Supporting Informations

Pd(II)-Catalyzed *ortho*-Halogenation of 2-Arylbenzothiazole and 2,3-Diarylquinoxaline

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Contents:

Instrumentation and Chemicals:

All the reagents were commercial grade and purified according to the established procedures. Organic extracts were dried over anhydrous sodium sulphate. Solvents were removed in a rotary evaporator under reduced pressure. Silica gel (60-120 mesh size) was used for the column chromatography. Reactions were monitored by TLC on silica gel 60 F_{254} (0.25mm). NMR spectra were recorded in $CDCl_3$ with tetramethylsilane as the internal standard for ^1H NMR (400 and 600 MHz) $CDCl_3$ solvent as the internal standard for ^{13}C NMR (100 and 150 MHz). MS spectra were recorded using ESI mode. IR spectra were recorded in KBr or neat.

Experimental procedure:

*(A) Synthesis of 2-(benzo[d]thiazol-2-yl)-3-bromophenyl benzoate (**1a**) from 2-(benzo[d]thiazol-2-yl)phenyl benzoate (**1**).*

To an oven-dried 25 mL round bottom flask were added 2-(benzo[*d*]thiazol-2-yl)phenyl benzoate (**1**) (0.083g, 0.25 mmol), *N*-bromosuccinamide (0.053g, 0.3 mmol), $Pd(OAc)_2$ (0.003g, 0.013 mmol), para-toluenesulfonic acid (0.024g, 0.13 mmol) and 1,2-dichloroethane (2.0 mL). Then the reaction mixture was refluxed in an oil bath preheated to 90 ^oC. After completion of the reaction (7 h) excess solvent was evacuate under reduced pressure. The product was extracted with ethyl acetate (3 x 10 mL) and the combined organic layer was washed carefully with saturated sodium bicarbonate solution (10 mL), dried over anhydrous sodium sulphate (Na_2SO_4), and evaporated under reduced pressure. The crude product so obtained was purified by silica gel column chromatography (hexane / ethyl acetate, 10:0.3) to give pure 2-(benzo[*d*]thiazol-2-yl)-3-bromophenyl benzoate (**1a**) (0.081g, yield 79%). The identity and purity of the product was confirmed by spectroscopic analysis.

Mechanistic Investigation:

ESI-MS study for the detection of reaction intermediates during *o*-bromination

In order to detect the intermediate species in the reaction mixture an electrospray mass spectrometry was performed. In this study, an oven-dried flask was charged with 2-(benzo[*d*]thiazol-2-yl)phenyl benzoate (**1**) (0.083g, 0.25 mmol), *N*-bromosuccinamide (0.053g, 0.3 mmol), $Pd(OAc)_2$ (0.003g, 0.013 mmol), para-toluenesulfonic acid (0.024g, 0.13 mmol) and 1,2-dichloroethane (2.0 mL). Then the reaction mixture was stirred in an oil bath at 90 ^oC. After 0.5 h of reaction, aliquot (100 μL) was withdrawn and diluted with acetonitrile (1 mL). A 20 μL of the diluted solution was injected to run ESI-MS analysis. Various cationic and neutral Pd species were detected in the ESI-MS analysis as shown below in Figure S1. The o-brominated product, cationic and neutral Pd-species observed in the spectrum are as follows: peaks at m/z 411.9857 corresponding to 2-(benzo[*d*]thiazol-2-yl)-3-bromophenyl benzoate (**1a**) (Figure S1), at m/z 614.8975 corresponding to $[C_{24}H_{16}BrN_2O_4Pd(IV)S]^+$ (**A**) (Figure S1), at m/z 846.9437 corresponding to $[C_{40}H_{24}BrN_2O_4Pd(IV)S_2]^+$ (**B**) (Figure S1), at m/z 962.8334 corresponding to $[C_{48}H_{32}N_4O_8Pd(IV)S_2]$ (**C**) (Figure S1).

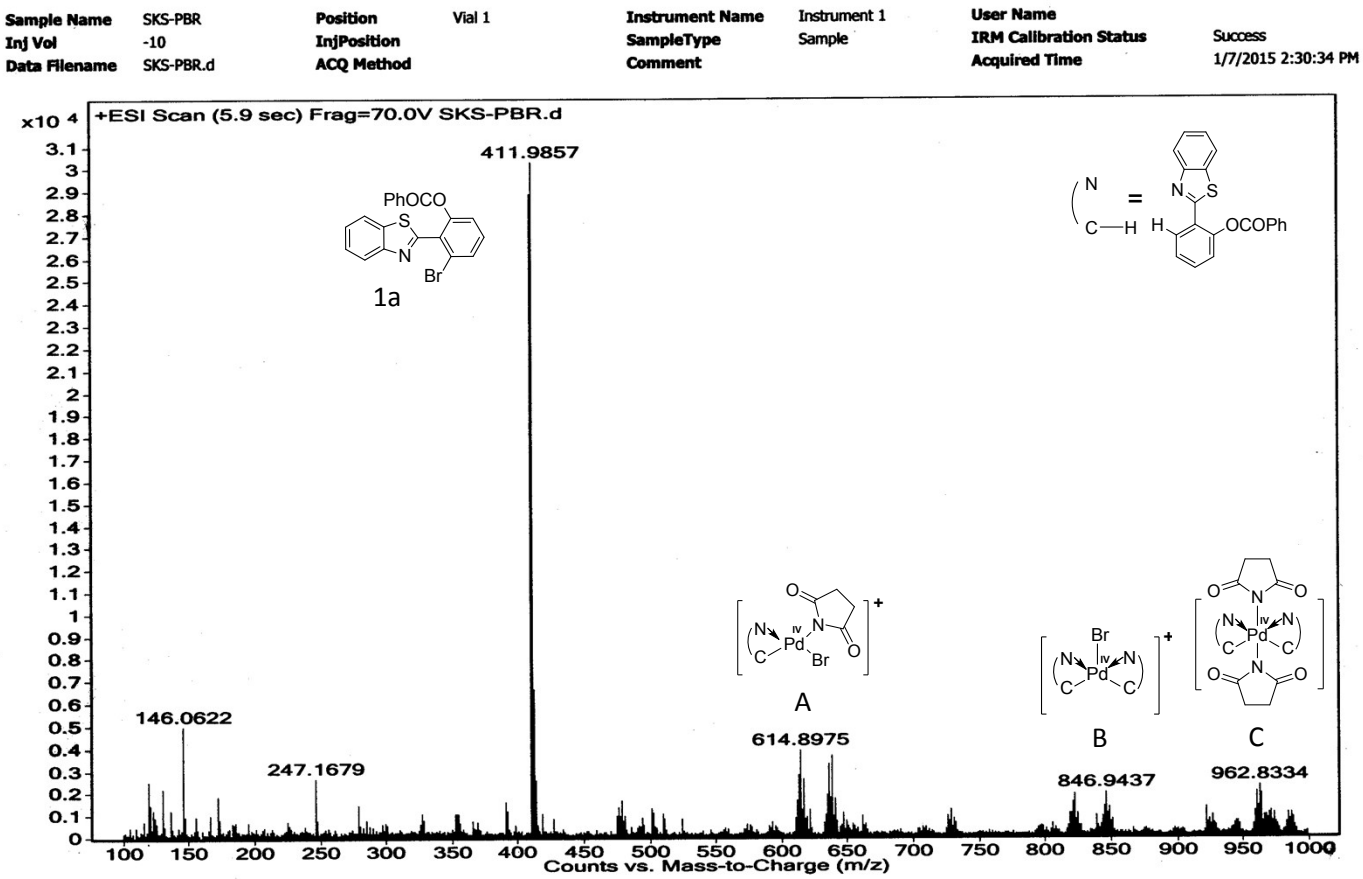


Figure S1. ESI-MS spectrum of the reaction mixture

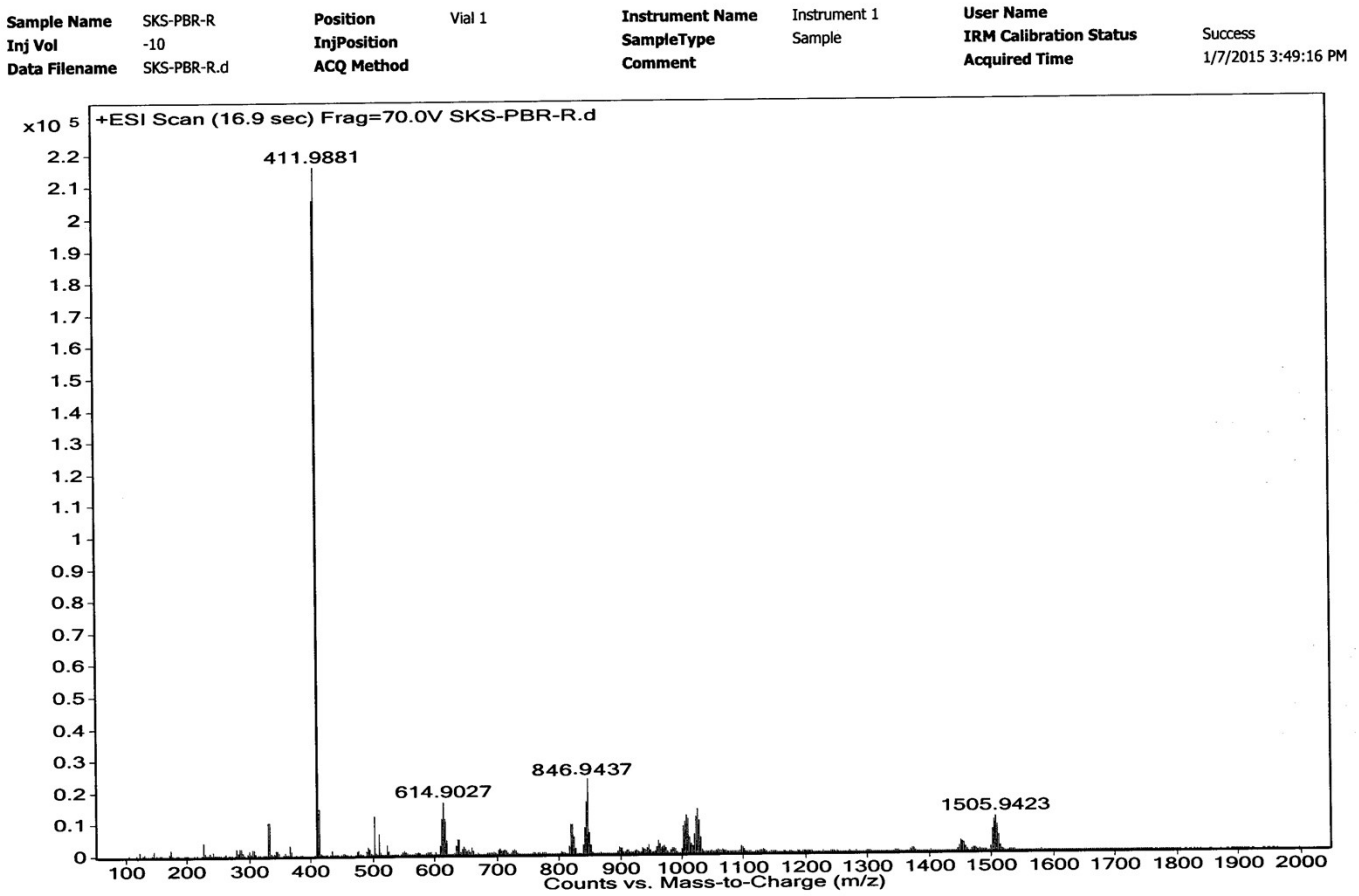
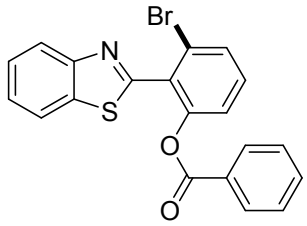


Figure S2. ESI-MS spectrum of the reaction mixture

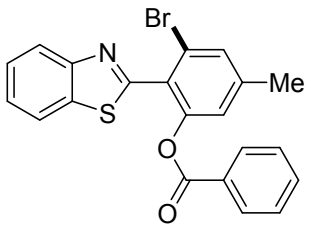
Spectral Data:

2-(Benzo[*d*]thiazol-2-yl)-3-bromophenyl benzoate (1a):



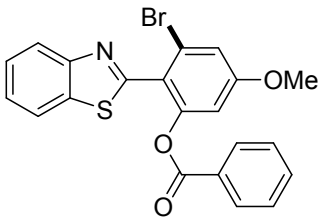
Gummy solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.06 (d, 1H, J = 8.0 Hz), 7.88–7.85 (m, 3H), 7.66 (d, 1H, J = 7.6 Hz), 7.50–7.42 (m, 3H), 7.40–7.36 (m, 2H), 7.29 (t, 2H, J = 7.6 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 164.7, 161.8, 153.0, 150.4, 136.3, 133.9, 131.8, 130.8, 130.3, 129.0, 128.7, 128.6, 126.3, 125.7, 124.3, 123.9, 122.6, 121.7; IR (KBr, cm^{-1}): 3059, 2914, 2853, 1741, 1598, 1565, 1518, 1441, 1428, 1313, 1261, 1221, 1175, 1137, 1077, 1055, 1023, 962, 873, 855, 760, 729, 707; HRMS (ESI) calcd for $C_{20}H_{12}BrNO_2S$ (M + H$^+$) 409.9850, found 409.9858.

2-(Benzo[*d*]thiazol-2-yl)-3-bromo-5-methylphenyl benzoate (2a):



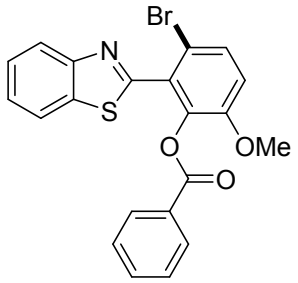
Gummy solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.03 (d, 1H, J = 8.4 Hz), 7.87–7.84 (m, 3H), 7.50–7.45 (m, 3H), 7.37 (t, 1H, J = 7.6 Hz), 7.30 (t, 2H, J = 8.0 Hz), 7.18 (s, 1H), 2.44 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 164.9, 161.9, 153.1, 150.2, 142.9, 136.5, 133.8, 131.6, 130.3, 128.9, 128.6, 126.2, 126.1, 125.6, 123.9, 123.8, 123.3, 121.7, 21.4; IR (KBr, cm^{-1}): 3061, 2919, 2845, 1741, 1610, 1555, 1451, 1432, 1313, 1237, 1176, 1128, 1077, 1058, 1024, 863, 821, 760, 729, 706; HRMS (ESI) calcd for $C_{21}H_{14}BrNO_2S$ (M + H$^+$) 424.0007, found 424.0013.

