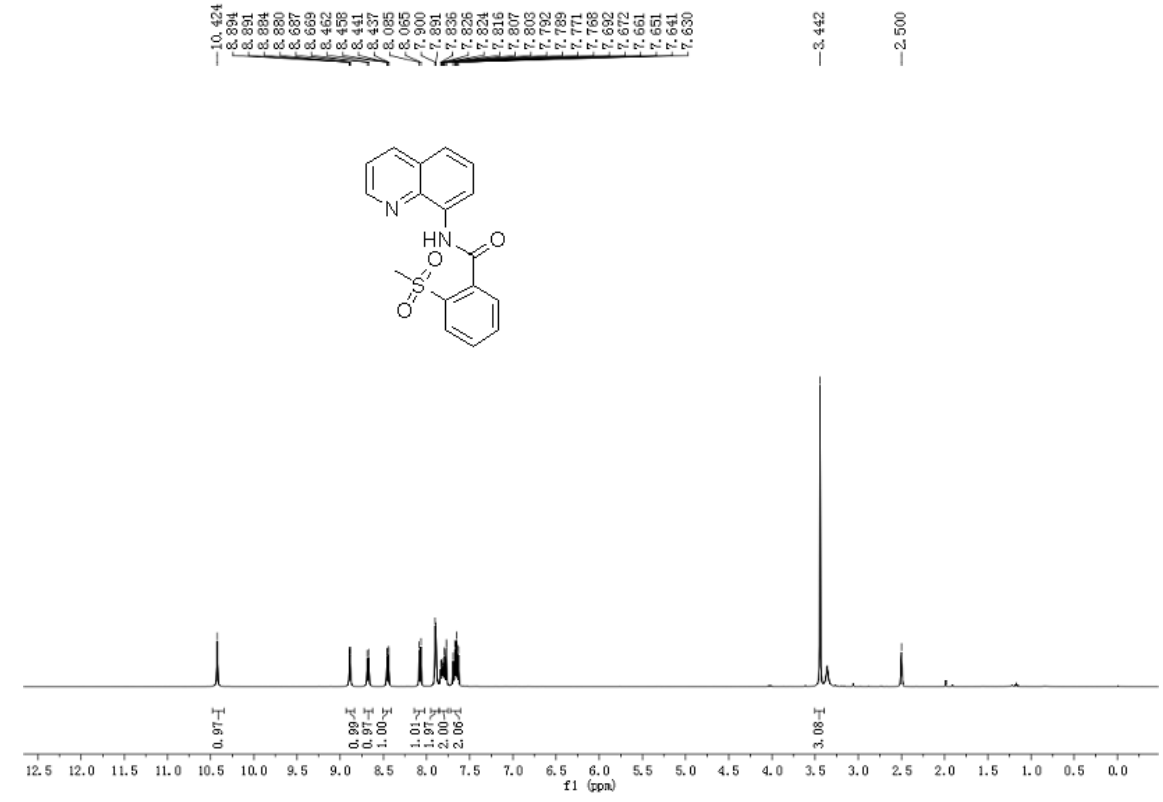

10.115
8.732
8.713
8.625
8.617
8.565
8.409
8.407
8.389
8.307
8.289
8.286
8.068
8.046
7.968
7.964
7.958
7.947
7.938
7.882
7.862
7.841
7.826
7.822
7.808
7.804
7.789
7.778
7.774
7.766
7.747
7.706
7.686
7.669
7.653
7.634
7.573
7.565
7.554
7.544
7.534
2.500

