Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

An efficient synthesis of sulfonated quinoline diones by copper catalyzed sulfonylation of activated alkenes with sulfonylhydrazides

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List of contents

A General information

All melting points (mp) were measured on a melting point apparatus with a microscope and a hot stage and were uncorrected. ^{1}H-NMR spectra were determined

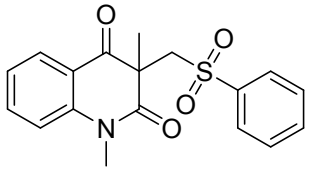
in $CDCl_3$ on a Bruker 400 spectrometer and chemical shifts were reported in parts per million from internal TMS (δ). Data for ^{1}H-NMR are recorded as follows: chemical shift (δ, ppm), multiplicity (integration, s=singlet, d=doublet, dd=doublets, t=triplet, q=quartet, m=multiplet or unresolved, coupling constants (s) in Hertz). ^{13}C-NMR spectra were obtained by using the same NMR spectrometers. High-resolution mass spectra (HRMS) was performed with 200-300 mesh silica gel using flash column techniques. All of the reagents obtained commercially were used directly unless otherwise noted.

B Experiment procedure and characterization data for products

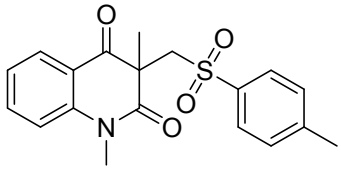
a General procedure for the synthesis of sulfonated quinoline diones

To a suspention of N-(2-cyanophenyl) acrylamides **1** (0.3 mmol), $(NH_4)_2S_2O_8$ (0.90 mmol), CuI (0.06 mmol) in CH_3CN/H_2O (2/1, 5.0 mL) was added sulfonohydrazides **2** (0.45 mmol) at room temperature, the solution was stirred at 80^{o}C for 12h. Water (10 mL) was added to the solution and the mixture was extracted with DCM (2x10 mL). The combined organic phase was dried over Na_2SO_4. After removal of solvents with a rotary evaporator, the residue was purified on a silica gel column with petroleum ether and ethyl acetate as eluent to afford the desired product **3**.

b Characterization data

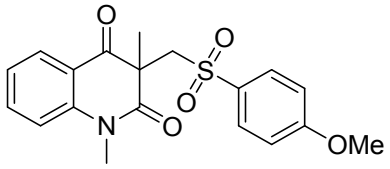


1,3-dimethyl-3-((phenylsulfonyl)methyl)quinoline-2,4(1H,3H)-dione (3a): 95% yield, white solid, mp = 118-120 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 7.6 Hz, 1H), 7.85 (d, *J* = 7.6 Hz, 2H), 7.71-7.61 (m, 2H), 7.56-7.52 (m, 2H), 7.27-7.21(m, 2H), 4.25 (s, 2H), 3.55 (s, 3H), 1.43 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.2, 171.7, 143.1, 141.6, 136.5, 133.6, 129.0, 128.7, 127.8, 123.3, 119.2, 115.2, 62.2, 55.3, 30.1, 25.9. HRMS (ESI): m/z calcd for $C_{18}H_{18}NO_4S$ $[M+H]^+$: 344.0951; found: 344.0957.

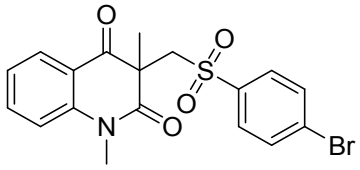


1,3-dimethyl-3-(tosylmethyl)quinoline-2,4(1H,3H)-dione (3b): 92% yield, white solid, mp = 167-169 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12-8.10 (m, 1H), 7.72 (d, *J*

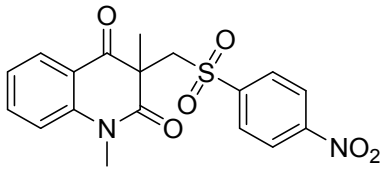
= 8.0 Hz, 2H), 7.69-7.67 (m, 1H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.26-7.21 (m, 2H), 4.23 (s, 2H), 3.55 (s, 3H), 2.44 (s, 3H), 1.43 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ194.2, 171.7, 144.5, 143.2, 138.7, 136.5, 129.6, 128.7, 127.8, 123.3, 119.3, 115.1, 62.4, 55.2, 30.1, 25.9, 21.6. HRMS (ESI): m/z calcd for $C_{19}H_{20}NO_4S$ $[M+H]^+$: 358.1108; found: 358.1114.



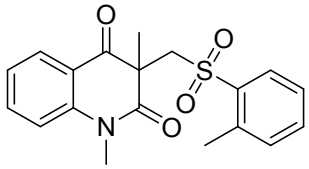
3-(((4-methoxyphenyl)sulfonyl)methyl)-1,3-dimethylquinoline-2,4(1H,3H)-dione (3c): 98% yield, white solid, mp = 145-147 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.8 Hz, 1H), 7.76 (d, *J* = 8.8 Hz, 2H), 7.70-7.66 (m, 1H), 7.25-7.20 (m, 2H), 6.98 (d, *J* = 8.8 Hz, 2H), 4.22 (s, 2H), 3.87 (s, 3H), 3.55 (s, 3H), 1.42 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.3, 171.7, 163.6, 143.2, 136.5, 133.2, 130.0, 128.6, 123.3, 119.3, 115.1,114.2, 62.7, 55.7, 55.2, 30.1, 25.9. HRMS (ESI): m/z calcd for $C_{19}H_{20}NO_5S$ $[M+H]^+$: 374.1057; found: 374.1064.



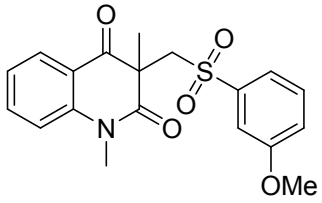
3-(((4-bromophenyl)sulfonyl)methyl)-1,3-dimethylquinoline-2,4(1H,3H)-dione (3d): 84% yield, white solid, mp = 173-175 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 6.8 Hz, 1H), 7.73-7.67 (m, 5H), 7.27-7.23 (m, 2H), 4.25 (s, 2H), 3.56 (s, 3H), 1.43 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.2, 171.6, 143.1, 140.6, 136.6, 132.3, 129.5, 128.9, 128.7, 123.4, 119.2, 115.2, 62.1, 55.6, 30.2, 25.8. HRMS (ESI): m/z calcd for $C_{18}H_{17}BrNO_3$ $[M+H]^+$: 422.0056; found: 422.0068.



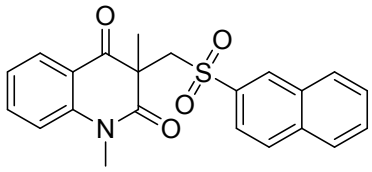
1,3-dimethyl-3-(((4-nitrophenyl)sulfonyl)methyl)quinoline-2,4(1H,3H)-dione (3e): 83% yield, white solid, mp = 190-192 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41-8.38 (m, 2H), 8.10-8.06 (m, 3H), 7.75-7.70 (m, 1H), 7.29-7.25 (m, 2H), 4.31 (s, 2H), 3.58 (s, 3H), 1.45 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.2, 171.6, 150.7, 147.2, 143.0, 136.8, 129.4, 128.7, 124.2, 123.6, 119.1, 115.3, 61.7, 56.0, 30.2, 25.7. HRMS (ESI): m/z calcd for $C_{18}H_{17}N_2O_6S$ $[M+H]^+$: 389.0802; found: 389.0811.



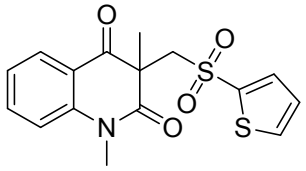
1,3-dimethyl-3-((o-tolylsulfonyl)methyl)quinoline-2,4(1H,3H)-dione (3f): 81% yield, white solid, mp = 142-144 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 7.6 Hz, 1H), 7.71-7.65 (m, 3H), 7.51-7.48 (m, 1H), 7.35-7.21 (m, 3H), 4.28 (s, 2H), 3.51 (s, 3H), 2.75 (s, 3H), 1.45 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.0, 171.5, 143.1, 139.8, 137.5, 136.5, 133.5, 132.5, 129.2, 128.7, 126.2, 123.3, 119. 3, 115.1, 61.7, 54.7, 30.1, 26.0, 20.5. HRMS (ESI): m/z calcd for $C_{19}H_{20}NNO_4S$ $[M+H]^+$: 358.1108; found: 358.1116.



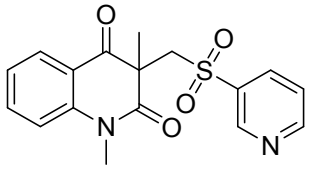
3-(((3-methoxyphenyl)sulfonyl)methyl)-1,3-dimethylquinoline-2,4(1H,3H)-dione (3g): 93% yield, white solid, mp = 143-145 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.8 Hz, 1H), 7.68 (t, *J* = 8.6 Hz, 1H), 7.43-7.41 (m, 2H), 7.34 (s, 1H), 7.25-7.20 (m, 2H), 7.16-7.13 (m, 1H), 4.24 (s, 2H), 3.86 (s, 3H), 3.54 (s, 3H), 1.43 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.2, 171.6, 159.8, 143.1, 142.6, 136.5, 130.1, 128.6, 123.3, 120.3, 119.9, 119.2, 115.2, 112.2, 62.3, 55.7, 55.2, 30.1, 25.9. HRMS (ESI): m/z calcd for $C_{19}H_{20}NO_5S$ $[M+H]^+$: 374.1057; found: 374.1066.



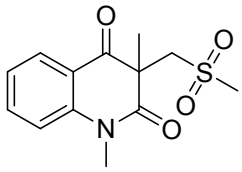
1,3-dimethyl-3-((naphthalen-2-ylsulfonyl)methyl)quinoline-2,4(1H,3H)-dione (3h): 91% yield, yellow solid, mp = 135-137 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (s, 1H), 8.09 (dd, *J* = 7.6 Hz, *J* = 1.6 Hz, 1H), 7.99 (d, *J* = 8.8 Hz, 1H), 7.94-7.91 (m, 2H), 7.87 (dd, *J* = 8.4 Hz, *J* = 1.6 Hz, 1H), 7.70-7.58 (m, 3H), 7.24-7.20 (m, 2H), 4.32 (s, 2H), 3.52 (s, 3H), 1.44 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.2, 171.6, 143.2, 138.2, 136.6, 135.3, 132.0, 129.6, 129.5, 129.4, 129.2, 128.7, 128.0, 127.5, 123.3, 122.6, 119.3, 115.2, 62.3, 55.2, 30.1, 26.1. HRMS (ESI): m/z calcd for $C_{22}H_{20}BrNO_4S$ $[M+H]^+$: 394.1108; found: 394.1117.



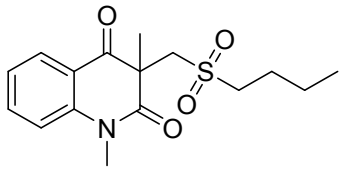
1,3-dimethyl-3-((thiophen-2-ylsulfonyl)methyl)quinoline-2,4(1H,3H)-dione (3i): 74% yield, yellow solid, mp = 174-176 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (dd, *J* = 7.6 Hz, *J* = 1.2 Hz, 1H), 7.71-7.62 (m, 3H), 7.23 (t, *J* = 8.4 Hz, 2H), 7.12 (t, *J* = 4.4 Hz, 1H), 4.38 (s, 2H), 3.55 (s, 3H), 1.45 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.2, 171.6, 143.1, 142.8, 136.6, 134.0, 133.9, 128.7, 127.6, 123.4, 119.2, 115.2, 63.4, 55.5, 30.2, 25.9. HRMS (ESI): m/z calcd for $C_{16}H_{16}NO_4S_2$ $[M+H]^+$: 350.0515; found: 350.0524.



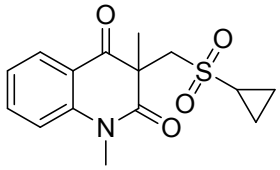
1,3-dimethyl-3-((pyridin-3-ylsulfonyl)methyl)quinoline-2,4(1H,3H)-dione (3j): 72% yield, light yellow solid, mp = 146-148 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.03 (s, 1H), 8.85 (d, *J* = 3.6 Hz, 1H), 8.11(q, *J* = 7.9 Hz, 2H), 7.70 (t, *J* = 7.8 Hz, 1H), 7.52-7.48 (m, 1H), 7.28-7.22 (m, 2H), 4.29 (s, 2H), 3.55 (s, 3H), 1.43 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.2, 171.6, 154.0, 149.0, 143.0, 138.2, 136.7, 135.7, 128.7, 123.6, 123.5, 119.1, 115.3, 62.2, 55.8, 30.2, 25.7. HRMS (ESI): m/z calcd for $C_{17}H_{17}N_2O_4S$ $[M+H]^+$: 345.0904; found: 345.0909.



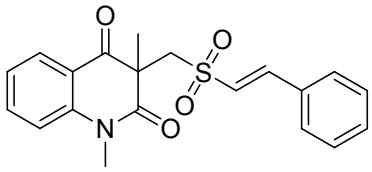
1,3-dimethyl-3-((methylsulfonyl)methyl)quinoline-2,4(1H,3H)-dione (3k): 62% yield, white solid, mp = 132-134 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (dd, *J* = 8.1 Hz, *J* = 1.6 Hz, 1H), 7.70-7.66 (m, 1H), 7.26-7.22 (m, 2H), 4.16 (s, 2H), 3.54 (s, 3H), 3.04 (s, 3H), 1.46 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.7, 172.0, 143.0, 136.5, 128.7, 123.4, 119.1, 115.2, 59.9, 56.0, 45.2, 30.2, 25.5. HRMS (ESI): m/z calcd for $C_{13}H_{16}NO_4S$ $[M+H]^+$: 282.0795; found: 282.0801.



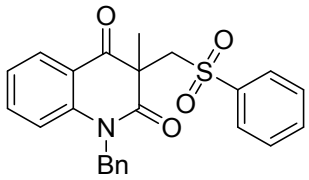
3-((butylsulfonyl)methyl)-1,3-dimethylquinoline-2,4(1H,3H)-dione (3l): 63% yield, white solid, mp = 108-110 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 5.6 Hz, 1H), 7.67-7.65 (m, 1H), 7.23-7.21 (m, 2H), 4.09 (s, 2H), 3.53 (s, 3H), 3.13-3.05 (m, 2H), 1.88-1.77 (m, 2H), 1.54-1.41 (m, 5H), 1.03-0.94 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.8, 172.1, 143.0, 136.5, 128.6, 123.3, 119.1, 115.1, 58.2, 56.8, 55.7, 30.1, 25.6, 23.8, 21.6, 13.6. HRMS (ESI): m/z calcd for $C_{16}H_{22}NO_4S$ $[M+H]^+$: 324.1264; found: 324.1272.



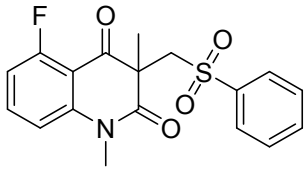
3-((cyclopropylsulfonyl)methyl)-1,3-dimethylquinoline-2,4(1H,3H)-dione (3m): 73% yield, white solid, mp = 153-155 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 7.1 Hz, 1H), 7.68-7.65 (m, 1H), 7.23-7.19 (m, 2H), 4.21 (s, 2H), 3.53 (s, 3H), 2.63 (bs, 1H), 1.46 (s, 3H), 1.20 (bs, 2H), 1.10 (d, *J* = 8.1 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.8, 172.1, 143.0, 136.5, 128.6, 123.3, 119.1, 115.1, 59.9, 55.7, 33.3, 30.1, 25.6, 5.1, 5.0. HRMS (ESI): m/z calcd for $C_{15}H_{18}NO_4S$ $[M+H]^+$: 308.0951; found: 308.0959.