2-(Benzo[*d*]thiazol-2-yl)-3-bromo-5-methoxyphenyl benzoate (3a):



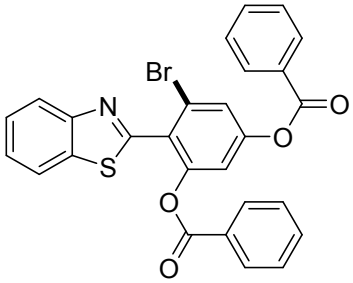
Solid; M.p. 155 ^{o}C–157 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.01 (d, 1H, J = 8.4 Hz), 7.87 (d, 2H, J = 8.0 Hz), 7.83 (d, 1H, J = 7.6 Hz), 7.49–7.41 (m, 2H), 7.35 (t, 1H, J = 7.6 Hz), 7.29 (t, 2H, J = 7.4 Hz), 7.21 (s, 1H), 6.92 (s, 1H), 3.86 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 164.7, 161.9, 161.7, 152.9, 151.1, 136.5, 133.9, 130.3, 128.8, 128.6, 126.2, 125.6, 124.6, 123.8, 121.6, 121.3, 116.9, 108.8, 56.1; IR (KBr, cm^{-1}): 3075, 2958, 1747, 1609, 1564, 1523, 1461, 1452, 1425, 1316, 1241, 1202, 1176, 1117, 1075, 1054, 1039, 1023, 965, 863, 814, 761, 731; HRMS (ESI) calcd for $C_{21}H_{14}BrNO_3S$ (M + H$^+$) 439.9956, found 439.9965.

2-(Benzo[*d*]thiazol-2-yl)-3-bromo-6-methoxyphenyl benzoate (4a):



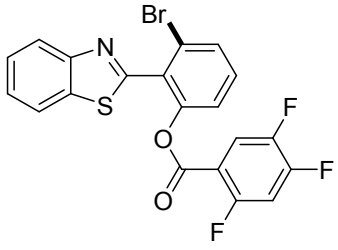
Solid; M.p. 183 °C–186 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.05 (d, 1H, J = 8.0 Hz), 7.95 (d, 2H, J = 7.6 Hz), 7.83 (d, 1H, J = 8.0 Hz), 7.58 (d, 1H, J = 8.8 Hz), 7.50–7.42 (m, 2H), 7.37–7.30 (m, 3H), 7.02 (d, 1H, J = 9.2 Hz), 3.82 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 164.2, 161.7, 153.1, 151.5, 140.1, 136.4, 133.7, 130.9, 130.4, 130.0, 128.7, 128.6, 126.2, 125.7, 123.9, 121.7, 115.1, 113.8, 56.6; IR (KBr, cm^{-1}): 3058, 2923, 2851, 1742, 1598, 1572, 1558, 1524, 1466, 1451, 1438, 1298, 1258, 1244, 1221, 1196, 1100, 1076, 1055, 1021, 994, 869, 801, 760, 731, 706; HRMS (ESI) calcd for $C_{21}H_{14}BrNO_3S$ (M + H$^+$) 439.9956, found 439.9959.

4-(Benzo[*d*]thiazol-2-yl)-5-bromo-1,3-phenylene dibenzoate (5a):



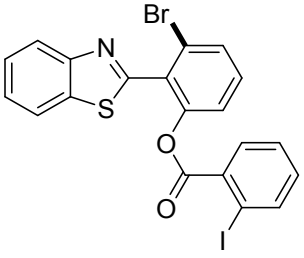
Solid; M.p. 115 °C–117 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.21 (d, 2H, J = 7.6 Hz), 8.05 (d, 1H, J = 8.4 Hz), 7.89 (d, 1H, J = 8.4 Hz), 7.85 (d, 2H, J = 8.0 Hz), 7.67 (t, 1H, J = 7.4 Hz), 7.64 (s, 1H), 7.54 (t, 2H, J = 7.8 Hz), 7.49–7.46 (m, 2H), 7.43–7.38 (m, 2H), 7.30 (t, 2H, J = 8.0 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 164.4, 161.3, 153.1, 152.6, 150.8, 136.5, 134.3, 134.0, 130.6, 130.4, 128.9, 128.8, 128.7, 128.6, 126.6, 126.3, 125.8, 124.4, 124.3, 124.0, 121.7, 116.8; IR (KBr, cm^{-1}): 3055, 2913, 2842, 1742, 1601, 1558, 1507, 1450, 1431, 1409, 1256, 1240, 1132, 1076, 1059, 1024, 951, 886, 754, 695; HRMS (ESI) calcd for $C_{27}H_{16}BrNO_4S$ (M + H$^+$) 530.0061, found 530.0071.

2-(Benzo[*d*]thiazol-2-yl)-3-bromophenyl 2,4,5-trifluorobenzoate (6a):



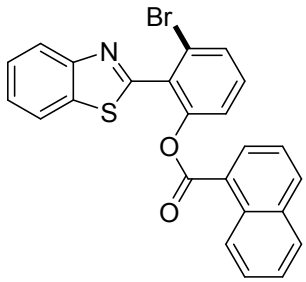
Solid; M.p. 120 °C–123 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.03 (d, 1H, J = 8.0 Hz), 7.89 (d, 1H, J = 8.0 Hz), 7.67 (d, 1H, J = 8.0 Hz), 7.56–7.49 (m, 1H), 7.47 (d, 1H, J = 8.8 Hz), 7.43–7.41 (m, 2H), 7.37 (t, 1H, J = 7.8 Hz), 6.90–6.84 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 161.5, 160.3, 152.9, 149.7, 136.3, 131.9, 131.3, 128.9, 126.5, 125.9, 124.4, 123.9, 122.4, 121.8, 120.5, 120.3, 107.6, 107.4, 107.3, 107.1; IR (KBr, cm^{-1}): 3065, 2923, 2847, 1746, 1623, 1595, 1566, 1522, 1446, 1422, 1341, 1253, 1237, 1191, 1145, 1045, 959, 893, 859, 846, 814, 772, 764, 749, 720, 702; HRMS (ESI) calcd for $C_{20}H_9BrF_3NO_2S$ (M + H$^+$) 463.9567, found 463.9574.

2-(Benzo[*d*]thiazol-2-yl)-3-bromophenyl 2-iodobenzoate (7a):



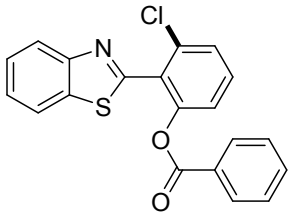
Gummy solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.08 (d, 1H, J = 8.0 Hz), 7.89 (t, 2H, J = 7.4 Hz), 7.66 (d, 1H, J = 8.0 Hz), 7.50–7.38 (m, 5H), 7.12 (t, 1H, J = 7.6 Hz), 7.04 (t, 1H, J = 7.6 Hz); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 164.3, 161.8, 153.1, 150.2, 141.8, 136.5, 133.5, 133.1, 131.9, 131.7, 131.2, 129.2, 128.0, 126.4, 125.9, 124.4, 124.0, 122.7, 121.8, 94.9; IR (KBr, cm^{-1}): 3060, 2922, 2851, 1750, 1581, 1559, 1440, 1428, 1313, 1280, 1216, 1172, 1125, 1071, 1036, 1010, 961, 871, 760, 737; HRMS (ESI) calcd for $C_{20}H_{11}BrINO_2S$ (M + H$^+$) 535.8817, found 535.8828.

2-(Benzo[*d*]thiazol-2-yl)-3-bromophenyl 1-naphthoate (8a):



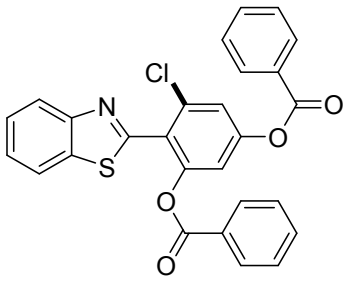
Gummy solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.74 (d, 1H, J = 9.6 Hz), 8.06 (d, 1H, J = 8.4 Hz), 7.95–7.90 (m, 2H), 7.85–7.79 (m, 2H), 7.69 (d, 1H, J = 8.0 Hz), 7.49–7.42 (m, 5H), 7.36 (t, 1H, J = 7.6 Hz), 7.25 (t, 1H, J = 7.8 Hz); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 165.3, 162.1, 153.1, 150.6, 136.5, 134.6, 133.9, 131.9, 131.6, 131.5, 130.9, 129.4, 128.7, 128.3, 126.6, 126.3, 125.8, 125.7, 125.1, 124.5, 124.4, 123.9, 122.9, 121.8; IR (KBr, cm^{-1}): 3050, 2959, 2926, 2847, 1736, 1593, 1564, 1507, 1441, 1428, 1277, 1229, 1158, 1109, 1076, 981, 961, 881, 811, 779, 761, 728, 699; HRMS (ESI) calcd for $C_{24}H_{14}BrNO_2S$ (M + H$^+$) 460.0007, found 460.0001.

2-(Benzo[*d*]thiazol-2-yl)-3-chlorophenyl benzoate (1b):



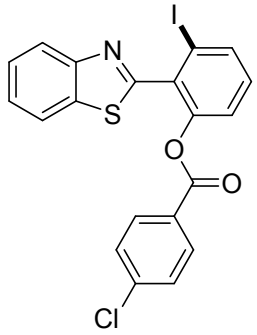
Gummy solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.00 (d, 1H, J = 8.0 Hz), 7.89 (d, 2H, J = 8.4 Hz), 7.84 (d, 1H, J = 8.0 Hz), 7.51–7.45 (m, 3H), 7.42 (d, 1H, J = 7.2 Hz), 7.36 (d, 1H, J = 8.0 Hz), 7.34–7.28 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 164.8, 160.2, 152.9, 150.4, 136.2, 135.0, 133.8, 131.5, 130.3, 128.7, 128.6, 127.7, 127.1, 126.2, 125.7, 123.8, 122.1, 121.6; IR (KBr, cm^{-1}): 3061, 2914, 2845, 1741, 1599, 1569, 1518, 1445, 1430, 1313, 1262, 1222, 1176, 1125, 1077, 1056, 1023, 964, 892, 855, 760, 729, 705; HRMS (ESI) calcd for $C_{20}H_{12}ClNO_2S$ (M + H$^+$) 366.0355, found 366.0362.

4-(Benzo[*d*]thiazol-2-yl)-5-chloro-1,3-phenylene dibenzoate (5b):



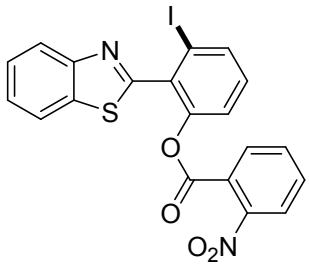
Solid; M.p. 135 °C–138 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.19 (d, 2H, J = 8.0 Hz), 7.99 (d, 1H, J = 8.0 Hz), 7.89–7.86 (m, 3H), 7.65 (t, 1H, J = 7.4 Hz), 7.54–7.49 (m, 3H), 7.47–7.42 (m, 2H), 7.39–7.36 (m, 2H), 7.30 (t, 2H, J = 7.8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 164.4, 164.3, 159.7, 153.1, 152.4, 150.9, 136.4, 135.5, 134.3, 133.9, 130.5, 130.4, 128.9, 128.8, 128.7, 126.3, 125.8, 124.7, 123.9, 121.7, 121.4, 116.3; IR (KBr, cm^{-1}): 3110, 3061, 2920, 2844, 1743, 1735, 1602, 1572, 1507, 1451, 1431, 1412, 1314, 1260, 1196, 1133, 1078, 1060, 1024, 1001, 984, 953, 880, 840, 795, 754, 721, 711, 695; HRMS (ESI) calcd for $C_{27}H_{16}ClNO_4S$ (M + H$^+$) 486.0567, found 486.0576.

2-(Benzo[*d*]thiazol-2-yl)-3-iodophenyl 4-chlorobenzoate (9c):



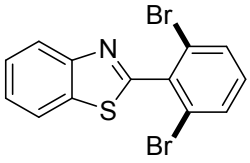
Gummy solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.01 (d, 1H, J = 8.4 Hz), 7.85 (d, 1H, J = 7.6 Hz), 7.80 (d, 1H, J = 8.0 Hz), 7.68 (d, 2H, J = 7.6 Hz), 7.43 (t, 1H, J = 7.6 Hz), 7.36–7.32 (m, 2H), 7.23–7.18 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 164.4, 163.9, 152.9, 149.4, 140.5, 137.4, 136.3, 132.6, 132.4, 131.6, 129.1, 127.2, 126.5, 125.9, 124.0, 123.2, 121.8, 98.9; IR (KBr, cm^{-1}): 3064, 2923, 2850, 1742, 1592, 1560, 1514, 1487, 1438, 1426, 1401, 1312, 1259, 1220, 1172, 1127, 1090, 1059, 1013, 961, 845, 774, 751, 728; HRMS (ESI) calcd for $C_{20}H_{11}ClINO_2S$ (M + H$^+$) 491.9322, found 491.9332.

2-(Benzo[*d*]thiazol-2-yl)-3-iodophenyl 2-nitrobenzoate (10c):



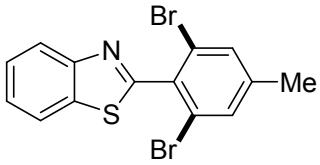
Gummy solid; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 8.14 (d, 1H, J = 8.4 Hz), 7.96–7.94 (m, 3H), 7.56–7.52 (m, 3H), 7.47 (t, 1H, J = 7.4 Hz), 7.41 (t, 1H, J = 7.8 Hz), 7.33 (t, 1H, J = 8.0 Hz), 7.17 (d, 1H, J = 7.8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 164.3, 163.9, 153.0, 148.8, 147.4, 137.9, 136.4, 133.5, 132.7, 132.6, 132.1, 129.5, 127.2, 126.6, 126.0, 124.4, 124.1, 122.9, 121.9, 98.8; IR (KBr, cm^{-1}): 3118, 3054, 1759, 1595, 1558, 1532, 1482, 1438, 1426, 1348, 1312, 1281, 1216, 1174, 1126, 1098, 1052, 1033, 961, 909, 869, 852, 761, 729; HRMS (ESI) calcd for $C_{20}H_{11}IN_2O_4S$ (M + H$^+$) 502.9562, found 502.9565.