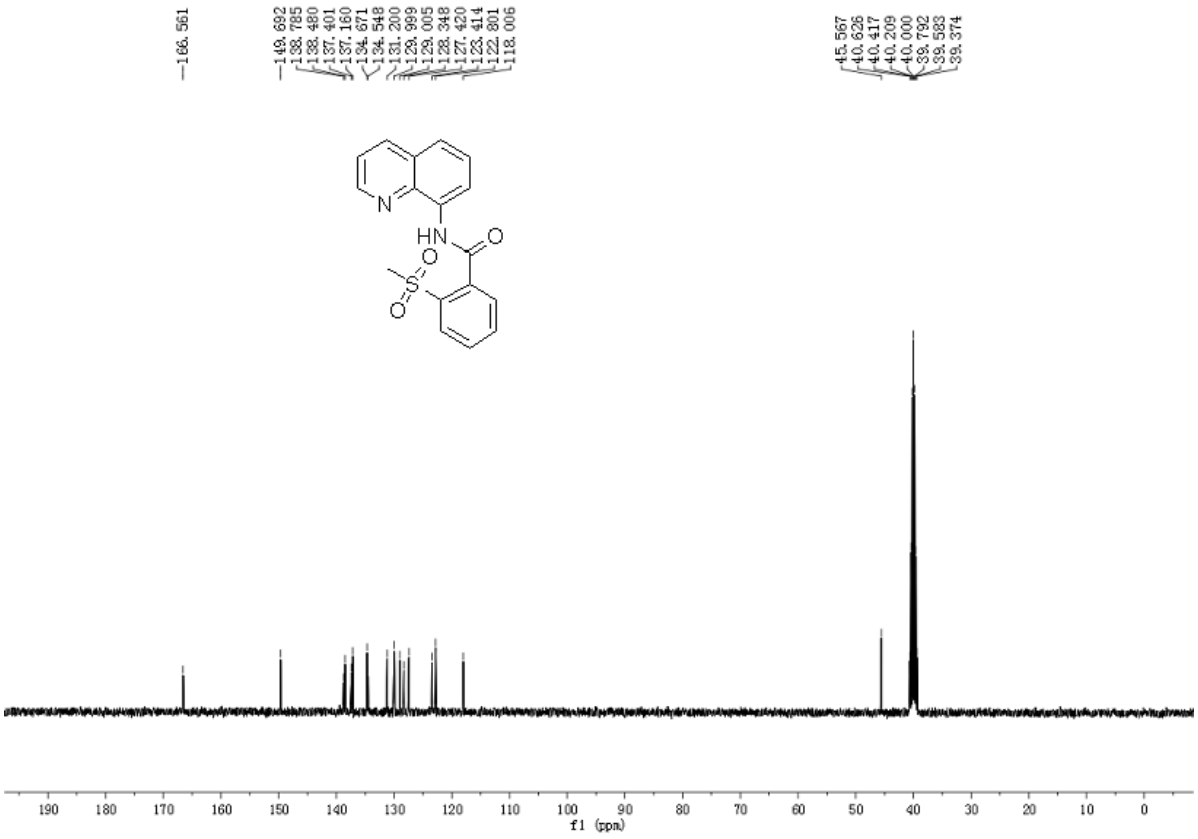

HN
O
N
O=S=O
1.01
1.03
1.02
1.01
1.00
1.00
1.01
2.03
5.04
2.09
1.97
2.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

