Supporting Information for:

TBAI-HBr system mediated generation of various thioethers with benzenesulfonyl chlorides in PEG_{400}

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General methods

^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.

1-(p-tolylthio)naphthalene-2,7-diol (3aa)[1]:

Yield 84 %； White solid

^1H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, J = 8.0 Hz, 1H), 7.68 (d, J = 8.0 Hz, 1H), 7.52 (s, 1H), 7.19-7.14 (m, 2H), 6.97-6.90 (m, 5H), 5.13 (s, 1H), 2.23 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.4, 155.5, 137.4, 135.7, 132.5, 131.7, 130.7, 129.9, 126.4, 124.8, 115.2, 114.3, 110.3, 107.3, 20.8.

1-(phenylthio)naphthalene-2,7-diol (3ba):

Yield 86 %； White solid

^1H NMR (400 MHz, $CDCl_3$) δ 7.84-7.81 (m, 1H), 7.74-7.70 (m, 1H), 7.51(d, J = 8.0 Hz, 1H), 7.27-7.20 (m, 5H), 7.01-6.98 (m, 3H), 5.14 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.7, 155.5, 137.4, 135.1, 132.7, 130.7, 129.2, 126.1, 125.8, 124.7, 115.3, 114.3, 107.2, 106.2.

1-((4-bromophenyl)thio)naphthalene-2,7-diol (3ca) :

Yield 87 %； White solid

^1H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, J = 8.0 Hz, 1H), 7.71 (d, J = 8.0 Hz, 1H), 7.46 (s, 1H), 7.28 (d, J = 8.0Hz, 1H), 7.17 (d, J = 12.0 Hz, 2H), 7.05 (s, 1H), 6.97 (d, J = 8.0 Hz, 1H), 6.86 (d, J = 8.0 Hz, 2H), 5.15 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.7, 155.8, 137.1, 136.7, 134.4, 132.9, 132.2, 130.8, 127.7, 115.4, 114.4, 114.3, 107.0, 106.

1-((4-methoxyphenyl)thio)naphthalene-2,7-diol (3da) :

Yield 81 %； White solid

^1H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, J = 8.0 Hz, 1H), 7.68 (d, J = 4.0 Hz, 1H), 7.56 (d, J = 4.0 Hz, 1H), 7.28 (d, J = 8.0 Hz, 1H), 7.17-7.13 (m, 1H), 6.99-6.96 (m, 3H), 6.71-6.69 (m, 2H), 5.58 (s, 1H), 3.68 (d, J = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 158.2, 157.3, 137.2, 132.4, 130.7, 130.4, 128.5, 125.9, 124.7, 115.3, 115.0, 114.2, 108.0, 107.3

6-bromo-1-(phenylthio)naphthalen-2-ol (3ab) [1]:

Yield 92 %； White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, J = 12.0 Hz, 1H), 7.93 (s, 1H), 7.77 (d, J = 8.0 Hz, 1H), 7.54-7.51 (m, 1H), 7.33 (d, J = 8.0 Hz, 1H), 7.20 (s, 1H), 6.98 (d, J = 12.0 Hz, 2H), 6.91 (d, J = 12.0 Hz, 2H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.7, 155.8, 137.1, 136.7, 134.4, 132.9, 132.2, 130.8, 127.7, 115.4, 114.3, 114.2, 107.0, 105.9.

4-(p-tolylthio)benzene-1,3-diol (3ac)[2]:

Yield 90 %；Brown solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (d, J = 8.0 Hz, 1H), 6.96 (d, J = 8.0 Hz, 2H), 6.89 (d, J = 8.0 Hz, 2H), 6.53 (s, 1H), 6.48 (s, 1H), 6.37 (d, J = 8.0 Hz, 1H), 5.18 (s, 1H), 2.19 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 158.4, 138.0, 135.9, 132.9, 129.9, 126.7, 109.1, 107.8, 102.4, 20.85.

4-(phenylthio)benzene-1,3-diol (3bc)[2]:

Yield 89 %；Brown solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (d, J = 8.0 Hz, 1H), 7.16-7.12 (m, 2H), 7.06-7.05 (m, 1H), 6.97 (d, J = 8.0 Hz, 2H), 6.50 (d, J = 8.0 Hz, 2H), 6.39 (d, J = 8.0 Hz, 1H), 5.29 (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.

4-((4-bromophenyl)thio)benzene-1,3-diol (3cc)[2]:

Yield 87 %；Brown solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.25 (m, 3H), 6.89 (d, J = 8.0 Hz, 2H), 6.57 (s, 1H), 6.48 (d, J = 12.0 Hz, 2H), 5.47 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.5, 158.5, 138.1, 136.1, 132.1, 127.7, 119.6, 109.4, 106.8, 102.6.

4-((4-methoxyphenyl)thio)benzene-1,3-diol (3dc):

Yield 82 %；Brown solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41-7.37 (m, 1H), 7.09-7.05 (m, 2H), 6.79 (s, 2H), 6.67 (d, J = 8.0 Hz, 1H), 6.54 (d, J = 8.0 Hz, 1H), 6.43 (s, 1H), 5.51 (s, 1H), 3.76 (d, J = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 158.2, 137.7, 129.7, 129.0, 127.1, 114.9, 109.0, 102.3, 101.7, 55.4.

(2,4-dimethoxyphenyl)(p-tolyl)sulfane (3ad)[3]:

Yield 87 %；White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27-7.23 (m, 1H), 7.11-7.06 (m, 4H), 6.52-6.46 (m, 2H), 3.82 (d, J = 8.0 Hz, 6H), 2.29 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.4, 159.8, 135.7, 135.4, 133.4, 129.6, 129.1, 114.1, 105.4, 99.3, 55.9, 55.4, 20.9.

(2,4-dimethoxyphenyl)(phenyl)sulfane (3bd)[3]:

Yield 87 %；White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35-7.32 (m, 1H)，7.20-7.18 (m, 2H), 7.13-7.11 (m, 3H), 6.52-6.47 (m, 2H), 3.80 (d, J = 8.0 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.8, 160.4, 137.8, 136.8, 128.7, 127.7, 125.4, 112.3, 105.4, 99.3, 55.9, 55.5.

(4-bromophenyl)(2,4-dimethoxyphenyl)sulfane (3cd):

Yield 86 %；White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, J = 8.0 Hz, 1H), 7.30 (d, J = 8.0 Hz, 2H), 6.96 (d, J = 8.0 Hz, 2H),

6.52-6.49 (m, 2H), 3.81 (d, J = 16.0 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.3, 160.6, 137.5, 137.2, 131.7, 128.9, 118.9, 111.3, 105.5, 99.4, 55.9, 55.5.

(2,4-dimethoxyphenyl)(4-methoxyphenyl)sulfane (3dd)[3]:

Yield 81 %；White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 (d, J = 8.0 Hz, 2H), 7.07 (d, J = 8.0 Hz, 1H), 6.83(d, J = 8.0 Hz, 2H), 6.48 (s, 1H), 6.44-6.41 (m, 1H), 3.83 (s, 3H), 7.79 (d, J = 8.0 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7, 158.9, 158.8, 133.4, 132.6, 126.4, 115.8, 114.7, 105.3, 99.1, 55.9, 55.4, 55.3.

p-tolyl(2,4,6-trimethoxyphenyl)sulfane (3ae)[2]:

Yield 88 %；White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.96 (s, 4H), 6.20 (d, J = 8.0 Hz, 2H), 3.86 (s, 3H), 3.80 (d, J = 8.0 Hz, 6H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.7, 162.5, 135.1, 134.1, 129.2, 126.1, 110.0, 91.3, 56.3, 55.4, 20.8.

phenyl(2,4,6-trimethoxyphenyl)sulfane (3be)[2]:

Yield 89 %；White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.13 (d, J = 8.0 Hz, 2H), 7.03 (s, 3H), 6.21 (s, 2H), 3.85 (s, 3H), 3.80 (s, 3H), 2.79 (s, 3H); ^{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,

(4-bromophenyl)(2,4,6-trimethoxyphenyl)sulfane (3ce)[2]:

Yield 91 %；White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 (d, J = 8.0 Hz, 2H), 6.88 (d, J = 8.0 Hz, 2H), 6.21 (s, 2H), 3.86 (s, 3H), 3.80 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.1, 162.4, 138.2, 131.4, 127.3, 117.8, 109.0, 91.2, 56.3, 55.4.

(4-methoxyphenyl)(2,4,6-trimethoxyphenyl)sulfane (3de)[4]:

Yield 85 %；White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.06 (d, J = 8.0 Hz, 2H), 6.73 (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 162.6, 162.3, 157.6, 129.3, 128.6, 114.2, 100.7, 91.3, 56.2, 55.4, 55.2.

3,5-dimethyl-4-(p-tolylthio)phenol (3af):

Yield 81 %；White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.98 (d, J = 8.0 Hz, 2H), 6.81(d, J = 4.0 Hz, 2H), 6.67 (s, 2H), 4.93 (s, 1H), 2.37 (s, 6H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.0, 145.8, 135.0, 134.2, 129.6, 125.4, 122.1, 115.3, 21.9, 20.8.

4-((4-bromophenyl)thio)-3,5-dimethylphenol (3cf):

Yield 83 %；White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28-7.26 (m, 2H), 6.77-6.75 (m, 2H), 6.68 (s, 2H), 4.88 (s, 1H), 2.35 (s, 6H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 156.4, 145.9, 138.0, 131.8, 128.9, 126.7, 117.9, 115.5, 21.8.

4-((4-methoxyphenyl)thio)-3,5-dimethylphenol (3df) :

Yield 80 %； White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.81 (d, J = 12.0 Hz, 2H), 6.68 (d, J = 12.0 Hz, 2H), 6.58 (s, 2H), 4.93 (s, 1H), 3.67 (s, 3H), 2.3 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.3, 130.9, 128.6, 125.9, 124.7, 123.0, 120.9, 119.7, 111.5.

2-(p-tolylthio)-1H-indole (5aa)[5]:

Yield 82 %； White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (s, 1H), 7.61 (d, J = 8.0 Hz, 1H), 7.44-7.40 (m, 2H), 7.25-7.23 (m, 1H), 7.17-7.13 (m, 1H), 7.03 (d, J = 8.0 Hz, 2H), 6.96 (d, J = 8.0 Hz, 2H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.5, 135.5, 134.6, 130.4, 129.5, 129.1, 126.3, 123.0, 120.8, 120.0, 111.5, 103.6, 20.8.

2-(phenylthio)-1H-indole (5ba)[5]:

Yield 78 %； White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (s, 1H), 7.61 (d, J = 8.0 Hz, 1H), 7.47-7.41 (m, 2H), 7.28-7.24 (m, 2H), 7.18-7.02 (m, 5H).

2-((4-bromophenyl)thio)-1H-indole (5ca)[5]:

Yield 81 %； White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (s, 1H), 7.56 (d, J = 8.0 Hz, 1H), 7.46-7.42 (m, 2H), 7.29-7.23 (m, 3H), 7.19-7.15 (m, 1H), 6.95 (d, J = 12.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.6, 136.1, 131.6, 130.7, 128.8, 127.4, 123.2, 121.1, 119.5, 118.3, 111.7, 101.4.

2-((4-methoxyphenyl)thio)-1H-indole (5da)[5]:

Yield 76%； White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (s, 1H), 7.58 (d, J = 8.0 Hz, 1H), 7.25-7.20 (m, 4H), 7.16-7.05 (m, 4H)， 3.47(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.3, 136.4, 129.7, 129.3, 128.7, 127.2, 126.6, 125.0, 123.8, 121.1, 119.9, 111.1, 100.8.

2-(o-tolylthio)-1H-indole (5ea):

Yield 79 %； White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (s, 1H), 7.57 (s, 1H), 7.42 (s, 2H), 7.24 (d, J = 8.0 Hz, 1H), 7.13 (d, J = 8.0 Hz, 2H), 6.71 (s, 1H), 2.48 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.2, 136.6, 134.4, 130.7, 129.8, 129.2, 126.2, 125.3, 124.5, 123.0, 120.9, 119.7, 111.6, 102.7, 19.9.

2-((4-nitrophenyl)thio)-1H-indole (5fa)[5]:

Yield 71 %； Yellow solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (s, 1H), 7.99 (d, J = 8.0 Hz, 2H), 7.53-7.48 (m, 3H), 7.33-7.29 (m, 1H), 7.25-7.11 (m, 1H), 7.13 (d, J = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.1, 145.0, 136.4, 131.2, 128.4, 125.1, 123.8, 123.5, 121.4, 119.2, 111.9, 100.4.

2-phenyl-3-(p-tolylthio)imidazo[1,2-a]pyridine (5ab)[6]:

Yield 69 %；White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ8.27 (d, J = 8.0 Hz, 1H), 8.21 (d, J = 8.0 Hz, 2H), 7.72 (d, J = 8.0 Hz, 1H), 7.45-7.25 (m, 4H), 7.01 (d, J = 8.0 Hz, 2H), 6.91 (d, J = 8.0 Hz, 2H), 6.85 (t, J = 8.0 Hz, 1H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.2, 151.2, 147.0, 136.0, 133.4, 131.5, 130.2, 128.5, 128.4, 126.6, 125.8, 124.5, 117.6, 113.0, 106.5, 20.9.

2-phenyl-3-(phenylthio)imidazo[1,2-a]pyridine (5bb)[6]:

Yield 64 %；White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, J = 8.0 Hz, 1H), 8.20 (d, J = 8.0 Hz, 2H), 7.74 (d, J = 8.0 Hz, 1H), 7.45-7.42 (m, 2H), 7.39-7.31 (m, 2H), 7.22-7.19 (m, 2H), 7.15-7.11 (m, 1H), 7.00 (d, J = 8.0 Hz, 2H), 6.88-6.85 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.3, 147.1, 135.1, 133.2, 129.4, 128.6, 128.4, 128.3, 126.8, 126.1, 125.6, 124.5, 117.6, 113.4, 106.2.

3-((4-bromophenyl)thio)-2-phenylimidazo[1,2-a]pyridine (5cb)[6]:

Yield 65 %；White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ8.22 (d, J = 8.0 Hz, 1H), 8.17 (d, J = 8.0 Hz, 2H), 7.73 (d, J = 12.0 Hz, 1H), 7.45-7.25 (m, 6H), 6.88-6.83 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.7, 147.2, 134.4, 133.1, 132.5, 128.8, 128.5, 128.3, 127.1, 126.9, 124.3, 119.8, 117.8, 113.3, 105.6.

methyl 3-(p-tolylthio)indolizine-1-carboxylate (5ac)[7]:

Yield 73 %；White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27-8.24 (m, 2H), 7.65 (s, 1H), 7.17-7.13 (m, 1H), 6.98 (d, J = 8.0 Hz, 2H), 6.77-6.74 (m, 1H), 3.91(s, 3H), 2.23 (s, 3H);

methyl 3-(phenylthio)indolizine-1-carboxylate (5bc)[7]:

Yield 61 %；White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27-8.25 (m, 2H), 7.68 (s, 1H), 7.20-7.17 (m, 3H), 7.13-7.09 (m, 1H), 6.95 (d, J = 8.0 Hz, 2H), 6.80-6.77 (m, 1H), 3.92 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.8, 138.4, 136.5, 129.2, 126.5, 125.9, 124.5, 124.1, 119.8, 113.2, 110.5, 104.43, 50.8.

methyl 3-((4-bromophenyl)thio)indolizine-1-carboxylate (5cc)[7]:

Yield 69 %；White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, J = 8.0 Hz, 1H), 8.21 (s, 1H), 7.67 (s, 1H), 7.29 (d, J = 8.0 Hz, 2H), 7.21 (s, 1H), 6.85-6.81 (m, 3H), 3.92 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.7, 136.6, 133.0, 130.3, 125.3, 124.8, 122.4, 117.9, 117.8, 111.5, 107, 102.6, 49.2.

3-methyl-1-phenyl-4-(p-tolylthio)-1H-pyrazol-5-ol (7aa)[8]:

Yield 82 %；White solid

^{1}H NMR (400 MHz, ^{d6}DMSO) δ 12.1 (s, 1H), 7.71 (d, J = 8.0 Hz, 2H), 7.46-7.42 (m, 2H), 7.26 (d, J = 8.0 Hz, 1H), 7.07 (d, J = 8.0 Hz, 2H), 6.96 (d, J = 8.0 Hz, 2H), 2.48 (s, 3H), 2.21 (s, 3H); ^{13}C NMR (100 MHz, ^{d6}DMSO) δ 156.1, 152.4, 138.7, 135.2, 134.8, 130.1, 129.3, 126.1, 125.8, 121.2, 87.1, 20.8, 12.8.

3-methyl-1-phenyl-4-(phenylthio)-1H-pyrazol-5-ol (7ba):

Yield 80 %；White solid

^{1}H NMR (400 MHz, ^{d6}DMSO) δ 12.2 (s, 1H), 7.72 (d, J = 8.0 Hz, 2H), 7.47-7.43 (m, 2H), 7.28-7.24 (m, 3H), 7.11-7.05 (m, 3H), 2.10 (s, 1H); ^{13}C NMR (100 MHz, ^{d6}DMSO) δ 157.4, 152.5, 138.8, 138.6, 129.5, 129.4, 126.2, 125.4, 121.1, 121.0, 88.4, 12.7.

4-((4-bromophenyl)thio)-3-methyl-1-phenyl-1H-pyrazol-5-ol (7ca)[8]:

Yield 87 %；Brown solid

^{1}H NMR (400 MHz, ^{d6}DMSO) δ 12.28 (s, 1H), 7.73 (d, J = 8.0 Hz, 2H), 7.47-7.42 (m, 4H), 7.27-7.23 (m, 1H), 7.01 ((d, J = 8.0 Hz, 2H), 2.11 (s, 3H); ^{13}C NMR (100 MHz, ^{d6}DMSO) δ 152.9, 138.6, 132.2, 129.4, 127.3, 126.2, 121.2, 118.1, 12.7.

4-((4-fluorophenyl)thio)-3-methyl-1-phenyl-1H-pyrazol-5-ol (7da)[8]:

Yield 75 %；White solid

^{1}H NMR (400 MHz, ^{d6}DMSO) δ 7.74 (d, J = 8.0 Hz, 2H), 7.46-7.43 (m, 2H), 7.26-7.23 (m, 1H), 7.12 (d, J = 4.0 Hz, 4H), 2.13 (s, 3H); ^{13}C NMR (100 MHz, ^{d6}DMSO) δ 161.9, 159.6, 157.4, 152.4, 138.5, 134.3, 134.2, 129.4, 129.3, 127.7, 127.6, 126.2, 121.2, 120.9, 116.6, 116.4, 12.7.

4-((4-chlorophenyl)thio)-3-methyl-1-phenyl-1H-pyrazol-5-ol (7ea)[8]:

Yield 85 %；White solid

^{1}H NMR (400 MHz, ^{d6}DMSO) δ 12.19 (s, 1H), 7.74 (d, J = 8.0 Hz, 2H), 7.47-7.43 (m, 2H), 7.32-7.23 (m, 3H), 7.08 (d, J = 12.0 Hz, 2H), 2.11 (s, 3H); ^{13}C NMR (100 MHz, ^{d6}DMSO) δ 152.3, 138.5, 138.0, 129.9, 129.4, 129.3, 129.2, 129.1, 127.0, 126.2, 125.3, 121.2, 120.7, 118.4, 12.7.

3-methyl-1-phenyl-4-(o-tolylthio)-1H-pyrazol-5-ol (7fa)[8]:

Yield 81 %；White solid

^{1}H NMR (400 MHz, ^{d6}DMSO) δ 7.72 (d, J = 8.0 Hz, 2H), 7.47 (d, J = 8.0 Hz, 2H), 7.31 (d, J = 8.0 Hz, 1H), 7.19 (d, J = 4.0 Hz, 1H), 7.16 (d, J = 4.0 Hz, 1H), 7.07 (d, J = 8.0 Hz, 1H), 7.01 (d, J = 8.0 Hz, 1H), 6.74 (d, J = 8.0 Hz, 1H), 2.36 (s, 3H), 2.10 (s, 3H); ^{13}C NMR (100 MHz, ^{d6}DMSO) δ 157.4, 152.6, 138.6, 137.7, 134.0, 130.1, 129.4, 127.0, 126.2, 125.0, 124.1, 121.2, 87.4, 19.7, 12.7.

