The first catalytic asymmetric thioacetalization by chiral phosphoric acid catalysis

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Supporting Information

Contents

General: Reactions were monitored by thin layer chromatography using UV light to visualize the course of reaction. Purification of reaction products was carried out by flash chromatography on silica gel. Chemical yields refer to pure isolated substances. The $[\alpha]_D$ was recorded using PolAAr 3005 High Accuracy Polarimeter. Infrared (IR) spectra were obtained using a Nicolet Nexus 670 FT-IR spectrometer. ^{1}H, ^{13}C and ^{19}F NMR spectra were obtained using a Bruker DPX-400 spectrometer. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard. The following abbreviations were used to designate chemical shift multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, h = heptet, m = multiplet, br = broad. Coupling constants (*J*) are reported in Hertz.

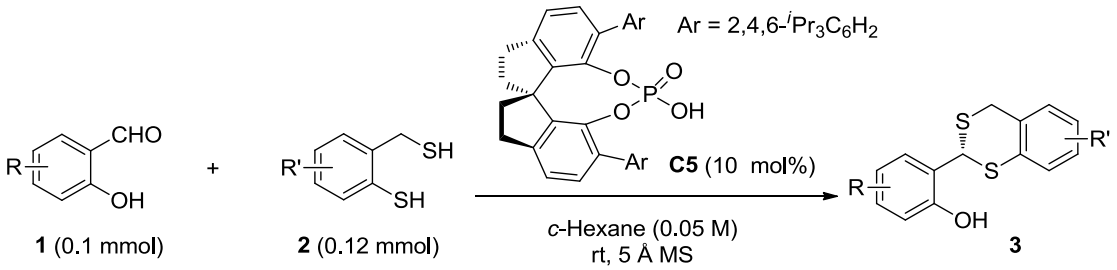
All reactions were run in air except noted. Anhydrous *n*-hexane, toluene and *c*-hexane were prepared by distillation over sodium-benzophenone ketyl prior to use. Powdered 5Å molecular sieve was purchased from Aldrich and activated by heating at 150 ^{o}C under vacumm for 12 hours before using.The chiral phosphoric acid **C1**-**C5** were purchased from *Daicel Chiral Technologies (China) Co., Ltd.* The salicylaldehydes **1** were purchased from *Accela ChemBio Co. Ltd* and *Shanghai Darui Finechemical Co. Ltd*. and used after purification. The dithiols **2** and **4** were prepared according to the literature report.[1]

List of abbreviation:

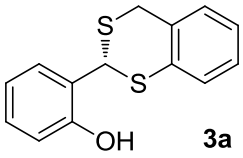
Entry	Chemical name	Abbreviation
1	Petroleum ether	PE
2	Molecular sieve	MS

[1] (a) E. Klingsberg and A. M.Schreiber, *J. Am. Chem. Soc.*, 1962, **84**, 2941; (b) A. G. Hortmann, A. J. Aron and A. K. Bhattacharya, *J. Org. Chem.*, 1978, **43**, 3374; (c) A. Schöberl, and H. Gräfje, *Justus Liebigs Ann. Chem.*, 1958, **614**, 66.

1. General procedure for the thioacetalization reaction.

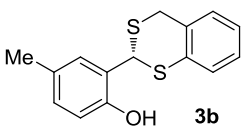


To a 5 mL vial were added chiral catalyst C**5** (7.2 mg, 0.01 mmol) and salicylaldehyde **1** (0.1 mmol), and then 100 mg activated 5Å MS was added, followed by the addition of 2.0 mL of anhydrous *c*-hexane. The reaction mixture was stirred at room temperature for about 20 minutes before adding dithiols **2** (0.12 mmol). The resulting mixture was stirred at room temperature till full conversion of **1** by TLC analysis and the reaction mixture was directly subjected to flash column chromatography to afford products **3** using PE/CH_2Cl_2 = 2:1 to 0:1 as eluent.



3a

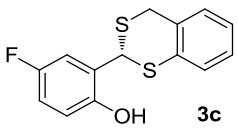
Column chromatography afforded product **3a** in 85% yield as pale yellow oil, HPLC analysis (Chiralpak AD-H, ^{i}PrOH/hexane = 15/85, 1.0 mL/min, 230 nm, t_r (minor) = 12.349 min, t_r (major) = 16.488 min) gave the isomeric composition of the product: 90% ee, $[\alpha]^{20}_D$ = +56.7 (c = 0.37, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35-7.31 (m, 2H), 7.28-7.18 (m, 4H), 6.91-6.87 (m, 2H), 6.18 (s, 1H), 5.72 (s, 1H), 4.01, 3.97 (AB, *J* = 14.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.54, 135.19, 134.43, 130.27, 129.87, 129.61, 128.63, 127.81, 126.49, 123.04, 120.86, 117.46, 48.00, 33.94. IR (KBr): 2919, 1595, 1487, 1456, 1348, 1272, 1227, 1088, 1039, 754 cm^{-1}. GC-MS: 260 (M^+, 30), 227 (100), 207 (54), 165 (14), 153 (26), 137 (51), 122 (45), 121 (54), 78 (27). HRMS (EI): Exact mass calcd for $C_{14}H_{12}OS_2$ $[M]^+$: 260.0330, Fou1nd: 260.0329.



3b

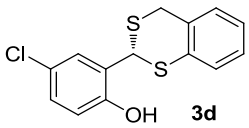
Column chromatography afforded product **3b** in 96% yield as pink oil, HPLC analysis (Chiralpak AD-H ^{i}PrOH/hexane = 15/85, 1.0 mL/min, 230 nm, t_r (minor) = 12.777 min, t_r (major) = 18.277 min) gave the isomeric composition of the product: 91% ee, $[\alpha]^{20}_D$ = +84.2 (c = 0.99, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34-7.32 (m, 1H), 7.27-7.19 (m, 3H), 7.14-7.13 (m, 1H), 7.04-7.01 (m, 1H), 6.78 (d, *J* = 8.4 Hz, 1H), 6.01 (s,

1H), 5.68 (s, 1H), 4.01, 3.96 (AB, *J* = 14.8 Hz, 2H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.23, 135.37, 134.36, 130.85, 130.17, 130.13, 129.54, 128.63, 127.75, 126.40, 122.53, 117.32, 48.12, 34.13, 20.40. IR (KBr): 3347, 2920, 1502, 1467, 1274, 1256, 1199, 1095, 813, 757, 738 cm^{-1}. GC-MS: 274(M^+, 45), 241 (100), 208 (11), 153 (76), 121 (41), 91 (11), 78 (16). HRMS (EI): Exact mass calcd for $C_{15}H_{14}OS_2$ $[M]^+$: 274.0486, Found: 274.0484.



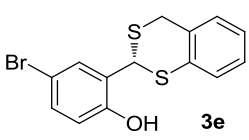
3c

Column chromatography afforded product **3c** in 88% yield as pink oil, HPLC analysis (Chiralpak AS-H, ^{i}PrOH/hexane = 10/90, 1.0 mL/min, 230 nm, t_r (minor) = 14.998 min, t_r (major) = 17.311 min) gave the isomeric composition of the product: 88% ee, $[\alpha]^{20}_D$ = +72.1 (c = 1.06, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35-7.33 (m, 1H), 7.30-7.20 (m, 3H), 7.07-7.04 (m, 1H), 6.94-6.89 (m, 1H), 6.83-6.80 (m, 1H), 5.95 (s, 1H), 5.67 (s, 1H), 3.98, 3.94 (AB, *J* = 14.8 Hz, 2H); ^{19}F NMR (376 MHz, $CDCl_3$): δ -122.82 (s, 1F); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.69 (d, *J* = 238 Hz), 150.21 (d, *J* = 2.3 Hz), 134.98, 134.57, 129.88, 128.55, 127.94, 126.81, 125.06 (d, *J* = 7.2 Hz), 118.26 (d, *J* = 8.0 Hz), 116.51 (d, *J* = 23 Hz), 116.15 (d, *J* = 24 Hz), 47.00, 33.52. IR (KBr): 3335, 2920, 1496, 1436, 1345, 1226, 1166, 812, 739 cm^{-1}. GC-MS: 278 (M^+, 36), 245 (100), 212 (6), 155 (43), 134 (16), 121 (63), 78 (18). HRMS (EI): Exact mass calcd for $C_{14}H_{11}OFS_2$ $[M]^+$: 278.0235, Found: 278.0232.



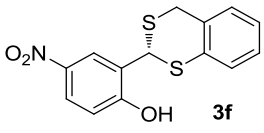
3d

Column chromatography afforded product **3d** in 97% yield as colorless oil, HPLC analysis (Chiralpak AD-H, ^{i}PrOH/hexane = 25/75, 1.0 mL/min, 230 nm, t_r (minor) = 6.160 min, t_r (major) = 7.893 min) gave the isomeric composition of the product: 84% ee, $[\alpha]^{20}_D$ = +65.4 (c = 0.99, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35-7.33 (m, 1H), 7.30-7.22 (m, 4H), 7.17-7.15 (m, 1H), 6.80 (d, *J* = 4.2 Hz, 1H), 6.23 (s, 1H), 5.64 (s, 1H), 3.98, 3.93 (AB, *J* = 14.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.02, 134.99, 134.63, 129.92, 129.88, 129.50, 128.54, 127.96, 126.86, 125.52, 125.11, 118.68, 47.23, 33.68. IR (KBr): 3380, 2918, 1482, 1415, 1271, 1224, 1109, 815, 756, 741, 646 cm^{-1}. GC-MS: 296 ($M[^{37}Cl]^+$, 14), 294 ($M[^{35}Cl]^+$, 36), 263 (36), 261 (100), 226 (37), 171 (41), 153 (33), 122 (49), 121 (77), 78 (22). HRMS (EI): Exact mass calcd for $C_{14}H_{11}{}^{35}ClOS_2$ $[M]^+$: 293.9940, Found: 293.9937.



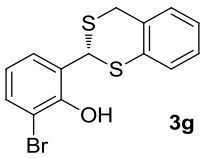
3e

Column chromatography afforded product **3e** in 91% yield as pale yellow solid, M.p. = 88-90 ^{o}C. HPLC analysis (Chiralpak AD-H, ^{i}PrOH/hexane = 25/75, 1.0 mL/min, 230 nm, t_r (minor) = 6.560 min, t_r (major) = 8.609 min) gave the isomeric composition of the product: 86% ee, $[\alpha]^{20}_{D}$ = +75.3 (c = 1.35, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.43 (d, *J* = 2.4 Hz, 1H), 7.35-7.20 (m, 5H), 6.75 (d, *J* = 8.4 Hz, 1H), 6.32 (s, 1H), 5.64 (s, 1H), 3.98, 3.93 (AB, *J* = 14.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.56, 134.99, 134.63, 132.84, 132.36, 129.89, 128.53, 127.95, 126.86, 125.56, 119.09, 112.62, 47.14, 33.72. IR (KBr): 3414, 1638, 1480, 1410, 1271, 1103, 624 cm^{-1}. GC-MS: 340 (M[^{80}Br]$^{+}$, 29), 338 (M[^{79}Br]$^{+}$, 28), 307 (80), 305 (78), 226 (69), 217 (32), 215 (30), 153 (45), 122 (61), 121 (100), 78 (30). HRMS (EI): Exact mass calcd for $C_{14}H_{11}{}^{79}BrOS_2$ [M]$^{+}$: 337.9435, Found: 337.9438.



3f

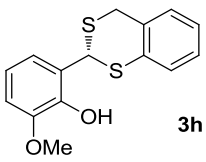
Column chromatography afforded product **3f** in 94% yield as yellow solid, M.p. = 145-147 ^{o}C. HPLC analysis (Chiralpak AD-H, ^{i}PrOH/hexane = 25/75, 1.0 mL/min, 230 nm, t_r (minor) = 5.570 min, t_r (major) = 7.274 min) gave the isomeric composition of the product: 87% ee, $[\alpha]^{20}_{D}$ = +99.3 (c = 1.22, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.23 (d, *J* = 1.6 Hz, 1H), 8.13-8.10 (m, 1H), 7.37-7.24 (m, 5H), 6.96 (d, *J* = 9.2 Hz, 1H), 5.74 (s, 1H), 4.01, 3.96 (AB, *J* = 14.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.02, 141.23, 135.77, 133.90, 130.38, 128.48, 128.22, 127.48, 126.14, 125.87, 124.84, 117.63, 46.88, 33.55. IR (KBr): 3268, 1589, 1516, 1480, 1434, 1336, 1278, 1074, 830, 740, 636 cm^{-1}. HRMS (EI): Exact mass calcd for $C_{14}H_{11}NO_3S_2$ [M]$^{+}$: 305.0180, Found: 305.0181.



3g

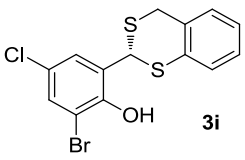
Column chromatography afforded product **3g** in 93% yield as white solid, M.p. = 111-113 ^{o}C. HPLC analysis (Chiralpak AS-H, ^{i}PrOH/hexane = 10/90, 1.0 mL/min, 230 nm, t_r (minor) = 14.957 min, t_r (major) = 17.463 min) gave the isomeric composition of the product: 92% ee, $[\alpha]^{20}_{D}$ = +78.0 (c = 0.78, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.41-7.39 (m, 2H), 7.31-7.17 (m, 4H), 6.77 (t, *J* = 8.0 Hz, 1H), 5.99 (s, 1H), 5.95 (s, 1H), 3.98, 3.91 (AB, *J* = 14.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.34, 135.26, 134.71, 131.85, 129.73, 129.01, 128.40, 127.67, 126.97, 126.41, 121.63, 110.77, 44.46, 33.35. IR (KBr): 3498, 1594, 1450, 1320, 1238, 1179, 1065, 771, 745, 649 cm^{-1}. GC-MS: 340 (M[^{80}Br]$^{+}$, 38), 338 (M[^{79}Br]$^{+}$, 35),

307 (94), 305 (91), 226 (89), 217 (29), 215 (28), 153 (57), 122 (68), 121 (100), 78 (31). HRMS (EI): Exact mass calcd for $C_{14}H_{11}{}^{79}BrOS_2$ $[M]^+$: 337.9435, Found: 337.9437.



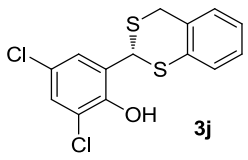
3h

Column chromatography afforded product **3h** in 95% yield as white solid, M.p. = 125-127 ^oC. HPLC analysis (Chiralpak AS-H, ^{i}PrOH/hexane = 15/85, 1.0 mL/min, 230 nm, t_r (minor) = 17.181 min, t_r (major) = 21.674 min) gave the isomeric composition of the product: 94% ee, $[\alpha]^{20}_D$ = +88.9 (c = 1.16, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.30-7.14 (m, 5H), 6.85-6.78 (m, 2H), 6.00 (s, 1H), 5.96 (s, 1H), 4.01, 3.93 (AB, *J* = 14.8 Hz, 2H), 3.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 146.30, 142.79, 135.39, 134.57, 129.29, 128.49, 127.44, 125.87, 124.76, 121.09, 119.83, 110.34, 56.15, 43.49, 33.76. IR (KBr): 3485, 2943, 1479, 1362, 1267, 1066, 765, 742 cm^{-1}. GC-MS: 290 (M, 47), 257 (100), 226 (31), 197 (13), 167 (37), 153 (34), 121 (30), 78 (10). HRMS (EI): Exact mass calcd for $C_{15}H_{14}O_2S_2$ $[M]^+$: 290.0435, Found: 290.0432.



3i

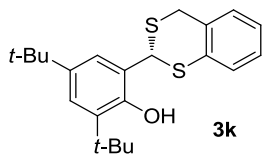
Column chromatography afforded product **3i** in 96% yield as pale yellow solid, M.p. = 70-74 ^oC. HPLC analysis (Chiralpak AD-H, ^{i}PrOH/hexane = 5/95, 1.0 mL/min, 230 nm, t_r (minor) = 19.747 min, t_r (major) = 18.767 min) gave the isomeric composition of the product: 92% ee, $[\alpha]^{20}_D$ = +65.0 (c = 1.32, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39-7.38 (m, 1H), 7.34-7.29 (m, 3H), 7.26-7.23 (m, 2H), 5.94 (s, 1H), 5.88 (s, 1H), 3.95, 3.90 (AB, *J* = 14.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.17, 136.23, 134.12, 131.06, 130.23, 129.00, 128.51, 128.25, 127.86, 126.94, 125.86, 110.80, 44.13, 33.19. IR (KBr): 3466, 2924, 1461, 1412, 1313, 1246, 1182, 1146, 873, 745, 550 cm^{-1}. GC-MS: 374 (35), 372 (25), 341 (84), 339 (61), 260 (43), 251 (20), 153 (48), 122 (69), 121 (100), 78 (29). HRMS (EI): Exact mass calcd for $C_{14}H_{10}{}^{79}Br^{35}ClOS_2$ $[M]^+$: 371.9045, Found: 371.9051.



3j

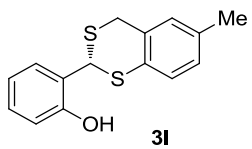
Column chromatography afforded product **3j** in 98% yield as pale yellow solid, M.p. = 110-112 ^oC. HPLC analysis (Chiralpak AD-H, ^{i}PrOH/hexane = 5/95, 1.0 mL/min, 230 nm, t_r (minor) undetected, t_r (major) = 19.933 min) gave the isomeric composition of the product: >99% ee, $[\alpha]^{20}_D$ = +78.5 (c = 1.18, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.33-7.29 (m, 3H), 7.26-7.23 (m, 3H), 5.96 (s, 1H), 5.88 (s, 1H), 3.95, 3.90 (AB, *J*

= 14.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.31, 136.24, 134.15, 130.23, 128.74, 128.30, 128.26, 127.86, 126.95, 125.47, 120.78, 43.79, 33.22. IR (KBr): 3487, 2923, 1465, 1317, 1246, 1155, 874, 752 cm^{-1}. GC-MS: 328 (M^+, 35), 297 (62), 295 (88), 260 (43), 205 (22), 153 (44), 121 (100), 78 (29). HRMS (EI): Exact mass calcd for $C_{14}H_{10}{}^{35}Cl_2OS_2$ $[M]^+$: 327.9550, Found: 327.9543.



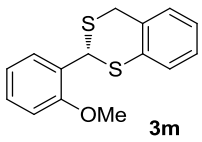
3k

Column chromatography afforded product **3k** in 73% yield as pale yellow oil. HPLC analysis (Chiralpak OD-H, ^{i}PrOH/hexane = 3/97, 0.8 mL/min, 230 nm, t_r (minor) = 7.587 min, t_r (major) = 7.860 min) gave the isomeric composition of the product: 96% ee, $[\alpha]^{20}_D$ = +48.9 (c = 0.89, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.30-7.26 (m, 2H), 7.21-7.13 (m, 3H), 7.01-7.00 (m, 1H), 6.49 (s, 1H), 5.53 (s, 1H), 4.00, 3.89 (AB, *J* = 14.4 Hz, 2H), 1.36 (s, 9 H), 1.20 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.20, 142.25, 137.70, 135.72, 134.37, 129.82, 128.76, 127.85, 126.66, 125.39, 124.59, 121.08, 51.43, 35.21, 34.42, 34.34, 31.56, 29.87. IR (KBr): 3441, 2957, 1478, 1362, 1226, 1201, 738 cm^{-1}. GC-MS: 328 (M^+, 62), 339 (89), 283 (24), 249 (100), 235 (29), 193 (13), 153 (37), 57 (90). HRMS (EI): Exact mass calcd for $C_{22}H_{28}OS_2$ $[M]^+$: 372.1582, Found: 372.1585.



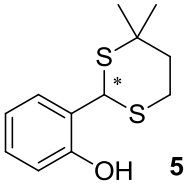
3l

Column chromatography afforded product **3l** in 87% yield as pale yellow oil. HPLC analysis (Chiralpak AD-H, ^{i}PrOH/hexane = 15/85, 1.0 mL/min, 230 nm, t_r (minor) = 13.527 min, t_r (major) = 24.363 min) gave the isomeric composition of the product: 86% ee, $[\alpha]^{20}_D$ = +52.8 (c = 0.94, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.30-7.21 (m, 4H), 7.12 (s, 1H), 7.08-7.06 (m, 1H), 6.90-6.86 (m, 2H), 5.65 (s, 1H), 4.00, 3.90 (AB, *J* = 14.4 Hz, 2H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.69, 136.82, 134.98, 131.66, 130.28, 129.91, 129.82, 129.27, 128.67, 123.00, 120.82, 117.59, 48.60, 33.87, 21.05. IR (KBr): 3443, 1628, 1595, 1484, 1087, 752, 535 cm^{-1}. GC-MS: 274 (M^+, 12), 272 (100), 239 (52), 207 (44), 167 (52), 139 (46), 91 (34). HRMS (EI): Exact mass calcd for $C_{15}H_{14}OS_2$ $[M]^+$: 274.0486, Found: 274.0489.



3m

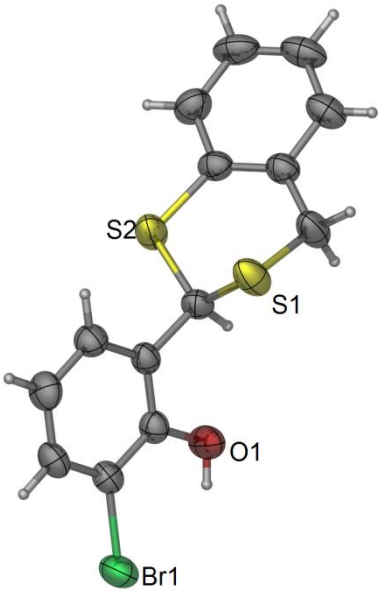
Column chromatography afforded product **3m** in 26% yield as pale yellow oil. HPLC analysis (Chiralpak AD-H, ^{i}PrOH/hexane = 15/85, 1.0 mL/min, 230 nm, t_r (minor) = 5.613 min, t_r (major) = 6.247 min) gave the isomeric composition of the product: 73% ee, $[\alpha]^{20}_{D}$ = +45.4 (c = 0.48, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.57 (dd, *J* = 7.6 Hz, *J* = 1.2 Hz, 1H), 7.29-7.23 (m, 3H), 7.20-7.15 (m, 2H), 6.94 (t, *J* = 7.6 Hz, 1H), 6.89 (d, *J* = 8.4 Hz, 1H), 6.04 (s, 1H), 4.01, 3.91 (AB, *J* = 14.8 Hz, 2H), 3.87 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.07, 135.44, 134.32, 129.41, 129.22, 129.20, 128.54, 127.42, 127.38, 125.77, 120.78, 110.69, 55.72, 43.16, 33.69. IR (KBr): 2932, 1459, 1289, 1254, 1140, 865, 653 cm^{-1}. GC-MS: 274 (M^+, 32), 241 (100), 226 (23), 153 (30), 121 (33), 107 (17), 91 (28). HRMS (EI): Exact mass calcd for $C_{15}H_{14}OS_2$ $[M]^+$: 274.0486, Found: 274.0489.



5

Column chromatography afforded product **5** in 72% yield as white solid, M.p. = 101-103 ^{o}C. HPLC analysis (Chiralpak AD-H+AD-H, ^{i}PrOH/hexane = 15/85, 0.7 mL/min, 230 nm, t_r (minor) = 22.036 min, t_r (major) = 20.901 min) gave the isomeric composition of the product: 55% ee, $[\alpha]^{20}_{D}$ = +19.0 (c = 0.67, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.28-7.25 (m, 1H), 7.22-7.20 (m, 1H), 6.90-6.85 (m, 2H), 6.45 (s, 1H), 5.48 (s, 1H), 3.30-3.22 (m, 1H), 2.83 (dt, *J* = 14.8 Hz, *J* = 4.0 Hz, 1H), 1.95-1.89 (m, 2H), 1.49 (s, 3H), 1.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.08, 130.21, 129.39, 122.69, 120.74, 117.55, 44.44, 42.80, 38.44, 31.77, 27.52, 26.11. IR (KBr): 2959, 2926, 1595, 1499, 1457, 1272, 1229, 1084, 765 cm^{-1}. GC-MS: 240 (M^+, 85), 175 (41), 138 (100), 119 (50), 107 (34), 68 (33). HRMS (EI): Exact mass calcd for $C_{12}H_{16}OS_2$ $[M]^+$: 240.0643, Found: 240.0648.

2. Single-Crystal X-ray Crystallography of product 3g



Data intensity of $C_{14}H_{11}BrOS_2$ **(3g)** was collected using a Bruker SMART APEX II (Mo radiation) at 296 K in a nitrogen stream. Data collection and reduction were done by using the Bruker ApexII software package. The structures were solved by direct methods and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for non-H atoms using SHELX-97. Hydrogen atoms were added at their geometrically idea positions and refined isotropically. Crystal data for **3g**: $C_{14}H_{11}BrOS_2$, T = 296(2) K, Orthorhombic, P2(1)2(1)2(1). a = 5.9198(2) Å, b = 8.4943(4) Å, c = 26.9054(11) Å, alpha = 90 deg, beta = 90 deg, gamma = 90 deg. V = 1352.93(10) Å^3. Z = 4, d_{calc} = 1.666 mg/m^3. Total number of reflections 15751/[R(int) = 0.0358], R_1 = 0.0316, wR_2 = 0.0630 (all data), GOF = 1.037, and 163 parameter.