2-(2,6-Dibromophenyl)benzo[*d*]thiazole (11a):



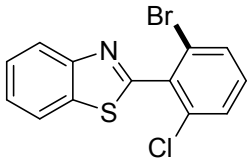
Gummy solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.18 (d, 1H, J = 8.0 Hz), 7.98 (d, 1H, J = 7.6 Hz), 7.67 (d, 2H, J = 8.0 Hz), 7.57 (t, 1H, J = 7.8 Hz), 7.49 (t, 1H, J = 7.6 Hz), 7.22 (t, 1H, J = 8.0 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 165.5, 152.9, 136.4, 135.9, 132.3, 132.1, 126.4, 125.9, 124.7, 124.2, 121.9; IR (KBr, cm^{-1}): 3072, 2959, 2917, 2848, 1575, 1594, 1549, 1514, 1546, 1420, 1316, 1243, 1228, 1195, 1185, 1147, 1123, 1081, 1067, 1015, 962, 941, 900, 852, 776, 765, 741, 730, 724, 707; HRMS (ESI) calcd for $C_{13}H_7Br_2NS$ (M + H$^+$) 369.8723, found 369.8716.

2-(2,6-Dibromo-4-methylphenyl)benzo[*d*]thiazole (12a):



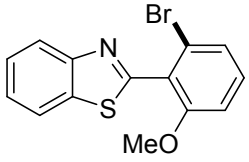
Solid; M.p. 84 ^{o}C–86 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.15 (d, 1H, J = 8.0 Hz), 7.95 (d, 1H, J = 8.0 Hz), 7.53 (t, 1H, J = 7.8 Hz), 7.48–7.43 (m, 3H), 2.38 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 165.7, 152.9, 143.3, 136.5, 132.9, 132.7, 130.1, 126.4, 125.9, 124.1, 121.9, 20.9; IR (KBr, cm^{-1}): 3058, 2954, 2921, 2850, 1597, 1526, 1485, 1431, 1379, 1311, 1228, 1195, 1084, 1065, 964, 850, 817, 759, 743, 728, 707; HRMS (ESI) calcd for $C_{14}H_9Br_2NS$ (M + H$^+$) 383.8880, found 383.8872.

2-(2-Bromo-6-chlorophenyl)benzo[*d*]thiazole (13a):



Gummy solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.17 (d, 1H, J = 8.0 Hz), 7.95 (d, 1H, J = 8.0 Hz), 7.59 (d, 1H, J = 8.8 Hz), 7.53 (t, 1H, J = 7.6 Hz), 7.47–7.43 (m, 2H), 7.25 (t, 1H, J = 8.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 163.8, 152.9, 136.4, 135.6, 134.2, 131.9, 131.5, 128.9, 126.4, 125.9, 124.8, 124.1, 121.8; IR (KBr, cm^{-1}): 3055, 2918, 2858, 1579, 1553, 1516, 1456, 1428, 1313, 1240, 1225, 1194, 1091, 1072, 962, 776, 762, 741, 728, 707; HRMS (ESI) calcd for $C_{13}H_7Br_2ClNS$ (M + H$^+$) 323.9249, found 323.9253.

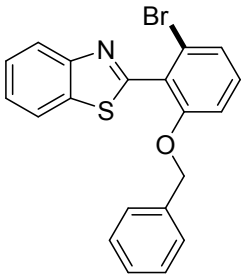
2-(2-Bromo-6-methoxyphenyl)benzo[*d*]thiazole (14a):



Gummy solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.14 (d, 1H, J = 7.6 Hz), 7.93 (d, 1H, J = 8.0 Hz), 7.51 (t, 1H, J = 7.4 Hz), 7.42 (t, 1H, J = 7.4 Hz), 7.30–7.28 (m, 2H), 6.94 (t, 1H, J = 4.2 Hz), 3.74 (s,

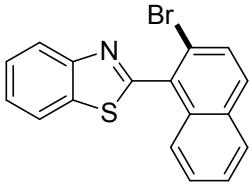
3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 163.8, 159.2, 153.3, 136.7, 132.1, 126.1, 125.5, 125.1, 124.7, 124.5, 123.9, 121.7, 110.3, 56.4; IR (KBr, cm^{-1}): 3061, 2967, 2938, 2835, 1587, 1567, 1518, 1460, 1429, 1312, 1267, 1240, 1221, 1184, 1148, 1125, 1083, 1033, 959, 852, 777, 760, 741, 729; HRMS (ESI) calcd for $C_{14}H_{10}BrNOS$ (M + H^+) 319.9744, found 319.9740.

2-(2-(Benzyloxy)-6-bromophenyl)benzo[*d*]thiazole (15a):



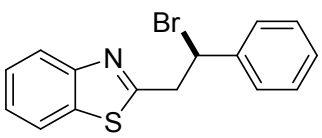
Gummy solid; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 8.17 (d, 1H, J = 8.4 Hz), 7.95 (d, 1H, J = 8.4 Hz), 7.52 (t, 1H, J = 7.4 Hz), 7.44 (t, 1H, J = 7.4 Hz), 7.30 (d, 1H, J = 8.4 Hz), 7.25–7.21 (m, 6H), 6.95 (d, 1H, J = 8.4 Hz), 5.09 (s, 2H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 163.7, 158.2, 153.3, 136.7, 136.3. 131.9, 128.8, 128.7, 128.0, 126.9, 126.1, 125.5, 125.2, 124.7, 123.9, 121.8, 112.1, 70.9; IR (KBr, cm^{-1}): 3064, 3031, 2934, 2870, 1587, 1567, 1518, 1496, 1440, 1380, 1311, 1267, 1238, 1222, 1147, 1125, 1080, 1023, 960, 868, 834, 775, 759, 730; HRMS (ESI) calcd for $C_{20}H_{14}BrNOS$ (M + H^+) 396.0057, found 396.0063.

2-(2-Bromonaphthalen-1-yl)benzo[*d*]thiazole (16a):



Gummy solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.14 (d, 1H, J = 8.0 Hz), 7.98 (d, 1H, J = 8.0 Hz), 7.94 (d, 1H, J = 8.4 Hz), 7.88 (d, 1H, J = 8.4 Hz), 7.83 (d, 1H, J = 7.8 Hz), 7.72 (d, 1H, J = 7.2 Hz), 7.56–7.50 (m, 2H), 7.44 (t, 1H, J = 7.6 Hz), 7.32 (t, 1H, J = 7.8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.2, 153.2, 136.9, 136.1, 134.4, 131.9, 131.8, 131.6, 130.1, 128.9, 126.9, 126.4, 125.4, 125.1, 123.7, 121.6, 119.7; IR (KBr, cm^{-1}): 3054, 3000, 2970, 2914, 1509, 1493, 1448, 1433, 1357, 1343, 1311, 1278, 1248, 1180, 1106, 1067, 1013, 946, 877, 825, 814, 762, 730, 698; HRMS (ESI) calcd for $C_{17}H_{10}BrNS$ (M + H^+) 339.9795, found 339.9801.

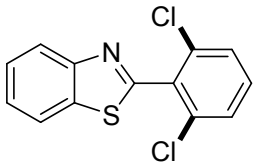
2-(2-Bromo-2-phenylethyl)benzo[*d*]thiazole (17a):



Gummy solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.03 (d, 1H, J = 8.4 Hz), 7.87 (d, 1H, J = 8.0 Hz), 7.49 (t, 1H, J = 7.6 Hz), 7.42 (t, 1H, J = 7.6 Hz), 7.31–7.24 (m, 5H), 5.52 (t, 1H, J = 7.6 Hz),

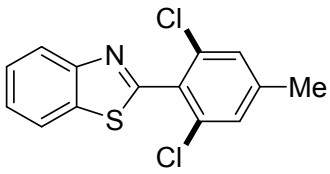
3.87–3.81 (m, 1H), 3.66–3.59 (m, 1H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 170.7, 152.8, 137.2, 135.8, 129.5, 128.8, 127.5, 126.6, 126.0, 123.8, 122.0, 49.2, 45.2; IR (KBr, cm^{-1}): 3058, 3028, 2926, 2847, 1603, 1558, 1496, 1454, 1434, 1313, 1243, 1178, 1075, 1030, 1013, 930, 758, 729, 699; HRMS (ESI) calcd for $C_{15}H_{12}BrNS$ (M + H$^+$) 317.9952, found 317.9957.

2-(2,6-Dichlorophenyl)benzo[*d*]thiazole (11b):



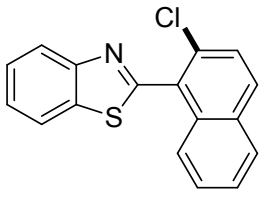
Gummy solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.16 (d, 1H, J = 8.0 Hz), 7.96 (d, 1H, J = 8.4 Hz), 7.55 (t, 1H, J = 7.8 Hz), 7.48–7.43 (m, 3H), 7.36 (t, 1H, J = 8.0 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 162.3, 153.1, 136.5, 135.8, 132.6, 131.7, 128.4, 126.5, 125.9, 124.2, 121.9; IR (KBr, cm^{-1}): 3058, 2924, 2853, 1582, 1558, 1516, 1457, 1431, 1311, 1241, 1224, 1191, 1106, 1076, 1013, 964, 788, 759, 743, 729, 699; HRMS (ESI) calcd for $C_{13}H_7Cl_2NS$ (M + H$^+$) 279.9754, found 279.9758.

2-(2,6-Dichloro-4-methylphenyl)benzo[*d*]thiazole (12b):



Gummy solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.17 (d, 1H, J = 8.0 Hz), 7.97 (d, 1H, J = 8.0 Hz), 7.55 (t, 1H, J = 7.8 Hz), 7.47 (t, 1H, J = 7.6 Hz), 7.27 (s, 2H), 2.39 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 162.5, 153.2, 142.6, 136.6, 135.3, 129.5, 129.0, 126.4, 125.9, 124.1, 121.8, 21.2; IR (KBr, cm^{-1}): 3067, 2951, 2918, 1603, 1546, 1524, 1451, 1441, 1430, 1388, 1311, 1279, 1244, 1224, 1201, 1159, 1096, 1070, 1037, 1012, 964, 908, 850, 803, 797, 754, 724, 707; HRMS (ESI) calcd for $C_{14}H_9Cl_2NS$ (M + H$^+$) 293.9911, found 293.9904.

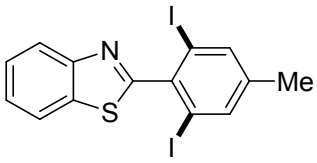
2-(2-Chloronaphthalen-1-yl)benzo[*d*]thiazole (16b):



Gummy solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.13 (d, 1H, J = 8.4 Hz), 8.04 (d, 1H, J = 8.0 Hz), 7.96 (d, 1H, J = 8.0 Hz), 7.87 (d, 1H, J = 8.4 Hz), 7.71 (d, 1H, J = 7.2 Hz), 7.61–7.53 (m, 3H), 7.48–7.42 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.8, 153.2, 136.8, 135.9, 131.8, 131.6, 131.0, 130.8, 130.2, 129.1, 128.3, 126.6, 126.5, 125.4, 125.2, 123.7, 121.6; IR (KBr, cm^{-1}): 3055, 2924, 2844, 1516, 1496, 1451, 1362, 1344, 1327, 1312, 1278,

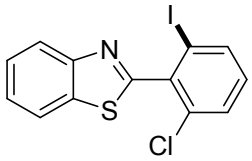
1199, 1110, 1067, 1013, 959, 884, 820, 758, 728, 705; HRMS (ESI) calcd for $C_{17}H_{10}ClNS$ ($M + H^+$) 296.0300, found 296.0296.

2-(2,6-Diiodo-4-methylphenyl)benzo[*d*]thiazole (12c):



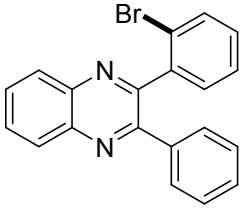
Gummy solid; ^1H NMR ($CDCl_3$, 400 MHz): δ 8.16 (d, 1H, J = 8.4 Hz), 7.94 (d, 1H, J = 8.0 Hz), 7.76 (s, 2H), 7.54 (t, 1H, J = 7.8 Hz), 7.46 (t, 1H, J = 7.6 Hz), 2.31 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 171.1, 152.7, 143.5, 139.9, 139.7, 136.5, 126.5, 126.0, 124.3, 122.0, 97.0, 20.4; IR (KBr, cm^{-1}): 3058, 2919, 2859, 1581, 1518, 1455, 1438, 1426, 1372, 1314, 1242, 1229, 1192, 1159, 1125, 1080, 1056, 1011, 957, 851, 758, 728; HRMS (ESI) calcd for $C_{14}H_9I_2NS$ ($M + H^+$) 477.8623, found 477.8632.

2-(2-Chloro-6-iodophenyl)benzo[*d*]thiazole (13c):



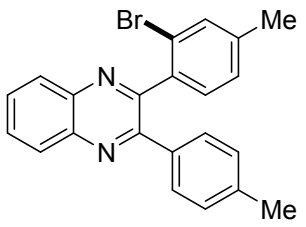
Gummy solid; ^1H NMR ($CDCl_3$, 400 MHz): δ 8.17 (d, 1H, J = 8.4 Hz), 7.96 (d, 1H, J = 8.0 Hz), 7.68 (d, 1H, J = 8.4 Hz), 7.54 (t, 1H, J = 7.6 Hz), 7.49–7.44 (m, 2H), 7.09 (t, 1H, J = 8.0 Hz); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 166.7, 152.9, 137.9, 137.8, 136.5, 134.5, 131.9, 129.7, 126.5, 126.0, 124.3, 121.9, 99.3; IR (KBr, cm^{-1}): 3062, 2923, 2845, 1575, 1548, 1514, 1455, 1423, 1314, 1277, 1240, 1224, 1197, 1149, 1124, 1083, 1066, 1016, 959, 853, 775, 759, 738, 728; HRMS (ESI) calcd for $C_{13}H_7ClINS$ ($M + H^+$) 371.9110, found 371.9117.

