Supporting Information

Palladium-catalyzed *S*-benzylation of unprotected mercaptobenzoic acid with benzyl alcohols in water

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General procedure: A mixture of mercaptobenzoic acid **1** (1 mmol), palladium(II) acetate (12 mg, 0.05 mmol), sodium diphenylphosphinobenzene-3-sulfonate (TPPMS, 36 mg, 0.1 mmol) and benzyl alcohol **2** (5 mmol) in H_2O (4 mL) was heated for 24-48 h in sealed tube. After cooling, the reaction mixture was poured into water and extracted with EtOAc. The organic layer was washed with brine, dried over $MgSO_4$ and concentrated in vacuo. The residue was washed with hexanes, then purified by flash column chromatography (silica gel, hexanes/EtOAc) to give desired product **3**.

4-Benzylthiobenzoic acid 3a (Table 1, entry 1) [1]

Following the general procedure, **3a** was obtained as a white solid. mp 188-190 °C; IR (KBr) (cm^{-1}) 3401, 2925, 1676, 1589, 1419, 1289; ^{1}H NMR (400 MHz, DMSO-d_6): δ 4.35 (s, 2H), 7.23 (t, *J*=7.2 Hz, 1H), 7.32 (dd, *J*=7.2, 7.2 Hz, 2H), 7.41 (d, *J*=7.2 Hz, 2H), 7.42 (d, *J*=8.4 Hz, 2H), 7.82 (d, *J*=8.4 Hz, 2H), 12.9 (brs, 1H); ^{13}C NMR (400 MHz, DMSO-d_6): δ 35.3, 126.4, 127.2, 127.4, 128.5, 128.8, 129.7, 136.8, 143.0, 166.9; MS (EI): *m/z* (%) 244 (M^+, 35.0), 91 (100).

3-Benzylthiobenzoic acid 3b (Table 2, entry 1) [2]

Following the general procedure, **3b** was obtained as a white solid. mp 129-131 °C; IR (KBr) (cm^{-1}) 2847, 1689, 1579, 1433, 1288; ^{1}H NMR (400 MHz, DMSO-d_6): δ 4.30 (s, 2H), 7.23 (t, *J*=7.2 Hz, 1H), 7.30 (t, *J*=7.2 Hz, 2H), 7.35-7.39 (m, 2H), 7.42 (t, *J*=8.0 Hz, 1H), 7.55-7.60 (m, 1H), 7.73 (dt, *J*=8.0, 1.2 Hz, 1H), 7.84 (t, *J*=1.6 Hz, 1H), 13.1 (brs, 1H); ^{13}C NMR (400 MHz, DMSO-d_6): δ 36.4, 126.7, 127.1, 128.4, 128.6, 128.8, 129.2, 131.5, 132.3, 136.9, 137.1, 166.8; MS(EI): *m/z* (%) 244 (M^+, 67.1), 91 (100).

2-Benzylthiobenzoic acid 3c (Table 2, entry 2) [2]

Following the general procedure, **3c** was obtained as a white solid. mp 187-189 °C; IR (KBr) (cm^{-1}) 3413, 2920, 1674, 1459, 1411, 1262; ^{1}H NMR (400 MHz, DMSO-d_6): δ 4.21 (s, 2H), 7.18-7.23 (m, 1H), 7.27 (t, *J*=6.0 Hz, 1H), 7.34 (t, *J*=7.2 Hz, 2H), 7.40-7.60 (m, 2H), 7.48-7.52 (m, 2H), 7.89 (d, *J*=7.6 Hz, 1H), 13.0 (brs, 1H); ^{13}C NMR (400 MHz, DMSO-d_6): δ 35.7, 124.0, 125.7, 127.1, 127.6, 128.5, 129.2, 130.9, 132.3, 136.6, 141.2, 167.4; MS(EI): *m/z* (%) 244 (M^+, 25.1), 91 (100).

2-Benzylthio-5-fluorobenzoic acid 3d (Table 2, entry 3) [3]

Following the general procedure, **3d** was obtained as a white solid. mp 153-155 °C; IR (KBr) (cm^{-1}) 3034, 2912, 1690, 1465, 1424, 1246; ^{1}H NMR (400 MHz, DMSO-d_6): δ 4.21 (s, 2H), 7.27 (t, *J*=7.2 Hz, 1H), 7.34 (t, *J*=7.2 Hz, 2H), 7.38-7.44 (m, 3H), 7.51 (dd, *J*=9.0, 5.2 Hz, 1H), 7.63 (dd, *J*=9.0, 2.8 Hz, 1H), 13.4 (brs, 1H); ^{13}C NMR (400 MHz, DMSO-d_6): δ 36.1, 117.0, 117.3, 119.3, 119.5, 127.2, 128.3, 128.4, 128.5, 129.1, 129.9, 130.0, 136.2, 136.5, 157.8, 160.2, 166.4; MS(EI): *m/z* (%) 262 (M^+, 18.7), 91 (100).

2-Benzylthio-5-chlorobenzoic acid 3e (Table 2, entry 4) [4]

Following the general procedure, **3e** was obtained as a white solid. mp 162-164 °C; IR (KBr) (cm^{-1}) 2924, 1681, 1462, 1317, 1250; ^{1}H NMR (400 MHz, DMSO-d_6): δ 4.23 (s, 2H), 7.27 (t, *J*=7.2 Hz, 1H), 7.34 (t, *J*=6.0 Hz, 2H), 7.43 (d, *J*=7.2 Hz, 2H), 7.51 (d, *J*=8.6 Hz, 1H), 7.58 (dd, *J*=8.6, 2.4 Hz, 1H), 7.84 (d, *J*= 2.4 Hz, 1H), 13.4 (brs, 1H); ^{13}C NMR (400 MHz, DMSO-d_6): δ 35.7, 127.3, 127.7, 128.5, 129.1, 130.1, 131.9, 136.3, 140.2, 166.2; MS (EI): *m/z* (%) 280 (M^++2, 13.3), 278 (M^+, 35.8), 91 (100).

4-(4-Methylbenzylthio)benzoic acid 3f (Table 3, entry 1) [5]

Following the general procedure, **3f** was obtained as a white solid. mp 210-212 °C; IR (KBr) (cm^{-1}) 2916, 1681, 1588, 1418, 1288; ^{1}H NMR (400 MHz, DMSO-d_6): δ 2.26 (s, 3H), 4.30 (s, 2H), 7.11 (d, *J*=8.0 Hz, 2H), 7.29 (d, *J*=8.0 Hz, 2H), 7.41 (d, *J*=8.4 Hz, 2H), 7.82 (d, *J*=8.4 Hz, 2H), 12.9 (brs, 1H); ^{13}C NMR (400 MHz, DMSO-d_6): δ 20.6, 35.1, 126.4, 127.3, 128.7, 129.0, 129.7, 133.6, 136.4, 143.1, 166.9; MS (EI): *m/z* (%) 258 (M^+, 13.9), 105 (100).

4-(4-Ethylbenzylthio)benzoic acid 3g (Table 3, entry 2) [6]

Following the general procedure, **3g** was obtained as a white solid. mp 203-205 °C; IR (KBr) (cm^{-1}) 2963, 1680, 1587, 1417, 1288; ^{1}H NMR (400 MHz, DMSO-d_6): δ 1.15 (t, *J*=8.0 Hz, 3H), 2.56 (q, *J*=8.0 Hz, 2H), 4.31 (s, 2H), 7.15 (d, *J*=8.0 Hz, 2H), 7.32 (d, *J*=8.0 Hz, 2H), 7.41 (d, *J*=8.4 Hz, 2H), 7.83 (d, *J*=8.4 Hz, 2H), 12.9 (brs, 1H); ^{13}C NMR (400 MHz, DMSO-d_6): δ 15.5, 27.8, 35.0, 126.3, 127.3, 127.9, 128.8, 129.7, 133.9, 142.8, 143.2, 167.0; MS(EI): *m/z* (%) 272 (M^+, 12.4), 119 (100).

