Electronic Supplementary Material (ESI) for ChemComm.


# Supporting Information

# Synthesis of Polysubstituted Cyclic 1,2-Diketones Enabled by Iterative Sulfoxide-Mediated Arylation

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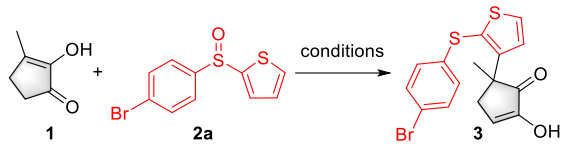
## I. General Information

Unless otherwise stated. All solvents were distilled from appropriate drying agents prior to use. All reagents were used as received from commercial suppliers unless otherwise indicated. Cyclic 1,2-Diketones [1] and sulfoxides[2] were prepared according to reported procedures. Reactions were monitored using Thin Layer Chromatography (TLC) carried out on Merck silica gel plates (60F-254) using UV light as the visualizing agent and High Performance Liquid Chromatography (HPLC) with UV detection at 254 nm. For HPLC yields, UV response factors relative to an internal standard (1-nitronaphthalene). Flash column chromatography was performed using silica gel 60 (200-300 mesh). HRMS data were recorded on Agilent 6500 QTOFMS-ESI or Waters GCT Premier TOFMS-EI. All $^{1}$H NMR, $^{13}$C NMR spectra were recorded on Bruker DRX-600 and AMX-400 instruments. Chemical shifts were given in parts per million (ppm, δ), referenced to the solvent peak of $CDCl_3$, defined at δ = 7.26 ($^{1}$H NMR), defined at δ = 77.16 ($^{13}$C NMR). Coupling constants were quoted in Hz (J). $^{1}$H NMR Spectroscopy splitting patterns were designated as singlet (s), doublet (d), triplet (t), quartet (q). Splitting patterns that could not be interpreted or easily visualized were designated as multiplet (m) or broad (br).

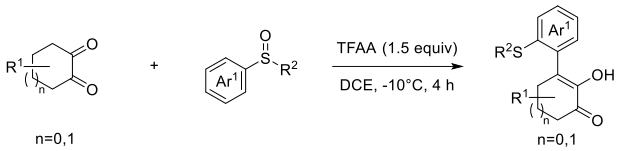
## II. General Program for the Reaction of 1,2-Diketone with Sulfoxide

**Table S1. Optimization of Reaction Conditions**[a]



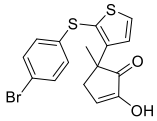

| entry | anhydride | solvent | conc. (M) | T (°C) | time (h) | yield (%)[b] |
|---|---|---|---|---|---|---|
| **1** | TFAA | DCE | 0.1 | 80 | 12 | 28 |
| **2** | TFAA | DCE | 0.125 | 80 | 12 | 61 |
| **3** | TFAA | DCE | 0.2 | 80 | 12 | 36 |
| **4** | TFAA | DCE | 0.125 | 25 | 12 | 79 |
| **5** | $Tf_2O$ | DCE | 0.125 | 25 | 12 | trace |
| **6** | **TFAA** | **DCE** | **0.125** | **-10** | **4** | **92** |
| **7** | TFAA | DCE | 0.125 | -30 | 4 | 77 |
| **8** | TFAA | DCE | 0.125 | 0 | 4 | 82 |
| **9** | TFAA | DCE | 0.125 | 30 | 4 | 67 |
| **10** | TFAA | DCE | 0.125 | -10 | 3 | 81 |
| **11** | TFAA | DCE | 0.125 | -10 | 8 | 82 |
| **12** | TFAA | MeCN | 0.125 | -10 | 4 | 88 |
| **13** | TFAA | DCM | 0.125 | -10 | 4 | 81 |

[a]The reactions were run with **1** (0.15 mmol), **2** (0.1 mmol), and TFAA (0.15 mmol). [b]Yields were determined by HPLC analysis.




TFAA (0.15 mmol, 1.5 equiv) was added to a solution of cyclic 1,2-diketones[1] (0.15 mmol, 1.5 equiv) and sulfoxide[2] (0.1 mmol, 1 equiv) in DCE (0.8 mL, 0.125 M) at -10 °C. After 4 hours, the reaction mixture was concentrated under reduced pressure and purified by column chromatography (eluent: petroleum ether/ethyl acetate = 9/1) to afford product.

**5-(2-((4-Bromophenyl)thio)thiophen-3-yl)-2-hydroxy-5-methylcyclopent-2-en-1-one (3)**



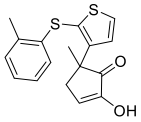
White solid, 34.7 mg, 91% yield. ($R_f$ = 0.59, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.49 (d, *J* = 5.6 Hz, 1H), 7.34 (d, *J* = 8.5 Hz, 2H), 7.19 (d, *J* = 5.6 Hz, 1H), 6.91 (d, *J* = 8.5 Hz, 2H), 6.35 (t, *J* = 3.1 Hz, 1H), 5.55 (s, 1H), 2.68 (dd, *J* = 17.9, 2.8 Hz, 1H), 2.60 (dd, *J* = 17.9, 3.3 Hz, 1H), 1.57 (s, 3H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 205.6, 150.4, 150.2, 136.8, 131.9, 130.6, 129.0, 128.5, 127.8, 125.7, 124.8, 47.3, 41.4, 26.1.

HRMS-ESI (m/z) $[M-H]^-$ calculated for $C_{16}H_{12}BrO_2S_2$ 378.9468, found 378.9453.

**2-Hydroxy-5-methyl-5-(2-(*o*-tolylthio)thiophen-3-yl)cyclopent-2-en-1-one (4)**



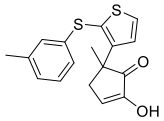
White solid, 28.5 mg, 90% yield. ($R_f$ = 0.62, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.47 (d, *J* = 5.6 Hz, 1H), 7.21 (d, *J* = 5.6 Hz, 1H), 7.13 – 7.10 (m, 1H), 7.07 – 7.02 (m, 2H), 6.75 (dd, *J* = 7.2, 2.0 Hz, 1H), 6.32 (t, *J* = 3.1 Hz, 1H), 5.72 (s, 1H), 2.80 (dd, *J* = 17.9, 2.9 Hz, 1H), 2.58 (dd, *J* = 17.9, 3.4 Hz, 1H), 2.33 (s, 3H), 1.57 (s, 3H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 204.2, 148.9, 147.9, 135.9, 133.2, 128.3, 126.9, 124.9, 124.5, 124.33, 124.25, 123.9, 123.3, 45.7, 39.4, 24.4, 18.0.

**HRMS-ESI (m/z)** $[M-H]^-$ calculated for $C_{17}H_{15}O_2S_2$ 315.0519, found 315.0516.

**2-Hydroxy-5-methyl-5-(2-(*m*-tolylthio)thiophen-3-yl)cyclopent-2-en-1-one (5)**



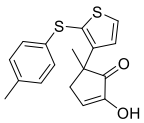
White solid, 30.6 mg, 97% yield. ($R_f$ = 0.61, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.44 (d, *J* = 5.6 Hz, 1H), 7.18 (d, *J* = 5.6 Hz, 1H), 7.12 (t, *J* = 7.7 Hz, 1H), 6.95 (d, *J* = 7.5 Hz, 1H), 6.92 (s, 1H), 6.86 (dd, *J* = 7.9, 0.5 Hz, 1H), 6.34 (t, *J* = 3.1 Hz, 1H), 5.69 (s, 1H), 2.76 (dd, *J* = 17.9, 2.9 Hz, 1H), 2.60 (dd, *J* = 17.9, 3.4 Hz, 1H), 2.28 (s, 3H), 1.57 (s, 3H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 205.9, 150.4, 149.5, 138.7, 138.1, 130.1, 128.7, 128.3, 127.2, 126.9, 126.0, 125.8, 123.8, 47.4, 41.2, 26.1, 21.4.

**HRMS-ESI (m/z)** $[M+H]^+$ calculated for $C_{17}H_{17}O_2S_2$ 317.0664, found 317.0663.

**2-Hydroxy-5-methyl-5-(2-(*p*-tolylthio)thiophen-3-yl)cyclopent-2-en-1-one (6)**



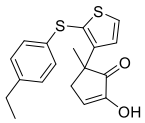
White solid, 27.5 mg, 87% yield. ($R_f$ = 0.63, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.42 (d, *J* = 5.6 Hz, 1H), 7.16 (d, *J* = 5.6 Hz, 1H), 7.05 (d, *J* = 8.1 Hz, 2H), 7.01 – 6.98 (m, 2H), 6.35 (t, *J* = 3.1 Hz, 1H), 5.69 (s, 1H), 2.74 (dd, *J* = 17.9, 2.9 Hz, 1H), 2.60 (dd, *J* = 17.9, 3.4 Hz, 1H), 2.29 (s, 3H), 1.57 (s, 3H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 205.8, 150.3, 149.1, 136.1, 134.6, 129.7, 128.2, 127.2, 126.6, 125.7, 125.6, 47.3, 41.3, 26.2, 20.9.

**HRMS-ESI (m/z)** $[M-H]^-$ calculated for $C_{17}H_{15}O_2S_2$ 315.0519, found 315.0521.

**5-(2-((4-Ethylphenyl)thio)thiophen-3-yl)-2-hydroxy-5-methylcyclopent-2-en-1-one (7)**



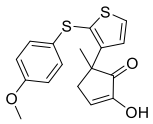
White solid, 31.8 mg, 96% yield. ($R_f$ = 0.65, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.42 (d, *J* = 5.6 Hz, 1H), 7.16 (d, *J* = 5.6 Hz, 1H), 7.09 – 7.06 (m, 2H), 7.04 – 7.00 (m, 2H), 6.35 (t, *J* = 3.1 Hz, 1H), 5.77 (s, 1H), 2.75 (dd, *J* = 17.9, 2.9 Hz, 1H), 2.60 (dd, *J* = 17.9, 3.4 Hz, 1H), 2.59 (q, *J* = 7.6 Hz, 2H), 1.57 (s, 3H), 1.20 (t, 3H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 205.9, 150.4, 149.1, 142.4, 134.8, 129.8, 128.5, 128.2, 127.2, 126.6, 125.8, 47.3, 41.3, 28.3, 26.2, 15.4.

**HRMS-ESI (m/z)** [M-H]$^-$ calculated for $C_{18}H_{17}O_2S_2$ 329.0675, found 329.0668.

**2-Hydroxy-5-(2-((4-methoxyphenyl)thio)thiophen-3-yl)-5-methylcyclopent-2-en-1-one (8)**



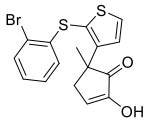
White solid, 32.2 mg, 97% yield. ($R_f$ = 0.61, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.37 (d, *J* = 5.6 Hz, 1H), 7.14 – 7.09 (m, 3H), 6.83 – 6.78 (m, 2H), 6.38 (t, *J* = 3.1 Hz, 1H), 5.71 (s, 1H), 3.77 (s, 3H), 2.75 (dd, *J* = 17.9, 2.9 Hz, 1H), 2.60 (dd, *J* = 17.9, 3.4 Hz, 1H), 1.57 (s, 3H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 206.1, 158.7, 150.5, 148.1, 129.9, 129.1, 128.3, 128.2, 128.1, 125.8, 114.6, 55.3, 47.3, 41.3, 26.0.

**HRMS-ESI (m/z)** [M-H]$^-$ calculated for $C_{17}H_{15}O_3S_2$ 331.0468, found 331.0460.

**5-(2-((2-Bromophenyl)thio)thiophen-3-yl)-2-hydroxy-5-methylcyclopent-2-en-1-one (9)**

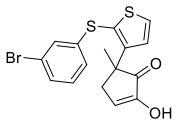


White solid, 32.0 mg, 84% yield. ($R_f$ = 0.60, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.54 (d, *J* = 5.6 Hz, 1H), 7.47 (dd, *J* = 7.9, 0.8 Hz, 1H), 7.25 (d, *J* = 5.6 Hz, 1H), 7.18 – 7.12 (m, 1H), 6.98 (td, *J* = 7.9, 1.3 Hz, 1H), 6.66 (dd, *J* = 8.0, 1.2 Hz, 1H), 6.37 (t, *J* = 3.1 Hz, 1H), 5.30 (s, 1H), 2.82 (dd, *J* = 18.0, 2.9 Hz, 1H), 2.65 (dd, *J* = 17.9, 3.3 Hz, 1H), 1.57 (s, 3H)；**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 205.8, 150.9, 150.8, 139.9, 132.5, 131.3, 128.9, 127.7, 126.8, 126.7, 126.5, 123.7, 119.6, 47.42, 41.2, 26.1.

**HRMS-ESI (m/z)** [M-H]$^-$ calculated for $C_{16}H_{12}BrO_2S_2$ 378.9468, found 378.9474.

**5-(2-((3-Bromophenyl)thio)thiophen-3-yl)-2-hydroxy-5-methylcyclopent-2-en-1-one (10)**



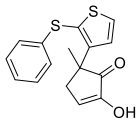
White solid, 36.2 mg, 95% yield. ($R_f$ = 0.58, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.52 (dd, *J* = 5.6, 0.7 Hz, 1H), 7.28 (dd, *J* = 3.8, 2.9 Hz, 1H), 7.25 – 7.18 (m, 2H), 7.11 (t, *J* = 7.9 Hz, 1H), 7.03 – 6.95 (m, 1H), 6.38 (dd, *J* = 4.5, 1.8 Hz, 1H), 5.63 (s, 1H), 2.71 (dd, *J* = 17.9, 2.8 Hz, 1H), 2.61 (dd, *J* = 17.9, 3.3 Hz, 1H), 1.59 (s, 3H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 205.7, 150.5, 150.4, 140.7, 130.9, 130.2, 129.0, 128.8, 128.7, 125.8, 124.9, 123.9, 122.9, 47.3, 41.3, 26.1.

**HRMS-ESI (m/z)** $[M+H]^+$ calculated for $C_{16}H_{14}BrO_2S_2$ 380.9613, found 380.9602.

**2-Hydroxy-5-methyl-5-(2-(phenylthio)thiophen-3-yl)cyclopent-2-en-1-one (11)**



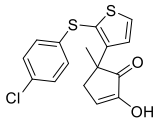
White solid, 29.0 mg, 96% yield. ($R_f$ = 0.60, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.46 (d, *J* = 5.6 Hz, 1H), 7.23 (dd, *J* = 10.9, 4.6 Hz, 2H), 7.19 (d, *J* = 5.6 Hz, 1H), 7.14 (dd, *J* = 10.6, 4.2 Hz, 1H), 7.08 – 7.05 (m, 2H), 6.33 (t, *J* = 3.1 Hz, 1H), 2.73 (dd, *J* = 17.9, 2.9 Hz, 1H), 2.59 (dd, *J* = 17.9, 3.4 Hz, 1H), 1.57 (s, 3H).

**$^{13}$C NMR** (150 MHz, CDCl3) δ 205.8, 150.4, 149.7, 138.33, 130.2, 128.9, 128.4, 126.6, 125.9, 125.7, 125.5, 47.3, 41.2, 26.1.

**HRMS-ESI (m/z)** $[M-H]^-$ calculated for $C_{16}H_{13}O_2S_2$ 301.0362, found 301.0358.

**5-(2-((4-Chlorophenyl)thio)thiophen-3-yl)-2-hydroxy-5-methylcyclopent-2-en-1-one (12)**



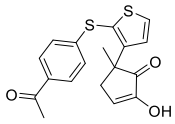
White solid, 29.3 mg, 87% yield. ($R_f$ = 0.64, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.49 (d, *J* = 5.6 Hz, 1H), 7.25 – 7.15 (m, 3H), 7.04 – 6.98 (m, 2H), 6.37 (t, *J* = 3.1 Hz, 1H), δ 2.69 (dd, *J* = 17.9, 2.9 Hz, 1H), 2.59 (dd, *J* = 17.9, 3.4 Hz, 1H), 1.58 (s, 3H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 206.0, 150.6, 150.3, 136.9, 131.9, 130.5, 129.0, 128.6, 127.8, 126.0, 124.7, 47.3, 41.4, 26.0.

**HRMS-ESI (m/z)** $[M-H]^-$ calculated for $C_{16}H_{12}ClO_2S_2$ 334.9973, found 334.9970.

**5-(2-((4-Acetylphenyl)thio)thiophen-3-yl)-2-hydroxy-5-methylcyclopent-2-en-1-one (13)**



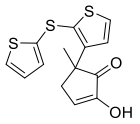
White solid, 31.7 mg, 92% yield. ($R_f$ = 0.64, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.86 – 7.73 (m, 2H), 7.53 (d, *J* = 5.6 Hz, 1H), 7.23 (d, *J* = 5.6 Hz, 1H), 7.10 – 7.00 (m, 2H), 6.32 (t, *J* = 3.1 Hz, 1H), 5.50 (s, 1H), 2.71 (dd, *J* = 17.9, 2.9 Hz, 1H), 2.60 (dd, *J* = 17.9, 3.4 Hz, 1H), 2.54 (s, 3H), 1.57 (s, 3H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 205.4, 197.1, 151.0, 150.4, 145.3, 134.5, 131.3, 128.83, 128.76, 125.6, 125.4, 122.9, 47.3, 41.4, 26.5, 26.0.

**HRMS-ESI (m/z)** $[M-H]^-$ calculated for $C_{18}H_{15}O_3S_2$ 343.0468, found 343.0460.

**2-Hydroxy-5-methyl-5-(2-(thiophen-2-ylthio)thiophen-3-yl)cyclopent-2-en-1-one (14)**



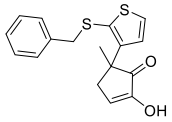
White solid, 24.6 mg, 80% yield. ($R_f$ = 0.62, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.35 – 7.28 (m, 2H), 7.10 (dd, *J* = 3.6, 1.2 Hz, 1H), 7.05 (d, *J* = 5.5 Hz, 1H), 6.93 (dd, *J* = 5.3, 3.6 Hz, 1H), 6.51 (t, *J* = 3.1 Hz, 1H), 5.73 (s, 1H), 2.91 (dd, *J* = 18.0, 2.9 Hz, 1H), 2.71 (dd, *J* = 18.0, 3.4 Hz, 1H), 1.60 (s, 3H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 206.1, 150.5, 146.6, 135.2, 131.9, 130.0, 129.3, 128.8, 127.8, 127.4, 126.2, 47.3, 41.4, 26.2.

**HRMS-ESI (m/z)** $[M+H]^+$ calculated for $C_{14}H_{13}O_2S_3$ 309.0072, found 309.0066.

**5-(2-(Benzylthio)thiophen-3-yl)-2-hydroxy-5-methylcyclopent-2-en-1-one (15)**



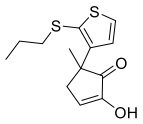

White solid, 28.7 mg, 91% yield. ($R_f$ = 0.62, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.29 (d, J = 5.5 Hz, 1H), 7.28 – 7.26 (m, 2H), 7.24 (m, 1H), 7.21 – 7.17 (m, 2H), 7.04 (d, J = 5.5 Hz, 1H), 6.41 (t, J = 3.1 Hz, 1H), 5.56 (s, 1H), 3.86 (d, *J* = 12.3 Hz, 1H), 3.83 (d, *J* = 12.3 Hz, 1H), 2.62 (dd, *J* = 17.8, 2.9 Hz, 1H), 2.57 (dd, *J* = 17.8, 3.4 Hz, 1H), 1.54 (s, 3H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 206.4, 150.4, 148.5, 136.9, 129.3, 128.7, 128.5, 127.7, 127.4, 125.6, 125.5, 47.3, 43.6, 42.0, 26.1.

**HRMS-ESI (m/z)** $[M-H]^-$ calculated for $C_{17}H_{15}O_2S_2$ 315.0519, found 315.0515.

**2-Hydroxy-5-methyl-5-(2-(propylthio)thiophen-3-yl)cyclopent-2-en-1-one (16)**



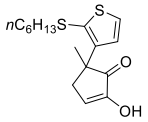

Yellow oil, 26.3 mg, 98% yield. ($R_f$ = 0.65, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.28 (d, *J* = 5.5 Hz, 1H), 7.04 (d, *J* = 5.6 Hz, 1H), 6.46 (t, *J* = 3.1 Hz, 1H), 5.65 (s, 1H), δ 2.86 (dd, *J* = 17.8, 2.9 Hz, 1H), 2.71 – 2.60 (m, 3H), 1.66 – 1.58 (m, 2H), 1.57 (s, 3H), 0.97 (t, *J* = 7.4 Hz, 3H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 206.5, 150.6, 147.2, 130.2, 127.7, 125.4, 125.2, 47.3, 41.9, 41.0, 26.1, 22.7, 13.3.

**HRMS-ESI (m/z)** $[M-H]^-$ calculated for $C_{13}H_{15}O_2S_2$ 267.0519, found 267.0517.

**5-(2-(Hexylthio)thiophen-3-yl)-2-hydroxy-5-methylcyclopent-2-en-1-one (17)**



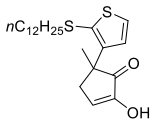

Yellow oil, 29.5 mg, 96% yield. ($R_f$ = 0.63, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.29 – 7.26 (m, 1H), 7.04 (d, *J* = 5.5 Hz, 1H), 6.45 (t, *J* = 3.0 Hz, 1H), 5.60 (s, 1H), δ 2.86 (dd, *J* = 17.8, 2.7 Hz, 1H), 2.73 – 2.62 (m, 3H), 1.61 – 1.54 (m,5H), 1.39 – 1.32 (m, 2H), 1.31 – 1.22 (m, 4H), 0.88 (t, *J* = 6.9 Hz, 3H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 206.4, 150.6, 147.2, 130.2, 127.7, 125.3, 125.1, 47.3, 41.9, 39.1, 31.4, 29.2, 28.3, 25.9, 22.5, 14.0.

**HRMS-ESI (m/z)** $[M-H]^-$ calculated for $C_{16}H_{21}O_2S_2$ 309.0988, found 309.0980.

**5-(2-(Dodecylthio)thiophen-3-yl)-2-hydroxy-5-methylcyclopent-2-en-1-one (18)**



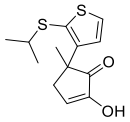
White solid, 38.6 mg, 97% yield. ($R_f$ = 0.64, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.28 (d, *J* = 5.5 Hz, 1H), 7.04 (d, *J* = 5.5 Hz, 1H), 6.45 (s, 1H), 5.57 (s, 1H), 2.86 (dd, *J* = 17.8, 2.8 Hz, 1H), 2.73 – 2.61 (m, 3H), 1.60 – 1.58 (m, 1H), 1.57 (s, 3H), 1.38 – 1.22 (m, 19H), 0.88 (t, *J* = 7.0 Hz, 3H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 206.4, 150.6, 147.2, 130.3, 127.7, 127.6, 125.2, 47.3, 41.9, 39.1, 31.9, 29.6, 29.62, 29.58, 29.5, 29.34, 29.28, 29.2, 28.7, 26.0, 22.7, 14.1.

**HRMS-ESI (m/z)** [M-H]$^-$ calculated for $C_{22}H_{33}O_2S_2$ 393.1927, found 393.1916.

**2-Hydroxy-5-(2-(isopropylthio)thiophen-3-yl)-5-methylcyclopent-2-en-1-one (19)**



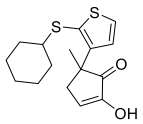
Yellow oil, 25.7 mg, 96% yield. ($R_f$ = 0.66, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.30 (d, *J* = 5.6 Hz, 1H), 7.07 (d, *J* = 5.6 Hz, 1H), 6.46 (t, *J* = 3.1 Hz, 1H), 5.55 (s, 1H), 3.06 – 2.95 (m, 1H), 2.88 (dd, *J* = 17.8, 2.8 Hz, 1H), 2.65 (dd, *J* = 17.8, 3.4 Hz, 1H), 1.28 (d, *J* = 6.7 Hz, 3H),1.57 (s, 3H), 1.21 (d, *J* = 6.8 Hz, 3H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 206.5, 150.5, 148.0, 129.2, 127.8, 125.4, 125.2, 47.3, 41.9, 26.1, 23.3, 22.7.

**HRMS-ESI (m/z)** [M-H]$^-$ calculated for $C_{13}H_{15}O_2S_2$ 267.0519, found 267.0513.

**5-(2-(Cyclohexylthio)thiophen-3-yl)-2-hydroxy-5-methylcyclopent-2-en-1-one (20)**



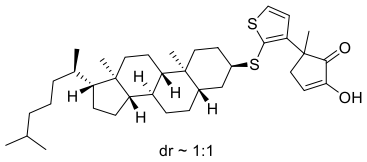
Yellow oil, 28.3 mg, 92% yield. ($R_f$ = 0.65, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.28 (d, *J* = 5.6 Hz, 1H), 7.07 (d, *J* = 5.6 Hz, 1H), 6.46 (t, *J* = 3.1 Hz, 1H), 5.63 (s, 1H), 2.88 (dd, *J* = 17.8, 2.8 Hz, 1H), 2.80 – 2.71 (m, 1H), 2.65 (dd, *J* = 17.8, 3.4 Hz, 1H), 2.08 – 1.95 (m, 1H), 1.94 – 1.82 (m, 1H), 1.80 – 1.67 (m, 2H), 1.59 (d, *J* = 4.4 Hz, 1H), 1.57 (s, 3H), 1.40 – 1.32 (m, 1H), 1.31 – 1.20 (m, 4H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 206.5, 150.6, 147.7, 128.9, 127.7, 125.4, 50.4, 47.3, 41.9, 33.5, 33.0, 26.1, 26.1, 25.9, 25.7.

**HRMS-ESI (m/z)** [M-H]$^-$ calculated for $C_{16}H_{19}O_2S_2$ 307.0832, found 307.0829.

**5-(2-(((3*R*,5*S*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-10,13-dimethyl-17-((*R*)-6-methylheptan-2-yl)hexadecahydro-1H-cyclopenta[*a*]phenanthren-3-yl)thio)thiophen-3-yl)-2-hydroxy-5-methylcyclopent-2-en-1-one (21)**



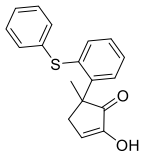
White solid, 44.1 mg, 74% yield. ($R_f$ = 0.66, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.30 (d, *J* = 5.6 Hz, 2H), δ 7.09 (d, *J* = 5.6 Hz, 1H), 7.08 (d, *J* = 5.6 Hz, 1H), 6.49 (m, 2H), 5.68 (s, 1H), 5.62 (s, 1H), 3.25 (d, *J* = 10.5 Hz, 2H), 2.87 (m, 2H), 2.67 (dd, *J* = 17.7, 3.4 Hz, 2H), 2.00 (m, 2H), 1.92 – 1.75 (m, 7H), 1.74 – 1.63 (m, 6H), 1.59 (s, 6H), 1.52 – 1.47 (m, 8H), 1.39 – 1.32 (m, 5H), 1.30 – 1.21 (m, 10H), 1.19 – 1.10 (m, 12H), 1.08 – 0.97 (m, 8H), 0.93 – 0.88 (m, 22H), 0.78 (s, 6H), 0.67 (s, 6H).

**$^{13}$C NMR** (151 MHz, $CDCl_3$) δ 206.61, 206.60, 150.58, 150.5, 147.84, 147.75, 129.99, 129.97, 127.75, 127.72, 127.71, 127.68, 125.32, 125.27, 56.5, 56.3, 54.2, 50.3, 50.1, 47.3, 42.6, 42.03, 42.01, 40.9, 40.5, 40.0, 39.5, 36.23, 36.20, 35.8, 35.48, 35.47, 33.6, 33.4, 33.2, 33.1, 32.0, 31.9, 28.4, 28.3, 28.0, 26.8, 26.4, 26.13, 26.10, 24.2, 23.9, 22.9, 22.6, 20.8, 18.7, 12.1, 11.9.

**HRMS-ESI (m/z)** $[M+H]^+$ calculated for $C_{37}H_{57}O_2S_2$ 597.3794, found 597.3764.

**2-Hydroxy-5-methyl-5-(2-(phenylthio)phenyl)cyclopent-2-en-1-one (22)**



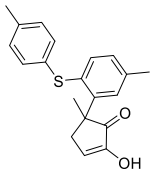

White solid, 26.9 mg, 91% yield. ($R_f$ = 0.59, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.54 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.39 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.35 – 7.31 (m, 1H), 7.26 – 7.20 (m, 3H), 7.18 – 7.13 (m, 1H), 7.09 (m, 2H), 6.31 (t, *J* = 3.1 Hz, 1H), 5.61 (s, 1H), 2.76 (dd, *J* = 17.7, 2.6 Hz, 1H), 2.60 (dd, *J* = 17.7,1H), 1.61 (s, 3H);

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 206.1, 150.7, 145.4, 137.4, 136.6, 133.3, 129.0, 128.8, 128.4, 128.2, 126.3, 123.4, 123.2, 50.4, 41.3, 25.3.

**HRMS-ESI (m/z)** $[M+H]^+$ calculated for $C_{18}H_{17}O_2S$ 297.0944, found 297.0939.

**2-Hydroxy-5-methyl-5-(5-methyl-2-(*p*-tolylthio)phenyl)cyclopent-2-en-1-one (23)**



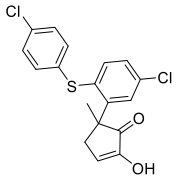

White solid, 30.5 mg, 94% yield. ($R_f$ = 0.60, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.35 (d, *J* = 1.3 Hz, 1H), 7.27 (d, *J* = 8.0 Hz, 1H), 7.09 – 7.04 (m, 1H), 7.03 (d, *J* = 8.0 Hz, 2H), 6.99 –6.97 (m, 2H), 6.31 (t, *J* = 3.1 Hz, 1H), 5.61 (s, 1H), 2.75 (dd, *J* = 17.7, 2.6 Hz, 1H), 2.54 (dd, *J* = 17.7, 3.5 Hz, 1H), 2.39 (s, 3H), 2.31 (s, 3H), 1.62 (s, 3H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 206.2, 150.7, 145.1, 138.3, 136.6, 136.0, 134.2, 130.1, 129.7, 129.3, 128.9, 128.7, 123.3, 50.4, 41.4, 25.4, 21.4, 21.0.

**HRMS-ESI (m/z)** $[M+H]^+$ calculated for $C_{20}H_{21}O_2S$ 325.1257, found 325.1250.

**5-(5-Chloro-2-((4-chlorophenyl)thio)phenyl)-2-hydroxy-5-methylcyclopent-2-en-1-one (24)**



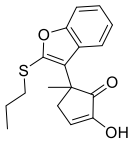

White solid, 27.4 mg, 75% yield. ($R_f$ = 0.58, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.51 (d, J = 2.1 Hz, 1H), 7.27 (d, J = 8.2 Hz, 1H), 7.23 (dd, J = 8.3, 2.2 Hz, 1H), 7.20 (d, J = 8.6 Hz, 2H), 7.00 (d, J = 8.6 Hz, 2H), 6.33 (t, J = 3.1 Hz, 1H), 5.55 (s, 1H), 2.70 (dd, J = 17.8, 2.4 Hz, 1H), 2.57 (dd, J = 17.8, 3.4 Hz, 1H), 1.58 (s, 3H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 205.4, 150.7, 147.2, 137.5, 135.3, 134.9, 132.7, 131.5, 130.1, 129.3 129.2, 128.5, 123.4, 50.3, 41.1, 25.3.

**HRMS-ESI (m/z)** $[M+H]^+$ calculated for $C_{18}H_{15}Cl_2O_2S$ 365.0164, found 365.0164.

**2-Hydroxy-5-methyl-5-(2-(propylthio)benzofuran-3-yl)cyclopent-2-en-1-one (25)**



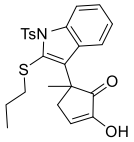

White solid, 26.6 mg, 88% yield. ($R_f$ = 0.61, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.40 (t, *J* = 7.8 Hz, 2H), 7.26 – 7.21 (m, 1H), 7.17 – 7.12 (m, 1H), 6.54 (t, *J* = 3.1 Hz, 1H), 5.85 (s, 1H), 2.97 –2.88 (m, 3H), 2.72 (dd, *J* = 18.0, 3.3 Hz, 1H), 1.82 (s, 3H), 1.70 – 1.62 (m, 2H), 1.00 (t, *J* = 7.4 Hz, 3H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 205.8, 155.5, 150.6, 146.9, 128.0, 126.1, 124.5, 124.1, 122.6, 120.3, 111.1, 45.4, 41.1, 37.0, 24.5, 23.2, 13.3.

**HRMS-ESI (m/z)** $[M+H]^+$ calculated for $C_{17}H_{19}O_3S$ 303.1049, found 303.1047.

**2-Hydroxy-5-methyl-5-(2-(propylthio)-1-tosyl-1H-indol-3-yl)cyclopent-2-en-1-one (26)**



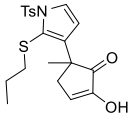

White solid, 36.7 mg, 80% yield. ($R_f$ = 0.60, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 8.38 (d, *J* = 8.6 Hz, 1H), 7.68 (d, *J* = 8.4 Hz, 2H), 7.61 (d, *J* = 8.1 Hz, 1H), 7.36 – 7.31 (m, 1H), 7.23 – 7.18 (m, 1H), 7.16 (d, *J* = 8.2 Hz, 2H), 6.36 (t, *J* = 3.0 Hz, 1H), 2.98 – 2.88 (m, 1H), 2.84 – 2.76 (m, 1H), 2.70 (dd, *J* = 17.6, 3.3 Hz, 1H), 2.66 (dd, *J* = 17.6, 2.7 Hz, 1H), 2.34 (s, 3H), 1.77 (s, 3H), 1.60 – 1.52 (m, 2H), 0.97 (t, *J* = 7.4 Hz, 3H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 205.8, 150.6, 144.7, 138.7, 135.7, 133.3, 129.5, 129.1, 129.0, 127.1, 125.4, 123.7, 123.5, 120.6, 116.2, 47.0, 42.3, 40.6, 24., 22.04, 21.6, 13.5.

**HRMS-ESI (m/z)** $[M+Na]^+$ calculated for $C_{24}H_{25}NaO_4S_2$ 478.1117, found 478.1104.

**2-Hydroxy-5-methyl-5-(2-(propylthio)-1-tosyl-1H-pyrrol-3-yl)cyclopent-2-en-1-one (27)**



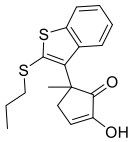

White solid, 24.3 mg, 60% yield. ($R_f$ = 0.61, petroleum ether/ethyl acetate = 9/1)

$^1$H NMR (600 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.4 Hz, 2H), 7.48 (d, *J* = 3.7 Hz, 1H), 7.27 (d, *J* = 7.4 Hz, 2H), 6.40 (t, *J* = 3.1 Hz, 1H), 6.34 (d, *J* = 3.7 Hz, 1H), 5.56 (s, 1H), 2.71 – 2.63 (m, 3H), 2.55 (dd, *J* = 17.7, 3.4 Hz, 1H), 2.40 (s, 3H), 1.50 (m, 2H), 1.44 (s, 3H), 0.93 (t, J = 7.4 Hz, 3H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 206.2, 150.4, 145.0, 139.8, 135.9, 129.6, 127.9, 125.2, 125.0, 119.7, 111.2, 45.1, 42.3, 29.7, 25.2, 21.9, 21.6, 13.4.

**HRMS-ESI (m/z)** $[M+H]^+$ calculated for $C_{20}H_{24}NO_4S_2$ 406.1141, found 406.1126.

**2-Hydroxy-5-methyl-5-(2-(propylthio)benzo[*b*]thiophen-3-yl)cyclopent-2-en-1-one (28)**



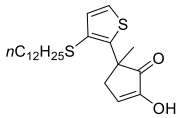

White solid, 30.2 mg, 95% yield. ($R_f$ = 0.61, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.73 – 7.66 (m, 1H), 7.64 – 7.54 (m, 1H), 7.27 (m, 1H), 7.26 – 7.24 (m, 1H), 6.46 (t, *J* = 3.1 Hz, 1H), 6.00 (s, 1H), δ 2.96 (dd, *J* = 17.8, 2.9 Hz, 1H), 2.92 – 2.81 (m, 2H), 2.77 (dd, *J* = 17.8, 3.3 Hz, 1H), 1.92 (s, 3H), 1.73 – 1.60 (m, 2H), 1.00 (t, *J* = 7.4 Hz, 3H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 206.2, 150.9, 140.8, 139.1, 138.3, 133.7, 124.5, 124.2, 124.1, 122.8, 122.0, 49.4, 41.1, 40.9, 25.4, 22.7, 13.4.

**HRMS-ESI (m/z)** $[M+H]^+$ calculated for $C_{17}H_{19}O_2S_2$ 319.0821, found 319.0816.

**5-(3-(Dodecylthio)thiophen-2-yl)-2-hydroxy-5-methylcyclopent-2-en-1-one (29)**



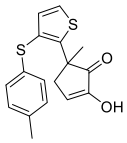

White solid, 31.5 mg, 80% yield, ($R_f$ = 0.62, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.17 (d, *J* = 5.3 Hz, 1H), 7.02 (d, *J* = 5.3 Hz, 1H), 6.49 (t, *J* = 3.1 Hz, 1H), 5.70 (s, 1H), 2.96 (dd, *J* = 17.8, 2.8 Hz, 1H), 2.78 – 2.58 (m, 3H), 1.64 (s, 3H), 1.60 – 1.48 (m, 2H), 1.41 – 1.19 (m, 18H), 0.90 (t, *J* = 6.8 Hz, 3H).

**$^{13}$C NMR** (100 MHz, $CDCl_3$) δ 205.1, 150.4, 145.7, 131.9, 127.7, 125.4, 122.8, 47.4, 41.7, 36.1, 31.9, 29.67, 29.66, 29.62, 29.56, 29.5, 29.4, 29.2, 28.8, 26.5, 22.7, 14.2.

**HRMS-ESI (m/z)** $[M+H]^+$ calculated for $C_{22}H_{35}O_2S_2$ 395.2073, found 395.2059.

**2-Hydroxy-5-methyl-5-(3-(*p*-tolylthio)thiophen-2-yl)cyclopent-2-en-1-one (30)**




White solid, 31.0 mg, 98% yield. ($R_f$ = 0.62, petroleum ether/ethyl acetate = 9/1)

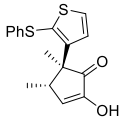
**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.19 (d, *J* = 5.3 Hz, 1H), 7.04 (d, *J* = 8.1 Hz, 2H), 6.97 (d, *J* = 8.2

Hz, 2H), 6.91 (d, *J* = 5.3 Hz, 1H), 6.42 (t, *J* = 3.1 Hz, 1H), 5.76 (s, 1H), 2.87 (dd, *J* = 17.9, 2.8 Hz, 1H), 2.69 (dd, *J* = 17.9, 3.4 Hz, 1H), 2.28 (s, 3H), 1.64 (s, 3H).

**$^{13}$C NMR** (100 MHz, $CDCl_3$) δ 204.7, 150.3, 148.4, 135.9, 133.7, 133.6, 129.7, 127.9, 126.0, 125.2, 123.3, 47.5, 41.5, 26.7, 21.0.

**HRMS-ESI (m/z)** $[M+H]^+$ calculated for $C_{17}H_{17}O_2S_2$ 317.0664, found 317.0654.

**2-Hydroxy-4,5-dimethyl-5-(2-(phenylthio)thiophen-3-yl)cyclopent-2-en-1-one (31)**



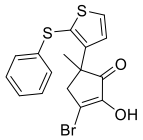

White solid, 23.4 mg, 74% yield. ($R_f$ = 0.60, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.48 (d, *J* = 5.6 Hz, 1H), 7.26 (t, *J* = 7.7 Hz, 2H), 7.19 – 7.14 (m, 1H), 7.11 (dd, *J* = 4.7, 3.2 Hz, 3H), 6.23 (d, *J* = 2.5 Hz, 1H), 5.54 (s, 1H), 2.95 (qd, *J* = 7.4, 2.6 Hz, 1H), 1.43 (s, 3H), 1.11 (d, *J* = 7.4 Hz, 3H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 206.2, 150.1, 150.0, 138.0, 130.8, 130.2, 128.8, 128.5, 126.9, 126.1, 125.6, 51.0, 43.6, 20.9, 14.6.

**HRMS-ESI (m/z)** $[M+H]^+$ calculated for $C_{17}H_{17}O_2S_2$ 317.0664, found 317.0656.

**3-Bromo-2-hydroxy-5-methyl-5-(2-(phenylthio)thiophen-3-yl)cyclopent-2-en-1-one (32)**



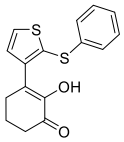

White solid, 30.5 mg, 80% yield. ($R_f$ = 0.62, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.48 (d, *J* = 5.6 Hz, 1H), 7.26 (m, 2H), 7.19 (d, *J* = 5.6 Hz, 1H), 7.16 (d, *J* = 7.4 Hz, 1H), 7.12 – 7.08 (m, 2H), 6.07 (s, 1H), 3.08 (d, *J* = 17.2 Hz, 1H), 2.87 (d, *J* = 17.2 Hz, 1H), 1.64 (s, 3H).

**$^{13}$C NMR** (151 MHz, $CDCl_3$) δ 200.8, 148.9, 148.4, 137.7, 130.3, 129.0, 128.3, 126.8, 126.2, 123.9, 49.3, 48.4, 25.7.

**HRMS-ESI (m/z)** $[M+Na]^+$ calculated for $C_{16}H_{13}BrNaO_2S_2$ 402.9433, found 402.9431.

**2-Hydroxy-3-(2-(phenylthio)thiophen-3-yl)cyclohex-2-en-1-one (33)**



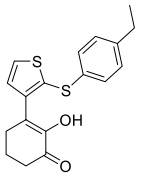

White solid, 22.6 mg, 75% yield. ($R_f$ = 0.60, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.45 (d, *J* = 5.5 Hz, 1H), 7.25 – 7.21 (m, 3H), 7.19 – 7.12 (m, 3H), 6.39 (s, 1H), 2.78 (t, *J* = 5.9 Hz, 2H), 2.55 (dd, *J* = 14.7, 7.8 Hz, 2H), 2.03 – 1.99 (m, 2H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 195.2, 144.0, 143.1, 138.2, 129.6, 129.4, 129.0, 127.3, 126.2, 125.6, 36.1, 29.4, 22.9.

**HRMS-ESI (m/z)** $[M+H]^+$ calculated for $C_{16}H_{15}O_2S_2$ 303.0508, found 303.0503.

**3-(2-((4-Ethylphenyl)thio)thiophen-3-yl)-2-hydroxycyclohex-2-en-1-one (34)**



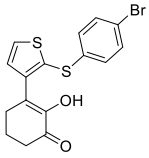
Colorless oil, 24.8 mg, 75% yield. ($R_f$ = 0.61, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.44 (d, *J* = 5.5 Hz, 1H), 7.23 (d, *J* = 5.5 Hz, 1H), δ 7.15 (d, *J* = 8.3 Hz, 1H), 7.12 – 7.09 (m, 3H), 6.41 (s, 1H), 2.82 (t, *J* = 5.9 Hz, 2H), 2.65 – 2.55 (m, 4H), 2.09 – 2.01 (m, 2H), 1.22 (t, *J* = 7.6 Hz, 3H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 195.2, 144.0, 142.8, 142.4, 134.7, 130.1, 129.4, 129.0, 128.6, 128.0, 125.8, 36.1, 29.4, 28.4, 23.0, 15.5.

**HRMS-ESI (m/z)** $[M+Na]^+$ calculated for $C_{18}H_{18}NaO_2S_2$ 353.0640, found 353.0635.

**3-(2-((4-Bromophenyl)thio)thiophen-3-yl)-2-hydroxycyclohex-2-en-1-one (35)**



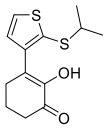
White solid, 22.9 mg, 60% yield. ($R_f$ = 0.61, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 5.5 Hz, 1H), 7.37 – 7.32 (m, 2H), 7.22 (d, *J* = 5.5 Hz, 1H), 7.03 – 6.97 (m, 2H), 6.38 (s, 1H), 2.75 (t, *J* = 5.9 Hz, 2H), 2.60 – 2.52 (m, 2H), 2.05 – 2.01 (m, 2H).

**$^{13}$C NMR** (100 MHz, $CDCl_3$) δ 195.1, 144.1, 143.8, 137.7, 132.2, 130.0, 129.6, 128.5, 127.7, 125.2, 119.9, 36.1, 29.5, 22.9.

**HRMS-ESI (m/z)** $[M+H]^+$ calculated for $C_{16}H_{14}BrO_2S_2$ 380.9613, found 380.9600.

**2-Hydroxy-3-(2-(isopropylthio)thiophen-3-yl)cyclohex-2-en-1-one (36)**



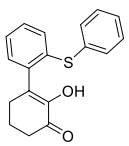
Yellow solid, 17.5 mg, 65% yield. ($R_f$ = 0.60, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.35 (d, *J* = 5.5 Hz, 1H), 7.12 (d, *J* = 5.5 Hz, 1H), 6.34 (s, 1H), 3.21 – 3.17 (m, 1H), 2.86 (t, *J* = 5.9 Hz, 2H), 2.65 – 2.59 (m, 2H), 2.10 (m, 2H), 1.24 (d, *J* = 6.7 Hz, 6H).

**$^{13}$C NMR** (151 MHz, $CDCl_3$) δ 195.3, 144.0, 142.2, 131.4, 129.2, 128.0, 126.8, 42.5, 36.2, 29.9, 23.06, 23.00.

**HRMS-ESI (m/z)** $[M+Na]^+$ calculated for $C_{13}H_{16}NaO_2S_2$ 291.0484, found 291.0493.

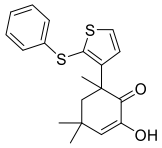
**2-Hydroxy-2'-(phenylthio)-5,6-dihydro-[1,1'-biphenyl]-3(4H)-one (37)**



Yellow solid, 17.8 mg, 60% yield. ($R_f$ = 0.60, petroleum ether/ethyl acetate = 9/1)

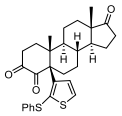
**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.32 (m, 5H), 7.24 (m, 4H), 6.15 (s, 1H), 2.69 (t, *J* = 5.7 Hz, 2H), 2.64 – 2.58 (m, 2H), 2.12 (dt, *J* = 12.5, 6.2 Hz, 2H).
**$^{13}$C NMR** (151 MHz, $CDCl_3$) δ 195.2, 143.7, 139.4, 136.0, 133.8, 132.7, 130.9, 130.5, 129.1, 129.0, 128.8, 127.5, 127.0, 36.1, 30.3, 22.9.
**HRMS-ESI (m/z)** $[M+Na]^+$ calculated for $C_{18}H_{16}NaO_2S$ 319.0763, found 319.0768.

**2-Hydroxy-4,4,6-trimethyl-6-(2-(phenylthio)thiophen-3-yl)cyclohex-2-en-1-one (38)**



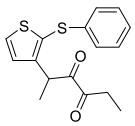

White solid, 28.9 mg, 84% yield. ($R_f$ = 0.60, petroleum ether/ethyl acetate = 9/1)
**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.41 (d, *J* = 5.6 Hz, 1H), 7.24 (d, *J* = 7.8 Hz, 2H), 7.18 – 7.09 (m, 3H), 6.88 (d, *J* = 5.6 Hz, 1H), 6.01 (s, 1H), 5.84 (s, 1H), 2.60 (d, *J* = 14.2 Hz, 1H), 1.87 (d, *J* = 14.2 Hz, 1H), 1.65 (s, 3H), 1.16 (s, 3H), 0.74 (s, 3H).
**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 197.9, 151.0, 144.3, 138.3, 130.2, 128.9, 128.4, 126.8, 126.5, 126.1, 125.2, 49.9, 47.4, 32.1, 31.8, 29.3, 26.6.
**HRMS-ESI (m/z)** $[M+H]^+$ calculated for $C_{19}H_{21}O_2S_2$ 345.0977, found 345.0964.

**(8*R*,9*S*,10*R*,13*S*,14*S*)-10,13-dimethyl-2-(2-(phenylthio)thiophen-3-yl)dodecahydro-1H-cyclopenta[a]phenanthrene-3,4,17(2H)-trione (39)**




Green solid, 37.4 mg, 76% yield. ($R_f$ = 0.40, petroleum ether/ethyl acetate = 9/1)
**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.53 (d, *J* = 5.7 Hz, 1H), 7.28 – 7.24 (m, 2H), 7.22 (m, 1H), 7.11 (d, *J* = 5.7 Hz, 1H), 6.84 – 6.79 (m, 2H), 2.95 (dd, *J* = 20.2, 6.5 Hz, 1H), 2.64 (m, 1H), 2.51 (d, *J* = 13.4 Hz, 1H), 2.42 (dd, *J* = 19.4, 8.7 Hz, 1H), 2.23 (td, *J* = 13.6, 3.6 Hz, 1H), 2.13 – 2.00 (m, 2H), 1.95 – 1.84 (m, 2H), 1.76 – 1.48 (m, 7H), 1.22 – 1.11 (m, 3H), 0.99 (s,3H), 0.87 (s, 3H).
**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 220.1, 194.3, 188.1, 153.3, 135.5, 131.3, 130.9, 128.9, 127.0, 126.3, 125.3, 61.8, 51.0, 47.3, 46.3, 40.4, 35.8, 34.5, 34.05, 31.6, 31.2, 27.5, 27.1, 21.7, 21.0, 18.7, 13.6.
**HRMS-ESI (m/z)** $[M+Na]^+$ calculated for $C_{29}H_{32}NaO_3S_2$ 515.1685, found 515.1674.

**2-(2-(Phenylthio)thiophen-3-yl)hexane-3,4-dione (40)**

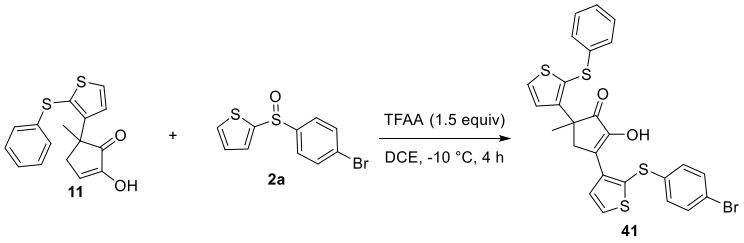



Yellow oil, 9.1 mg, 30% yield. ($R_f$ = 0.75, petroleum ether/ethyl acetate = 9/1)
**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.49 (d, *J* = 5.5 Hz, 1H), 7.27 – 7.22 (m, 2H), 7.18 – 7.14 (m, 1H), 7.11 (m, 2H), 7.05 (d, *J* = 5.5 Hz, 1H), 5.00 (q, *J* = 7.1 Hz, 1H), 2.81 – 2.73 (m, 1H), 2.47 – 2.38 (m, 1H), 1.36 (d, *J* = 7.1 Hz, 3H), 0.97 (t, *J* = 7.2 Hz, 3H).
**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 200.0, 199.0, 145.3, 138.1, 130.6, 129.1, 127.6, 127.2, 126.9, 126.1, 39.7, 30.1, 16.9, 6.8.
**HRMS-ESI (m/z)** $[M+Na]^+$ calculated for $C_{16}H_{16}NaO_2S_2$ 327.0484, found 327.0480.

## III. Procedure for Multi-Step Substituted Cyclic 1.2-Diketones

TFAA (0.15 mmol, 1.5 equiv) was added to a solution of cyclic 1,2-diketones (0.15 mmol, 1.5equiv) and sulfoxide (0.1 mmol, 1 equiv) in DCE (0.8 mL, 0.125 M) at -10 ℃. After 4 hours, the reaction mixture was concentrated under reduced pressure and purified by column chromatography (eluent: petroleum ether and ethyl acetate = 9/1) to afford product.

**3-(2-((4-Bromophenyl)thio)thiophen-3-yl)-2-hydroxy-5-methyl-5-(2-(phenylthio)thiophen-3-yl)cyclopent-2-en-1-one (41)**



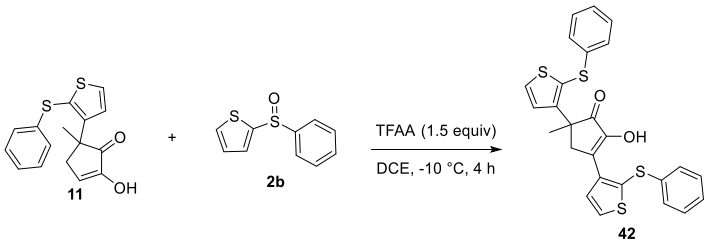

Yellow solid, 40.4 mg, 70% yield. ($R_f$ = 0.62, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.84 (d, *J* = 5.6 Hz, 1H), 7.48 (d, *J* = 5.6 Hz, 1H), 7.45 (d, *J* = 5.6 Hz, 1H), 7.35 – 7.30 (m, 2H), 7.19 (d, *J* = 5.6 Hz, 1H), 7.12 (t, *J* = 7.5 Hz, 2H), 7.06 (t, *J* = 7.3 Hz, 1H), 7.00 – 6.96 (m, 2H), 6.91 – 6.86 (m, 2H), 6.30 (s, 1H), 3.40 (d, *J* = 17.2 Hz, 1H), 3.18 (d, *J* = 17.2 Hz, 1H), 1.53 (s, 3H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 205.1, 149.8, 145.9, 139.4, 138.1, 138.0, 132.2, 130.9, 130.6, 130.2, 130.0, 129.0, 128.8, 128.5, 128.3, 126.7, 126.0, 125.5, 120.0, 46.5, 43.6, 26.3.

**HRMS-ESI (m/z)** $[M+Na]^+$ calculated for $C_{26}H_{19}BrNaO_2S_4$ 592.9343, found 592.9317.

**2-Hydroxy-5-methyl-3,5-bis(2-(phenylthio)thiophen-3-yl)cyclopent-2-en-1-one(42)**



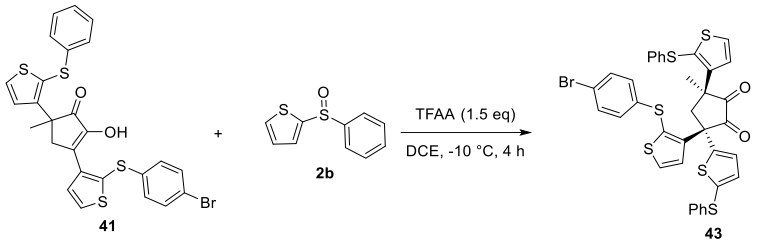

Yellow solid, 32.1 mg, 65% yield. ($R_f$ = 0.61, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 5.6 Hz, 1H), 7.45 (d, *J* = 5.6 Hz, 1H), 7.44 (d, *J* = 5.6 Hz, 1H), 7.23 (d, *J* = 7.7 Hz, 2H), 7.19 (d, *J* = 5.6 Hz, 1H), 7.18 – 7.14 (m, 1H), 7.12 (d, *J* = 7.6 Hz, 2H), 7.09 – 7.03 (m, 3H), 7.03 – 6.98 (m, 2H), 6.22 (s, 1H), 3.42 (d, *J* = 17.3 Hz, 1H), 3.25 (d, *J* = 17.3 Hz, 1H), 1.52 (s, 3H).

**$^{13}$C NMR** (100 MHz, $CDCl_3$) δ 205.2, 149.9, 145.9, 138.9, 138.5, 138.1, 131.6, 130.6, 130.3, 130.1, 129.5, 129.2, 128.8, 128.6, 127.1, 126.7, 126.3, 125.9, 125.4, 46.5, 43.6, 26.2.

**HRMS-ESI (m/z)** $[M+Na]^+$ calculated for $C_{26}H_{20}NaO_2S_4$ 515.0238, found 515.0230.

**(3*S*,5*S*)-3-(2-((4-Bromophenyl)thio)thiophen-3-yl)-5-methyl-3-(5-(phenylthio)thiophen-2-yl)-5-(2-(phenylthio)thiophen-3-yl)cyclopentane-1,2-dione (43)**



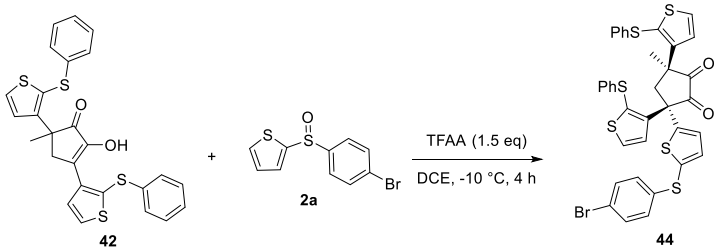

Yellow solid, 50.3 mg, 66% yield. ($R_f$ = 0.63, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.45 (d, *J* = 5.6 Hz, 1H), 7.37 (d, *J* = 5.6 Hz, 1H), 7.26 (d, *J* = 5.2 Hz, 1H), 7.28 – 7.14 (m, 10H), 7.04 (d, *J* = 3.8 Hz, 1H), 7.01 – 6.94 (m, 4H), 6.69 (d, *J* = 8.5 Hz, 2H), 3.79 (d, *J* = 14.6 Hz, 1H), 3.20 (d, *J* = 14.6 Hz, 1H), 1.53 (s, 3H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 200.8, 197.2, 152.2, 151.3, 147.8, 137.5, 137.1, 135.9, 135.4, 134.0, 131.9, 131.0, 130.9, 129.14, 129.08, 129.0, 128.6, 127.9, 127.6, 127.5, 126.6, 126.4, 126.2, 125.0, 124.4, 120.3, 52.6, 49.7, 47.2, 25.8.

**HRMS-ESI (m/z)** $[M+Na]^+$ calculated for $C_{36}H_{25}BrNaO_2S_6$ 782.9254, found 782.9243.

**(3*R*,5*R*)-3-(5-((4-Bromophenyl)thio)thiophen-2-yl)-5-methyl-3,5-bis(2-(phenylthio)thiophen-3-yl)cyclopentane-1,2-dione (44)**



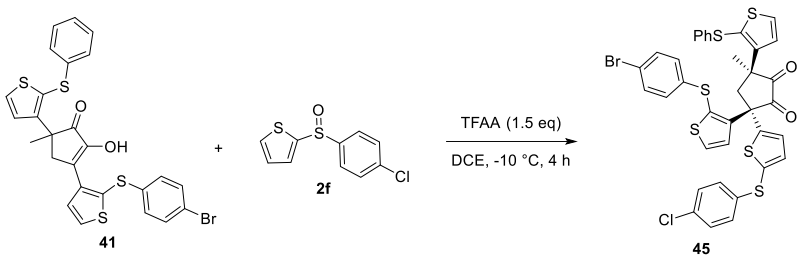

Yellow solid, 41.9 mg, 55% yield. ($R_f$ = 0.64, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.44 (d, *J* = 5.6 Hz, 1H), 7.37 (d, *J* = 5.6 Hz, 1H), 7.36 (d, *J* = 8.6 Hz, 2H), 7.28 (d, *J* = 5.5 Hz, 1H), 7.24 (t, *J* = 7.7 Hz, 2H), 7.20 – 7.12 (m, 4H), 7.06 (d, *J* = 3.8 Hz, 1H), 7.06 – 7.03 (m, 2H), 7.00 (d, *J* = 3.8 Hz, 1H), 6.98 – 6.95 (m, 2H), 6.92 (d, *J* = 5.6 Hz, 1H), 6.85 (m, 2H), 3.75 (d, *J* = 14.6 Hz, 1H), 3.23 (d, *J* = 14.6 Hz, 1H), 1.50 (s, 3H).

**$^{13}$C NMR** (151 MHz, $CDCl_3$) δ 200.6, 197.3, 151.8, 151.2, 148.7, 137.3, 137.0, 136.4, 136.0, 132.6, 132.1, 131.0, 130.5, 129.1, 129.1, 128.9, 128.70, 128.67, 127.6, 126.4, 126.3, 126.2, 126.1, 125.4, 124.9, 120.4, 52.6, 49.7, 47.2, 25.8.

**HRMS-ESI (m/z)** $[M+Na]^+$ calculated for $C_{36}H_{25}BrNaO_2S_6$ 782.9254, found 784.9260.

**(3*S*,5*S*)-3-(2-((4-Bromophenyl)thio)thiophen-3-yl)-3-(5-((4-chlorophenyl)thio)thiophen-2-yl)-5-methyl-5-(2-(phenylthio)thiophen-3-yl)cyclopentane-1,2-dione (45)**



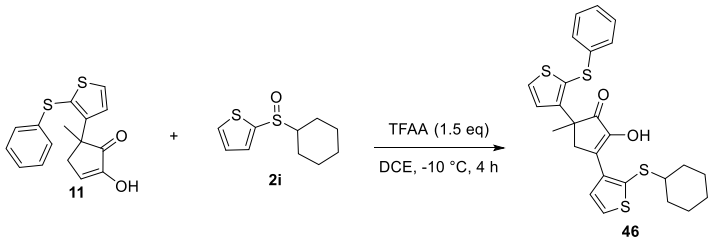

Yellow solid, 55.7 mg, 70% yield. ($R_f$ = 0.64, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.46 (d, *J* = 5.6 Hz, 1H), 7.37 (d, *J* = 5.6 Hz, 1H), 7.26 – 7.17 (m, 7H), 7.15 (t, *J* = 7.3 Hz, 1H), 7.11 (d, *J* = 8.6 Hz, 2H), 7.02 (d, *J* = 3.8 Hz, 1H), 6.95 (m, 4H), 6.66 (d, *J* = 8.6 Hz, 2H), 3.76 (d, *J* = 14.6 Hz, 1H), 3.20 (d, *J* = 14.6 Hz, 1H), 1.50 (s, 3H).

**$^{13}$C NMR** (151 MHz, $CDCl_3$) δ 200.6, 197.2, 152.0, 151.4, 148.3, 137.1, 136.0, 135.9, 135.6, 133.3, 132.7, 131.9, 131.1, 131.0, 129.3, 129.2, 129.1, 128.9, 128.7, 127.6, 127.5, 126.5, 126.1, 124.9, 124.4, 120.3, 52.6, 49.7, 47.2, 25.8.