Table 1. Crystal data and structure refinement for z.

Identification code	z
Empirical formula	$C_{14}H_{11}BrOS_2$
Formula weight	339.26
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 5.9198(2) Å alpha = 90 deg.
	b = 8.4943(4) Å beta = 90 deg.
	c = 26.9054(11) Å gamma = 90 deg.

Volume	1352.93(10) Å^3
Z, Calculated density	4, 1.666 Mg/m^3
Absorption coefficient	3.330 mm^{-1}
F(000)	680
Crystal size	0.46 x 0.33 x 0.21 mm
Theta range for data collection	1.51 to 25.00 deg.
Limiting indices	-7<=h<=7, -10<=k<=10, -32<=l<=31
Reflections collected / unique	15751 / 2386 [R(int) = 0.0358]
Completeness to theta = 25.00	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.5414 and 0.3095
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2386 / 0 / 163
Goodness-of-fit on F^2	1.037
Final R indices [I>2sigma(I)]	R_1 = 0.0266, wR_2 = 0.0608
R indices (all data)	R_1 = 0.0316, wR_2 = 0.0630
Absolute structure parameter	0.000(9)
Largest diff. peak and hole	0.520 and -0.191 e. Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for z. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Br(1)	1205(1)	3595(1)	526(1)	62(1)
S(1)	-482(2)	7636(1)	-1417(1)	56(1)
S(2)	-3665(2)	4959(1)	-1627(1)	54(1)
O(1)	1490(4)	4029(3)	-614(1)	58(1)
C(1)	517(6)	7196(4)	-2033(1)	60(1)
C(2)	-1243(5)	6539(3)	-2381(1)	44(1)
C(3)	-1025(7)	6911(4)	-2885(1)	57(1)
C(4)	-2558(7)	6411(5)	-3232(1)	63(1)
C(5)	-4353(7)	5494(5)	-3089(1)	64(1)
C(6)	-4585(6)	5082(4)	-2594(1)	58(1)
C(7)	-3043(5)	5598(4)	-2239(1)	43(1)

C(8)	-1272(6)	5640(3)	-1267(1)	42(1)
C(9)	-1821(5)	5523(3)	-718(1)	39(1)
C(10)	-3750(5)	6221(3)	-523(1)	47(1)
C(11)	-4187(5)	6160(4)	-17(1)	52(1)
C(12)	-2706(6)	5395(4)	297(1)	47(1)
C(13)	-804(5)	4691(3)	100(1)	42(1)
C(14)	-340(5)	4738(3)	-408(1)	39(1)

Table 3. Bond lengths [Å] and angles [deg] for z.

Br(1)-C(13)	1.896(3)
S(1)-C(1)	1.798(3)
S(1)-C(8)	1.804(3)
S(2)-C(7)	1.772(3)
S(2)-C(8)	1.811(3)
O(1)-C(14)	1.357(3)
O(1)-H(1C)	0.8200
C(1)-C(2)	1.508(4)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(2)-C(7)	1.386(4)
C(2)-C(3)	1.399(4)
C(3)-C(4)	1.369(5)
C(3)-H(3A)	0.9300
C(4)-C(5)	1.373(5)
C(4)-H(4A)	0.9300
C(5)-C(6)	1.386(5)
C(5)-H(5A)	0.9300
C(6)-C(7)	1.391(4)
C(6)-H(6A)	0.9300
C(8)-C(9)	1.514(4)
C(8)-H(8A)	0.9800
C(9)-C(14)	1.382(4)
C(9)-C(10)	1.390(4)
C(10)-C(11)	1.385(4)

C(10)-H(10A)	0.9300
C(11)-C(12)	1.381(4)
C(11)-H(11A)	0.9300
C(12)-C(13)	1.381(4)
C(12)-H(12A)	0.9300
C(13)-C(14)	1.395(4)
C(1)-S(1)-C(8)	95.59(15)
C(7)-S(2)-C(8)	103.70(14)
C(14)-O(1)-H(1C)	109.5
C(2)-C(1)-S(1)	114.9(2)
C(2)-C(1)-H(1A)	108.5
S(1)-C(1)-H(1A)	108.5
C(2)-C(1)-H(1B)	108.5
S(1)-C(1)-H(1B)	108.5
H(1A)-C(1)-H(1B)	107.5
C(7)-C(2)-C(3)	118.0(3)
C(7)-C(2)-C(1)	125.0(2)
C(3)-C(2)-C(1)	117.0(3)
C(4)-C(3)-C(2)	122.0(4)
C(4)-C(3)-H(3A)	119.0
C(2)-C(3)-H(3A)	119.0
C(3)-C(4)-C(5)	119.9(3)
C(3)-C(4)-H(4A)	120.1
C(5)-C(4)-H(4A)	120.1
C(4)-C(5)-C(6)	119.3(3)
C(4)-C(5)-H(5A)	120.3
C(6)-C(5)-H(5A)	120.3
C(5)-C(6)-C(7)	121.1(3)
C(5)-C(6)-H(6A)	119.5
C(7)-C(6)-H(6A)	119.5
C(2)-C(7)-C(6)	119.8(3)
C(2)-C(7)-S(2)	126.4(2)
C(6)-C(7)-S(2)	113.9(3)
C(9)-C(8)-S(1)	109.7(2)
C(9)-C(8)-S(2)	109.4(2)

S(1)-C(8)-S(2)	112.49(16)
C(9)-C(8)-H(8A)	108.4
S(1)-C(8)-H(8A)	108.4
S(2)-C(8)-H(8A)	108.4
C(14)-C(9)-C(10)	119.8(3)
C(14)-C(9)-C(8)	119.0(3)
C(10)-C(9)-C(8)	121.1(3)
C(11)-C(10)-C(9)	120.6(3)
C(11)-C(10)-H(10A)	119.7
C(9)-C(10)-H(10A)	119.7
C(12)-C(11)-C(10)	120.1(3)
C(12)-C(11)-H(11A)	120.0
C(10)-C(11)-H(11A)	120.0
C(13)-C(12)-C(11)	119.1(3)
C(13)-C(12)-H(12A)	120.5
C(11)-C(12)-H(12A)	120.5
C(12)-C(13)-C(14)	121.7(3)
C(12)-C(13)-Br(1)	119.5(2)
C(14)-C(13)-Br(1)	118.8(2)
O(1)-C(14)-C(9)	118.3(2)
O(1)-C(14)-C(13)	123.0(3)
C(9)-C(14)-C(13)	118.8(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3) for z. The anisotropic displacement factor exponent takes the form: $-2\ pi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
Br(1)	65(1)	78(1)	43(1)	13(1)	1(1)	11(1)
S(1)	76(1)	55(1)	38(1)	-4(1)	-1(1)	-21(1)
S(2)	54(1)	71(1)	38(1)	-2(1)	-1(1)	-22(1)
O(1)	51(1)	83(2)	40(1)	0(1)	6(1)	20(1)
C(1)	66(2)	78(2)	37(2)	1(2)	1(2)	-26(2)
C(2)	49(2)	50(2)	34(2)	-2(1)	-1(1)	2(2)

C(3)	76(2)	56(2)	38(2)	2(1)	2(2)	2(2)
C(4)	87(3)	69(2)	34(2)	-1(2)	-8(2)	12(2)
C(5)	68(3)	82(2)	42(2)	-14(2)	-19(2)	15(2)
C(6)	48(2)	74(2)	51(2)	-11(2)	-6(2)	-3(2)
C(7)	45(2)	49(2)	35(2)	-6(1)	-4(1)	8(1)
C(8)	44(2)	49(2)	32(2)	-2(1)	-3(2)	-3(2)
C(9)	41(2)	44(2)	33(2)	-3(1)	3(1)	-6(1)
C(10)	46(2)	48(2)	46(2)	2(1)	0(2)	5(2)
C(11)	50(2)	54(2)	51(2)	-7(2)	13(2)	7(2)
C(12)	56(2)	49(2)	36(2)	-1(1)	11(2)	-2(2)
C(13)	46(2)	41(2)	38(2)	1(1)	4(1)	-1(1)
C(14)	40(2)	42(2)	37(2)	-6(1)	4(1)	-1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å ^{2} x 10^3) for z.

	x	y	z	U(eq)
H(1C)	2241	3608	-395	87
H(1A)	1126	8152	-2178	72
H(1B)	1745	6444	-2008	72
H(3A)	198	7516	-2988	68
H(4A)	-2383	6693	-3564	76
H(5A)	-5403	5153	-3323	77
H(6A)	-5790	4451	-2496	69
H(8A)	18	4952	-1337	50
H(10A)	-4756	6733	-733	56
H(11A)	-5478	6635	110	62
H(12A)	-2987	5354	637	56

Table 6. Torsion angles [deg] for z.

C(8)-S(1)-C(1)-C(2)	61.7(3)
S(1)-C(1)-C(2)-C(7)	-32.1(4)
S(1)-C(1)-C(2)-C(3)	148.0(3)
C(7)-C(2)-C(3)-C(4)	1.8(5)

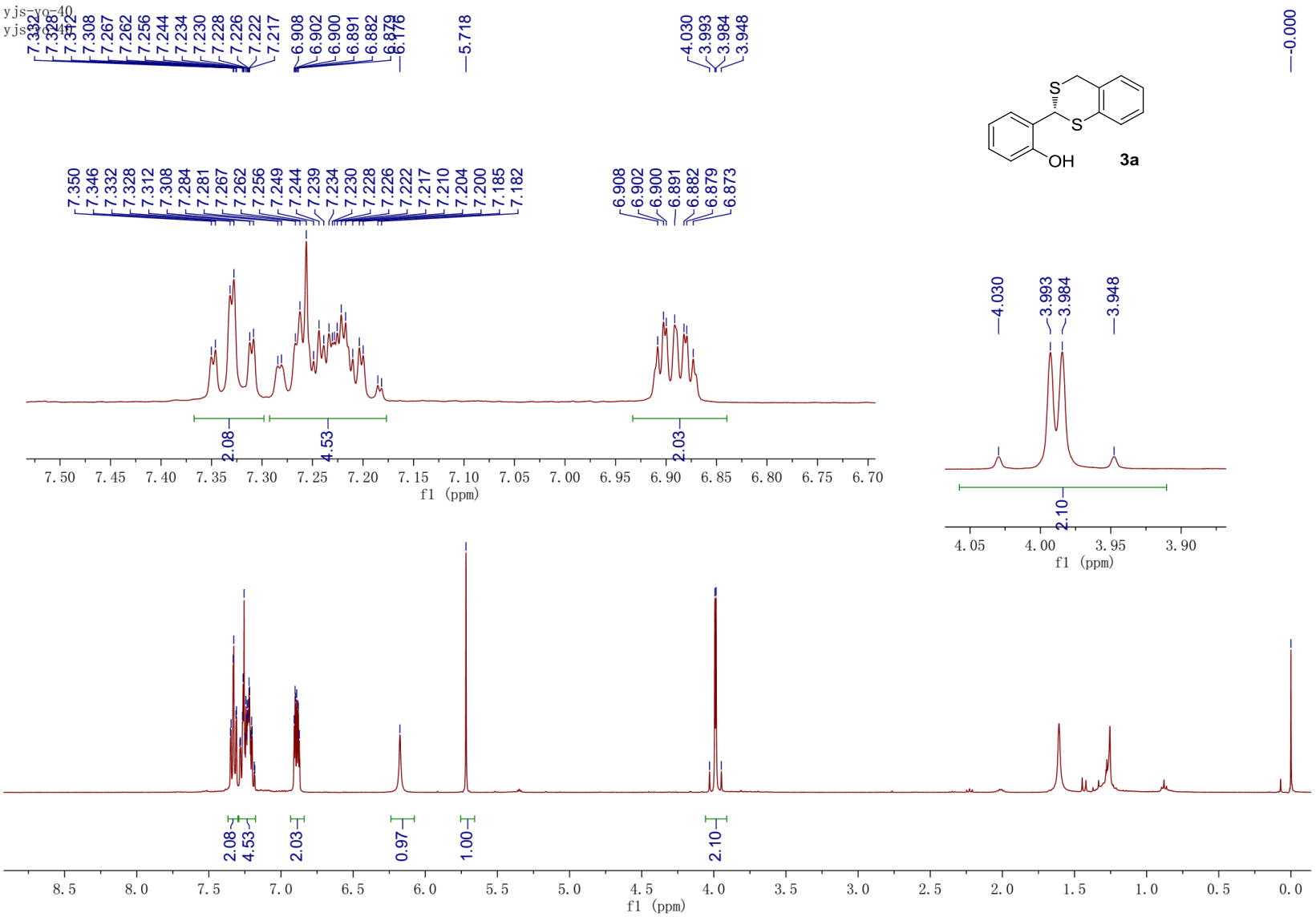
C(1)-C(2)-C(3)-C(4)	-178.3(3)
C(2)-C(3)-C(4)-C(5)	-1.1(5)
C(3)-C(4)-C(5)-C(6)	-0.2(5)
C(4)-C(5)-C(6)-C(7)	0.7(5)
C(3)-C(2)-C(7)-C(6)	-1.2(4)
C(1)-C(2)-C(7)-C(6)	178.9(3)
C(3)-C(2)-C(7)-S(2)	179.6(2)
C(1)-C(2)-C(7)-S(2)	-0.3(5)
C(5)-C(6)-C(7)-C(2)	0.0(5)
C(5)-C(6)-C(7)-S(2)	179.3(3)
C(8)-S(2)-C(7)-C(2)	-6.0(3)
C(8)-S(2)-C(7)-C(6)	174.8(2)
C(1)-S(1)-C(8)-C(9)	169.6(2)
C(1)-S(1)-C(8)-S(2)	-68.3(2)
C(7)-S(2)-C(8)-C(9)	166.6(2)
C(7)-S(2)-C(8)-S(1)	44.4(2)
S(1)-C(8)-C(9)-C(14)	-108.5(3)
S(2)-C(8)-C(9)-C(14)	127.7(2)
S(1)-C(8)-C(9)-C(10)	69.9(3)
S(2)-C(8)-C(9)-C(10)	-53.9(3)
C(14)-C(9)-C(10)-C(11)	1.0(4)
C(8)-C(9)-C(10)-C(11)	-177.3(3)
C(9)-C(10)-C(11)-C(12)	-0.3(4)
C(10)-C(11)-C(12)-C(13)	-0.3(4)
C(11)-C(12)-C(13)-C(14)	0.2(4)
C(11)-C(12)-C(13)-Br(1)	-178.5(2)
C(10)-C(9)-C(14)-O(1)	178.0(3)
C(8)-C(9)-C(14)-O(1)	-3.6(4)
C(10)-C(9)-C(14)-C(13)	-1.2(4)
C(8)-C(9)-C(14)-C(13)	177.3(3)
C(12)-C(13)-C(14)-O(1)	-178.6(3)
Br(1)-C(13)-C(14)-O(1)	0.1(4)
C(12)-C(13)-C(14)-C(9)	0.6(4)
Br(1)-C(13)-C(14)-C(9)	179.3(2)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for z [Å and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