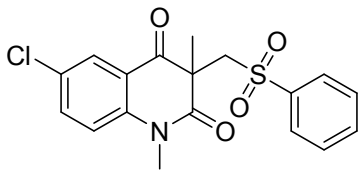
(E)-1,3-dimethyl-3-((styrylsulfonyl)methyl)quinoline-2,4(1H,3H)-dione (3n): 23% yield, yellow solid, mp = 63-65 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 11.4 Hz, 1H), 7.71-7.65 (m, 1H), 7.53-7.40 (m, 6H), 7.26-7.21 (m, 2H), 6.92 (d, *J* = 15.2 Hz, 1H), 4.23 (s, 2H), 3.54 (s, 3H), 1.48 (s, 3H). HRMS (ESI): m/z calcd for $C_{20}H_{20}NO_4S$ $[M+H]^+$: 370.1108; found: 370.1118.



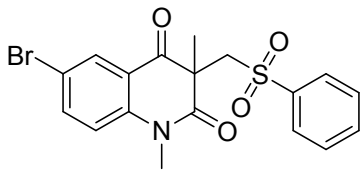
1-benzyl-3-methyl-3-((phenylsulfonyl)methyl)quinoline-2,4(1H,3H)-dione (3p): 81% yield, light yellow solid, mp = 163-165 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (dd, *J* = 9.2 Hz, *J* = 1.2 Hz, 1H), 7.89 (d, *J* = 7.5 Hz, 2H), 7.63 (t, *J* = 7.5 Hz, 1H), 7.56-7.49 (m, 3H), 7.40-7.33 (m, 4H), 7.28-7.25 (m, 1H), 7.18 (t, *J* = 7.3 Hz, 1H), 7.11 (d, *J* = 8.3 Hz, 1H), 5.40 (t, *J* = 17.5 Hz, 2H), 4.35 (s, 2H), 1.53 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.1, 172.3, 142.3, 141.8, 136.4, 135.9, 133.6, 129.0, 129.0, 128.8, 127.8, 127.4, 126.4, 123.4, 119.4, 116.2, 62.1, 55.8, 46.4, 25.9. HRMS (ESI): m/z calcd for $C_{24}H_{22}NO_4S$ $[M+H]^+$: 420.1264; found: 420.1274.



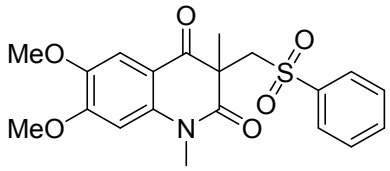
5-fluoro-1,3-dimethyl-3-((phenylsulfonyl)methyl)quinoline-2,4(1H,3H)-dione (3r): 93% yield, white solid, mp = 138-140 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 7.5 Hz, 2H), 7.65-7.52 (m, 4H), 7.05 (d, *J* = 8.7 Hz, 1H), 6.91 (t, *J* = 9.5 Hz, 1H), 4.21 (q, *J* = 13.1 Hz, 2H), 3.54 (s, 3H), 1.43 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.5, 171.3, 162.7 (d, $^1J_{FC}$ = 267.1 Hz, 1C), 144.2 (d, $^3J_{FC}$ = 3.1 Hz, 1C), 141.7, 136.8 (d, $^3J_{FC}$ = 11.9 Hz, 1C), 133.6, 129.1, 127.8, 111.5 (d, $^2J_{FC}$ = 21.4 Hz, 1C), 111.1 (d, $^4J_{FC}$ = 3.6 Hz, 1C), 109.0 (d, $^2J_{FC}$ = 9.0 Hz, 1C), 61.7, 56.4, 31.0, 25.4. HRMS (ESI): m/z calcd for $C_{18}H_{17}FNO_4S$ $[M+H]^+$: 362.0857; found: 362.0867.



6-chloro-1,3-dimethyl-3-((phenylsulfonyl)methyl)quinoline-2,4(1H,3H)-dione (3s): 93% yield, white solid, mp = 142-144 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 2.8 Hz, 1H), 7.85-7.80 (m, 2H), 7.66-7.58 (m, 2H), 7.57-7.51 (m, 2H), 7.20 (d, *J* = 8.9 Hz, 1H), 4.23 (m, 2H), 3.52 (s, 3H), 1.42 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.3, 171.4, 141.7, 141.4, 136.1, 133.7, 129.1, 129.0, 128.0, 127.7, 62.3, 55.3, 30.3, 25.7. HRMS (ESI): m/z calcd for $C_{18}H_{17}ClNO_4S$ $[M+H]^+$: 378.0561; found: 378.0570.



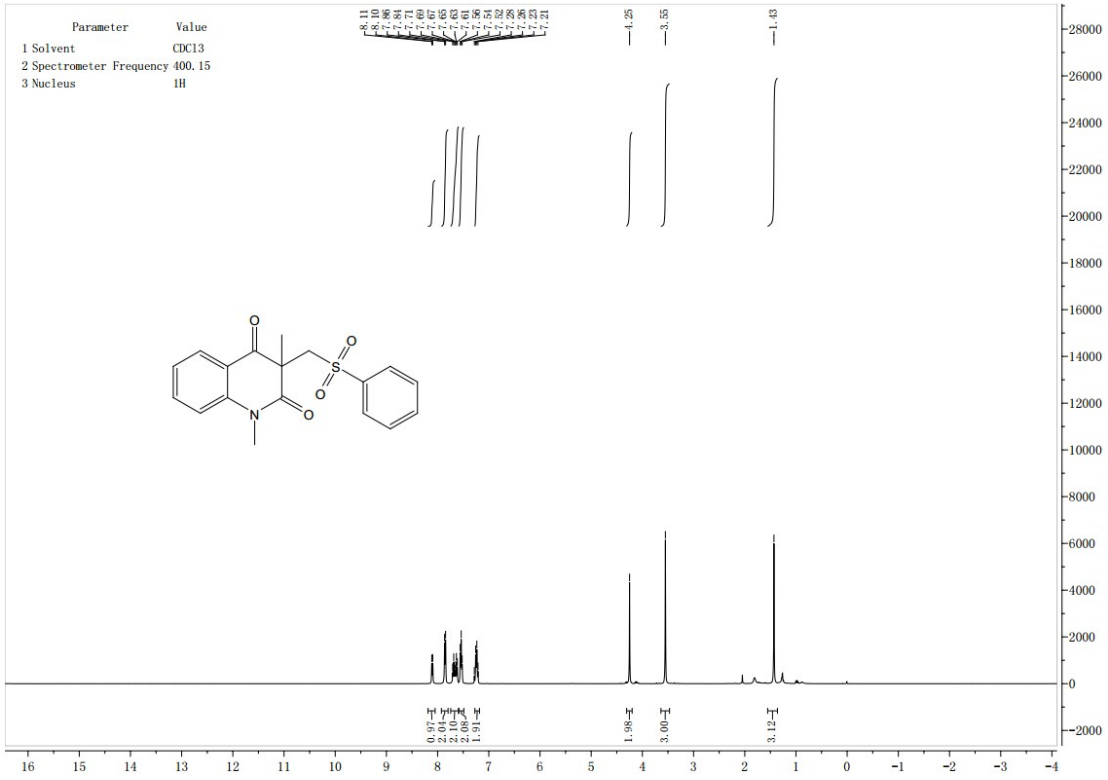
6-bromo-1,3-dimethyl-3-((phenylsulfonyl)methyl)quinoline-2,4(1H,3H)-dione (3t): 85% yield, light yellow solid, mp = 148-150 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, *J* = 2.5 Hz, 1H), 7.83 (d, *J* = 7.7 Hz, 2H), 7.76 (dd, *J* = 8.7 Hz, *J* = 2.5 Hz, 1H), 7.65 (t, *J* = 7.3 Hz, 2H), 7.55 (t, *J* = 7.7 Hz, 2H), 7.15 (d, *J* = 8.7 Hz, 1H), 4.24 (dd, *J* = 13.9 Hz, *J* = 1.7 Hz, 2H), 3.53 (s, 3H), 1.42 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.2, 171.4, 142.1, 141.4, 139.0, 133.7, 131.1, 129.1, 127.8, 120.5, 117.2, 116.4, 62.3, 55.3, 30.3, 25.7. HRMS (ESI): m/z calcd for $C_{18}H_{17}BrNO_4S$ $[M+H]^+$: 422.0056; found: 422.0069.

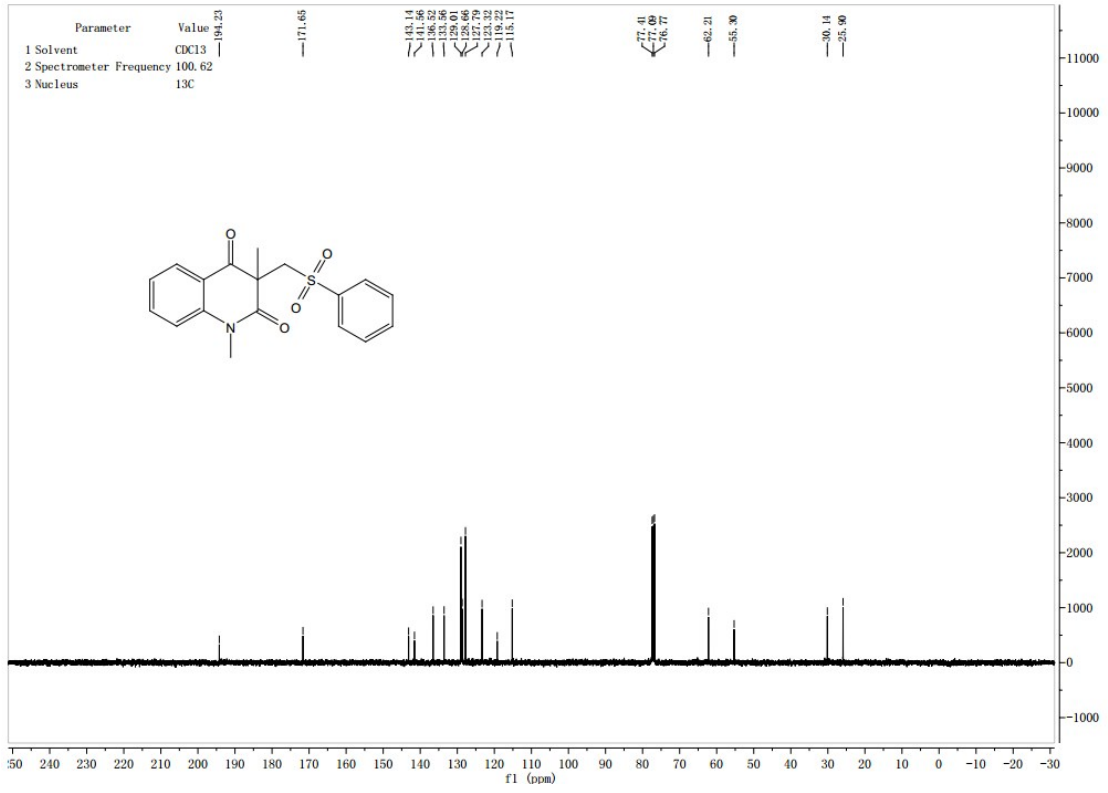


6,7-dimethoxy-1,3-dimethyl-3-((phenylsulfonyl)methyl)quinoline-2,4(1H,3H)-dione (3u): 71% yield, light yellow solid, mp = 186-188 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.9 Hz, 2H), 7.62 (t, *J* = 7.3 Hz, 1H), 7.55-7.50 (m, 3H), 6.67 (s, 1H), 4.20 (dd, *J* = 14.1 Hz, *J* = 3.9 Hz, 2H), 4.02 (s, 3H), 3.94 (s, 3H), 3.54 (s, 3H), 1.42 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.8, 172.1, 156.0, 145.4, 141.4, 139.4, 133.5, 129.0, 127.8, 111.9, 109.2, 98.4, 62.3, 56.4, 54.5, 30.2, 26.5. HRMS (ESI): m/z calcd for $C_{20}H_{22}NO_6S$ $[M+H]^+$: 404.1162; found: 404.1173.

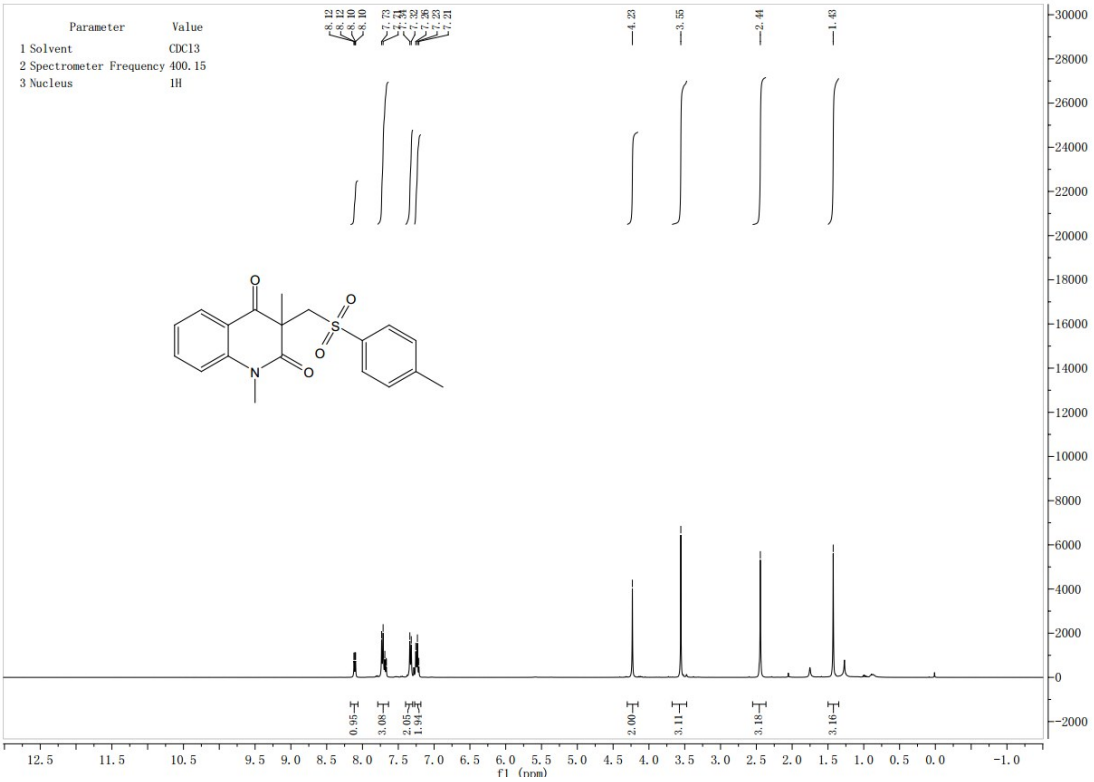
NMR Spectra:

3a





3b


Parameter Value
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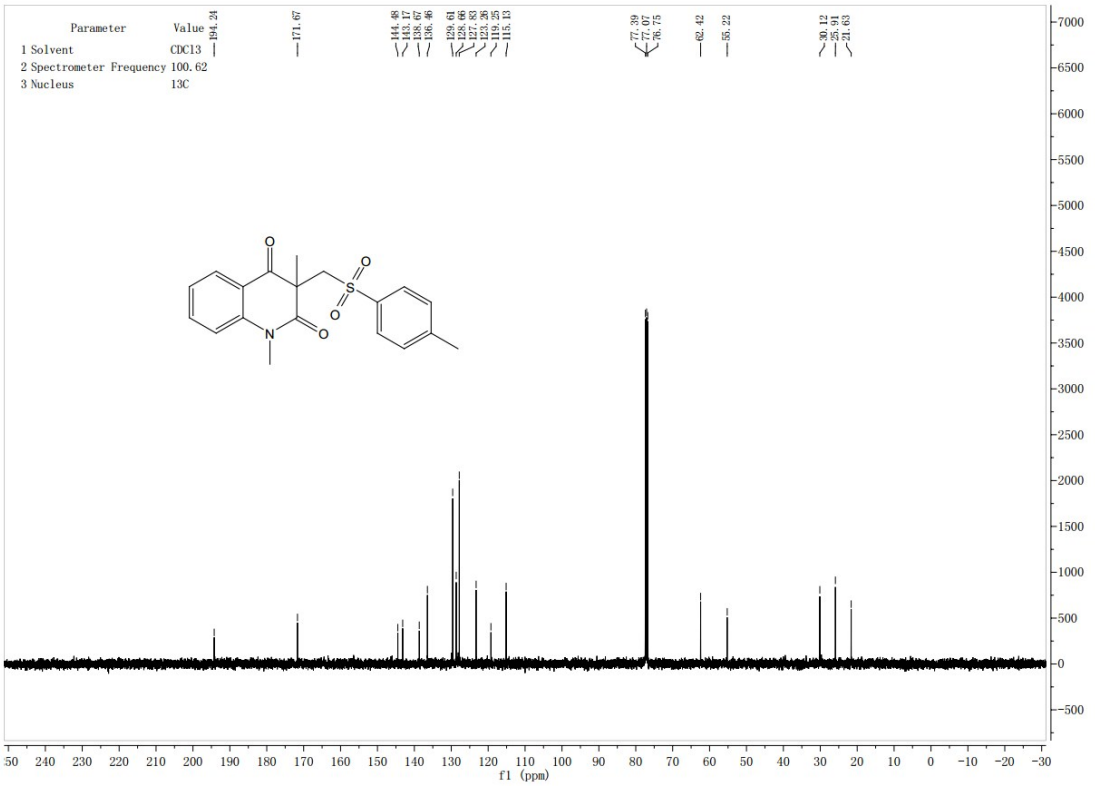
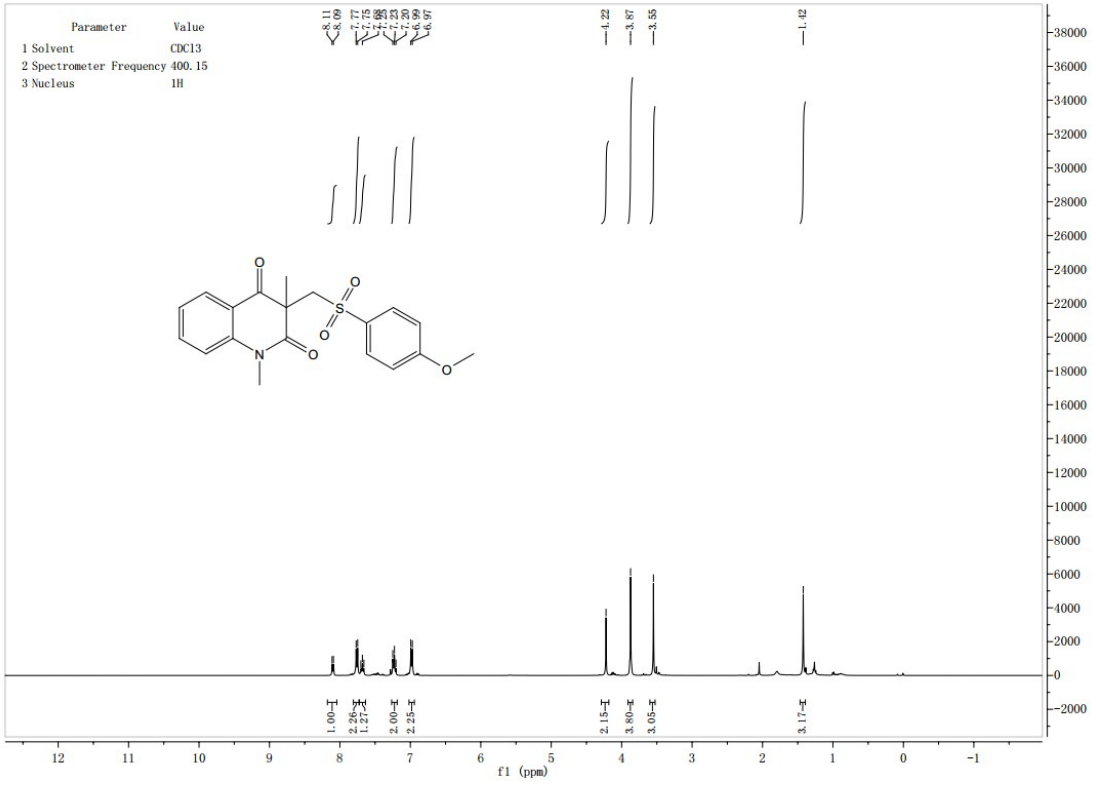
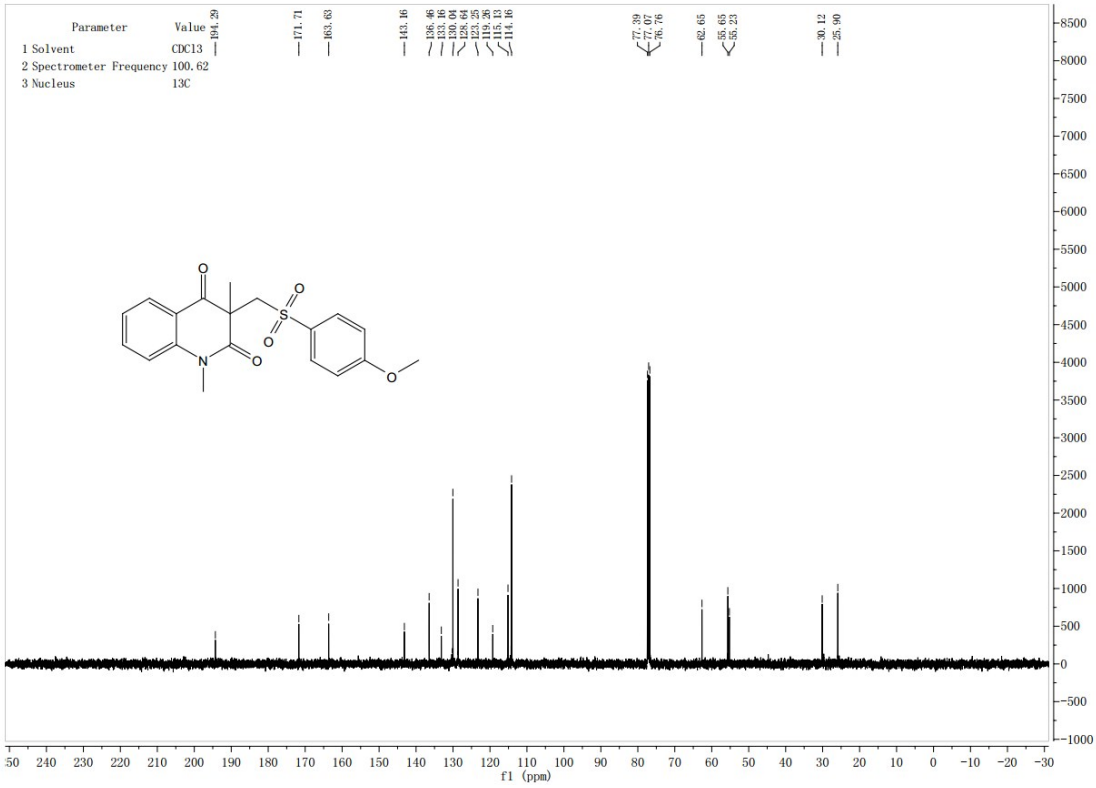
2 Spectrometer Frequency 400.15
3 Nucleus 1H
8.12
8.12
8.10
8.10
7.73
7.71
7.34
7.32
7.26
7.23
7.21
4.23
3.55
2.44
1.43
0.95
3.08
2.05
1.94
2.00
3.11
3.18
3.16
f1 (ppm)


Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 100.62
3 Nucleus 13C
194.24
171.67
144.48
143.17
138.67
136.46
129.61
128.66
127.83
123.36
115.25
113.13
77.39
77.07
76.75
62.42
55.22
30.12
25.91
21.63
f1 (ppm)

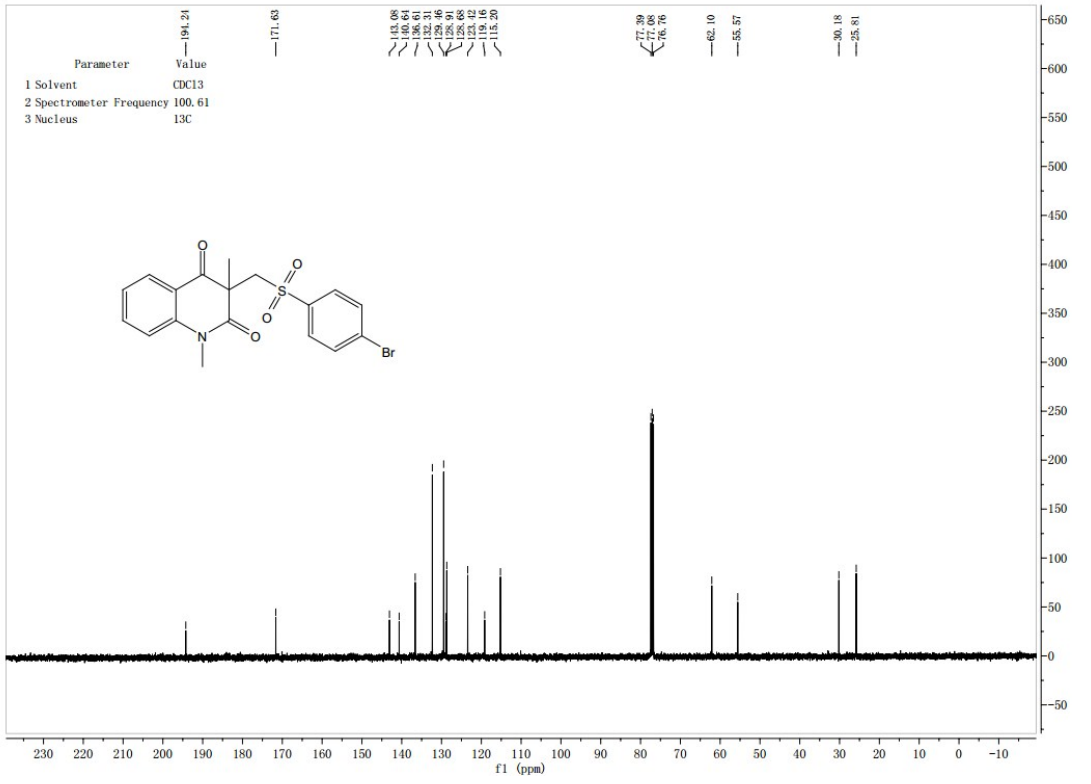
3c


Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 400.15
3 Nucleus 1H
8.11
8.09
7.77
7.75
7.68
7.66
7.23
7.20
6.99
6.97
4.22
3.87
3.55
1.42
1.00
2.26
1.27
2.00
2.25
2.15
3.80
3.05
3.17
f1 (ppm)

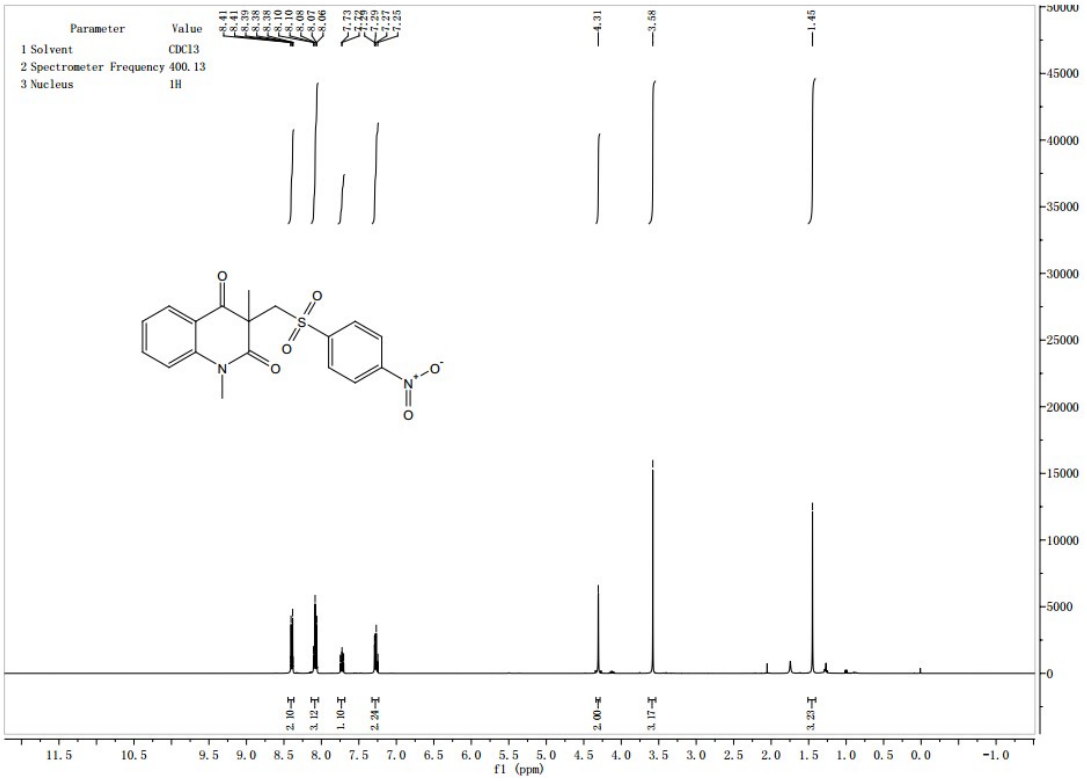

Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 100.62
3 Nucleus 13C
194.29
171.71
163.63
143.16
136.46
133.16
130.04
128.64
123.25
119.26
115.13
114.16
77.39
77.07
76.76
62.65
55.65
55.23
30.12
25.90
f1 (ppm)

3d


Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 400.13
3 Nucleus 1H
8.11
8.09
7.73
7.71
7.69
7.68
7.67
7.28
7.26
7.24
7.23
4.25
3.56
1.43
0.97
5.08
2.14
2.00
3.00
3.09
Br
f1 (ppm)


Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 100.61
3 Nucleus 13C
194.24
171.63
143.08
140.61
136.61
132.31
129.46
128.91
128.68
123.42
119.16
115.20
77.39
77.08
76.76
62.10
55.57
30.18
25.81
Br
f1 (ppm)