**HRMS-ESI (m/z)** $[M+Na]^+$ calculated for $C_{36}H_{24}BrClNaO_2S_6$ 818.8865, found 818.8879.

**3-(2-(Cyclohexylthio)thiophen-3-yl)-2-hydroxy-5-methyl-5-(2-(phenylthio)thiophen-3-yl)cyclopent-2-en-1-one (46)**



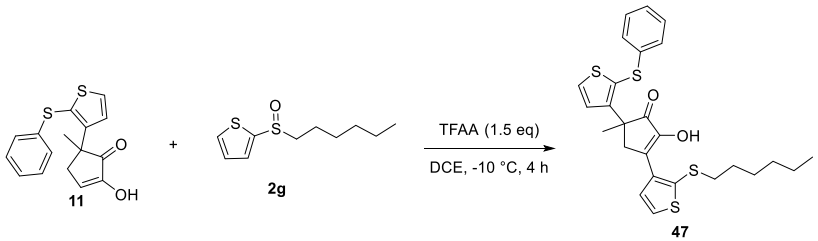

Yellow oil, 34.9 mg, 70% yield. ($R_f$ = 0.64, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.54 (d, *J* = 5.6 Hz, 1H), 7.46 (d, *J* = 5.6 Hz, 1H), 7.33 (d, *J* = 5.6 Hz, 1H), 7.25 (d, *J* = 5.6 Hz, 1H), 7.15 (t, *J* = 7.6 Hz, 2H), 7.10 – 7.03 (m, 3H),6.44 (s. 1H) 3.41 (d, *J* = 17.2 Hz, 1H), 3.33 (d, *J* = 17.2 Hz, 1H), 2.96 – 2.84 (m, 1H), 1.90 (m, 2H), 1.76 – 1.66 (m, 2H), 1.64 (s, 3H),1.58 (m, 1H), 1.34 – 1.28 (m, 2H), 1.25 – 1.18 (m, 3H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 204.9, 149.9, 145.4, 138.2, 138.1, 132.9, 132.2, 130.0, 129.8, 128.8, 128.6, 128.0, 126.8, 126.0, 125.7, 51.6, 46.7, 44.7, 33.0, 26.4, 26.0, 25.5.

**HRMS-ESI (m/z)** $[M+Na]^+$ calculated for $C_{26}H_{26}NaO_2S_4$ 521.0708, found 521.0695.

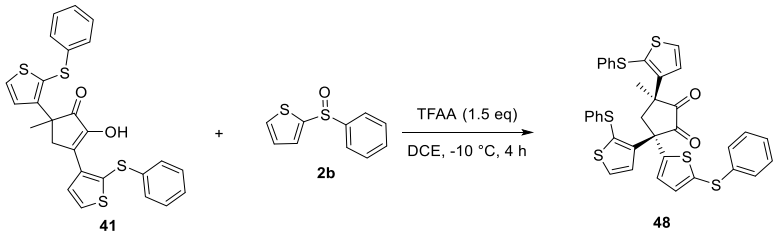
**3-(2-(Hexylthio)thiophen-3-yl)-2-hydroxy-5-methyl-5-(2-(phenylthio)thiophen-3-yl)cyclopent-2-en-1-one (47)**




Yellow oil, 32.5 mg, 65% yield. ($R_f$ = 0.63, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.68 (d, *J* = 5.6 Hz, 1H), 7.46 (d, *J* = 5.6 Hz, 1H), 7.29 (d, *J* = 5.6 Hz, 1H), 7.26 (m, 1H), 7.18 – 7.10 (m, 2H), 7.10 – 7.01 (m, 3H), 6.71 (s, 1H), 3.45 (d, *J* = 17.2 Hz, 1H), 3.36 (d, *J* = 17.2 Hz, 1H), 2.79 – 2.69 (m, 2H), 1.66 (s, 3H), 1.60 – 1.52 (m, 2H), 1.40 – 1.32 (m, 2H), 1.31 – 1.21 (m, 4H), 0.89 (t, *J* = 7.1 Hz, 3H).
**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 205.1, 150.0, 145.5, 138.3, 136.4, 135.5, 132.6, 130.08, 130.07, 128.8, 128.7, 126.78, 126.76, 125.9, 125.6, 46.7, 44.5, 39.5, 31.4, 29.2, 28.4, 26.5, 22.6, 14.1.
**HRMS-ESI (m/z)** $[M+Na]^+$ calculated for $C_{26}H_{28}NaO_2S_4$ 523.0864, found 523.1041.

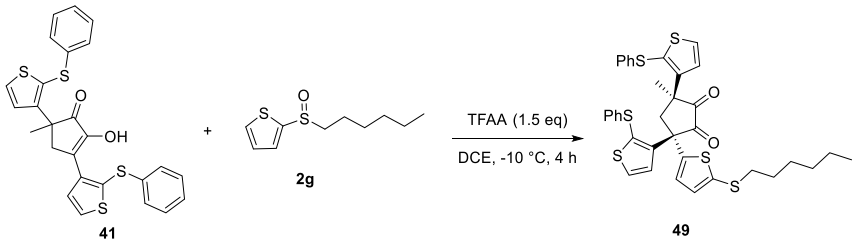
**(3*R*,5*R*)-3-Methyl-5-(5-(phenylthio)thiophen-2-yl)-3,5-bis(2-(phenylthio)thiophen-3-yl)cyclopentane-1,2-dione (48)**



41 48

Yellow solid, 44.4 mg, 65% yield. ($R_f$ = 0.64, petroleum ether/ethyl acetate = 9/1)
**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.43 (d, *J* = 5.6 Hz, 1H), 7.35 (d, *J* = 5.6 Hz, 1H), 7.27 (d, *J* = 5.6 Hz, 1H), 7.26 – 7.20 (m, 4H), 7.19 – 7.10 (m, 7H), 7.05 (d, *J* = 3.8 Hz, 1H), 6.97 (d, *J* = 3.8 Hz, 1H), 6.95 (d, *J* = 7.7 Hz, 2H), 6.91 (d, *J* = 5.6 Hz, 1H), 6.83 (d, *J* = 7.4 Hz, 2H), 3.78 (d, *J* = 14.6 Hz, 1H), 3.19 (d, *J* = 14.6 Hz, 1H), 1.51 (s, 3H).
**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 200.1, 197.3, 152.2, 151.2, 148.0, 137.7, 137.4, 136.5, 135.7, 133.4, 131.0, 130.6, 129.1, 129.1, 128.9, 128.8, 128.7, 127.8, 127.6, 126.5, 126.4, 126.3, 126.12, 126.05, 125.1, 124.9, 52.6, 49.7, 47.3, 25.8.
**HRMS-ESI (m/z)** $[M+Na]^+$ calculated for $C_{36}H_{26}NaO_2S_6$ 705.0149, found 705.0141.

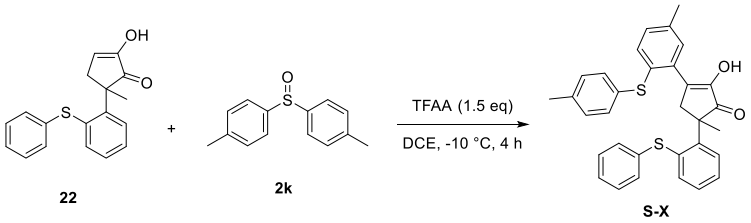
**(3*R*,5*R*)-3-(5-(Hexylthio)thiophen-2-yl)-5-methyl-3,5-bis(2-(phenylthio)thiophen-3-yl)cyclopentane-1,2-dione (49)**



41 49

Yellow oil, 36.6 mg, 53% yield. ($R_f$ = 0.63, petroleum ether/ethyl acetate = 9/1)
**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.42 (d, *J* = 5.6 Hz, 1H), 7.33 (d, *J* = 5.6 Hz, 1H), 7.27 (d, *J* = 5.6 Hz, 1H), 7.22 (t, *J* = 7.8 Hz, 2H), 7.18 – 7.09 (m, 4H), 6.99 – 6.94 (m, 2H), 6.88 (d, *J* = 5.8 Hz, 1H), 6.88 (d, *J* = 3.6 Hz, 1H), 6.86 (d, *J* = 3.7 Hz, 1H), 6.83 (d, *J* = 7.3 Hz, 2H), 3.83 (d, *J* = 14.5 Hz, 1H), 3.18 (d, *J* = 14.5 Hz, 1H), 2.77 (t, *J* = 7.3 Hz, 2H), 1.65 – 1.55 (m, 3H), 1.52 (s, 3H), 1.42 – 1.35 (m, 2H), 1.34 – 1.31 (m, 1H), 1.25 (m, 2H), 0.89 (t, *J* = 7.0 Hz, 3H).
**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 201.0, 197.3, 152.6, 151.1, 145.2, 137.5, 137.4, 136.6, 132.7, 130.8, 130.4, 129.04, 128.99, 128.9, 128.4, 127.7, 126.34, 126.26, 126.11, 126.08, 125.0, 124.9, 52.6, 49.6, 47.2, 38.7, 31.3, 29.3, 28.1, 25.9, 22.5, 14.0.
**HRMS-ESI (m/z)** $[M+Na]^+$ calculated for $C_{36}H_{34}NaO_2S_6$ 713.0775, found 713.0759.

**2-Hydroxy-5-methyl-3-(5-methyl-2-(*p*-tolylthio)phenyl)-5-(2-(phenylthio)phenyl)cyclopent-2-en-1-one (S-X)**




22 2k S-X

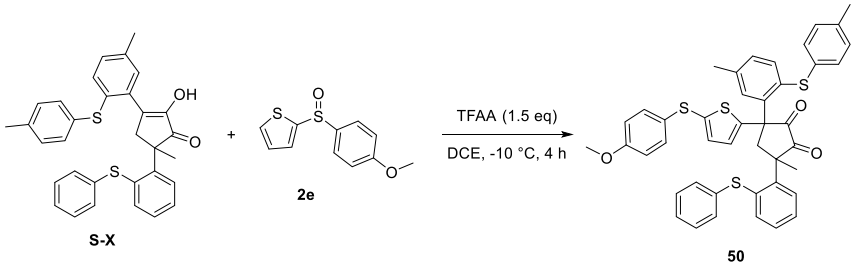
Yellow solid, 35.6 mg, 70% yield. ($R_f$ = 0.65, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.60 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.45 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.38 (m, 1H), 7.34 – 7.29 (m, 1H), 7.28 – 7.22 (m, 3H), 7.18 (m, 1H), 7.16 – 7.11 (m, 4H), 7.09 (m, 3H), 6.94 (d, *J* = 1.3 Hz, 1H), 5.95 (s, 1H), 3.19 (d, *J* = 17.0 Hz, 1H), 2.93 (d, *J* = 17.0 Hz, 1H), 2.33 (s, 3H), 2.32 (s, 3H), 1.62 (s, 3H).

**$^{13}$C NMR** (151 MHz, $CDCl_3$) δ 205.1, 146.9, 145.6, 137.9, 137.5, 136.8, 136.64, 136.62, 136.0, 133.2, 132.9, 130.9, 130.3, 130.1, 130.0, 129.9, 129.6, 129.0, 128.7, 128.53, 128.46, 128.2, 126.1, 50.4, 45.7, 25.0, 21.1, 21.0.

**HRMS-ESI (m/z)** $[M+Na]^+$ calculated for $C_{32}H_{28}NaO_2S_2$ 531.1423, found 531.1428.

**3-(5-(4-Methoxyphenyl)thiophen-2-yl)-5-methyl-3-(5-methyl-2-(*p*-tolylthio)phenyl)-5-(2-(phenylthio)phenyl)cyclopentane-1,2-dione (50)**




S-X 2e 50

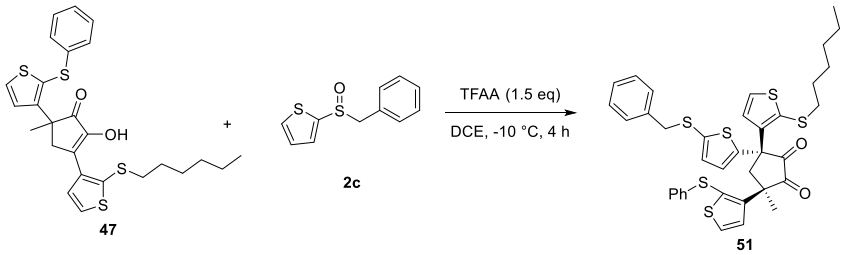
Yellow oil, 52.3 mg, 75% yield. ($R_f$ = 0.60, petroleum ether/ethyl acetate = 15/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.70 (dd, *J* = 8.1, 1.1 Hz, 1H), 7.34 – 7.26 (m, 3H), 7.26 – 7.24 (m, 1H), 7.24 – 7.14 (m, 4H), 7.13 – 7.05 (m, 3H), 7.03 – 6.90 (m, 6H), 6.82 – 6.77 (m, 2H), 6.74 (d, *J* = 8.2 Hz, 2H), 4.17 (d, *J* = 14.9 Hz, 1H), 3.77 (s, 3H), 2.88 (d, *J* = 14.9 Hz, 1H), 2.28 (s, 3H), 2.27 (s, 3H), 1.73 (s, 3H).

**$^{13}$C NMR** (151 MHz, $CDCl_3$) δ 199.1, 195.7, 159.1, 147.5, 147.3, 138.2, 136.9, 136.5, 136.2, 136.1, 135.7, 135.6, 133.8, 132.1, 131.8, 131.7, 131.2, 129.8, 129.7, 129.6, 129.3, 129.1, 128.7, 128.4, 128.2, 127.9, 127.63, 127.55, 126.8, 114.8, 55.4, 55.2, 50.7, 49.3, 25.5, 21.5, 21.1.

**HRMS-ESI (m/z)** $[M+H]^+$ calculated for $C_{46}H_{37}O_3S_4$ 729.1620, found 729.1621.

**(3R,5R)-3-(5-(Benzylthio)thiophen-2-yl)-3-(2-(hexylthio)thiophen-3-yl)-5-methyl-5-(2-(phenylthio)thiophen-3-yl)cyclopentane-1,2-dione (51)**



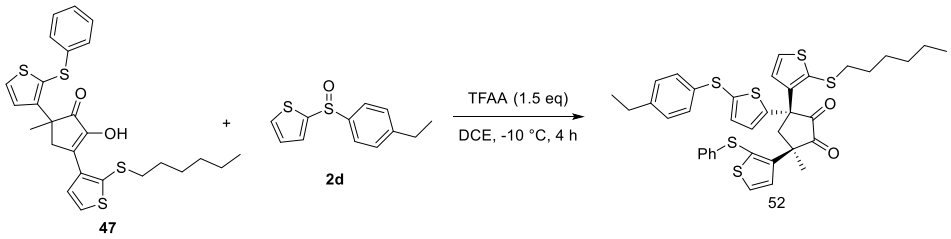

Yellow oil, 40.9 mg, 58% yield. ($R_f$ = 0.65, petroleum ether/ethyl acetate = 15/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.47 (d, *J* = 5.6 Hz, 1H), 7.39 (d, *J* = 5.6 Hz, 1H), 7.24 (m, 2H), 7.19 (t, *J* = 7.1 Hz, 2H), 7.14 (m, 5H), 7.10 – 7.05 (m, 2H), 6.90 (d, *J* = 3.8 Hz, 1H), 6.83 (d, *J* = 3.7 Hz, 1H), 6.35 (d, *J* = 5.5 Hz, 1H), 3.96 (s, 2H), 3.78 (d, *J* = 14.4 Hz, 1H), 3.02 (d, *J* = 14.5 Hz, 1H), 2.47 – 2.36 (m, 2H), 1.52 – 1.46 (m, 2H), 1.44 (s, 3H), 1.33 – 1.25 (m, 6H), 0.90 (t, *J* = 7.1 Hz, 3H).

**$^{13}$C NMR** (151 MHz, $CDCl_3$) δ 200.0, 198.8, 154.4, 149.6, 146.7, 138.4, 137.2, 135.0, 134.7, 130.5, 129.10, 129.02, 128.70, 128.67, 128.4, 128.2, 127.9, 127.6, 127.3, 126.3, 126.1, 125.9, 52.2, 50.6, 48.0, 43.4, 38.2, 31.3, 28.6, 28.4, 26.1, 22.5, 14.1.

**HRMS-ESI (m/z)** $[M+Na]^+$ calculated for $C_{37}H_{36}NaO_2S_6$ 727.0932, found 727.0957.

**(3R,5R)-3-(5-((4-Ethylphenyl)thio)thiophen-2-yl)-3-(2-(hexylthio)thiophen-3-yl)-5-methyl-5-(2-(phenylthio)thiophen-3-yl)cyclopentane-1,2-dione (52)**



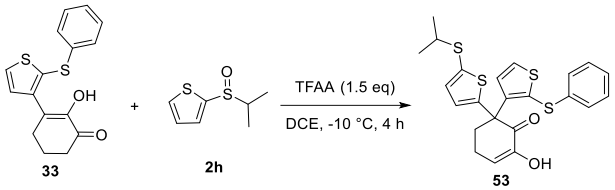

Yellow oil, 55.1 mg, 60% yield. ($R_f$ = 0.66, petroleum ether/ethyl acetate = 15/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.46 (d, *J* = 5.6 Hz, 1H), 7.38 (d, *J* = 5.6 Hz, 1H), 7.21 (m, 2H), 7.19 – 7.16 (m, 2H), 7.14 (m, 2H), 7.11 (m, 3H), 7.05 (m, 3H), 6.50 (d, *J* = 5.6 Hz, 1H), 3.82 (d, *J* = 14.5 Hz, 1H), 3.10 (d, *J* = 14.5 Hz, 1H), 2.60 (q, *J* = 7.6 Hz, 2H), 2.45 – 2.36 (m, 2H), 1.52 (s, 3H), 1.33 – 1.23 (m, 8H), 1.20 (t, *J* = 7.6 Hz, 3H), 0.90 (t, *J* = 7.1 Hz, 3H).

**$^{13}$C NMR** (151 MHz, $CDCl_3$) δ 200.2, 198.8, 153.9, 149.8, 147.6, 143.1, 138.2, 135.0, 134.5, 134.1, 130.5, 129.1, 128.8, 128.7, 128.5, 128.44, 128.40, 127.91, 127.89, 126.3, 126.1, 125.8, 52.4, 50.4, 47.9, 38.2, 31.3, 28.6, 28.40, 28.39, 26.0, 22.5, 15.5, 14.1.

**HRMS-ESI (m/z)** $[M+Na]^+$ calculated for $C_{38}H_{38}NaO_2S_6$ 741.1088, found 741.1103.

**2-Hydroxy-6-(5-(isopropylthio)thiophen-2-yl)-6-(2-(phenylthio)thiophen-3-yl)cyclohex-2-en-1-one (53)**



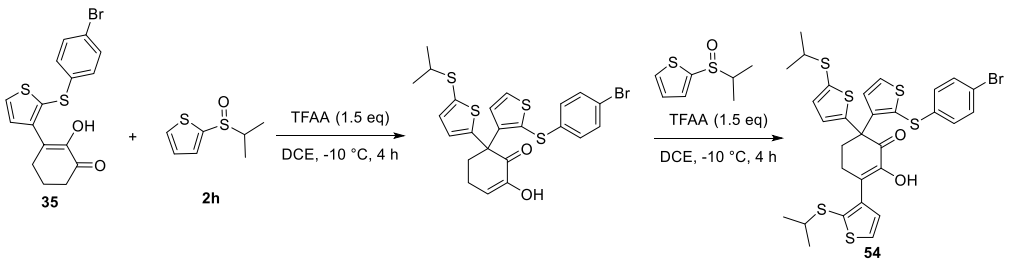

Yellow oil, 22.5 mg, 49% yield. ($R_f$ = 0.62, petroleum ether/ethyl acetate = 9/1)

**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.32 (d, *J* = 5.6 Hz, 1H), 7.25 (t, *J* = 7.6 Hz, 2H), 7.19 – 7.13 (m, 3H), 7.02 (d, *J* = 3.7 Hz, 1H), 6.79 (d, *J* = 3.7 Hz, 1H), 6.45 (d, *J* = 5.6 Hz, 1H), 6.05 – 5.99 (m, 2H), 3.19 – 3.11 (m, 1H), 3.07 – 3.00 (m, 1H), 2.60 – 2.47 (m, 2H), 2.34 – 2.24 (m, 1H), 1.28 (d, *J* = 6.7 Hz, 6H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 193.5, 149.1, 146.7, 146.0, 138.0, 134.9, 133.8, 130.7, 129.7, 129.3, 128.9, 127.2, 127.2, 126.3, 117.1, 55.0, 41.7, 36.4, 23.1, 21.4.

**HRMS-ESI (m/z)** $[M+Na]^+$ calculated for $C_{23}H_{22}NaO_2S_4$ 481.0395, found 481.0385.

**6-(2-((4-Bromophenyl)thio)thiophen-3-yl)-2-hydroxy-6-(5-(isopropylthio)thiophen-2-yl)-3-(2-(isopropylthio)thiophen-3-yl)cyclohex-2-en-1-one (54)**




Yellow oil, 45.1 mg, 65% yield. ($R_f$ = 0.63, petroleum ether/ethyl acetate = 9/1)

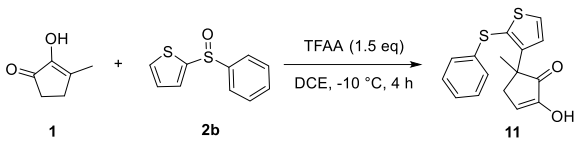
**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.40 – 7.34 (m, 3H), 7.32 (d, *J* = 5.5 Hz, 1H), 7.13 (d, *J* = 5.5 Hz, 1H), 7.02 (d, *J* = 3.6 Hz, 1H), 7.01 (d, *J* = 8.5 Hz, 2H), 6.84 (d, *J* = 3.7 Hz, 1H), 6.58 (d, *J* = 5.6 Hz, 1H), 6.35 (s, 1H), 3.19 – 3.08 (m, 2H), 3.08 – 2.95 (m, 2H), 2.77 (m, 1H), 2.64 (m 1H), 1.29 (d, *J* = 6.7 Hz, 6H), 1.11 (m, 6H).

**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 193.1, 149.3, 146.2, 143.7, 141.9, 137.3, 134.7, 134.1, 131.9, 131.6, 120.0, 129.6, 129.3, 128.7, 128.0, 127.2, 126.4, 125.4, 120.2, 54.5, 42.4, 41.6, 36.4, 26.7, 23.1, 23.1, 22.90, 22.89.

**HRMS-ESI (m/z)** $[M+Na]^+$ calculated for $C_{30}H_{29}BrNaO_2S_6$ 714.9567, found 714.9562.

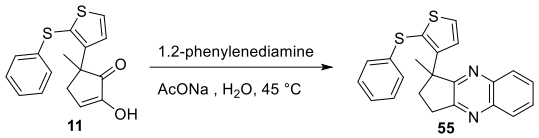
## IV. Gram-Scale Reaction and Derivatization of Compound 11

### 1. Gram-scale reaction




TFAA (7.5 mmol, 1.0655 mL) was added to a solution of cyclic 1,2-diketones **1** (7.5 mmol, 855 mg) and sulfoxide **2b** (5 mmol, 1.050 g) in DCE (40 mL, 0.125 M) at -10 ℃. After 4 hours, the reaction mixture was concentrated under reduced pressure and purified by column chromatography (eluent: petroleum ether/ethyl acetate = 9/1) to afford product **11** (1.420 g, 94%) as a white solid.

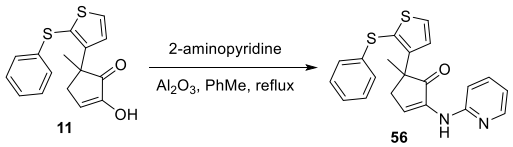
### 2. Synthesis for 1-methyl-1-(2-(phenylthio)thiophen-3-yl)-2,3-dihydro-1H-cyclopenta[*b*]quinoxaline (55)




A 25 mL round-bottomed flask was charged with a solution of the appropriate 1,2-dicarbonyl compound **11** (0.1 mmol) in $H_2O$ (3 mL). To this solution was added the respective 1.2-diphenylamine (0.888 mmol) and the mixture was stirred at 45 ℃. After 12h, the crude mixture was extracted with $CH_2Cl_2$ (3 × 10 mL). The combined organic layers were dried ($MgSO_4$) and after filtration, the solvent was removed to give the desired product.

Yellow solid, 35.2 mg, 94% yield. ($R_f$ = 0.64, petroleum ether/ethyl acetate = 9/1)
**$^1$H NMR** (400 MHz, $CDCl_3$) δ 7.95 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.80 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.59 (ddd, *J* = 8.3, 7.0, 1.5 Hz, 1H), 7.55 – 7.49 (m, 1H), 7.47 (d, *J* = 5.6 Hz, 1H), 7.25 (d, *J* = 5.6 Hz, 1H), 6.97 (t, *J* = 7.6 Hz, 2H), 6.90 – 6.83 (m, 1H), 6.82 – 6.77 (m, 2H), 3.35 – 3.12 (m, 2H), 2.82 (ddd, *J* = 13.2, 9.4, 7.6 Hz, 1H), 2.46 – 2.31 (m, 1H), 1.83 (s, 3H).
**$^{13}$C NMR** (100 MHz, $CDCl_3$) δ 165.1, 159.9, 153.6, 141.7, 141.5, 137.9, 123.0, 129.2, 129.0, 128.9, 128.5, 128.42, 128.39, 125.8, 125.7, 125.1, 48.6, 38.8, 30.0, 27.6.
**HRMS-ESI (m/z)** $[M+H]^+$ calculated for $C_{22}H_{19}N_2S_2$ 375.0984, found 375.0973.

### 3. Synthesis for 5-methyl-5-(2-(phenylthio)thiophen-3-yl)-2-(pyridin-2-ylamino)cyclopent-2-en-1-one (56)

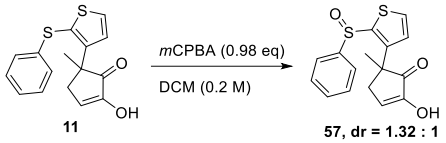



In a 38 mL round bottom flask, equipped with a condenser, 2-hydroxy-5-methyl-5-(2-(phenylthio)thiophen-3-yl)cyclopent-2-en-1-one **11** (60 mg, 0.2 mmol) , 2-aminopyridine (18.8 mg, 0.2 mmol), alumina (0.2 g) and toluene (4 mL) was stirred and heated to reflux for 36 h. Upon reaction completion, alumina was removed by filtration and washed with EtOAc (2 x 10 mL). The

organic phases were combined and concentrated under vacuum and the residue was purified by flash chromatography eluting with hexane/EtOAc (10:1 v/v) to give **56** (41.6 mg, 55%) as an oil.

Yellow oil, 41.6 mg, 55% yield. ($R_f$ = 0.65, petroleum ether/ethyl acetate = 9/1)
**$^1$H NMR** (600 MHz, $CDCl_3$) δ 8.26 (dd, *J* = 5.0, 1.2 Hz, 1H), 7.58 (t, *J* = 3.2 Hz, 1H), 7.49 (ddd, *J* = 8.9, 7.3, 1.9 Hz, 1H), 7.45 (d, *J* = 5.6 Hz, 1H), 7.22 (d, *J* = 5.6 Hz, 1H), 7.18 (t, *J* = 7.6 Hz, 2H), 7.11 (t, *J* = 7.3 Hz, 1H), 7.05 (dd, *J* = 5.2, 3.3 Hz, 2H), 6.88 (s, 1H), 6.79 – 6.74 (m, 1H), 6.69 (d, *J* = 8.3 Hz, 1H), 2.96 (dd, *J* = 18.1, 3.0 Hz, 1H), 2.80 (dd, *J* = 18.1, 3.4 Hz, 1H), 1.62 (s, 3H).
**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 206.4, 154.5, 150.2, 147.8, 138.4, 137.4, 136.0, 130.0, 129.7, 128.8, 128.7, 126.8, 125.9, 125.5, 115.4, 110.8, 47.5, 44.0, 26.4.
**HRMS-ESI (m/z)** $[M+H]^+$ calculated for $C_{21}H_{19}N_2OS_2$ 379.0933, found 379.0924.

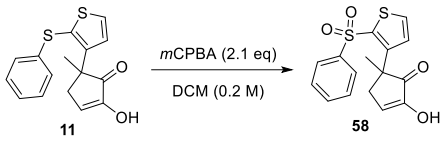
## 4. Synthesis for 2-hydroxy-5-methyl-5-(2-(phenylsulfinyl)thiophen-3-yl)cyclopent-2-en-1-one (57)




A solution of **11** (0.1 mmol, 1.0 equiv) in dichloromethane (0.5 mL, 0.2 M) was cooled to 0 ℃. After addition of m-CPBA (0.98 equiv) the solution was stirred for overnight The reaction mixture was washed with saturated $NaHCO_3$ solution, dried over anhydrous magnesium sulfate and the solvent was removed under reduced pressure. The crude product was purified by flash chromatography on silica gel using a mixture of petroleum ether and ethyl acetate to afford the product **57** (dr = 1.32:1).

White solid, 29.3 mg, 92% yield. ($R_f$ = 0.2, petroleum ether/ethyl acetate = 1/1)
**$^1$H NMR** (600 MHz, $CDCl_3$) δ 7.68 (dd, *J* = 6.5, 3.0 Hz, 2H), 7.61 (dd, *J* = 6.5, 3.0 Hz, 2H), 7.52 (d, *J* = 5.2 Hz, 1H), 7.50 – 7.47 (m, 4H), 7.46 – 7.41 (m, 3H), 7.10 (d, *J* = 5.2 Hz, 1H), 7.02 (d, *J* = 5.3 Hz, 1H), 6.60 (t, *J* = 3.1 Hz, 1H), 6.51 (t, *J* = 3.1 Hz, 1H), 3.12 (dd, *J* = 18.5, 2.6 Hz, 1H), 3.09 (dd, *J* = 19.2, 2.7 Hz, 1H), 2.94 (dd, *J* = 18.1, 3.3 Hz, 1H), 2.77 (dd, *J* = 18.3, 3.4 Hz, 1H), 1.71 (s, 3H), 1.66 (s, 3H).
**$^{13}$C NMR** (150 MHz, $CDCl_3$) δ 206.3, 204.8, 151.0, 150.9, 150.1, 149.0, 144.5, 144.0, 143.3, 142.3, 132.3, 131.9, 131.3, 131.1, 129.2, 129.1, 127.67, 127.66, 127.6, 127.5, 124.9, 124.8, 47.8, 47.7, 42.7, 41.9, 28.1, 26.4.
**HRMS-ESI (m/z)** $[M+ Na]^+$ calculated for $C_{16}H_{14}NaO_3S_2$ 341.0277, found 341.0269.

## 5. Synthesis for 2-hydroxy-5-methyl-5-(2-(phenylsulfonyl)thiophen-3-yl)cyclopent-2-en-1-one (58)

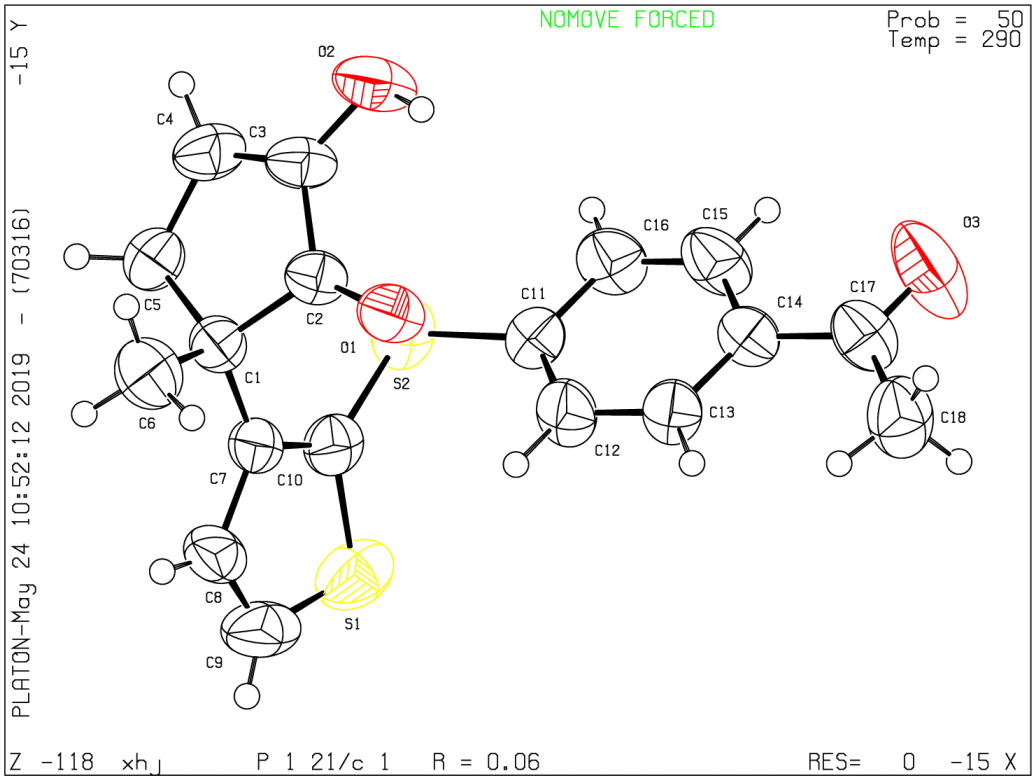



A solution of **11** (0.1 mmol, 1.0 equiv) in dichloromethane (0.5 mL, 0.2 M) was cooled to 0 ℃. After addition of m-CPBA (2.1 equiv) the solution was stirred for overnight. The reaction mixture

was washed with saturated $NaHCO_3$ solution, dried over anhydrous magnesium sulfate and the solvent was removed under reduced pressure. The crude product was purified by flash chromatography on silica gel using a mixture of petroleum ether and ethyl acetate to afford the product.

White solid, 30 mg, 90% yield. ($R_f$ = 0.25, petroleum ether/ethyl acetate = 1/1)
**$^1$H NMR** (600 MHz, DMSO) δ 9.57 (s, 1H), 8.07 (d, *J* = 5.3 Hz, 1H), 7.86 (d, *J* = 7.4 Hz, 2H), 7.72 (t, *J* = 7.4 Hz, 1H), 7.65 (t, *J* = 7.8 Hz, 2H), 7.23 (d, *J* = 5.3 Hz, 1H), 6.34 (t, *J* = 3.1 Hz, 1H), 2.63 (dd, *J* = 17.6, 2.7 Hz, 1H), 2.55 (dd, *J* = 17.6, 3.4 Hz, 1H), 1.48 (s, 3H).
**$^{13}$C NMR** (151 MHz, DMSO) δ 204.7, 151.8, 149.2, 142.3, 136.5, 134.2, 134.1, 131.0, 130.0, 127.6, 126.4, 47.8, 41.3, 27.4.
**HRMS-ESI (m/z)** $[M+Na]^+$ calculated for $C_{16}H_{14}NaO_4S_2$ 357.0226, found 357.0234.

## V. X-Ray Crystal Data of 13, 39, 45.

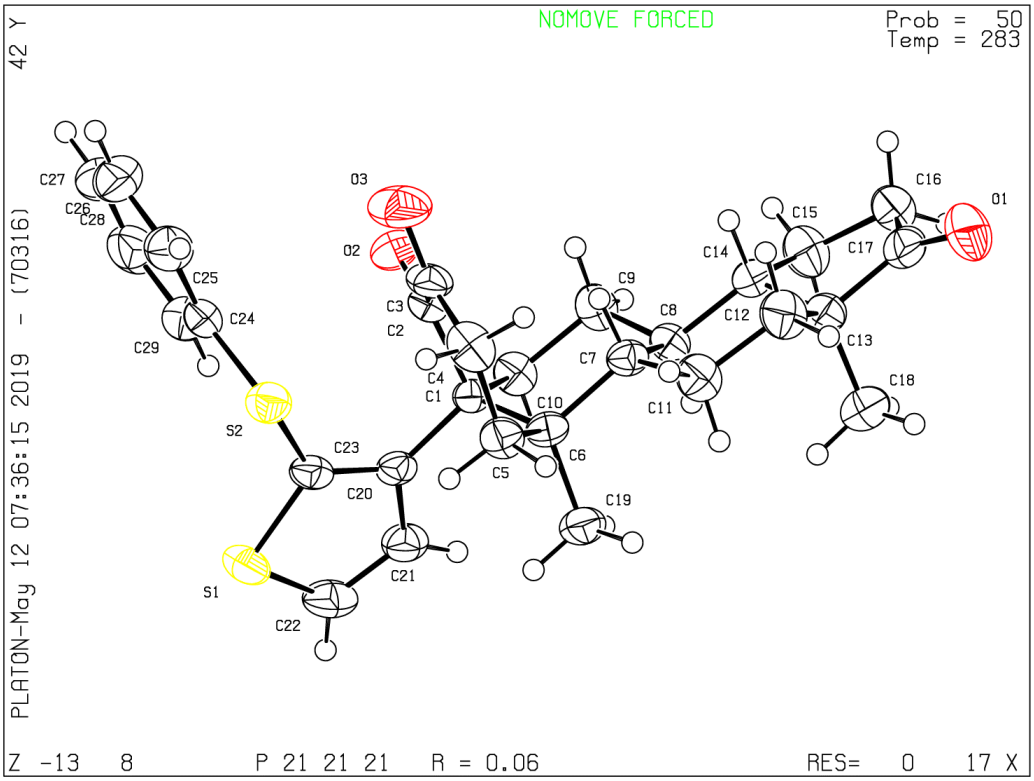



**CCDC 1938311**

X-ray structure and CCDC number of compound **13**.

| | |
|---|---|
| Crystal data and structure refinement for **13** | |
| Identification code | **13** |
| Empirical formula | $C_{18}H_{16}O_3S_2$ |
| Formula weight | 344.43 |
| Temperature | 290(2) K |
| Wavelength | 0.71073 A |
| Crystal system, space group | ?, ? |
| Unit cell dimensions | a = 7.2857(4) A alpha = 90 deg.<br>b = 11.4124(6) A beta = 94.519(2) deg.<br>c = 20.6457(11) A gamma = 90 deg. |
| Volume | 1711.30(16) A^3 |
| Z, Calculated density | 4, 1.337 Mg/m^3 |
| Absorption coefficient | 0.322 mm^-1 |
| F(000) | 720 |
| Crystal size | ? x ? x ? mm |
| Theta range for data collection | 2.67 to 27.55 deg. |
| Limiting indices | -9<=h<=9, -14<=k<=14, -26<=l<=26 |
| Reflections collected / unique | 23912 / 3953 [R(int) = 0.0369] |

| | |
|---|---|
| Completeness to theta = 27.55 | 99.8 % |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 3953 / 0 / 208 |
| Goodness-of-fit on F^2 | 1.042 |
| Final R indices [I>2sigma(I)] | R1 = 0.0696, wR2 = 0.1676 |
| R indices (all data) | R1 = 0.1090, wR2 = 0.1974 |
| Largest diff. peak and hole | 0.406 and -0.434 e.A^-3 |



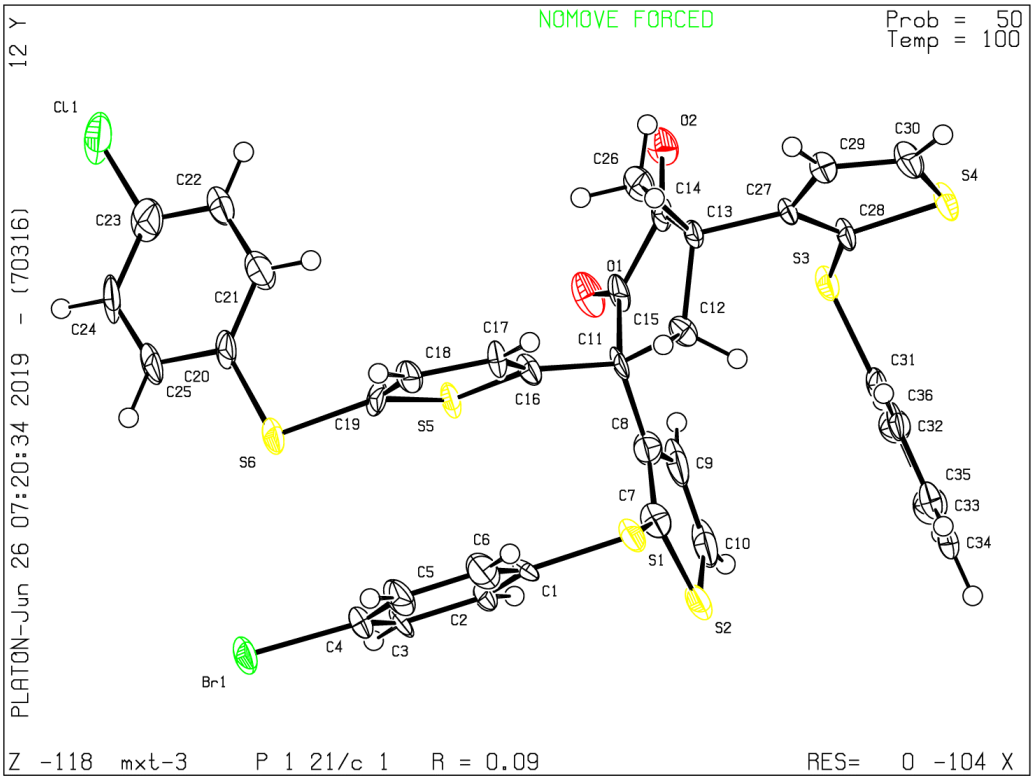

**CCDC 1938322**

X-ray structure and CCDC number of compound **39**.

Crystal data and structure refinement for **39**

| | |
|---|---|
| Identification code | **39** |
| Empirical formula | $C_{29}H_{32}O_3S_2$ |
| Formula weight | 492.66 |
| Temperature/K | 283.47 |
| Crystal system | orthorhombic |
| Space group | $P2_12_12_1$ |
| a/Å | 9.2472(8) |
| b/Å | 13.6858(14) |
| c/Å | 19.2652(15) |
| α/° | 90 |
| β/° | 90 |
| γ/° | 90 |
| Volume/Å$^3$ | 2438.1(4) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.342 |
| μ/mm$^{-1}$ | 0.249 |

| | |
|---|---|
| F(000) | 1048.0 |
| Crystal size/$mm^3$ | 0.12 × 0.10 × 0.09 |
| Radiation | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 4.886 to 55.01 |
| Index ranges | -12 ⩽ h ⩽ 9, -16 ⩽ k ⩽ 17, -20 ⩽ l ⩽ 24 |
| Reflections collected | 12728 |
| Independent reflections | 5440 [$R_{int}$ = 0.0486, $R_{sigma}$ = 0.1016] |
| Data/restraints/parameters | 5440/0/309 |
| Goodness-of-fit on $F^2$ | 1.047 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0638, $wR_2$ = 0.1100 |
| Final R indexes [all data] | $R_1$ = 0.1475, $wR_2$ = 0.1418 |
| Largest diff. peak/hole / e $Å^{-3}$ | 0.41/-0.55 |
| Flack parameter | 0.00(5) |




**CCDC 1938323**

X-ray structure and CCDC number of compound **45**.

Crystal data and structure refinement for **45**

| | |
|---|---|
| Identification code | **45** |
| Empirical formula | $C_{36}H_{24}BrClO_2S_6$ |
| Formula weight | 796.27 |
| Temperature/K | 100.00(10) |
| Crystal system | monoclinic |
| Space group | $P2_1/c$ |
| a/Å | 18.920(3) |
| b/Å | 6.6165(9) |
| c/Å | 29.427(4) |
| α/° | 90 |
| β/° | 91.184(14) |
| γ/° | 90 |
| Volume/Å$^3$ | 3682.9(9) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.436 |

| | |
|---|---|
| $\mu/mm^{-1}$ | 1.560 |
| F(000) | 1616.0 |
| Crystal size/$mm^3$ | 0.12 × 0.11 × 0.1 |
| Radiation | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 4.306 to 50 |
| Index ranges | $-21 \leq h \leq 22$, $-7 \leq k \leq 6$, $-34 \leq l \leq 34$ |
| Reflections collected | 14585 |
| Independent reflections | 6482 [$R_{int}$ = 0.0832, $R_{sigma}$ = 0.1180] |
| Data/restraints/parameters | 6482/38/416 |
| Goodness-of-fit on $F^2$ | 1.042 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0851, $wR_2$ = 0.2035 |
| Final R indexes [all data] | $R_1$ = 0.1201, $wR_2$ = 0.2325 |
| Largest diff. peak/hole / e $Å^{-3}$ | 1.51/-1.50 |

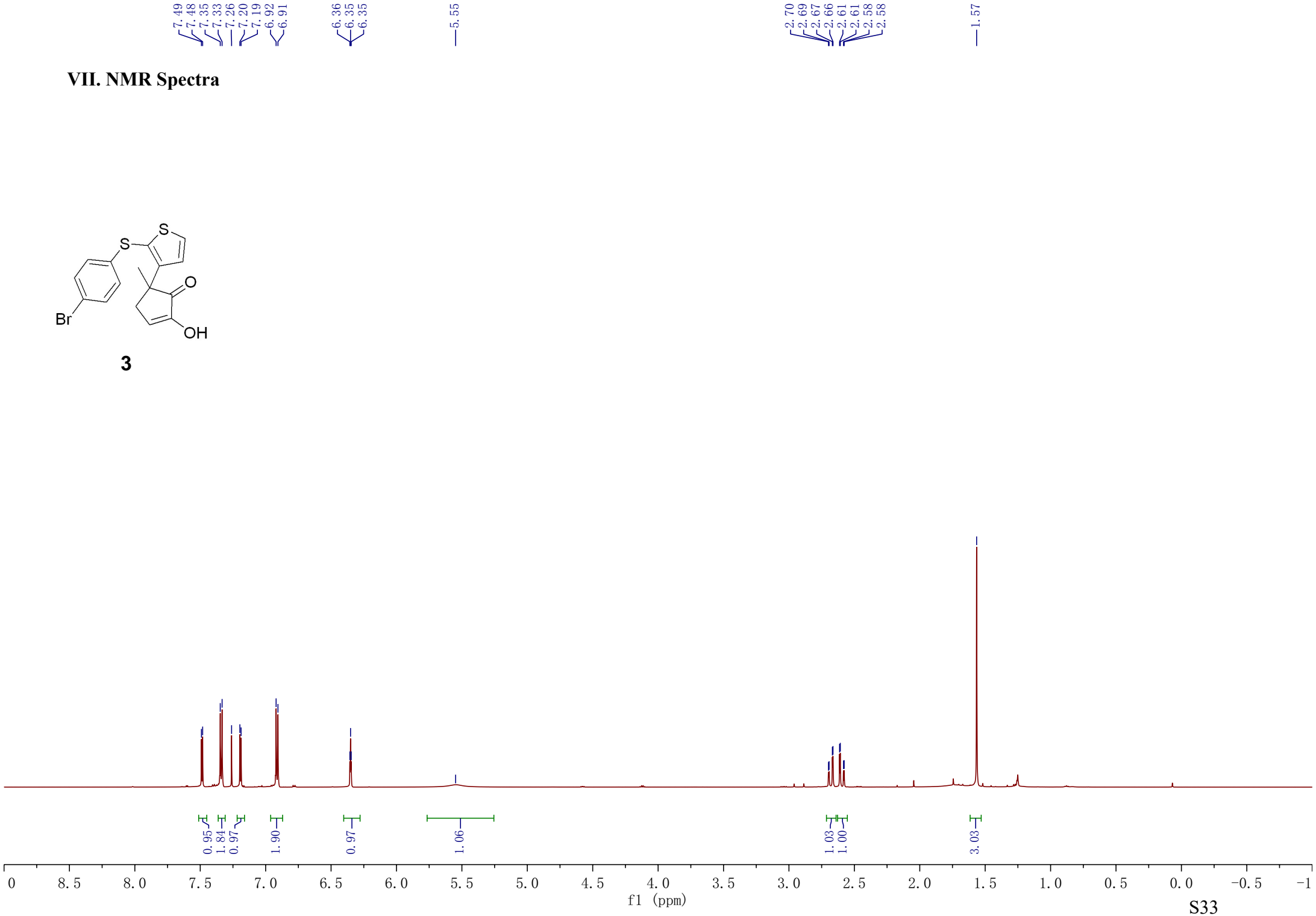
## VI. References

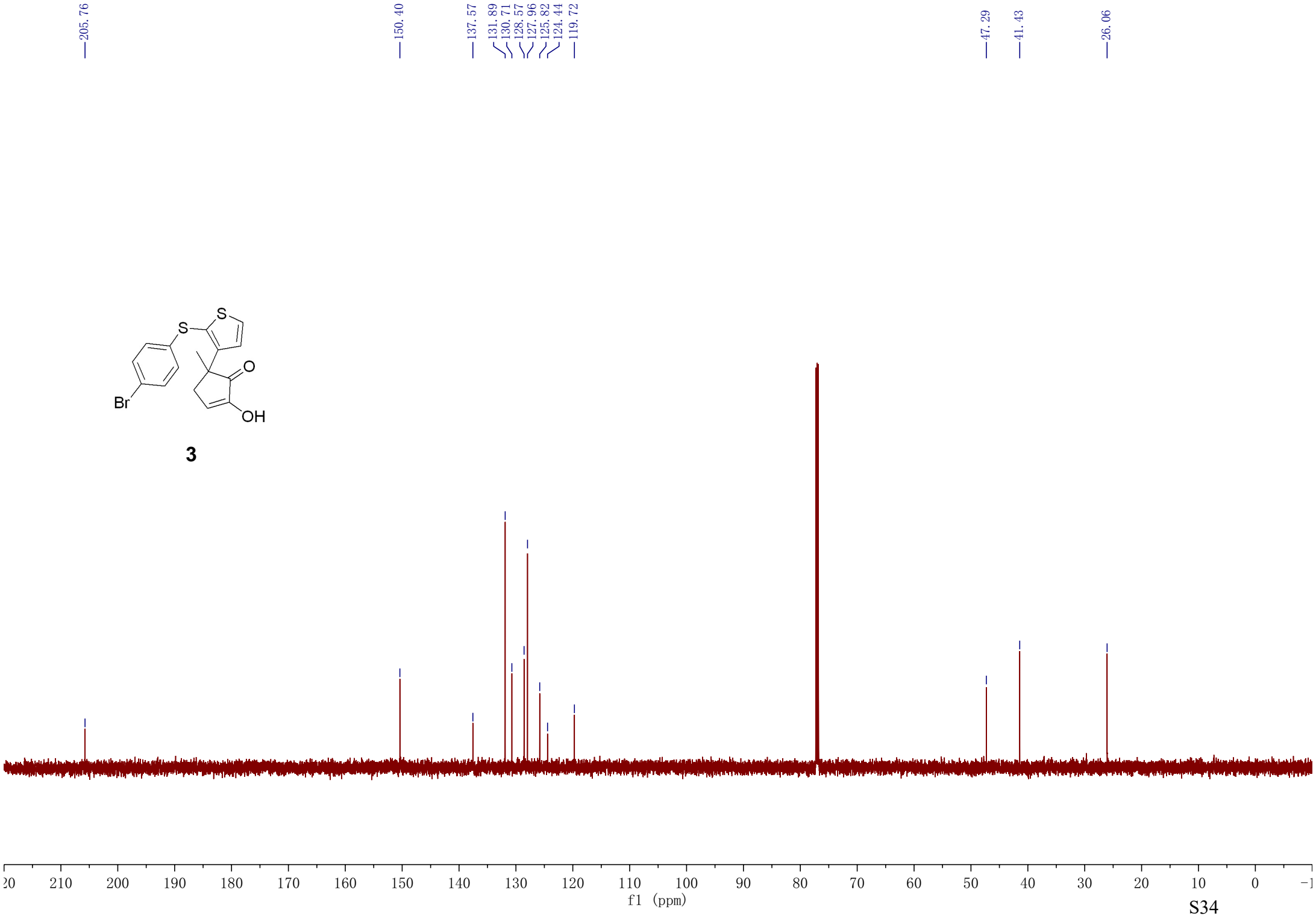
1. Paju, A.; Kanger, T.; Muurisepp, A.-M.; Aid, T.; Pehk, T.; Lopp, M. *Tetrahedron*, **2014**, *70*, 5845.
2. (*a*) Xu, H-J.; Zhao, X-Y.; Fu, Y.; Feng, Y-S. *Synlett*, **2008**, *19*, 3063; (*b*) Yanagi, T.; Otsuka, S.; Kasuga, Y.; Fujimoto, K.; Murakami, K.; Nogi, K.; Yorimisu, H.; Osuka, A. *J. Am. Chem. Soc.*, **2016**, *138*, 14582.

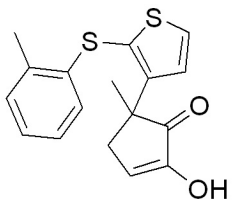
## VII. NMR Spectra



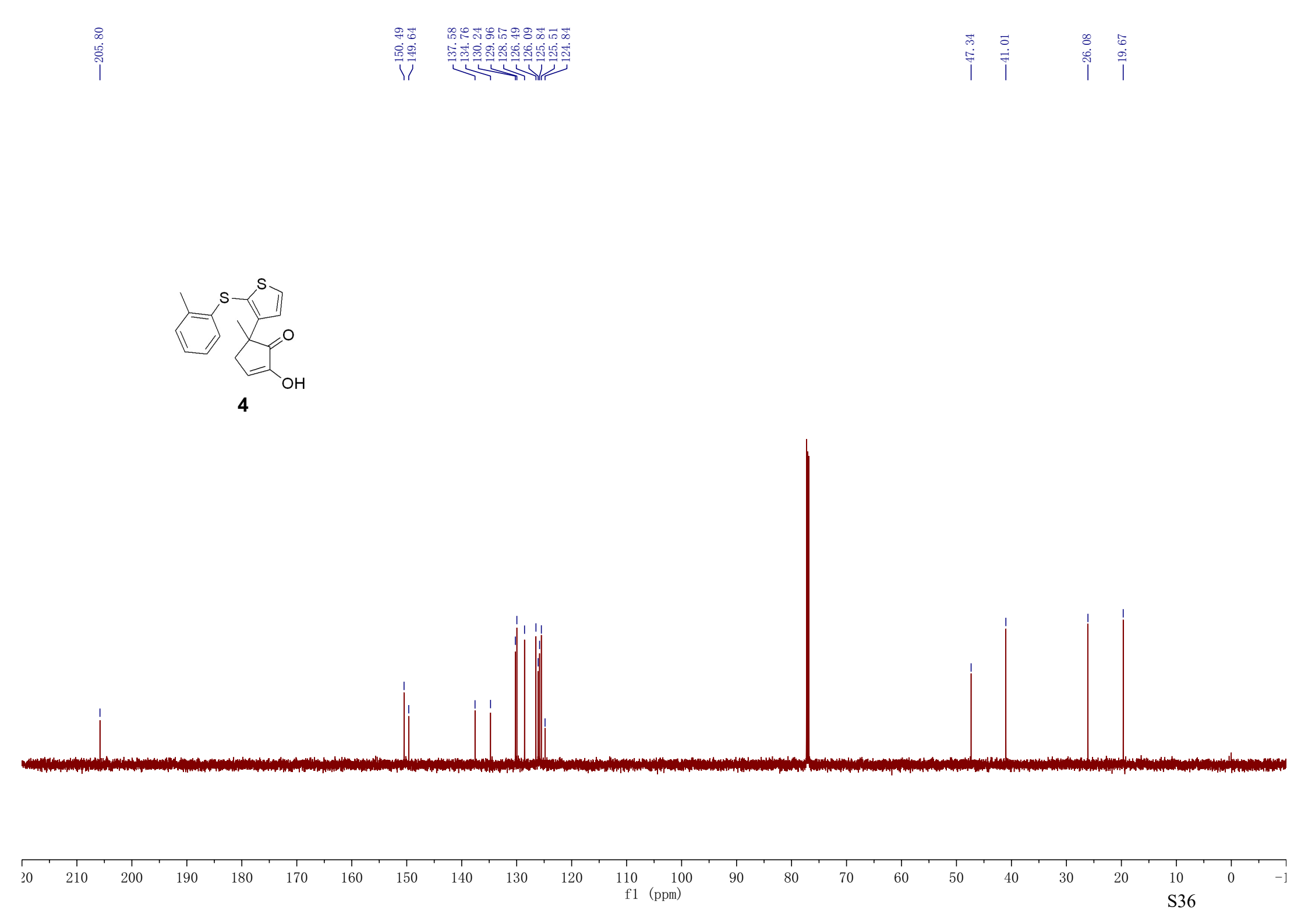

**3**

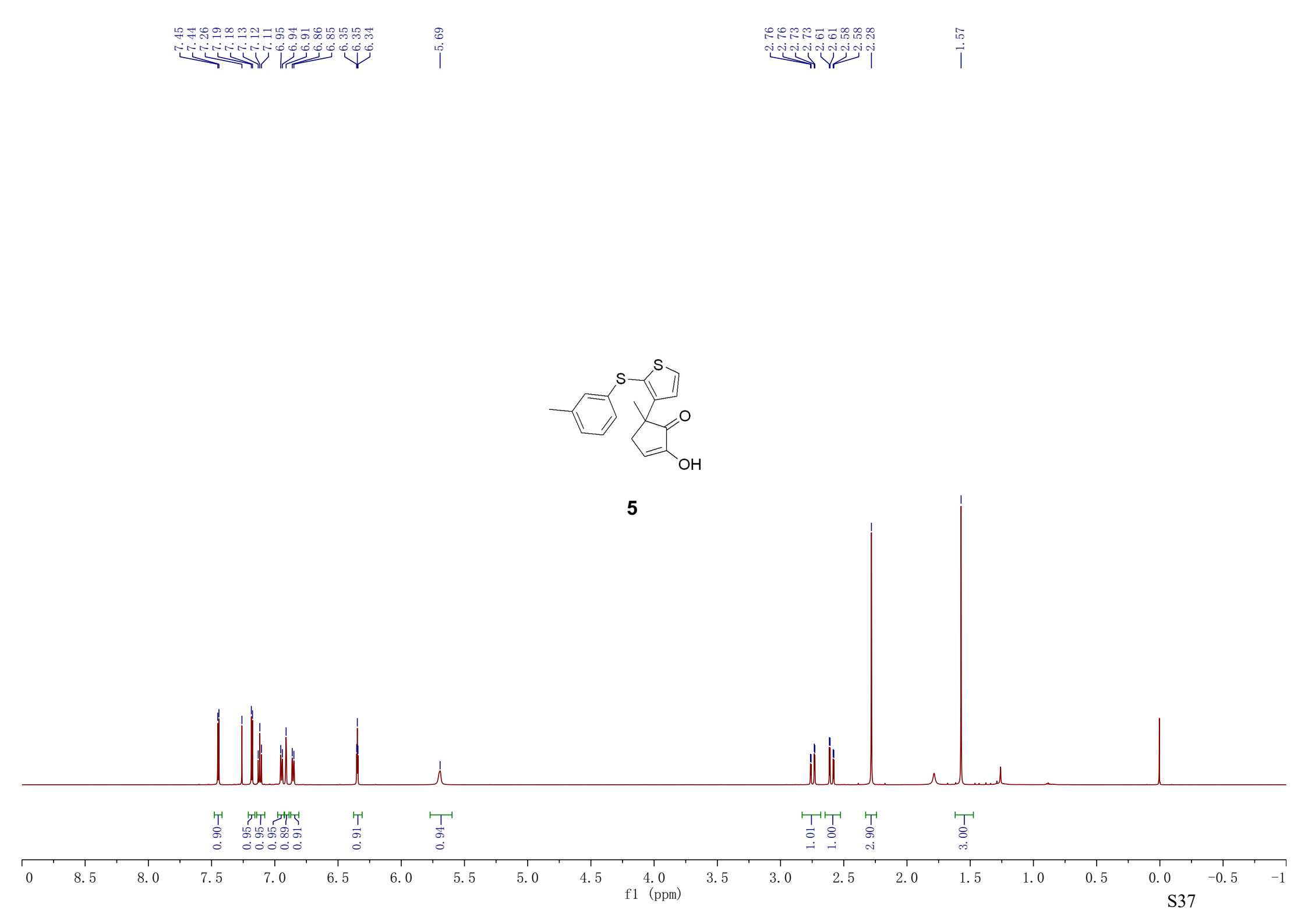



205.76
150.40
137.57
131.89
130.71
128.57
127.96
125.82
124.44
119.72
47.29
41.43
26.06
S
S
O
Br
OH
3
f1 (ppm)




**4**


205.80
150.49
149.64
137.58
134.76
130.24
129.96
128.57
126.49
126.09
125.84
125.51
124.84
47.34
41.01
26.08
19.67
S
S
O
OH
4
f1 (ppm)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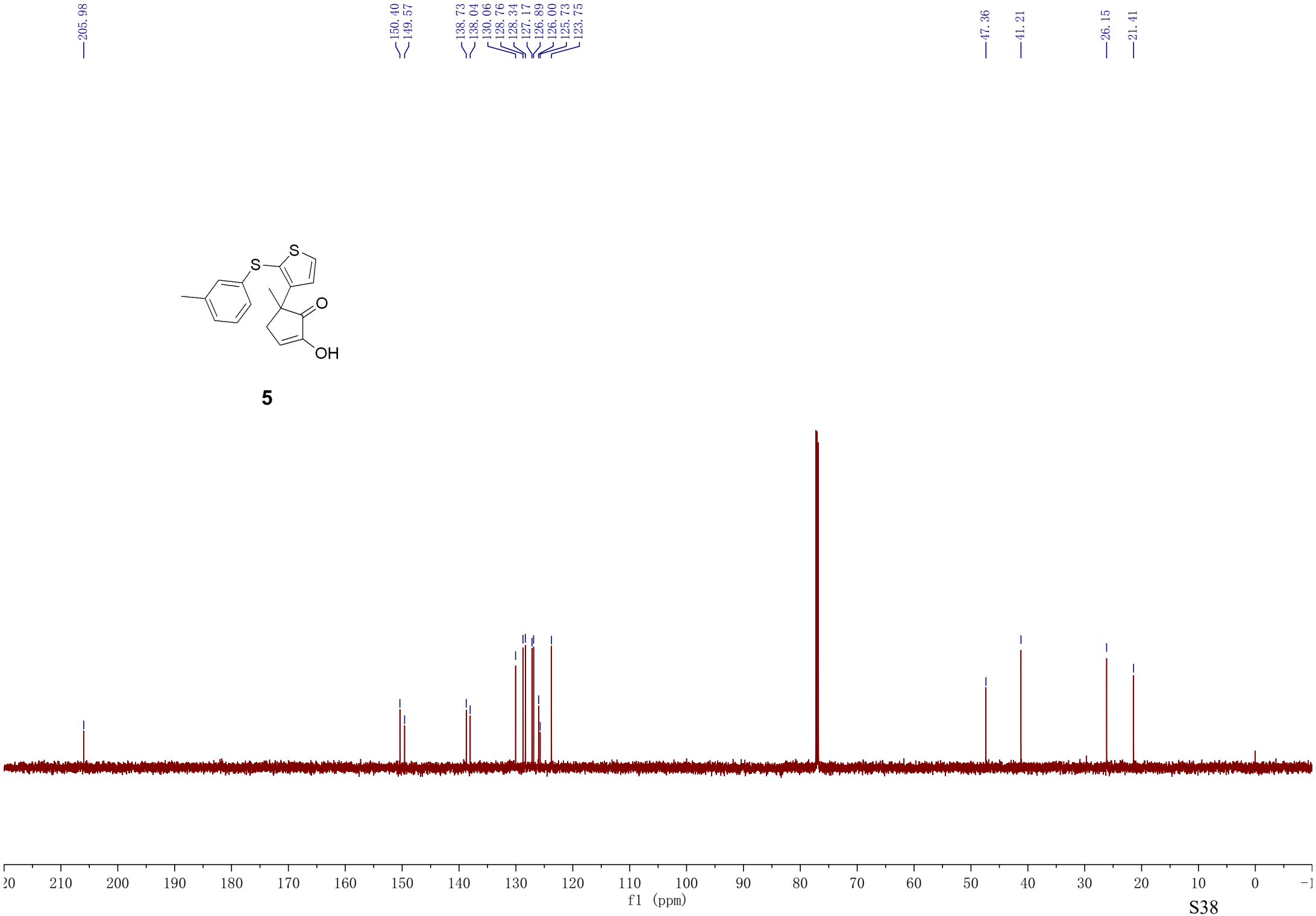
7.44
7.26
7.19
7.18
7.13
7.12
7.11
6.95
6.94
6.91
6.86
6.85
6.35
6.35
6.34
5.69
2.76
2.76
2.73
2.73
2.61
2.58
2.58
2.28
1.57
S
S
O
OH
5
0.90
0.95
0.95
0.95
0.89
0.91
0.91
0.94
1.01
1.00
2.90
3.00
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

