Supporting Information to

Highly Mono-selective *ortho*-Methylthiolation of Benzamides via Cobalt-catalyzed sp^2 C-H activation

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Table of Contents

3.4 Removal of directing group

4. Characterization data of products

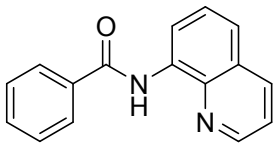
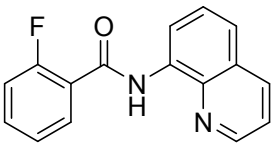
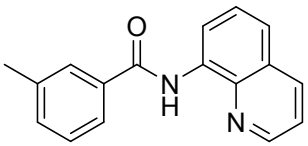
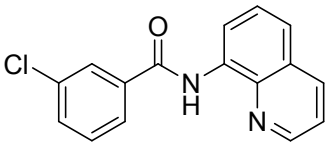
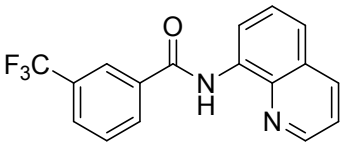
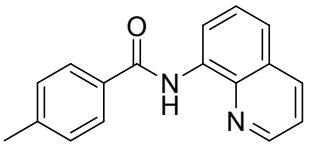
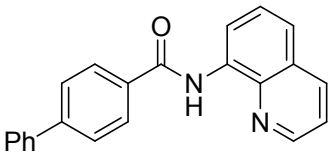
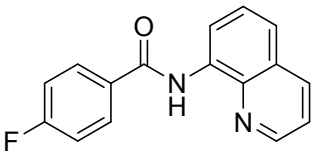
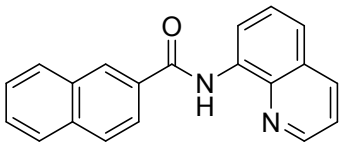
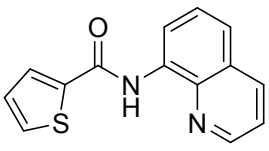
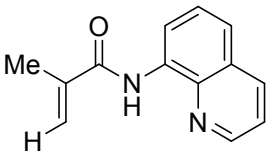
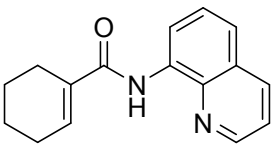
1. General information

^{1}H NMR, ^{13}C NMR and ^{19}F NMR were recorded in $CDCl_3$ at room temperature on the Varian INOVA-400 spectrometer (400 MHz, ^{1}H). The ^{1}H NMR 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). High-resolution mass spectral (HRMS) analyses were carried out using a TOF MS instrument with an ESI source.

Unless otherwise noted, all reagents were obtained from commercial suppliers and used without further purification. Anhydrous $Co(acac)_3$ 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

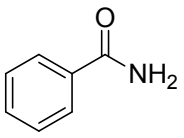
All benzamides were synthesized from the corresponding benzoic acids or benzoyl chlorides and 8-aminoquinoline. The deuterated amides were synthesized according to a literature method, spectral properties are consistent with literature values.[1] The following amides were synthesized according to literature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

3. Co-catalyzed methylthiolation of benzamides

3.1 Optimization of reaction conditions

Scheme S1 ineffective directing groups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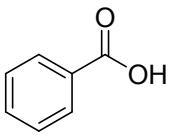
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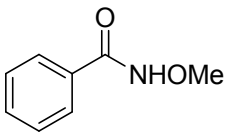
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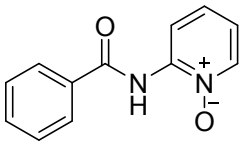
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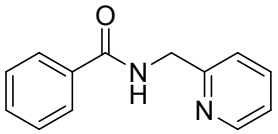
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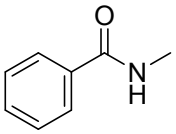
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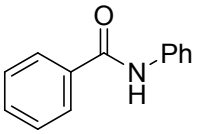
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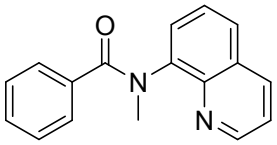
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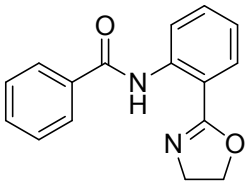
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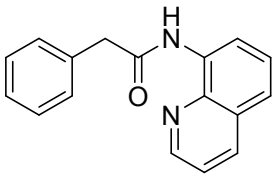
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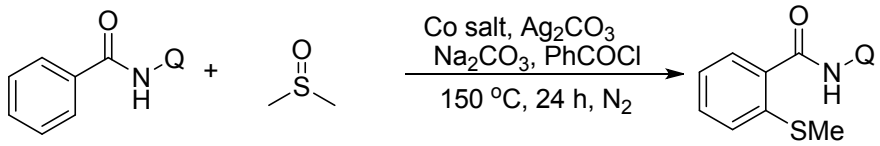
Table S1. screaning of Co salts [a]

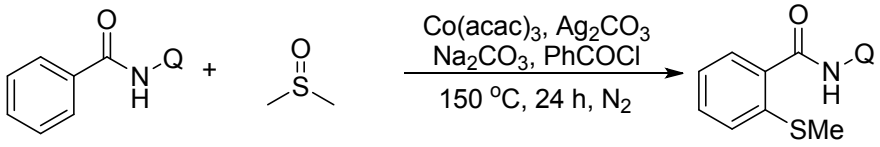


1a **2** **3b**

Entry	Co salts	yield[b] (%)
1	$Co(OAc)_2$	27
2	$Co(CO)_3$	<5
3	$CoCl_2$	ND
4	$CoBr_2$	ND
5	$CoSO_4$	ND
6	$Co(oxalate)_2$	trace
7	$Co(NO_3)_2.6H_2O$	ND
8	$Co(acac)_2$	13

[a] Reaction conditions: amide **1a** (0.2 mmol), **2** (2 mL), Co salt (0.04 mmol), Ag_2CO_3 (0.4 mmol), Na_2CO_3 (0.4 mmol), PhCOCl (0.4 mmol), 150 °C, under N_2 for 24 h; [b] isolated yield.

Table S2. screaning of different purity of $Co(acac)_3$ [a]

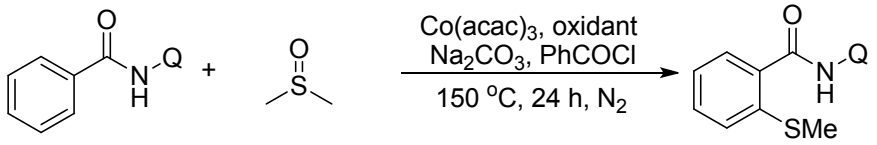


1a **2** **3b**

Entry	purity/$Co(acac)_3$	yield[b] (%)
1	97%	76
2	98%	78
3	>98%	78

[a] Reaction conditions: amide **1a** (0.2 mmol), **2** (2 mL), $Co(acac)_3$ 0.04 mmol), Ag_2CO_3 (0.4 mmol), Na_2CO_3 (0.4 mmol), PhCOCl (0.4 mmol), 150 °C, under N_2 for 24 h; [b] isolated yield.

Table S3. screaning of oxidant [a]

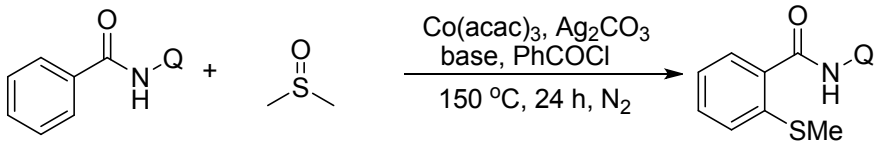


1a **2** **3b**

Entry	oxidant	yield[b] (%)
1	$Mn(OAc)_2$	ND
2	NMO	ND
3	O_2 (1 atm)	ND
4	Ag_2O	71
5	AgOAc	56
6	$AgCF_3CO_2$	64

[a] Reaction conditions: amide **1a** (0.2 mmol), **2** (2 mL), $Co(acac)_3$ (0.04 mmol), oxidant (0.4 mmol), Na_2CO_3 (0.4 mmol), PhCOCl (0.4 mmol), 150 °C, under N_2 for 24 h; [b] isolated yield.

Table S4. screaning of base [a]

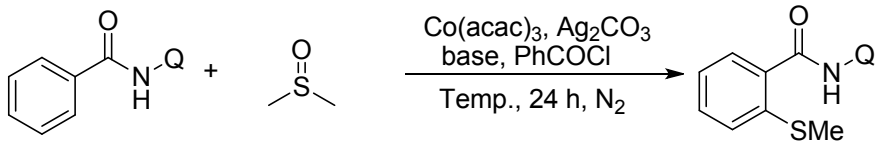


1a **2** **3b**

Entry	base	yield[b] (%)
1	K_2CO_3	41
2	NaOPiv	43
3	KOAc	45
4	Cs_2CO_3	54
5	*t*-BuOK	<5

[a] Reaction conditions: amide **1a** (0.2 mmol), **2** (2 mL), $Co(acac)_3$ (0.04 mmol), Ag_2CO_3 (0.4 mmol), base (0.4 mmol), PhCOCl (0.4 mmol), 150 °C, under N_2 for 24 h; [b] isolated yield.

Table S5. screaning of temperature [a]

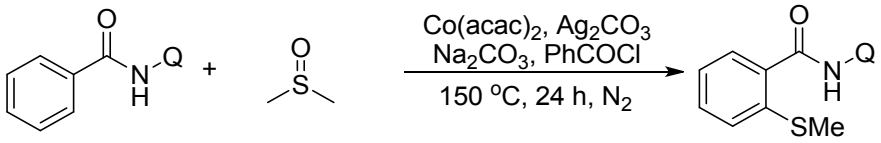


1a **2** **3b**

Entry	Temp. (°C)	yield[b] (%)
1	R.T.	trace
2	60	<5
3	80	<5
4	100	<10
5	120	21
6	150	78

[a] Reaction conditions: amide **1a** (0.2 mmol), **2** (2 mL), $Co(acac)_3$ (0.04 mmol), Ag_2CO_3 (0.4 mmol), Na_2CO_3 (0.4 mmol), PhCOCl (0.4 mmol), under N_2 for 24 h; [b] isolated yield.

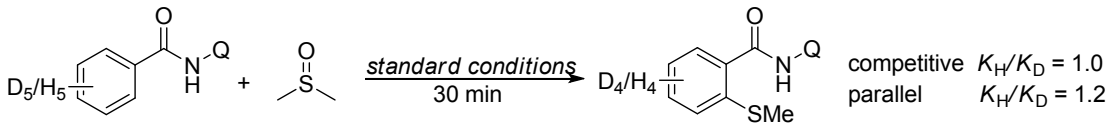
3.2 General procedure for Co-catalyzed *ortho*-methylthiolation of Benzamides with DMSO:



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

Benzamide **1a** (0.2 mmol, 49.6 mg), anhydrous $Co(acac)_3$ (14 mg, 0.04 mmol), Ag_2CO_3 (110 mg, 0.4 mmol), Na_2CO_3 (42 mg, 0.4 mmol), PhCOCl (56 mg, 0.4 mmol) and anhydrous DMSO (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 N_2 and stirred at 150 °C for 24 h. After the completion of the reaction, the solvent was evaporated under reduced pressure. 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 (8/1 to 6/1) gave the desired product **3a** as a white solid (45.9 mg, 78% yield).

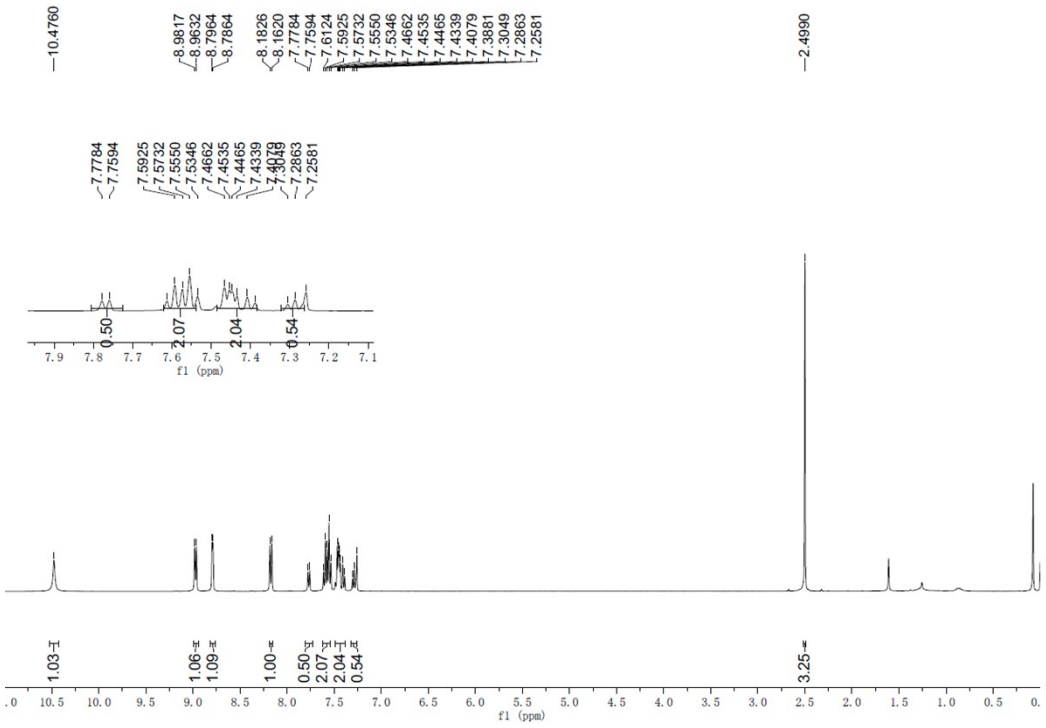
3.3 Deuterium-labeling experiments:



1a: 1a-*d*$_5$ = 1: 1 **2** **3a/3a-d$_4$**

Intermolecular competition KIE Following general procedure: **1a** (50 mg, 0.2 mmol), **1a'-*d*$_5$** (51 mg, 0.2 mmol), $Co(acac)_3$ (28 mg, 0.08 mmol), Ag_2CO_3 (220 mg, 0.8 mmol), Na_2CO_3 (84 mg, 0.8 mmol), PhCOCl (112 mg, 0.8 mmol) and anhydrous DMSO (4 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 N_2 and stirred at 150 °C for 30 min. The product was separated by column chromatography to give the desired product less than 10 % yield. The KIE value was calculated as $k_H/k_D = 1.0$.

Intermolecular parallel KIE Following general procedure:**1a** (50 mg, 0.2 mmol) or **1a'-*d*$_5$** (51 mg, 0.2 mmol), $Co(acac)_3$ (14 mg, 0.04 mmol), Ag_2CO_3 (110 mg, 0.4 mmol), Na_2CO_3 (42 mg, 0.4 mmol), PhCOCl (56 mg, 0.4 mmol) and anhydrous DMSO (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 N_2 and stirred at 150 °C for 30 min. The product was separated by column chromatography to give the desired product less than 12 % yield. The KIE value was calculated as $k_H/k_D = 1.2$.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7.4339
7.4079
7.3881
7.3049
7.2863
7.2581
2.4990
0.50
2.07
2.04
0.54
f1 (ppm)
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1.06
1.09
1.00
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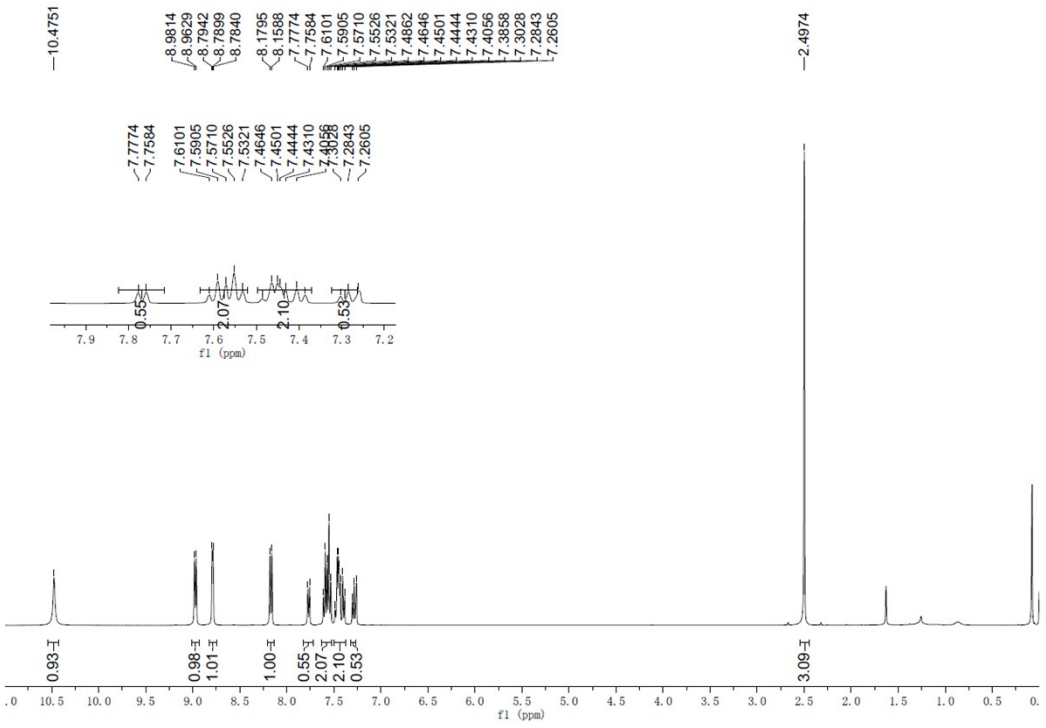
f1 (ppm)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2.10
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f1 (ppm)
0.93
0.98
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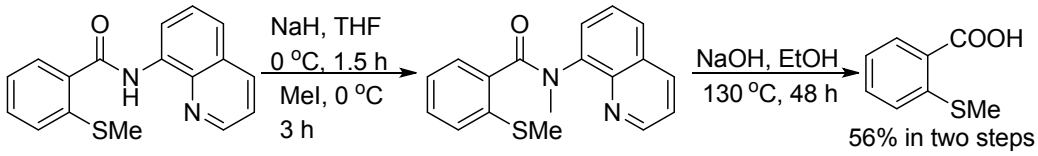
2.10
0.53
3.09
f1 (ppm)

3.4 Removal of the 8-aminoquinoline Auxiliary:

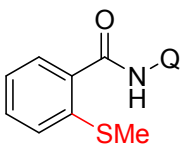


Eq. 5

2-(methylthio)-N-(quinolin-8-yl)benzamide **3a** (294 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 1.5 h. MeI (710 mg, 5 mmol) was added dropwise over 5 min, and reaction mixture was stirred for additional 3 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 to give intermediate **6** as a yellow solid (246 mg, 80%).Intermediate **6** (154 mg, 0.5 mmol) and NaOH (307 mg, 7.5 mmol) were dissolved in EtOH (5 ml). The resulting mixture was stirred at 130 °C for 48 hours. After that, reaction mixture was diluted with EtOAc (100 mL) and 1N HCl (30mL) 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 faint yellow solid (56%). Its spectral properties are consistent with literature values.

4 Characterization data of products

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

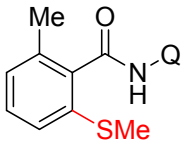


3a

78% yield (45.9 mg); White solid, mp: 113–115 °C (from ethyl acetate/petroleum ether = 12:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.47 (s, 1H), 8.97 (d, J = 7.3 Hz, 1H), 8.79 (d, J = 7.2 Hz, 1H), 8.17 (d, J = 8.2 Hz, 1H), 7.77 (d, J = 7.5 Hz, 1H), 7.61–7.53 (m, 2H), 7.48–7.39 (m, 3H), 7.30–7.26

(m, 1H), 2.50 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.5, 148.2, 138.7, 138.7, 136.3, 135.3, 134.6, 130.9, 128.1, 128.0, 127.4, 126.9, 124.9, 121.8, 121.6, 116.8, 16.5; HRMS (ESI) calcd for $C_{17}H_{15}N_2OS[M + H]^+$ 295.0905, Found 295.0888.

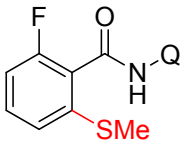
2-methyl-6-(methylthio)-N-(quinolin-8-yl)benzamide (**3b**)



3b

73% yield (45.0 mg); colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.99 (s, 1H), 9.02 (d, J = 7.3 Hz, 1H), 8.75 (d, J = 3.1 Hz, 1H), 8.18 (d, J = 8.2 Hz, 1H), 7.63–7.56 (m, 2H), 7.46–7.42 (m, 1H), 7.33–7.30 (m, 1H), 7.26–7.24 (m, 1H), 7.12 (d, J = 7.4 Hz, 1H), 2.47 (s, 3H), 2.44 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.2, 148.3, 138.5, 138.2, 136.3, 135.6, 135.6, 134.6, 129.5, 128.0, 127.8, 127.5, 125.6, 122.0, 121.6, 116.9, 19.5, 17.5; HRMS (ESI) calcd for $C_{18}H_{17}N_2OS[M + H]^+$ 309.1062, Found 309.1033.

2-fluoro-6-(methylthio)-N-(quinolin-8-yl)benzamide (**3c**)

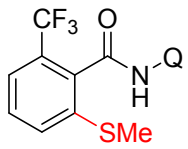


3c

67% yield (41.8 mg); White solid, mp: 118–120 ^{o}C (from ethyl acetate/petroleum ether = 12:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.29 (s, 1H), 8.99 (d, J = 7.0 Hz, 1H), 8.79 (d, J = 1.6 Hz, 1H), 8.17 (d, J = 8.2 Hz, 1H), 7.62–7.55 (m, 2H), 7.47–7.37 (m, 2H), 7.14 (d, J = 8.0 Hz, 1H), 6.99 (t, J = 8.8 Hz, 1H), 2.49 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.1, 159.6 (d, J = 247.9 Hz), 148.3, 140.9 (d, J = 3.5 Hz), 138.5, 136.3, 134.3, 131.2 (d, J = 9.2 Hz), 130.1, 128.2 (d, J = 47.2 Hz), 127.4, 122.2, 122.1 (d, J = 3.0 Hz), 121.6, 117.1, 112.5 (d, J = 22.7 Hz), 16.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -114.0; HRMS (ESI) calcd for $C_{17}H_{14}FN_2OS[M + H]^+$ 313.0811, Found

313.0803.

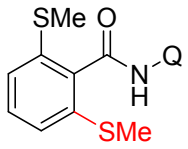
2-(methylthio)-N-(quinolin-8-yl)-6-(trifluoromethyl)benzamide (**3d**)



3d

63% yield (45.6 mg); White solid, mp: 132–134 °C (from ethyl acetate/petroleum ether = 12:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.05 (s, 1H), 8.98 (d, J = 7.0 Hz, 1H), 8.75 (s, 1H), 8.18 (d, J = 8.2 Hz, 1H), 7.63–7.53 (m, 5H), 7.46–7.43 (m, 1H), 2.50 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.1, 148.3, 138.7, 138.5, 136.3, 135.5 (q, J = 1.8 Hz), 134.1, 131.1, 129.8, 128.1 (q, J = 31.7 Hz), 128.0, 127.4, 123.5 (q, J = 272.7 Hz), 123.2 (q, J = 4.7 Hz), 122.3, 121.7, 117.1, 17.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.08; HRMS (ESI) calcd for $C_{18}H_{14}F_3N_2OS[M + H]^+$ 363.0779, Found 363.0757.

2,6-bis(methylthio)-N-(quinolin-8-yl)benzamide (**3e**)

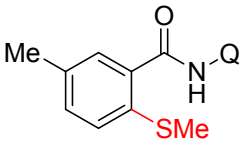


3e

61% yield (41.5 mg); White solid, mp: 123–125 °C (from ethyl acetate/petroleum ether = 12:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.04 (s, 1H), 9.03 (d, J = 7.4 Hz, 1H), 8.75 (d, J = 3.2 Hz, 1H), 8.16 (d, J = 8.2 Hz, 1H), 7.63–7.54 (m, 2H), 7.43 (dd, J = 8.2, 4.1 Hz, 1H), 7.36 (t, J = 7.9 Hz, 1H), 7.26–7.21 (m, 2H), 2.47 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.6, 148.2, 138.6, 137.8, 136.9, 136.3, 134.4, 129.9, 128.0, 127.5, 125.0, 122.0, 121.6, 117.1, 17.3; HRMS (ESI) calcd for $C_{18}H_{17}N_2OS_2[M + H]^+$ 341.0782, Found 341.0764.

5-methyl-2-(methylthio)-N-(quinolin-8-yl)benzamide (**3f**)

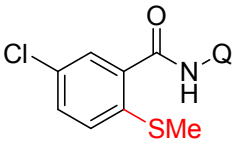
77% yield (47.4 mg); White solid, mp: 130–132 °C (from ethyl acetate/petroleum ether = 12:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.48 (s, 1H),



3f

8.97 (d, J = 7.4 Hz, 1H), 8.79 (d, J = 3.7 Hz, 1H), 8.16 (d, J = 8.2 Hz, 1H), 7.60–7.52 (m, 3H), 7.44 (dd, J = 8.1, 4.1 Hz, 1H), 7.32–7.25 (m, 2H), 2.47 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.7, 148.2, 138.6, 136.3, 135.7, 135.2, 134.6, 134.4, 131.7, 128.9, 127.9, 127.8, 127.4, 121.8, 121.6, 116.8, 20.8, 17.1; HRMS (ESI) calcd for $C_{18}H_{17}N_2OS[M + H]^+$ 309.1062, Found 309.1055.