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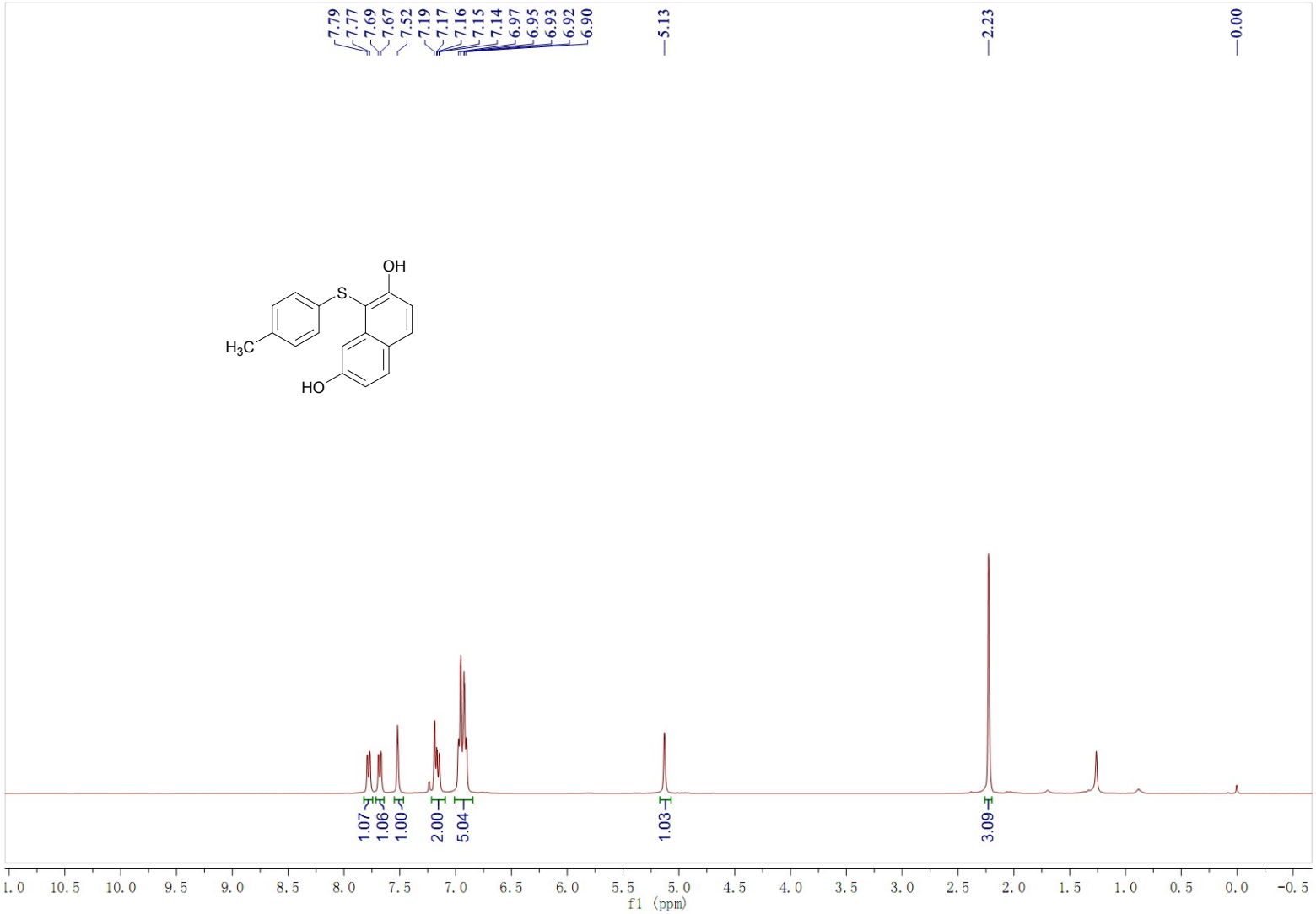
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6.93
6.92
6.90
5.13
2.23
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H3C
HO
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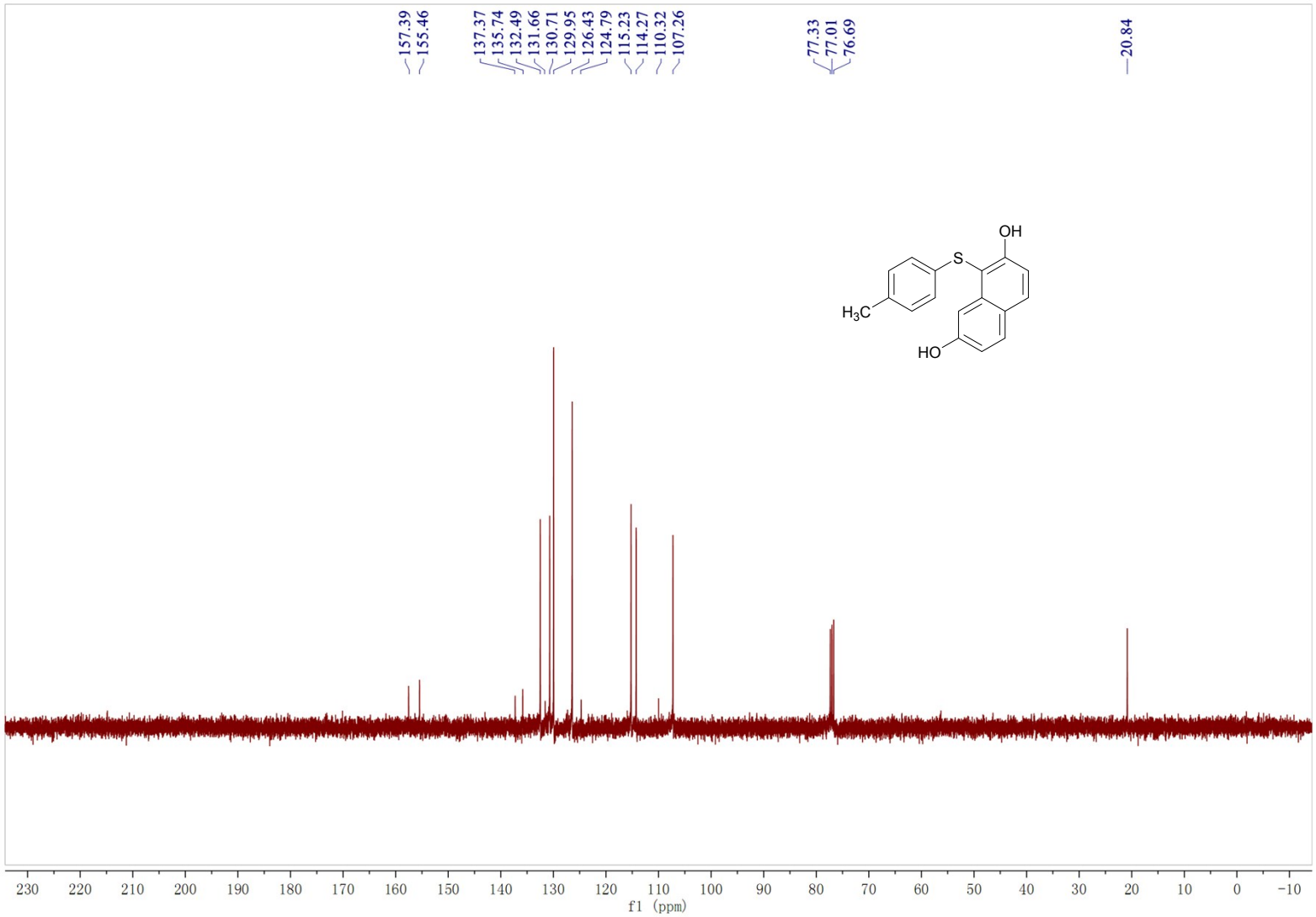
1.06
1.00
2.00
5.04
1.03
3.09
f1 (ppm)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110.32
107.26
77.33
77.01
76.69
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OH
S
H3C
HO
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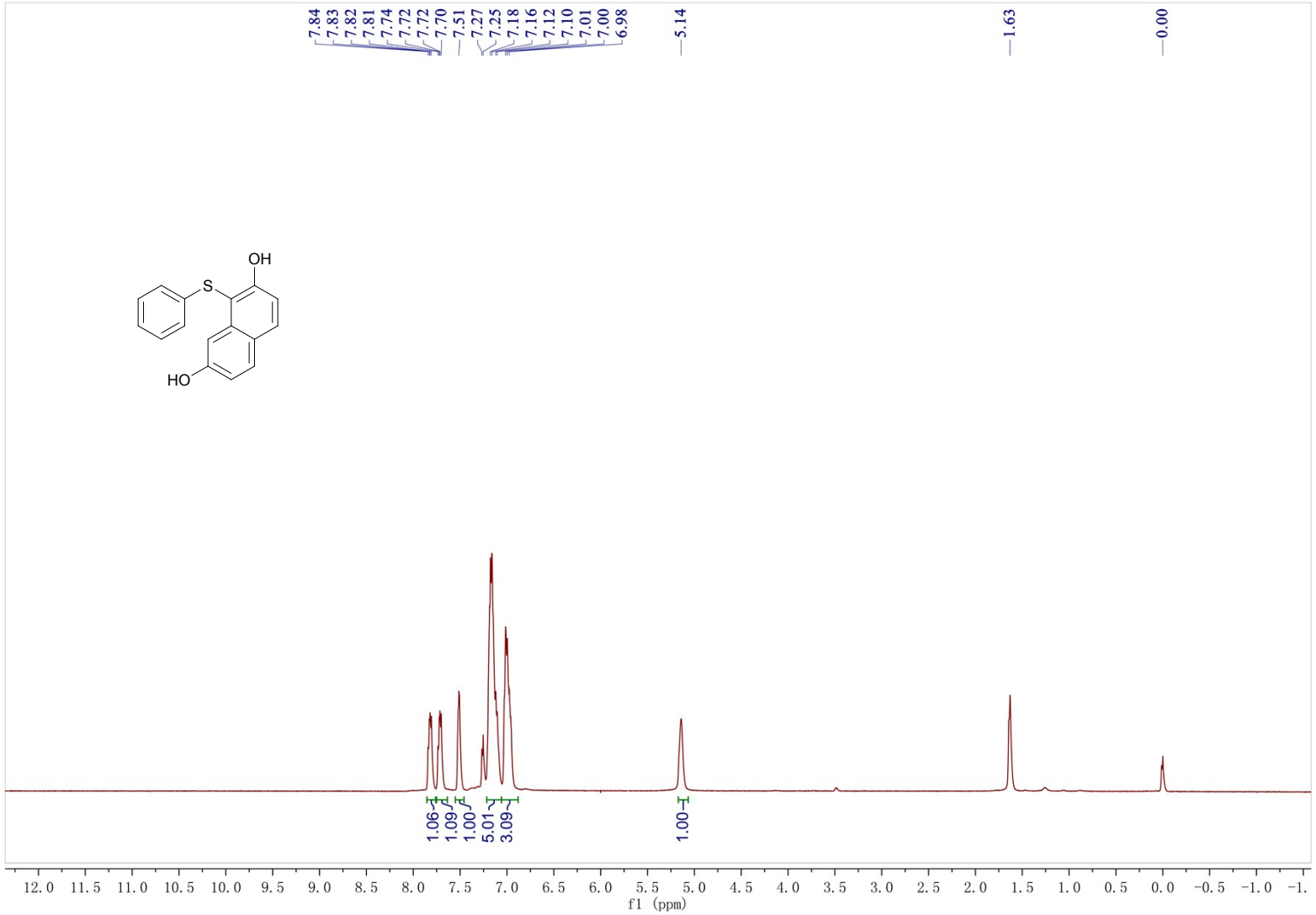
f1 (ppm)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7.18
7.16
7.12
7.10
7.01
7.00
6.98
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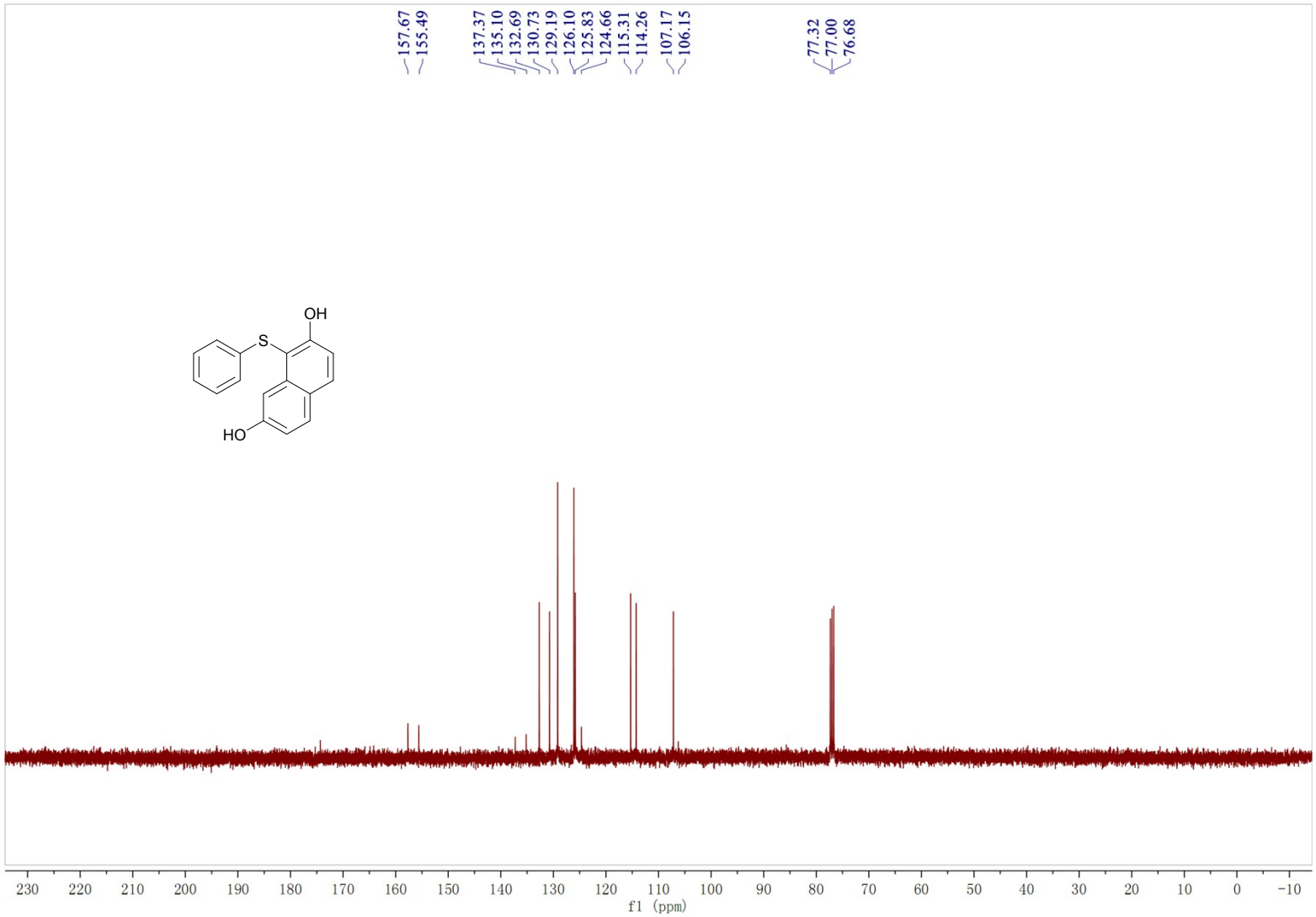
S
HO
1.06
1.09
1.00
5.01
3.09
1.00
f1 (ppm)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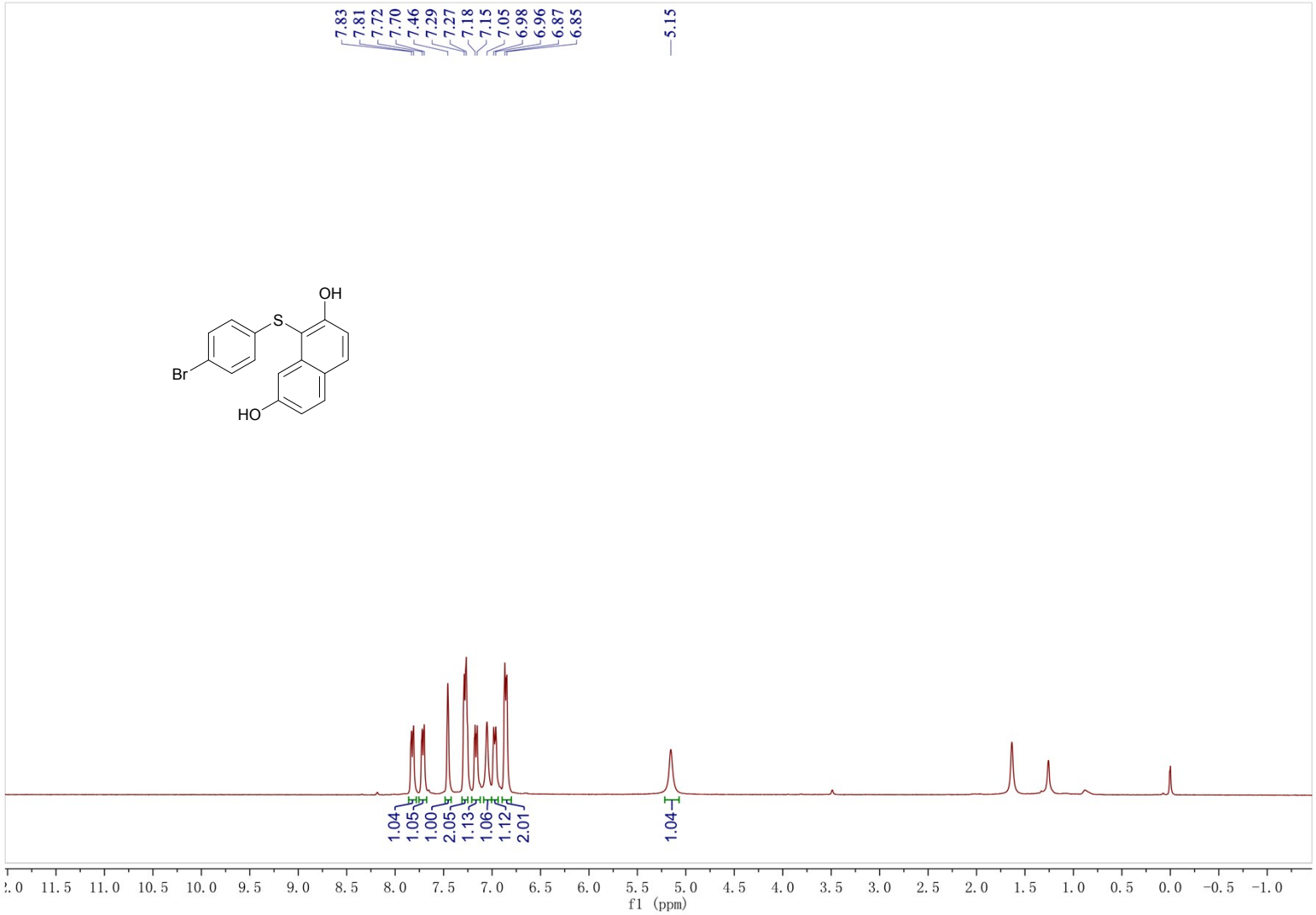
f1 (ppm)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6.87
6.85
5.15
OH
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Br
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1.05
1.00
2.05
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1.06
1.12
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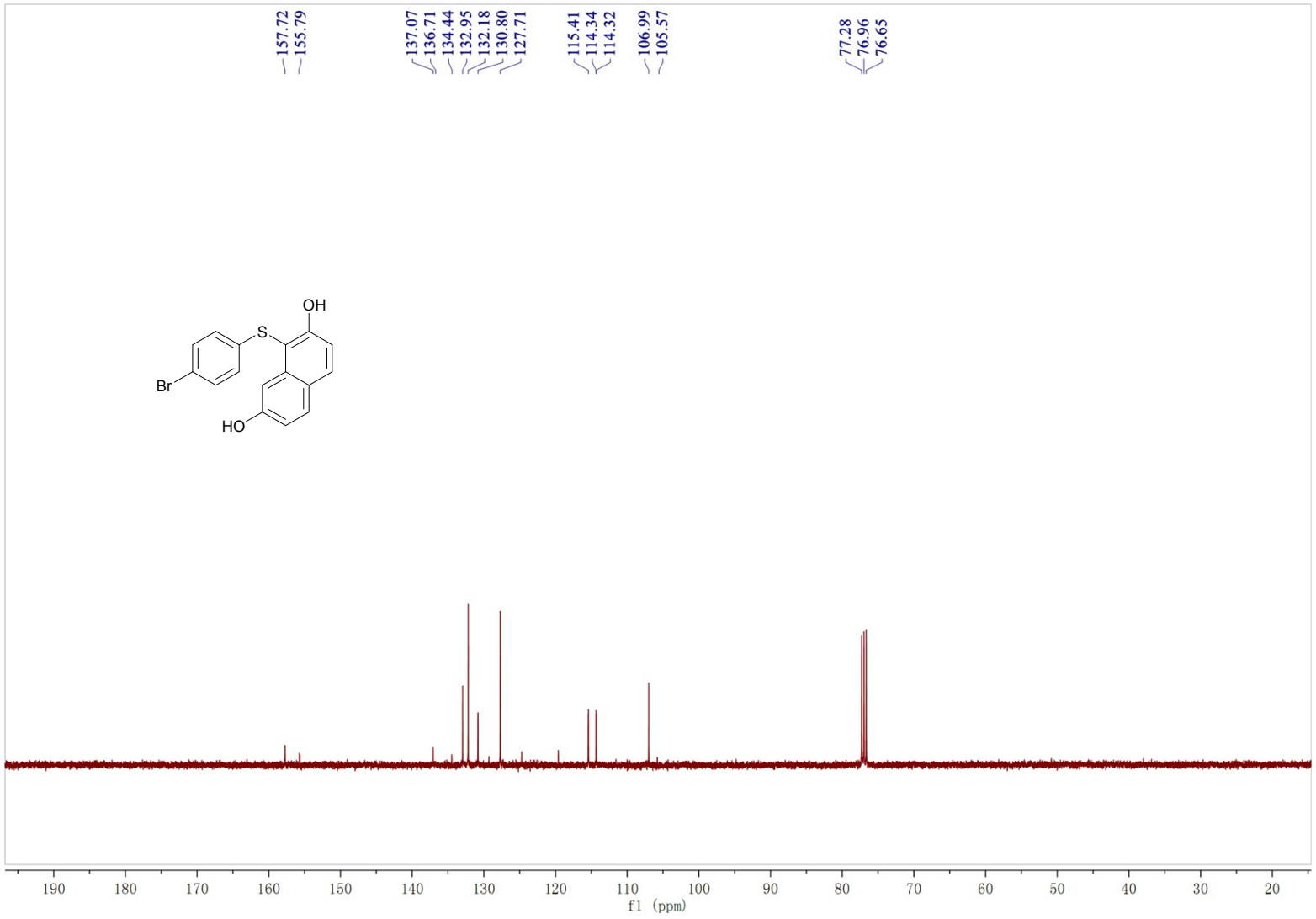
1.04
f1 (ppm)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77.28
76.96
76.65
OH
S
Br
HO
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90
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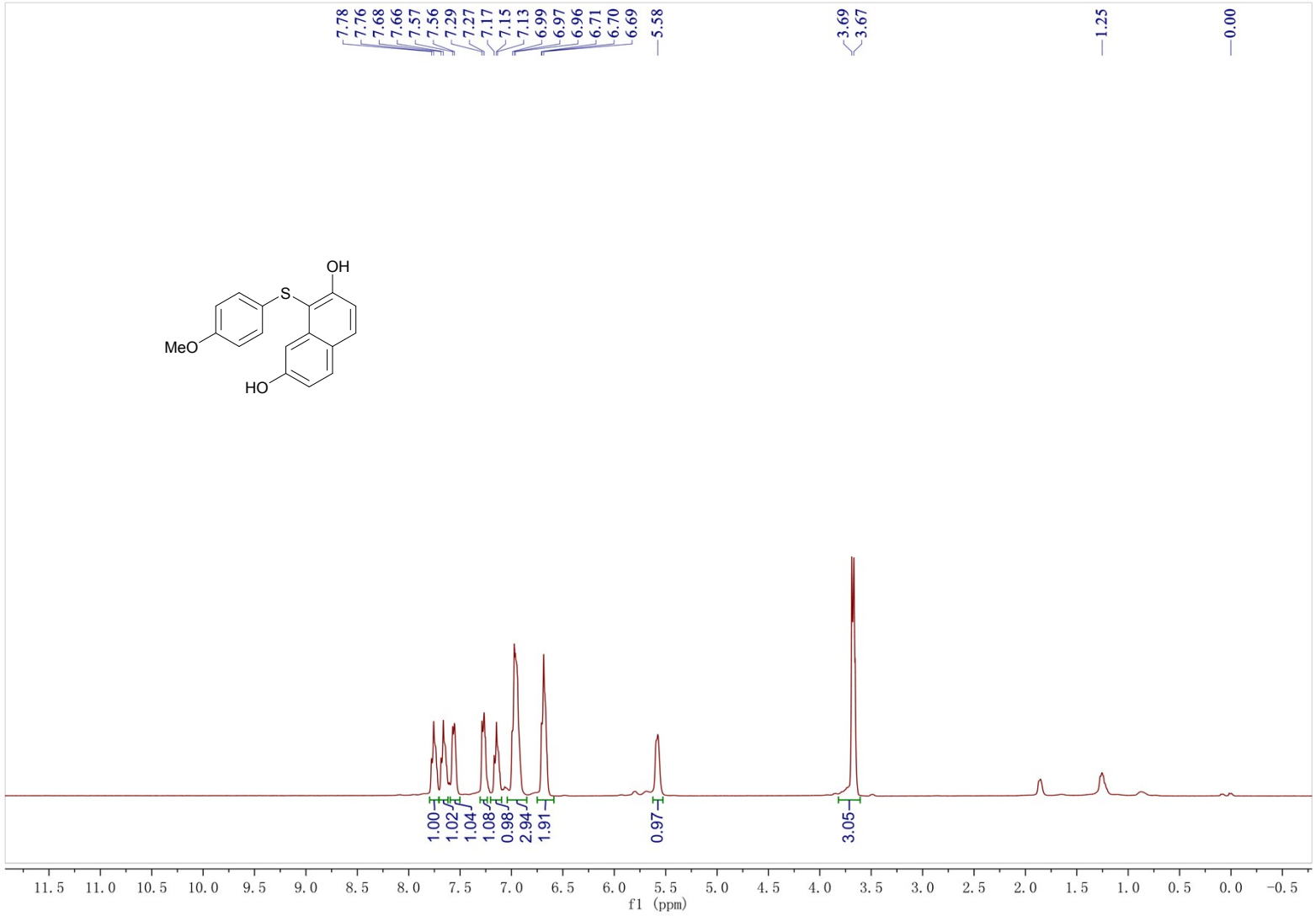
70
60
50
40
30
20
f1 (ppm)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6.96
6.71
6.70
6.69
5.58
3.69
3.67
1.25
0.00
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S
MeO
HO
1.00
1.02
1.04
1.08
0.98
2.94
1.91
0.97
3.05
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5
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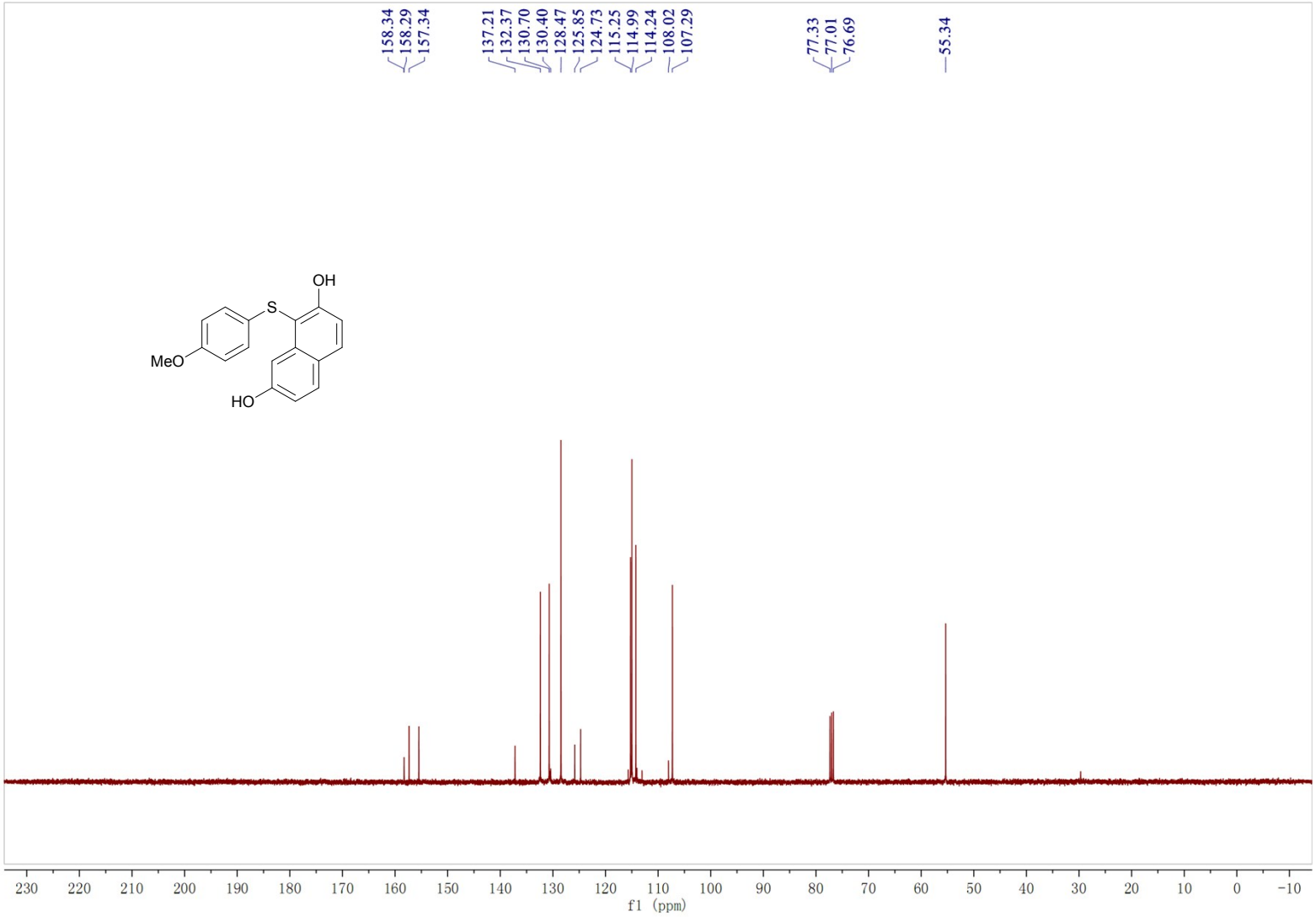
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108.02
107.29
77.33
77.01
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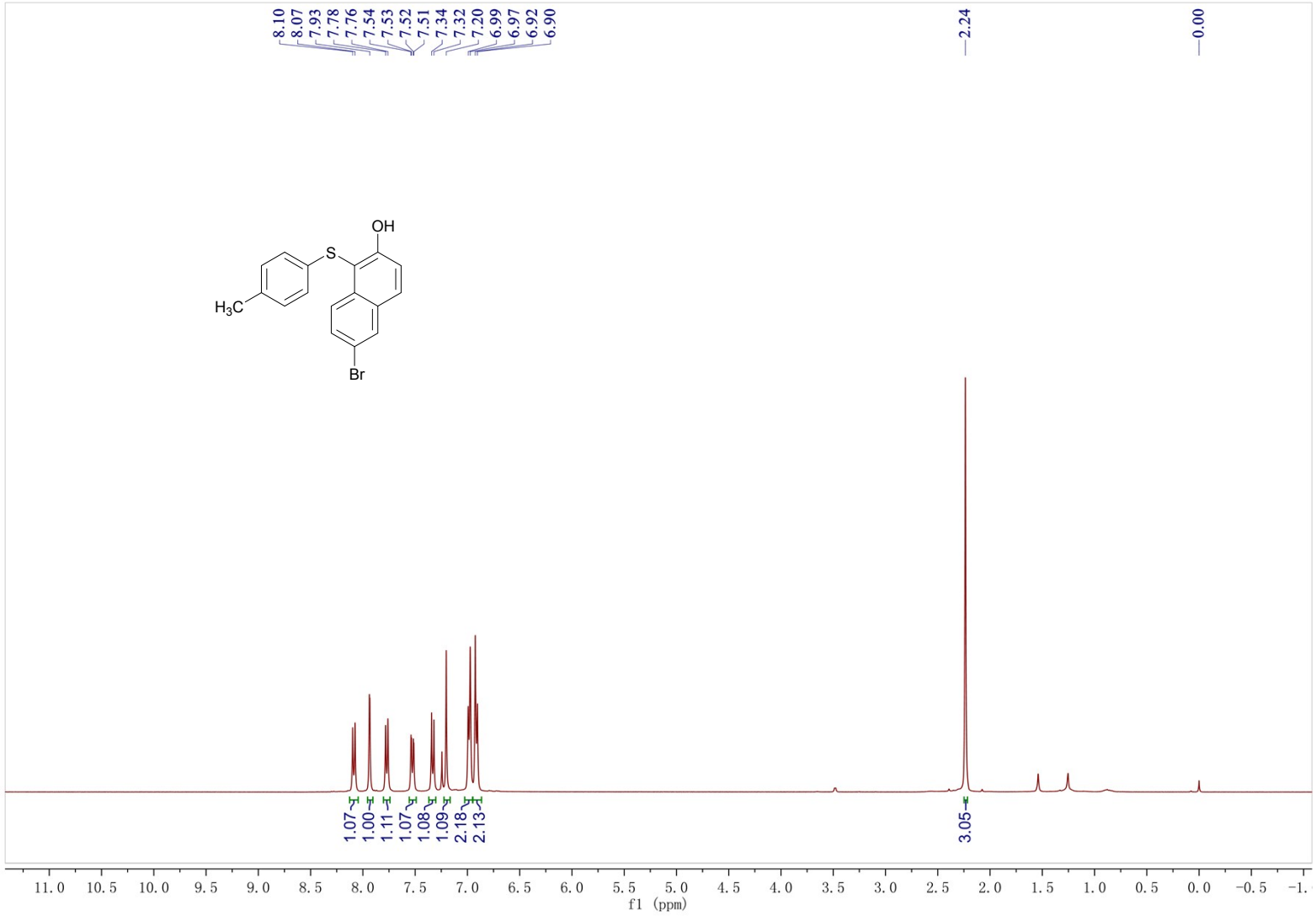
OH
S
MeO
HO
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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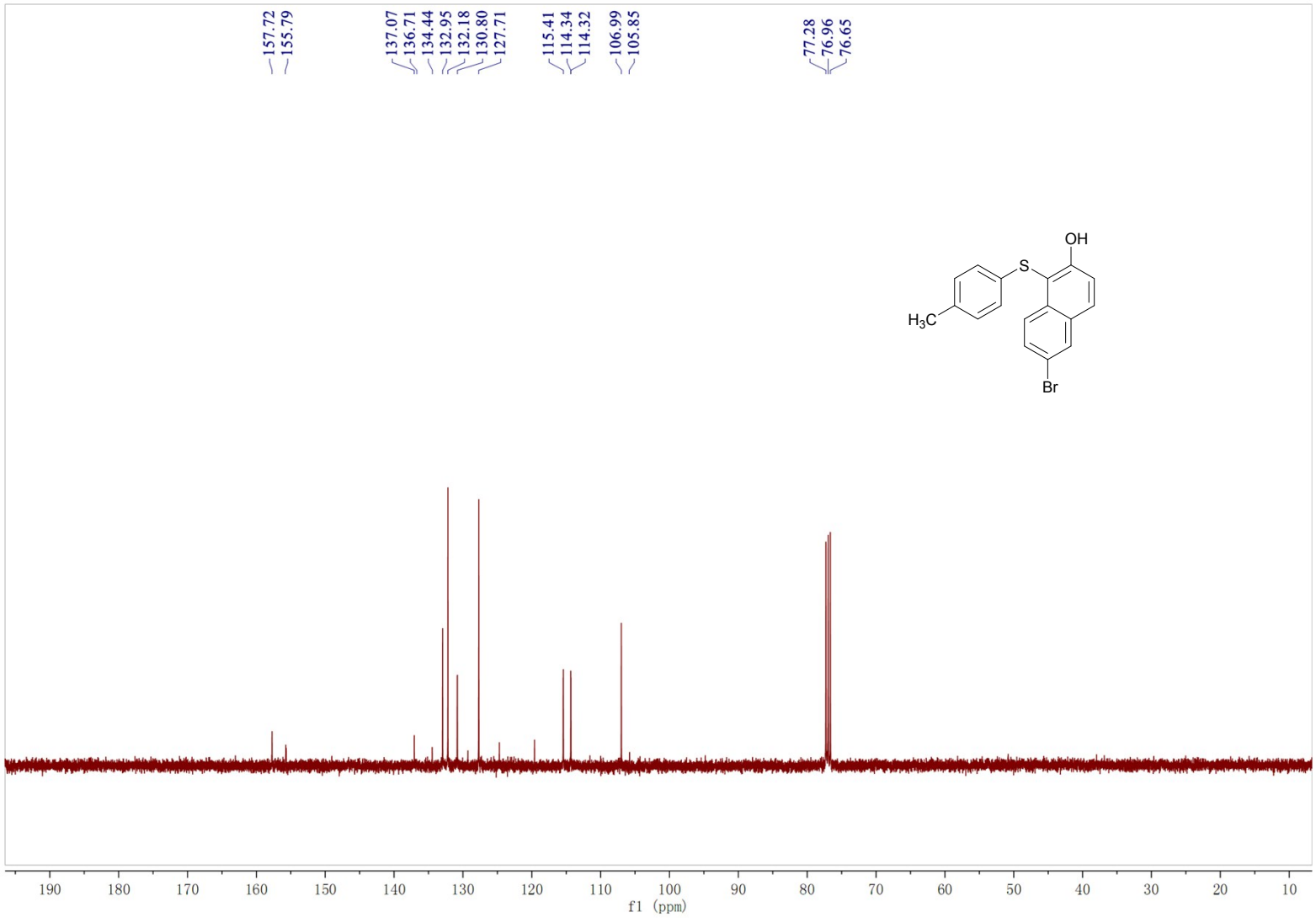
6.99
6.97
6.92
6.90
2.24
0.00
OH
S
H3C
Br
1.07
1.00
1.11
1.07
1.08
1.09
2.18
2.13
3.05
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.
f1 (ppm)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114.32
106.99
105.85
77.28
76.96
76.65
OH
S
H3C
Br
190
180
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140
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120
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100
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80
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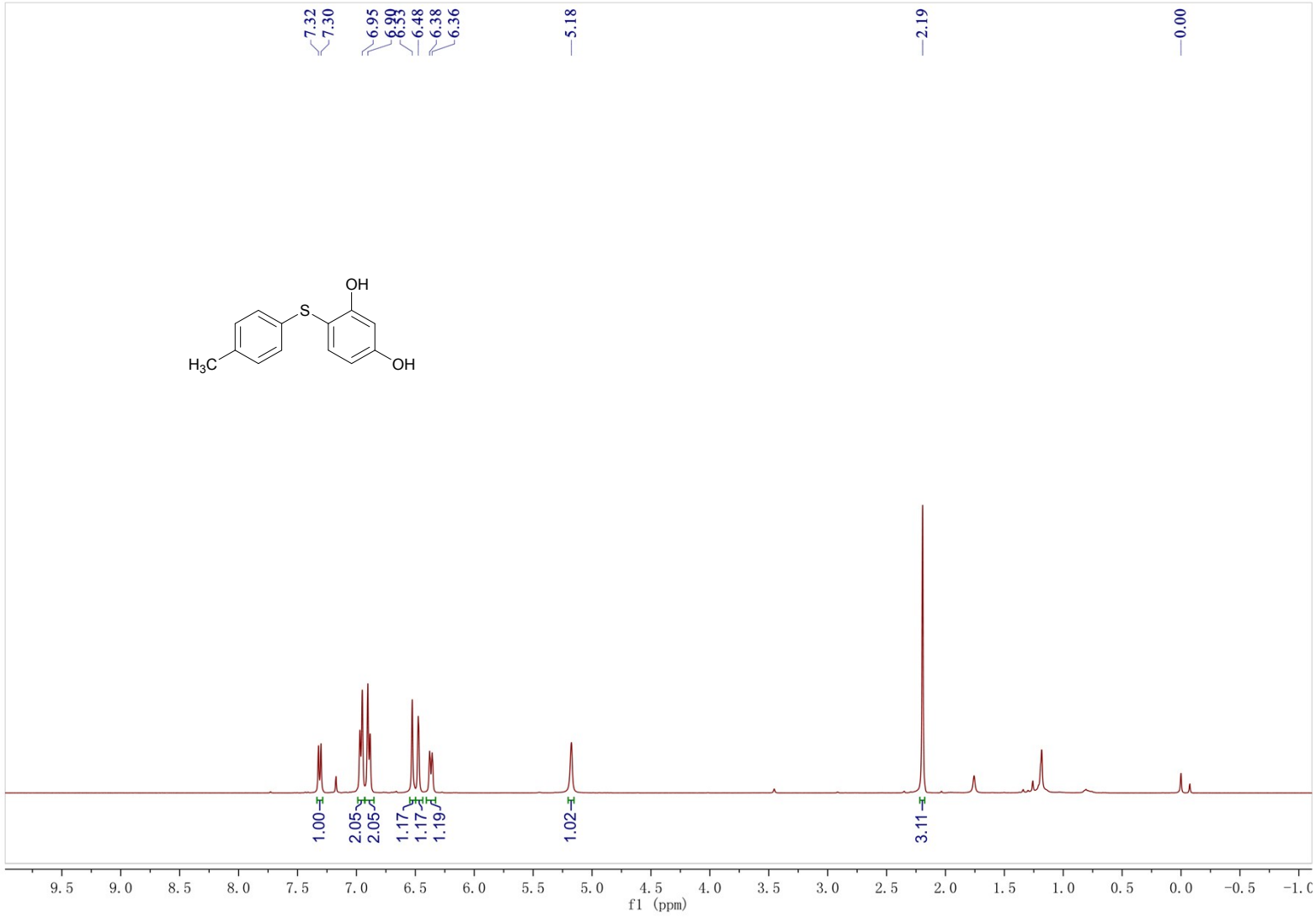
60
50
40
30
20
10
f1 (ppm)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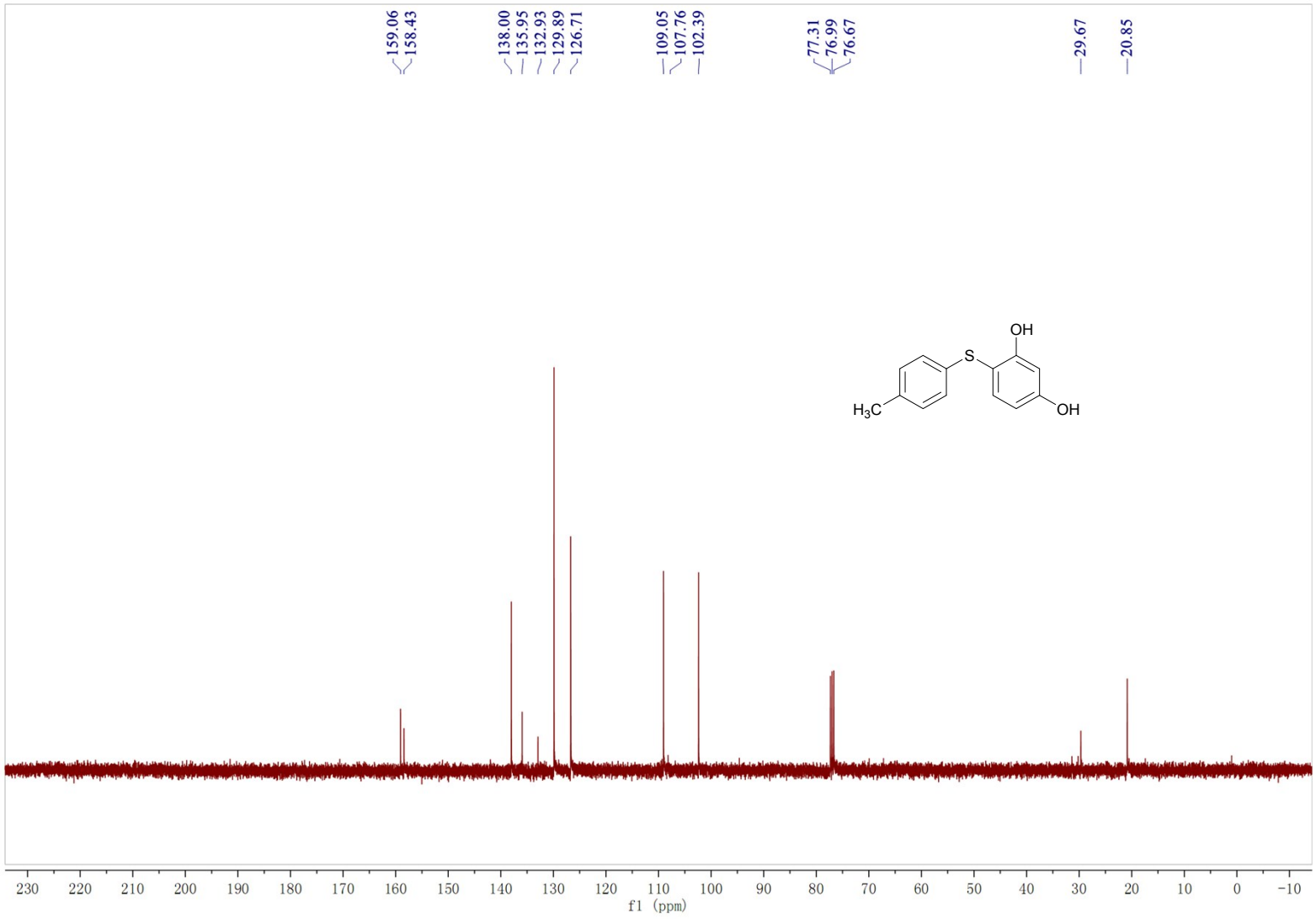
H3C
OH
1.00
2.05
2.05
1.17
1.17
1.19
1.02
3.11
f1 (ppm)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S
H3C
OH
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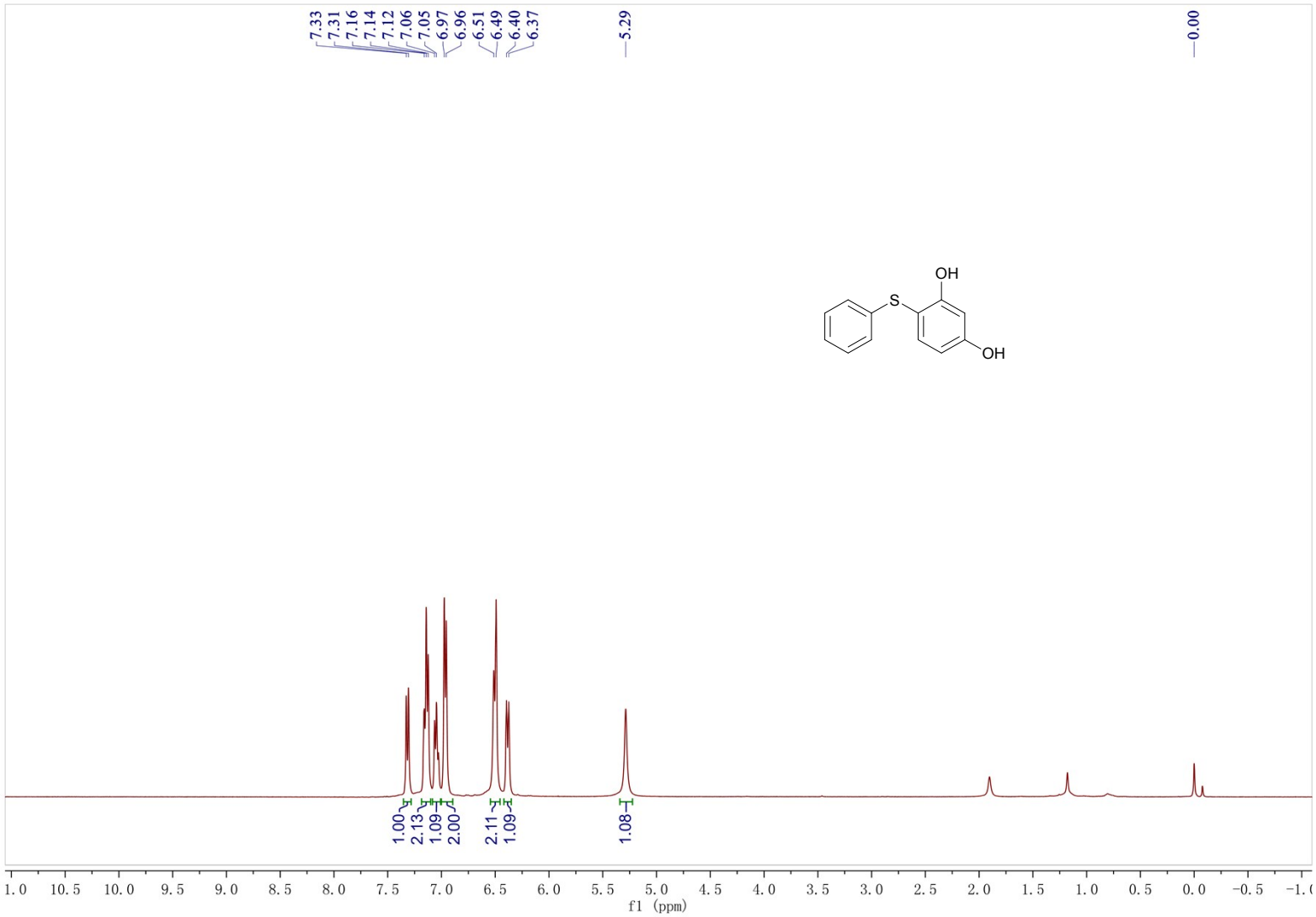
f1 (ppm)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6.97
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6.37
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OH
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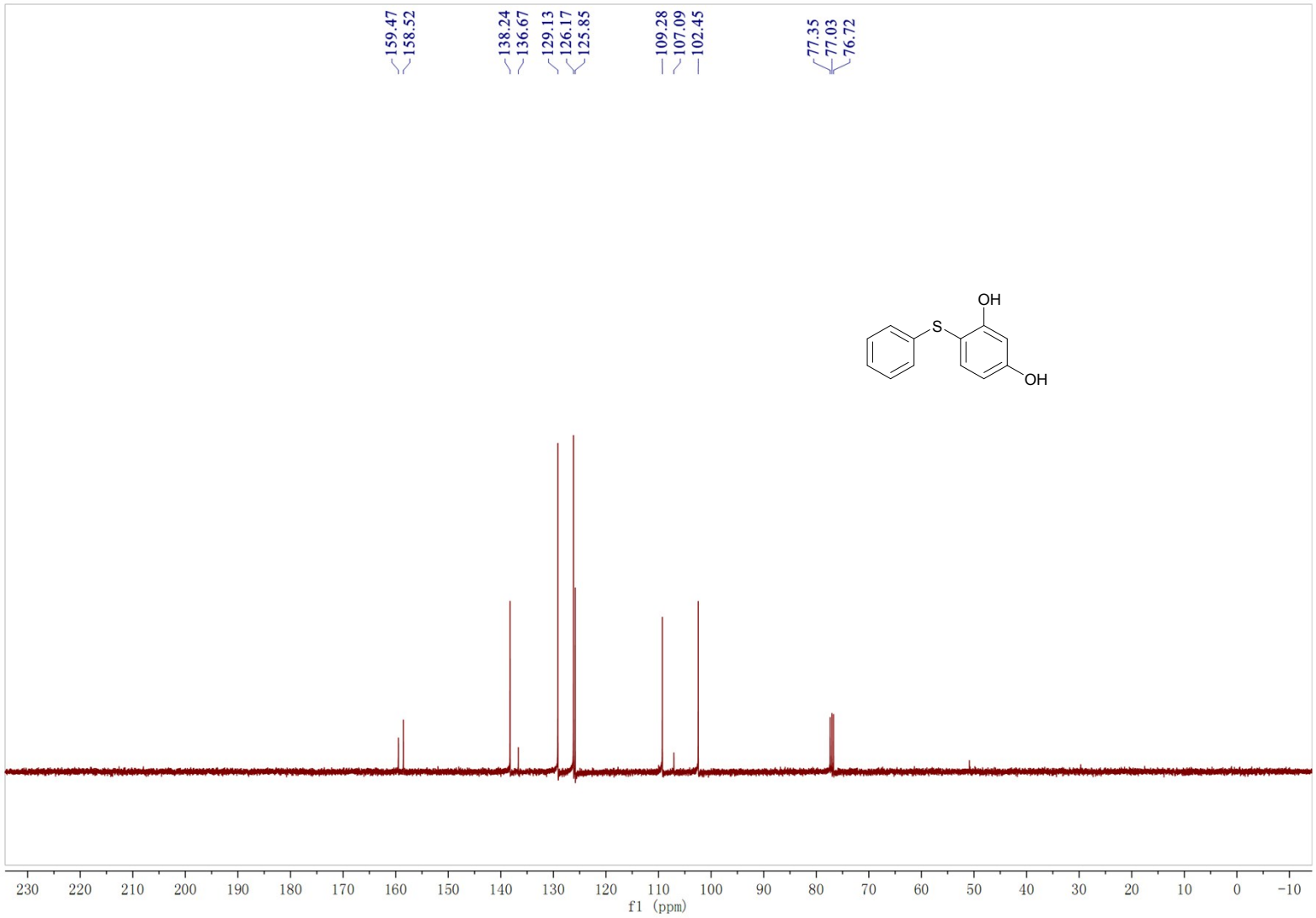
2.13
1.09
2.00
2.11
1.09
1.08
f1 (ppm)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OH
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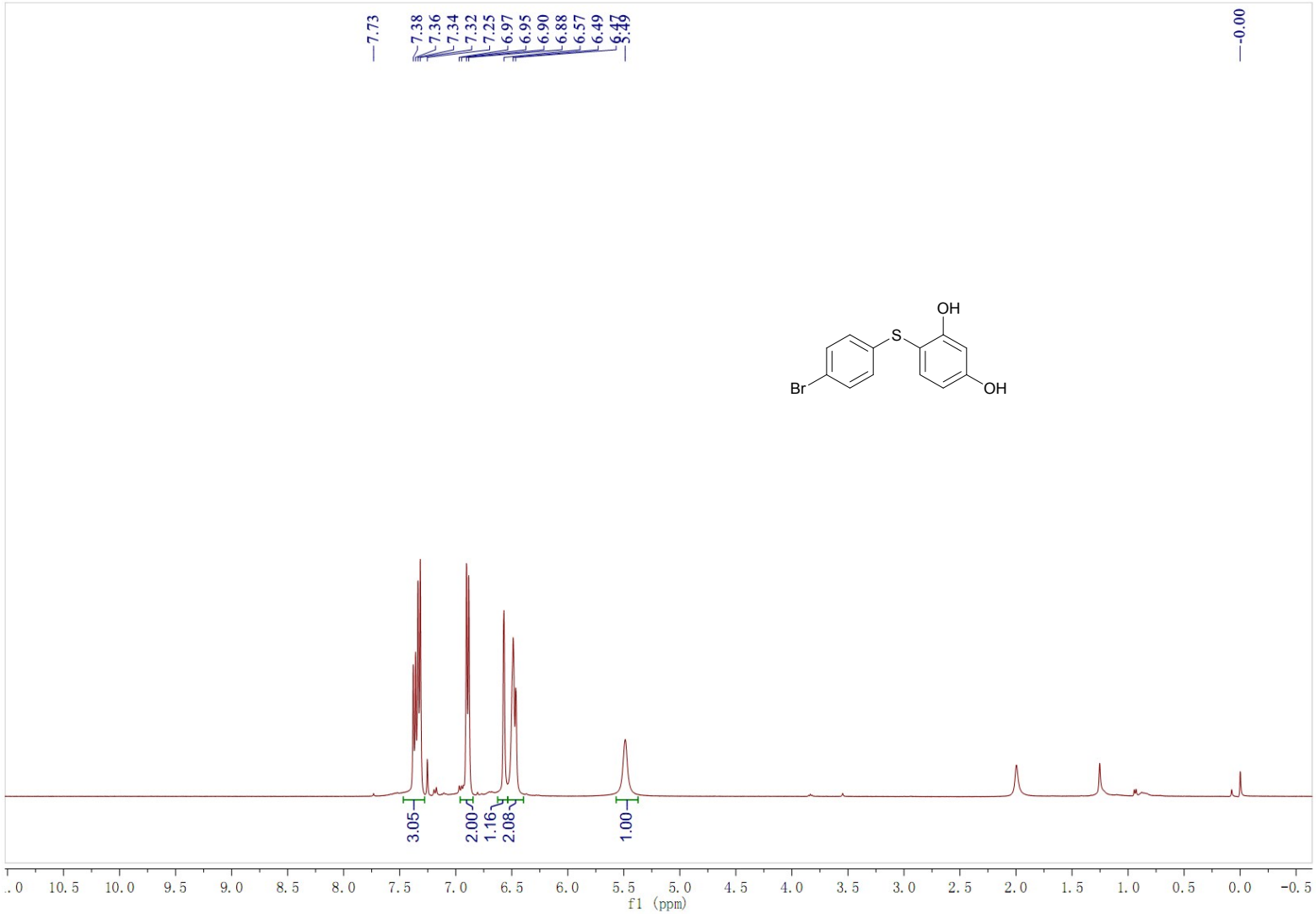
f1 (ppm)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OH
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2.08
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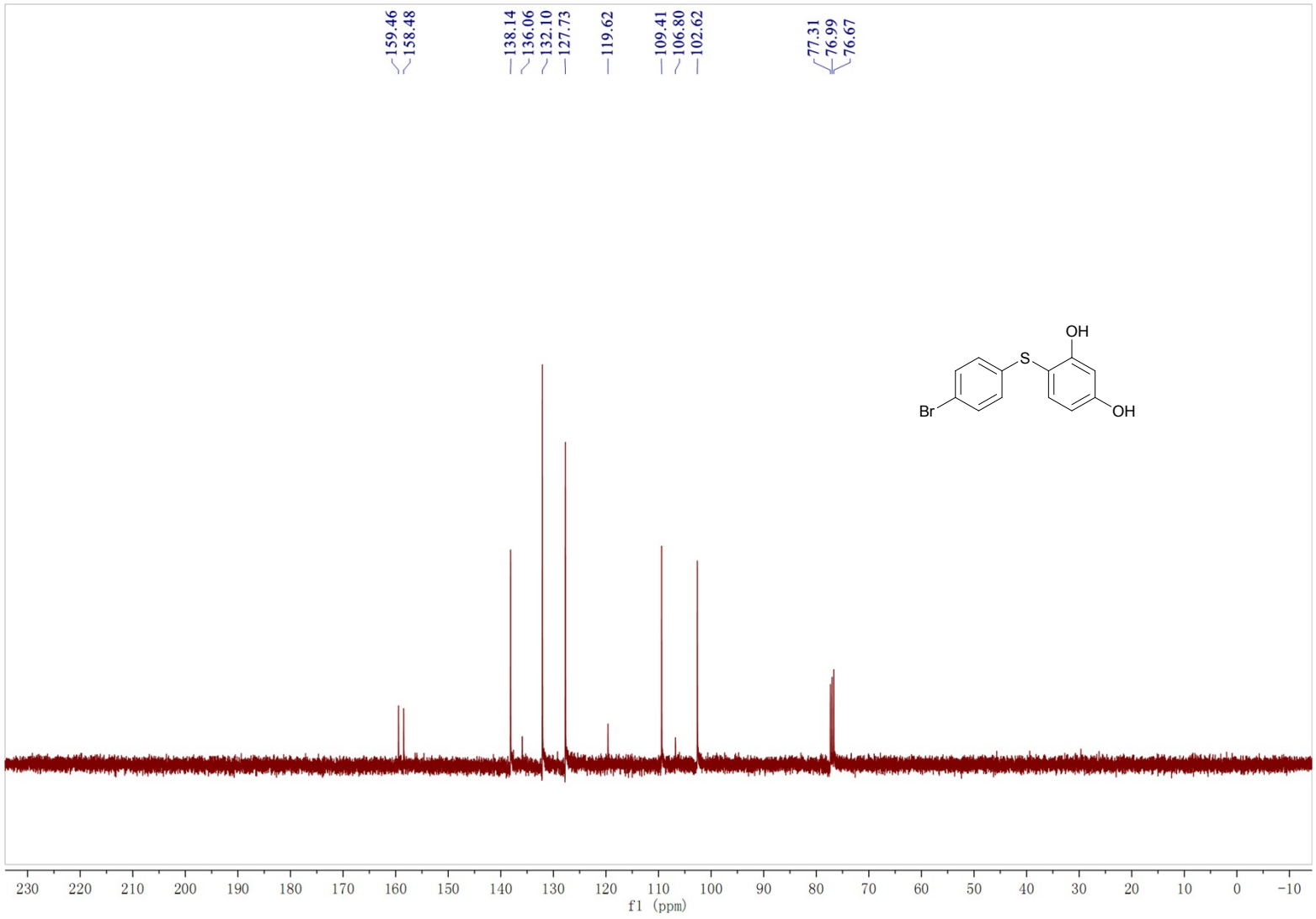
f1 (ppm)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OH
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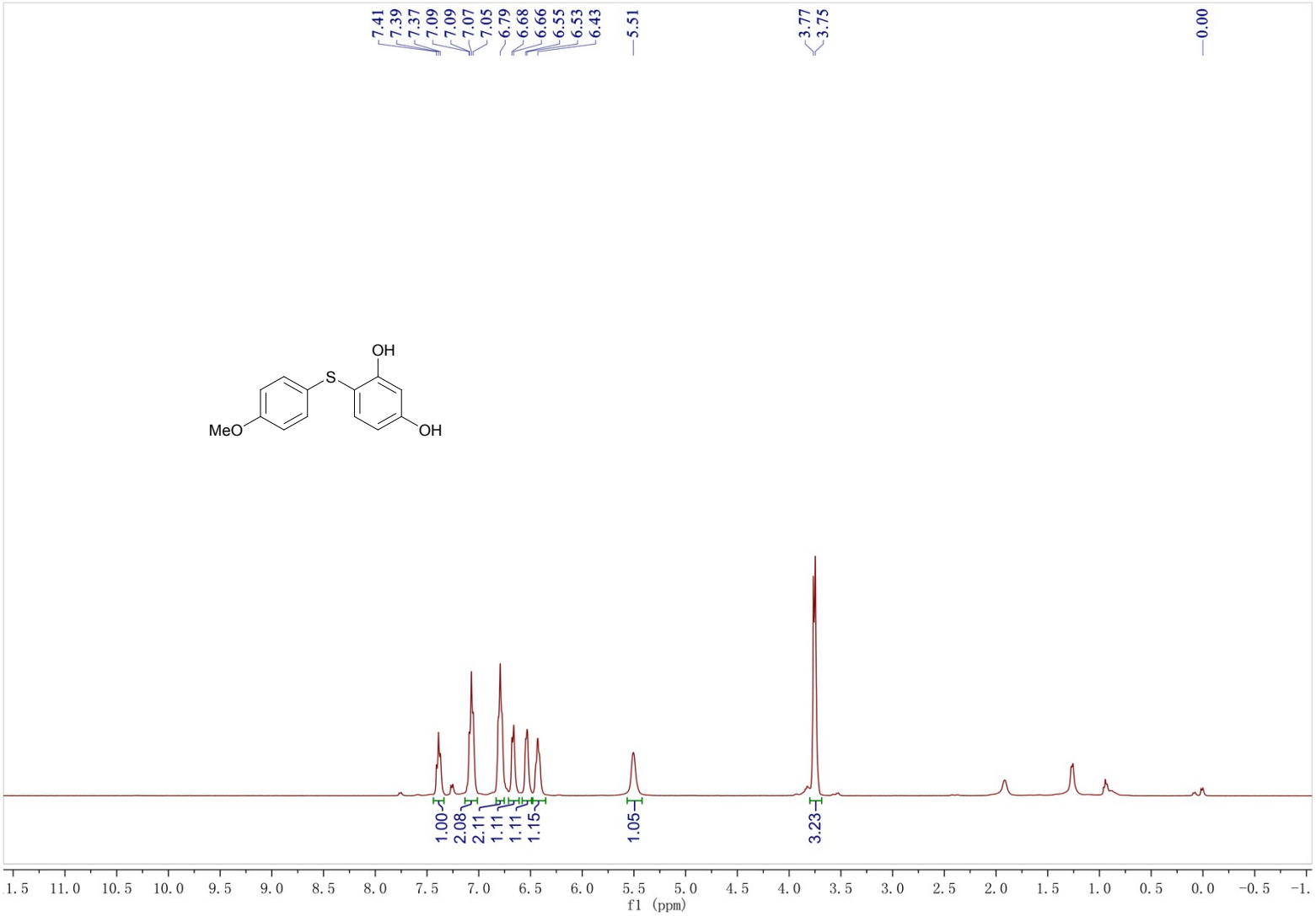
f1 (ppm)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5.51
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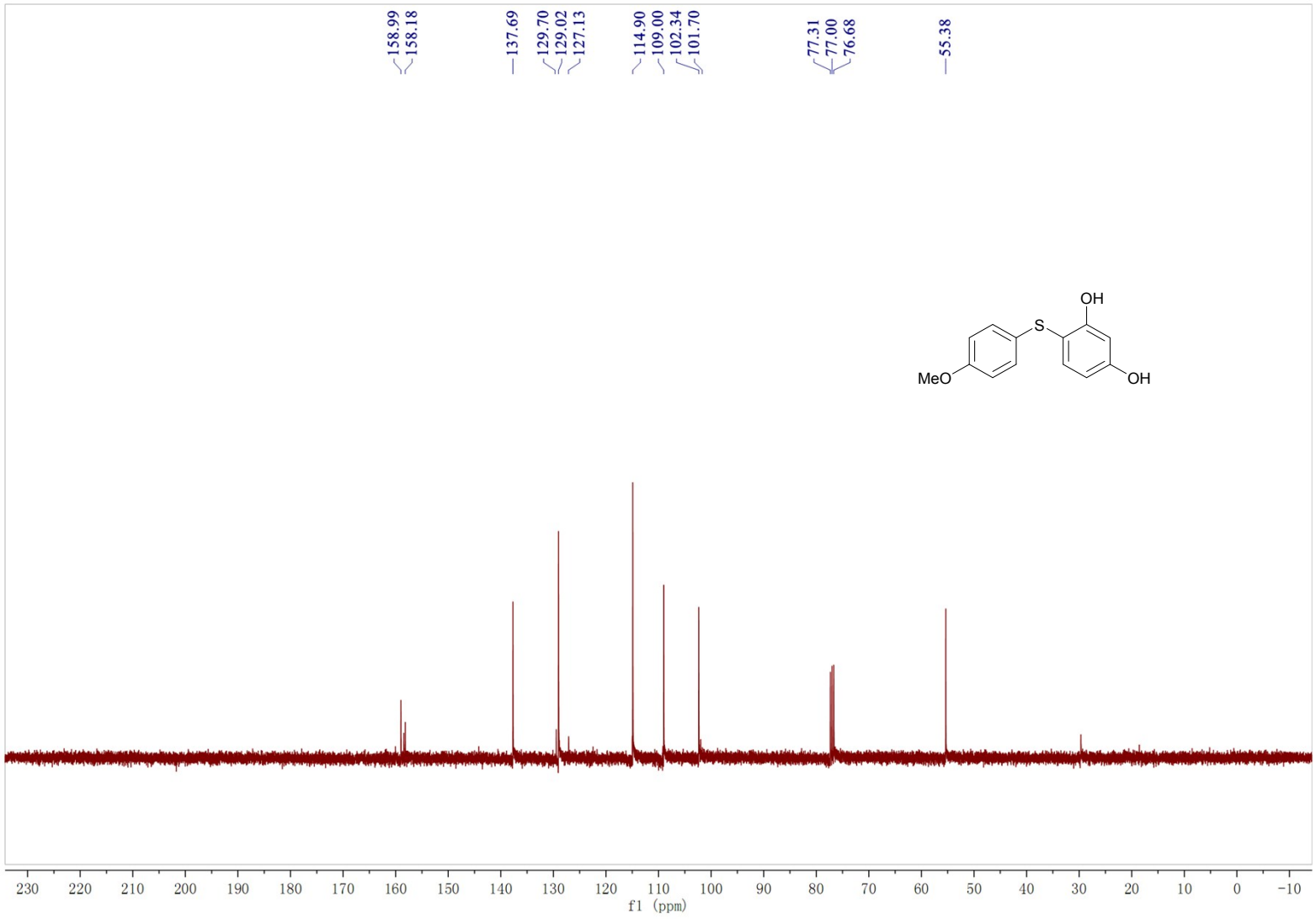
3.23
f1 (ppm)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101.70
77.31
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OH
S
MeO
OH
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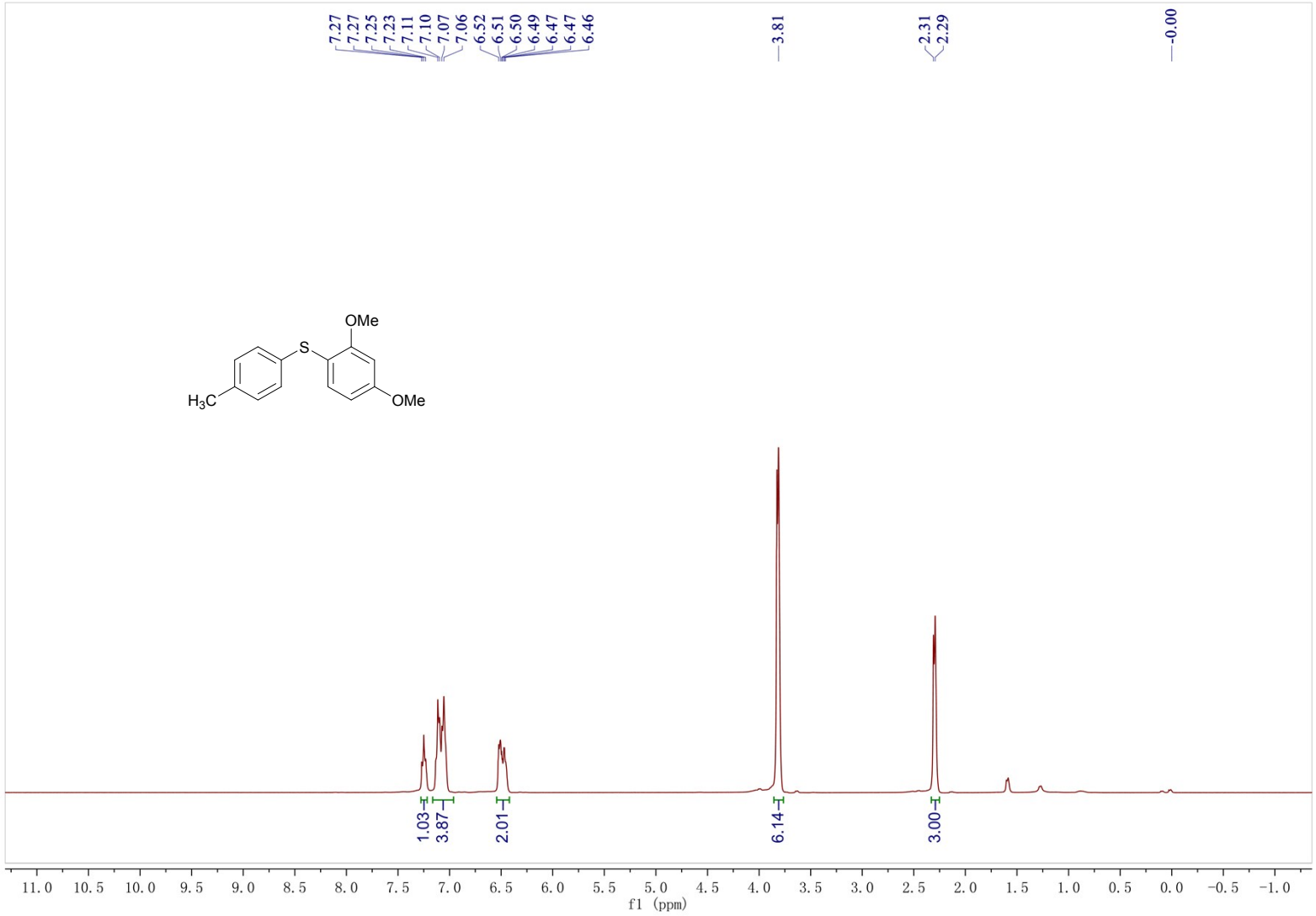
f1 (ppm)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7.10
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7.06
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6.51
6.50
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6.47
6.47
6.46
3.81
2.31
2.29
0.00
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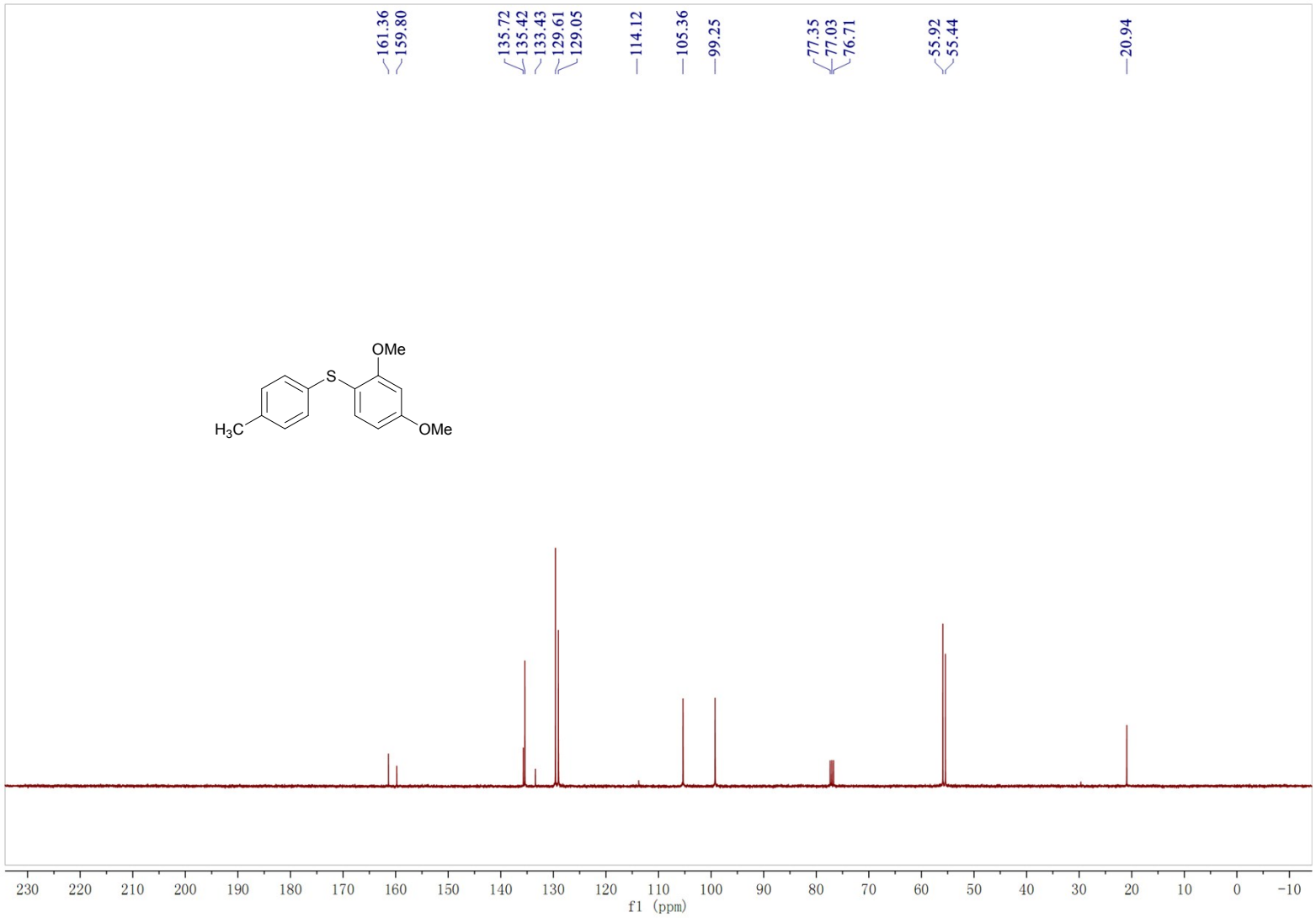
S
H3C
OMe
1.03
3.87
2.01
6.14
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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77.35
77.03
76.71
55.92
55.44
20.94
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S
OMe
H3C
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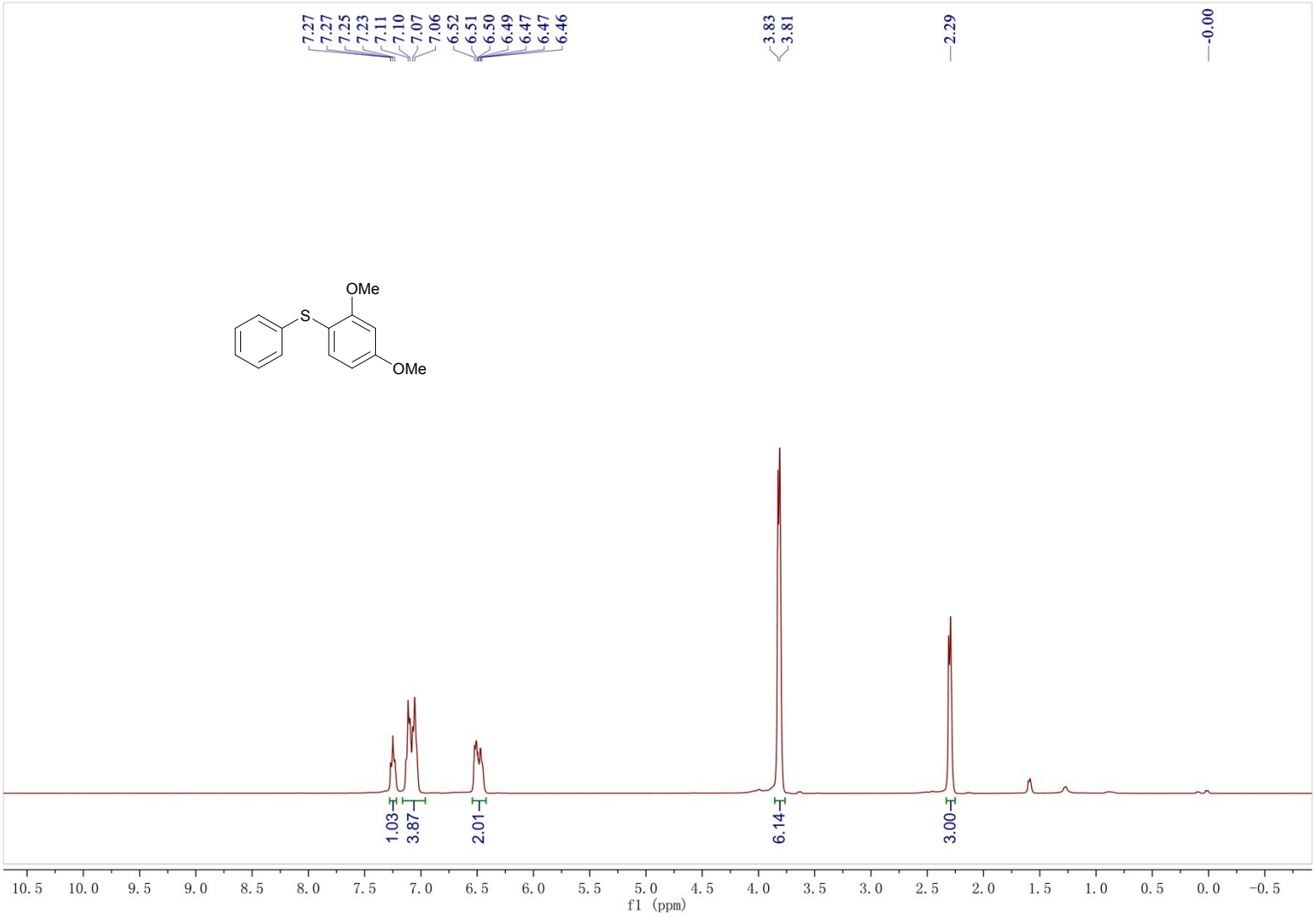
f1 (ppm)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7.11
7.10
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6.51
6.50
6.49
6.47
6.47
6.46
3.83
3.81
2.29
-0.00
OMe
S
OMe
1.03
3.87
2.01
6.14
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
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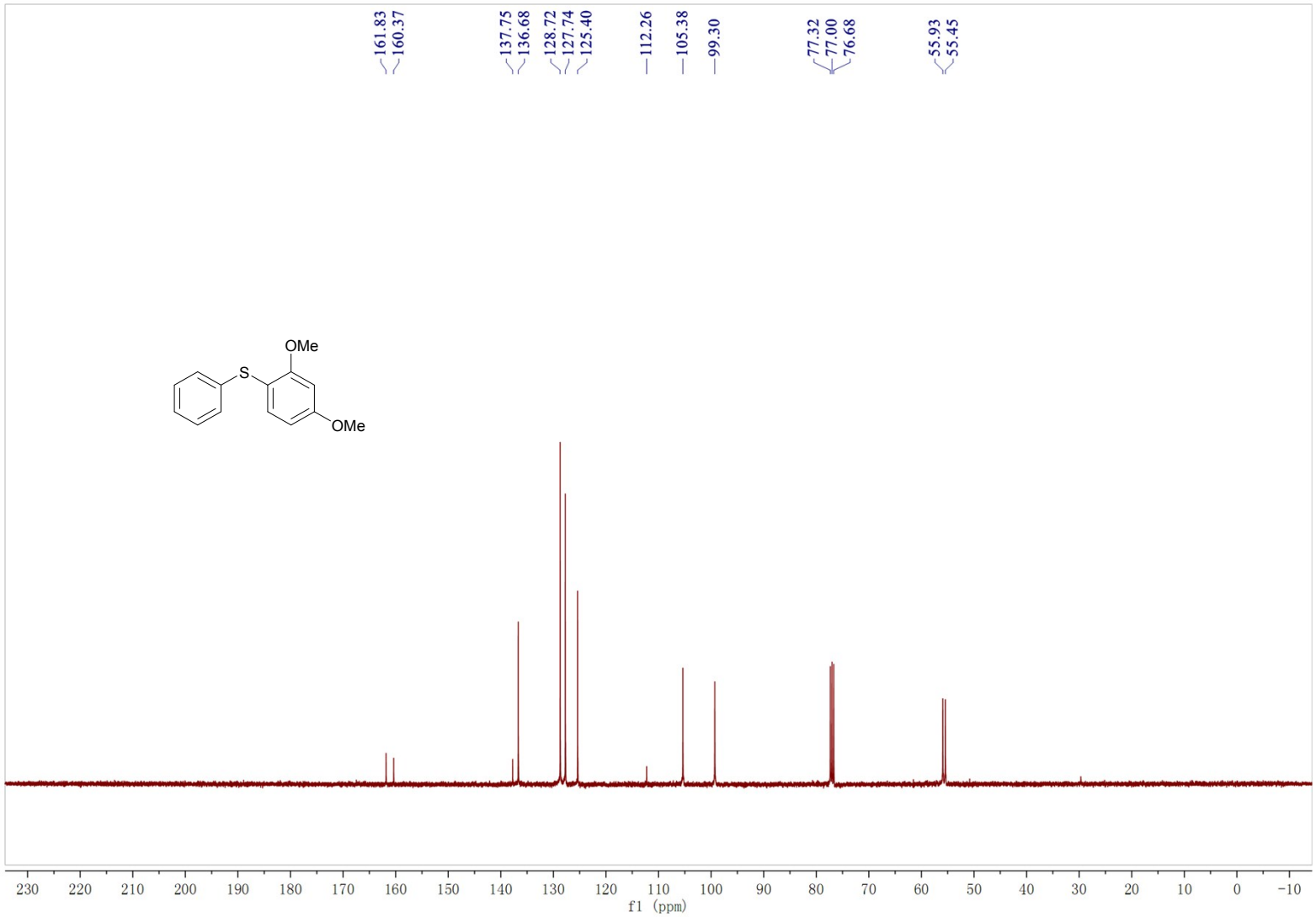
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77.32
77.00
76.68
55.93
55.45
OMe
S
OMe
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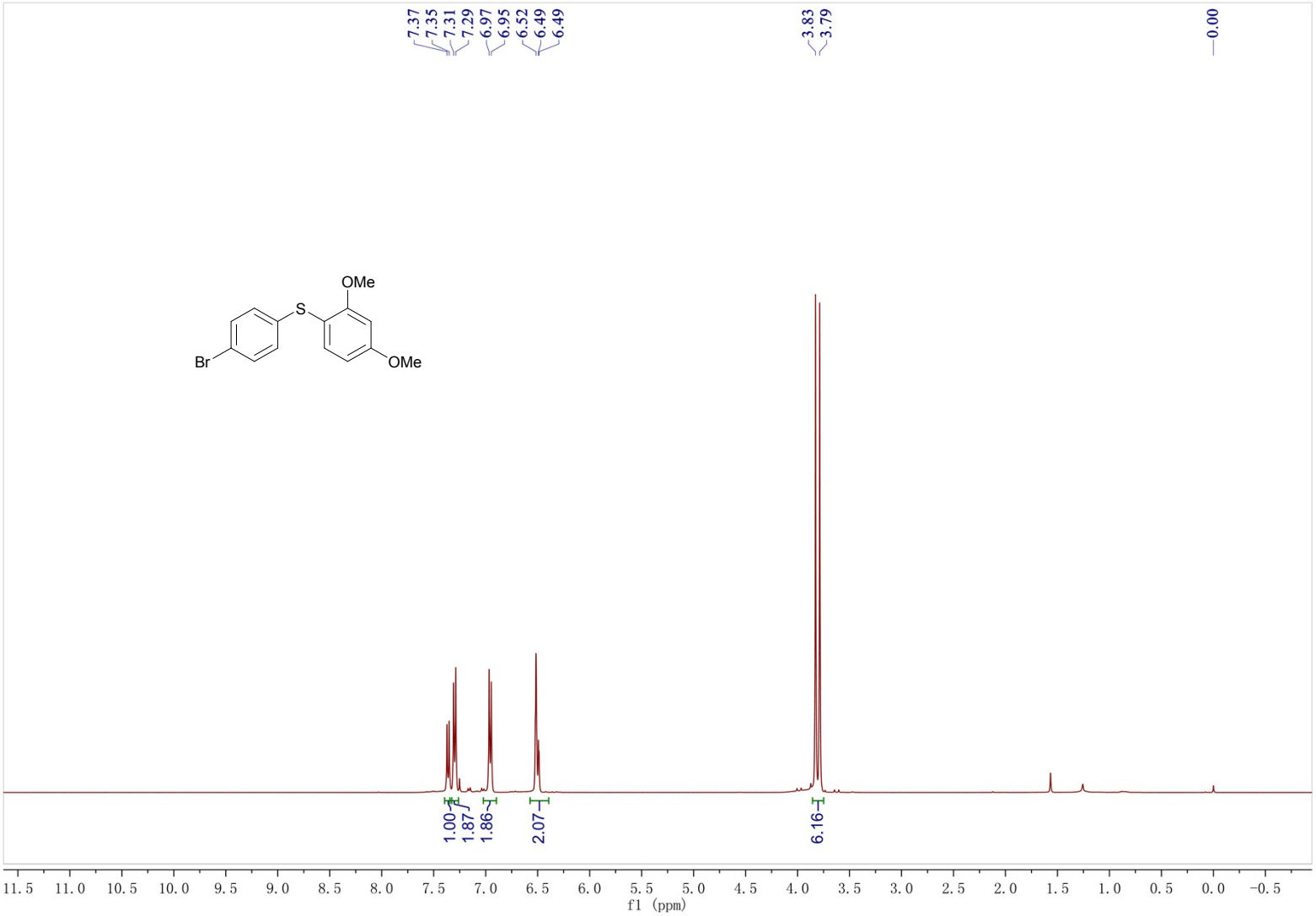
f1 (ppm)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3.79
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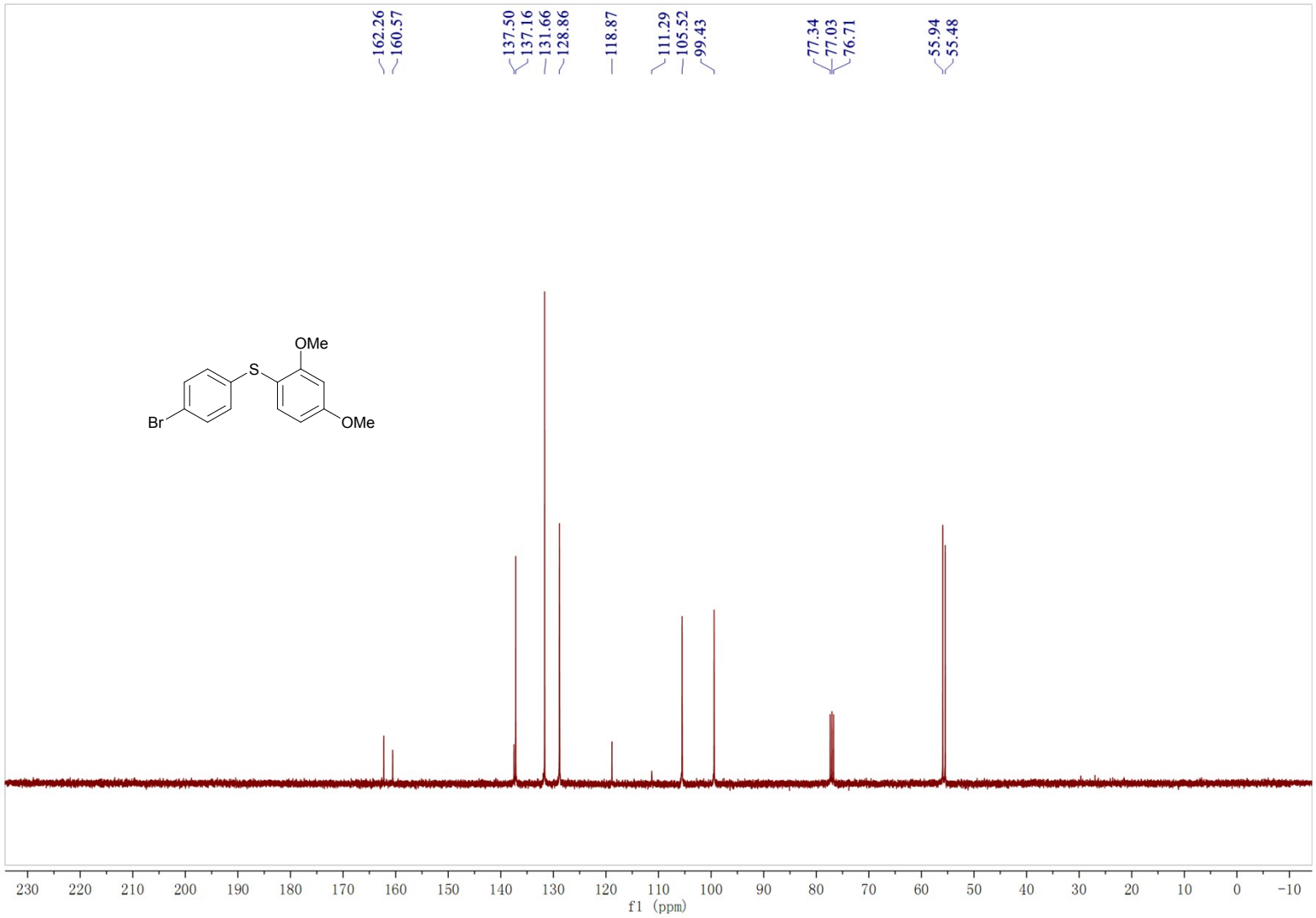
OMe
S
Br
OMe
1.00
1.87
1.86
2.07
6.16
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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111.29
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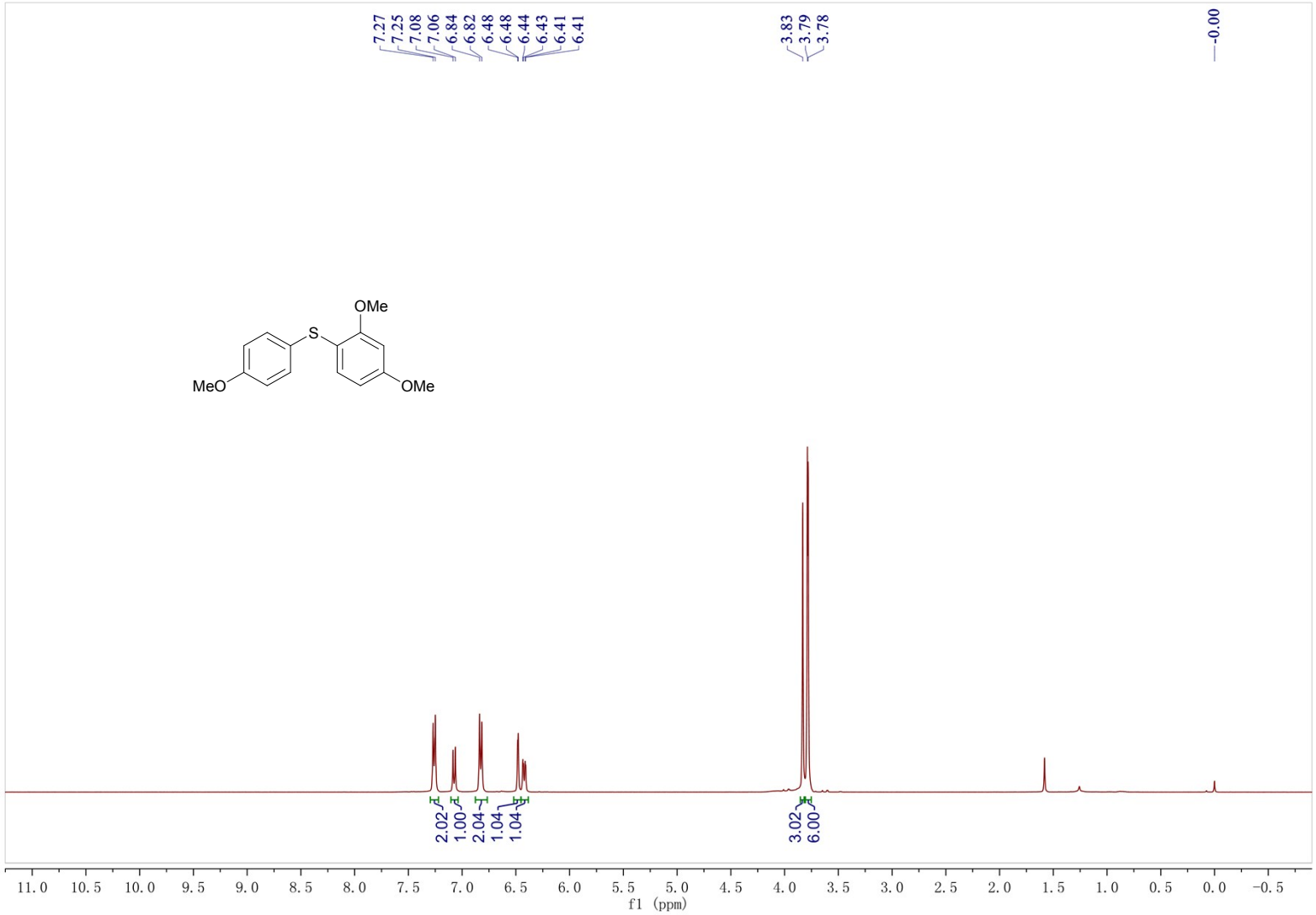
99.43
77.34
77.03
76.71
55.94
55.48
OMe
S
Br
OMe
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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6.43
6.41
6.41
3.83
3.79
3.78
-0.00
OMe
S
MeO
OMe
2.02
1.00
2.04
1.04
1.04
3.02
6.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.0
2.5
2.0
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1.0
0.5
0.0
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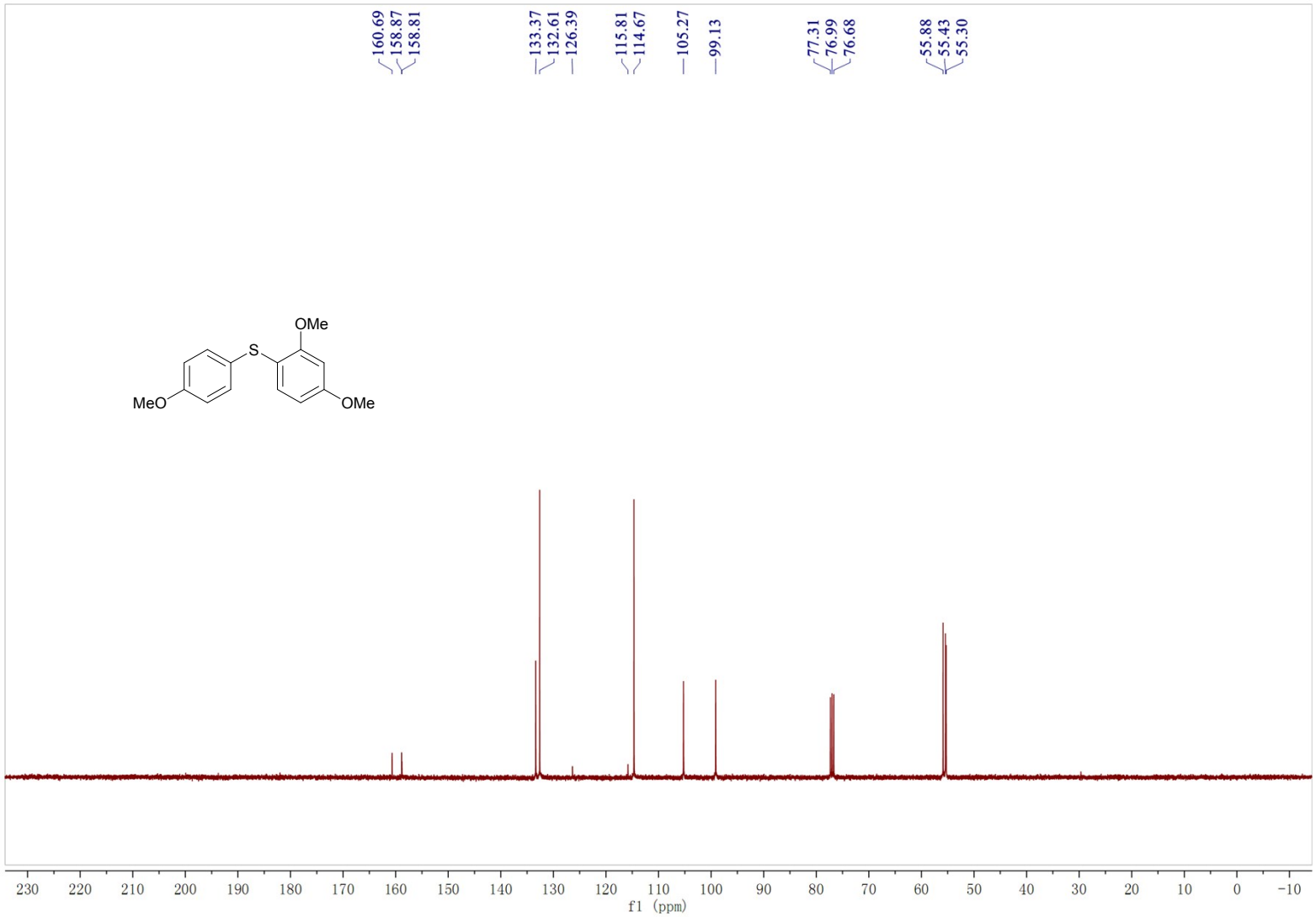
f1 (ppm)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77.31
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76.68
55.88
55.43
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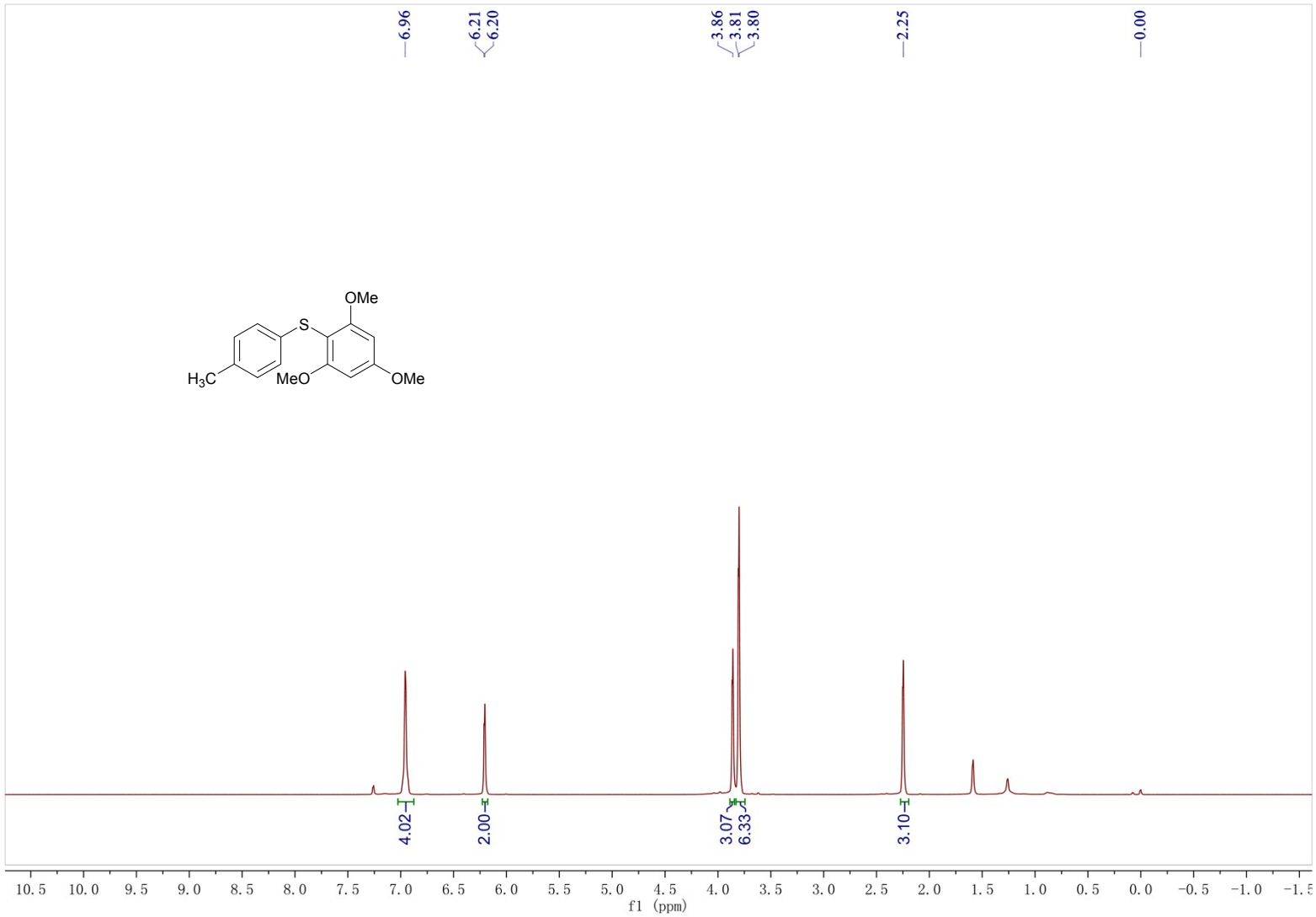
OMe
S
MeO
OMe
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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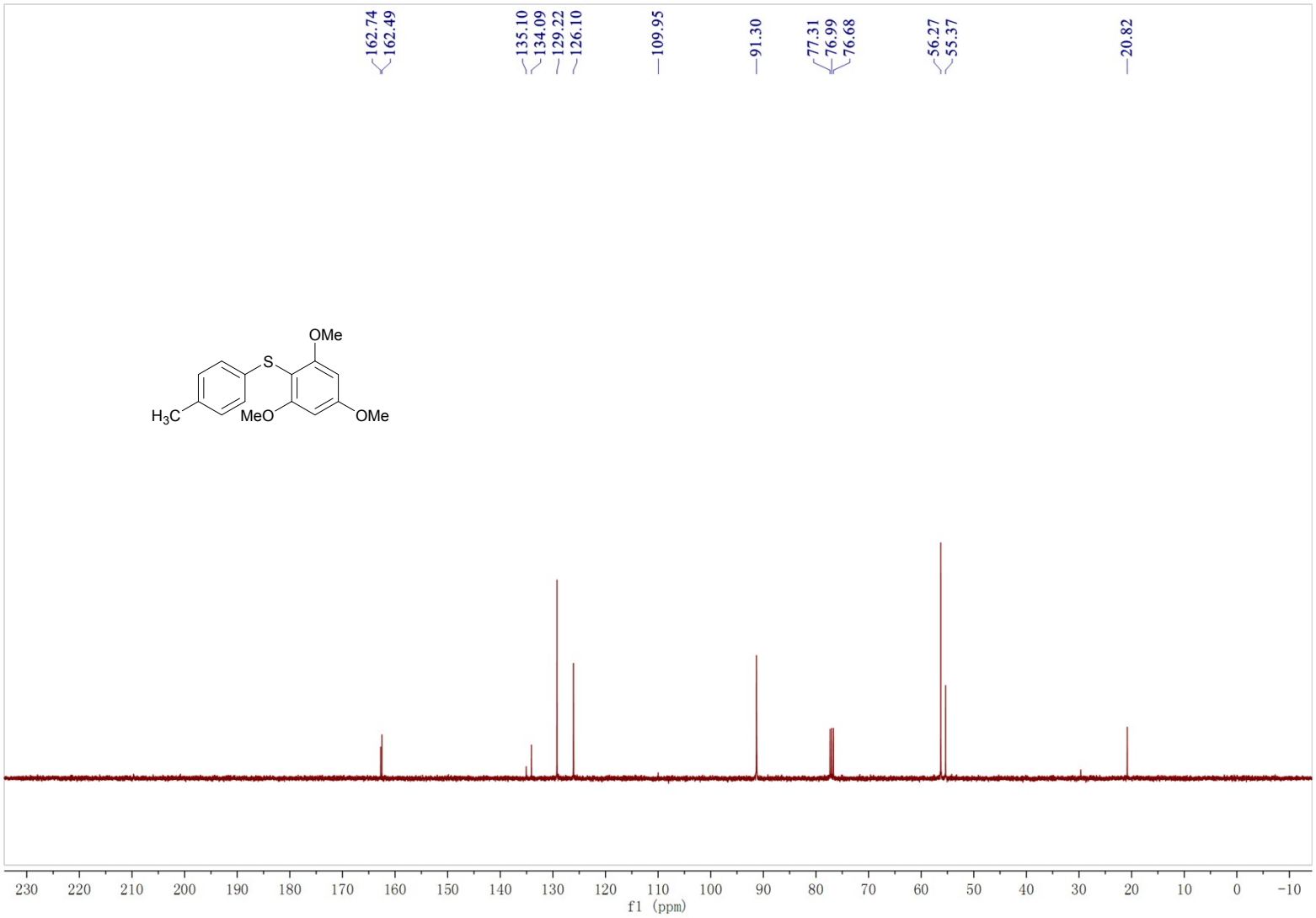
S
H3C
MeO
OMe
4.02
2.00
3.07
6.33
3.10
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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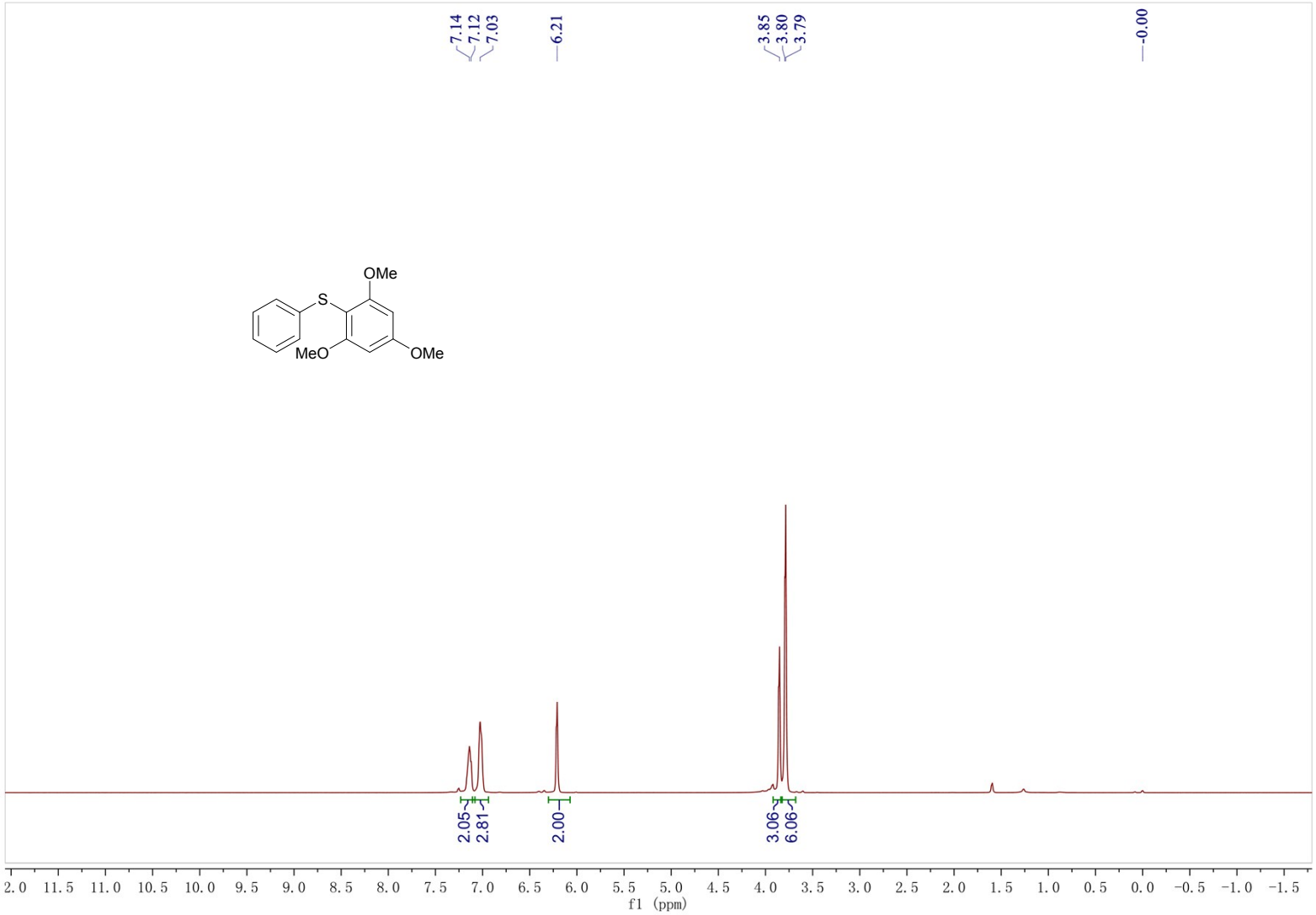
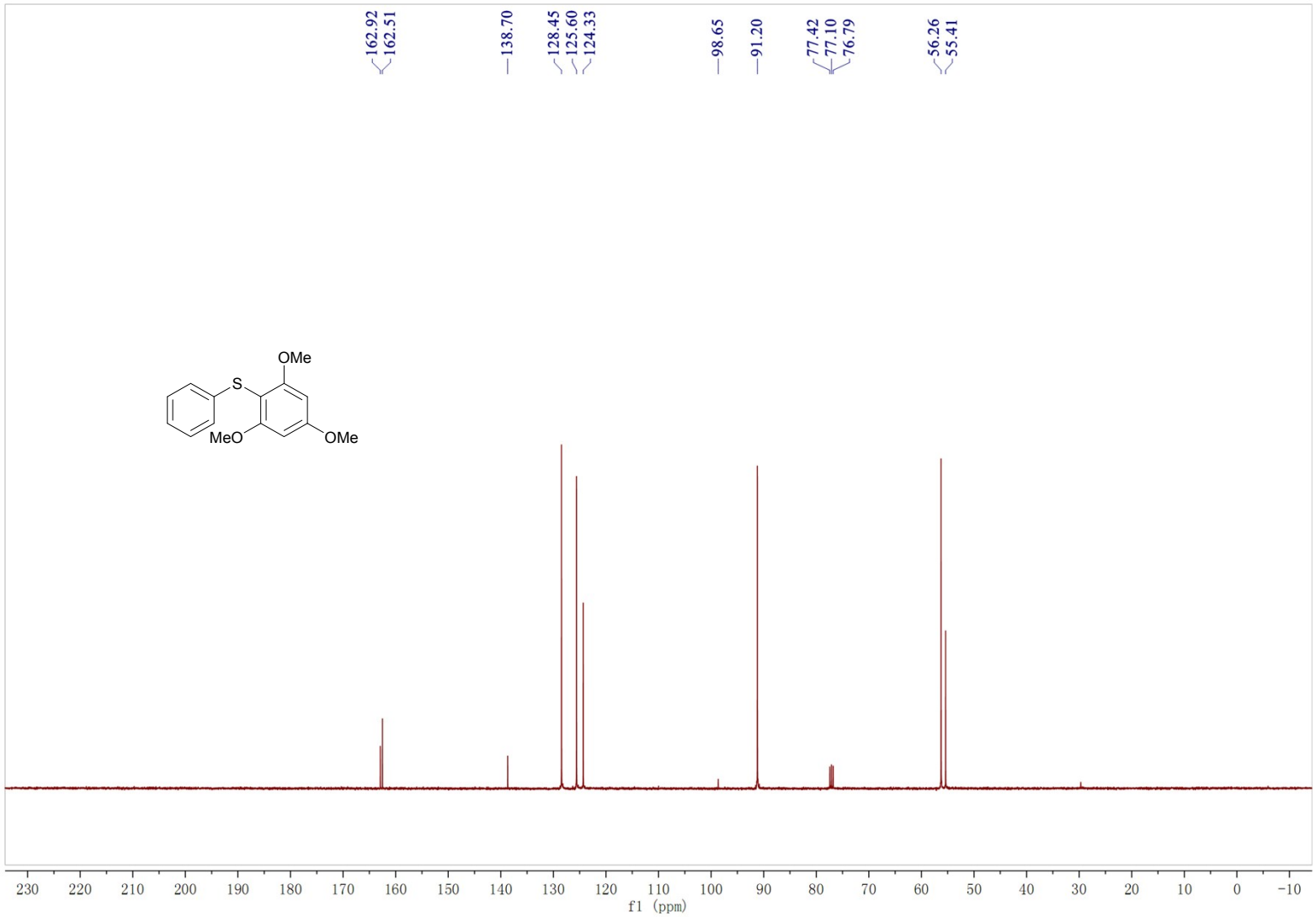
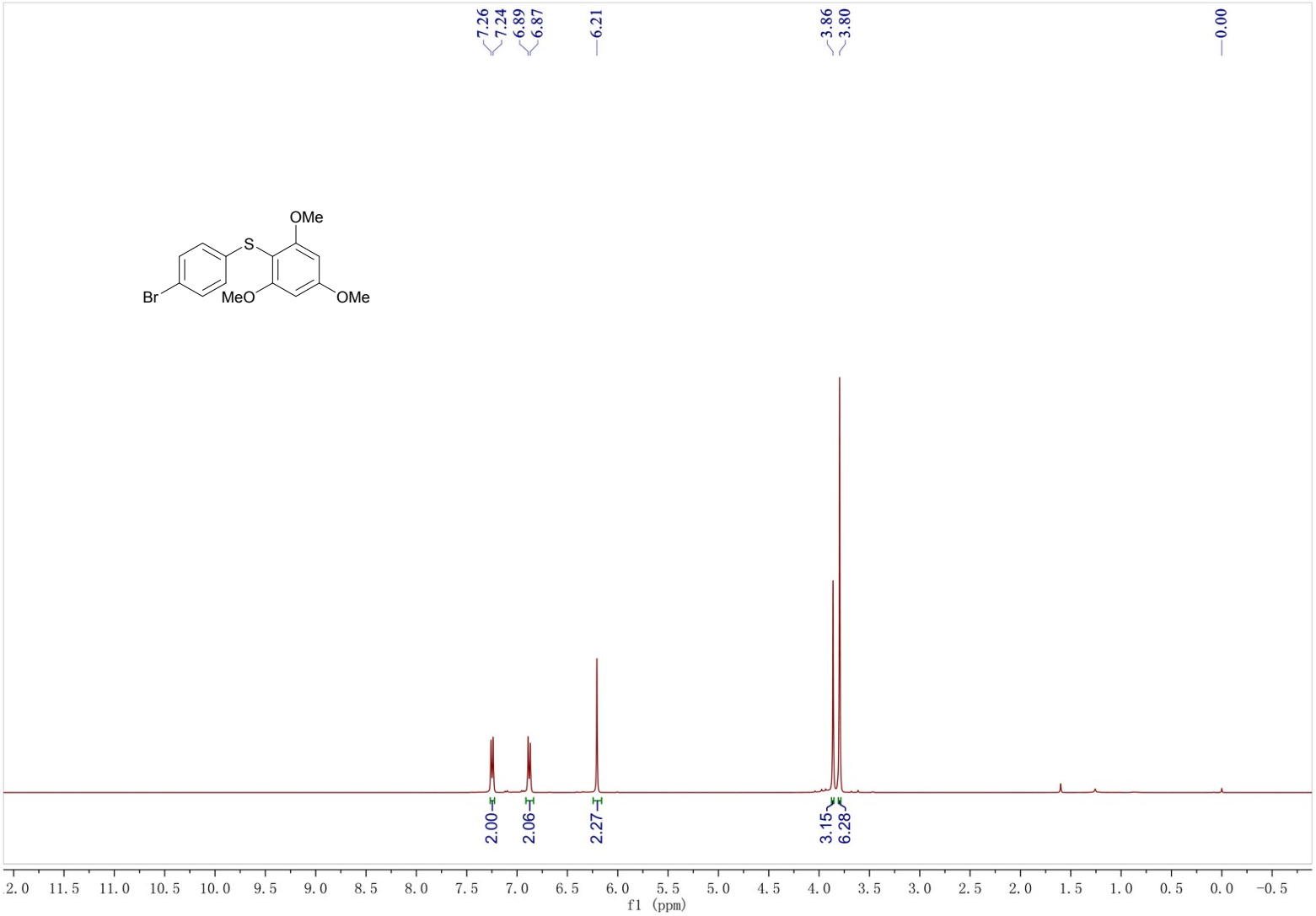
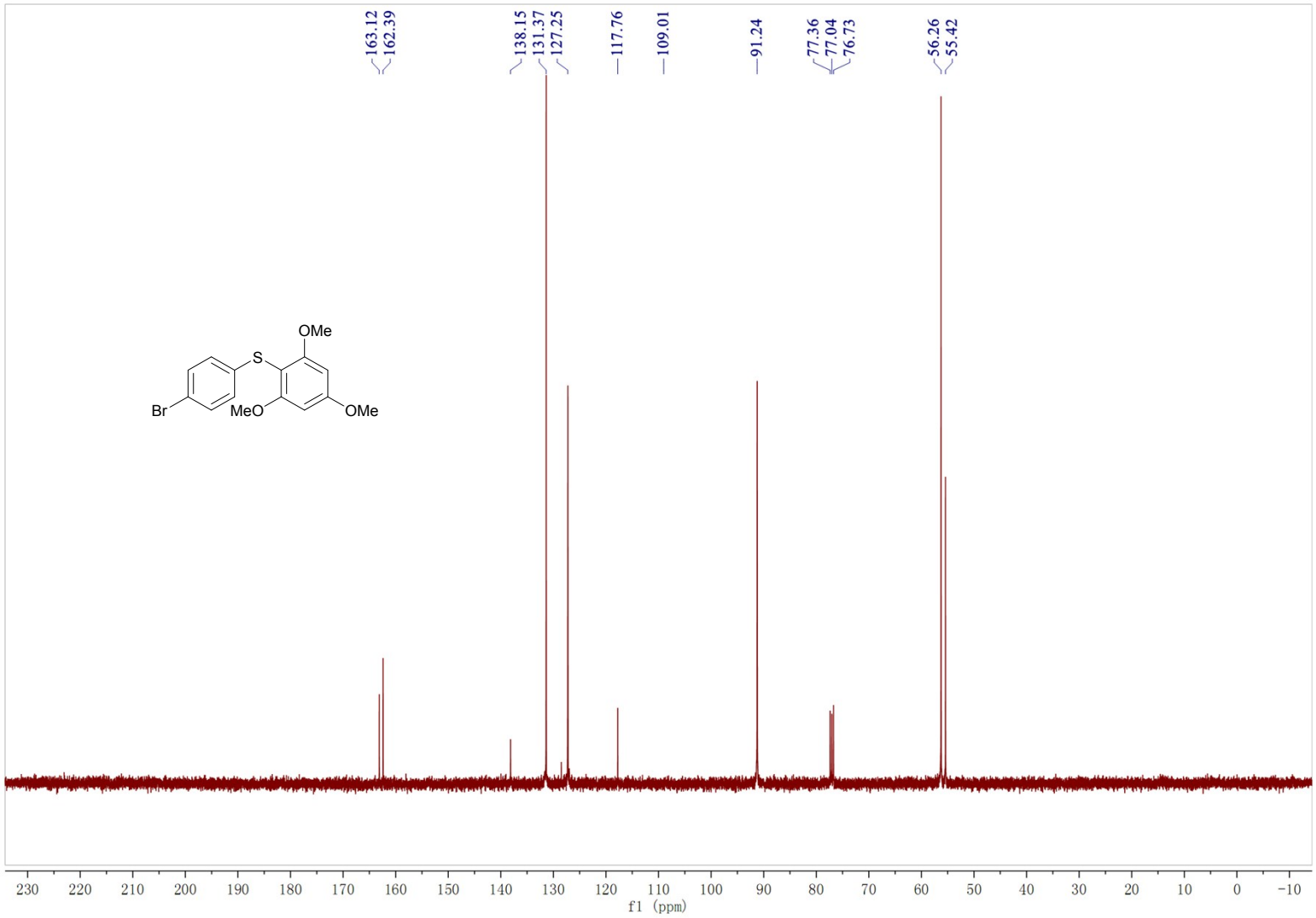
76.68
56.27
55.37
20.82
OMe
S
H3C
MeO
OMe
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.14
7.12
7.03
6.21
3.85
3.80
3.79
0.00
OMe
S
MeO
OMe
2.05
2.81
2.00
3.06
6.06
f1 (ppm)


