Supporting Information for:

Iodine-Mediated Thiolation of Phenol/Phenylamine Derivatives and Sodium Arylsulfinates in Neat Water

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General Information

^1H and ^{13}C NMR spectra were recorded on Bruker Ascend™ 400(400 MHz) using tetramethylsilane as an internal reference. NMR multiplicities are abbreviated as follows: s = singlet, d = doublet, m = multiplet, br = broad signal. Chemical shifts (δ) and coupling constants (J) were expressed in ppm and Hz, respectively.

1f-1g were prepared according to the literature procedure.[1] The rest of chemicals were purchased from the Sinopharm Chemical Reagent Co., Adamas, Aladdin and TCI used as received.

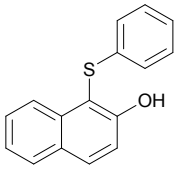
General Procedure for the Synthesis of the Desired Thioethers 3

Iodine (76.1 mg, 0.3 mmol) was added to a solution of 2-Naphthol **2** (0.3 mmol), sodium benzenesulfinates **1** (0.36 mmol) and triphenylphosphine(94.4 mg, 0.36 mmol) in H_2O (2 mL), and the reaction mixture was stirred under reflux conditions for 10 h. The reaction mixture was quenched by the addition of saturated sodium thiosulfate solution. Further stirring was followed by extraction with EtOAc (3×20 mL). The combined organic extracts were dried ($MgSO_4$), filtered, and concentrated (aspirator). The residue was purified by column chromatography using ethyl acetate / petroleum ether as eluent to afford the corresponding product **3**.

General Procedure for the Synthesis of the Desired Thioethers 5

Iodine (76.1 mg, 0.3 mmol) was added to a solution of Phenol/Amine **4** (0.36 mmol), sodium benzenesulfinates 1 (0.3 mmol) and triphenylphosphine(94.4 mg, 0.36 mmol) in H_2O (2 mL), and the reaction mixture was stirred under reflux conditions for 8-12 h. The reaction mixture was quenched by the addition of saturated sodium thiosulfate solution. Further stirring was followed by extraction with EtOAc (3×20 mL). The combined organic extracts were dried ($MgSO_4$), filtered, and concentrated (aspirator). The residue was purified by column chromatography using ethyl acetate / petroleum ether as eluent to afford the corresponding product **5**.

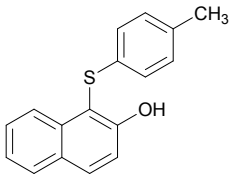
Analytical Data for the Products Shown in Tables 2 and 3



3a

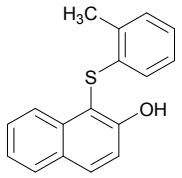
3a,[2] Yellow solid (62.0 mg, 82% yield). ^1H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, J = 8.0 Hz, 1H), 7.92 (d, J =

8.0 Hz, 1H), 7.83 (d, J = 4.0 Hz, 1H), 7.52−7.50 (m, 1H), 7.39−7.36 (m, 2H), 7.20 (s, 3H), 7.13−7.12 (m, 1H), 7.07−7.05 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.0, 135.5, 135.4, 132.8, 129.5, 129.2, 128.6, 127.9, 126.4, 125.9, 124. 7, 123.8, 116.9, 108.1.



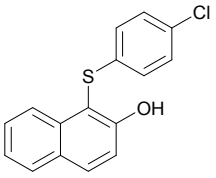
3b

3b,[2] Yellow solid (71.1 mg, 89% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, J = 8.0 Hz, 1H), 7.93−7.91 (d, J = 8.0 Hz, 1H), 7.84 (d, J = 8.0 Hz, 1H), 7.55−7.51 (m, 1H), 7.42−7.38 (m, 2H), 7.31 (s, 1H),7.01 (s, 4H), 2.27 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.9, 135.9, 135.5, 132.7, 131.8, 130.0, 129.5, 128.6, 127.9, 126.8, 124.7, 123.9, 116.9, 108.7, 20.9.



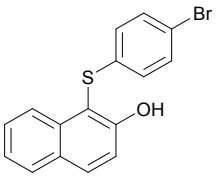
3c

3c,[2] Yellow solid (66.0 mg, 83% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, J = 12.0 Hz, 1H), 7.96 (d, J = 12.0 Hz, 1H), 7.86 (d, J = 8.0 Hz, 1H), 7.54−7.50 (m, 1H), 7.43−7.39 (m, 2H), 7.23 (d, J = 4.0 Hz, 1H), 7.15 (s, 1H), 7.07−7.03 (m, 1H), 6.91−6.88 (m, 1H), 6.45 (d, J = 8.0 Hz, 1H), 2.64 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.2, 135.6, 135.2, 134.4, 132.8, 130.4, 129.6, 128.7, 127.9, 126.8, 125.5, 124.8, 124.7, 123.9, 116.9, 107.4, 20.1.



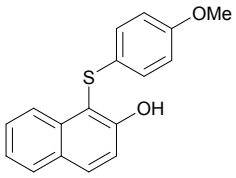
3d

3d,[2] Yellow solid (72.9 mg, 85% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, J = 8.0 Hz, 1H), 7.92 (d, J = 8.0 Hz, 1H), 7.82 (d, J = 8.0 Hz, 1H), 7.52−7.49 (m, 1H), 7.40−7.33 (m, 2H), 7.15−7.11 (m, 3H), 6.95−6.93 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.0, 135.2, 133.9, 133.1, 131.9, 129.5, 129.3, 128.6, 128.1, 127.6, 124.4, 124.0, 116.9, 107.6.



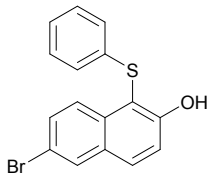
3e

3e, [2] Yellow solid (85.9 mg, 87% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14−8.12 (d, J = 8.0 Hz, 1H), 7.92 (d, J = 12.0 Hz, 1H), 7.80 (d, J = 8.0 Hz, 1H), 7.50−7.46 (m, 1H), 7.38−7.31 (m, 2H), 7.28−7.24 (m, 2H), 7.08 (s, 1H), 6.86 (d, J = 4.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.0, 135.1, 134.6, 133.1, 132.1, 129.5, 128.6, 128.1, 127.9, 124.4, 124.0, 119.6, 116.9, 107.4.



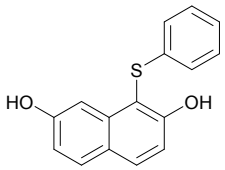
3f

3f, [2] Yellow solid (68.5 mg, 81% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, J = 12.0 Hz, 1H), 7.92 (d, J = 8.0 Hz, 1H), 7.84 (d, J = 8.0 Hz, 1H), 7.55−7.51 (m, 1H), 7.42−7.38 (m, 3H), 7.31 (d, J = 4Hz, 2H), 7.01 (d, 2H), 2.27 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.5, 156,7, 135.4, 132.5, 129.5, 128.8, 128.5, 127.8, 125.9, 124.7, 123.7, 116.8, 114.9, 109.9, 55.3..



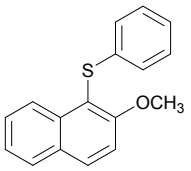
3h

3h, [2] White solid (94.0 mg, 91% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, J = 12 Hz, 1H), 7.94 (d, J = 12.0 Hz, 1H), 7.78 (d, J = 8.0 Hz, 1H), 7.54−7.51 (m, 1H), 7.33 (d, J = 8.0 Hz, 1H), 7.20-7.14 (m, 4H), 6.99 (d, J = 8.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.3, 135.2, 134.1, 131.7, 131.1, 131.0,130.4, 129.3, 126.6, 126.4.0, 126.1, 118.0, 117.6, 109.2, 20.9.



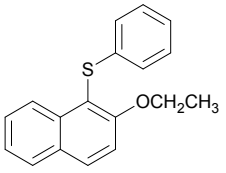
3i

3i, [2] white solid (71.0 mg, 88% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84-7.81 (m, 1H), 7.73−7.70 (m, 1H), 7.51 (s, 1H), 7.18−7.10 (m, 4H), 7.00 (m, 3H), 5.14 (s, 1H), 1.63(s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.7, 155.6, 137.3, 135.2, 132.7, 132. 7, 130.7, 129.2, 126.1, 125.8, 115.3, 114.3, 107.2.



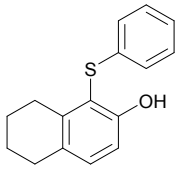
3j

3j, [2] Yellow oil (59.6 mg, 71% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49−8.47 (d, J = 8.0 Hz, 1H), 7.98 (d, J = 8.0 Hz, 1H), 7.83 (d, J = 8.0 Hz, 1H), 7.52−7.49 (m, 1H), 7.41−7.36 (m, 2H), 7.15−7.02(m, 4H), 3.98 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.3,136.3,132.1,129.6,128.7,128.3,127.8,126.3,125.5,124.8,124.1,113.4,56.9,29.7.



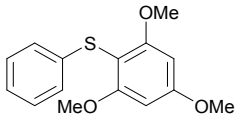
3k

3k, [2] colourless oil (66.2 mg, 73% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56−8.54 (d, J = 8.0 Hz, 1H), 7.95 (d, J = 8.0 Hz, 1H), 7.83 (d, J = 8.0 Hz, 1H), 7.58−7.52 (m, 1H), 7.43−7.40 (m, 1H), 7.36−7.32 (m, 1H),7.17−7.06 (m,4H), 4.23−4.18 (m, 2H), 1.35−1.31 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.6, 136.4, 135.2, 131.6, 129.5, 128.6, 128.2, 127.5, 126.8, 125.5, 124.8, 124.1, 114.9, 66.5, 14.8.



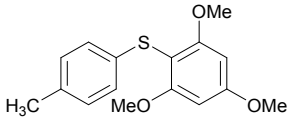
3l

3l, [2] Colourless oil (40.0 mg, 52% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24−7.21 (m, 3H), 7.14 (d, J = 4Hz,1H), 7.08 (d, J = 8 Hz,2H), 6.78 (s, 1H), 6.24 (s, 1H), 2.77-2.69 (m, 4H), 1.78 (s, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.9, 142.1, 137.0, 136.5, 130.2, 129.1, 126.5,125.8, 115.2, 112.9, 29.6,28.4, 23.2, 22.9.



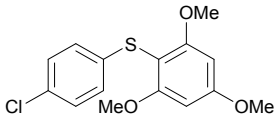
5aa

5aa,[3] white solid (66.3 mg, 80% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.15-7.14 (d, J = 4.0 Hz, 2H), 7.03 (d, J = 7 Hz, 3H), 3.86 (s, 3H), 3.78 (s, 6H) ; ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.9, 162.5 , 138.7, 128.5, 125.6, 124.3, 98.7, 91.2, 56.3, 55.4.



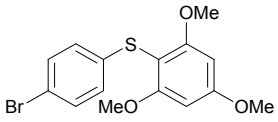
5ba

5ba, [3] white solid (123.4 mg, 86% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.95 (d, J = 2.0 Hz, 4H), 6.20 (s, 2H), 3.85 (s, 3H), 3.79 (s, 6H), 2.24 (s, 3H) ; ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.6, 162.3, 135.0, 134.1, 129.3, 125.9, 99.3, 91.2, 56.3, 55.4, 20.9 .



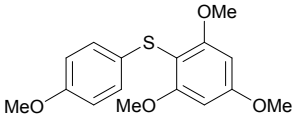
5ca

5ca, [3] white solid (76.3 mg, 82% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.10 (d, J = 8.0 Hz, 2H), 6.94 (d, J = 12 Hz, 2H), 6.20 (s, 2H), 3.86 (s, 3H), 3.80 (s, 6H) ; ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.1, 162.4, 137.7, 130.4, 128.5, 126.9, 110.3, 91.2, 56.2, 55.4.



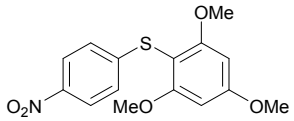
5da

5da, [3] white solid (85.0 mg, 80% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.24 (d, J = 8 Hz, 2H), 6.86 (d, J = 8 Hz, 2H), 6.19 (s, 2H), 3.85 (s, 3H), 3.79 (s, 6H) ; ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.0, 162.4, 138.1, 131.4, 127.2, 117.8, 98.0, 91.2, 56.3, 55.4.



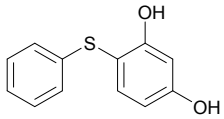
5ea

5ea,[4] white soild (75.3 mg, 82% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.06 (d, J = 4 Hz, 2H), 6.72 (d, J = 8.0 Hz, 2H), 6.18 (s,2H), 3.83(s, 3H)，3.80 (s,6H), 3.72 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.6, 152.3, 157.5, 129.2, 128.6, 114.2, 91.2, 56.3, 55.4, 55.3.



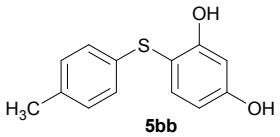
5fa

5fa,[4] yellow solid (75.1 mg, 78% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98 (d, J = 8.0 Hz, 2H), 7.03 (d, J = 8.0 Hz, 2H), 6.22(s, 2H), 3.87(s, 3H), 3.79(s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.4, 152.4, 149.5, 144.6, 124.8, 123.7, 95.9, 91.3, 56.3, 55.5.



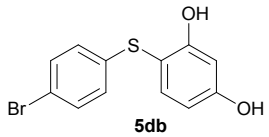
5ab

5ab,[3] gray solid (58.9 mg, 90% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40 (d, J = 8 Hz, 1H), 7.25-7.21 (m, 2H), 7.15–7.11 (m, 1H), 7.05 (d, J = 1.0, 8 Hz, 2H), 6.59 (d, J = 8 Hz, 2 H), 6.47 (d, J = 8 Hz, 1H) 5.37(s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.5, 158.5, 138.2, 136.7, 129.1, 126.2, 125.9, 109.3, 107.1, 102.5.



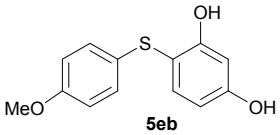
5bb

5bb,[3] brown solid (64.1 mg, 92% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39 (d, J = 8 Hz, 1H), 7.04 (d, J = 8.0 Hz, 2H), 6.97 (d, J = 8.0 Hz, 2H), 6.63 (s, 1H), 6.56 (d, J = 2.5 Hz, 1H), 6.45 (m, 1H), 5.48 (s, 1H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.1 , 158.4, 138.1, 136.0, 133.0, 130.0, 126.7, 109.3, 108.1, 102.5, 20.9 .



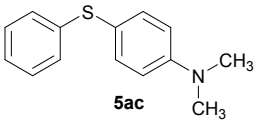
5db

5db, [3] brown solid (78.1 mg, 88% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38-7.25 (m, 3H), 6.89 (d, J = 4.0 Hz, 2H), 6.57 (s, 1H), 6.48 (d, J = 8 Hz, 2H), 5.49 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.6, 158.5, 138.2, 135.8, 132.1, 127.7, 119.6, 109.5, 106.6, 102.6 .



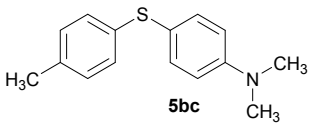
5eb

5eb, white soild (64.7 mg, 87% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38-7.25 (m, 3H), 6.89 (d, J = 4 Hz, 2H), 6.57 (s, 1H), 6.48 (d, J = 8 Hz, 2H), 5.49 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): 158.9, 158.3, 137.7, 129.4, 128.9,127.1, 114.9, 109.0, 102.3, 55.4.



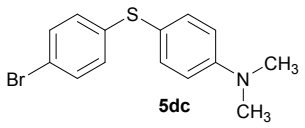
5ac

5ac,[3] yellow solid (57.0 mg, 83% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40 (d, J=4Hz, 2H), 7.21 (d,J=8 Hz, 2H), 7.10 (d, J= 4 Hz, 3H), 6.71 (d, J= 4Hz, 2H), 3.00 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.5, 139.9, 136.1, 128.7, 126.8, 124.9, 117.1, 112.9, 40.3 .



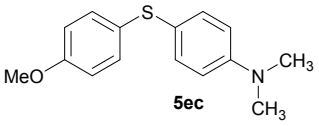
5bc

5bc, [3] yellow solid (72.9 mg, 87% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37-7.35 (m, 2H), 7.13 (d, J = 8.5 Hz, 2H), 7.04 (d, J = 4.0 Hz, 4H), 6.69 (m, 2H), 3.97 (s, 6H), 2.28 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.4, 138.1, 135.5, 129.5, 127.7, 118.5, 112.9, 40.2, 20.8.



5dc

5dc, [3] white solid (77.4 mg, 84% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.36 (d, J = 8.0 Hz, 2H), 7.29 (d, J = 8.0 Hz, 2H), 6.94 (d, J = 8.0 Hz, 2H), 6.69 (d, J = 8.0 Hz, 2H), 2.99 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.7, 139.9, 136.2, 131.6, 128.2, 118.4 , 117.9, 112.9 , 40.2.



5ec

5ec, yellow oil (63.7 mg, 82% yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.33 (d, J = 8.0 Hz, 2H), 7.21 (d, J = 8.0 Hz, 2H), 6.81 (d, J = 8.0 Hz, 2H), 6.68 (d, J = 8.0 Hz, 2H), 3.77(s,3H), 2.96 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): 158.3, 150.1, 134.3, 133.7, 132.7, 130.9, 114.6, 113.0, 55.3, 40.4.

References

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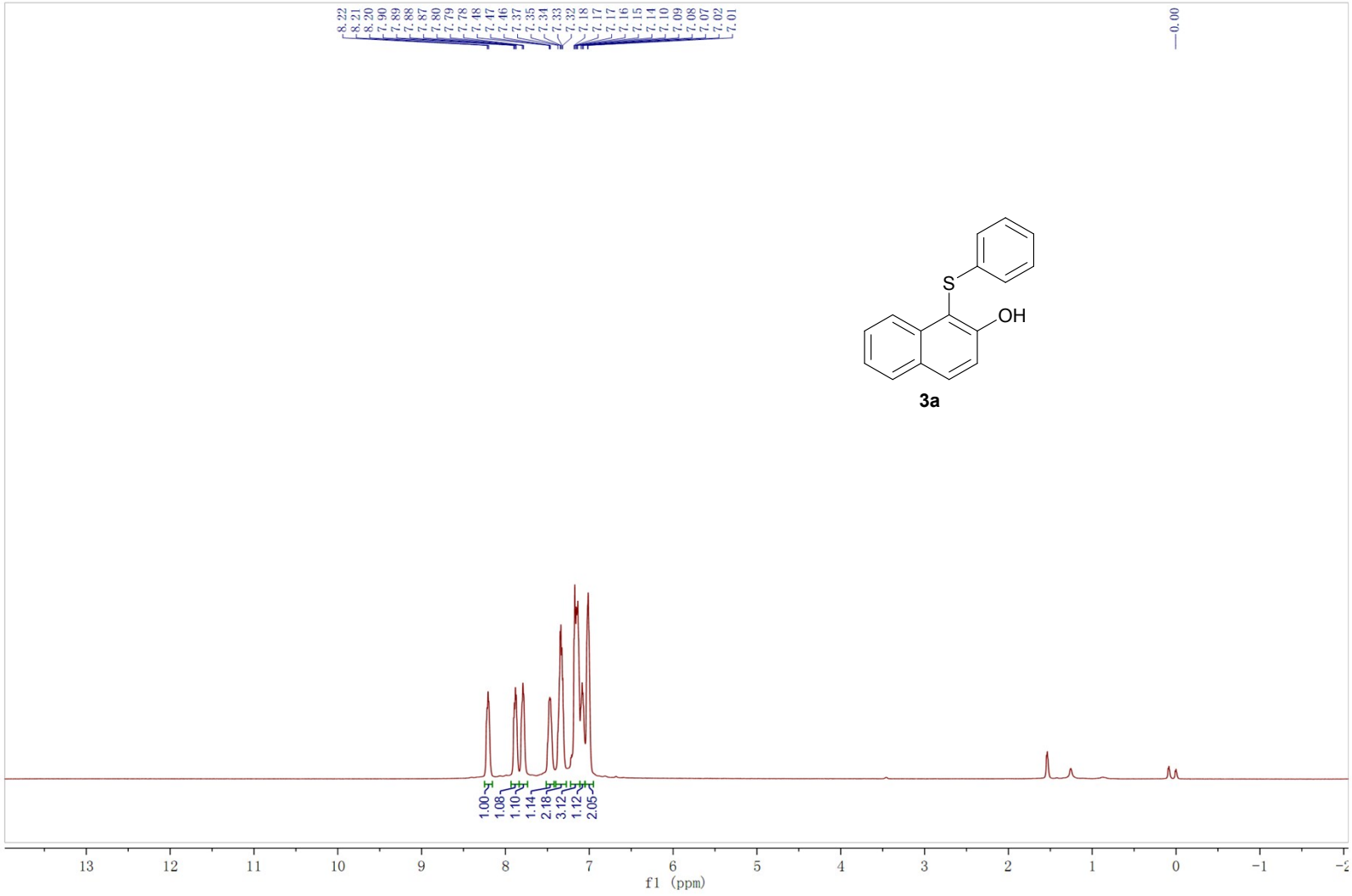
[2] X. Kang, R. Yan, G. Yu, X. Pang, X. Liu, X. Li, L. Xiang and G. Huang, *J. Org. Chem.*, 2014, **79**, 10605-10610.

[3] S. K. R. Parumala and R. K. Peddinti, *Green. Chem.*, 2015, **17**, 4068–4072**.**