4-(4-Methoxybenzylthio)benzoic acid 3h (Table 3, entry 3) [7]

Following the general procedure, **3h** was obtained as a white solid. mp 200-202 °C; IR (KBr) (cm^{-1}) 2955, 1683, 1589, 1505, 1419, 1294; ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.72 (s, 3H), 4.29 (s, 2H), 6.87 (d, *J*=8.8 Hz, 2H), 7.33 (d, *J*=8.8 Hz, 2H), 7.40 (d, *J*=8.8 Hz, 2H), 7.83 (d, *J*=8.4 Hz, 2H), 12.9 (brs, 1H); ^{13}C NMR (400 MHz, DMSO-d_6): δ 34.8, 55.0, 113.9, 126.4, 127.3, 128.4, 129.7, 130.0, 143.3, 158.4, 166.9; MS (EI): *m/z* (%) 274 (M^+, 9.4), 121 (100).

4-(2-Methylbenzylthio)benzoic acid 3i (Table 3, entry 4) [8]

Following the general procedure, **3i** was obtained as a white solid. mp 173-175 °C; IR (KBr) (cm^{-1}) 2866, 1678, 1587, 1415, 1286; ^{1}H NMR (400 MHz, DMSO-d_6): δ 2.38 (s, 3H), 4.33 (s, 2H), 7.10-7.25 (m, 3H), 7.32 (d, *J*=7.2 Hz, 1H), 7.44 (d, *J*=8.0 Hz, 2H), 7.86 (d, *J*=8.0 Hz, 2H), 12.9 (brs, 1H); ^{13}C NMR (400 MHz, DMSO-d_6): δ 18.7, 34.1, 126.0, 126.6, 127.5, 127.6, 129.7, 130.4, 134.1, 136.7, 143.3, 167.0; MS(EI): *m/z* (%) 258 (M^+, 16.7), 105 (100).

4-(4-Fluorobenzylthio)benzoic acid 3j (Table 3, entry 5) [9]

Following the general procedure, **3j** was obtained as an off-white solid. mp 197-199 °C; IR (KBr) (cm^{-1})

2821, 1675, 1589, 1503, 1415, 1286; ^{1}H NMR (400 MHz, DMSO-d_6): δ 4.35 (s, 2H), 7.14 (d, *J*=8.8 Hz, 2H), 7.42 (d, *J*=8.4 Hz, 2H), 7.45 (dd, *J*=8.8, 5.6 Hz, 2H), 7.83 (d, *J*=8.4 Hz, 2H), 12.9 (brs, 1H); ^{13}C NMR (400 MHz, DMSO-d_6): δ 34.5, 115.1, 115.4, 126.5, 127.5, 129.7, 130.8, 133.0, 133.1, 142.7, 160.1, 162.5, 166.9; MS (EI): *m/z* (%) 262 (M^+, 48.7), 109 (100).

4-(4-Bromobenzylthio)benzoic acid 3k (Table 3, entry 6) [1]

Following the general procedure, **3k** was obtained as a white solid. mp 222-224 °C; IR (KBr) (cm^{-1}) 2879, 1684, 1589, 1419, 1291; ^{1}H NMR (400 MHz, DMSO-d_6): δ 4.34 (s, 2H), 7.38 (d, *J*=8.4 Hz, 2H), 7.41 (d, *J*=8.0 Hz, 2H), 7.50 (d, *J*=8.4 Hz, 2H), 7.83 (d, *J*=8.4 Hz, 2H), 12.9 (brs, 1H); ^{13}C NMR (400 MHz, DMSO-d_6): δ 34.5, 120.3, 126.6, 127.6, 129.7, 131.0, 131.3, 136.5, 142.5, 166.9; MS(EI): *m/z* (%) 324 (M^++2, 17.8), 322 (M^+, 17.2), 169 (100).

4-(3-Bromobenzylthio)benzoic acid 3l (Table 3, entry 7) [10]

Following the general procedure, **3l** was obtained as a white solid. mp 162-164 °C; IR (KBr) (cm^{-1}) 2830, 1678, 1588, 1419, 1291; ^{1}H NMR (400 MHz, DMSO-d_6): δ 4.36 (s, 2H), 7.28 (t, *J*=7.6 Hz, 1H), 7.40-7.46 (m, 4H), 7.63 (s, 1H), 7.83 (d, *J*=8.4 Hz, 2H), 12.9 (brs, 1H); ^{13}C NMR (400 MHz, DMSO-d_6): δ 34.5, 121.6, 126.7, 127.6, 127.9, 129.7, 130.1, 130.6, 131.5, 139.9, 142.3, 166.9; MS (EI): *m/z* (%) 324 (M^++2, 36.0), 322 (M^+, 35.1), 169 (100).

4-(4-Chlorobenzylthio)benzoic acid 3m (Table 3, entry 8) [11]

Following the general procedure, **3m** was obtained as a white solid. mp 210-212 °C; IR (KBr) (cm^{-1}) 2842, 1685, 1589, 1419, 1295; ^{1}H NMR (400 MHz, DMSO-d_6): δ 4.36 (s, 2H), 7.34-7.46 (m, 6H), 7.83 (d, *J*=8.0 Hz, 2H), 12.9 (brs, 1H); ^{13}C NMR (400 MHz, DMSO-d_6): δ 34.5, 126.6, 127.6, 128.4, 129.7, 130.7, 131.8, 136.1, 142.5, 166.9; MS(EI): *m/z* (%) 280 (M^++2, 6.6), 278 (M^+, 17.2), 125 (100).

4-(1-Phenylethylthio)benzoic acid 3n (Table 4, entry 1)

Following the general procedure, **3n** was obtained as a white solid. mp 172-174 °C; IR (KBr) (cm^{-1}) 3430, 2974, 2920, 1683, 1591, 1426, 1301; ^{1}H NMR (400 MHz, DMSO-d_6): δ 1.59 (d, *J*=6.8 Hz, 3H), 4.81 (q, *J*=6.8 Hz, 1H), 7.23 (t, *J*=7.2 Hz, 1H), 7.32 (t, *J*=7.2 Hz, 2H), 7.40 (d, *J*=8.4 Hz, 2H), 7.45 (d, *J*=7.2 Hz, 2H), 7.80 (d, *J*=8.4 Hz, 2H), 12.9 (brs, 1H); ^{13}C NMR (400 MHz, DMSO-d_6): δ 22.3, 44.6, 127.2, 127.3, 127.9, 128.2, 128.5, 129.6, 142.0, 142.5, 166.9; MS (EI): *m/z* (%) 258 (M^+, 57.5), 105 (100); Anal. Calcd for $C_{15}H_{14}O_2S$: C, 69.74; H, 5.46. Found: C, 69.61; H, 5.44.

4-(1-Phenylpropylthio)benzoic acid 3o (Table 4, entry 2)

Following the general procedure, **3o** was obtained as a white solid. mp 150-152 °C; IR (KBr) (cm^{-1}) 2973, 1684, 1592, 1424, 1296; ^{1}H NMR (400 MHz, DMSO-d_6): δ 0.80-0.90 (m, 3H), 1.80-2.00 (m, 2H),

4.50-4.60 (m, 1H), 7.20-7.26 (m, 1H), 7.31 (t, *J*=6.8 Hz, 2H), 7.36-7.44 (m, 4H), 7.78 (dd, *J*=8.8, 2.4 Hz, 2H), 12.9 (brs, 1H); ^{13}C NMR (400 MHz, DMSO-d_6): δ 11.9, 29.2, 51.4, 127.2, 127.7, 127.8, 128.1, 128.4, 129.6, 141.2, 142.1, 166.9; MS (EI): *m/z* (%) 272 (M^+, 24.1), 91 (100); Anal. Calcd for $C_{16}H_{16}O_2S$: C, 70.56; H, 5.92. Found: C, 70.32; H, 5.92.

4-(1,2,3,4-Tetrahydronaphthalen-1-ylthio)benzoic acid 3p (Table 4, entry 3)

Following the general procedure, **3p** was obtained as an off-white solid. mp 169-171 °C; IR (KBr) (cm^{-1}) 2936, 1684, 1590, 1418, 1286; ^{1}H NMR (400 MHz, DMSO-d_6): δ 1.70-1.80 (m, 1H), 1.90-2.10 (m, 3H), 2.65-2.85 (m, 2H), 4.98 (s, 1H), 7.10-7.20 (m, 3H), 7.38 (d, *J*=7.2 Hz, 1H), 7.53 (d, *J*=8.0 Hz, 2H), 7.90 (dd, *J*=8.4, 1.2 Hz, 2H), 12.9 (brs, 1H); ^{13}C NMR (400 MHz, DMSO-d_6): δ 18.2, 27.9, 28.3, 44.6, 125.7, 127.2, 128.0, 129.1, 129.9, 130.4, 134.3, 137.5, 142.6, 166.9; MS (EI): *m/z* (%) 284 (M^+, 6.0), 131 (100); Anal. Calcd for $C_{17}H_{16}O_2S$: C, 71.80; H, 5.67. Found: C, 71.75; H, 5.70.