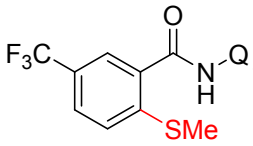
5-chloro-2-(methylthio)-N-(quinolin-8-yl)benzamide (**3g**)



3g

74% yield (48.5 mg); White solid, mp: 128–130 °C (from ethyl acetate/petroleum ether = 12:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.46 (s, 1H), 8.93 (d, J = 6.9 Hz, 1H), 8.81 (s, 1H), 8.18 (d, J = 8.1 Hz, 1H), 7.73 (s, 1H), 7.61–7.55 (m, 2H), 7.48–7.40 (m, 2H), 7.32 (d, J = 8.5 Hz, 1H), 2.49 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.1, 148.4, 138.6, 136.9, 136.7, 136.3, 134.2, 131.0, 130.8, 128.4, 128.1, 127.9, 127.4, 122.2, 121.7, 116.9, 16.7; HRMS (ESI) calcd for $C_{17}H_{14}ClN_2OS[M + H]^+$ 329.0515, Found 329.0497.

2-(methylthio)-N-(quinolin-8-yl)-5-(trifluoromethyl)benzamide (**3h**)

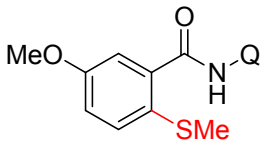


3h

71% yield (51.4 mg); White solid, mp: 134–136 °C (from ethyl acetate/petroleum ether = 12:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.46 (s, 1H), 8.93 (d, J = 6.9 Hz, 1H), 8.81 (d, J = 3.8 Hz, 1H), 8.18 (d, J = 8.2 Hz, 1H), 7.97 (s, 1H), 7.68 (d, J = 8.3 Hz, 1H), 7.63–7.54 (m, 2H), 7.48–7.43 (m, 2H), 2.53 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.1, 148.4, 143.9, 138.6, 136.3, 135.0, 134.1, 127.9, 127.3, 127.3, 126.8 (q, J = 32.2 Hz), 125.9, 124.9 (q, J = 3.7 Hz), 123.8 (q, J = 270.2 Hz), 122.3, 121.7, 117.0, 15.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.3; HRMS (ESI) calcd for $C_{18}H_{14}F_3N_2OS[M$

+ H]$^+$ 363.0779, Found 363.0769.

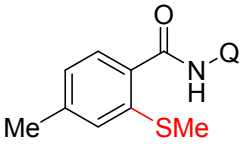
5-methoxy-2-(methylthio)-N-(quinolin-8-yl)benzamide (**3i**)



3i

81% yield (52.5 mg); White solid, mp: 140–142 °C (from ethyl acetate/petroleum ether = 8:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.65 (s, 1H), 8.97 (d, J = 7.4 Hz, 1H), 8.79 (d, J = 4.0 Hz, 1H), 8.17 (d, J = 8.2 Hz, 1H), 7.61–7.53 (m, 2H), 7.46–7.41 (m, 2H), 7.34 (s, 1H), 7.01 (d, J = 8.7 Hz, 1H), 3.86 (s, 3H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.3, 158.3, 148.3, 138.7, 138.5, 136.3, 134.6, 131.9, 128.0, 127.4, 127.3, 121.9, 121.6, 117.1, 116.8, 114.0, 55.6, 18.7; HRMS (ESI) calcd for $C_{18}H_{17}N_2O_2S$[M + H]$^+$ 325.1011, Found 325.1003.

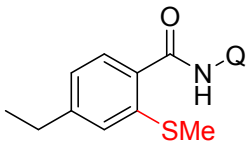
4-methyl-2-(methylthio)-N-(quinolin-8-yl)benzamide (**3j**)



3j

79% yield (48.7 mg); White solid, mp: 124–126 °C (from ethyl acetate/petroleum ether = 12:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.51 (s, 1H), 8.96 (d, J = 7.4 Hz, 1H), 8.80 (s, 1H), 8.17 (d, J = 8.2 Hz, 1H), 7.70 (d, J = 7.7 Hz, 1H), 7.61–7.53 (m, 2H), 7.48–7.44 (m, 1H), 7.19 (s, 1H), 7.09 (d, J = 7.7 Hz, 1H), 2.50 (s, 3H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.5, 148.2, 141.3, 138.7, 138.7, 136.3, 134.7, 132.2, 128.2, 128.0, 127.5, 127.3, 125.7, 121.7, 121.6, 116.7, 21.6, 16.5; HRMS (ESI) calcd for $C_{18}H_{17}N_2OS$[M + H]$^+$ 309.1062, Found 309.1095.

4-ethyl-2-(methylthio)-N-(quinolin-8-yl)benzamide (**3k**)

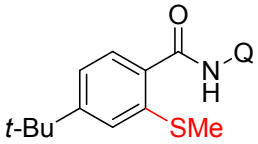


3k

76% yield (48.9 mg); White solid, mp: 129–131 °C (from ethyl acetate/petroleum ether = 12:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.51 (s, 1H), 8.97 (d, J = 7.4 Hz, 1H), 8.79 (d, J = 1.4 Hz, 1H), 8.17 (d, J = 8.1 Hz, 1H), 7.72 (d, J = 7.8 Hz, 1H), 7.59–7.53 (m, 2H), 7.47–7.42 (m, 1H), 7.22 (s, 1H),

7.12 (d, J = 7.7 Hz, 1H), 2.72 (q, J = 7.4 Hz, 2H), 2.51 (s, 3H), 1.29 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.5, 148.2, 147.6, 138.7, 138.6, 136.3, 134.7, 132.5, 128.3, 128.0, 127.5, 126.4, 124.5, 121.7, 121.6, 116.7, 28.9, 16.6, 15.4; HRMS (ESI) calcd for $C_{19}H_{19}N_2OS[M + H]^+$ 323.1218, Found 323.1205.

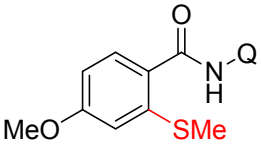
4-(tert-butyl)-2-(methylthio)-N-(quinolin-8-yl)benzamide (**3l**)



3l

74% yield (51.8 mg); White solid, mp: 135–137 °C (from ethyl acetate/petroleum ether = 12:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.54 (s, 1H), 8.98 (d, J = 7.4 Hz, 1H), 8.79 (d, J = 1.8 Hz, 1H), 8.17 (d, J = 8.2 Hz, 1H), 7.74 (d, J = 8.0 Hz, 1H), 7.61–7.53 (m, 2H), 7.46–7.44 (m, 2H), 7.32 (d, J = 8.0 Hz, 1H), 2.52 (s, 3H), 1.38 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.5, 154.3, 148.2, 138.7, 137.9, 136.3, 134.7, 132.6, 128.2, 128.0, 127.5, 124.5, 122.4, 121.7, 121.6, 116.7, 35.2, 31.1, 16.9; HRMS (ESI) calcd for $C_{21}H_{23}N_2OS[M + H]^+$ 351.1531, Found 351.1504.

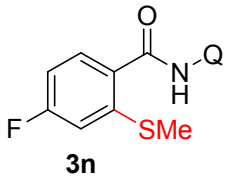
4-methoxy-2-(methylthio)-N-(quinolin-8-yl)benzamide (**3m**)



3m

82% yield (53.1 mg); White solid, mp: 142–144 °C (from ethyl acetate/petroleum ether = 8:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.52 (s, 1H), 8.95 (d, J = 7.5 Hz, 1H), 8.80 (d, J = 4.0 Hz, 1H), 8.17 (d, J = 8.2 Hz, 1H), 7.80 (d, J = 8.5 Hz, 1H), 7.60–7.51 (m, 2H), 7.45 (dd, J = 8.1, 4.1 Hz, 1H), 6.89 (s, 1H), 6.79 (d, J = 8.5 Hz, 1H), 3.89 (s, 3H), 2.49 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.0, 161.6, 148.2, 141.6, 138.7, 136.3, 134.8, 130.0, 128.0, 127.5, 127.1, 121.5, 121.5, 116.6, 112.7, 109.2, 55.5, 16.4; HRMS (ESI) calcd for $C_{18}H_{17}N_2O_2S[M + H]^+$ 325.1011, Found 325.0999.

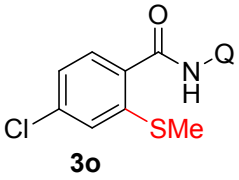
4-fluoro-2-(methylthio)-N-(quinolin-8-yl)benzamide (**3n**)



3n

73% yield (45.6 mg); White solid, mp: 131–133 °C (from ethyl acetate/petroleum ether = 12:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.45 (s, 1H), 8.93 (d, J = 7.2 Hz, 1H), 8.80 (d, J = 2.0 Hz, 1H), 8.18 (d, J = 8.2 Hz, 1H), 7.81–7.77 (m, 1H), 7.61–7.54 (m, 2H), 7.46 (dd, J = 7.8, 4.0 Hz, 1H), 7.06 (d, J = 10.0 Hz, 1H), 6.95 (t, J = 8.1 Hz, 1H), 2.49 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.5, 164.2 (d, J = 250.8 Hz), 148.3, 142.8 (d, J = 8.4 Hz), 138.6, 136.4, 134.4, 130.3 (d, J = 2.1 Hz), 130.1 (d, J = 9.3 Hz), 128.0, 127.4, 121.9, 121.7, 116.8, 113.0 (d, J = 24.5 Hz), 111.4 (d, J = 21.7 Hz), 16.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ -108.4; HRMS (ESI) calcd for $C_{17}H_{14}FN_2OS[M + H]^+$ 313.0811, Found 313.0784.

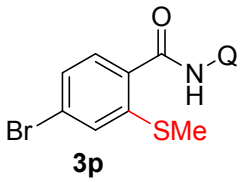
4-chloro-2-(methylthio)-N-(quinolin-8-yl)benzamide (**3o**)



3o

70% yield (45.9 mg); White solid, mp: 132–134 °C (from ethyl acetate/petroleum ether = 12:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.46 (s, 1H), 8.93 (d, J = 7.0 Hz, 1H), 8.80 (d, J = 1.3 Hz, 1H), 8.19 (d, J = 8.2 Hz, 1H), 7.71 (d, J = 8.1 Hz, 1H), 7.61–7.55 (m, 2H), 7.48–7.46 (m, 1H), 7.32 (s, 1H), 7.25 (d, J = 8.8 Hz, 1H), 2.50 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.5, 148.3, 141.4, 138.6, 137.3, 136.4, 134.3, 132.8, 129.2, 127.9, 127.4, 125.9, 124.7, 122.0, 121.7, 116.8, 16.3; HRMS (ESI) calcd for $C_{17}H_{14}ClN_2OS[M + H]^+$ 329.0515, Found 329.0499.

4-bromo-2-(methylthio)-N-(quinolin-8-yl)benzamide (**3p**)

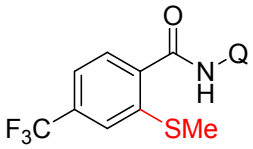


3p

63% yield (46.9 mg); White solid, mp: 136–138 °C (from ethyl acetate/petroleum ether = 12:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.46 (s, 1H), 8.93 (d, J = 7.0 Hz, 1H), 8.80 (d, J = 1.7 Hz, 1H), 8.19 (d, J = 8.1

Hz, 1H), 7.65–7.55 (m, 3H), 7.48–7.46 (m, 2H), 7.41 (d, J = 8.1 Hz, 1H), 2.50 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.5, 148.3, 138.6, 136.4, 134.3, 133.4, 129.4, 128.8, 128.0, 127.7, 127.4, 125.6, 124.7, 122.0, 121.7, 116.8, 16.3; HRMS (ESI) calcd for $C_{17}H_{14}BrN_2OS[M + H]^+$ 373.0010, Found 372.9986.

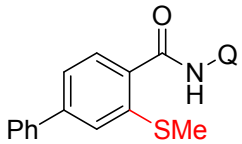
2-(methylthio)-N-(quinolin-8-yl)-4-(trifluoromethyl)benzamide (**3q**)



3q

67% yield (48.5 mg); White solid, mp: 141–143 °C (from ethyl acetate/petroleum ether = 12:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.47 (s, 1H), 8.94 (d, J = 6.5 Hz, 1H), 8.82 (s, 1H), 8.19 (d, J = 8.1 Hz, 1H), 7.97 (s, 1H), 7.69 (d, J = 8.3 Hz, 1H), 7.64–7.55 (m, 2H), 7.49–7.44 (m, 2H), 2.53 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.1, 148.4, 143.9, 138.6, 136.4, 135.1, 134.2, 128.0, 127.4, 127.3, 126.9 (q, J = 32.9 Hz), 126.0, 124.9 (q, J = 3.7 Hz), 123.8 (q, J = 270.2 Hz), 122.3, 121.8, 117.0, 16.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.3; HRMS (ESI) calcd for $C_{18}H_{14}F_3N_2OS[M + H]^+$ 363.0779, Found 363.0757.

3-(methylthio)-N-(quinolin-8-yl)-[1,1'-biphenyl]-4-carboxamide (**3r**)

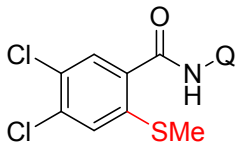


3r

72% yield (53.3 mg); White solid, mp: 143–145 °C (from ethyl acetate/petroleum ether = 12:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.58 (s, 1H), 8.99 (d, J = 7.3 Hz, 1H), 8.82 (d, J = 1.7 Hz, 1H), 8.19 (d, J = 8.2 Hz, 1H), 7.87 (d, J = 7.8 Hz, 1H), 7.67–7.55 (m, 5H), 7.50–7.41 (m, 5H), 2.57 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.3, 148.3, 144.0, 140.1, 139.4, 138.7, 136.4, 134.6, 133.7, 129.0, 128.7, 128.1, 128.0, 127.5, 127.3, 125.6, 123.8, 121.8, 121.6, 116.8, 16.6; HRMS (ESI) calcd for $C_{23}H_{19}N_2OS[M + H]^+$

371.1218, Found 371.1207.

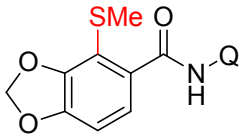
4,5-dichloro-2-(methylthio)-N-(quinolin-8-yl)benzamide (**3s**)



3s

63% yield (45.6 mg); White solid, mp: 136–138 °C (from ethyl acetate/petroleum ether = 12:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.47 (s, 1H), 8.90 (d, J = 5.7 Hz, 1H), 8.82 (s, 1H), 8.20 (d, J = 8.4 Hz, 1H), 7.84 (s, 1H), 7.59–7.55 (m, 2H), 7.48 (dd, J = 7.3, 3.8 Hz, 1H), 7.41 (s, 1H), 2.50 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.2, 148.4, 139.0, 138.6, 136.4, 134.1, 130.8, 129.8, 129.6, 128.9, 128.0, 127.4, 127.4, 122.3, 121.8, 117.0, 16.6; HRMS (ESI) calcd for $C_{17}H_{13}Cl_2N_2OS[M + H]^+$ 363.0126, Found 363.0121.

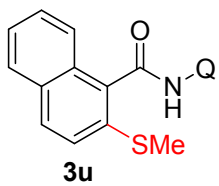
4-(methylthio)-N-(quinolin-8-yl)benzo[d][1,3]dioxole-5-carboxamide (**3t**)



3t

77% yield (52.1 mg); White solid, mp: 147–149 °C (from ethyl acetate/petroleum ether = 8:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.64 (s, 1H), 8.95 (d, J = 7.1 Hz, 1H), 8.80 (d, J = 3.6 Hz, 1H), 8.18 (d, J = 8.2 Hz, 1H), 7.62–7.53 (m, 2H), 7.46 (dd, J = 8.1, 4.1 Hz, 1H), 7.40 (d, J = 8.0 Hz, 1H), 6.85 (d, J = 8.0 Hz, 1H), 6.12 (s, 2H), 2.54 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.5, 154.9, 148.9, 148.2, 138.7, 136.3, 134.8, 134.3, 133.2, 128.0, 127.5, 123.5, 121.7, 121.6, 116.8, 107.5, 100.7, 18.2; HRMS (ESI) calcd for $C_{18}H_{15}N_2O_3S[M + H]^+$ 339.0803, Found 339.0691.

2-(methylthio)-N-(quinolin-8-yl)-1-naphthamide (**3u**)

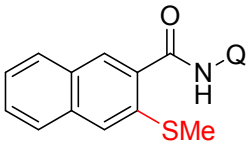


3u

69% yield (47.5 mg); White solid, mp: 152–154 °C (from ethyl acetate/petroleum ether = 12:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.17 (s, 1H), 9.15 (d, J = 7.5 Hz, 1H), 8.68 (d, J = 4.0 Hz, 1H), 8.17 (d, J = 8.2

Hz, 1H), 7.98 (d, J = 8.2 Hz, 1H), 7.91 (d, J = 8.7 Hz, 1H), 7.86 (d, J = 8.1 Hz, 1H), 7.66 (t, J = 7.9 Hz, 1H), 7.60–7.57 (m, 2H), 7.50–7.47 (m, 2H), 7.41 (dd, J = 8.2, 4.1 Hz, 1H), 2.57 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.8, 148.3, 138.5, 136.3, 135.4, 134.5, 132.9, 131.7, 130.5, 129.9, 128.0, 127.7, 127.5, 126.1, 126.1, 124.8, 122.1, 121.6, 117.0, 17.8; HRMS (ESI) calcd for $C_{21}H_{17}N_2OS[M + H]^+$ 345.1062, Found 345.1050.

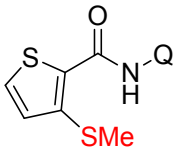
3-(methylthio)-N-(quinolin-8-yl)-2-naphthamide (**3v**)



3v

72% yield (49.5 mg); White solid, mp: 163–165 °C (from ethyl acetate/petroleum ether = 12:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.57 (s, 1H), 9.01 (d, J = 7.3 Hz, 1H), 8.81 (s, 1H), 8.25 (s, 1H), 8.20 (d, J = 8.2 Hz, 1H), 7.91 (d, J = 8.0 Hz, 1H), 7.82 (d, J = 8.1 Hz, 1H), 7.73 (s, 1H), 7.65–7.55 (m, 3H), 7.51–7.45 (m, 2H), 2.61 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.5, 148.3, 138.7, 136.4, 135.1, 134.7, 134.5, 133.9, 130.3, 128.4, 128.1, 128.1, 128.0, 127.5, 126.7, 126.0, 124.8, 121.9, 121.7, 116.9, 16.7; HRMS (ESI) calcd for $C_{21}H_{17}N_2OS[M + H]^+$ 345.1062, Found 345.1036.

3-(methylthio)-N-(quinolin-8-yl)thiophene-2-carboxamide (**3w**)

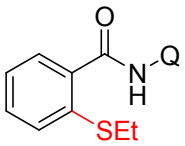


3w

56% yield (33.6 mg); White solid, mp: 106–108 °C (from ethyl acetate/petroleum ether = 12:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.49 (s, 1H), 8.91 (d, J = 7.3 Hz, 1H), 8.85 (d, J = 3.8 Hz, 1H), 8.16 (d, J = 8.2 Hz, 1H), 7.60–7.50 (m, 3H), 7.45 (dd, J = 8.0, 4.1 Hz, 1H), 7.15 (d, J = 5.1 Hz, 1H), 2.62 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ

160.2, 148.3, 139.0, 136.3, 136.2, 134.9, 134.7, 130.6, 129.3, 128.0, 127.4, 121.8, 121.5, 117.3, 18.9; HRMS (ESI) calcd for $C_{15}H_{13}N_2OS_2[M + H]^+$ 301.0469, Found 301.0442.

2-(ethylthio)-N-(quinolin-8-yl)benzamide (**3x**)



3x

72% yield (44.4 mg); White solid, mp: 123–125 °C (from ethyl acetate/petroleum ether = 12:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.55 (s, 1H), 8.98 (d, J = 7.4 Hz, 1H), 8.78 (d, J = 3.6 Hz, 1H), 8.17 (d, J = 8.2 Hz, 1H), 7.78 (d, J = 7.6 Hz, 1H), 7.61–7.53 (m, 2H), 7.48–7.42 (m, 3H), 7.31 (t, J = 7.3 Hz, 1H), 2.99 (q, J = 7.3 Hz, 2H), 1.33 (t, J = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 148.2, 138.7, 136.6, 136.4, 136.3, 134.7, 130.7, 129.2, 128.5, 128.0, 127.4, 125.6, 121.8, 121.6, 116.8, 27.9, 13.8; HRMS (ESI) calcd for $C_{18}H_{17}N_2OS[M + H]^+$ 309.1062, Found 309.1041.

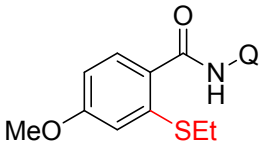
2-(ethylthio)-5-methyl-N-(quinolin-8-yl)benzamide (**3y**)

3y

70% yield (45.1 mg); White solid, mp: 126–128 °C (from ethyl acetate/petroleum ether = 12:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.60 (s, 1H), 8.98 (d, J = 7.4 Hz, 1H), 8.79 (d, J = 3.7 Hz, 1H), 8.16 (d, J = 8.2 Hz, 1H), 7.60–7.53 (m, 3H), 7.44 (dd, J = 8.2, 4.1 Hz, 1H), 7.40 (d, J = 8.0 Hz, 1H), 7.24 (d, J = 8.8 Hz, 1H), 2.95 (q, J = 7.3 Hz, 2H), 2.40 (s, 3H), 1.29 (t, J = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.8, 148.2, 138.7, 137.5, 136.3, 136.3, 134.8, 131.7, 131.5, 130.8, 129.4, 128.0, 127.4, 121.8, 121.6, 116.9, 28.7, 20.9, 14.0; HRMS

(ESI) calcd for $C_{19}H_{19}N_2OS[M + H]^+$ 323.1218, Found 323.1194.

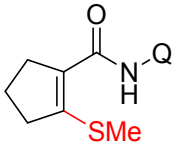
2-(ethylthio)-4-methoxy-N-(quinolin-8-yl)benzamide (**3z**)



3z

74% yield (50.0 mg); White solid, mp: 132–134 °C (from ethyl acetate/petroleum ether = 8:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.66 (s, 1H), 8.96 (d, J = 7.5 Hz, 1H), 8.80 (d, J = 3.5 Hz, 1H), 8.17 (d, J = 8.1 Hz, 1H), 7.82 (d, J = 8.5 Hz, 1H), 7.61–7.52 (m, 2H), 7.45 (dd, J = 8.2, 4.1 Hz, 1H), 6.97 (s, 1H), 6.82 (d, J = 8.6 Hz, 1H), 3.88 (s, 3H), 2.98 (q, J = 7.4 Hz, 2H), 1.35 (t, J = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.1, 161.3, 148.2, 139.2, 138.8, 136.3, 134.9, 130.5, 129.2, 128.3, 128.0, 127.5, 121.5, 116.7, 114.7, 110.2, 55.5, 27.7, 13.6; HRMS (ESI) calcd for $C_{19}H_{19}N_2O_2S[M + H]^+$ 339.1167, Found 339.1140.

2-(methylthio)-N-(quinolin-8-yl)cyclopent-1-enecarboxamide (**5a**)

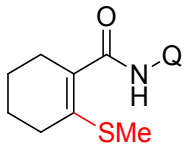


5a

77% yield (43.7 mg); colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.01 (s, 1H), 8.93 (d, J = 7.5 Hz, 1H), 8.79 (d, J = 4.1 Hz, 1H), 8.14 (d, J = 8.2 Hz, 1H), 7.56–7.41 (m, 3H), 2.99 (t, J = 7.1 Hz, 2H), 2.90 (t, J = 7.0 Hz, 2H), 2.40 (s, 3H), 2.19–2.08 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.0, 154.4, 148.0, 136.3, 134.8, 127.9, 127.5, 125.9, 121.4, 121.0, 116.3, 100.0, 37.1, 33.0, 22.1, 15.2; HRMS (ESI) calcd for $C_{16}H_{17}N_2OS[M + H]^+$ 285.1062, Found 285.1036.

2-(methylthio)-N-(quinolin-8-yl)cyclohex-1-enecarboxamide (**5b**)

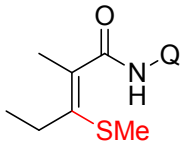
63% yield (37.5 mg); colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.18 (s, 1H), 8.90 (d, J = 7.5 Hz, 1H), 8.82–8.80 (m, 1H), 8.16 (d, J =



5b

8.2 Hz, 1H), 7.57–7.44 (m, 3H), 2.60–2.49 (m, 4H), 2.30 (s, 3H), 1.79–1.77 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.7, 148.1, 138.7, 136.3, 134.7, 132.8, 129.7, 128.2, 127.5, 121.5, 121.3, 116.6, 29.9, 27.9, 23.0, 21.9, 15.0; HRMS (ESI) calcd for $C_{17}H_{19}N_2OS[M + H]^+$ 299.1218, Found 299.1210.

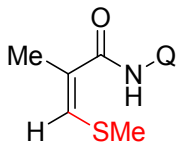
(Z)-2-methyl-3-(methylthio)-N-(quinolin-8-yl)pent-2-enamide (**5c**)



5c

61% yield (34.9 mg); colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.07 (s, 1H), 8.87 (d, J = 7.2 Hz, 1H), 8.81 (s, 1H), 8.16 (d, J = 8.2 Hz, 1H), 7.58–7.50 (m, 2H), 7.45 (dd, J = 7.7, 4.0 Hz, 1H), 2.47 (q, J = 7.4 Hz, 2H), 2.27 (s, 3H), 2.15 (s, 3H), 1.20 (t, J = 7.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.9, 148.1, 140.7, 138.6, 136.3, 134.7, 131.1, 128.0, 127.5, 121.5, 121.4, 116.5, 25.2, 17.0, 16.1, 12.7; HRMS (ESI) calcd for $C_{16}H_{19}N_2OS[M + H]^+$ 287.1218, Found 287.1236.