3. ^{1}H, ^{19}F, ^{13}C NMR spectra and HPLC spectra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2.10
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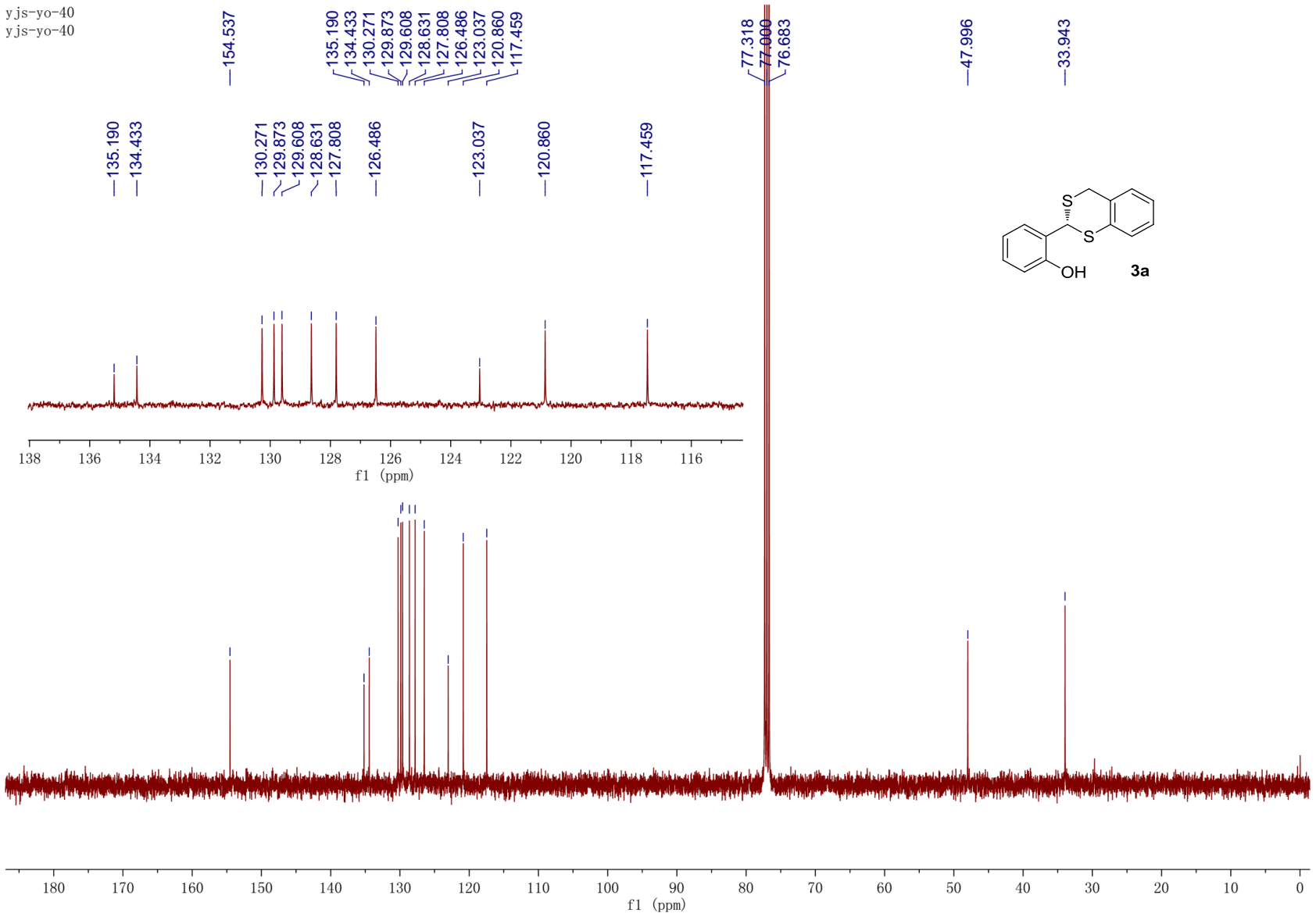
f1 (ppm)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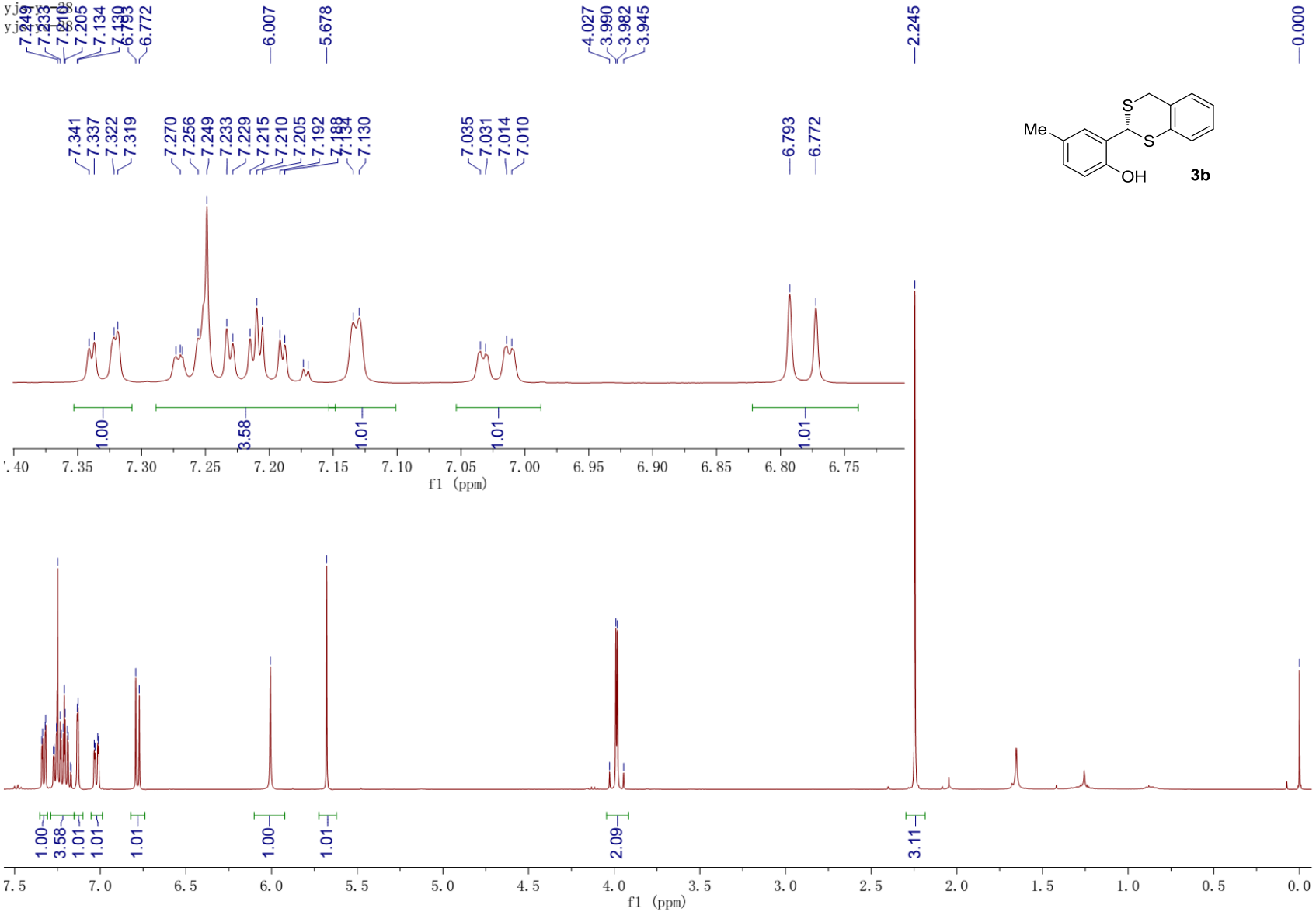
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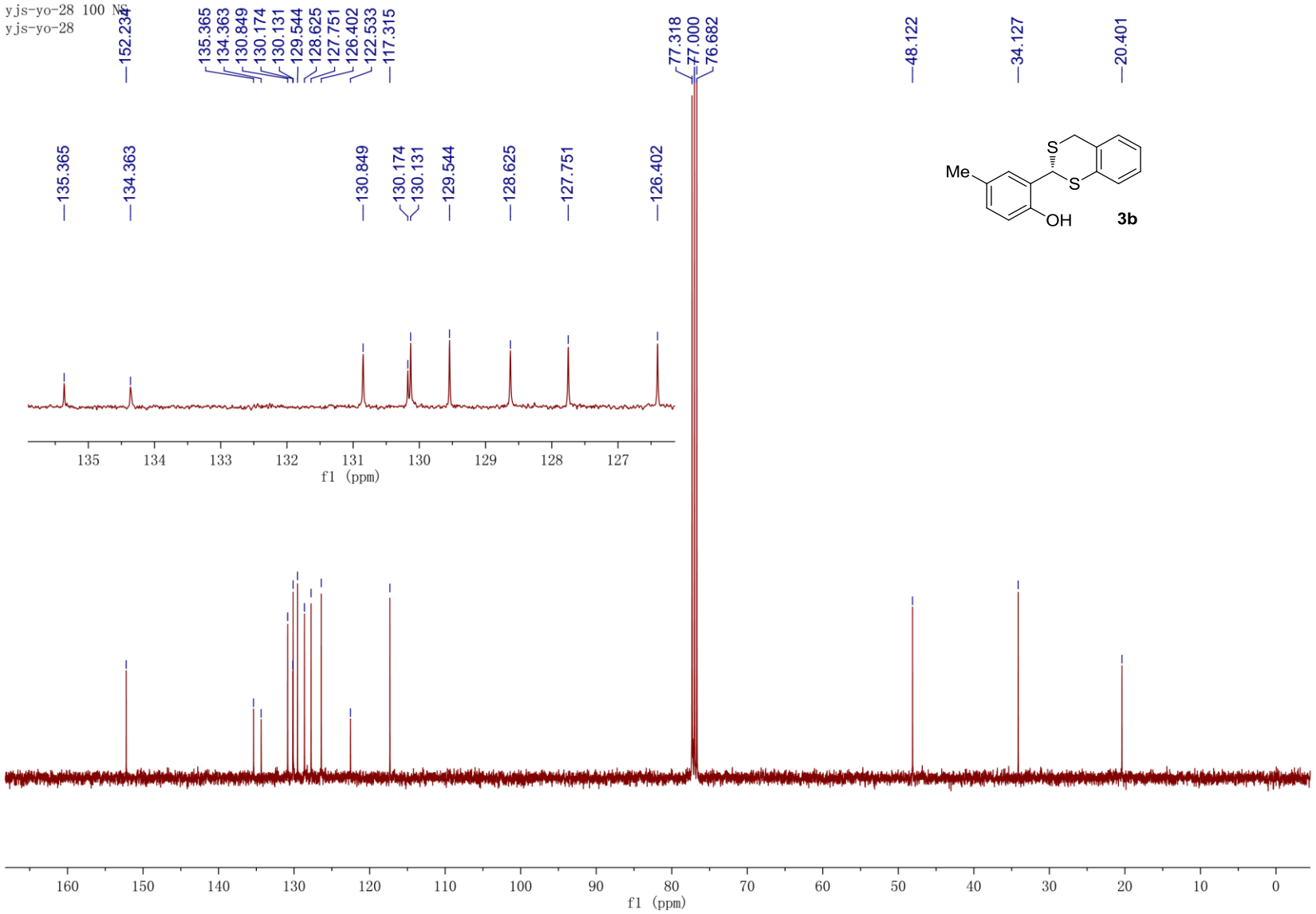
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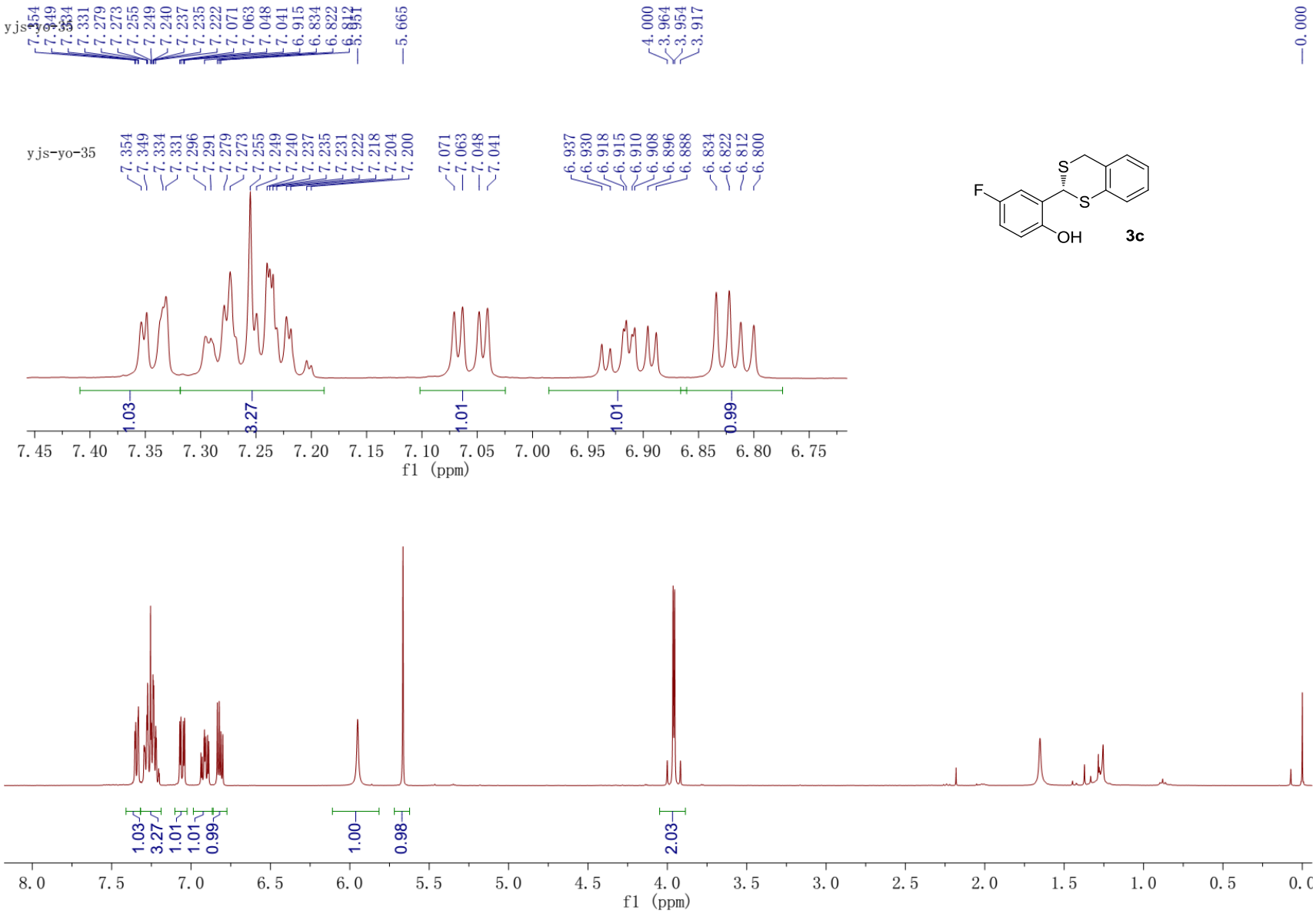
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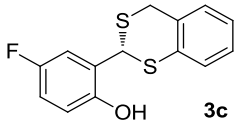
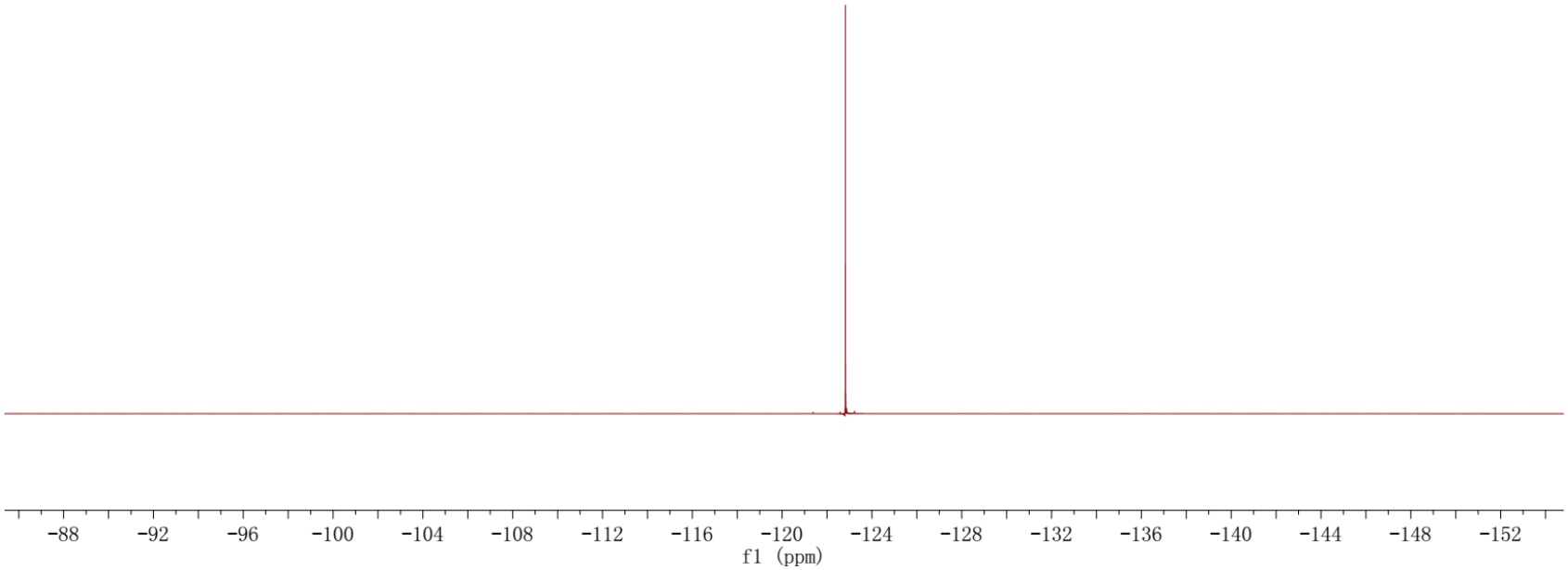
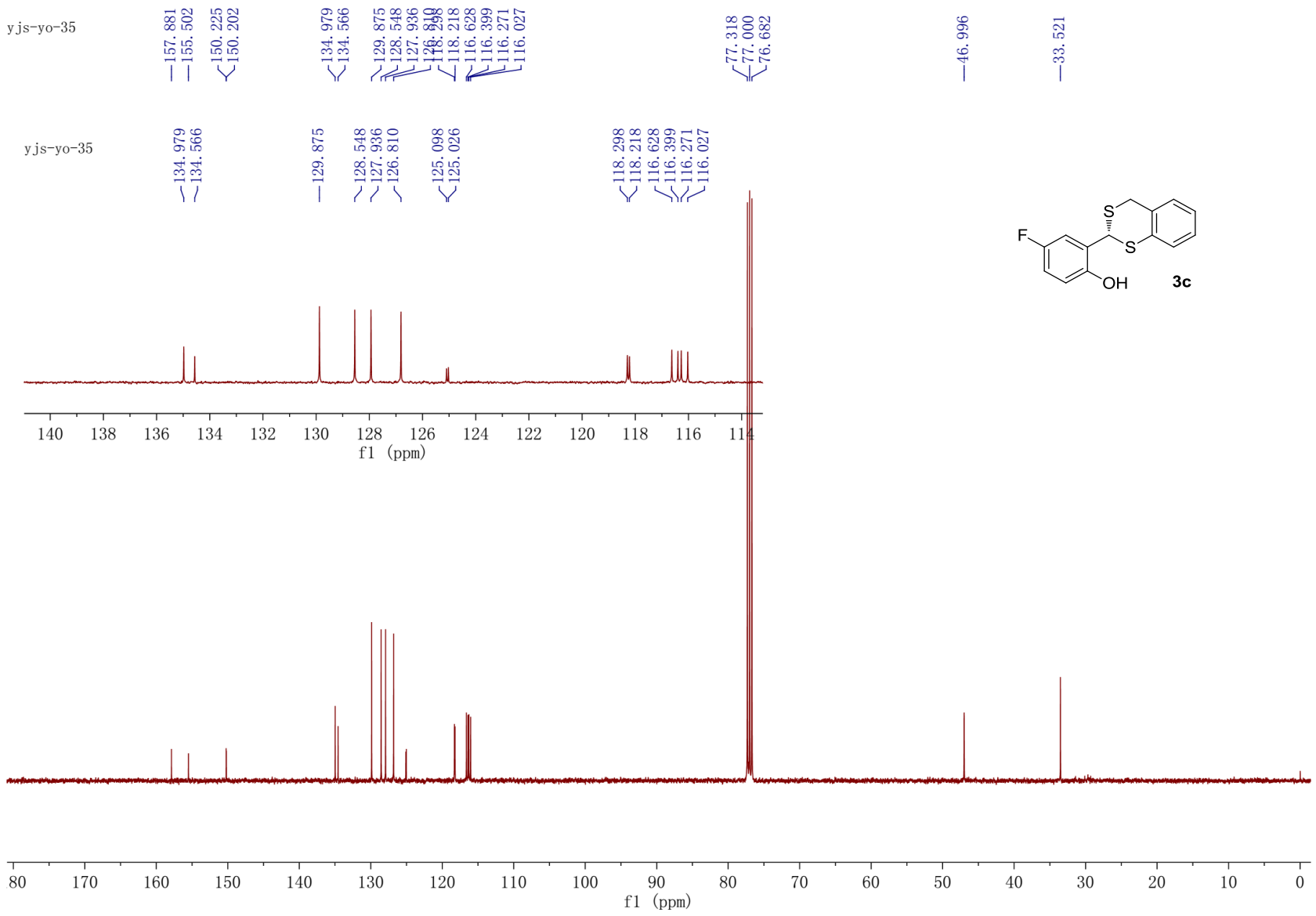
6.888
6.834
6.822
6.812
6.800
1.03
3.27
1.01
1.01
0.99
7.45 7.40 7.35 7.30 7.25 7.20 7.15 7.10 7.05 7.00 6.95 6.90 6.85 6.80 6.75
f1 (ppm)
F
S
S
OH
3c
1.03
3.27
1.01
1.01
0.99
1.00
0.98
2.03
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

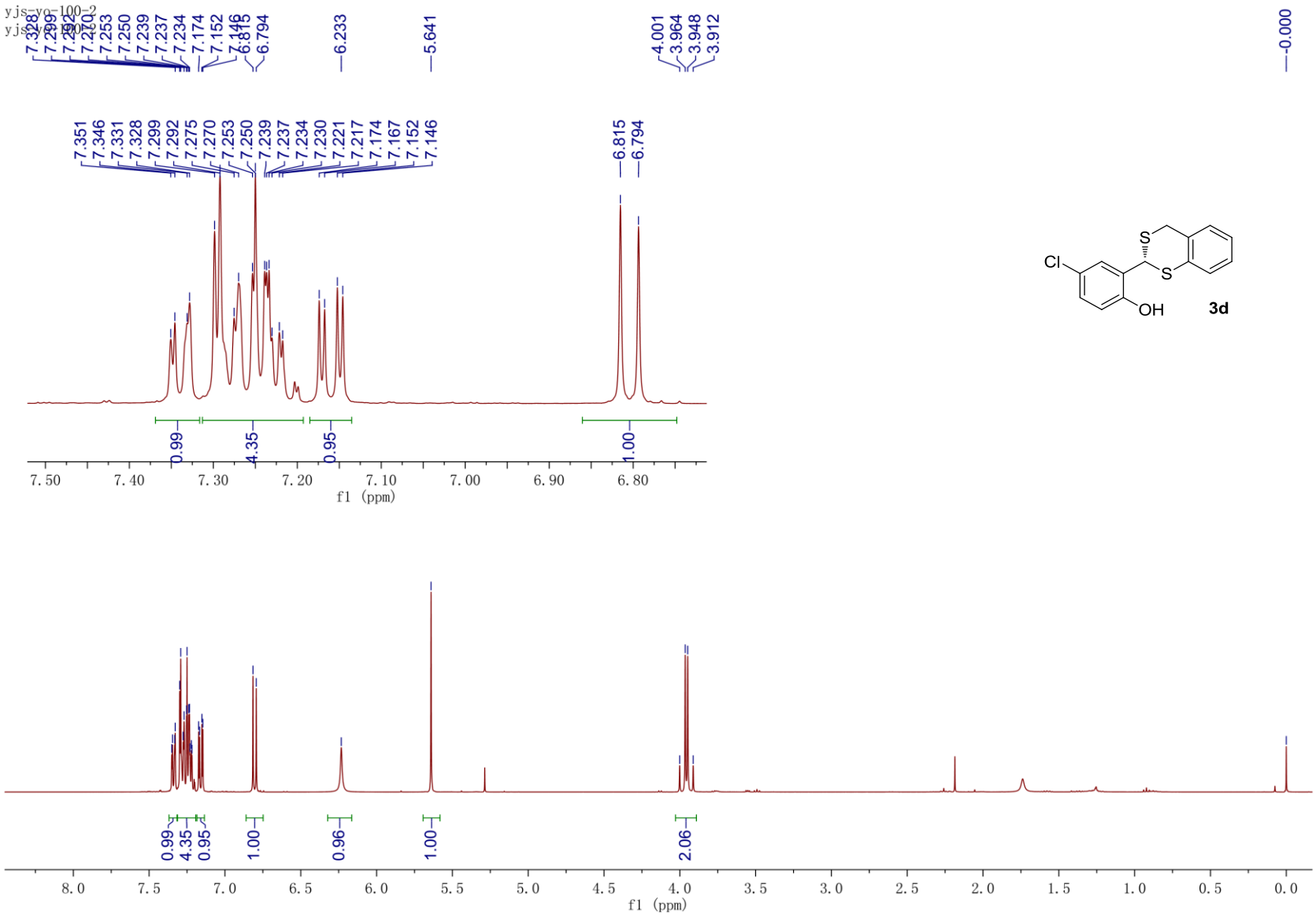
yjs-yo-35

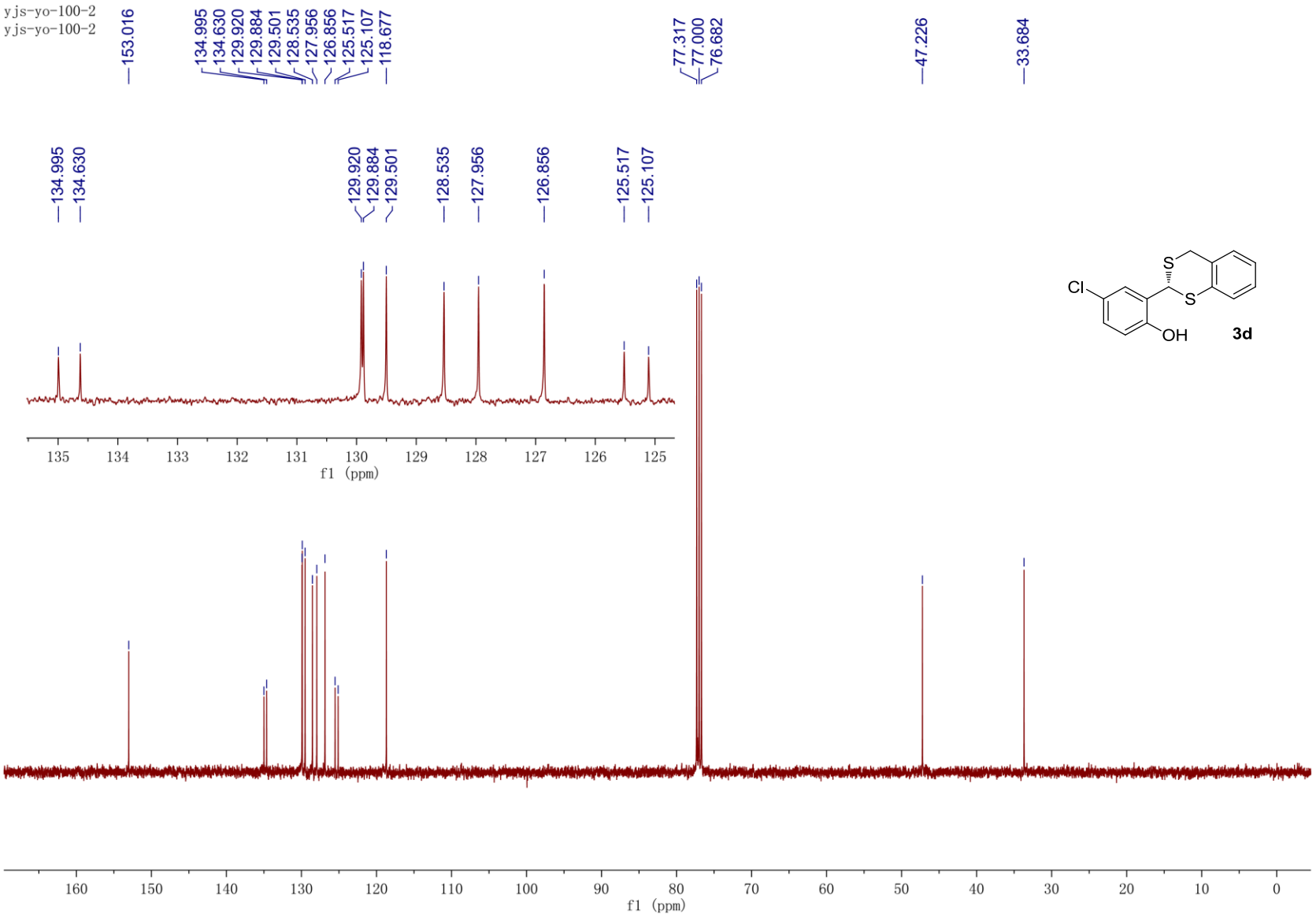

S
F
S
OH

3c

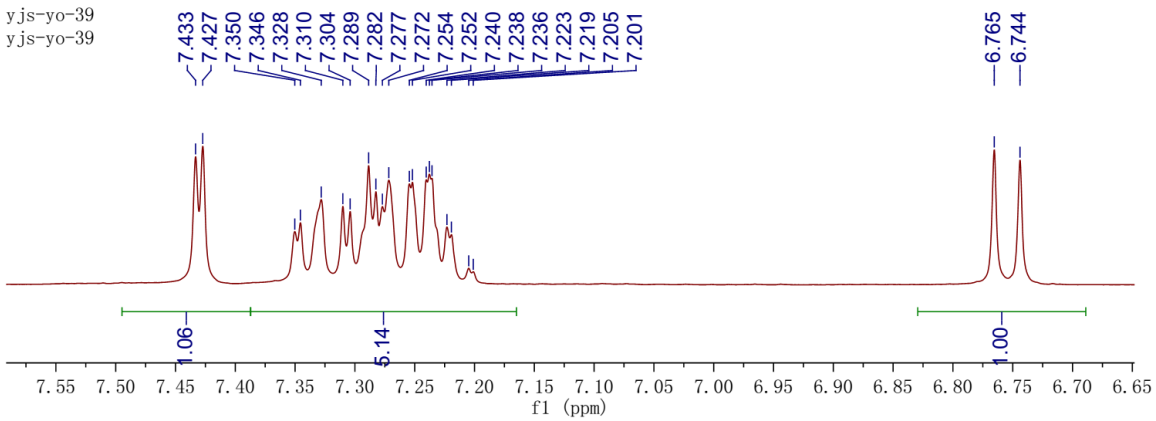

—122.819
-88
-92
-96
-100
-104
-108
-112
-116
-120
-124
-128
-132
-136
-140
-144
-148
-152
f1 (ppm)

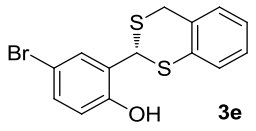

yjs-yo-35
157.881
155.502
150.225
150.202
134.979
134.566
129.875
128.548
127.936
126.810
125.098
125.026
118.298
118.218
116.628
116.399
116.271
116.027
77.318
77.000
76.682
46.996
33.521
yjs-yo-35
134.979
134.566
129.875
128.548
127.936
126.810
125.098
125.026
118.298
118.218
116.628
116.399
116.271
116.027
140 138 136 134 132 130 128 126 124 122 120 118 116 114
f1 (ppm)
F
S
S
OH
3c
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


yjs-yo-100-2
7.328
7.299
7.292
7.270
7.253
7.250
7.239
7.237
7.234
7.174
7.152
7.146
6.815
6.794
6.233
5.641
4.001
3.964
3.948
3.912
0.000
7.351
7.346
7.331
7.328
7.299
7.292
7.275
7.270
7.253
7.250
7.239
7.237
7.234
7.230
7.221
7.217
7.174
7.167
7.152
7.146
6.815
6.794
0.99
4.35
0.95
1.00
7.50
7.40
7.30
7.20
7.10
7.00
6.90
6.80
f1 (ppm)
Cl
S
S
OH
3d
0.99
4.35
0.95
1.00
0.96
1.00
2.06
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)

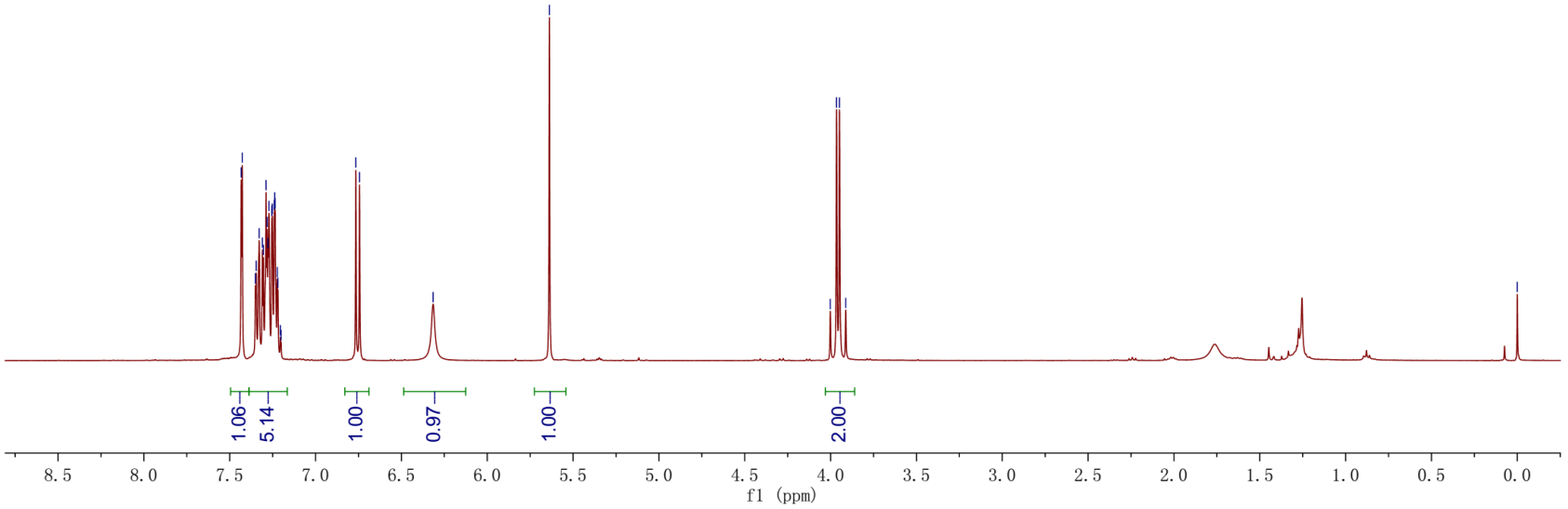

yjs-yo-100-2
yjs-yo-100-2
153.016
134.995
134.630
129.920
129.884
129.501
128.535
127.956
126.856
125.517
125.107
118.677
77.317
77.000
76.682
47.226
33.684
Cl
S
S
OH
3d
f1 (ppm)
f1 (ppm)