2-(2-Bromophenyl)-3-phenylquinoxaline (20a):



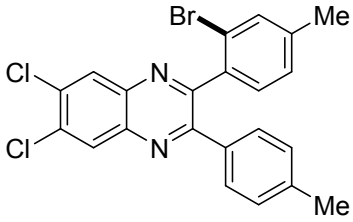
Gummy solid; ^1H NMR ($CDCl_3$, 400 MHz): δ 8.24 (d, 1H, J = 6.8 Hz), 8.19 (d, 1H, J = 7.6 Hz), 7.86–7.79 (m, 2H), 7.56–7.51 (m, 3H), 7.47 (d, 1H, J = 7.6 Hz), 7.39 (t, 1H, J = 7.4 Hz), 7.35–7.24 (m, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 153.7, 153.5, 141.9, 140.5, 138.5, 133.2, 131.6, 130.6, 130.4, 130.3, 129.8, 129.6, 129.5, 129.4, 129.1, 128.2, 127.7, 122.9; IR (KBr, cm^{-1}): 3059, 2928, 2850, 1631, 1563, 1558, 1477, 1431, 1395, 1345, 1261, 1215, 1126, 1077, 1055, 1026, 977, 802, 761, 730; HRMS (ESI) calcd for $C_{20}H_{13}BrN_2$ ($M + H^+$) 361.0340, found 361.0345.

2-(2-Bromo-4-methylphenyl)-3-(p-tolyl)quinoxaline (21a):



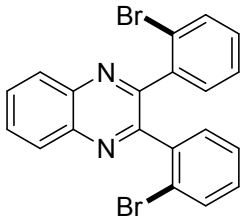
Gummy solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.19 (d, 1H, *J* = 8.4 Hz), 8.15 (d, 1H, *J* = 8.0 Hz), 7.80–7.73 (m, 2H), 7.41 (d, 2H, *J* = 8.0 Hz), 7.36–7.32 (m, 2H), 7.18 (d, 1H, *J* = 7.6 Hz), 7.08 (d, 2H, *J* = 8.0 Hz), 2.35 (s, 3H), 2.32 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 153.9, 153.6, 141.9, 140.8, 140.7, 139.0, 137.8, 135.8, 133.6, 131.3, 130.4, 129.9, 129.7, 129.5, 129.4, 128.9, 128.6, 122.5, 21.5, 21.2; IR (KBr, cm^{-1}): 3058, 3022, 2919, 2850, 1606, 1555, 1494, 1475, 1395, 1343, 1264, 1210, 1184, 1126, 1111, 1035, 1019, 977, 847, 821, 805, 762, 727, 709; HRMS (ESI) calcd for $C_{22}H_{17}BrN_2$ (M + H$^+$) 389.0653, found 389.0662.

2-(2-Bromo-4-methylphenyl)-6,7-dichloro-3-(p-tolyl)quinoxaline (22a):



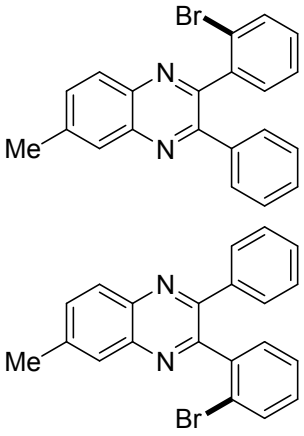
Gummy solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.31 (s, 1H), 8.27 (s, 1H), 7.41–7.37 (m, 3H), 7.32 (d, 1H, *J* = 7.6 Hz), 7.21 (d, 1H, *J* = 7.6 Hz), 7.09 (d, 2H, *J* = 8.0 Hz), 2.38 (s, 3H), 2.34 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 154.9, 154.6, 141.1, 140.7, 139.5, 135.1, 134.9, 134.4, 133.7, 131.1, 130.8, 130.1, 129.9, 129.7, 129.1, 128.7, 128.0, 122.3, 21.6, 21.2; IR (KBr, cm^{-1}): 3066, 3030, 2920, 2850, 1604, 1540, 1490, 1445, 1392, 1338, 1269, 1245, 1183, 1107, 1071, 1035, 1019, 964, 881, 855, 821, 800, 731, 705; HRMS (ESI) calcd for $C_{22}H_{15}BrCl_2N_2$ (M + H$^+$) 456.9874, found 456.9886.

2,3-Bis(2-bromophenyl)quinoxaline (20aa):



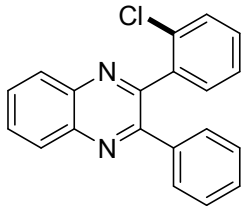
Gummy solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.26–8.23 (m, 2H), 7.88–7.86 (m, 2H), 7.54 (d, 2H, *J* = 7.6 Hz), 7.46 (d, 2H, *J* = 7.2 Hz), 7.26 (t, 2H, *J* = 7.6 Hz), 7.17 (t, 2H, *J* = 7.6 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 153.7, 141.3, 139.2, 132.9, 131.2, 130.8, 130.4, 129.6, 127.1, 123.0; IR (KBr, cm^{-1}): 3055, 2919, 1845, 1615, 1596, 1575, 1476, 1436, 1368, 1341, 1314, 1270, 1152, 1134, 1112, 1067, 1005, 979, 936, 879, 833, 814, 762, 726; HRMS (ESI) calcd for $C_{20}H_{12}Br_2N_2$ (M + H$^+$) 440.9425, found 440.9417.

2-(2-Bromophenyl)-6-methyl-3-phenylquinoxaline compound and 3-(2-Bromophenyl)-6-methyl-2-phenylquinoxaline (23a and 23a´):



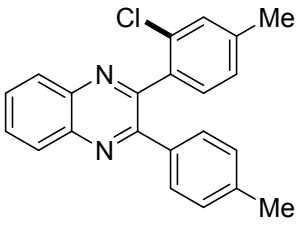
Gummy solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.11 (d, 1H, J = 8.4 Hz), 8.07 (d, 1H, J = 8.4 Hz), 8.00 (s, 1H), 7.96 (s, 1H), 7.64 (t, 2H, J = 9.2 Hz), 7.54–7.49 (m, 6H), 7.46–7.43 (m, 2H), 7.36 (t, 2H, J = 7.8 Hz), 7.31–7.22 (m, 8H), 2.62 (s, 3H), 2.61 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 153.6, 153.3, 152.9, 152.5, 142.0, 141.2, 140.9, 140.8, 140.6, 140.4, 139.3, 138.6, 133.1, 132.9, 132.6, 131.7, 131.6, 130.3, 129.79, 129.77, 129.1, 128.9, 128.89, 128.86, 128.3, 128.2, 128.1, 127.7, 127.1, 122.98, 122.90, 21.1; IR (KBr, cm^{-1}): 3058, 3022, 2921, 2844, 1618, 1595, 1587, 1559, 1488, 1428, 1344, 1263, 1243, 1219, 1199, 1183, 1158, 1137, 1119, 1079, 1070, 1040, 1024, 977, 883, 829, 805, 775, 763, 738, 710; HRMS (ESI) calcd for $C_{21}H_{15}BrN_2$ (M + H$^+$) 375.0497, found 375.0501.

2-(2-Chlorophenyl)-3-phenylquinoxaline (20b):



Gummy solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.23 (d, 1H, J = 8.4 Hz), 8.19 (d, 1H, J = 8.4 Hz), 7.85–7.79 (m, 2H), 7.53–7.50 (m, 3H), 7.37–7.27 (m, 6H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 154.1, 152.3, 141.9, 140.9, 138.7, 138.6, 133.1, 131.6, 130.6, 130.3, 130.2, 129.9, 129.6, 129.5, 129.4, 129.1, 128.3, 127.2; IR (KBr, cm^{-1}): 3056, 3030, 2915, 2853, 1558, 1543, 1478, 1442, 1433, 1395, 1346, 1263, 1219, 1126, 1079, 1045, 1024, 980, 915, 802, 763, 744, 730, 697; HRMS (ESI) calcd for $C_{20}H_{13}ClN_2$ (M + H$^+$) 317.0845, found 317.0851.

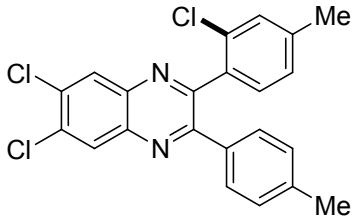
2-(2-Chloro-4-methylphenyl)-3-(p-tolyl)quinoxaline (21b):



Solid; M.p. 118 ^{o}C–121 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.20 (d, 1H, J = 8.0 Hz), 8.16 (d, 1H, J = 7.6 Hz), 7.83–7.74 (m, 2H), 7.43–7.38 (m, 3H), 7.17–7.14 (m, 2H), 7.09 (d, 2H, , J = 8.0 Hz), 2.37 (s, 3H), 2.33 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 154.1, 152.4, 141.9, 140.9, 140.6, 139.0, 135.9, 132.7, 131.3, 131.2, 130.4, 129.9, 129.5, 129.4, 129.3, 129.0, 128.1, 127.4, 21.5, 21.3; IR (KBr, cm^{-1}): 3060, 3028, 2919, 2855, 1609, 1475, 1392, 1340, 1220, 1210, 1185, 1126, 1075, 1037, 1020, 977, 956, 865, 821,

759, 730, 688; HRMS (ESI) calcd for $C_{22}H_{17}ClN_2$ (M + H^+) 345.1158, found 345.1165.

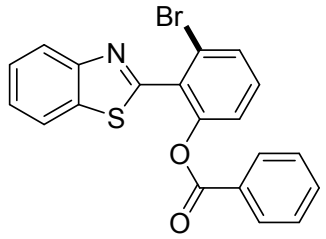
6,7-Dichloro-2-(2-chloro-4-methylphenyl)-3-(p-tolyl)quinoxaline (22b):

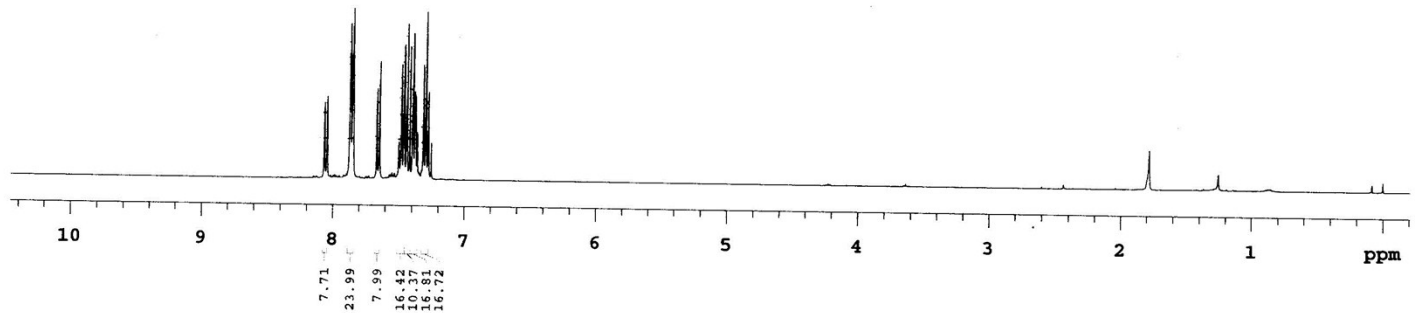


Gummy solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.31 (s, 1H), 8.26 (s, 1H), 7.39–7.36 (m, 3H), 7.18–7.14 (m, 2H), 7.09 (d, 2H, J = 8.4 Hz), 2.38 (s, 3H), 2.34 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 155.1, 153.5, 141.1, 140.7, 140.1, 139.6, 134.9, 134.4, 131.1, 131.0, 130.5, 130.1, 130.0, 129.9, 129.5, 129.1, 128.2, 127.5, 21.6, 21.3; IR (KBr, cm^{-1}): 3060, 3031, 2920, 2858, 1607, 1544, 1507, 1495, 1446, 1394, 1338, 1271, 1246, 1201, 1183, 1108, 1078, 1040, 1019, 964, 881, 820, 800, 732, 706; HRMS (ESI) calcd for $C_{22}H_{15}Cl_3N_2$ (M + H^+) 413.0379, found 413.0390.

Spectra

2-(Benzo[*d*]thiazol-2-yl)-3-bromophenyl benzoate (1a): ^{1}H NMR ($CDCl_3$, 400 MHz)





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Pulse 45.0 degrees
Acq. time 2.561 sec
Width 6398.0 Hz
32 repetitions