[4] T. Hostier, V. Ferey, G. Ricci, D. Gomez Pardo and J. Cossy, *Org. lett.*, 2015, **17**, 3898-3901.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7.18
7.17
7.17
7.16
7.15
7.14
7.10
7.09
7.08
7.07
7.02
7.01
0.00
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3a
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1.14
2.18
3.12
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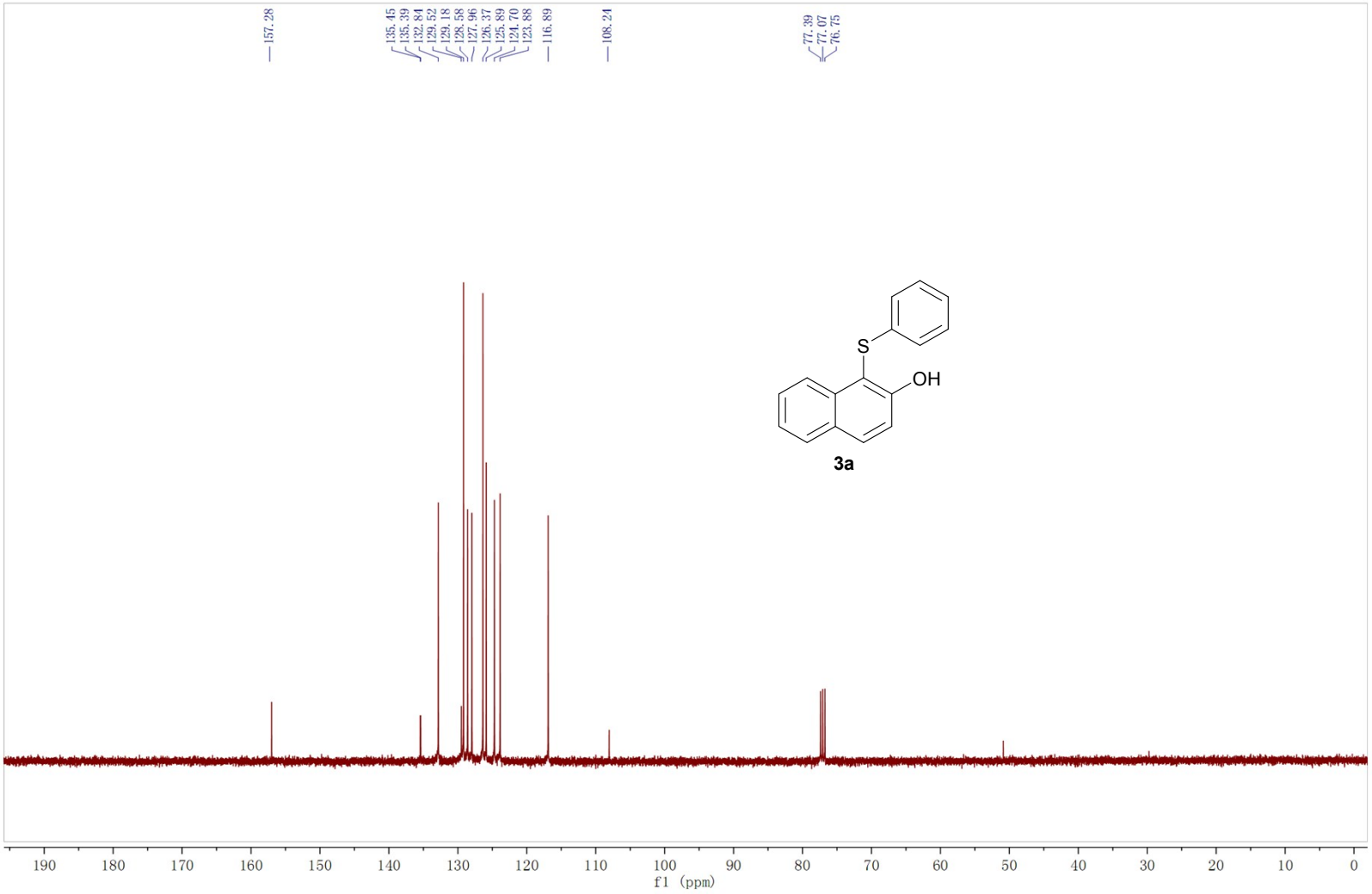
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76.75
S
OH
3a
190
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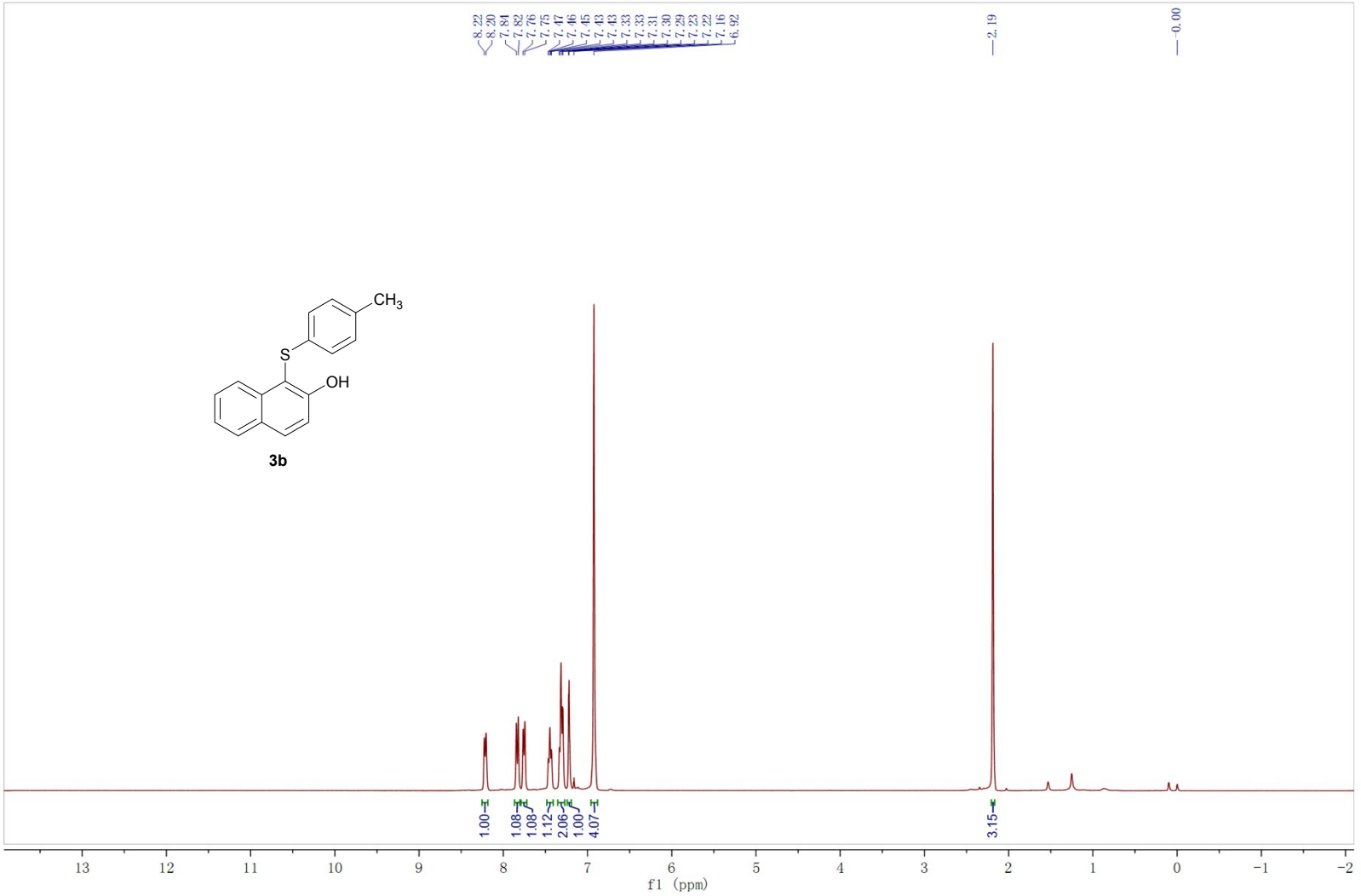
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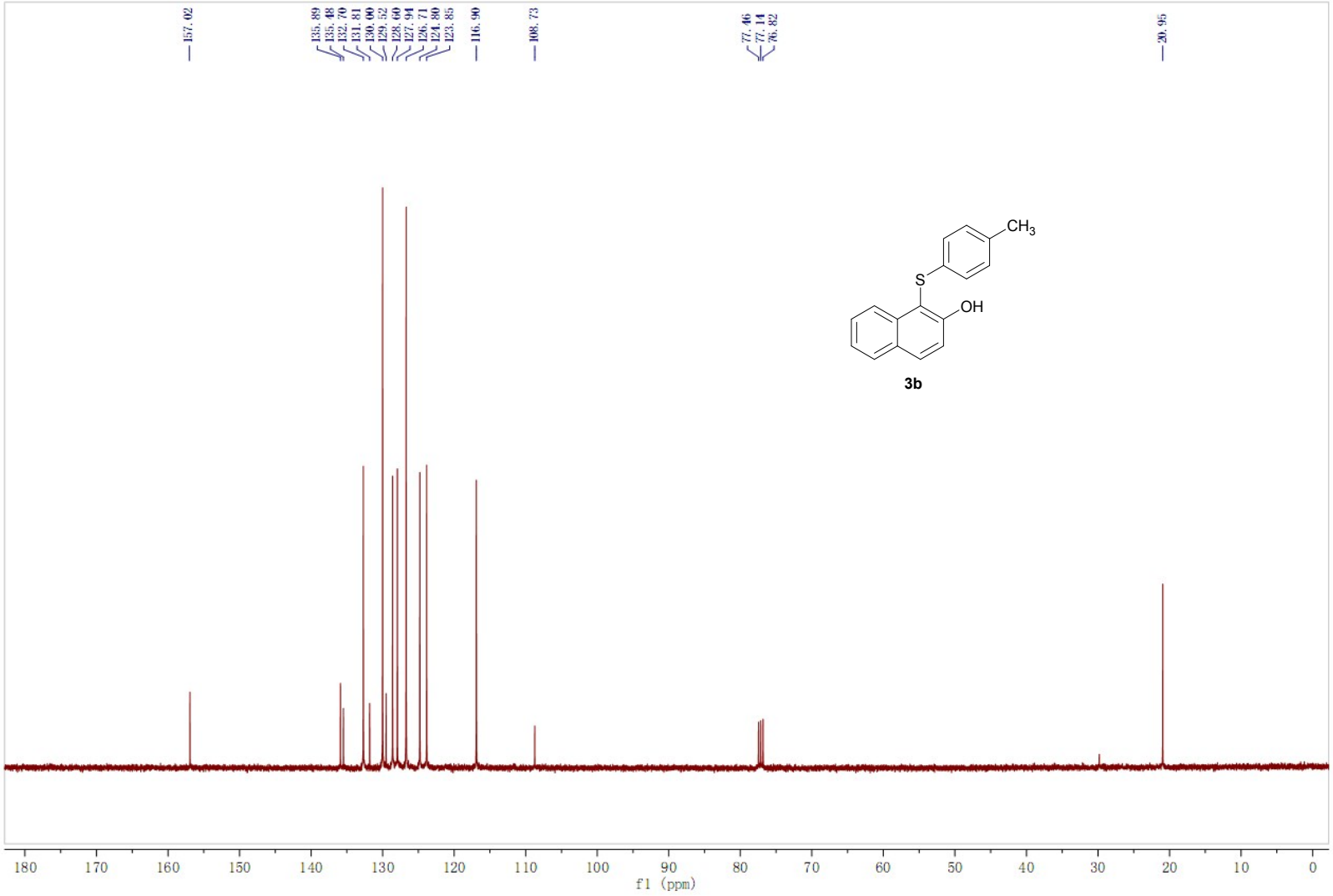
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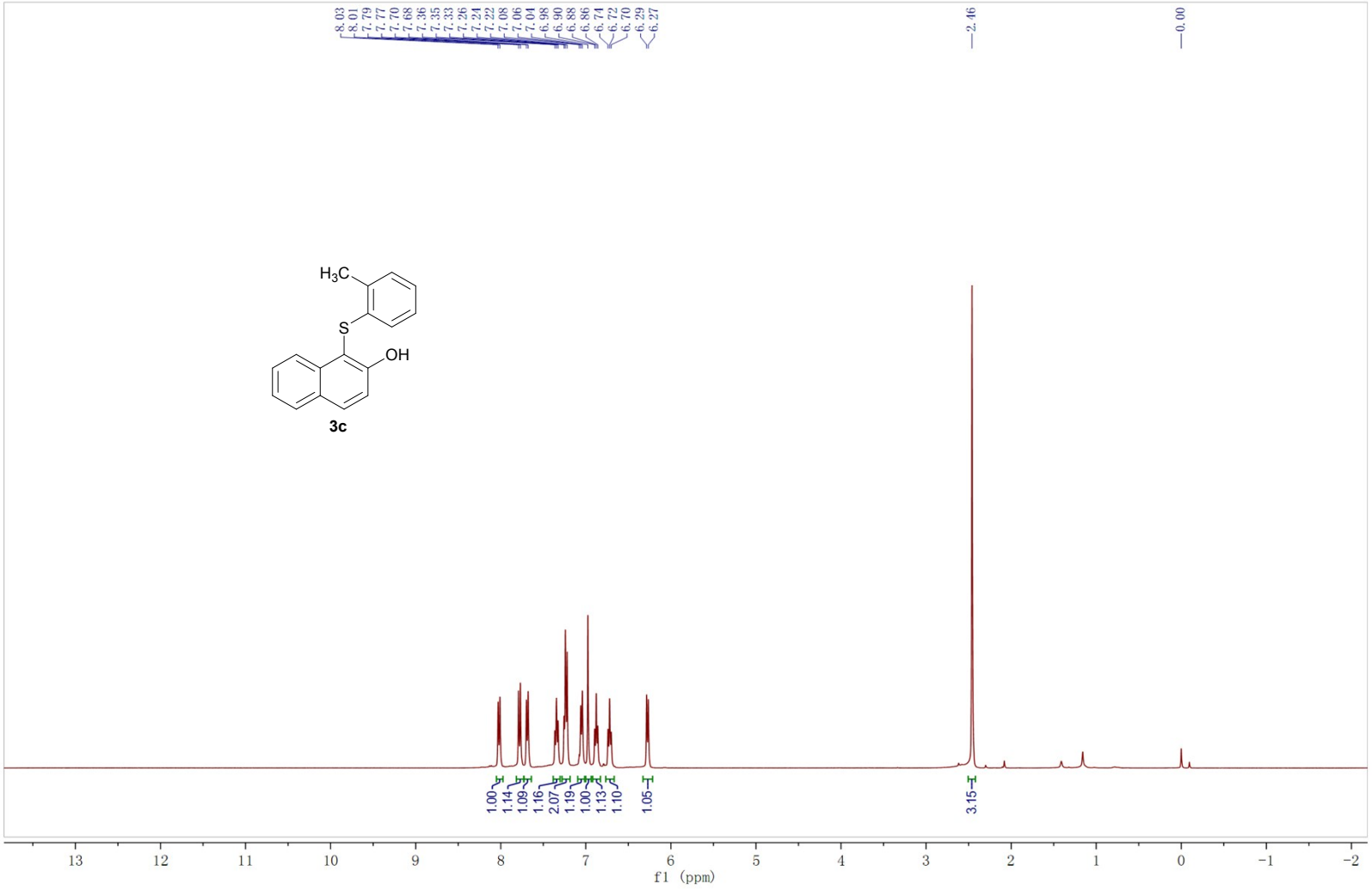
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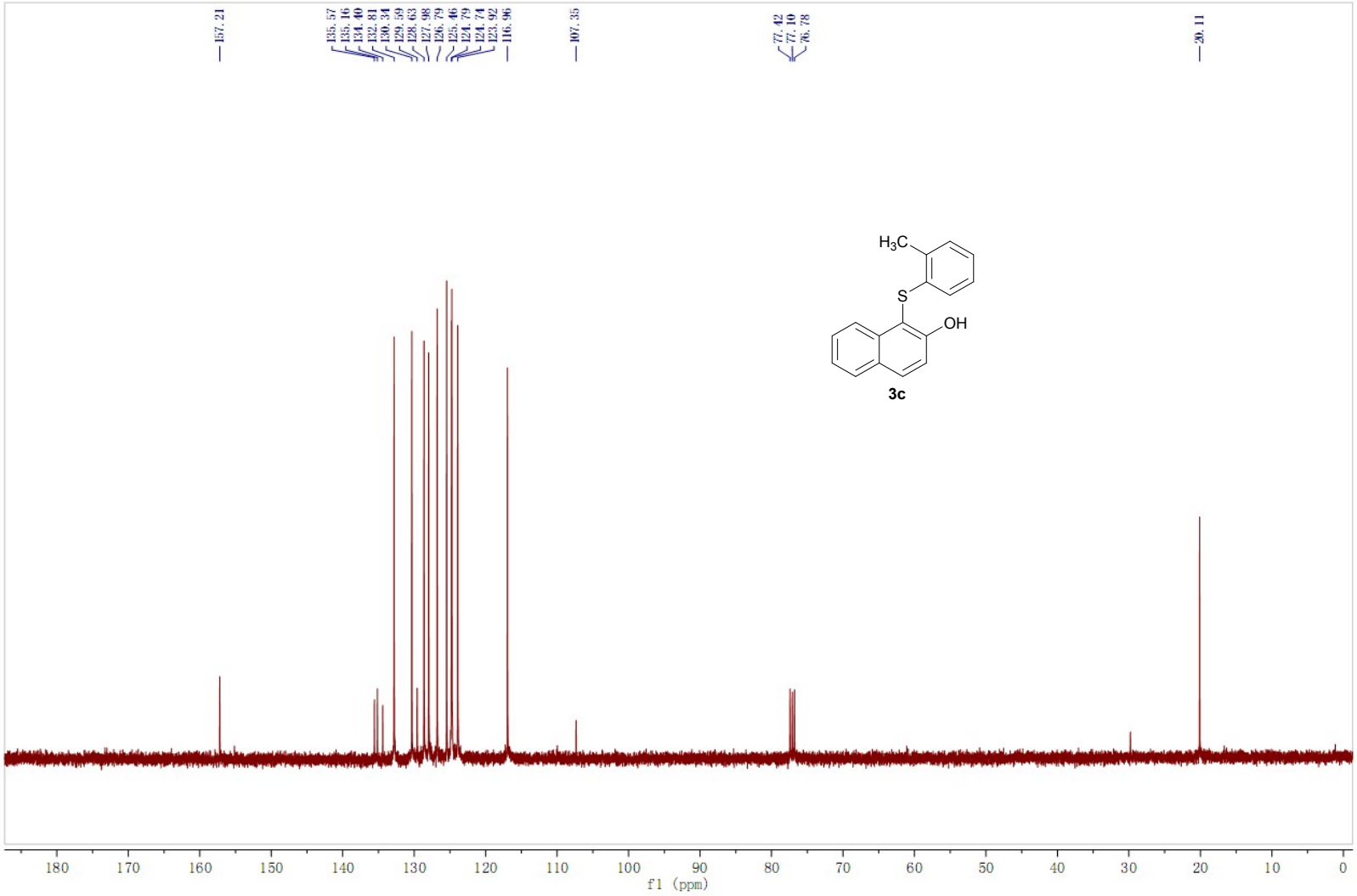
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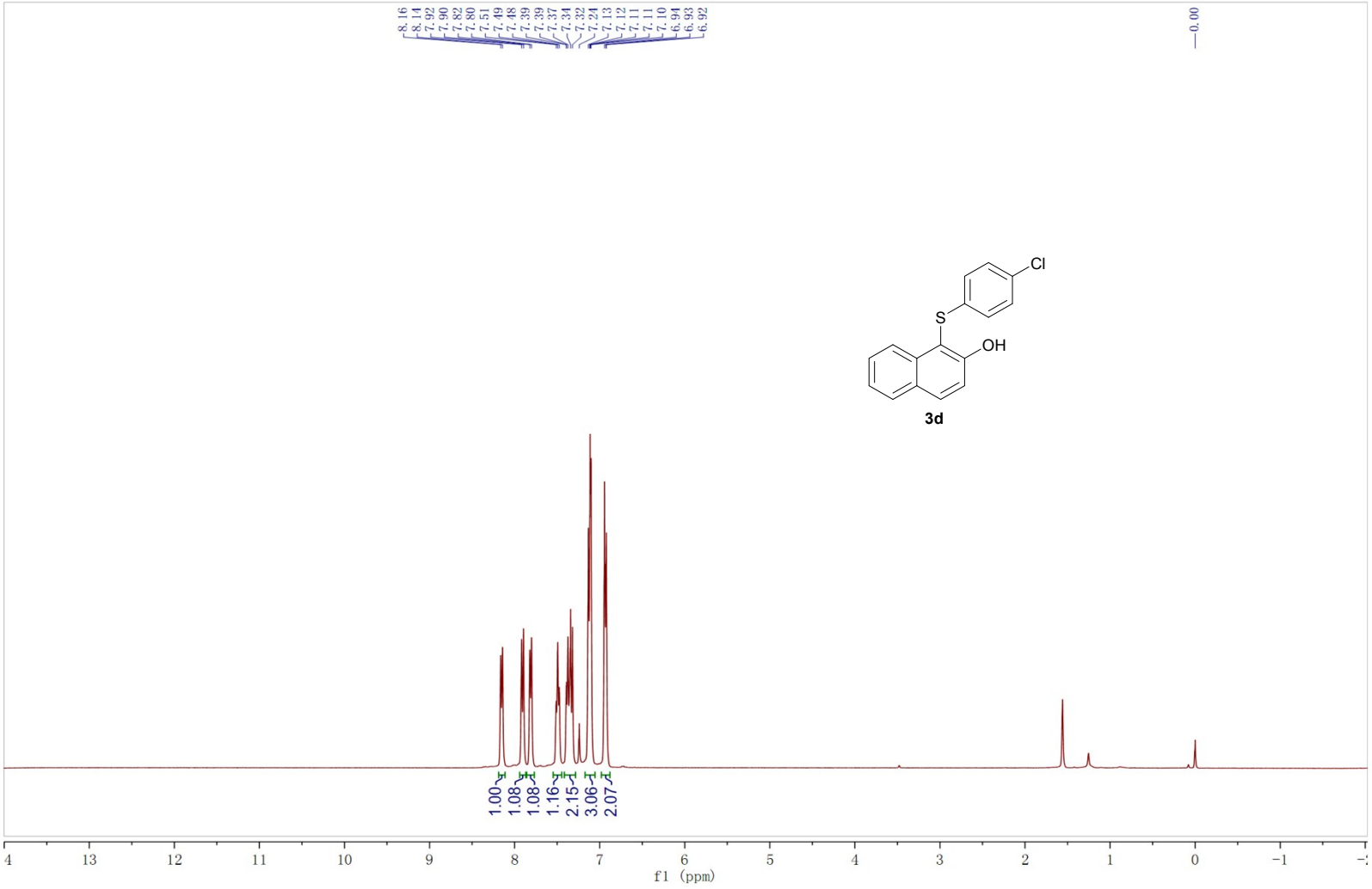