3e


Parameter Value
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2 Spectrometer Frequency 400.13
3 Nucleus 1H
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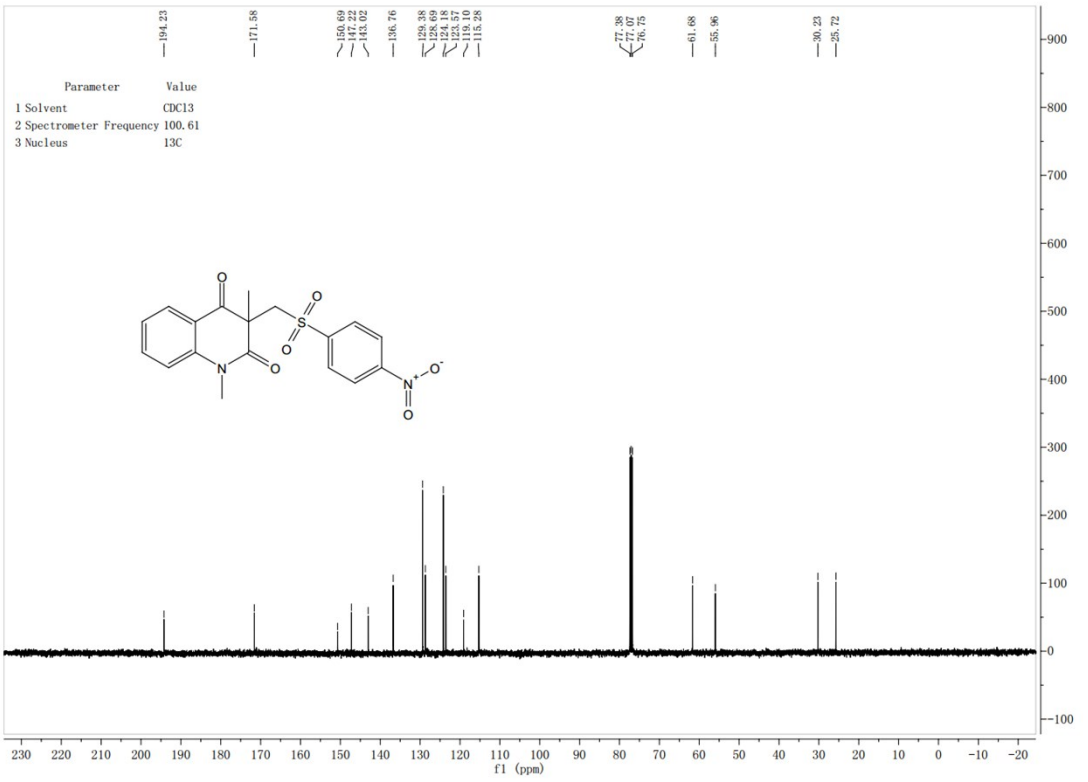
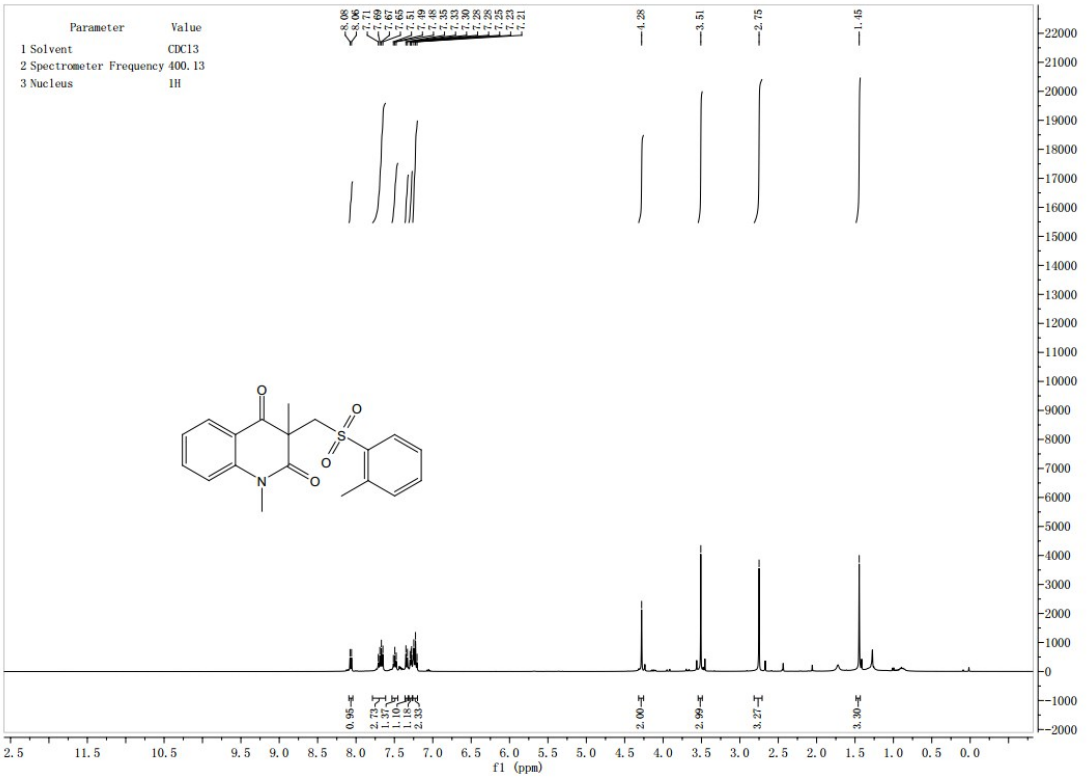
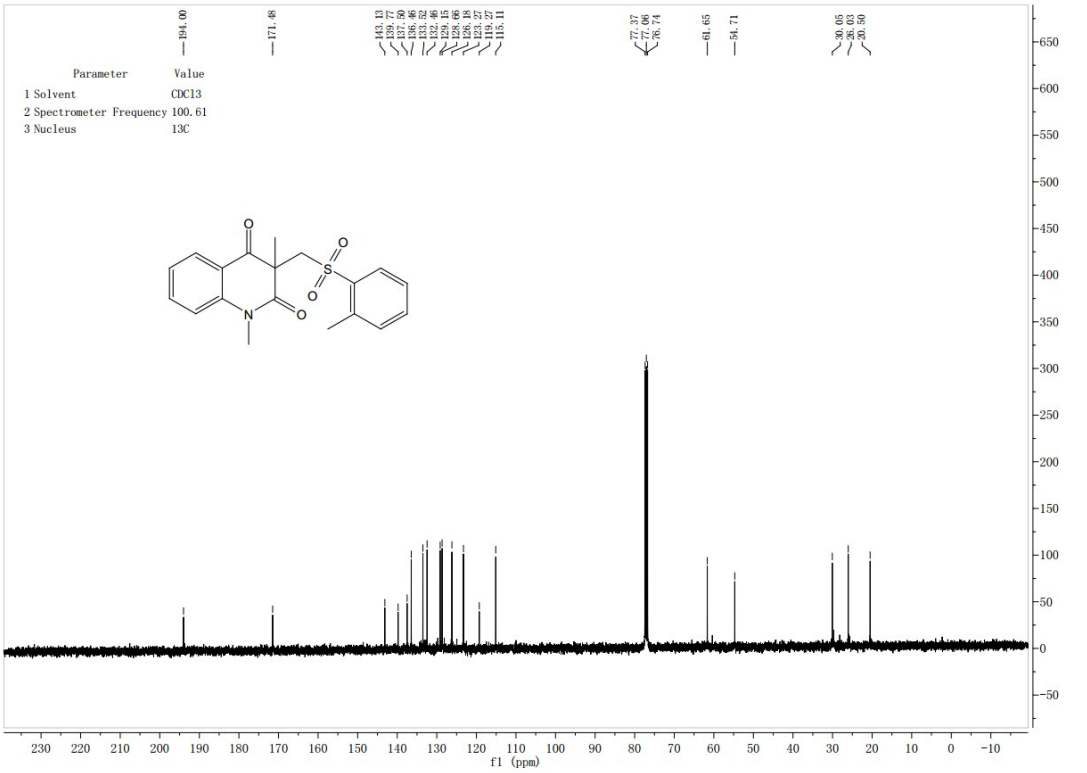
8.38
8.10
8.08
8.07
8.06
7.73
7.29
7.27
7.25
4.31
3.58
1.45
2.10
3.12
1.10
2.24
2.00
3.17
3.23
f1 (ppm)

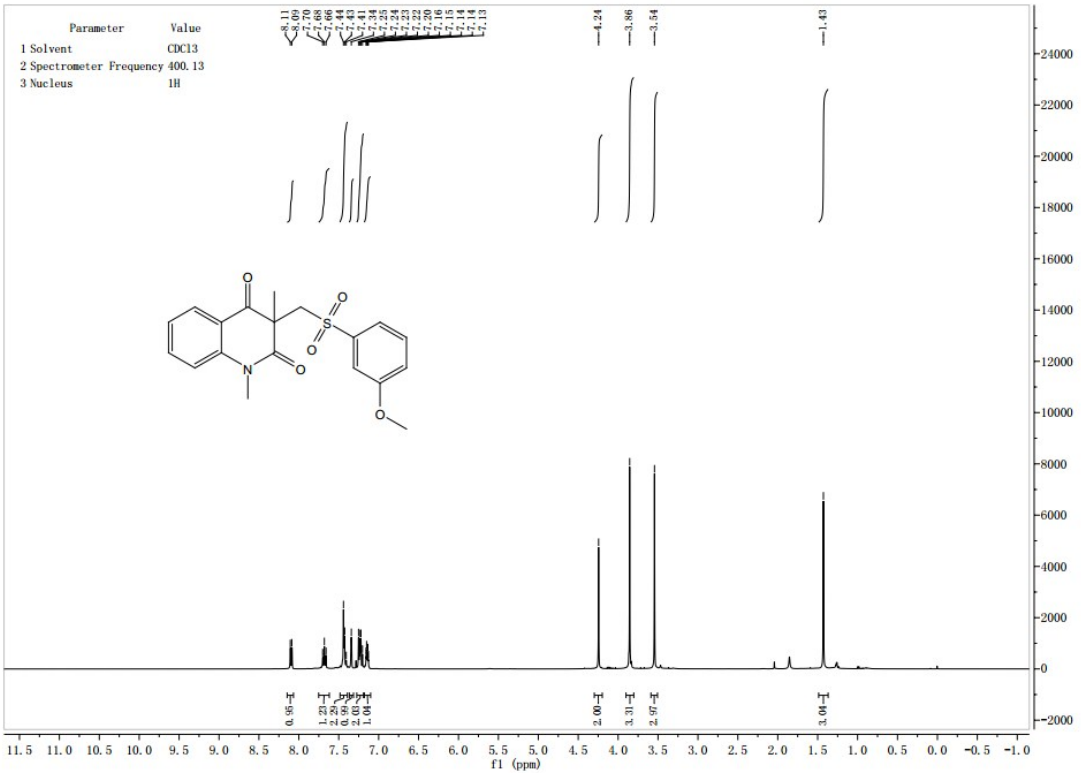

Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 100.61
3 Nucleus 13C
194.23
171.58
150.69
147.22
143.02
136.76
129.38
128.69
124.18
123.57
119.10
115.26
77.38
77.07
76.75
61.68
55.96
30.23
25.72
f1 (ppm)

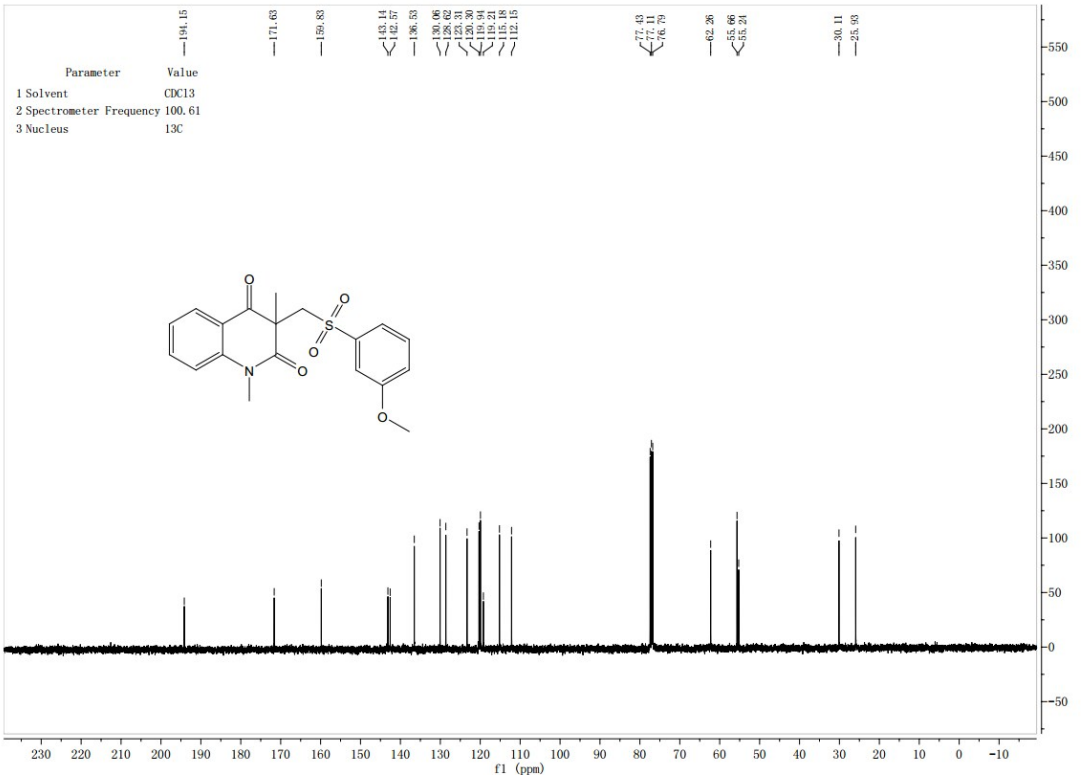
3f


Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 400.13
3 Nucleus 1H
f1 (ppm)


Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 100.61
3 Nucleus 13C
f1 (ppm)

3g


Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 400.13
3 Nucleus 1H
f1 (ppm)


Parameter Value
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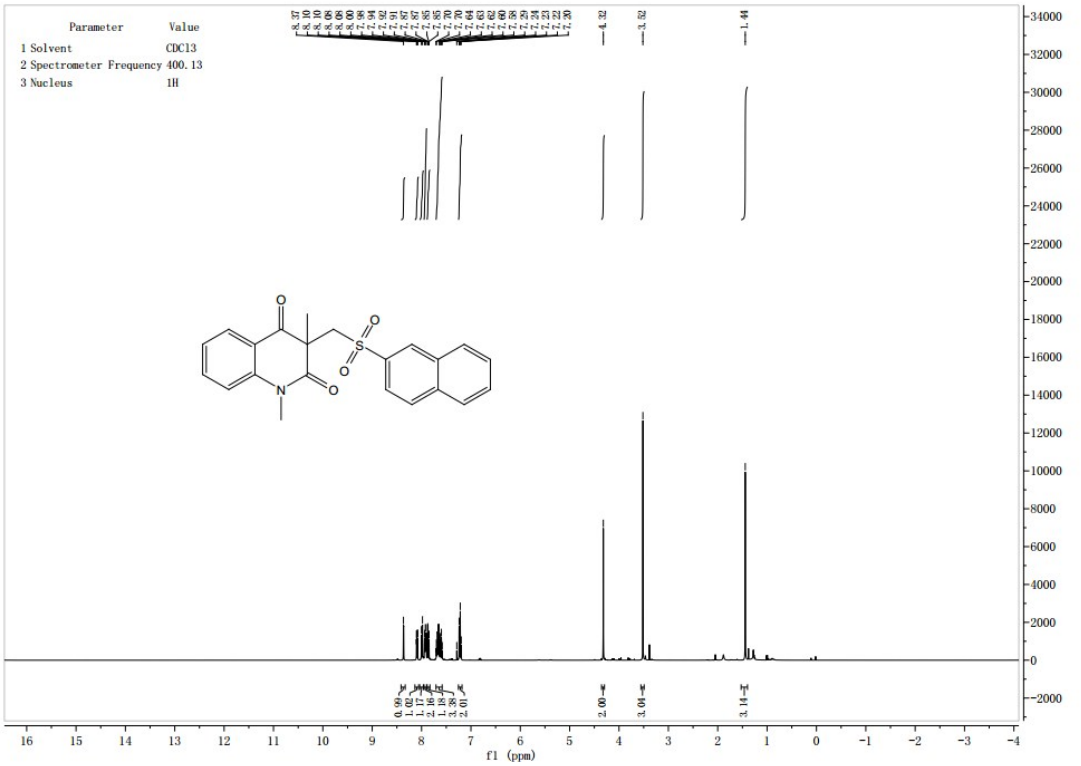
2 Spectrometer Frequency 100.61
3 Nucleus 13C
f1 (ppm)