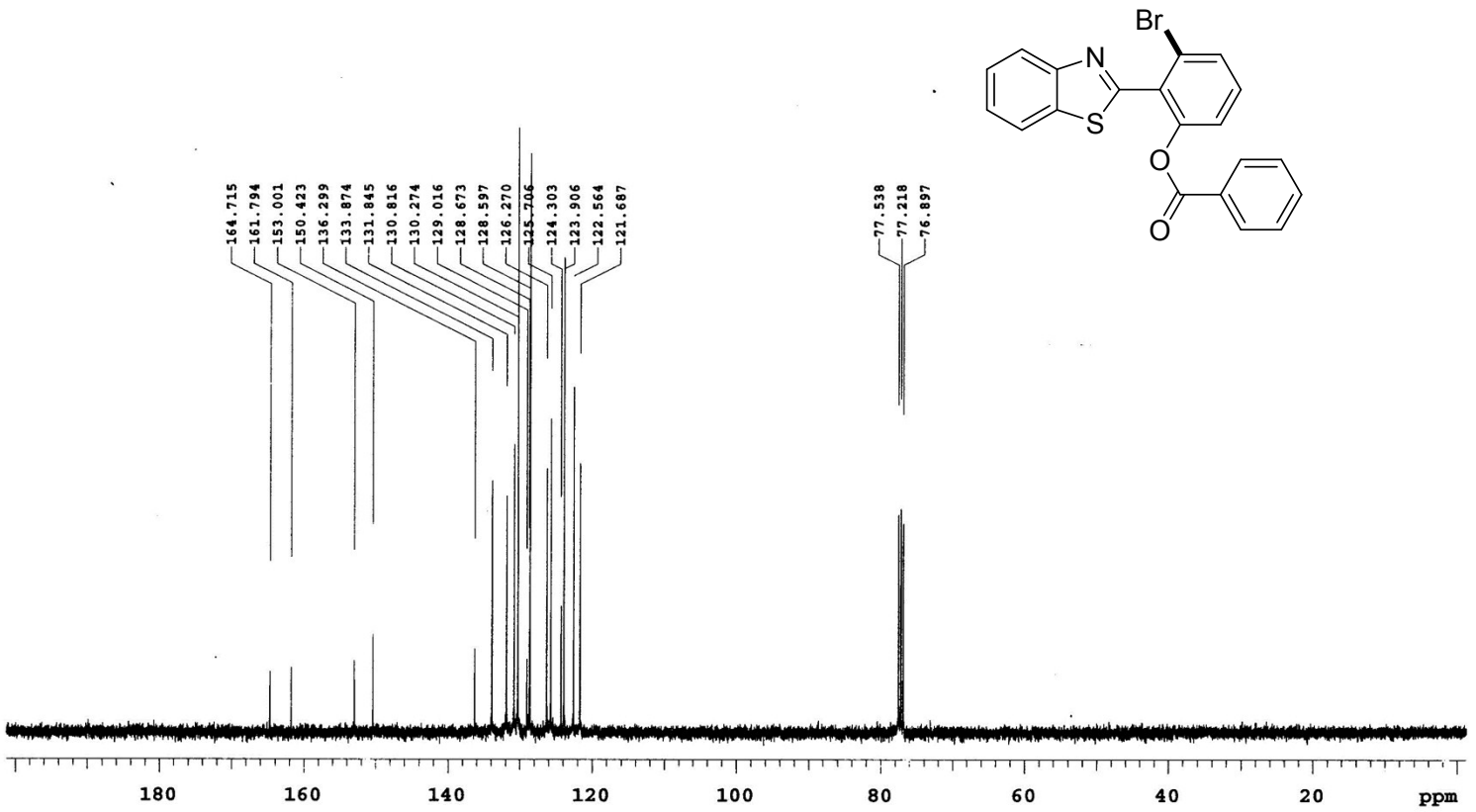
OBSERVE H1, 399.8509634

DATA PROCESSING
FT size 32768
Total time 1 minutes

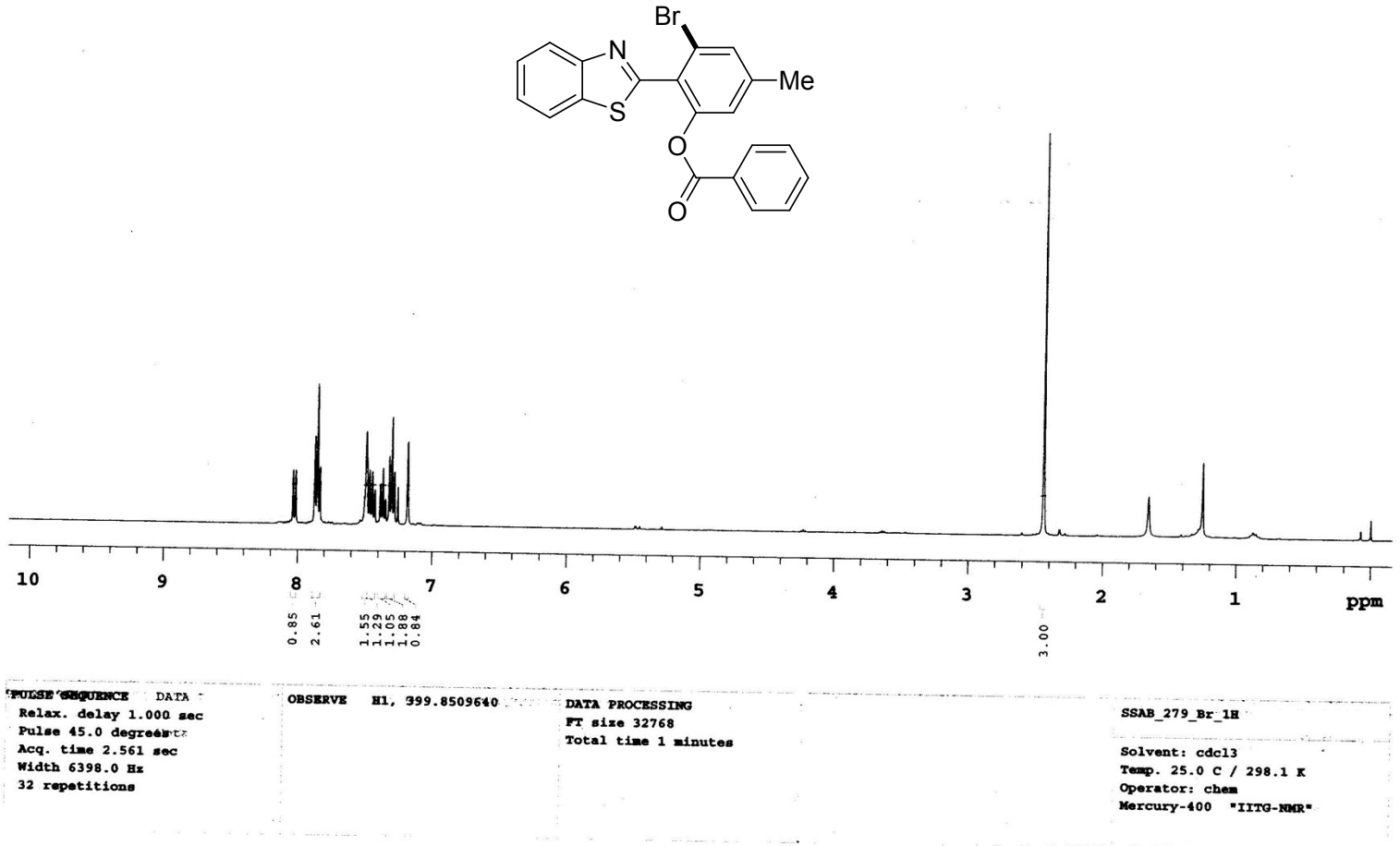
SSAB_256_Br-1H

Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: chem
Mercury-400 "IITG-NMR"

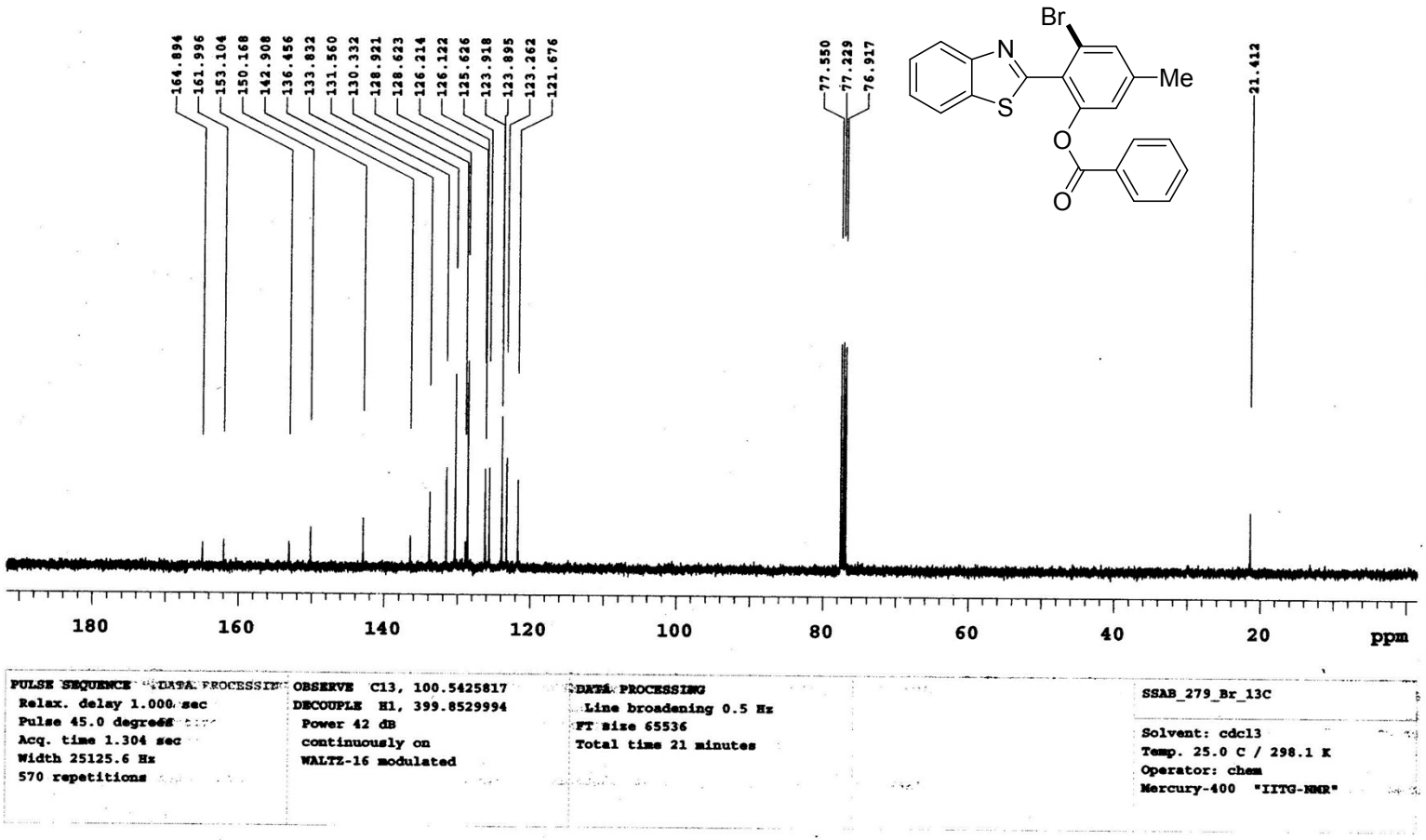
2-(Benzo[*d*]thiazol-2-yl)-3-bromophenyl benzoate (1a): ^{13}C NMR ($CDCl_3$, 100 MHz)



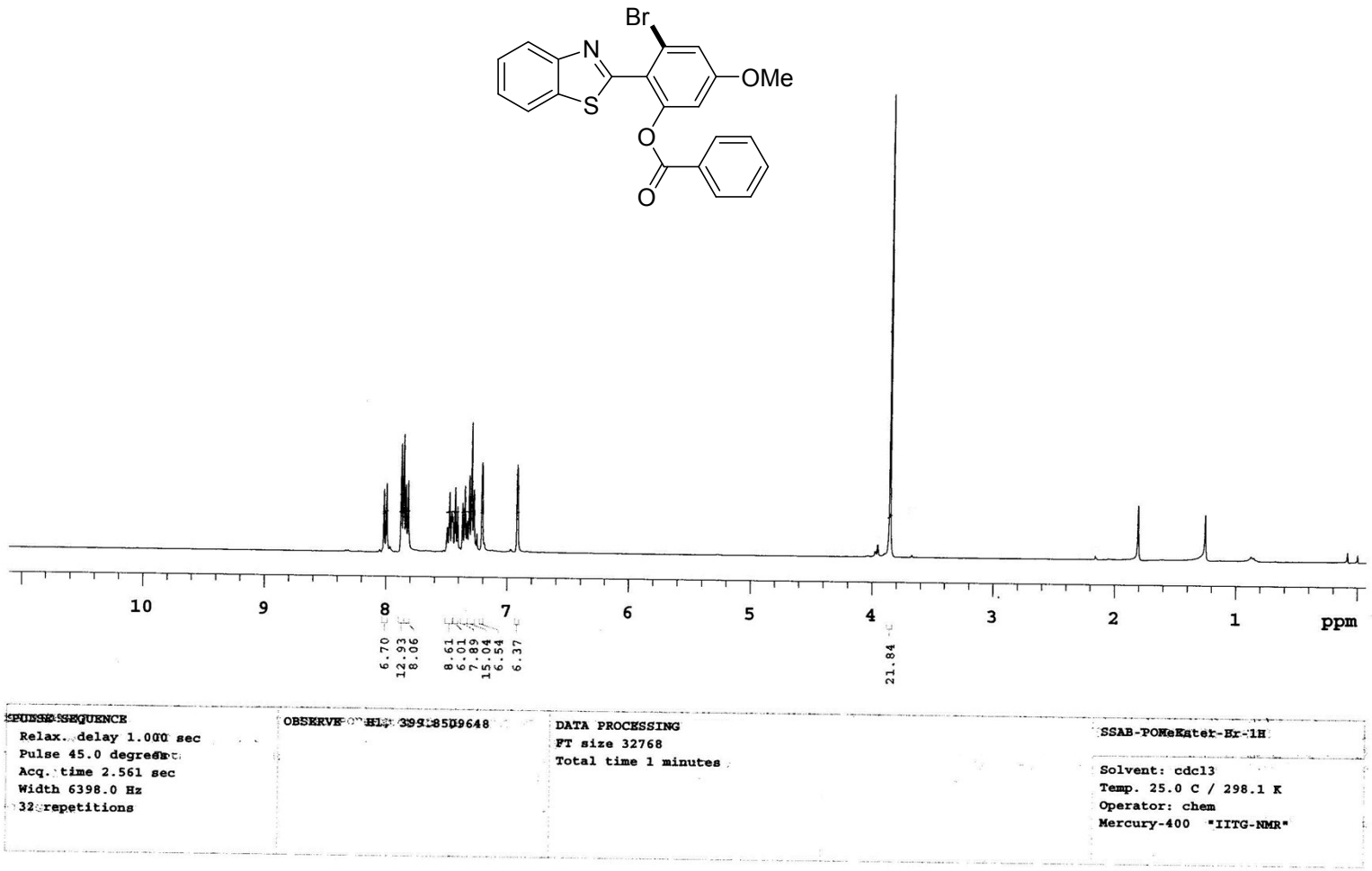
2-(Benzo[*d*]thiazol-2-yl)-3-bromo-5-methylphenyl benzoate (2a): ^{1}H NMR ($CDCl_3$, 400 MHz)