S
S
O
OH

**5**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150.40
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138.73
138.04
130.06
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128.34
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126.00
125.73
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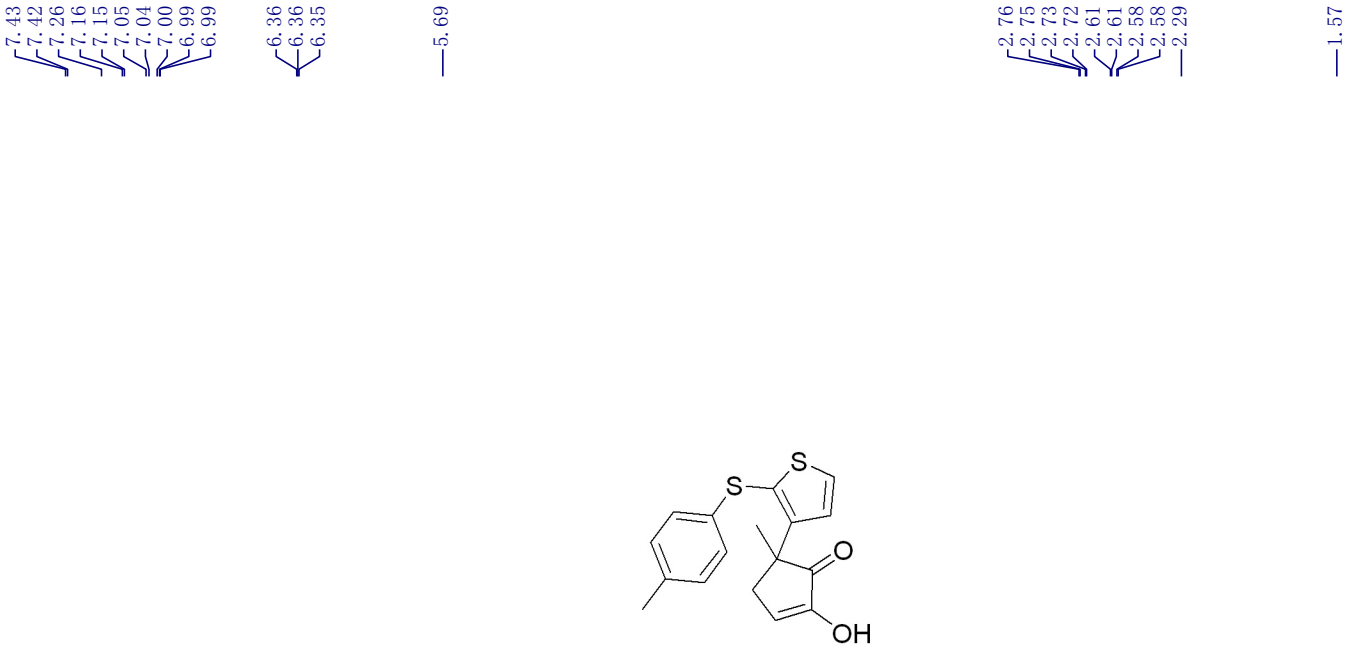
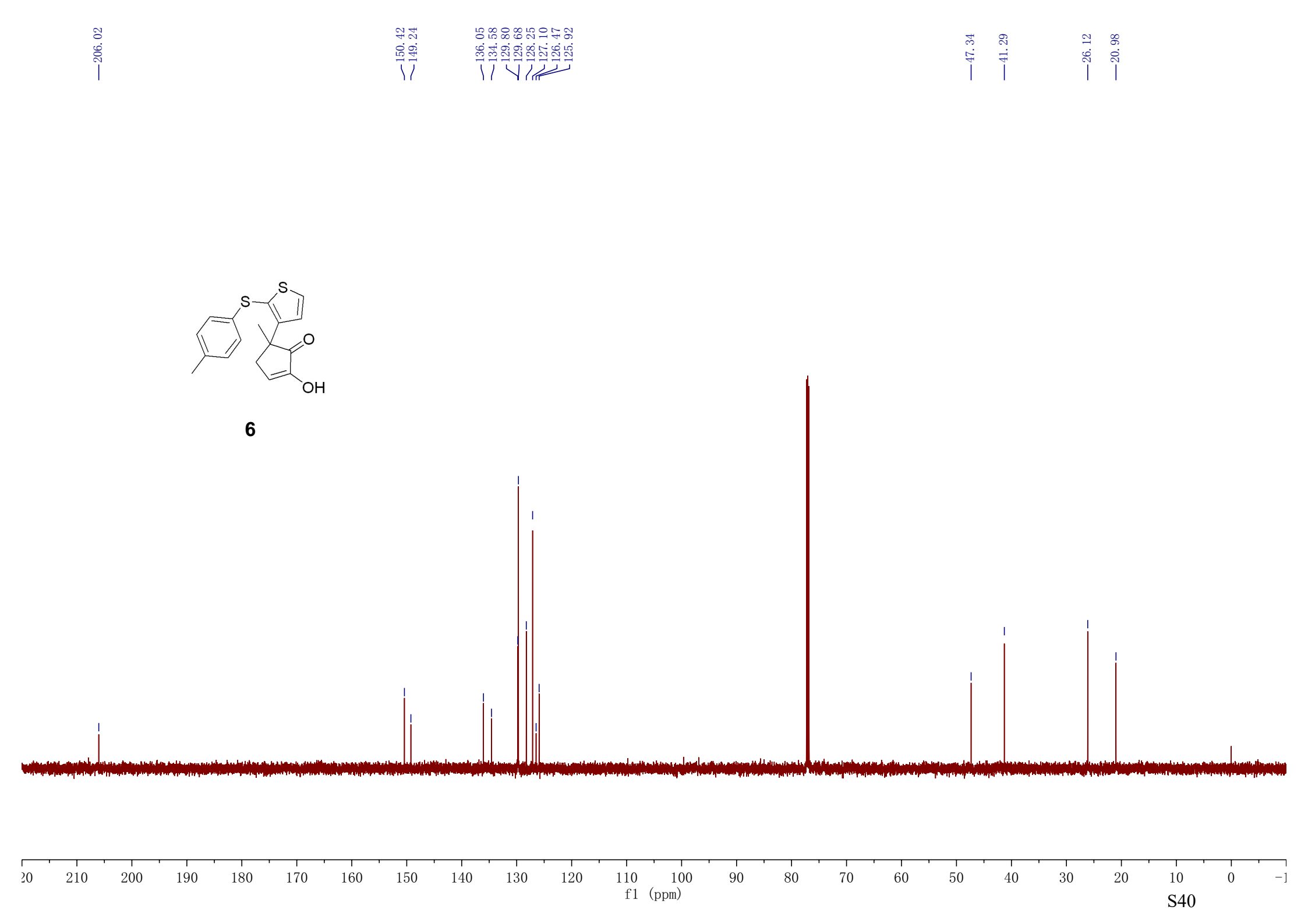
47.36
41.21
26.15
21.41
f1 (ppm)


7.43
7.42
7.26
7.16
7.15
7.05
7.04
7.00
6.99
6.99
6.36
6.36
6.35
5.69
2.76
2.75
2.73
2.72
2.61
2.61
2.58
2.58
2.29
1.57
S
S
O
OH
0.91
0.99
1.92
1.82
0.92
0.90
1.01
1.00
2.94
2.95
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

**6**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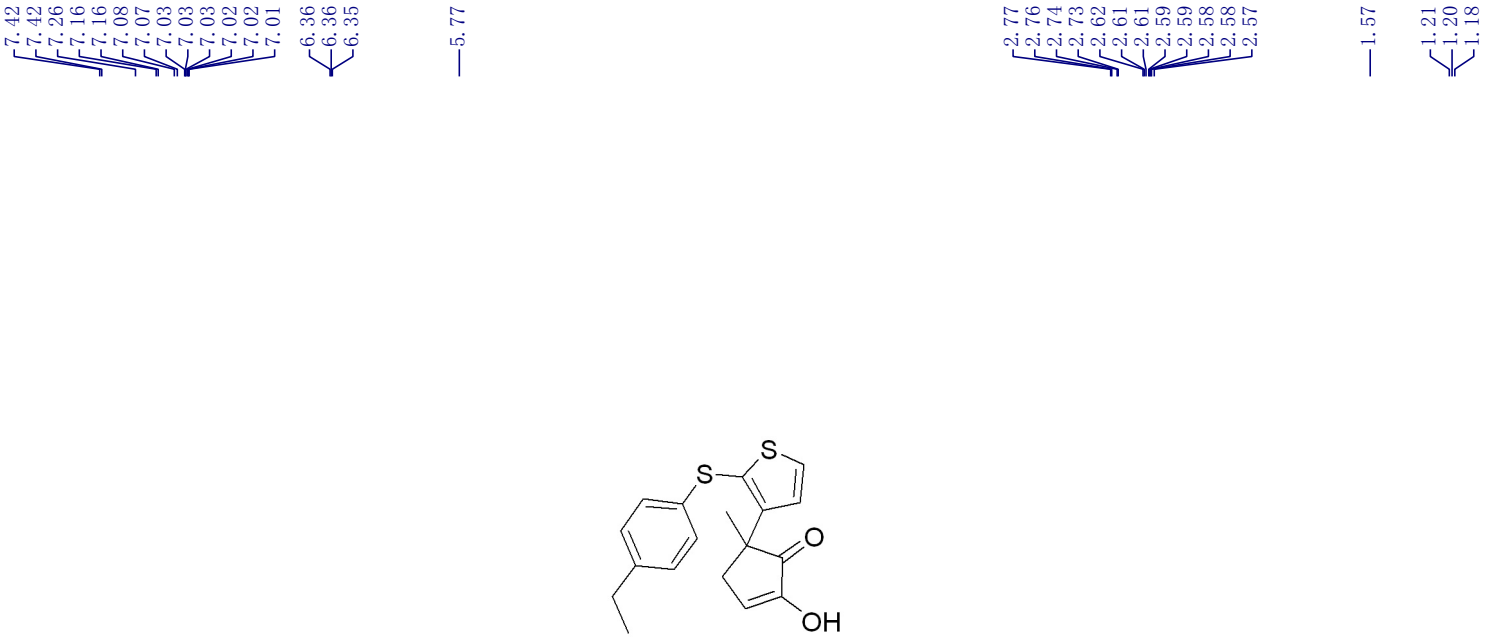
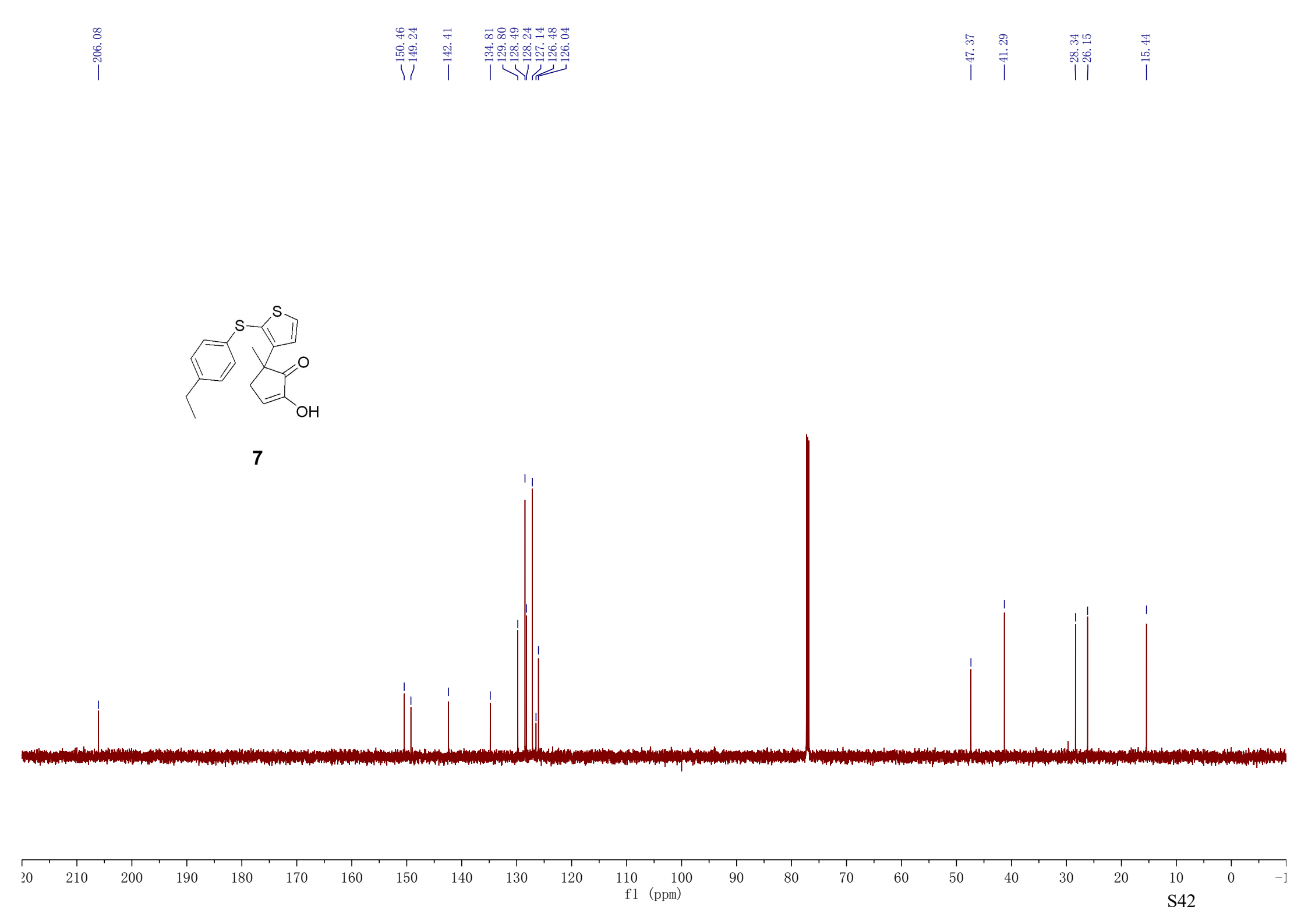
150.42
149.24
136.05
134.58
129.80
129.68
128.25
127.10
126.47
125.92
47.34
41.29
26.12
20.98
S
S
O
OH
6
f1 (ppm)


7.42
7.42
7.26
7.16
7.16
7.08
7.07
7.03
7.03
7.03
7.02
7.02
7.01
6.36
6.36
6.35
5.77
2.77
2.76
2.74
2.73
2.62
2.61
2.61
2.59
2.59
2.58
2.58
2.57
1.57
1.21
1.20
1.18
S
S
O
OH
0.95
1.10
2.01
1.94
0.99
1.00
1.12
3.13
3.04
3.04
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

**7**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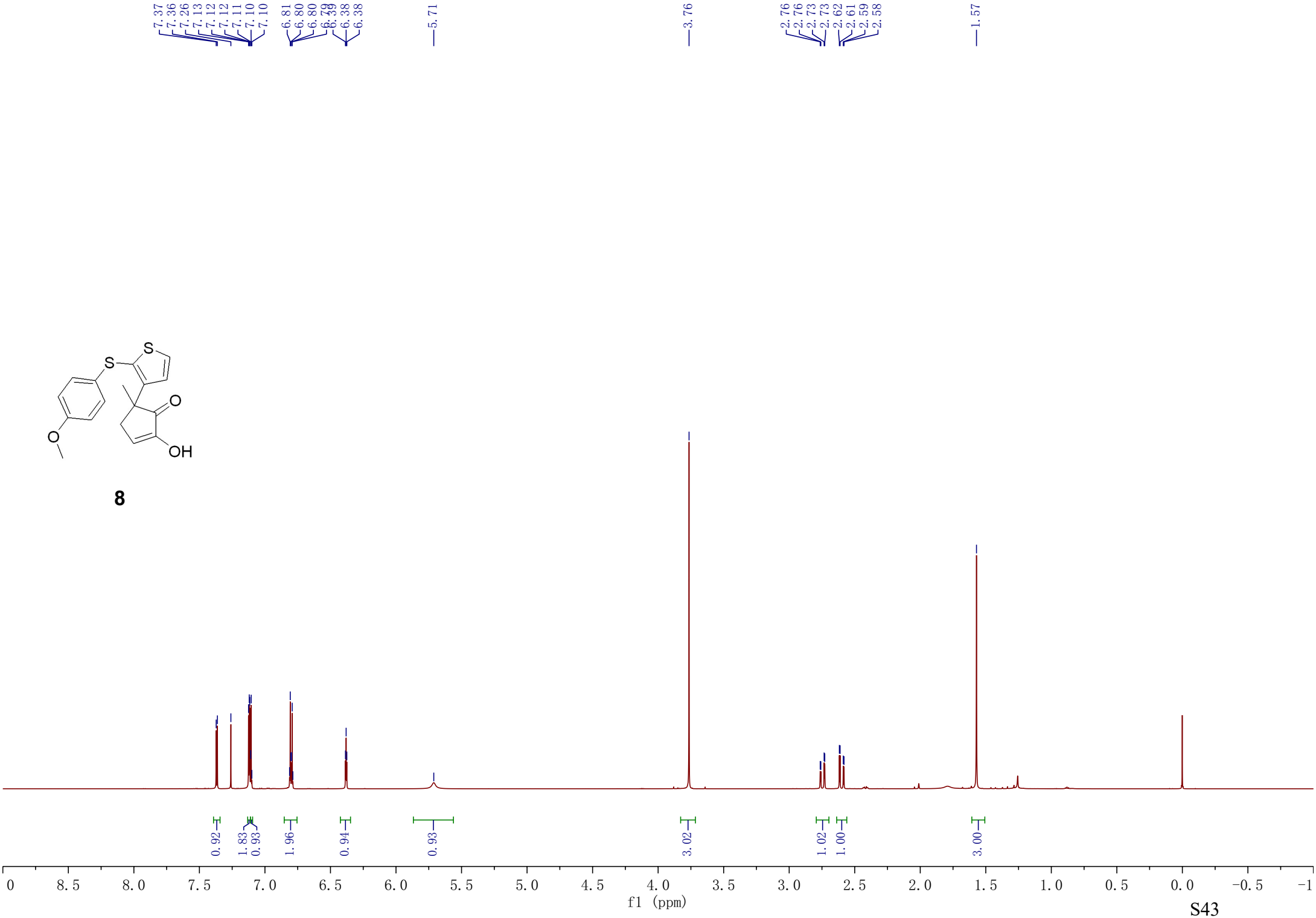
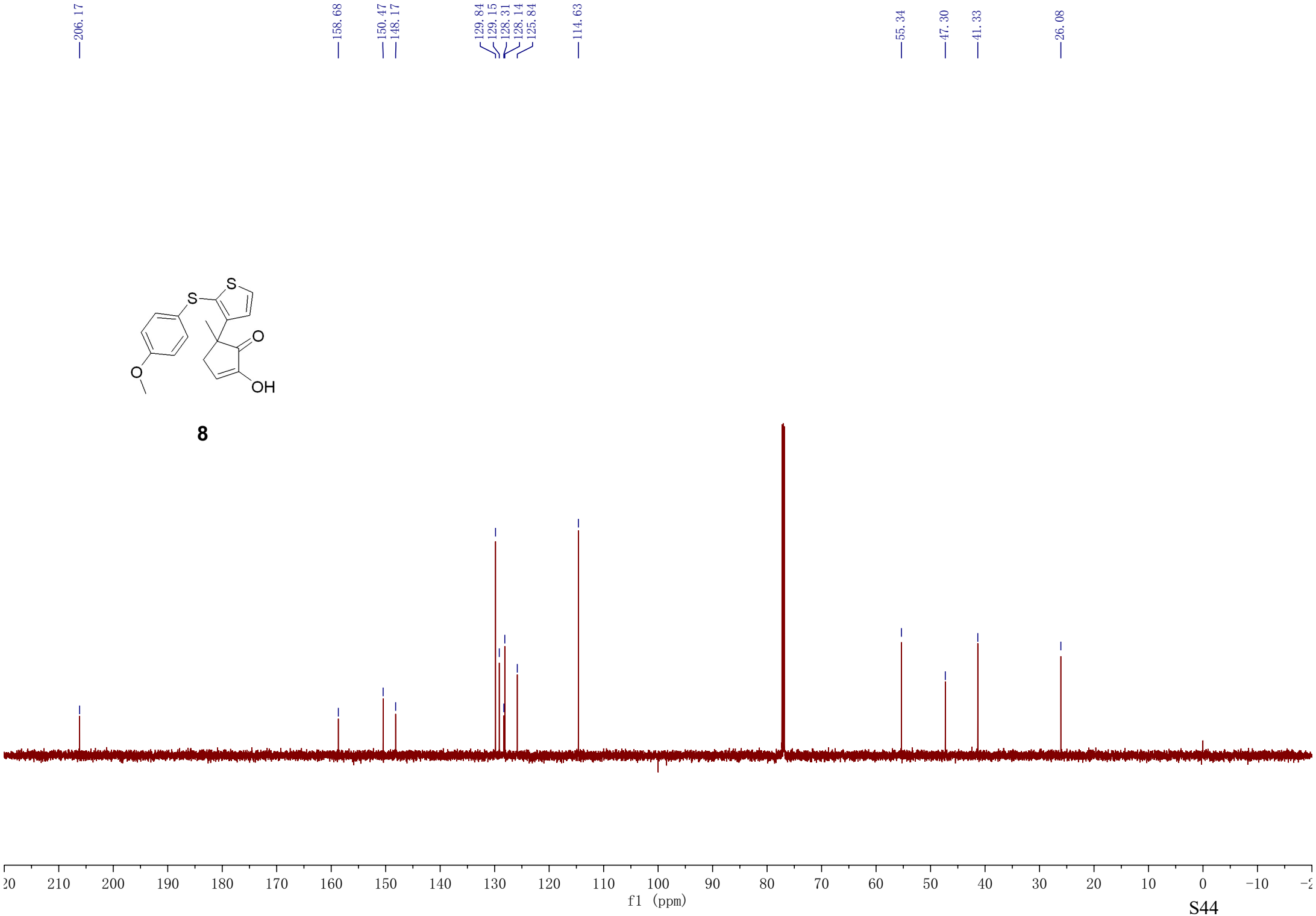
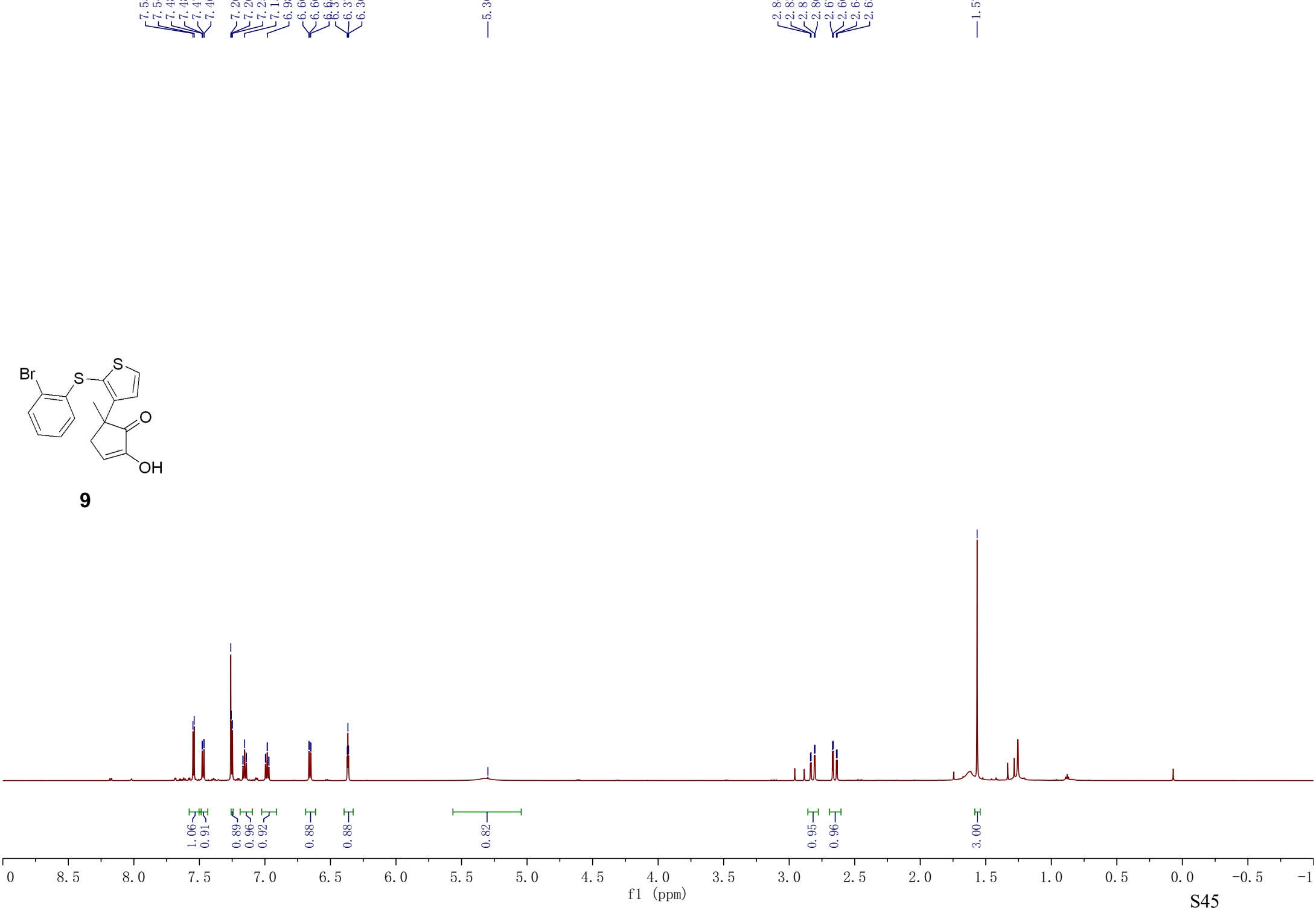
142.41
134.81
129.80
128.49
128.24
127.14
126.48
126.04
47.37
41.29
28.34
26.15
15.44
S
S
O
OH
7
f1 (ppm)

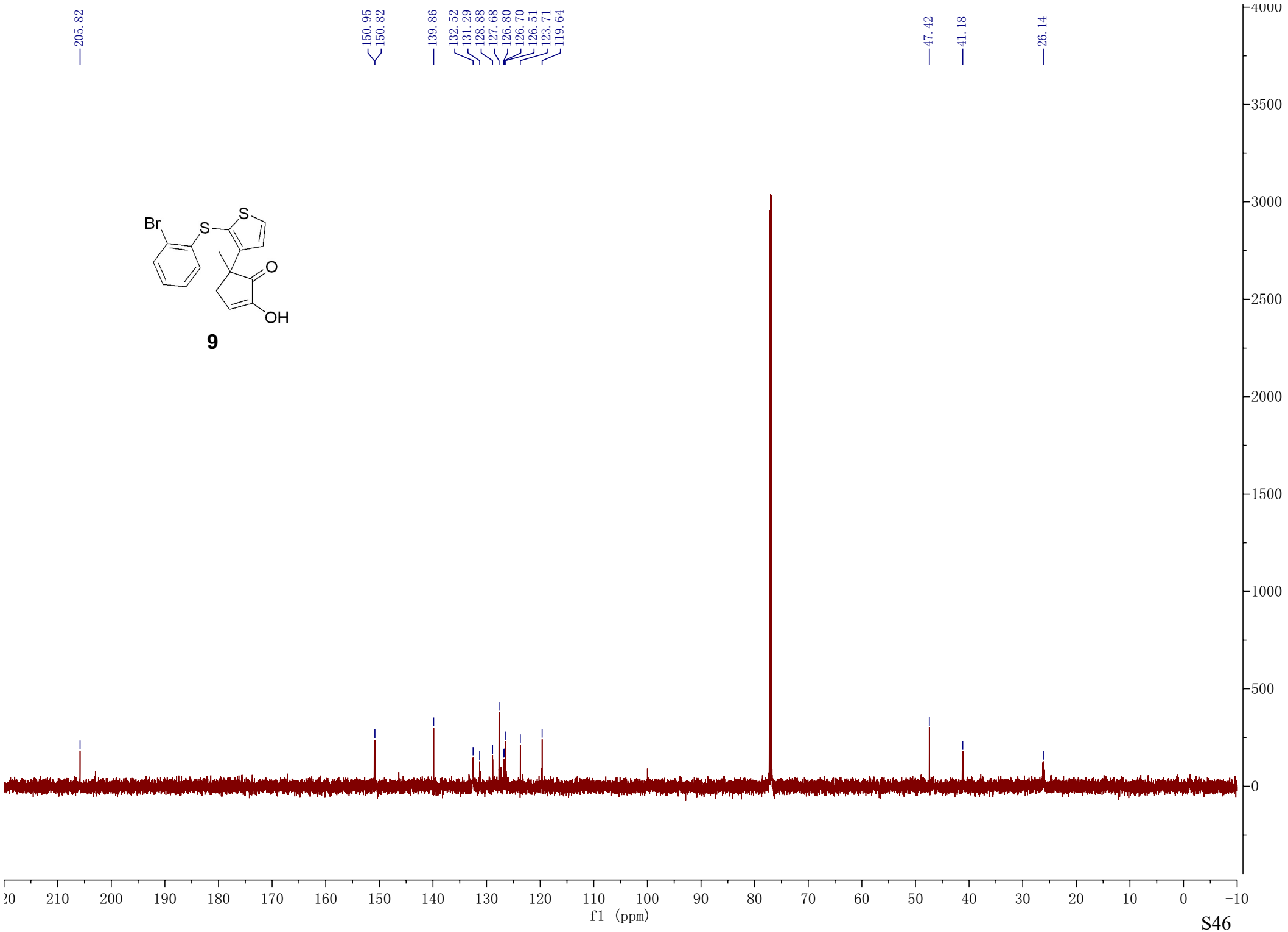
S
S
O
O
OH

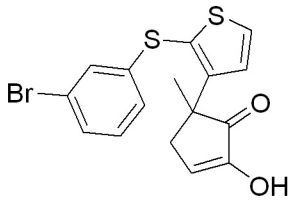
**8**


7.37
7.36
7.26
7.13
7.12
7.12
7.11
7.10
7.10
6.81
6.80
6.80
6.38
6.38
5.71
3.76
2.76
2.76
2.73
2.73
2.62
2.61
2.59
2.58
1.57
0.92
1.83
0.93
1.96
0.94
0.93
3.02
1.02
1.00
3.00
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

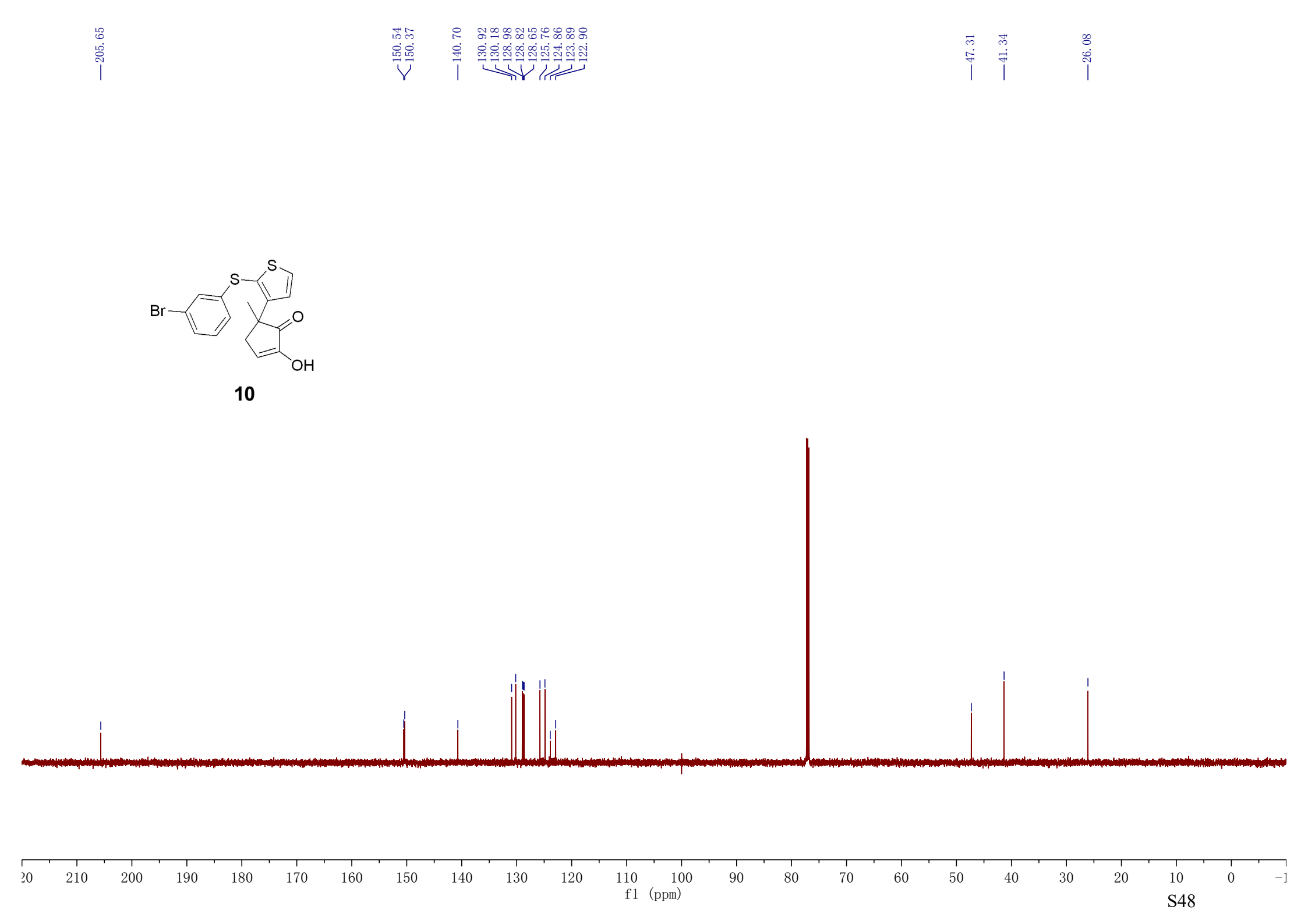

206.17
158.68
150.47
148.17
129.84
129.15
128.31
128.14
125.84
114.63
55.34
47.30
41.33
26.08
S
S
O
O
OH
8
f1 (ppm)

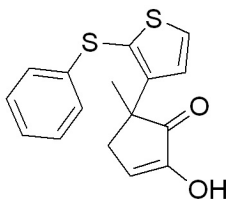

7.55
7.54
7.48
7.48
7.47
7.46
7.26
7.26
7.25
7.15
6.98
6.66
6.66
6.65
6.37
6.36
5.30
2.84
2.83
2.81
2.80
2.67
2.66
2.64
2.63
1.57
Br
S
S
O
OH
9
1.06
0.91
0.89
0.96
0.92
0.88
0.88
0.82
0.95
0.96
3.00
f1 (ppm)


205.82
150.95
150.82
139.86
132.52
131.29
128.88
127.68
126.80
126.70
126.51
123.71
119.64
47.42
41.18
26.14
Br
S
S
O
OH
9
4000
3500
3000
2500
2000
1500
1000
500
0
f1 (ppm)

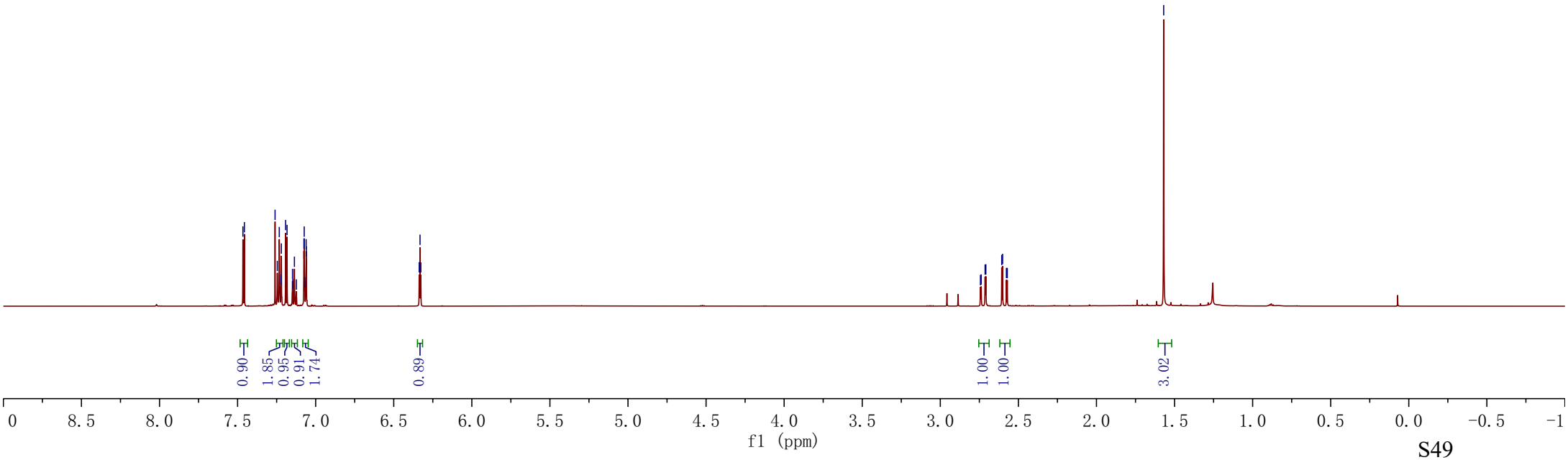


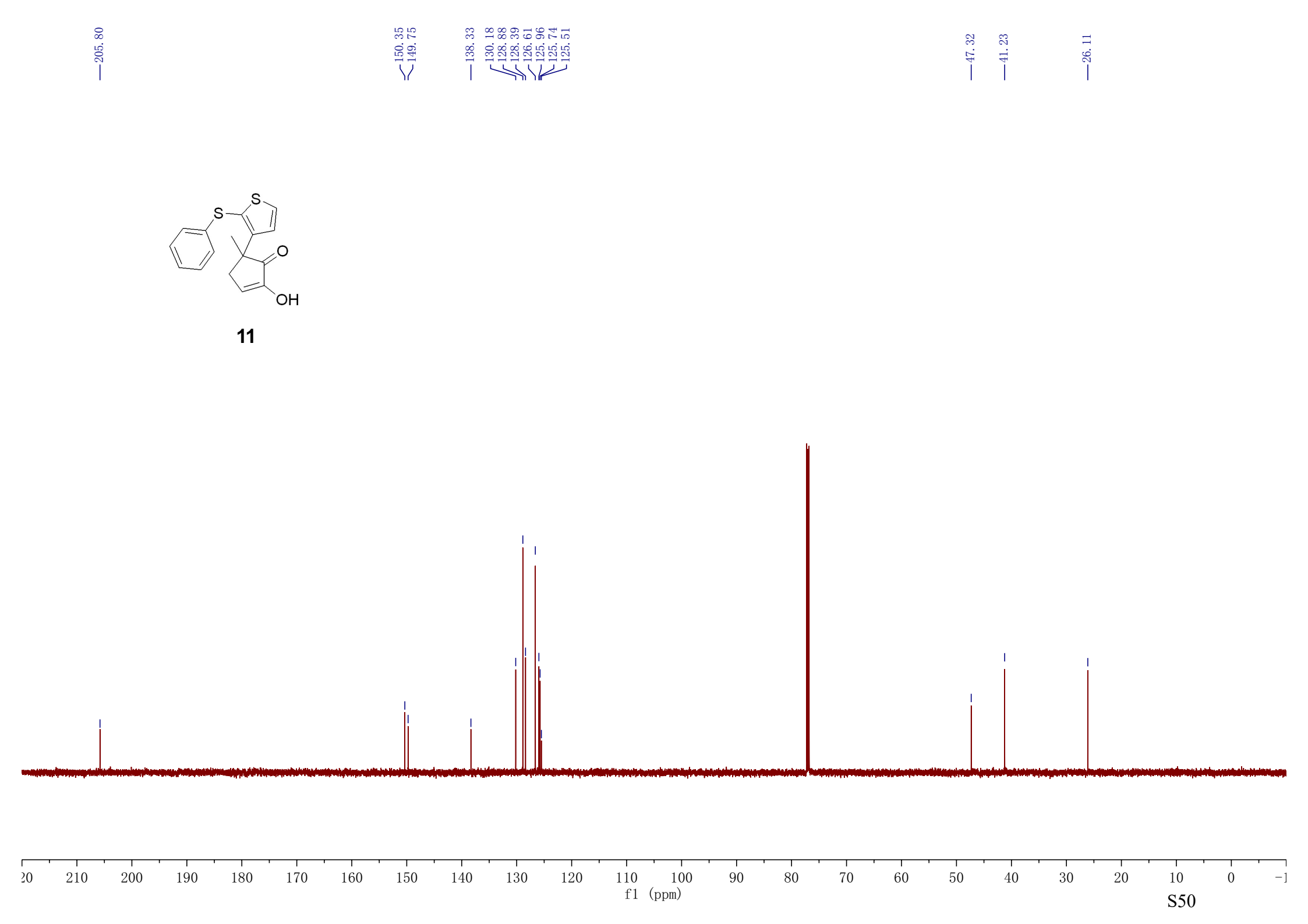

**10**


205.65
150.54
150.37
140.70
130.92
130.18
128.98
128.82
128.65
125.76
124.86
123.89
122.90
47.31
41.34
26.08
Br
S
S
O
OH
10
f1 (ppm)


S
S
O
OH

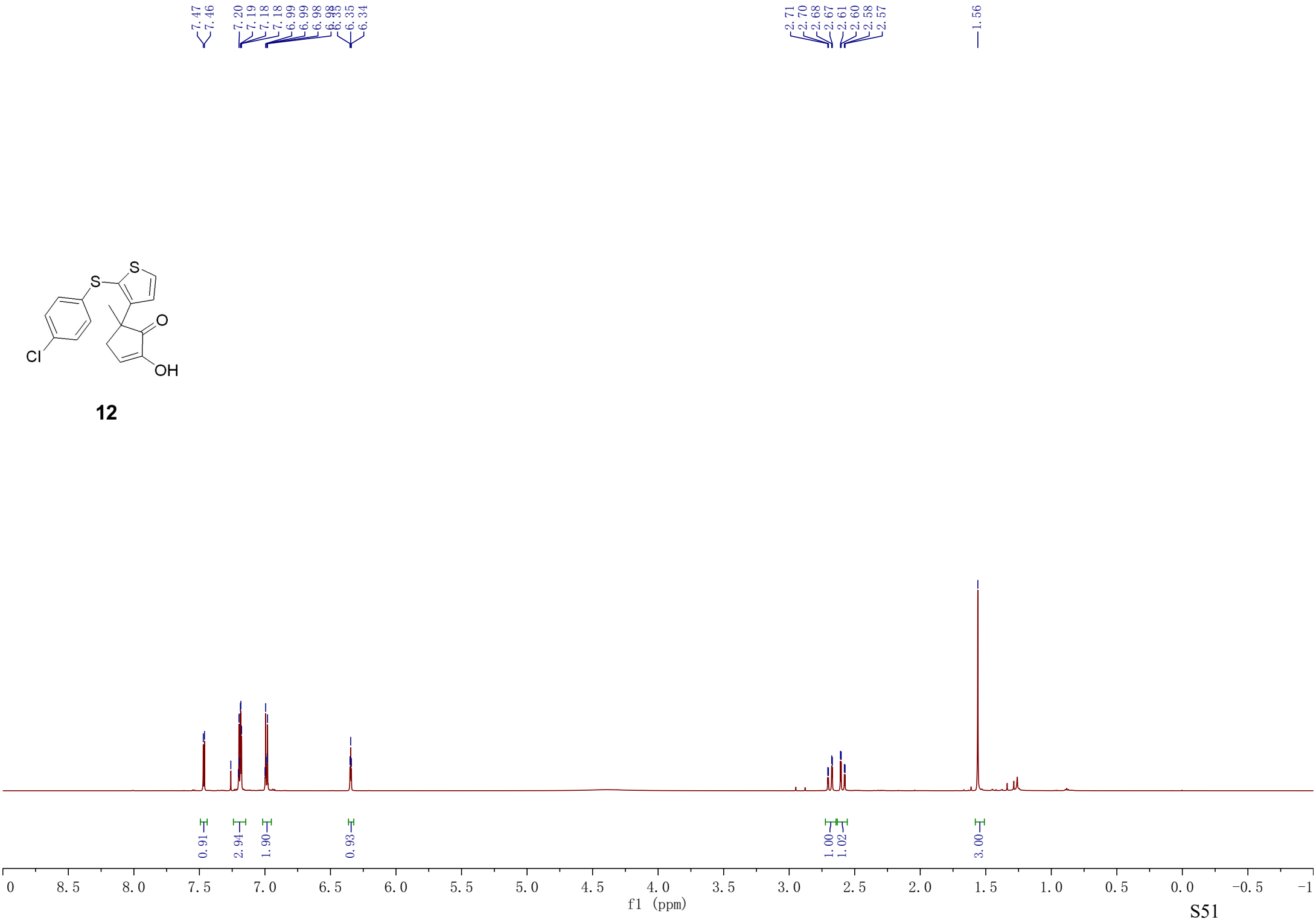
**11**

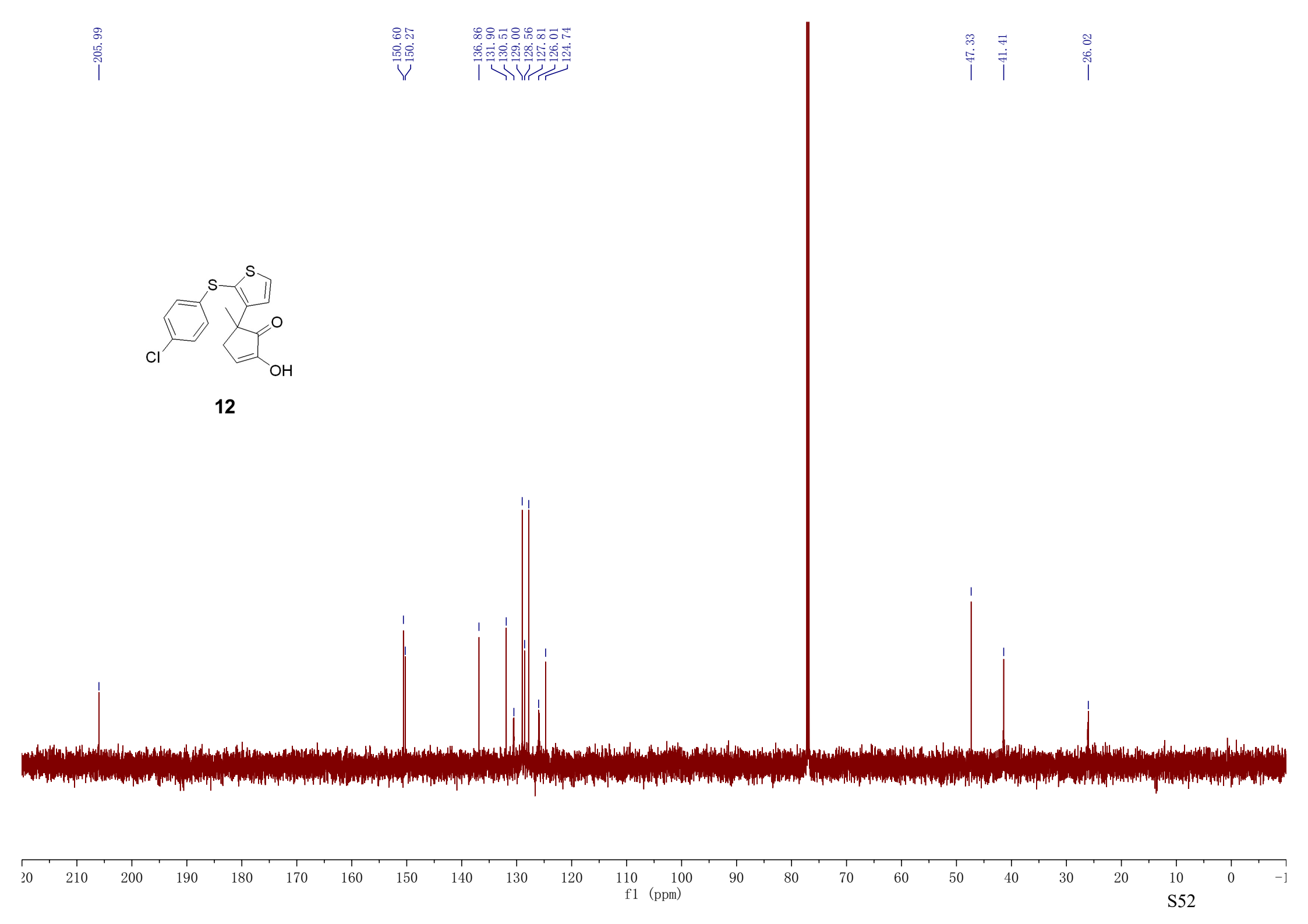

7.47
7.46
7.26
7.25
7.23
7.22
7.22
7.19
7.18
7.15
7.15
7.14
7.12
7.08
7.07
7.07
7.06
7.06
6.34
6.33
6.33
2.74
2.74
2.71
2.71
2.61
2.60
2.58
2.57
1.57
0.90
1.85
0.95
0.91
1.74
0.89
1.00
1.00
3.02
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


205.80
150.35
149.75
138.33
130.18
128.88
128.39
126.61
125.96
125.74
125.51
47.32
41.23
26.11
S
S
O
OH
11
f1 (ppm)

S
S
O
Cl
OH

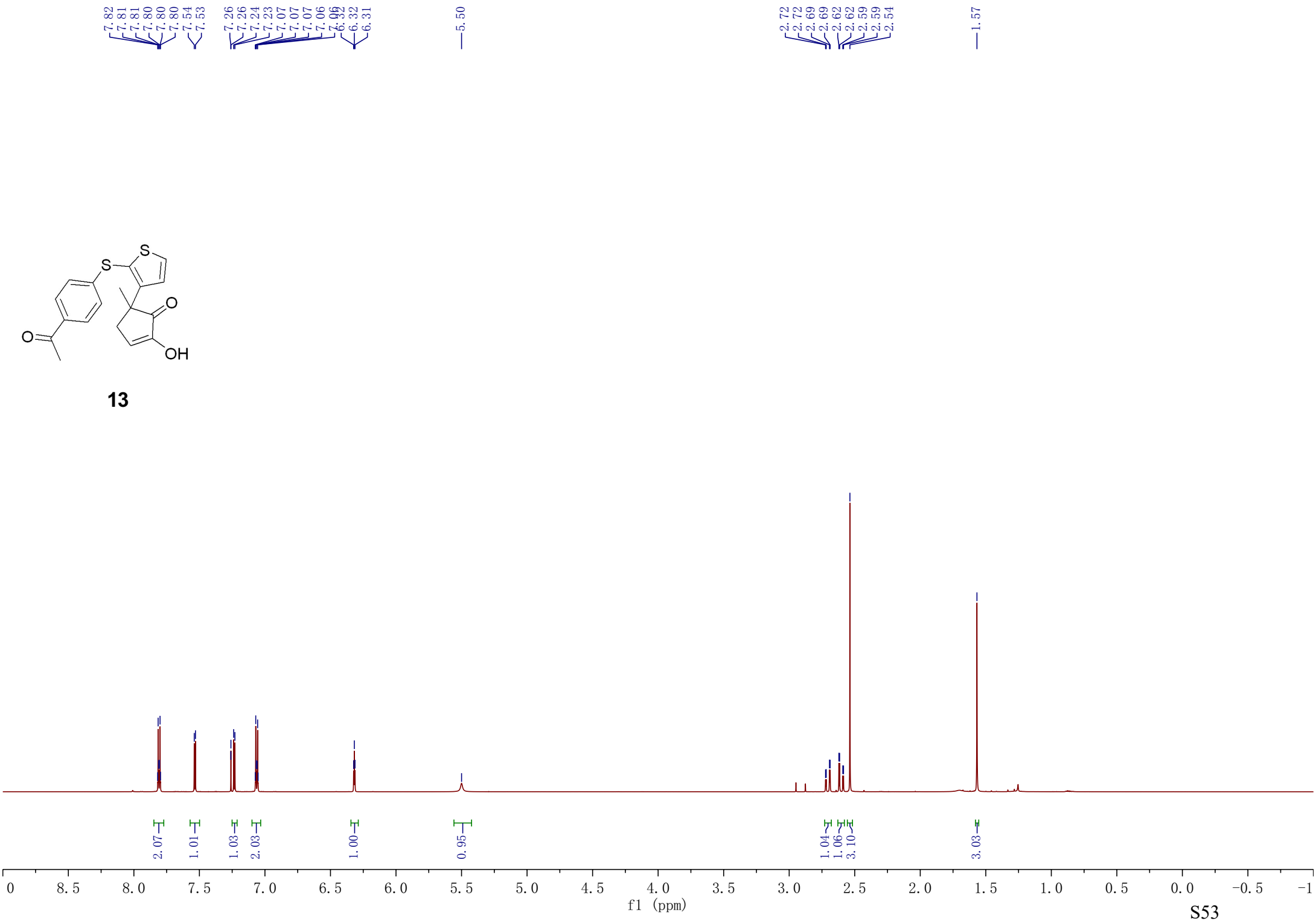
**12**

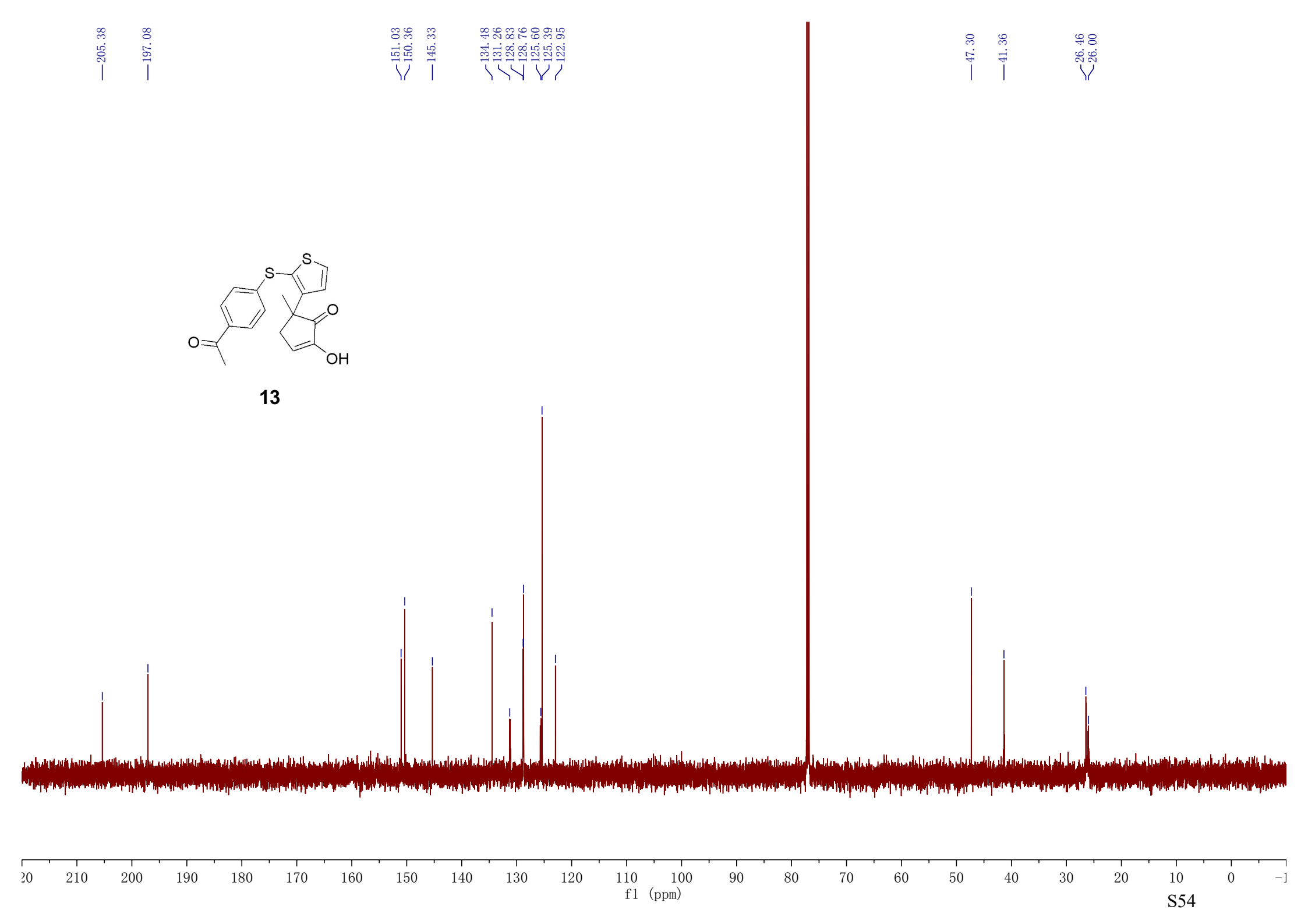

7.47
7.46
7.20
7.19
7.18
7.18
6.99
6.99
6.98
6.98
6.35
6.34
2.71
2.70
2.68
2.67
2.61
2.60
2.58
2.57
1.56
0.91
2.94
1.90
0.93
1.00
1.02
3.00
f1 (ppm)

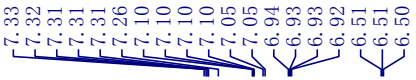

205.99
150.60
150.27
136.86
131.90
130.51
129.00
128.56
127.81
126.01
124.74
47.33
41.41
26.02
S
S
O
Cl
OH
12
f1 (ppm)

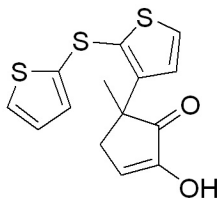
S
S
O
O
OH

**13**

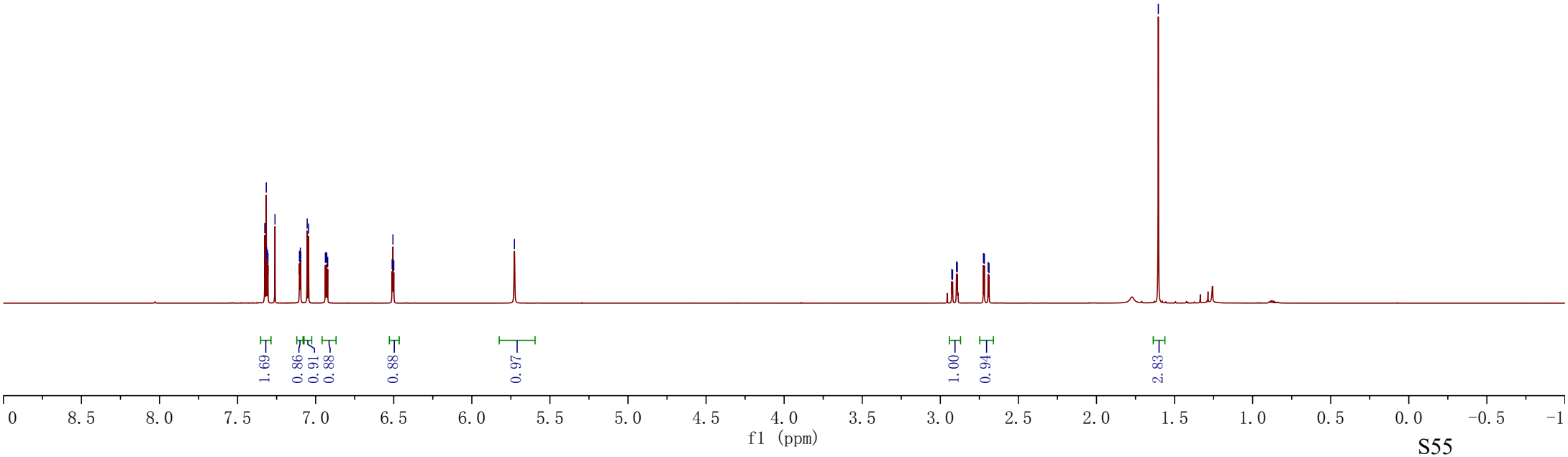

7.82
7.81
7.81
7.80
7.80
7.80
7.54
7.53
7.26
7.26
7.24
7.23
7.07
7.07
7.07
7.06
6.32
6.31
5.50
2.72
2.72
2.69
2.69
2.62
2.62
2.59
2.59
2.54
1.57
2.07
1.01
1.03
2.03
1.00
0.95
1.04
1.06
3.10
3.03
f1 (ppm)