4-(2,3-Dihydro-*1H*-inden-1-ylthio)benzoic acid 3q (Table 4, entry 4)

Following the general procedure, **3q** was obtained as an off-white solid. mp 183-185 °C; IR (KBr) (cm^{-1}) 2949, 1681, 1588, 1415, 1286; ^{1}H NMR (400 MHz, DMSO-d_6): δ 2.00-2.15 (m, 1H), 2.55-2.70 (m, 1H), 2.85-2.95 (m, 1H), 2.95-3.05 (m, 1H), 5.10-5.15 (m, 1H), 7.16-7.34 (m, 4H), 7.49 (d, *J*=8.4 Hz, 2H), 7.89 (d, *J*=8.4 Hz, 2H), 12.9 (brs, 1H); ^{13}C NMR (400 MHz, DMSO-d_6): δ 30.3, 33.2, 49.1, 124.7, 124.8, 126.6, 127.4, 127.7, 128.0, 129.8, 141.7, 143.1, 143.6, 166.9; MS (EI): *m/z* (%) 270 (M^+, 8.7), 117 (100); Anal. Calcd for $C_{16}H_{14}O_2S$: C, 71.08; H, 5.22. Found: C, 70.94; H, 5.27.

4-(Benzhydrylthio)benzoic acid 3r (Table 4, entry 5)

Following the general procedure, **3r** was obtained as an off-white solid. mp 179-181 °C; IR (KBr) (cm^{-1}) 3021, 1685, 1591, 1488, 1417, 1282; ^{1}H NMR (400 MHz, DMSO-d_6): δ 6.13 (s, 1H), 7.23 (t, *J*=7.2 Hz, 2H), 7.30-7.40 (m, 6H), 7.52 (d, *J*=7.6 Hz, 4H), 7.75 (d, *J*=8.4 Hz, 2H), 12.9 (brs, 1H); ^{13}C NMR (400 MHz, DMSO-d_6): δ 53.3, 127.4, 127.8, 128.0, 128.7, 129.6, 140.5, 142.2, 166.8; MS(EI): *m/z* (%) 320 (M^+, 2.1), 167 (100); Anal. Calcd for $C_{20}H_{16}O_2S$: C, 74.97; H, 5.03. Found: C, 74.87; H, 5.14.

4-(Thiophen-2-ylmethylthio)benzoic acid 3s (Table 4, entry 6) [12]

Following the general procedure, **3s** was obtained as an off-white solid. mp 136-138 °C; IR (KBr) (cm^{-1}) 2838, 1678, 1589, 1417, 1290; ^{1}H NMR (400 MHz, DMSO-d_6): δ 4.60 (s, 2H), 6.93 (dd, *J*=5.2, 3.6 Hz, 1H), 7.07 (d, *J*=3.6 Hz, 1H), 7.40 (dd, *J*=5.2, 1.2 Hz, 1H), 7.45 (d, *J*=8.4 Hz, 2H), 7.84 (d, *J*=8.0 Hz, 2H), 12.9 (brs, 1H); ^{13}C NMR (400 MHz, DMSO-d_6): δ 30.1, 125.6, 126.8, 126.9, 127.7, 129.7, 140.1, 142.2, 166.9; MS (EI): *m/z* (%) 250 (M^+, 30.7), 97 (100).

1) Ham, J.; Yang, I.; Kang, H. *J. Org. Chem.* 2004, **69**, 3236-3239.

2) Ko, J.; Ham. J.; Yang, I.; Chin, J.; Nam, S.-J.; Kang, H. *Tetrahedron Lett.* 2006, **47**, 7101-7106.

3) CAS Registry Number: 1275222-61-1

4) Lombardino, J. G.; Wiseman, E. H. *J. Med. Chem.* 1970, **13**, 206-210.

5) CAS Registry Number: 1041590-07-1

6) CAS Registry Number: 1272244-15-1

7) Glossop, P. A.; Millan, D. S.; Price, D. A. WO 2010136940.

8) CAS Registry Number: 1036434-06-6

9) CAS Registry Number: 1021000-75-8

10) CAS Registry Number: 1020937-60-3

11) CAS Registry Number: 1036468-71-9

12) CAS Registry Number: 1019372-72-5

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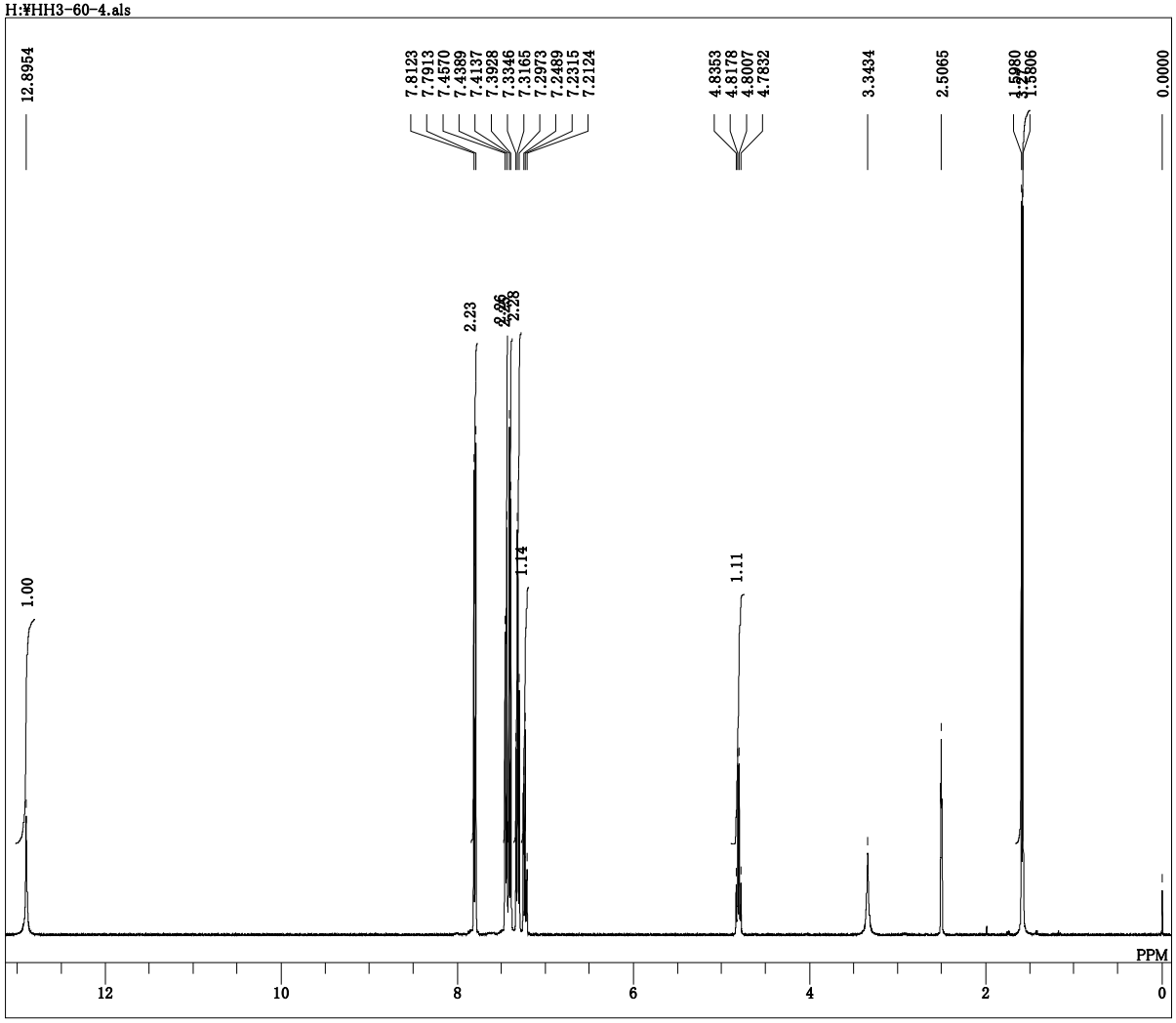