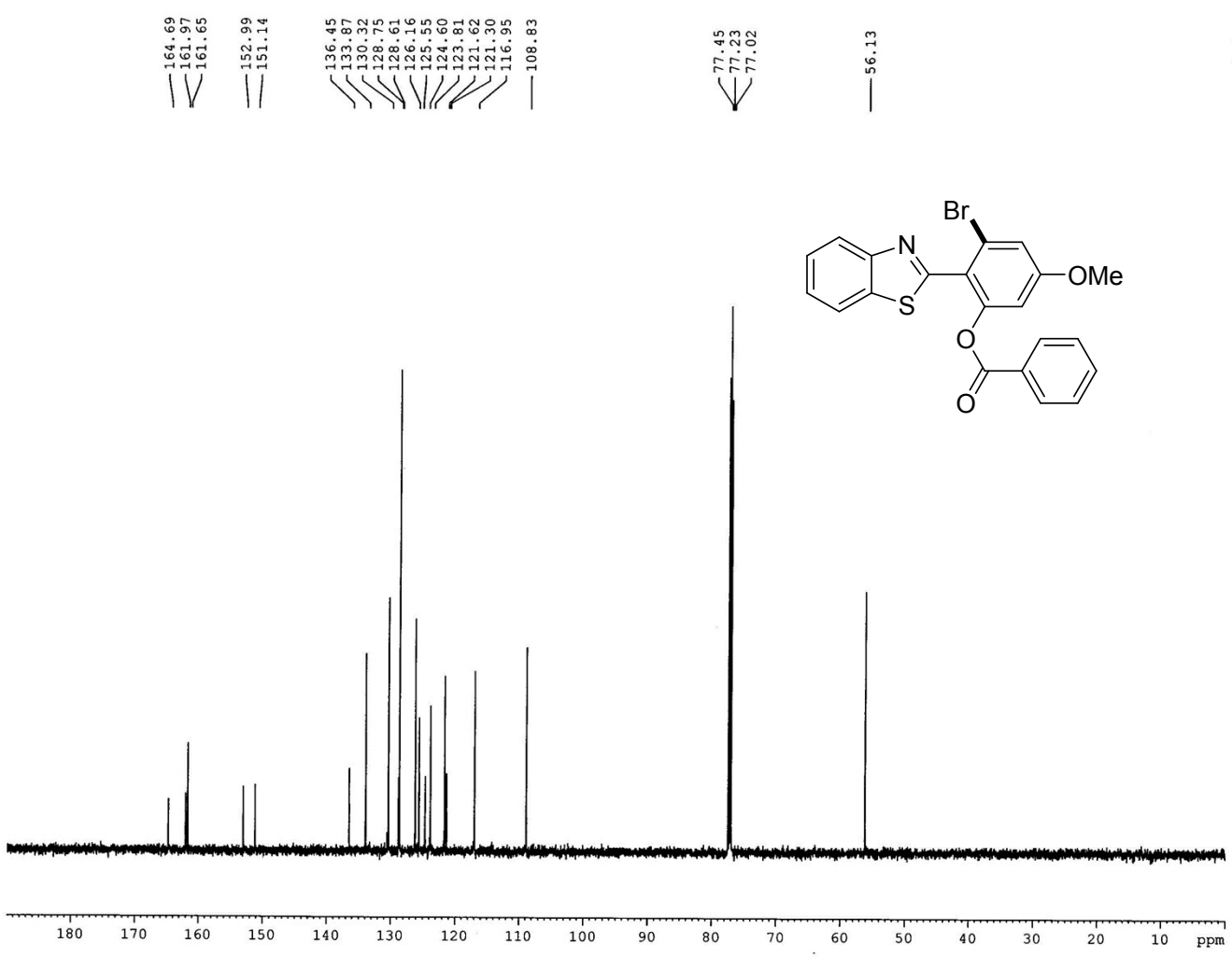
2-(Benzo[*d*]thiazol-2-yl)-3-bromo-5-methylphenyl benzoate (2a): ^{13}C NMR ($CDCl_3$, 100 MHz)



2-(Benzo[*d*]thiazol-2-yl)-3-bromo-5-methoxyphenyl benzoate (3a): ^{1}H NMR ($CDCl_3$, 400 MHz)



2-(Benzo[*d*]thiazol-2-yl)-3-bromo-5-methoxyphenyl benzoate (3a): ^{13}C NMR ($CDCl_3$, 150 MHz)



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PROCNO                   1

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PULPROG            zppg30
TD                  32768
SOLVENT             CDCl3
NS                    112
DS                      2
SWH             36057.691 Hz
FIDRES           1.100393 Hz
AQ               0.4543829 sec
RG                   65.24
DW                13.867 usec
DE                 6.50 usec
TE                 299.7 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          150.9279571 MHz
NUC1                   13C
P1                   10.50 usec
PLW1          95.00000000 W

======== CHANNEL f2 ========
SFO2          600.1724007 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2                70.00 usec
PLW2          21.00000000 W
PLW12          0.61714000 W
PLW13          0.30239999 W

F2 - Processing parameters
SI                    16384
SF            150.9128436 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
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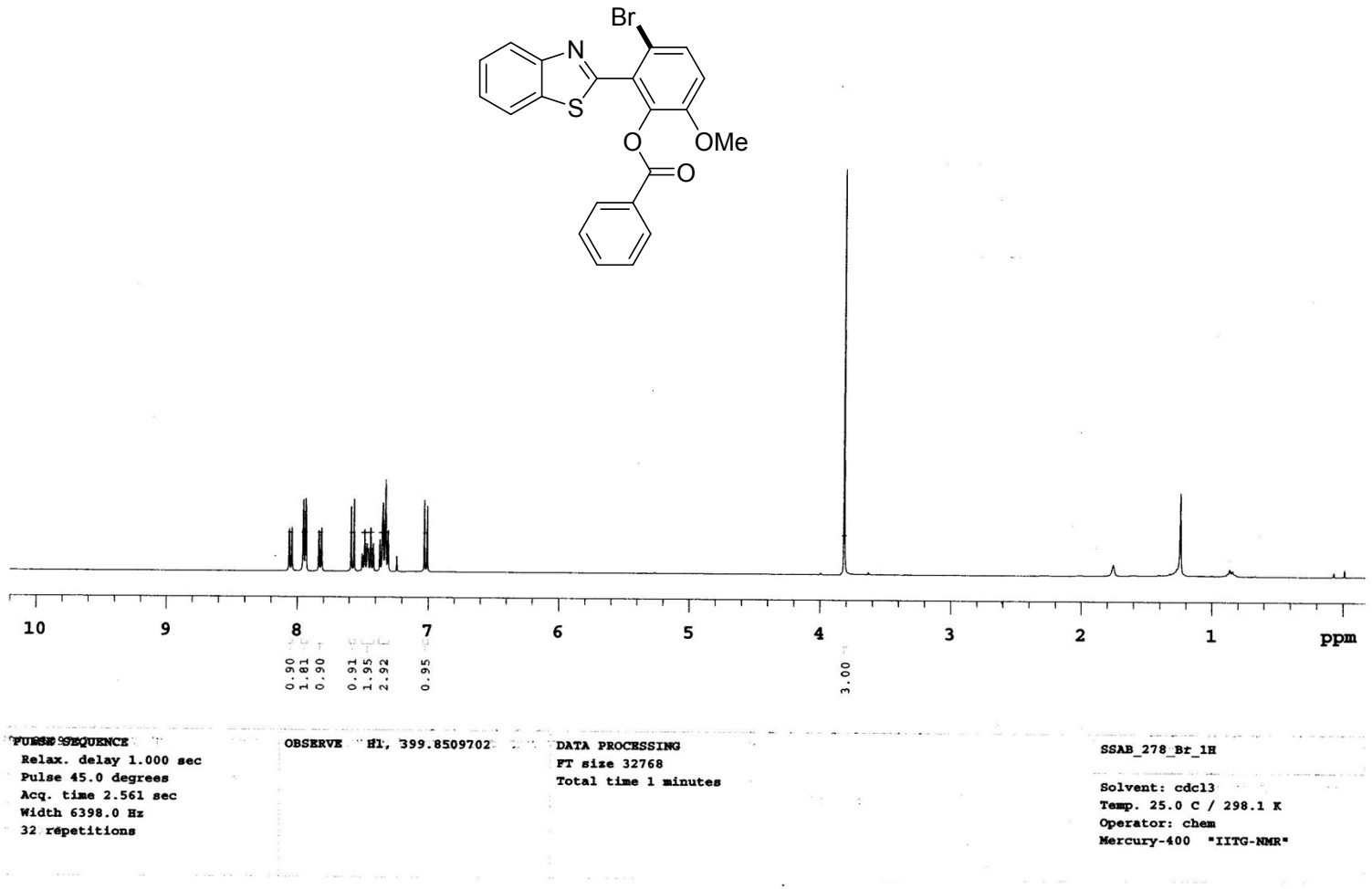
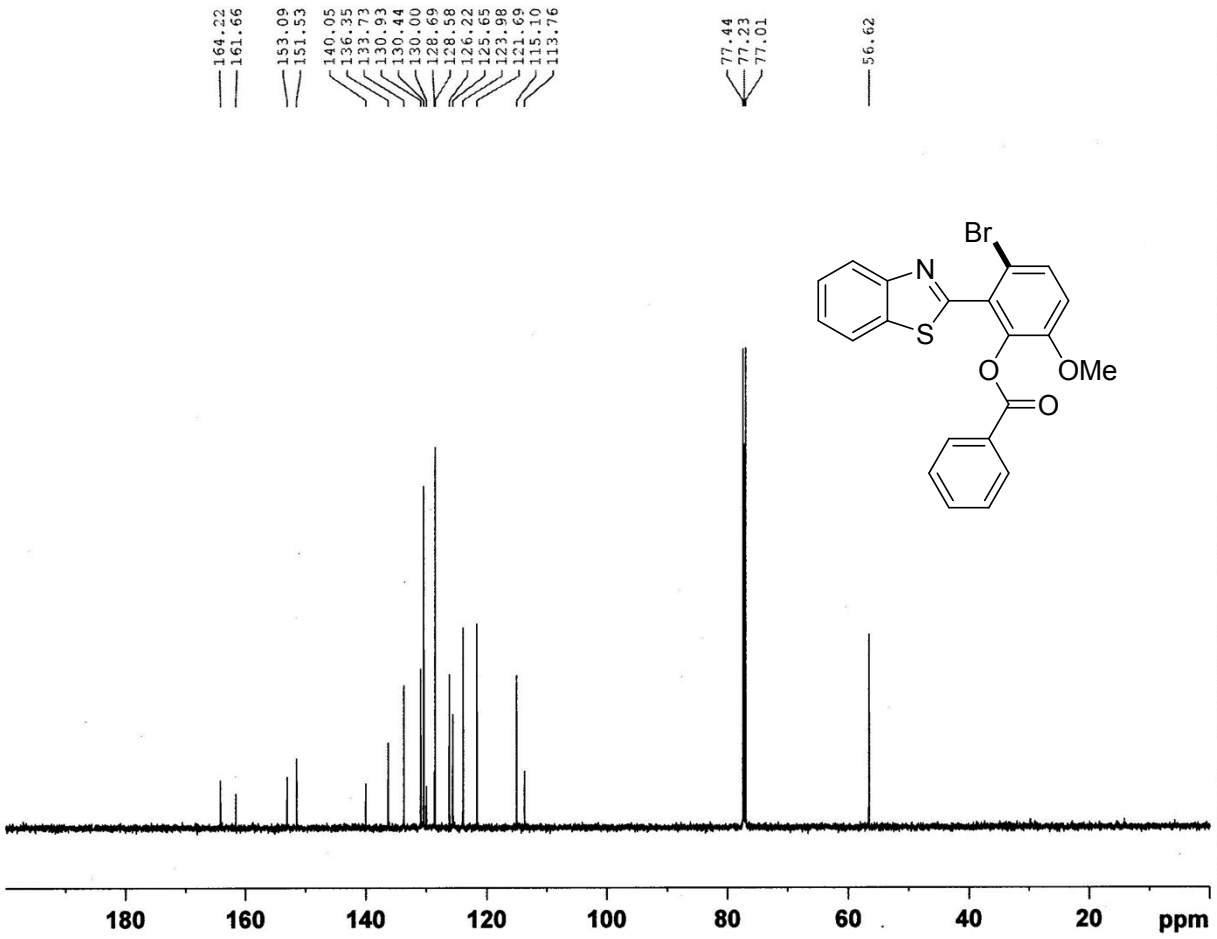
2-(Benzo[*d*]thiazol-2-yl)-3-bromo-6-methoxyphenyl benzoate (4a): ^{1}H NMR ($CDCl_3$, 400 MHz)



2-(Benzo[*d*]thiazol-2-yl)-3-bromo-6-methoxyphenyl benzoate (4a): ^{13}C NMR ($CDCl_3$, 150 MHz)



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Current Data Parameters
NAME      SSAB-278BR_13C
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
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PULPROG         zgpg30
TD              32768
SOLVENT          CDCl3
NS                 111
DS                   2
SWH          36057.691 Hz
FIDRES        1.100393 Hz
AQ           0.4543829 sec
RG               65.24
DW              13.867 usec
DE               6.50 usec
TE              301.2 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1       150.9279571 MHz
NUC1               13C
P1               10.50 usec
PLW1       95.00000000 W

======== CHANNEL f2 ========
SFO2       600.1724007 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            70.00 usec
PLW2       21.00000000 W
PLW12       0.61714000 W
PLW13       0.30239999 W