3h


Parameter Value
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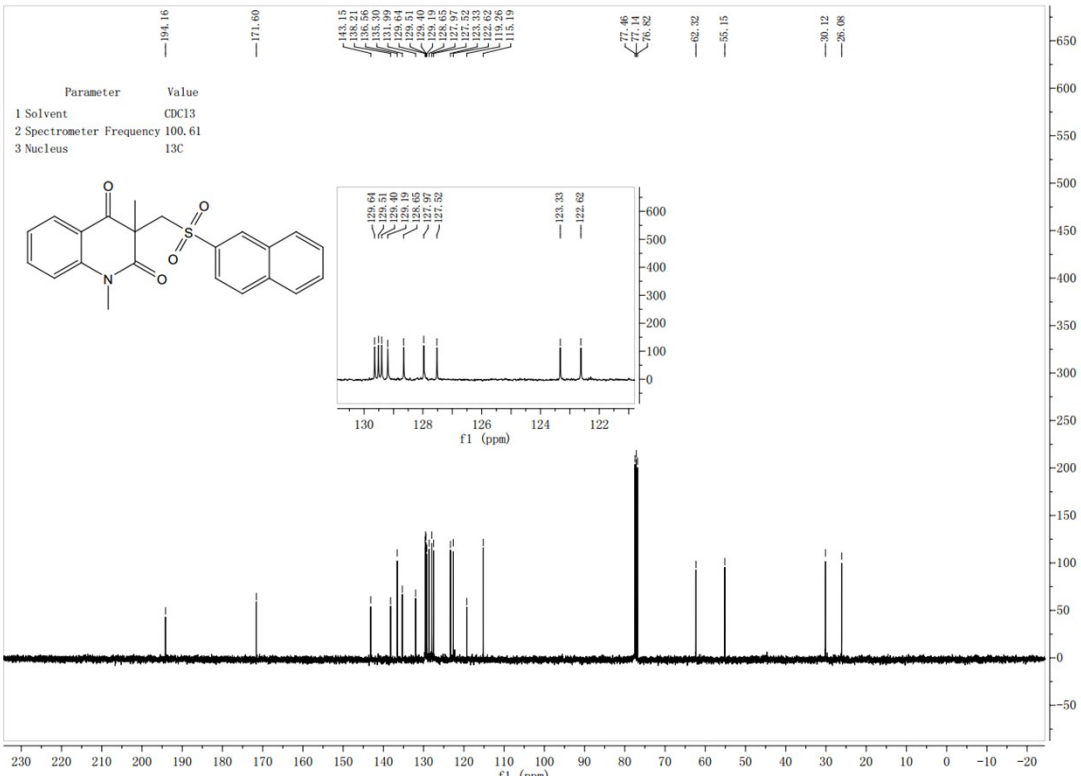
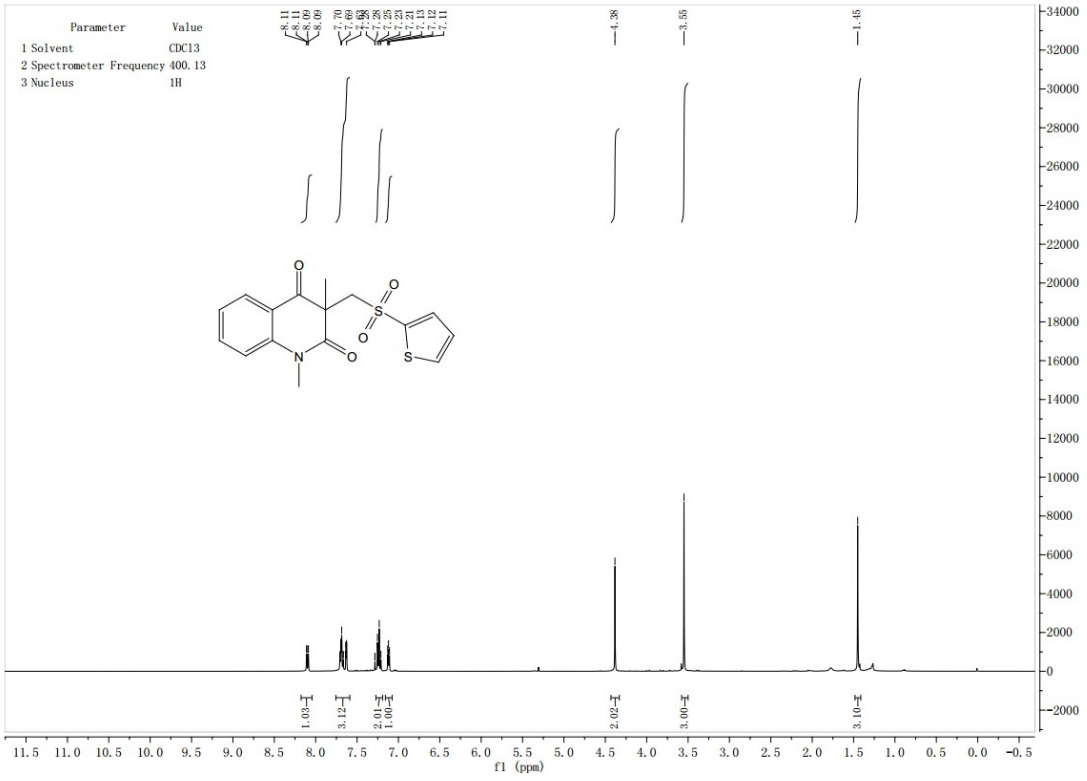
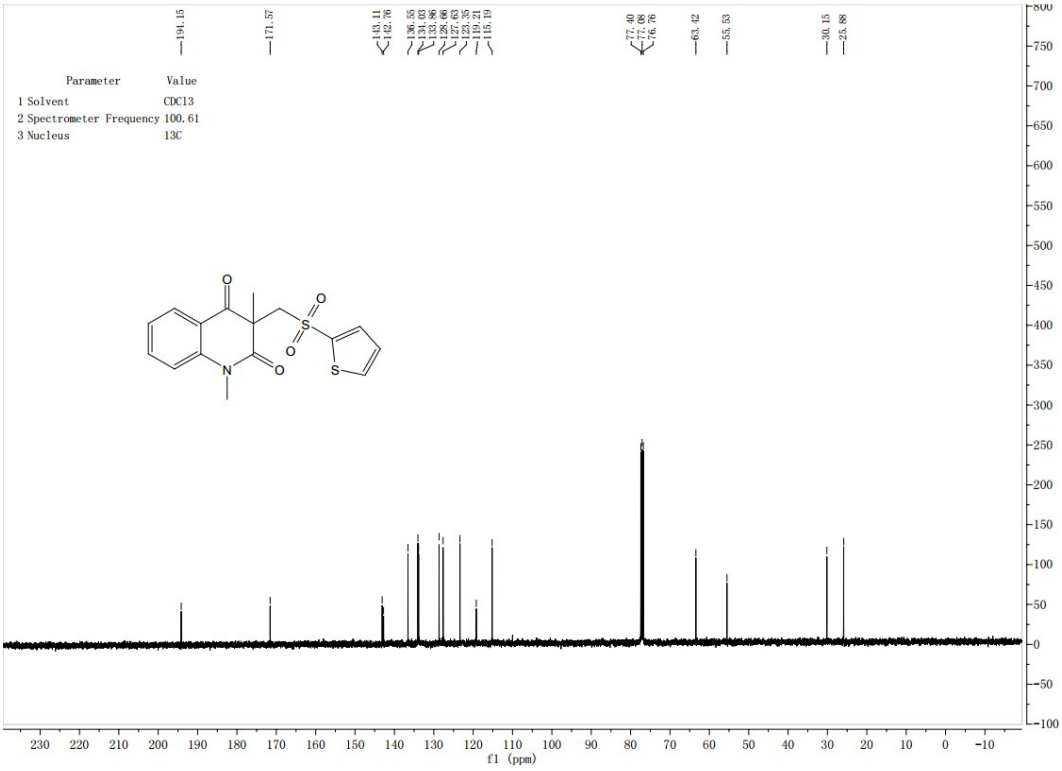
2 Spectrometer Frequency 400.13
3 Nucleus 1H
f1 (ppm)

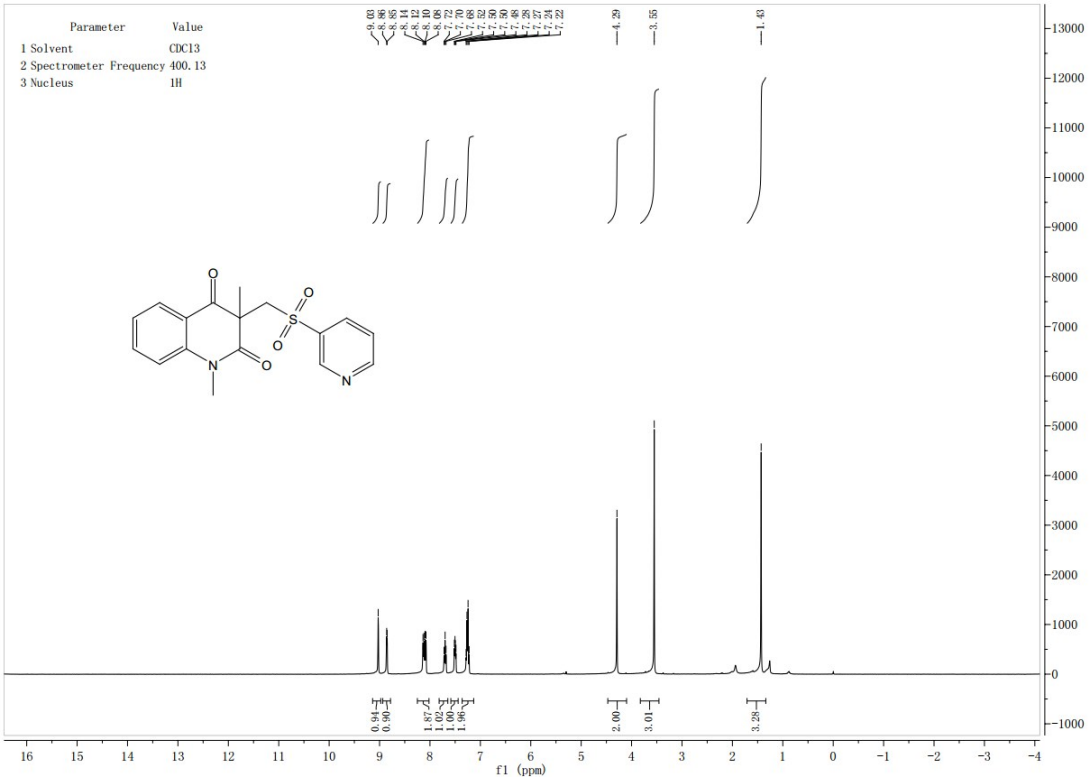

Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 100.61
3 Nucleus 13C
f1 (ppm)

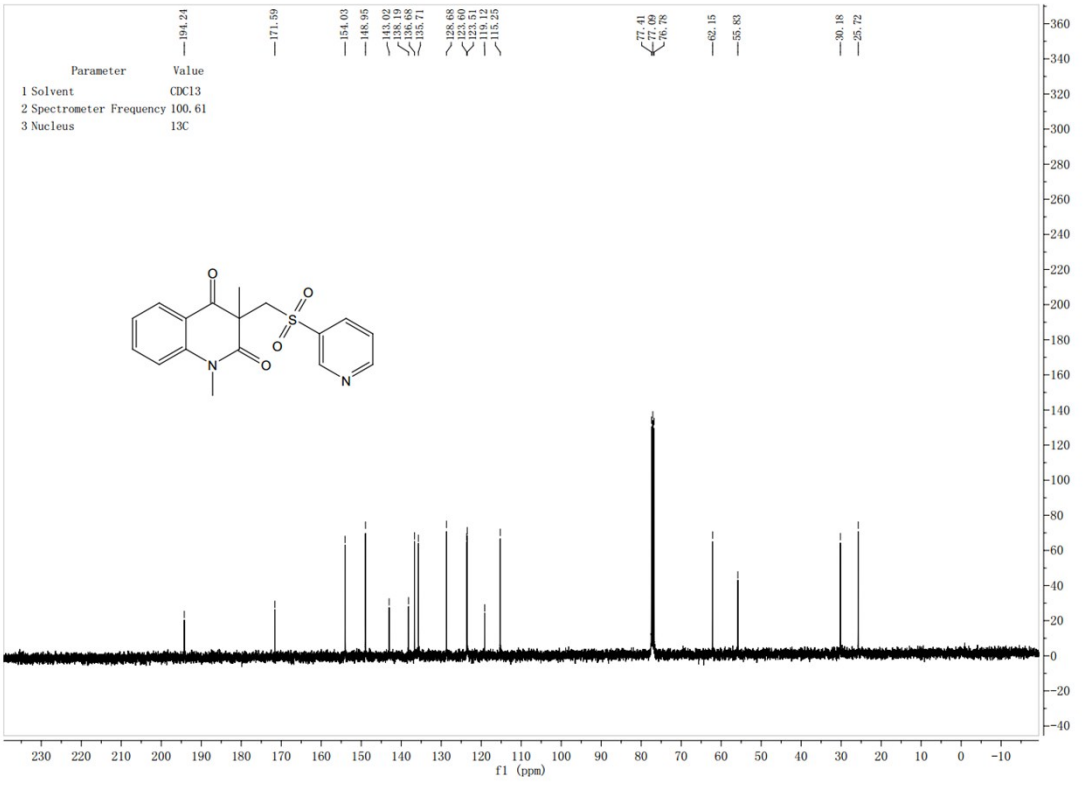
3i


Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 400.13
3 Nucleus 1H
8.11
8.09
7.70
7.69
7.28
7.25
7.23
7.21
7.13
7.12
7.11
4.38
3.55
1.45
1.03
3.12
2.01
1.00
2.02
3.00
3.10
f1 (ppm)


Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 100.61
3 Nucleus 13C
194.15
171.57
143.11
142.76
136.55
134.03
128.66
127.63
123.35
119.21
115.19
77.40
77.08
76.76
63.42
55.53
30.15
25.88
f1 (ppm)

3j


Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 400.13
3 Nucleus 1H
f1 (ppm)