162.92
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
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
3.86
3.80
0.00
OMe
S
Br
MeO
OMe
2.00
2.06
2.27
3.15
6.28
f1 (ppm)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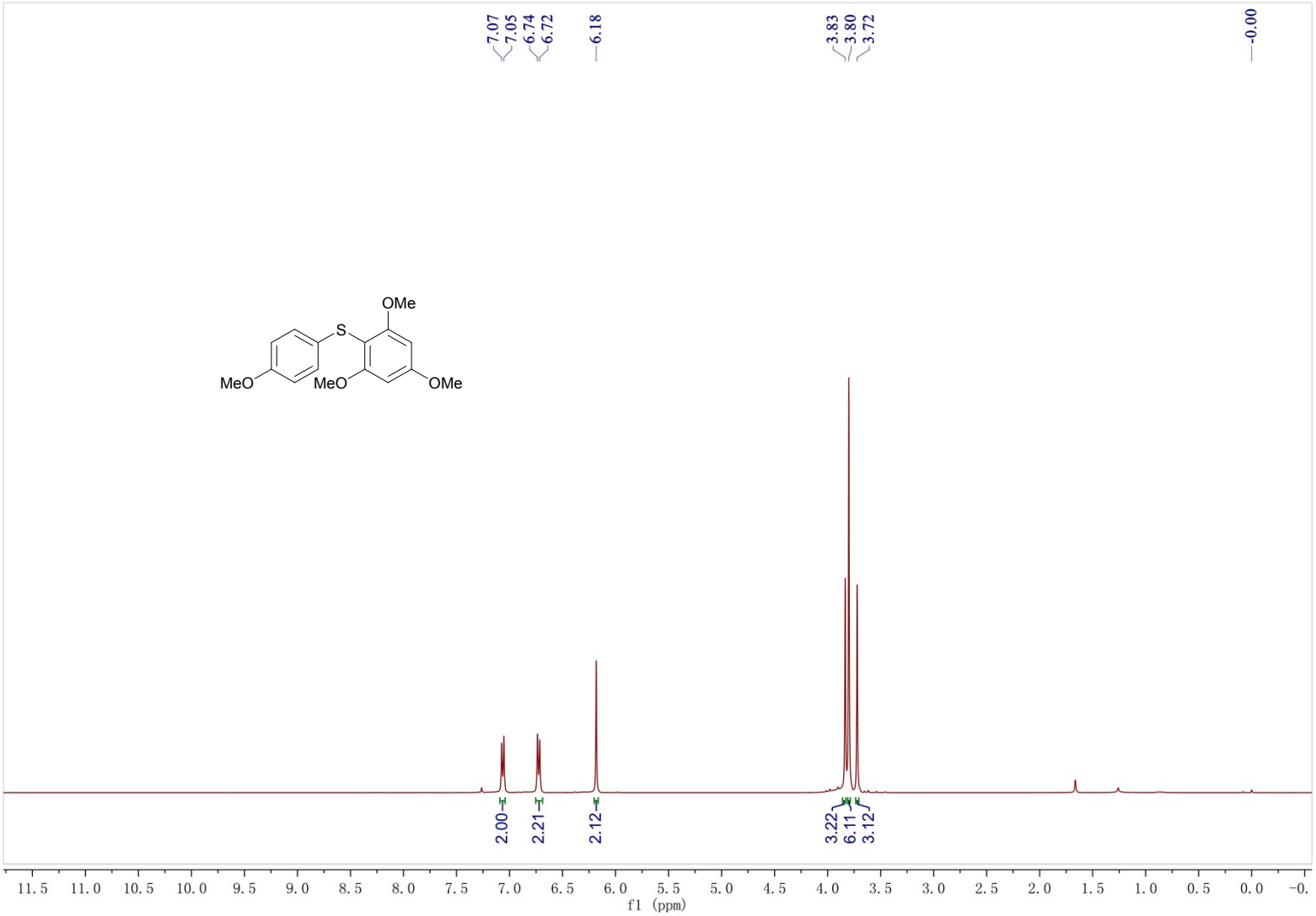
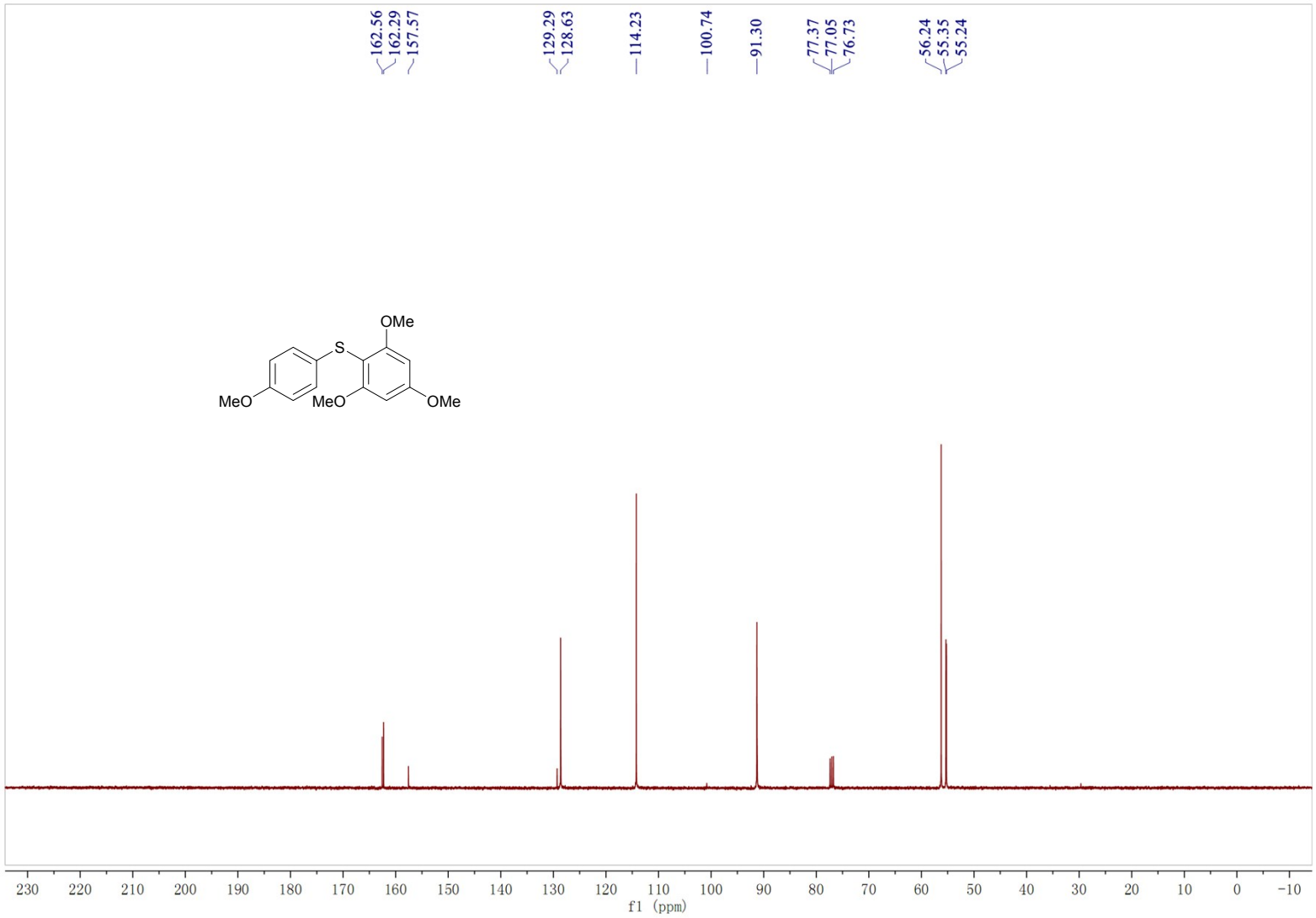
138.15
131.37
127.25
117.76
109.01
91.24
77.36
77.04
76.73
56.26
55.42
OMe
S
Br
MeO
OMe
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.07
7.05
6.74
6.72
6.18
3.83
3.80
3.72
-0.00
OMe
S
MeO
MeO
OMe
2.00
2.21
2.12
3.22
6.11
3.12
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)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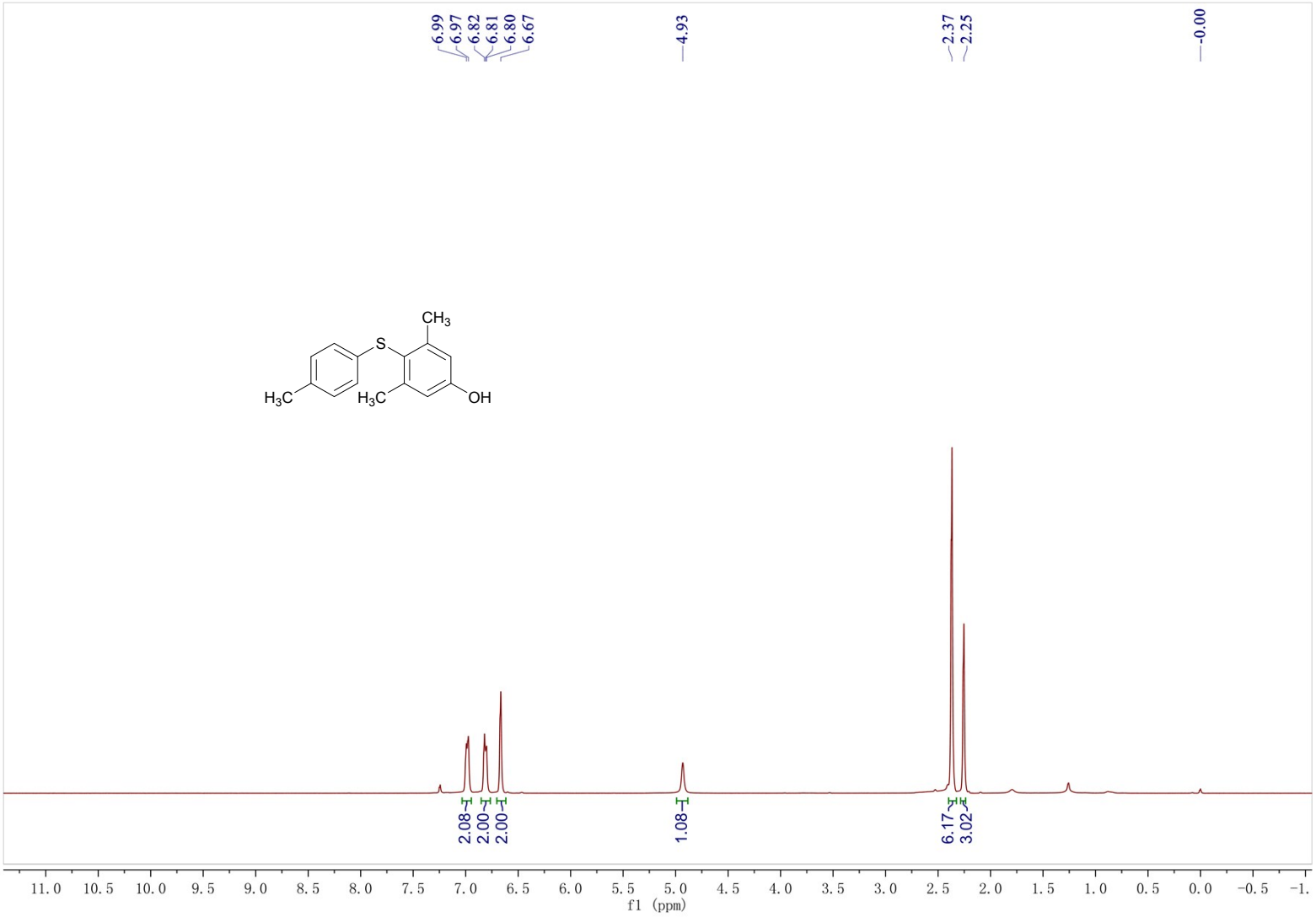
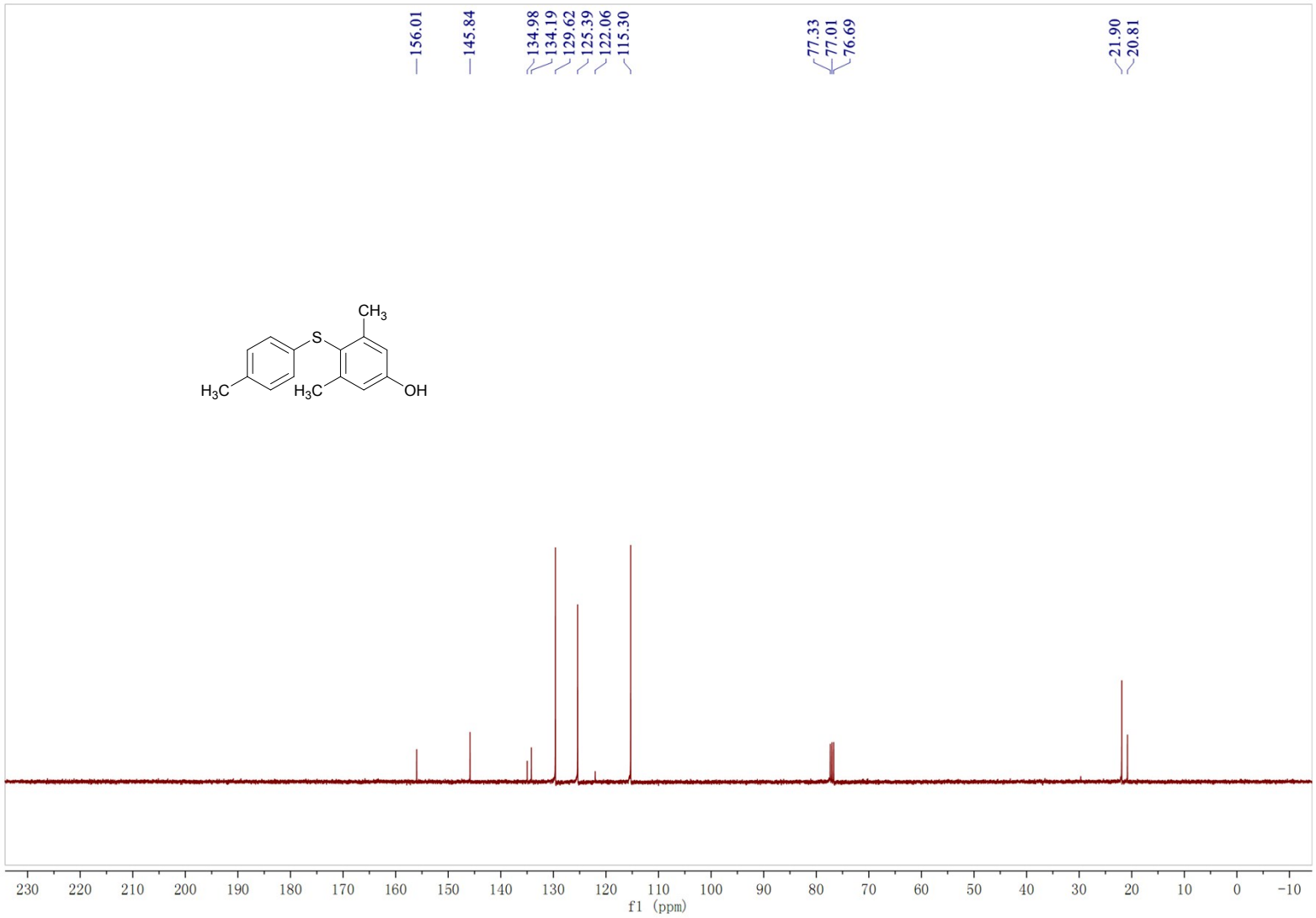
162.29
157.57
129.29
128.63
114.23
100.74
91.30
77.37
77.05
76.73
56.24
55.35
55.24
OMe
S
MeO
MeO
OMe
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