(Z)-2-methyl-3-(methylthio)-N-(quinolin-8-yl)acrylamide (**5d**)



5d

65% yield (33.5 mg); colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.26 (s, 1H), 8.93 (d, J = 7.3 Hz, 1H), 8.80 (d, J = 3.4 Hz, 1H), 8.16–8.11 (m, 1H), 7.54–7.44 (m, 3H), 6.74 (s, 1H), 2.37 (s, 3H), 2.29 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.7, 148.1, 144.3, 138.7, 136.3, 130.2, 128.5, 127.5, 122.3, 121.5, 121.3, 116.5, 19.9, 19.5; HRMS (ESI) calcd for $C_{14}H_{15}N_2OS[M + H]^+$ 259.0905, Found 259.0893.

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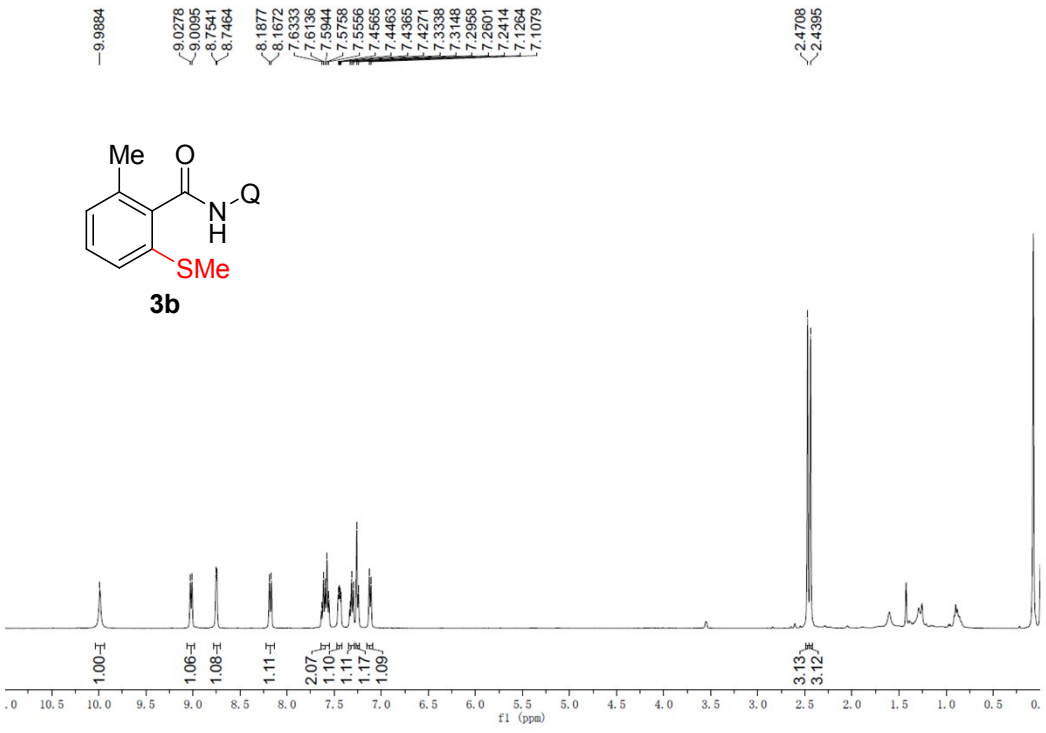
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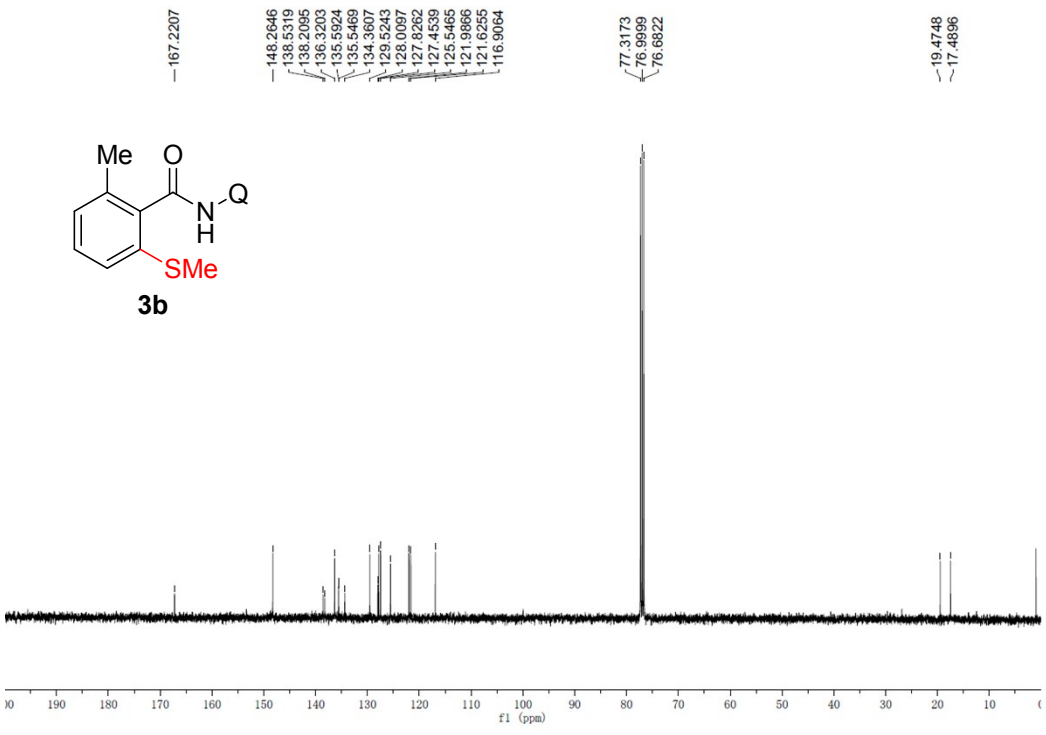
3b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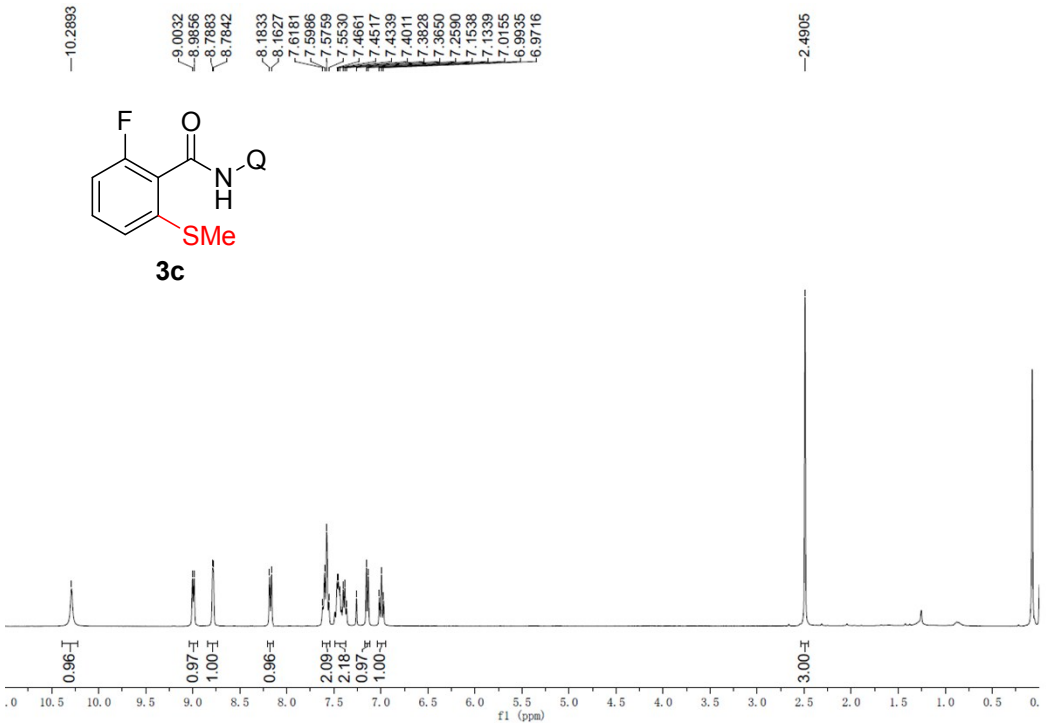
3b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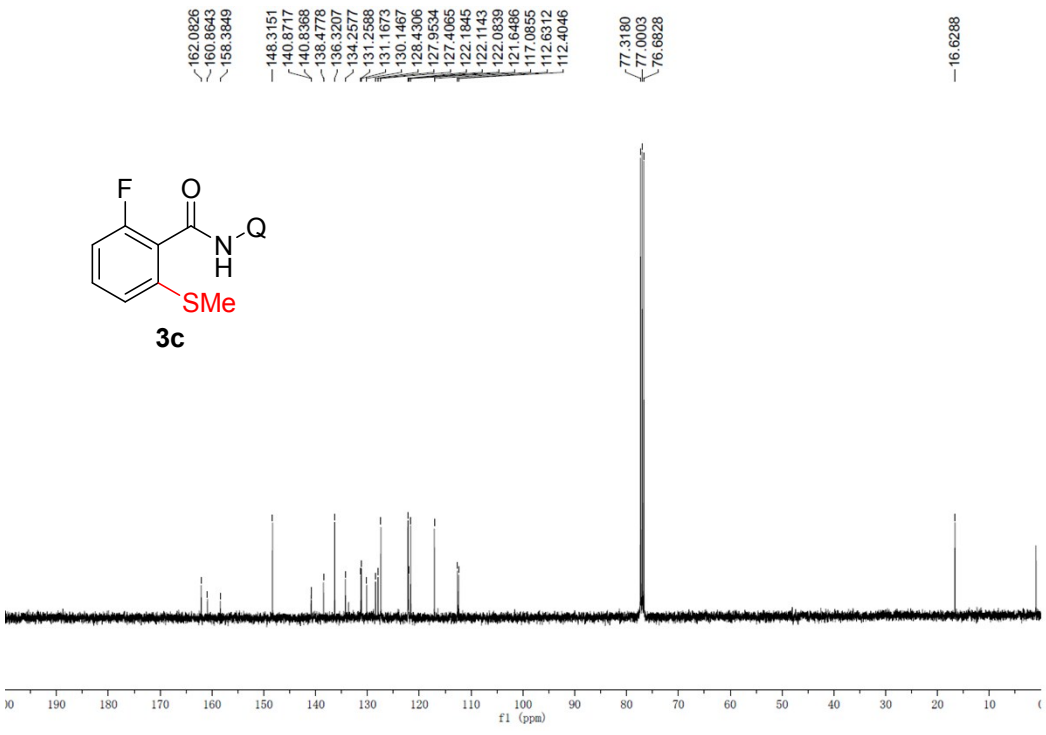
f1 (ppm)

3c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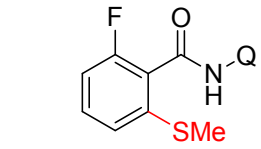
160.8643
158.3849
148.3151
140.8717
140.8368
138.4778
136.3207
134.2577
131.2588
131.1673
130.1467
128.4306
127.9534
127.4065
122.1845
122.1143
122.0839
121.6486
117.0855
112.6312
112.4046
77.3180
77.0003
76.6828
16.6288
F
O
N
H
Q
SMe
f1 (ppm)

3c


F
O
N
H
Q
SMe

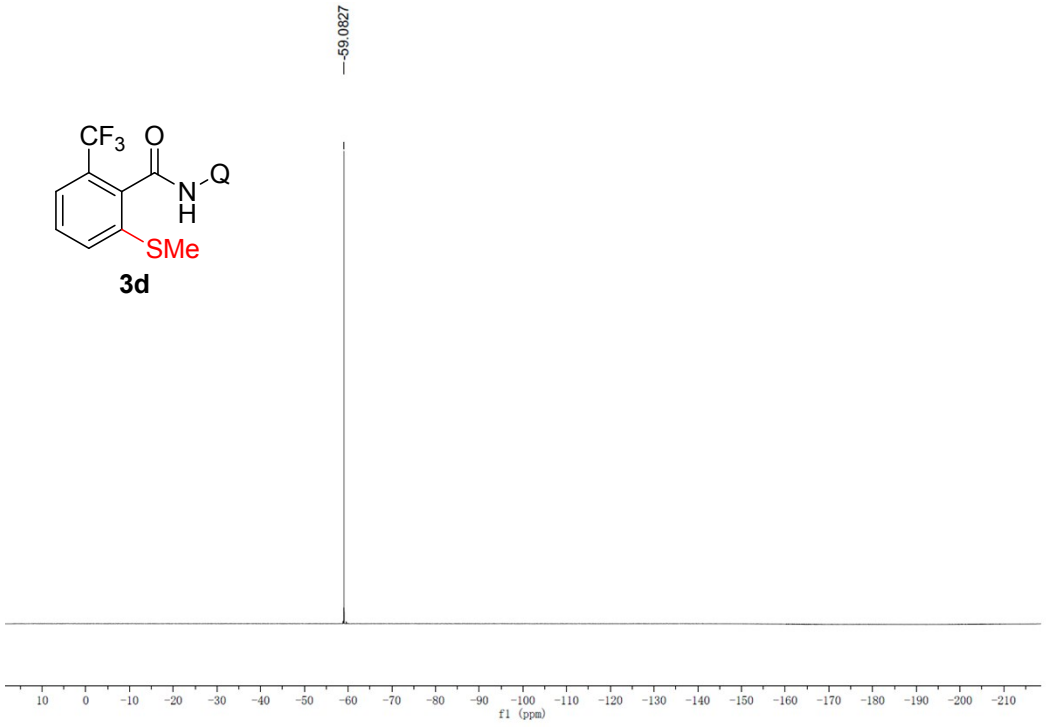
3c

-114.0211
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)

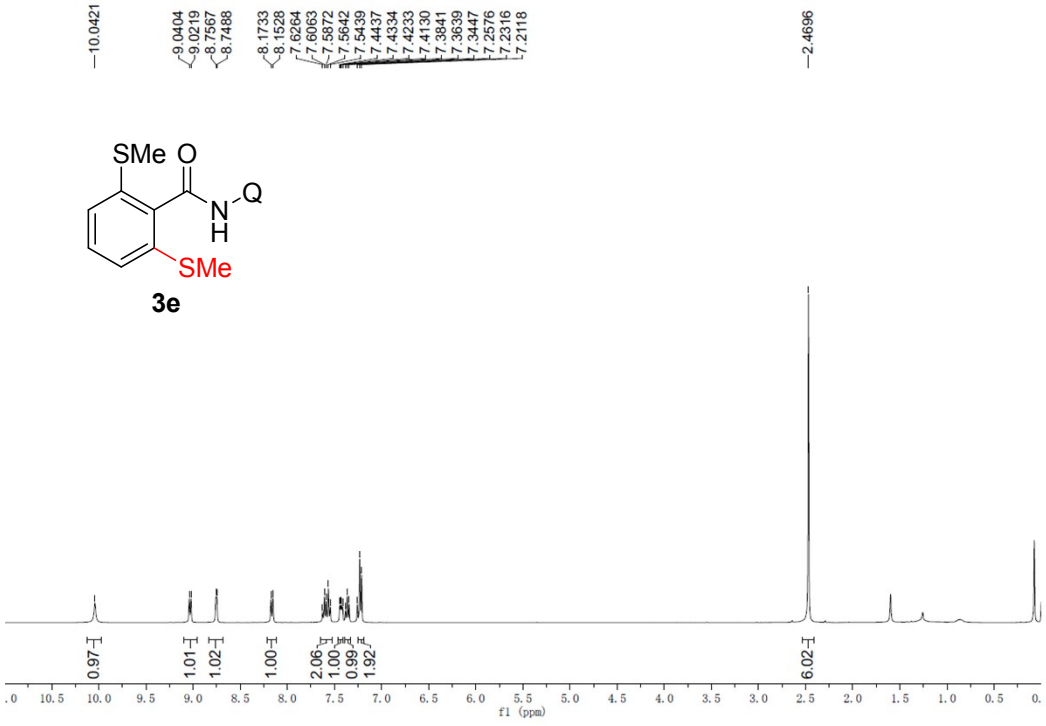

10.0481
8.9842
8.9666
8.7537
8.1878
8.1673
7.6334
7.6133
7.5913
7.5835
7.5611
7.5491
7.5289
7.4575
7.4462
7.4389
7.4279
2.4990
CF3
O
N
H
Q
SMe
0.99
1.00
1.00
0.99
5.09
1.11
3.01
f1 (ppm)
164.1359
148.3230
138.7174
138.4750
136.3388
135.4832
134.1454
131.1349
129.7595
128.2373
128.0053
127.9208
127.4497
124.8168
123.3099
123.2630
123.2161
123.1697
122.3185
122.0903
121.6633
77.3180
77.0004
76.6829
17.1974
f1 (ppm)

3d

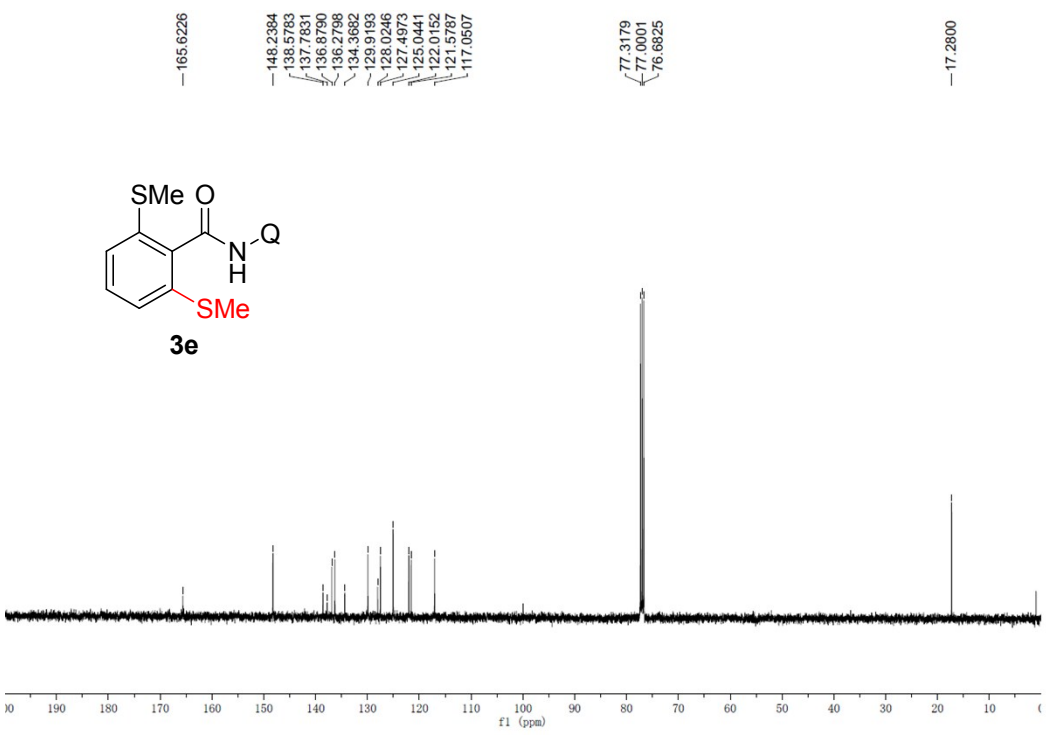
3d


-59.0827
CF3
O
N
H
Q
SMe
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)

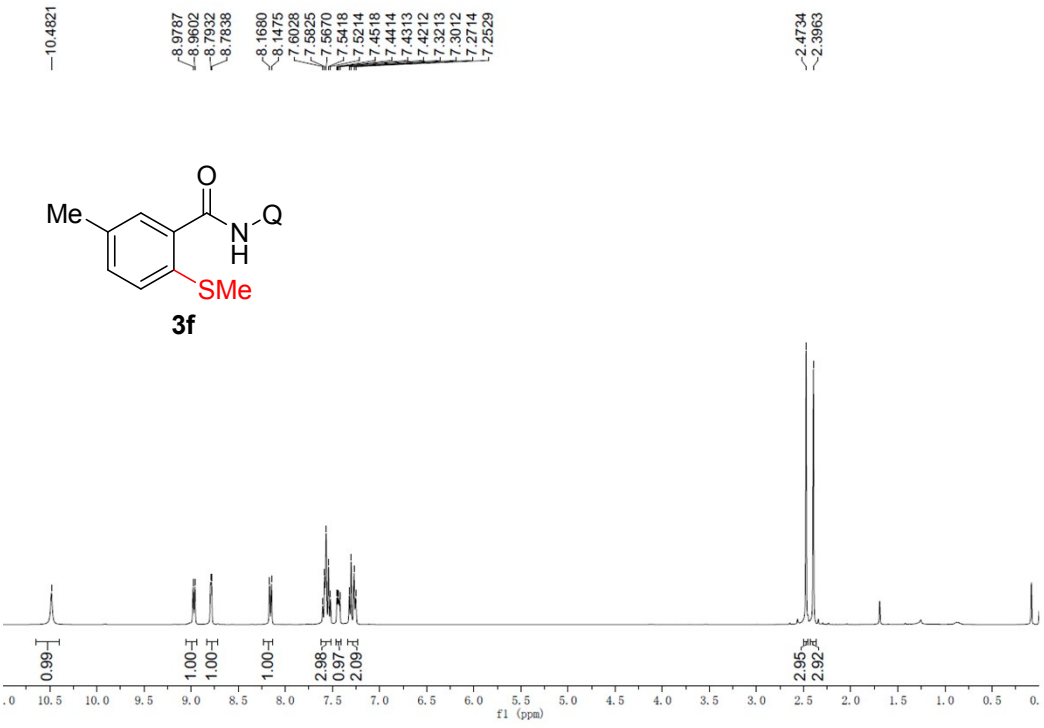
3d


10.0421
9.0404
9.0219
8.7567
8.7488
8.1733
8.1528
7.6264
7.6063
7.5872
7.5642
7.5439
7.4437
7.4334
7.4233
7.4130
7.3841
7.3639
7.3447
7.2576
7.2316
7.2118
2.4696
SMe
O
N
H
Q
SMe
0.97
1.01
1.02
1.00
2.06
1.00
0.99
1.92
6.02
f1 (ppm)

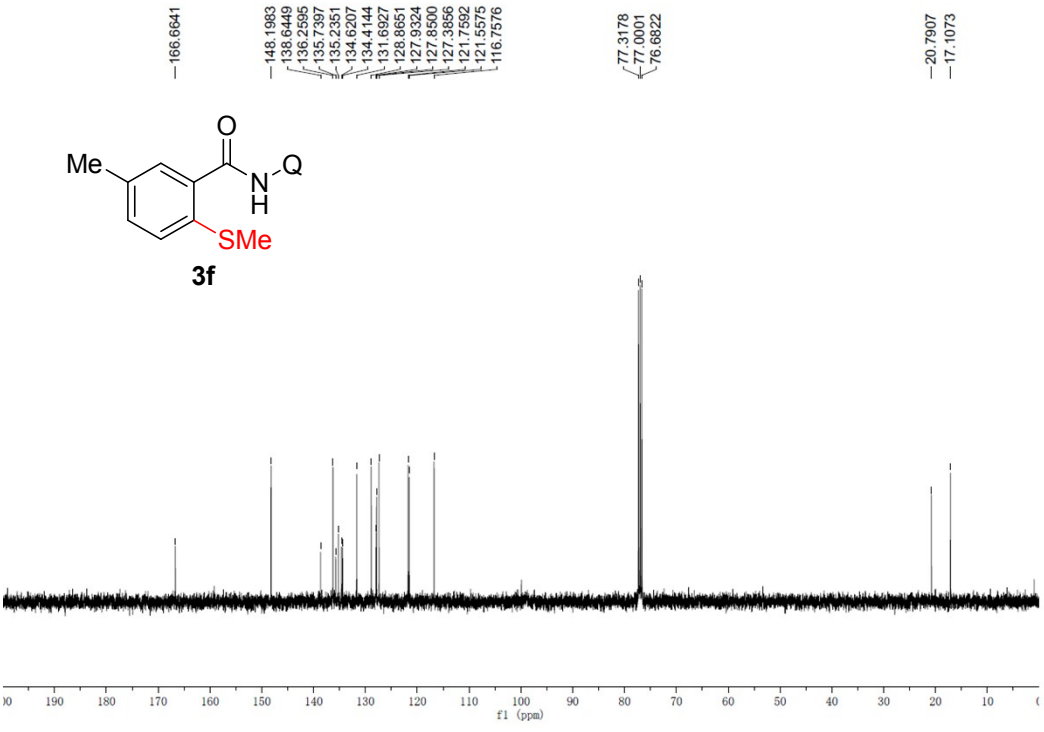
3e


165.6226
148.2384
138.5783
137.7831
136.8790
136.2798
134.3682
129.9193
128.0246
127.4973
125.0441
122.0152
121.5787
117.0507
77.3179
77.0001
76.6825
17.2800
SMe
O
N
H
Q
SMe
f1 (ppm)