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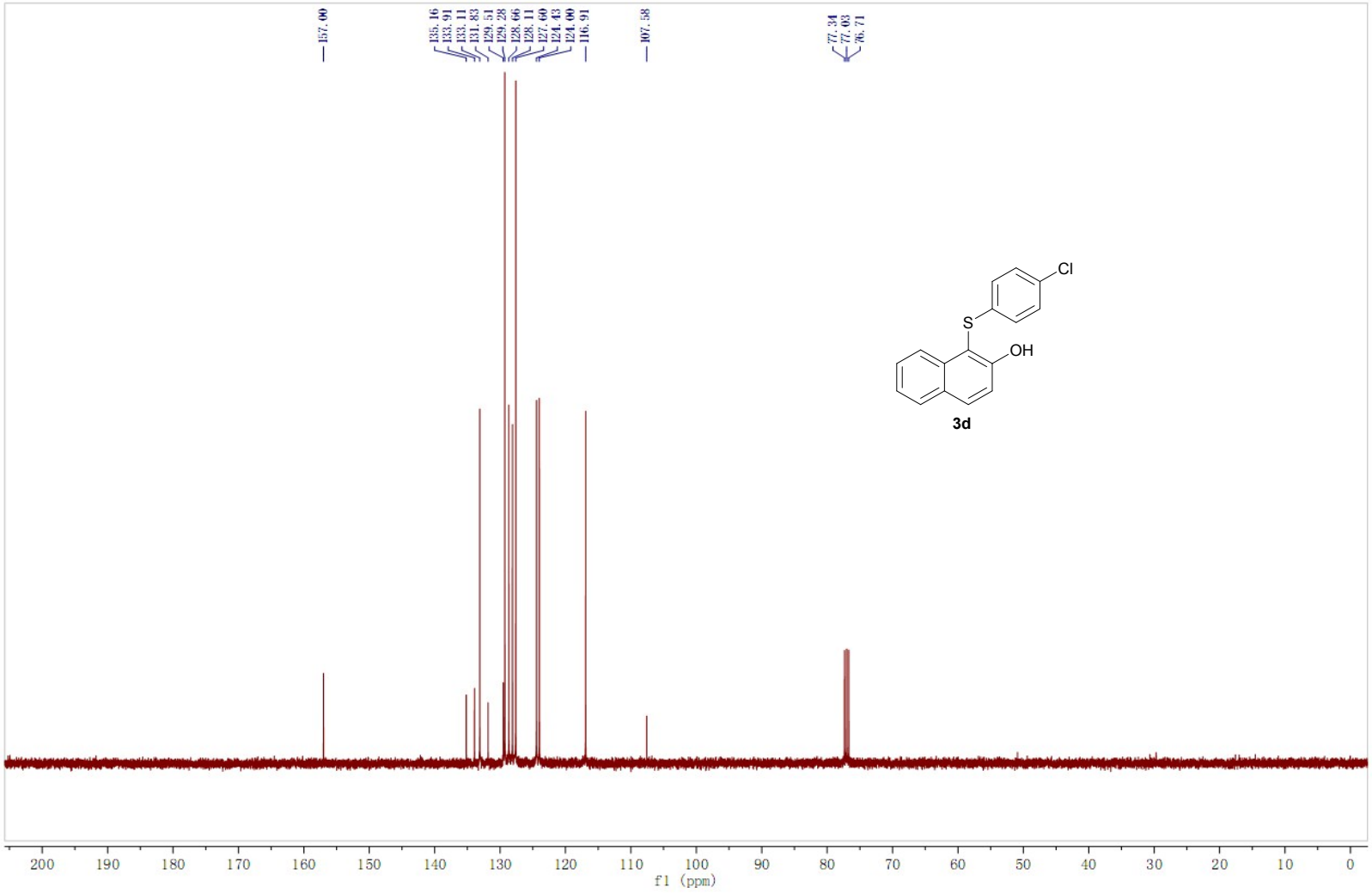
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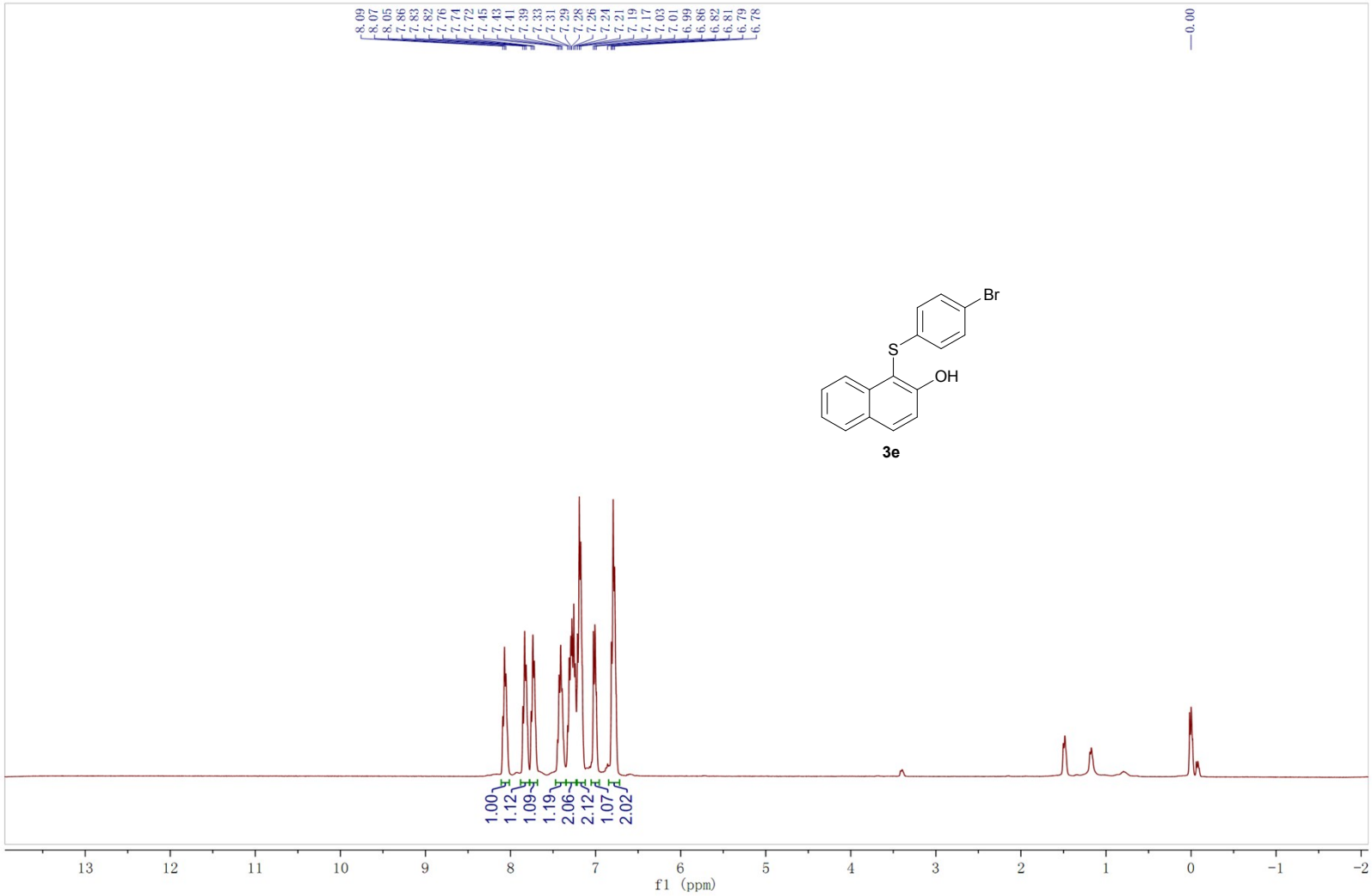
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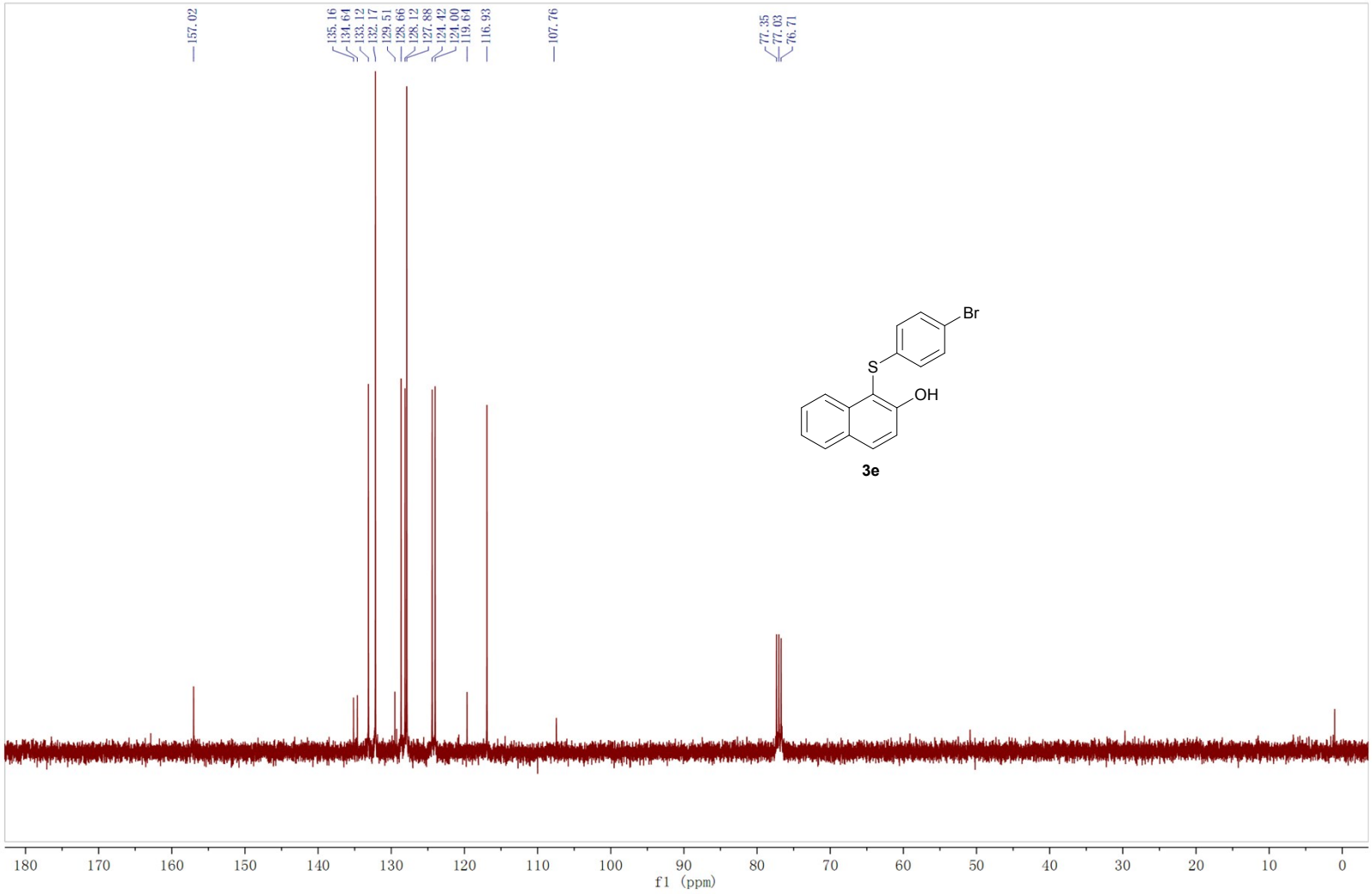
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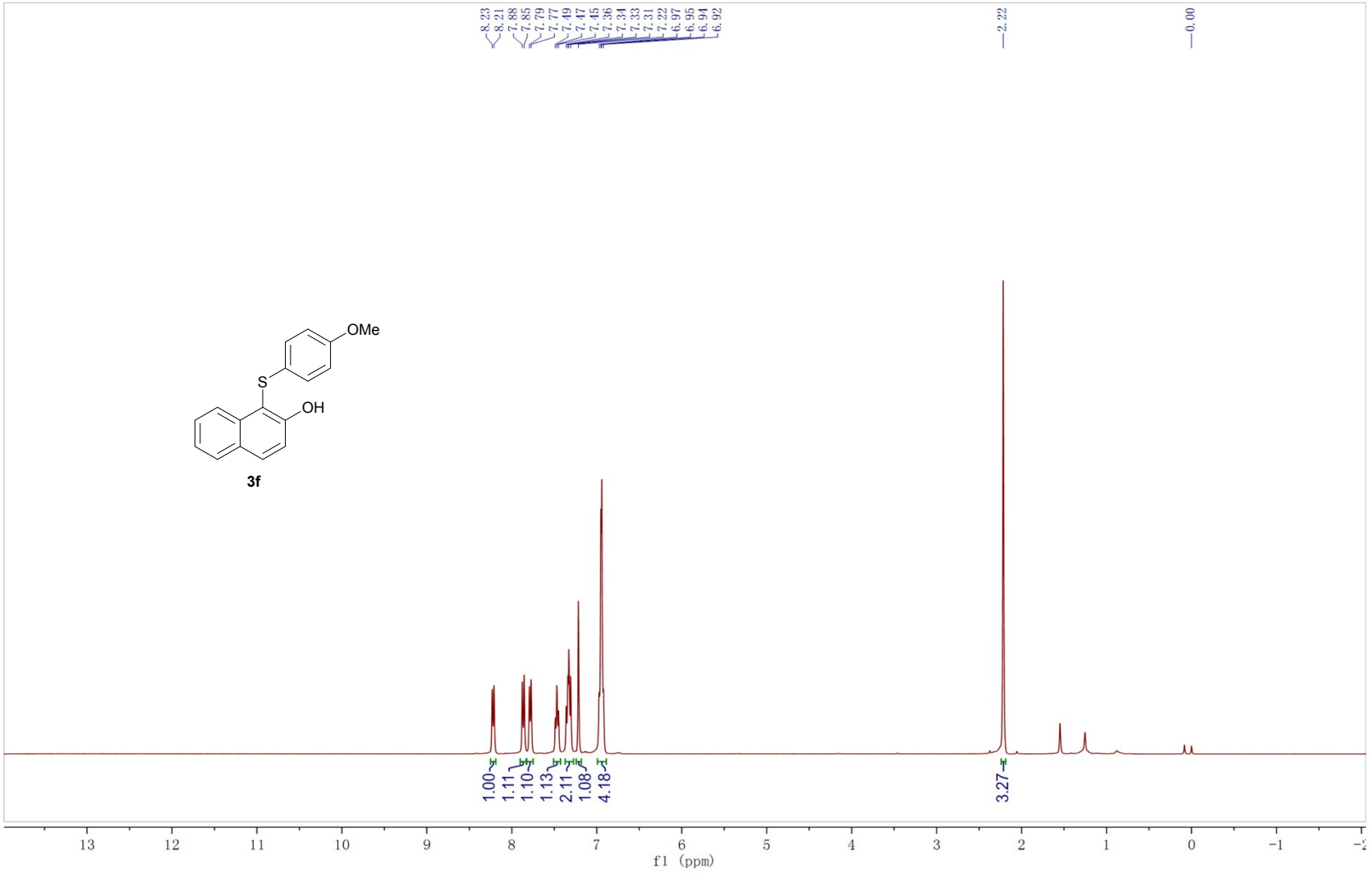
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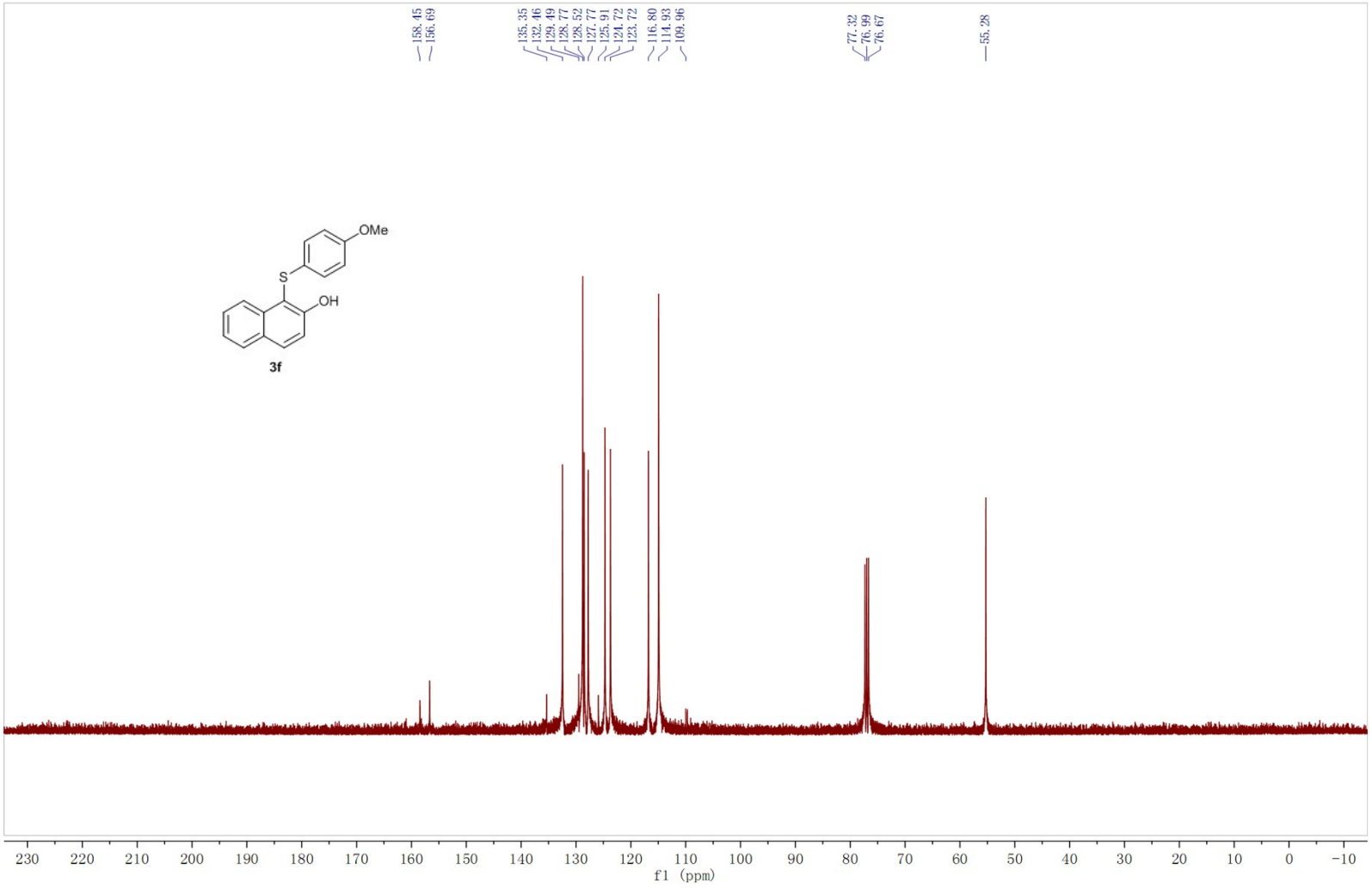
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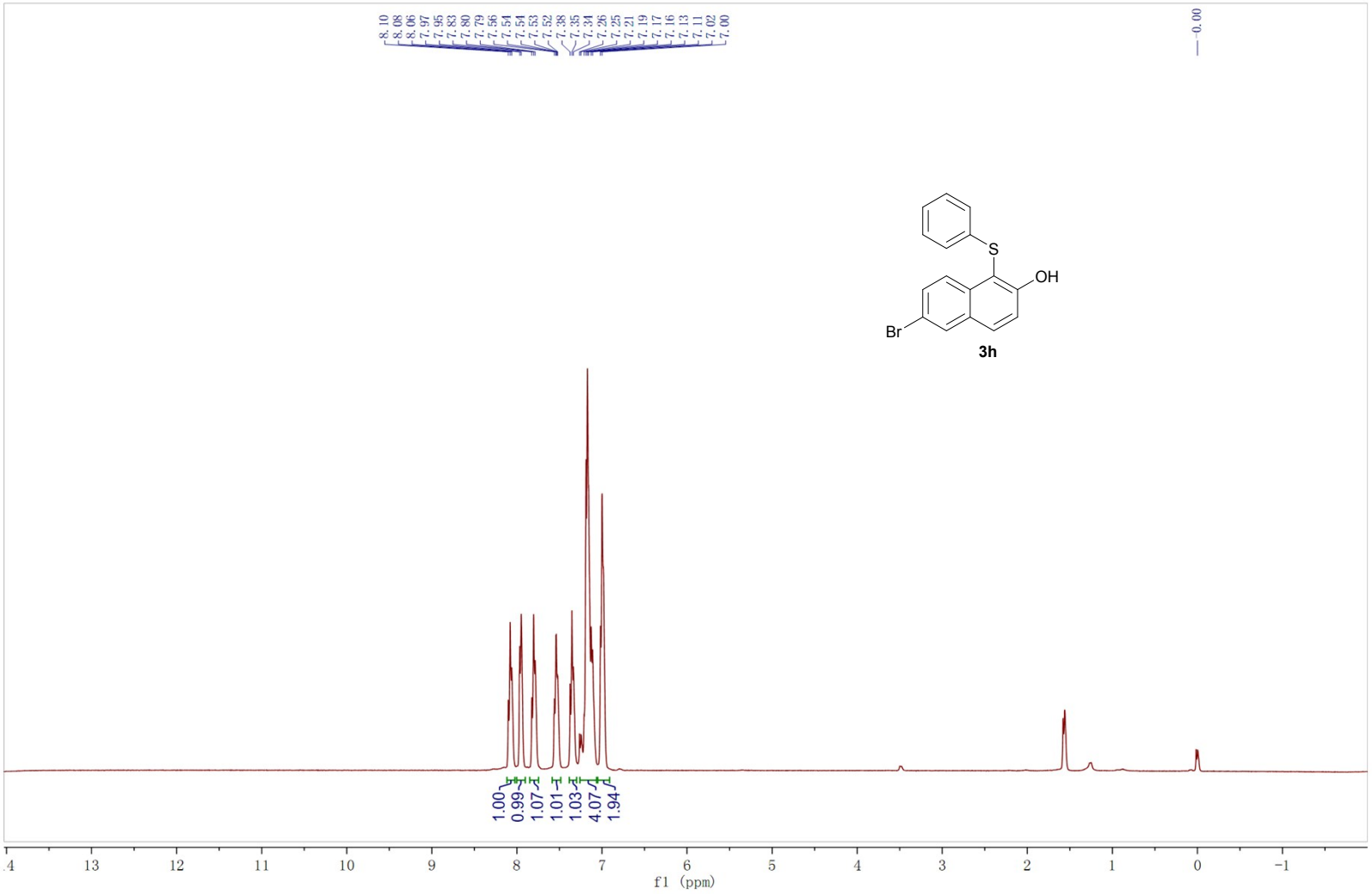
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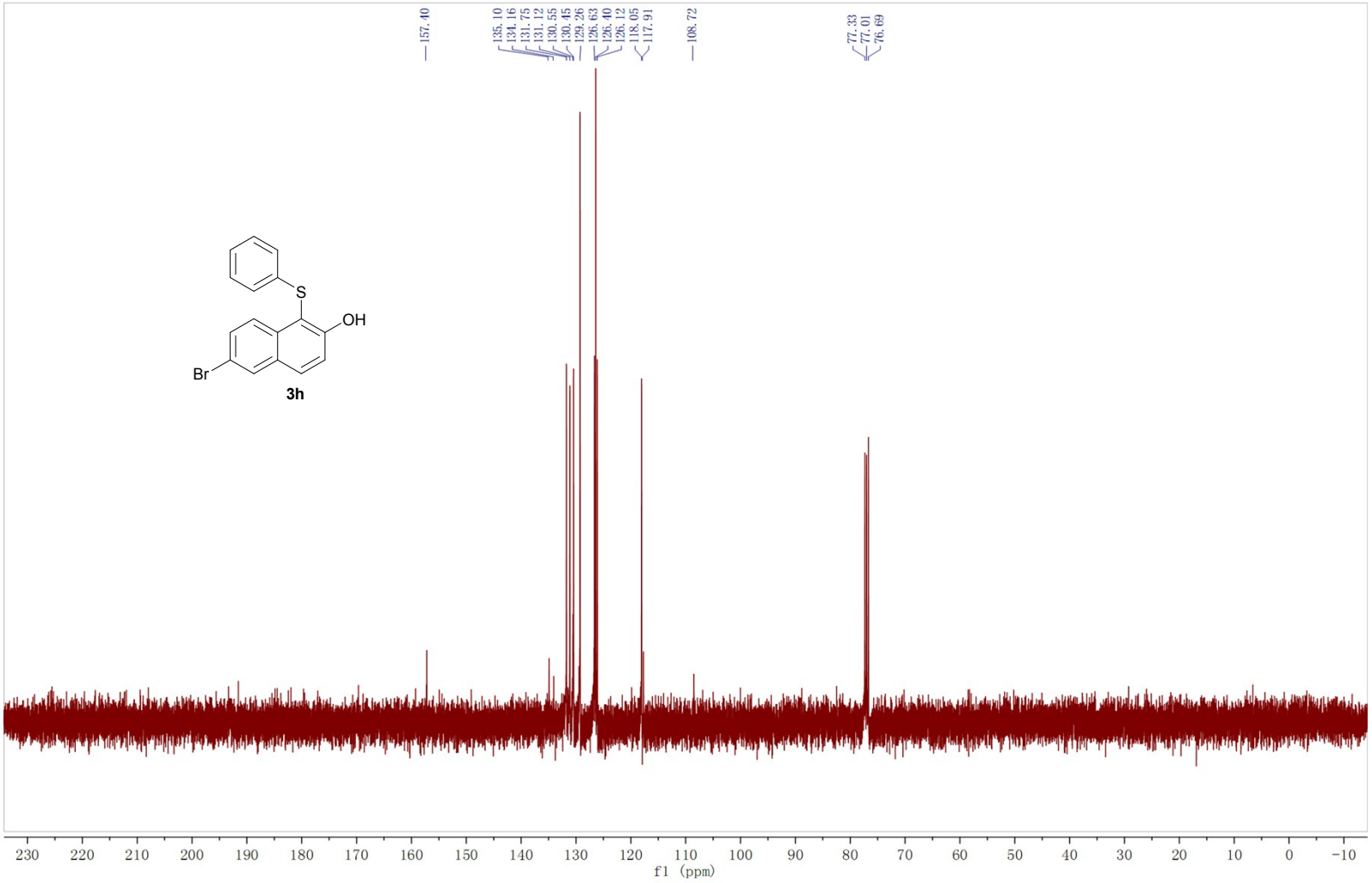
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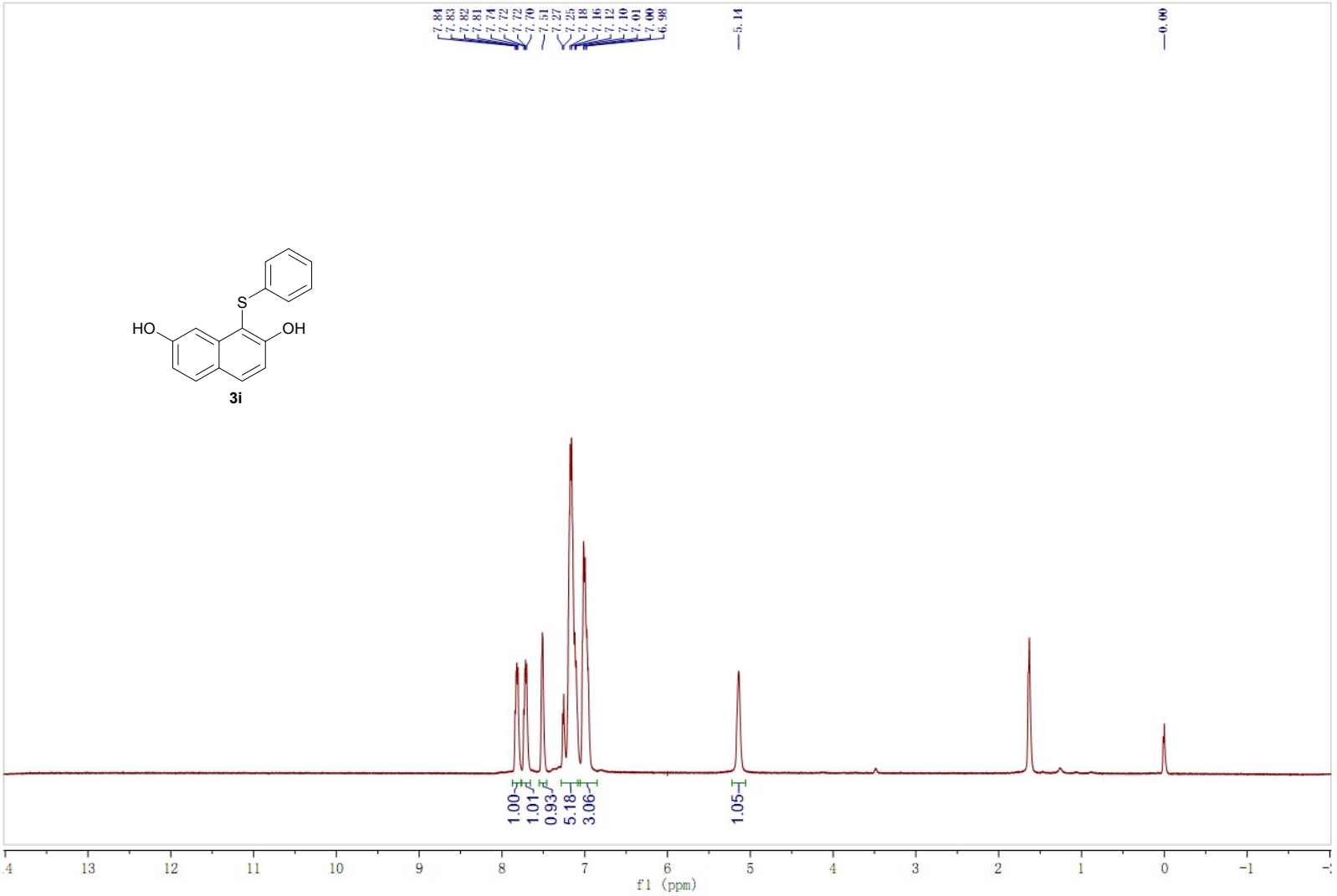
f1 (ppm)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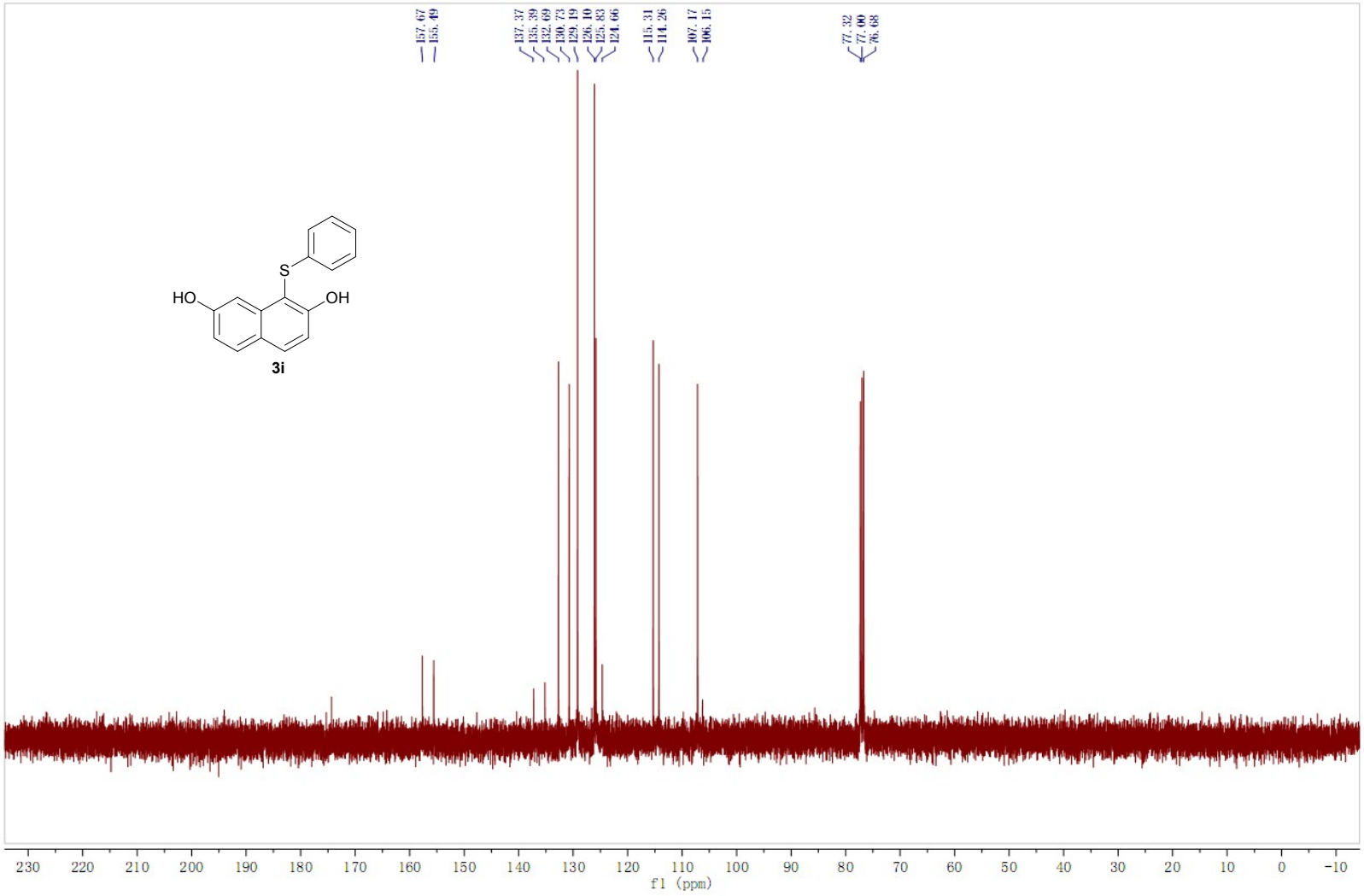
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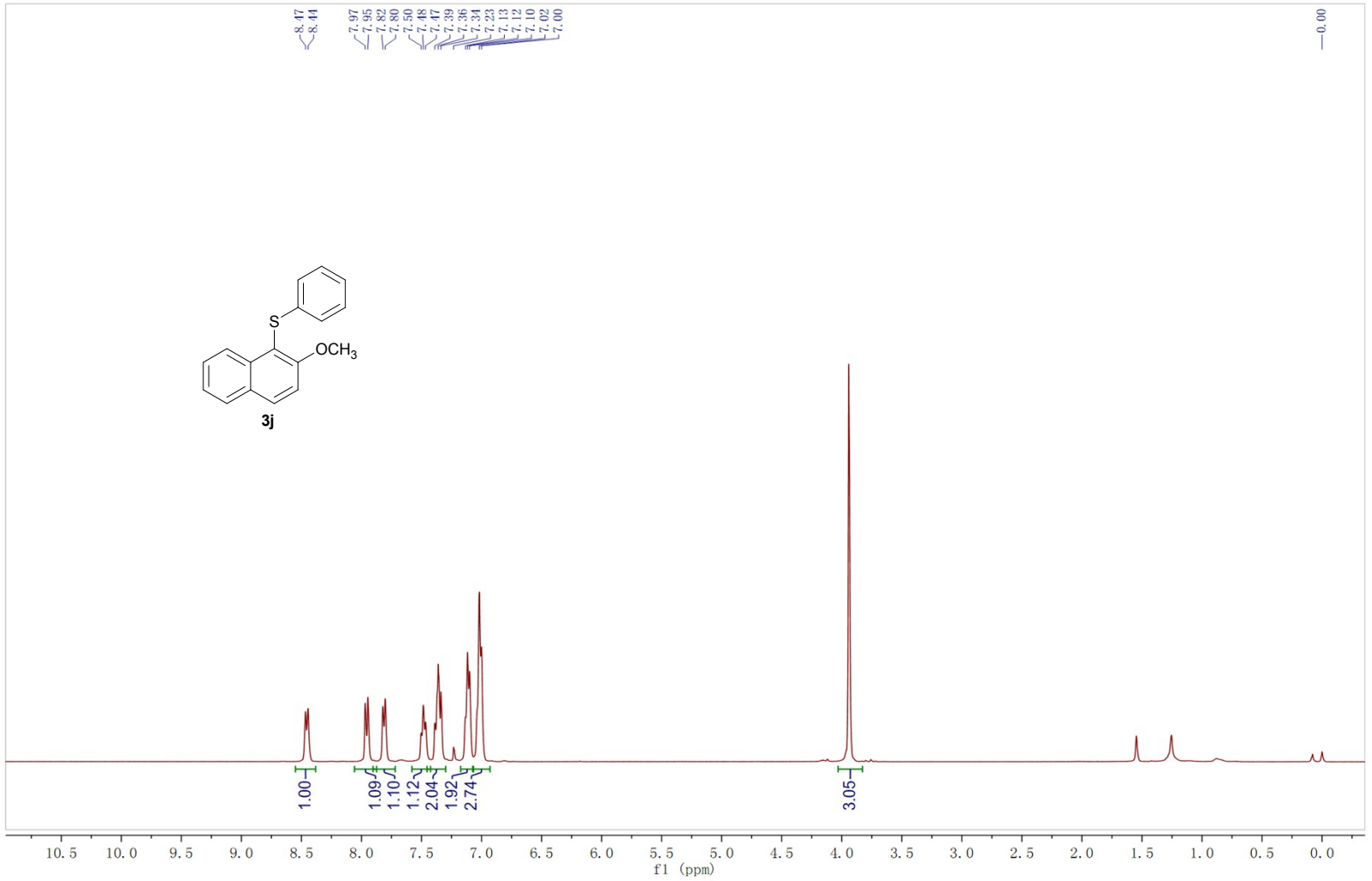
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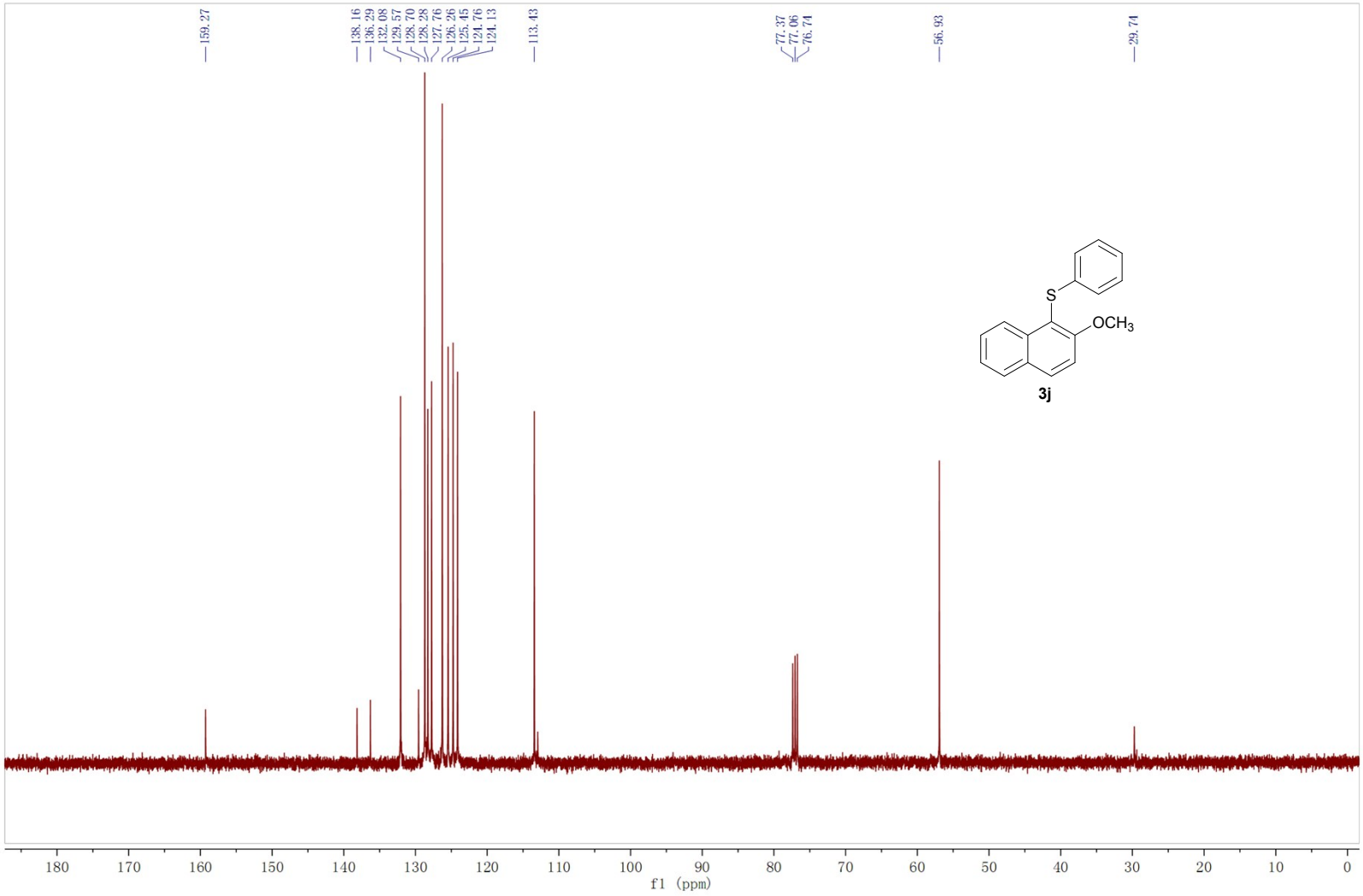