6.99
6.97
6.82
6.81
6.80
6.67
4.93
2.37
2.25
0.00
CH3
S
H3C
H3C
OH
2.08
2.00
2.00
1.08
6.17
3.02
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.
f1 (ppm)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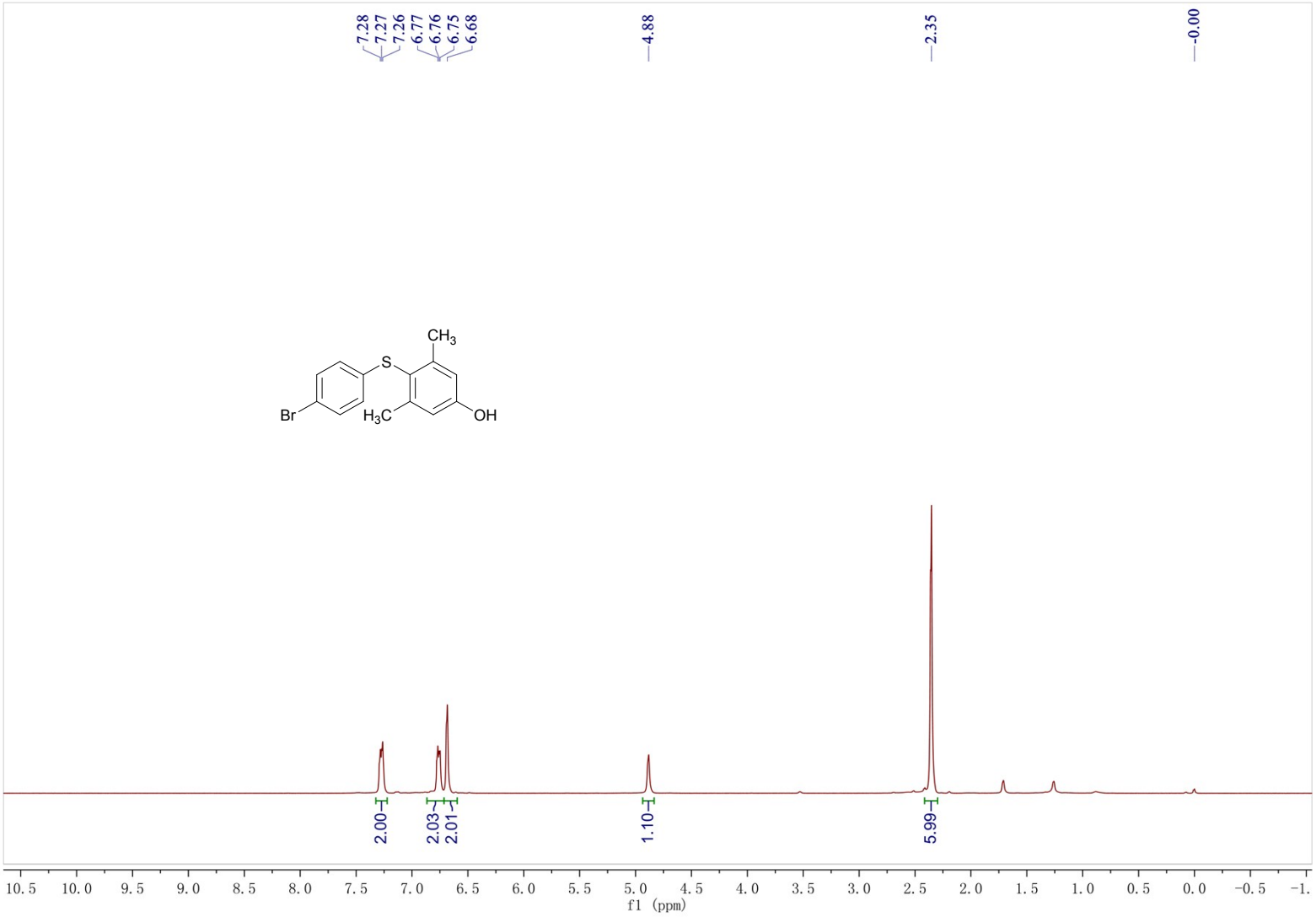
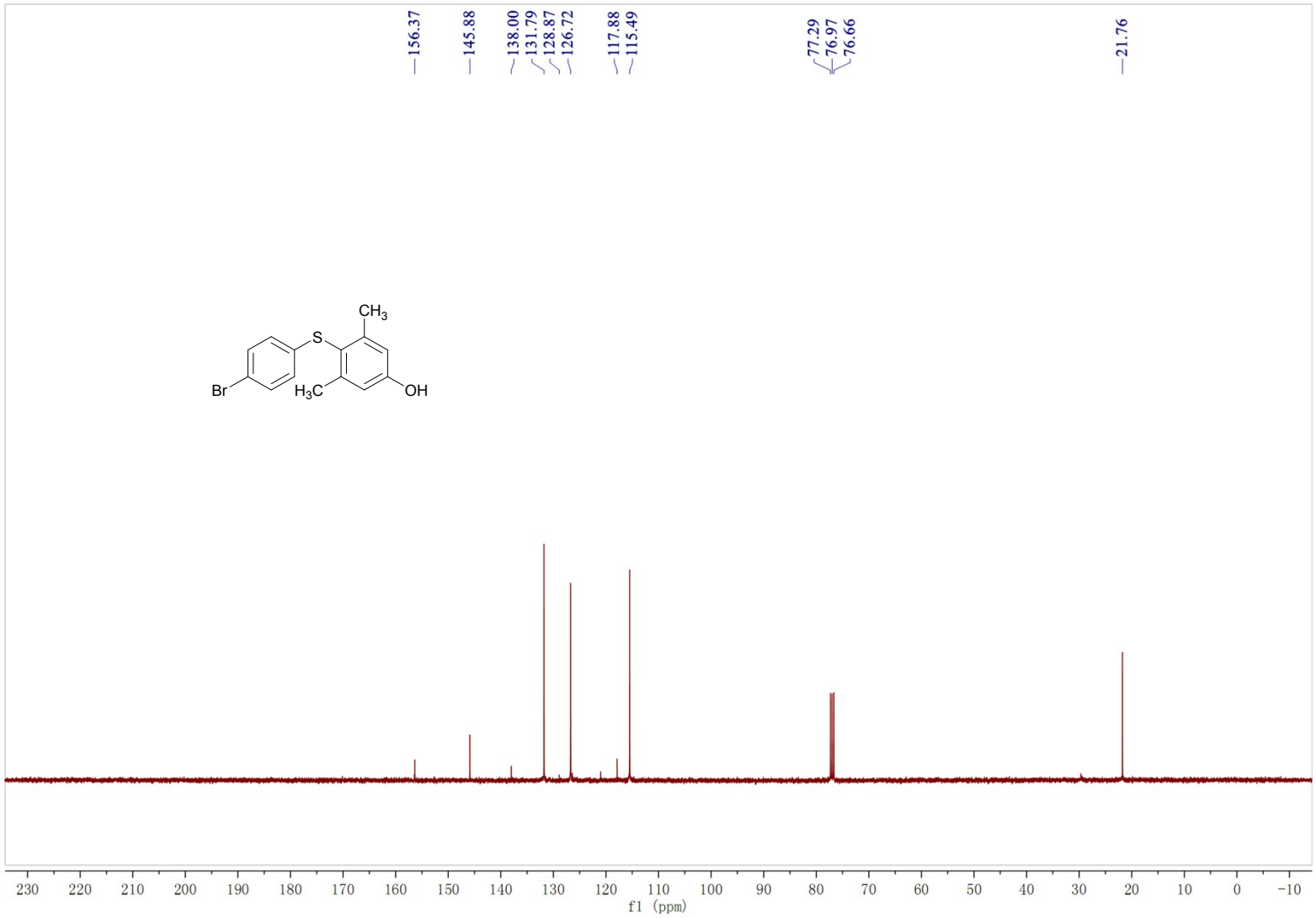
145.84
134.98
134.19
129.62
125.39
122.06
115.30
77.33
77.01
76.69
21.90
20.81
CH3
S
H3C
H3C
OH
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.28
7.27
7.26
6.77
6.76
6.75
6.68
4.88
2.35
0.00
CH3
S
Br
H3C
OH
2.00
2.03
2.01
1.10
5.99
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.
f1 (ppm)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145.88
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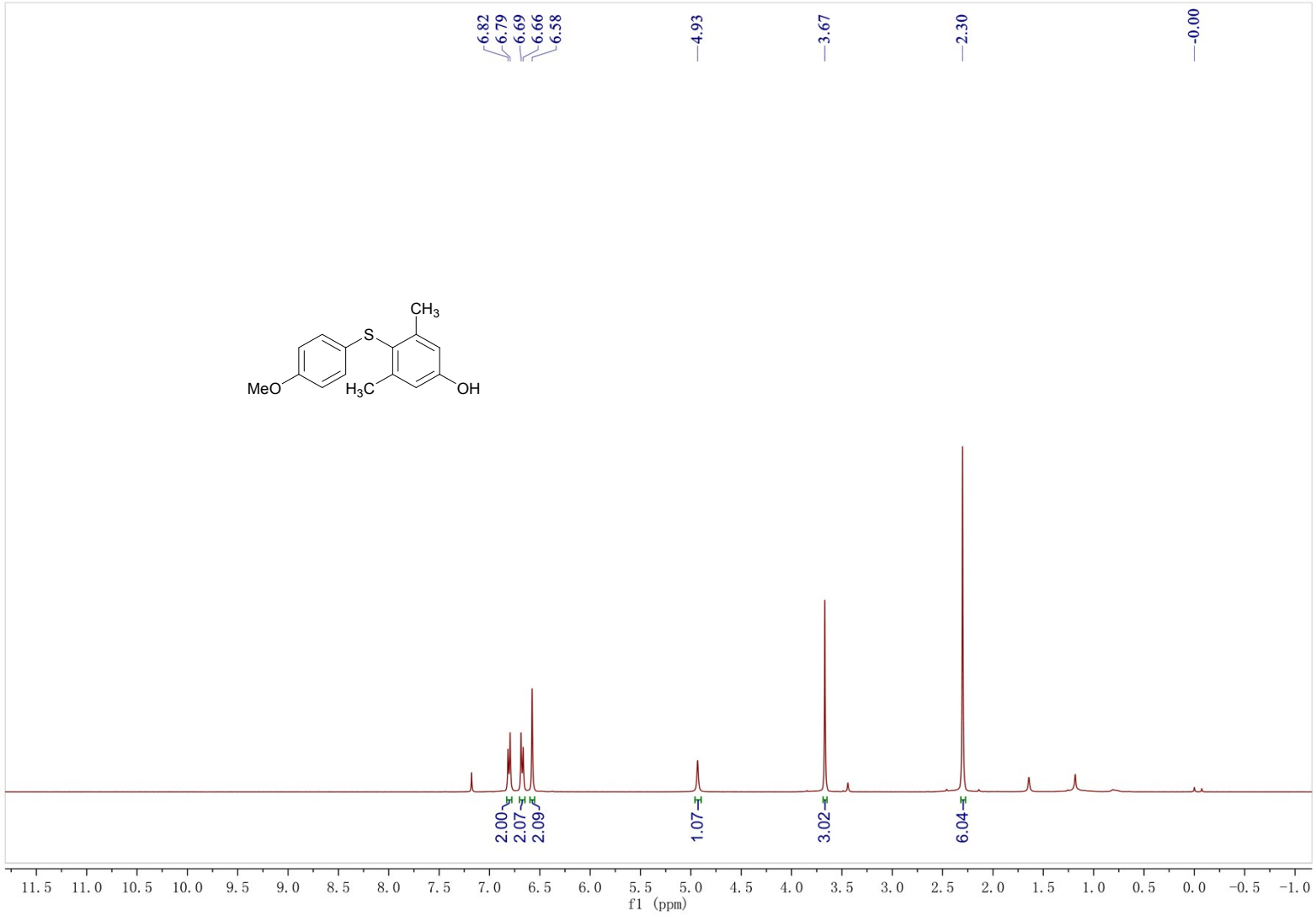
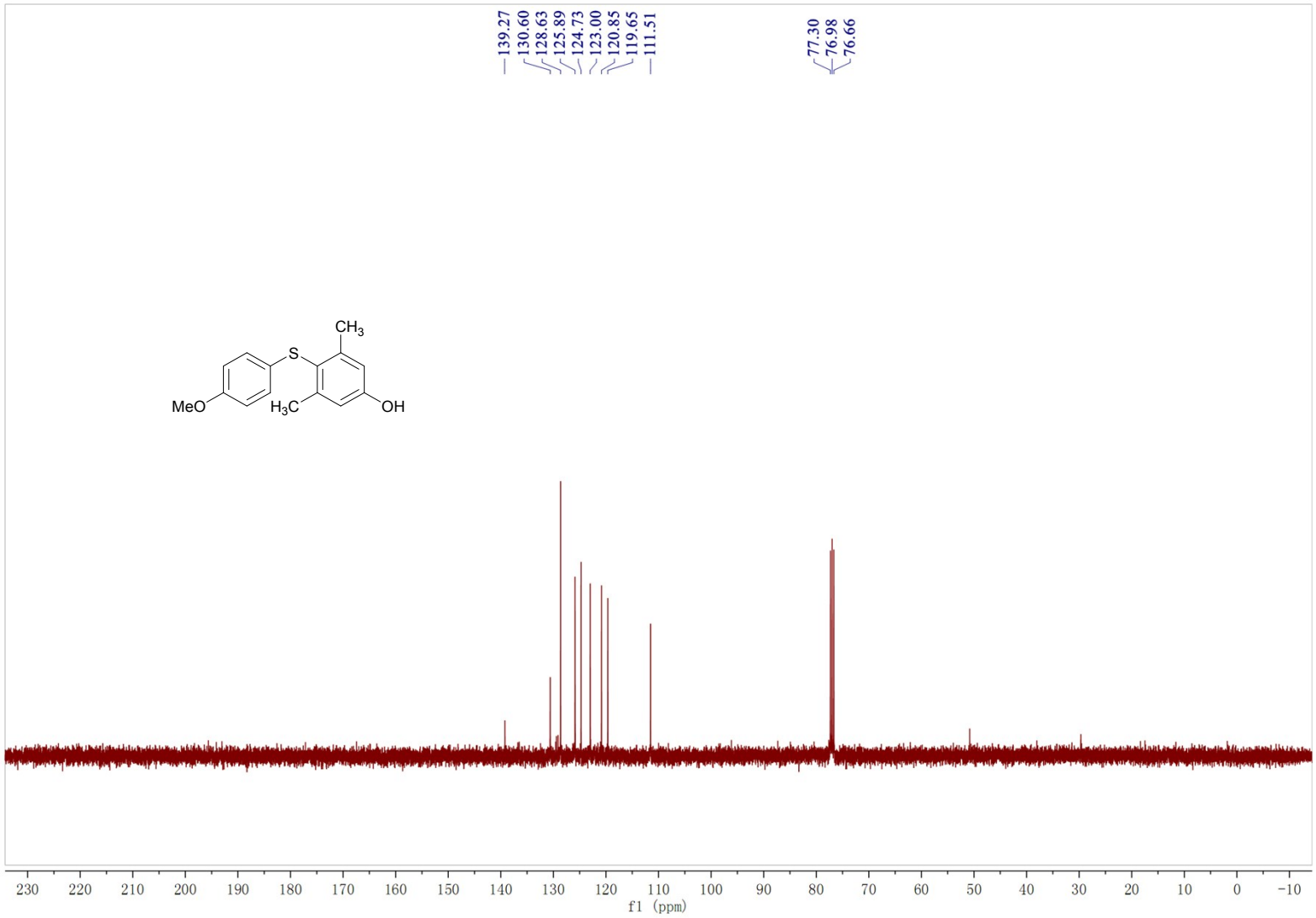
131.79
128.87
126.72
117.88
115.49
77.29
76.97
76.66
21.76
CH3
S
Br
H3C
OH
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