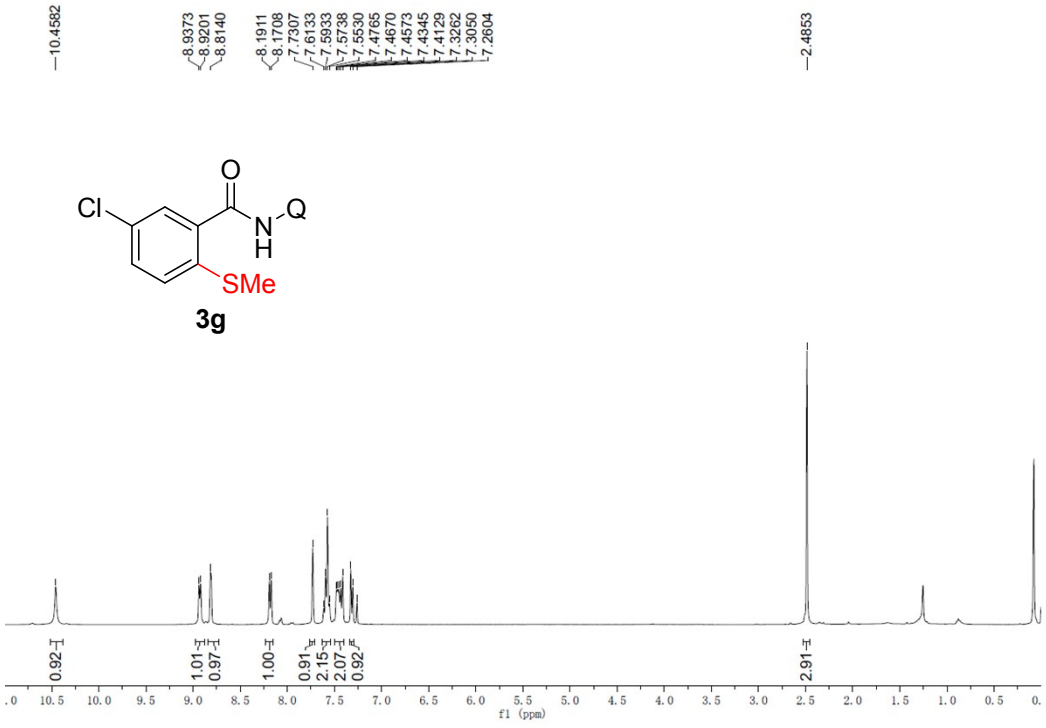
3e


10.4821
8.9787
8.9602
8.7932
8.7838
8.1680
8.1475
7.6028
7.5825
7.5670
7.5418
7.5214
7.4518
7.4414
7.4313
7.4212
7.3213
7.3012
7.2714
7.2529
2.4734
2.3963
Me
O
N
H
Q
SMe
0.99
1.00
1.00
1.00
2.98
0.97
2.09
2.95
2.92
f1 (ppm)

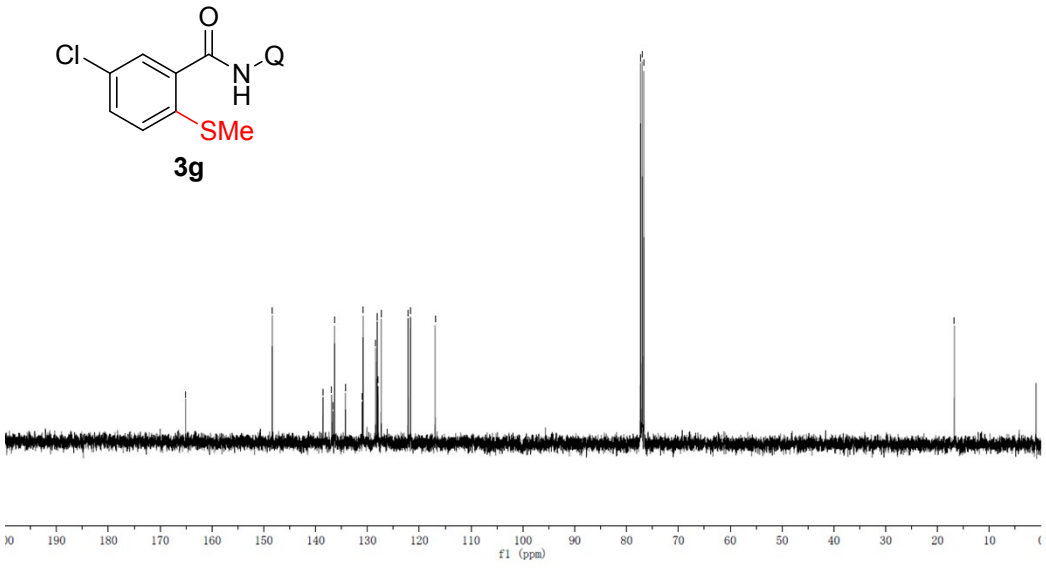
3f


166.6641
148.1983
138.6449
136.2595
135.7397
135.2351
134.6207
134.4144
131.6927
128.8651
127.9324
127.8500
127.3856
121.7592
121.5575
116.7576
77.3178
77.0001
76.6822
20.7907
17.1073
Me
O
N
H
Q
SMe
f1 (ppm)

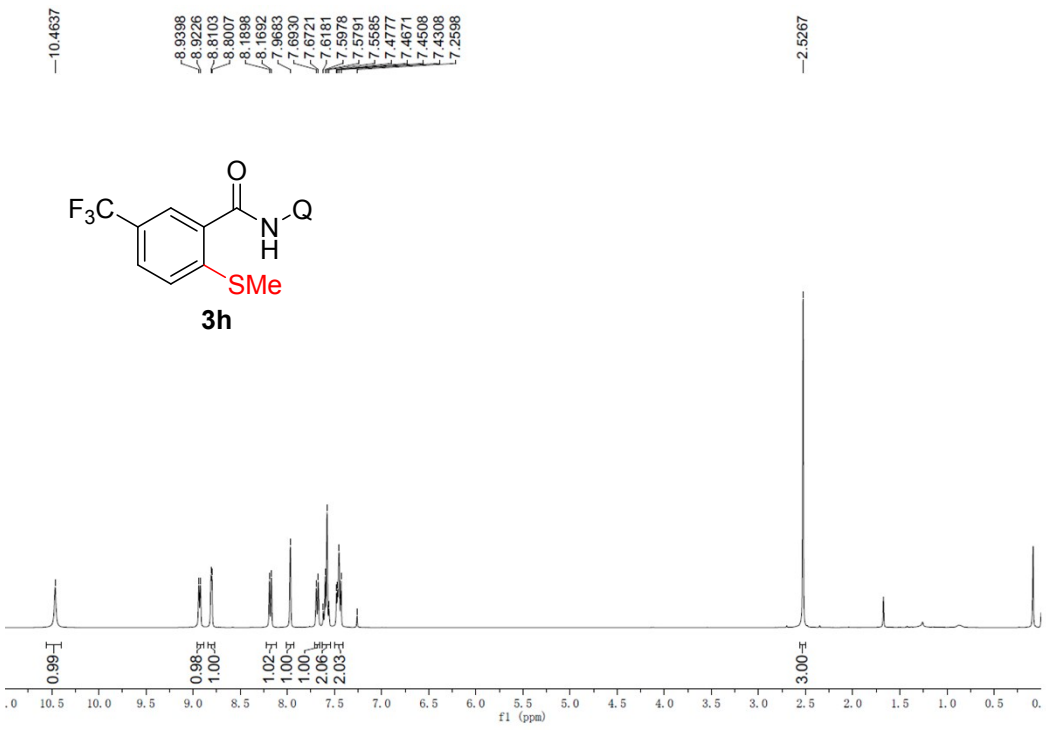
3f


10.4582
8.9373
8.9201
8.8140
8.1911
8.1708
7.7307
7.6133
7.5933
7.5738
7.5530
7.4765
7.4670
7.4573
7.4345
7.4129
7.3262
7.3050
7.2604
2.4853
Cl
O
N
Q
H
SMe
0.92
1.01
0.97
1.00
0.91
2.15
2.07
0.92
2.91
f1 (ppm)

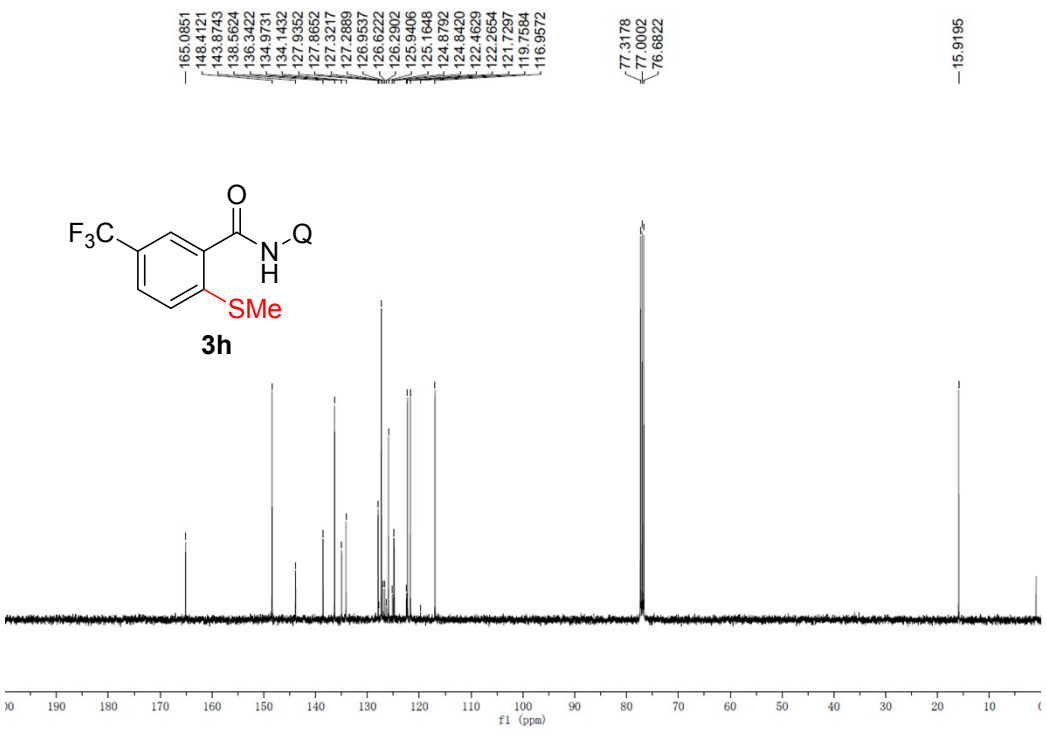
3g


165.0684
148.3569
138.5832
136.9006
136.6530
136.3433
134.2542
130.9950
130.8265
128.3855
128.1269
127.9393
127.3551
122.1600
121.7012
116.9364
77.3173
76.9995
76.6819
16.7411
Cl
O
N
Q
H
SMe
f1 (ppm)

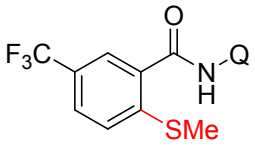
3g


10.4637
8.9398
8.9226
8.8103
8.8007
8.1898
8.1692
7.9683
7.6930
7.6721
7.6181
7.5978
7.5791
7.5585
7.4777
7.4671
7.4508
7.4308
7.2598
2.5267
F3C
O
N
H
Q
SMe
0.99
0.98
1.00
1.02
1.00
1.00
2.06
2.03
3.00
f1 (ppm)

3h

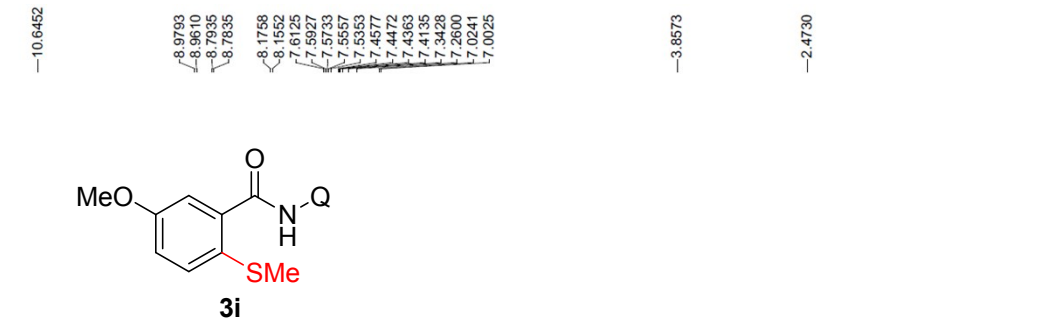

165.0851
148.4121
143.8743
138.5624
136.3422
134.9731
134.1432
127.9352
127.8652
127.3217
127.2889
126.9537
126.6222
126.2902
125.9406
125.1648
124.8792
124.8420
122.4629
122.2654
121.7297
119.7584
116.9572
77.3178
77.0002
76.6822
15.9195
F3C
O
N
H
Q
SMe
f1 (ppm)

3h


O
F3C
N
H
Q
SMe

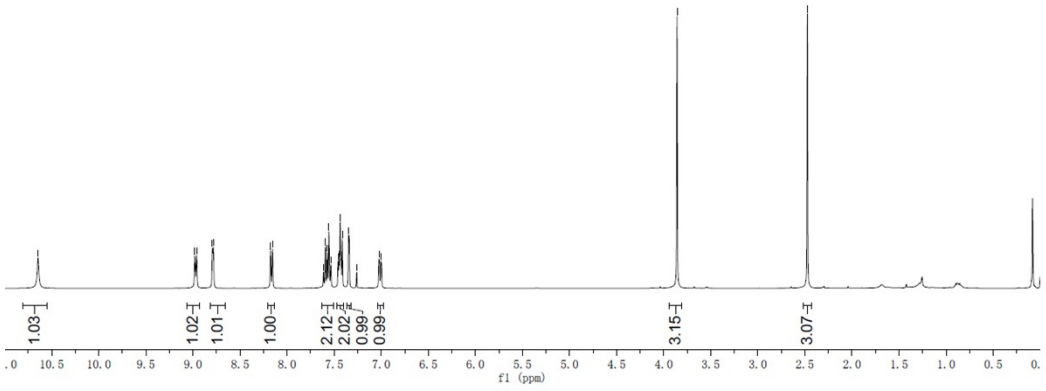
3h

-62.3155
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)

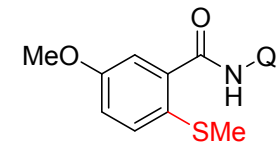

10.6452
8.9793
8.9610
8.7935
8.7835
8.1758
8.1552
7.6125
7.5927
7.5733
7.5557
7.5353
7.4577
7.4472
7.4363
7.4135
7.3428
7.2600
7.0241
7.0025
3.8573
2.4730

O
MeO
N
H
Q
SMe

3i

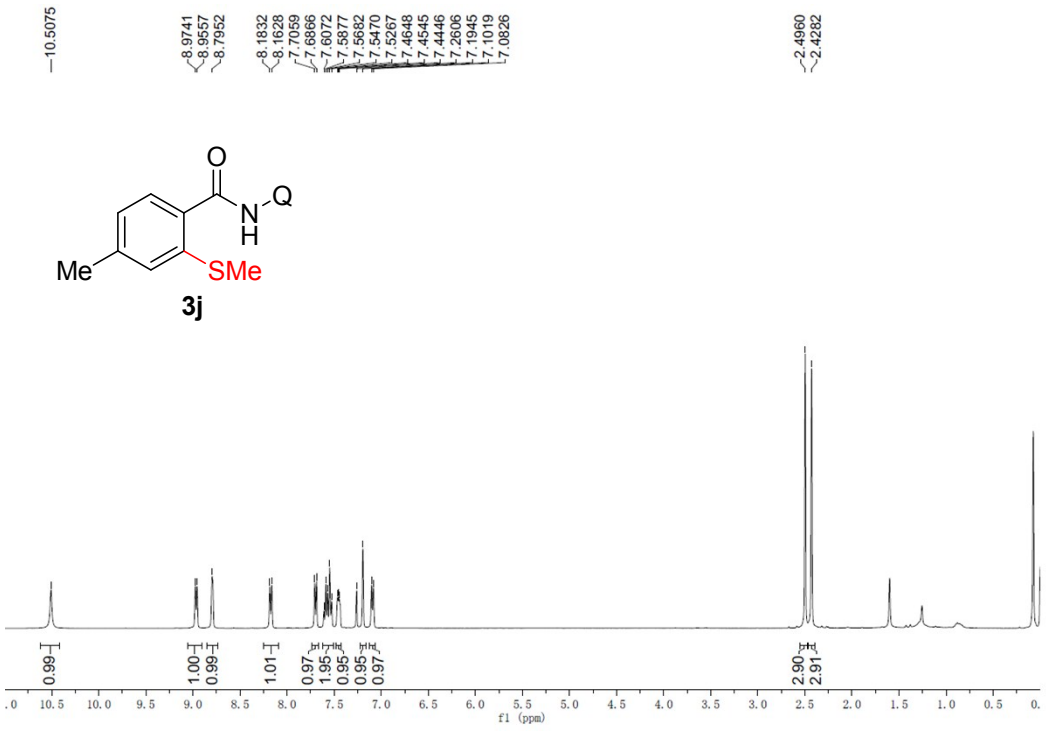

1.03
1.02
1.01
1.00
2.12
2.02
0.99
0.99
3.15
3.07
f1 (ppm)


166.3170
158.2537
148.2542
138.6992
138.4523
136.2517
134.6183
131.9111
127.9662
127.3725
127.2694
121.8990
121.6006
117.0627
116.8496
113.9893
77.3183
77.0005
76.6828
55.5733
18.7307

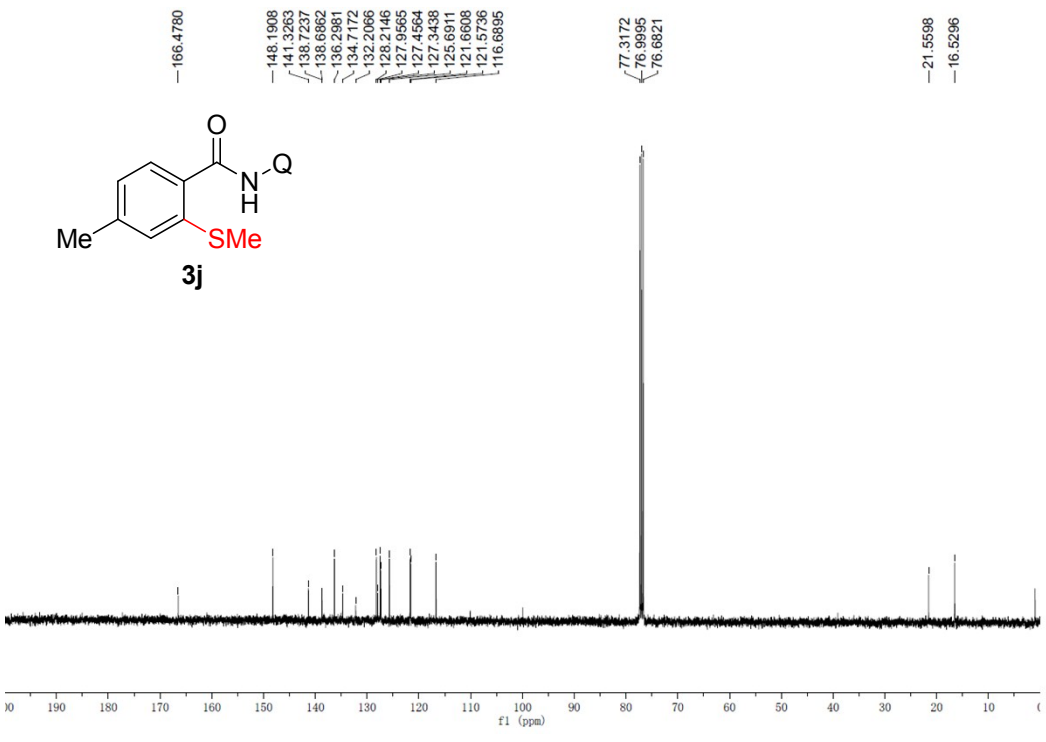

O
MeO
N
H
Q
SMe

3i

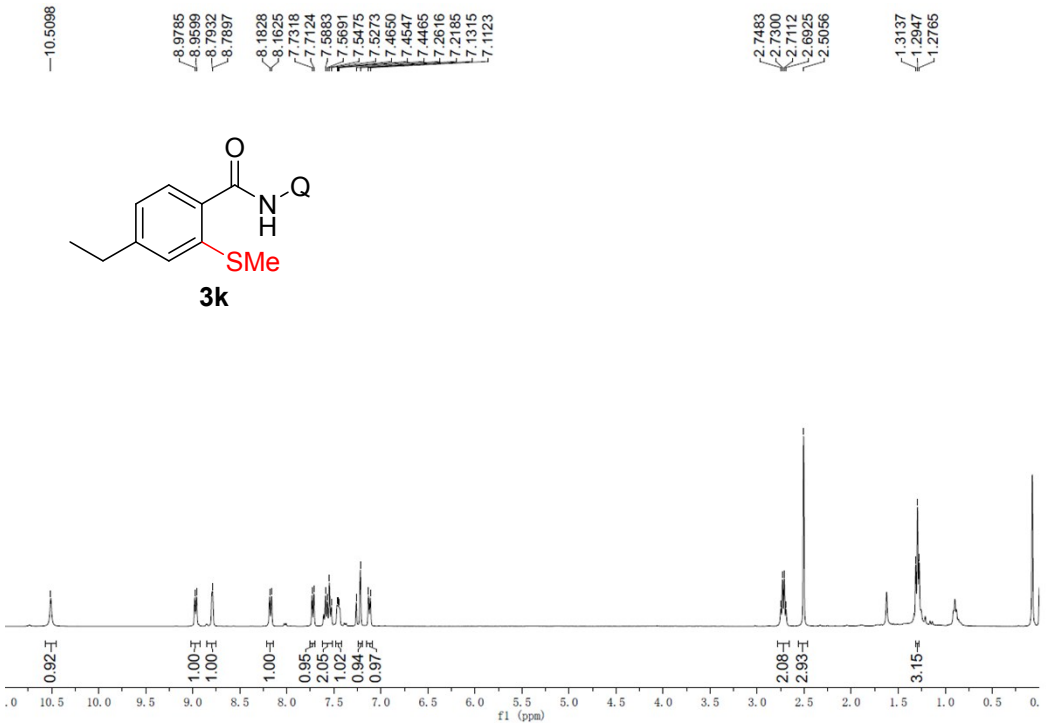
f1 (ppm)


10.5075
8.9741
8.9557
8.7952
8.1832
8.1628
7.7059
7.6866
7.6072
7.5877
7.5682
7.5470
7.5267
7.4648
7.4545
7.4446
7.2606
7.1945
7.1019
7.0826
2.4960
2.4282
O
N
Q
H
Me
SMe
0.99
1.00
0.99
1.01
0.97
1.95
0.95
0.95
0.97
2.90
2.91
f1 (ppm)

3j


166.4780
148.1908
141.3263
138.7237
138.6862
136.2981
134.7172
132.2066
128.2146
127.9565
127.4564
127.3438
125.6911
121.6608
121.5736
116.6895
77.3172
76.9995
76.6821
21.5598
16.5296
O
N
Q
H
Me
SMe
f1 (ppm)

3j


10.5098
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8.9599
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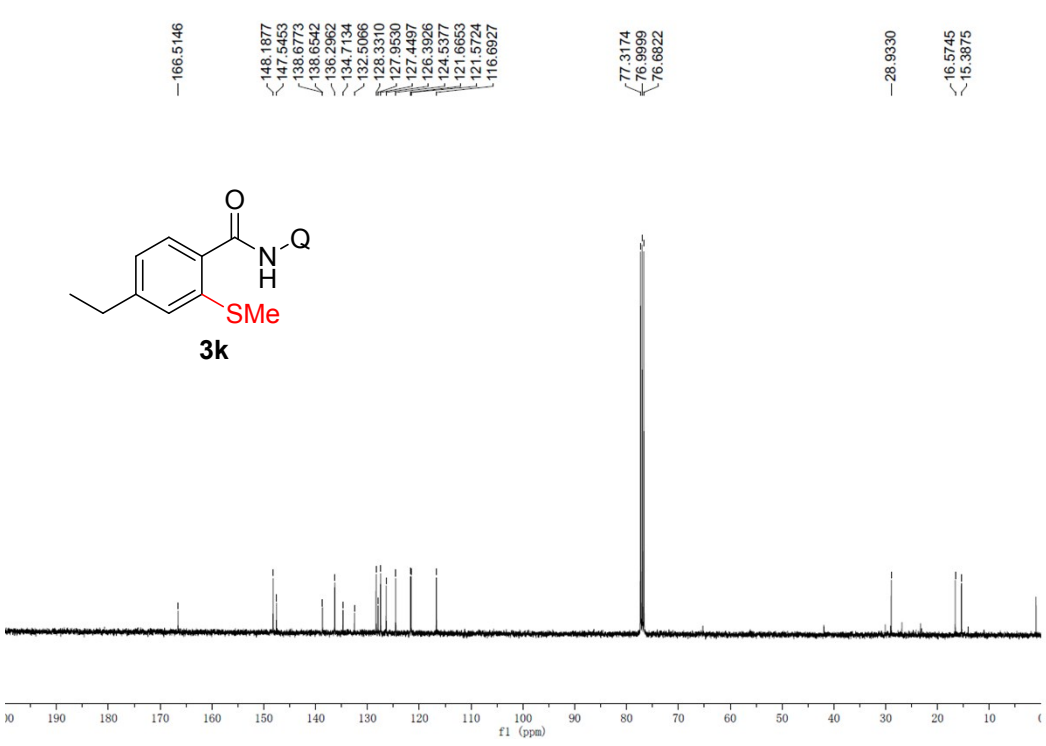
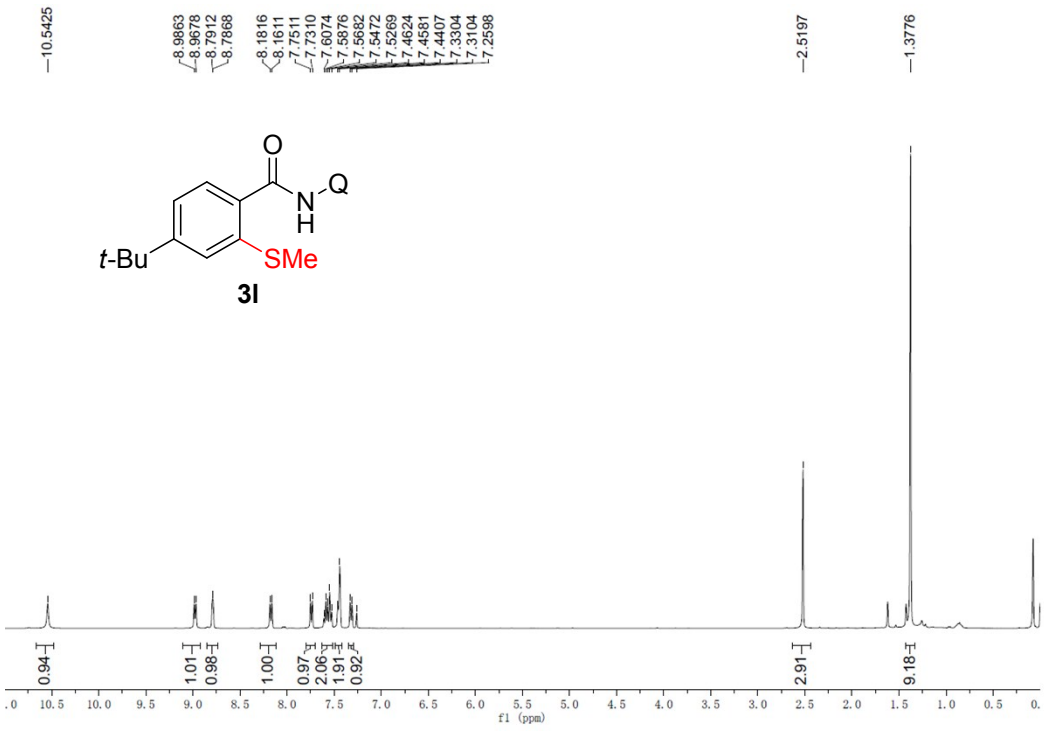
8.7897
8.1828
8.1625
7.7318
7.7124
7.5883
7.5691
7.5475
7.5273
7.4650
7.4547
7.4465
7.2616
7.2185
7.1315
7.1123
2.7483
2.7300
2.7112
2.6925
2.5056
1.3137
1.2947
1.2765
O
N
H
Q
SMe
0.92
1.00
1.00
1.00
0.95
2.05
1.02
0.94
0.97
2.08
2.93
3.15
f1 (ppm)