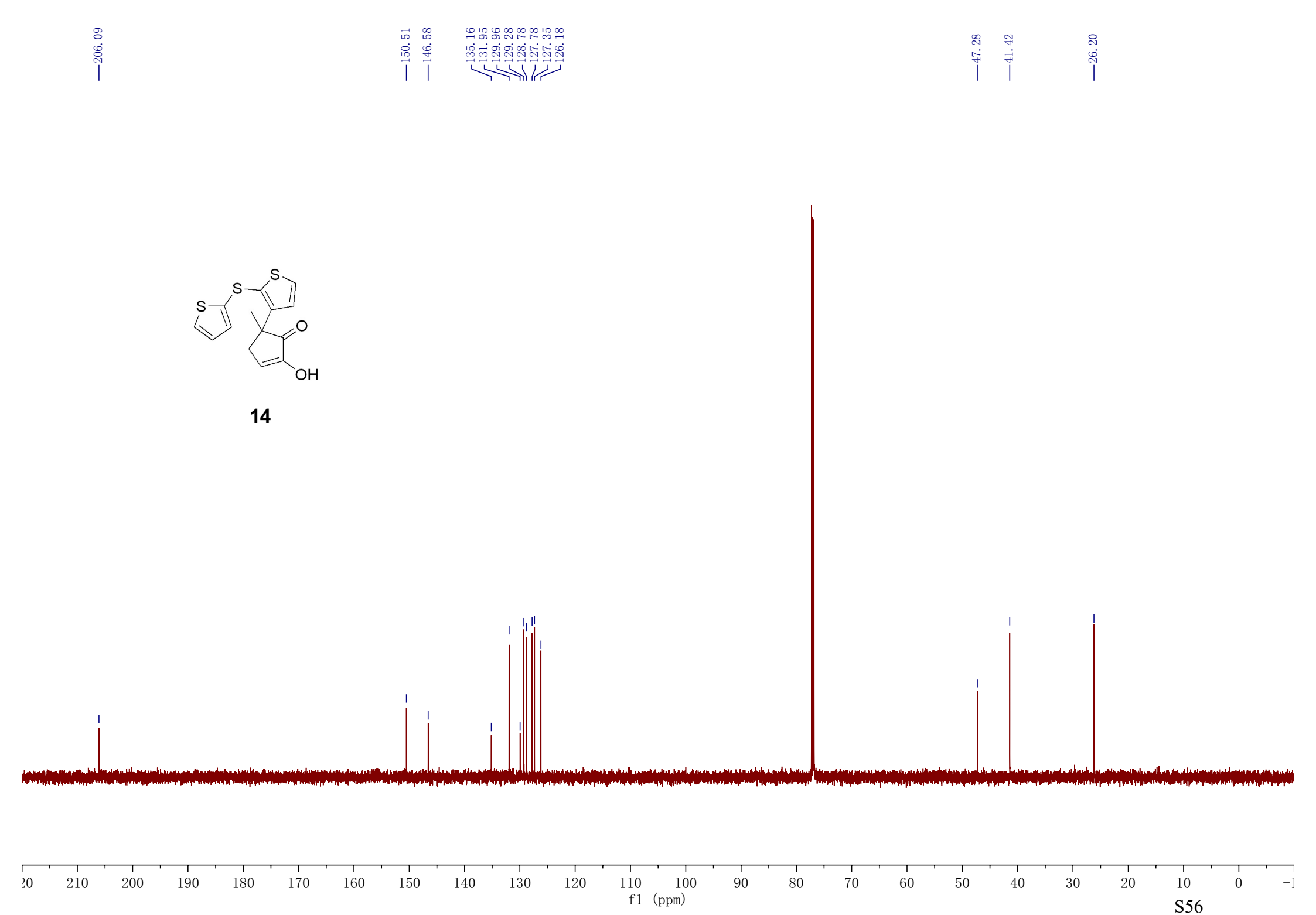

205.38
197.08
151.03
150.36
145.33
134.48
131.26
128.83
128.76
125.60
125.39
122.95
47.30
41.36
26.46
26.00
S
S
O
O
OH
13
f1 (ppm)

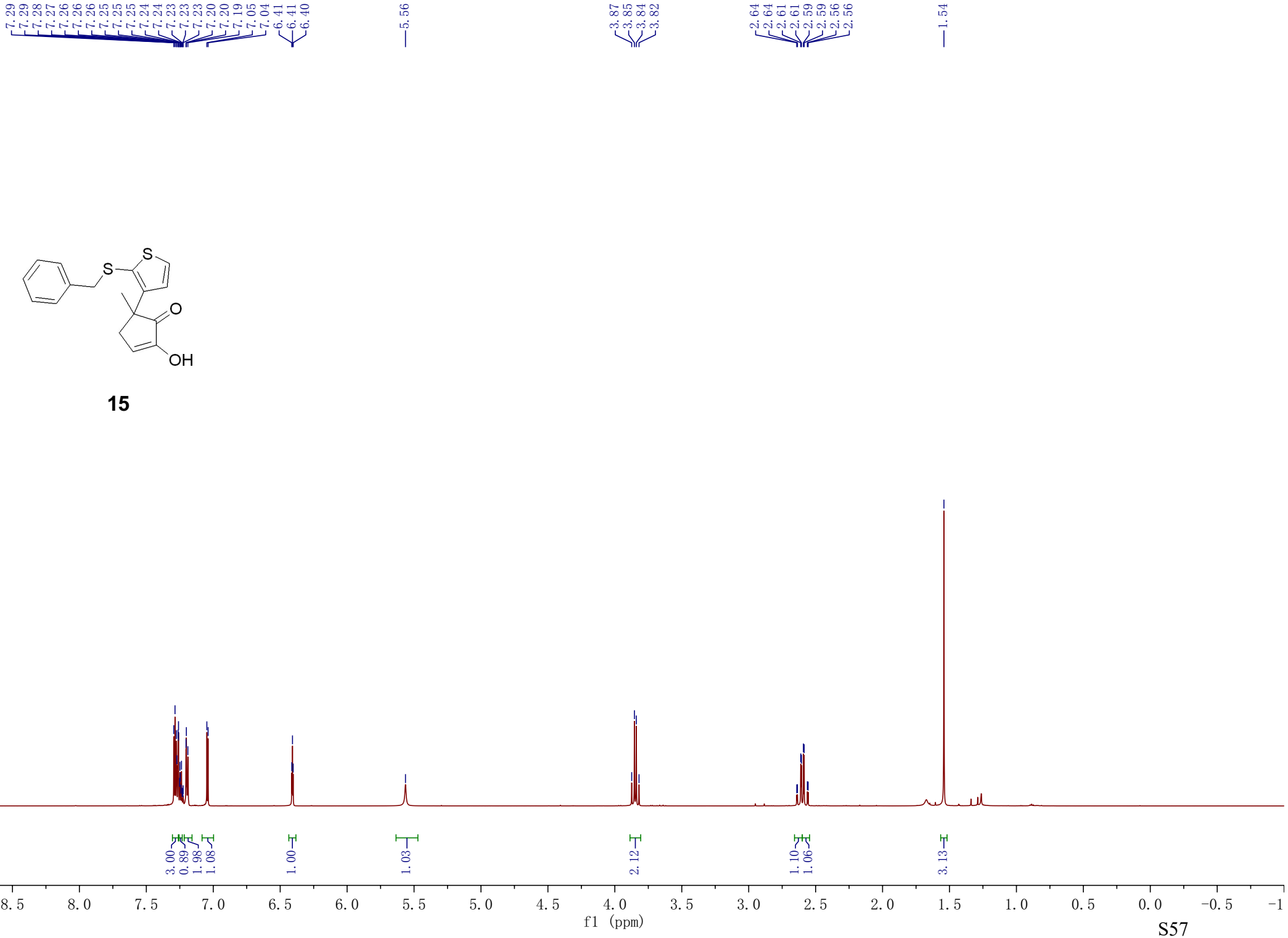

7.33
7.32
7.31
7.31
7.31
7.26
7.10
7.10
7.10
7.10
7.05
6.94
6.93
6.93
6.92
6.51
6.51
6.50
5.73
2.93
2.92
2.90
2.89
2.72
2.72
2.69
2.69
1.60

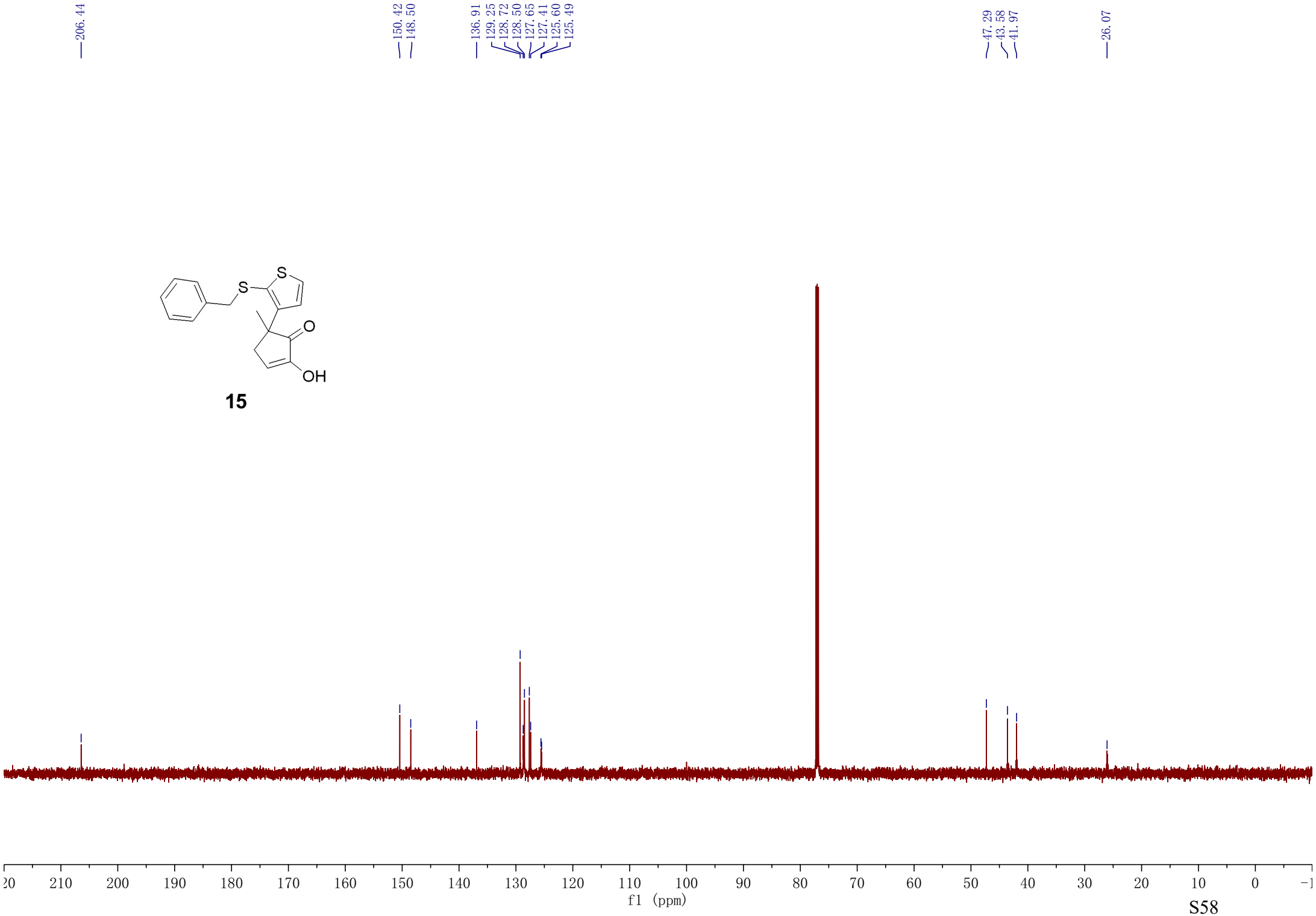

S
S
S
O
OH

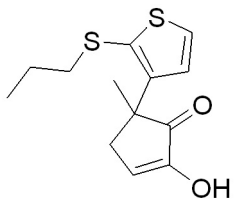
**14**


1.69
0.86
0.91
0.88
0.88
0.97
1.00
0.94
2.83
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


206.09
150.51
146.58
135.16
131.95
129.96
129.28
128.78
127.78
127.35
126.18
47.28
41.42
26.20
S
S
S
O
OH
14
f1 (ppm)

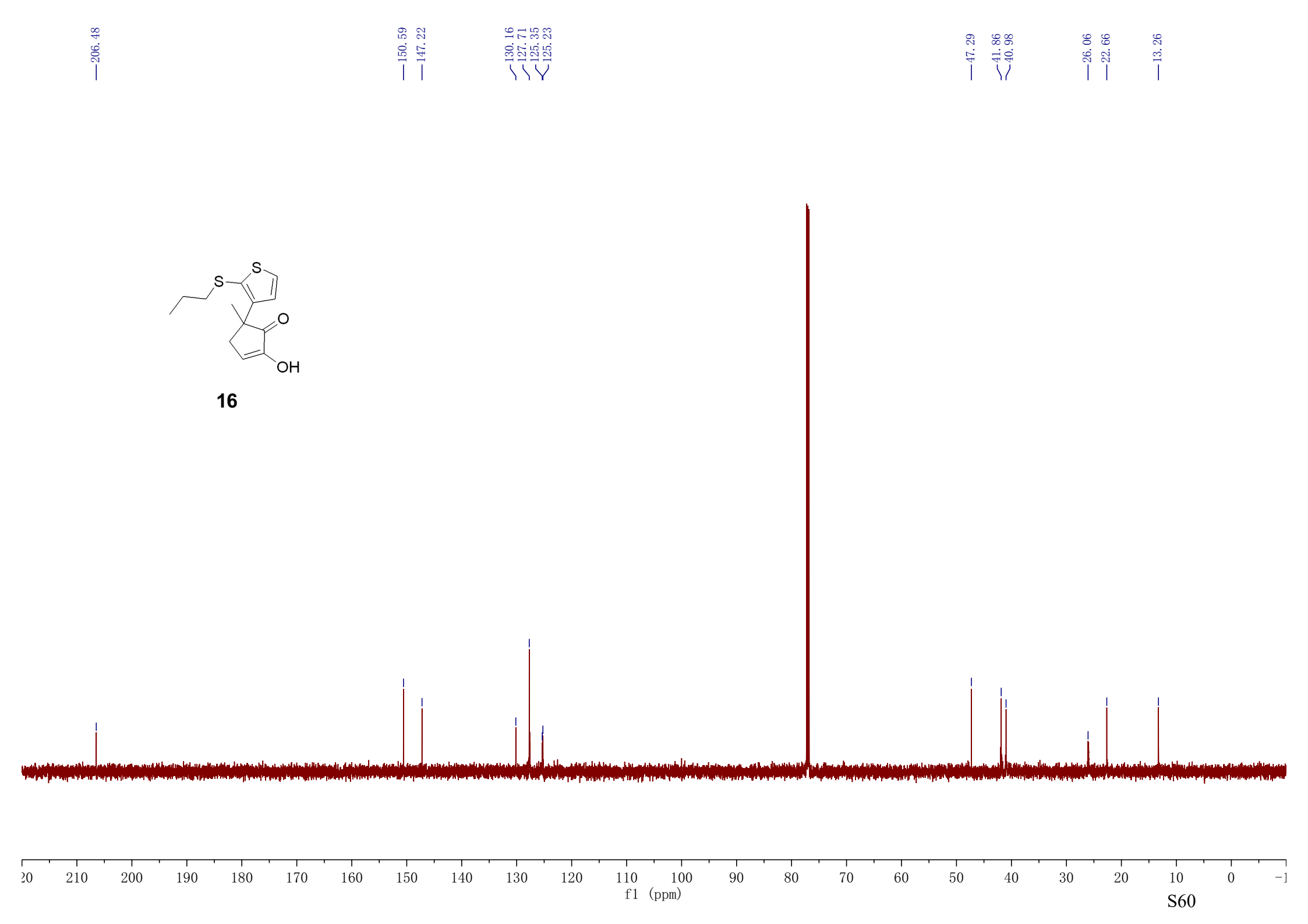

7.29
7.29
7.28
7.27
7.26
7.26
7.26
7.25
7.25
7.25
7.24
7.24
7.23
7.23
7.23
7.20
7.20
7.19
7.05
7.04
6.41
6.41
6.40
5.56
3.87
3.85
3.84
3.82
2.64
2.64
2.61
2.61
2.59
2.59
2.56
2.56
1.54
S
S
O
OH
15
3.00
0.89
1.98
1.08
1.00
1.03
2.12
1.10
1.06
3.13
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

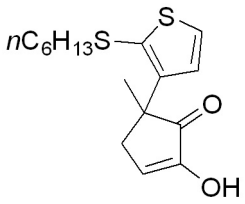

206.44
150.42
148.50
136.91
129.25
128.72
128.50
127.65
127.41
125.60
125.49
47.29
43.58
41.97
26.07
S
S
O
OH
15
f1 (ppm)


S
S
O
OH

**16**

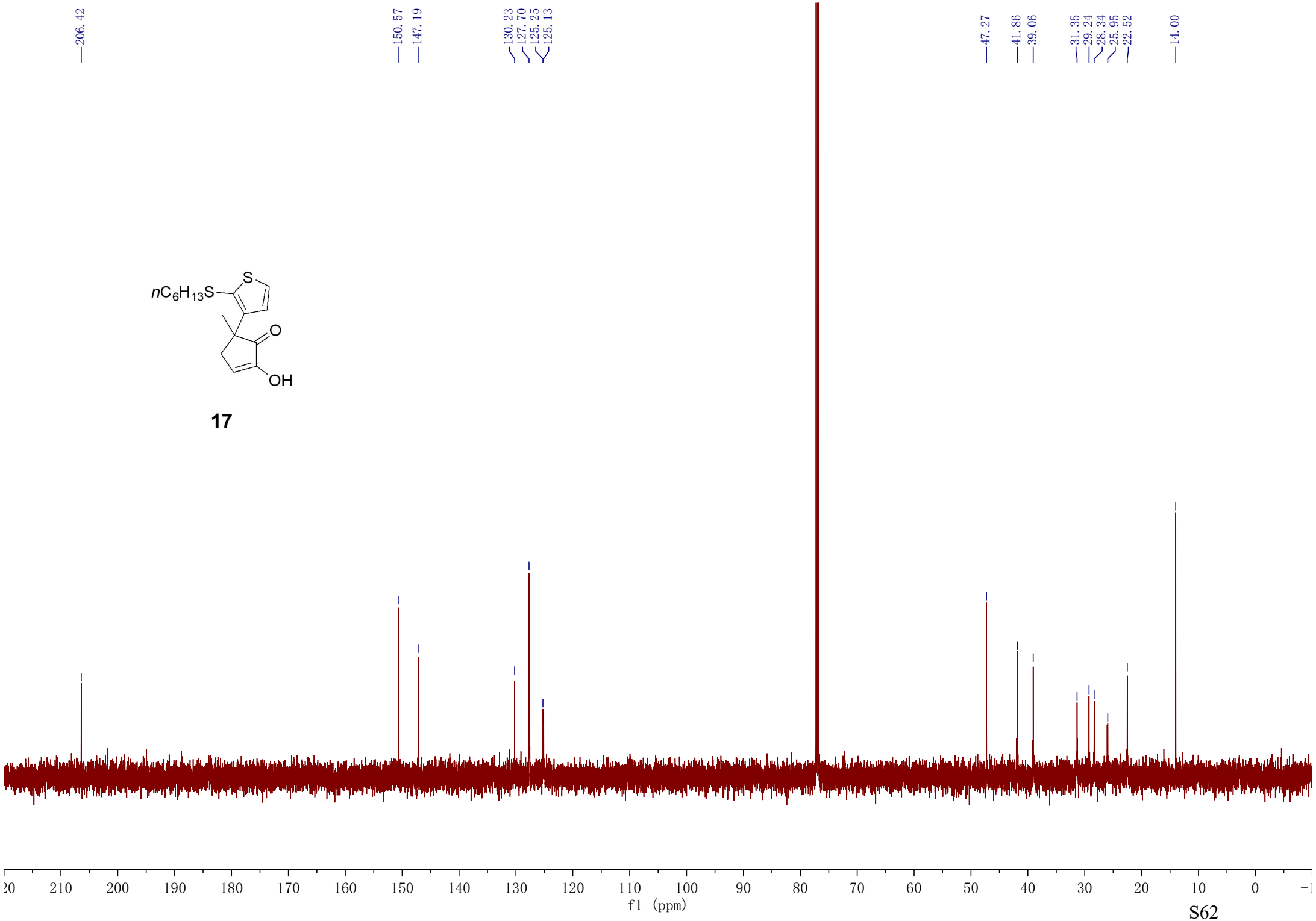
7.28
7.27
7.26
7.05
7.04
6.46
6.46
6.45
2.88
2.88
2.88
2.85
2.85
2.71
2.69
2.69
2.69
2.68
2.68
2.67
2.67
2.66
2.65
2.65
2.64
2.63
2.63
2.62
2.61
1.64
1.63
1.63
1.62
1.62
1.61
1.60
1.60
1.59
0.97
0.96
1.00
1.02
1.00
0.93
1.12
3.11
2.08
3.07
3.06
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

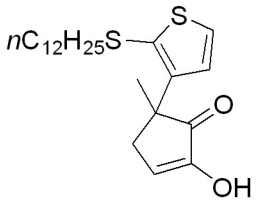

206.48
150.59
147.22
130.16
127.71
125.35
125.23
47.29
41.86
40.98
26.06
22.66
13.26
S
S
O
OH
16
f1 (ppm)


nC6H13S
S
O
OH

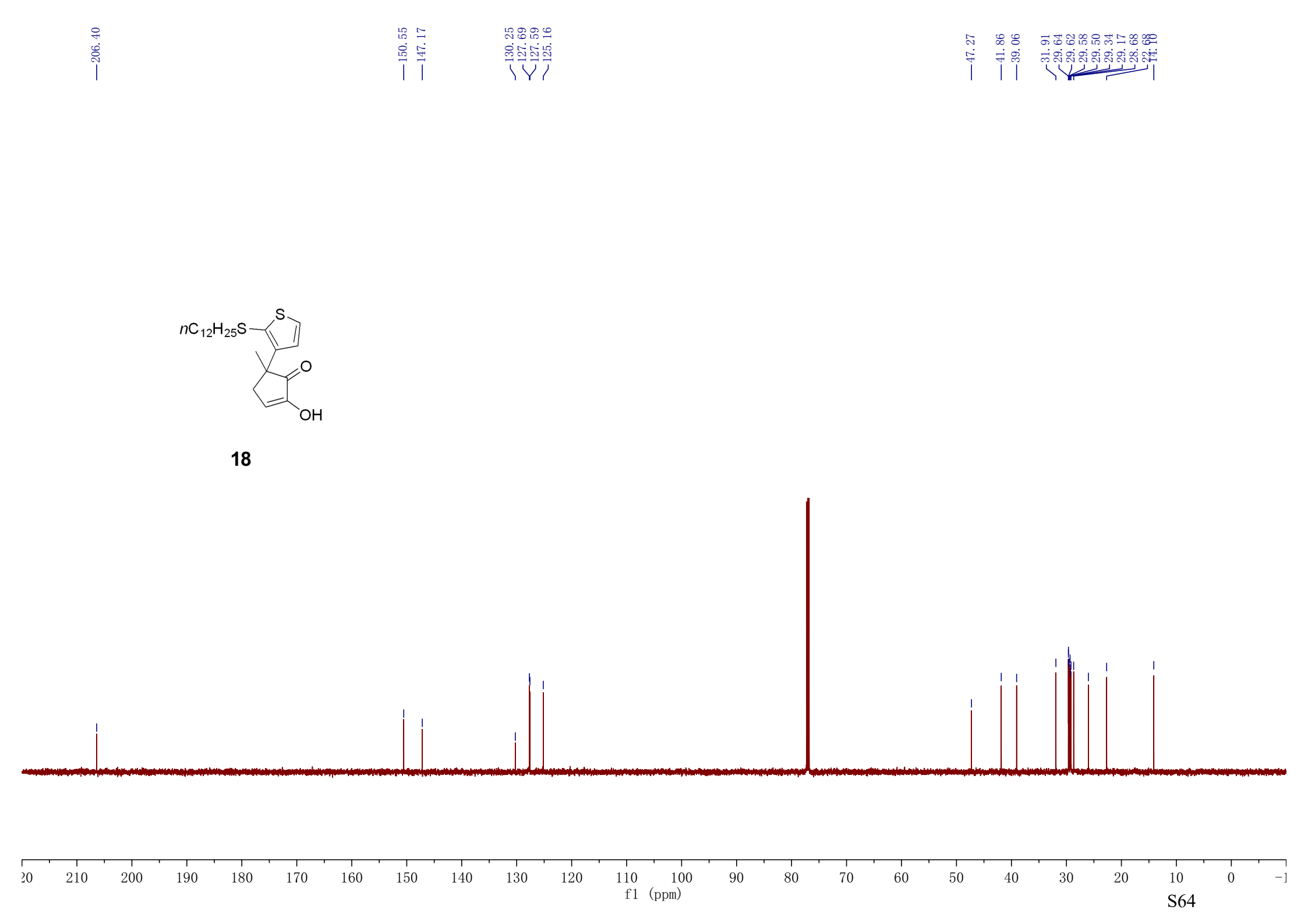
**17**

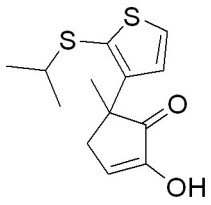
7.28
7.28
7.27
7.26
7.05
7.04
6.46
6.45
6.45
6.45
5.60
2.88
2.88
2.88
2.87
2.85
2.84
2.72
2.71
2.70
2.69
2.68
2.68
2.67
2.66
2.65
2.65
2.64
2.63
1.58
1.57
1.36
1.35
1.30
1.29
1.28
1.28
1.27
0.89
0.88
0.87
0.99
1.04
1.00
0.83
1.30
3.07
4.90
2.09
4.36
3.13
f1 (ppm)


206.42
150.57
147.19
130.23
127.70
125.25
125.13
47.27
41.86
39.06
31.35
29.24
28.34
25.95
22.52
14.00
nC6H13S
S
O
OH
17
f1 (ppm)

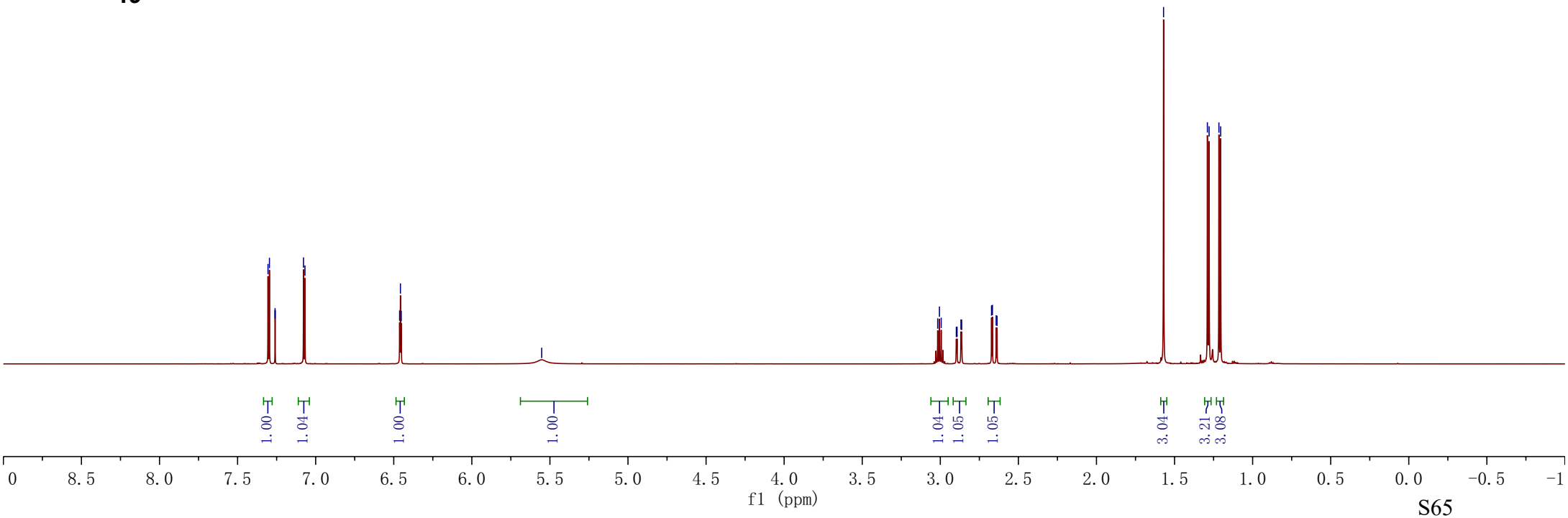


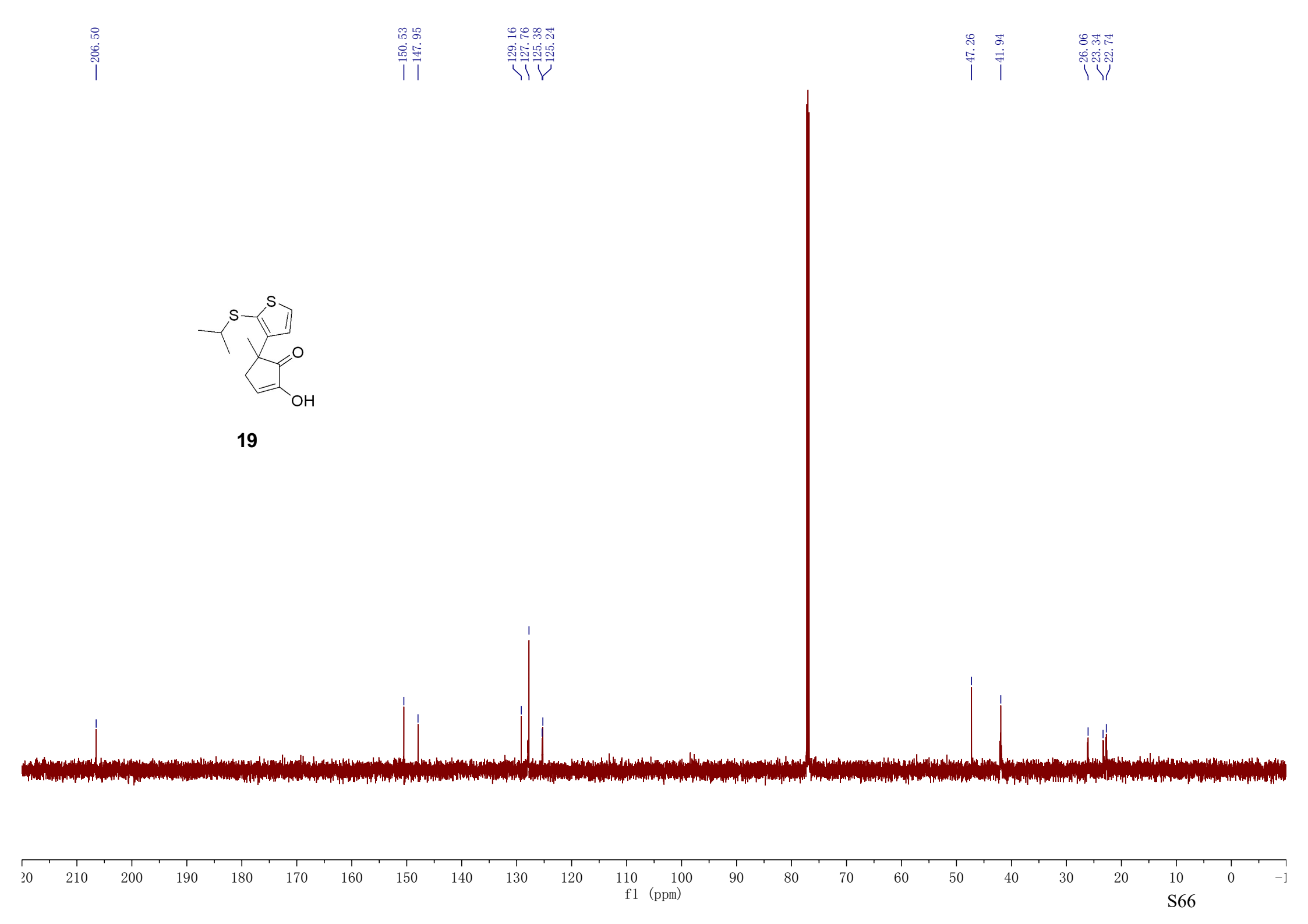

**18**

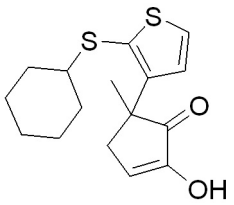

206.40
150.55
147.17
130.25
127.69
127.59
125.16
47.27
41.86
39.06
31.91
29.64
29.62
29.58
29.50
29.34
29.17
28.68
22.68
14.10
nC12H25S
S
O
OH
18
f1 (ppm)


S
S
O
OH

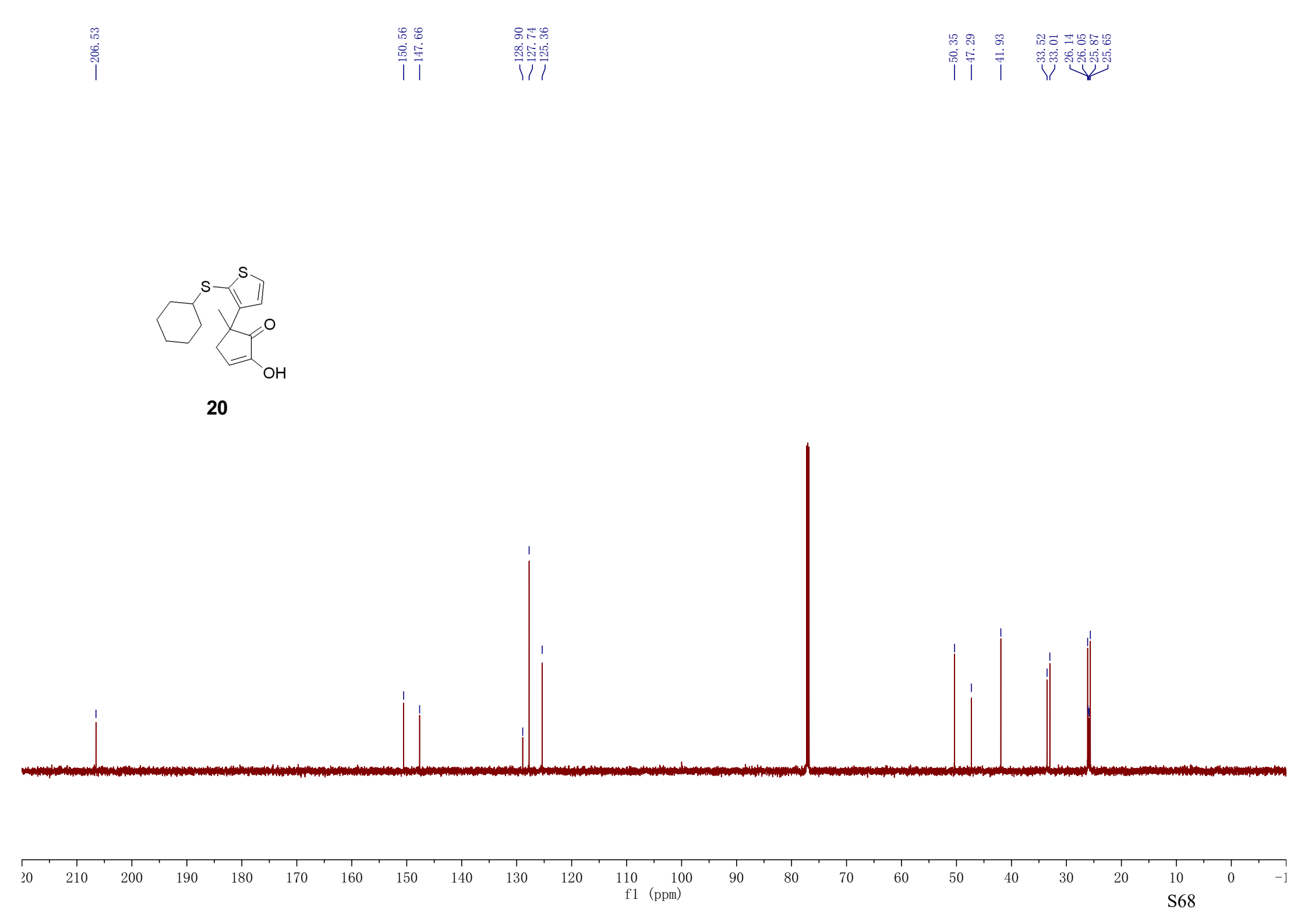
**19**

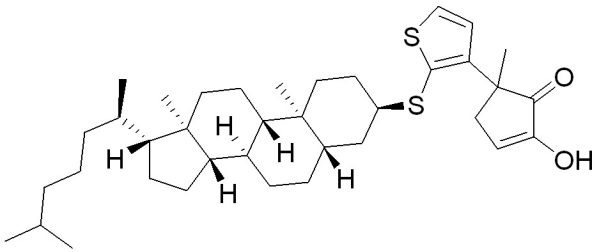

7.31
7.30
7.26
7.08
7.07
6.46
6.46
6.45
5.55
3.02
3.01
2.99
2.90
2.89
2.87
2.86
2.67
2.67
2.64
2.64
1.57
1.29
1.28
1.22
1.20
1.00
1.04
1.00
1.00
1.04
1.05
1.05
3.04
3.21
3.08
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


206.50
150.53
147.95
129.16
127.76
125.38
125.24
47.26
41.94
26.06
23.34
22.74
S
S
O
OH
19
f1 (ppm)

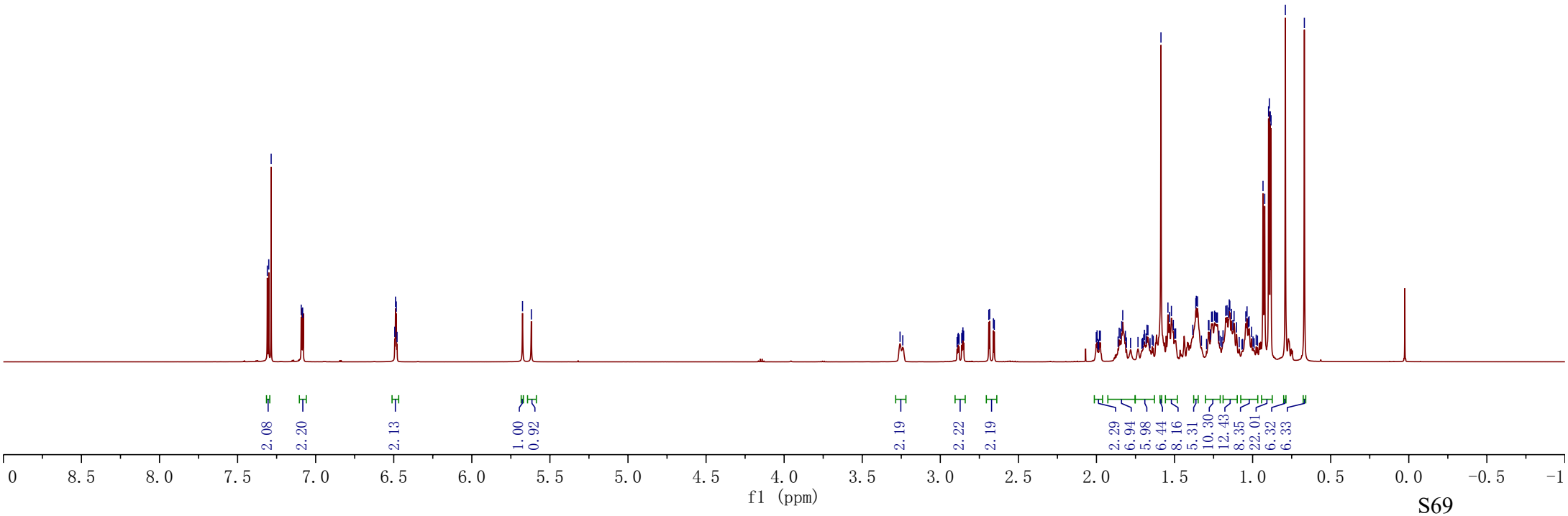


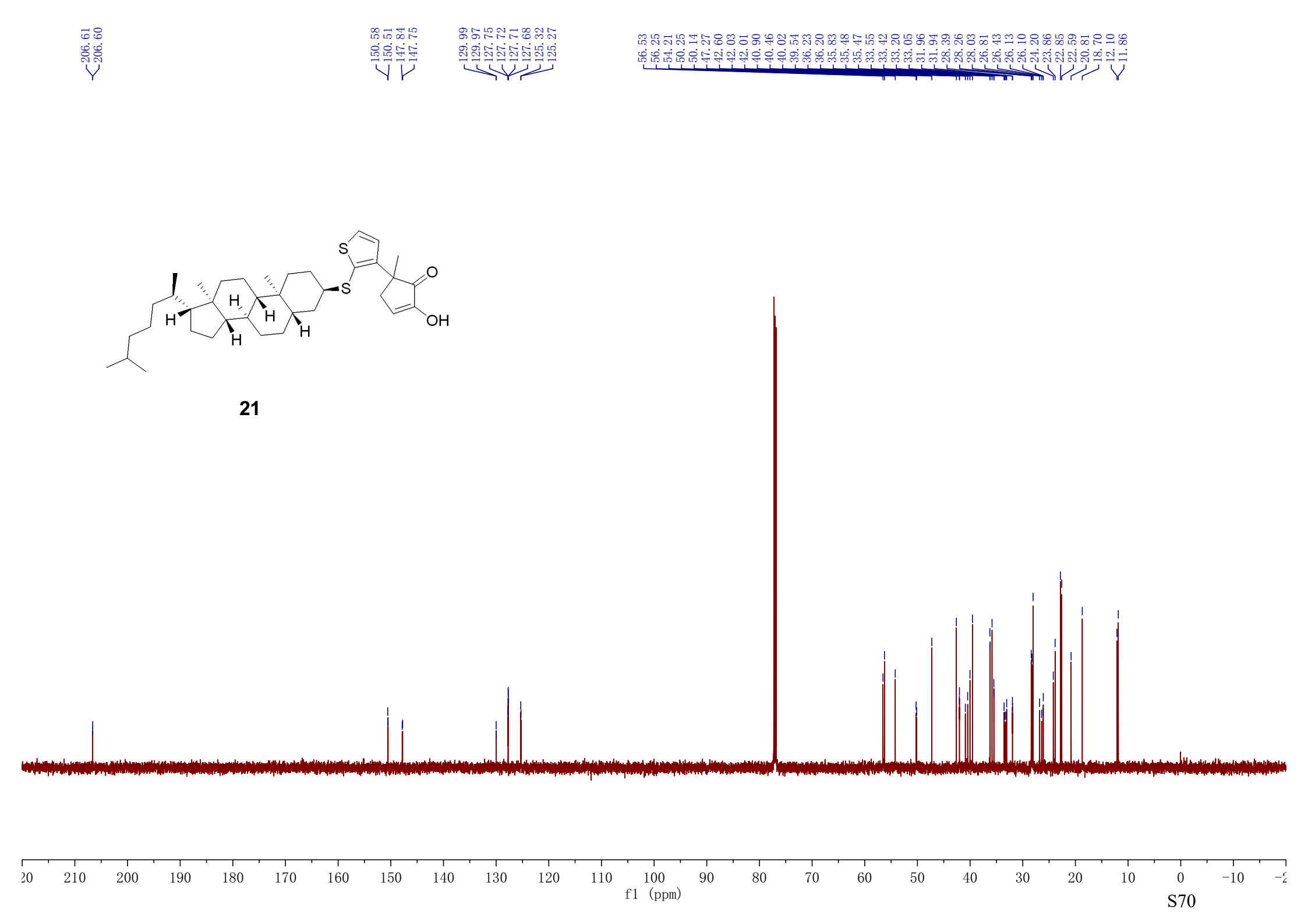

**20**

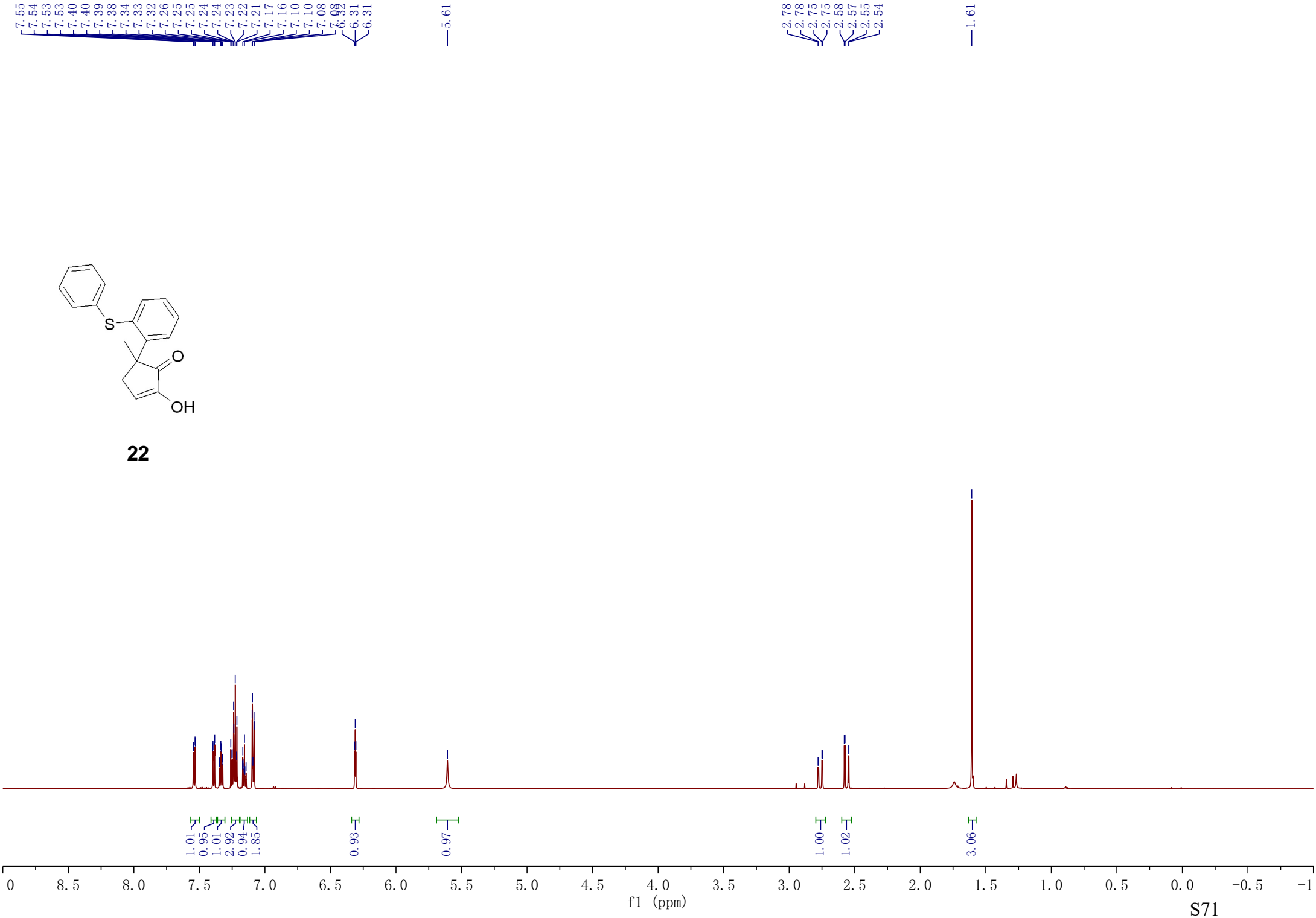

206.53
150.56
147.66
128.90
127.74
125.36
50.35
47.29
41.93
33.52
33.01
26.14
26.05
25.87
25.65
S
S
O
OH
20
f1 (ppm)


S
O
S
H
H
H
H
H
OH

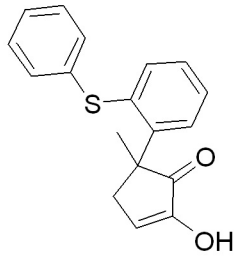
**21**


2.08
2.20
2.13
1.00
0.92
2.19
2.22
2.19
2.29
6.94
5.98
6.44
8.16
5.31
10.30
12.43
8.35
22.01
6.32
6.33
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


206.61
206.60
150.58
150.51
147.84
147.75
129.99
129.97
127.75
127.72
127.71
127.68
125.32
125.27
56.53
56.25
54.21
50.25
50.14
47.27
42.60
42.03
42.01
40.90
40.46
40.02
39.54
36.23
36.20
35.83
35.48
35.47
33.55
33.42
33.20
33.05
31.96
31.94
28.39
28.26
28.03
26.81
26.43
26.13
26.10
24.20
23.86
22.85
22.59
20.81
18.70
12.10
11.86
S
S
O
OH
H
H
H
H
21
f1 (ppm)


7.55
7.54
7.53
7.53
7.40
7.40
7.39
7.38
7.34
7.33
7.32
7.26
7.25
7.25
7.24
7.24
7.23
7.22
7.21
7.17
7.16
7.10
7.10
7.08
6.32
6.31
6.31
5.61
2.78
2.78
2.75
2.75
2.58
2.57
2.55
2.54
1.61
S
O
OH
22
1.01
0.95
1.01
2.92
0.94
1.85
0.93
0.97
1.00
1.02
3.06
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

206.08
150.69
145.40
137.40
136.57
133.27
128.98
128.76
128.44
128.19
126.28
123.36
123.22
50.43
41.29
25.34

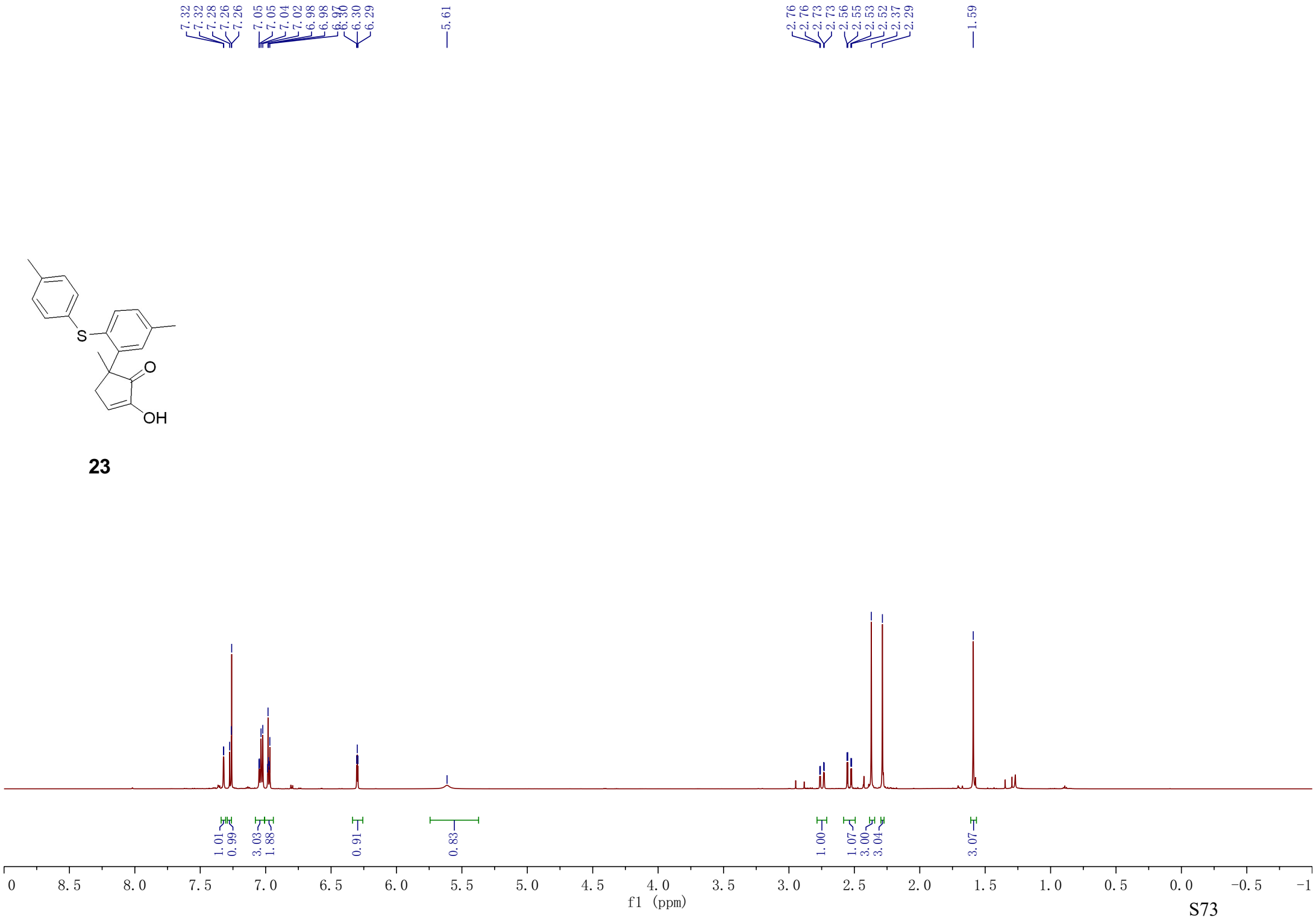



**22**

f1 (ppm)

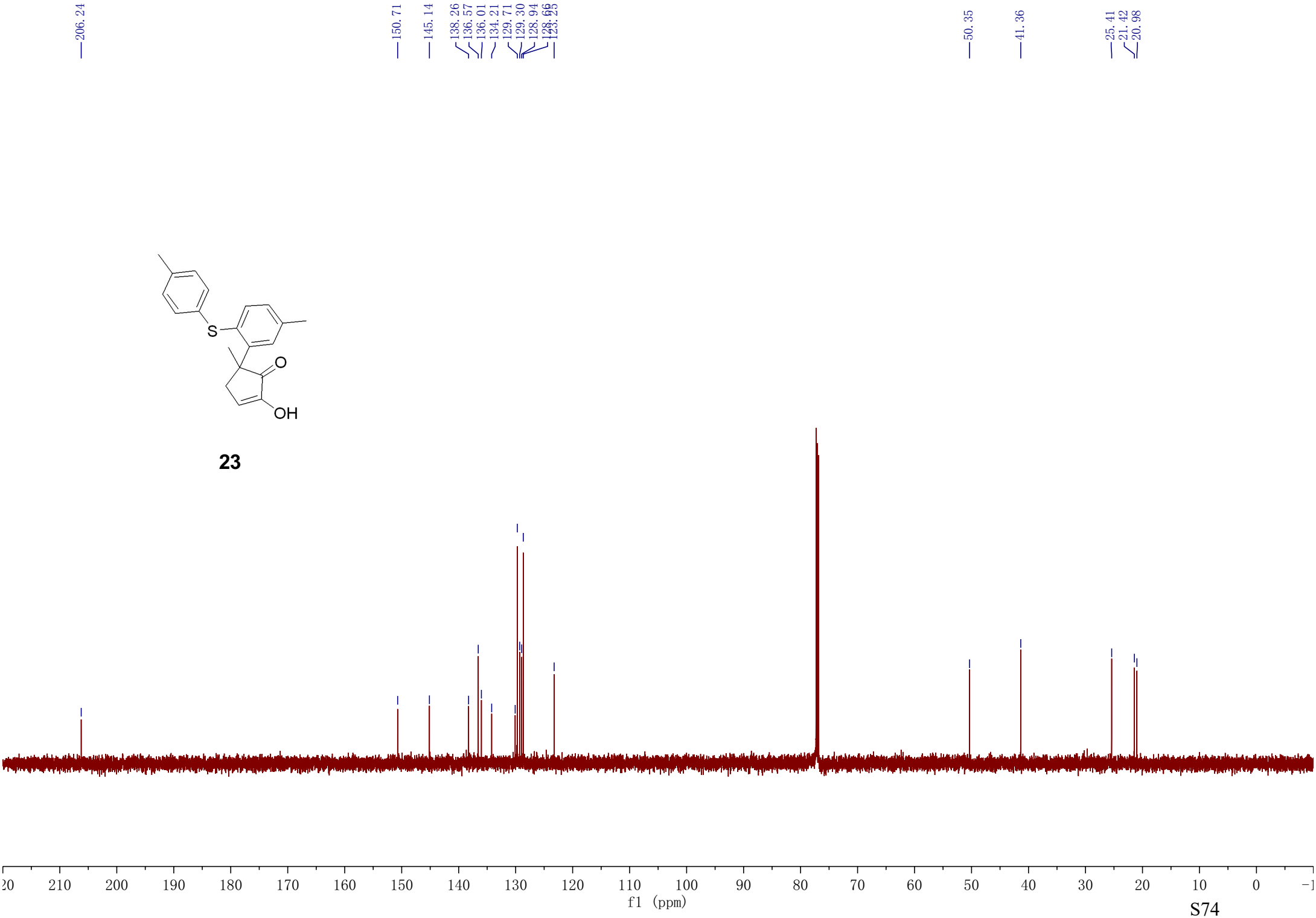
S
O
OH

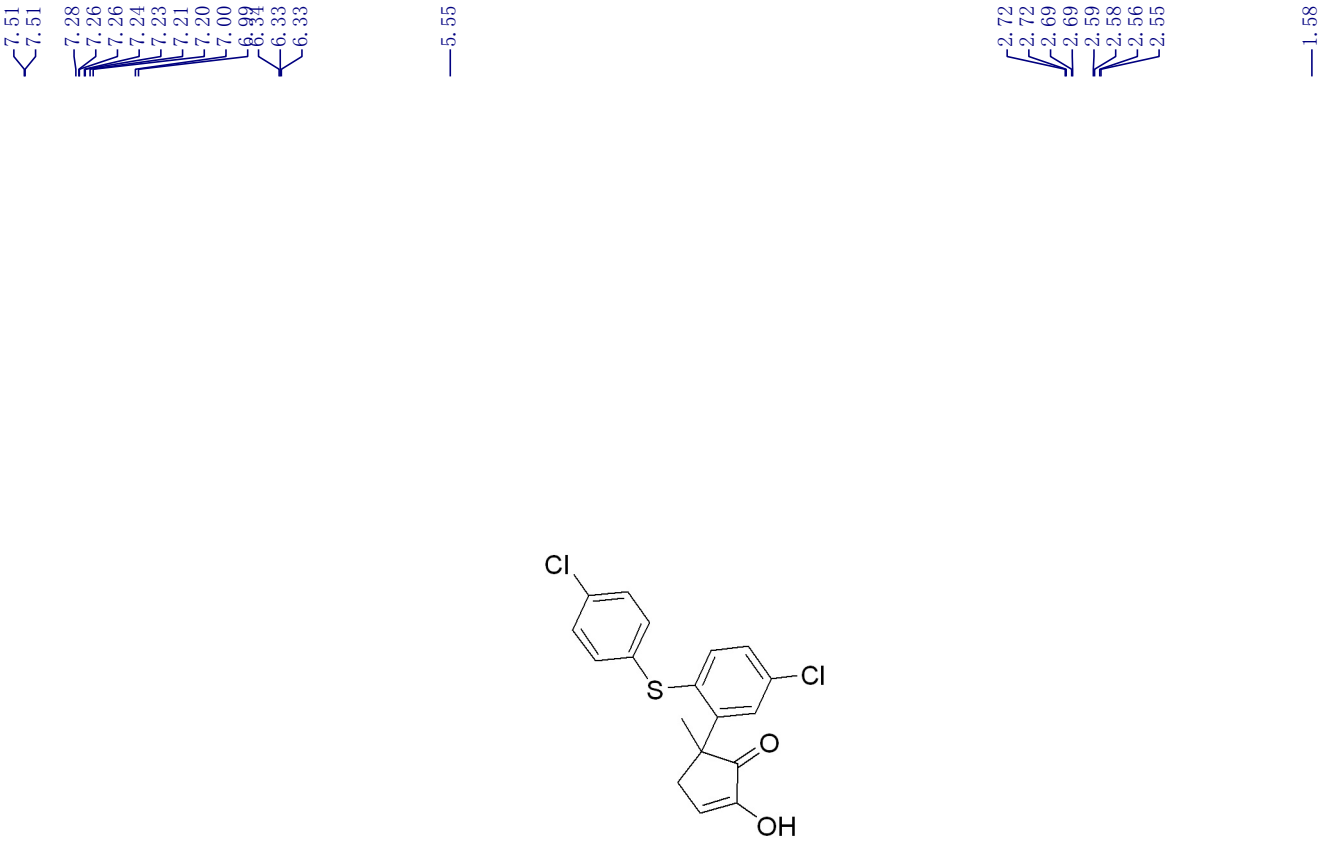
**23**


7.32
7.32
7.28
7.26
7.26
7.05
7.05
7.04
7.02
6.98
6.98
6.97
6.30
6.30
6.29
5.61
2.76
2.76
2.73
2.73
2.56
2.55
2.53
2.52
2.37
2.29
1.59
1.01
0.99
3.03
1.88
0.91
0.83
1.00
1.07
3.00
3.04
3.07
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