6.82
6.79
6.69
6.66
6.58
4.93
3.67
2.30
0.00
CH3
S
MeO
H3C
OH
2.00
2.07
2.09
1.07
3.02
6.04
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)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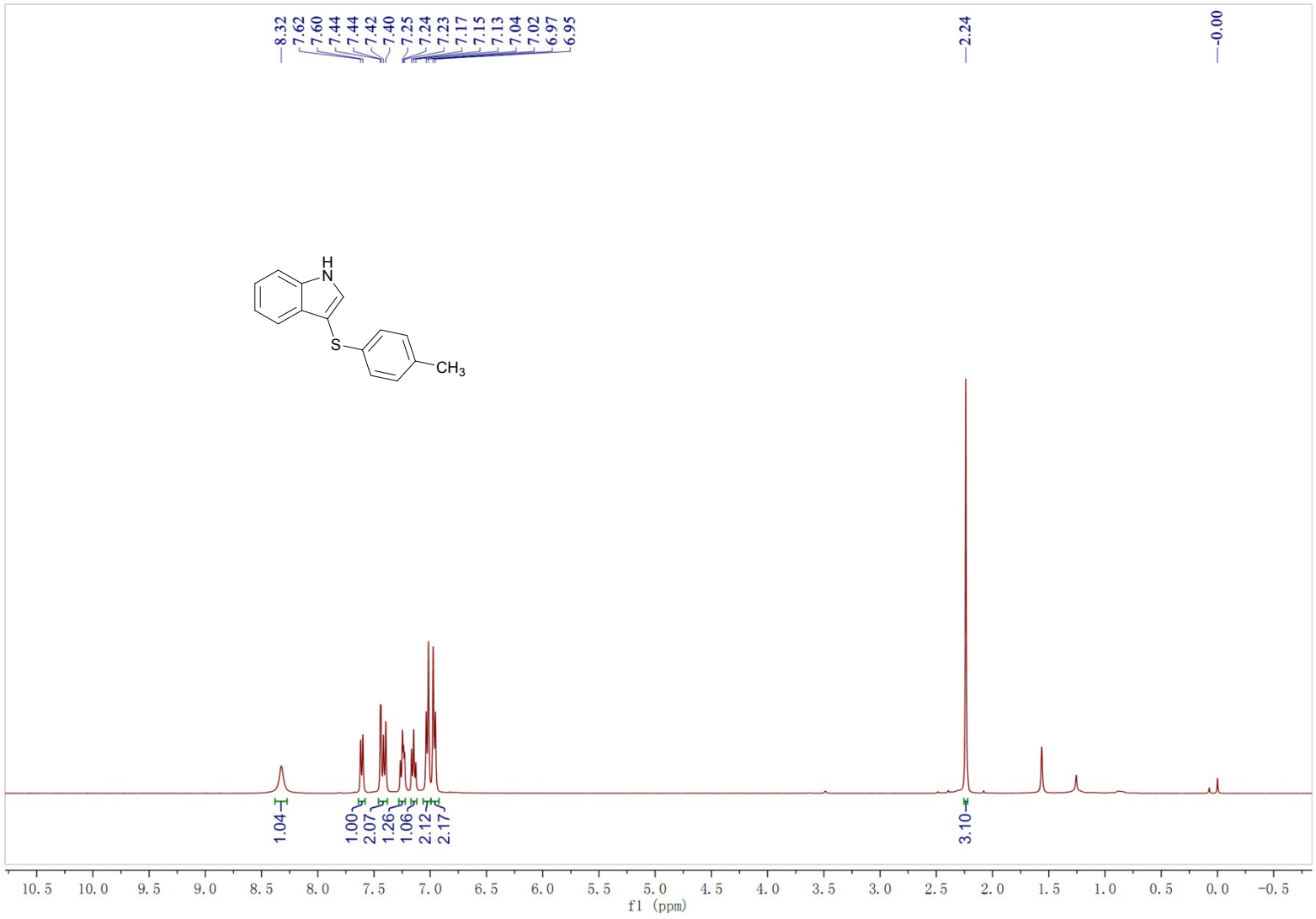
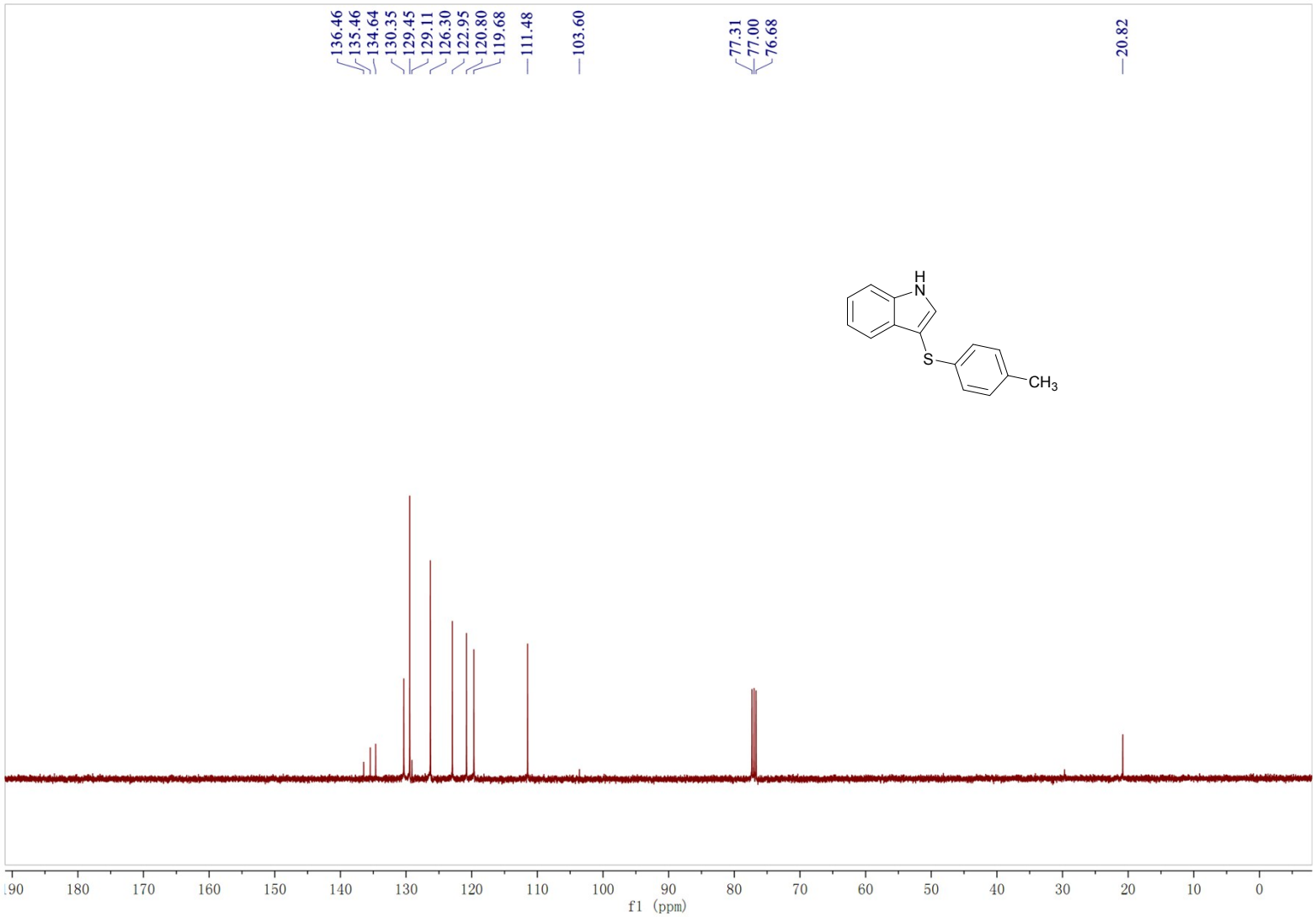
130.60
128.63
125.89
124.73
123.00
120.85
119.65
111.51
77.30
76.98
76.66
CH3
S
MeO
H3C
OH
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.32
7.62
7.60
7.44
7.44
7.42
7.40
7.25
7.24
7.23
7.17
7.15
7.13
7.04
7.02
6.97
6.95
2.24
-0.00
H
N
S
CH3
1.04
1.00
2.07
1.26
1.06
2.12
2.17
3.10
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)


136.46
135.46
134.64
130.35
129.45
129.11
126.30
122.95
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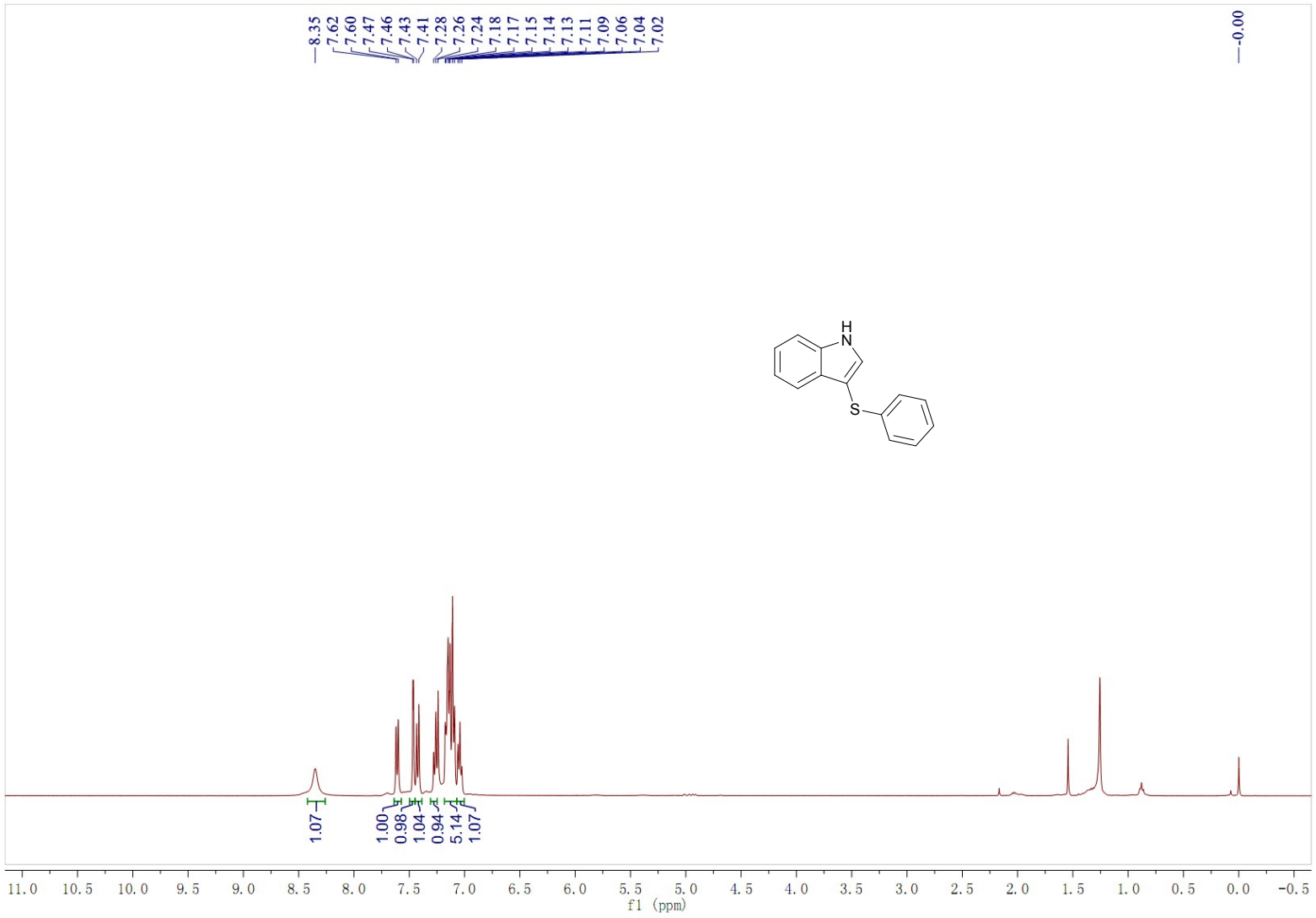
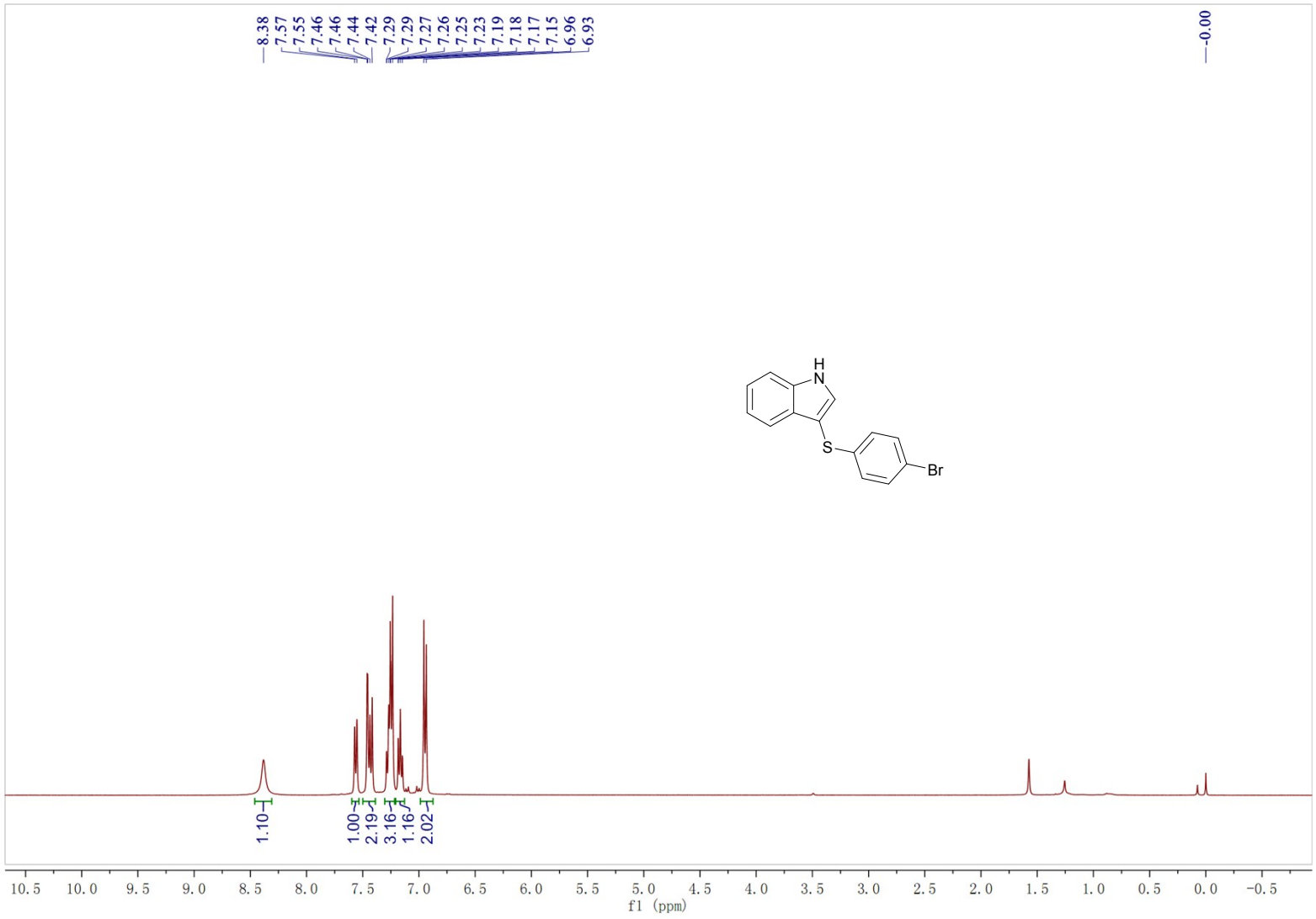
119.68
111.48
103.60
77.31
77.00
76.68
20.82
H
N
S
CH3
f1 (ppm)