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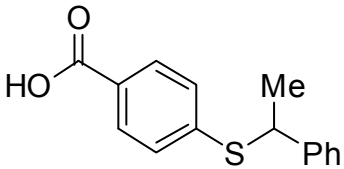

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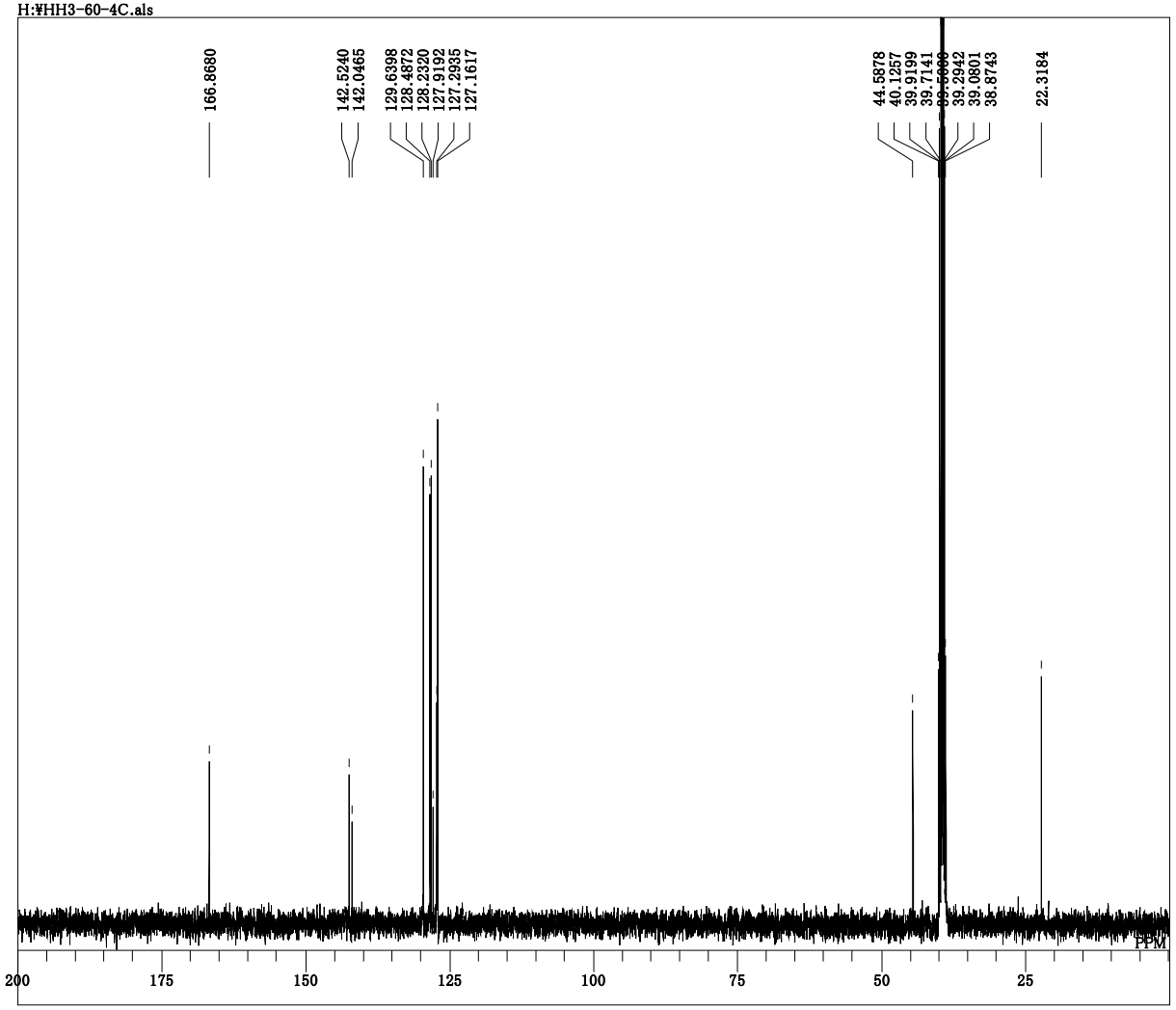

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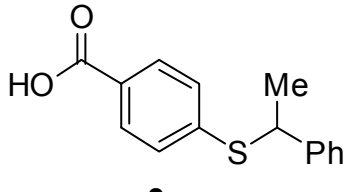

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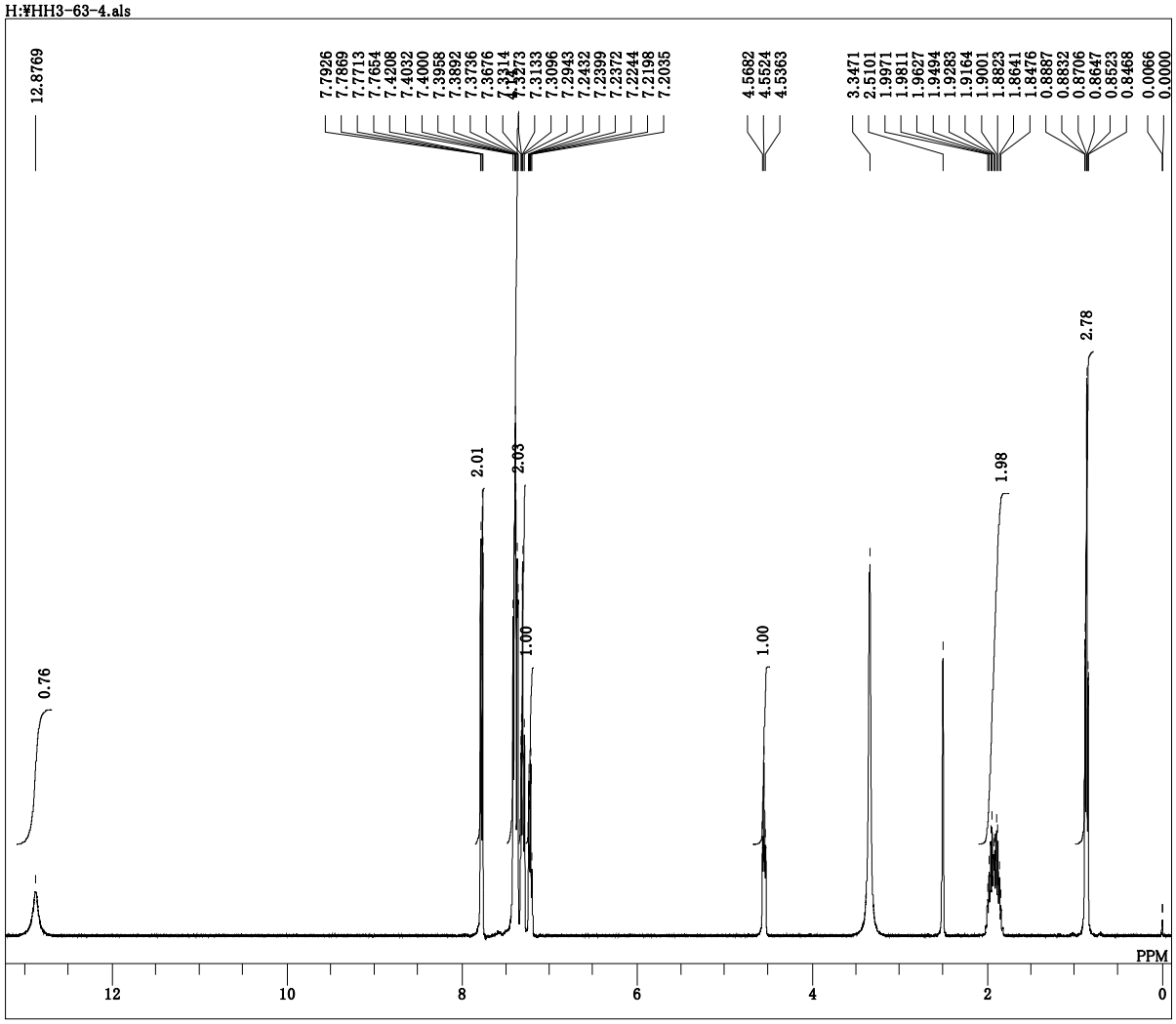