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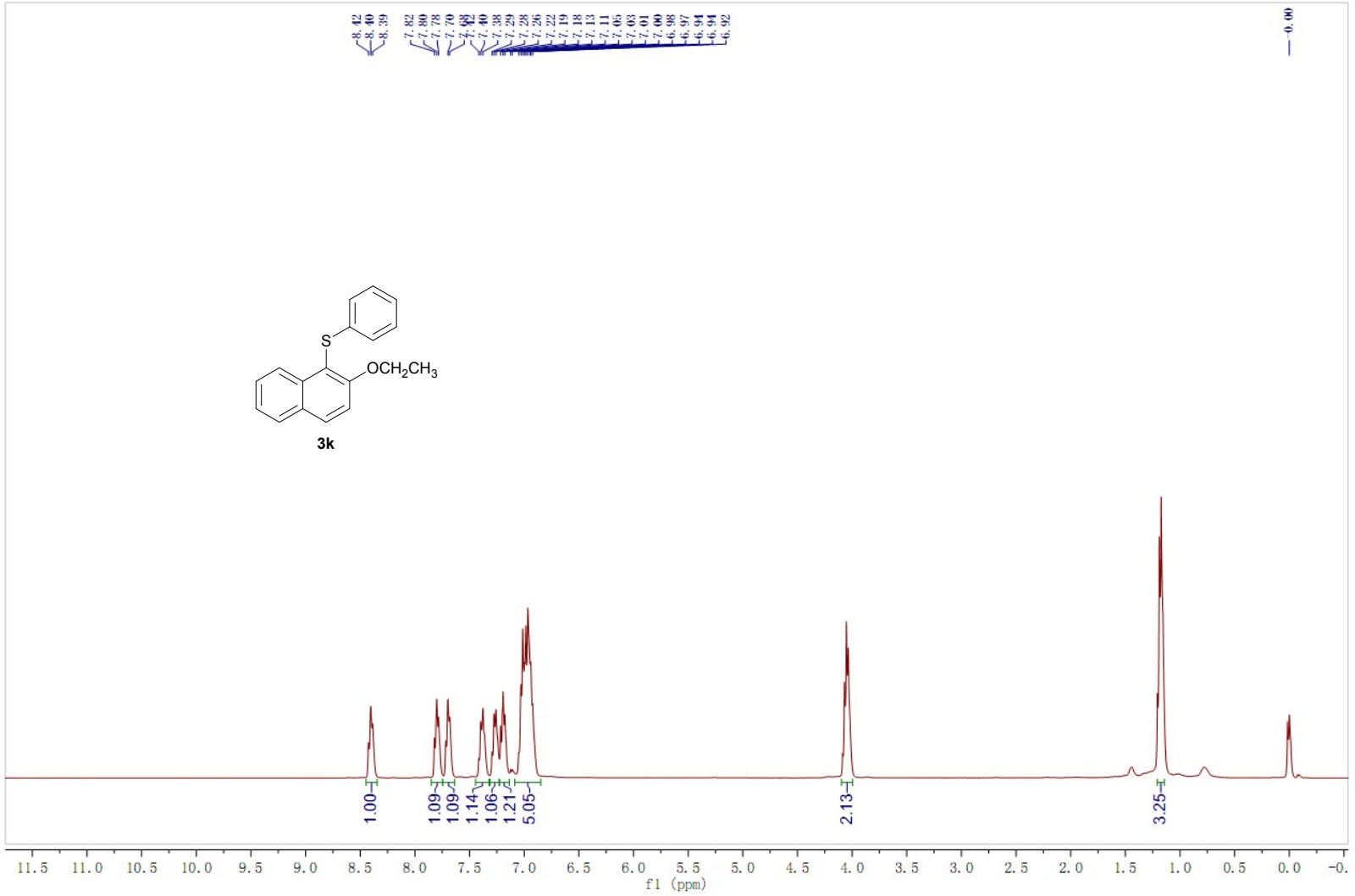
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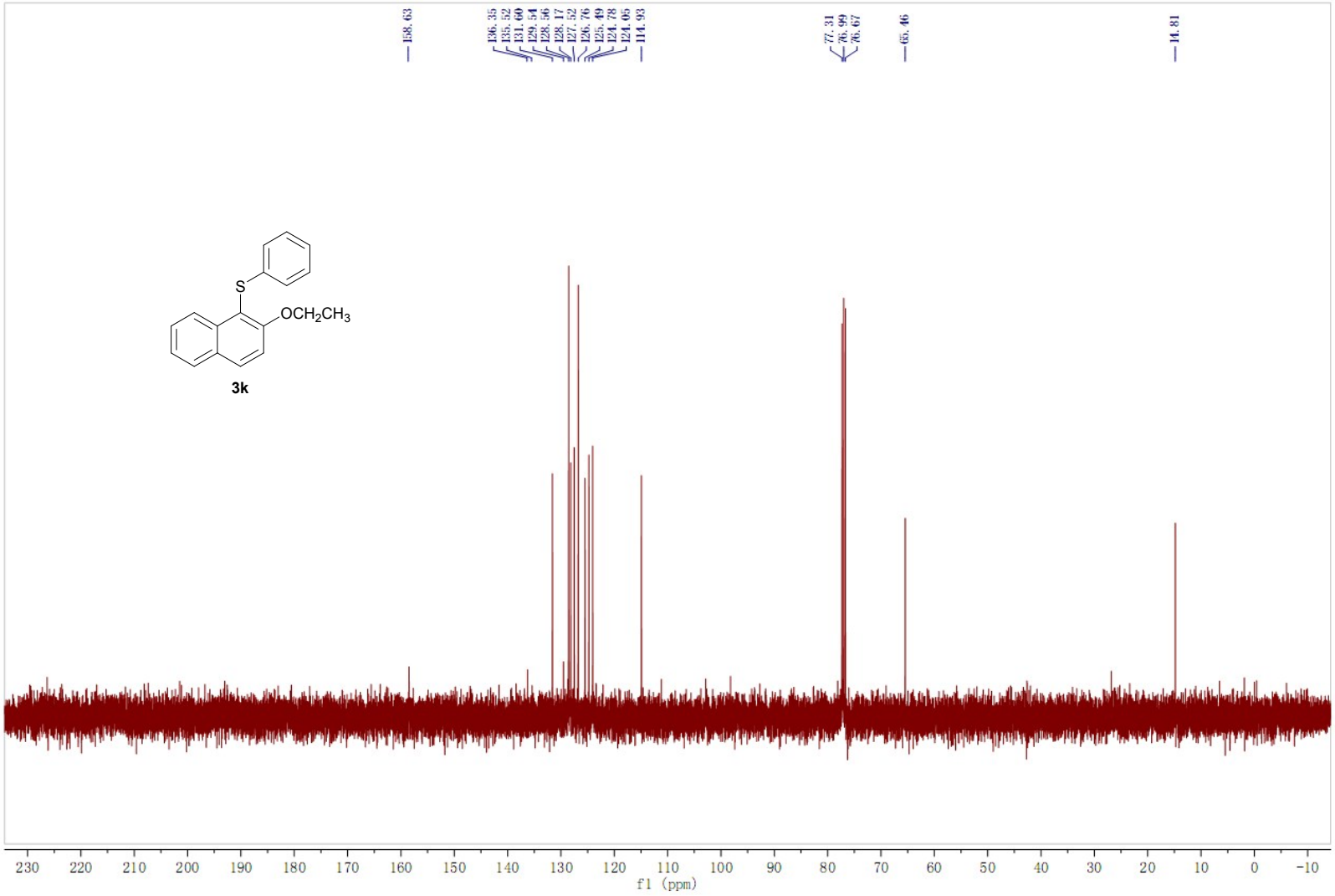
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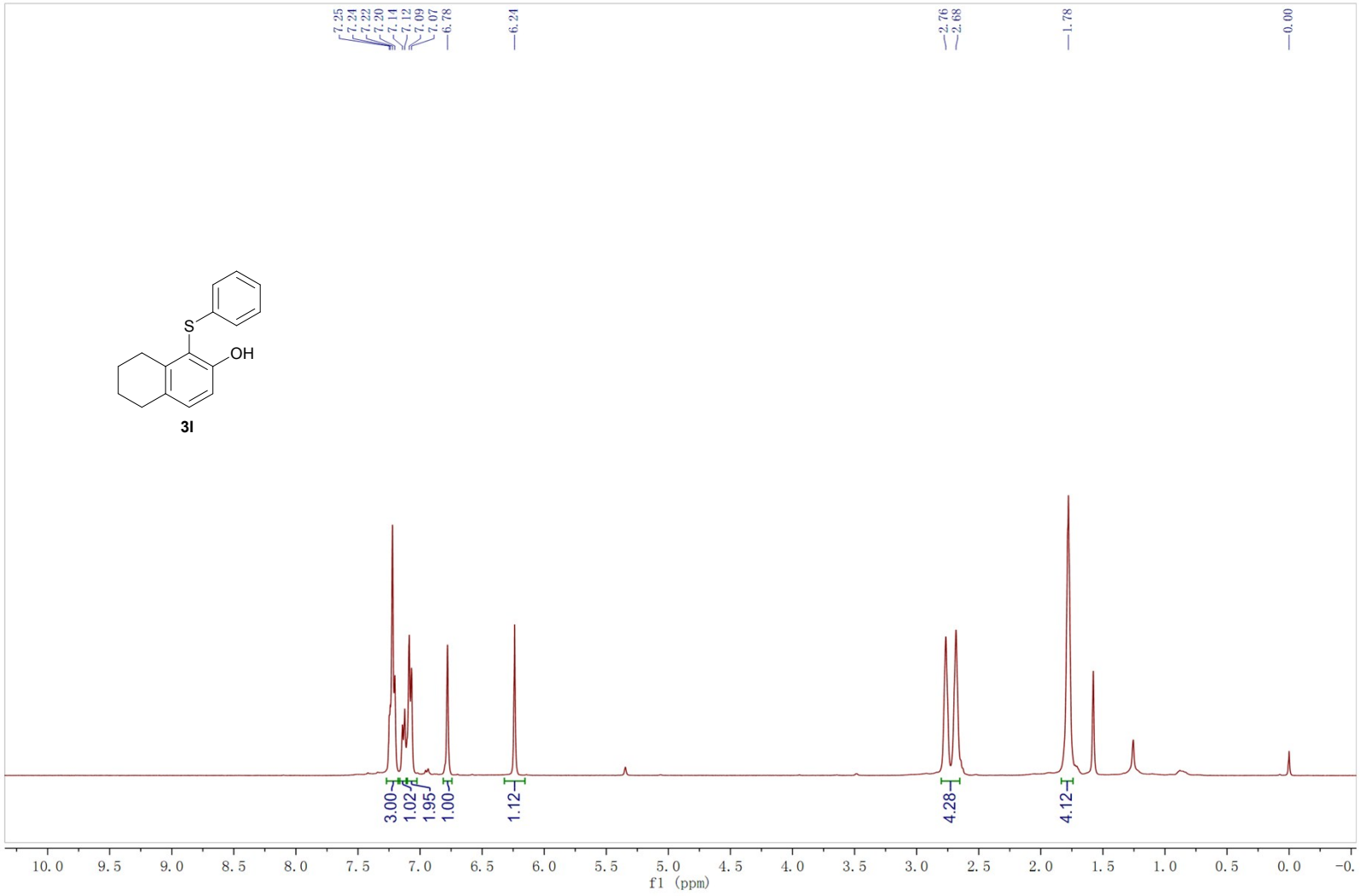
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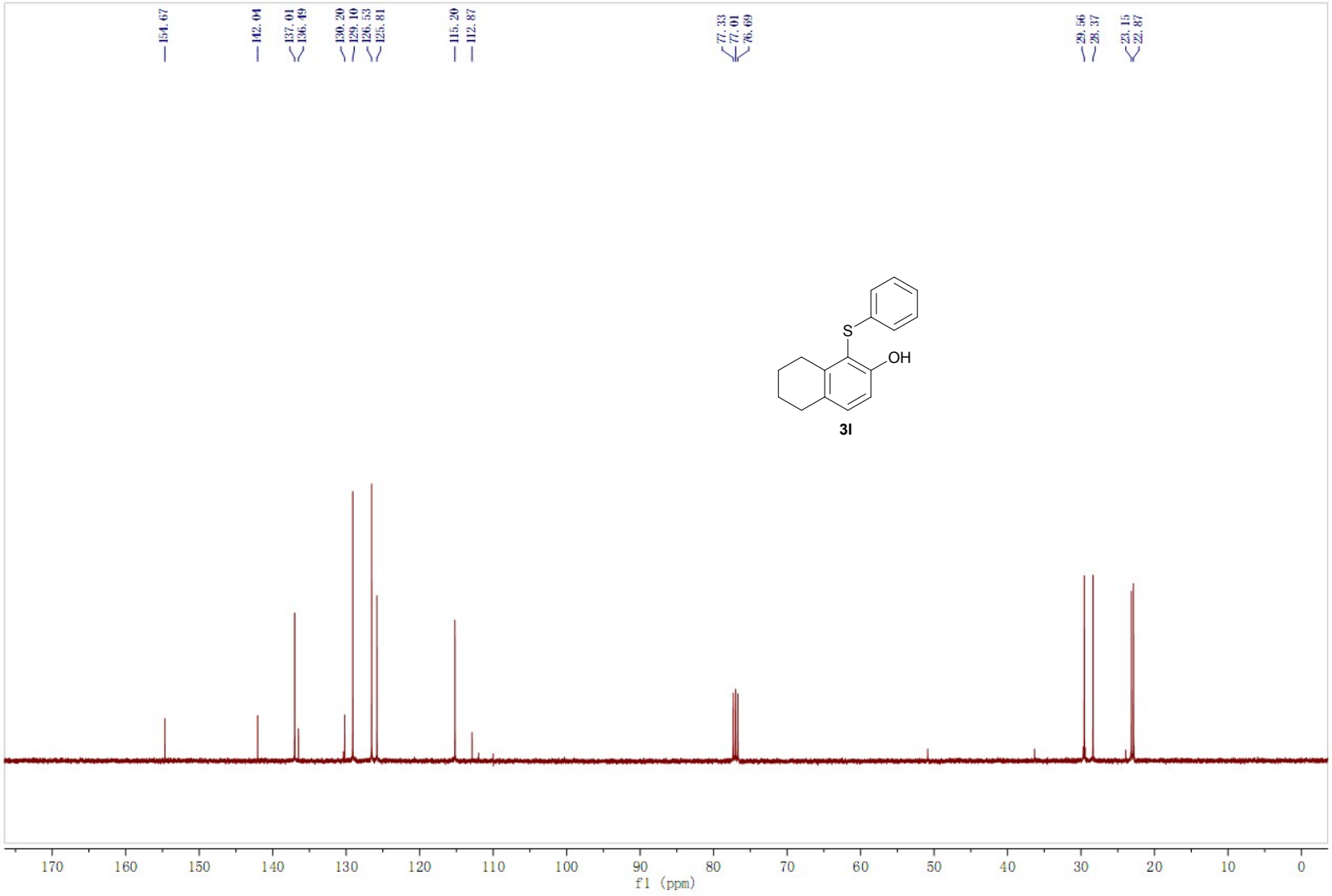
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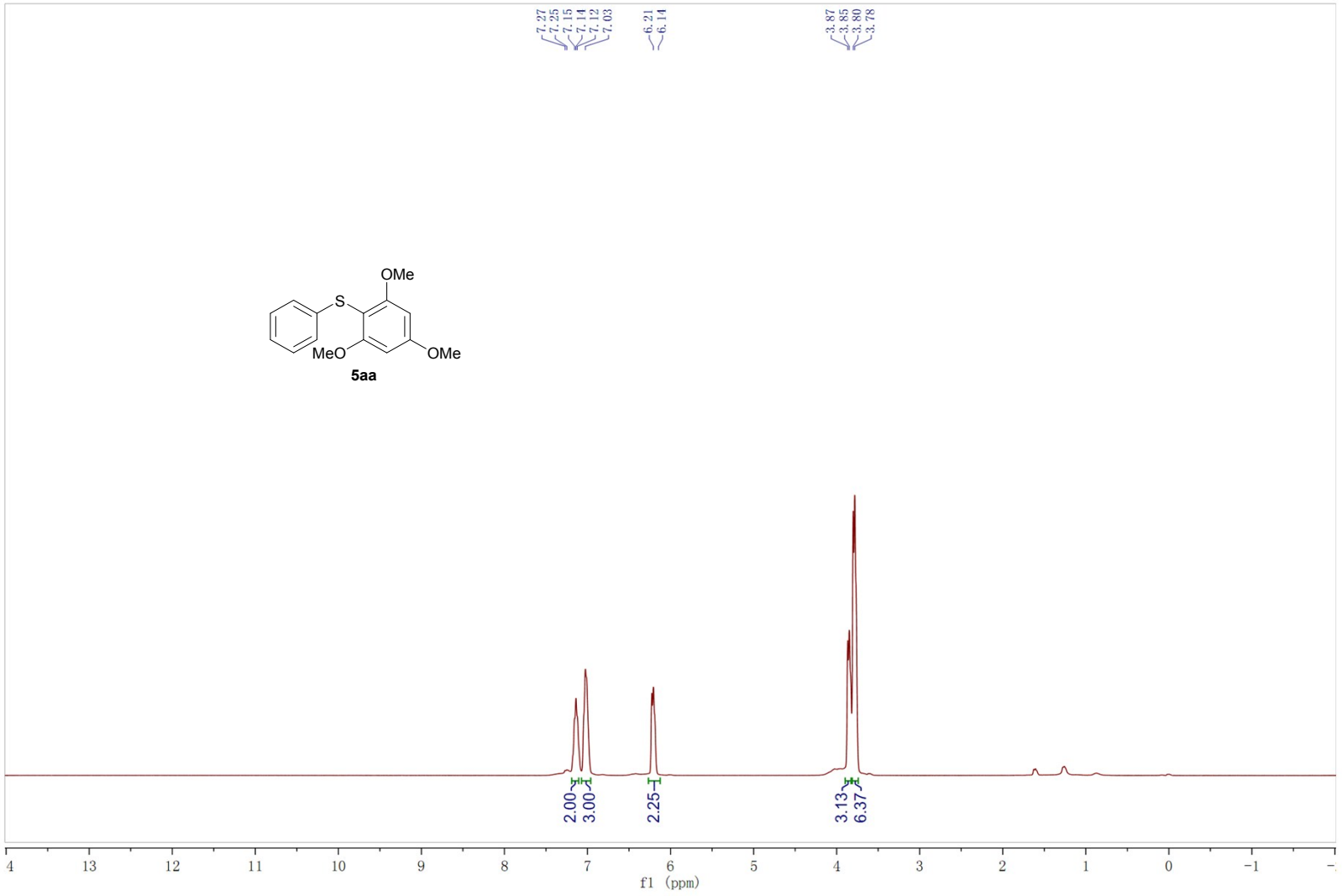
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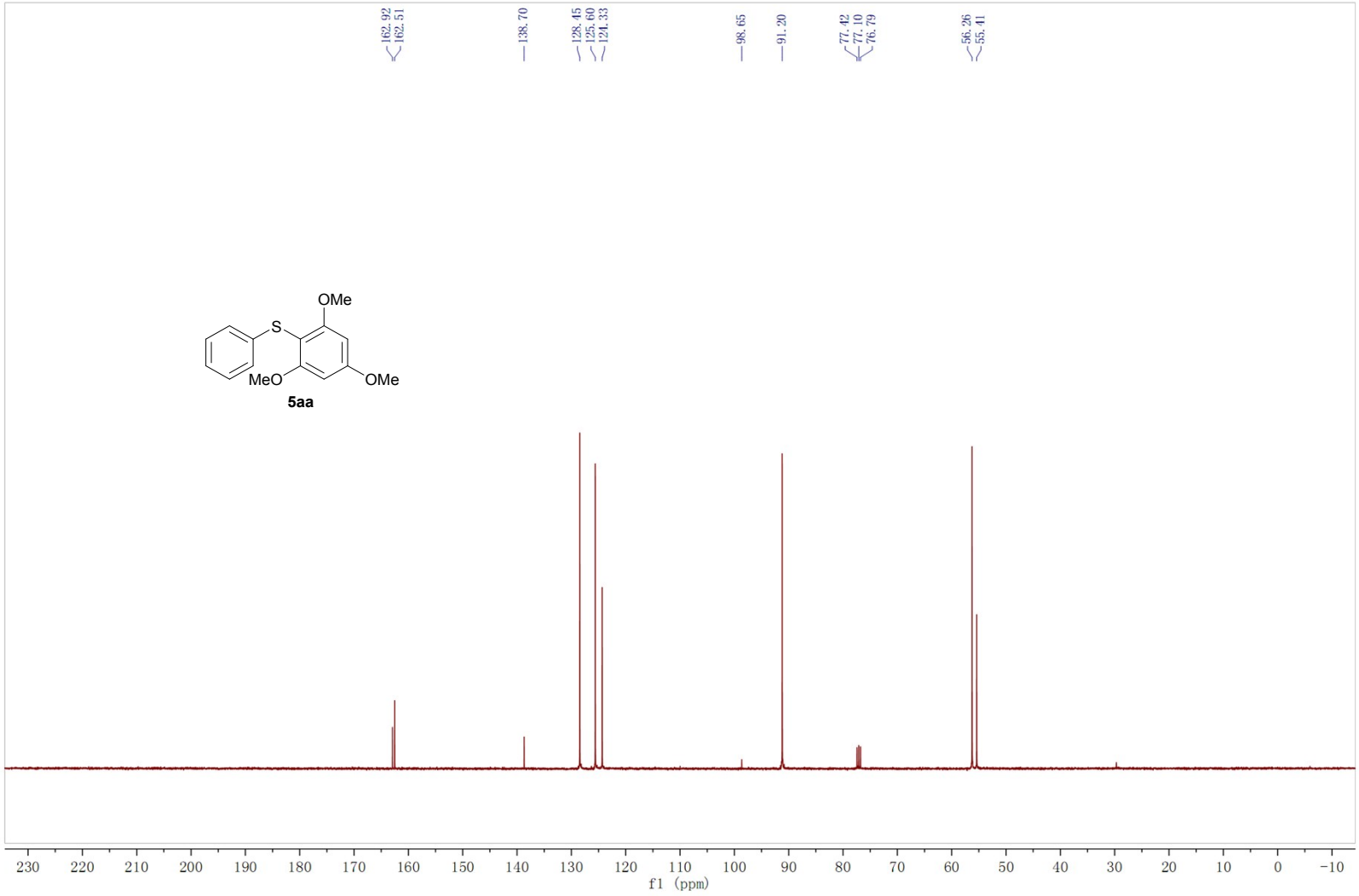
−1
f1 (ppm)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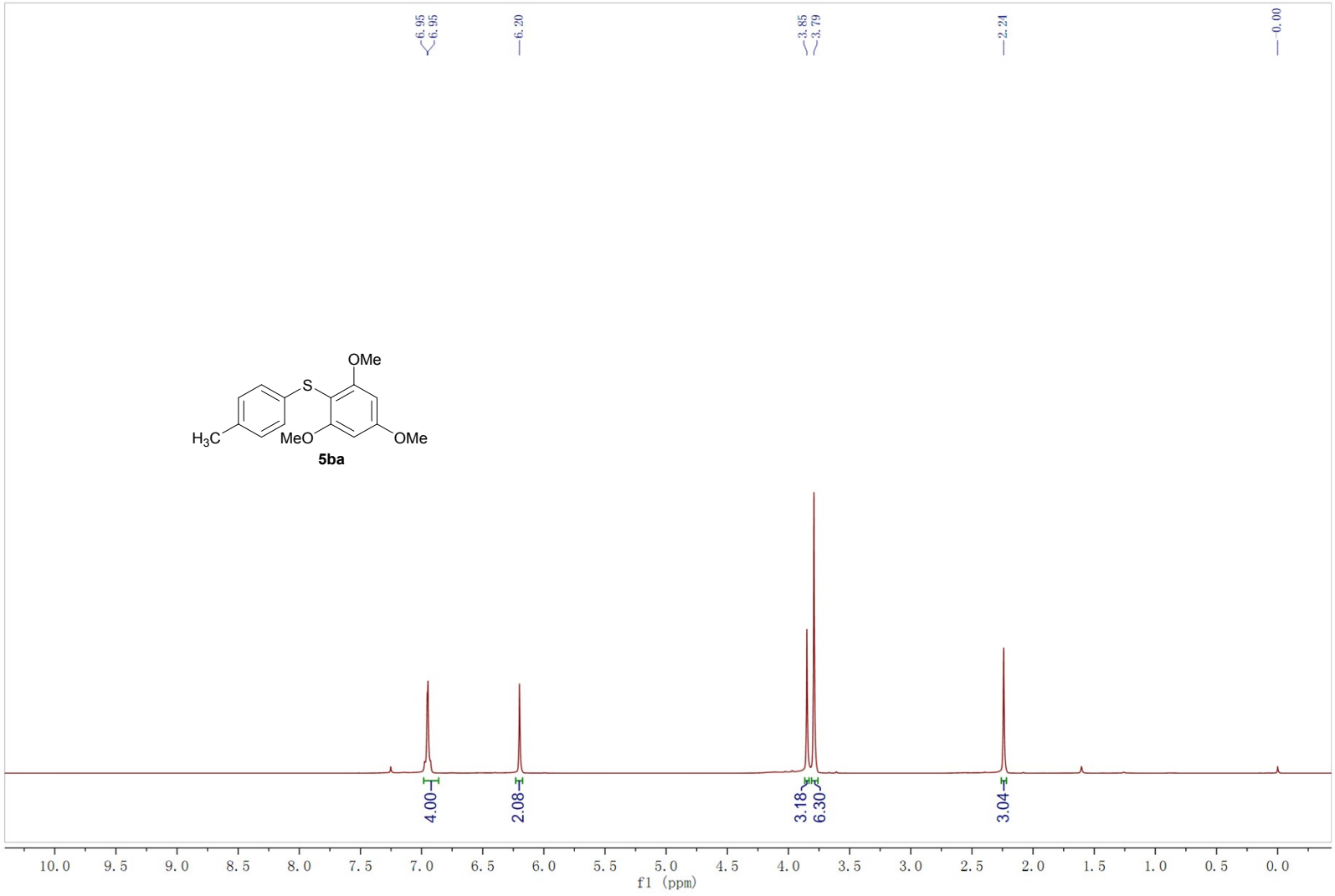
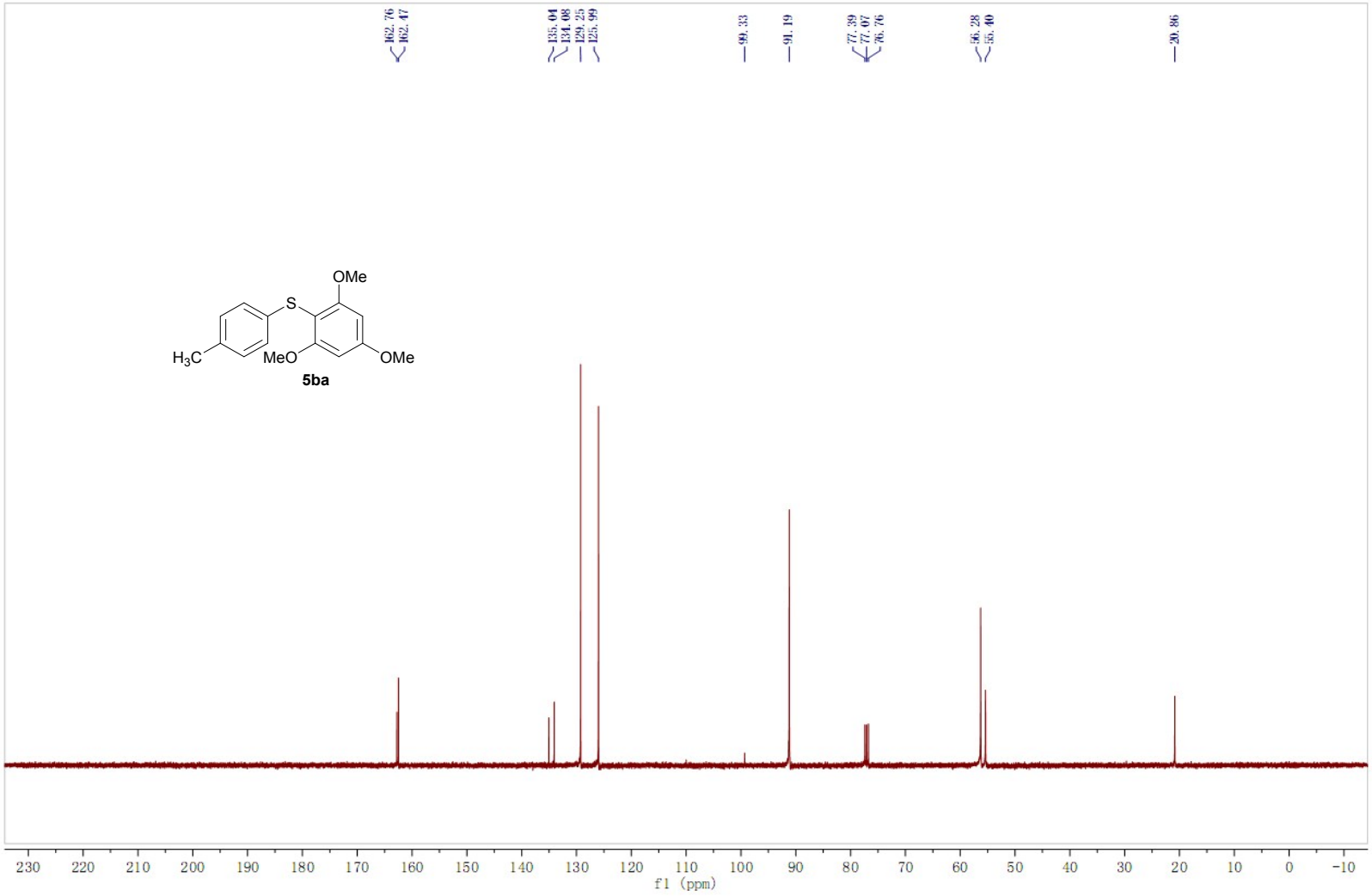
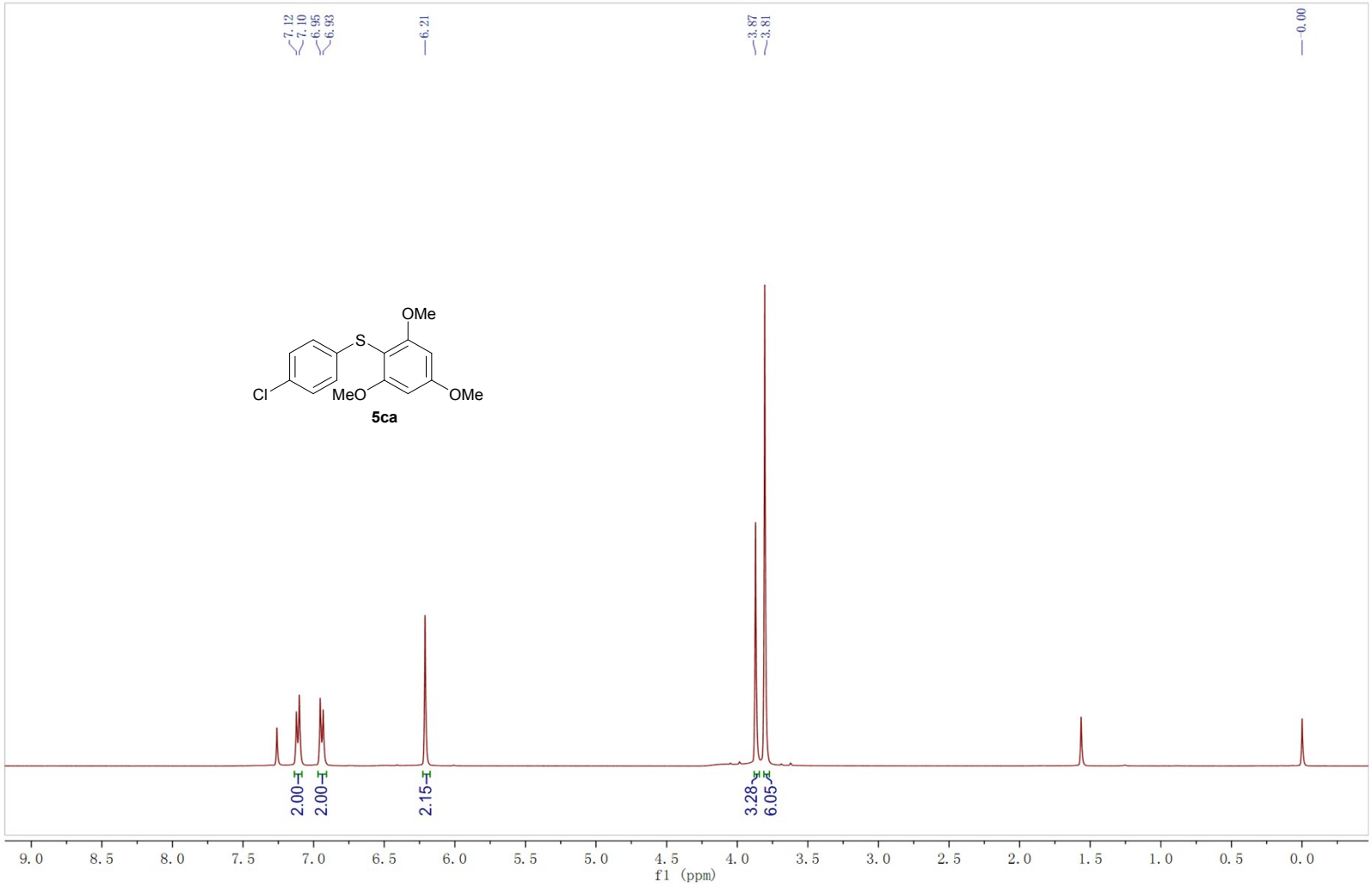
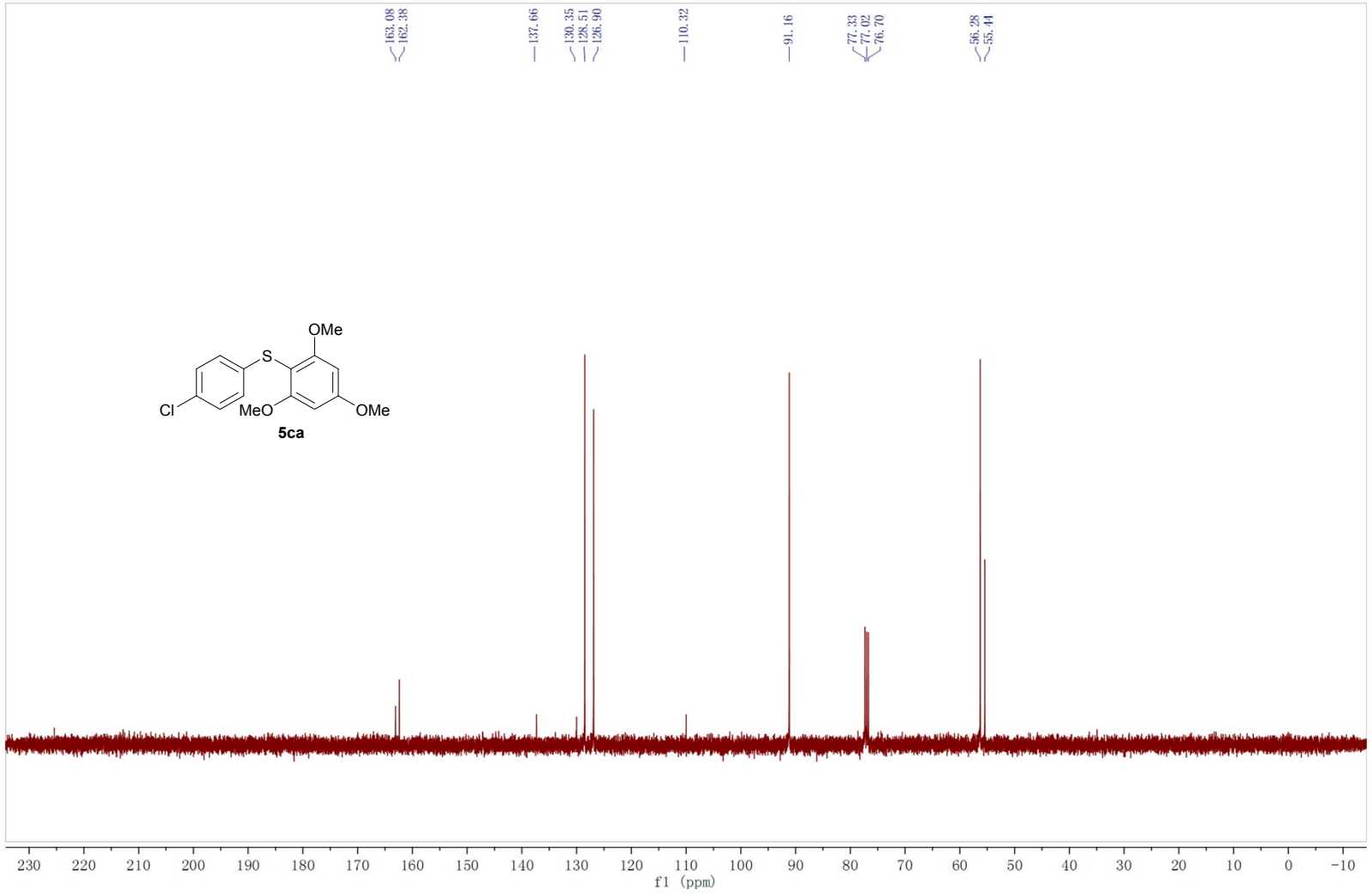
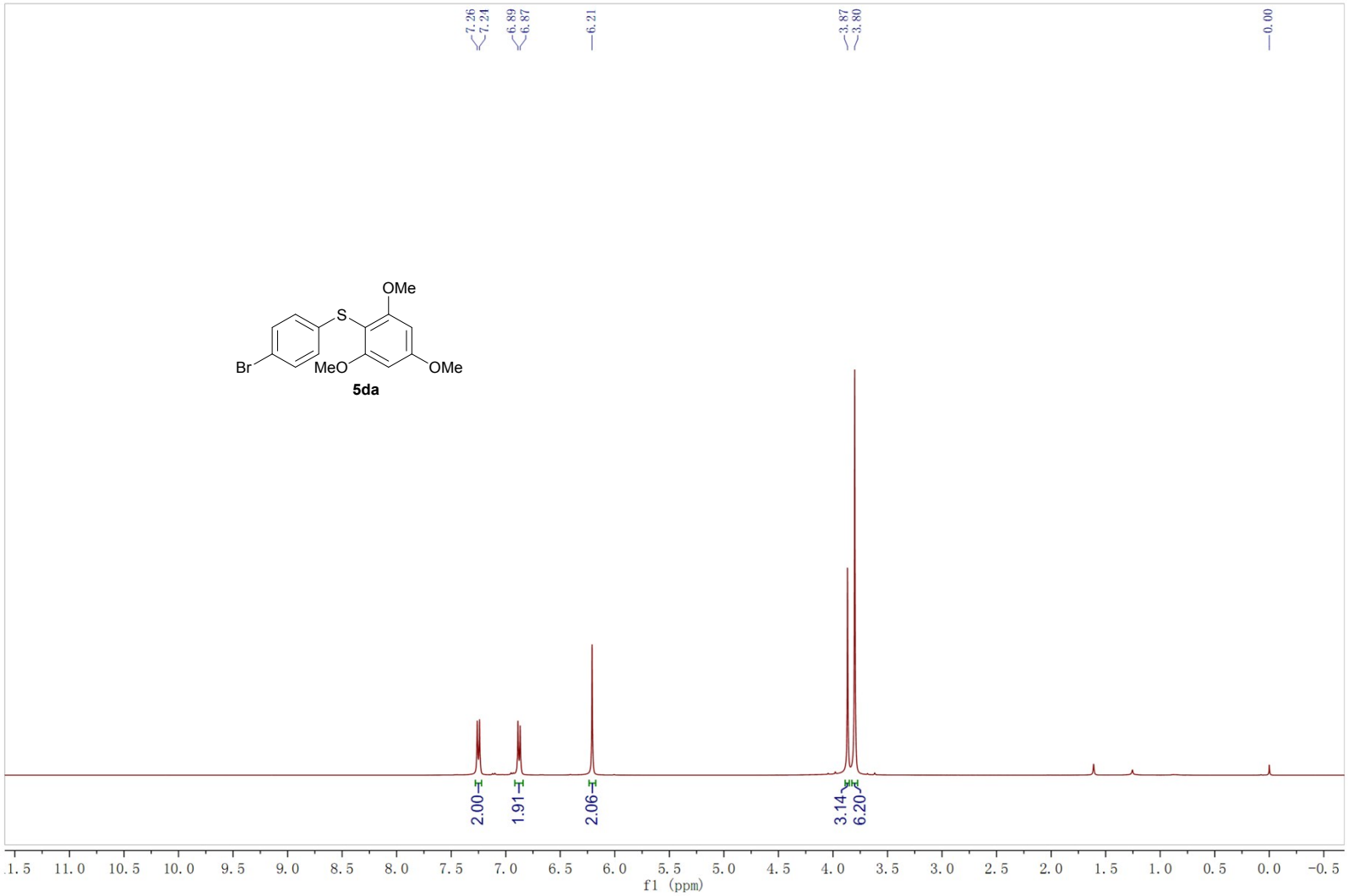
162.51
138.70
128.45
125.60
124.33
98.65
91.20
77.42
77.10
76.79
56.26
55.41
OMe
S
MeO
OMe
5aa
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