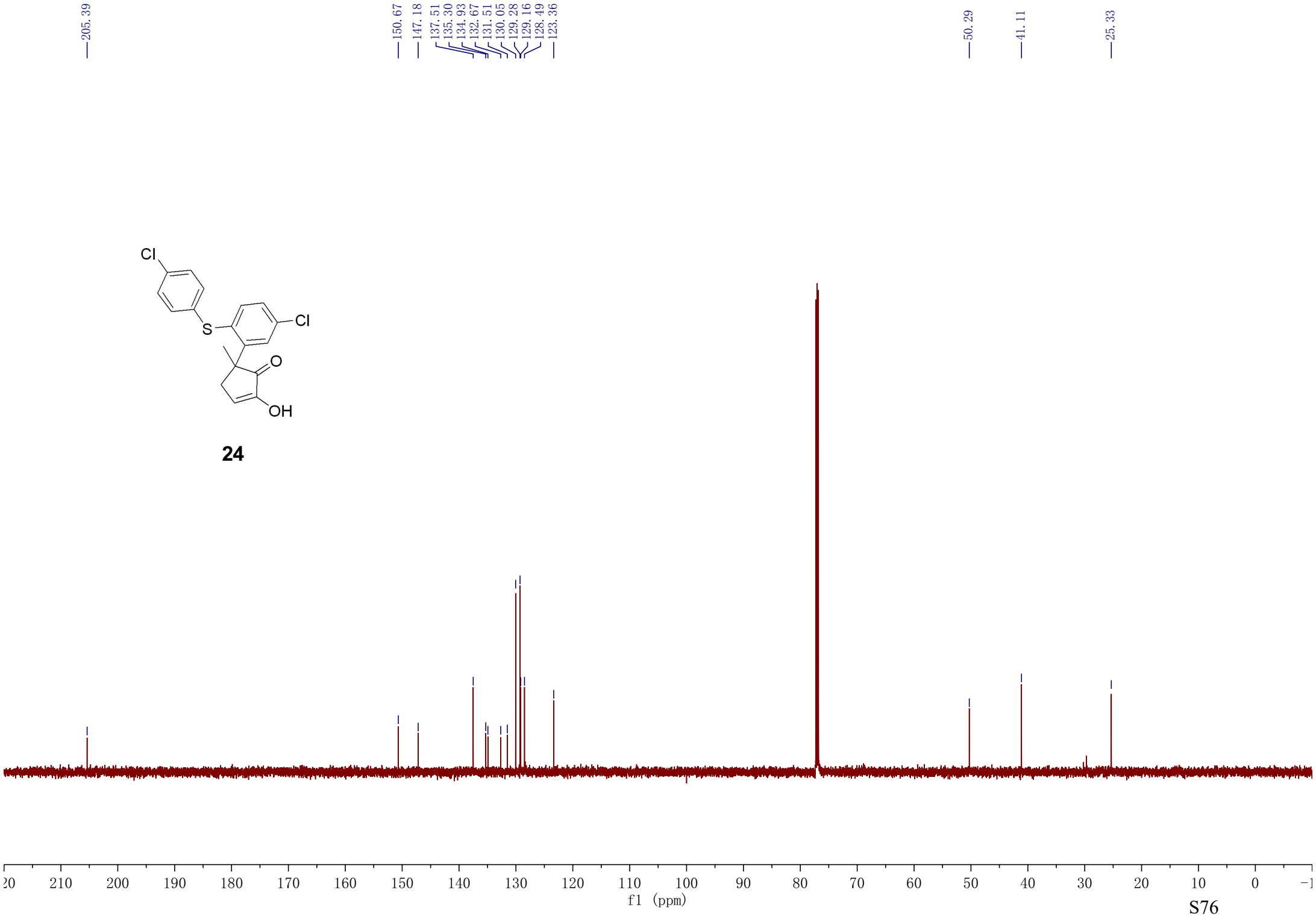
S
O
OH

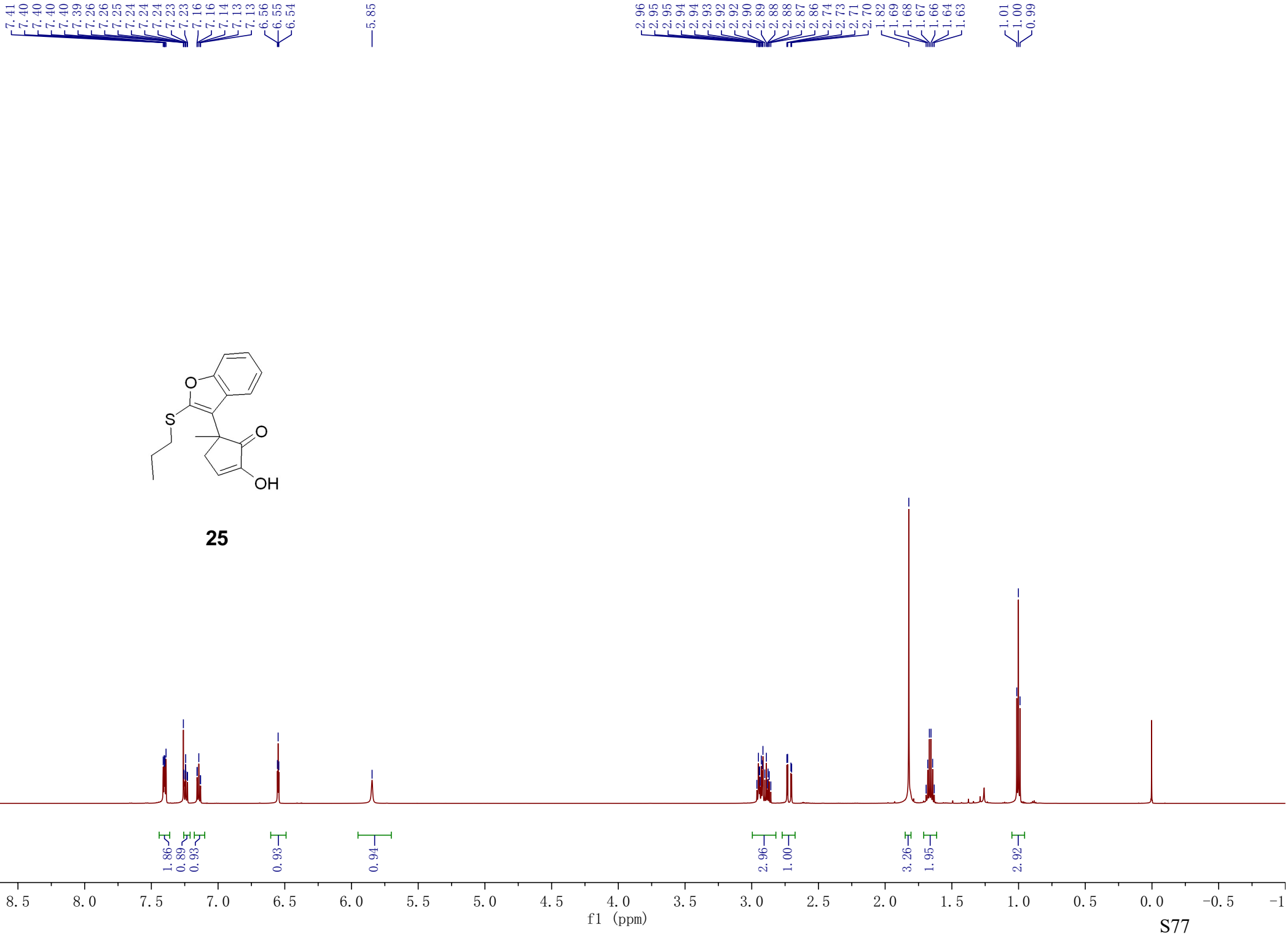
**23**

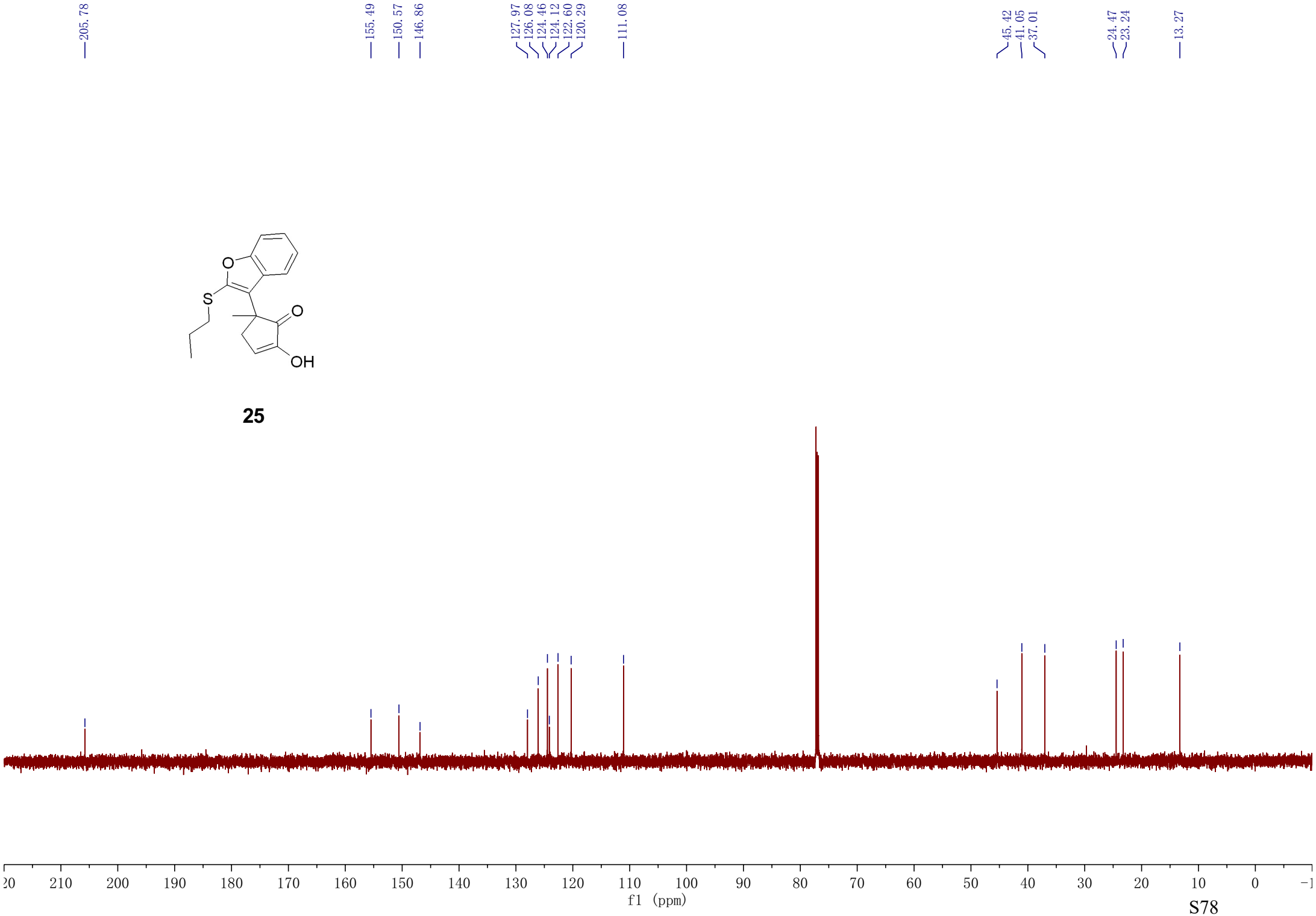

206.24
150.71
145.14
138.26
136.57
136.01
134.21
129.71
129.30
128.94
123.23
50.35
41.36
25.41
21.42
20.98
f1 (ppm)

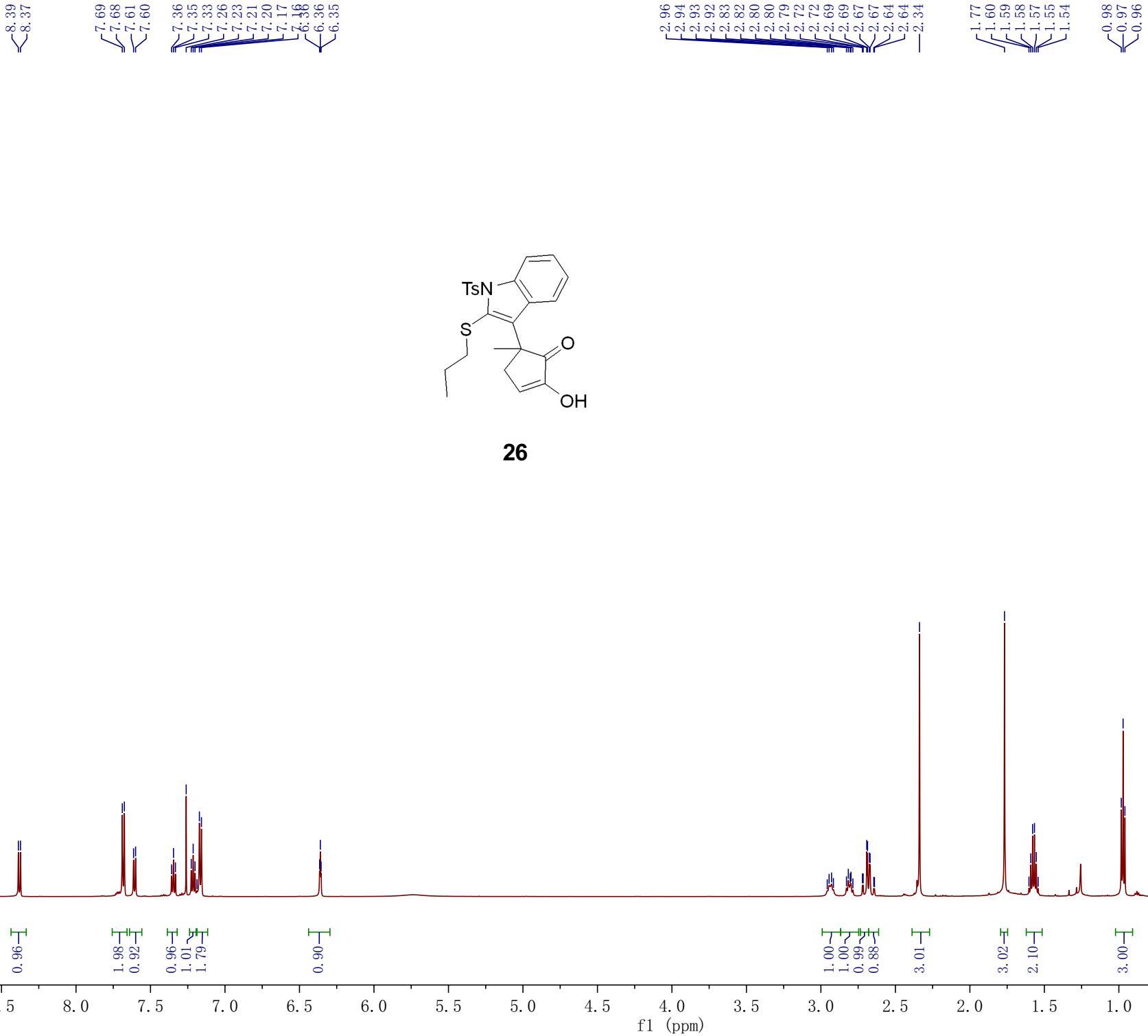

7.51
7.51
7.28
7.26
7.26
7.24
7.23
7.21
7.20
7.00
6.99
6.34
6.33
6.33
5.55
2.72
2.72
2.69
2.69
2.59
2.58
2.56
2.55
1.58
Cl
S
Cl
O
OH
0.91
1.10
0.59
2.12
1.75
0.94
0.96
1.00
1.05
3.00
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

**24**

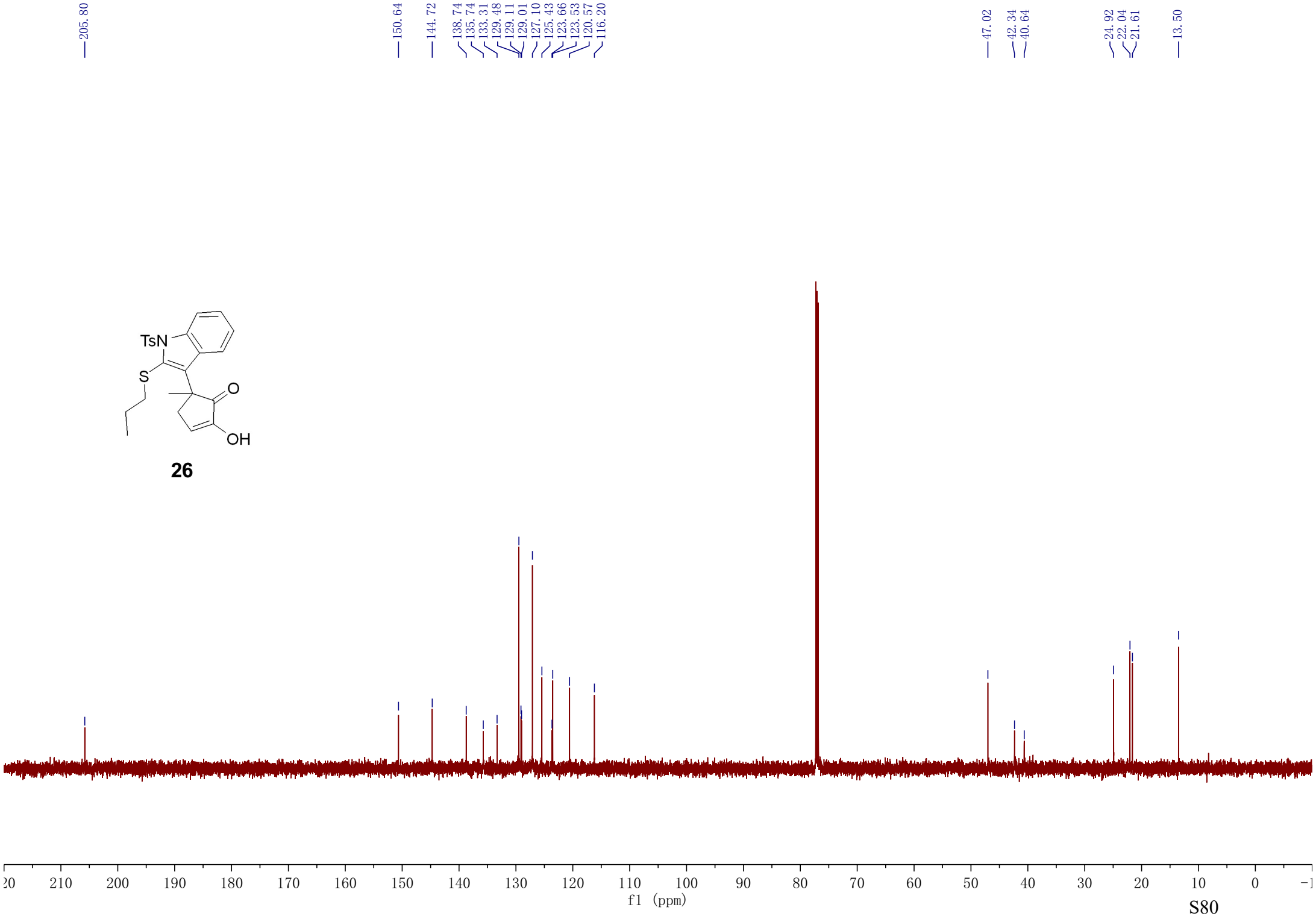

205.39
150.67
147.18
137.51
135.30
134.93
132.67
131.51
130.05
129.28
129.16
128.49
123.36
50.29
41.11
25.33
Cl
S
Cl
O
OH
24
f1 (ppm)

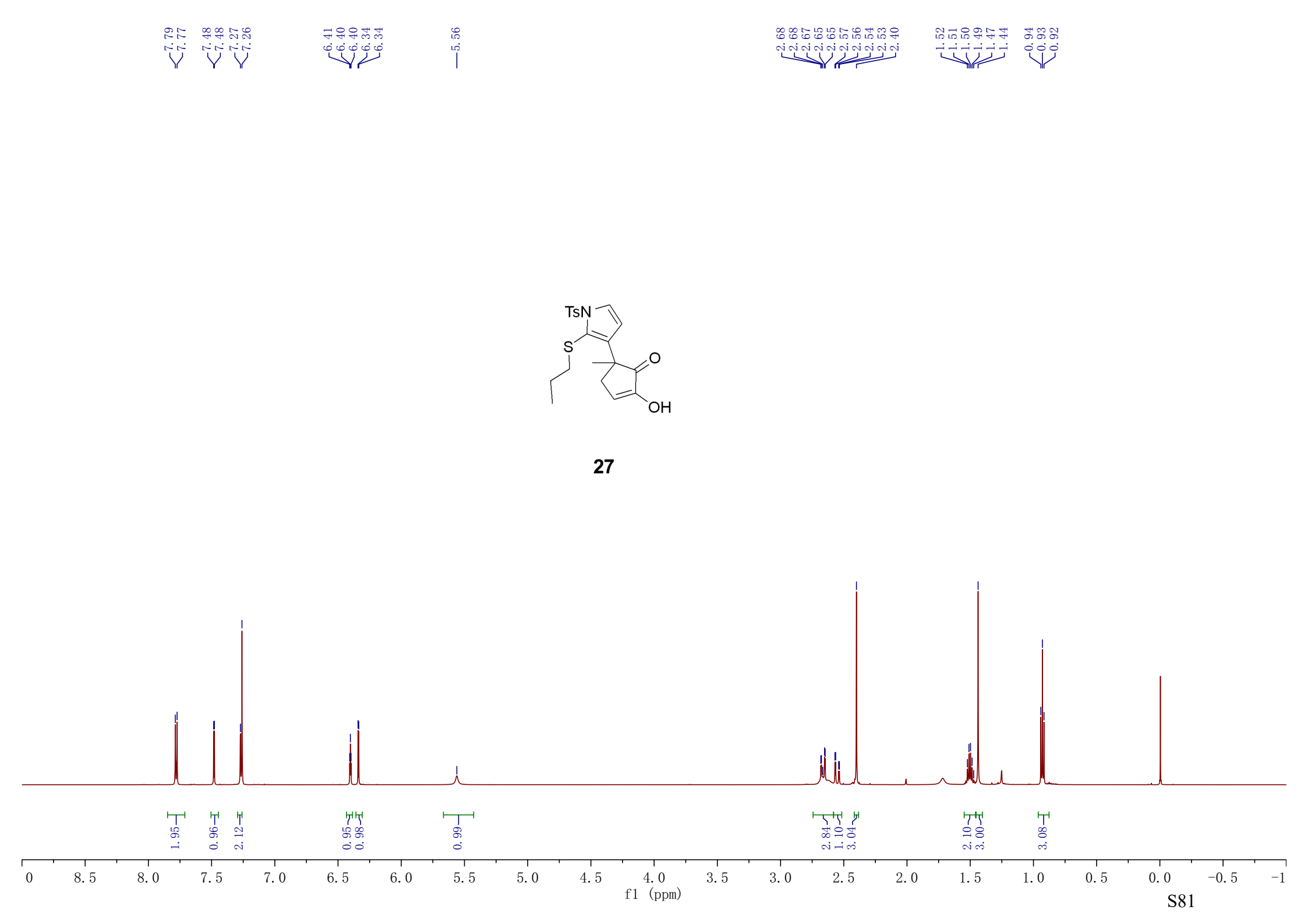

7.41
7.40
7.40
7.40
7.40
7.39
7.26
7.26
7.25
7.24
7.24
7.24
7.23
7.23
7.16
7.16
7.14
7.13
7.13
6.56
6.55
6.54
5.85
2.96
2.95
2.95
2.94
2.94
2.93
2.92
2.92
2.90
2.89
2.88
2.88
2.87
2.86
2.74
2.73
2.71
2.70
1.82
1.69
1.68
1.67
1.66
1.64
1.63
1.01
1.00
0.99
O
S
O
OH
25
1.86
0.89
0.93
0.93
0.94
2.96
1.00
3.26
1.95
2.92
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


205.78
155.49
150.57
146.86
127.97
126.08
124.46
124.12
122.60
120.29
111.08
45.42
41.05
37.01
24.47
23.24
13.27
O
S
O
OH
25
f1 (ppm)

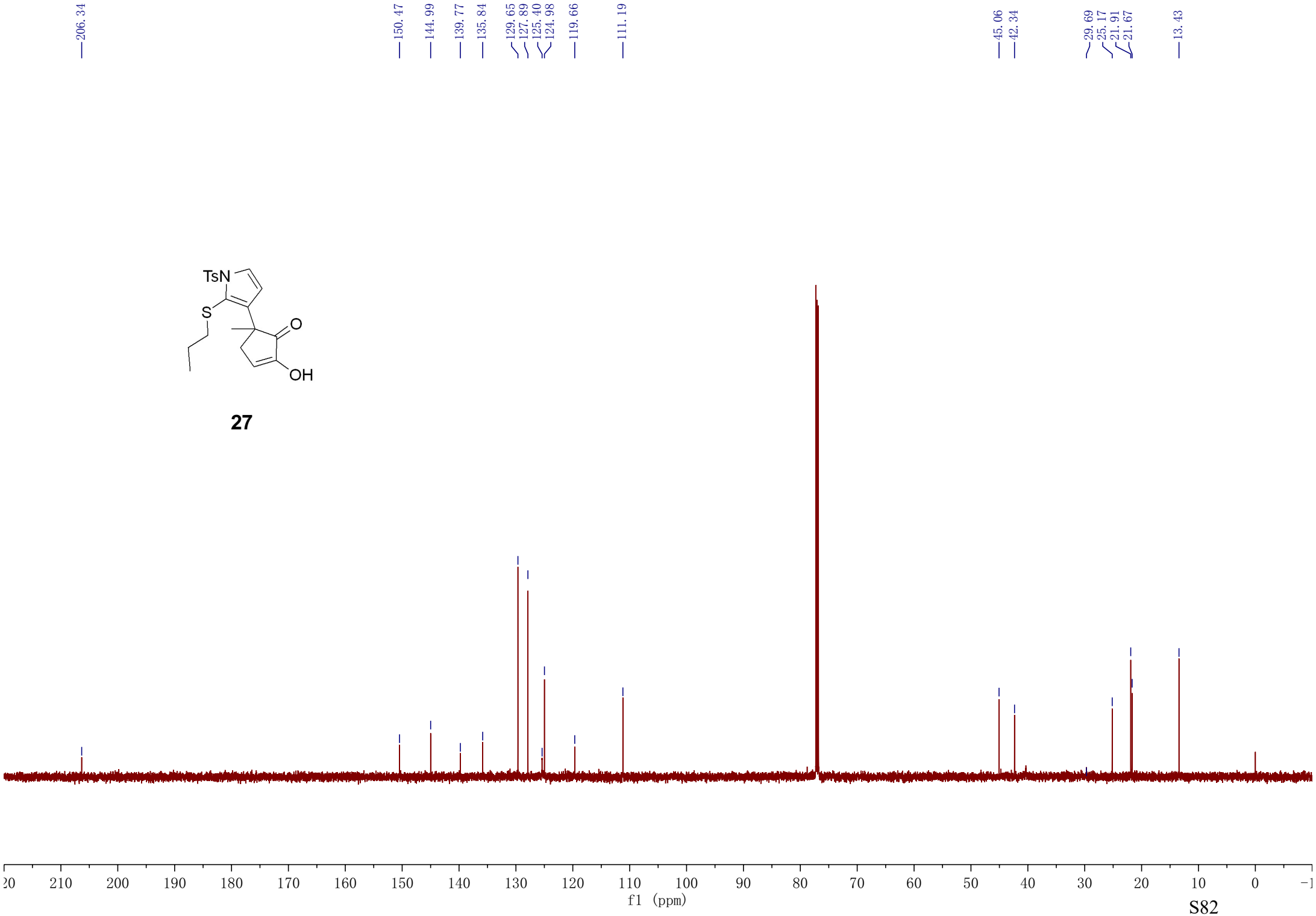

8.39
8.37
7.69
7.68
7.61
7.60
7.36
7.35
7.33
7.26
7.23
7.21
7.20
7.17
7.16
6.38
6.36
6.35
2.96
2.94
2.93
2.92
2.83
2.82
2.80
2.80
2.79
2.72
2.72
2.69
2.69
2.67
2.67
2.64
2.64
2.34
1.77
1.60
1.59
1.58
1.57
1.55
1.54
0.98
0.97
0.96
TsN
S
O
OH
0.96
1.98
0.92
0.96
1.01
1.79
0.90
1.00
1.00
0.99
0.88
3.01
3.02
2.10
3.00
f1 (ppm)

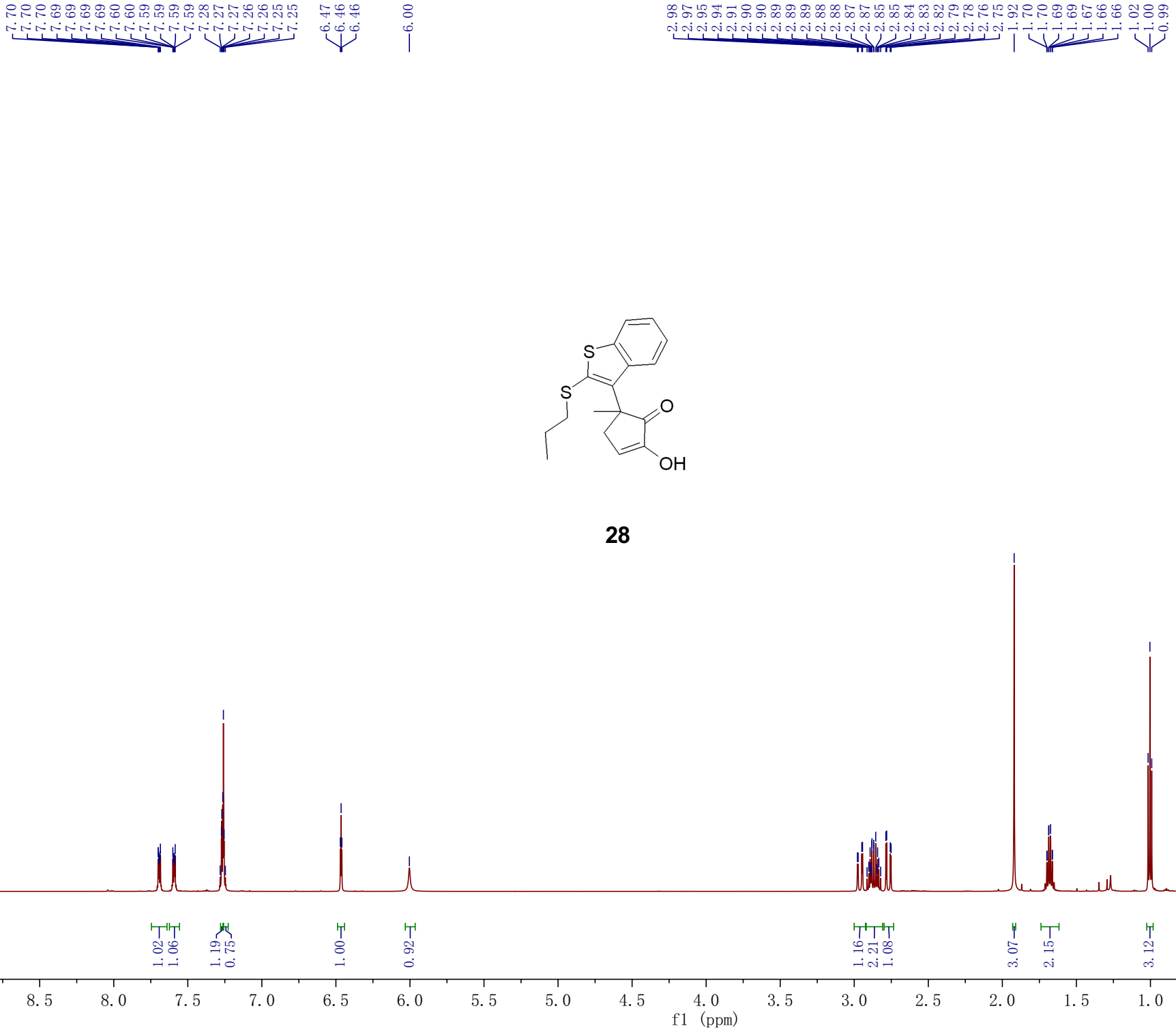
**26**


205.80
150.64
144.72
138.74
135.74
133.31
129.48
129.11
129.01
127.10
125.43
123.66
123.53
120.57
116.20
47.02
42.34
40.64
24.92
22.04
21.61
13.50
TsN
S
O
OH
26
f1 (ppm)


7.79
7.77
7.48
7.48
7.27
7.26
6.41
6.40
6.40
6.34
6.34
5.56
2.68
2.68
2.67
2.65
2.65
2.57
2.56
2.54
2.53
2.40
1.52
1.51
1.50
1.49
1.47
1.44
0.94
0.93
0.92
TsN
S
O
OH
1.95
0.96
2.12
0.95
0.98
0.99
2.84
1.10
3.04
2.10
3.00
3.08
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

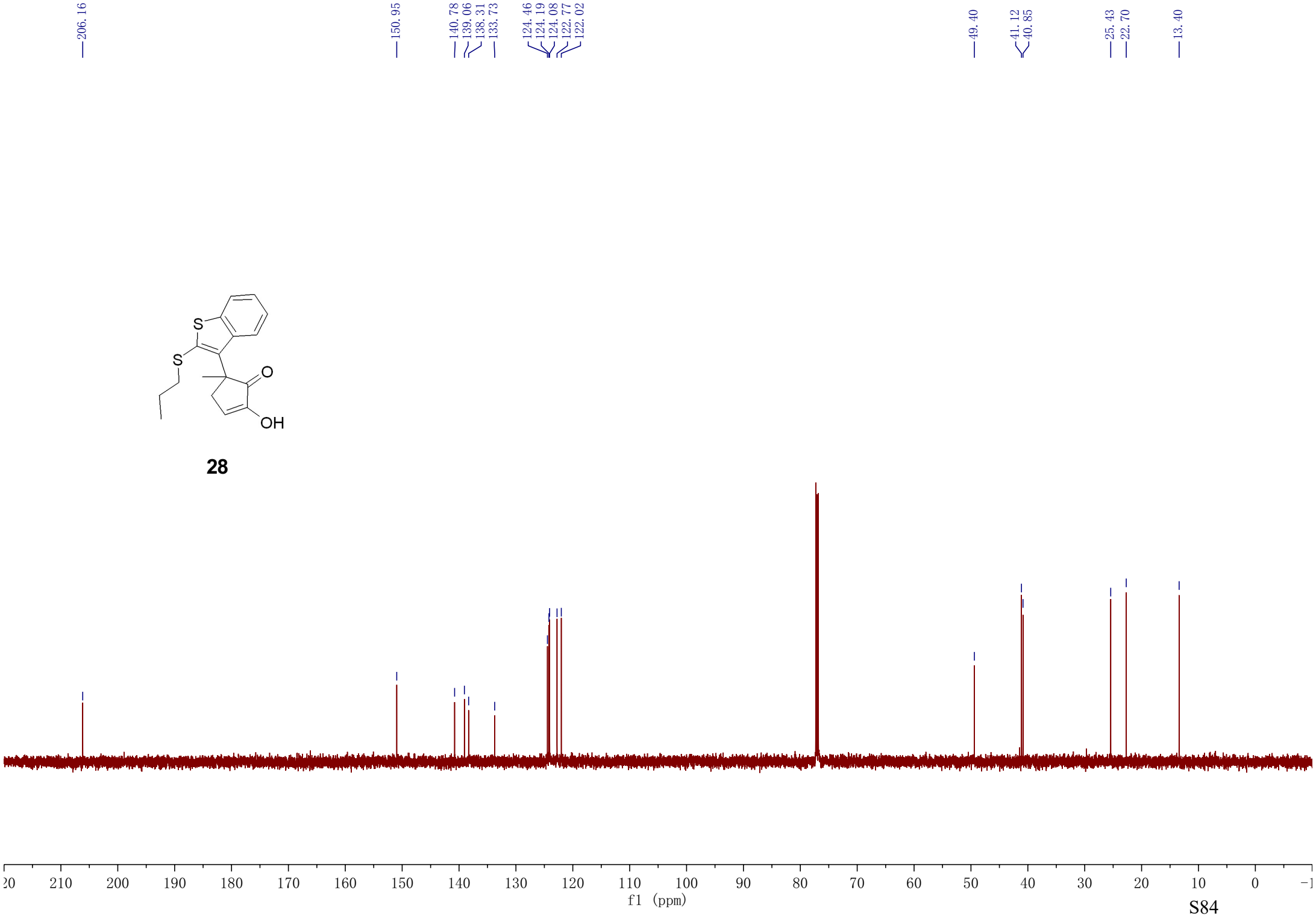
**27**

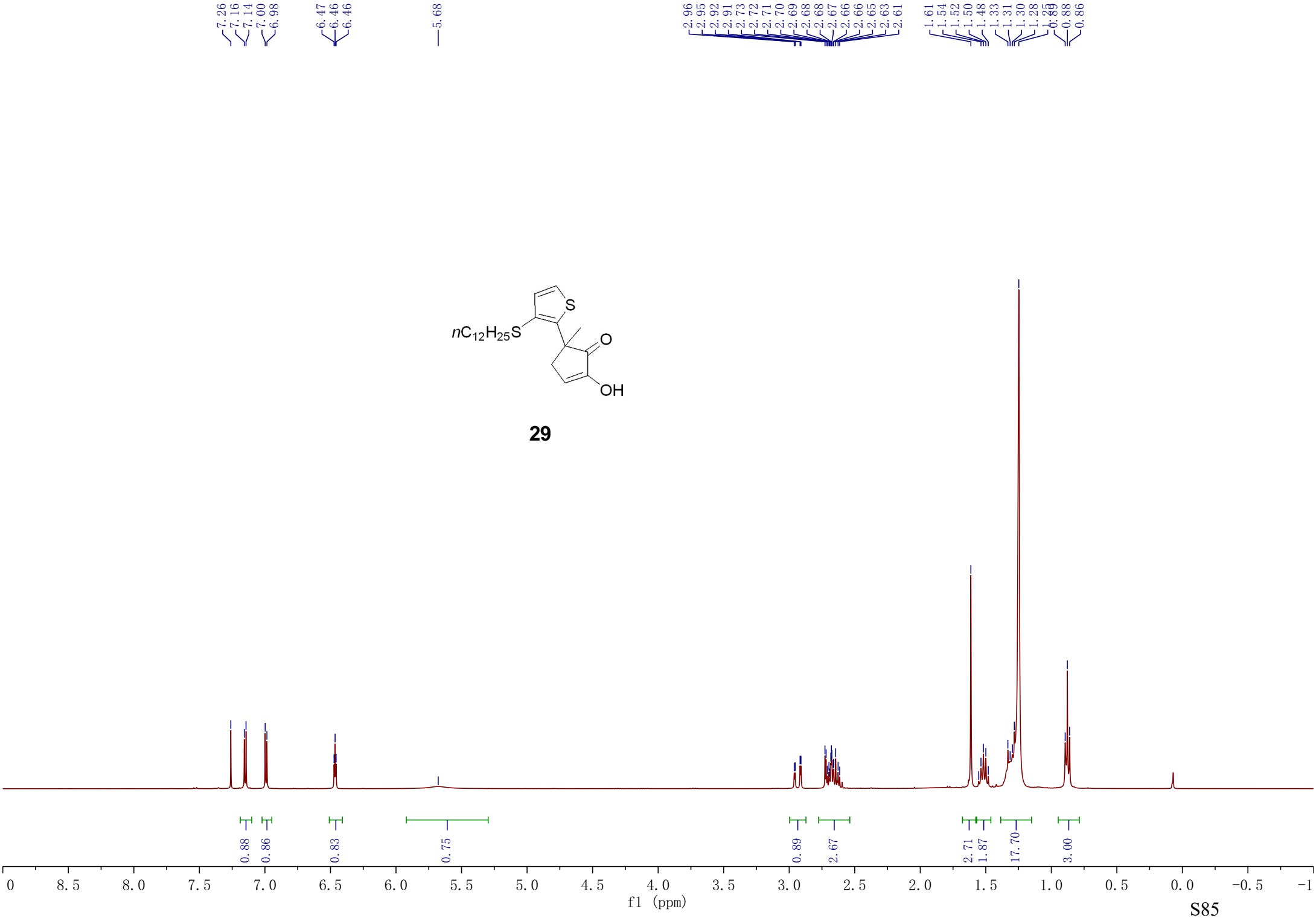

206.34
150.47
144.99
139.77
135.84
129.65
127.89
125.40
124.98
119.66
111.19
45.06
42.34
29.69
25.17
21.91
21.67
13.43
TsN
S
O
OH
27
f1 (ppm)

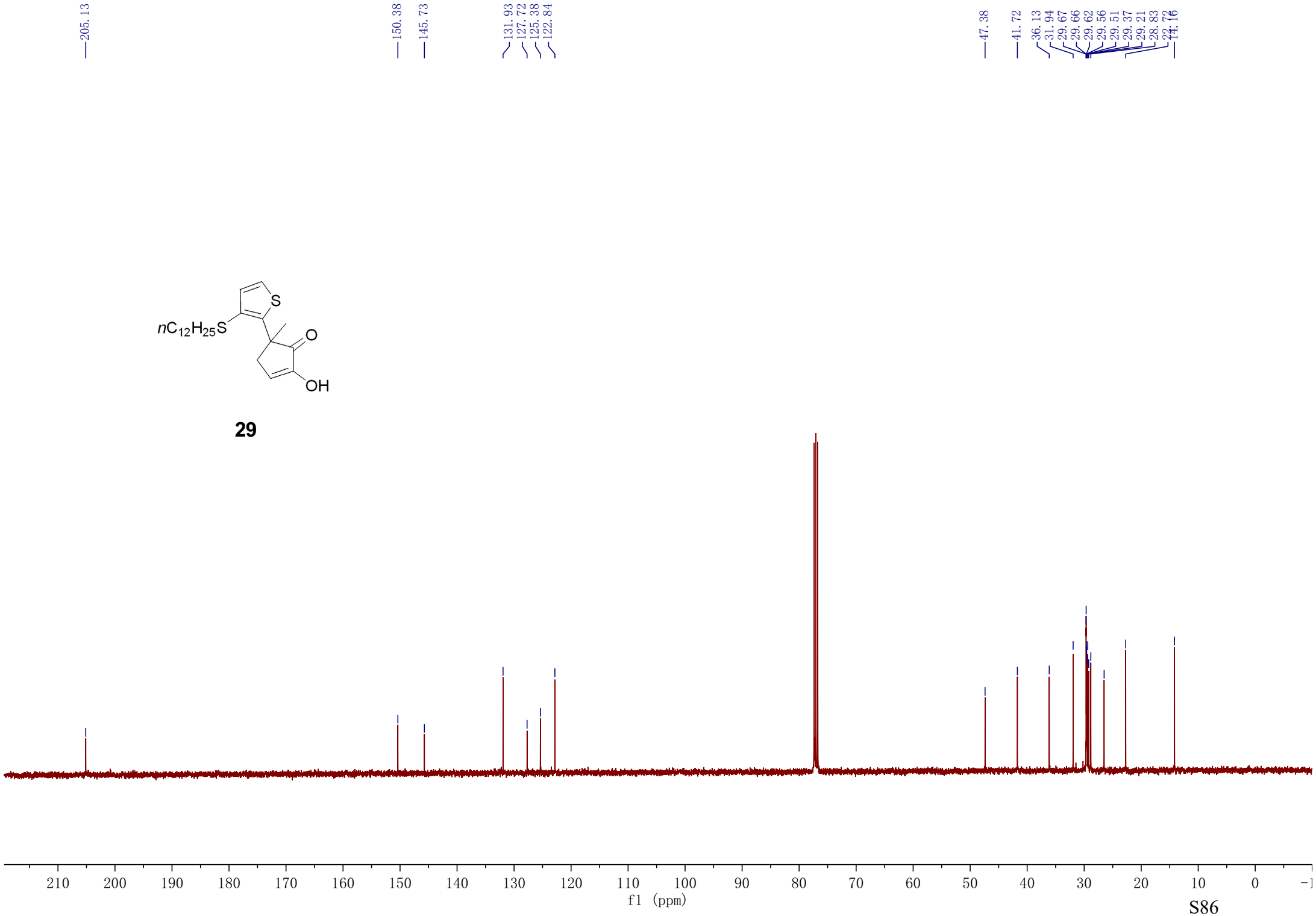

7.70 7.70 7.70 7.69 7.69 7.69 7.69 7.60 7.60 7.59 7.59 7.59 7.59 7.28 7.27 7.27 7.26 7.26 7.25 7.25
6.47 6.46 6.46
6.00
2.98 2.97 2.95 2.94 2.91 2.90 2.90 2.89 2.89 2.89 2.88 2.88 2.87 2.87 2.85 2.85 2.84 2.83 2.82 2.79 2.78 2.76 2.75
1.92
1.70 1.70 1.69 1.69 1.67 1.66 1.66
1.02 1.00 0.99
S
S
O
OH
28
1.02 1.06 1.19 0.75 1.00 0.92 1.16 2.21 1.08 3.07 2.15 3.12
0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

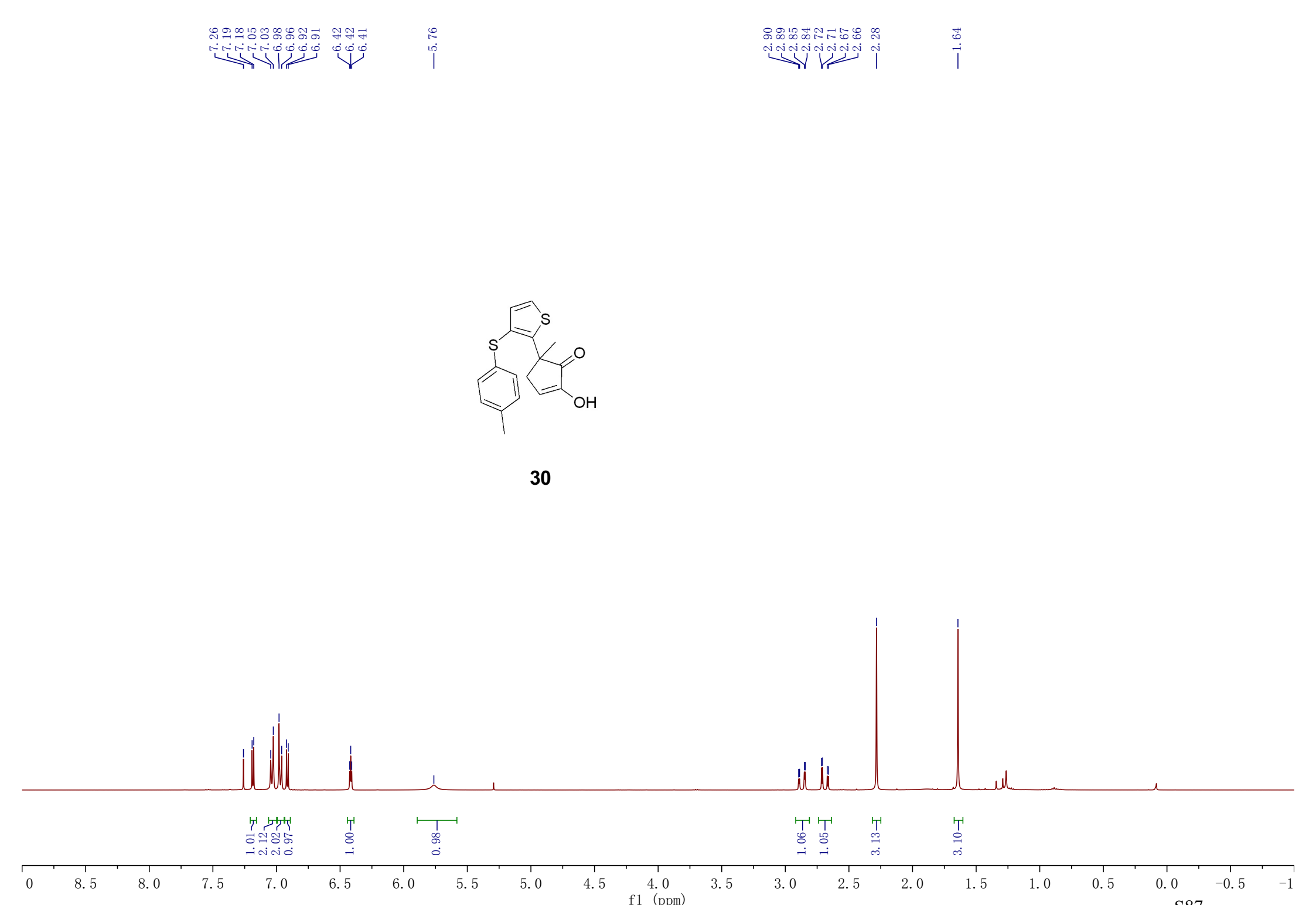
S
S
O
OH

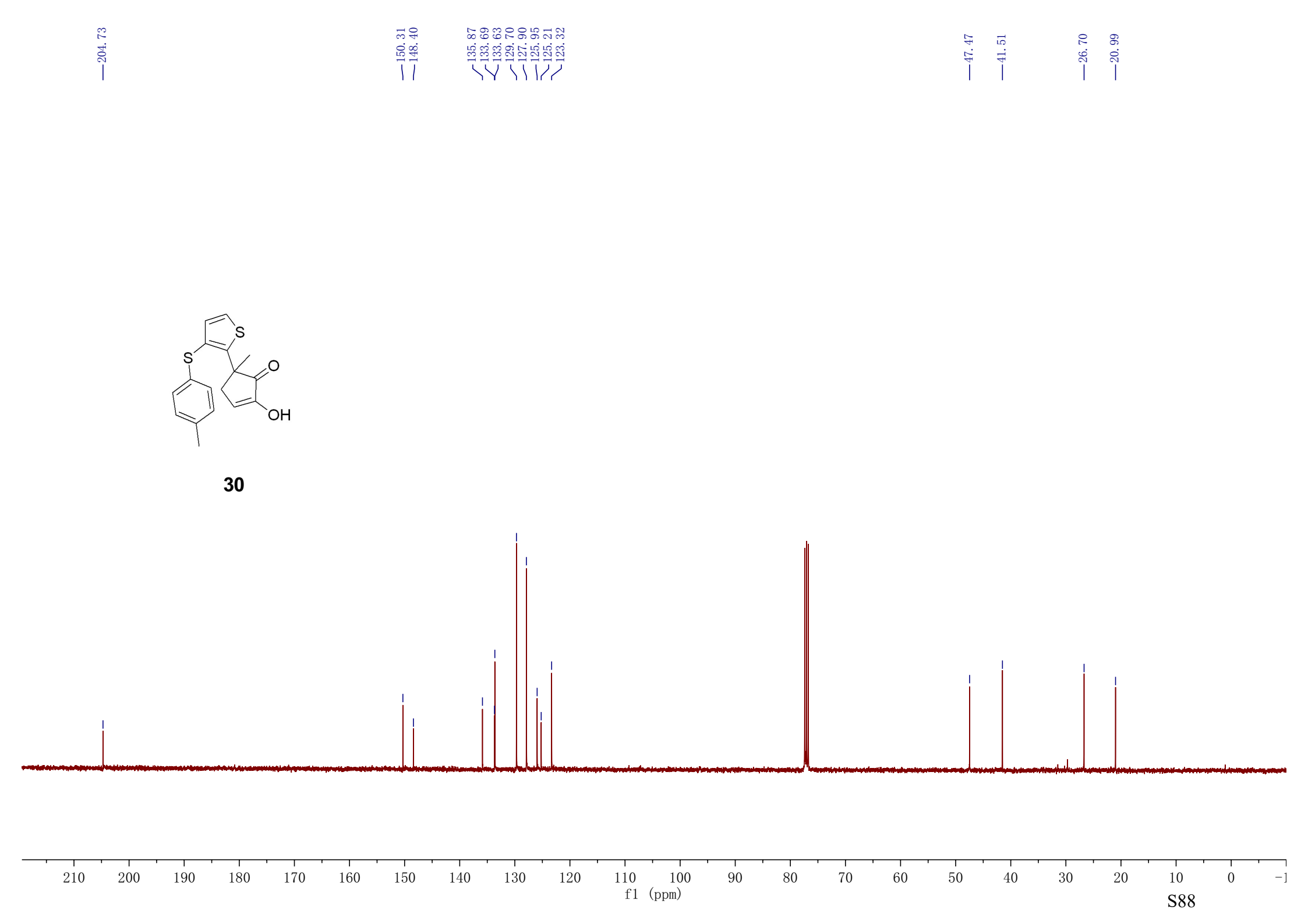
**28**

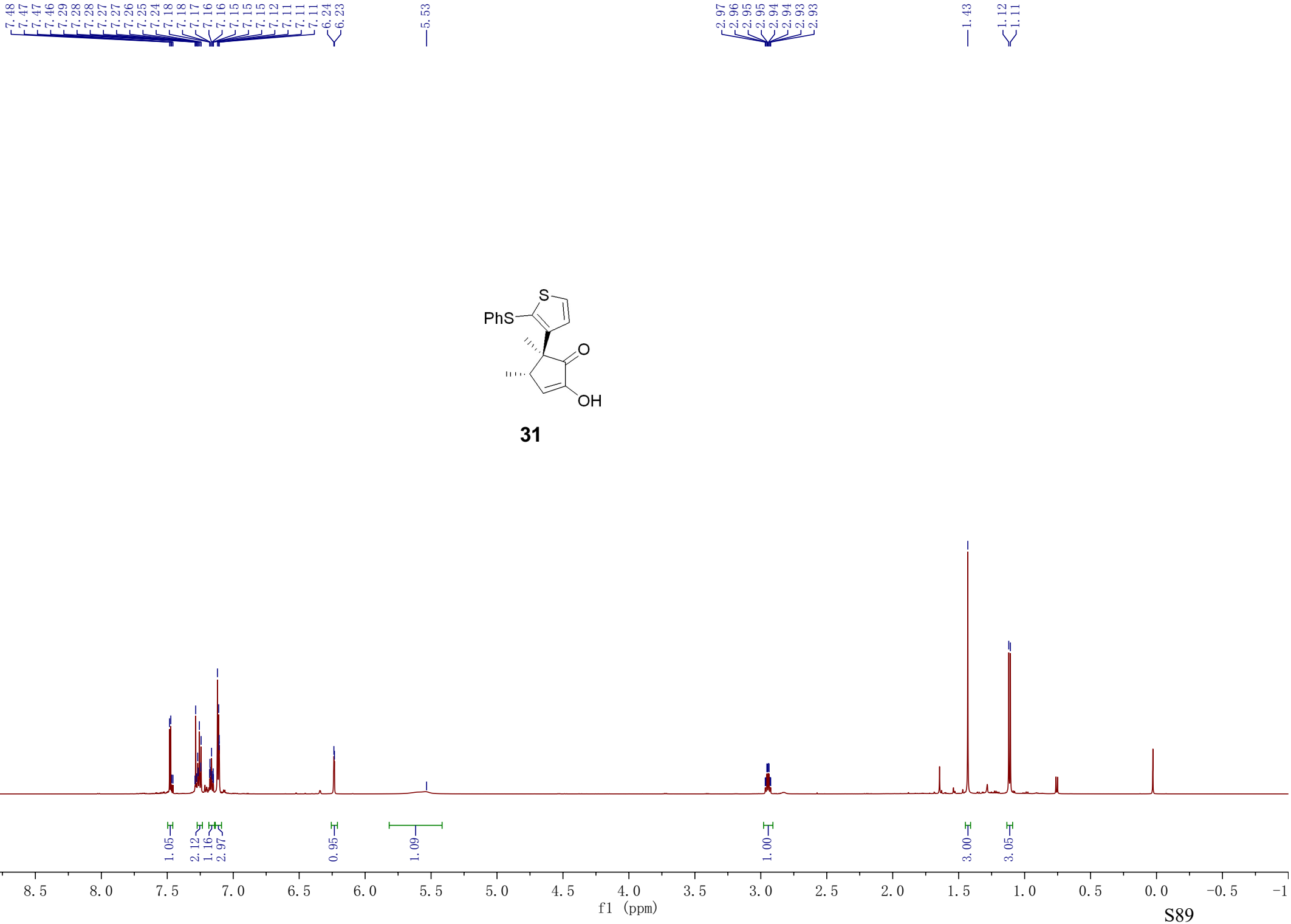

206.16
150.95
140.78
139.06
138.31
133.73
124.46
124.19
124.08
122.77
122.02
49.40
41.12
40.85
25.43
22.70
13.40
f1 (ppm)


7.26
7.16
7.14
7.00
6.98
6.47
6.46
6.46
5.68
2.96
2.95
2.92
2.91
2.73
2.72
2.71
2.70
2.69
2.68
2.68
2.67
2.66
2.66
2.65
2.63
2.61
1.61
1.54
1.52
1.50
1.48
1.33
1.31
1.30
1.28
0.89
0.88
0.86
S
nC12H25S
O
OH
29
0.88
0.86
0.83
0.75
0.89
2.67
2.71
1.87
17.70
3.00
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


205.13
150.38
145.73
131.93
127.72
125.38
122.84
47.38
41.72
36.13
31.94
29.67
29.66
29.62
29.56
29.51
29.37
29.21
28.83
22.72
14.16
S
nC12H25S
O
OH
29
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

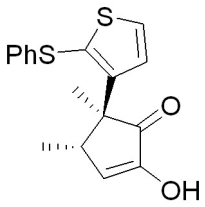

7.26
7.19
7.18
7.05
7.03
6.98
6.96
6.92
6.91
6.42
6.42
6.41
5.76
2.90
2.89
2.85
2.84
2.72
2.71
2.67
2.66
2.28
1.64
S
S
O
OH
30
1.01
2.12
2.02
0.97
1.00
0.98
1.06
1.05
3.13
3.10
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


204.73
150.31
148.40
135.87
133.69
133.63
129.70
127.90
125.95
125.21
123.32
47.47
41.51
26.70
20.99
S
S
O
OH
30
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.48
7.47
7.47
7.46
7.29
7.28
7.28
7.27
7.27
7.26
7.25
7.24
7.18
7.18
7.17
7.16
7.16
7.15
7.15
7.15
7.12
7.11
7.11
7.11
6.24
6.23
5.53
2.97
2.96
2.95
2.95
2.94
2.94
2.93
2.93
1.43
1.12
1.11
S
PhS
O
OH
1.05
2.12
1.16
2.97
0.95
1.09
1.00
3.00
3.05
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

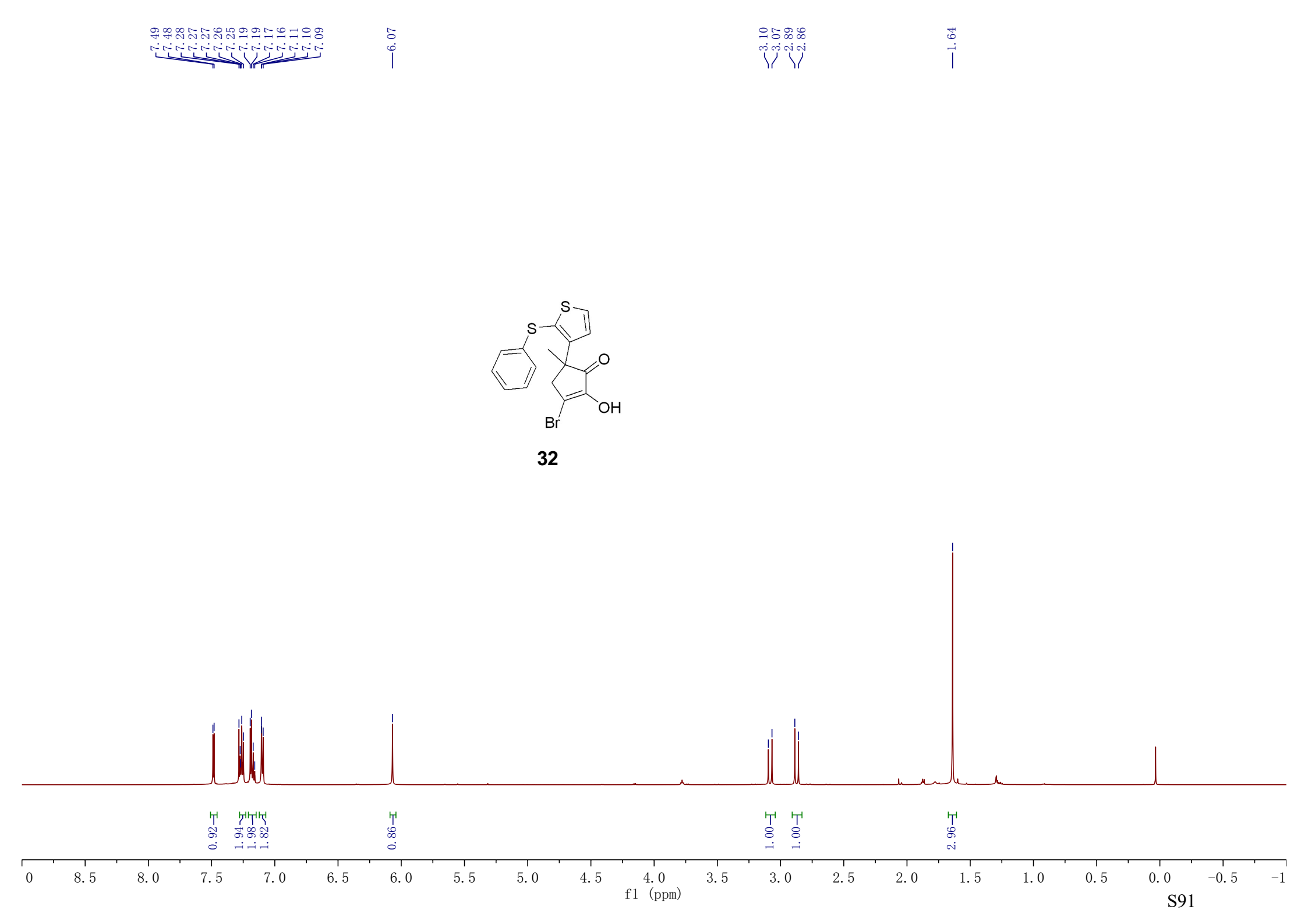
**31**

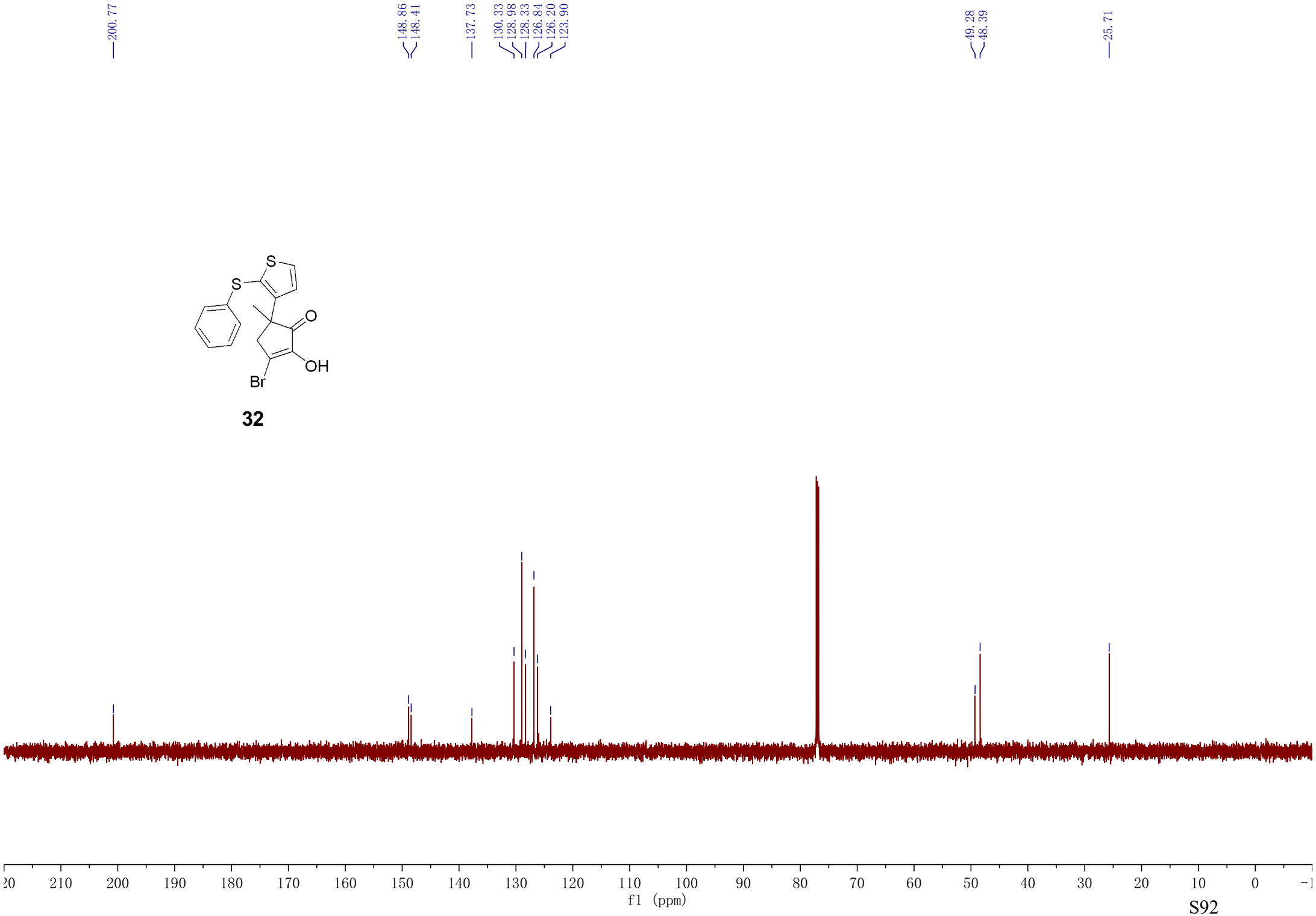
206.24
150.14
150.01
138.00
130.83
130.17
128.83
128.45
126.85
126.05
125.60
51.00
43.61
20.88
14.62