8.35
7.62
7.60
7.47
7.46
7.43
7.41
7.28
7.26
7.24
7.18
7.17
7.15
7.14
7.13
7.11
7.09
7.06
7.04
7.02
-0.00
H
N
S
1.07
1.00
0.98
1.04
0.94
5.14
1.07
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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7.57
7.55
7.46
7.46
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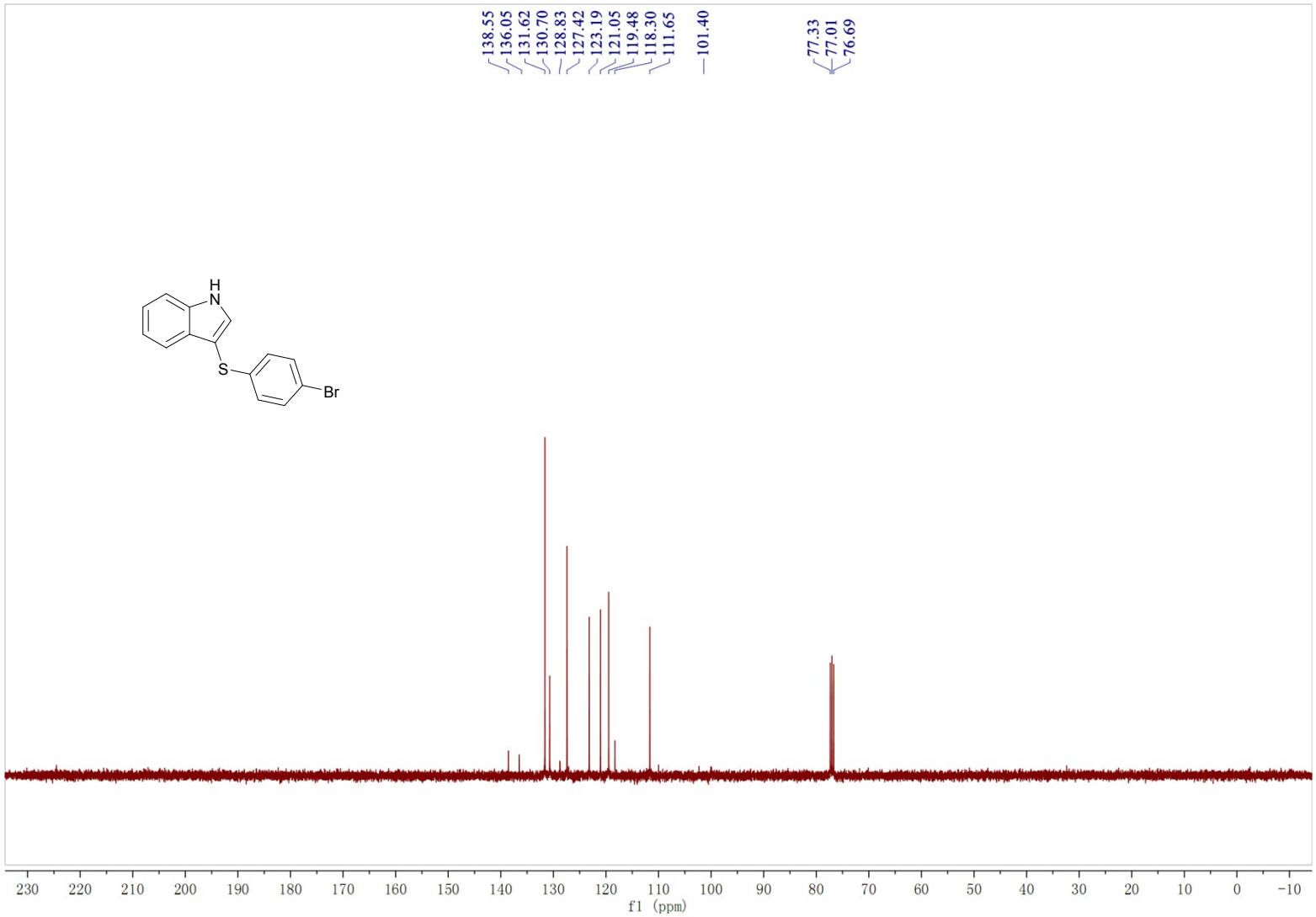
7.42
7.29
7.29
7.27
7.26
7.25
7.23
7.19
7.18
7.17
7.15
6.96
6.93
-0.00
H
N
S
Br
1.10
1.00
2.19
3.16
1.16
2.02
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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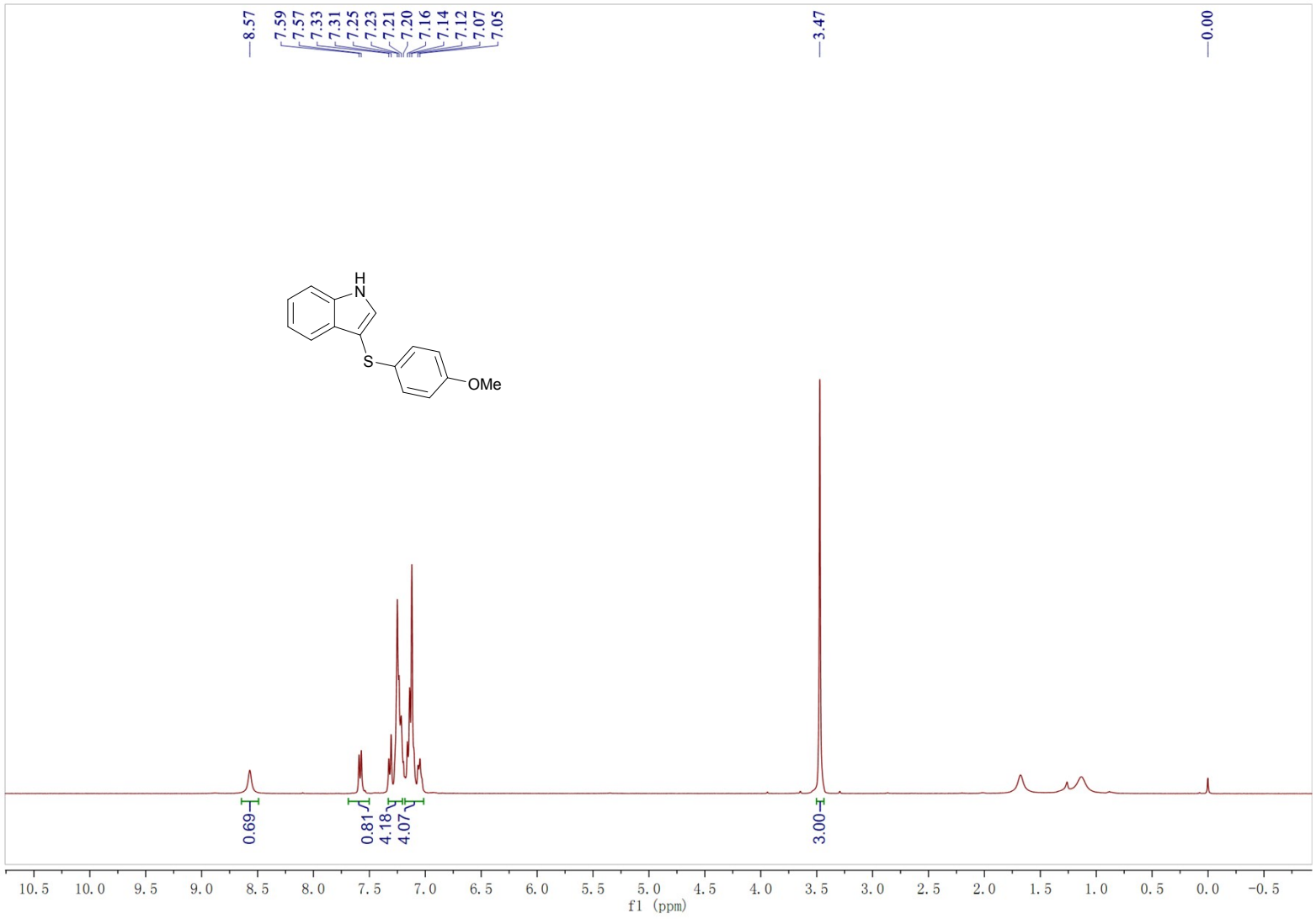
130.70
128.83
127.42
123.19
121.05
119.48
118.30
111.65
101.40
77.33
77.01
76.69
H
N
S
Br
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.57
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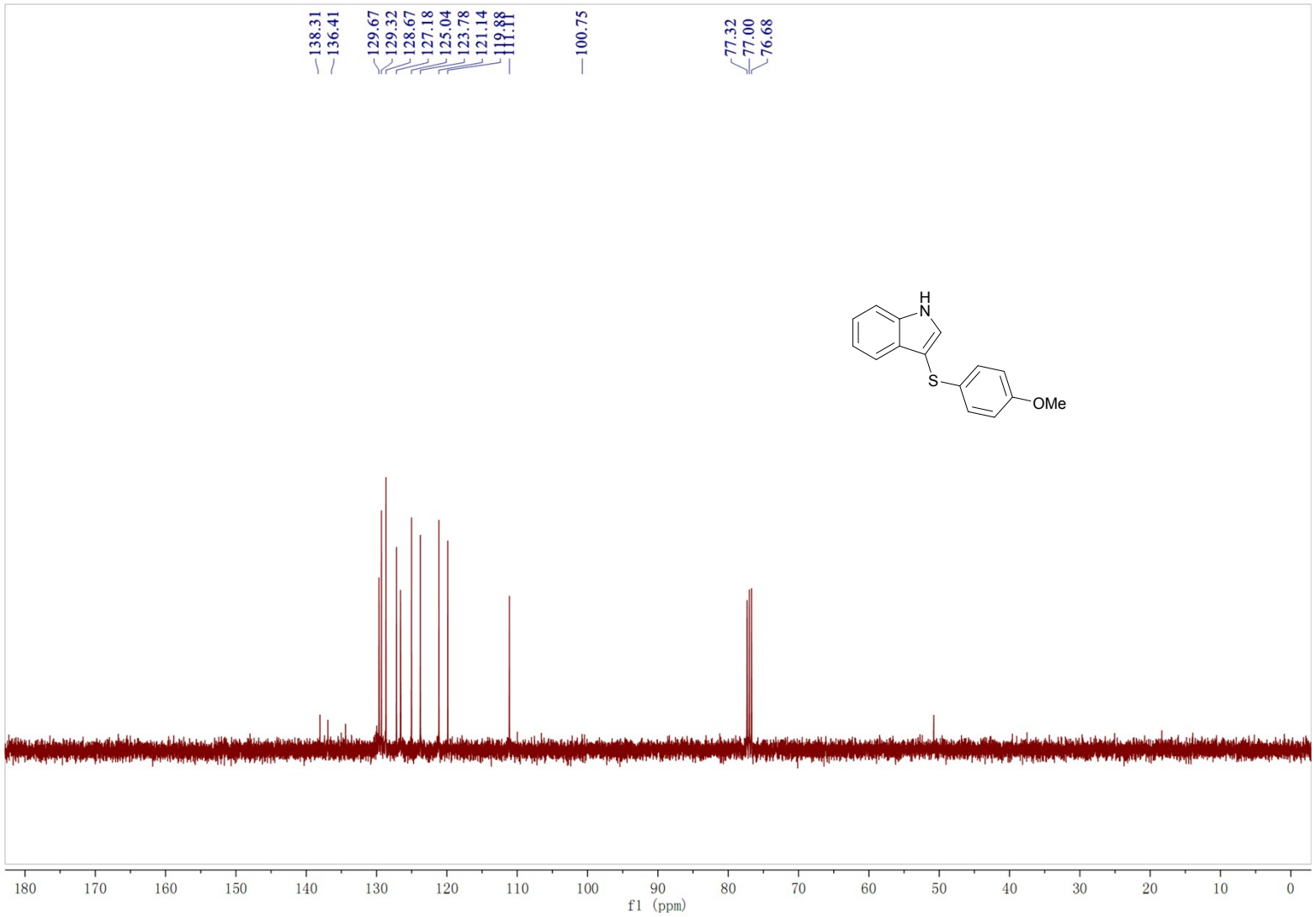
7.25
7.23
7.21
7.20
7.16
7.14
7.12
7.07
7.05
3.47
0.00
H
N
S
OMe
0.69
0.81
4.18
4.07
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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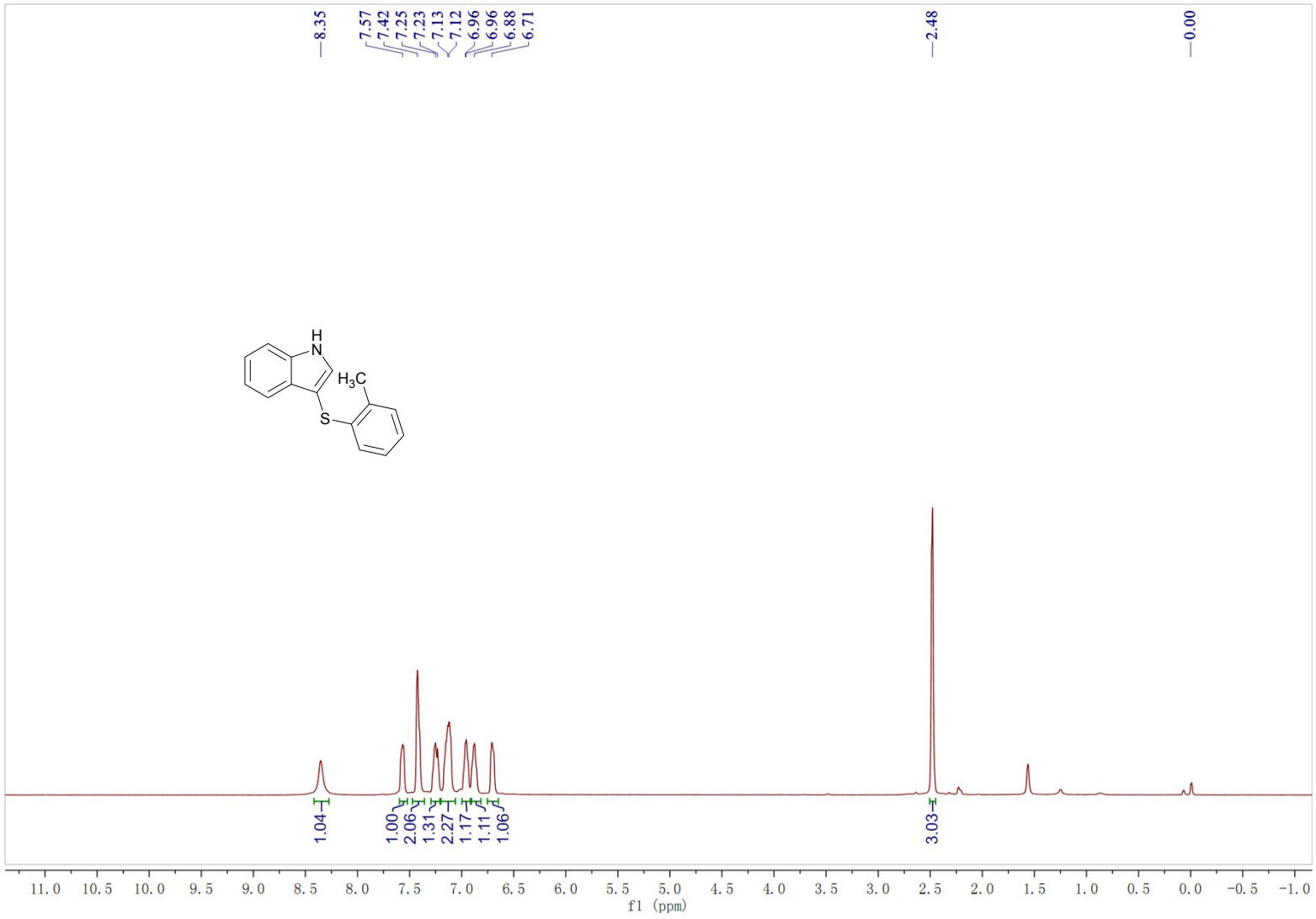
127.18
125.04
123.78
121.14
119.88
111.11
100.75
77.32
77.00
76.68
H
N
S
OMe
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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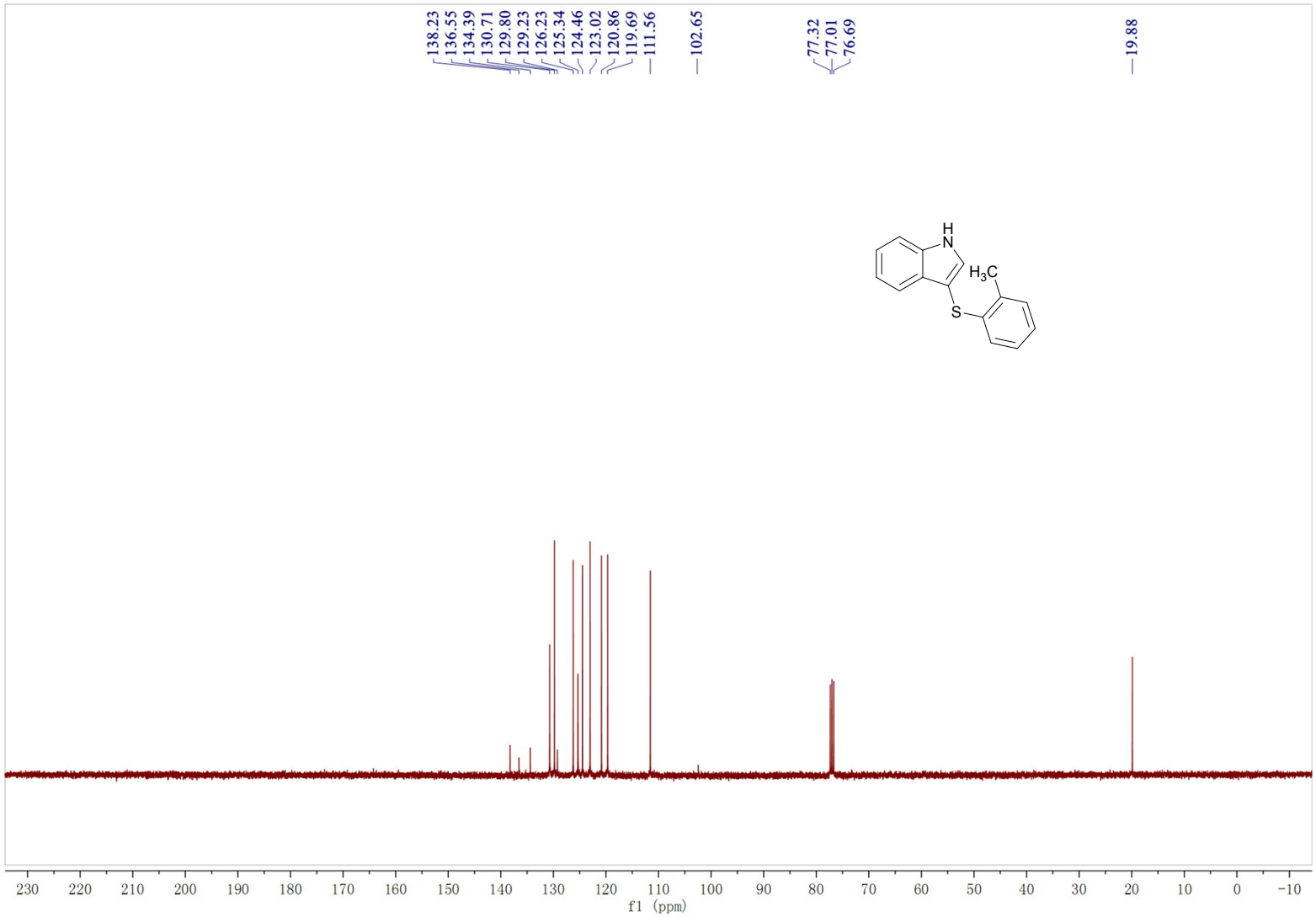
7.25
7.23
7.13
7.12
6.96
6.96
6.88
6.71
2.48
0.00
H
N
H3C
S
1.04
1.00
2.06
1.31
2.27
1.17
1.11
1.06
3.03
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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124.46
123.02
120.86
119.69
111.56
102.65
77.32
77.01
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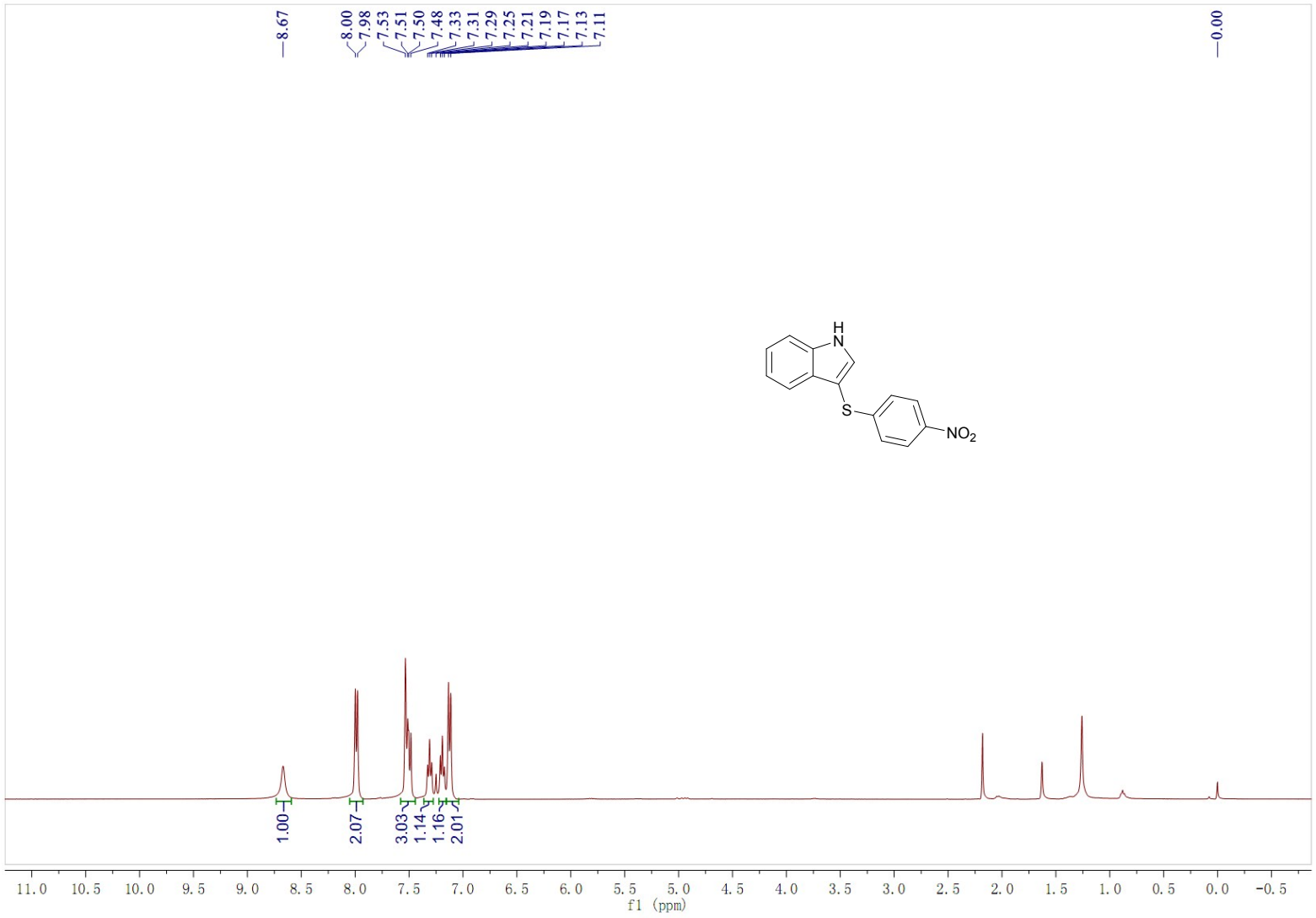
19.88
H
N
H3C
S
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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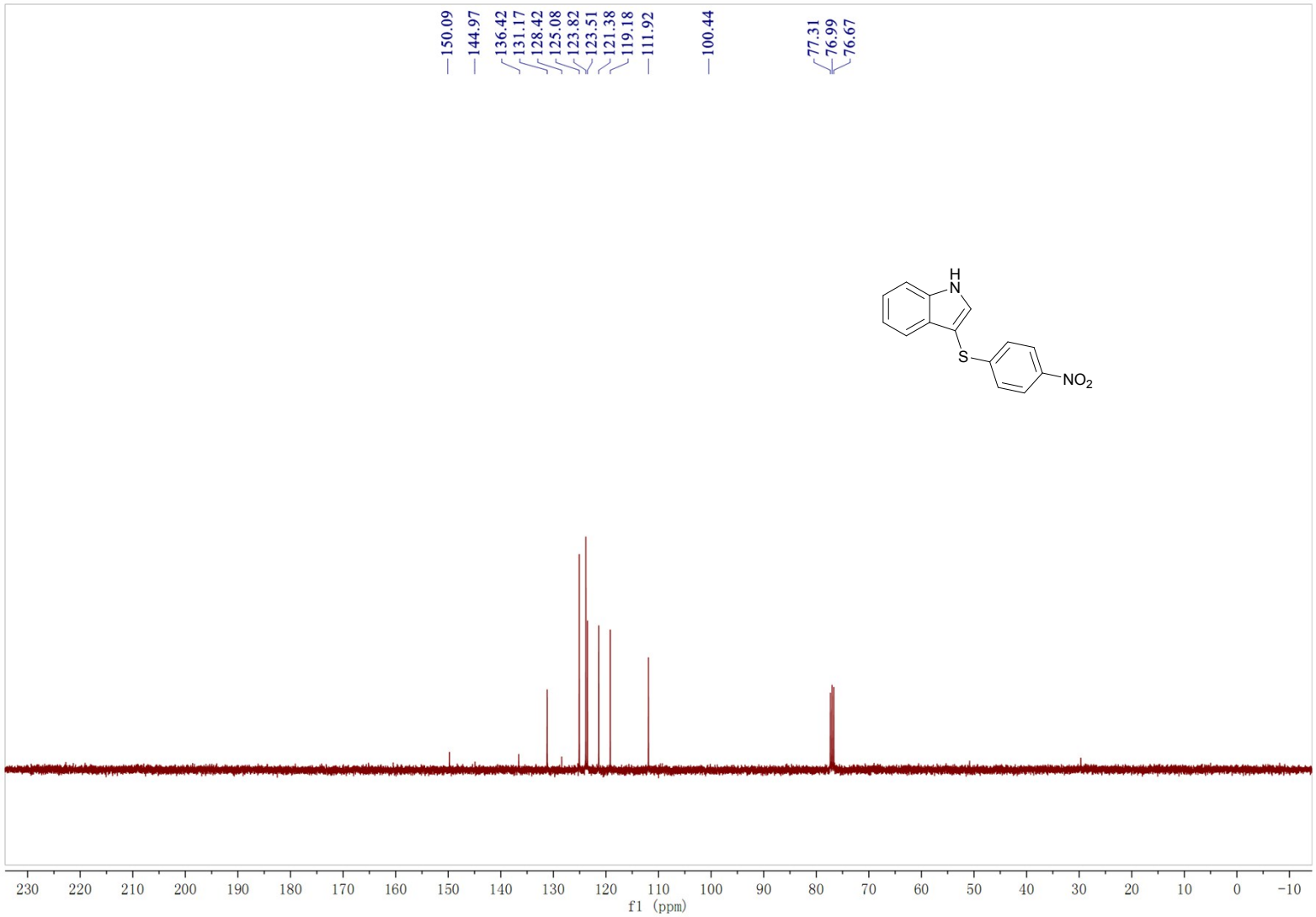
7.29
7.25
7.21
7.19
7.17
7.13
7.11
0.00
H
N
S
NO2
1.00
2.07
3.03
1.14
1.16
2.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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125.08
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123.51
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119.18
111.92
100.44
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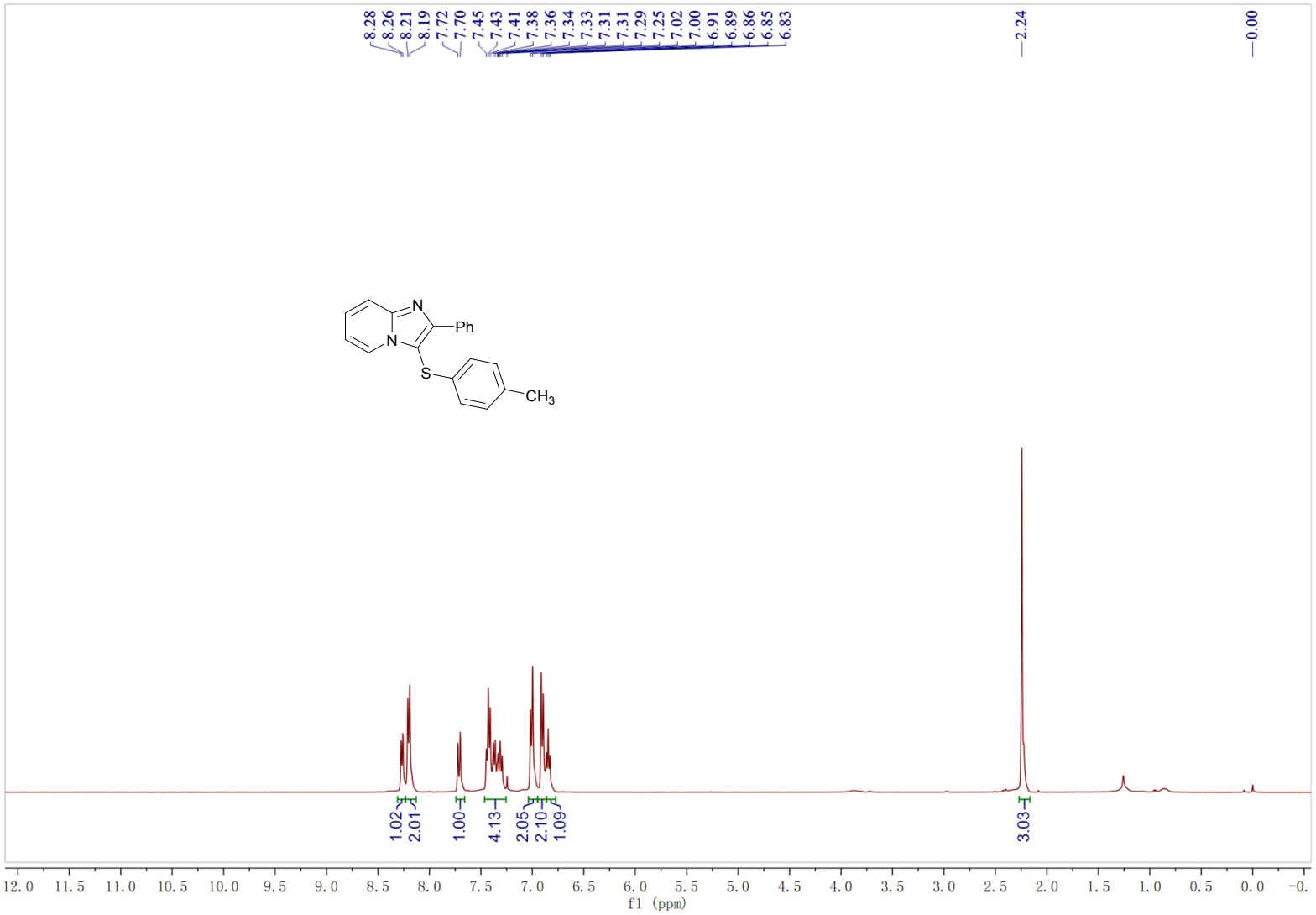
76.67
H
N
S
NO2
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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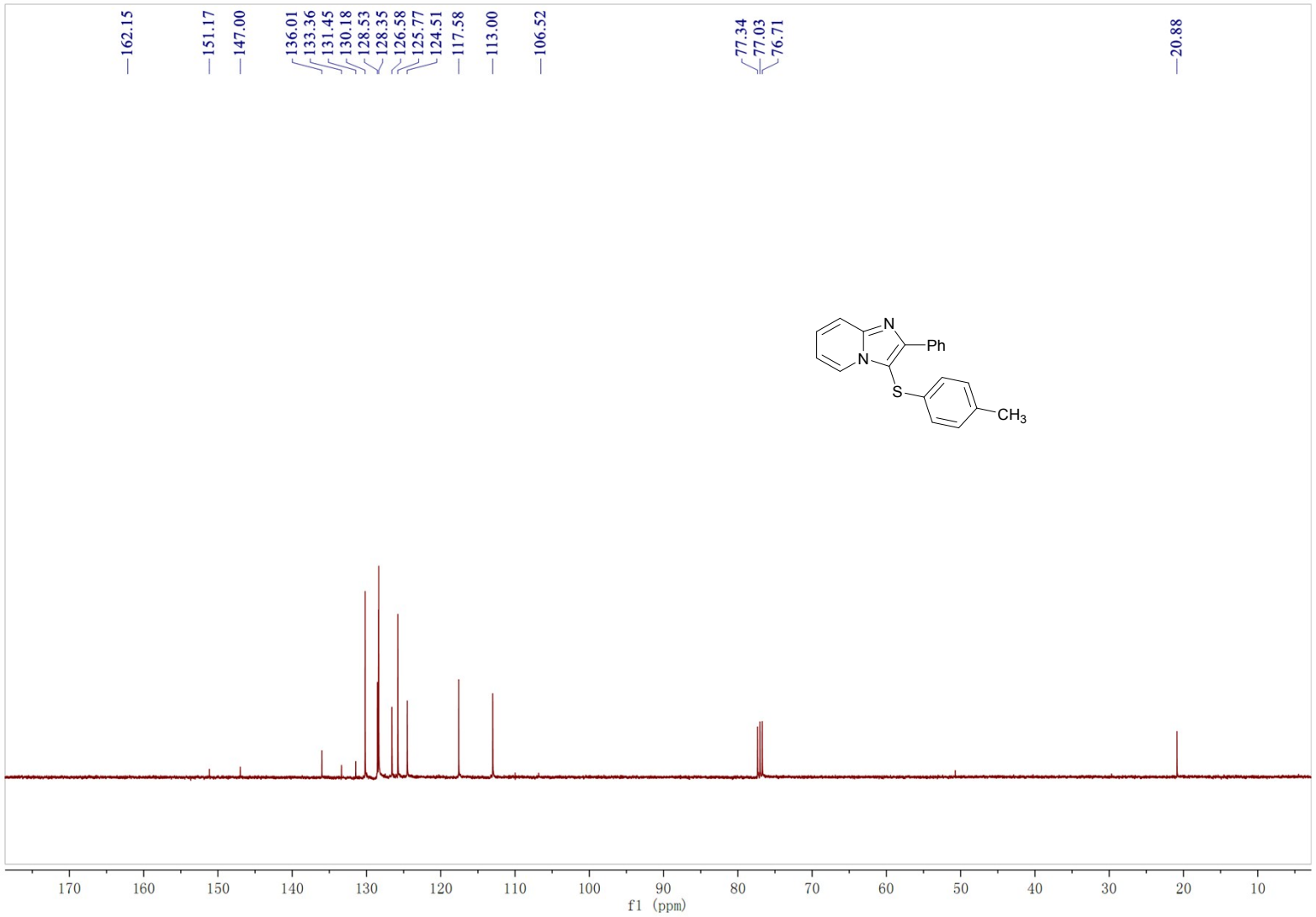
7.36
7.34
7.33
7.31
7.31
7.29
7.25
7.02
7.00
6.91
6.89
6.86
6.85
6.83
2.24
0.00
N
Ph
N
S
CH3
1.02
2.01
1.00
4.13
2.05
2.10
1.09
3.03
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)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126.58
125.77
124.51
117.58
113.00
106.52
77.34
77.03
76.71
20.88
N
N
Ph
S
CH3
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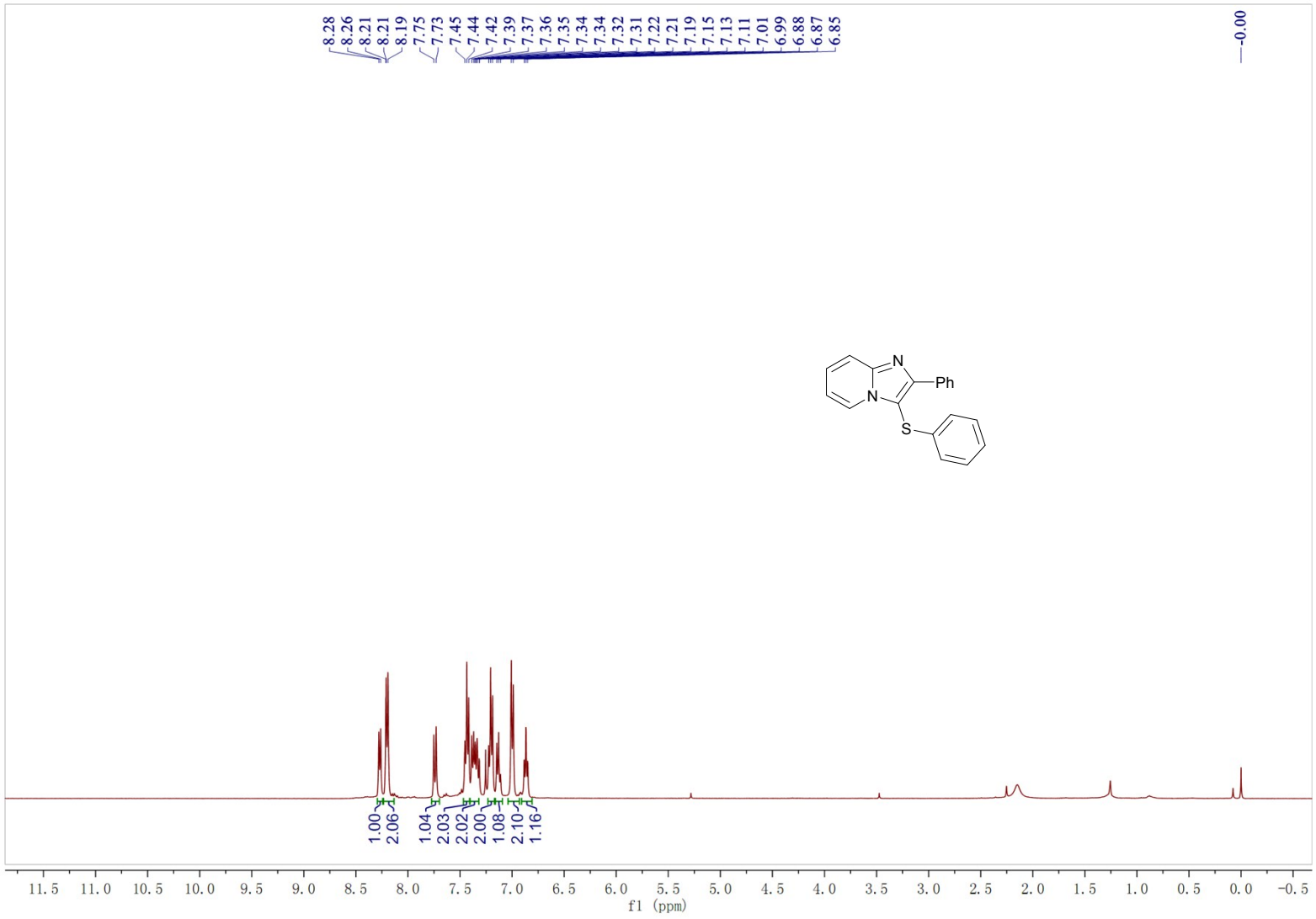
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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8.26
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8.21
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7.45
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7.42
7.39
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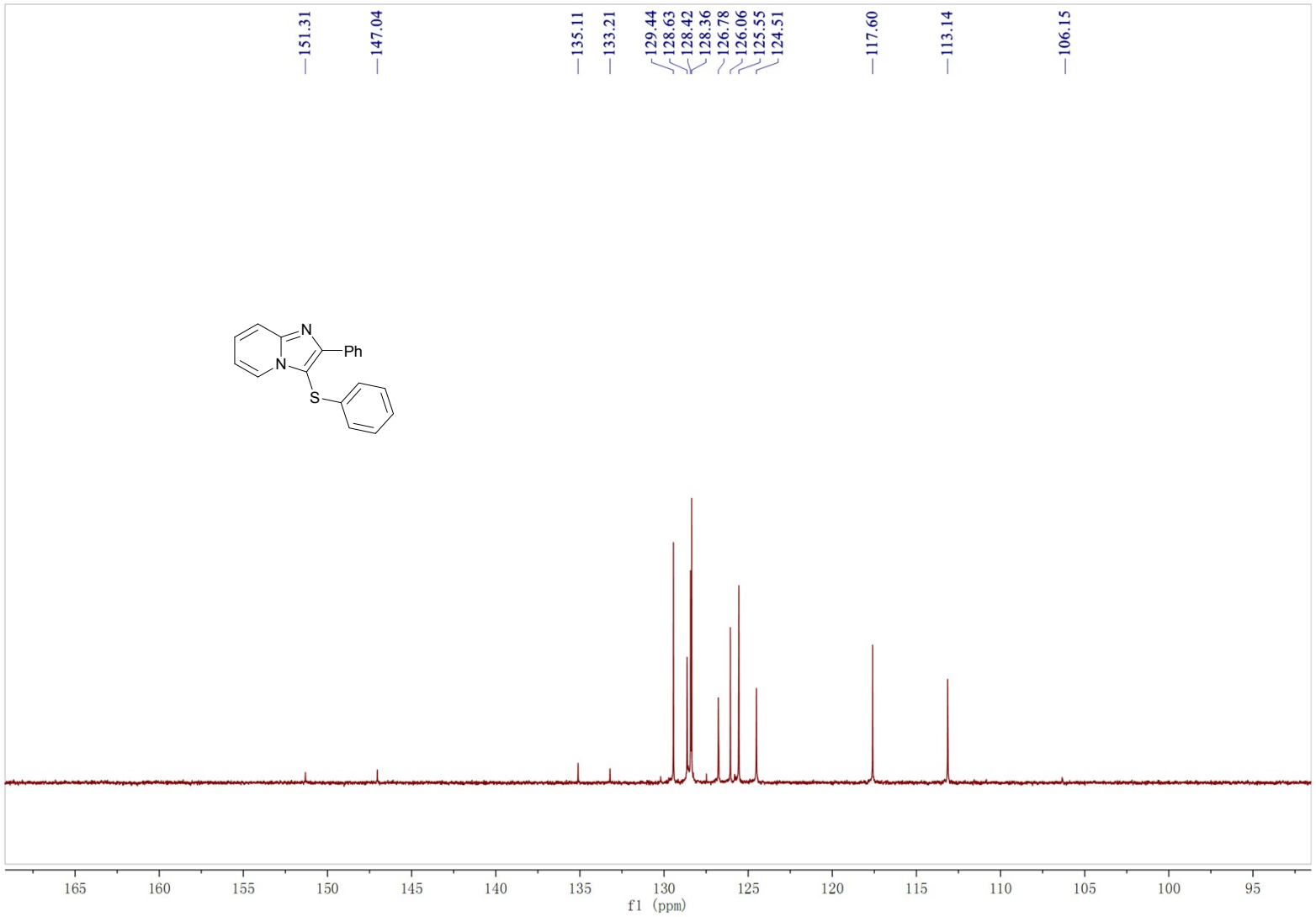
7.35
7.34
7.34
7.32
7.31
7.22
7.21
7.19
7.15
7.13
7.11
7.01
6.99
6.88
6.87
6.85
-0.00
N
N
Ph
S
1.00
2.06
1.04
2.03
2.02
2.00
1.08
2.10
1.16
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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128.42
128.36
126.78
126.06
125.55
124.51
117.60
113.14
106.15
N
N
Ph
S
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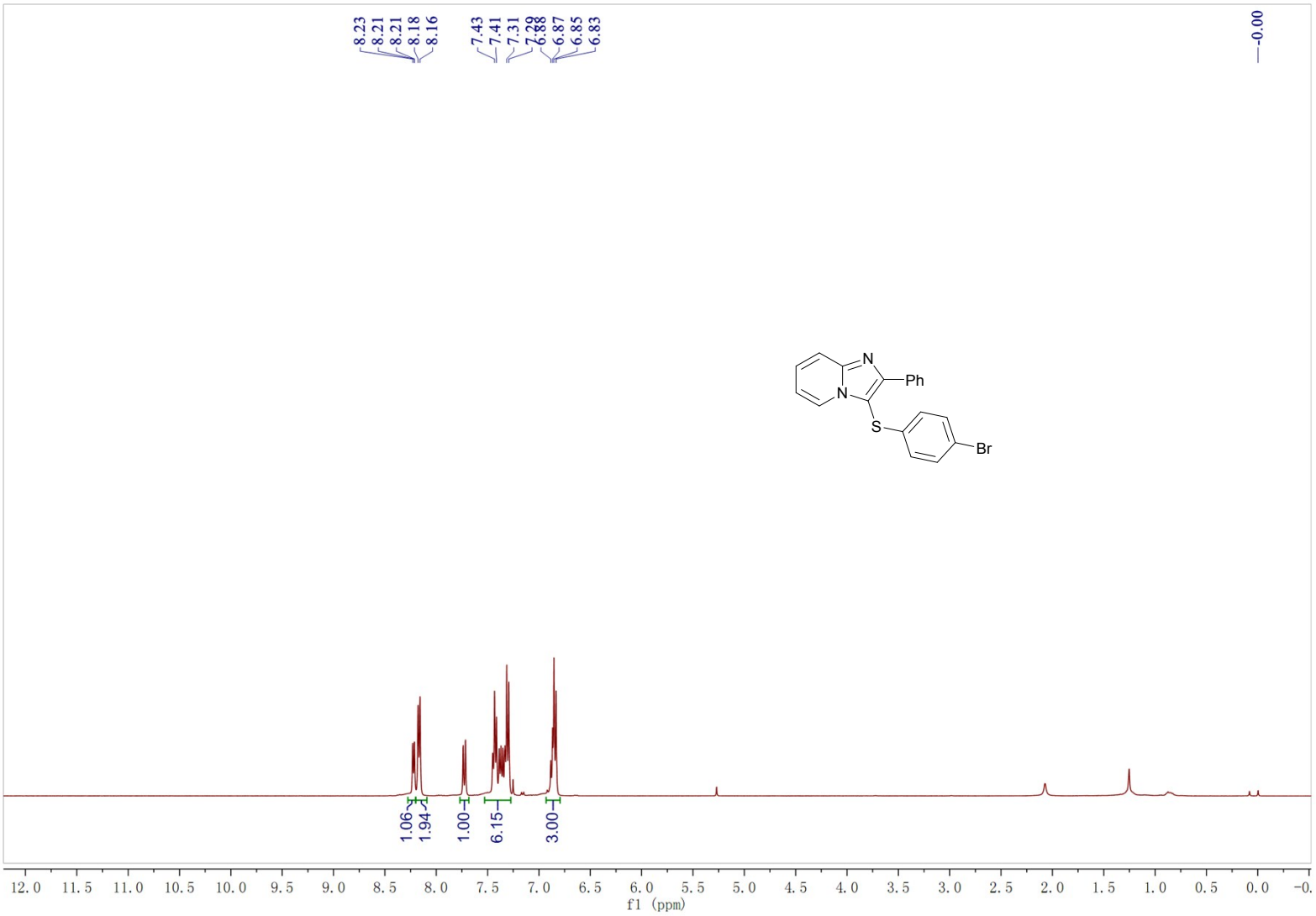
160
155
150
145
140
135
130
125
120
115
110
105
100
95
f1 (ppm)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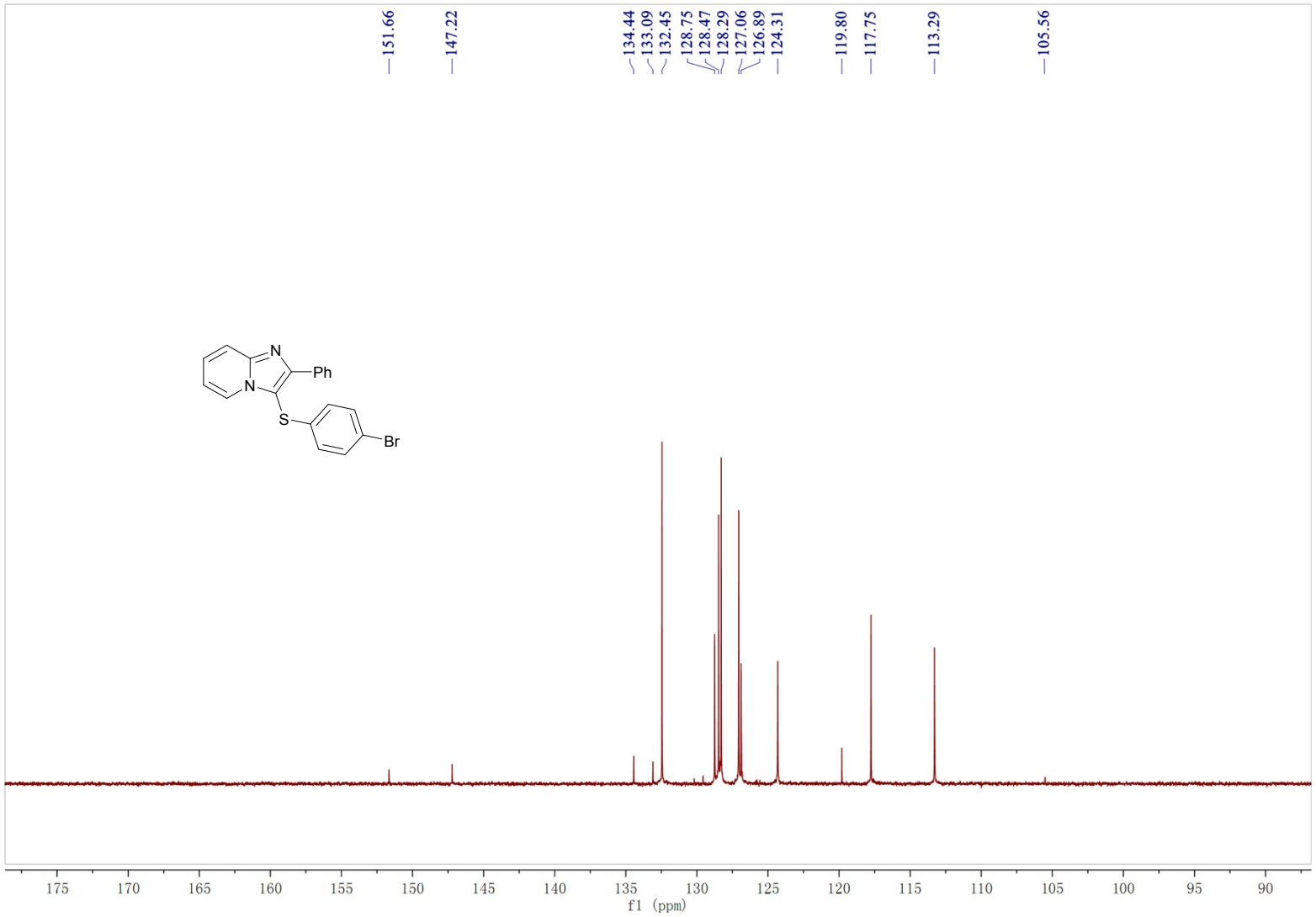
7.31
7.29
6.88
6.87
6.85
6.83
-0.00
N
Ph
N
S
Br
1.06
1.94
1.00
6.15
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)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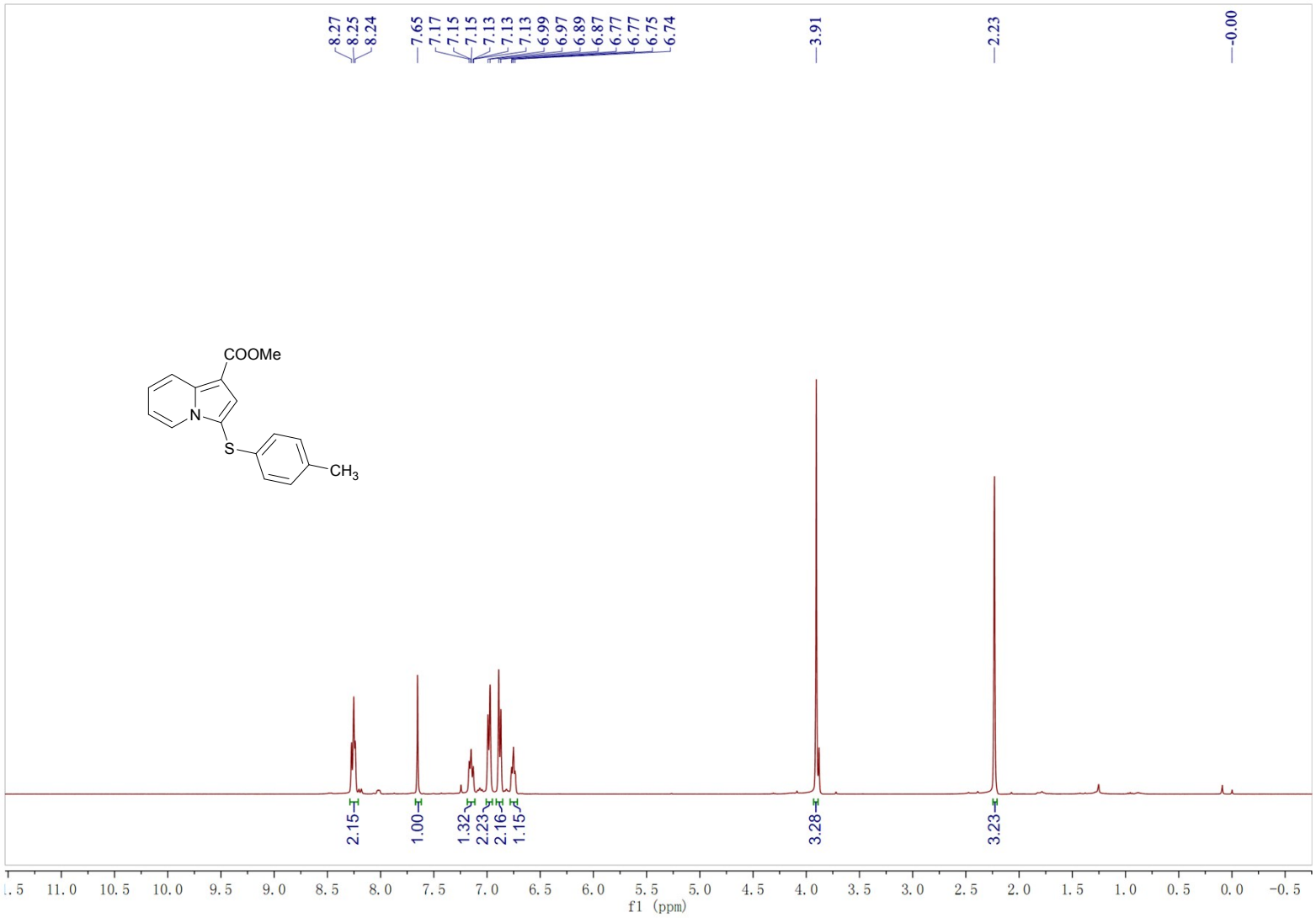
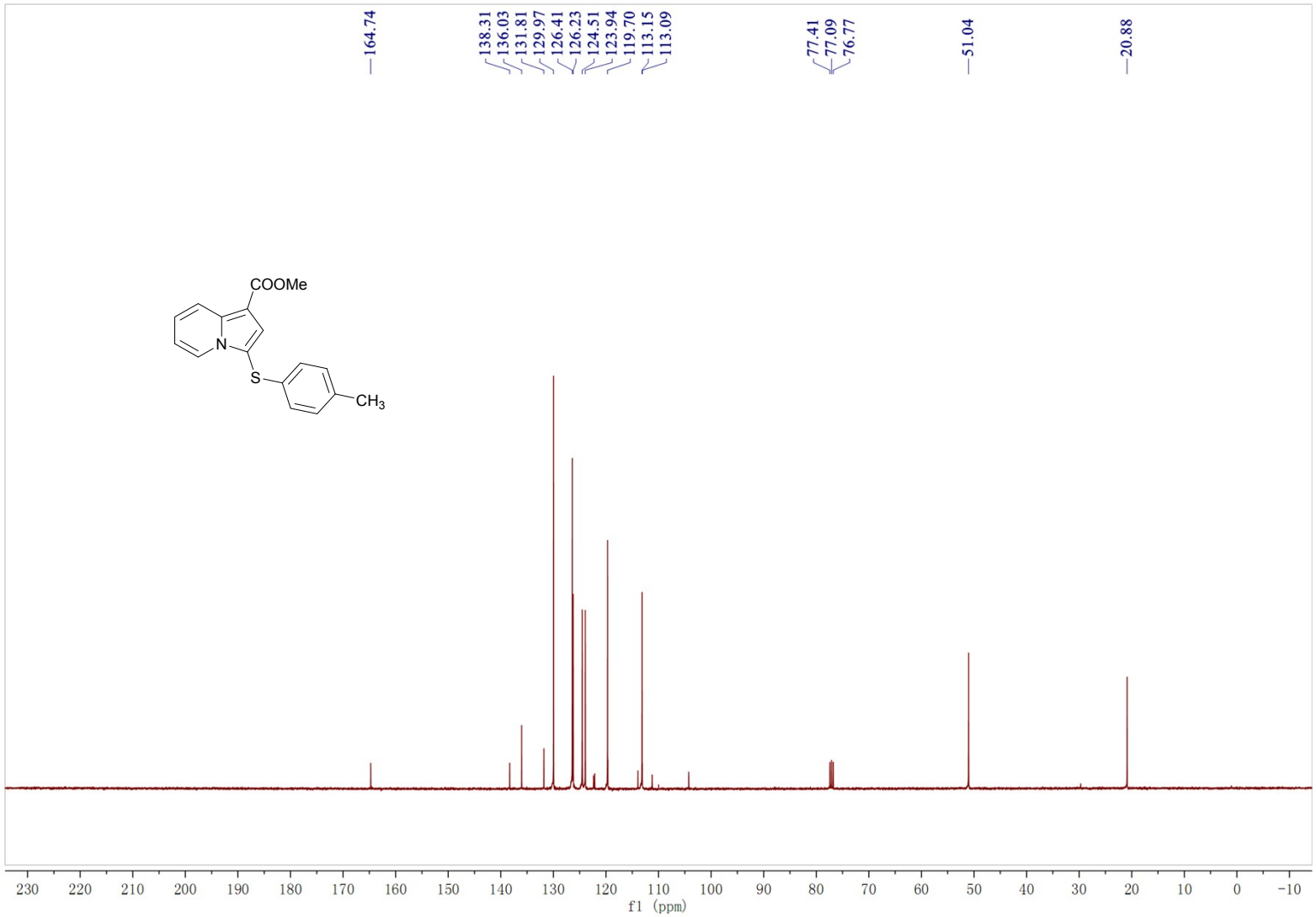
147.22
134.44
133.09
132.45
128.75
128.47
128.29
127.06
126.89
124.31
119.80
117.75
113.29
105.56
N
Ph
N
S
Br
175
170
165
160
155
150
145
140
135
130
125
120
115
110
105
100
95
90
f1 (ppm)