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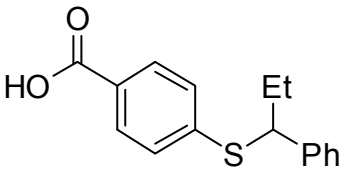

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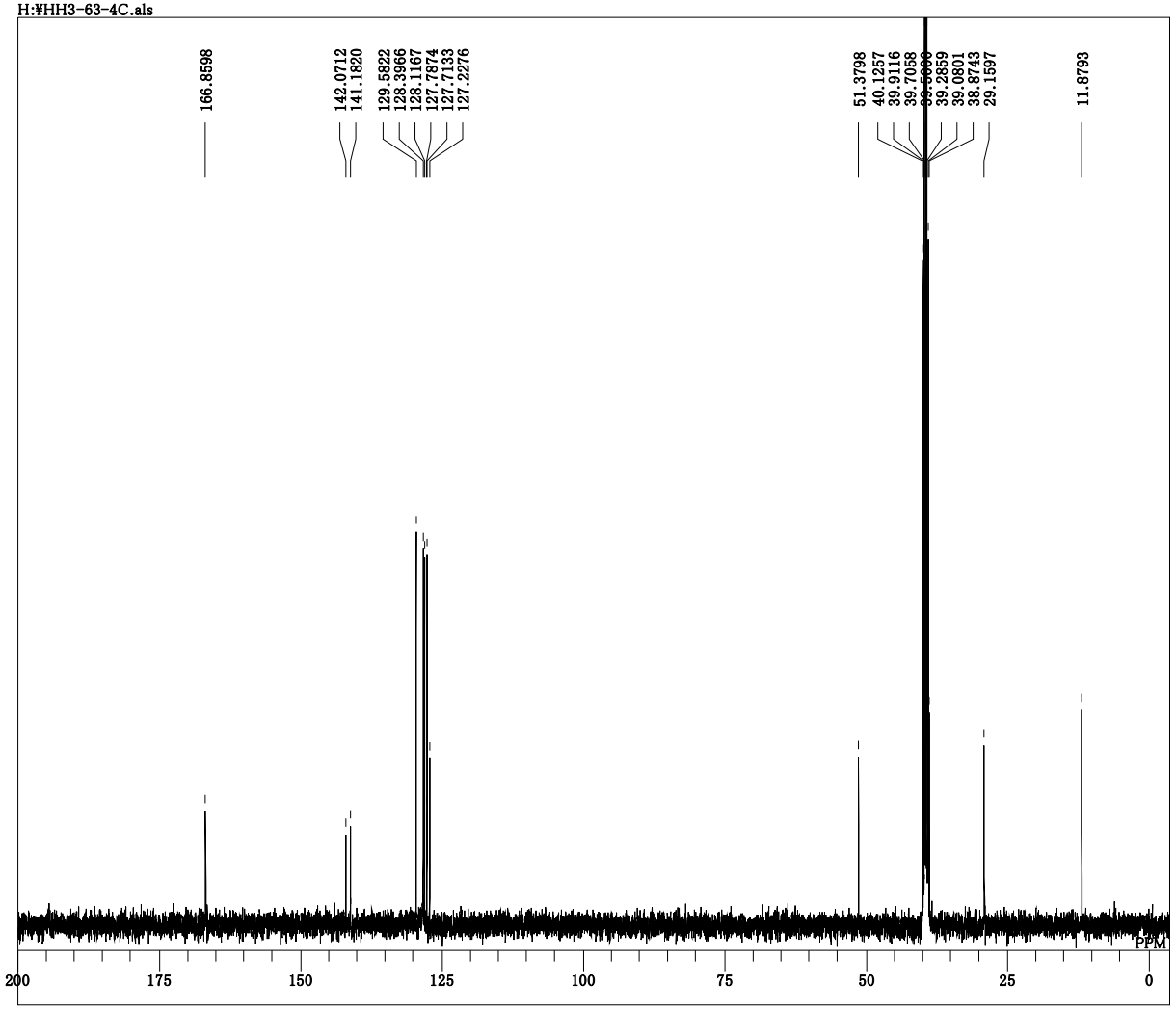

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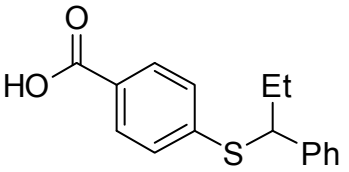
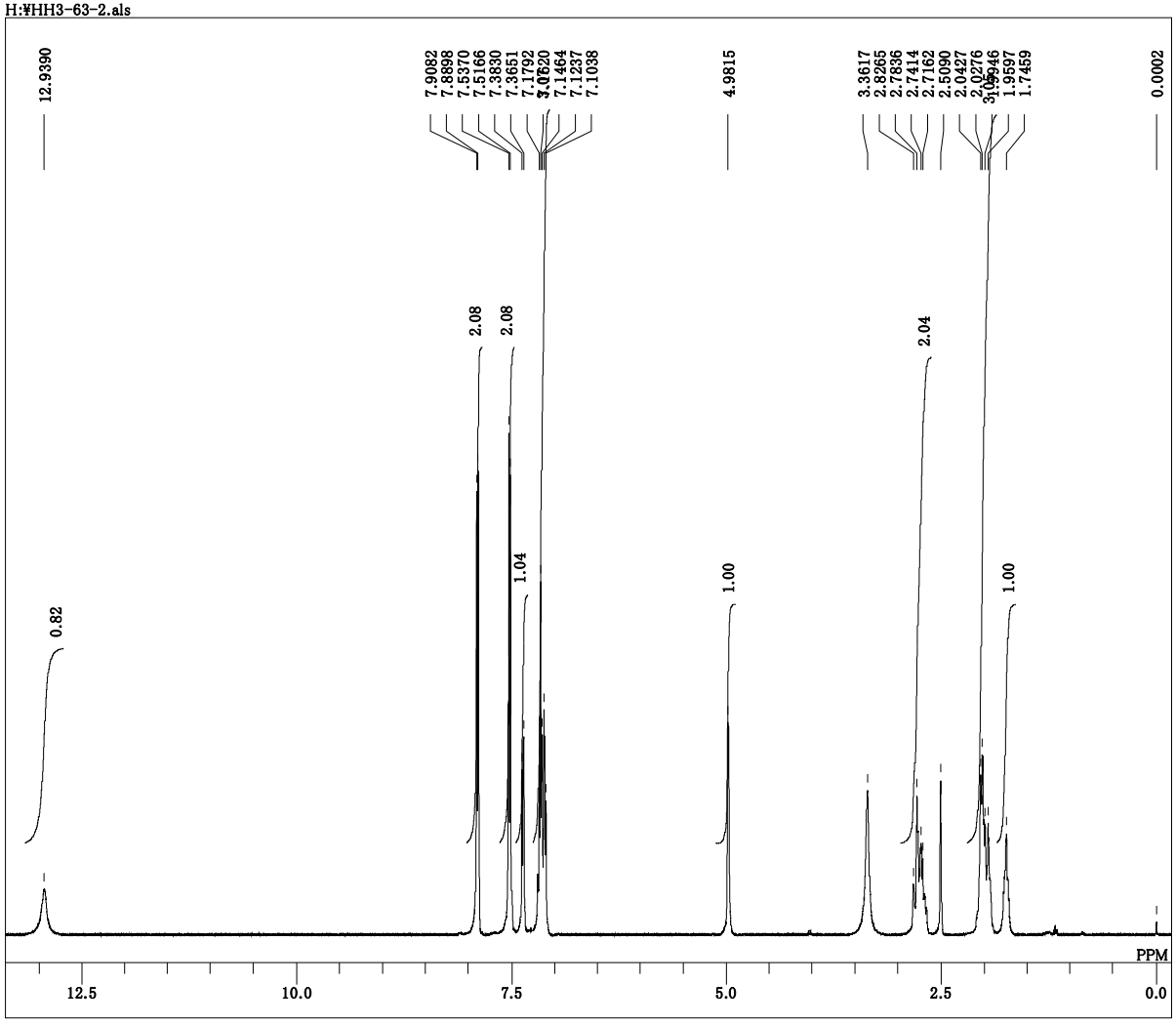