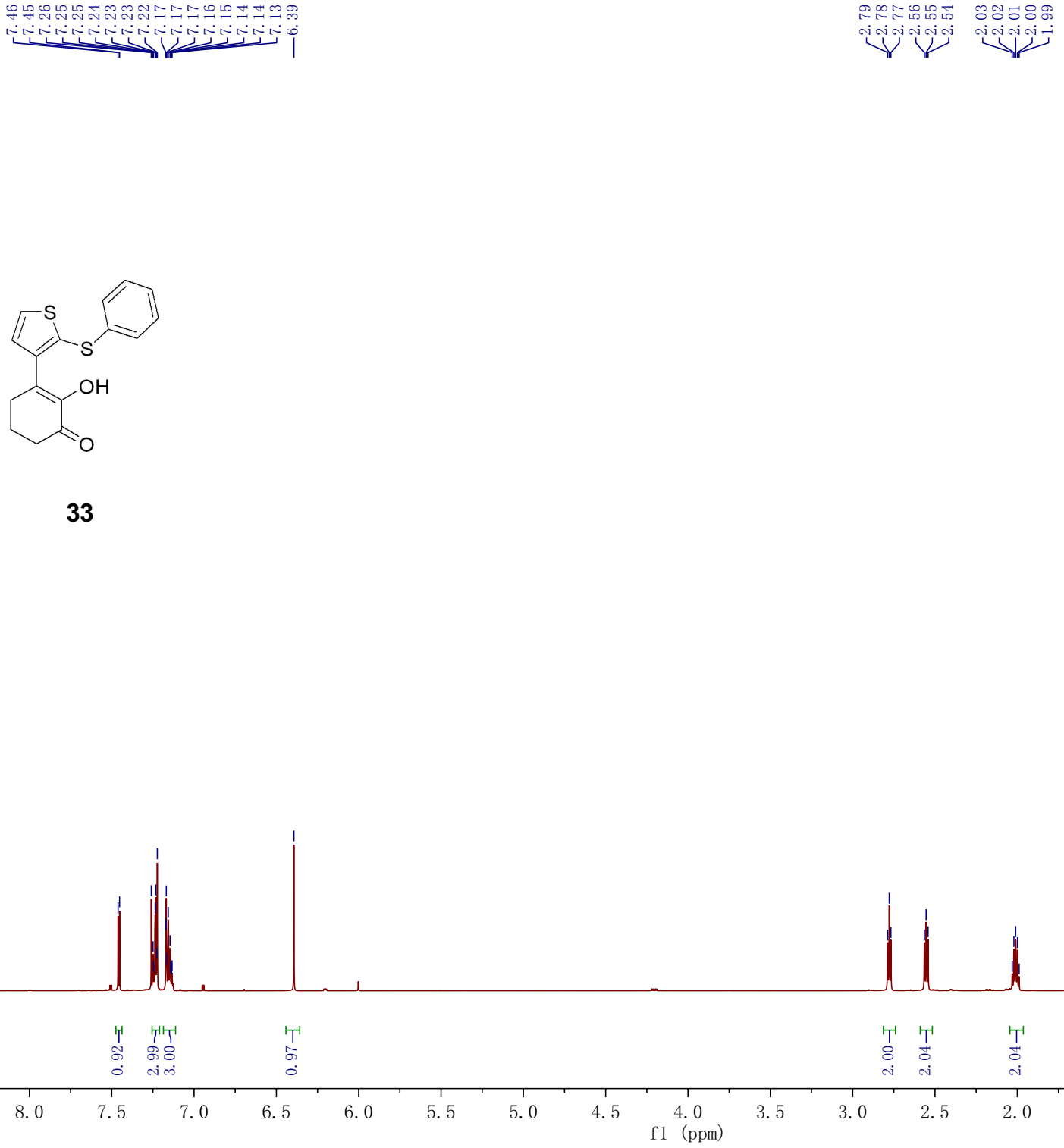

**31**

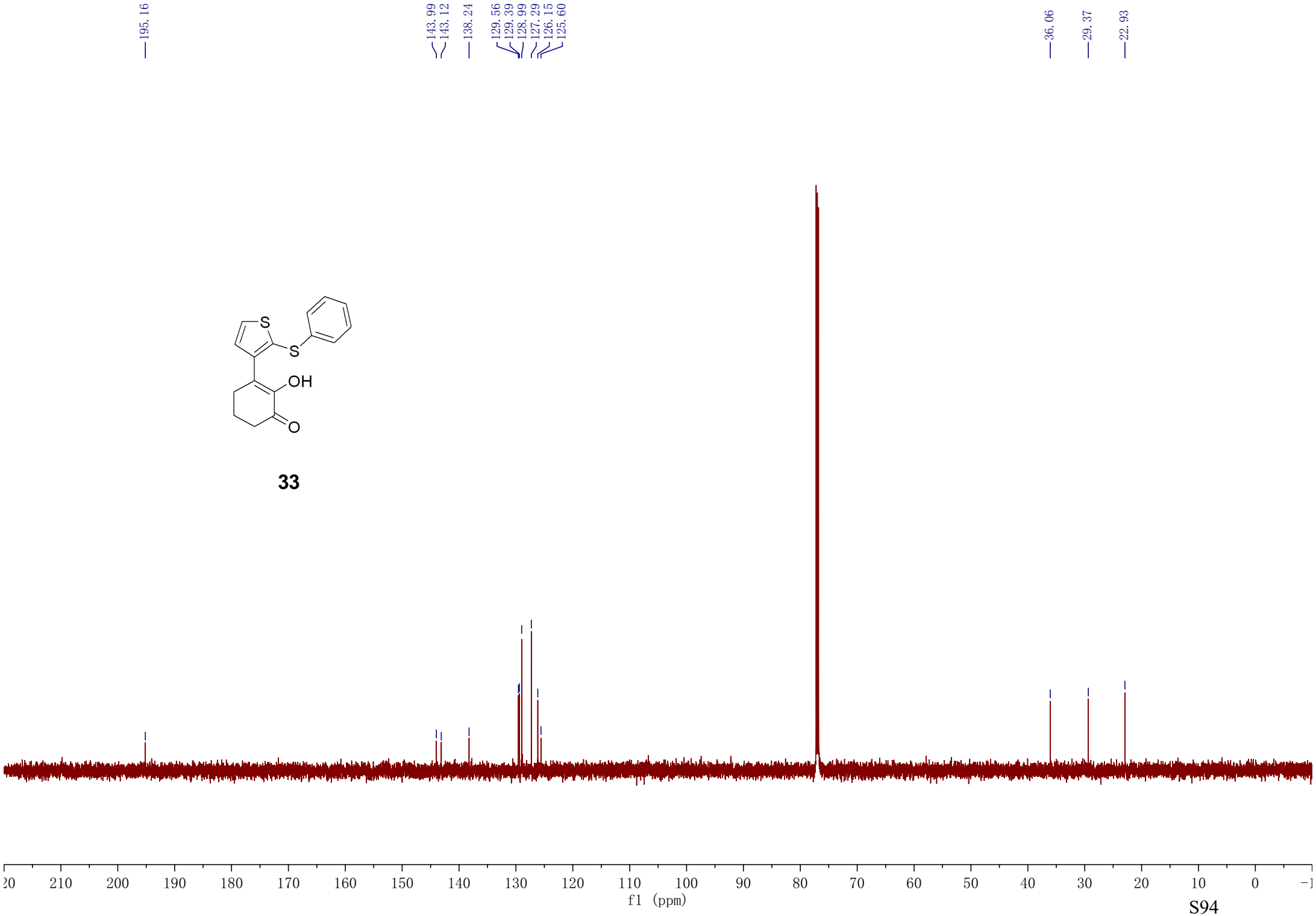
f1 (ppm)


7.49
7.48
7.28
7.27
7.27
7.26
7.25
7.19
7.19
7.17
7.16
7.11
7.10
7.09
6.07
3.10
3.07
2.89
2.86
1.64
S
S
O
OH
Br
32
0.92
1.94
1.98
1.82
0.86
1.00
1.00
2.96
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

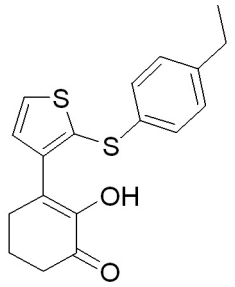

200.77
148.86
148.41
137.73
130.33
128.98
128.33
126.84
126.20
123.90
49.28
48.39
25.71
S
S
O
OH
Br
f1 (ppm)

**32**

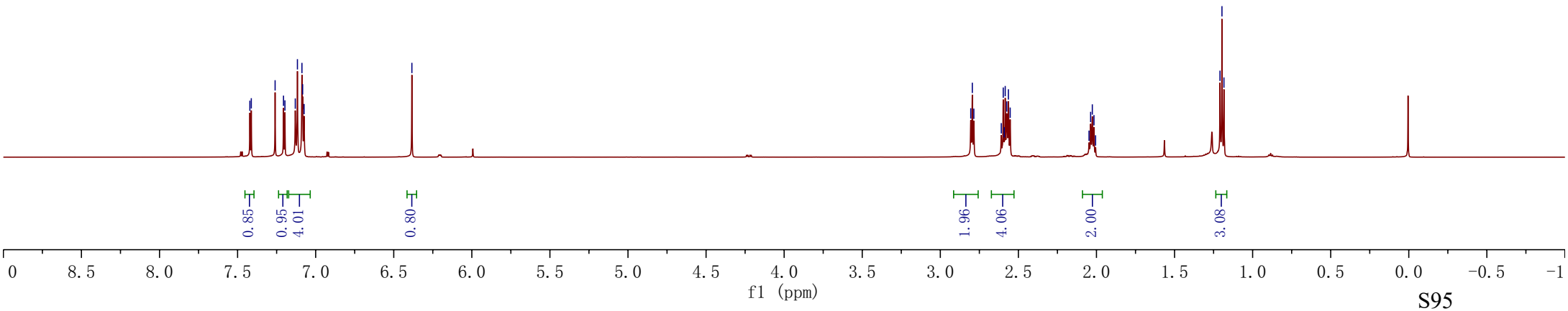

7.46
7.45
7.26
7.25
7.25
7.24
7.23
7.23
7.22
7.17
7.17
7.17
7.16
7.15
7.14
7.14
7.13
6.39
2.79
2.78
2.77
2.56
2.55
2.54
2.03
2.02
2.01
2.00
1.99
S
S
OH
O
33
0.92
2.99
3.00
0.97
2.00
2.04
2.04
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

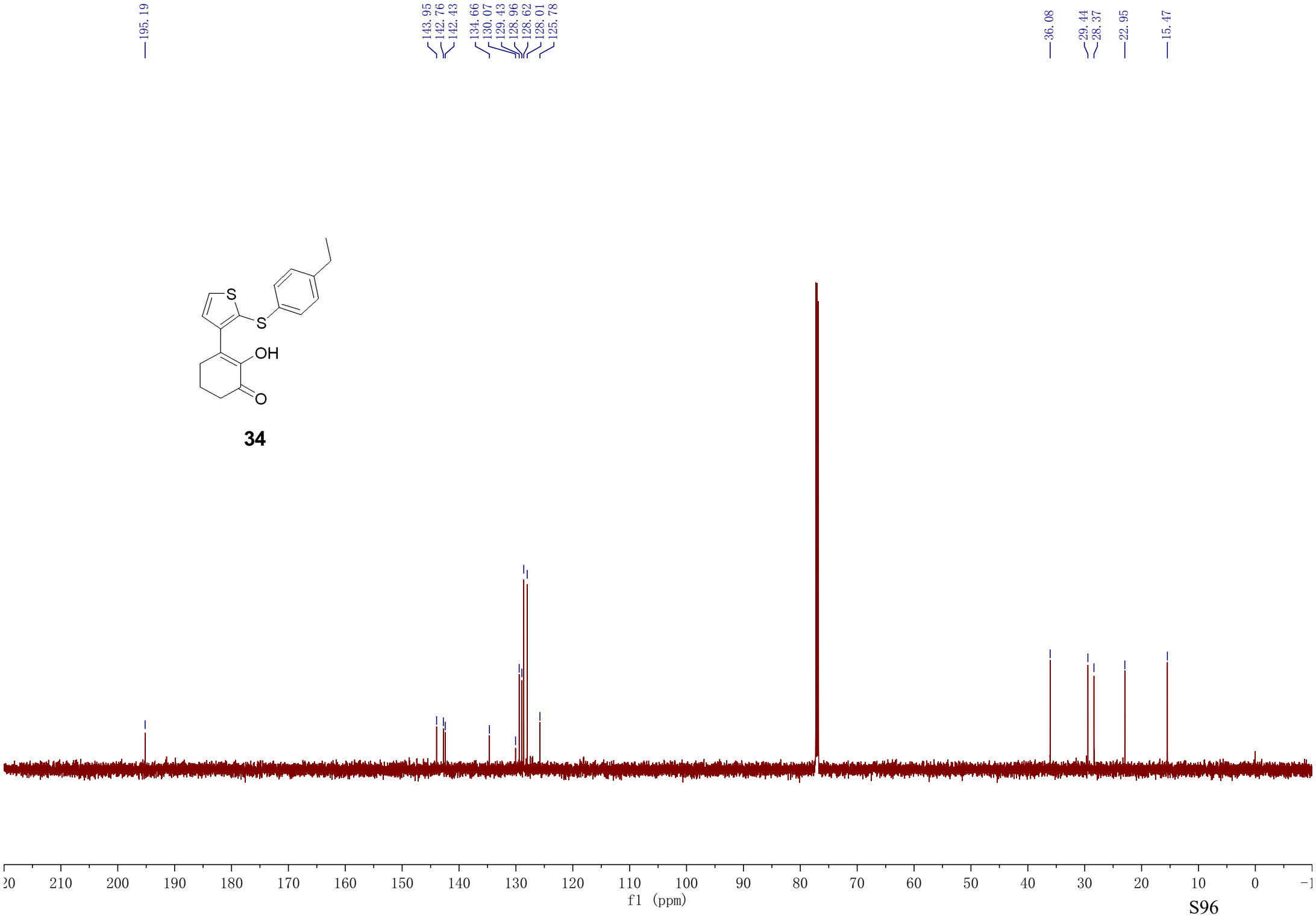

195.16
143.99
143.12
138.24
129.56
129.39
128.99
127.29
126.15
125.60
36.06
29.37
22.93
S
S
OH
O
33
f1 (ppm)

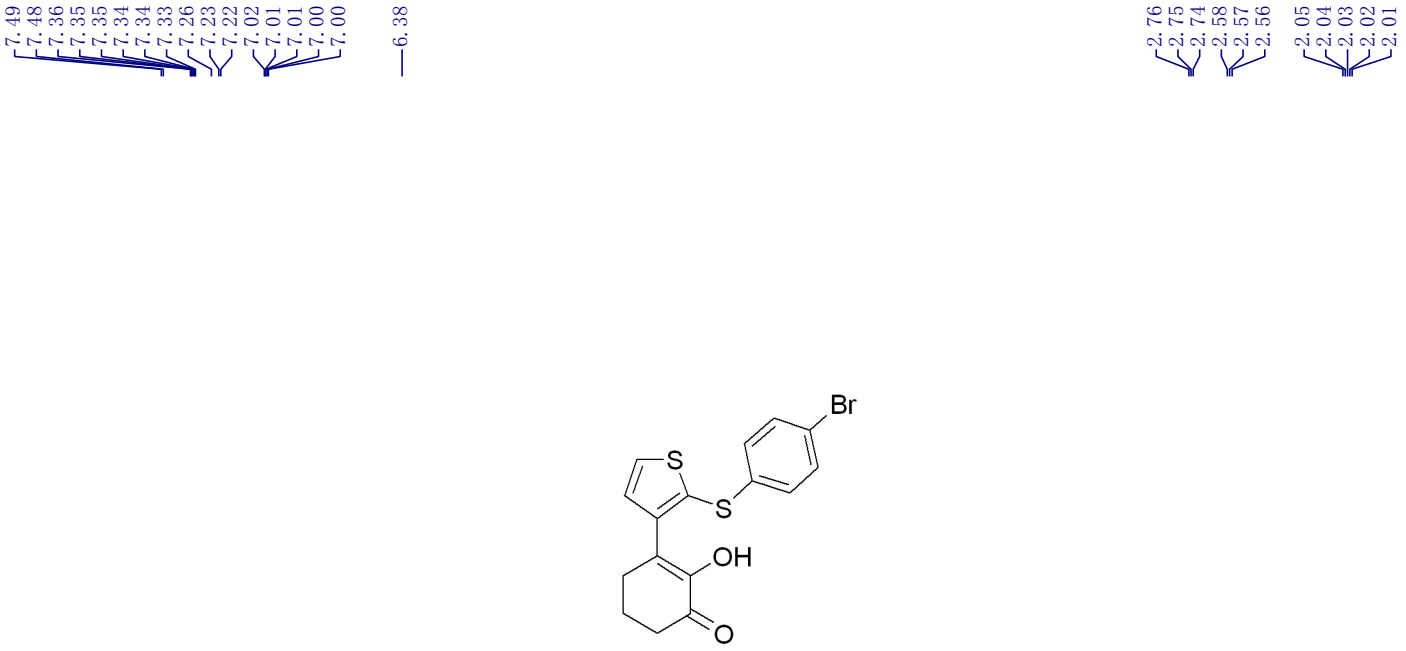

7.42
7.41
7.26
7.21
7.20
7.13
7.12
7.09
7.08
7.07
6.38
2.80
2.80
2.79
2.61
2.60
2.59
2.58
2.57
2.56
2.55
2.05
2.04
2.03
2.02
2.01
1.21
1.20
1.18


S
S
OH
O

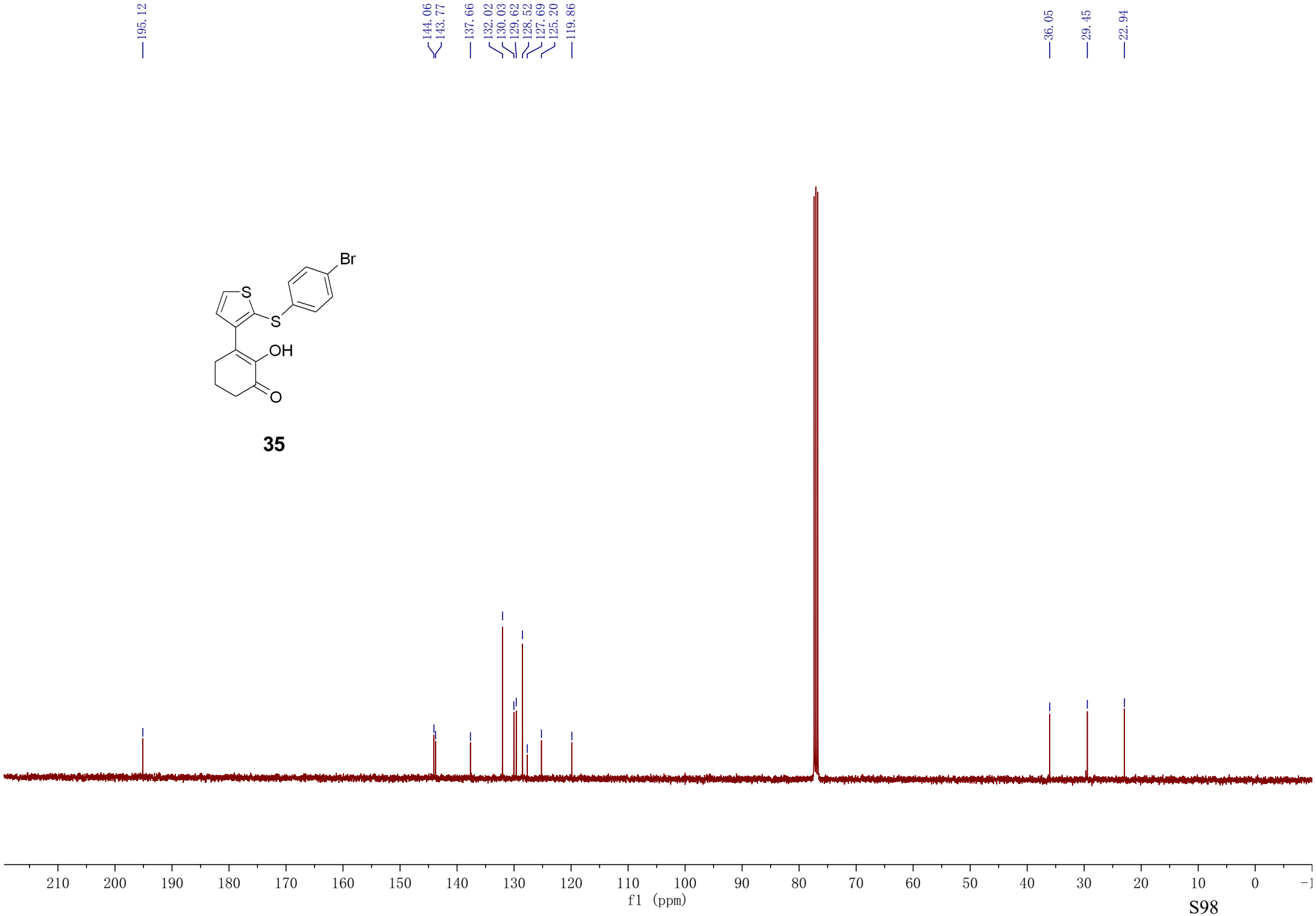
**34**

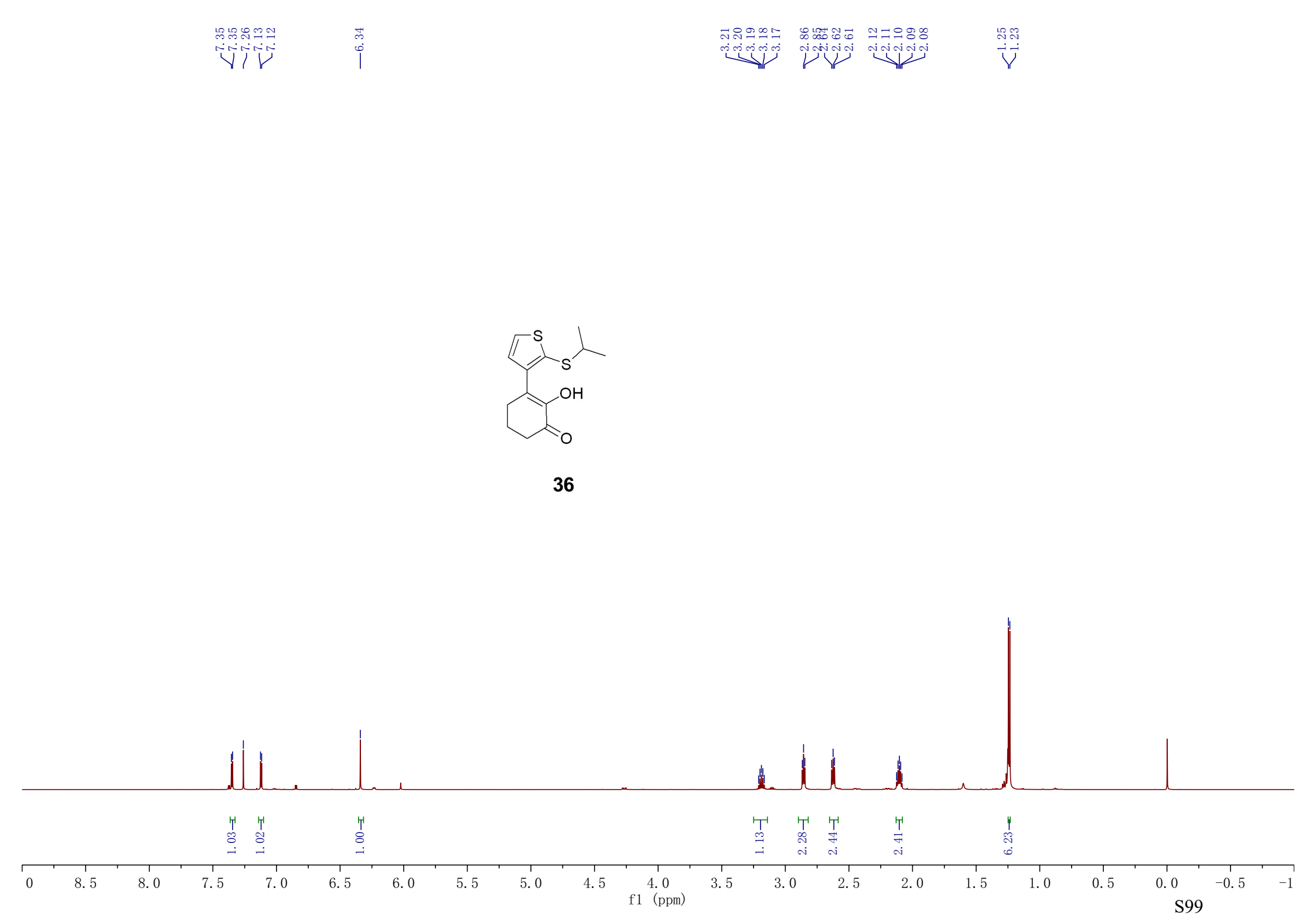

0.85
0.95
4.01
0.80
1.96
4.06
2.00
3.08
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

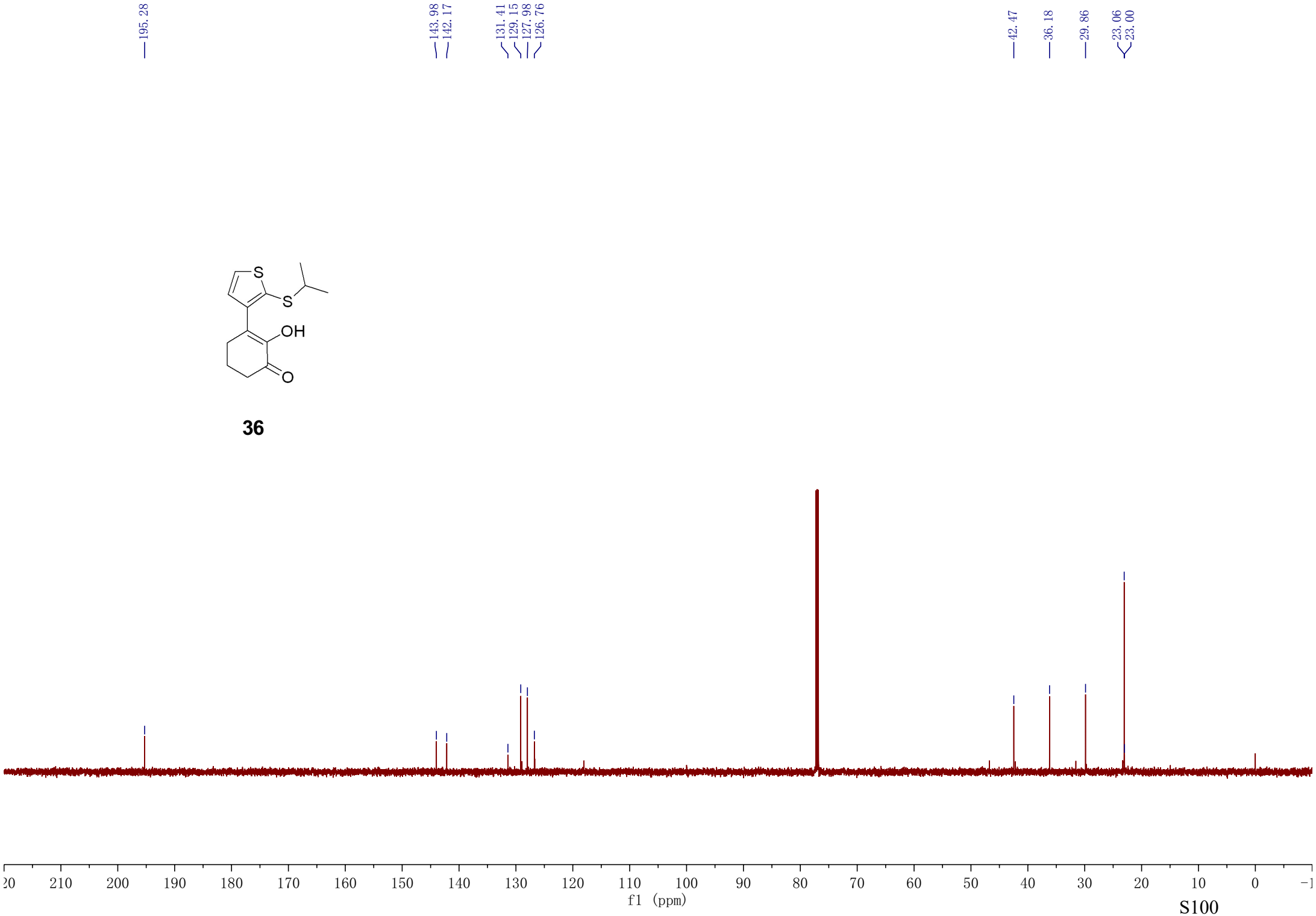

195.19
143.95
142.76
142.43
134.66
130.07
129.43
128.96
128.62
128.01
125.78
36.08
29.44
28.37
22.95
15.47
S
S
OH
O
34
f1 (ppm)


7.49
7.48
7.36
7.35
7.35
7.34
7.34
7.33
7.26
7.23
7.22
7.02
7.01
7.01
7.00
7.00
6.38
2.76
2.75
2.74
2.58
2.57
2.56
2.05
2.04
2.03
2.02
2.01
Br
S
S
OH
O
1.07
2.13
1.02
2.02
1.00
2.15
2.14
2.22
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

**35**

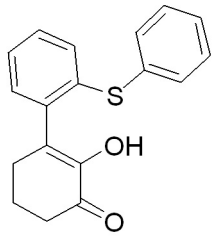

195.12
144.06
143.77
137.66
132.02
130.03
129.62
128.52
127.69
125.20
119.86
36.05
29.45
22.94
Br
S
S
OH
O
35
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.35
7.35
7.26
7.13
7.12
6.34
3.21
3.20
3.19
3.18
3.17
2.86
2.85
2.84
2.62
2.61
2.12
2.11
2.10
2.09
2.08
1.25
1.23
S
S
OH
O
36
1.03
1.02
1.00
1.13
2.28
2.44
2.41
6.23
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

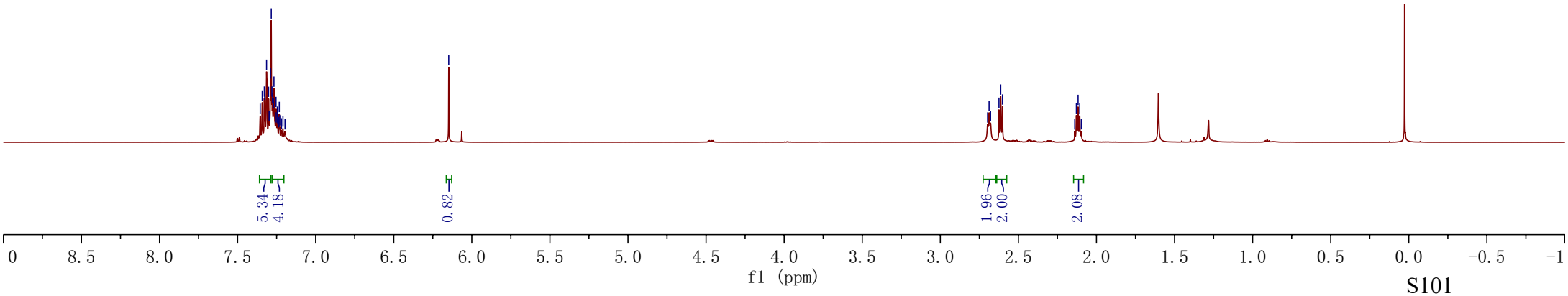

195.28
143.98
142.17
131.41
129.15
127.98
126.76
42.47
36.18
29.86
23.06
23.00
S
S
OH
O
f1 (ppm)

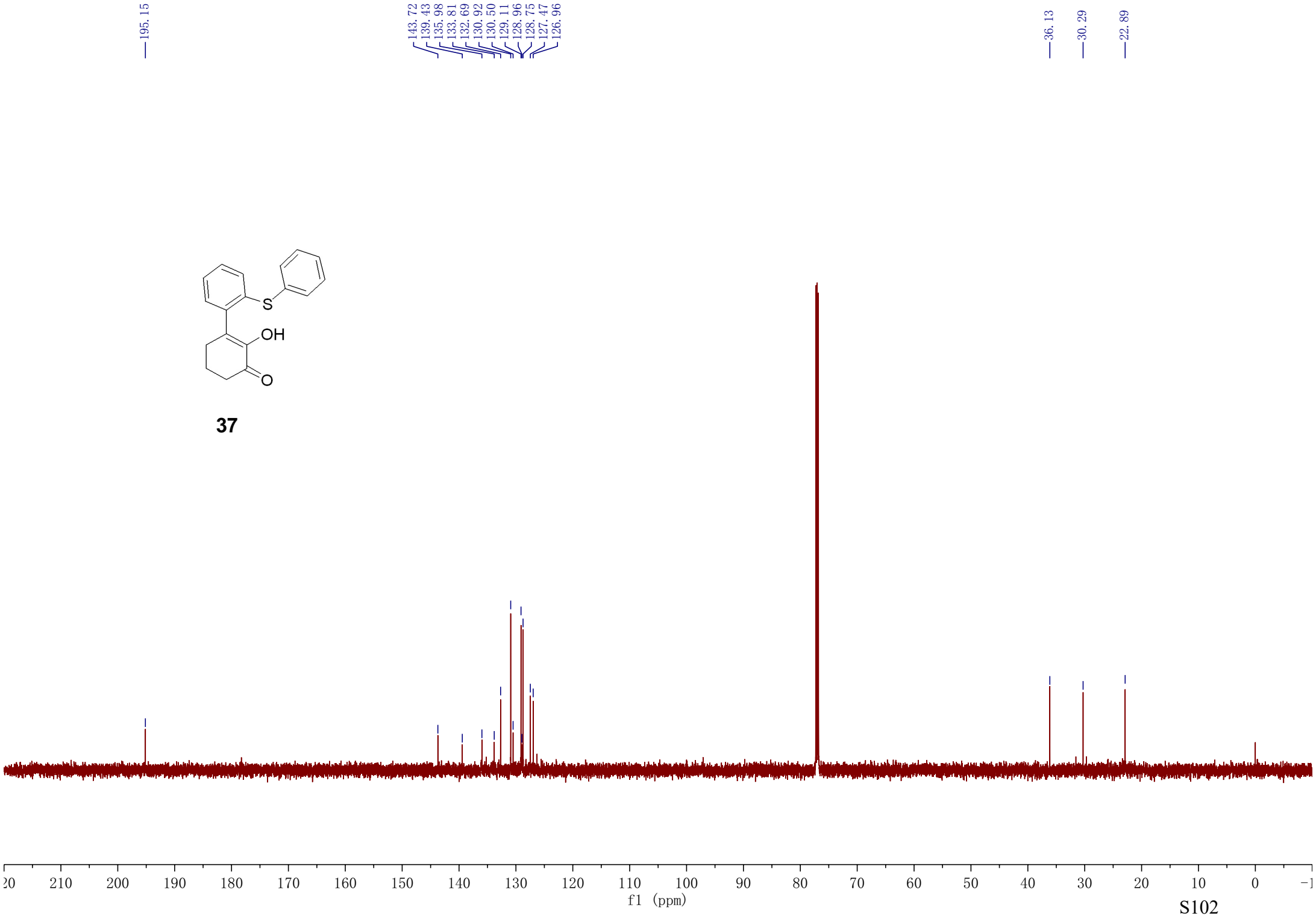
**36**

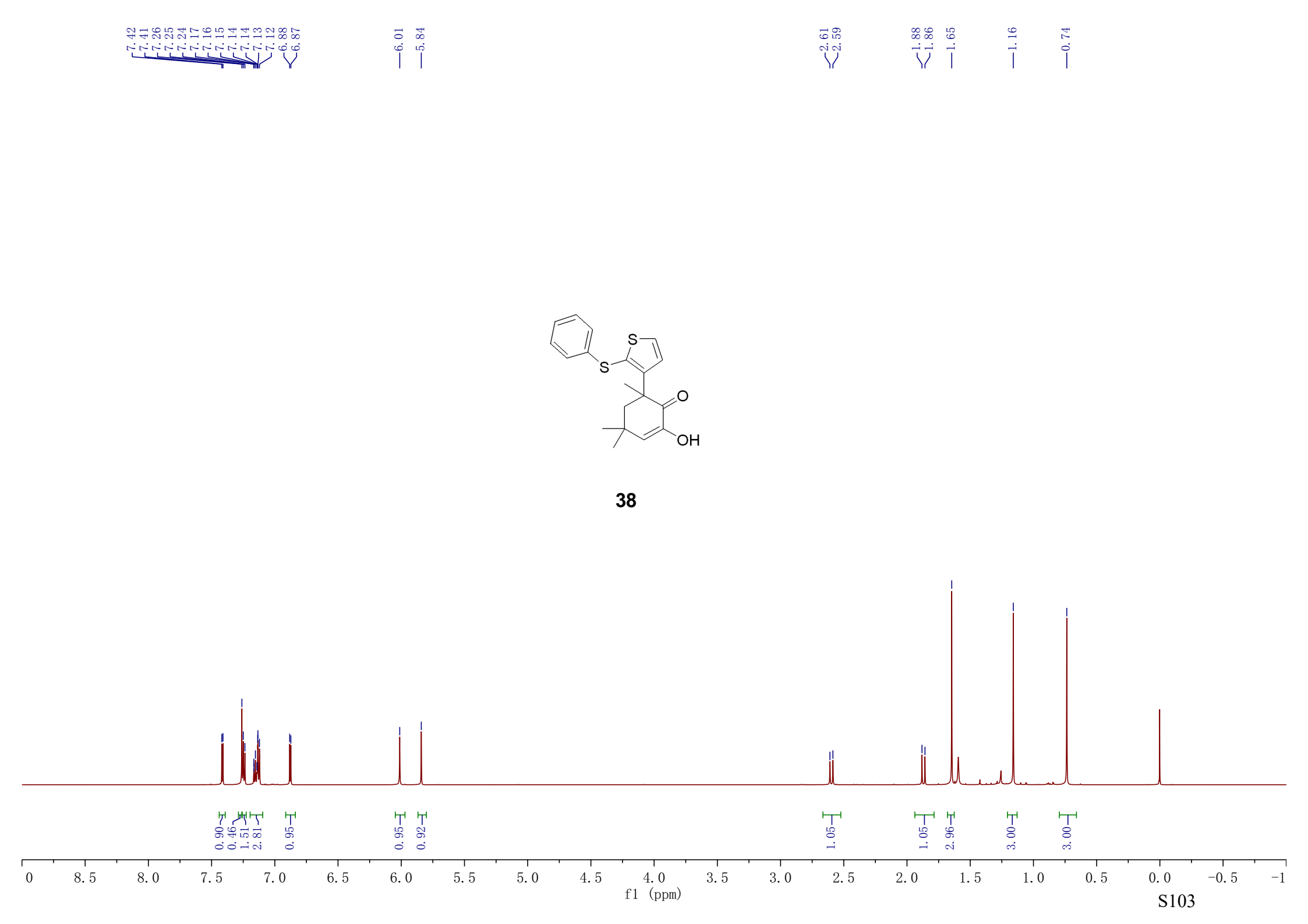

7.36
7.34
7.33
7.33
7.31
7.30
7.30
7.29
7.28
7.28
7.28
7.27
7.27
7.26
7.25
7.25
7.25
7.24
7.24
7.23
7.23
7.22
7.22
7.21
7.20
6.15
2.70
2.69
2.68
2.62
2.61
2.60
2.14
2.13
2.12
2.11
2.10


S
OH
O

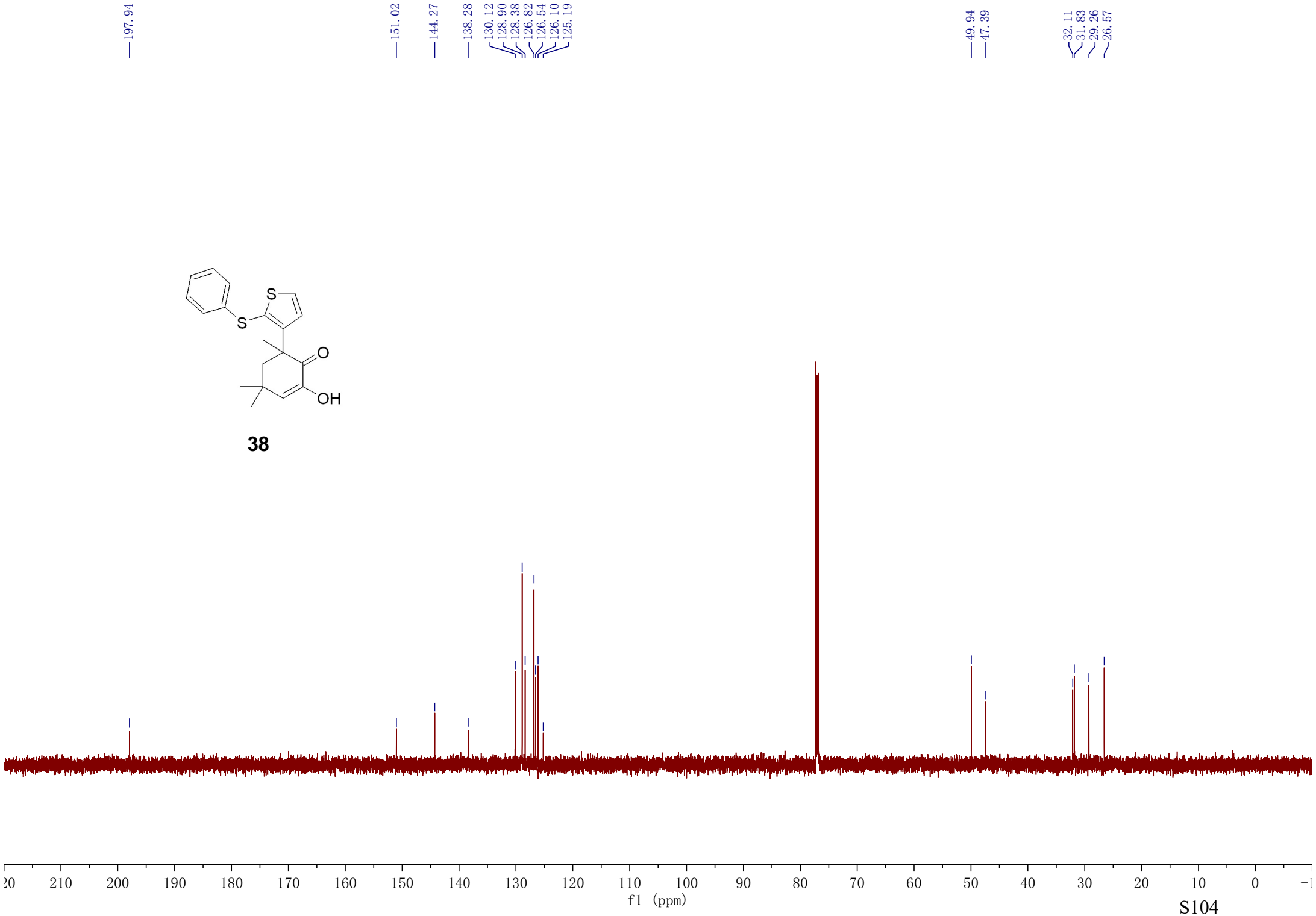
**37**

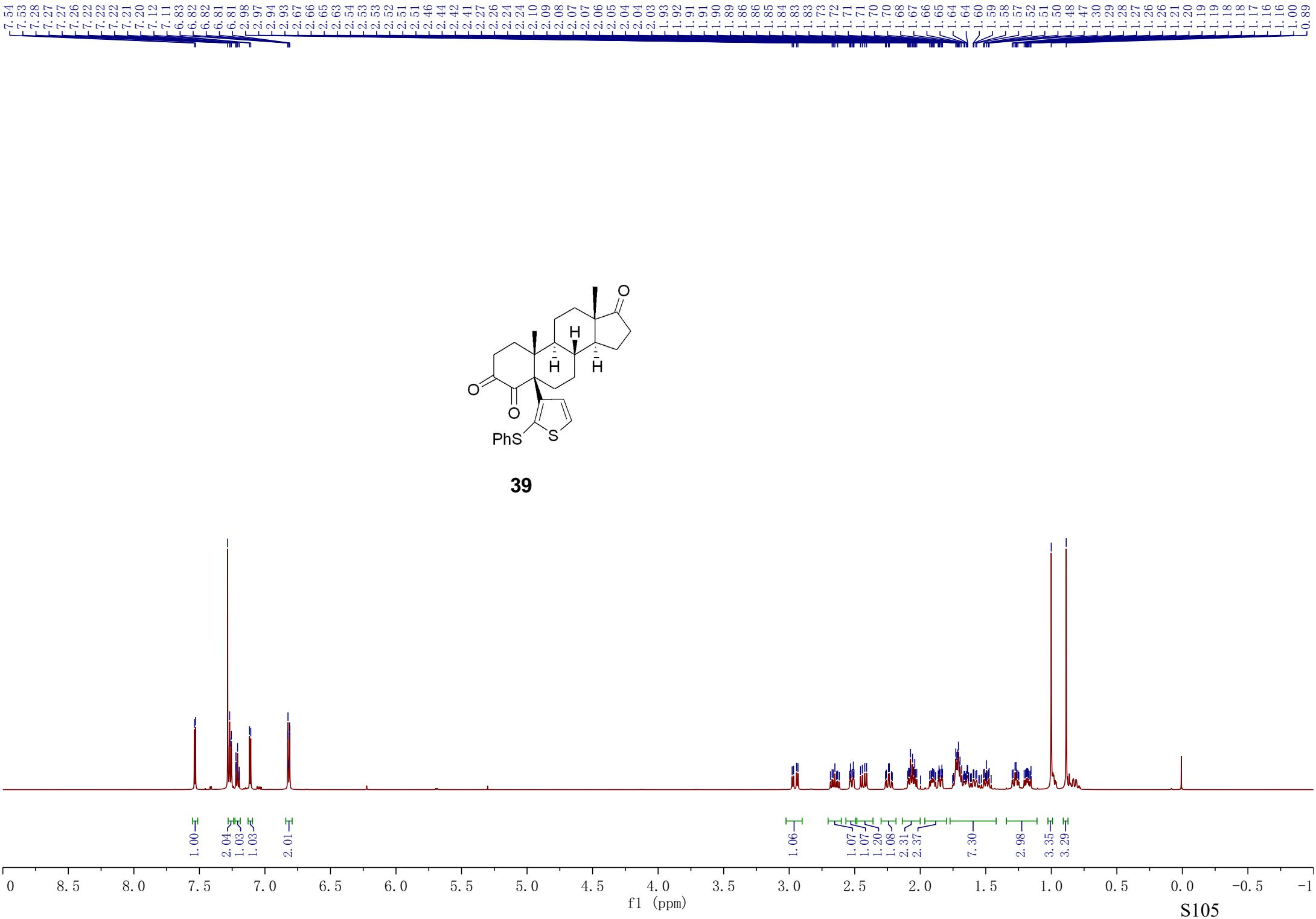

5.34
4.18
0.82
1.96
2.00
2.08
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


195.15
143.72
139.43
135.98
133.81
132.69
130.92
130.50
129.11
128.96
128.75
127.47
126.96
36.13
30.29
22.89
S
OH
O
37
f1 (ppm)


7.42
7.41
7.26
7.25
7.24
7.17
7.16
7.15
7.14
7.14
7.13
7.12
6.88
6.87
6.01
5.84
2.61
2.59
1.88
1.86
1.65
1.16
0.74
S
S
O
OH
0.90
0.46
1.51
2.81
0.95
0.95
0.92
1.05
1.05
2.96
3.00
3.00
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

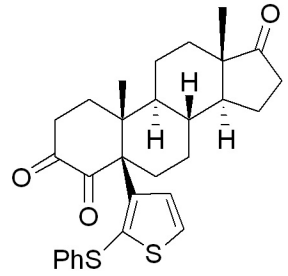
**38**


197.94
151.02
144.27
138.28
130.12
128.90
128.38
126.82
126.54
126.10
125.19
49.94
47.39
32.11
31.83
29.26
26.57
S
S
O
OH
38
f1 (ppm)

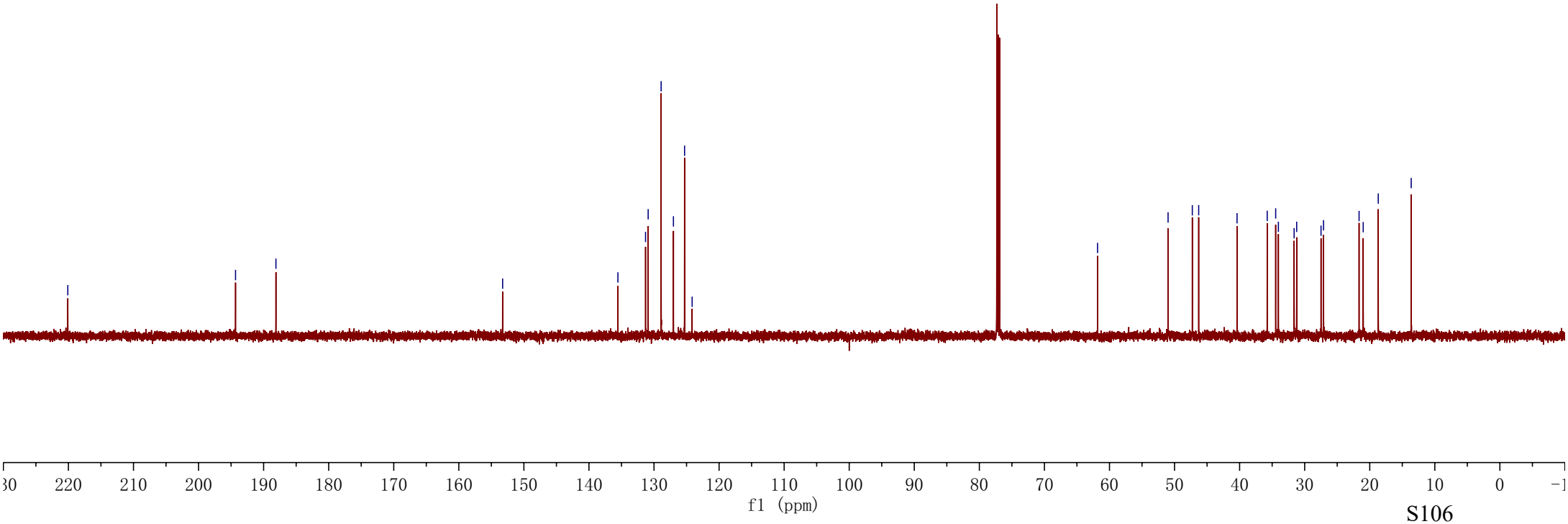

7.54 7.53 7.28 7.27 7.27 7.26 7.22 7.22 7.22 7.21 7.20 7.12 7.11 6.83 6.82 6.82 6.81 6.81 2.98 2.97 2.94 2.93 2.67 2.66 2.65 2.63 2.54 2.53 2.53 2.52 2.51 2.51 2.46 2.44 2.42 2.41 2.27 2.26 2.24 2.24 2.10 2.09 2.08 2.07 2.07 2.06 2.05 2.04 2.04 2.03 1.93 1.92 1.91 1.91 1.90 1.89 1.86 1.86 1.85 1.84 1.83 1.83 1.73 1.72 1.71 1.71 1.70 1.70 1.68 1.67 1.66 1.65 1.64 1.64 1.60 1.59 1.58 1.57 1.52 1.51 1.50 1.48 1.47 1.30 1.29 1.28 1.27 1.26 1.26 1.21 1.20 1.19 1.19 1.18 1.18 1.17 1.16 1.16 1.00 0.89
O
H
H
H
O
O
PhS
S
1.00 2.04 1.03 1.03 2.01 1.06 1.07 1.07 1.20 1.08 2.31 2.37 7.30 2.98 3.35 3.29
0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

**39**

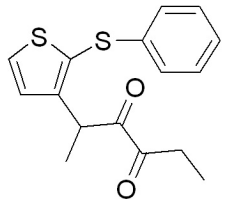
220.09
194.32
188.11
153.27
135.55
131.30
130.90
128.91
127.01
125.30
124.14
61.83
50.99
47.27
46.29
40.40
35.76
34.46
34.04
31.62
31.23
27.49
27.10
21.64
21.00
18.69
13.63



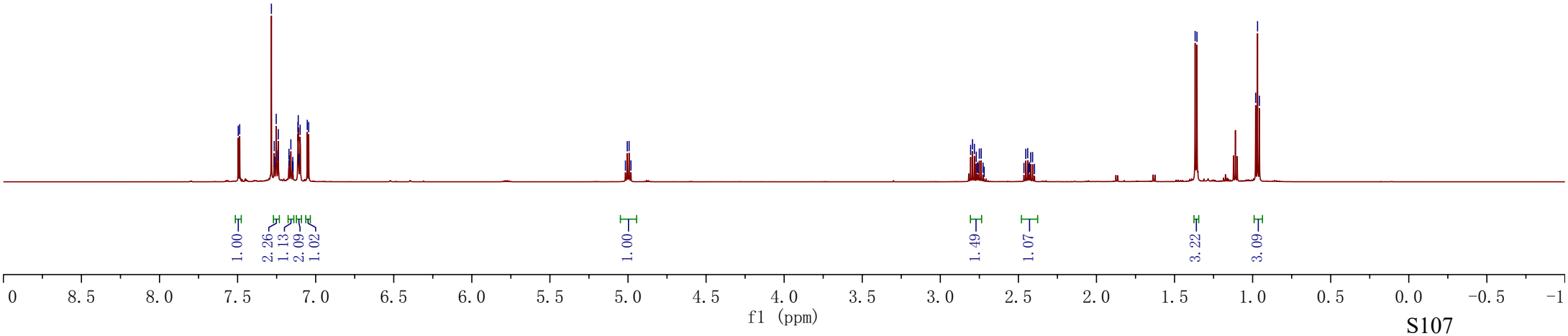

**39**

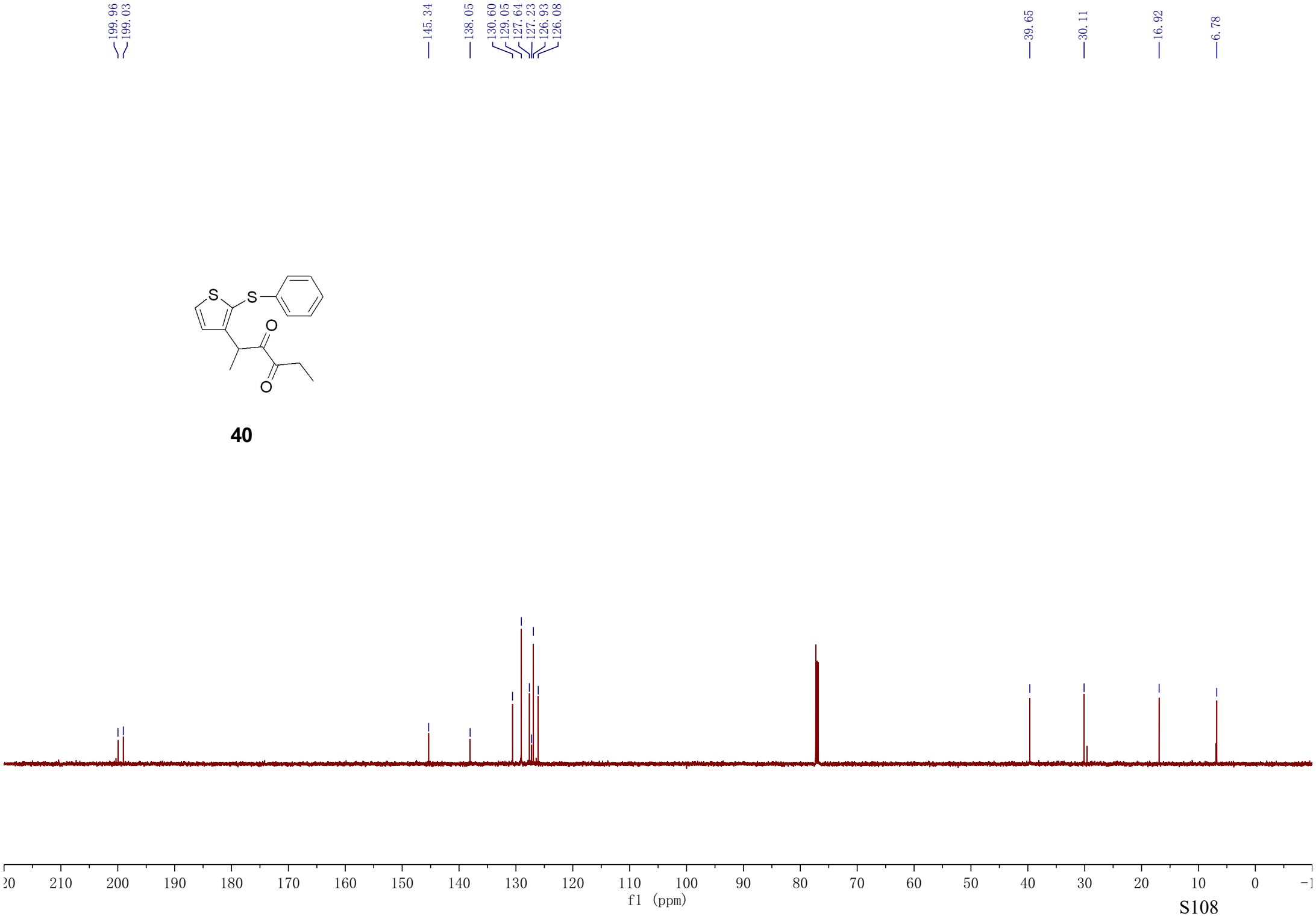



7.50
7.49
7.28
7.27
7.26
7.25
7.24
7.24
7.17
7.17
7.16
7.15
7.15
7.14
7.11
7.11
7.11
7.10
7.05
7.04
5.02
5.00
4.99
4.98
2.81
2.79
2.78
2.77
2.76
2.76
2.75
2.74
2.73
2.72
2.46
2.45
2.44
2.43
2.43
2.42
2.41
2.40
1.37
1.36
0.98
0.97
0.96