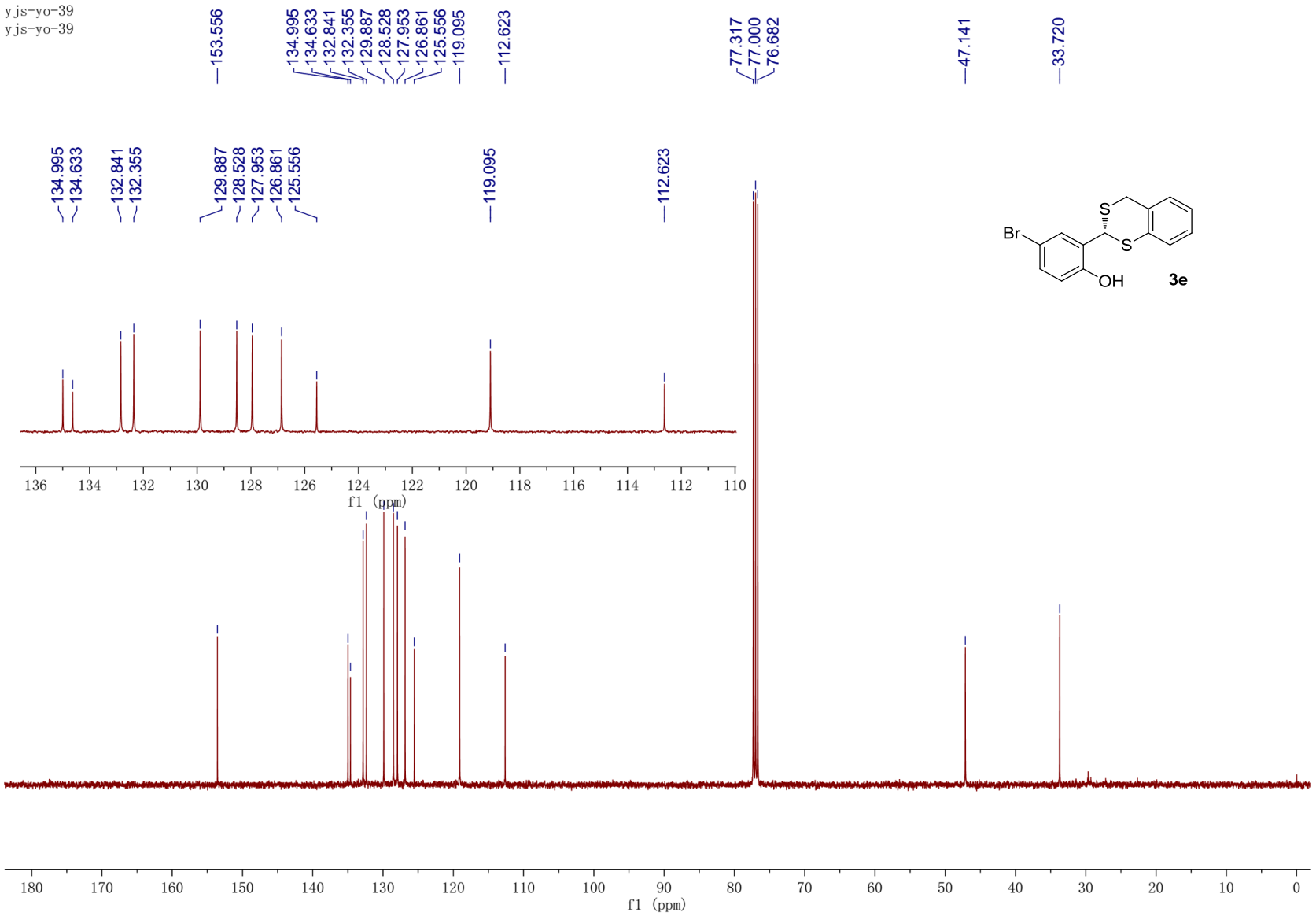

7.433
7.427
7.346
7.328
7.310
7.304
7.289
7.282
7.277
7.272
7.254
7.252
7.240
7.238
6.765
6.744
6.315
5.638
4.002
3.965
3.948
3.912
0.000

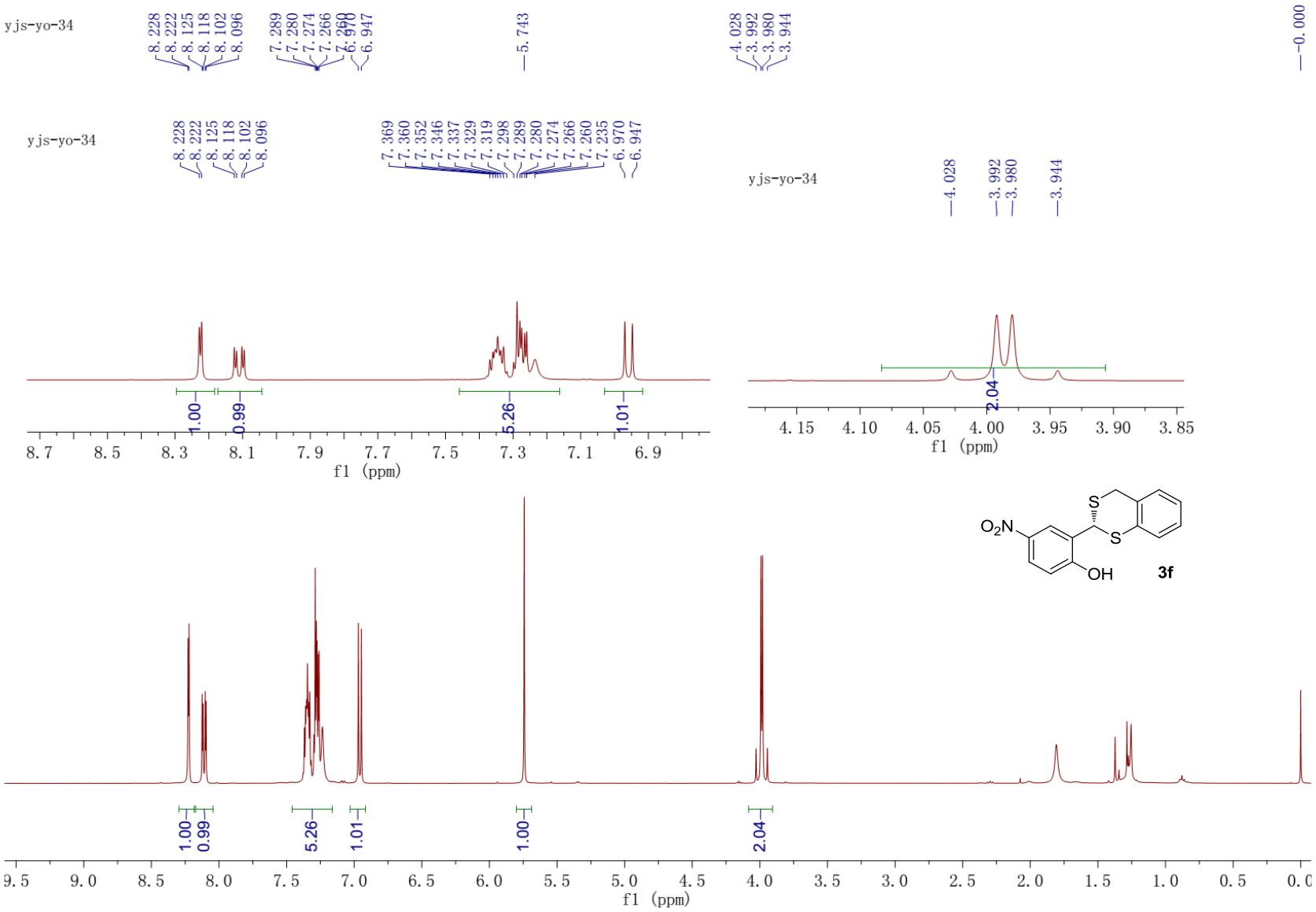

yjs-yo-39
yjs-yo-39
7.433
7.427
7.350
7.346
7.328
7.310
7.304
7.289
7.282
7.277
7.272
7.254
7.252
7.240
7.238
7.236
7.223
7.219
7.205
7.201
6.765
6.744
1.06
5.14
1.00
7.55 7.50 7.45 7.40 7.35 7.30 7.25 7.20 7.15 7.10 7.05 7.00 6.95 6.90 6.85 6.80 6.75 6.70 6.65
f1 (ppm)

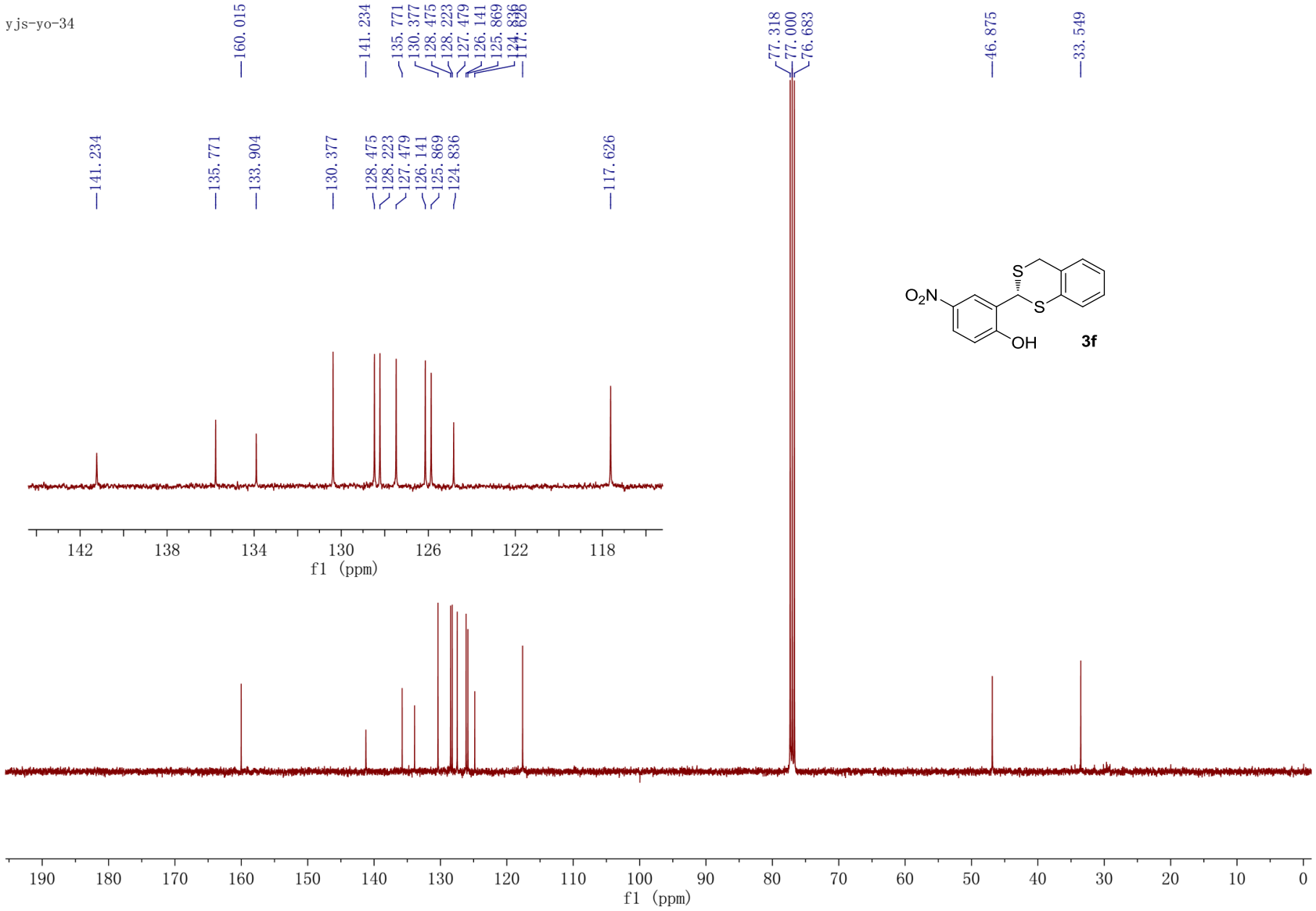

Br
S
S
OH

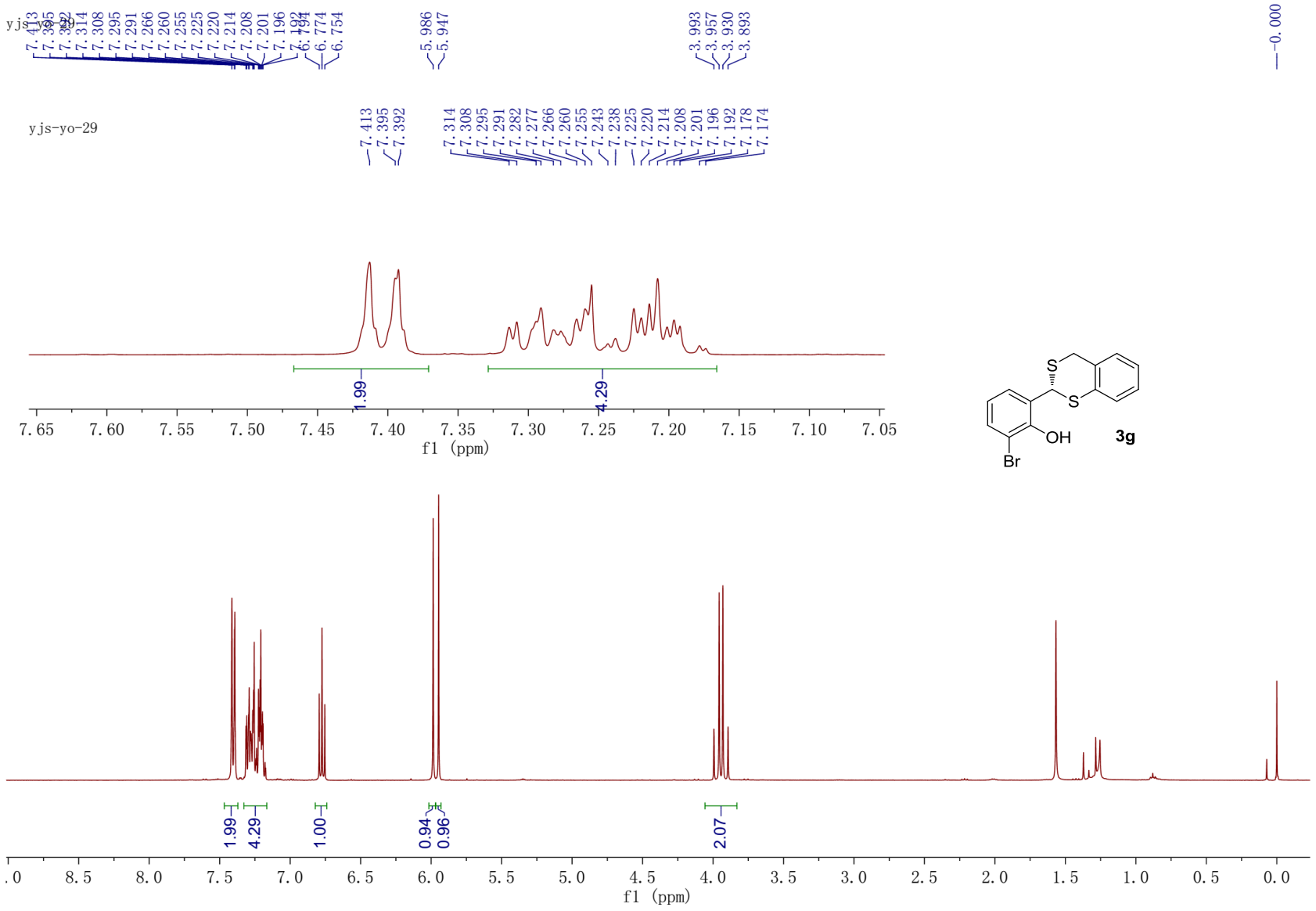
3e

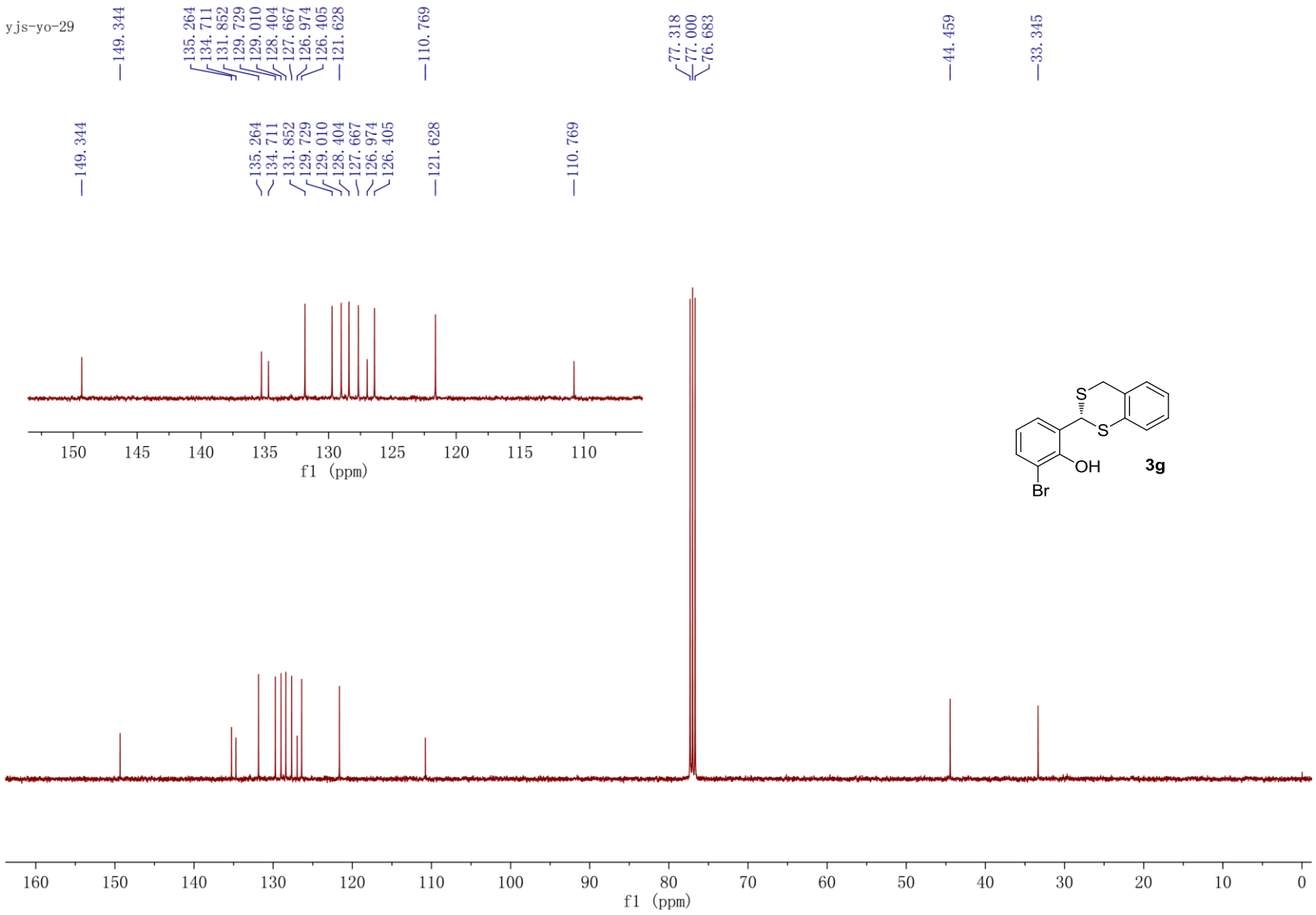

1.06
5.14
1.00
0.97
1.00
2.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

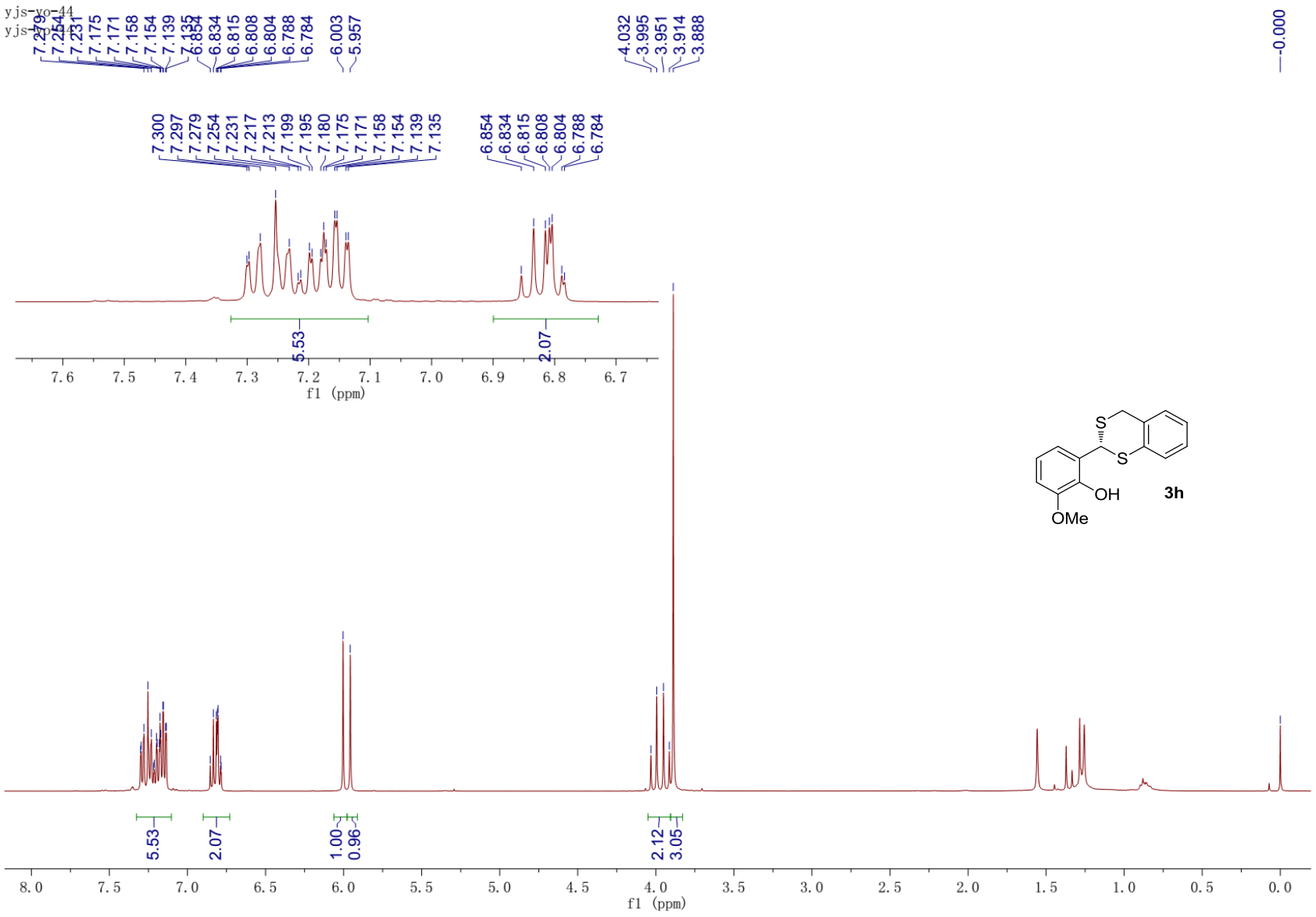

yjs-yo-39
yjs-yo-39
153.556
134.995
134.633
132.841
132.355
129.887
128.528
127.953
126.861
125.556
119.095
112.623
77.317
77.000
76.682
47.141
33.720
Br
S
S
OH
3e
f1 (ppm)
f1 (ppm)