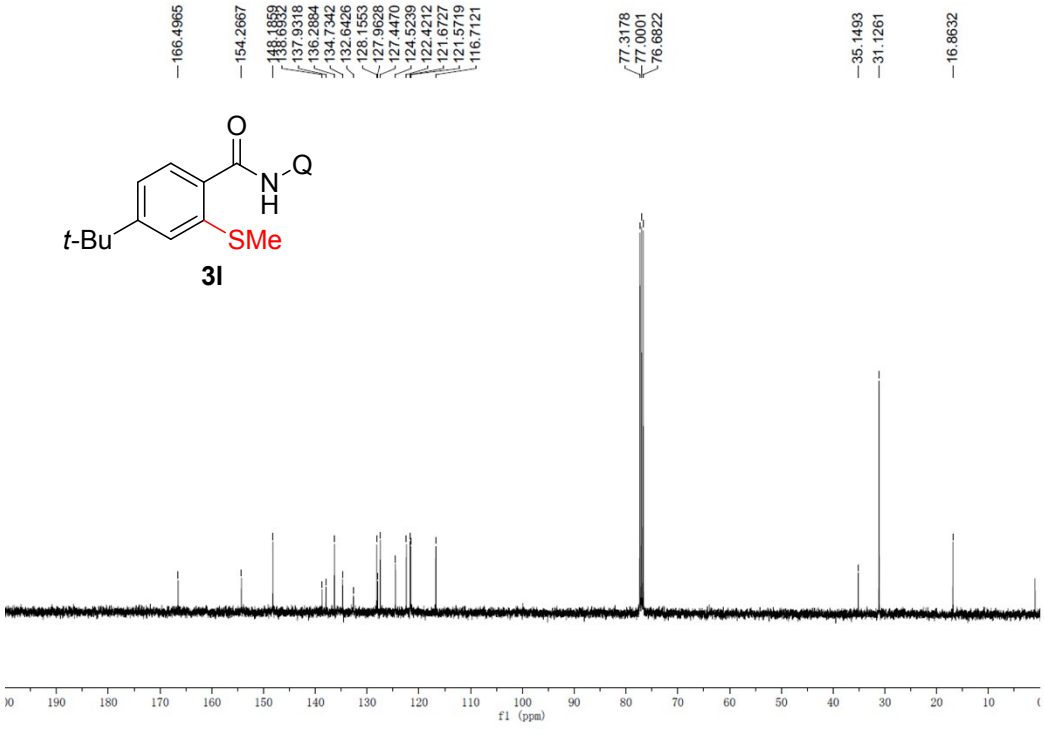
3k


166.5146
148.1877
147.5453
138.6773
138.6542
136.2962
134.7134
132.5066
128.3310
127.9530
127.4497
126.3926
124.5377
121.6653
121.5724
116.6927
77.3174
76.9999
76.6822
28.9330
16.5745
15.3875
O
N
H
Q
SMe
f1 (ppm)

3k


10.5425
8.9863
8.9678
8.7912
8.7868
8.1816
8.1611
7.7511
7.7310
7.6074
7.5876
7.5682
7.5472
7.5269
7.4624
7.4581
7.4407
7.3304
7.3104
7.2598
2.5197
1.3776
O
N
H
Q
t-Bu
SMe
0.94
1.01
0.98
1.00
0.97
2.06
1.91
0.92
2.91
9.18
f1 (ppm)

3l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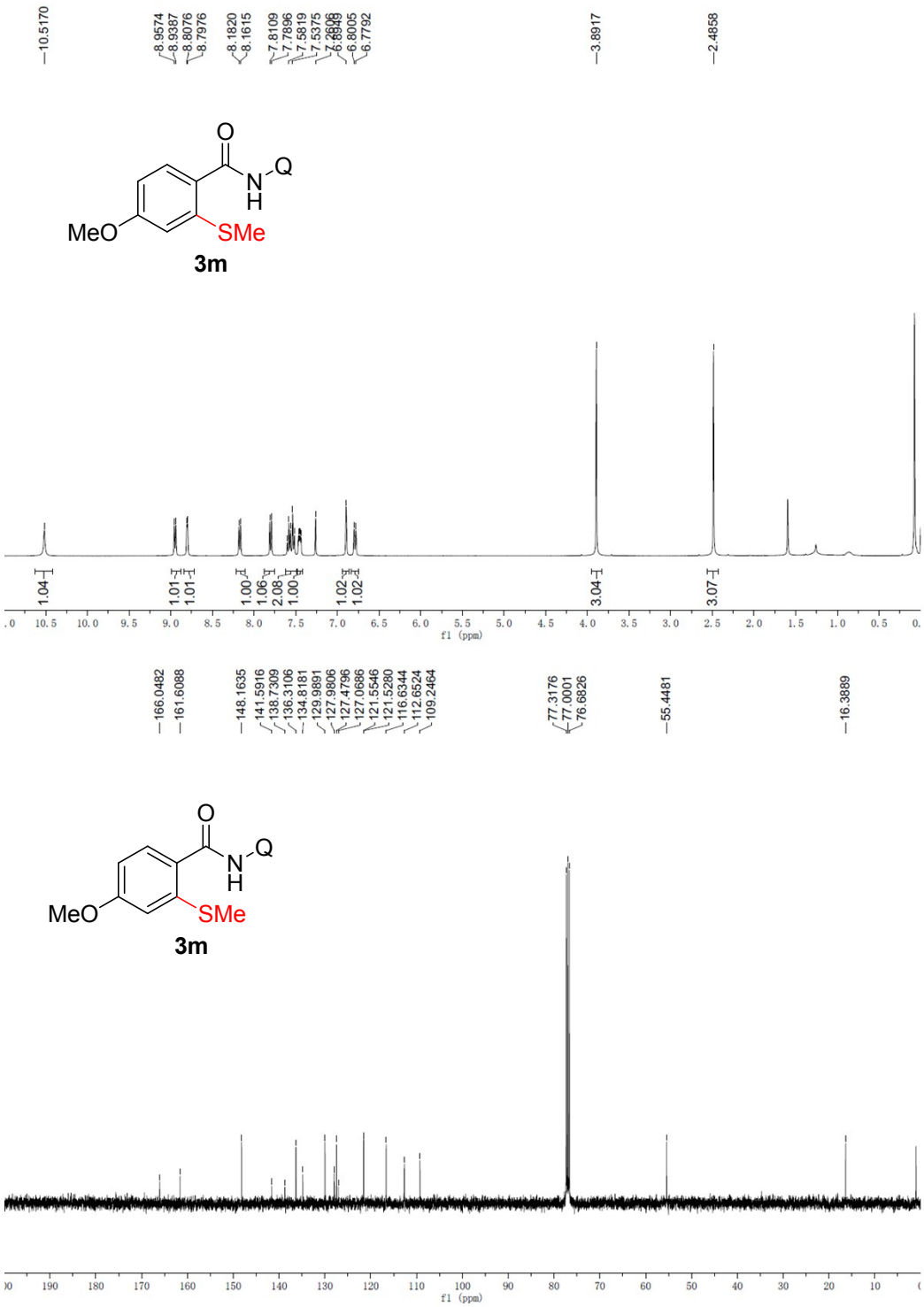
154.2667
148.1859
138.6932
137.9318
136.2884
134.7342
132.6426
128.1553
127.9628
127.4470
124.5239
122.4212
121.6727
121.5719
116.7121
77.3178
77.0001
76.6822
35.1493
31.1261
16.8632
O
N
H
Q
t-Bu
SMe
f1 (ppm)

3l


10.5170
8.9574
8.9387
8.8076
8.7976
8.1820
8.1615
7.8109
7.7896
7.5819
7.5375
7.2606
6.8949
6.8005
6.7792
3.8917
2.4858
O
N
H
Q
MeO
SMe
3m
1.04
1.01
1.01
1.00
1.06
2.08
1.00
1.02
1.02
3.04
3.07
f1 (ppm)
166.0482
161.6088
148.1635
141.5916
138.7309
136.3106
134.8181
129.9891
127.9806
127.4796
127.0686
121.5546
121.5280
116.6344
112.6524
109.2464
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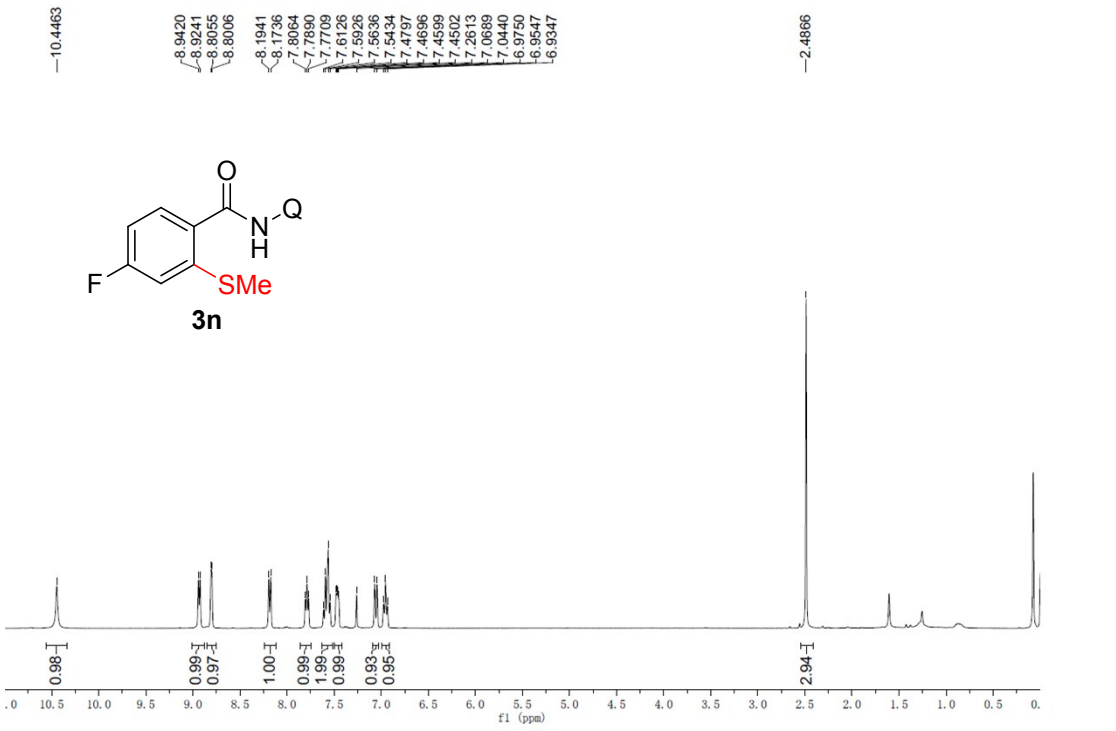
77.0001
76.6826
55.4481
16.3889
O
N
H
Q
MeO
SMe
3m
f1 (ppm)


10.4463
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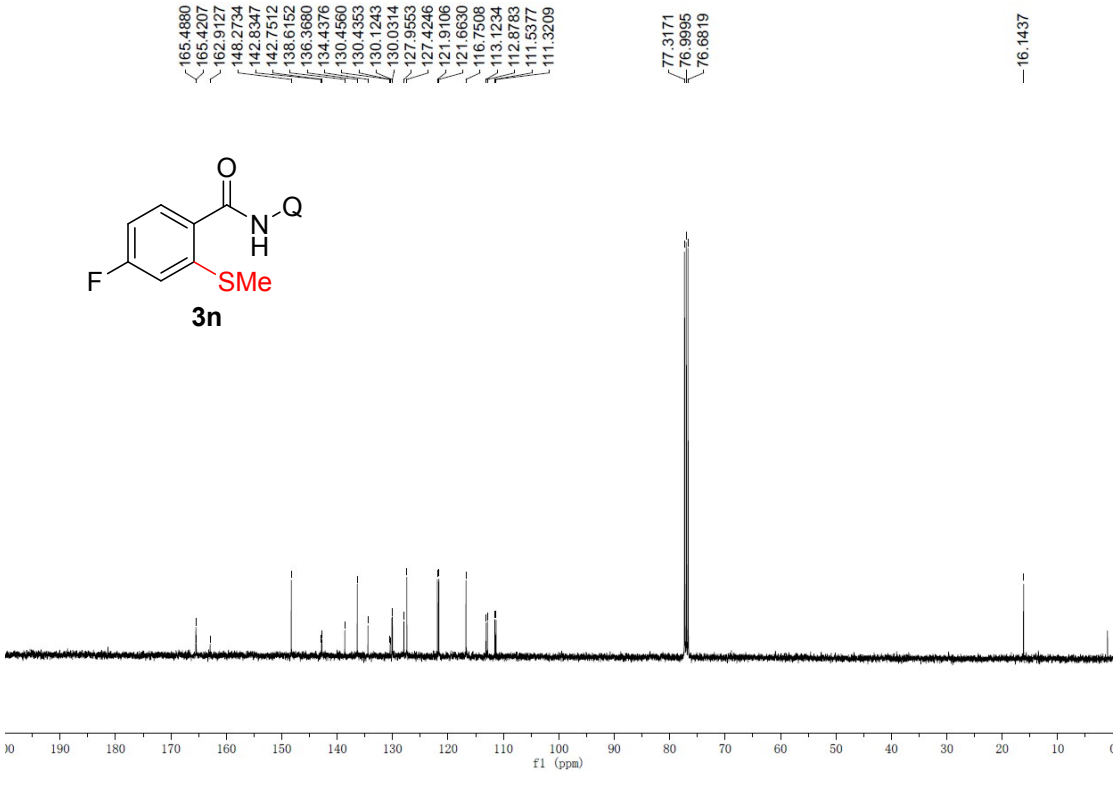
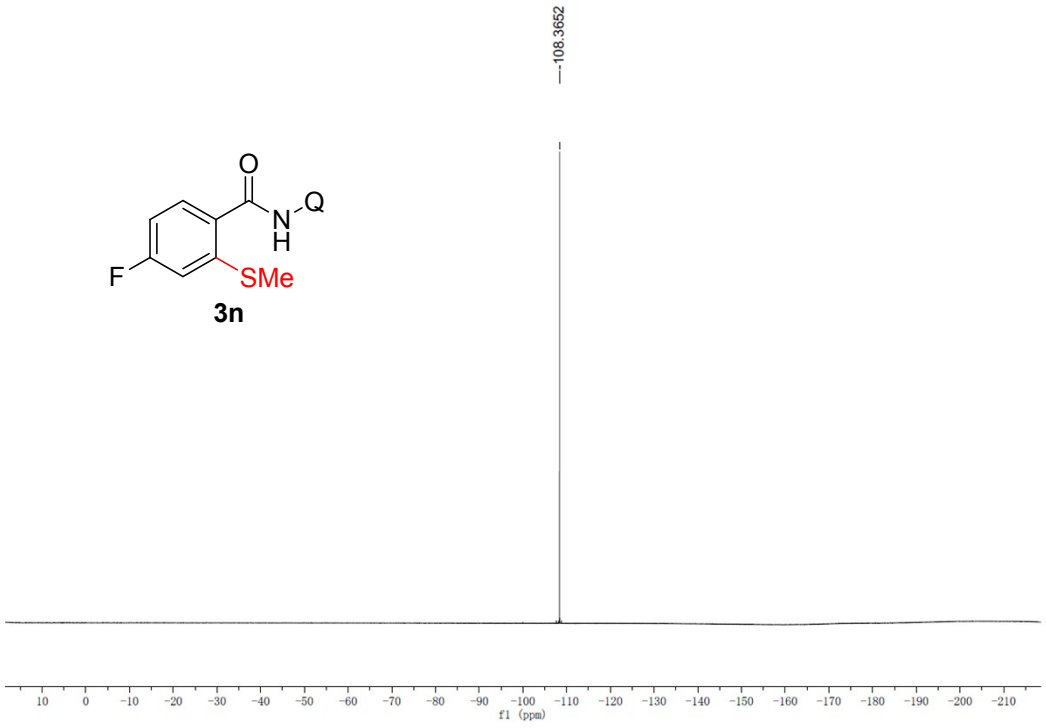
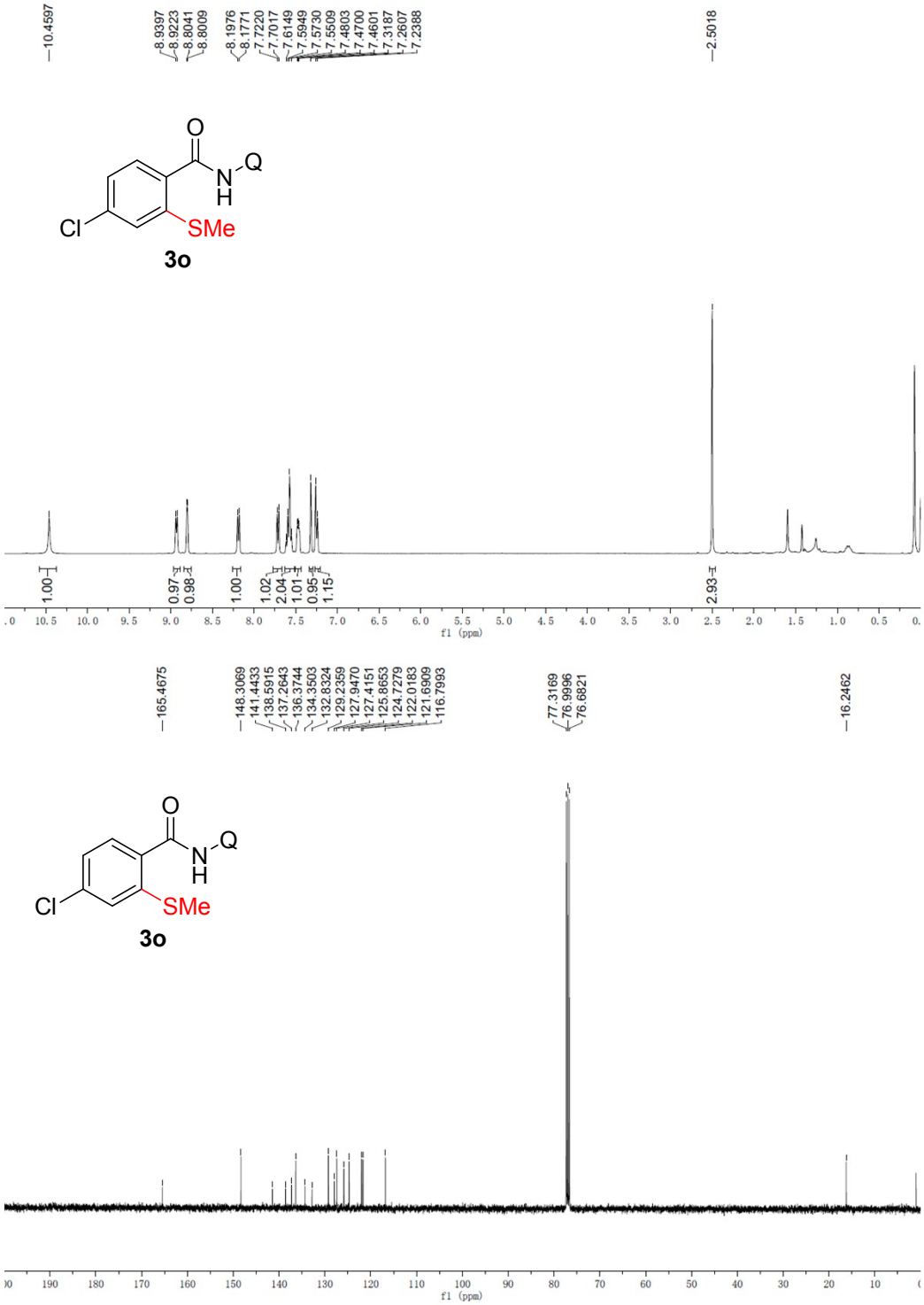
8.9241
8.8055
8.8006
8.1941
8.1736
7.8064
7.7890
7.7709
7.6126
7.5926
7.5636
7.5434
7.4797
7.4696
7.4599
7.4502
7.2613
7.0689
7.0440
6.9750
6.9547
6.9347
2.4866
O
N
Q
H
F
SMe
3n
0.98
0.99
0.97
1.00
0.99
1.99
0.99
0.93
0.95
2.94
f1 (ppm)


165.4880
165.4207
162.9127
148.2734
142.8347
142.7512
138.6152
136.3680
134.4376
130.4560
130.4353
130.1243
130.0314
127.9553
127.4246
121.9106
121.6630
116.7508
113.1234
112.8783
111.5377
111.3209
77.3171
76.9995
76.6819
16.1437
O
N
Q
H
F
SMe
3n
f1 (ppm)


-108.3652
O
N
H
Q
F
SMe
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)

3n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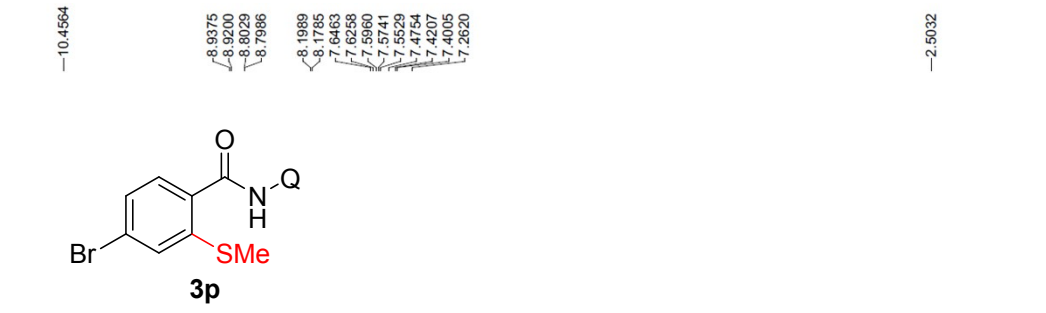
8.9223
8.8041
8.8009
8.1976
8.1771
7.7220
7.7017
7.6149
7.5949
7.5730
7.5509
7.4803
7.4700
7.4601
7.3187
7.2607
7.2388
2.5018
O
N
Q
H
Cl
SMe
3o
1.00
0.97
0.98
1.00
1.02
2.04
1.01
0.95
1.15
2.93
f1 (ppm)
165.4675
148.3069
141.4433
138.5915
137.2643
136.3744
134.3503
132.8324
129.2359
127.9470
127.4151
125.8653
124.7279
122.0183
121.6909
116.7993
77.3169
76.9996
76.6821
16.2462
O
N
Q
H
Cl
SMe
3o
f1 (ppm)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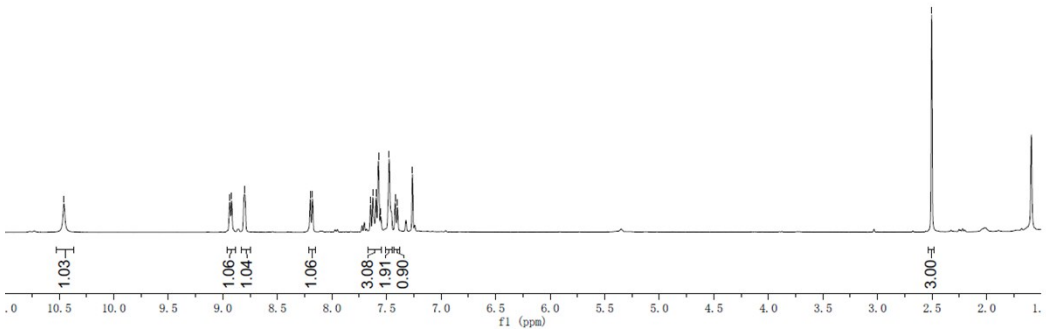
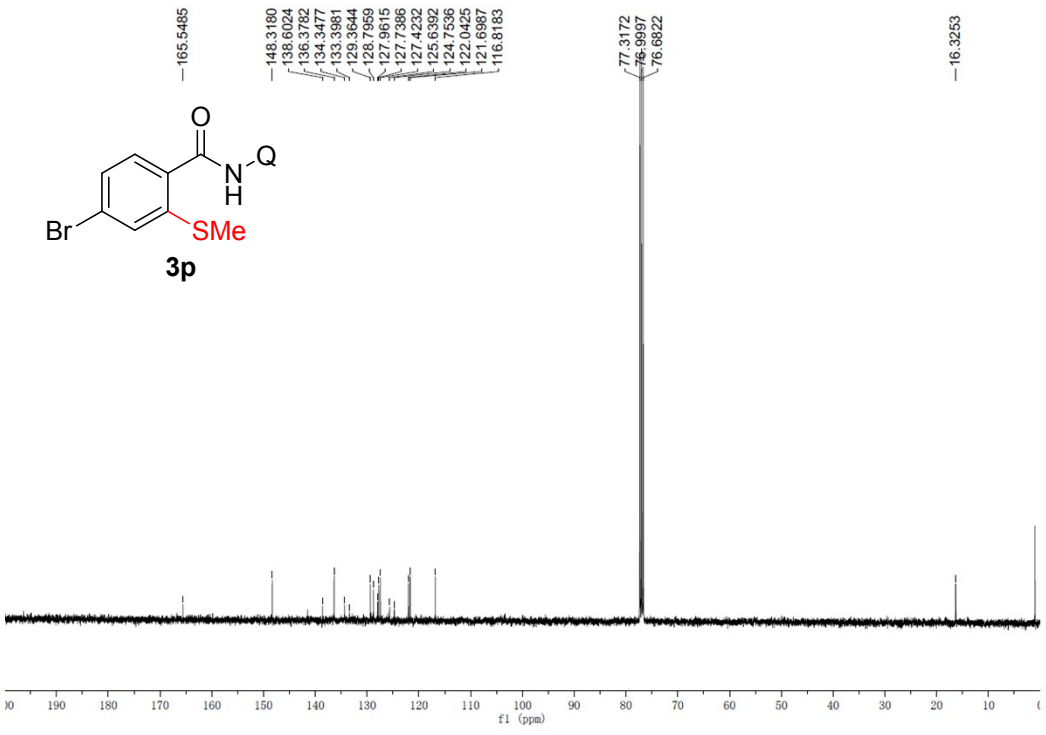
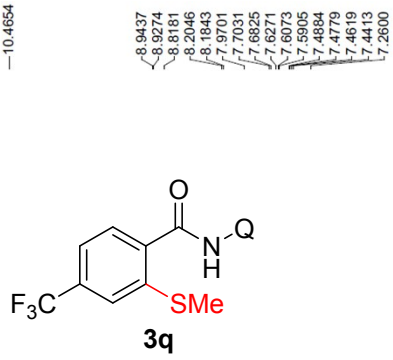
8.9375
8.9200
8.8029
8.7986
8.1989
8.1785
7.6463
7.6258
7.5960
7.5741
7.5529
7.4754
7.4207
7.4005
7.2620
2.5032
O
N
H
Q
Br
SMe