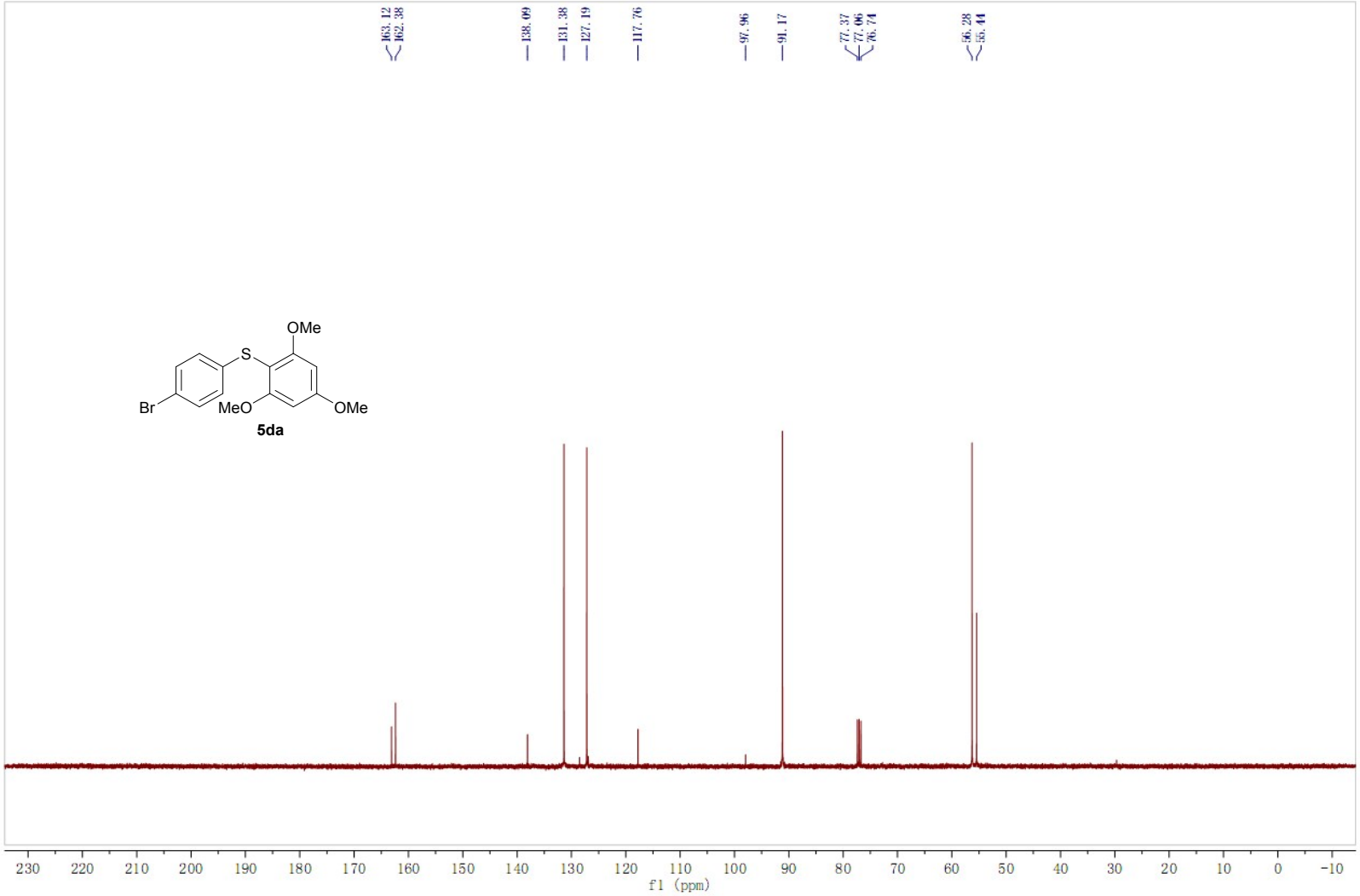

6.95
6.95
6.20
3.85
3.79
2.24
0.00
OMe
S
H3C
MeO
OMe
5ba
4.00
2.08
3.18
6.30
3.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


162.76
162.47
135.04
134.08
129.25
125.99
99.33
91.19
77.39
77.07
76.76
56.28
55.40
20.86
OMe
S
H3C
MeO
OMe
5ba
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.12
7.10
6.95
6.93
6.21
3.87
3.81
0.00
OMe
S
Cl
MeO
OMe
5ca
2.00
2.00
2.15
3.28
6.05
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