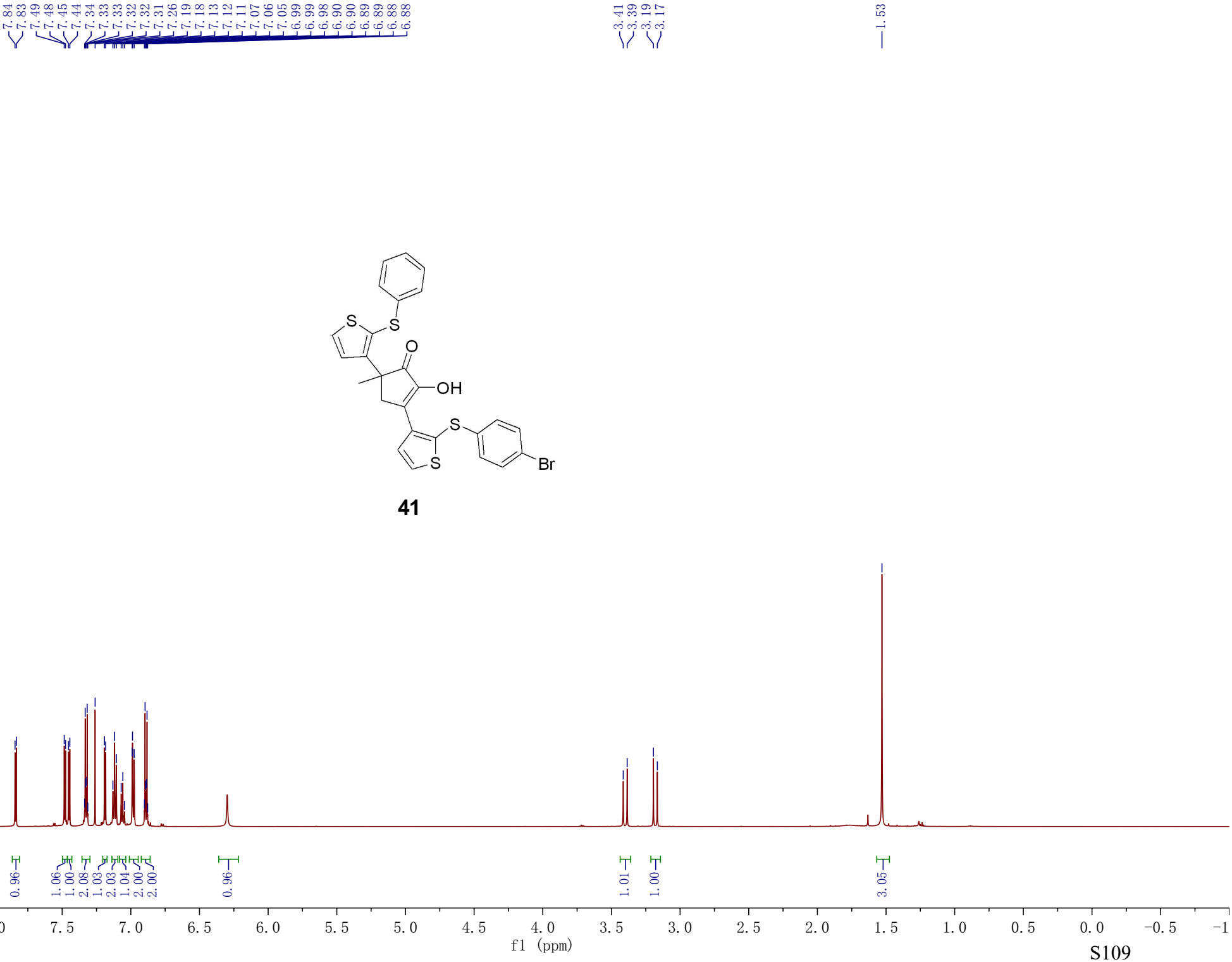

S
S
O
O

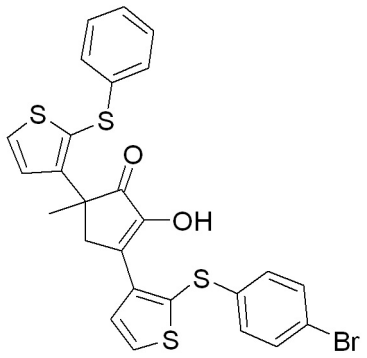
**40**


1.00
2.26
1.13
2.09
1.02
1.00
1.49
1.07
3.22
3.09
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


199.96
199.03
145.34
138.05
130.60
129.05
127.64
127.23
126.93
126.08
39.65
30.11
16.92
6.78
S
S
O
O
f1 (ppm)

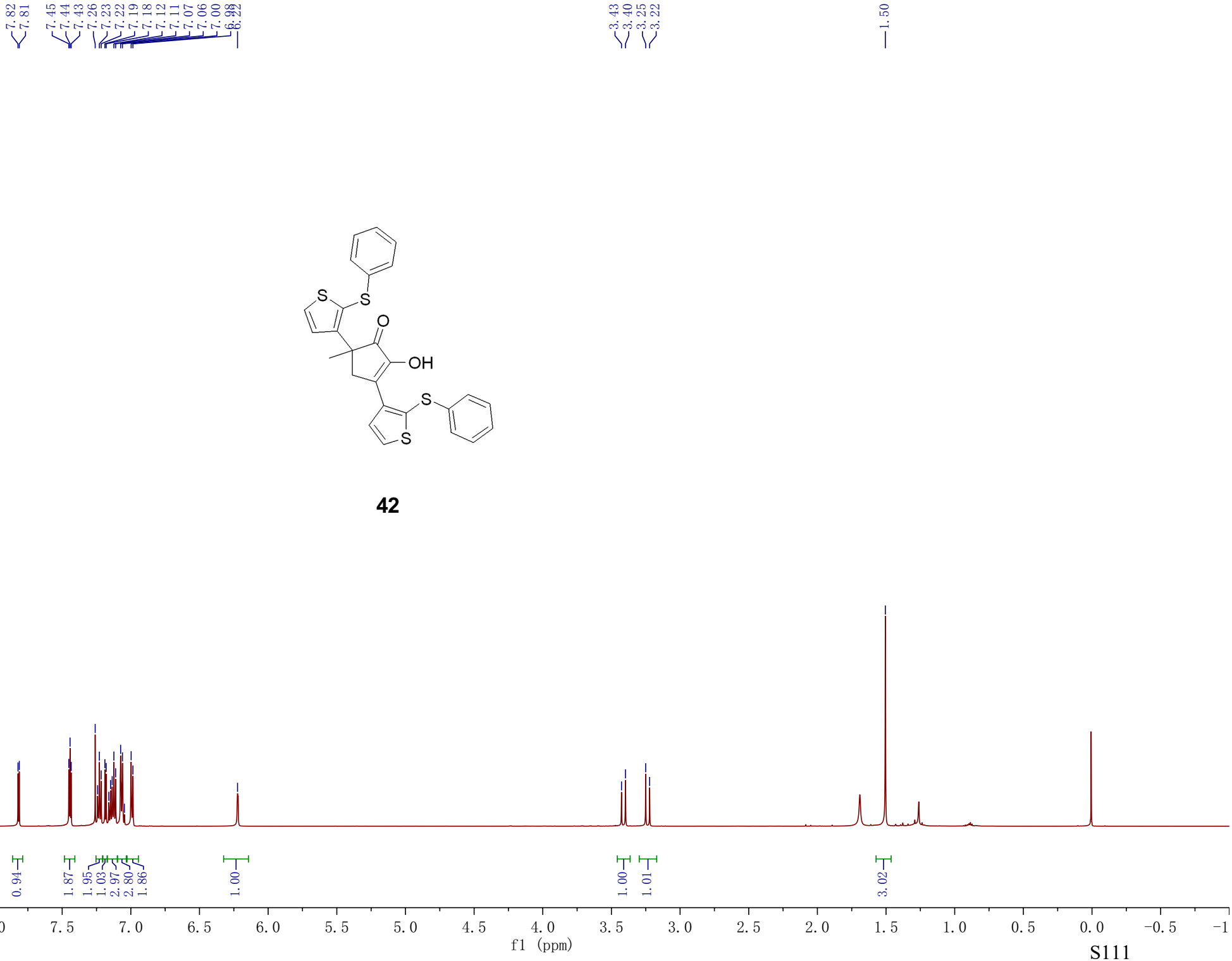
**40**


7.84
7.83
7.49
7.48
7.45
7.44
7.34
7.33
7.33
7.32
7.32
7.31
7.26
7.19
7.18
7.13
7.12
7.11
7.07
7.06
7.05
6.99
6.99
6.98
6.90
6.90
6.89
6.89
6.88
6.88
3.41
3.39
3.19
3.17
1.53
S
S
O
OH
S
S
Br
41
0.96
1.06
1.00
2.08
1.03
2.03
1.04
2.00
2.00
0.96
1.01
1.00
3.05
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

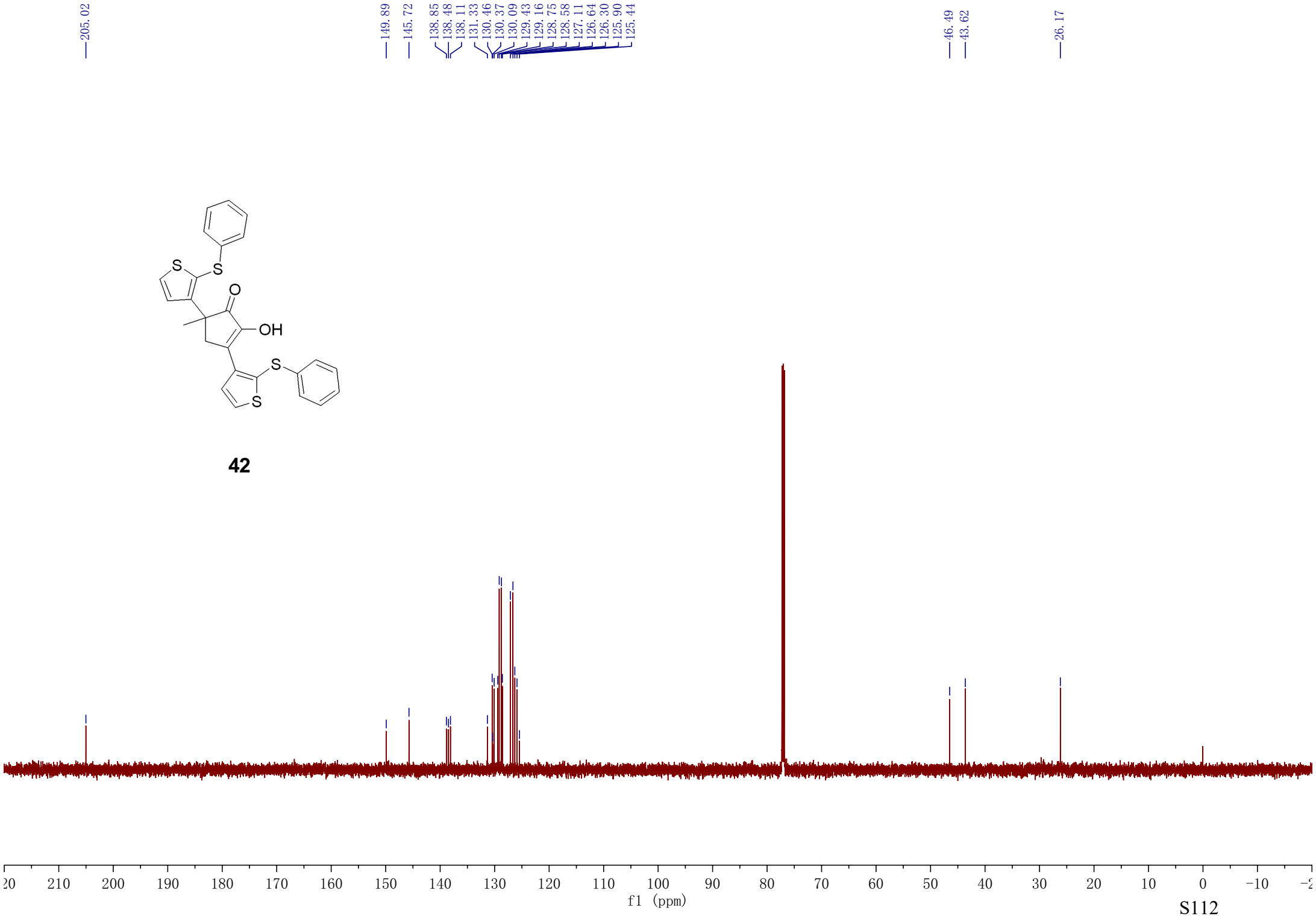

S
S
O
OH
S
S
Br

**41**

205.07
149.78
145.93
139.43
138.05
137.95
132.18
128.78
128.54
128.28
126.65
46.49
43.58
26.26
f1 (ppm)

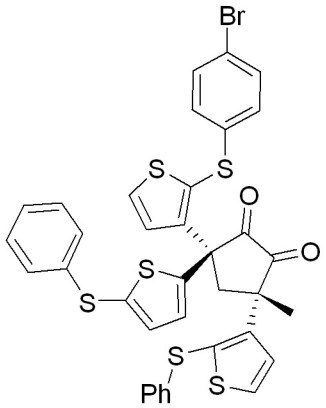

7.82
7.81
7.45
7.44
7.43
7.26
7.23
7.22
7.19
7.18
7.12
7.11
7.07
7.06
7.00
6.98
6.22
3.43
3.40
3.25
3.22
1.50
S
S
O
OH
S
S
0.94
1.87
1.95
1.03
2.97
2.80
1.86
1.00
1.00
1.01
3.02
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

**42**

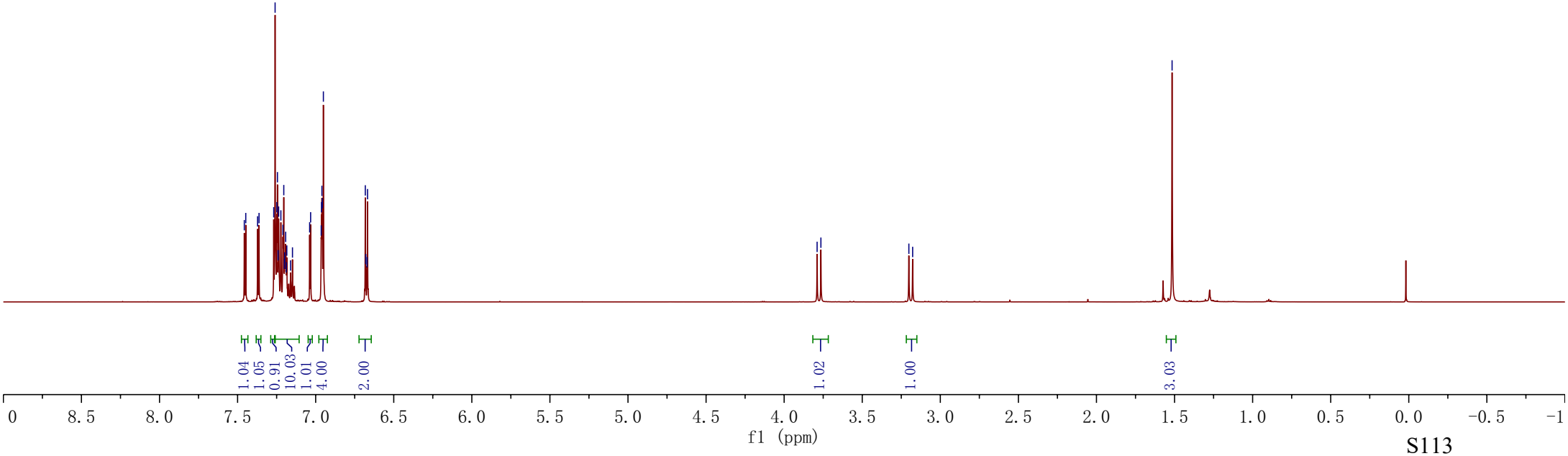

205.02
149.89
145.72
138.85
138.48
138.11
131.33
130.46
130.37
130.09
129.43
129.16
128.75
128.58
127.11
126.64
126.30
125.90
125.44
46.49
43.62
26.17
S
S
O
OH
S
S
42
f1 (ppm)

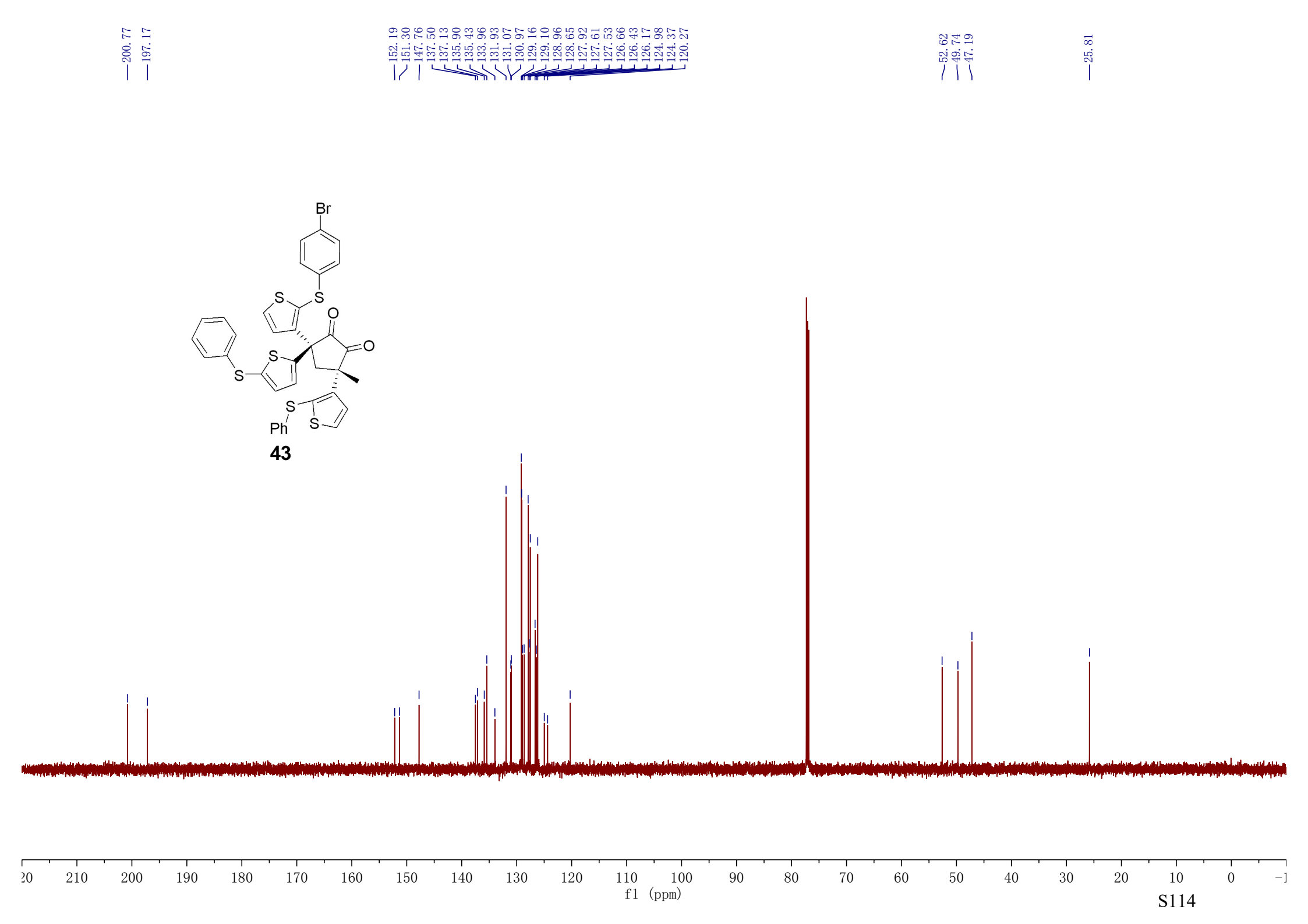

7.46
7.45
7.37
7.36
7.27
7.26
7.25
7.24
7.24
7.22
7.21
7.20
7.19
7.18
7.04
7.03
6.96
6.96
6.96
6.68
6.68
6.67
6.67

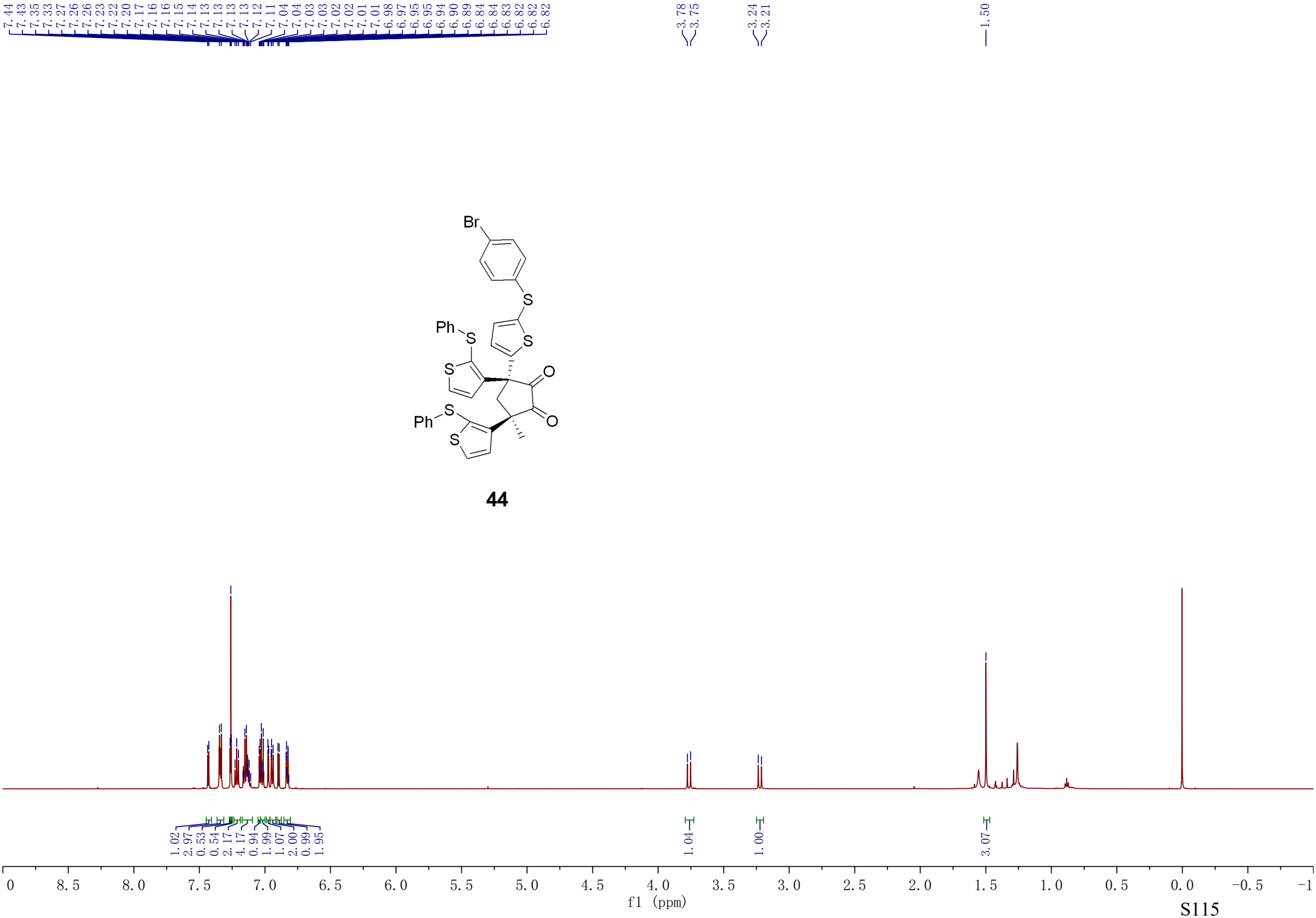

3.79
3.76
3.20
3.18
1.52


Br
S
S
O
O
S
S
S
Ph
S

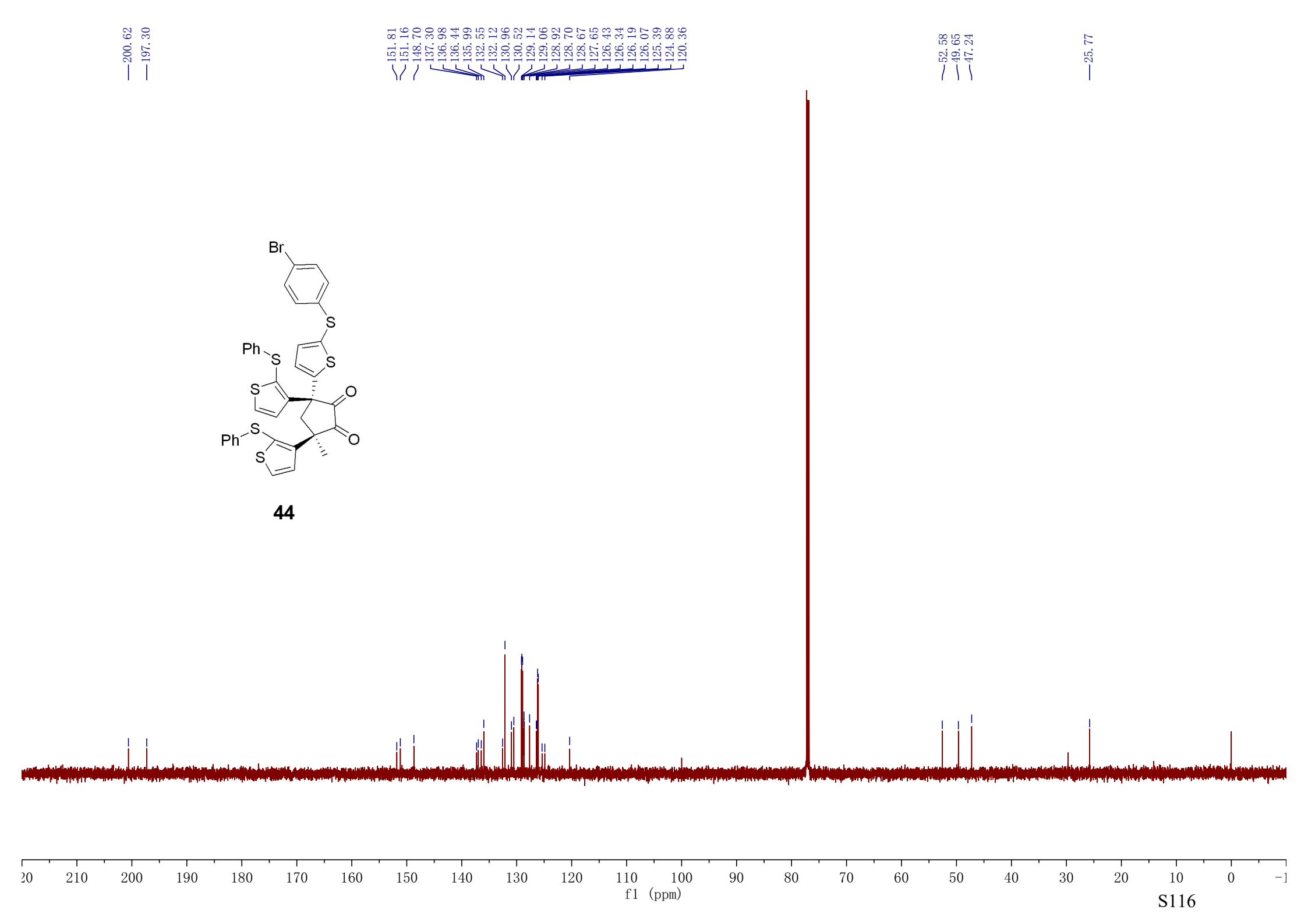
**43**


1.04
1.05
0.91
10.03
1.01
4.00
2.00
1.02
1.00
3.03
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


200.77
197.17
152.19
151.30
147.76
137.50
137.13
135.90
135.43
133.96
131.93
131.07
130.97
129.16
129.10
128.96
128.65
127.92
127.61
127.53
126.66
126.43
126.17
124.98
124.37
120.27
52.62
49.74
47.19
25.81
Br
S
S
O
O
S
S
S
S
Ph
43
f1 (ppm)


7.44
7.43
7.35
7.33
7.27
7.26
7.26
7.23
7.22
7.20
7.17
7.16
7.16
7.15
7.14
7.13
7.13
7.13
7.12
7.11
7.04
7.04
7.03
7.03
7.02
7.02
7.01
7.01
6.98
6.97
6.95
6.95
6.94
6.90
6.89
6.84
6.84
6.83
6.82
6.82
6.82
3.78
3.75
3.24
3.21
1.50
Br
S
Ph
S
S
S
O
O
Ph
S
S
1.02
2.97
0.53
0.54
2.17
4.17
0.94
1.99
1.07
2.00
0.99
1.95
1.04
1.00
3.07
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

**44**

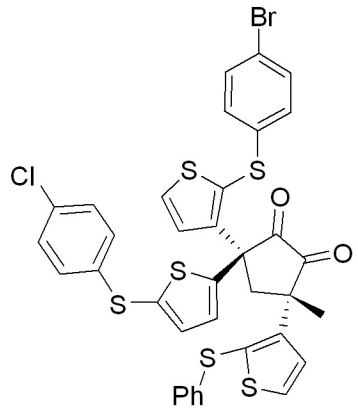

200.62
197.30
151.81
151.16
148.70
137.30
136.98
136.44
135.99
132.55
132.12
130.96
130.52
129.14
129.06
128.92
128.70
128.67
127.65
126.43
126.34
126.19
126.07
125.39
124.88
120.36
52.58
49.65
47.24
25.77
Br
S
Ph
S
S
S
O
O
Ph
S
S
44
f1 (ppm)


7.46
7.45
7.38
7.37
7.26
7.26
7.25
7.24
7.22
7.22
7.21
7.20
7.15
7.11
7.10
7.02
7.02
6.95
6.94
6.94
6.93
6.67
6.67
6.66
6.66
6.65
6.65

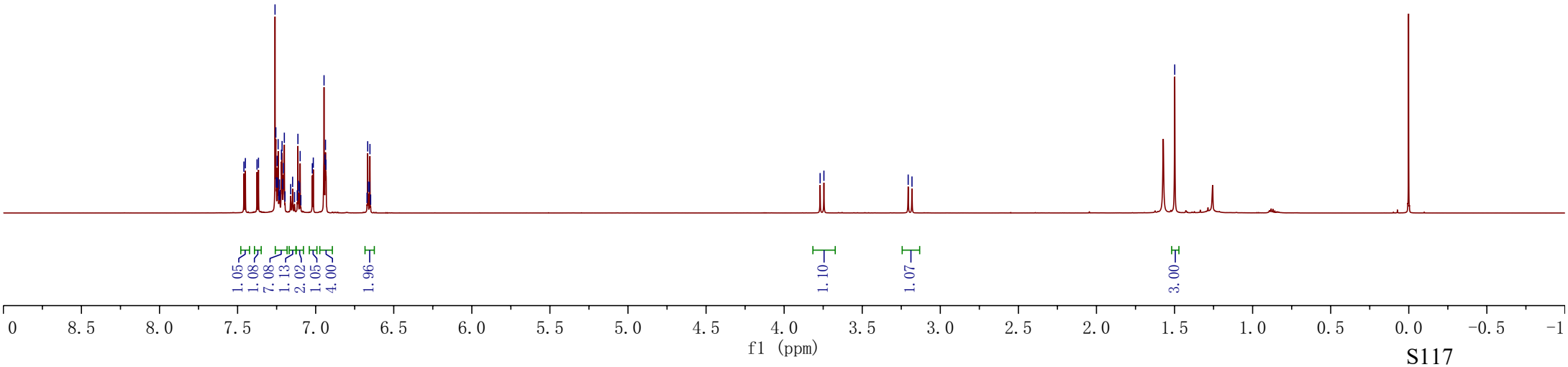

3.77
3.75


3.21
3.18

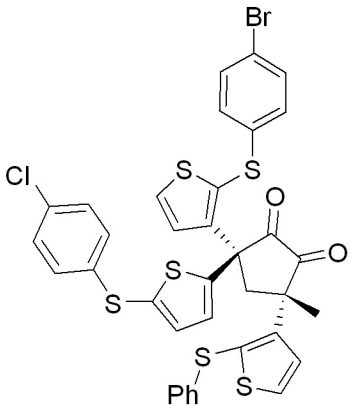

1.50


Br
Cl
S
S
O
O
S
S
S
Ph
S

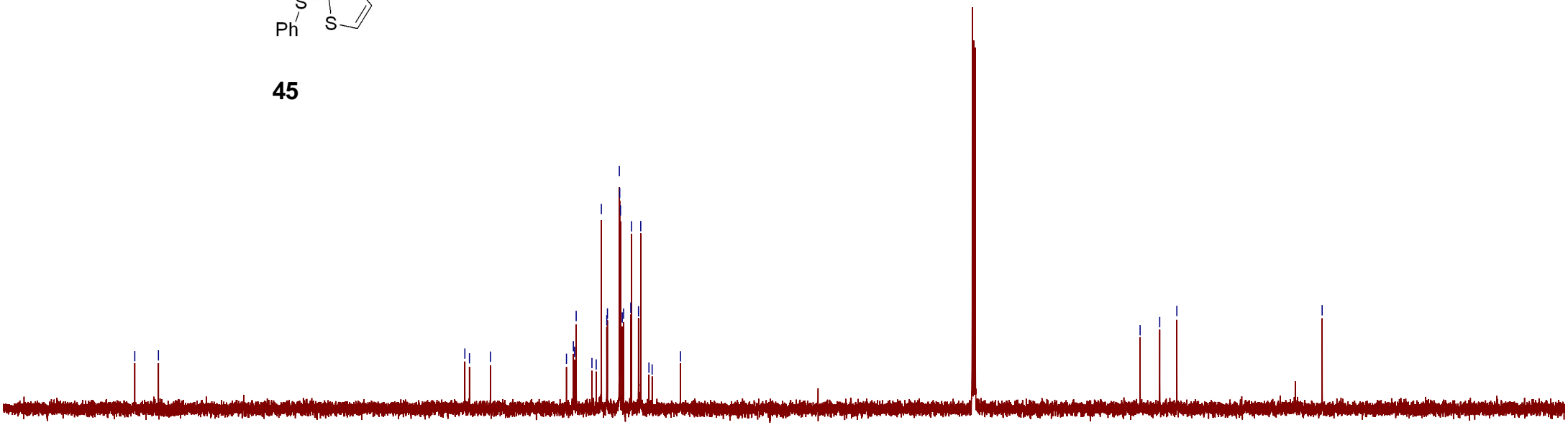
**45**

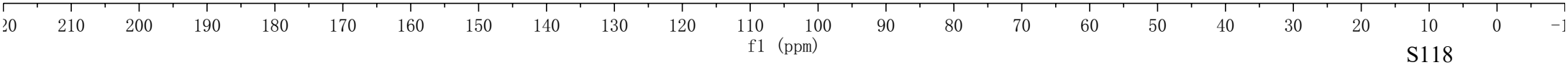

1.05
1.08
7.08
1.13
2.02
1.05
4.00
1.96
1.10
1.07
3.00
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

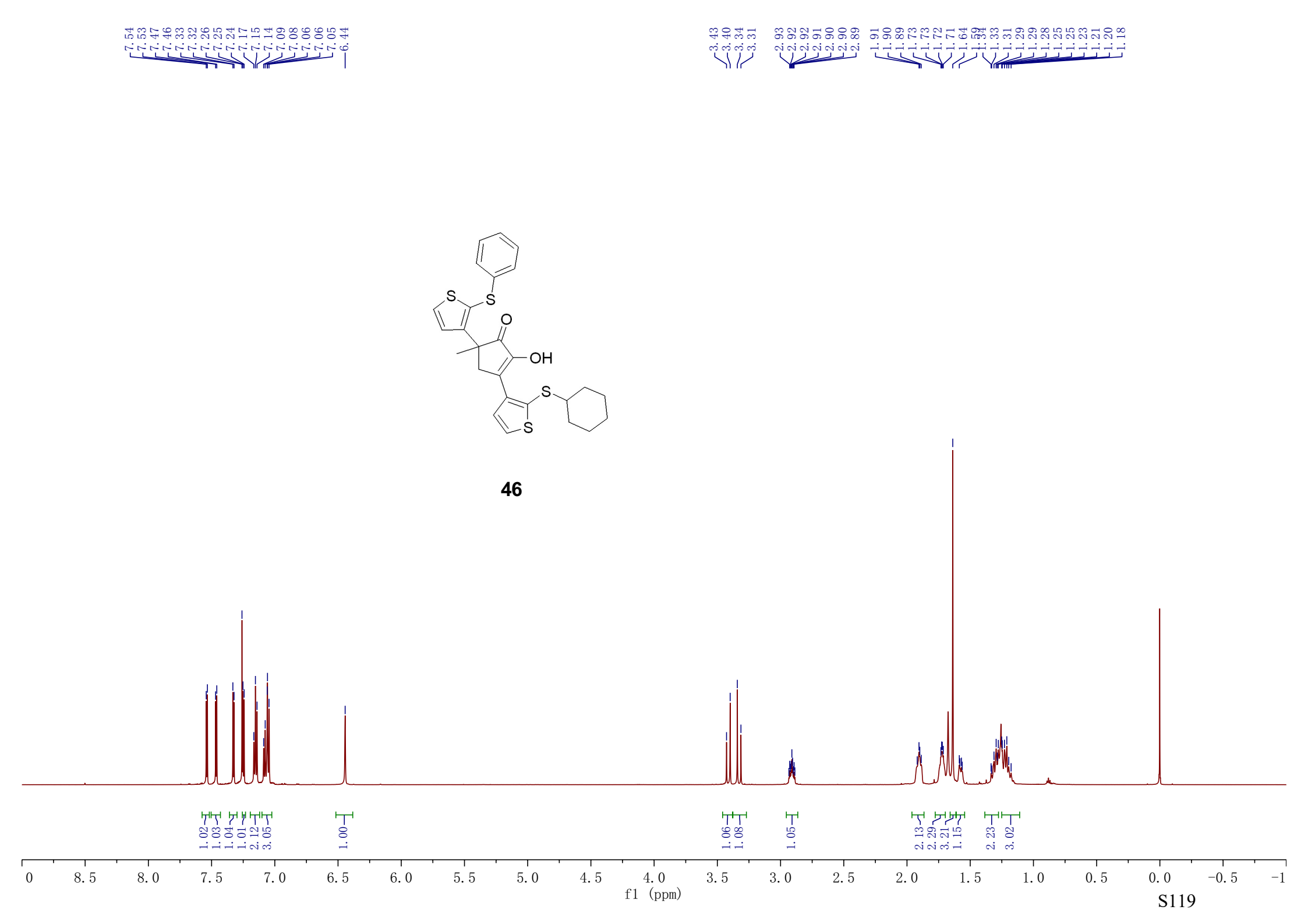
200.64
197.16
152.03
151.35
148.26
137.06
136.04
135.87
135.63
133.31
132.68
131.92
131.12
131.02
129.27
129.21
129.10
128.85
128.65
127.59
127.49
126.45
126.12
124.91
124.44
120.26
52.57
49.69
47.16
25.76

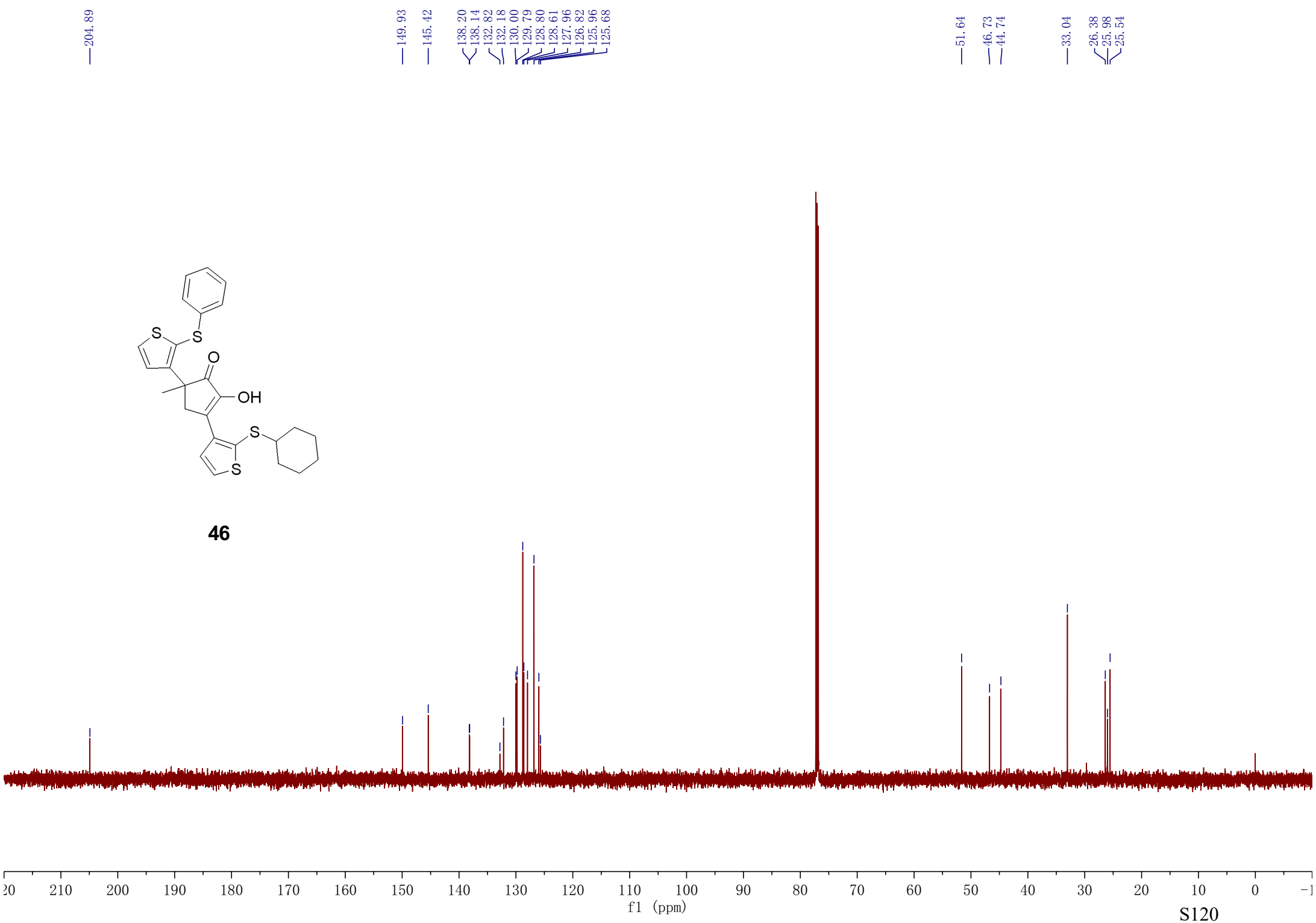


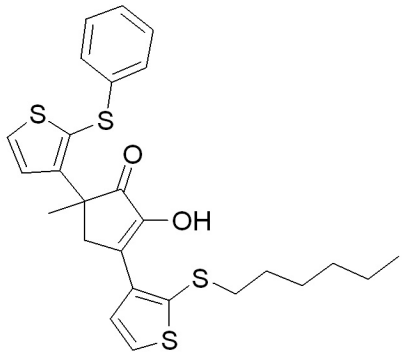

**45**






7.54
7.53
7.47
7.46
7.33
7.32
7.26
7.25
7.24
7.17
7.15
7.14
7.09
7.08
7.06
7.06
7.05
6.44
3.43
3.40
3.34
3.31
2.93
2.92
2.92
2.91
2.90
2.90
2.89
1.91
1.90
1.89
1.73
1.73
1.72
1.71
1.64
1.59
1.34
1.33
1.31
1.29
1.29
1.28
1.25
1.25
1.23
1.21
1.20
1.18
S
S
O
OH
S
S
46
1.02
1.03
1.04
1.01
2.12
3.05
1.00
1.06
1.08
1.05
2.13
2.29
3.21
1.15
2.23
3.02
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

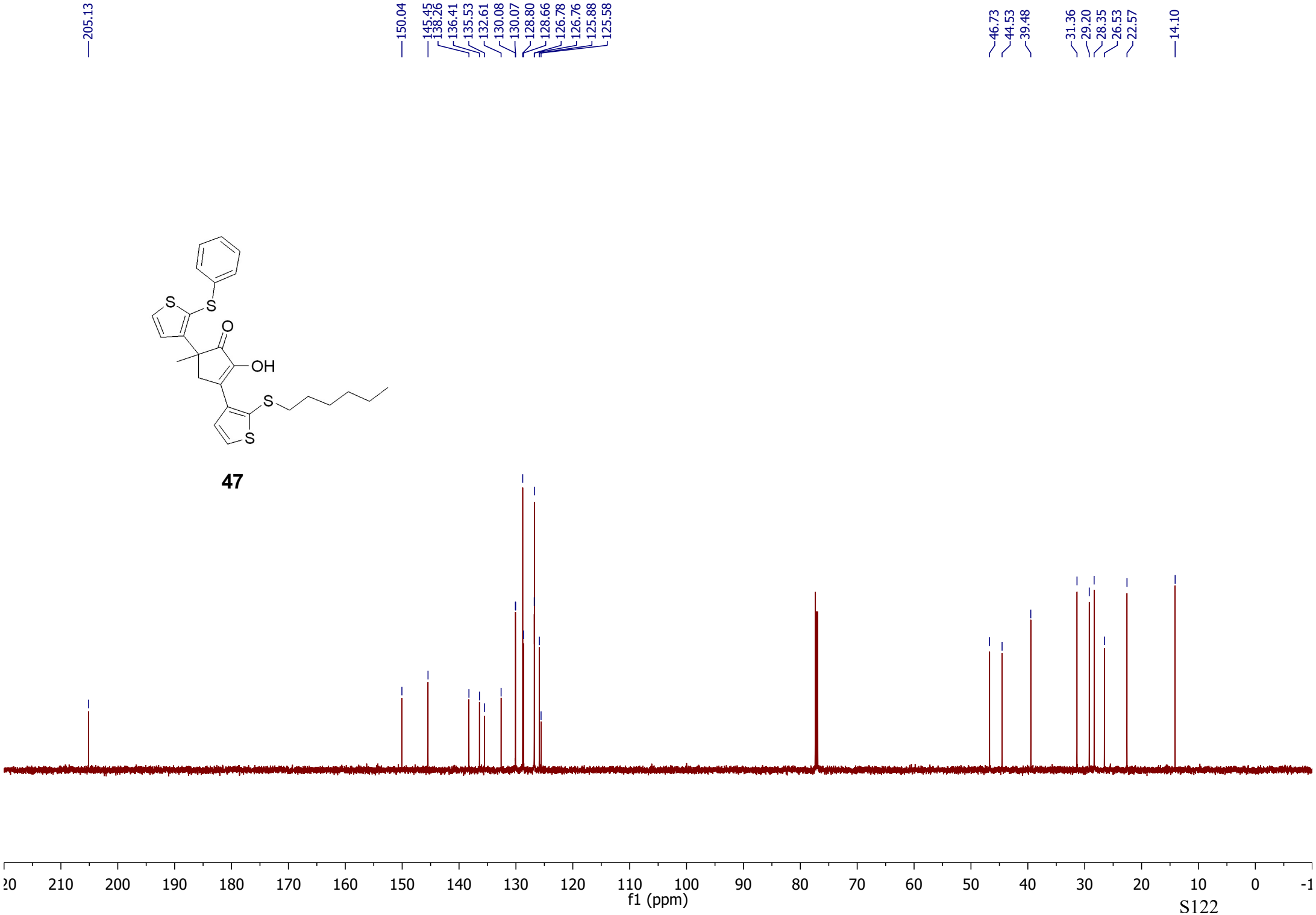

204.89
149.93
145.42
138.20
138.14
132.82
132.18
130.00
129.79
128.80
128.61
127.96
126.82
125.96
125.68
51.64
46.73
44.74
33.04
26.38
25.98
25.54
S
S
O
OH
S
S
46
f1 (ppm)

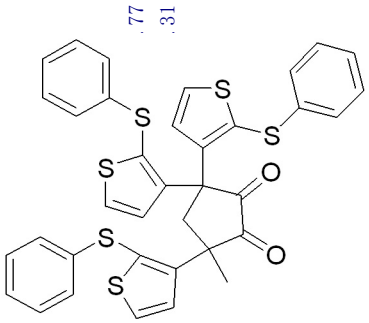



**47**

S
S
O
OH
S
S

**47**


205.13
150.04
145.45
138.26
136.41
135.53
132.61
130.08
130.07
128.80
128.66
126.78
126.76
125.88
125.58
46.73
44.53
39.48
31.36
29.20
28.35
26.53
22.57
14.10
f1 (ppm)



77.31

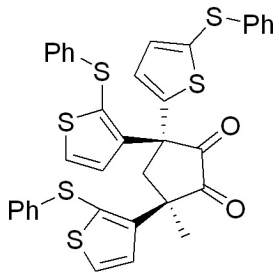
152.17
151.20
148.04
137.69
137.37
136.46
135.71
133.43
130.96
130.56
129.13
129.07
128.94
128.84
128.68
127.67
127.63
126.50
126.42
126.30
126.12
126.05
125.11
124.86

52.60
49.68
47.26

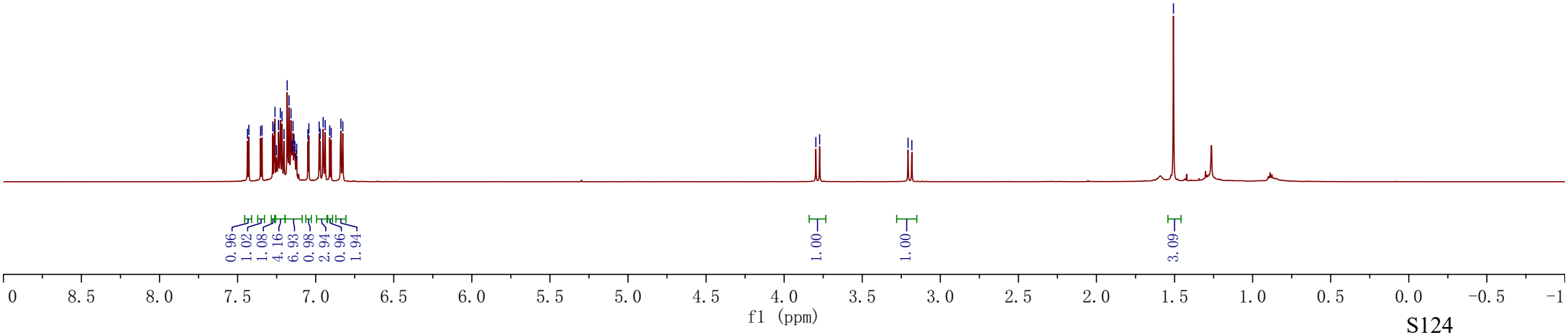
25.82

f1 (ppm)

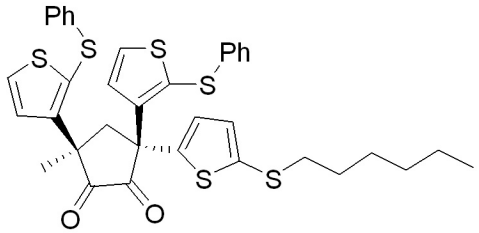

7.44
7.43
7.35
7.34
7.27
7.27
7.26
7.25
7.24
7.23
7.22
7.20
7.18
7.17
7.16
7.15
7.14
7.14
7.13
7.13
7.12
7.05
7.04
6.98
6.97
6.95
6.94
6.91
6.90
6.84
6.83
3.80
3.77
3.21
3.18
1.51


S
Ph
Ph
S
S
S
O
Ph
S
S
O

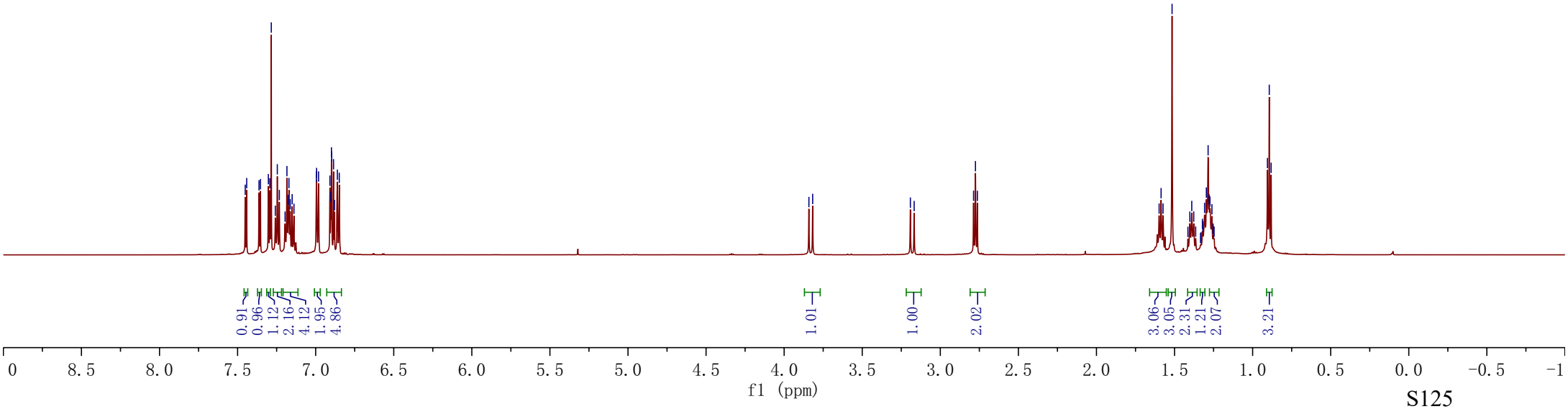
**48**

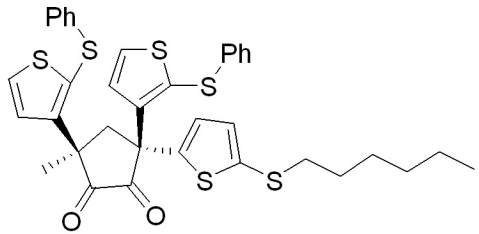

0.96
1.02
1.08
4.16
6.93
0.98
2.94
0.96
1.94
1.00
1.00
3.09
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


7.45
7.44
7.36
7.35
7.30
7.29
7.28
7.26
7.25
7.23
7.20
7.18
7.17
7.17
7.16
7.15
7.14
7.00
6.99
6.98
6.91
6.90
6.90
6.90
6.89
6.88
6.86
6.85
3.84
3.82
3.19
3.17
2.79
2.77
2.76
1.60
1.59
1.57
1.52
1.40
1.39
1.38
1.32
1.32
1.31
1.30
1.29
1.28
1.27
0.90
0.89
0.88


Ph
S
S
S
Ph
S
S
S
O
O

**49**

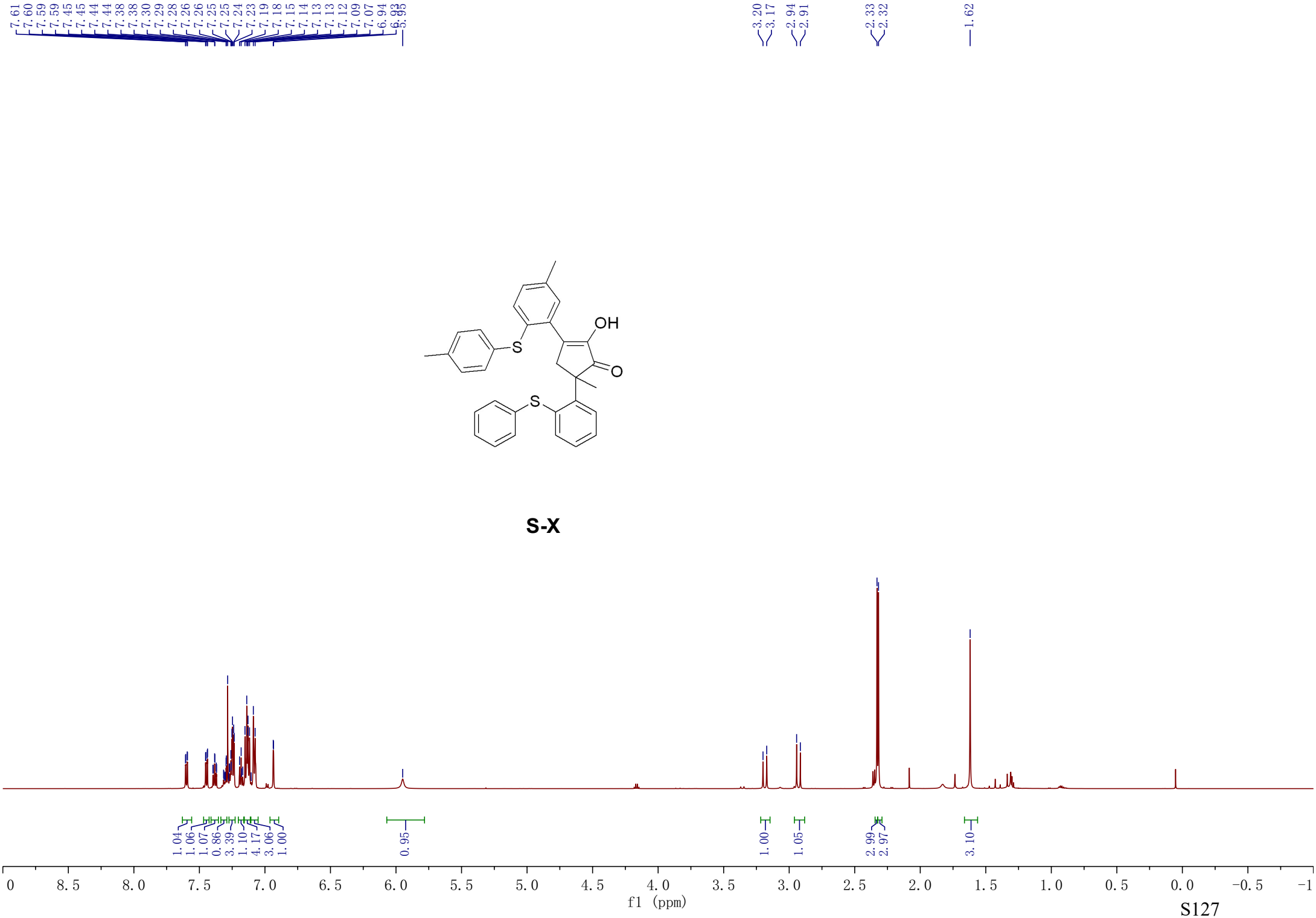

0.91
0.96
1.12
2.16
4.12
1.95
4.86
1.01
1.00
2.02
3.06
3.05
2.31
1.21
2.07
3.21
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)



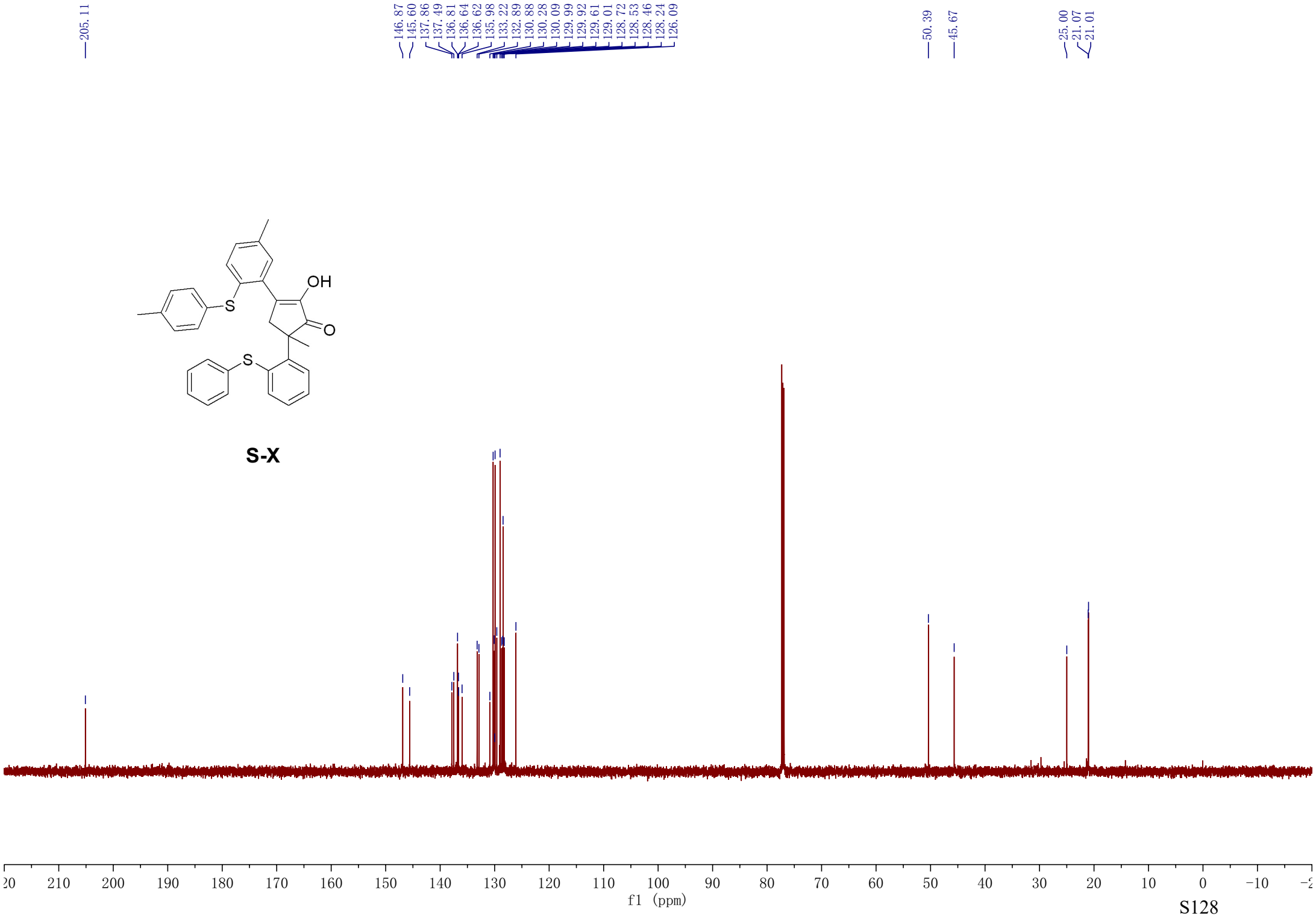

**49**

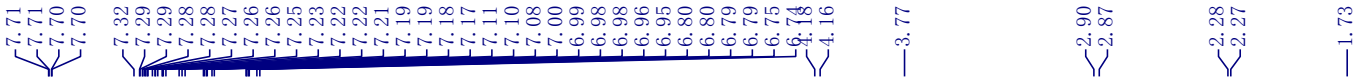
200.99
197.29
152.56
151.11
145.24
137.50
137.38
136.57
132.71
130.81
130.43
129.04
128.99
128.90
128.38
127.67
126.34
126.26
126.11
126.08
124.97
124.85
52.57
49.61
47.23
38.70
31.31
29.26
28.06
25.88
22.49
14.03

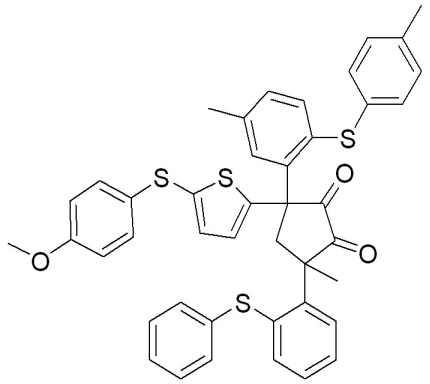
f1 (ppm)