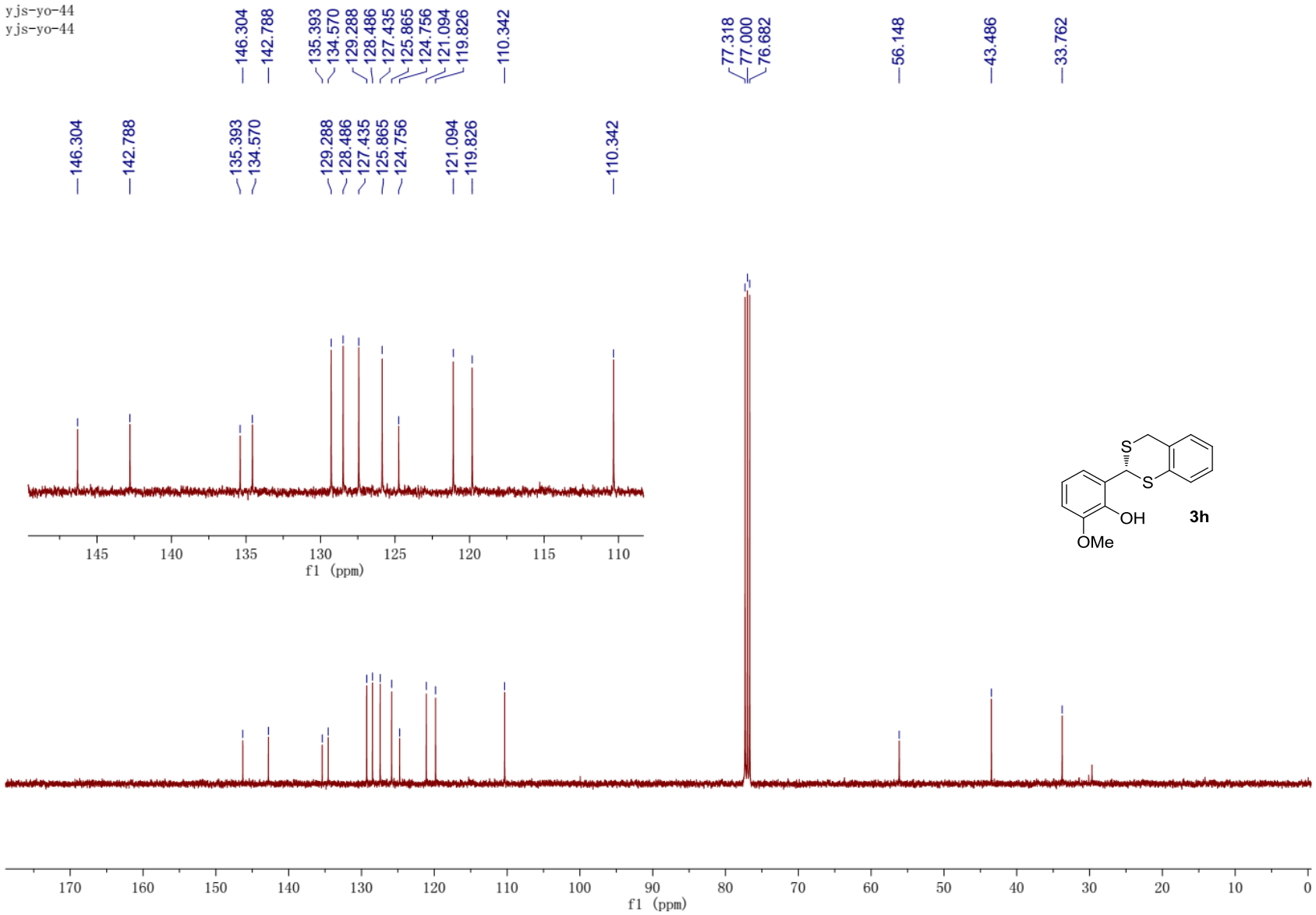

yjs-yo-34
8.228
8.222
8.125
8.118
8.102
8.096
7.289
7.280
7.274
7.266
6.970
6.947
5.743
4.028
3.992
3.980
3.944
0.000
yjs-yo-34
8.228
8.222
8.125
8.118
8.102
8.096
7.369
7.360
7.352
7.346
7.337
7.329
7.319
7.298
7.289
7.280
7.274
7.266
7.260
7.235
6.970
6.947
1.00
0.99
5.26
1.01
8.7
8.5
8.3
8.1
7.9
7.7
7.5
7.3
7.1
6.9
f1 (ppm)
yjs-yo-34
4.028
3.992
3.980
3.944
2.04
4.15
4.10
4.05
4.00
3.95
3.90
3.85
f1 (ppm)
O2N
S
S
OH
3f
1.00
0.99
5.26
1.01
1.00
2.04
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)

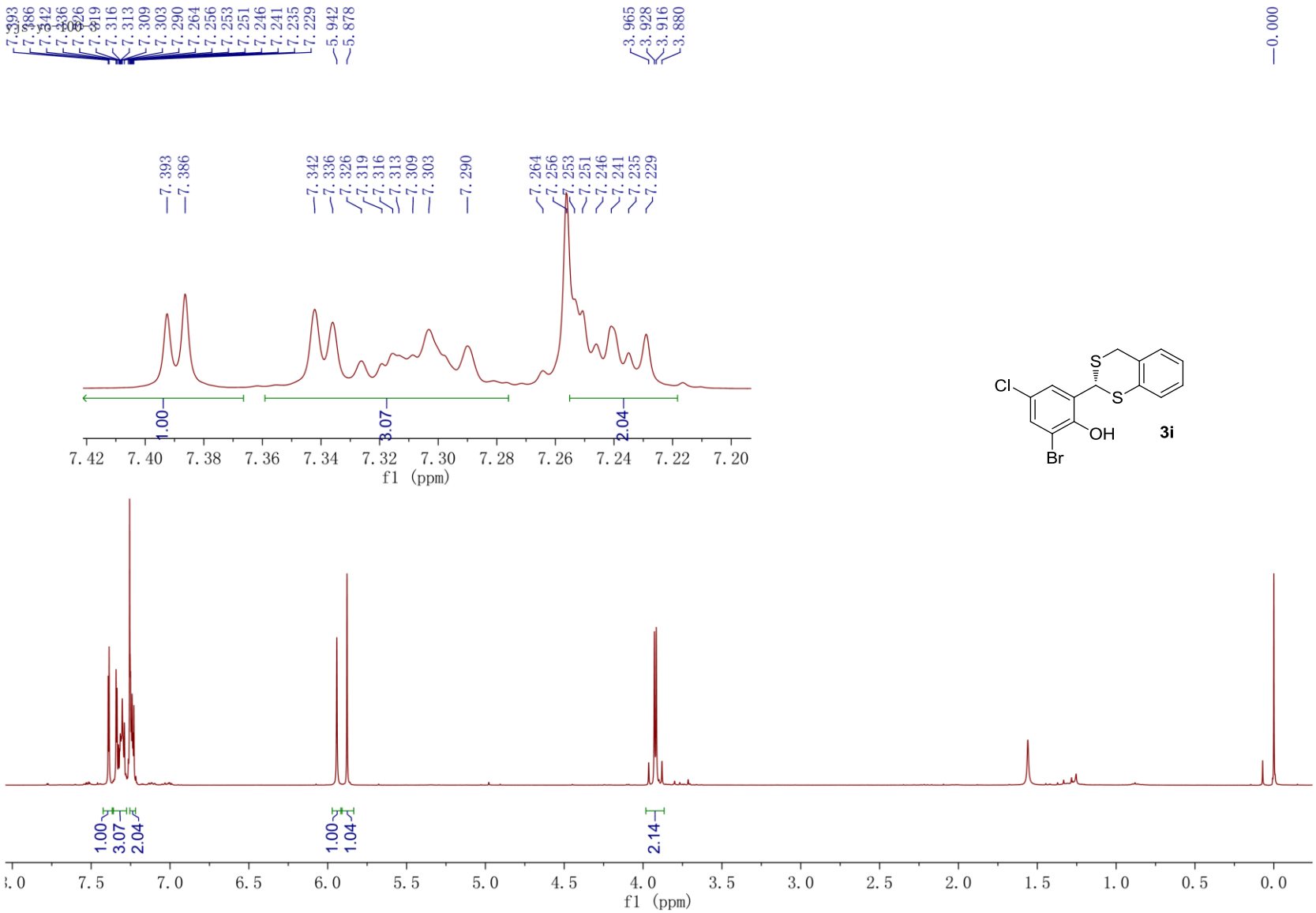

yjs-yo-34
160.015
141.234
135.771
130.377
128.475
128.223
127.479
126.141
125.869
124.836
117.626
77.318
77.000
76.683
46.875
33.549
141.234
135.771
133.904
130.377
128.475
128.223
127.479
126.141
125.869
124.836
117.626
142
138
134
130
126
122
118
f1 (ppm)
O2N
S
S
OH
3f
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

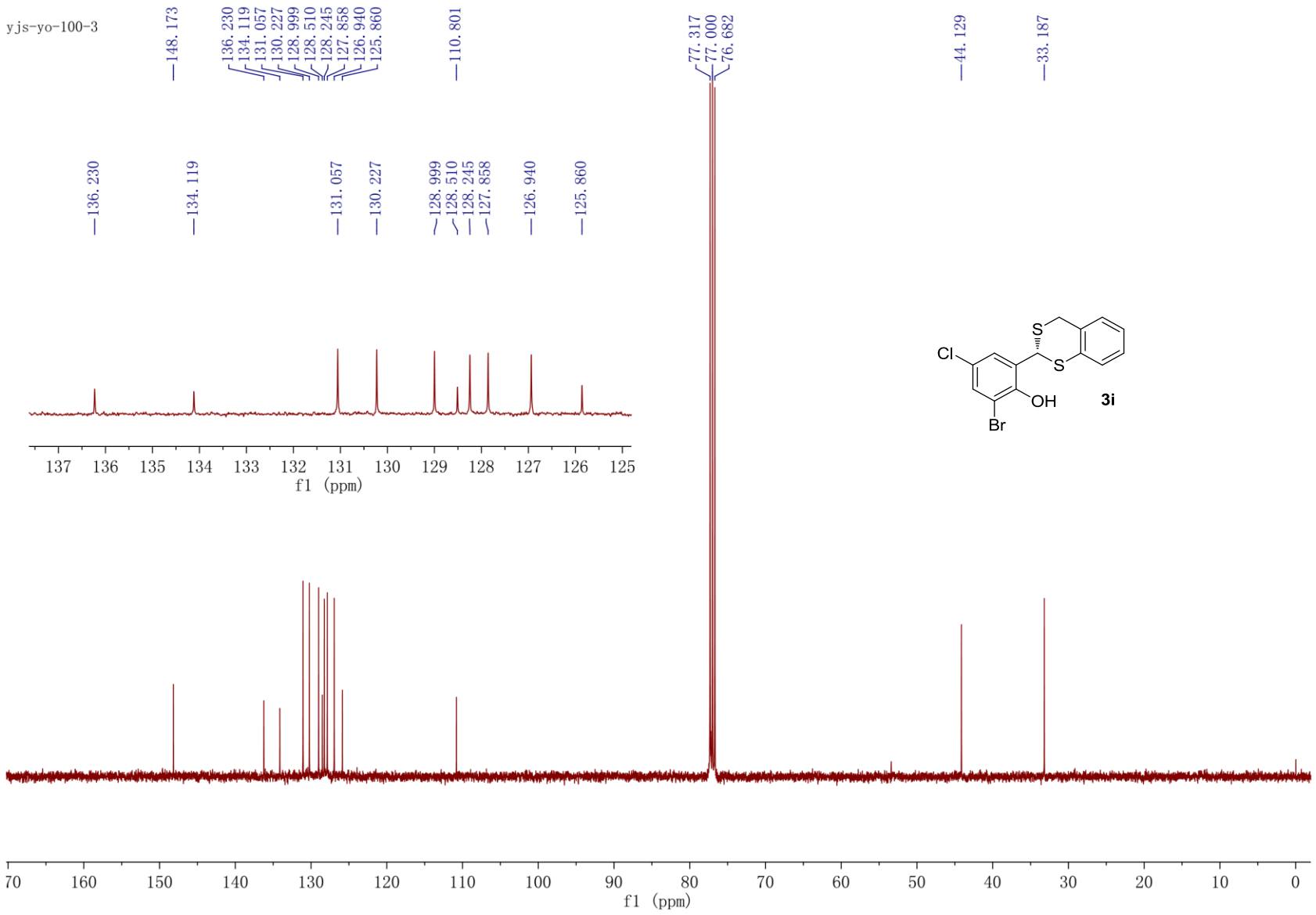

yjs-yo-29
7.413
7.395
7.392
7.314
7.308
7.295
7.291
7.282
7.277
7.266
7.260
7.255
7.243
7.238
7.225
7.220
7.214
7.208
7.201
7.196
7.192
7.178
7.174
6.774
6.754
5.986
5.947
3.993
3.957
3.930
3.893
-0.000
1.99
4.29
7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30 7.25 7.20 7.15 7.10 7.05
f1 (ppm)
S
S
OH
Br
3g
1.99
4.29
1.00
0.94
0.96
2.07
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)

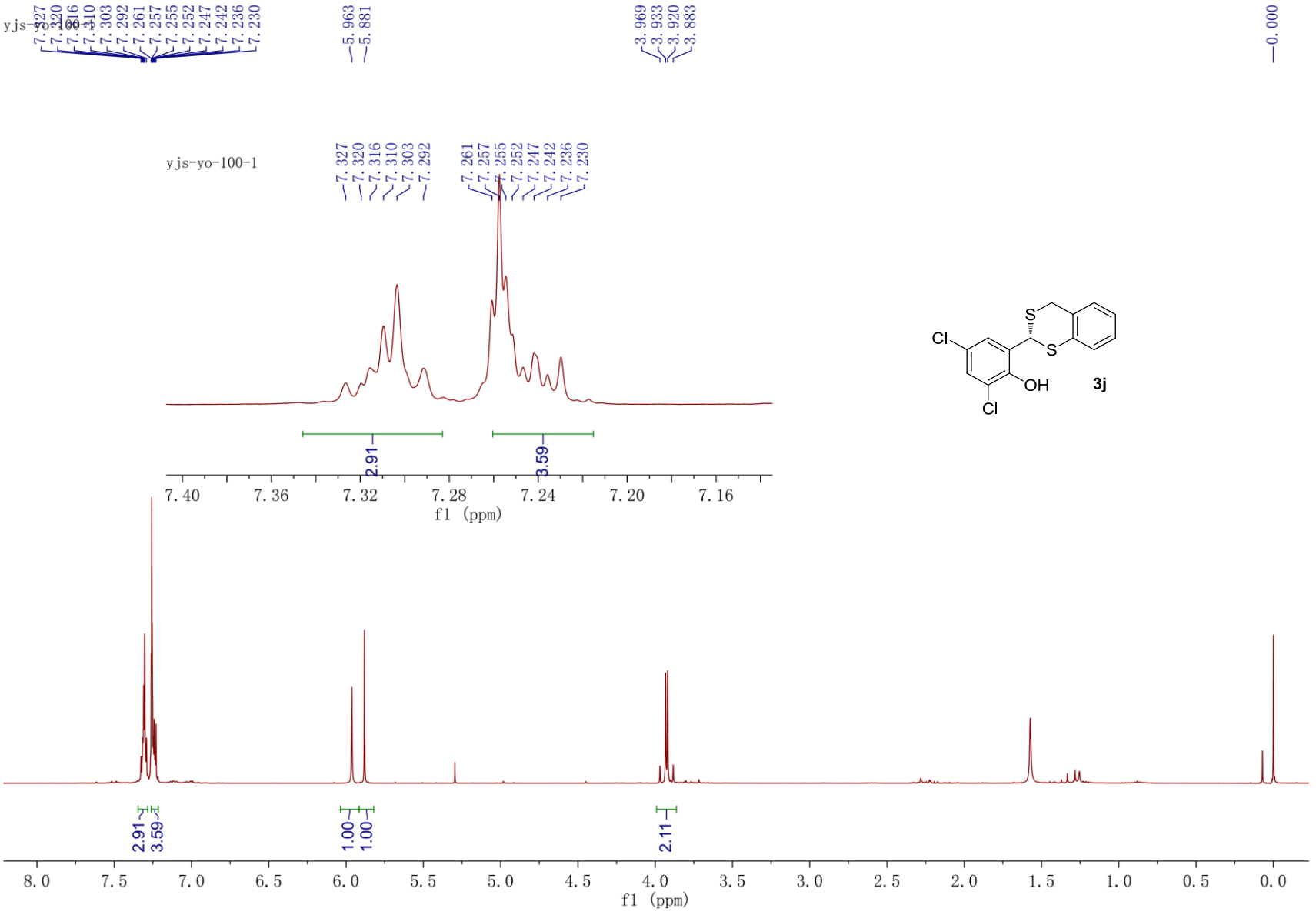

yjs-yo-29
149.344
135.264
134.711
131.852
129.729
129.010
128.404
127.667
126.974
126.405
121.628
110.769
77.318
77.000
76.683
44.459
33.345
f1 (ppm)
OH
Br
3g

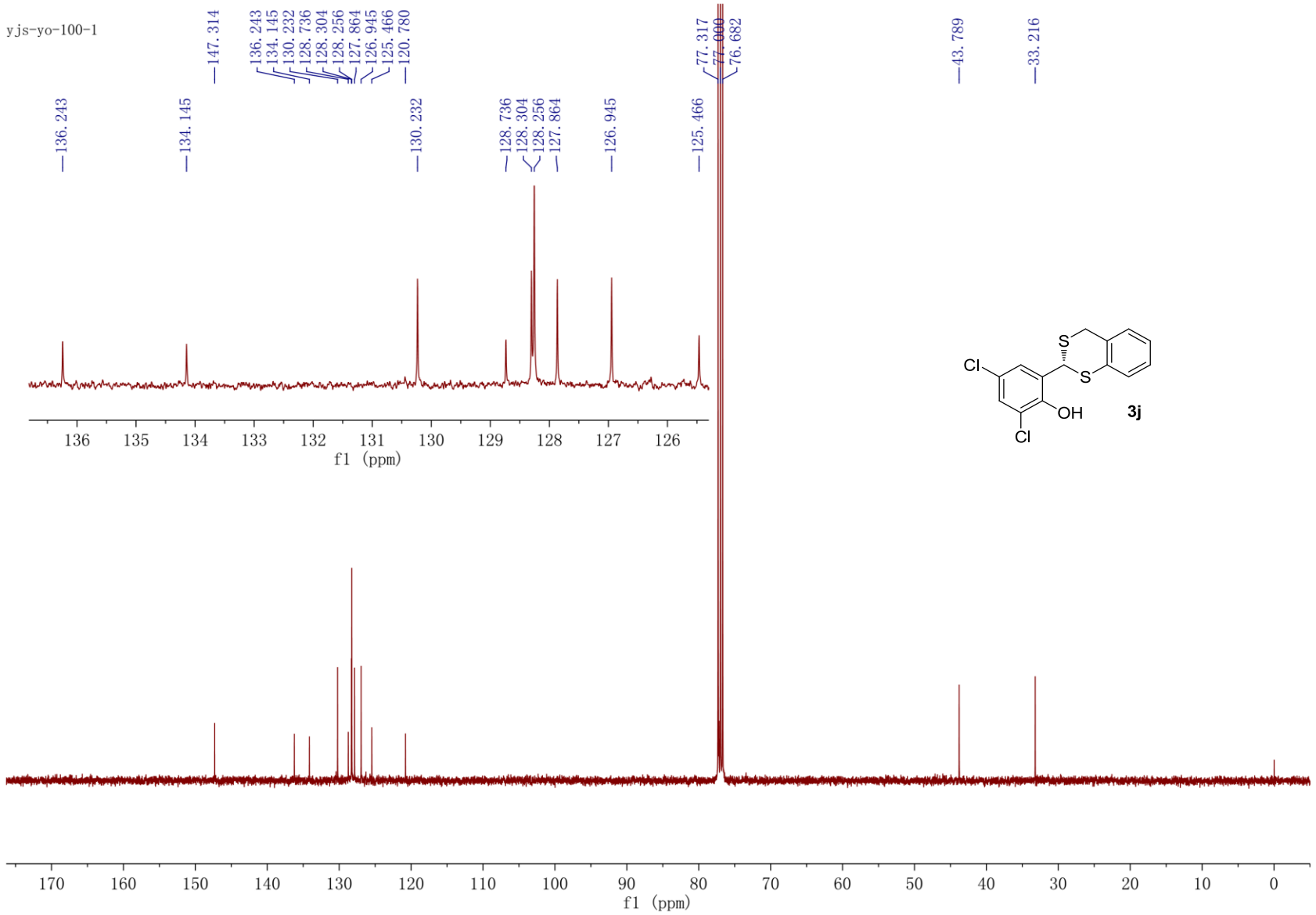

yjs-yo-44
yjs-yo-44
7.279
7.254
7.231
7.175
7.171
7.158
7.154
7.139
7.135
6.854
6.834
6.815
6.808
6.804
6.788
6.784
6.003
5.957
4.032
3.995
3.951
3.914
3.888
-0.000
7.300
7.297
7.279
7.254
7.231
7.217
7.213
7.199
7.195
7.180
7.175
7.171
7.158
7.154
7.139
7.135
6.854
6.834
6.815
6.808
6.804
6.788
6.784
5.53
2.07
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
f1 (ppm)
S
S
OH
OMe
3h
5.53
2.07
1.00
0.96
2.12
3.05
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)

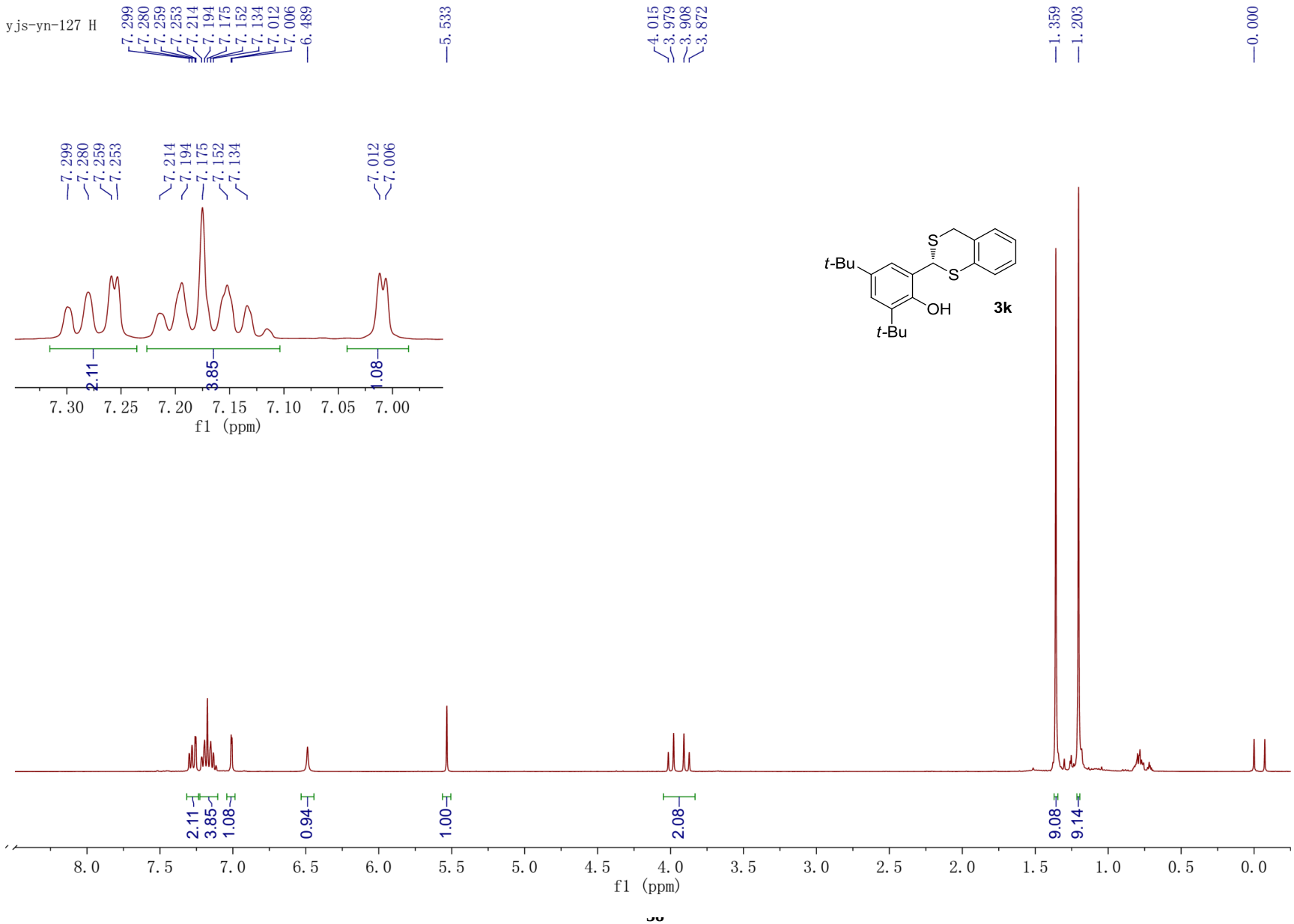

yjs-yo-44
yjs-yo-44
146.304
142.788
135.393
134.570
129.288
128.486
127.435
125.865
124.756
121.094
119.826
110.342
77.318
77.000
76.682
56.148
43.486
33.762
f1 (ppm)
OH
OMe
3h