8.27
8.25
8.24
7.65
7.17
7.15
7.15
7.13
7.13
7.13
6.99
6.97
6.89
6.87
6.77
6.77
6.75
6.74
3.91
2.23
-0.00
COOMe
N
S
CH3
2.15
1.00
1.32
2.23
2.16
1.15
3.28
3.23
f1 (ppm)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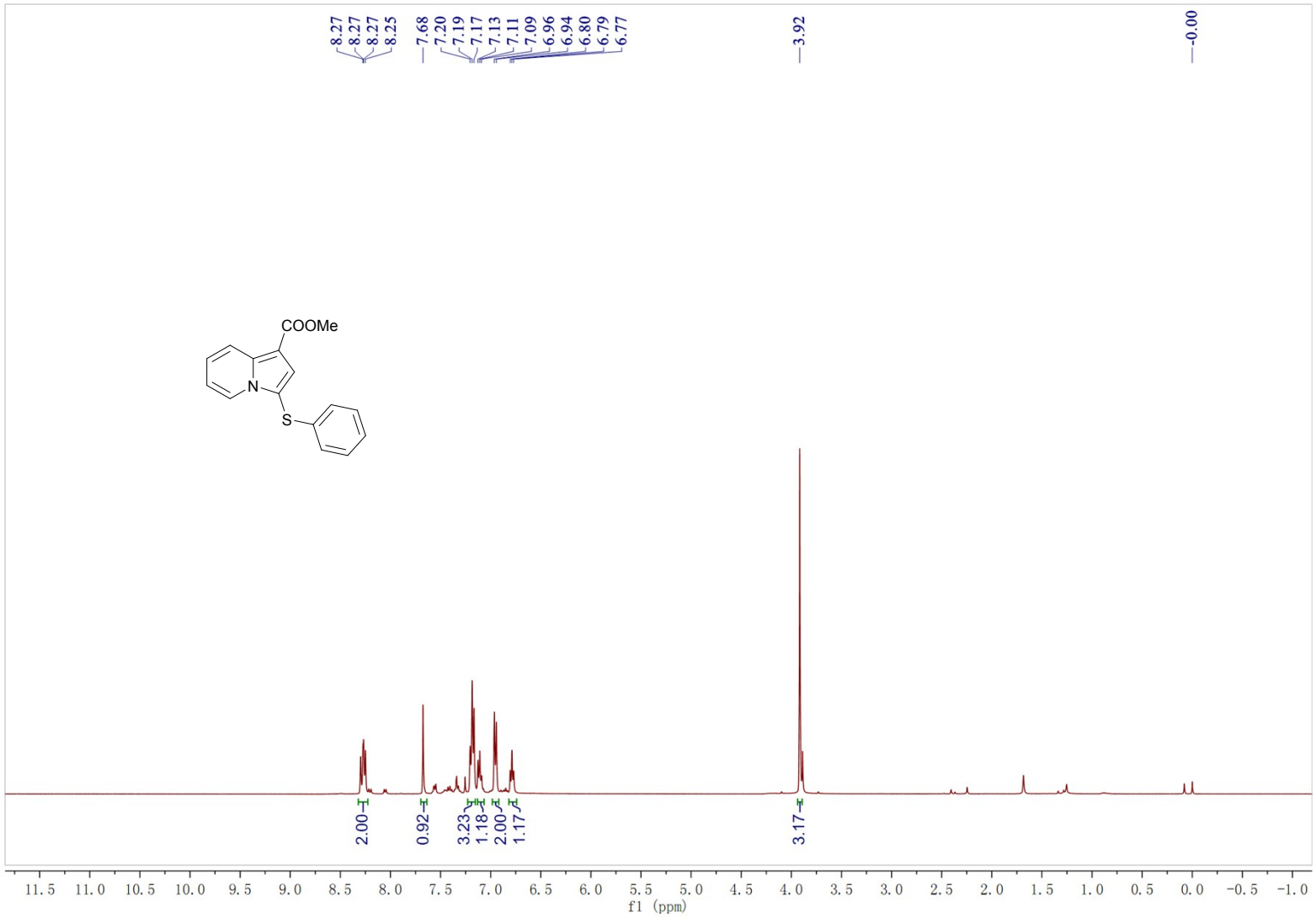
138.31
136.03
131.81
129.97
126.41
126.23
124.51
123.94
119.70
113.15
113.09
77.41
77.09
76.77
51.04
20.88
COOMe
N
S
CH3
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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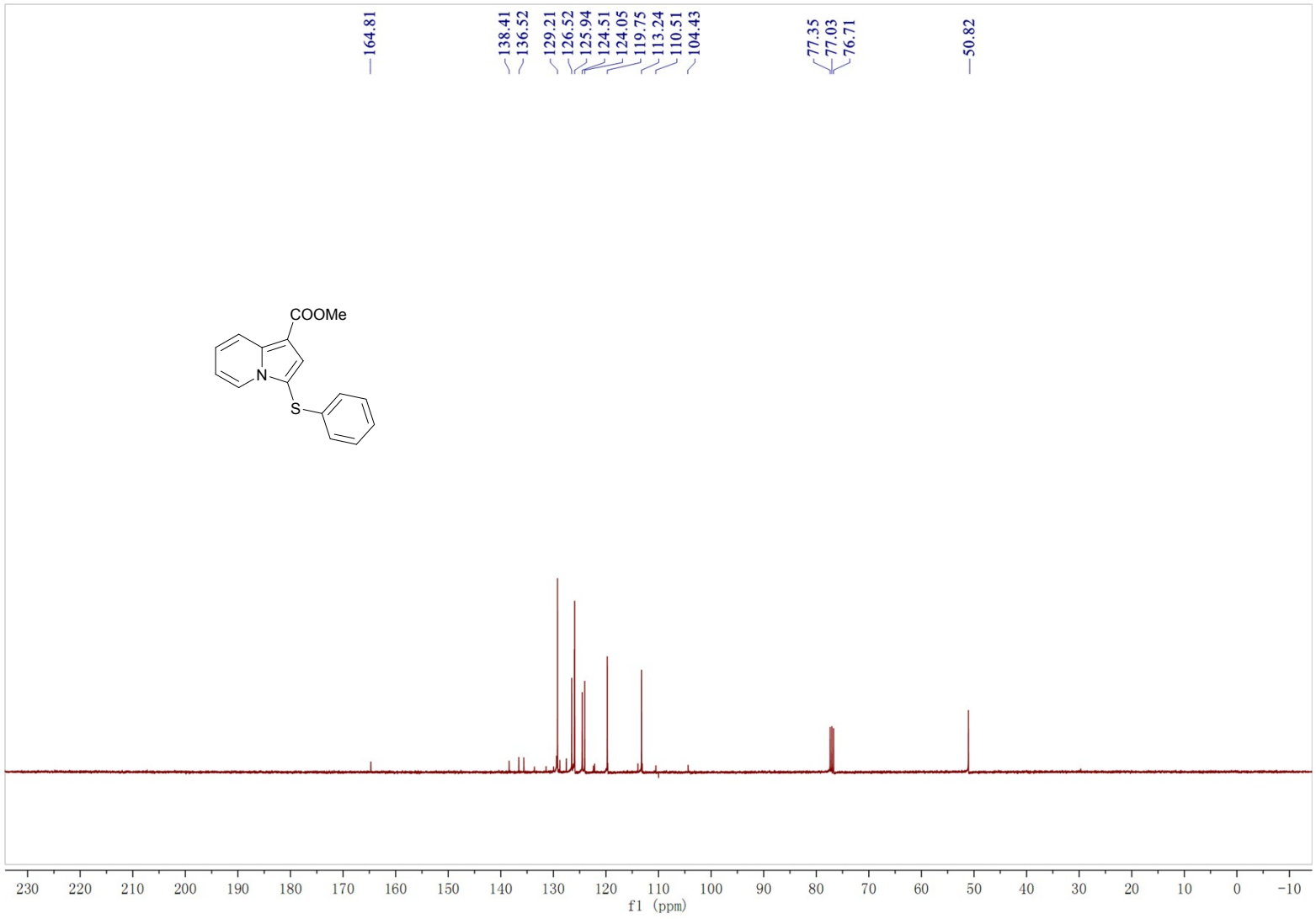
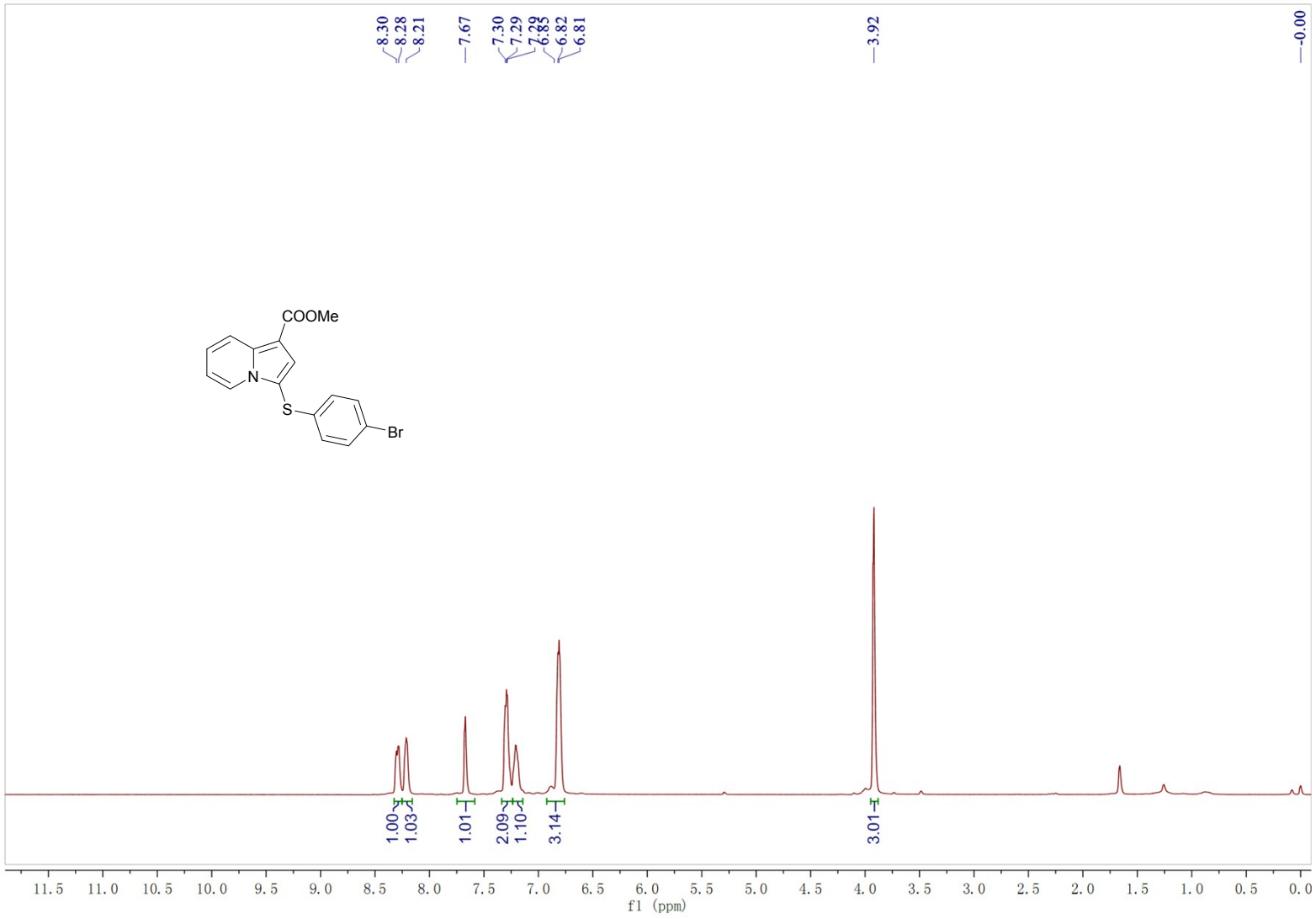
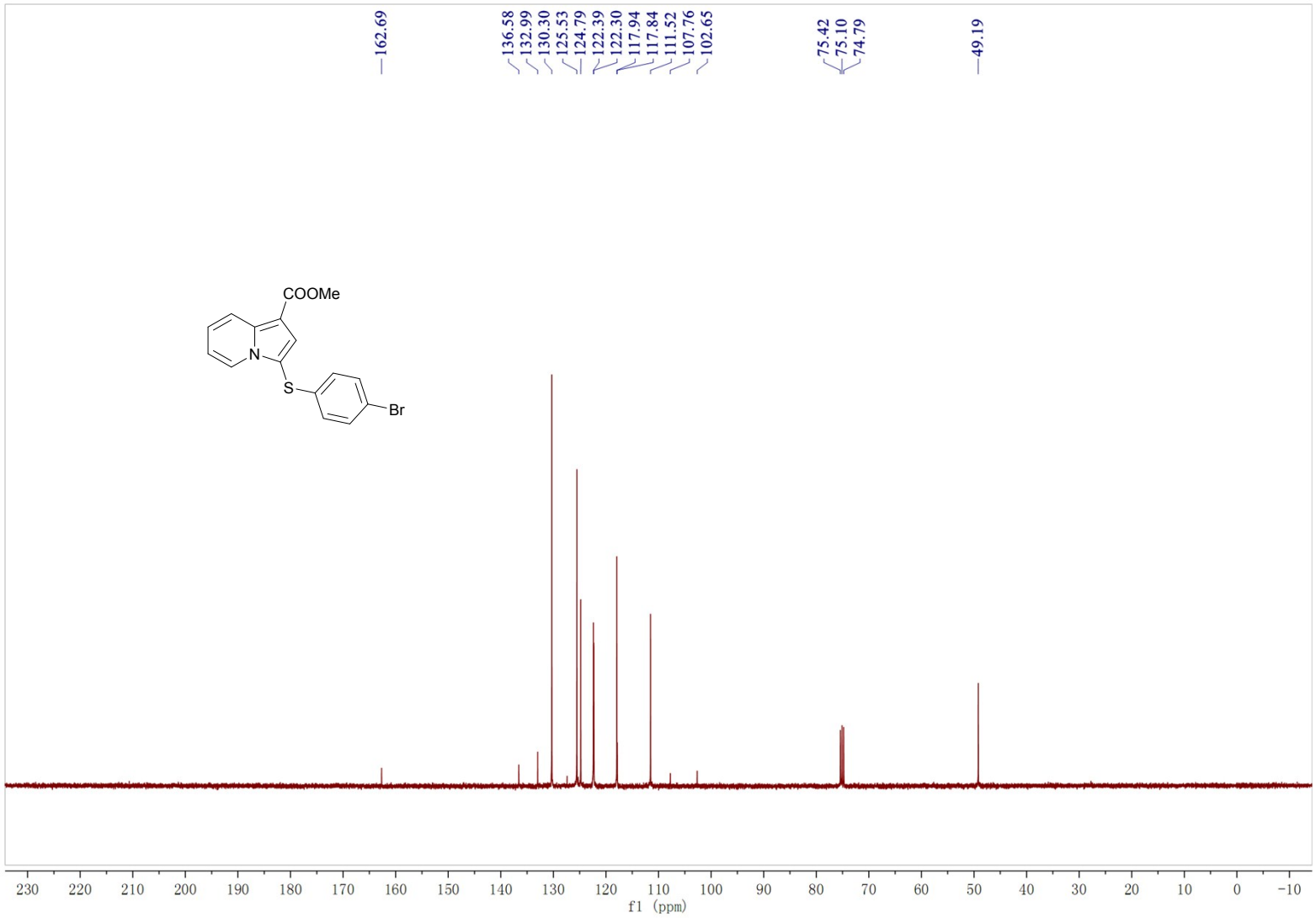
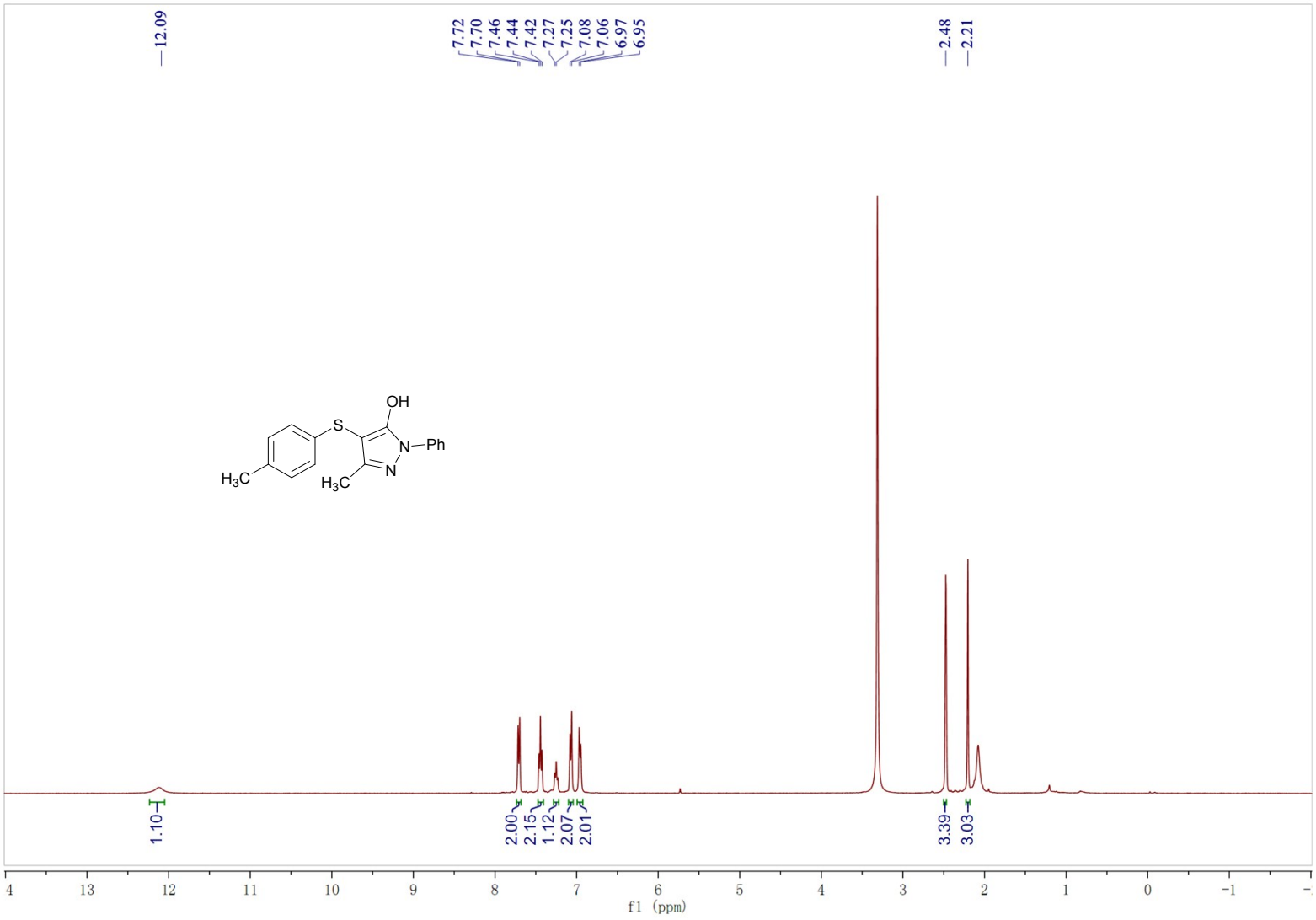
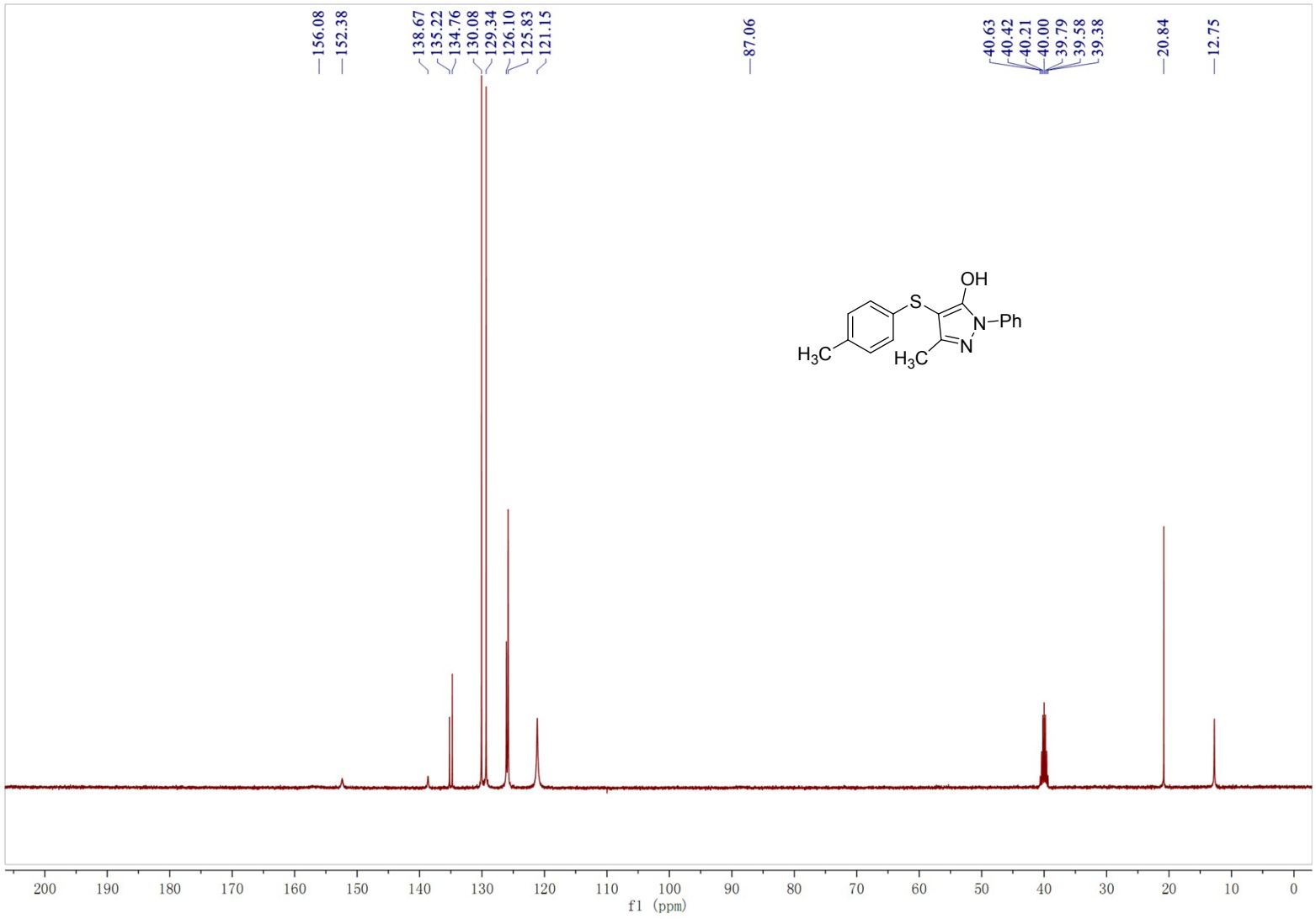
8.27
8.27
8.25
7.68
7.20
7.19
7.17
7.13
7.11
7.09
6.96
6.94
6.80
6.79
6.77
3.92
-0.00
COOMe
N
S
2.00
0.92
3.23
1.18
2.00
1.17
3.17
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