7.61
7.60
7.59
7.59
7.45
7.45
7.44
7.44
7.38
7.38
7.30
7.29
7.28
7.26
7.26
7.25
7.25
7.24
7.23
7.19
7.18
7.15
7.14
7.13
7.13
7.12
7.09
7.07
6.94
6.93
5.95
3.20
3.17
2.94
2.91
2.33
2.32
1.62
OH
S
O
S
1.04
1.06
1.07
0.86
3.39
1.10
4.17
3.06
1.00
0.95
1.00
1.05
2.99
2.97
3.10
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

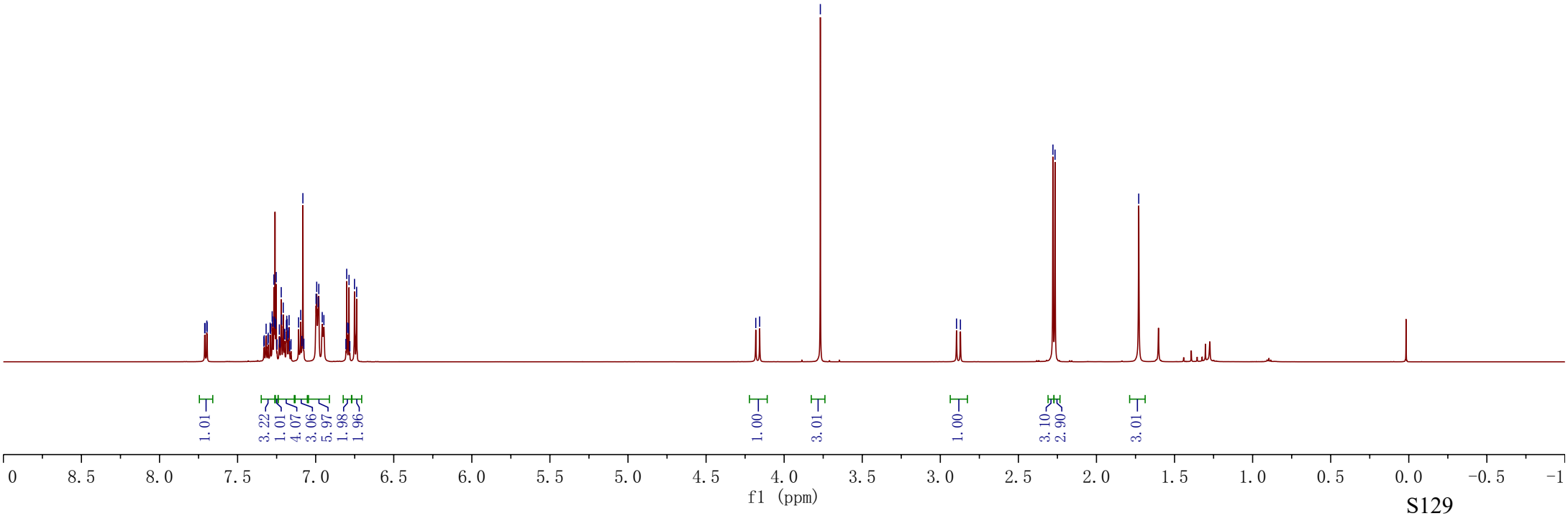
**S-X**

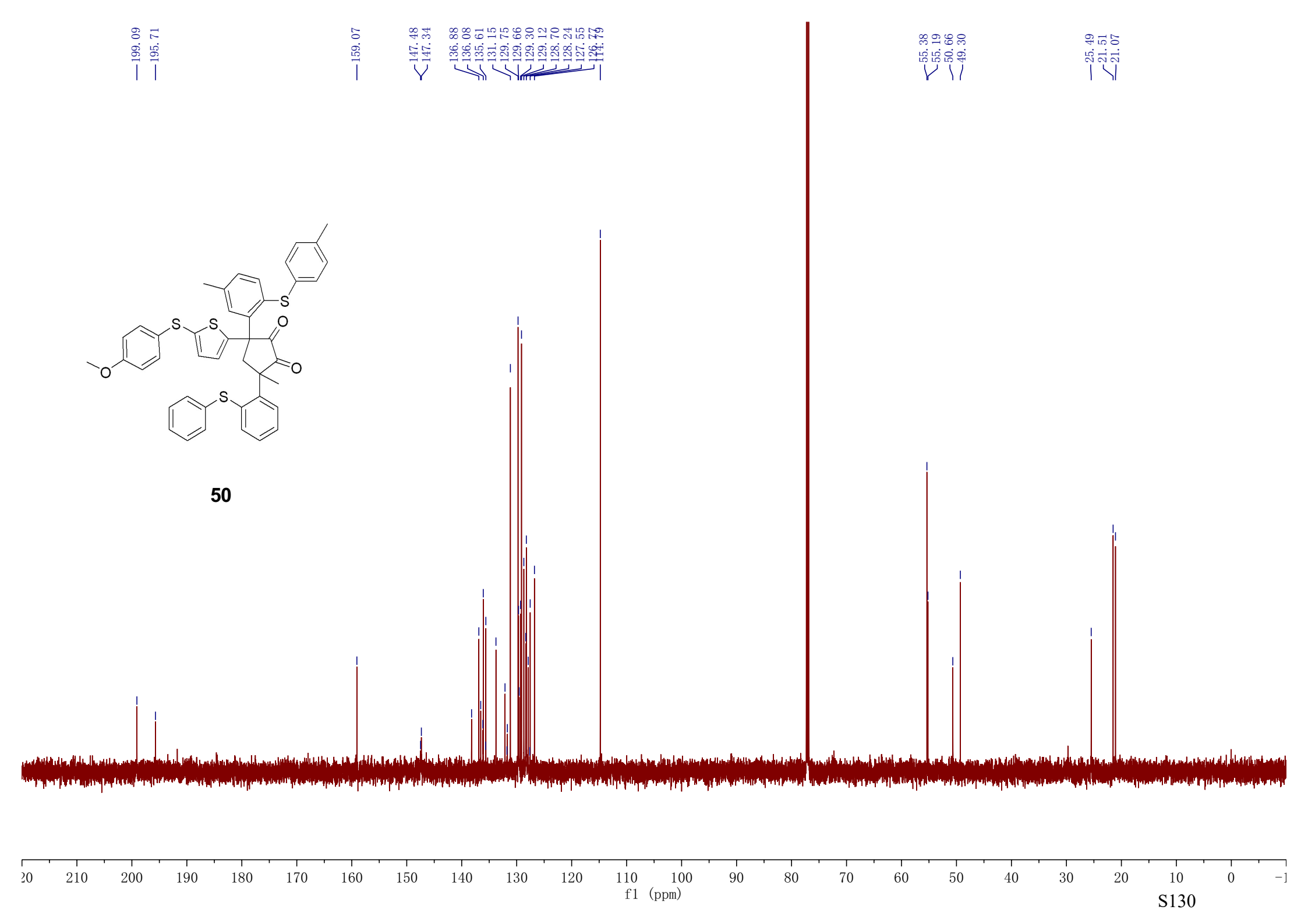

205.11
146.87
145.60
137.86
137.49
136.81
136.64
136.62
135.98
133.22
132.89
130.88
130.28
130.09
129.99
129.92
129.61
129.01
128.72
128.53
128.46
128.24
126.09
50.39
45.67
25.00
21.07
21.01
OH
S
O
S
S-X
f1 (ppm)


7.71
7.71
7.70
7.70
7.32
7.29
7.29
7.28
7.28
7.27
7.26
7.26
7.25
7.23
7.22
7.22
7.21
7.19
7.19
7.18
7.17
7.11
7.10
7.08
7.00
6.99
6.98
6.98
6.96
6.95
6.80
6.80
6.79
6.79
6.75
6.74
4.18
4.16
3.77
2.90
2.87
2.28
2.27
1.73

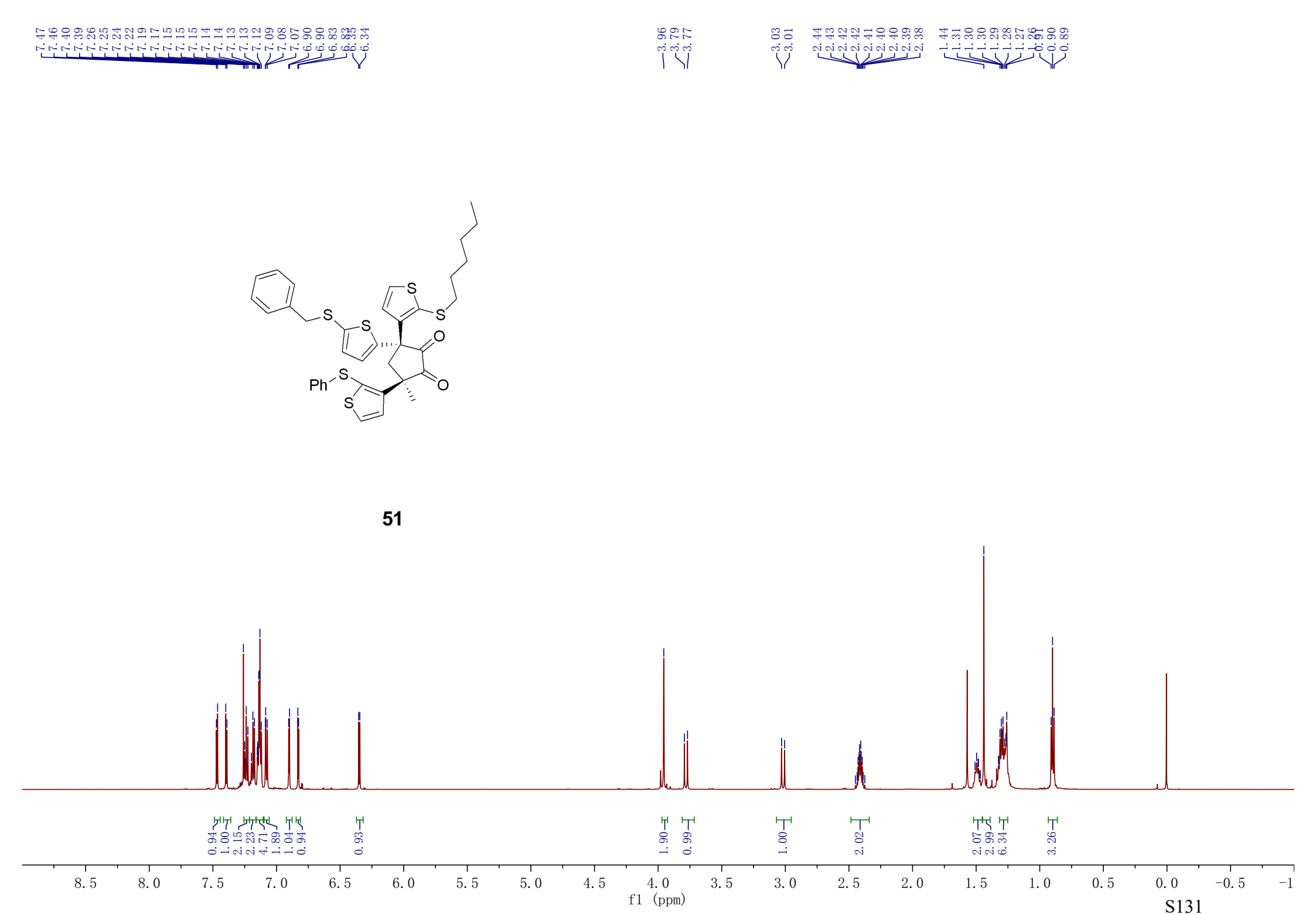

S
S
S
O
O
O
S

**50**

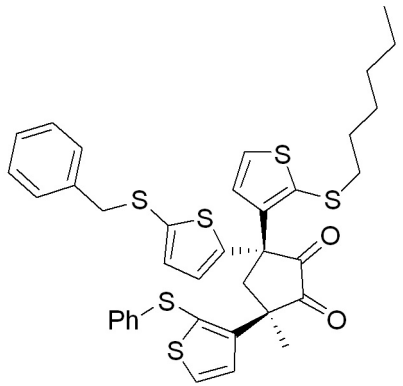

1.01
3.22
1.01
4.07
3.06
5.97
1.98
1.96
1.00
3.01
1.00
3.10
2.90
3.01
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


199.09
195.71
159.07
147.48
147.34
136.88
136.08
135.61
131.15
129.75
129.66
129.30
129.12
128.70
128.24
127.55
55.38
55.19
50.66
49.30
25.49
21.51
21.07
S
S
S
O
O
O
S
f1 (ppm)

**50**


7.47
7.46
7.40
7.39
7.26
7.25
7.24
7.22
7.19
7.17
7.15
7.15
7.14
7.14
7.13
7.13
7.12
7.09
7.08
7.07
6.90
6.90
6.83
6.83
6.35
6.34
3.96
3.79
3.77
3.03
3.01
2.44
2.43
2.42
2.42
2.41
2.40
2.40
2.39
2.38
1.44
1.31
1.30
1.30
1.29
1.28
1.27
1.26
0.91
0.90
0.89
S
S
S
S
S
O
O
Ph
S
S
0.94
1.00
2.15
2.23
4.71
1.89
1.04
0.94
0.93
1.90
0.99
1.00
2.02
2.07
2.99
6.34
3.26
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

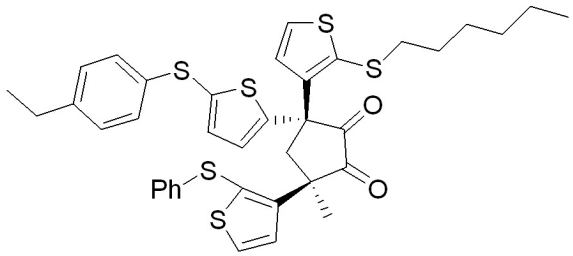
**51**



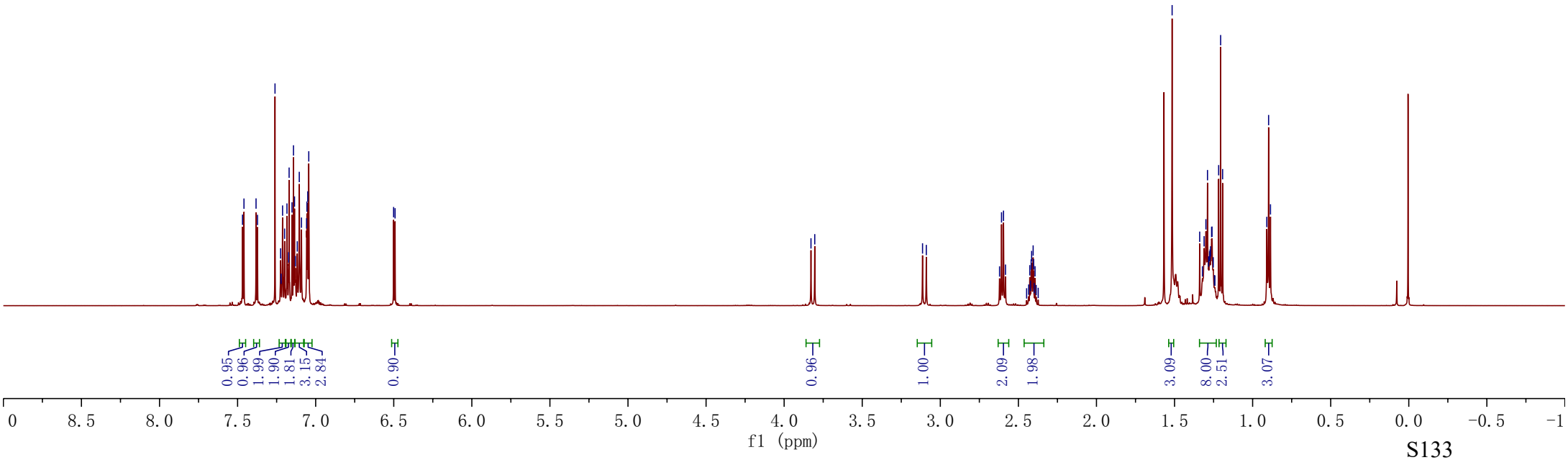

**51**

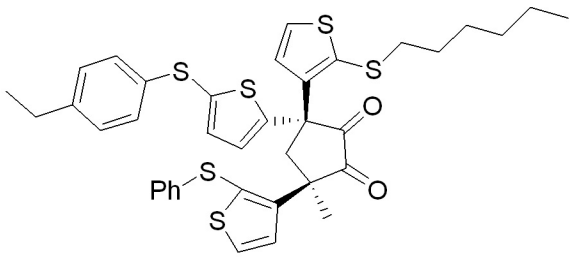
200.08
198.81
154.44
149.58
146.67
138.41
137.21
134.95
134.74
130.48
129.10
129.02
128.70
128.67
128.38
128.19
127.89
127.56
127.32
126.33
126.08
125.87
52.21
50.59
47.98
43.44
38.16
31.33
28.58
28.42
26.05
22.53
14.05

f1 (ppm)

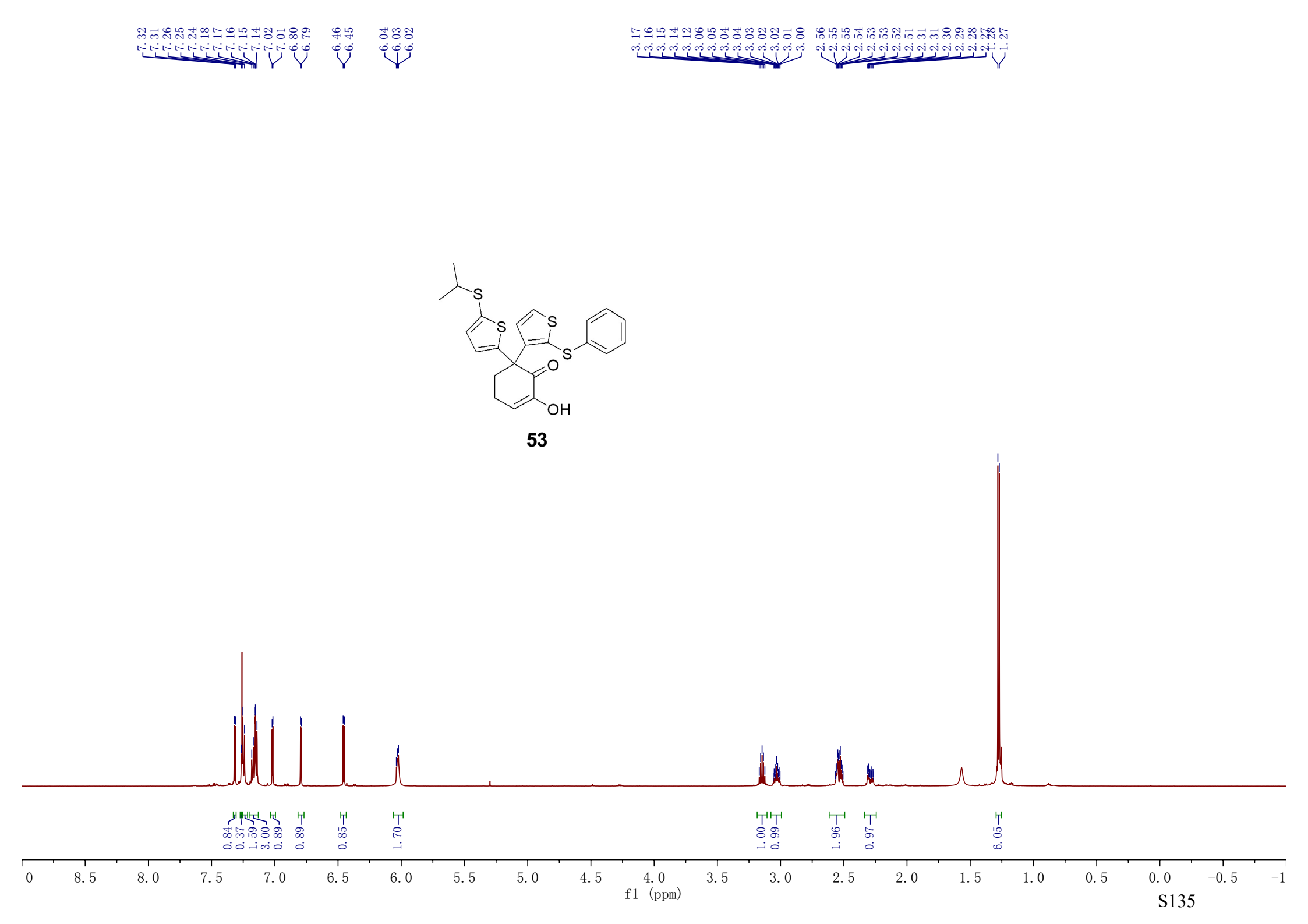



**52**

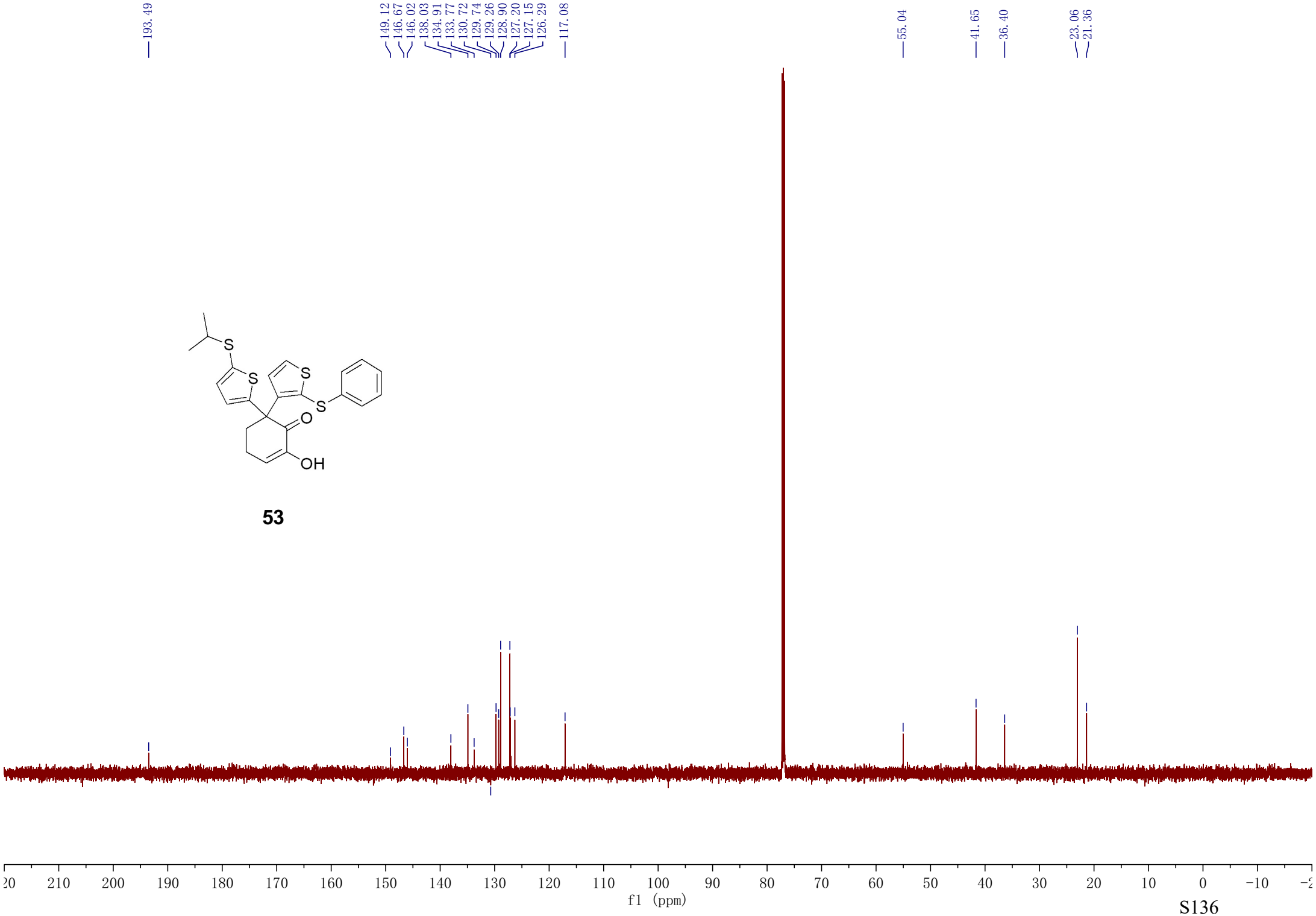


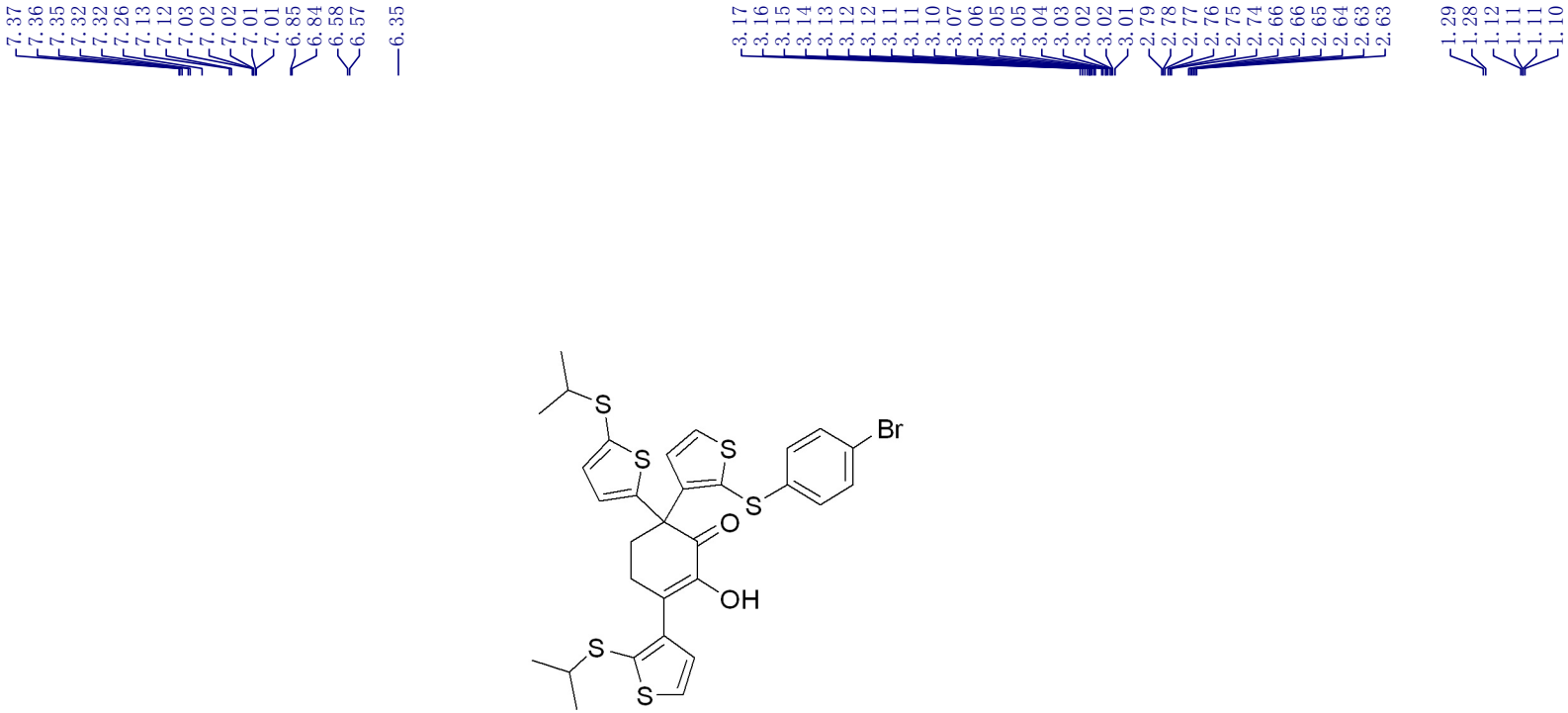



**52**

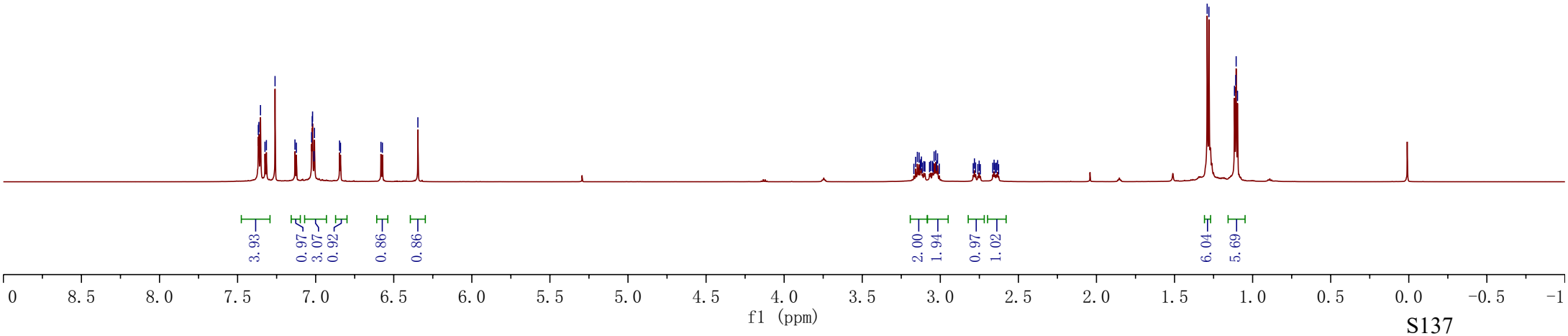

7.32
7.31
7.26
7.25
7.24
7.18
7.17
7.16
7.15
7.14
7.02
7.01
6.80
6.79
6.46
6.45
6.04
6.03
6.02
3.17
3.16
3.15
3.14
3.12
3.06
3.05
3.04
3.04
3.03
3.02
3.02
3.01
3.00
2.56
2.55
2.55
2.54
2.53
2.52
2.51
2.31
2.31
2.30
2.29
2.28
2.27
1.28
1.27
S
S
S
S
O
OH
0.84
0.37
1.59
3.00
0.89
0.89
0.85
1.70
1.00
0.99
1.96
0.97
6.05
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

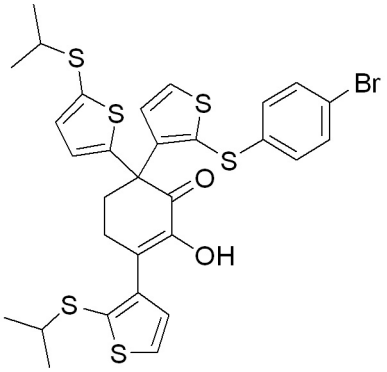
**53**


193.49
149.12
146.67
146.02
138.03
134.91
133.77
130.72
129.74
129.26
128.90
127.20
127.15
126.29
117.08
55.04
41.65
36.40
23.06
21.36
S
S
S
S
O
OH
53
f1 (ppm)


7.37
7.36
7.35
7.32
7.32
7.26
7.13
7.12
7.03
7.02
7.02
7.01
7.01
6.85
6.84
6.58
6.57
6.35
3.17
3.16
3.15
3.14
3.13
3.12
3.12
3.11
3.11
3.10
3.07
3.06
3.05
3.05
3.04
3.03
3.02
3.02
3.01
2.79
2.78
2.77
2.76
2.75
2.74
2.66
2.66
2.65
2.64
2.63
2.63
1.29
1.28
1.12
1.11
1.11
1.10
S
S
S
S
Br
O
OH
S
S

**54**

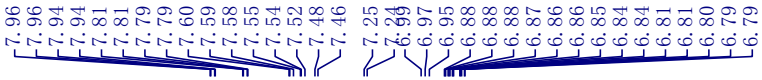

3.93
0.97
3.07
0.92
0.86
0.86
2.00
1.94
0.97
1.02
6.04
5.69
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)



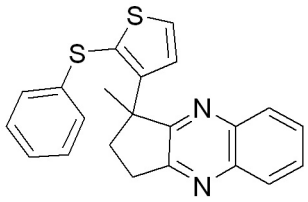

**54**

193.05
149.34
146.23
143.70
141.94
134.66
131.93
129.98
129.61
129.34
128.70
127.97
127.21
120.16
54.52
42.41
41.62
36.37
26.72
23.07
23.06
22.90
22.89

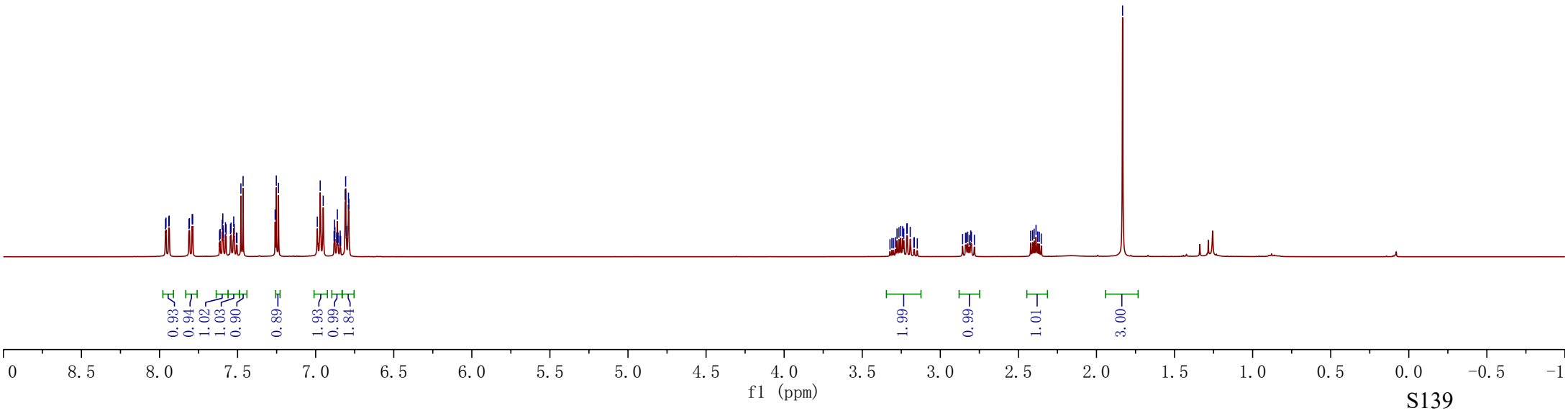
f1 (ppm)


7.96
7.96
7.94
7.94
7.81
7.81
7.79
7.79
7.60
7.59
7.58
7.55
7.54
7.52
7.48
7.46
7.25
7.24
6.97
6.95
6.88
6.88
6.87
6.86
6.86
6.85
6.84
6.84
6.81
6.81
6.80
6.79
6.79


3.32
3.31
3.30
3.29
3.28
3.26
3.25
3.24
3.23
3.21
3.21
3.19
3.17
3.17
3.15
2.83
2.82
2.81
2.41
2.40
2.39
2.38
2.37
2.35
1.83

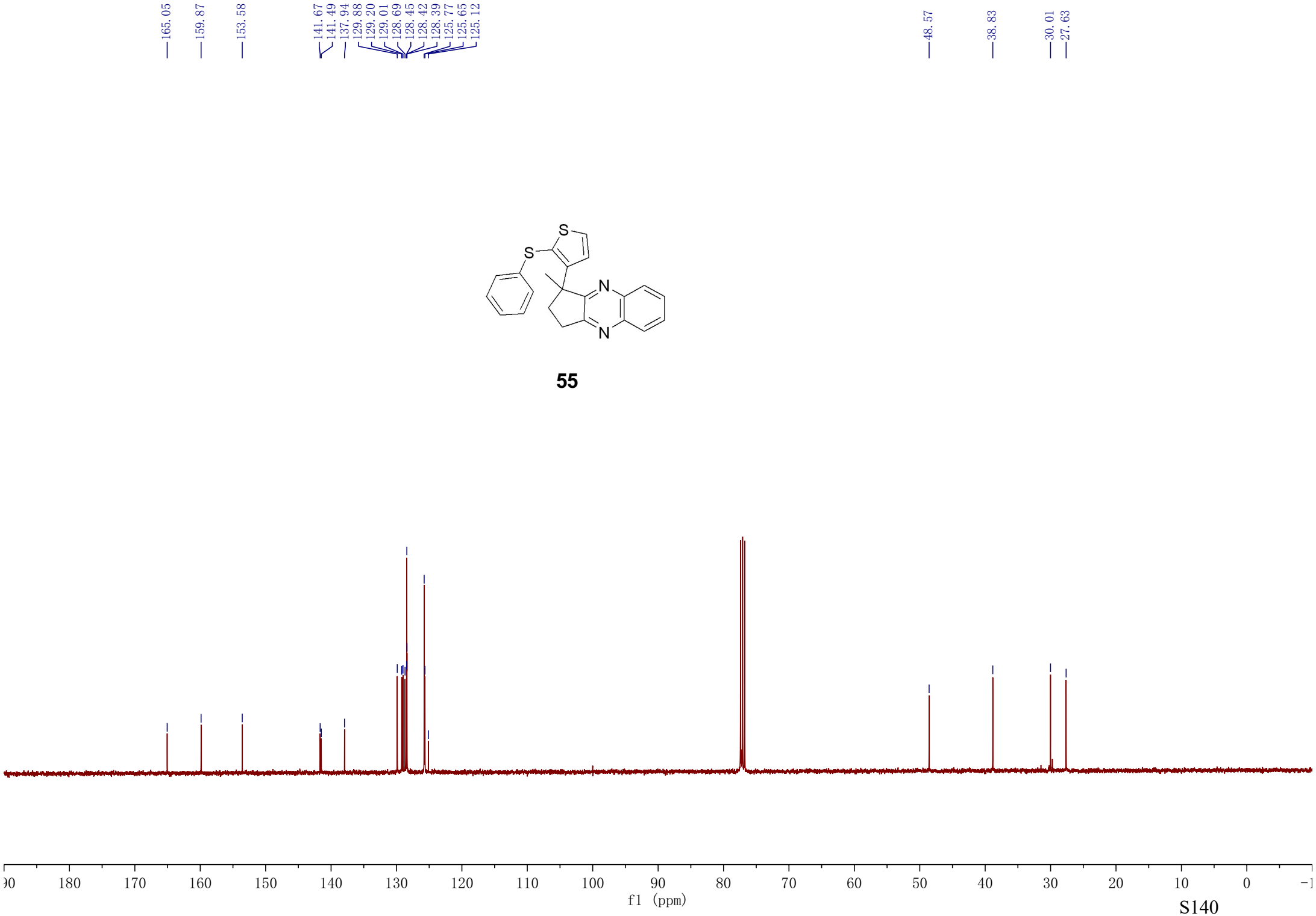

S
S
N
N

**55**

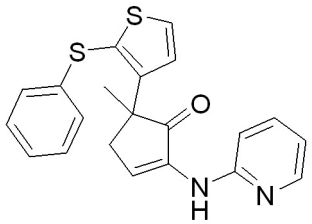

0.93
0.94
1.02
1.03
0.90
0.89
1.93
0.99
1.84
1.99
0.99
1.01
3.00
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

S
S
N
N

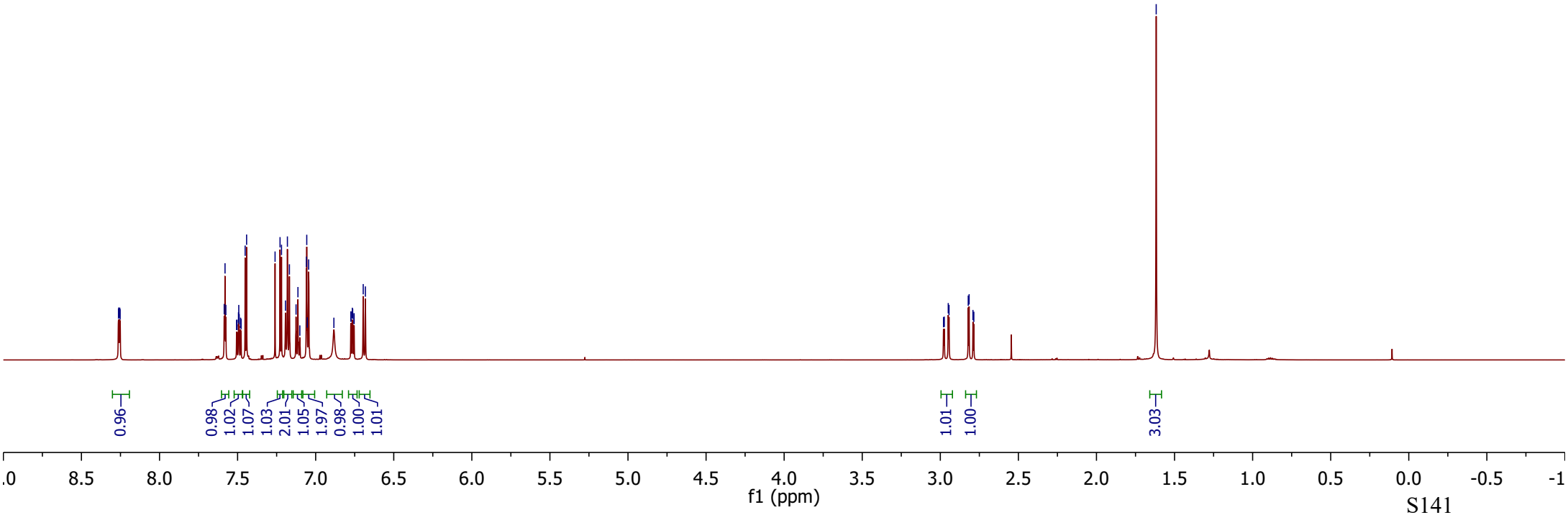
**55**


165.05
159.87
153.58
141.67
141.49
137.94
129.88
129.20
129.01
128.69
128.45
128.42
128.39
125.77
125.65
125.12
48.57
38.83
30.01
27.63
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.26
8.26
8.25
8.25
7.59
7.58
7.58
7.51
7.50
7.49
7.49
7.49
7.48
7.48
7.45
7.44
7.26
7.23
7.22
7.19
7.18
7.17
7.13
7.11
7.10
7.06
7.06
7.05
7.05
6.88
6.77
6.77
6.77
6.76
6.75
6.75
6.70
6.68
2.98
2.97
2.95
2.94
2.82
2.82
2.79
2.79
1.62

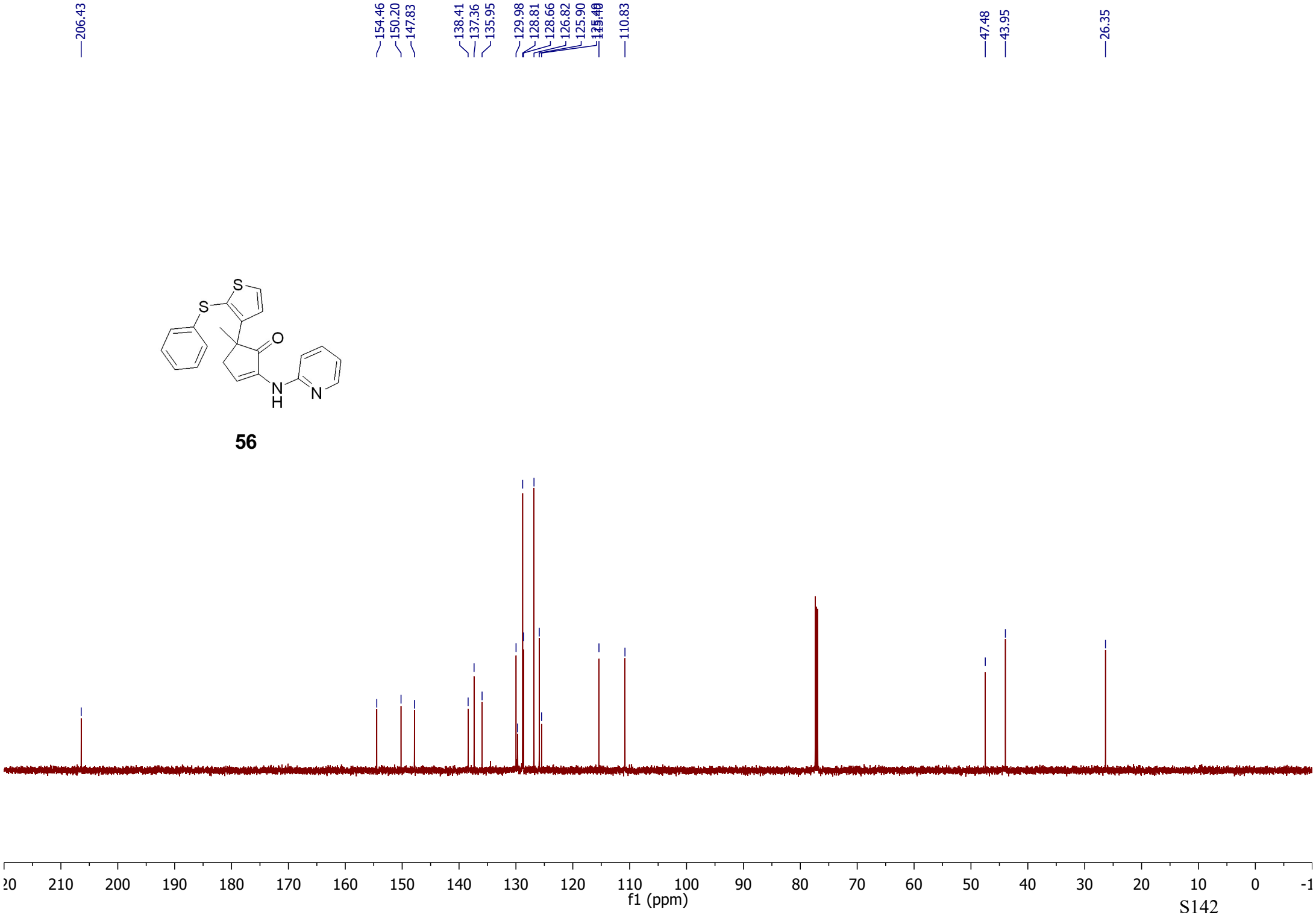

S
S
O
N
H
N

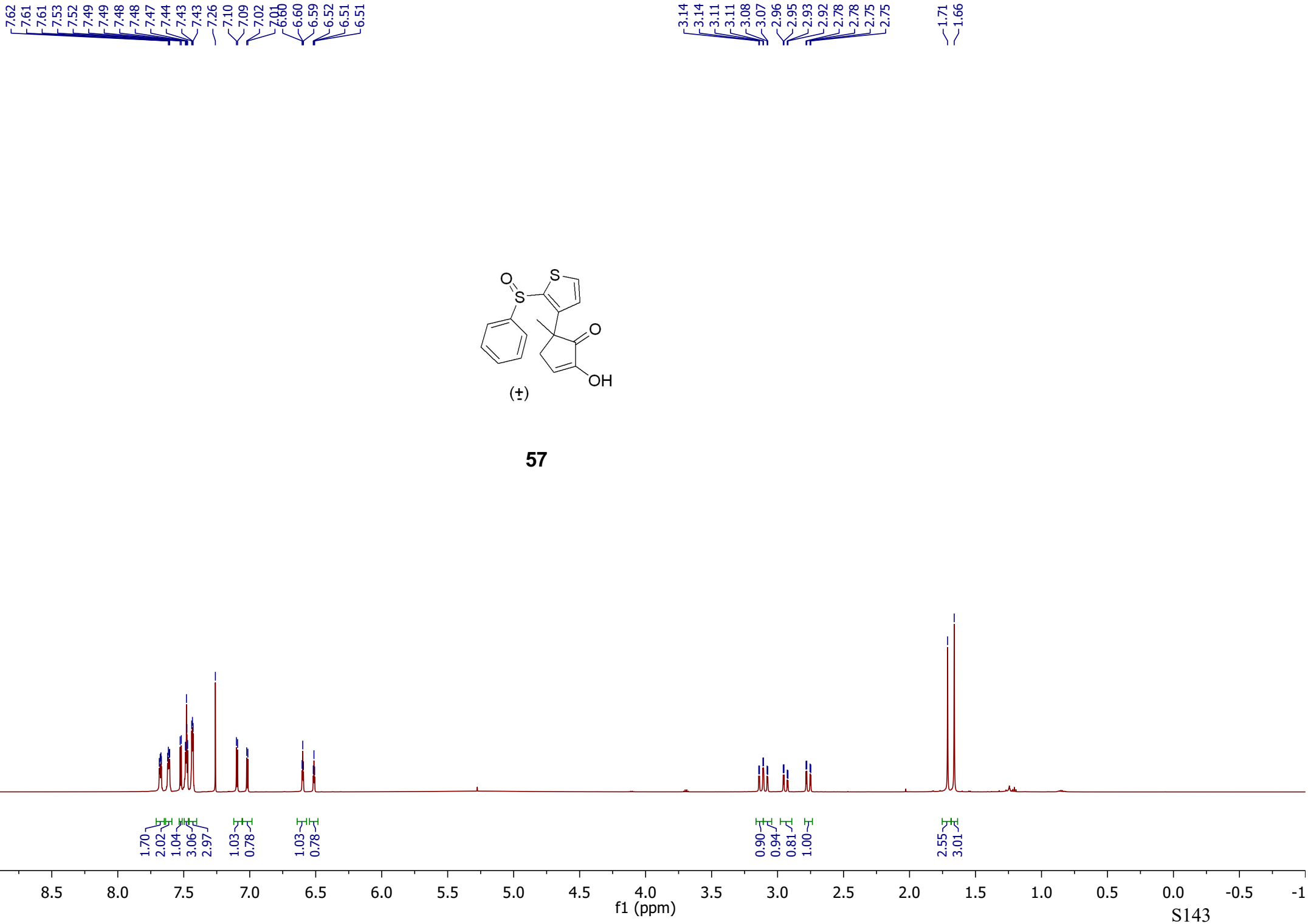
**56**


0.96
0.98
1.02
1.07
1.03
2.01
1.05
1.97
0.98
1.00
1.01
1.01
1.00
3.03
.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

S
S
O
N
H
N

**56**


206.43
154.46
150.20
147.83
138.41
137.36
135.95
129.98
128.81
128.66
126.82
125.90
110.83
47.48
43.95
26.35
f1 (ppm)


7.62
7.61
7.61
7.53
7.52
7.49
7.49
7.48
7.48
7.47
7.44
7.43
7.43
7.26
7.10
7.09
7.02
7.01
6.60
6.60
6.59
6.52
6.51
6.51
3.14
3.14
3.11
3.11
3.08
3.07
2.96
2.95
2.93
2.92
2.78
2.78
2.75
2.75
1.71
1.66
O
S
S
O
OH
(±)
1.70
2.02
1.04
3.06
2.97
1.03
0.78
1.03
0.78
0.90
0.94
0.81
1.00
2.55
3.01
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

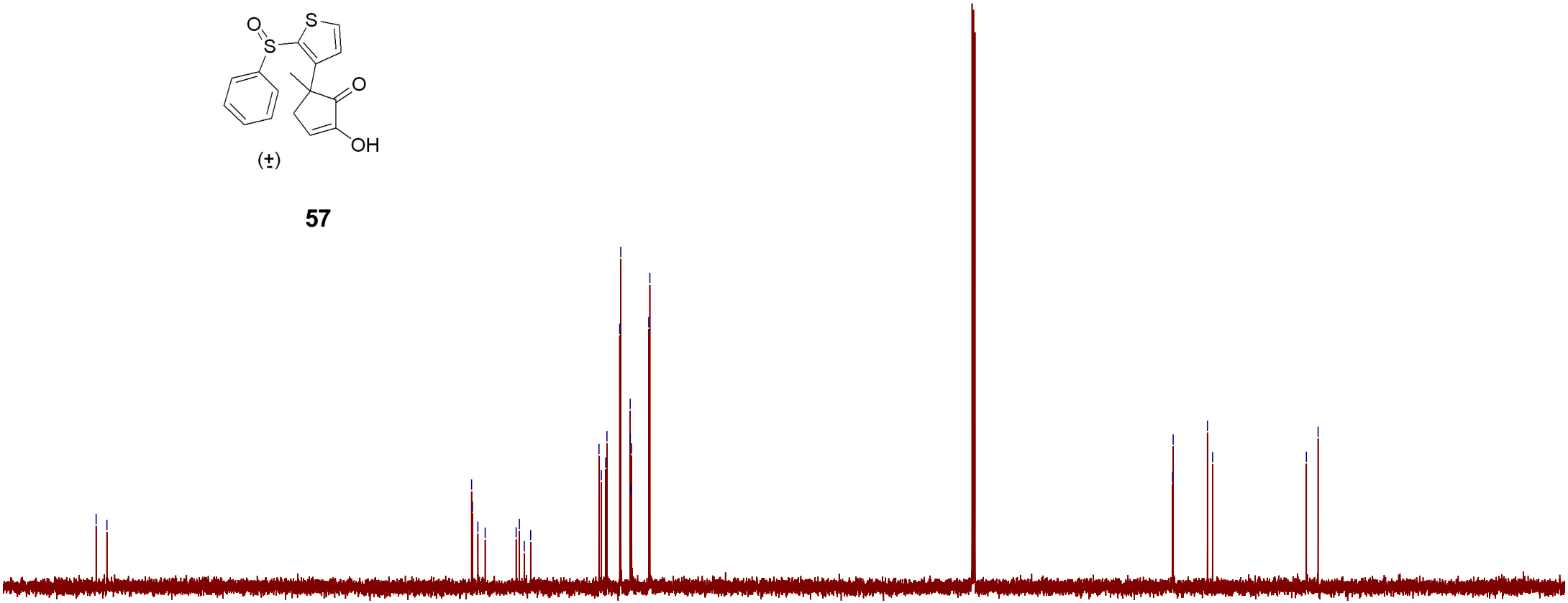
**57**

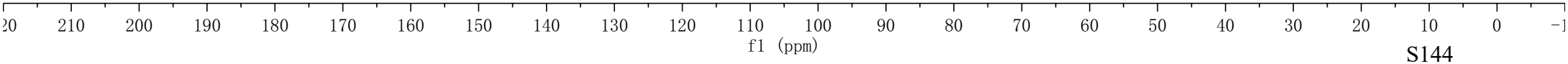
206.33
204.75
151.04
150.91
150.11
149.03
144.47
144.00
143.28
142.33
132.27
131.93
131.27
131.10
129.22
129.06
127.67
127.66
127.59
127.46
124.94
124.78
47.79
47.70
42.65
41.89
28.08
26.35

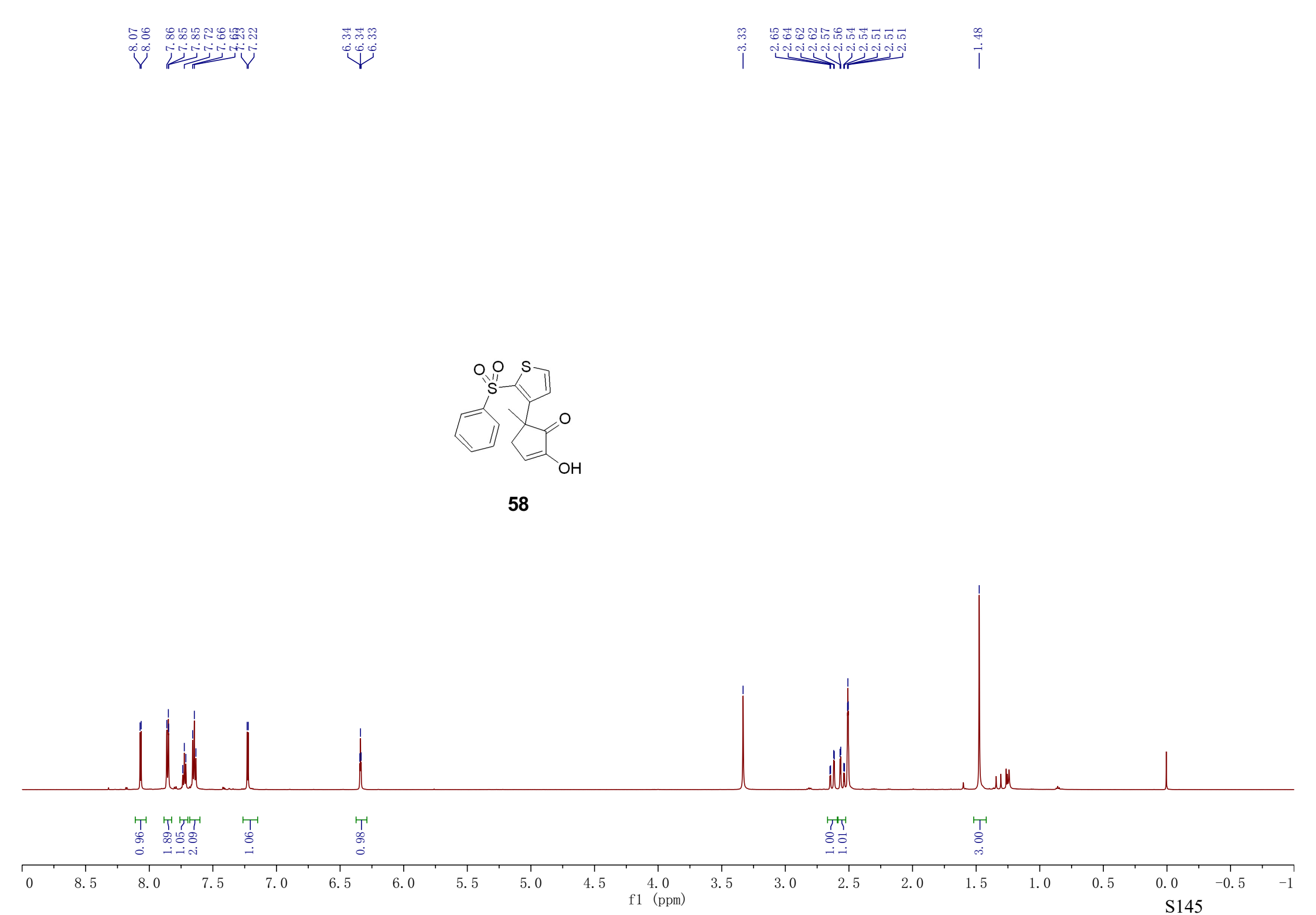


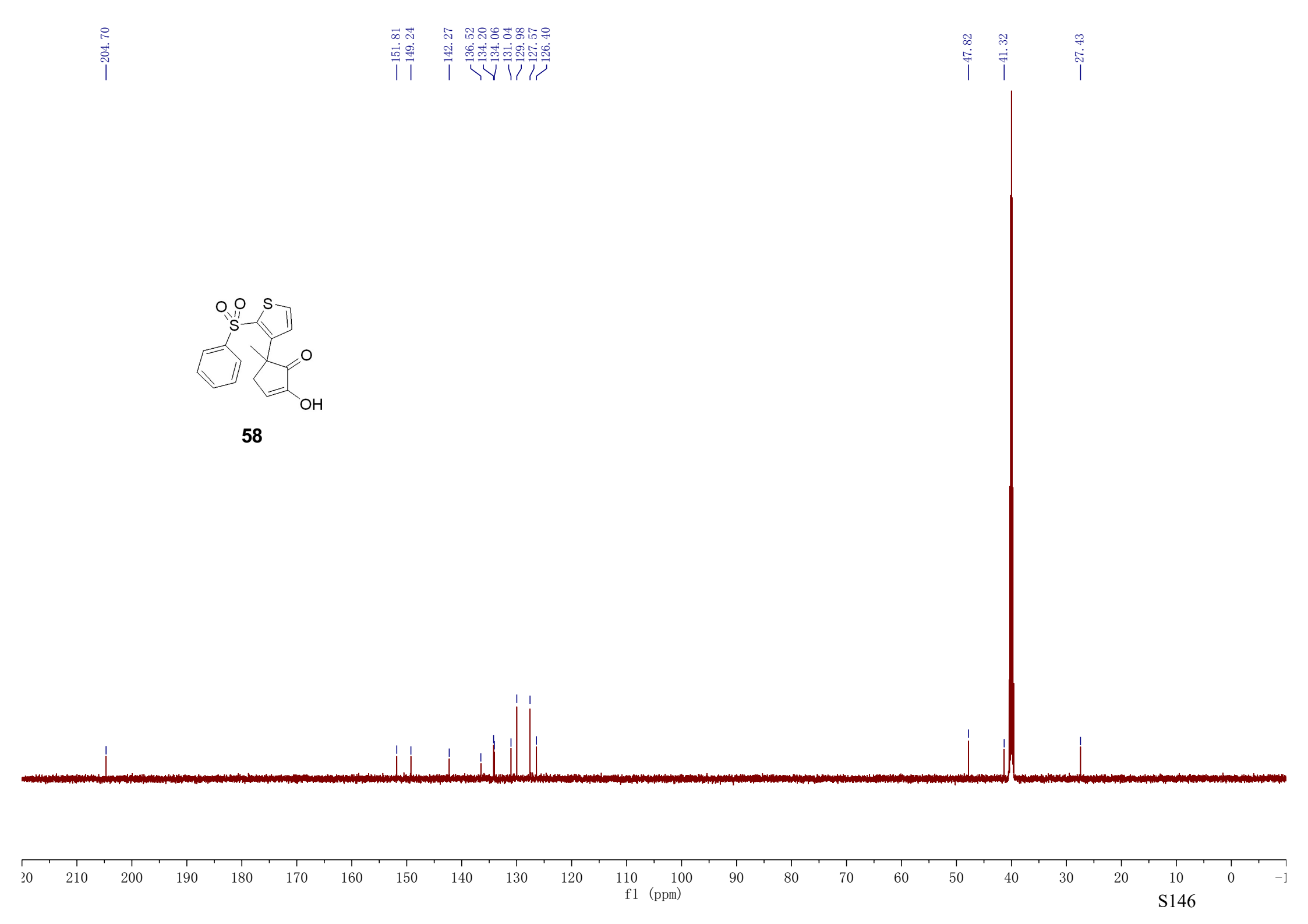

(±)

**57**






8.07
8.06
7.86
7.85
7.85
7.72
7.66
7.65
7.23
7.22
6.34
6.34
6.33
3.33
2.65
2.64
2.62
2.62
2.57
2.56
2.54
2.54
2.51
2.51
2.51
1.48
O
O
S
S
O
OH
58
0.96
1.89
1.05
2.09
1.06
0.98
1.00
1.01
3.00
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


204.70
151.81
149.24
142.27
136.52
134.20
134.06
131.04
129.98
127.57
126.40
47.82
41.32
27.43
O
O
S
S
O
OH
58
f1 (ppm)