7.393
7.386
7.342
7.336
7.326
7.319
7.316
7.313
7.309
7.303
7.290
7.264
7.256
7.253
7.251
7.246
7.241
7.235
7.229
5.942
5.878
3.965
3.928
3.916
3.880
0.000
1.00
3.07
2.04
f1 (ppm)
Cl
S
S
OH
Br
3i
1.00
3.07
2.04
1.00
1.04
2.14
f1 (ppm)

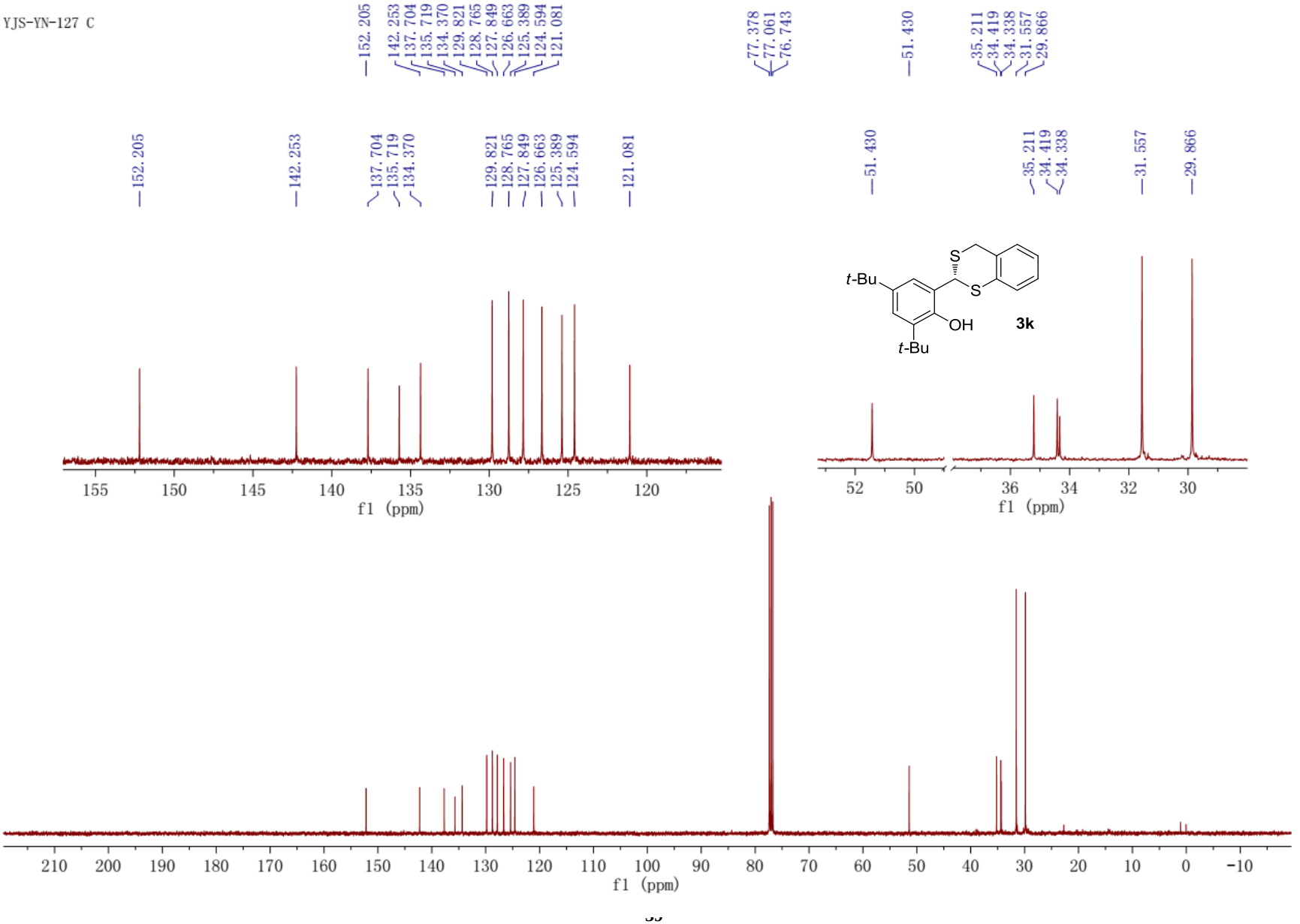

yjs-yo-100-3
148.173
136.230
134.119
131.057
130.227
128.999
128.510
128.245
127.858
126.940
125.860
110.801
77.317
77.000
76.682
44.129
33.187
f1 (ppm)
Cl
S
S
OH
Br
3i

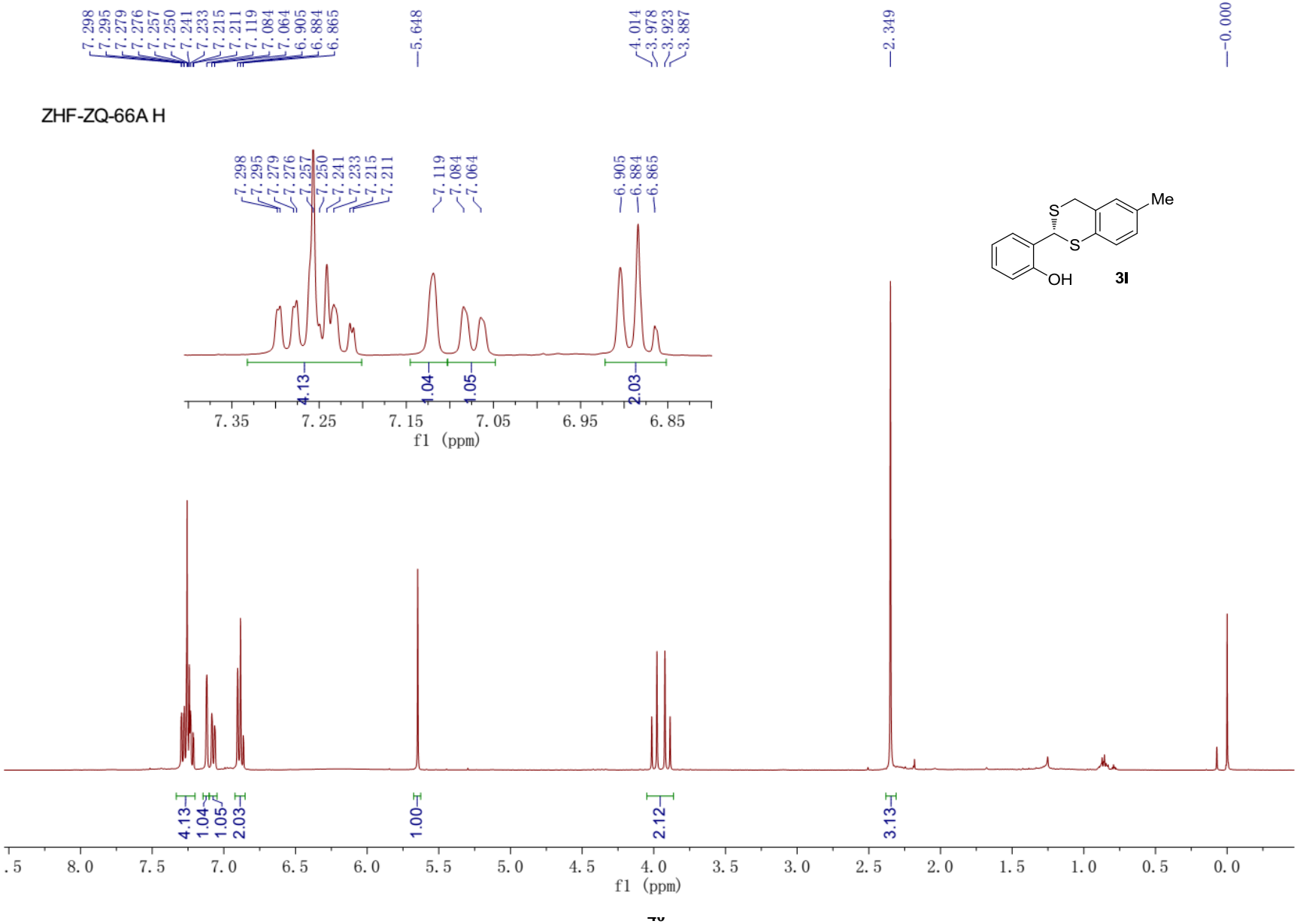

yjs-yo-100-1
7.327
7.320
7.316
7.310
7.303
7.292
7.261
7.257
7.255
7.252
7.247
7.242
7.236
7.230
5.963
5.881
3.969
3.933
3.920
3.883
0.000
2.91
3.59
7.40
7.36
7.32
7.28
7.24
7.20
7.16
f1 (ppm)
Cl
S
S
OH
Cl
3j
1.00
1.00
2.11
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

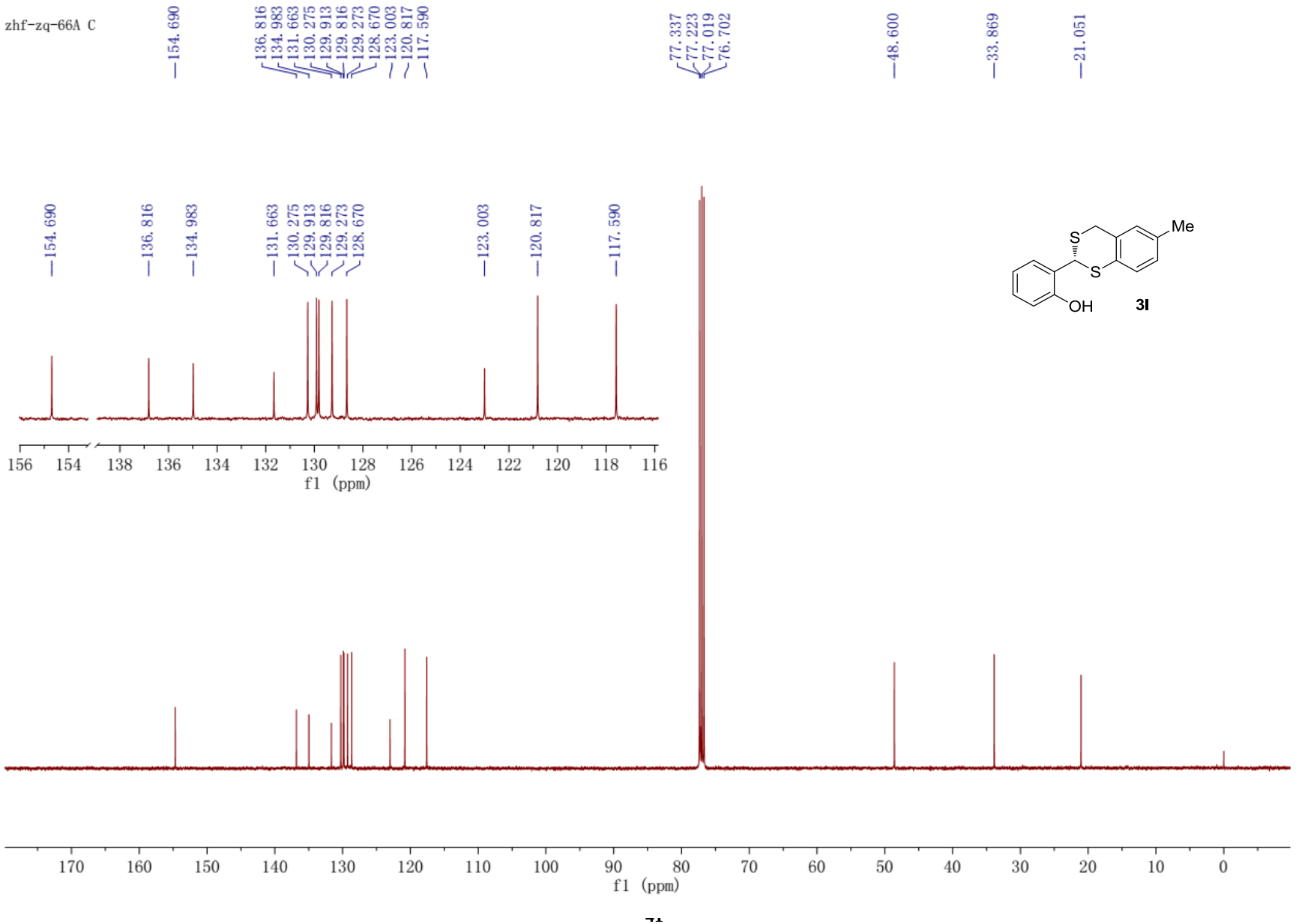

yjs-yo-100-1
147.314
136.243
134.145
130.232
128.736
128.304
128.256
127.864
126.945
125.466
120.780
77.317
77.000
76.682
43.789
33.216
f1 (ppm)
Cl
S
S
OH
Cl
3j

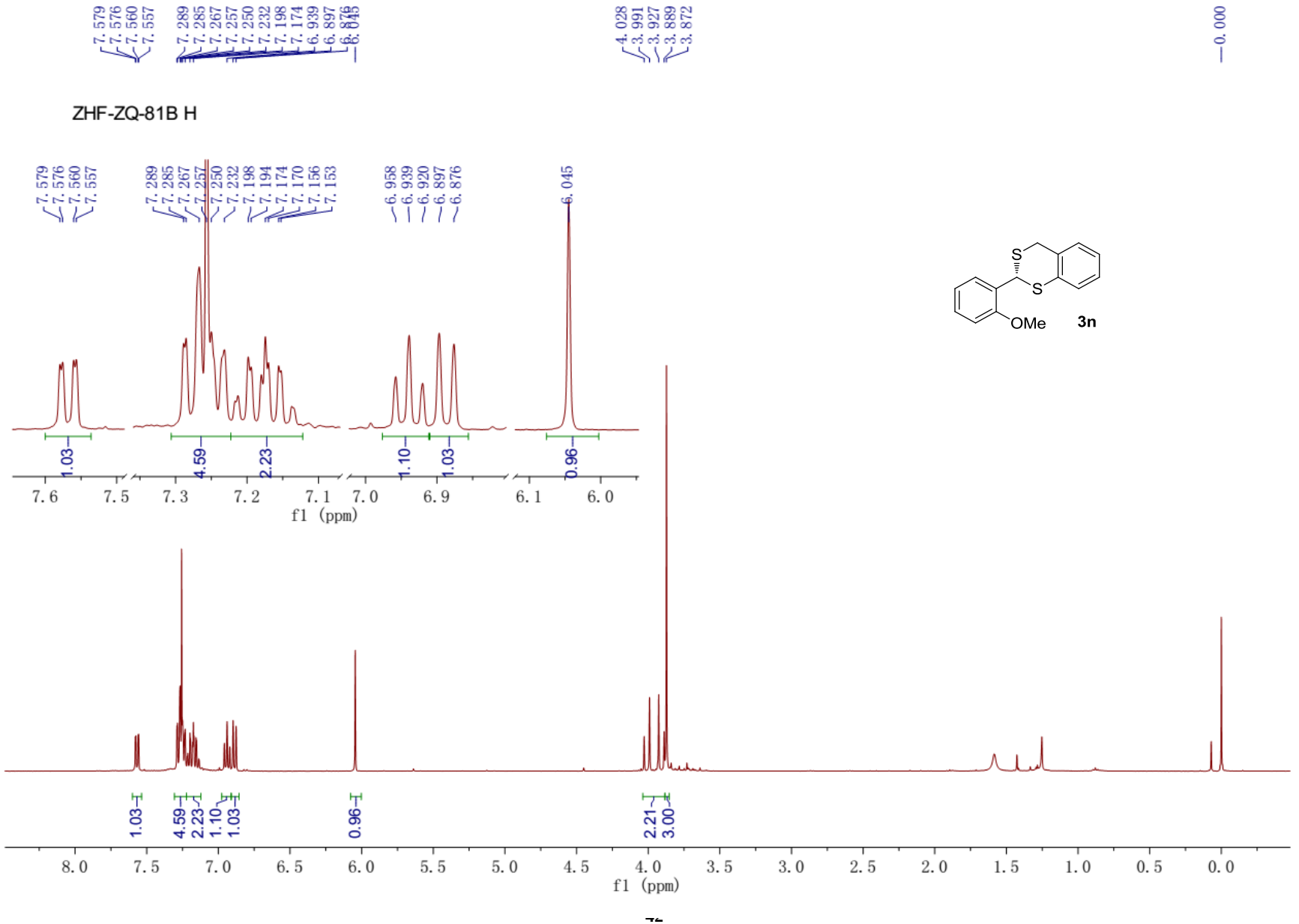

yjs-yn-127 H
7.299
7.280
7.259
7.253
7.214
7.194
7.175
7.152
7.134
7.012
7.006
6.489
5.533
4.015
3.979
3.908
3.872
1.359
1.203
0.000
t-Bu
S
S
OH
t-Bu
3k
2.11
3.85
1.08
0.94
1.00
2.08
9.08
9.14
f1 (ppm)

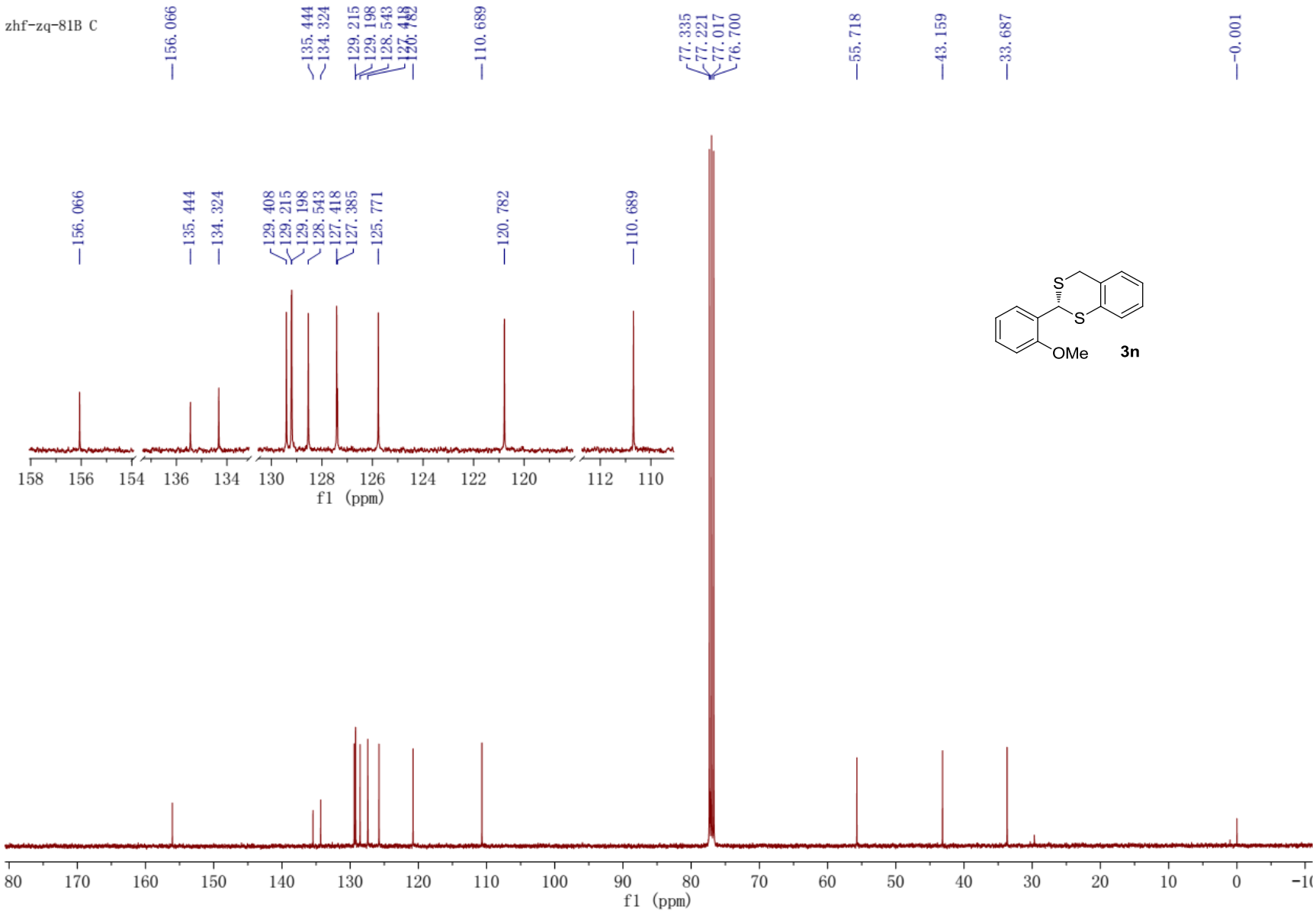
YJS-YN-127 C

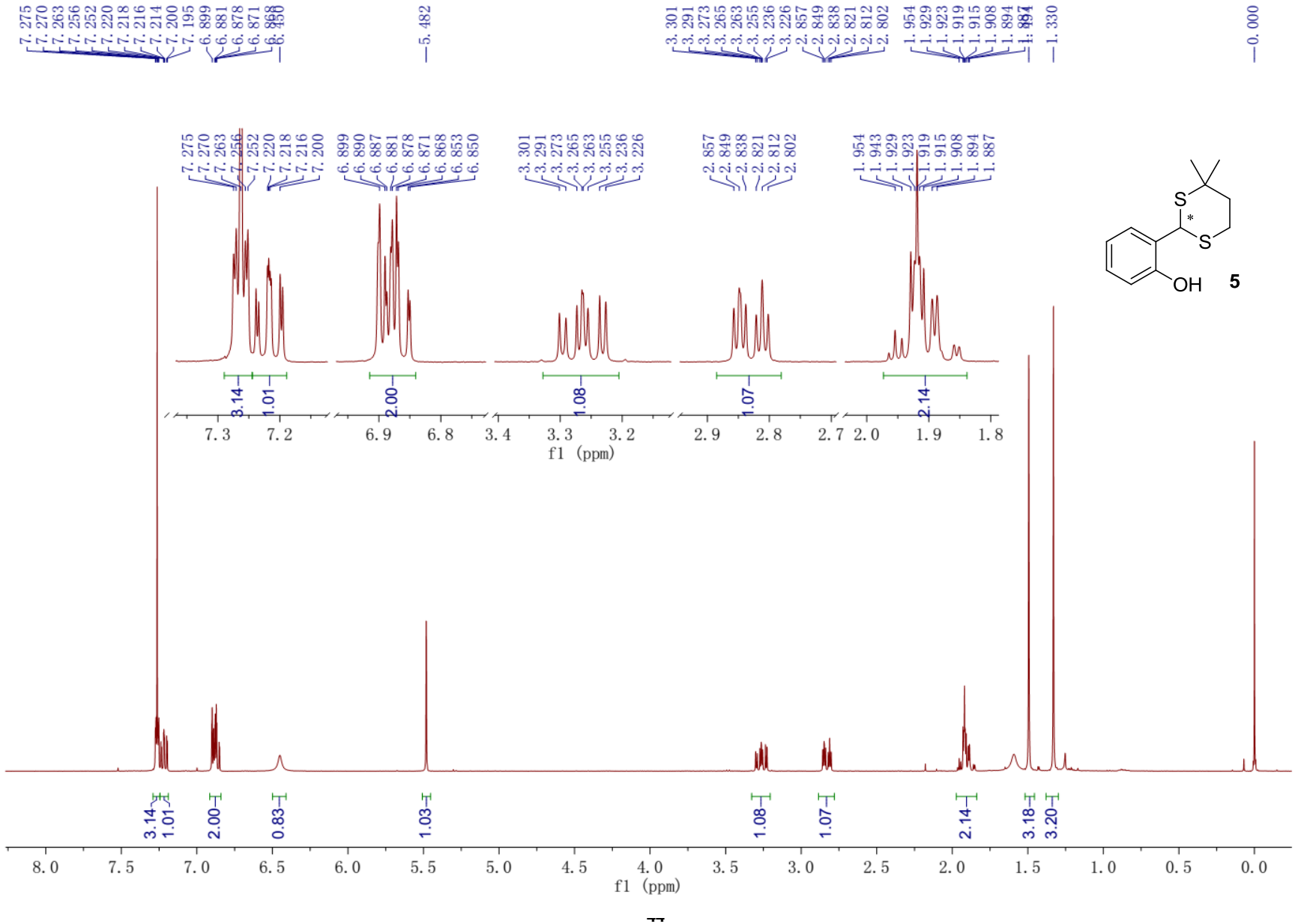

152.205
142.253
137.704
135.719
134.370
129.821
128.765
127.849
126.663
125.389
124.594
121.081
77.378
77.061
76.743
51.430
35.211
34.419
34.338
31.557
29.866
t-Bu
S
S
OH
t-Bu
3k
f1 (ppm)
f1 (ppm)
f1 (ppm)