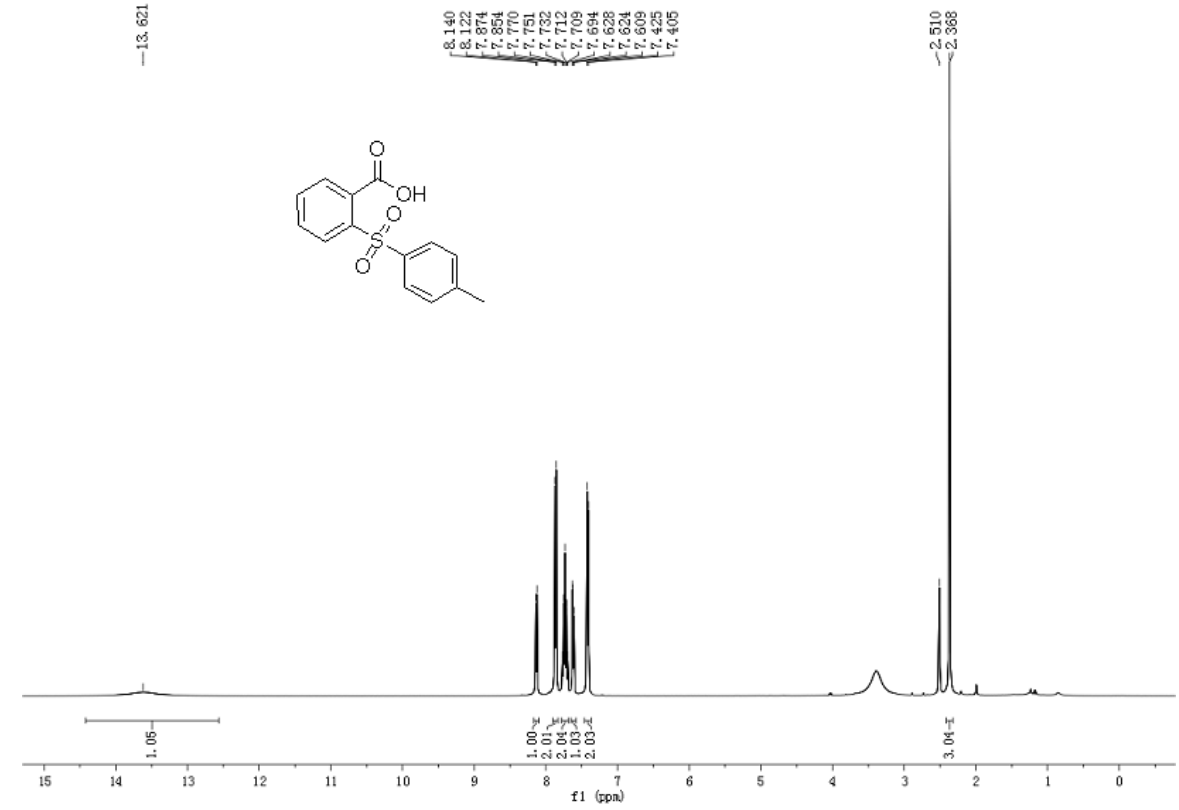

165.744
149.343
138.386
138.299
137.988
137.252
136.993
135.052
134.775
134.511
131.981
131.287
130.380
129.995
129.813
129.749
129.672
129.396
128.248
128.221
128.112
127.460
123.174
123.065
122.671
117.947
40.624
40.417
40.208
40.000
39.791
39.582
39.373
N
HN
O
O
S
O
f1 (ppm)