163.08
162.38
137.66
130.35
128.51
126.90
110.32
91.16
77.33
77.02
76.70
56.28
55.44
OMe
S
Cl
MeO
OMe
5ca
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.26
7.24
6.89
6.87
6.21
3.87
3.80
0.00
OMe
S
Br
MeO
OMe
5da
2.00
1.91
2.06
3.14
6.20
f1 (ppm)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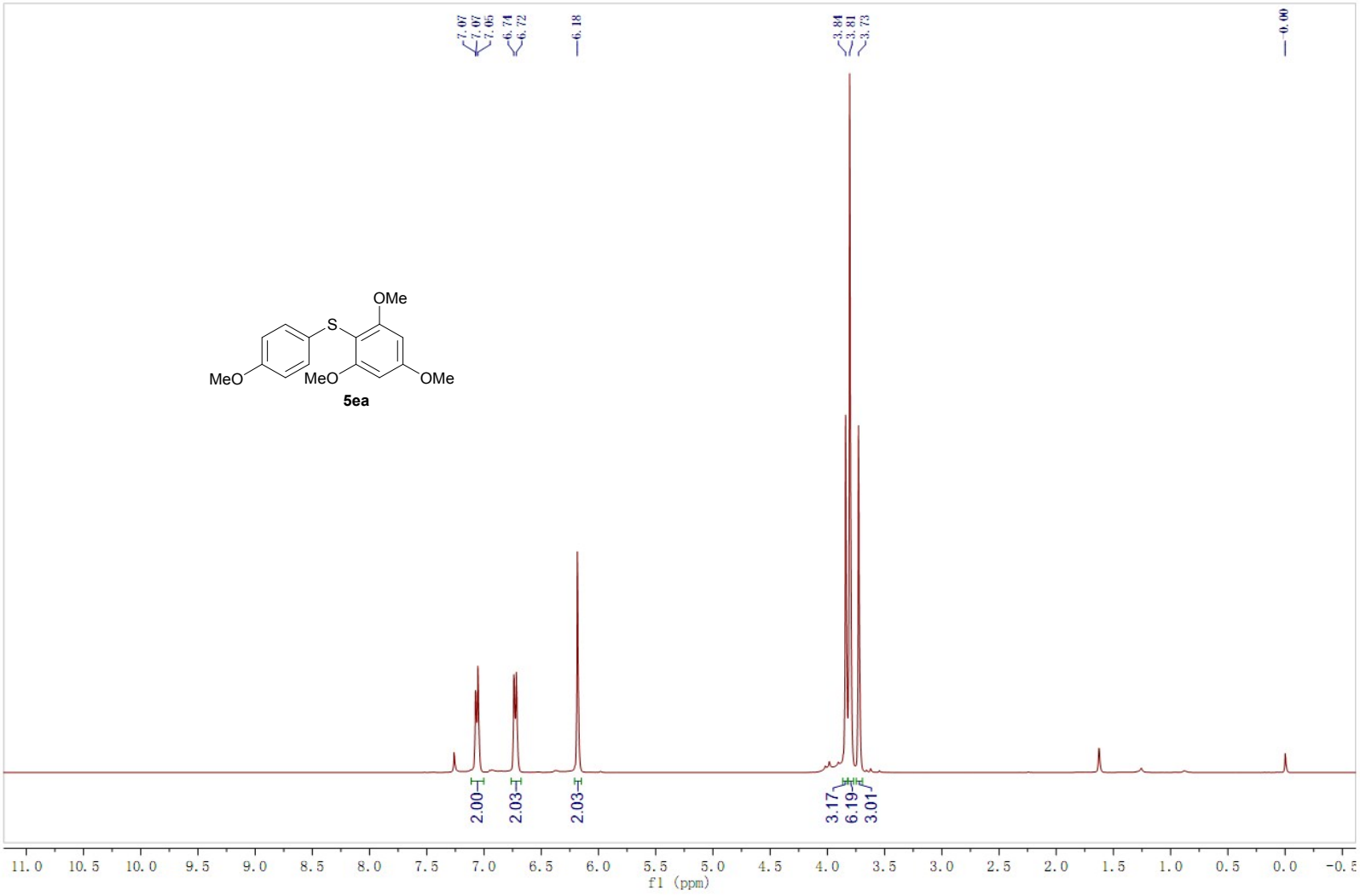
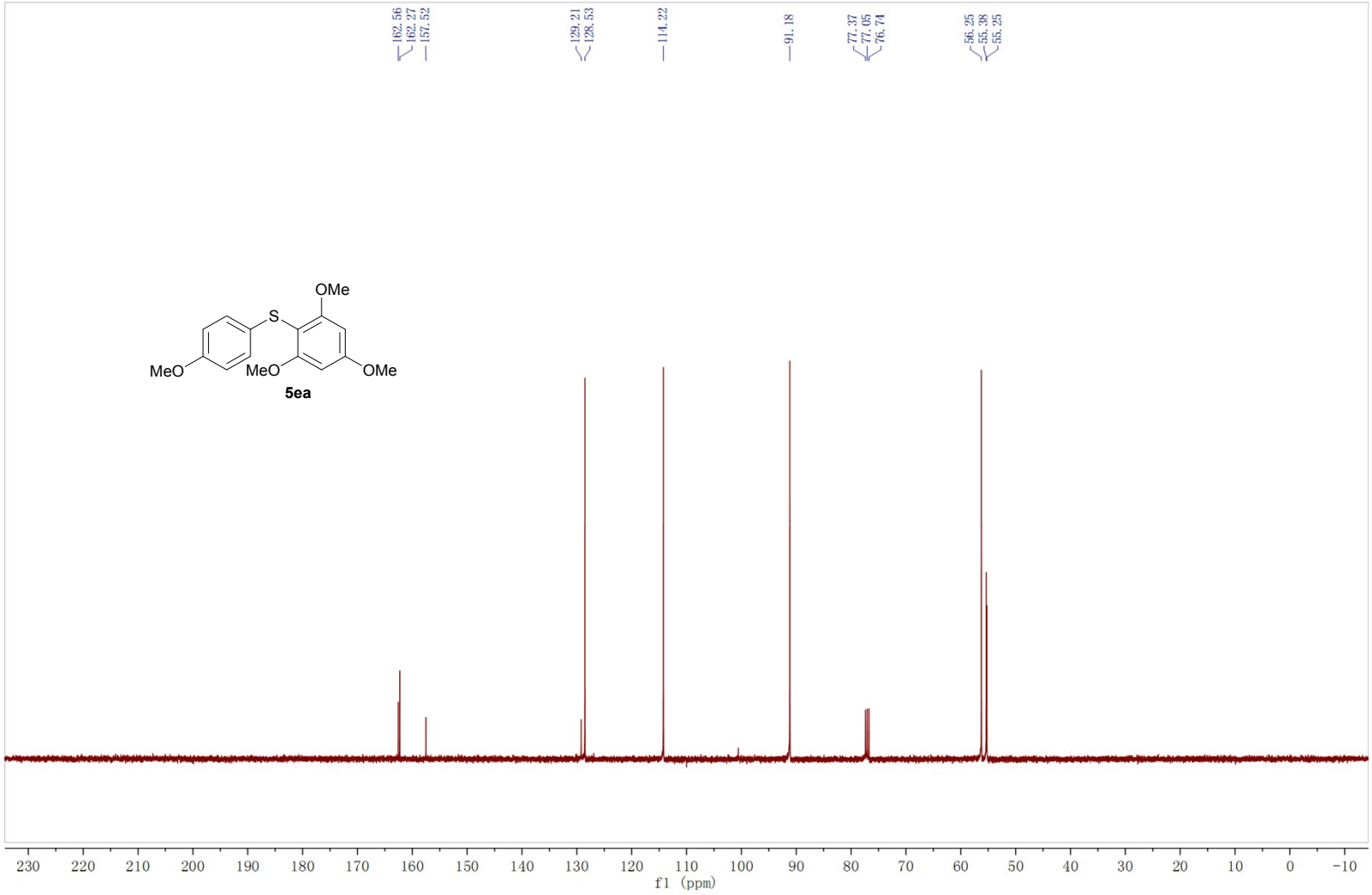
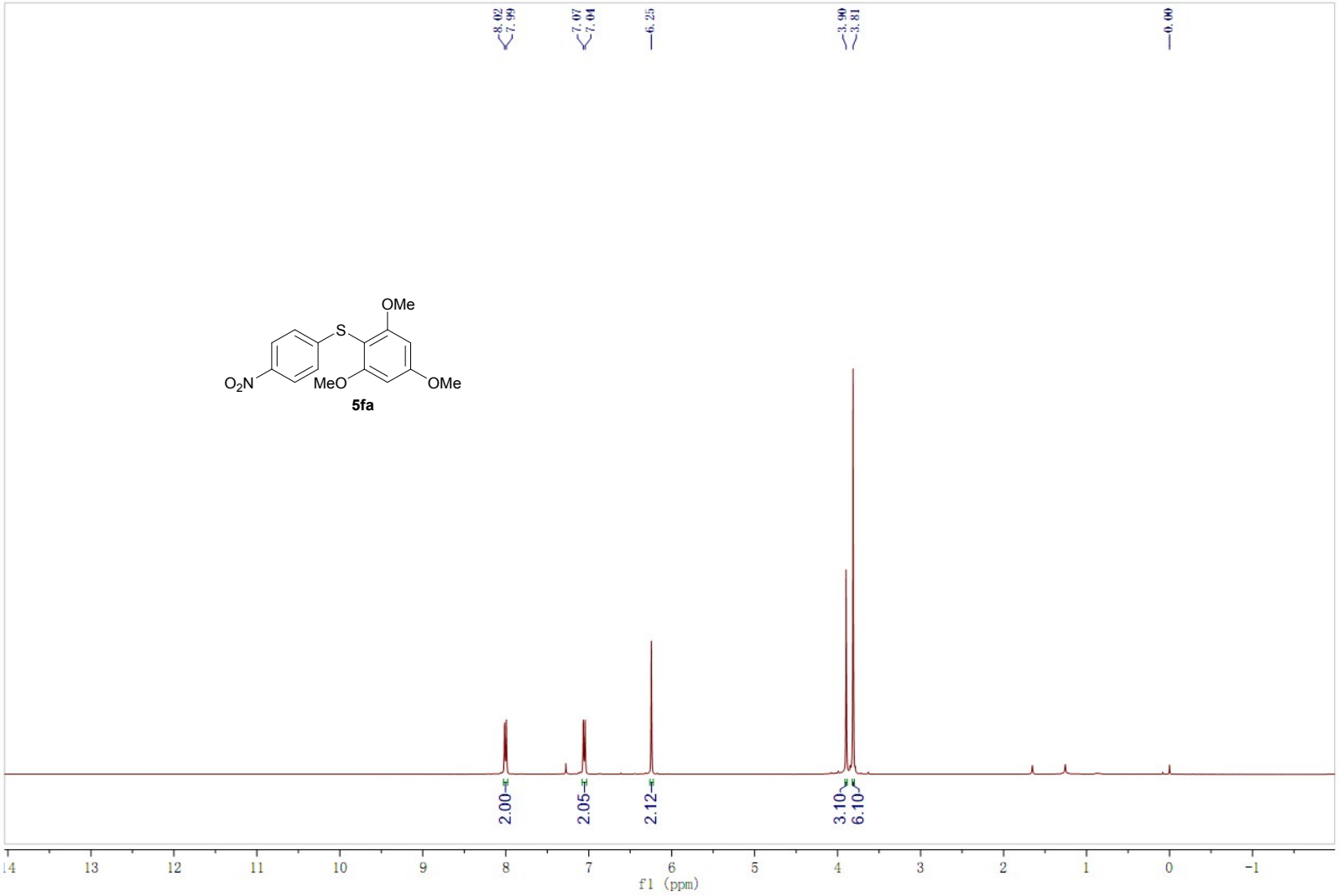
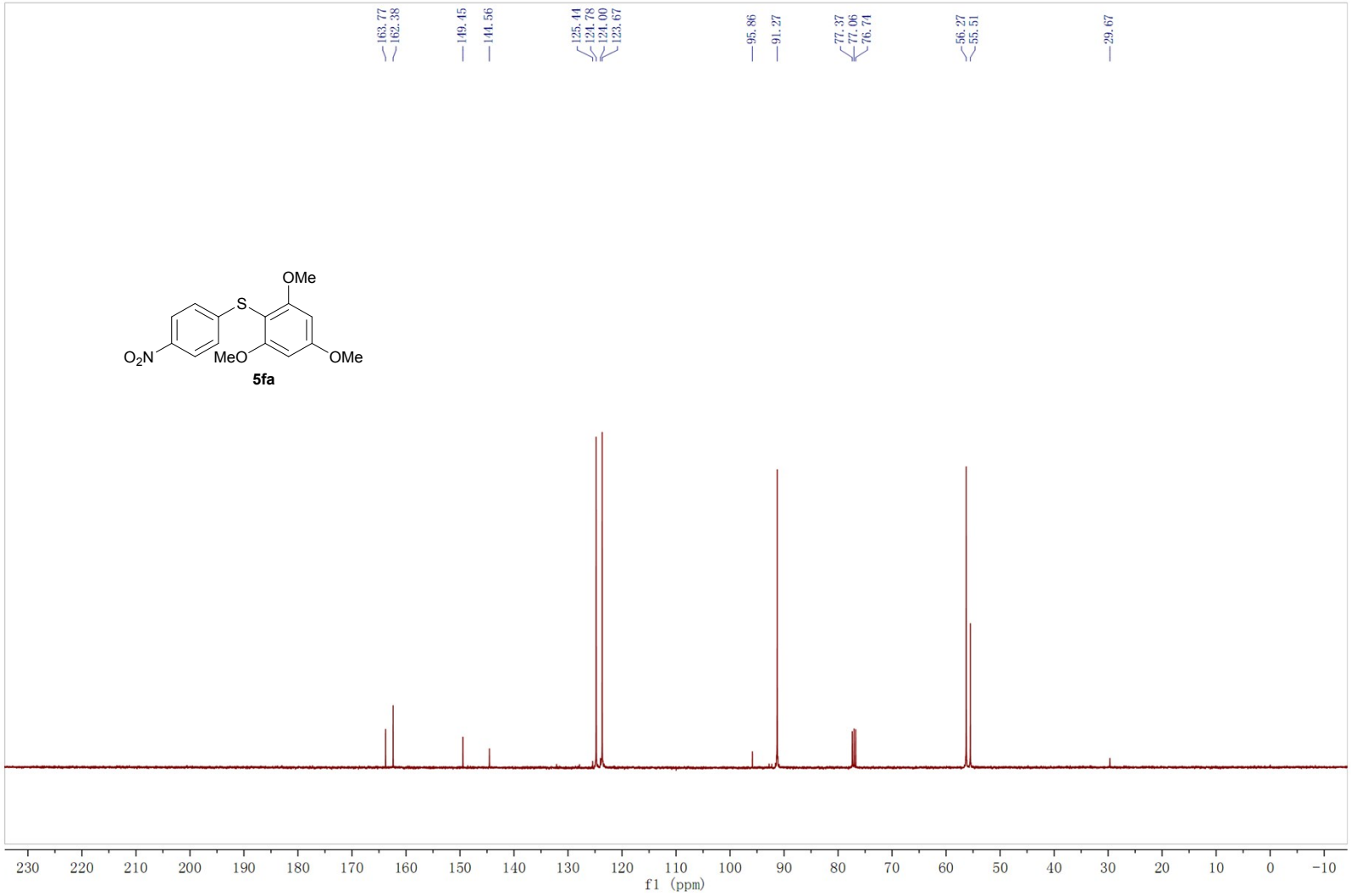
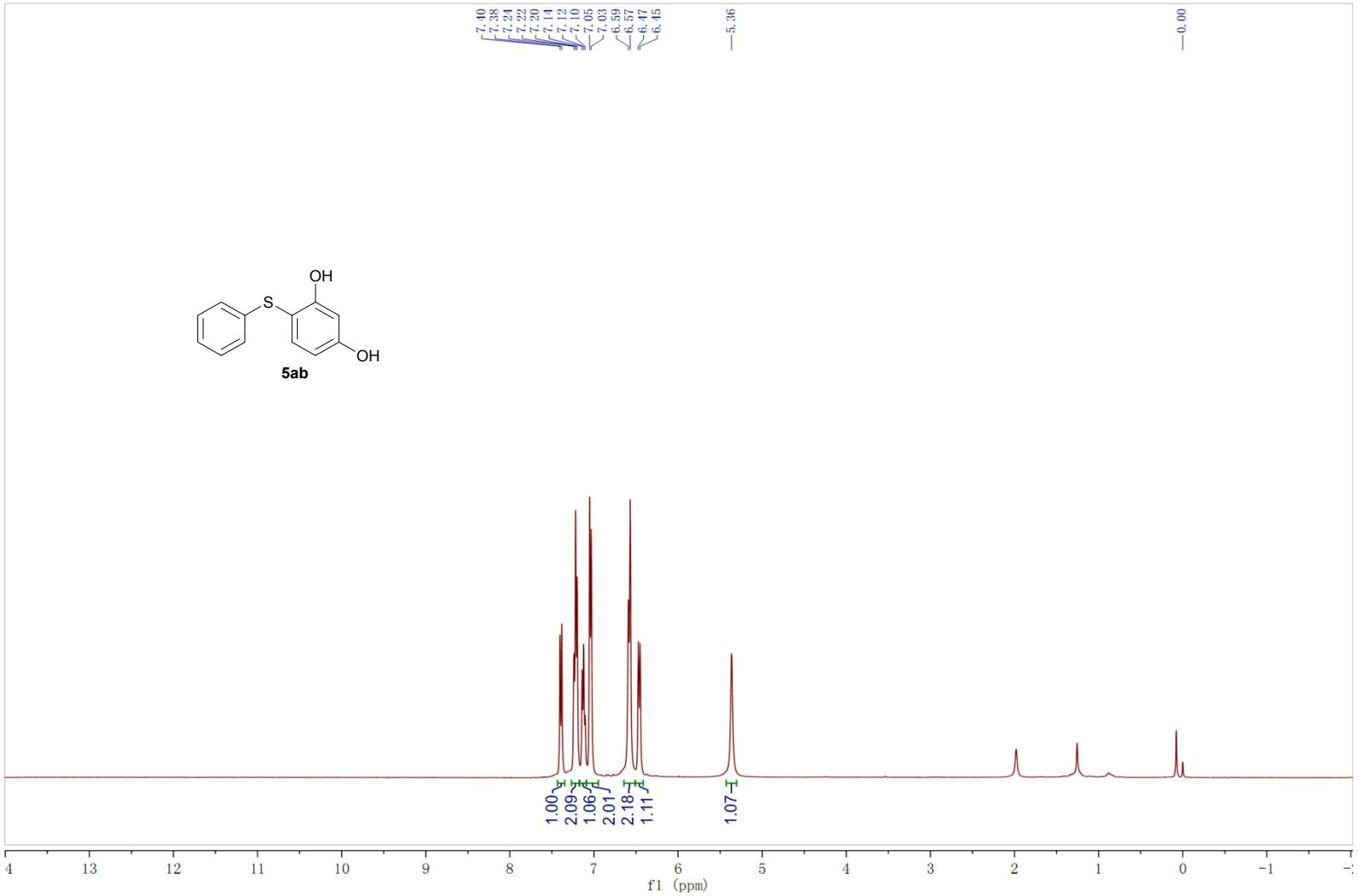
162.38
138.09
131.38
127.19
117.76
97.96
91.17
77.37
77.06
76.74
56.28
55.44
OMe
S
Br
MeO
OMe
5da
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

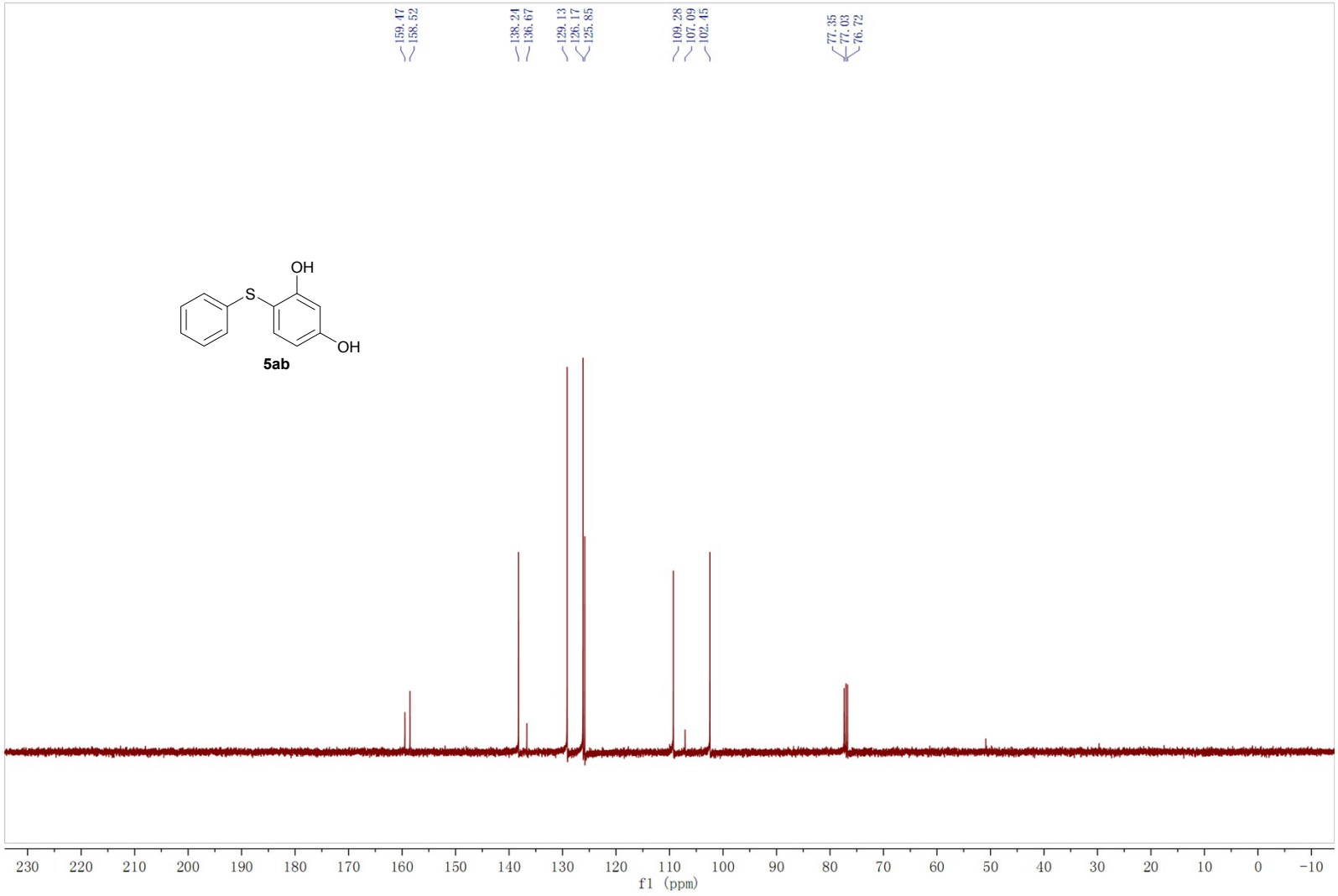

7.07
7.07
7.06
6.74
6.72
6.18
3.84
3.81
3.73
0.00
OMe
S
MeO
MeO
OMe
5ea
2.00
2.03
2.03
3.17
6.19
3.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

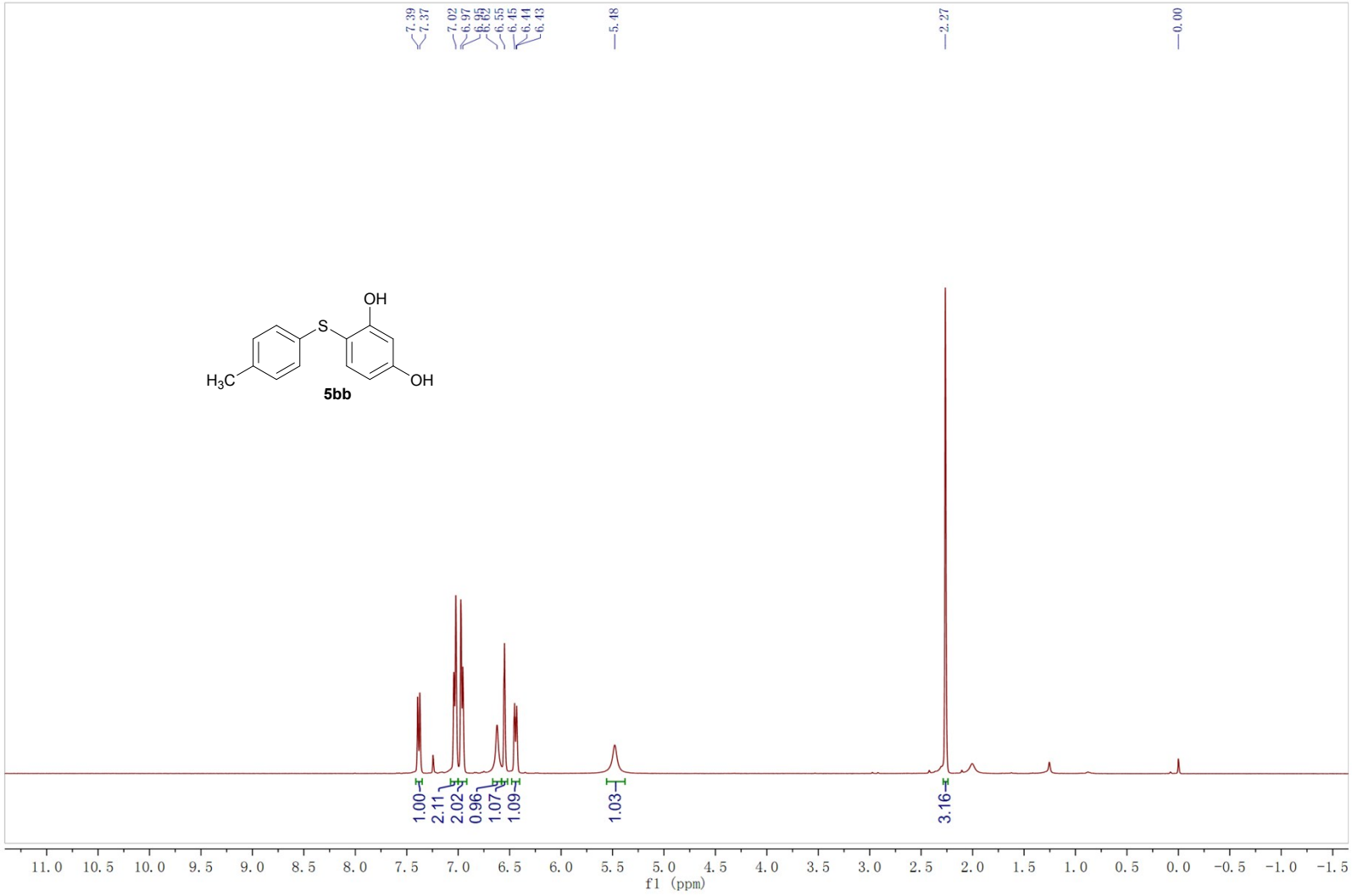

162.56
162.27
157.52
129.21
128.53
114.22
91.18
77.37
77.05
76.74
56.25
55.38
55.25
OMe
S
MeO
MeO
OMe
5ea
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