Parameter Value
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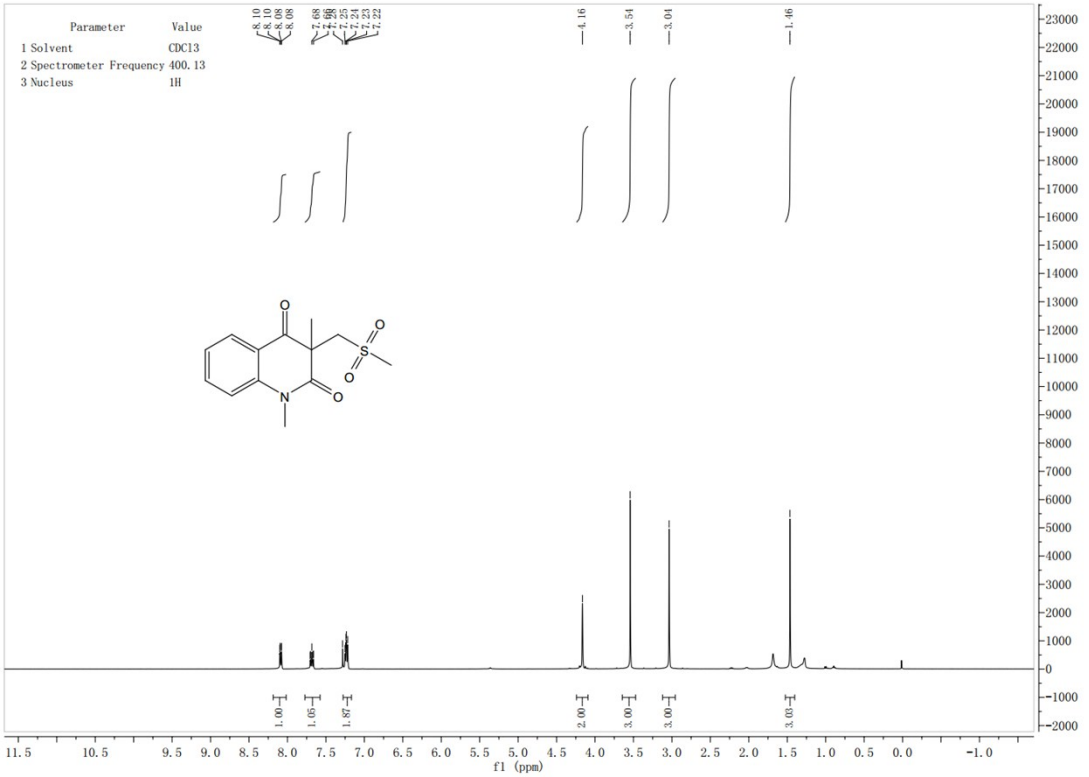
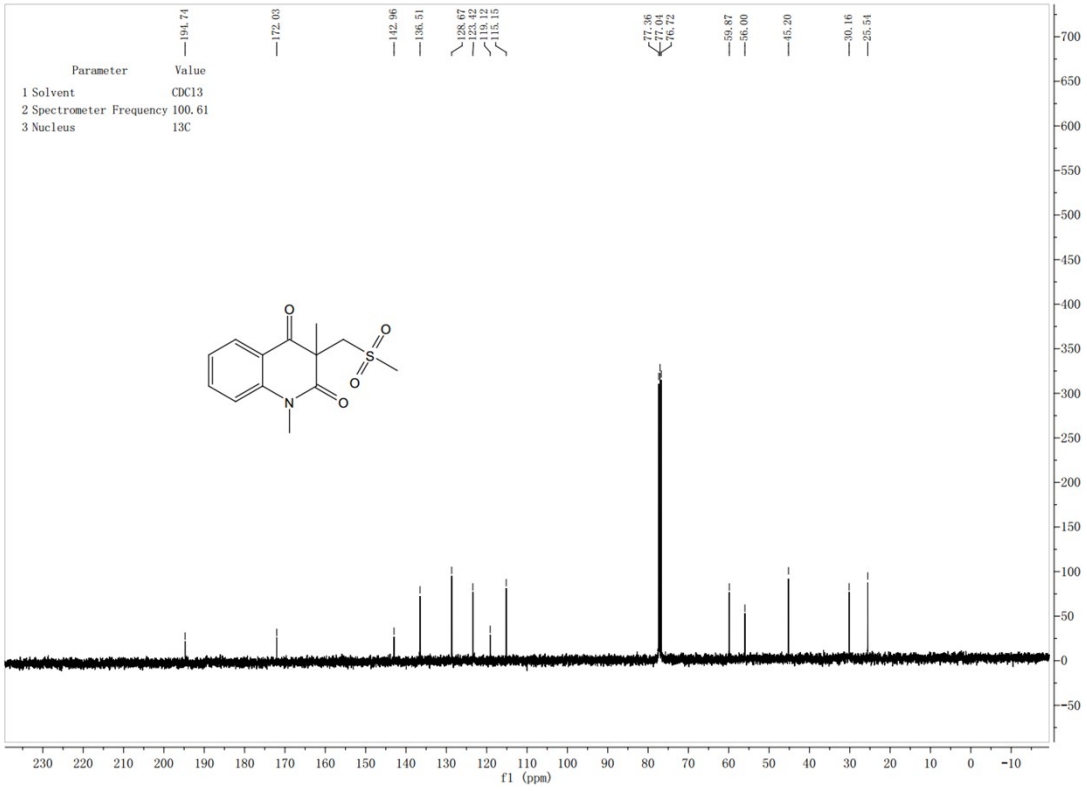
3 Nucleus 13C
f1 (ppm)

3k


Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 400.13
3 Nucleus 1H
8.10
8.08
7.68
7.25
7.24
7.23
7.22
4.16
3.54
3.04
1.46
1.00
1.05
1.87
2.00
3.00
3.00
3.03
f1 (ppm)


Parameter Value
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2 Spectrometer Frequency 100.61
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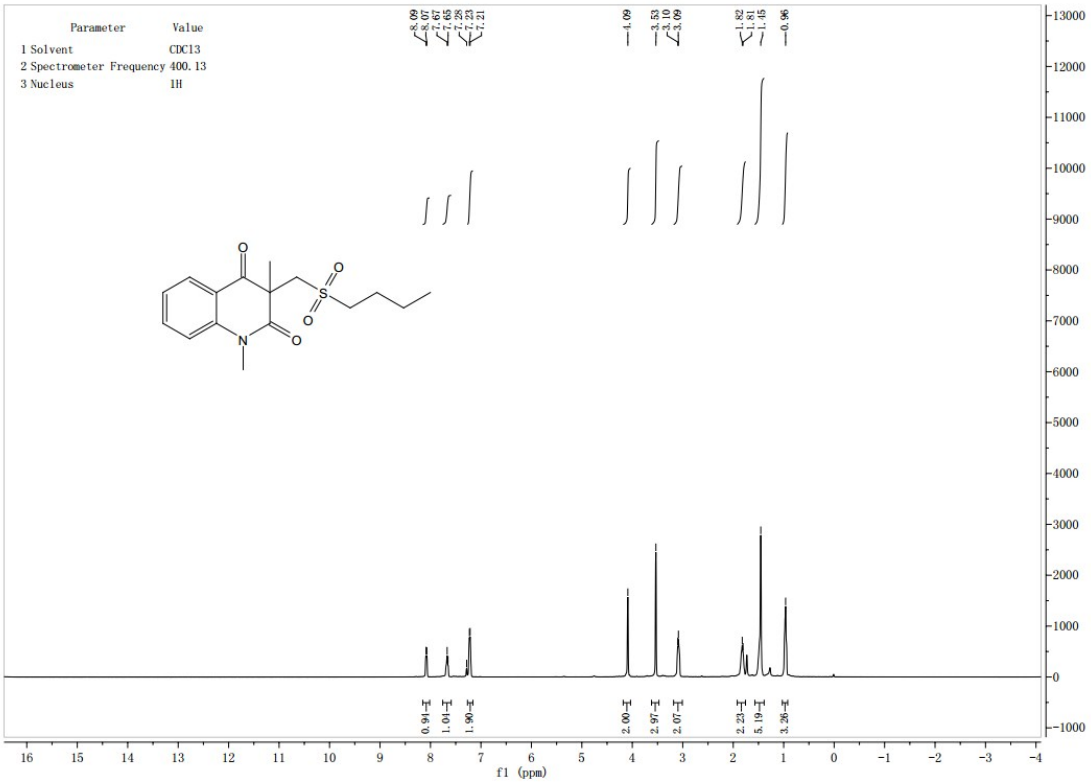
172.03
142.96
136.51
128.67
123.42
119.12
115.15
77.36
77.04
76.72
59.87
56.00
45.20
30.16
25.54
f1 (ppm)

3l


Parameter Value
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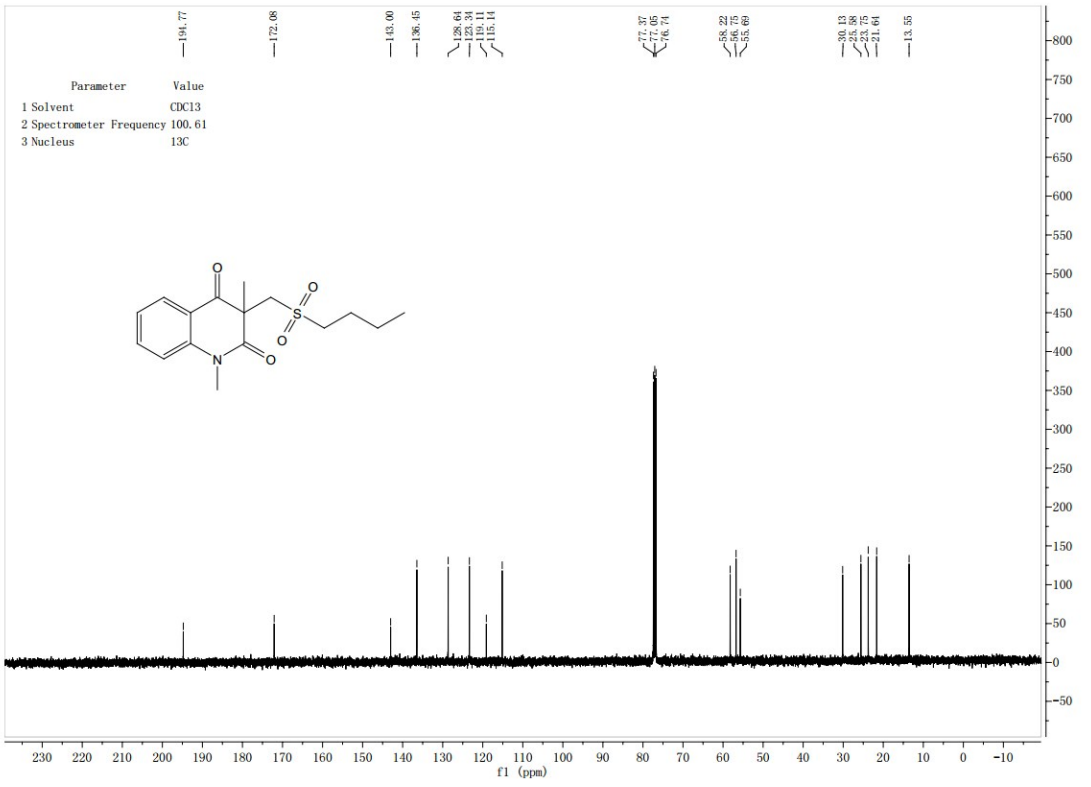
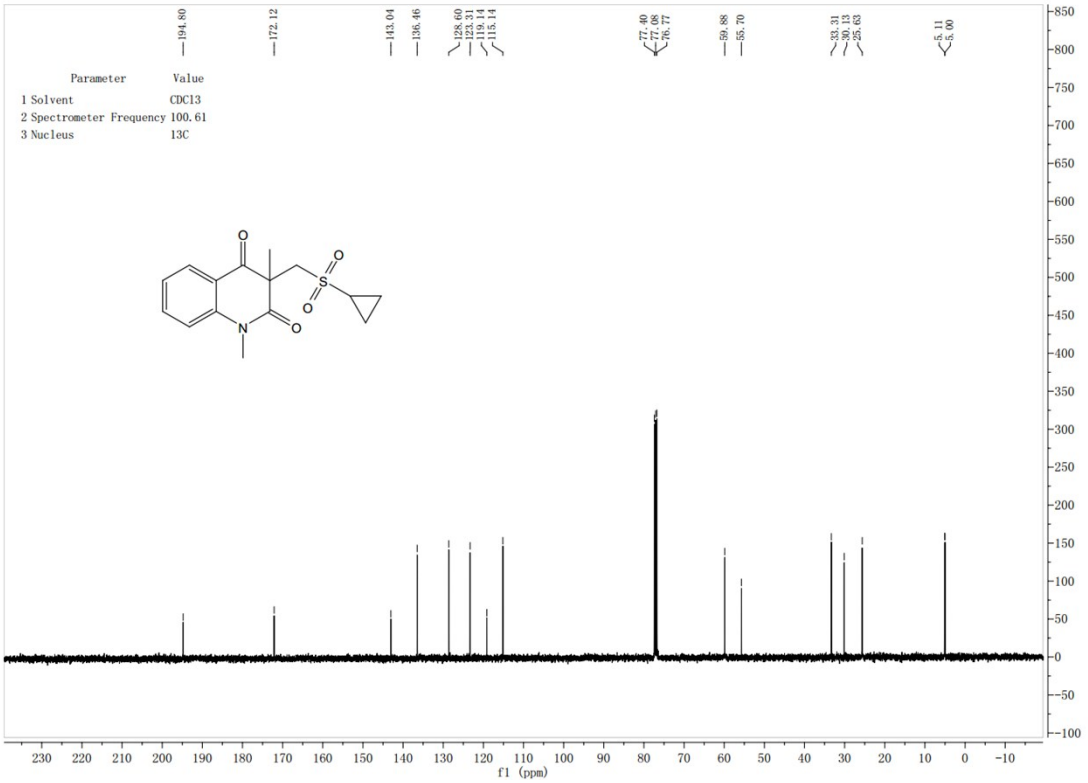
2 Spectrometer Frequency 400.13
3 Nucleus 1H
8.09
8.07
7.67
7.65
7.28
7.23
7.21
4.09
3.53
3.10
3.09
1.82
1.81
1.45
0.96
0.94
1.04
1.90
2.00
2.97
2.07
2.23
5.19
3.26
f1 (ppm)


194.77
172.08
143.00
136.45
128.64
123.34
119.11
115.14
77.37
77.05
76.74
58.22
56.75
55.69
30.13
25.58
23.75
21.64
13.55
Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 100.61
3 Nucleus 13C
f1 (ppm)

3m


Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 400.13
3 Nucleus 1H
8.09
8.07
7.68
7.66
7.65
7.28
7.23
7.21
7.19
4.21
3.53
2.63
1.46
1.20
1.01
0.99
0.95
0.99
1.95
2.00
2.99
1.01
3.05
2.14
2.16
f1 (ppm)


Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 100.61
3 Nucleus 13C
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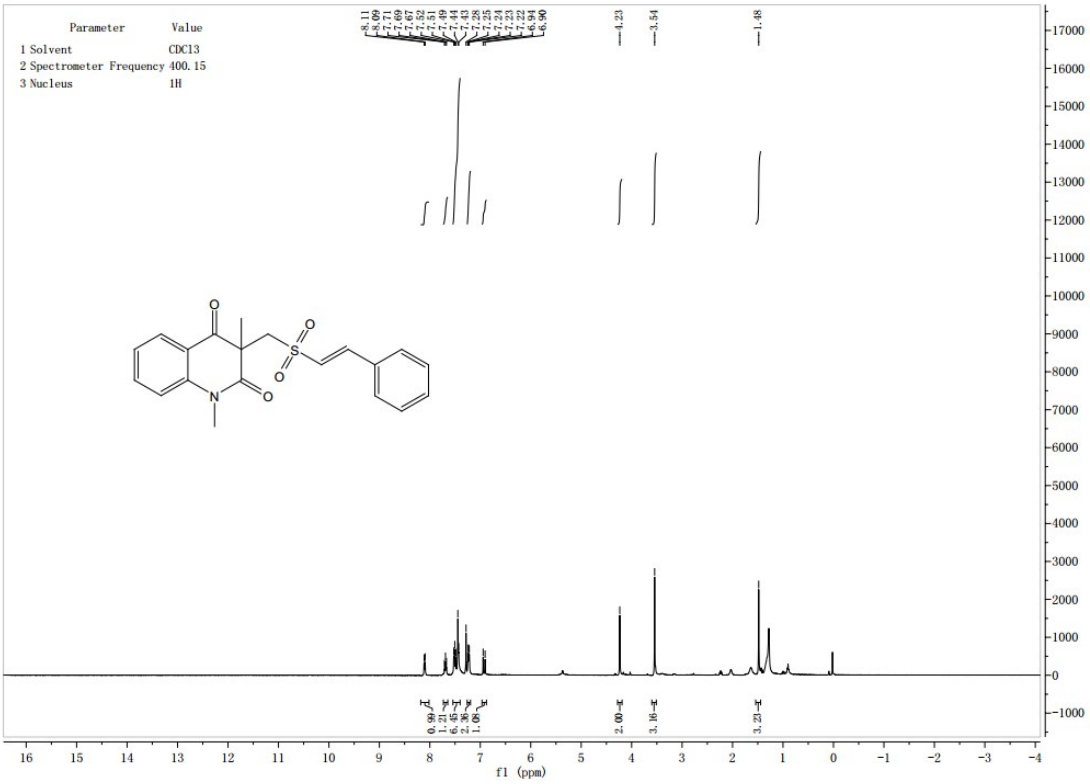
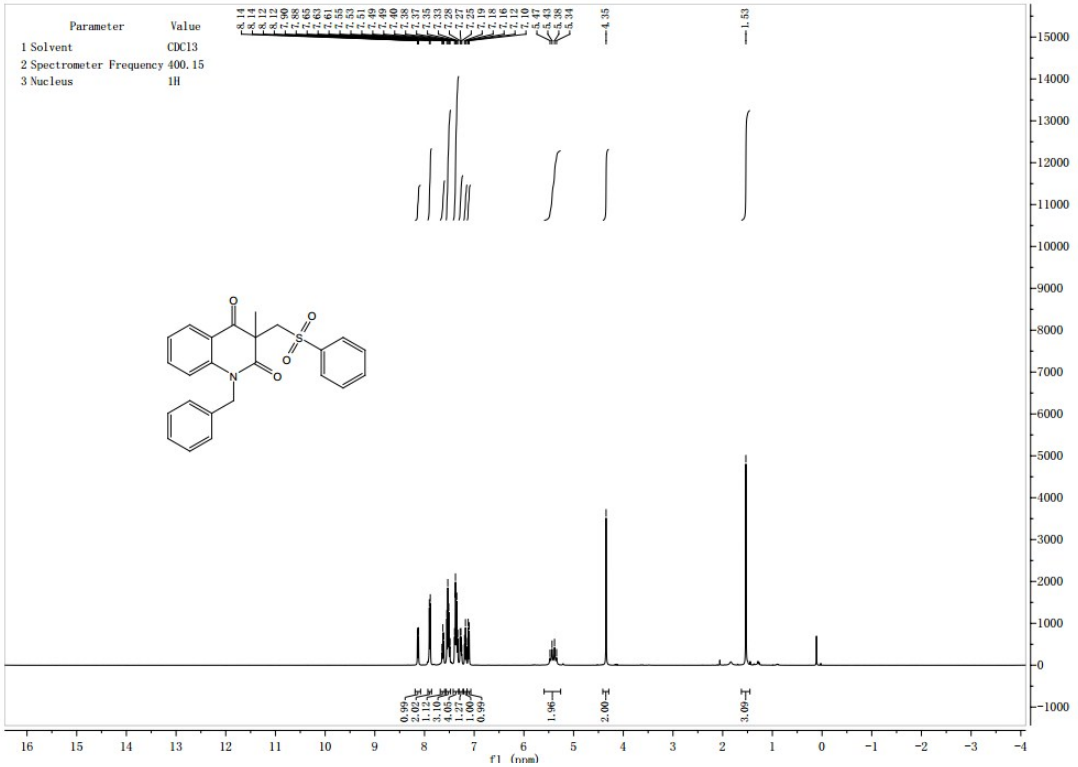
172.12
143.04
136.46
128.60
123.31
119.14
115.14
77.40
77.08
76.77
59.88
55.70
33.31
30.13
25.63
5.11
5.00
f1 (ppm)

3n


Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 400.15
3 Nucleus 1H
f1 (ppm)

3p


Parameter Value
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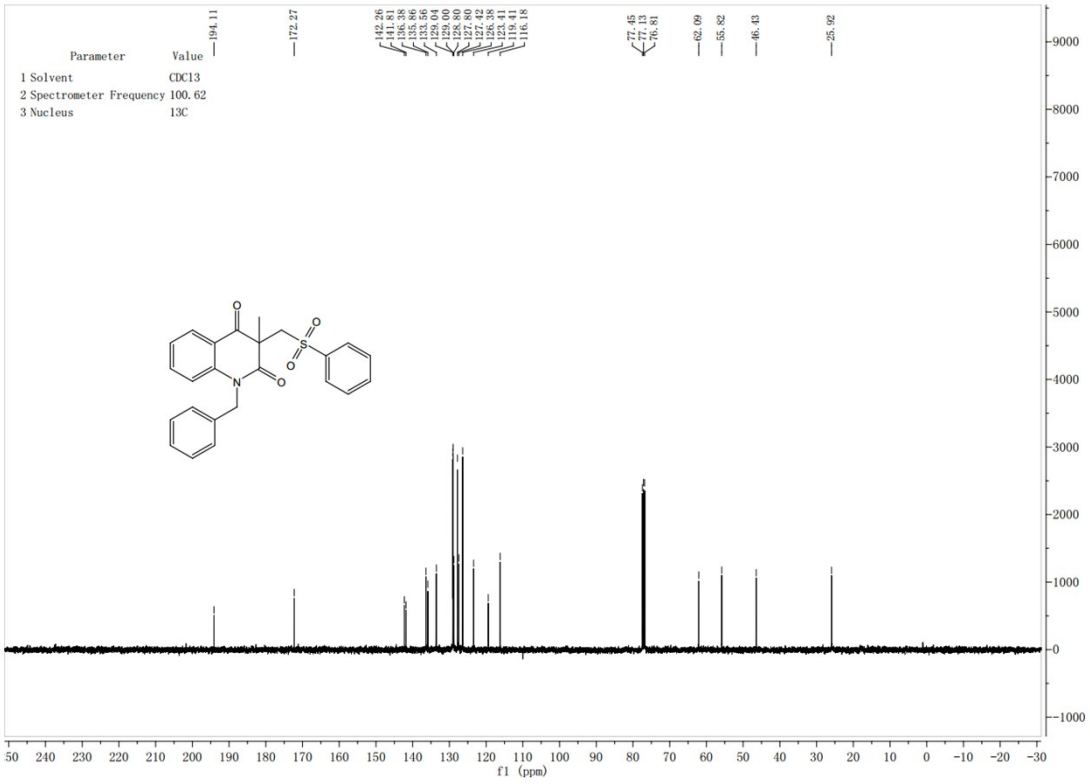
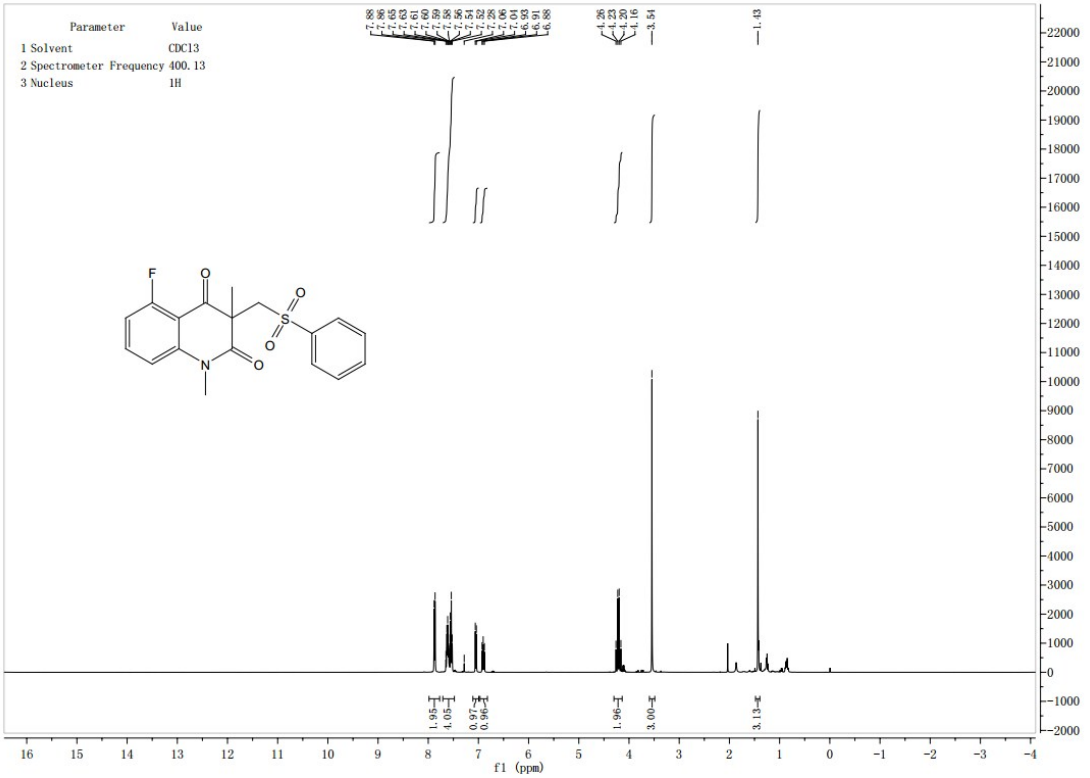
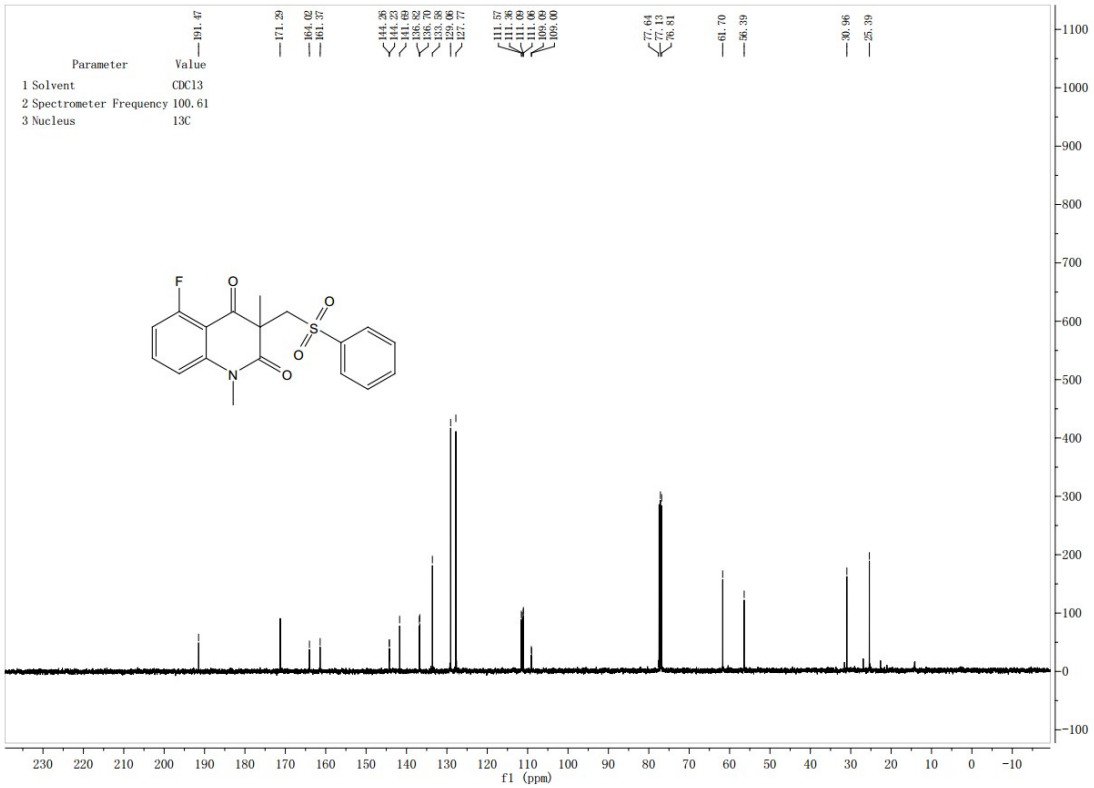
2 Spectrometer Frequency 400.15
3 Nucleus 1H
f1 (ppm)

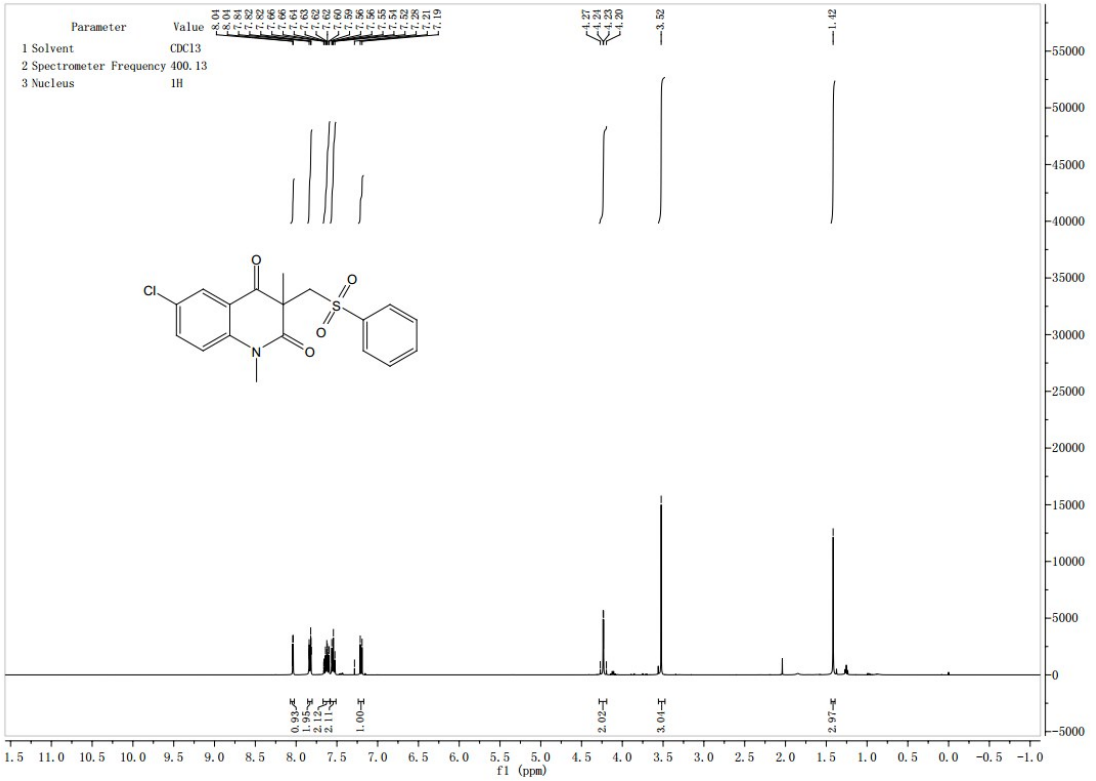

Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 100.62
3 Nucleus 13C
194.11
172.27
142.26
141.81
136.38
135.86
133.56
129.04
129.00
128.80
127.80
127.42
126.35
123.41
119.41
116.18
77.45
77.13
76.81
62.09
55.82
46.43
25.92
f1 (ppm)

3r


Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 400.13
3 Nucleus 1H
4.26
4.23
4.20
4.16
3.54
1.43
1.95
4.05
0.97
0.96
1.96
3.00
3.13
f1 (ppm)


Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 100.61
3 Nucleus 13C
191.47
171.29
164.02
161.37
144.26
144.23
141.69
136.82
136.70
133.38
129.86
127.77
111.57
111.36
111.09
111.06
109.09
109.00
77.64
77.13
76.81
61.70
56.39
30.96
25.39
F
O
O
S
O
N
O
f1 (ppm)

3s


Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 400.13
3 Nucleus 1H
8.04
8.01
7.84
7.82
7.82
7.66
7.66
7.64
7.63
7.62
7.62
7.60
7.59
7.56
7.56
7.55
7.54
7.52
7.26
7.21
7.19
4.27
4.24
4.23
4.20
3.52
1.42
Cl
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S
O
N
O
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1.95
2.12
1.00
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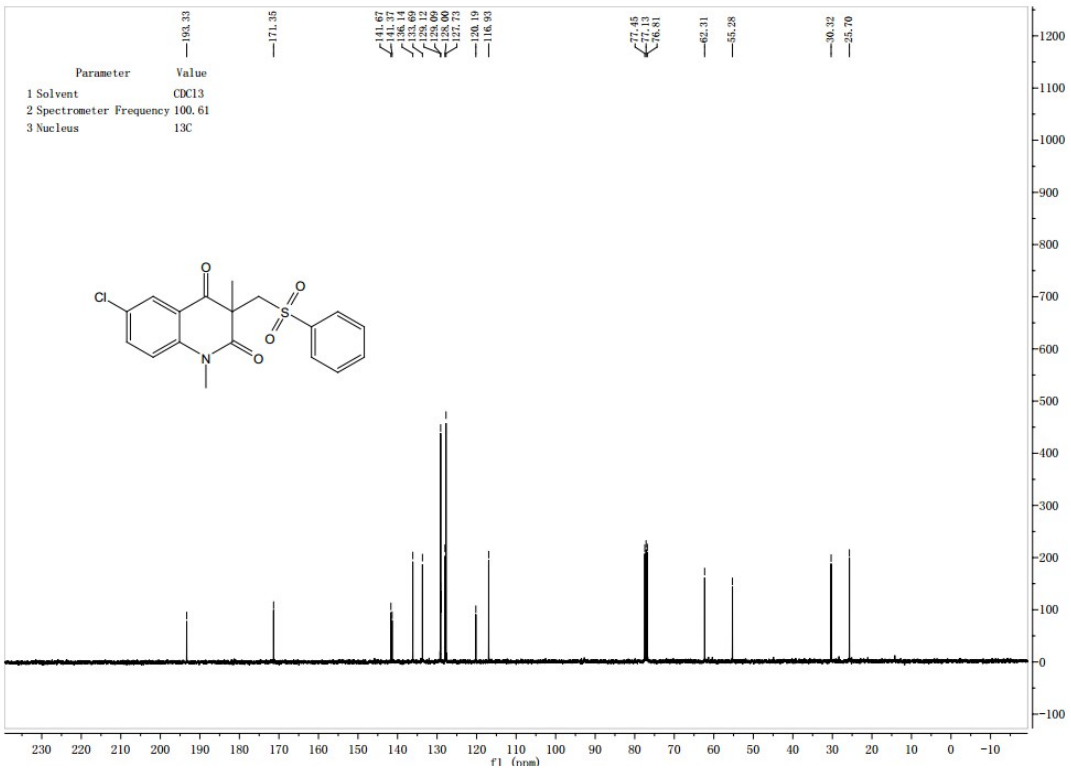
2.97
f1 (ppm)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77.13
76.81
62.31
55.28
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3 Nucleus 13C
Cl
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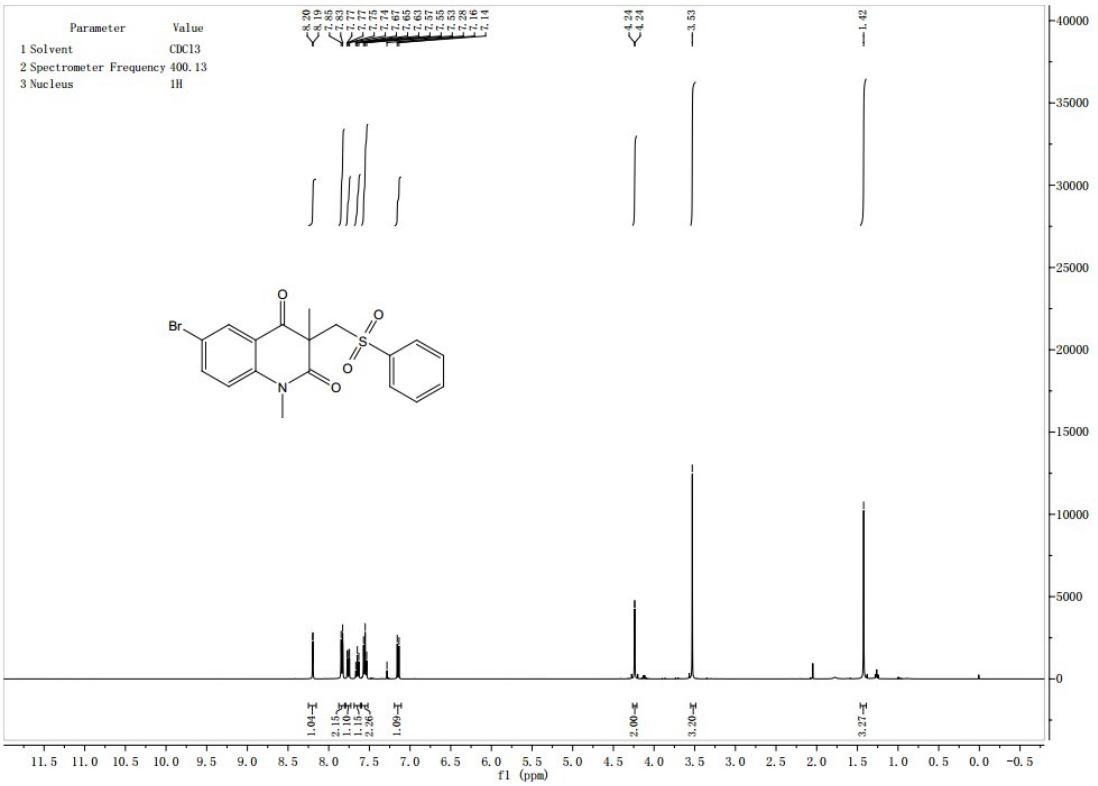
S
N
f1 (ppm)

3t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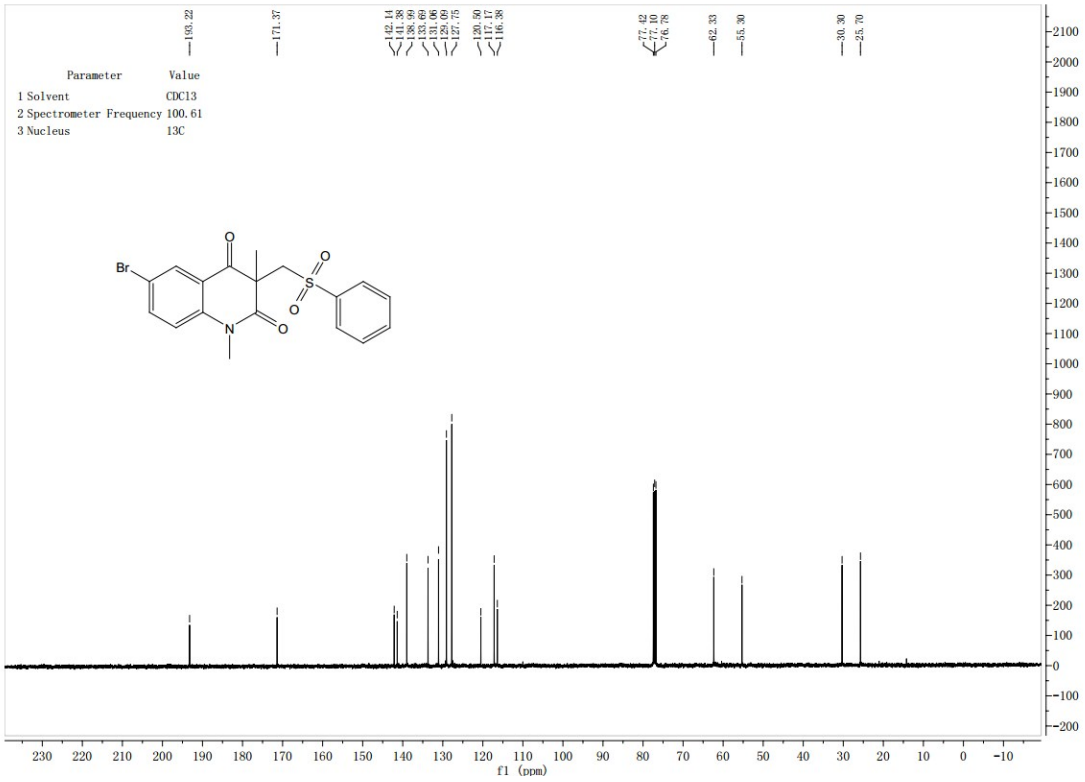
7.53
7.28
7.16
7.14
4.24
4.24
3.53
1.42
Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 400.13
3 Nucleus 1H
Br
O
S
N
1.04
2.15
1.10
1.15
2.26
1.09
2.00
3.20
3.27
f1 (ppm)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171.37
142.14
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138.64
133.69
131.06
129.09
127.75
120.50
117.17
116.38
77.42
77.10
76.78
62.33
55.30
30.30
25.70
Parameter Value
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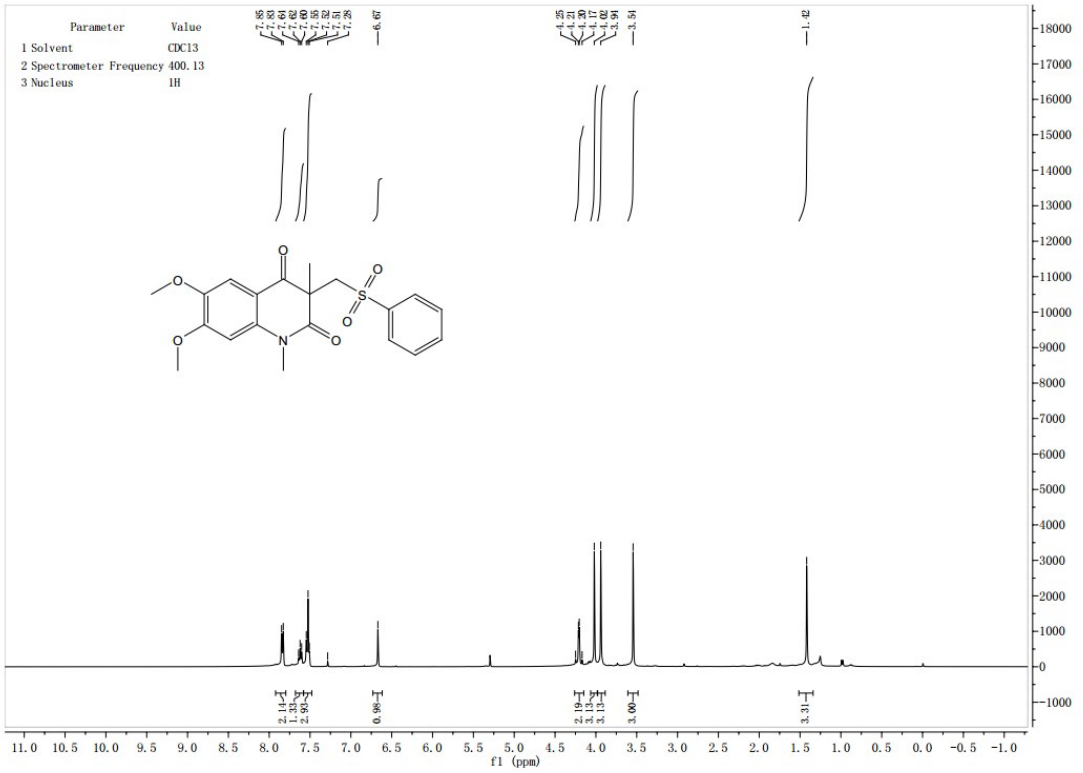
2 Spectrometer Frequency 100.61
3 Nucleus 13C
Br
O
S
N
f1 (ppm)

3u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7.83
7.65
7.62
7.60
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7.52
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7.28
6.67
4.25
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4.20
4.17
4.01
3.99
3.54
1.42
Parameter Value
1 Solvent CDC13
2 Spectrometer Frequency 400.13
3 Nucleus 1H
O
S
N
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1.33
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0.98
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3.13
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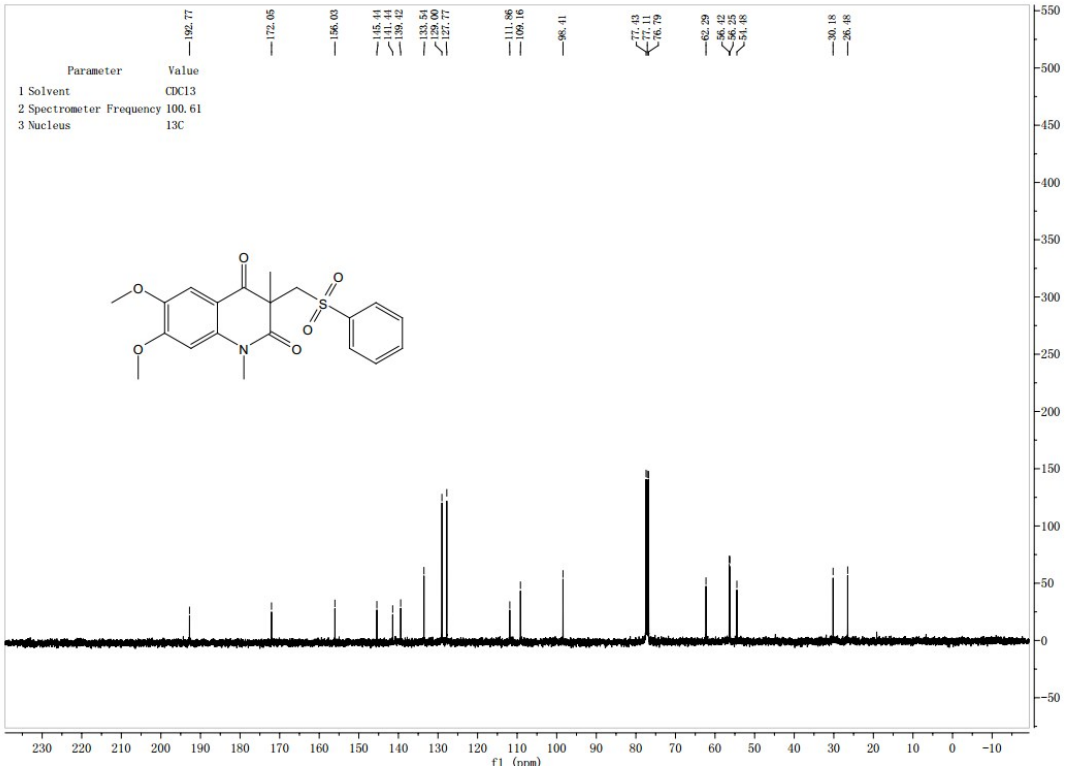
f1 (ppm)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156.03
145.44
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129.90
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111.86
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77.43
77.11
76.79
62.29
56.32
56.25
54.48
30.18
26.48
Parameter Value
1 Solvent CDCl3
2 Spectrometer Frequency 100.61
3 Nucleus 13C
O
O
O
S
O
O
N
O
f1 (ppm)