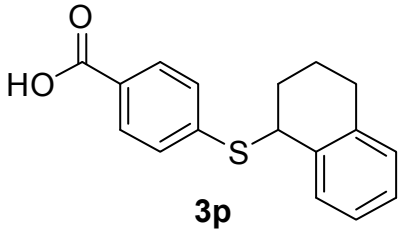
3o

HH3-63-2

H:¥HH3-63-2.als

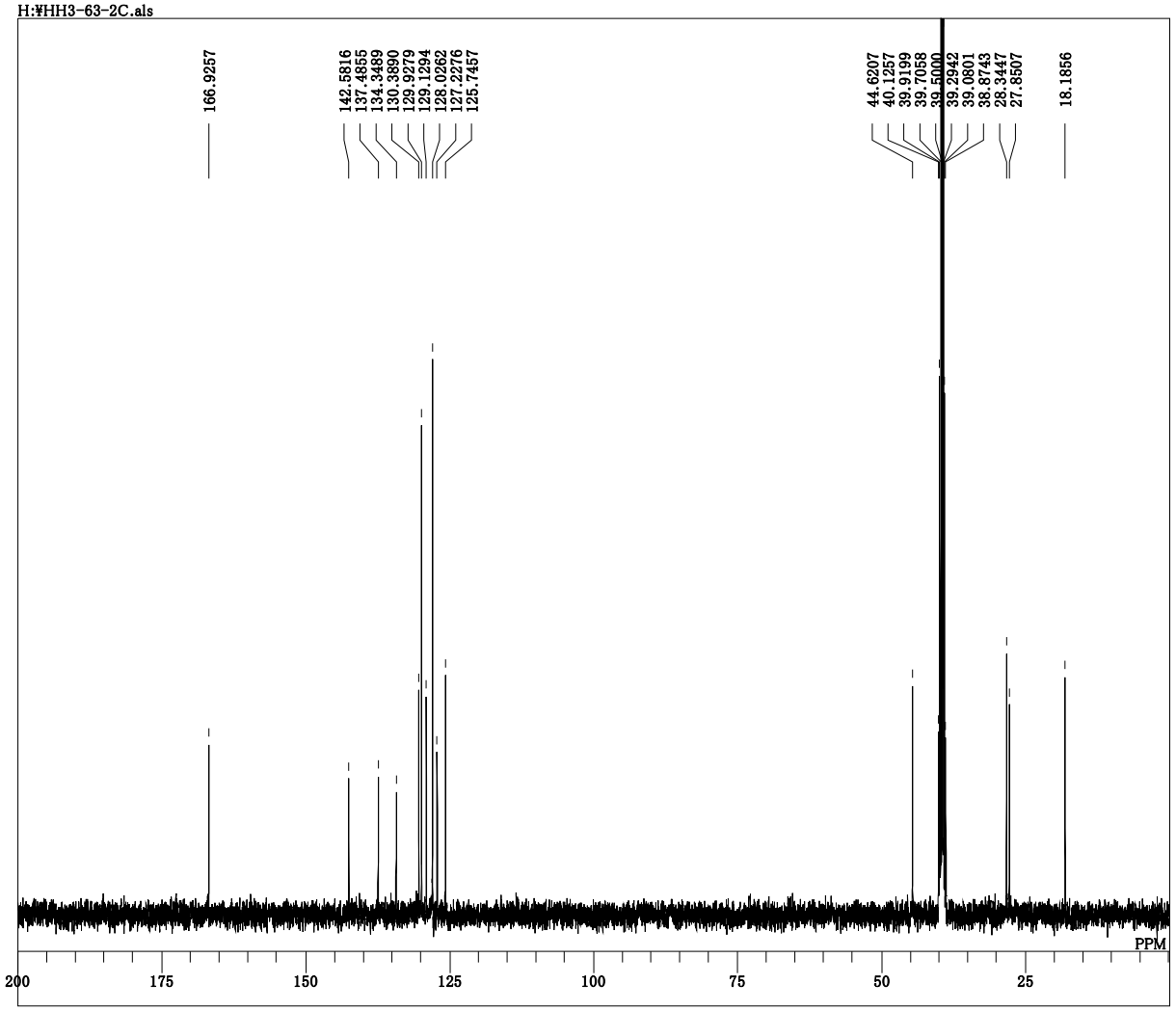


DFILE	HH3-63-2.als
COMNT	HH3-63-2
DATIM	Fri Oct 28 16:57:45 2011
OBNUC	1H
EXMOD	NON
OBFRQ	399.65 MHz
OBSET	124.00 KHz
OBFIN	11300.00 Hz
POINT	65536
FREQU	6006.01 Hz
SCANS	8
ACQTM	10.9117 sec
PD	1.0000 sec
PW1	5.50 usec
IRNUC	1H
CTEMP	22.9 c
SLVNT	DMSO
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	14

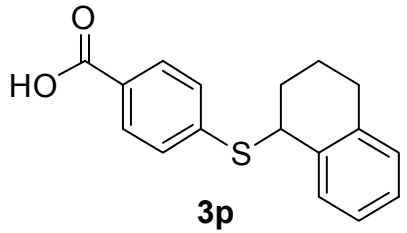


3p

HH3-63-2C



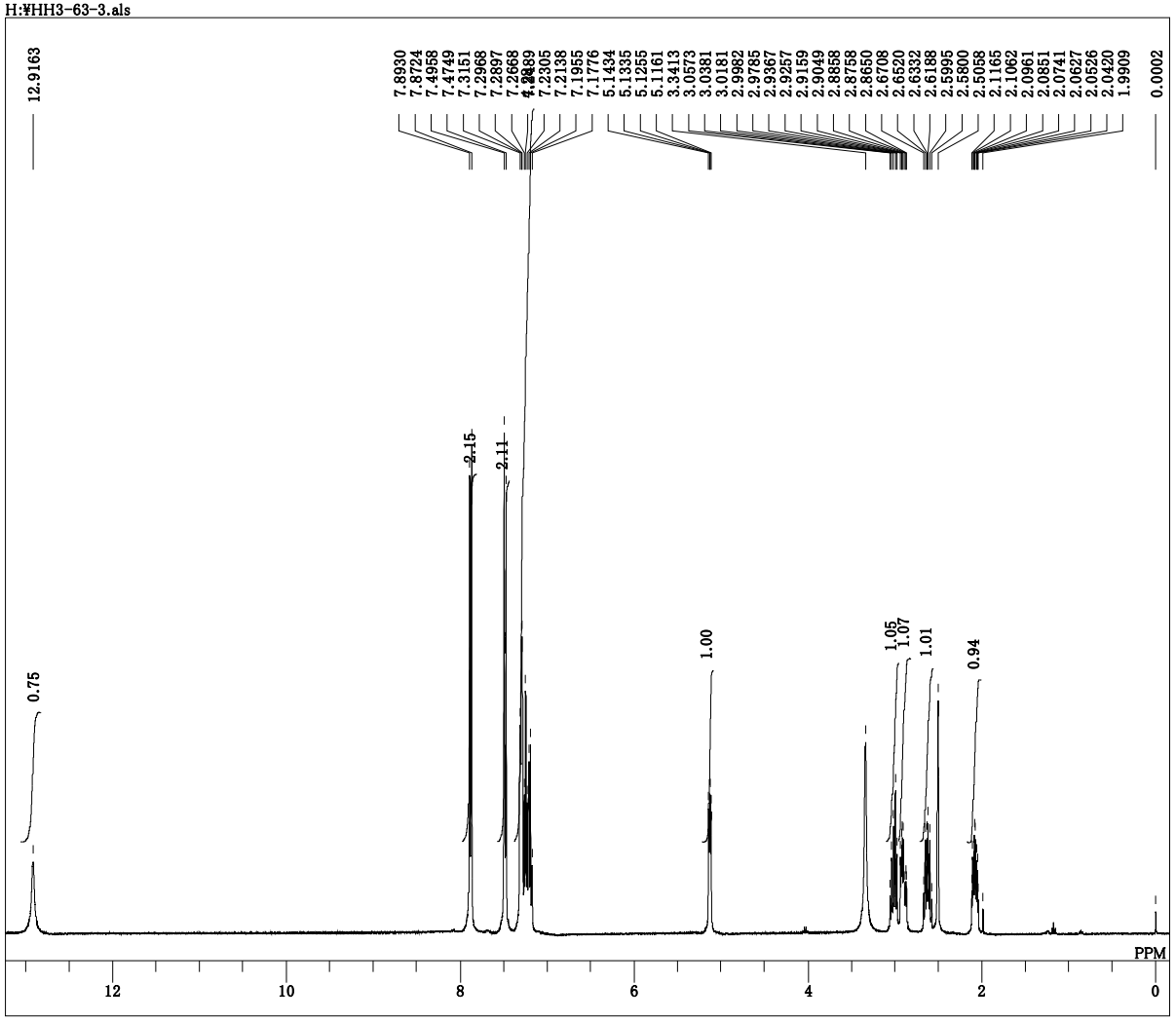
DFILE	HH3-63-2C.als
COMNT	HH3-63-2C
DATIM	Fri Oct 28 17:04:13 2011
OBNUC	13C
EXMOD	BCM
OBFRQ	100.40 MHz
OBSET	125.00 KHz
OBFIN	10500.00 Hz
POINT	32768
FREQU	27118.64 Hz
SCANS	111
ACQTM	1.2083 sec
PD	1.7920 sec
PW1	4.70 usec
IRNUC	1H
CTEMP	23.1 c
SLVNT	DMSO
EXREF	39.50 ppm
BF	1.20 Hz
RGAIN	24