7.298
7.295
7.279
7.276
7.257
7.250
7.241
7.233
7.215
7.211
7.119
7.084
7.064
6.905
6.884
6.865
5.648
4.014
3.978
3.923
3.887
2.349
0.000
ZHF-ZQ-66A H
4.13
1.04
1.05
2.03
1.00
2.12
3.13
f1 (ppm)
Me
S
S
OH
3l


zhf-zq-66A C
154.690
136.816
134.983
131.663
130.275
129.913
129.816
129.273
128.670
123.003
120.817
117.590
77.337
77.223
77.019
76.702
48.600
33.869
21.051
f1 (ppm)
Me
S
S
OH
3l


7.579
7.576
7.560
7.557
7.289
7.285
7.267
7.257
7.250
7.232
7.198
7.174
6.939
6.897
6.876
6.045
4.028
3.991
3.927
3.889
3.872
0.000
ZHF-ZQ-81B H
7.579
7.576
7.560
7.557
7.289
7.285
7.267
7.257
7.250
7.232
7.198
7.194
7.174
7.170
7.156
7.153
6.958
6.939
6.920
6.897
6.876
6.045
1.03
4.59
2.23
1.10
1.03
0.96
f1 (ppm)
S
S
OMe
3n
1.03
4.59
2.23
1.10
1.03
0.96
2.21
3.00
f1 (ppm)

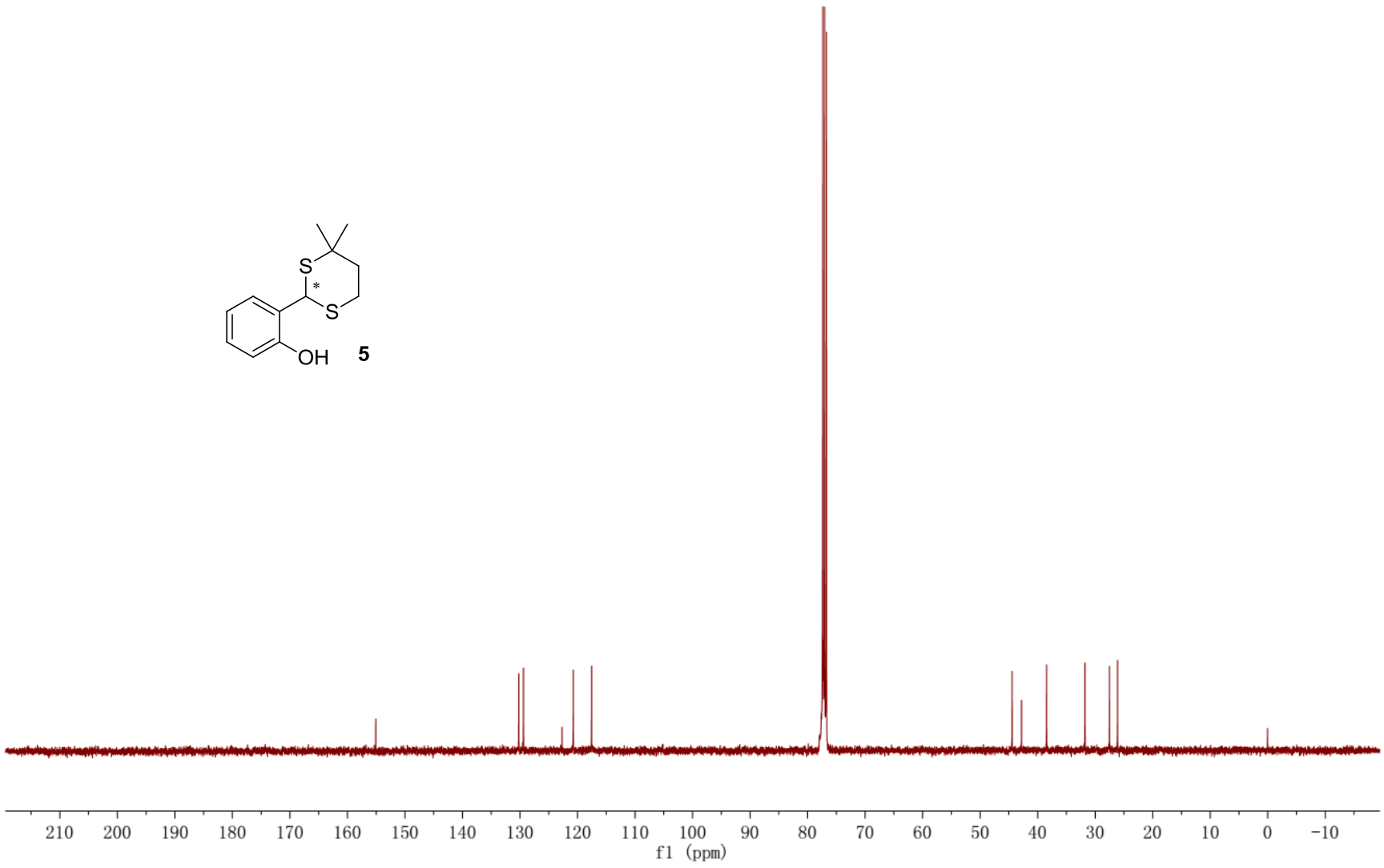

zhf-zq-81B C
156.066
135.444
134.324
129.215
129.198
128.543
127.418
127.385
125.771
120.782
110.689
77.335
77.221
77.017
76.700
55.718
43.159
33.687
-0.001
S
S
OMe
3n
f1 (ppm)


7.275
7.270
7.263
7.256
7.252
7.220
7.218
7.216
7.214
7.200
7.195
6.899
6.881
6.878
6.871
5.482
3.301
3.291
3.273
3.265
3.263
3.255
3.236
3.226
2.857
2.849
2.838
2.821
2.812
2.802
1.954
1.929
1.923
1.915
1.908
1.894
1.330
0.000
3.14
1.01
2.00
0.83
1.03
1.08
1.07
2.14
3.18
3.20
f1 (ppm)
S
S
OH
5

zhf-zq-111 C

155.076
130.212
129.392
122.691
120.736
117.553
77.363
77.249
77.045
76.728
44.442
42.805
38.444
31.773
27.519
26.113

5

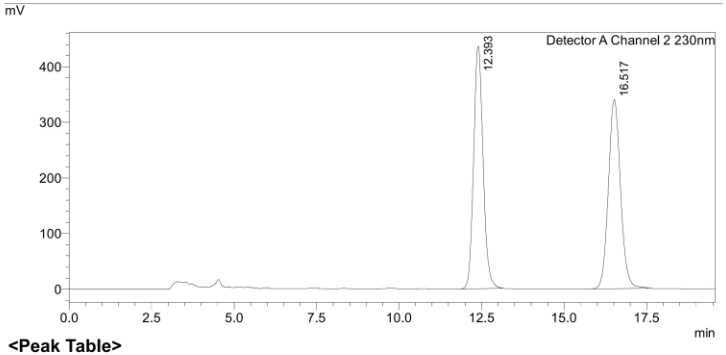


Analysis Report

<Sample Information>

Sample Name	: zhf-zo-86F		
Sample ID	:		
Data Filename	: yjs-yo-40-rac-ADH-85-15-1.0.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/26 16:15:00	Acquired by	: System Administrator
Date Processed	: 2015/6/26 16:34:36	Processed by	: System Administrator

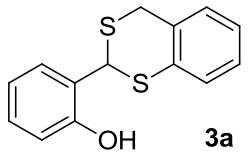
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	12.393	8679495	436030	49.853
2	16.517	8730723	339978	50.147
Total		17410218	776008	



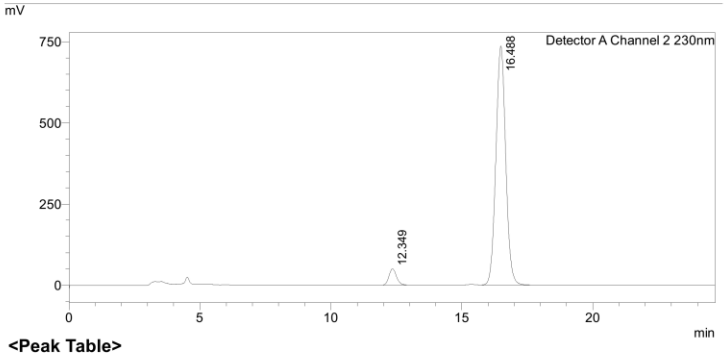
3a

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-40		
Sample ID	:		
Data Filename	: yjs-yo-40-asy-ADH-85-15-1.0.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/26 15:49:34	Acquired by	: System Administrator
Date Processed	: 2015/6/26 16:16:13	Processed by	: System Administrator

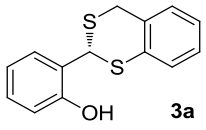
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	12.349	984533	50130	4.905
2	16.488	19088202	735493	95.095
Total		20072735	785623	



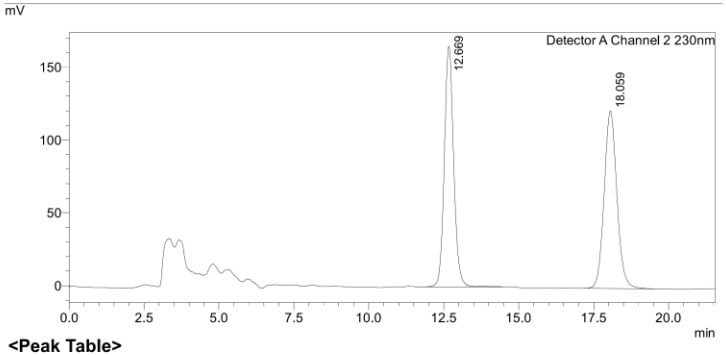
3a

Analysis Report

<Sample Information>

Sample Name	: yjs-yn-121-3rac		
Sample ID	:		
Data Filename	: yjs-yo-28-rac--ADH-85-15-1.0.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/20 11:17:45	Acquired by	: System Administrator
Date Processed	: 2015/6/25 22:16:44	Processed by	: System Administrator

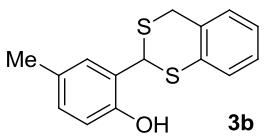
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	12.669	3565971	165115	49.659
2	18.059	3614876	121957	50.341
Total		7180847	287072	



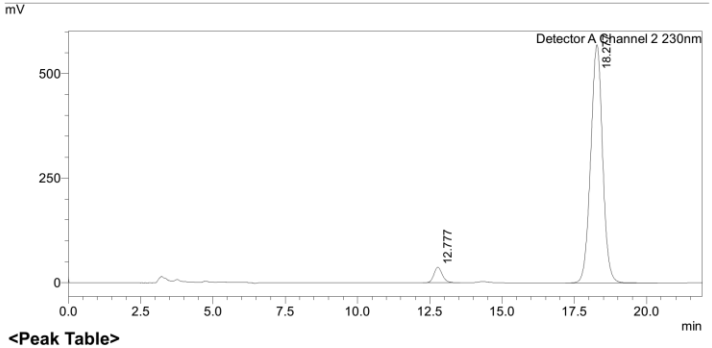
3b

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-28		
Sample ID	:		
Data Filename	: yjs-yo-28-ASY-ADH-85-15-1.0-44.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/20 10:08:27	Acquired by	: System Administrator
Date Processed	: 2015/6/20 10:32:02	Processed by	: System Administrator

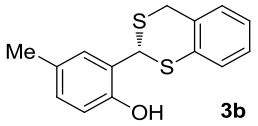
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	12.777	758015	37219	4.426
2	18.277	16368599	570315	95.574
Total		17126613	607534	



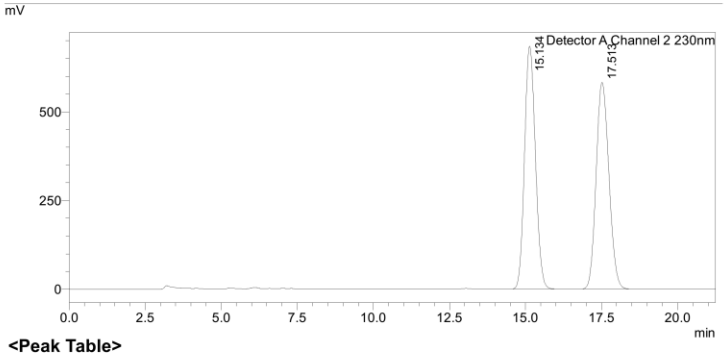
3b

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-38-2		
Sample ID	:		
Data Filename	: yjs-yo-38-2-rac-ASH-90-10-1.0.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/23 11:02:35	Acquired by	: System Administrator
Date Processed	: 2015/6/23 11:24:34	Processed by	: System Administrator

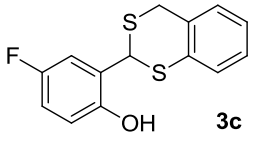
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	15.134	16982710	684435	49.928
2	17.513	17031775	582556	50.072
Total		34014485	1266991	



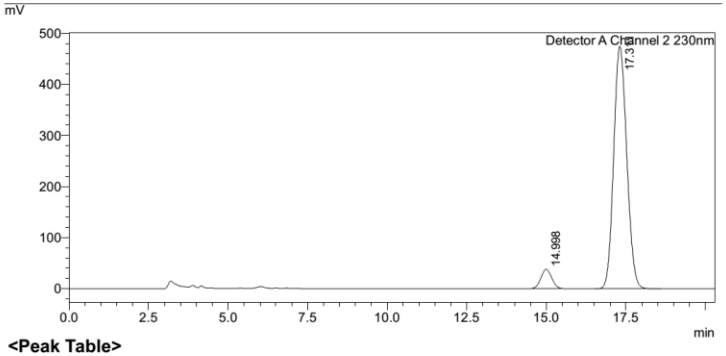
3c

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-35		
Sample ID	:		
Data Filename	: yjs-yo-35(5-F)-asy-ASH-90-10-1.0.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/23 14:24:44	Acquired by	: System Administrator
Date Processed	: 2015/6/23 14:45:41	Processed by	: System Administrator

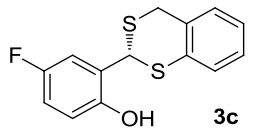
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

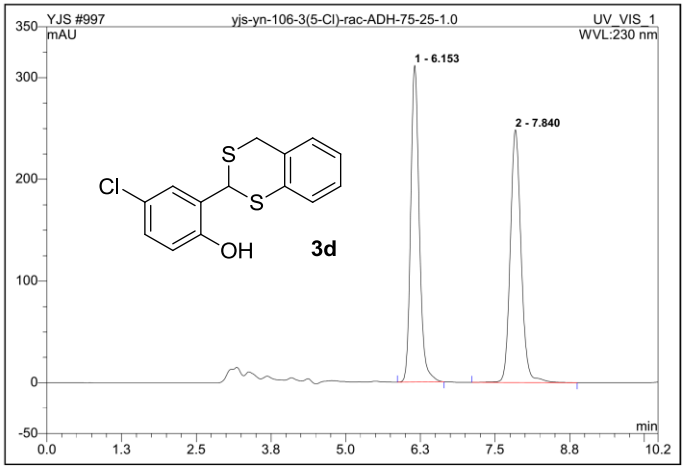
Peak#	Ret. Time	Area	Height	Conc.
1	14.998	877496	37514	6.070
2	17.311	13579618	474523	93.930
Total		14457114	512036	



3c

997 yjs-yn-106-3(5-Cl)-rac-ADH-75-25-1.0

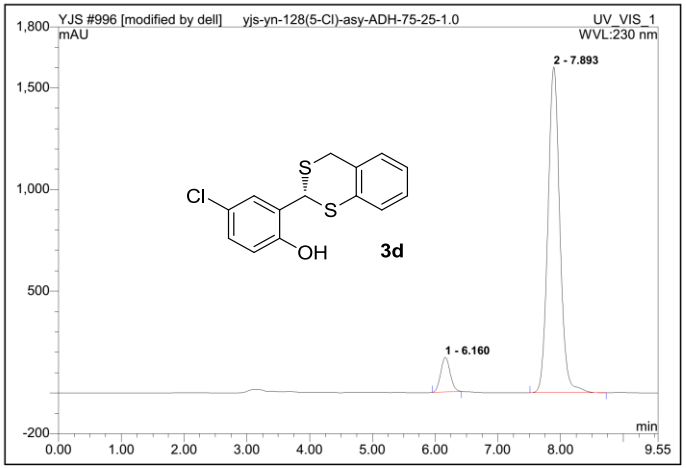
Sample Name:	**yjs-yn-106-3(5-Cl)-rac-ADH-75-25-1.0**	*Injection Volume:*	**20.0**
Vial Number:	**450**	*Channel:*	**UV_VIS_1**
Sample Type:	**standard**	*Wavelength:*	**230**
Control Program:	**YJS**	*Bandwidth:*	**n.a.**
Quantif. Method:	**YJS**	*Dilution Factor:*	**1.0000**
Recording Time:	**2015-5-29 15:33**	*Sample Weight:*	**1.0000**
Run Time (min):	**10.23**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	6.15	n.a.	311.445	51.715	49.79	n.a.	BMB
2	7.84	n.a.	248.625	52.154	50.21	n.a.	BMB
Total:			560.070	103.869	100.00	0.000	

996 yjs-yn-128(5-Cl)-asy-ADH-75-25-1.0

Sample Name:	**yjs-yn-128(5-Cl)-asy-ADH-75-25-1.0**	*Injection Volume:*	**20.0**
Vial Number:	**448**	*Channel:*	**UV_VIS_1**
Sample Type:	**standard**	*Wavelength:*	**230**
Control Program:	**YJS**	*Bandwidth:*	**n.a.**
Quantif. Method:	**YJS**	*Dilution Factor:*	**1.0000**
Recording Time:	**2015-5-29 15:11**	*Sample Weight:*	**1.0000**
Run Time (min):	**9.55**	*Sample Amount:*	**1.0000**



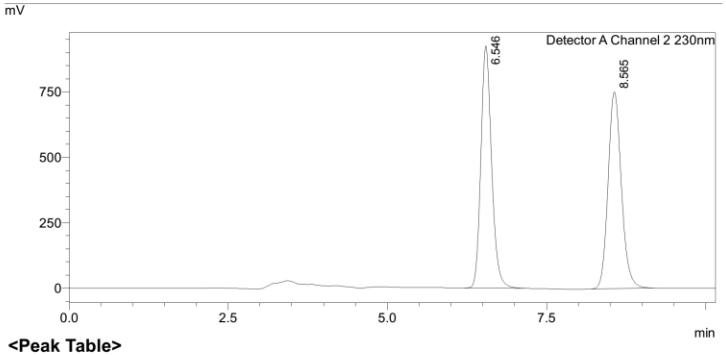
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	6.16	n.a.	170.362	29.679	7.76	n.a.	BMB*
2	7.89	n.a.	1602.314	352.778	92.24	n.a.	BMB*
Total:			1772.676	382.457	100.00	0.000	

Analysis Report

<Sample Information>

Sample Name	: yjs-yn-106-2		
Sample ID	:		
Data Filename	: yjs-yo-39-rac-ADH-75-25-1.0-48.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/25 22:03:39	Acquired by	: System Administrator
Date Processed	: 2015/6/25 22:13:49	Processed by	: System Administrator

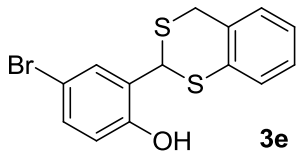
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	6.546	10902621	924675	49.979
2	8.565	10911897	752356	50.021
Total		21814518	1677031	



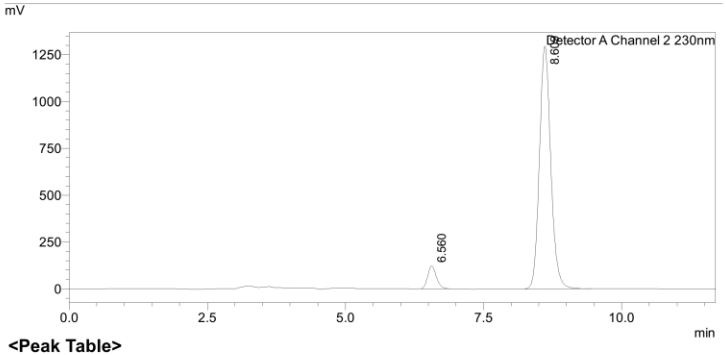
3e

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-39		
Sample ID	:		
Data Filename	: yjs-yo-39-asy-ADH-75-25-1.0.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/25 20:56:28	Acquired by	: System Administrator
Date Processed	: 2015/6/25 21:09:18	Processed by	: System Administrator

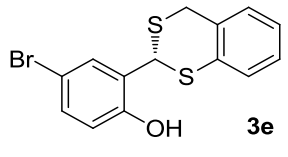
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	6.560	1335770	122041	6.742
2	8.609	18477268	1296300	93.258
Total		19813038	1418341	



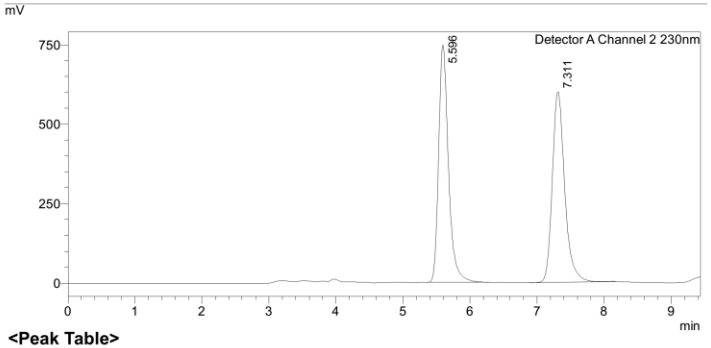
3e

Analysis Report

<Sample Information>

Sample Name	: yjs-yn-101-1		
Sample ID	:		
Data Filename	: yjs-yo-34-rac-ADH-75-25-1.0.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/23 20:17:16	Acquired by	: System Administrator
Date Processed	: 2015/6/23 20:27:53	Processed by	: System Administrator

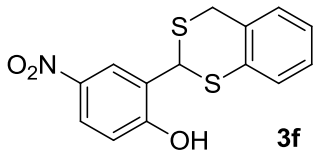
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	5.596	7623374	745762	49.784
2	7.311	7689561	599839	50.216
Total		15312934	1345601	



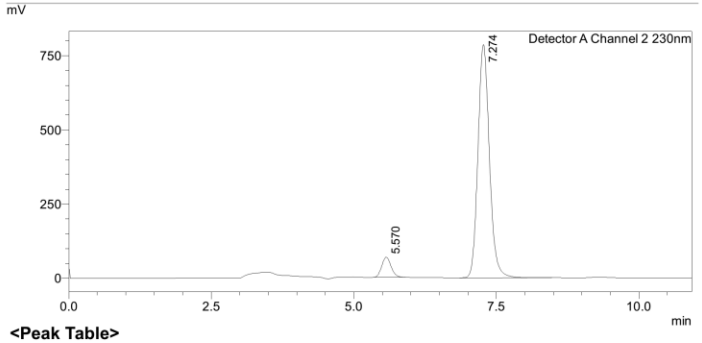
3f

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-34 asy		
Sample ID	:		
Data Filename	: yjs-yo-34-asy-ADH-75-25-1.0.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/23 20:05:12	Acquired by	: System Administrator
Date Processed	: 2015/6/23 20:23:47	Processed by	: System Administrator

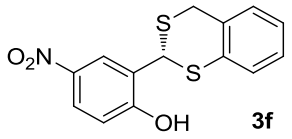
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	5.570	779239	67834	6.626
2	7.274	10981426	785910	93.374
Total		11760665	853743	



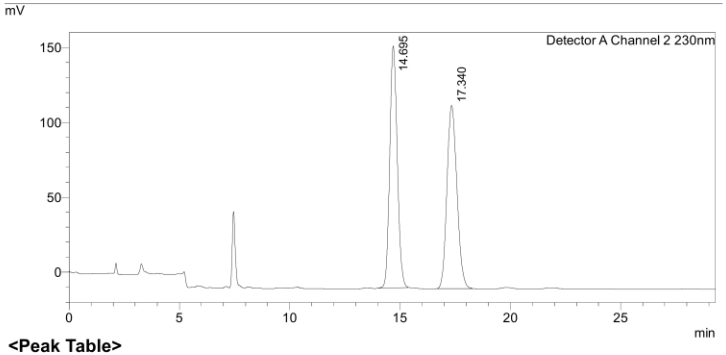
3f

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-29rac		
Sample ID	:		
Data Filename	: yjs-yo-29-rac-ASH-90-10-1.0-40.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/19 22:07:57	Acquired by	: System Administrator
Date Processed	: 2015/6/19 22:37:16	Processed by	: System Administrator

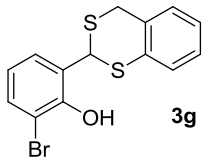
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	14.695	3837519	161450	49.955
2	17.340	3844457	122564	50.045
Total		7681977	284014	