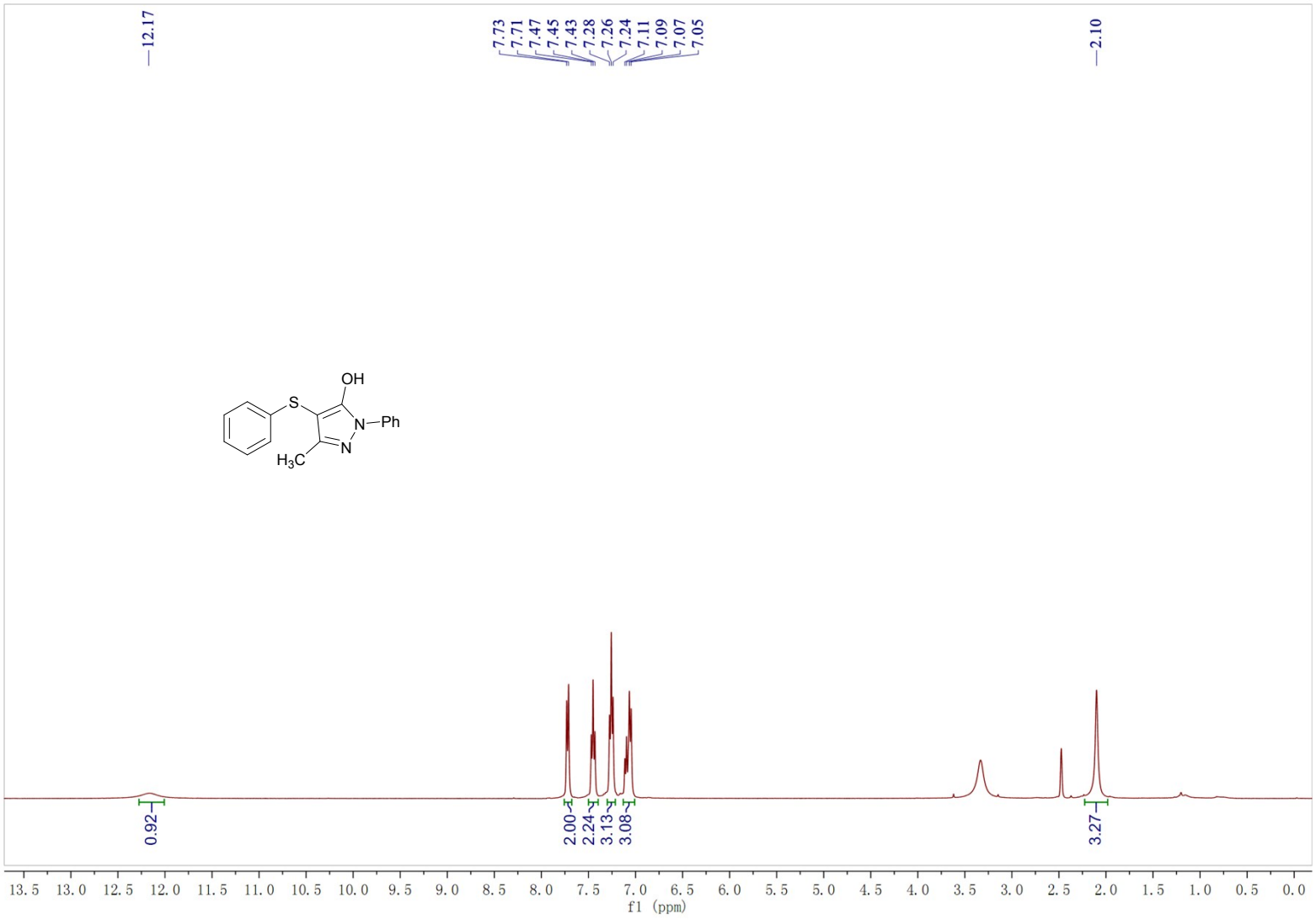

164.81
138.41
136.52
129.21
126.52
125.94
124.51
124.05
119.75
113.24
110.51
104.43
77.35
77.03
76.71
50.82
COOMe
N
S
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

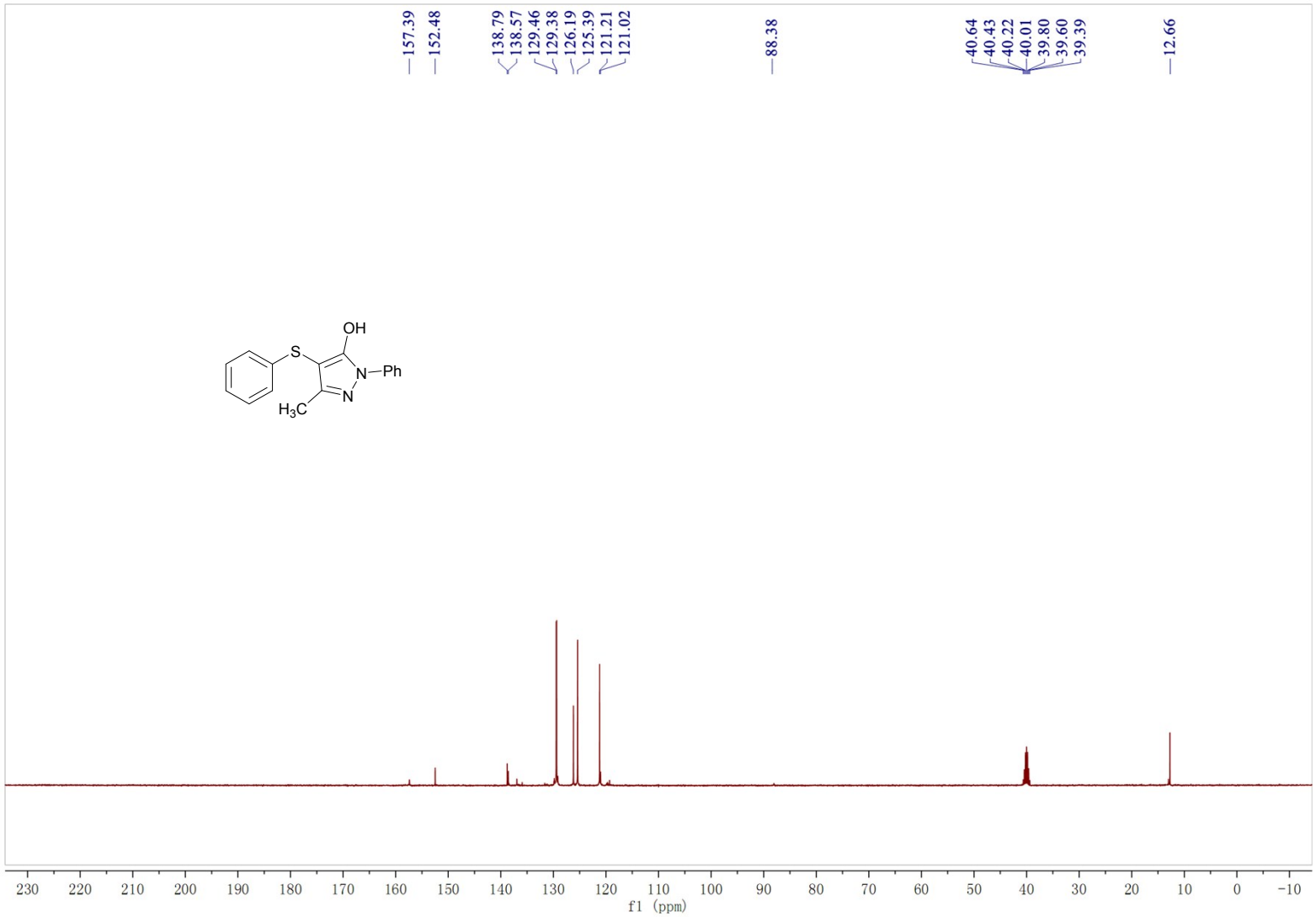

8.30
8.28
8.21
7.67
7.30
7.29
7.28
6.85
6.82
6.81
3.92
-0.00
COOMe
N
S
Br
1.00
1.03
1.01
2.09
1.10
3.14
3.01
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


162.69
136.58
132.99
130.30
125.53
124.79
122.39
122.30
117.94
117.84
111.52
107.76
102.65
75.42
75.10
74.79
49.19
COOMe
N
S
Br
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)


12.09
7.72
7.70
7.46
7.44
7.42
7.27
7.25
7.08
7.06
6.97
6.95
2.48
2.21
OH
S
N—Ph
N
H3C
H3C
1.10
2.00
2.15
1.12
2.07
2.01
3.39
3.03
f1 (ppm)


156.08
152.38
138.67
135.22
134.76
130.08
129.34
126.10
125.83
121.15
87.06
40.63
40.42
40.21
40.00
39.79
39.58
39.38
20.84
12.75
OH
S
N–Ph
N
H3C
H3C
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


12.17
7.73
7.71
7.47
7.45
7.43
7.28
7.26
7.24
7.11
7.09
7.07
7.05
2.10
OH
S
N—Ph
N
H3C
0.92
2.00
2.24
3.13
3.08
3.27
13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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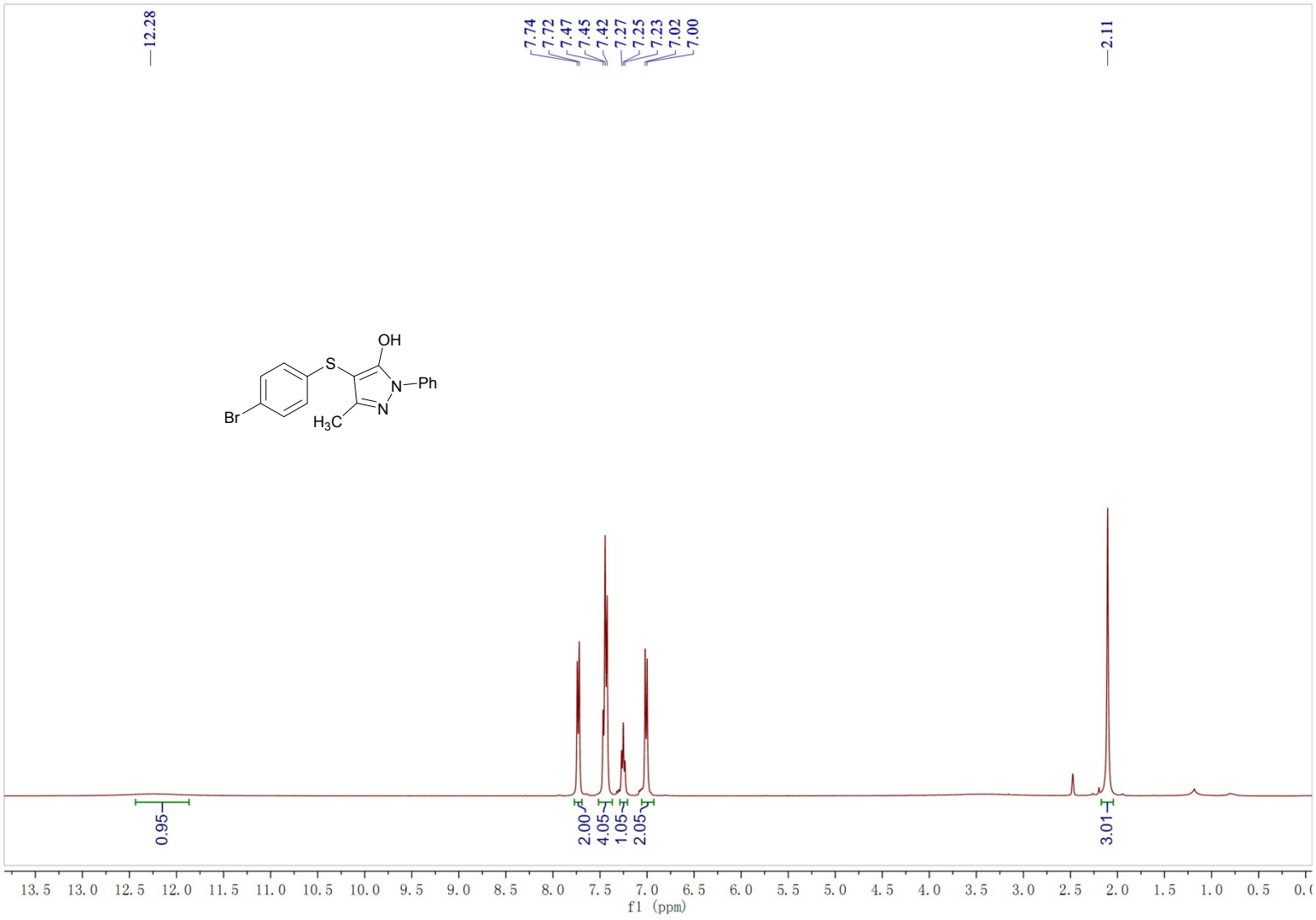
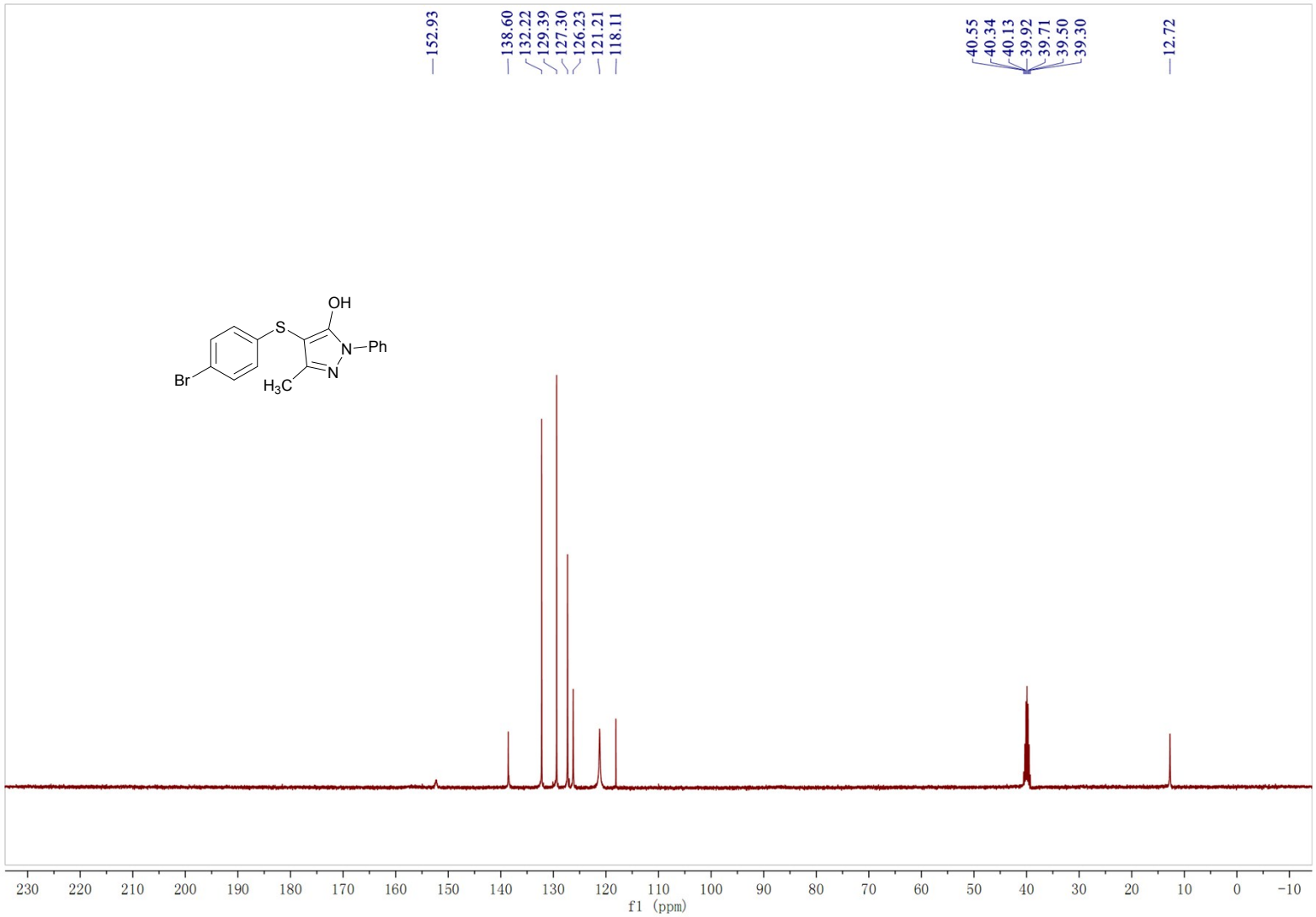
152.48
138.79
138.57
129.46
129.38
126.19
125.39
121.21
121.02
88.38
40.64
40.43
40.22
40.01
39.80
39.60
39.39
12.66
OH
S
N
Ph
N
H3C
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


12.28
7.74
7.72
7.47
7.45
7.42
7.27
7.25
7.23
7.02
7.00
2.11
OH
S
N
Ph
N
Br
H3C
0.95
2.00
4.05
1.05
2.05
3.01
f1 (ppm)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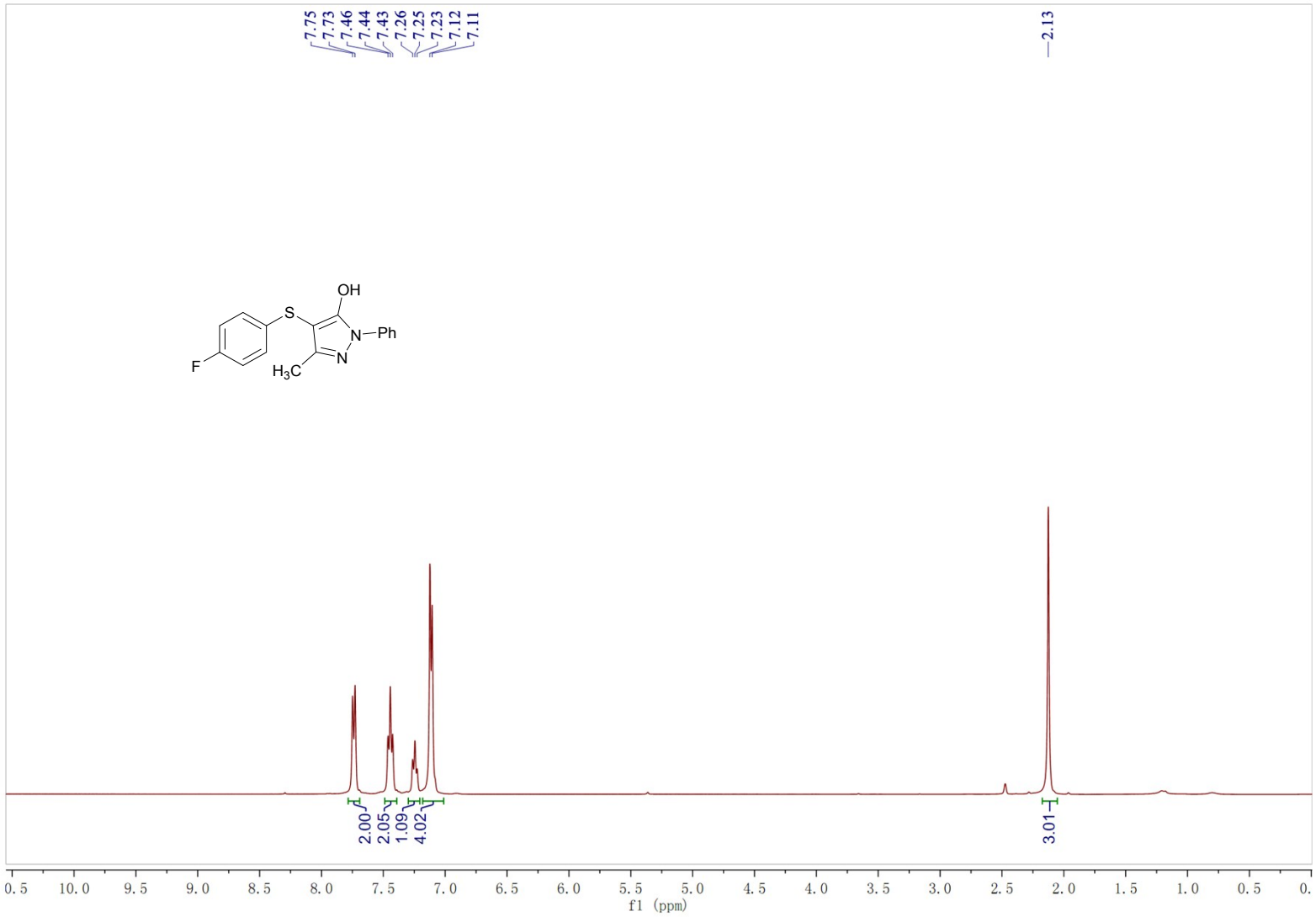
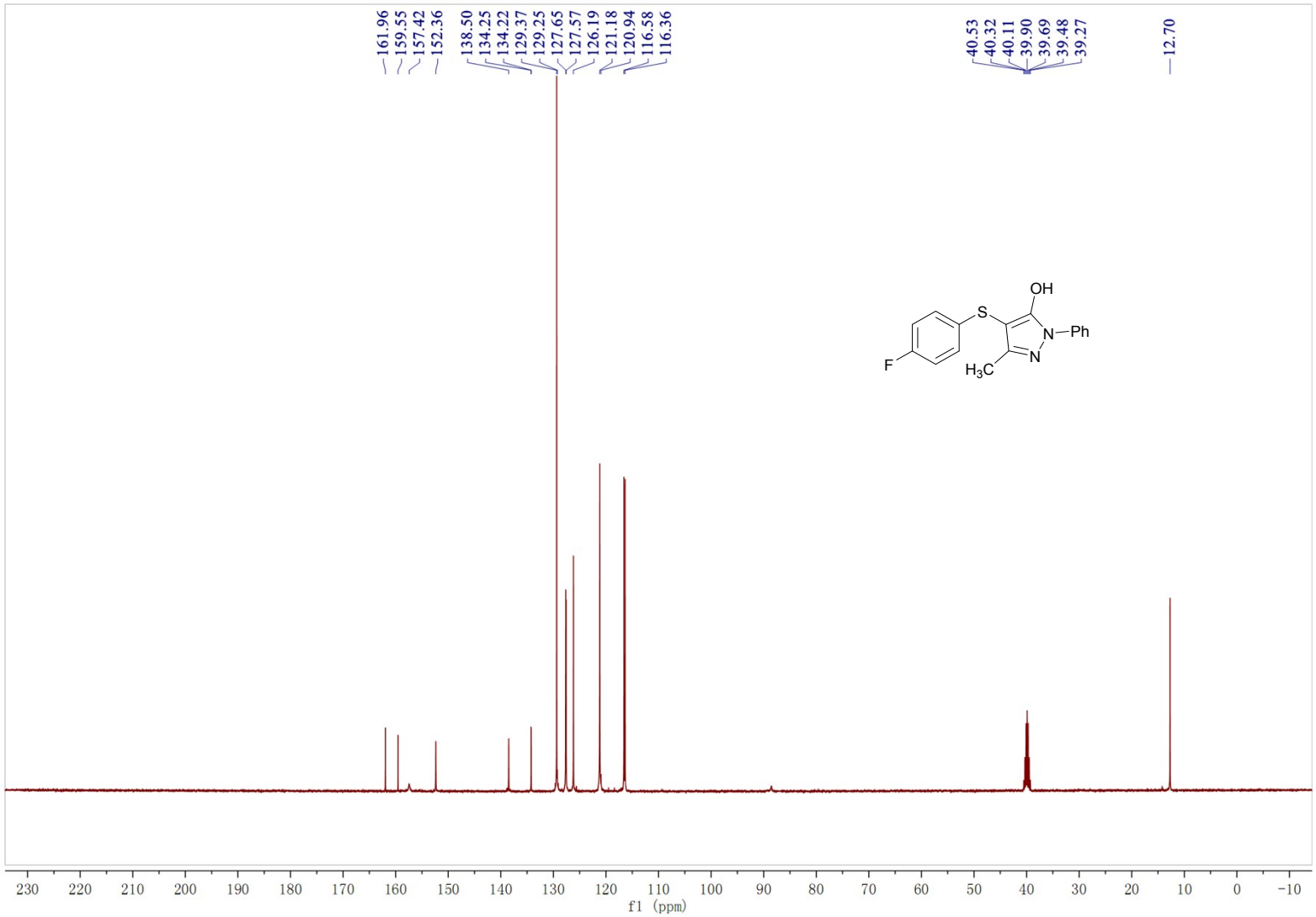
129.39
127.30
126.23
121.21
118.11
40.55
40.34
40.13
39.92
39.71
39.50
39.30
12.72
OH
S
N
Ph
N
Br
H3C
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.75
7.73
7.46
7.44
7.43
7.26
7.25
7.23
7.12
7.11
2.13
OH
S
N
Ph
N
F
H3C
2.00
2.05
1.09
4.02
3.01
f1 (ppm)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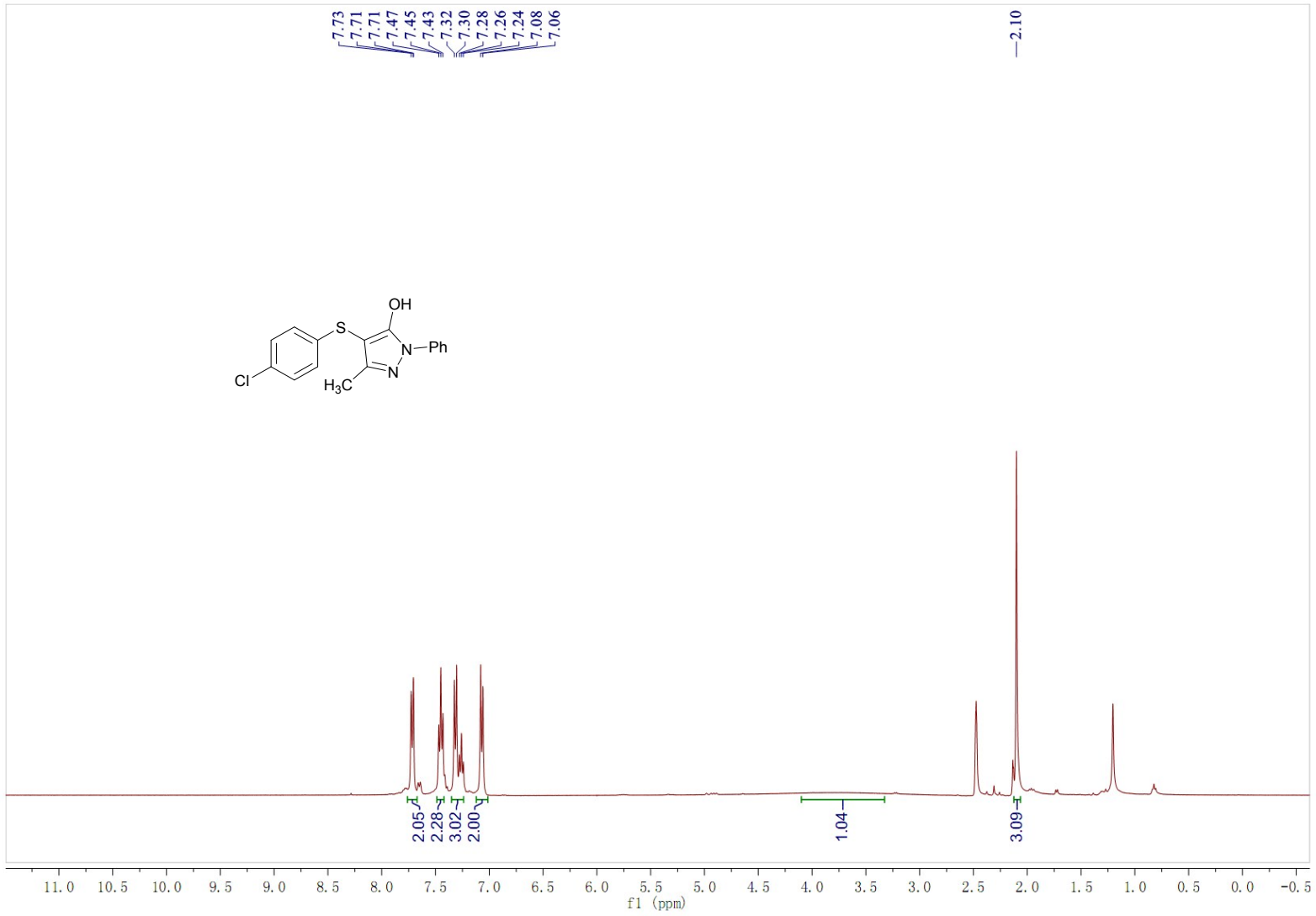
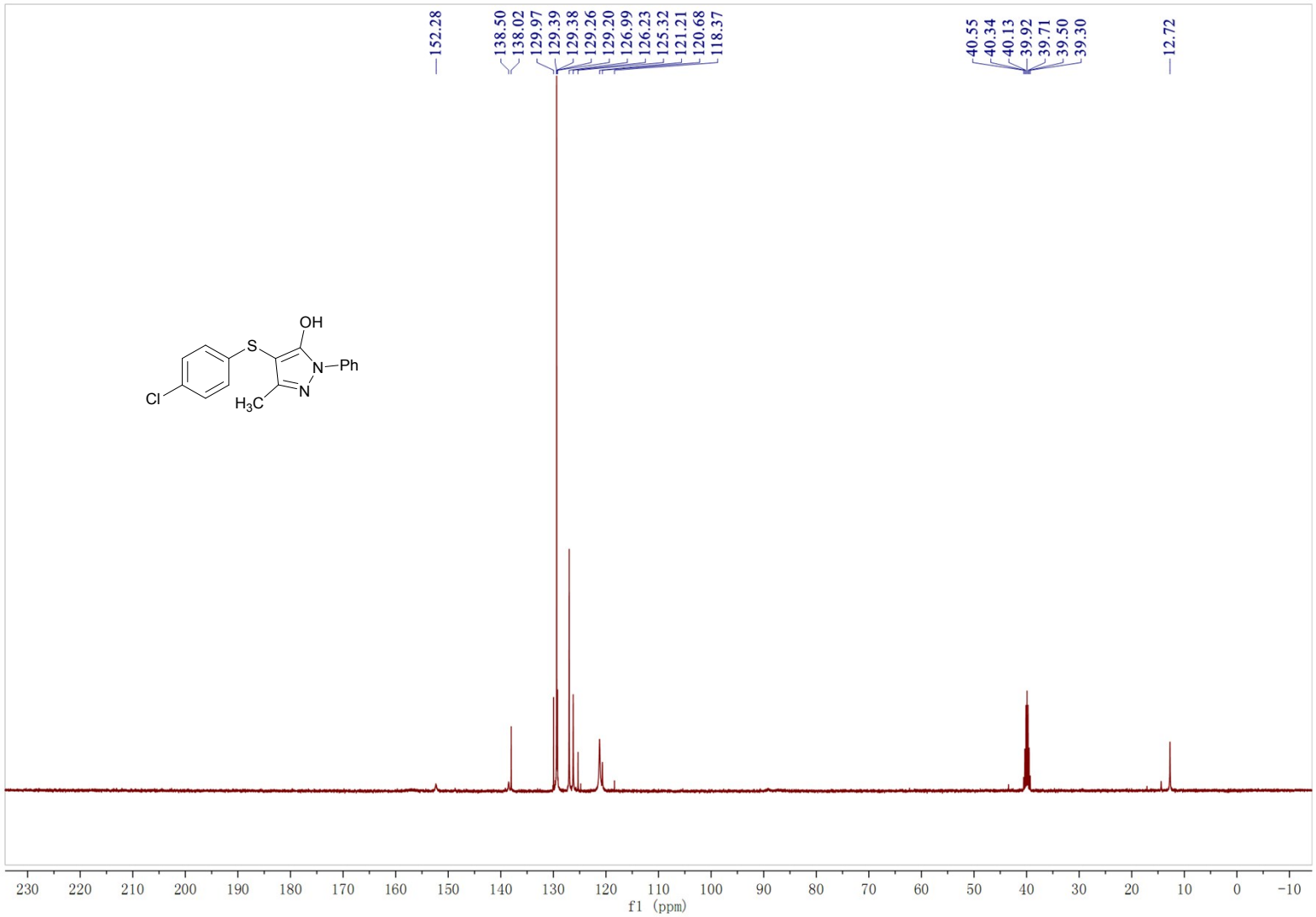
159.55
157.42
152.36
138.50
134.25
134.22
129.37
129.25
127.65
127.57
126.19
121.18
120.94
116.58
116.36
40.53
40.32
40.11
39.90
39.69
39.48
39.27
12.70
OH
S
N
Ph
N
F
H3C
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.73
7.71
7.71
7.47
7.45
7.43
7.32
7.30
7.28
7.26
7.24
7.08
7.06
2.10
OH
S
N—Ph
N
Cl
H3C
2.05
2.28
3.02
2.00
1.04
3.09
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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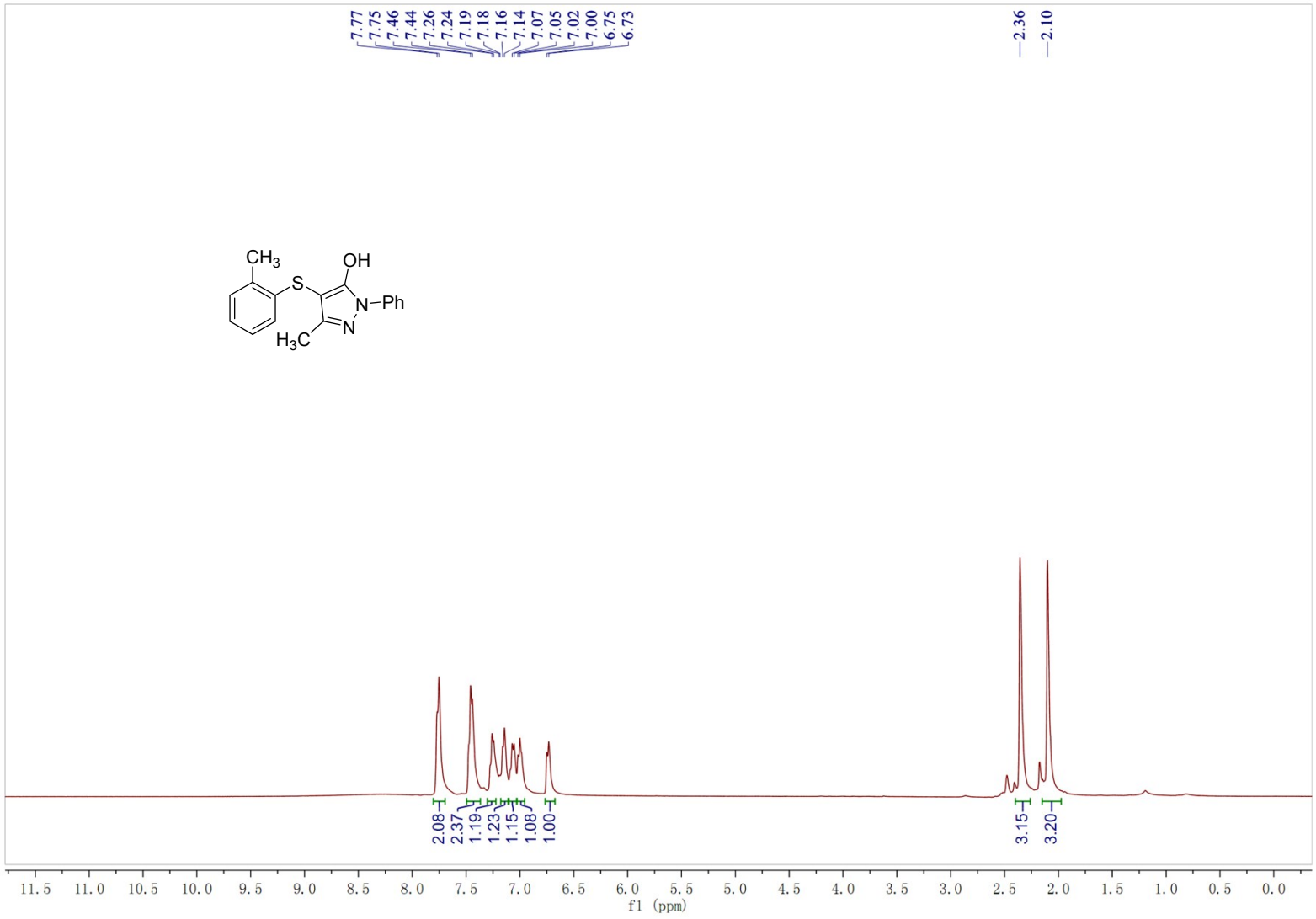
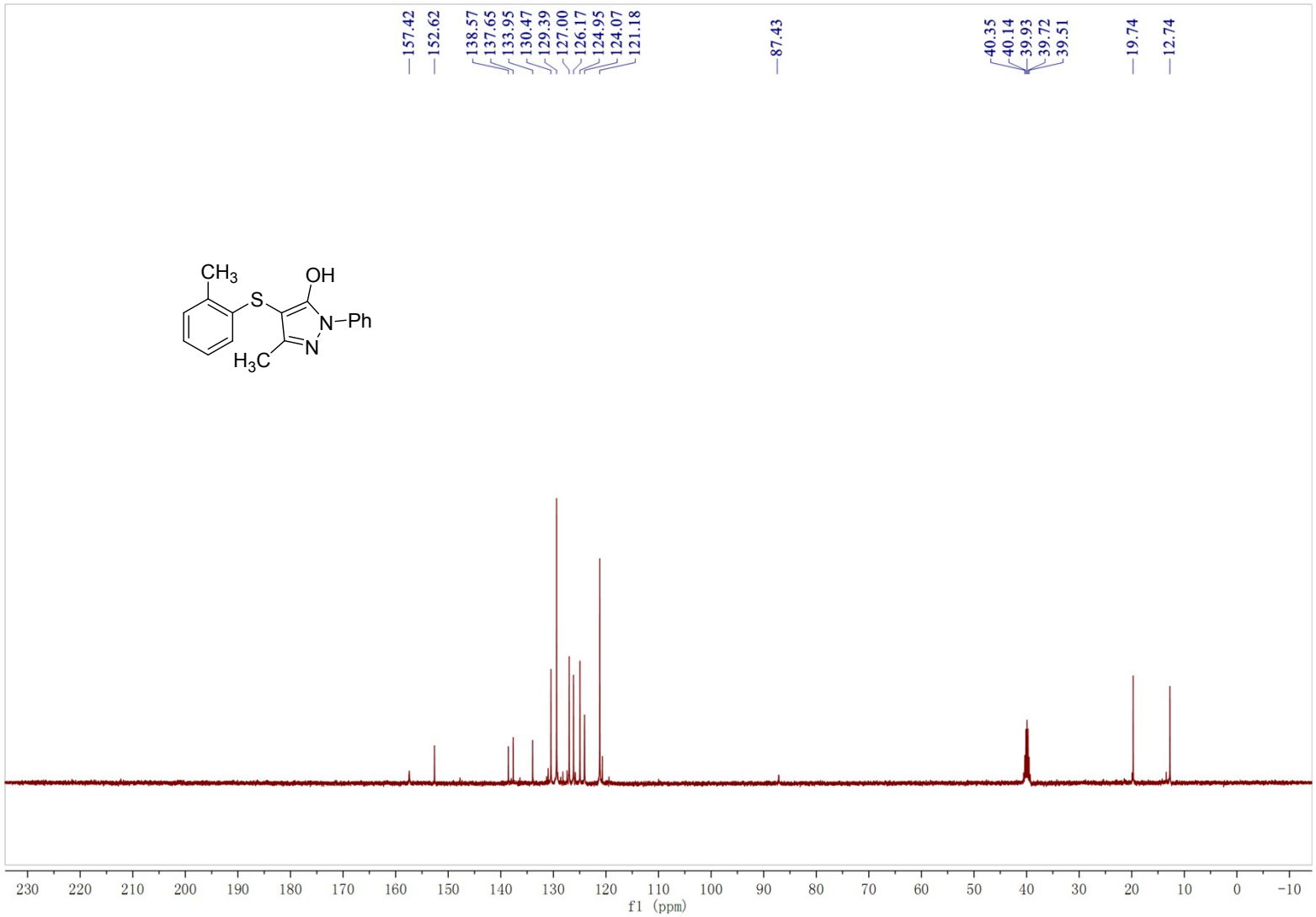
138.50
138.02
129.97
129.39
129.38
129.26
129.20
126.99
126.23
125.32
121.21
120.68
118.37
40.55
40.34
40.13
39.92
39.71
39.50
39.30
12.72
OH
S
N
Ph
N
Cl
H3C
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.77
7.75
7.46
7.44
7.26
7.24
7.19
7.18
7.16
7.14
7.07
7.05
7.02
7.00
6.75
6.73
2.36
2.10
CH3
S
OH
N–Ph
N
H3C
2.08
2.37
1.19
1.23
1.15
1.08
1.00
3.15
3.20
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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137.65
133.95
130.47
129.39
127.00
126.17
124.95
124.07
121.18
87.43
40.35
40.14
39.93
39.72
39.51
19.74
12.74
CH3
OH
S
N–Ph
N
H3C
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)