F2 - Processing parameters
SI                16384
SF         150.9128435 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
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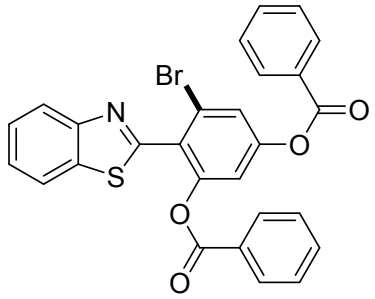
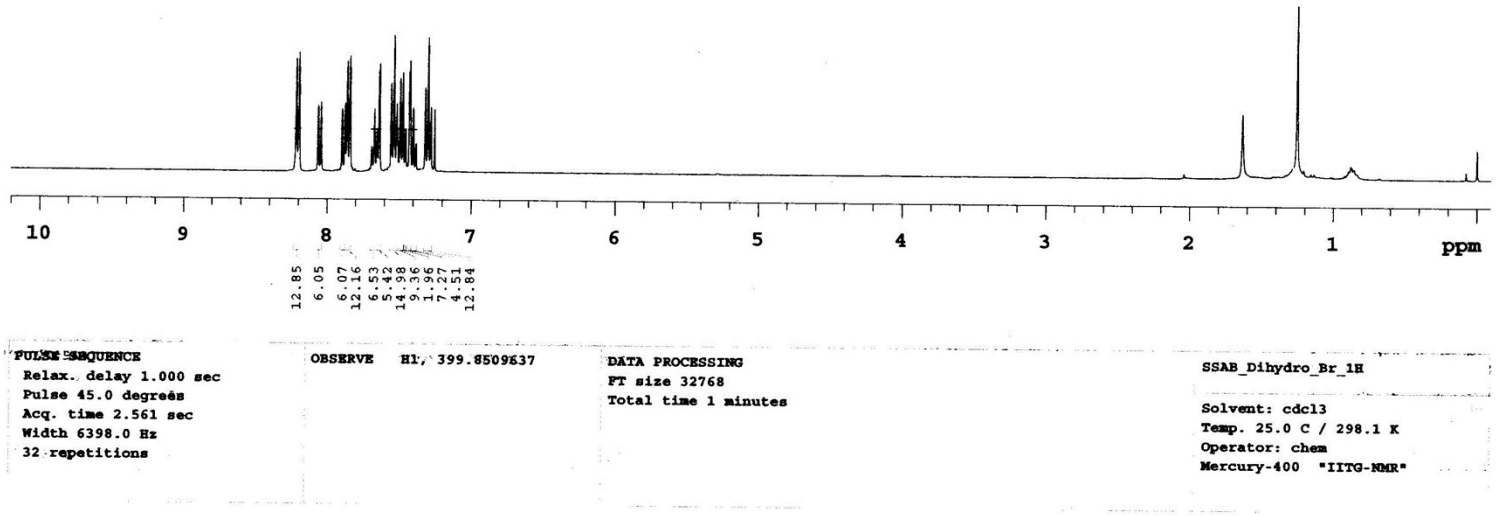
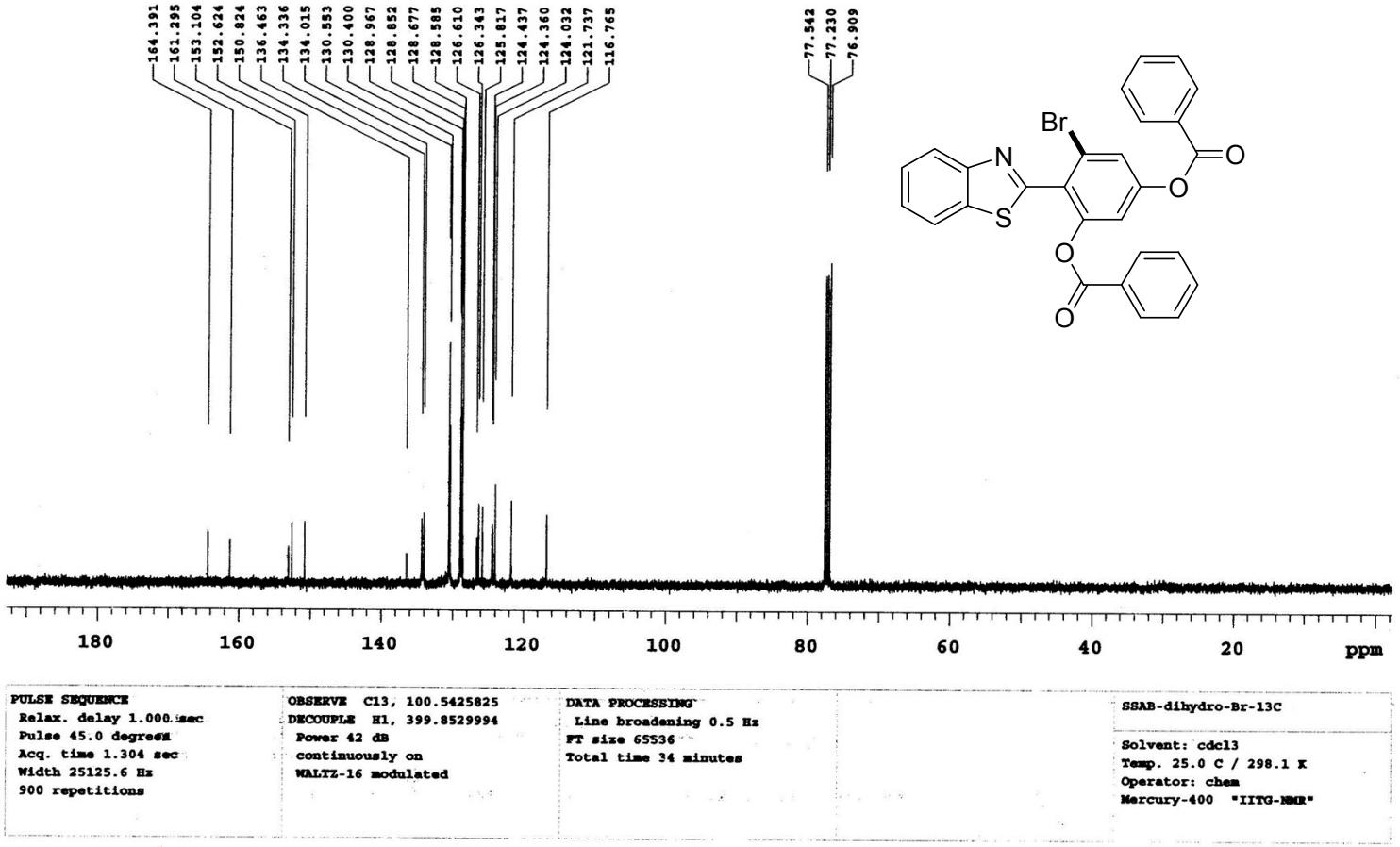
4-(Benzo[*d*]thiazol-2-yl)-5-bromo-1,3-phenylene dibenzoate (5a): ^{1}H NMR ($CDCl_3$, 400 MHz)

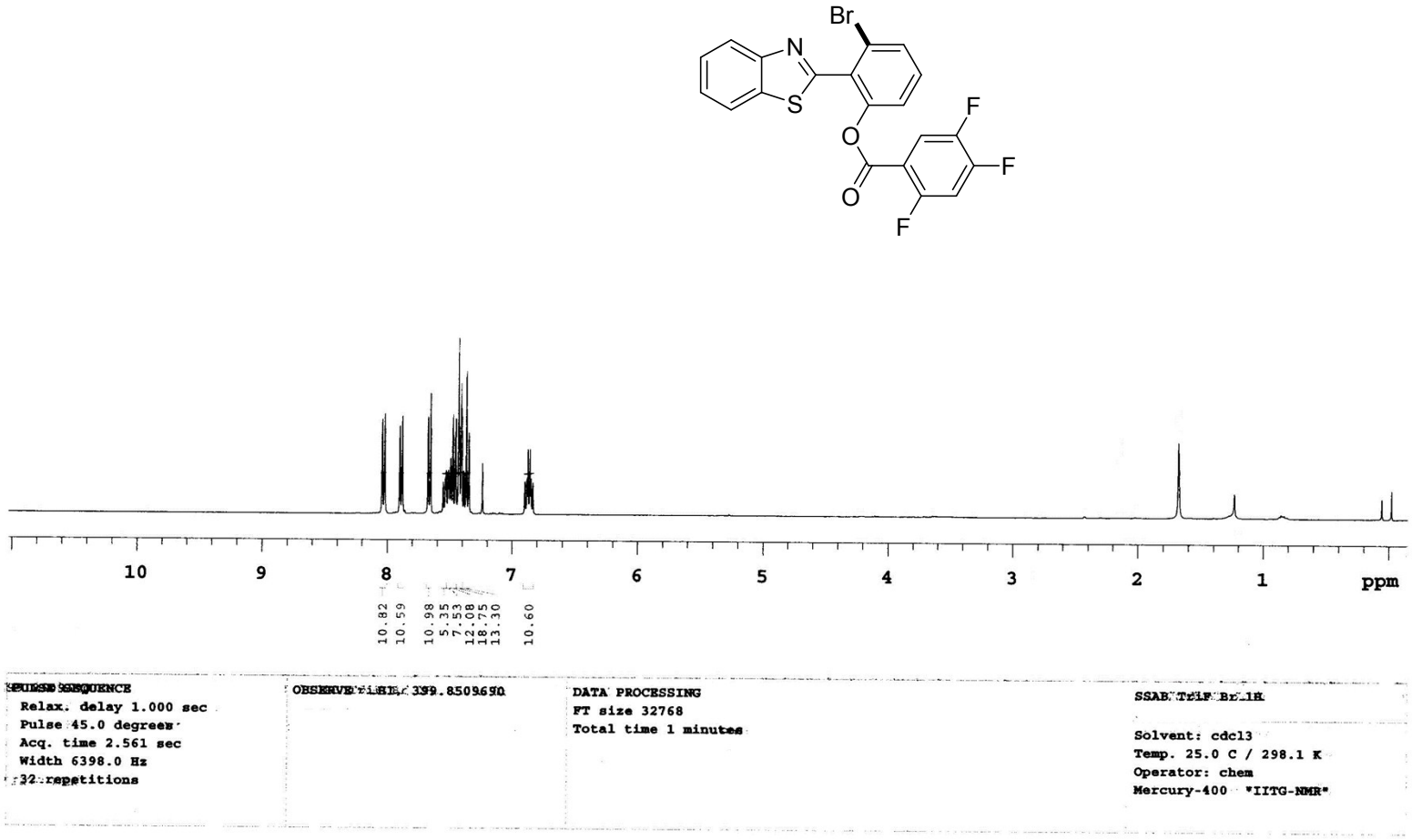




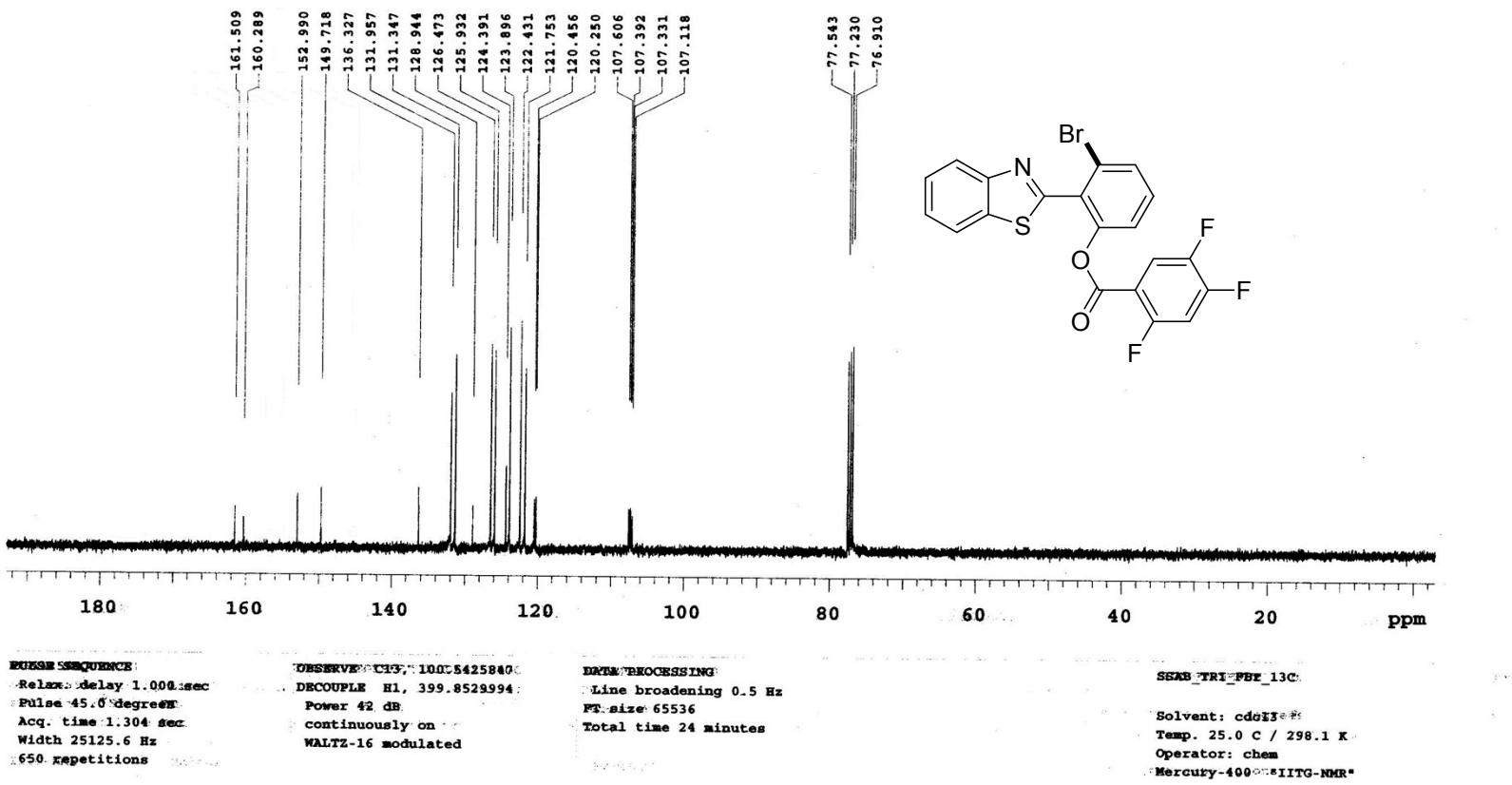
4-(Benzo[*d*]thiazol-2-yl)-5-bromo-1,3-phenylene dibenzoate (5a): ^{13}C NMR ($CDCl_3$, 100 MHz)



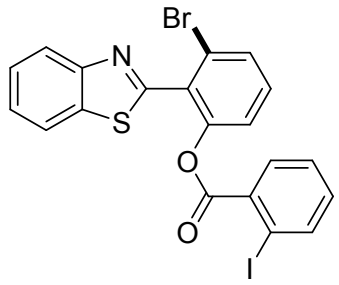
2-(Benzo[*d*]thiazol-2-yl)-3-bromophenyl 2,4,5-trifluorobenzoate (6a): ^{1}H NMR ($CDCl_3$, 400 MHz)