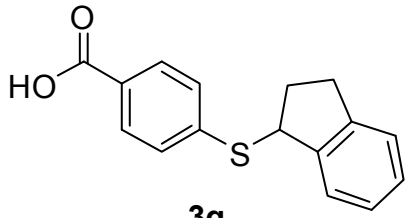
3p

HH3-63-3

H:¥HH3-63-3.als

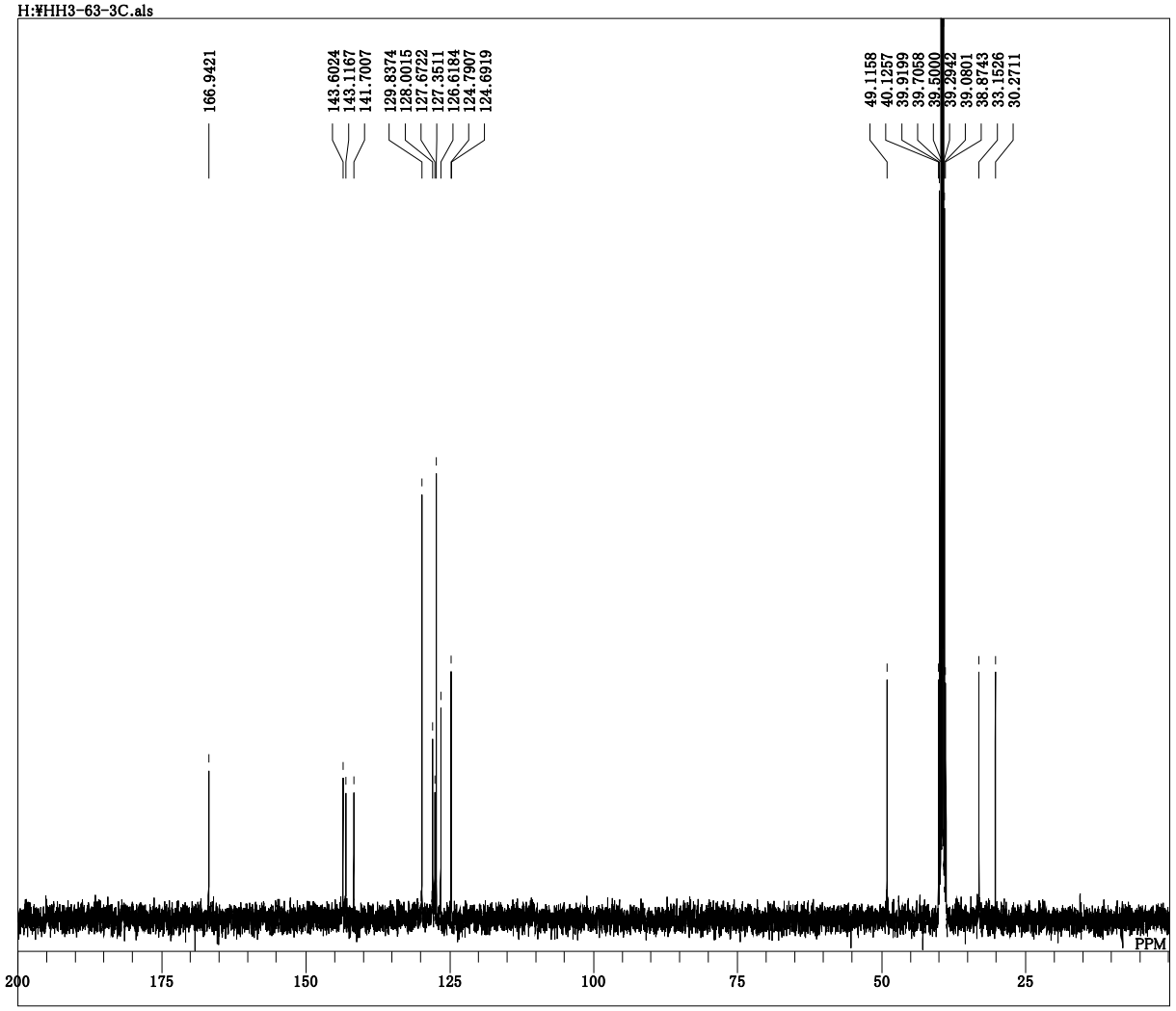


DFILE	HH3-63-3.als
COMNT	HH3-63-3
DATIM	Fri Oct 28 17:09:17 2011
OBNUC	1H
EXMOD	NON
OBFRQ	399.65 MHz
OBSET	124.00 KHz
OBFIN	11300.00 Hz
POINT	65536
FREQU	6006.01 Hz
SCANS	8
ACQTM	10.9117 sec
PD	1.0000 sec
PW1	5.50 usec
IRNUC	1H
CTEMP	23.0 c
SLVNT	DMSO
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	17