3p

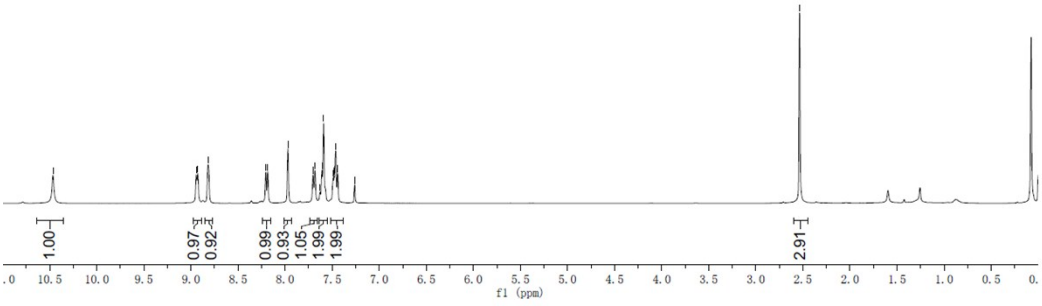

1.03
1.06
1.04
1.06
3.08
1.91
0.90
3.00
f1 (ppm)

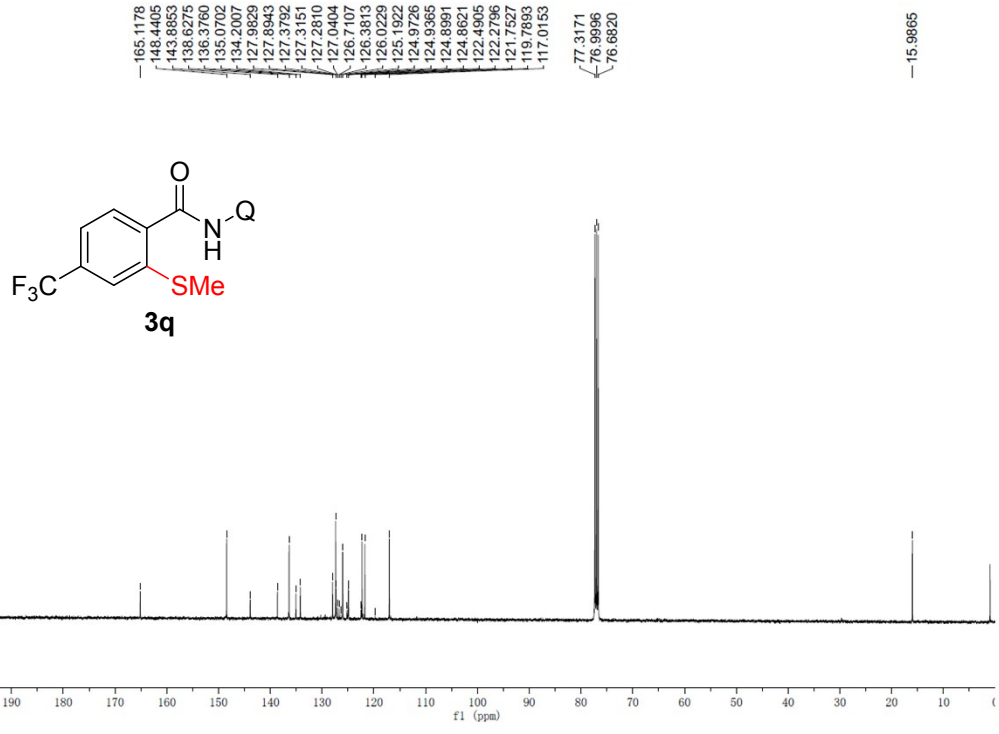

165.5485
148.3180
138.6024
136.3782
134.3477
133.3961
129.3644
128.7959
127.9615
127.7386
127.4232
125.6392
124.7536
122.0425
121.6987
116.8183
77.3172
76.9997
76.6822
16.3253
O
N
H
Q
Br
SMe
f1 (ppm)

3p

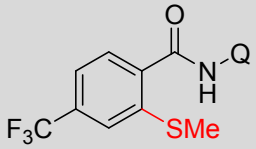

10.4654
8.9437
8.9274
8.8181
8.2046
8.1843
7.9701
7.7031
7.6825
7.6271
7.6073
7.5905
7.4884
7.4779
7.4619
7.4413
7.2600
2.5346
O
N
Q
H
F3C
SMe

3q

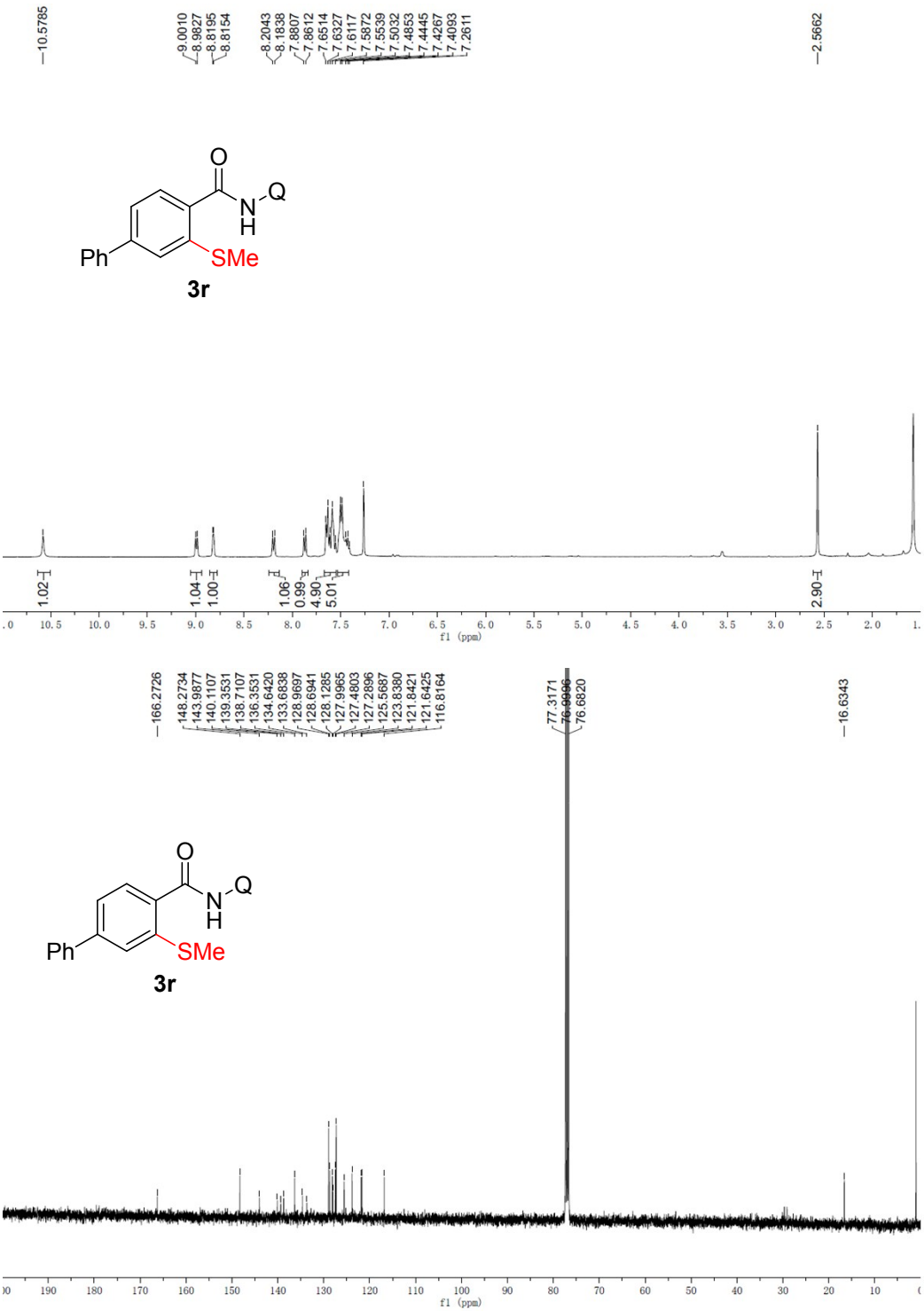

1.00
0.97
0.92
0.99
0.93
1.05
1.99
1.99
2.91
f1 (ppm)


165.1178
148.4405
143.8853
138.6275
136.3760
135.0702
134.2007
127.9829
127.8943
127.3792
127.3151
127.2810
127.0404
126.7107
126.3813
126.0229
125.1922
124.9726
124.9365
124.8991
124.8621
122.4905
122.2796
121.7527
119.7893
117.0153
77.3171
76.9996
76.6820
15.9865
O
N
Q
H
F3C
SMe
f1 (ppm)

3q



3q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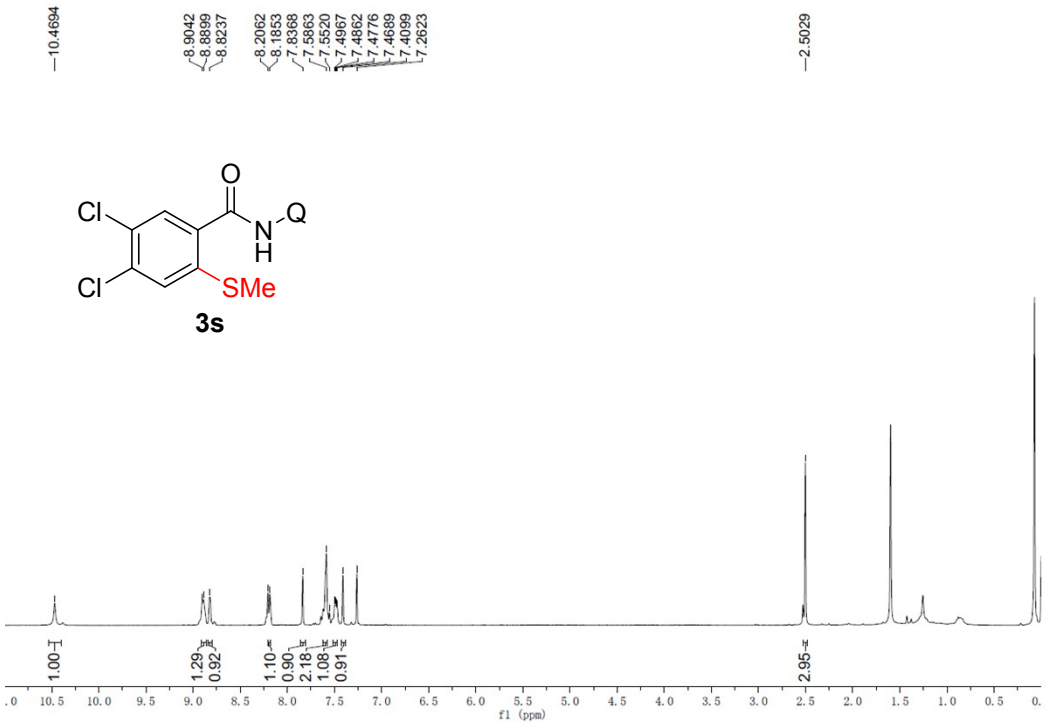
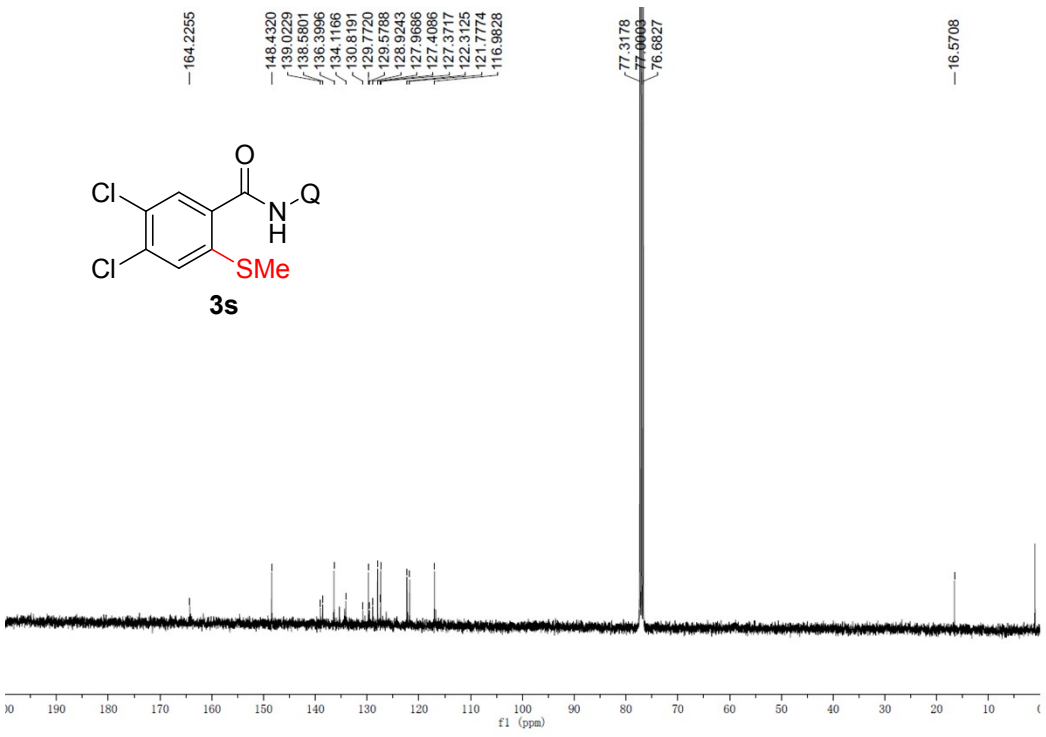
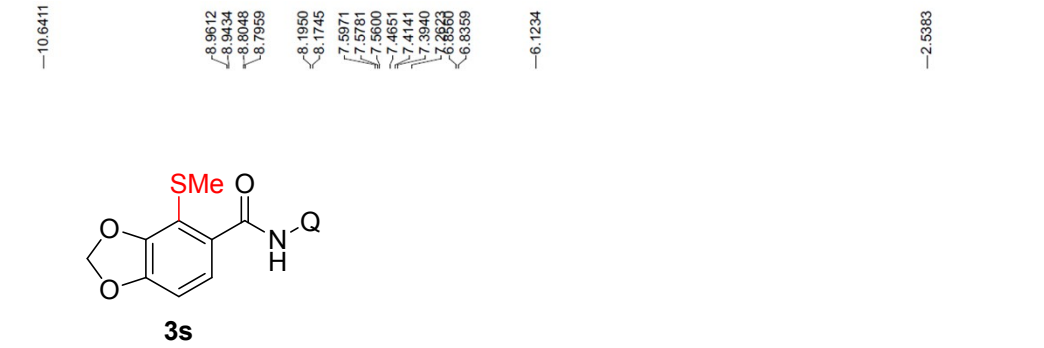
9.0010
8.9827
8.8195
8.8154
8.2043
8.1838
7.8807
7.8612
7.6514
7.6327
7.6117
7.5872
7.5539
7.5032
7.4853
7.4445
7.4267
7.4093
7.2611
2.5662
O
N
H
Q
Ph
SMe
3r
1.02
1.04
1.00
1.06
0.99
4.90
5.01
2.90
f1 (ppm)
166.2726
148.2734
143.9877
140.1107
139.3531
138.7107
136.3531
134.6420
133.6838
128.9697
128.6941
128.1285
127.9965
127.4803
127.2896
125.5687
123.8380
121.8421
121.6425
116.8164
77.3171
76.9996
76.6820
16.6343
O
N
H
Q
Ph
SMe
3r
f1 (ppm)


10.4694
8.9042
8.8899
8.8237
8.2062
8.1853
7.8368
7.5863
7.5520
7.4967
7.4862
7.4776
7.4689
7.4099
7.2623
2.5029
Cl
Cl
O
N
H
Q
SMe
1.00
1.29
0.92
1.10
0.90
2.18
1.08
0.91
2.95
f1 (ppm)

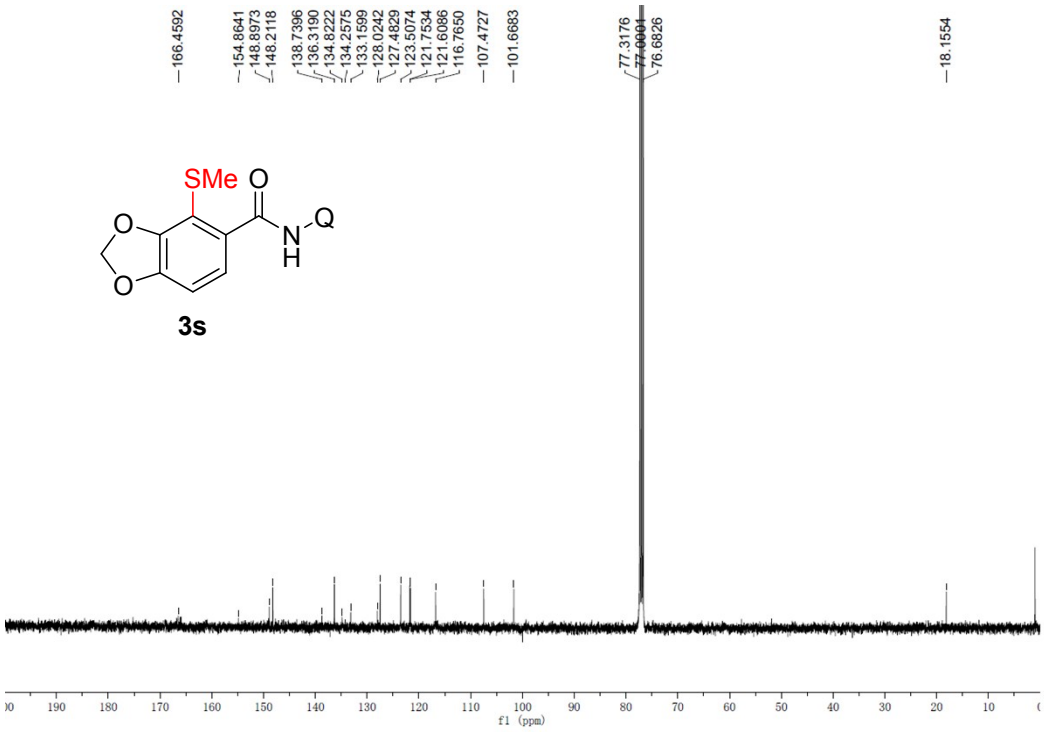
3s


164.2255
148.4320
139.0229
138.5801
136.3996
134.1166
130.8191
129.7720
129.5788
128.9243
127.9686
127.4086
127.3717
122.3125
121.7774
116.9828
77.3178
77.0003
76.6827
16.5708
Cl
Cl
O
N
H
Q
SMe
f1 (ppm)

3s


10.6411
8.9612
8.9434
8.8048
8.7959
8.1950
8.1745
7.5971
7.5781
7.5600
7.4651
7.4141
7.3940
6.8359
6.1234
2.5383
SMe
O
N
H
Q
O
O
1.07
1.03
1.00
1.19
2.12
1.08
1.08
1.08
1.91
2.95
f1 (ppm)

3s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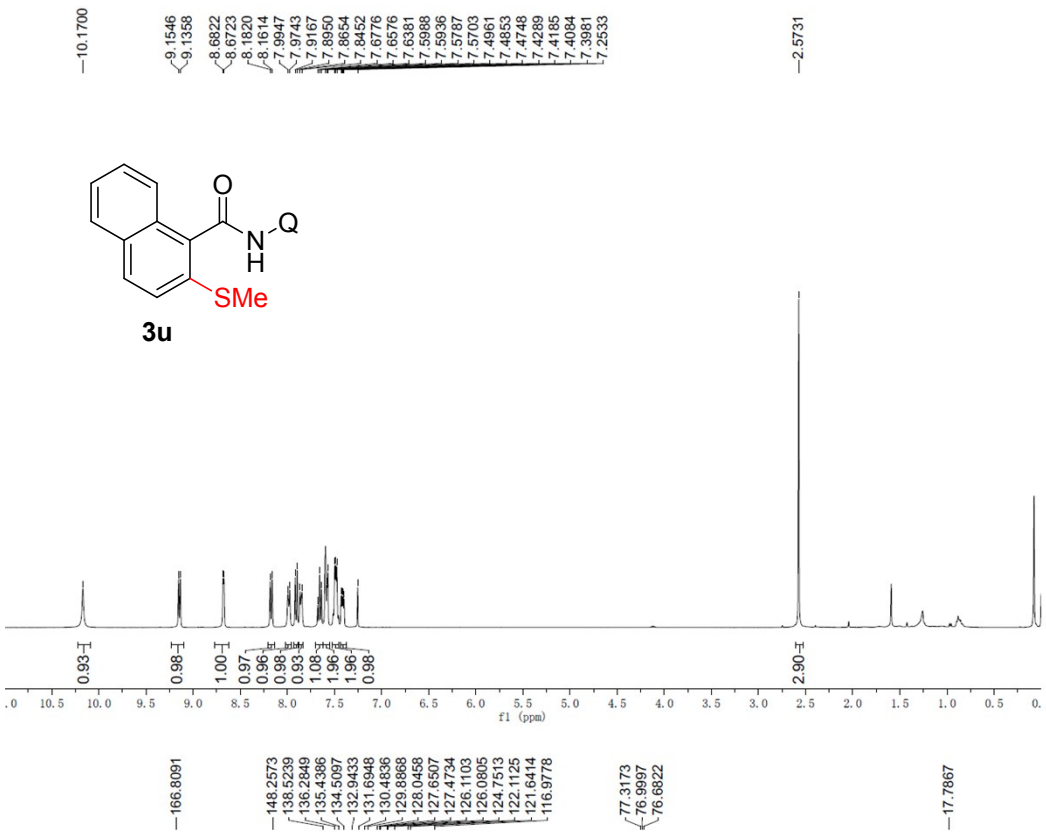
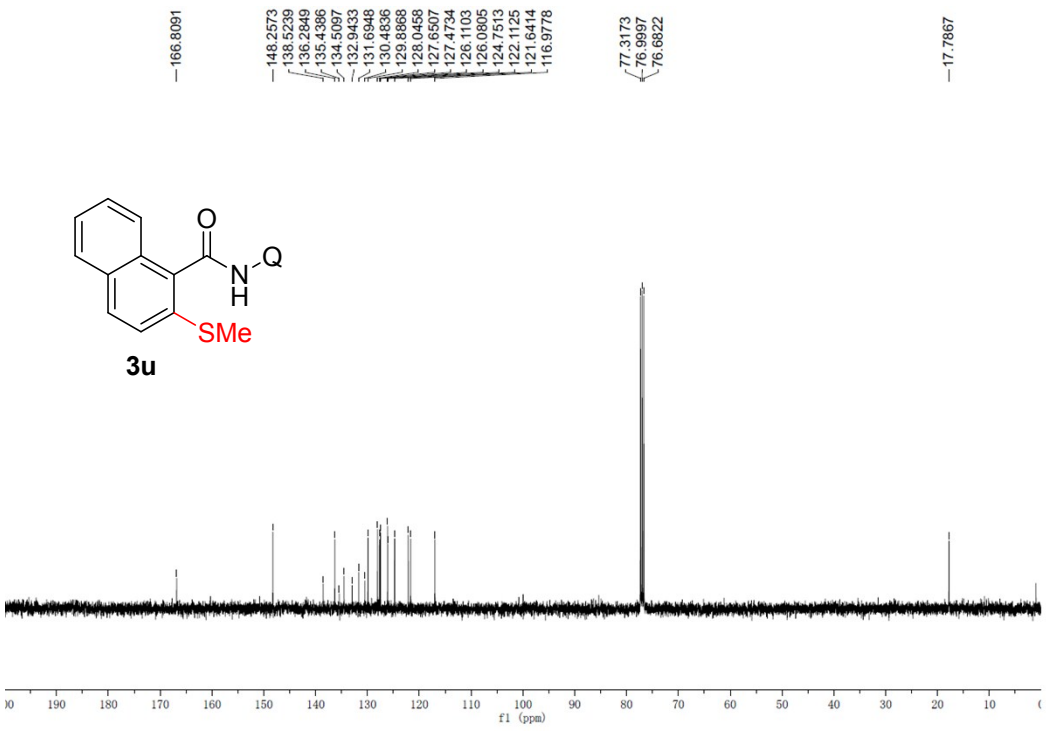
148.8973
148.2118
138.7396
136.3190
134.8222
134.2575
133.1599
128.0242
127.4829
123.5074
121.7534
121.6086
116.7650
107.4727
101.6683
77.3176
77.0001
76.6826
18.1554
SMe
O
N
H
Q
O
O
f1 (ppm)