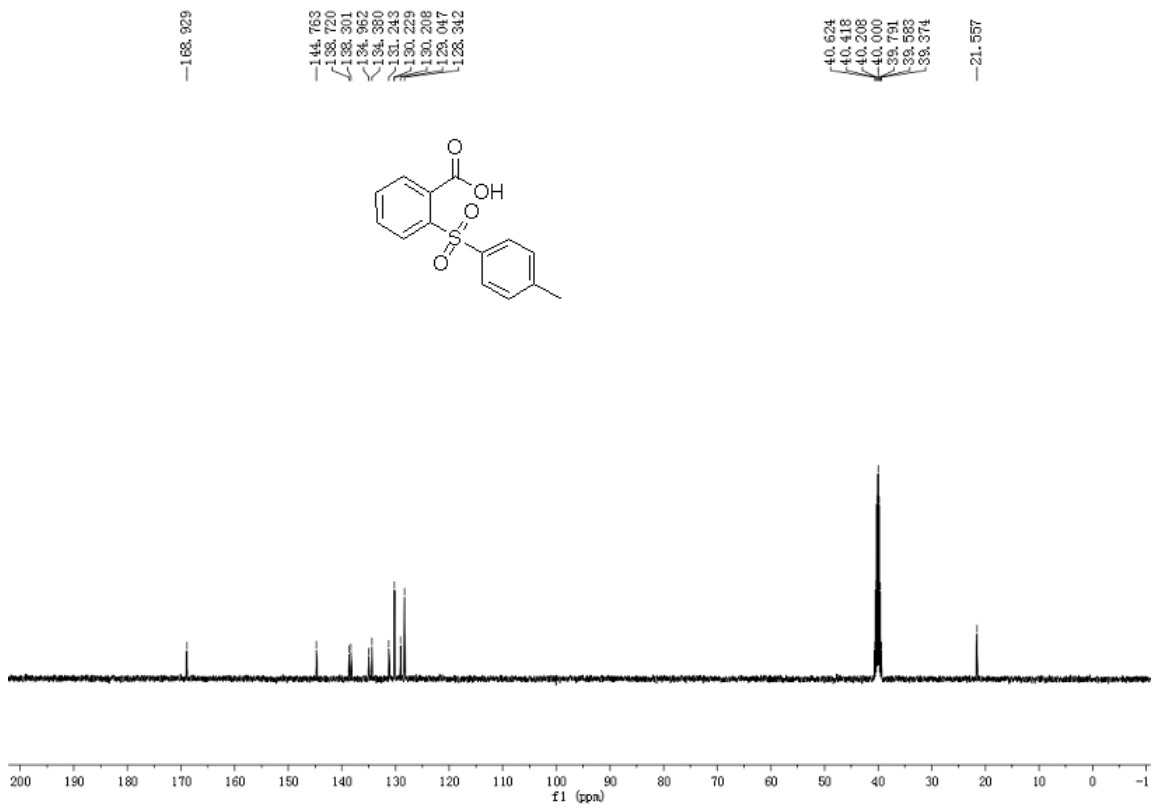

10.120
8.827
8.824
8.817
8.814
8.547
8.528
8.438
8.435
8.417
8.414
8.144
8.126
8.124
7.890
7.873
7.855
7.838
7.819
7.810
7.794
7.776
7.757
7.736
7.658
7.638
7.627
7.618
7.607
7.434
7.415
7.397
7.285
7.266
7.200
7.181
7.162
2.500
2.341
N
HN
O
O
S
O
Me
1.00
1.04
1.00
1.07
1.01
5.10
2.02
0.99
1.01
1.00
3.04
f1 (ppm)


164.990
149.539
137.445
137.125
134.715
134.238
133.044
129.833
129.750
129.640
127.429
126.733
122.215
40.627
40.419
40.209
40.000
39.792
39.584
39.372
20.044
HN
O
O
S
O
Me
N
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


10.424
8.894
8.891
8.884
8.880
8.687
8.669
8.462
8.458
8.441
8.437
8.085
8.065
7.900
7.891
7.836
7.826
7.824
7.816
7.807
7.803
7.792
7.789
7.771
7.768
7.692
7.672
7.661
7.651
7.641
7.630
3.442
2.500
HN
O
O
S
O
N
0.97
0.99
0.97
1.00
1.01
1.97
2.00
2.06
3.08
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


166.561
149.692
138.785
138.480
137.401
137.160
134.671
134.548
131.200
129.999
129.005
128.348
127.420
123.414
122.801
118.006
45.567
40.626
40.417
40.209
40.000
39.792
39.583
39.374
HN
O
O
S
O
f1 (ppm)


13.621
8.140
8.122
7.874
7.854
7.770
7.751
7.732
7.712
7.709
7.694
7.628
7.624
7.609
7.425
7.405
2.510
2.368
OH
O
O
S
O
1.05
1.00
2.01
2.04
1.03
2.03
3.04
f1 (ppm)


168.929
144.763
138.720
138.301
134.962
134.380
131.243
130.229
130.208
129.047
128.342
40.624
40.418
40.208
40.000
39.791
39.583
39.374
21.557
O
OH
O
S
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)