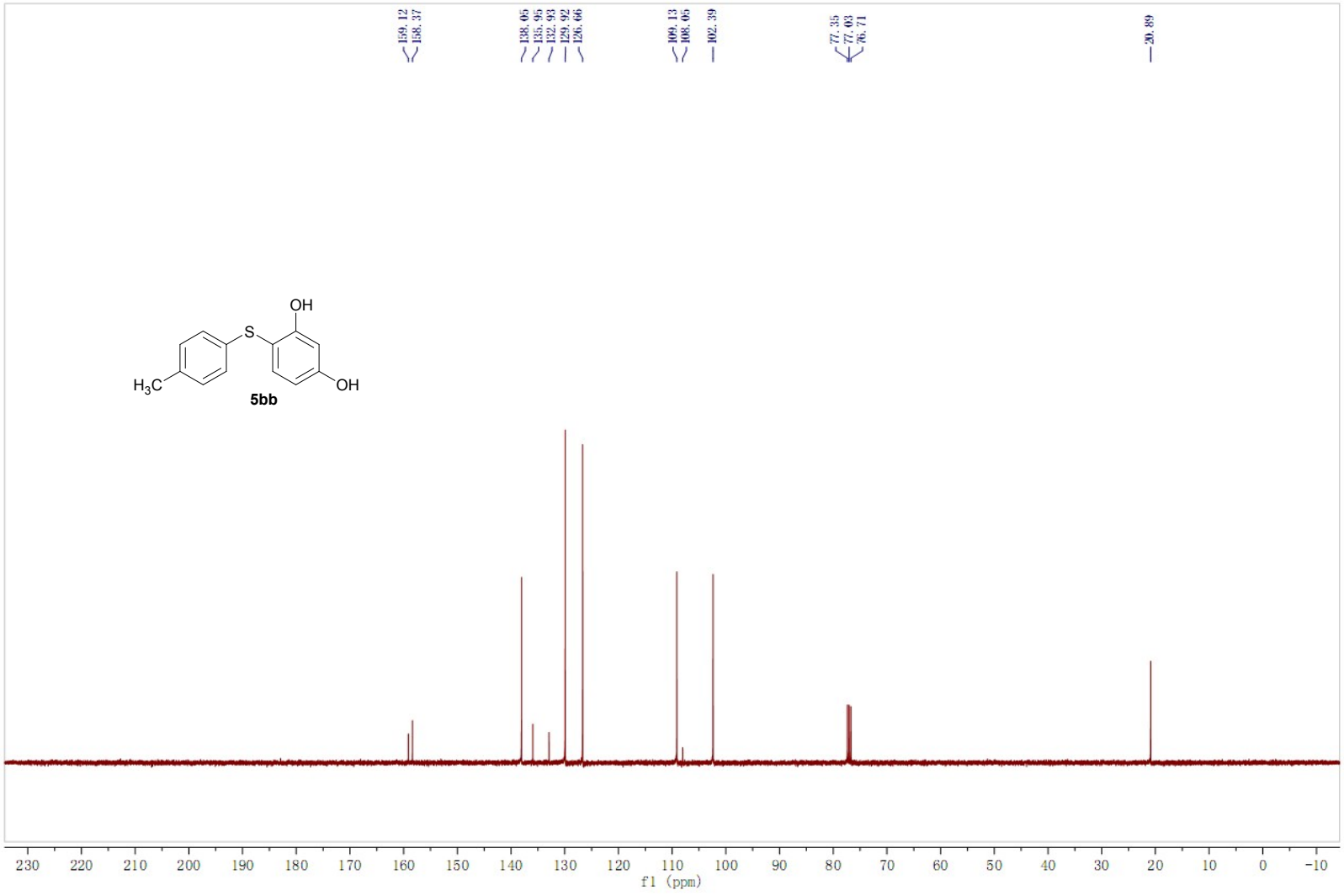

8.02
7.99
7.07
7.04
6.25
3.90
3.81
0.00
OMe
S
O_2N
MeO
OMe
5fa
2.00
2.05
2.12
3.10
6.10
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

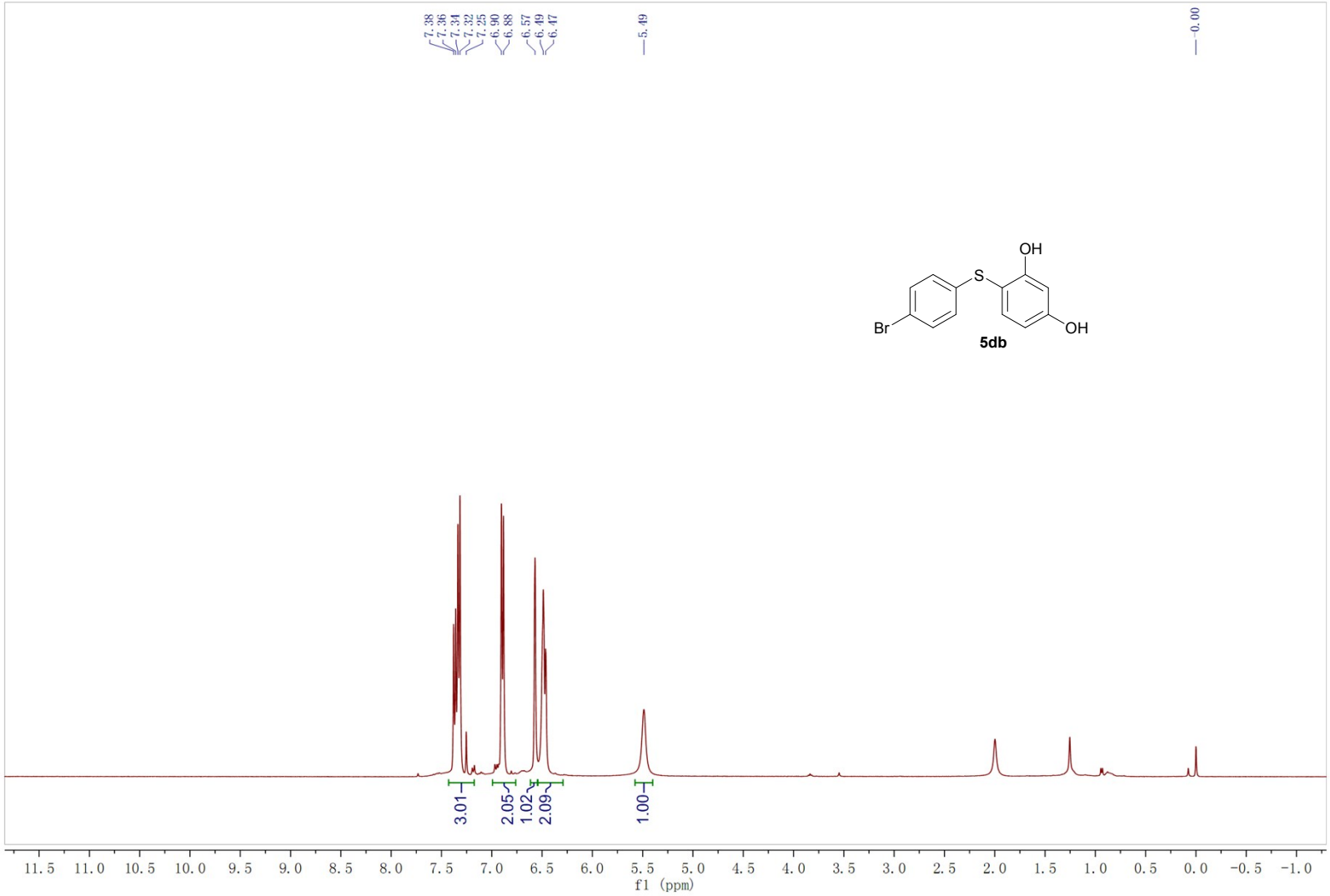

163.77
162.38
149.45
144.56
125.44
124.78
124.00
123.67
95.86
91.27
77.37
77.06
76.74
56.27
55.51
29.67
OMe
S
O2N
MeO
OMe
5fa
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

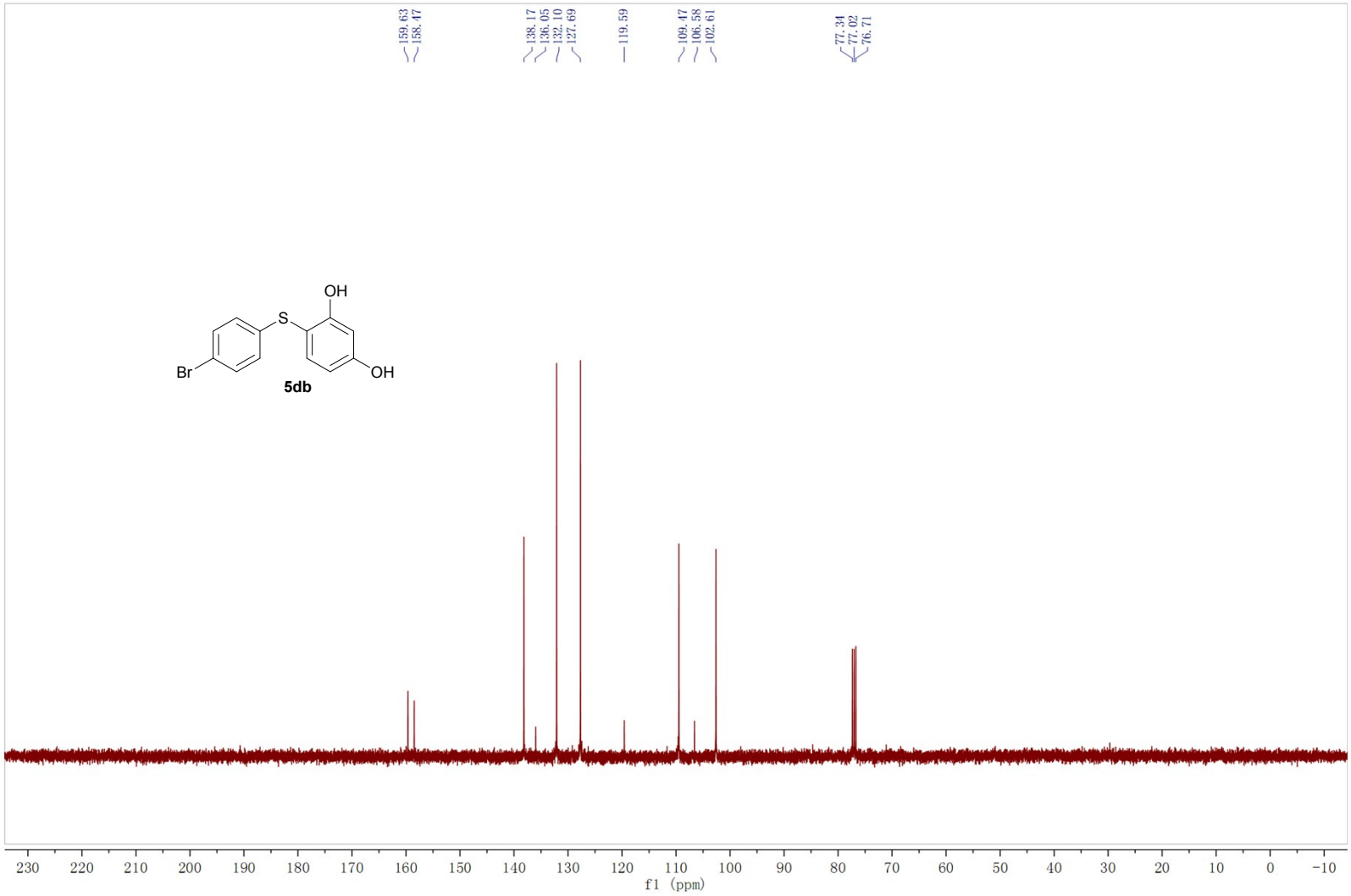

7.40
7.38
7.24
7.22
7.20
7.14
7.12
7.10
7.05
7.03
6.59
6.57
6.47
6.45
5.36
0.00
OH
S
OH
5ab
1.00
2.09
1.06
2.01
2.18
1.11
1.07
f1 (ppm)

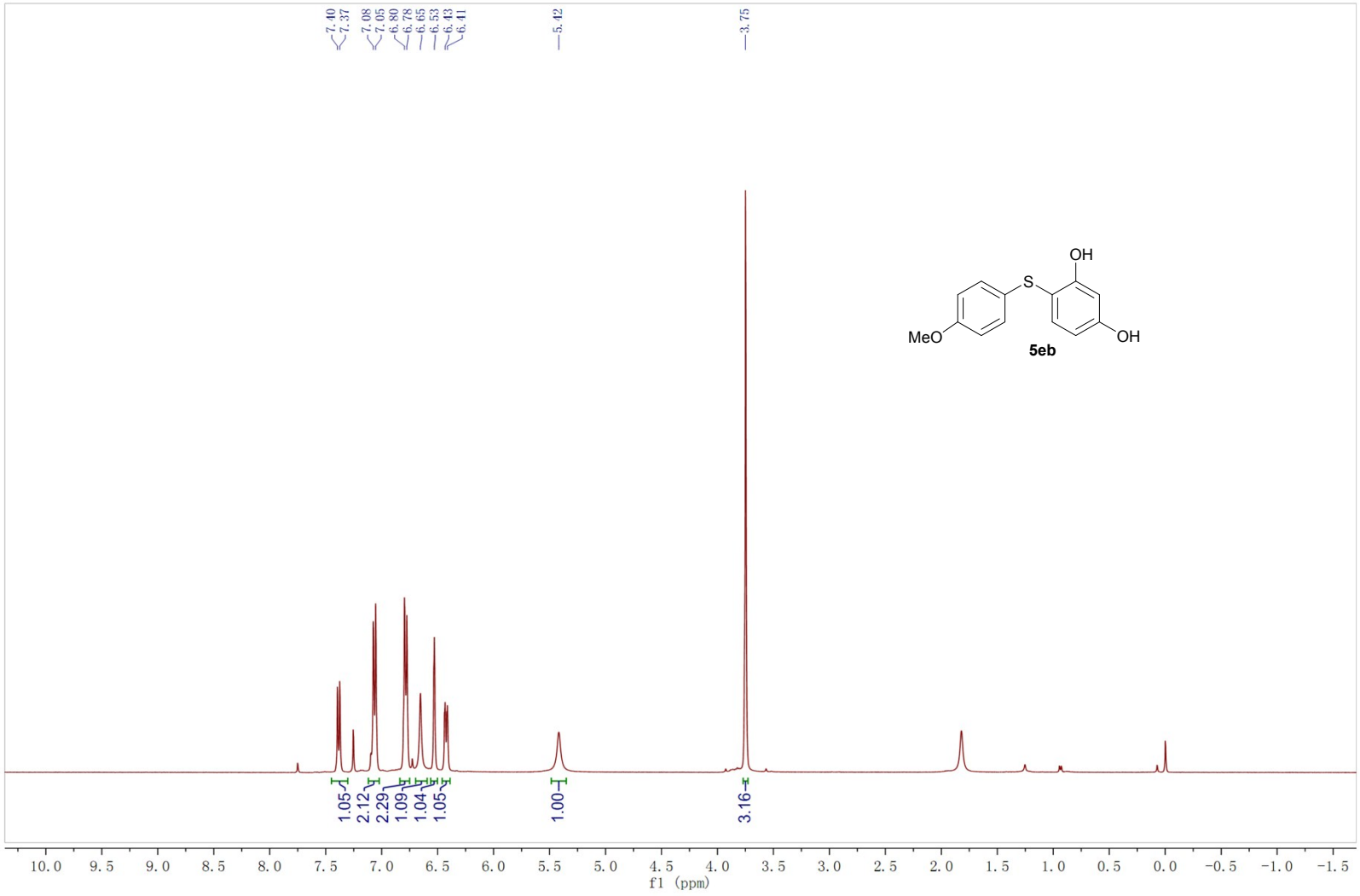

159.47
158.52
138.24
136.67
129.13
126.17
125.85
109.28
107.09
102.45
77.35
77.03
76.72
OH
S
OH
5ab
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

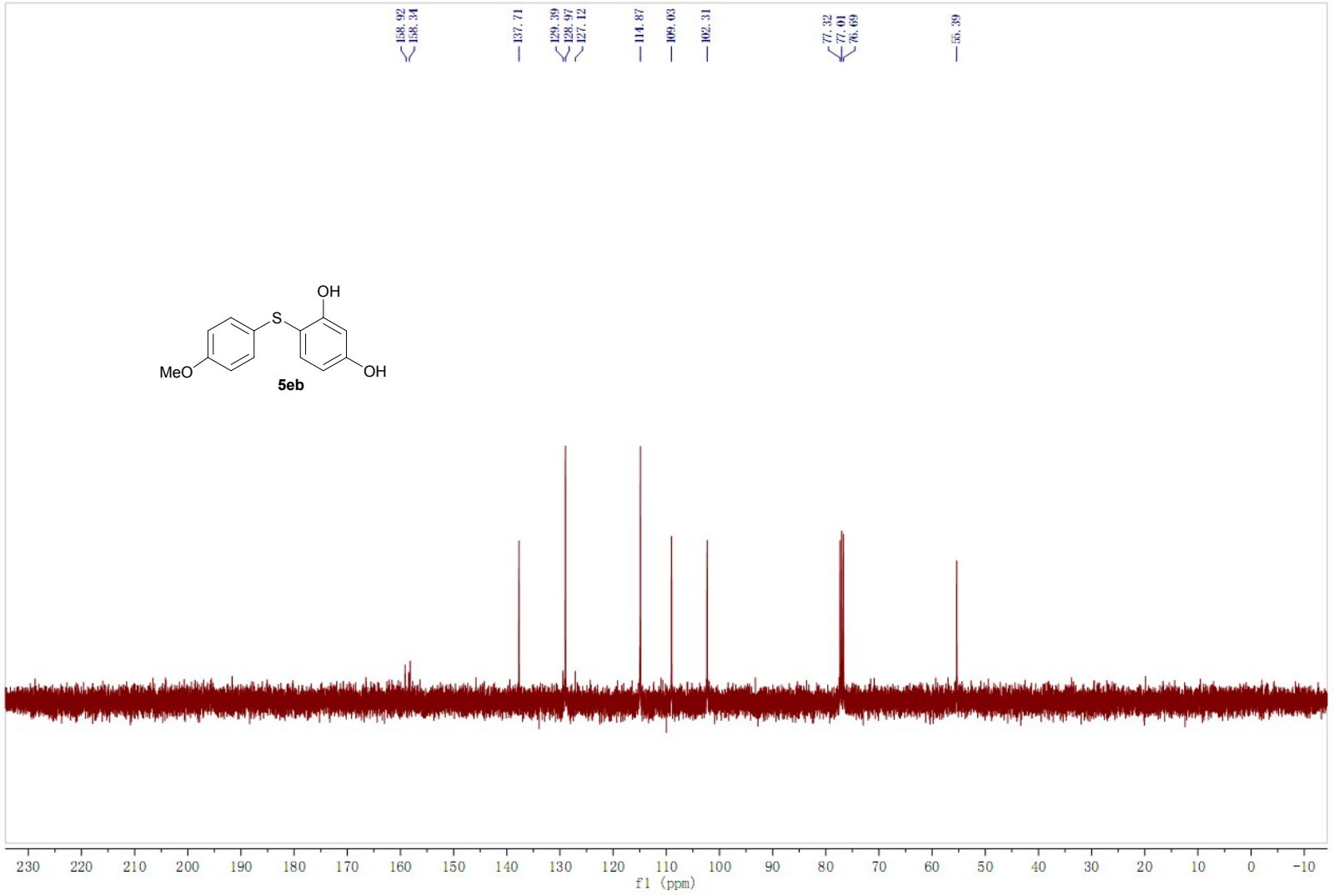

7.39
7.37
7.02
6.97
6.55
6.45
6.44
6.43
5.48
2.27
0.00
OH
S
OH
H3C
5bb
1.00
2.11
2.02
0.96
1.07
1.09
1.03
3.16
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)

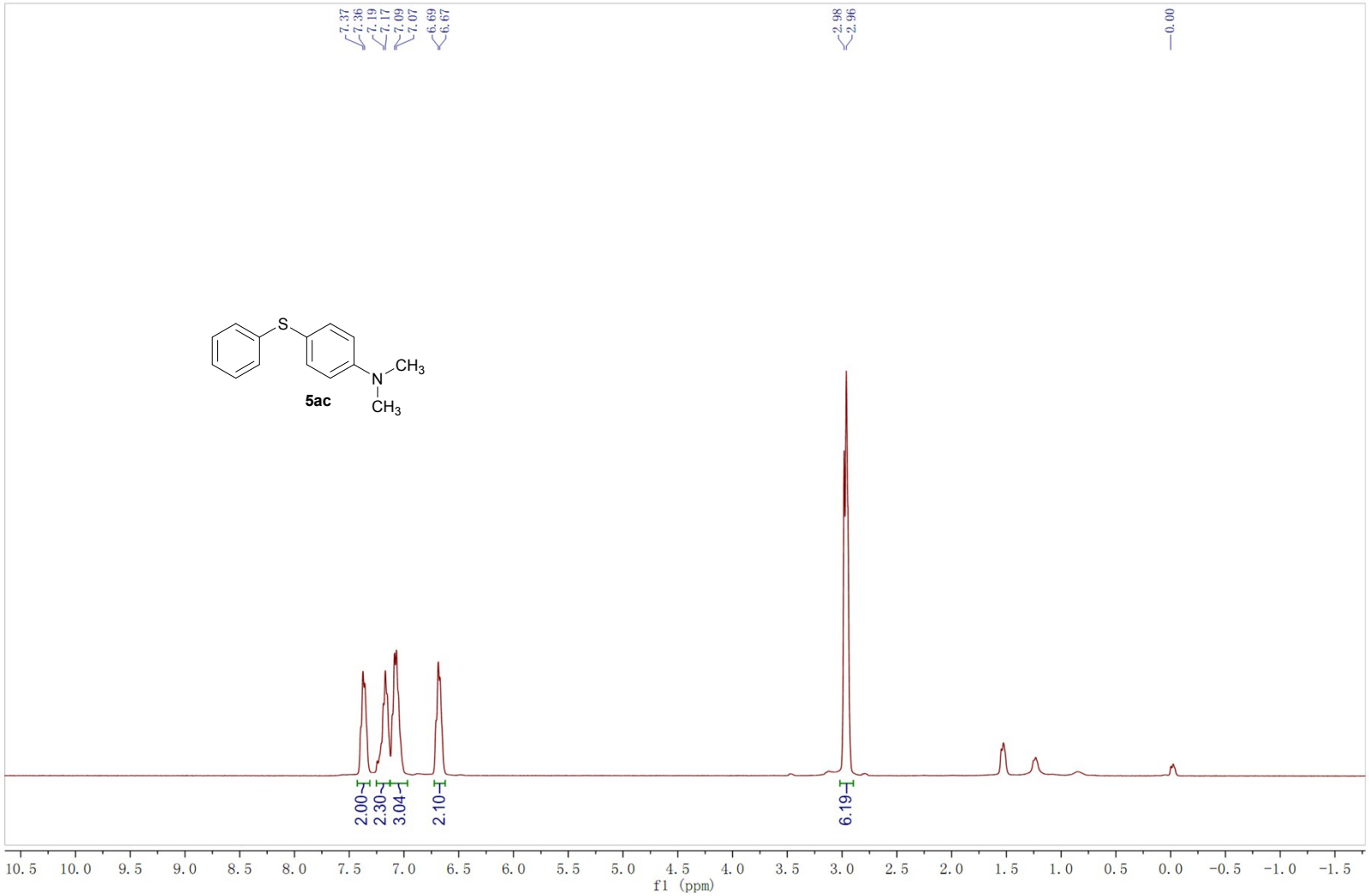

159.12
158.37
138.05
135.95
132.93
129.92
126.66
109.13
108.05
102.39
77.35
77.03
76.71
20.89
OH
S
OH
H3C
5bb
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

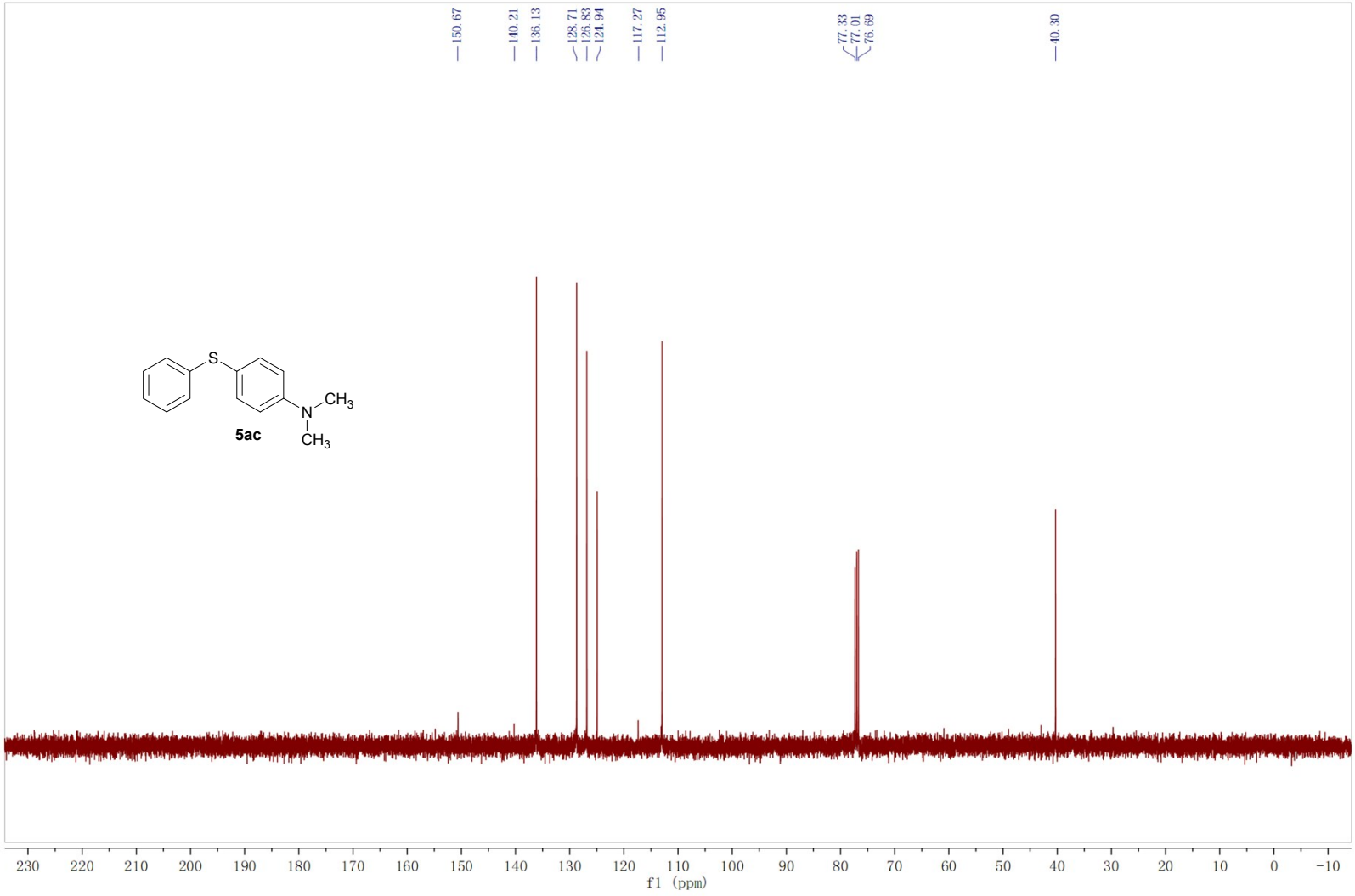

7.38
7.36
7.34
7.32
7.25
6.90
6.88
6.57
6.49
6.47
5.49
0.00
OH
S
Br
OH
5db
3.01
2.05
1.02
2.09
1.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