3s


10.1700
9.1546
9.1358
8.6822
8.6723
8.1820
8.1614
7.9947
7.9743
7.9167
7.8950
7.8654
7.8452
7.6776
7.6576
7.6381
7.5988
7.5936
7.5787
7.5703
7.4961
7.4853
7.4748
7.4289
7.4185
7.4084
7.3981
7.2533
2.5731
O
N
H
Q
SMe
0.93
0.98
1.00
0.97
0.96
0.98
0.93
1.08
1.96
1.96
0.98
2.90
f1 (ppm)

3u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138.5239
136.2849
135.4386
134.5097
132.9433
131.6948
130.4836
129.8868
128.0458
127.6507
127.4734
126.1103
126.0805
124.7513
122.1125
121.6414
116.9778
77.3173
76.9997
76.6822
17.7867
O
N
H
Q
SMe
f1 (ppm)

3u


10.5737
9.0219
9.0038
8.8060
8.2516
8.2079
8.1876
7.9222
7.9021
7.8253
7.8050
7.7297
7.6459
7.6257
7.6060
7.5878
7.5714
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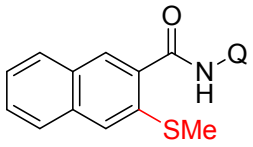
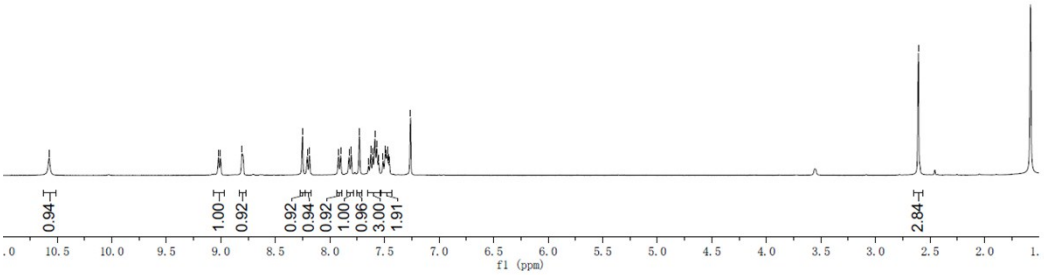
7.5130
7.4927
7.4829
7.4747
7.4630
7.4541
7.2612
2.6068


O
N
H
Q
SMe

3v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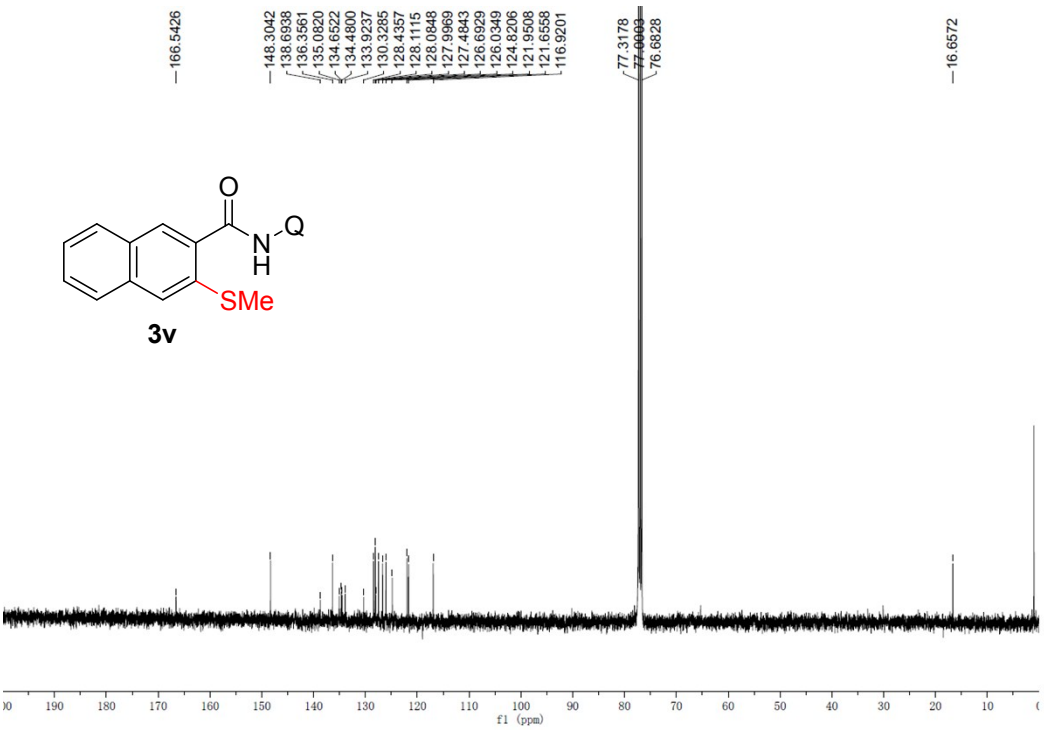
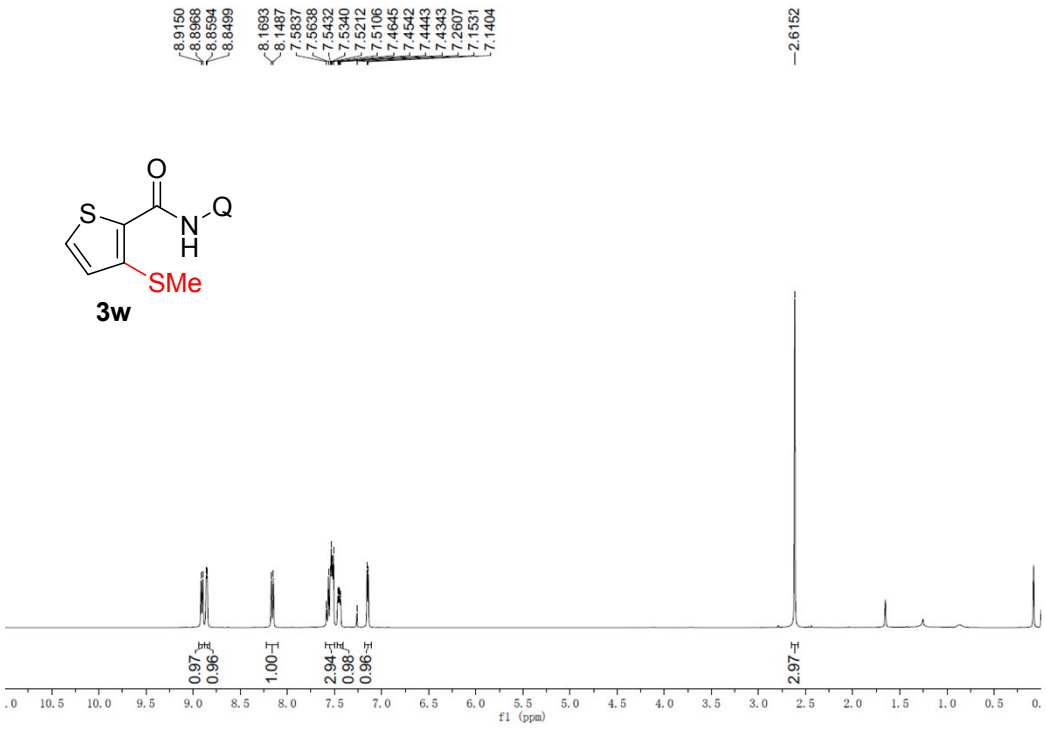
1.00
0.92
0.92
0.94
0.92
1.00
0.96
3.00
1.91
2.84
f1 (ppm)


166.5426
148.3042
138.6938
136.3561
135.0820
134.6522
134.4800
133.9237
130.3285
128.4357
128.1115
128.0848
127.9969
127.4843
126.6929
126.0349
124.8206
121.9508
121.6558
116.9201
77.3178
77.0000
76.6828
16.6572
f1 (ppm)

O
N
H
Q
SMe

3v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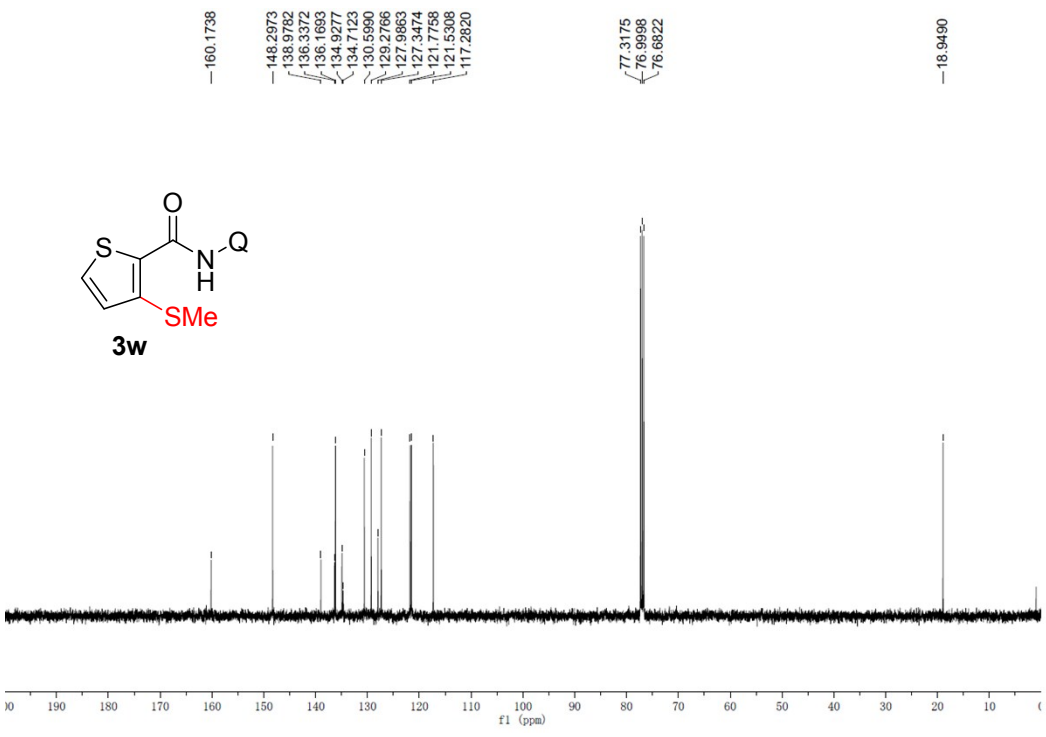
8.8968
8.8594
8.8499
8.1693
8.1487
7.5837
7.5638
7.5432
7.5340
7.5212
7.5106
7.4645
7.4542
7.4443
7.4343
7.2607
7.1531
7.1404
2.6152
O
S
N
H
Q
SMe
0.97
0.96
1.00
2.94
0.98
0.96
2.97
f1 (ppm)

3w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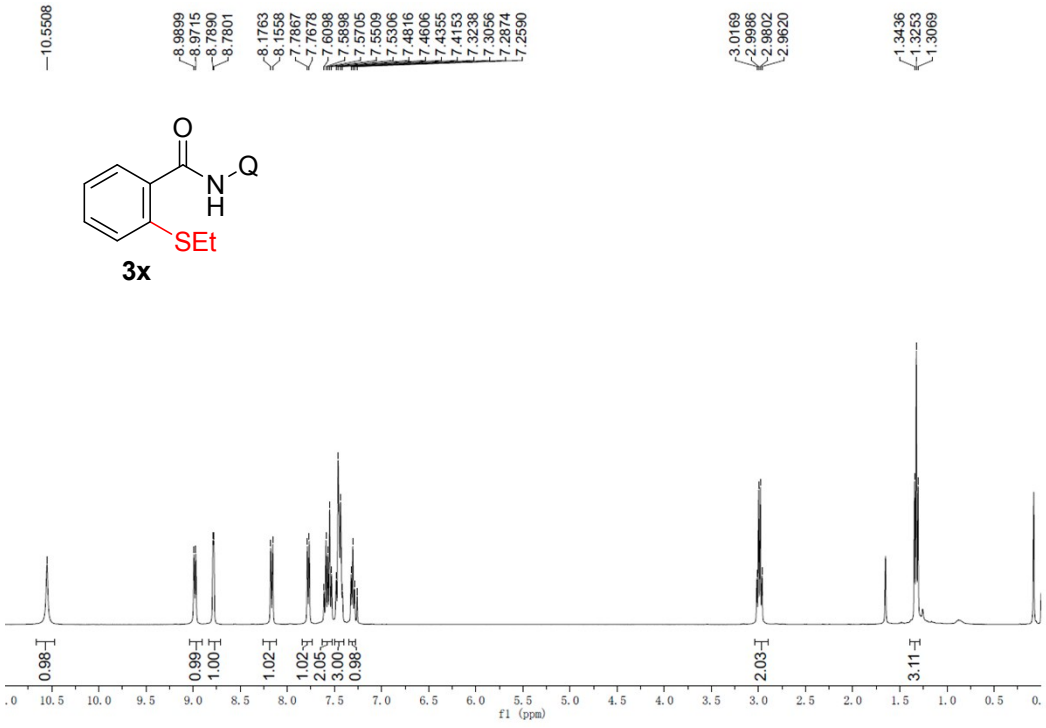
138.9782
136.3372
136.1693
134.9277
134.7123
130.5990
129.2766
127.9863
127.3474
121.7758
121.5308
117.2820
77.3175
76.9998
76.6822
18.9490
O
S
N
H
Q
SMe
f1 (ppm)

3w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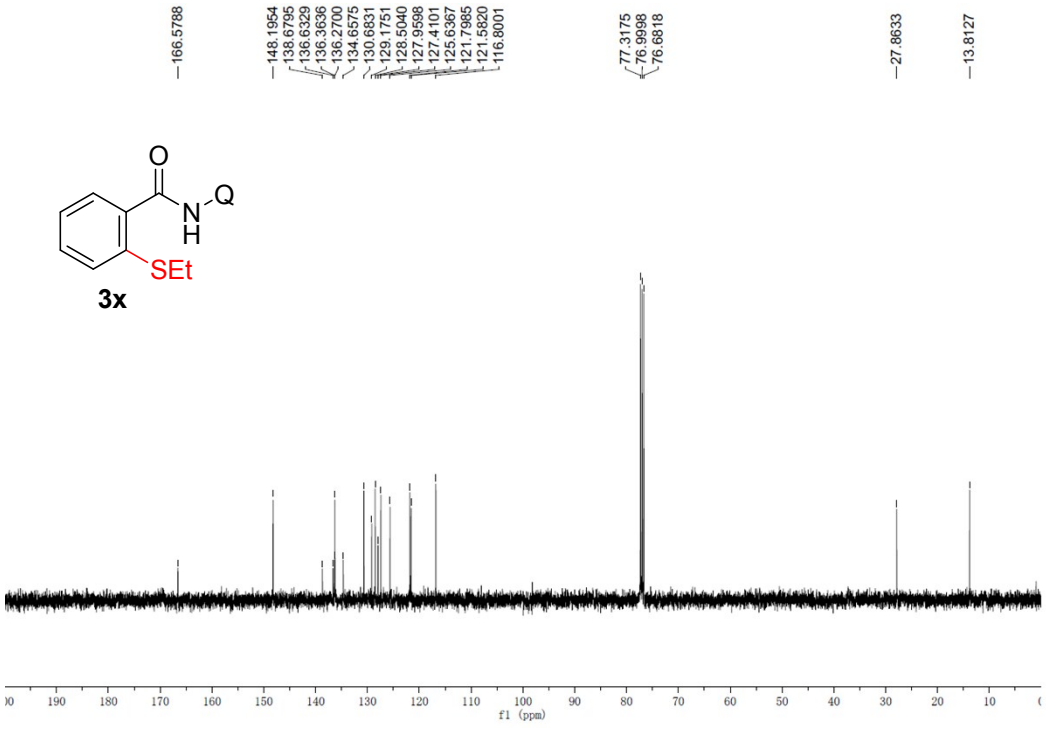
8.9715
8.7890
8.7801
8.1763
8.1558
7.7867
7.7678
7.6098
7.5898
7.5705
7.5509
7.5306
7.4816
7.4606
7.4355
7.4153
7.3238
7.3056
7.2874
7.2590
3.0169
2.9986
2.9802
2.9620
1.3436
1.3253
1.3069
O
N
H
Q
SEt
3x
0.98
0.99
1.00
1.02
1.02
2.05
3.00
0.98
2.03
3.11
f1 (ppm)


166.5788
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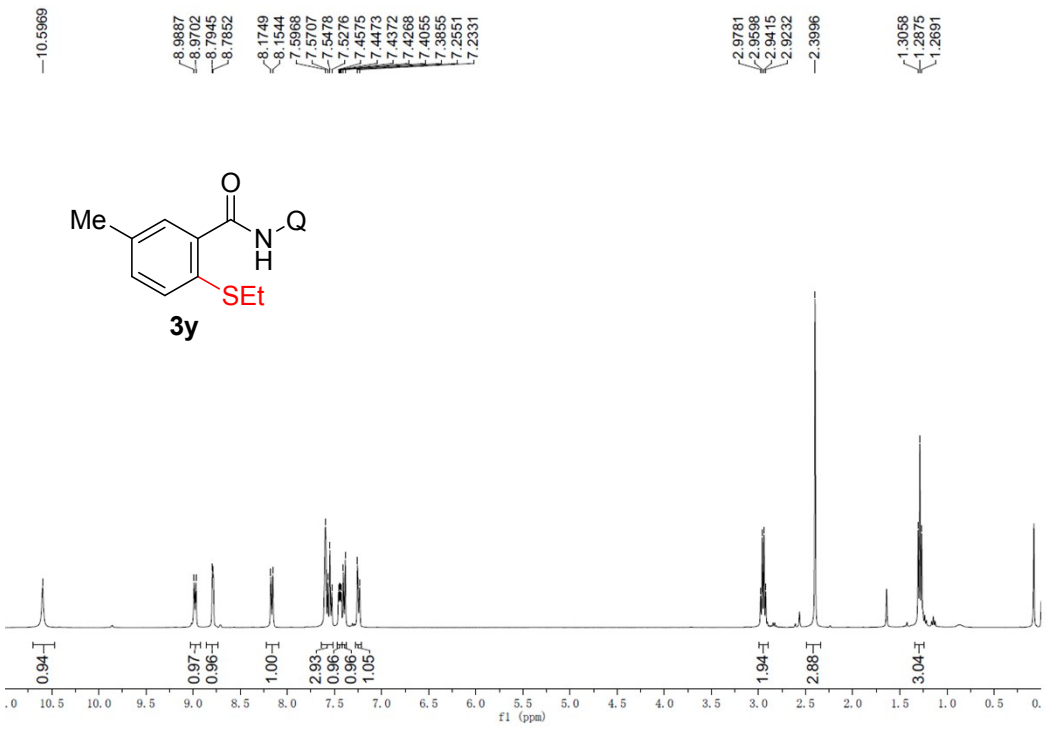
138.6795
136.6329
136.3636
136.2700
134.6575
130.6831
129.1751
128.5040
127.9598
127.4101
125.6367
121.7985
121.5820
116.8001
77.3175
76.9998
76.6818
27.8633
13.8127
O
N
H
Q
SEt
3x
f1 (ppm)


10.5969
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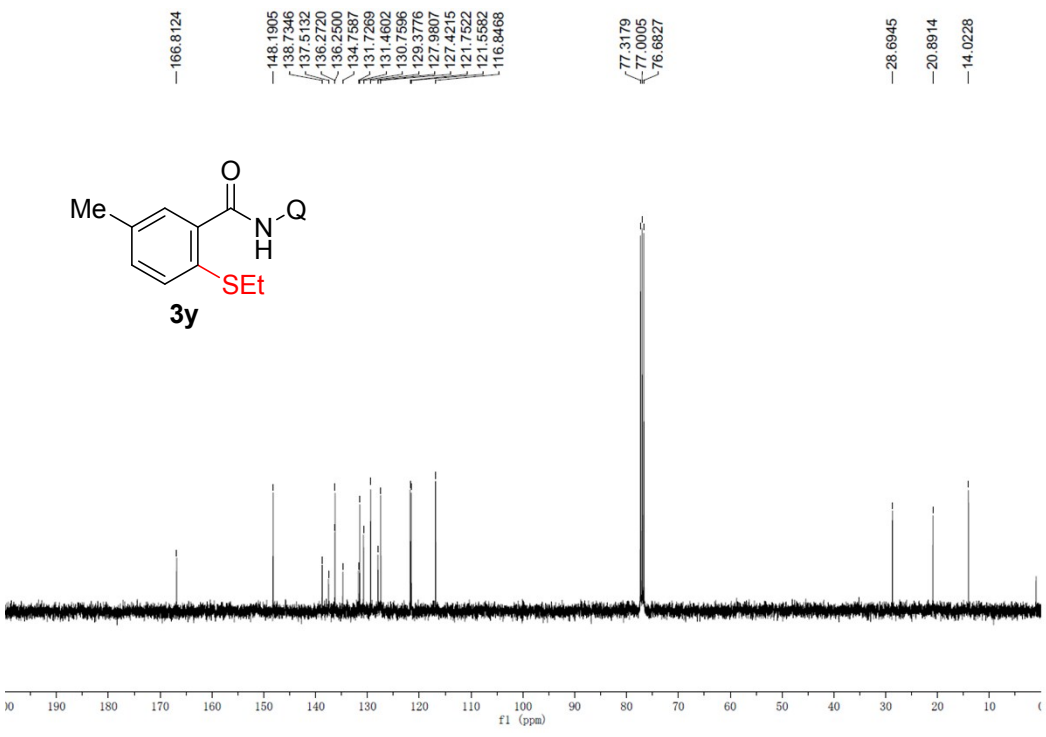
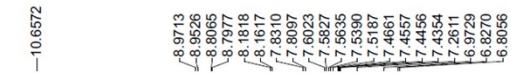
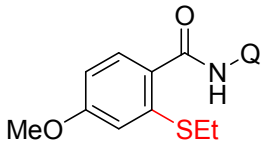
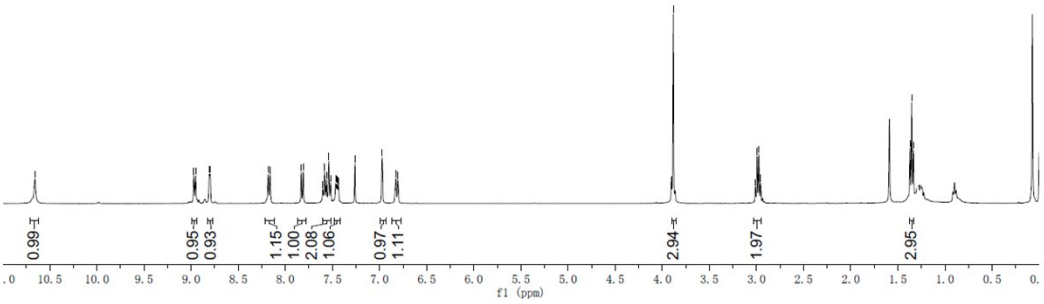
8.9702
8.7945
8.7852
8.1749
8.1544
7.5968
7.5707
7.5478
7.5276
7.4575
7.4473
7.4372
7.4268
7.4055
7.3855
7.2551
7.2331
2.9781
2.9598
2.9415
2.9232
2.3996
1.3058
1.2875
1.2691
Me
O
N
H
Q
SEt
3y
0.94
0.97
0.96
1.00
2.93
0.96
0.96
1.05
1.94
2.88
3.04
f1 (ppm)