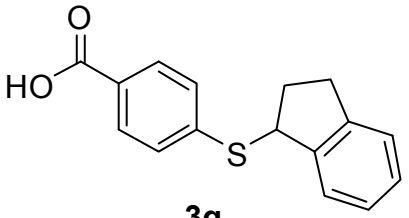


3q

HH3-63-3C



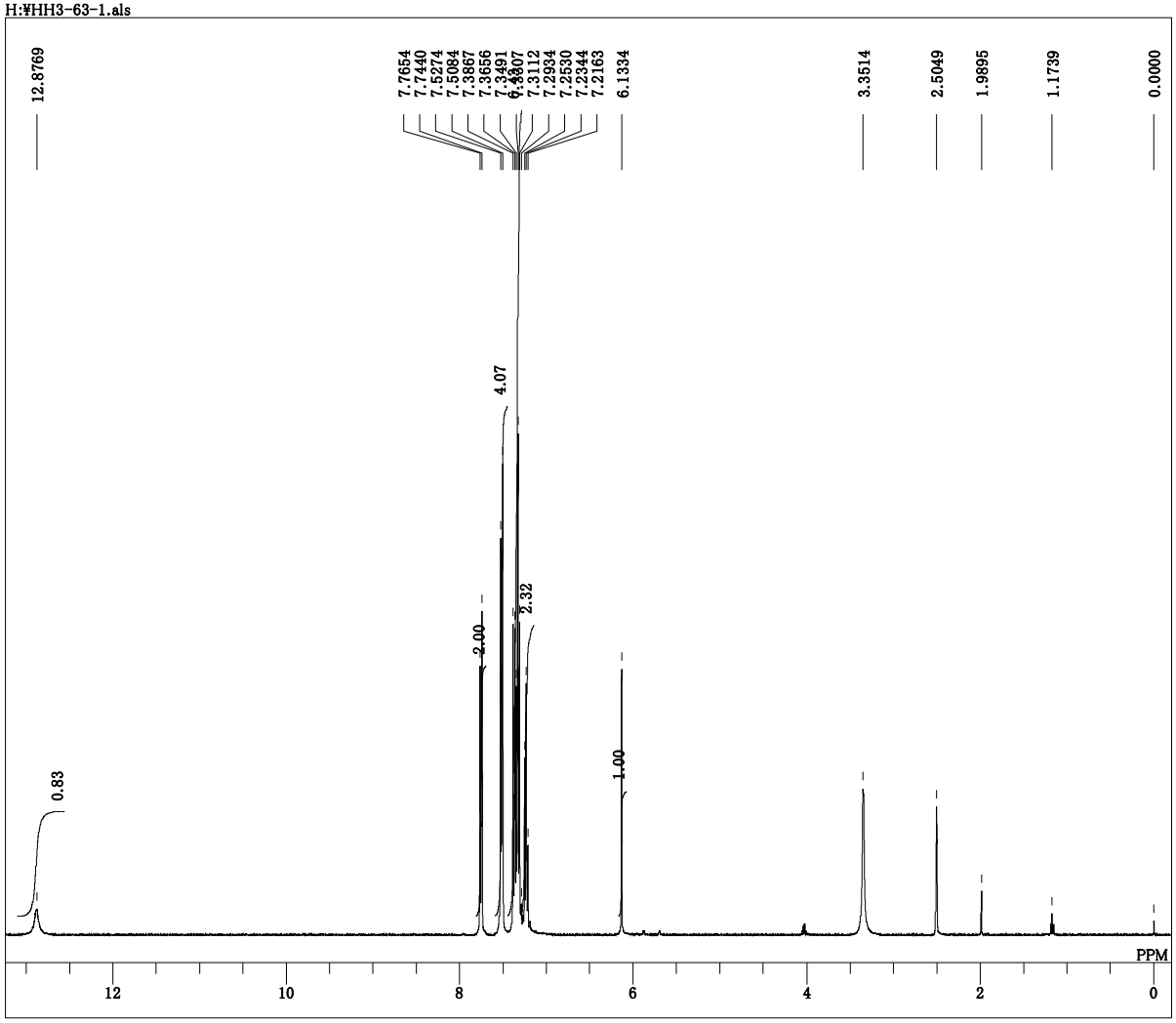
DFILE	HH3-63-3C.als
COMNT	HH3-63-3C
DATIM	Fri Oct 28 17:17:59 2011
OBNUC	13C
EXMOD	BCM
OBFRQ	100.40 MHz
OBSET	125.00 KHz
OBFIN	10500.00 Hz
POINT	32768
FREQU	27118.64 Hz
SCANS	157
ACQTM	1.2083 sec
PD	1.7920 sec
PW1	4.70 usec
IRNUC	1H
CTEMP	23.0 c
SLVNT	DMSO
EXREF	39.50 ppm
BF	1.20 Hz
RGAIN	24



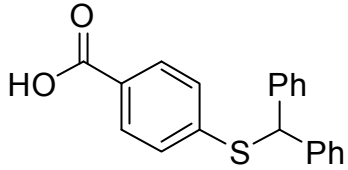
3q

HH3-63-1

H:¥HH3-63-1.als



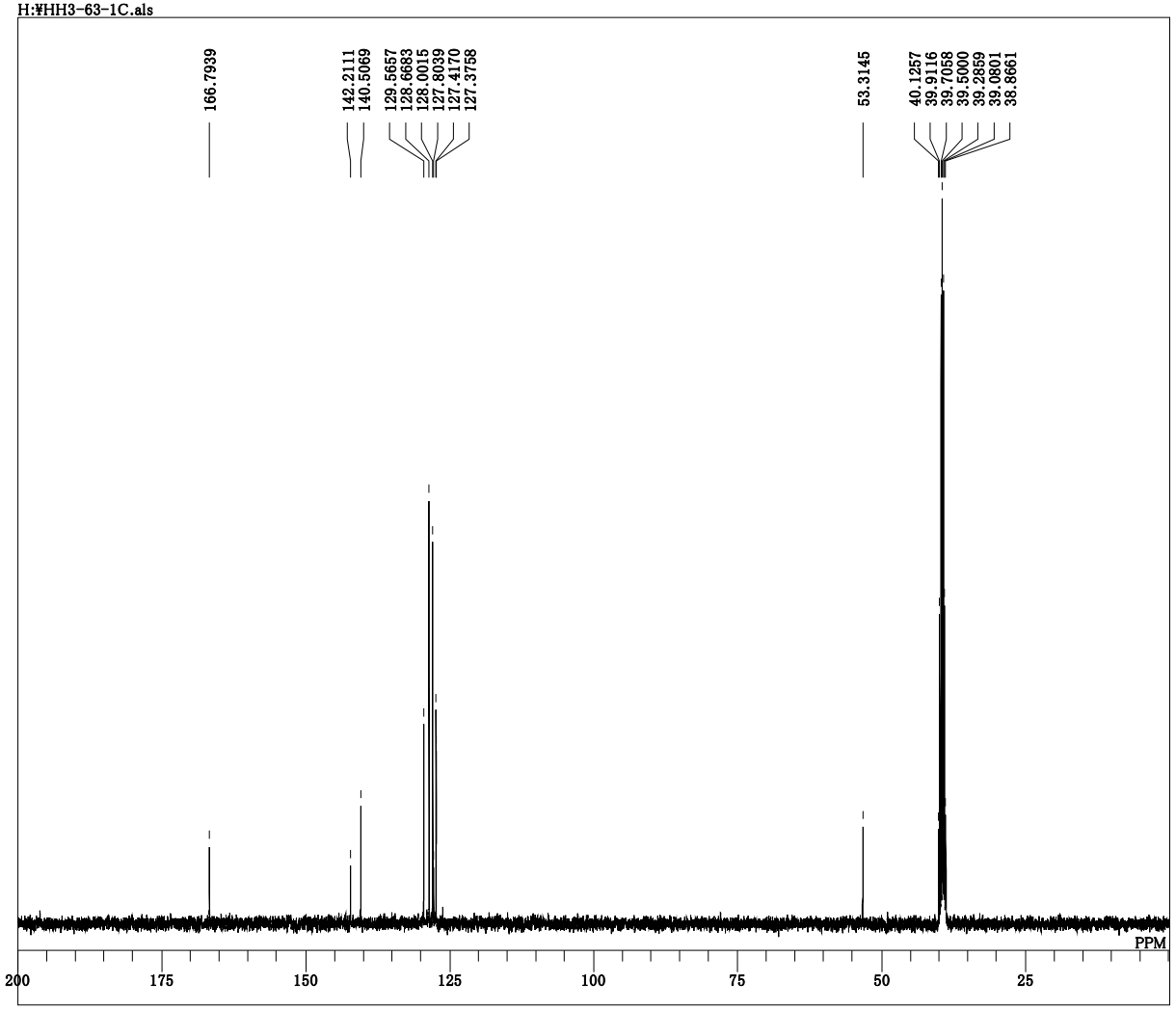
DFILE	HH3-63-1.als
COMNT	HH3-63-1
DATIM	Fri Oct 28 16:51:12 2011
OBNUC	1H
EXMOD	NON
OBFRQ	399.65 MHz
OBSET	124.00 KHz
OBFIN	11300.00 Hz
POINT	65536
FREQU	6006.01 Hz
SCANS	8
ACQTM	10.9117 sec
PD	1.0000 sec
PW1	5.50 usec
IRNUC	1H
CTEMP	23.2 c
SLVNT	DMSO
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	15



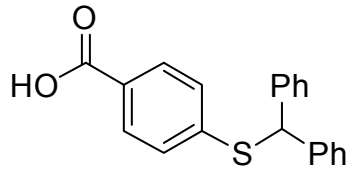
3r

HH3-63-1C

H:¥HH3-63-1C.als



DFILE	HH3-63-1C.als
COMNT	HH3-63-1C
DATIM	Fri Oct 28 16:47:59 2011
OBNUC	13C
EXMOD	BCM
OBFRQ	100.40 MHz
OBSET	125.00 KHz
OBFIN	10500.00 Hz
POINT	32768
FREQU	27118.64 Hz
SCANS	119
ACQTM	1.2083 sec
PD	1.7920 sec
PW1	4.70 usec
IRNUC	1H
CTEMP	23.6 c
SLVNT	DMSO
EXREF	39.50 ppm
BF	1.20 Hz
RGAIN	25



3r