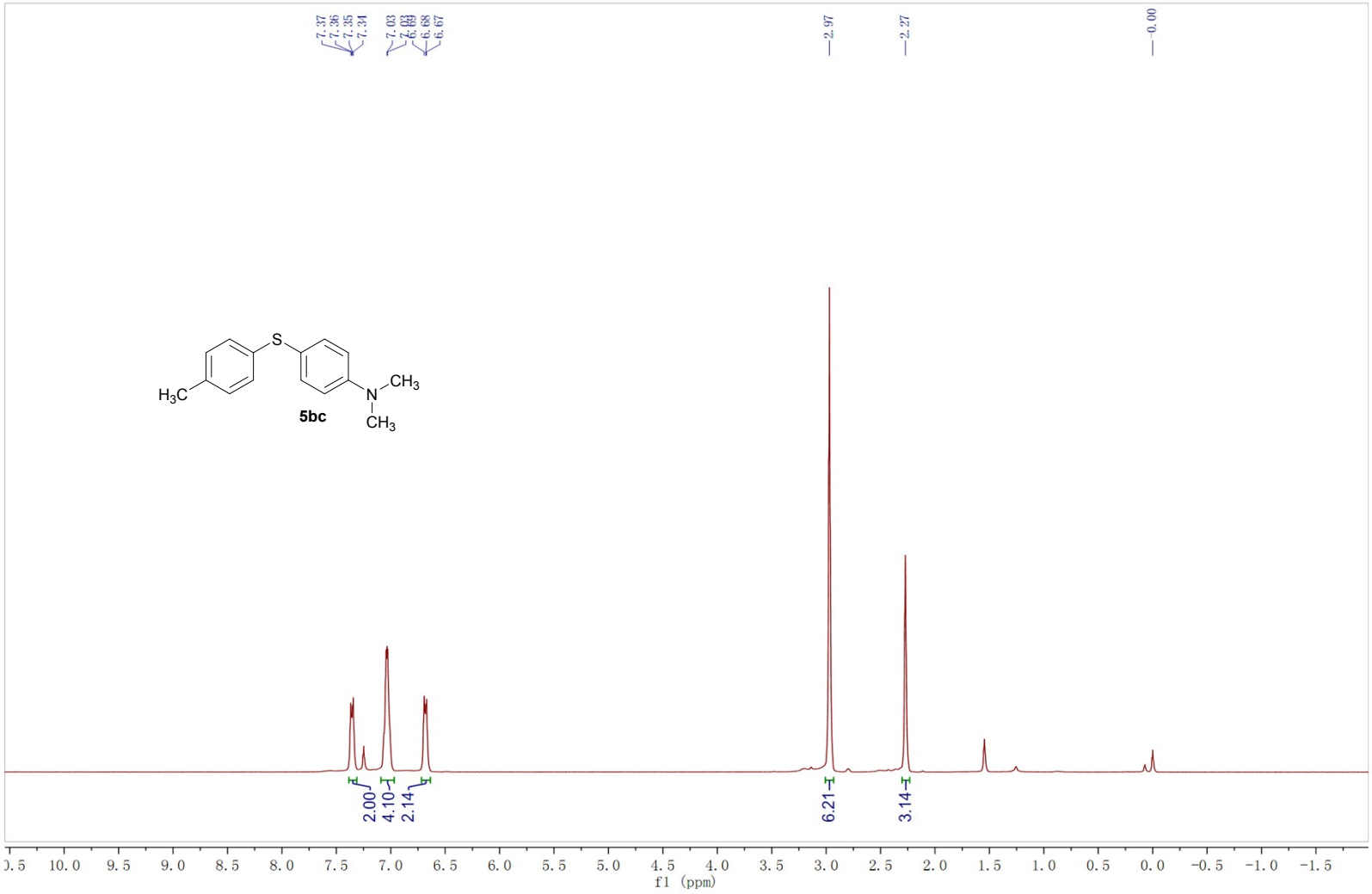

159.63
158.47
138.17
136.05
132.10
127.69
119.59
109.47
106.58
102.61
77.34
77.02
76.71
OH
S
Br
OH
5db
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

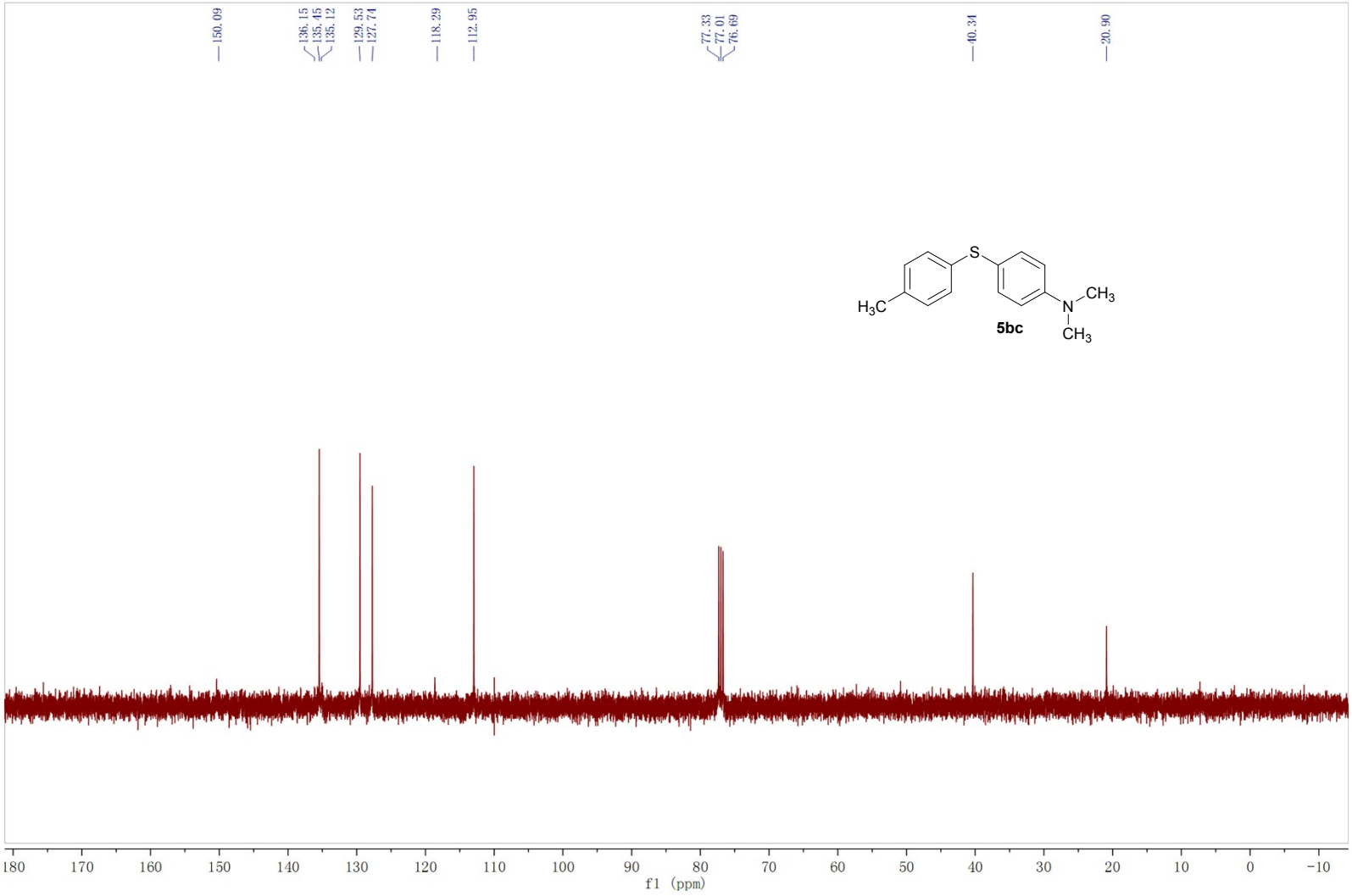

7.40
7.37
7.08
7.05
6.80
6.78
6.65
6.53
6.43
6.41
5.42
3.75
OH
S
MeO
OH
5eb
1.05
2.12
2.29
1.09
1.04
1.05
1.00
3.16
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)

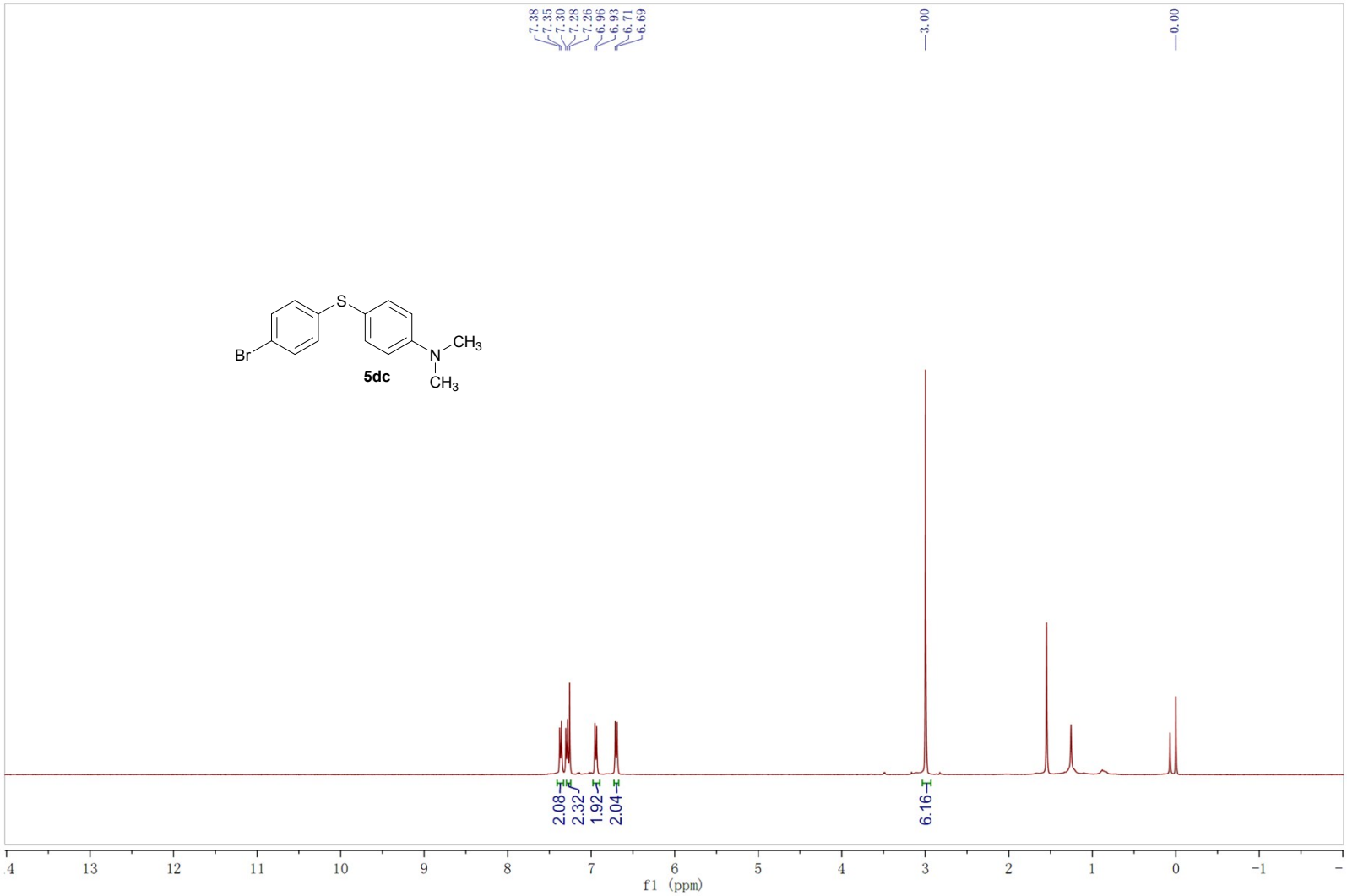

158.92
158.34
137.71
129.39
128.97
127.12
114.87
109.03
102.31
77.32
77.01
76.69
56.39
OH
S
MeO
OH
5eb
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

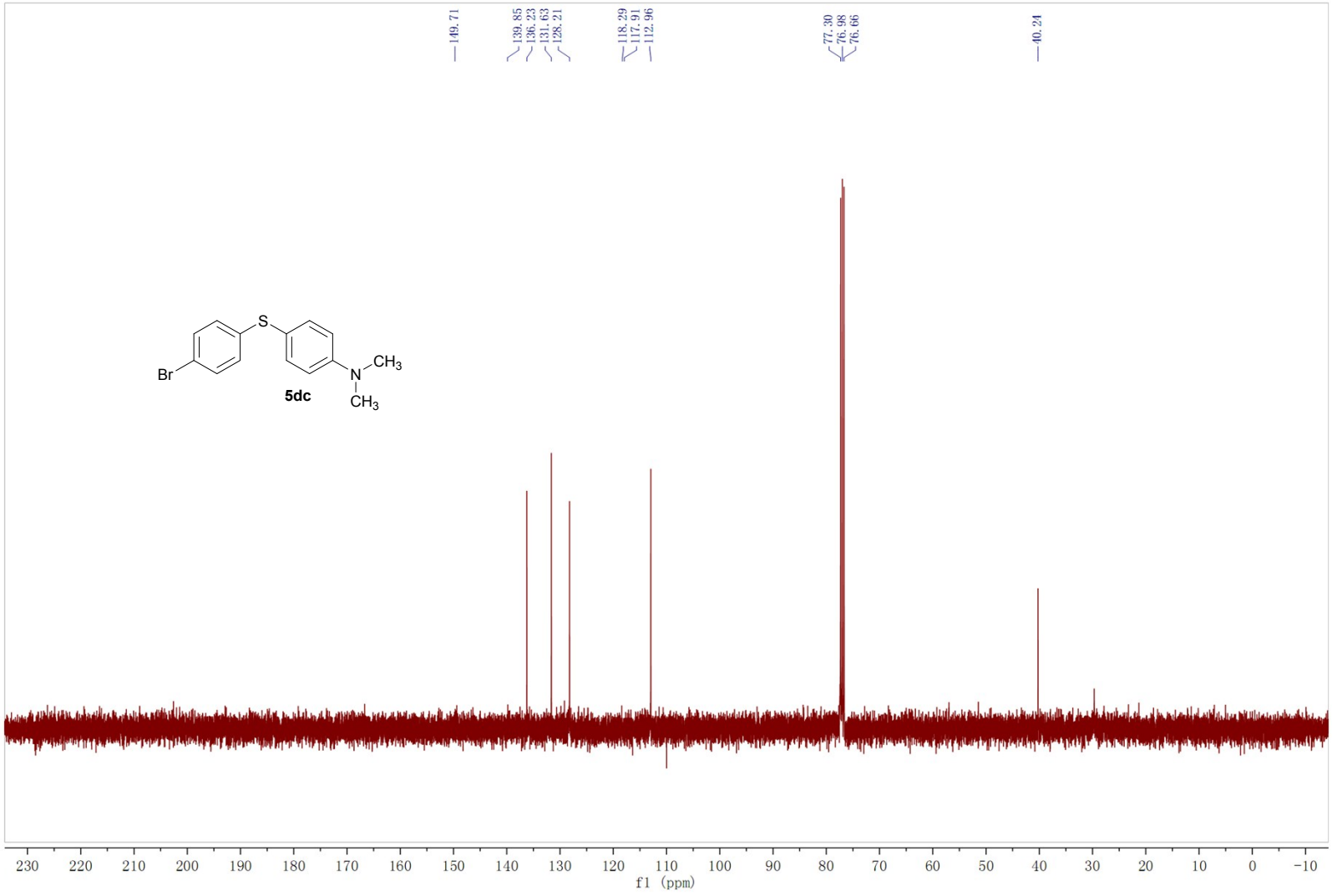

7.37
7.36
7.19
7.17
7.09
7.07
6.69
6.67
2.98
2.96
0.00
S
N
CH3
CH3
5ac
2.00
2.30
3.04
2.10
6.19
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)

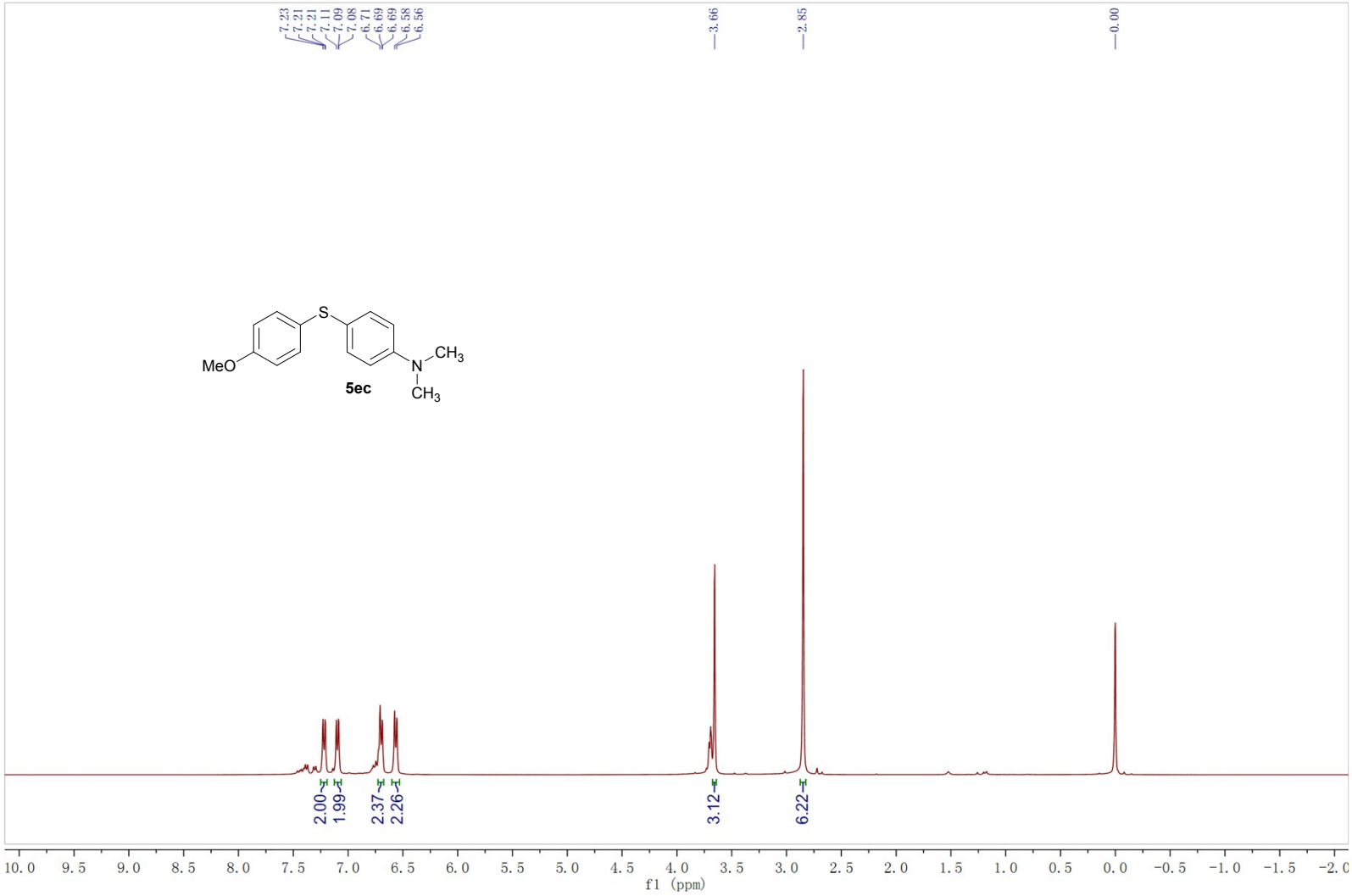

150.67
140.21
136.13
128.71
126.83
124.94
117.27
112.95
77.33
77.01
76.69
40.30
S
N
CH3
CH3
5ac
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

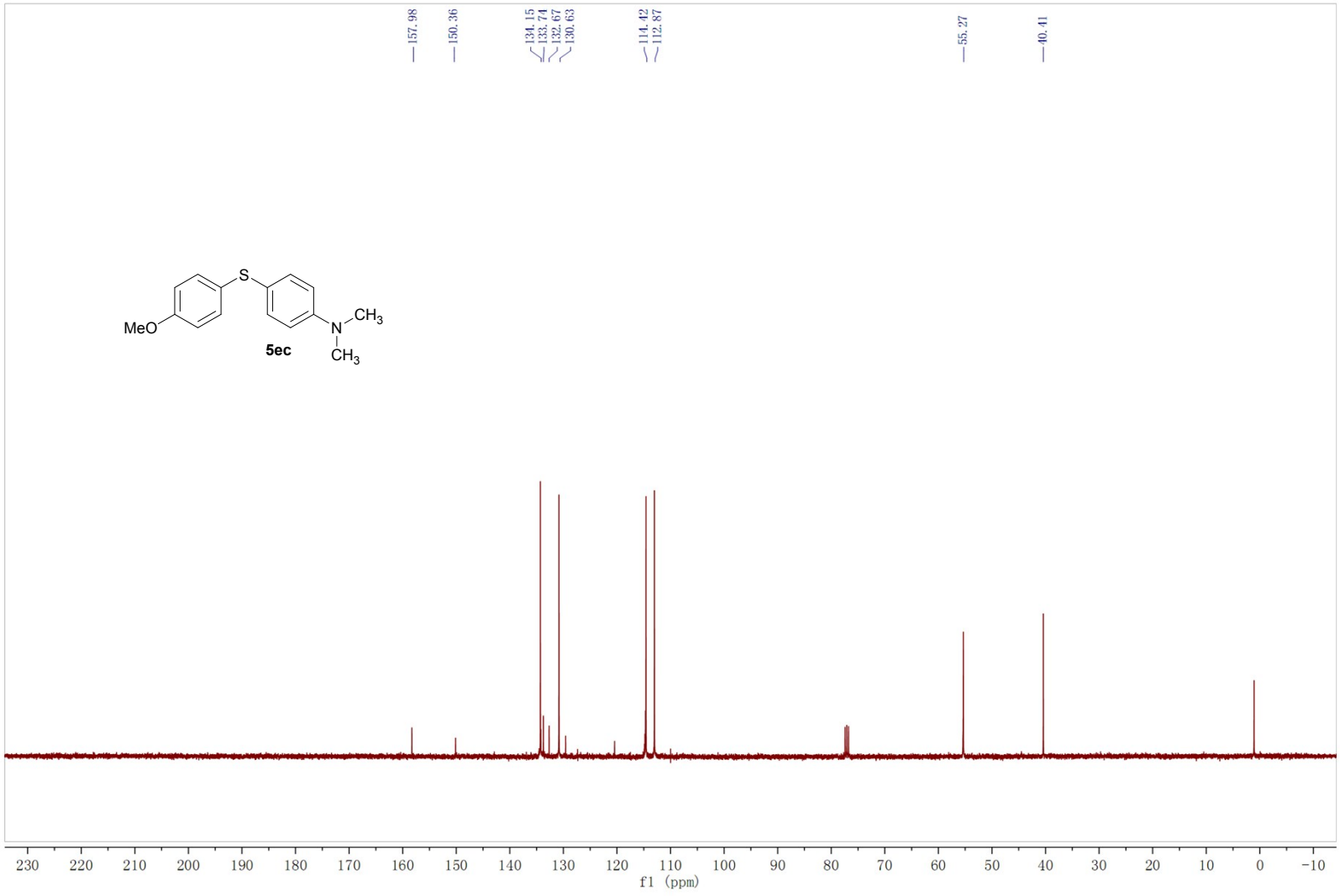

7.37
7.36
7.35
7.34
7.03
6.68
6.67
2.97
2.27
0.00
S
H3C
N
CH3
CH3
5bc
2.00
4.10
2.14
6.21
3.14
f1 (ppm)


150.09
136.15
135.45
135.12
129.53
127.74
118.29
112.95
77.33
77.01
76.69
40.34
20.90
S
H3C
N
CH3
CH3
5bc
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.38
7.35
7.30
7.28
7.26
6.96
6.93
6.71
6.69
3.00
0.00
Br
S
N
CH3
CH3
5dc
2.08
2.32
1.92
2.04
6.16
f1 (ppm)


149.71
139.85
136.23
131.63
128.21
118.29
117.91
112.96
77.30
76.98
76.66
40.24
Br
S
N
CH3
CH3
5dc
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.23
7.21
7.21
7.11
7.09
7.08
6.71
6.69
6.69
6.58
6.56
3.66
2.85
0.00
MeO
S
N
CH3
CH3
5ec
2.00
1.99
2.37
2.26
3.12
6.22
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)


157.98
150.36
134.15
133.74
132.67
130.63
114.42
112.87
55.27
40.41
MeO
S
N
CH3
CH3
5ec
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)