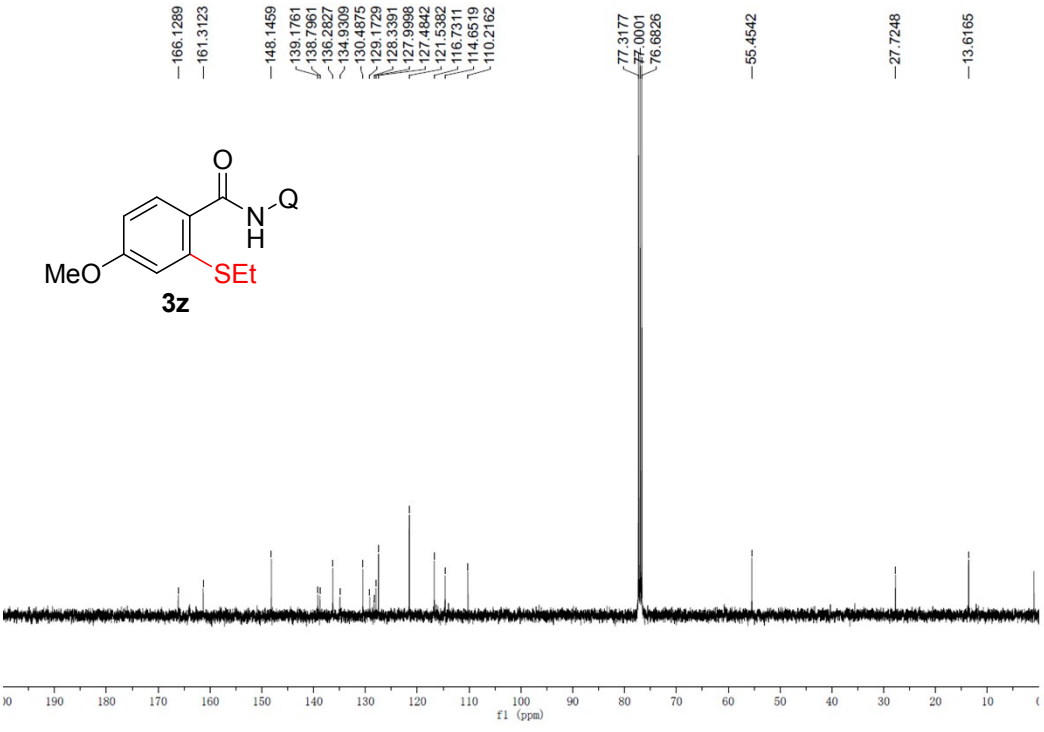

166.8124
148.1905
138.7346
137.5132
136.2720
136.2500
134.7587
131.7269
131.4602
130.7596
129.3776
127.9807
127.4215
121.7522
121.5582
116.8468
77.3179
77.0005
76.6827
28.6945
20.8914
14.0228
Me
O
N
H
Q
SEt
3y
f1 (ppm)


10.6572
8.9713
8.9526
8.8065
8.7977
8.1818
8.1617
7.8310
7.8097
7.6023
7.5827
7.5635
7.5390
7.5187
7.4661
7.4557
7.4456
7.4354
7.2611
6.9729
6.8270
6.8056
3.8831
3.0115
2.9931
2.9747
2.9560
1.3712
1.3528
1.3344


O
N
H
Q
MeO
SEt

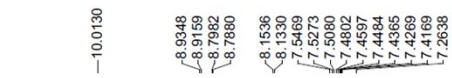
3z

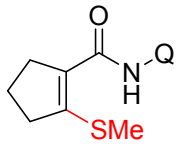

0.99
0.95
0.93
1.15
1.00
2.08
1.06
0.97
1.11
2.94
1.97
2.95
f1 (ppm)


166.1289
161.3123
148.1459
139.1761
138.7961
136.2827
134.9309
130.4875
129.1729
128.3391
127.9998
127.4842
121.5382
116.7311
114.6519
110.2162
77.3177
77.0001
76.6826
55.4542
27.7248
13.6165
f1 (ppm)

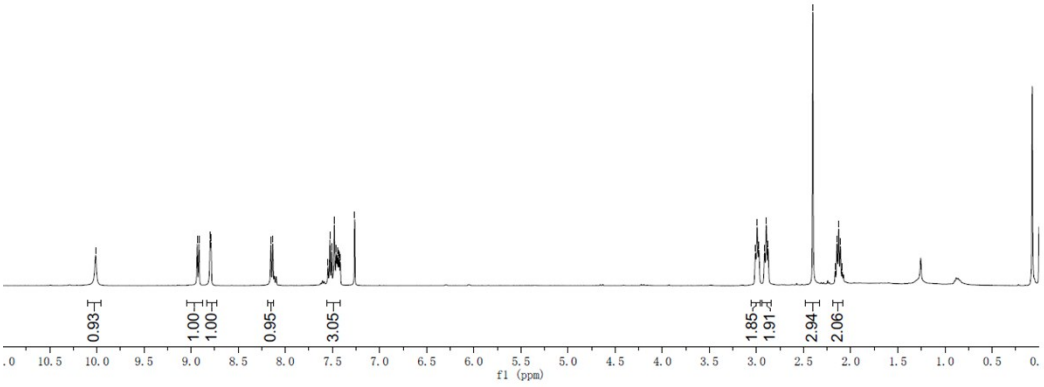
O
N
H
Q
MeO
SEt

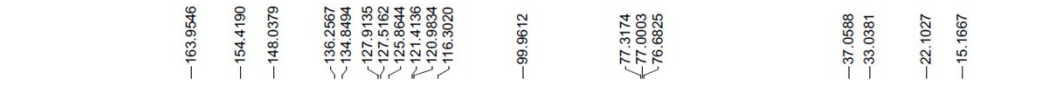
3z

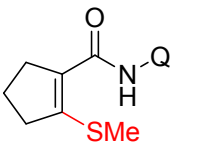

10.0130
8.9348
8.9159
8.7982
8.7880
8.1536
8.1330
7.5469
7.5273
7.5080
7.4802
7.4597
7.4484
7.4365
7.4269
7.4169
7.2638
3.0101
2.9926
2.9748
2.9130
2.8955
2.8780
2.4016
2.1641
2.1460
2.1273
2.1089
2.0900


O
N
H
Q
SMe

5a

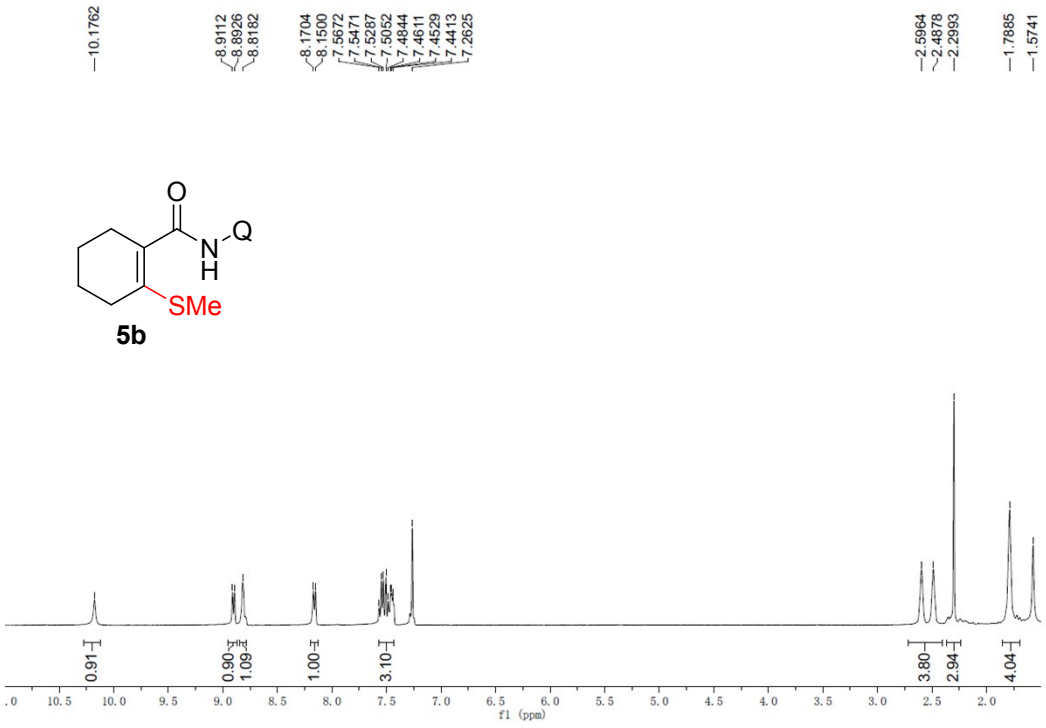

0.93
1.00
1.00
0.95
3.05
1.85
1.91
2.94
2.06
f1 (ppm)


163.9546
154.4190
148.0379
136.2567
134.8494
127.9135
127.5162
125.8644
121.4136
120.9834
116.3020
99.9612
77.3174
77.0003
76.6825
37.0588
33.0381
22.1027
15.1667

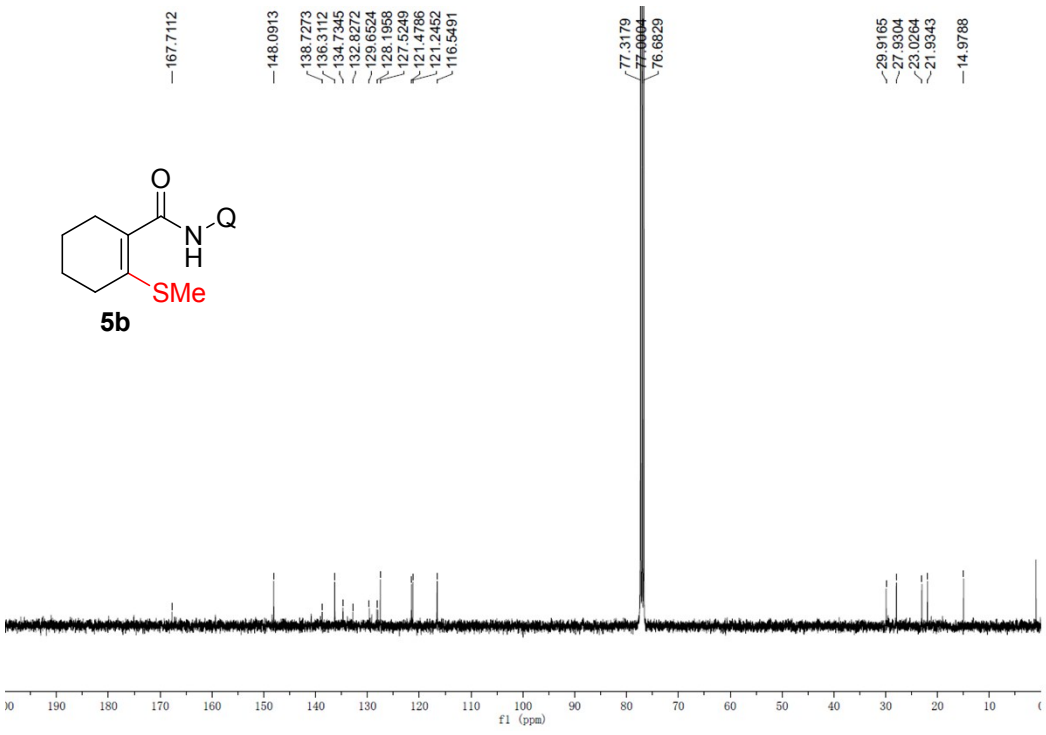

O
N
H
Q
SMe

5a

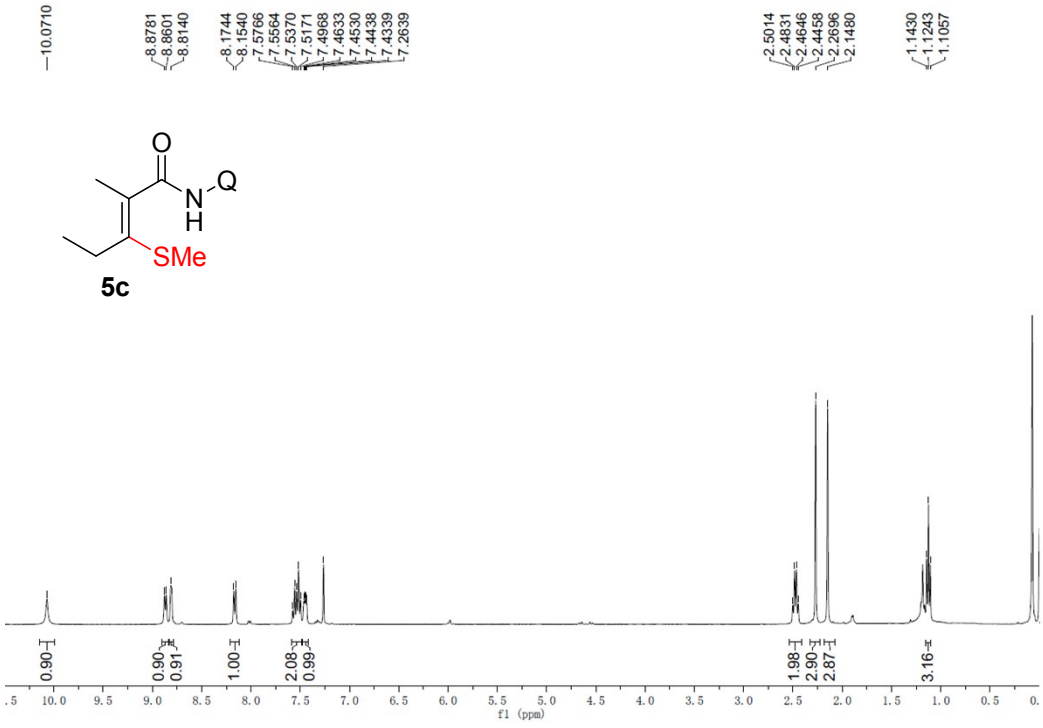
f1 (ppm)

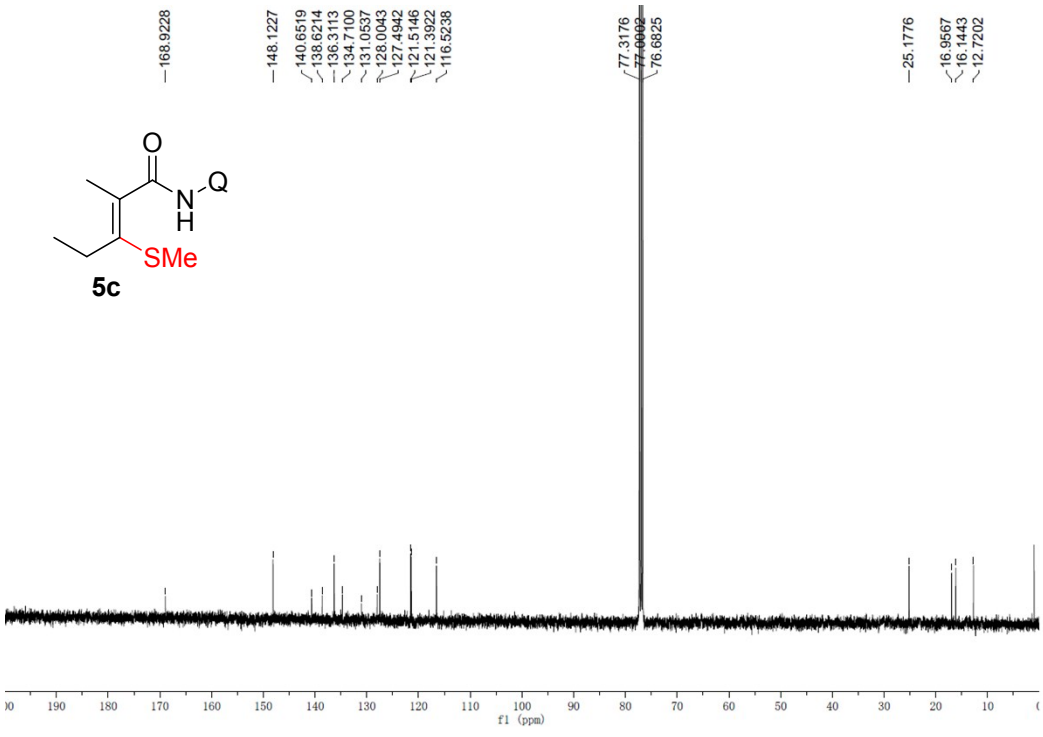

10.1762
8.9112
8.8926
8.8182
8.1704
8.1500
7.5672
7.5471
7.5287
7.5052
7.4844
7.4611
7.4529
7.4413
7.2625
2.5964
2.4878
2.2993
1.7885
1.5741
O
N
H
Q
SMe
0.91
0.90
1.09
1.00
3.10
3.80
2.94
4.04
f1 (ppm)

5b


167.7112
148.0913
138.7273
136.3112
134.7345
132.8272
129.6524
128.1958
127.5249
121.4786
121.2452
116.5491
77.3179
77.0004
76.6829
29.9165
27.9304
23.0264
21.9343
14.9788
O
N
H
Q
SMe
f1 (ppm)

5b


10.0710
8.8781
8.8601
8.8140
8.1744
8.1540
7.5766
7.5564
7.5370
7.5171
7.4968
7.4633
7.4530
7.4438
7.4339
7.2639
2.5014
2.4831
2.4646
2.4458
2.2696
2.1480
1.1430
1.1243
1.1057
O
N
H
Q
SMe
5c
0.90
0.90
0.91
1.00
2.08
0.99
1.98
2.90
2.87
3.16
f1 (ppm)


168.9228
148.1227
140.6519
138.6214
136.3113
134.7100
131.0537
128.0043
127.4942
121.5146
121.3922
116.5238
77.3176
77.0002
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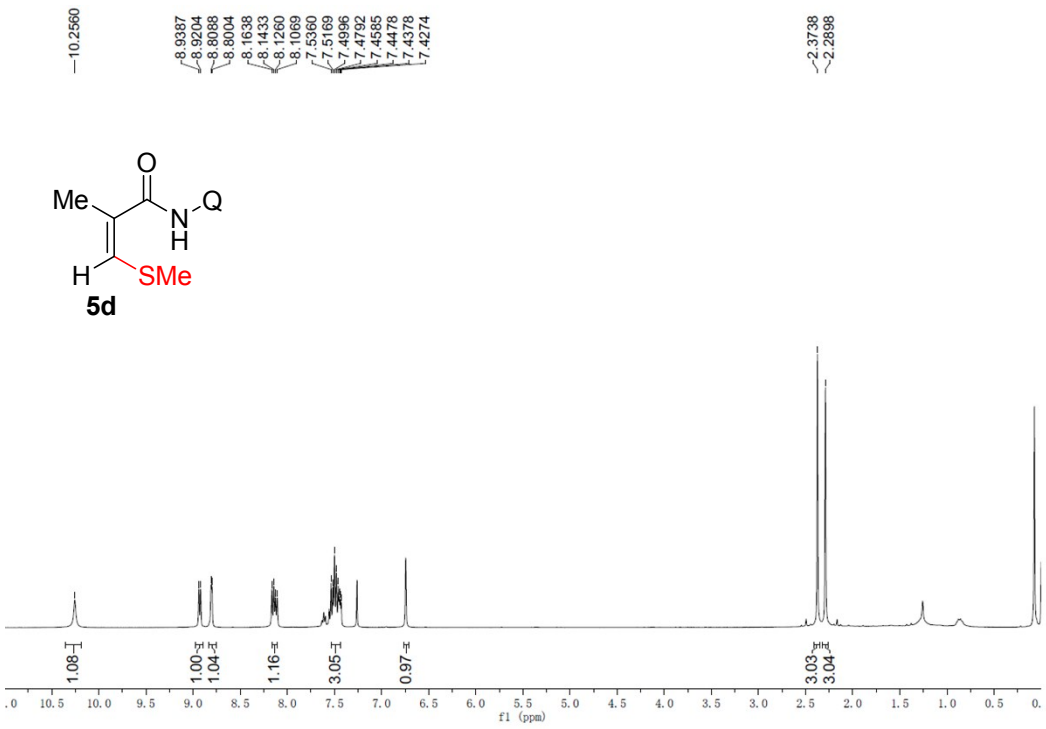
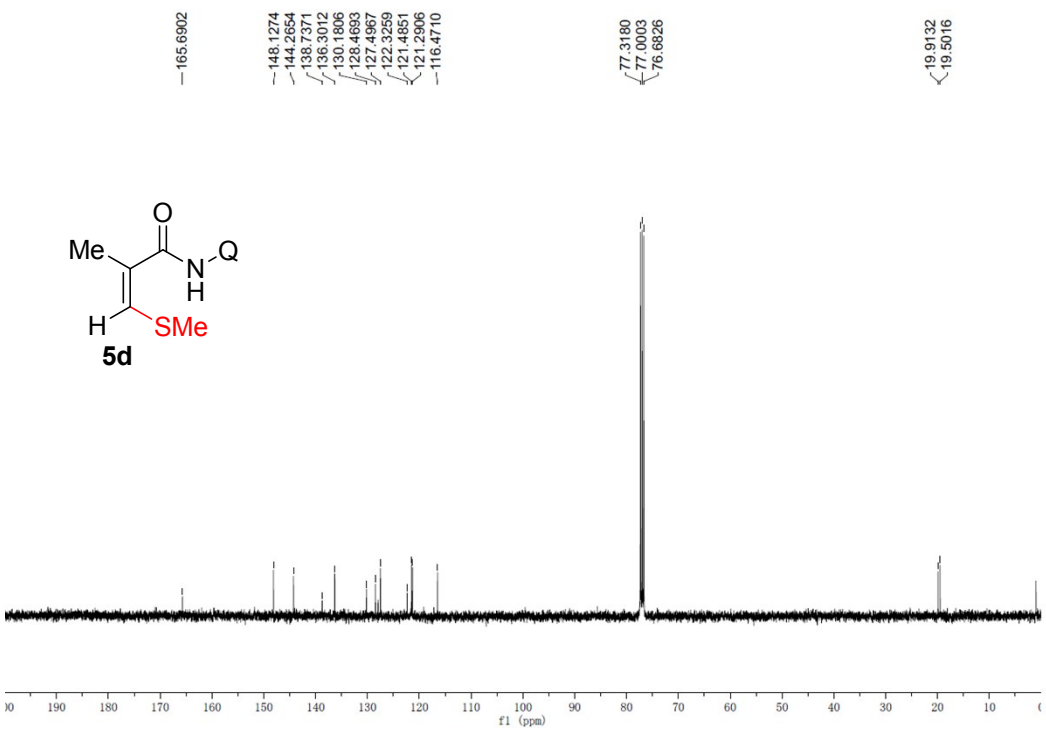
16.9567
16.1443
12.7202
O
N
H
Q
SMe
5c
f1 (ppm)


10.2560
8.9387
8.9204
8.8088
8.8004
8.1638
8.1433
8.1260
8.1069
7.5360
7.5169
7.4996
7.4792
7.4585
7.4478
7.4378
7.4274
2.3738
2.2898
1.08
1.00
1.04
1.16
3.05
0.97
3.03
3.04
f1 (ppm)

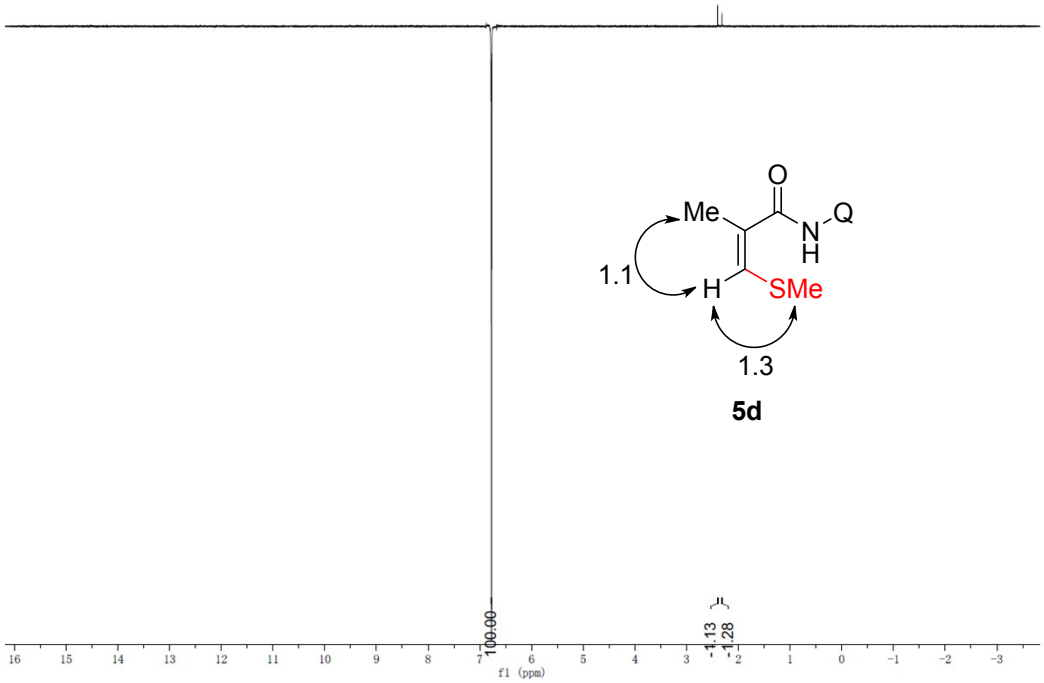
O
Me
N
H
Q
H
SMe

5d

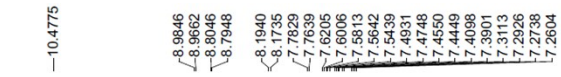

165.6902
148.1274
144.2654
138.7371
136.3012
130.1806
128.4693
127.4967
122.3259
121.4851
121.2906
116.4710
77.3180
77.0003
76.6826
19.9132
19.5016
f1 (ppm)

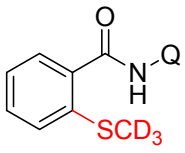
O
Me
N
H
Q
H
SMe

5d


Me
O
N
Q
H
1.1
H
SMe
1.3
100.00
1.13
1.28
f1 (ppm)

5d


10.4775
8.9846
8.9662
8.8046
8.7948
8.1940
8.1735
7.7829
7.7639
7.6205
7.6006
7.5813
7.5642
7.5439
7.4931
7.4748
7.4550
7.4449
7.4098
7.3901
7.3113
7.2926
7.2738
7.2604


O
N
Q
H
SCD3

3a-d3

0.95
0.97
1.04
1.00
0.98
2.02
1.91
0.99
1.10
f1 (ppm)