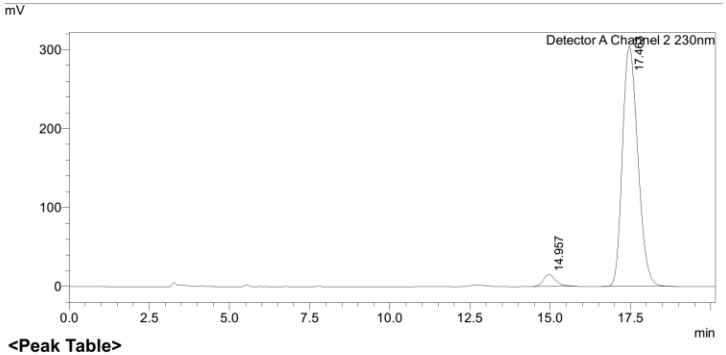
3g

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-29		
Sample ID	:		
Data Filename	: yjs-yo-29-ASY-ASH-90-10-1.0-42.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/6/20 8:57:00	Acquired by	: System Administrator
Date Processed	: 2015/6/20 9:32:17	Processed by	: System Administrator

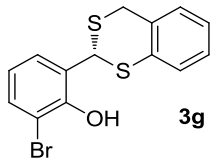
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	14.957	402307	15044	3.803
2	17.463	10175028	304394	96.197
Total		10577335	319439	



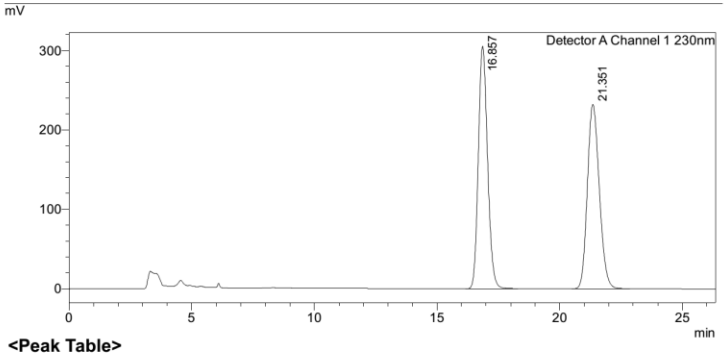
3g

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-38-1 rac		
Sample ID	:		
Data Filename	: yjs-yo-44-rac-ASH-85-15-1.0-41.lcd		
Method Filename	: 2.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/7/21 11:27:52	Acquired by	: System Administrator
Date Processed	: 2015/8/6 21:46:25	Processed by	: System Administrator

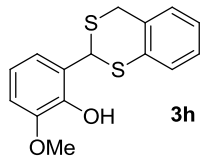
<Chromatogram>



<Peak Table>

Detector A Channel 1 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	16.857	7989244	305505	50.397
2	21.351	7863244	232283	49.603
Total		15852488	537788	



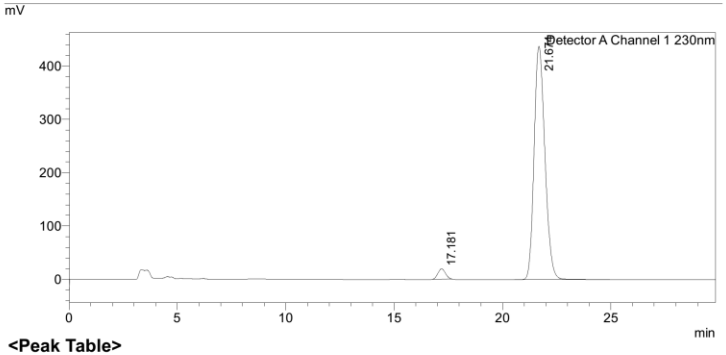
3h

Analysis Report

<Sample Information>

Sample Name	: yjs-yo-44 asy		
Sample ID	:		
Data Filename	: yjs-yo-44-asy-ASH-85-15-1.0-41.lcd		
Method Filename	: 2.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 2015/7/21 10:57:19	Acquired by	: System Administrator
Date Processed	: 2015/7/21 11:29:33	Processed by	: System Administrator

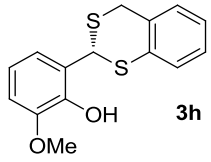
<Chromatogram>



<Peak Table>

Detector A Channel 1 230nm

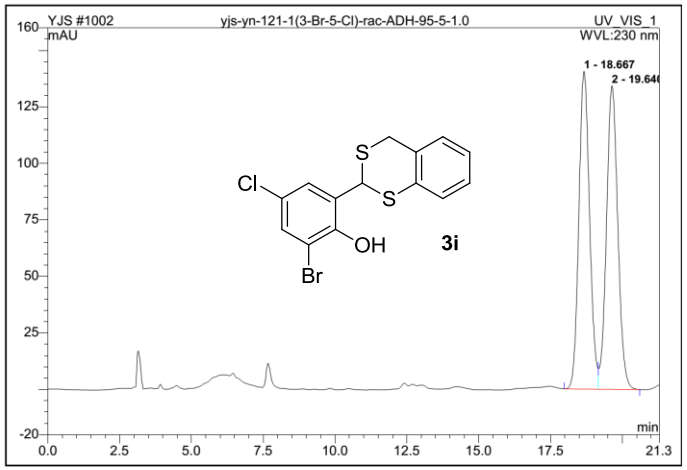
Peak#	Ret. Time	Area	Height	Conc.
1	17.181	474671	19547	3.013
2	21.674	15278478	437897	96.987
Total		15753149	457444	



3h

1002 yjs-yn-121-1(3-Br-5-Cl)-rac-ADH-95-5-1.0

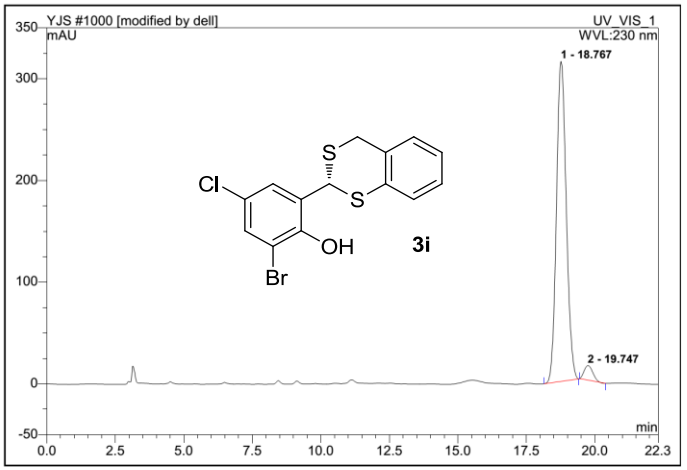
Sample Name:	**yjs-yn-121-1(3-Br-5-Cl)-rac-ADH-95-5-1.0**	*Injection Volume:*	**20.0**
Vial Number:	**455**	*Channel:*	**UV_VIS_1**
Sample Type:	**standard**	*Wavelength:*	**230**
Control Program:	**YJS**	*Bandwidth:*	**n.a.**
Quantif. Method:	**YJS**	*Dilution Factor:*	**1.0000**
Recording Time:	**2015-5-30 16:25**	*Sample Weight:*	**1.0000**
Run Time (min):	**21.28**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	18.67	n.a.	140.611	60.986	49.77	n.a.	BM
2	19.64	n.a.	134.326	61.559	50.23	n.a.	MB
Total:			274.937	122.545	100.00	0.000	

1000 yjs-yn-130(3-Br-5-Cl)-asy-ADH-95-5-1.0

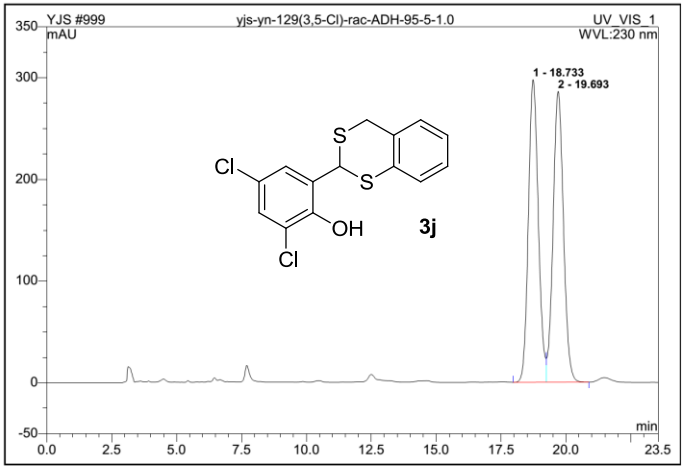
Sample Name:	**yjs-yn-130(3-Br-5-Cl)-asy-ADH-95-5-1.0**	*Injection Volume:*	**20.0**
Vial Number:	**453**	*Channel:*	**UV_VIS_1**
Sample Type:	**standard**	*Wavelength:*	**230**
Control Program:	**YJS**	*Bandwidth:*	**n.a.**
Quantif. Method:	**YJS**	*Dilution Factor:*	**1.0000**
Recording Time:	**2015-5-30 15:19**	*Sample Weight:*	**1.0000**
Run Time (min):	**22.31**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	18.77	n.a.	314.794	130.395	96.18	n.a.	BMB
2	19.75	n.a.	14.280	5.181	3.82	n.a.	BMB*
Total:			329.074	135.577	100.00	0.000	

999 yjs-yn-129(3,5-Cl)-rac-ADH-95-5-1.0

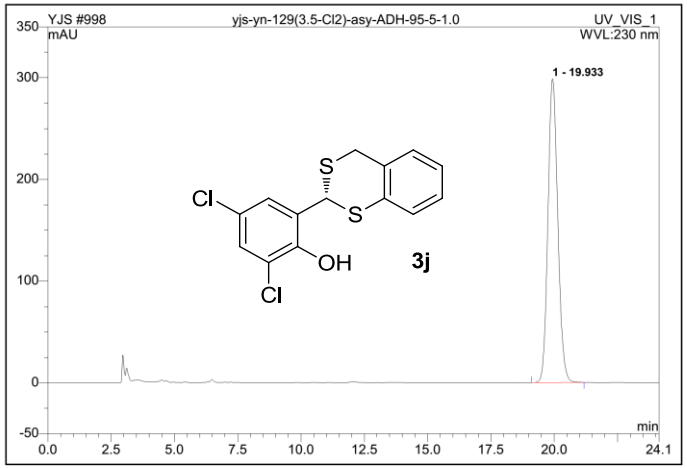
Sample Name:	**yjs-yn-129(3,5-Cl)-rac-ADH-95-5-1.0**	*Injection Volume:*	**20.0**
Vial Number:	**452**	*Channel:*	**UV_VIS_1**
Sample Type:	**standard**	*Wavelength:*	**230**
Control Program:	**YJS**	*Bandwidth:*	**n.a.**
Quantif. Method:	**YJS**	*Dilution Factor:*	**1.0000**
Recording Time:	**2015-5-30 14:55**	*Sample Weight:*	**1.0000**
Run Time (min):	**23.55**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	18.73	n.a.	297.724	131.670	49.72	n.a.	BM
2	19.69	n.a.	285.970	133.127	50.28	n.a.	MB
Total:			583.694	264.797	100.00	0.000	

998 yjs-yn-129(3.5-Cl2)-asy-ADH-95-5-1.0

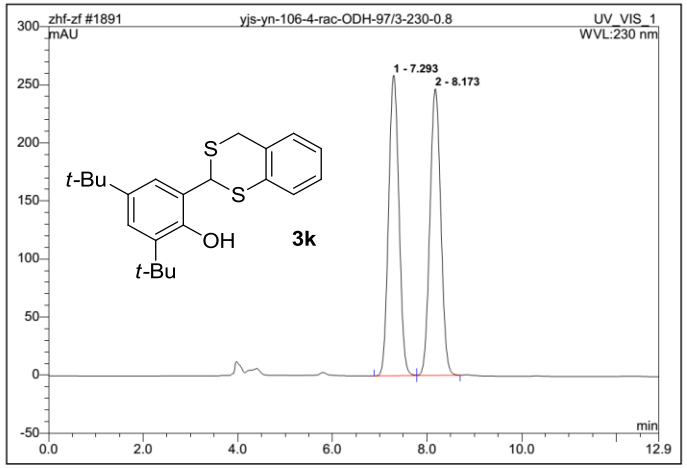
Sample Name:	**yjs-yn-129(3.5-Cl2)-asy-ADH-95-5-1.0**	*Injection Volume:*	**20.0**
Vial Number:	**451**	*Channel:*	**UV_VIS_1**
Sample Type:	**standard**	*Wavelength:*	**230**
Control Program:	**YJS**	*Bandwidth:*	**n.a.**
Quantif. Method:	**YJS**	*Dilution Factor:*	**1.0000**
Recording Time:	**2015-5-30 14:29**	*Sample Weight:*	**1.0000**
Run Time (min):	**24.14**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	19.93	n.a.	298.643	134.699	100.00	n.a.	BMB
Total:			298.643	134.699	100.00	0.000	

1891 yjs-yn-106-4-rac-ODH-97/3-230-0.8

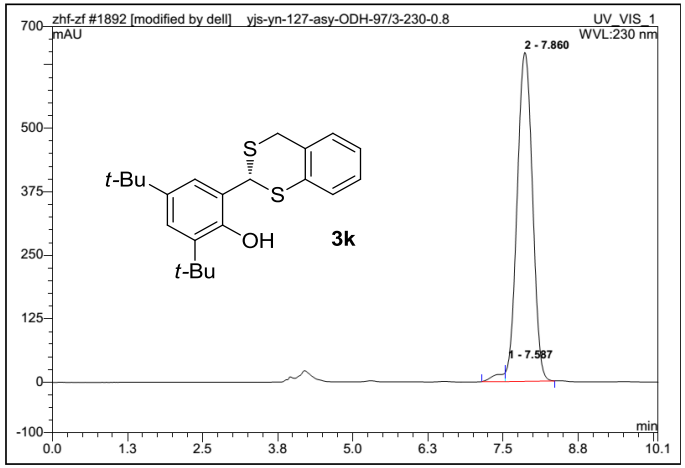
Sample Name:	**yjs-yn-106-4-rac-ODH-97/3-230-0.8**	*Injection Volume:*	**20.0**
Vial Number:	**999**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**zhf**	*Bandwidth:*	**n.a.**
Quantif. Method:	**zhf**	*Dilution Factor:*	**1.0000**
Recording Time:	**2015-11-27 10:28**	*Sample Weight:*	**1.0000**
Run Time (min):	**12.89**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	7.29	n.a.	258.743	65.685	50.04	n.a.	BM
2	8.17	n.a.	246.816	65.587	49.96	n.a.	MB
Total:			505.559	131.272	100.00	0.000	

1892 yjs-yn-127-asy-ODH-97/3-230-0.8

Sample Name:	**yjs-yn-127-asy-ODH-97/3-230-0.8**	*Injection Volume:*	**20.0**
Vial Number:	**999**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**zhf**	*Bandwidth:*	**n.a.**
Quantif. Method:	**zhf**	*Dilution Factor:*	**1.0000**
Recording Time:	**2015-11-27 10:51**	*Sample Weight:*	**1.0000**
Run Time (min):	**10.08**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	7.59	n.a.	38.837	3.724	1.90	n.a.	BM *
2	7.86	n.a.	647.525	191.749	98.10	n.a.	MB*
Total:			686.362	195.472	100.00	0.000	

SHIMADZU LabSolutions

Analysis Report

<Sample Information>

Sample Name	: ZHF-ZQ-066B		
Sample ID	:		
Data Filename	: zhf-zq-066B-rac-ADH-85-15-230-1.0.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 20 uL		
Date Acquired	: 2015/11/28 17:18:20	Acquired by	: System Administrator
Date Processed	: 2015/11/28 18:07:17	Processed by	: System Administrator

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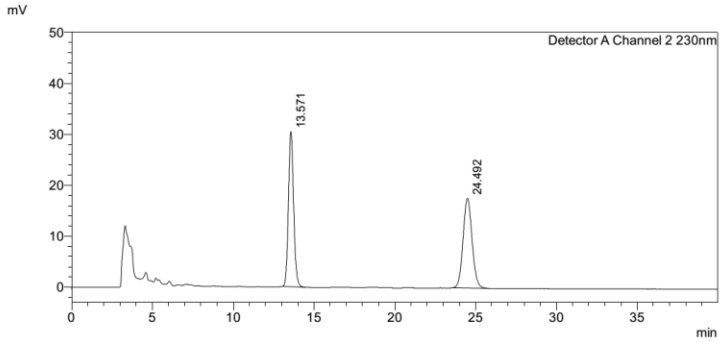
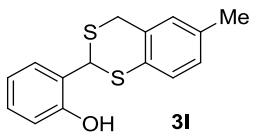


<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	13.571	678306	30450	49.905		M	
2	24.492	680893	17601	50.095		M	
Total		1359199	48051				



3l

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Analysis Report

<Sample Information>

Sample Name	: ZHF-ZQ-088-2		
Sample ID	:		
Data Filename	: zhf-zq-088-asy-ADH-85-15-230-1.1.lcd		
Method Filename	: chl-0128.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 20 uL		
Date Acquired	: 2015/11/28 15:58:24	Acquired by	: System Administrator
Date Processed	: 2015/11/28 16:46:56	Processed by	: System Administrator

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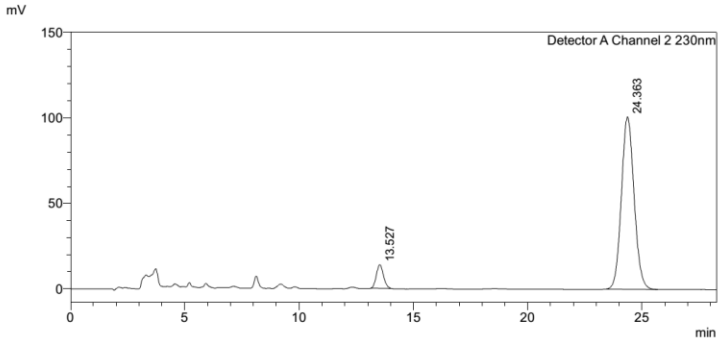
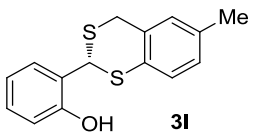


<Peak Table>

Detector A Channel 2 230nm

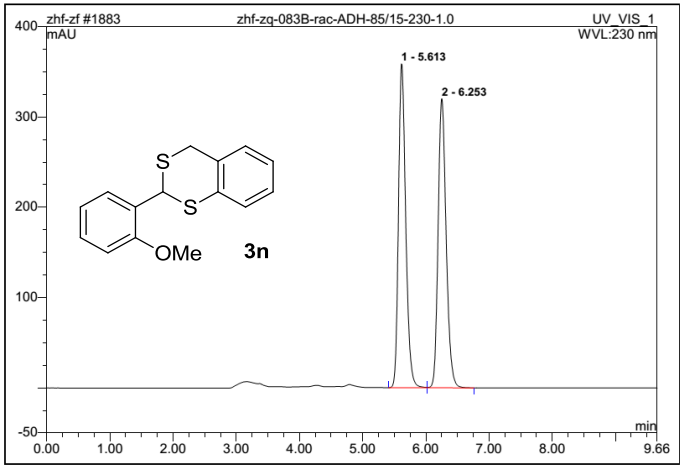
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	13.527	294405	13729	7.000		M	
2	24.363	3911304	100881	93.000		M	
Total		4205708	114610				



3l

1883 zhf-zq-083B-rac-ADH-85/15-230-1.0

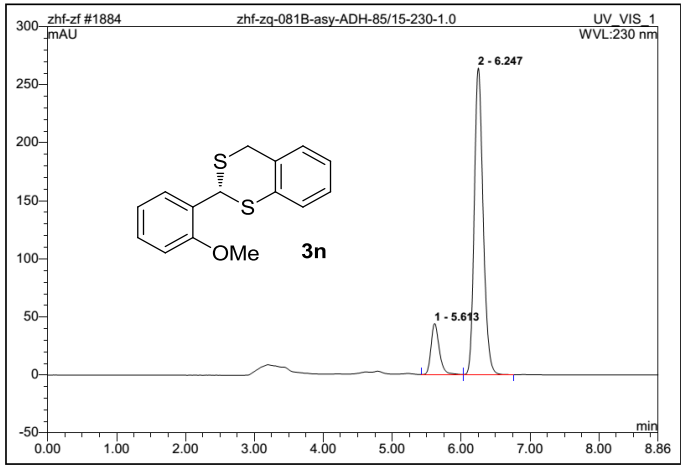
Sample Name:	**zhf-zq-083B-rac-ADH-85/15-230-1.0**	*Injection Volume:*	**20.0**
Vial Number:	**992**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**zhf**	*Bandwidth:*	**n.a.**
Quantif. Method:	**zhf**	*Dilution Factor:*	**1.0000**
Recording Time:	**2015-11-17 15:52**	*Sample Weight:*	**1.0000**
Run Time (min):	**9.66**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	5.61	n.a.	358.768	47.810	50.32	n.a.	BM
2	6.25	n.a.	319.982	47.206	49.68	n.a.	MB
Total:			678.750	95.016	100.00	0.000	

1884 zhf-zq-081B-asy-ADH-85/15-230-1.0

Sample Name:	**zhf-zq-081B-asy-ADH-85/15-230-1.0**	*Injection Volume:*	**20.0**
Vial Number:	**993**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**230**
Control Program:	**zhf**	*Bandwidth:*	**n.a.**
Quantif. Method:	**zhf**	*Dilution Factor:*	**1.0000**
Recording Time:	**2015-11-17 16:04**	*Sample Weight:*	**1.0000**
Run Time (min):	**8.86**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	5.61	n.a.	43.992	6.100	13.41	n.a.	BMB
2	6.25	n.a.	264.299	39.388	86.59	n.a.	BMB
Total:			308.291	45.488	100.00	0.000	

SHIMADZU LabSolutions

Analysis Report

<Sample Information>

Sample Name	: zhf-zq-111-rac--ADH-ADH-85-15-230-0.7		
Sample ID	:		
Data Filename	: zhf-zq-111-rac--ADH-ADH-85-15-230-0.7.lcd		
Method Filename	: WAC-93-FANFA.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 20 uL		
Date Acquired	: 2015/12/25 11:41:21	Acquired by	: System Administrator
Date Processed	: 2015/12/25 14:14:18	Processed by	: System Administrator

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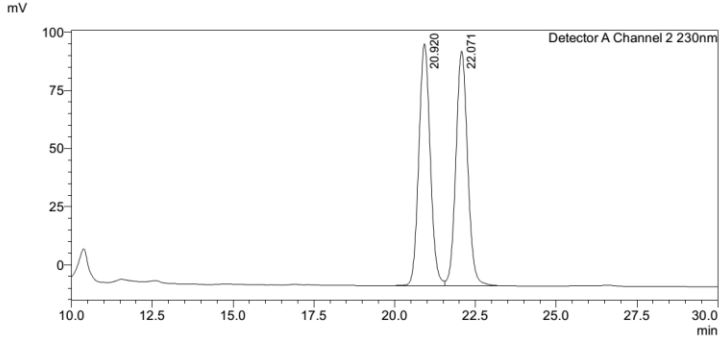
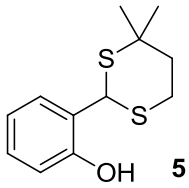


<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	20.920	2551324	104048	49.919		V	
2	22.071	2559554	100799	50.081		V	
Total		5110878	204847				



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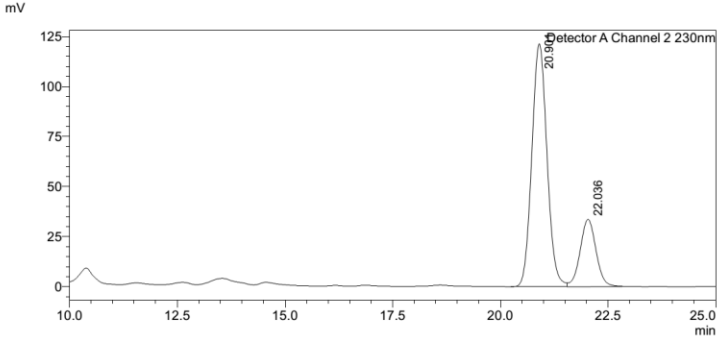
SHIMADZU LabSolutions

Analysis Report

<Sample Information>

Sample Name	: zhf-zq-112-asy--ADH-ADH-85-15-230-0.7		
Sample ID	:		
Data Filename	: zhf-zq-112-asy--ADH-ADH-85-15-230-0.7.lcd		
Method Filename	: WAC-93-FANFA.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 20 uL		
Date Acquired	: 2015/12/25 13:46:23	Acquired by	: System Administrator
Date Processed	: 2015/12/25 14:14:44	Processed by	: System Administrator

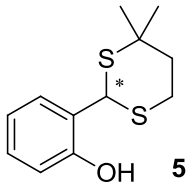
<Chromatogram>



<Peak Table>

Detector A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	20.901	2981681	121401	77.438			
2	22.036	868725	33638	22.562		V	
Total		3850406	155039				



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