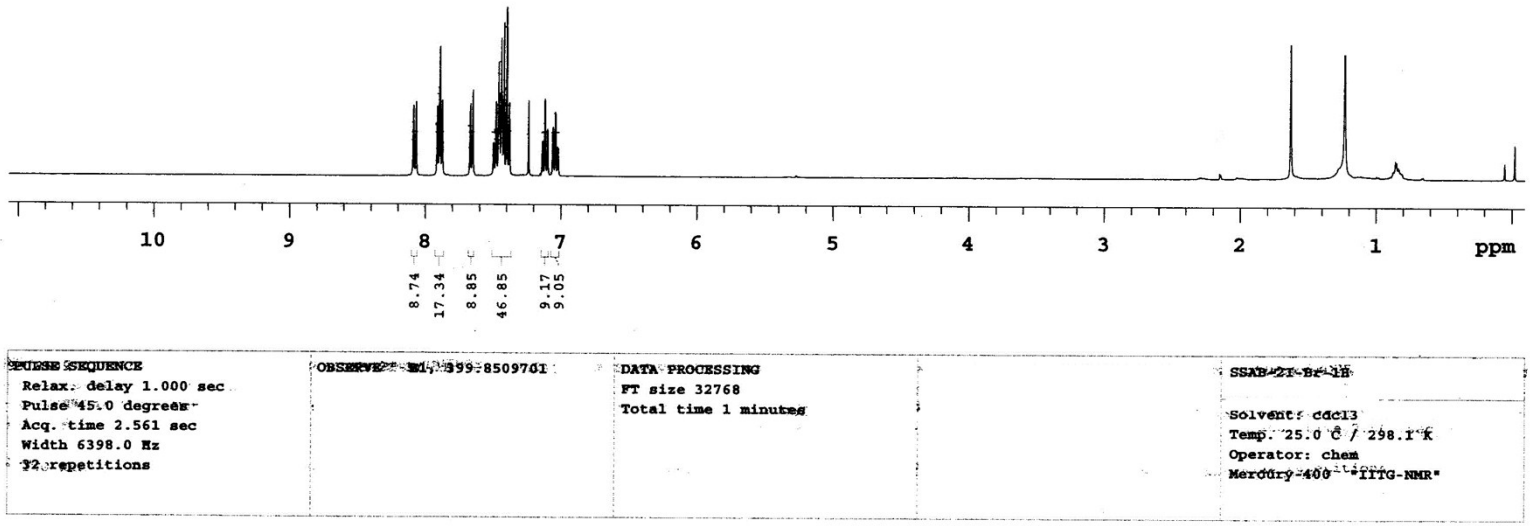


2-(Benzo[*d*]thiazol-2-yl)-3-bromophenyl 2,4,5-trifluorobenzoate (6a): ^{13}C NMR ($CDCl_3$, 100 MHz)

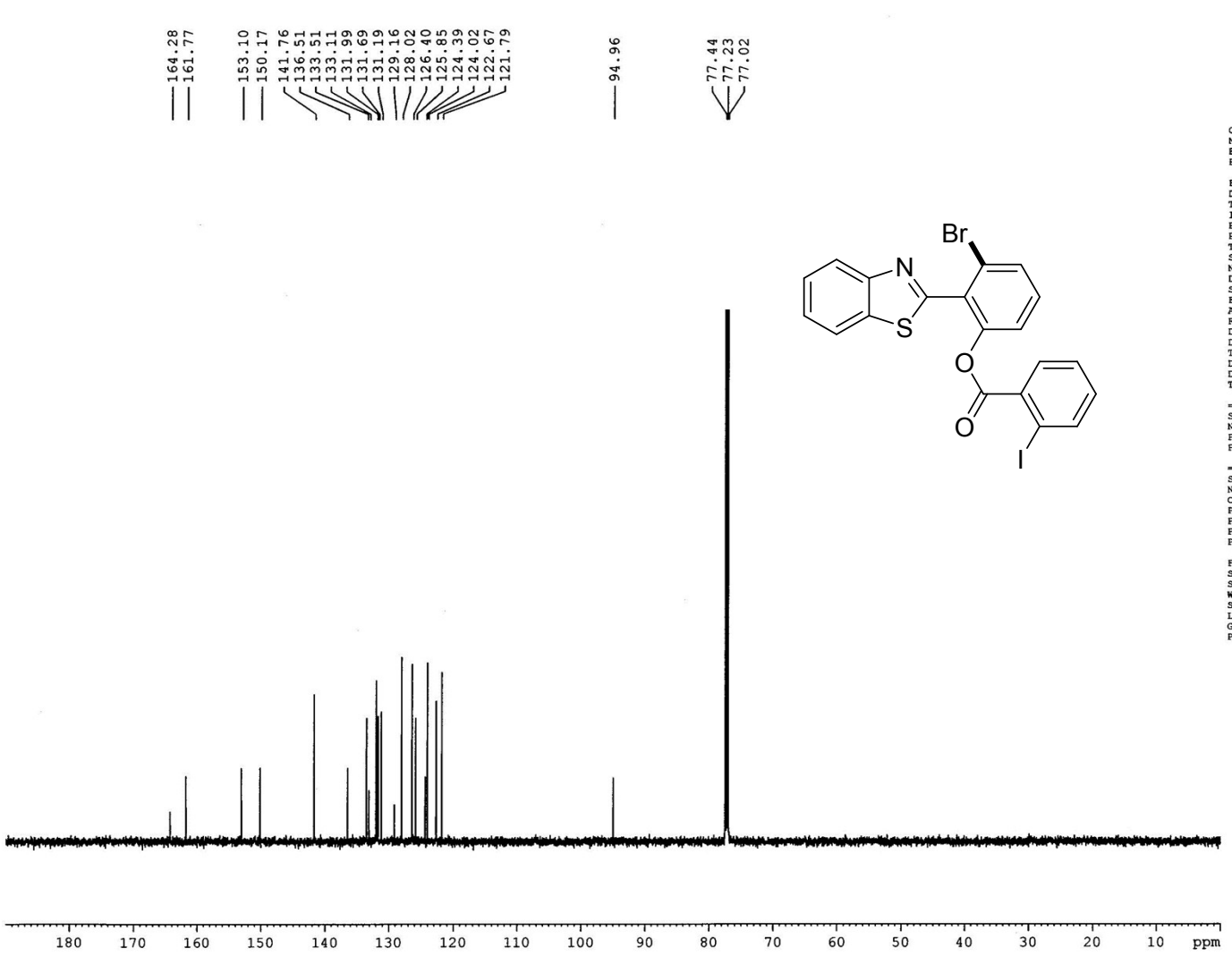


2-(Benzo[*d*]thiazol-2-yl)-3-bromophenyl 2-iodobenzoate (7a): ^{1}H NMR ($CDCl_3$, 400 MHz)





2-(Benzo[*d*]thiazol-2-yl)-3-bromophenyl 2-iodobenzoate (7a): ^{13}C NMR ($CDCl_3$, 150 MHz)

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TD              32768
SOLVENT           CDCl3
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FIDRES        1.100393 Hz
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RG                65.24
DW               13.867 usec
DE                6.50 usec
TE                299.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        150.9279571 MHz
NUC1                13C
P1                10.50 usec
PLW1        95.00000000 W

======== CHANNEL f2 ========
SFO2        600.1724007 MHz
NUC2                1H
CPDPRG[2          waltz16
PCPD2             70.00 usec
PLW2        21.00000000 W
PLW12        0.61714000 W
PLW13        0.30239999 W

F2 - Processing parameters
SI                 16384
SF          150.9128375 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
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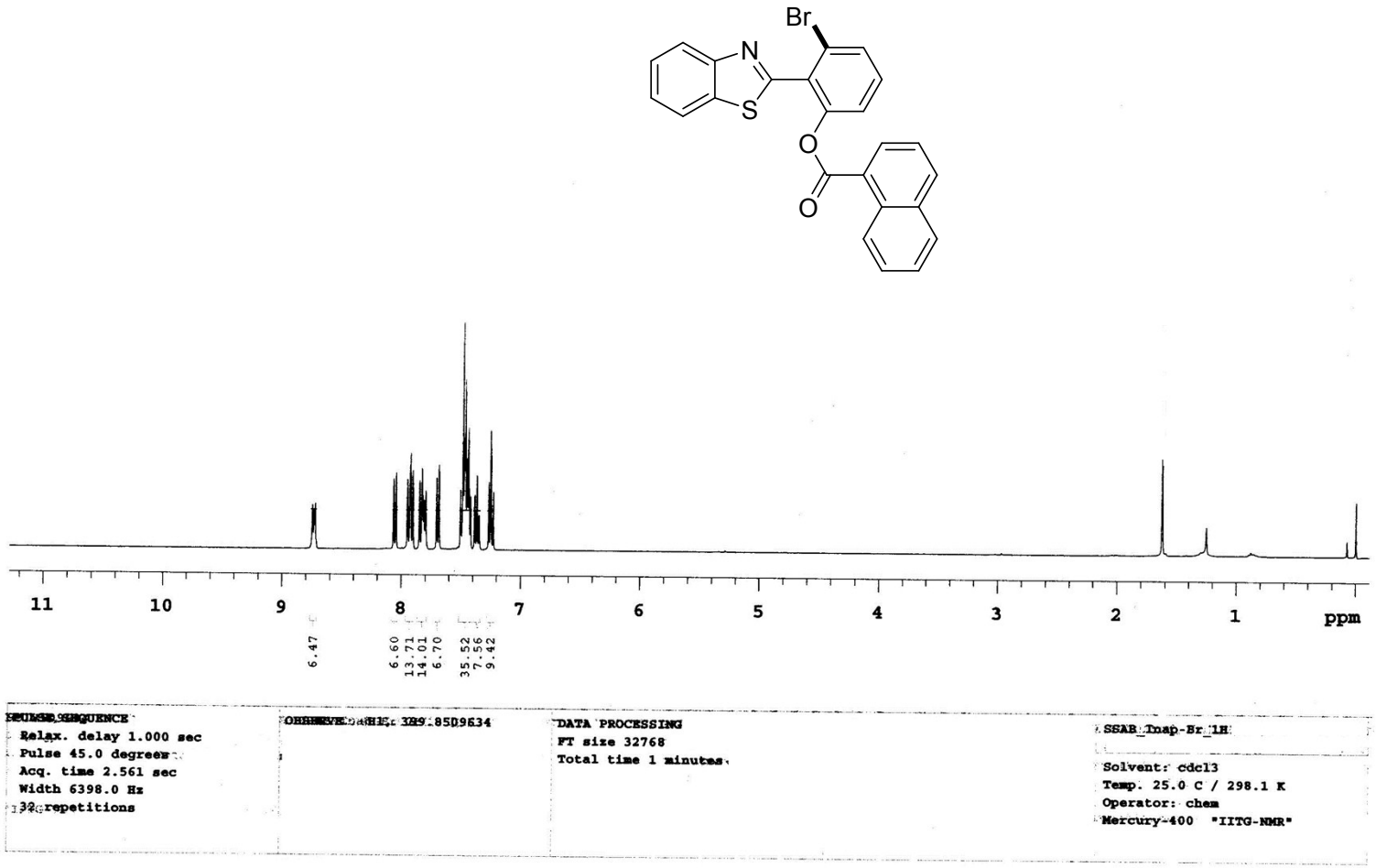
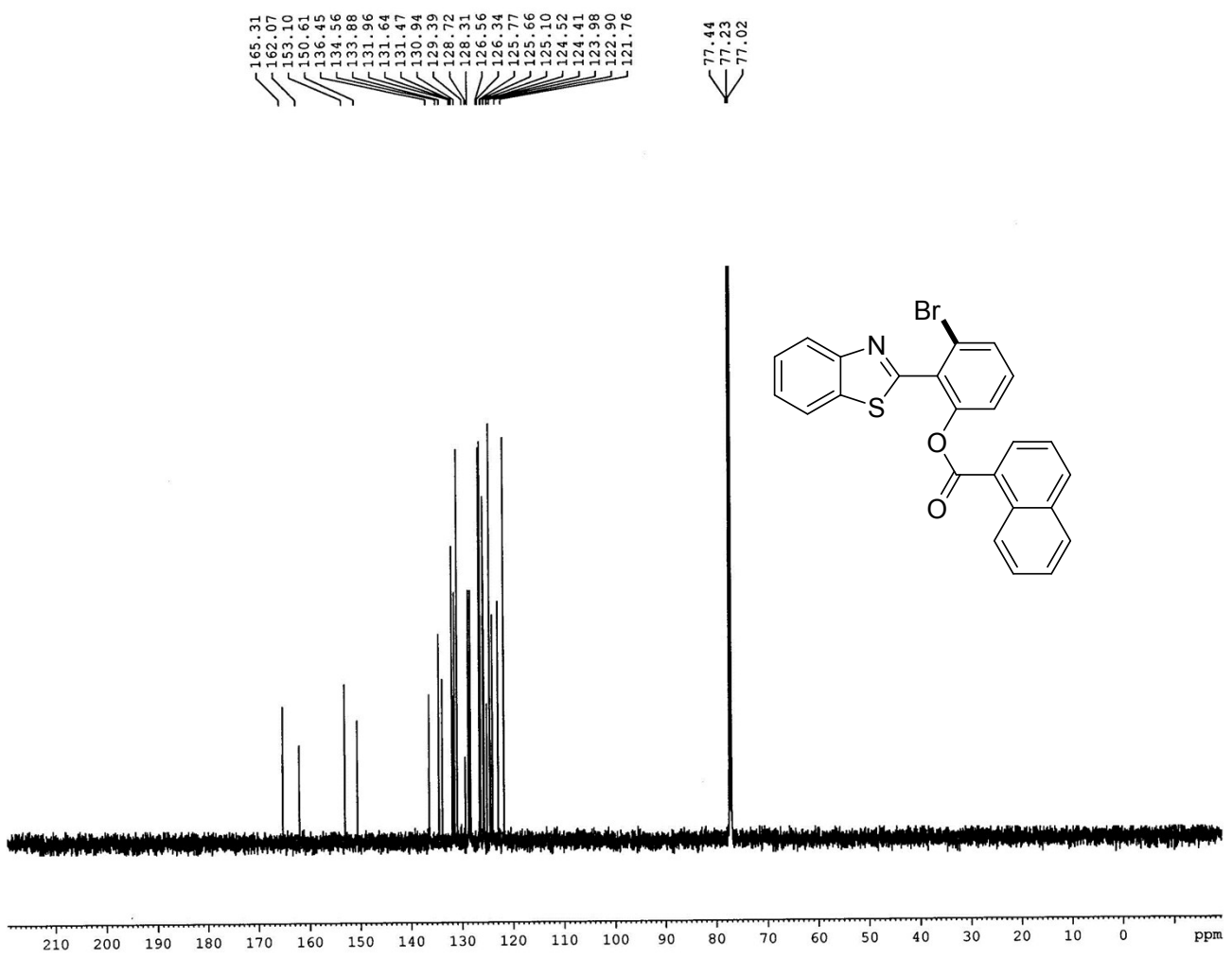
2-(Benzo[*d*]thiazol-2-yl)-3-bromophenyl 1-naphthoate (8a): ^{1}H NMR ($CDCl_3$, 400 MHz)



2-(Benzo[*d*]thiazol-2-yl)-3-bromophenyl 1-naphthoate (8a): ^{13}C NMR ($CDCl_3$, 150 MHz)



BRUKER

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Current Data Parameters
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EXPNO                  1
PROCNO                 1

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SWH           36057.691 Hz
FIDRES         1.100393 Hz
AQ             0.4543829 sec
RG                65.24
DW               13.867 usec
DE                6.50 usec
TE               299.6 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        150.9279571 MHz
NUC1               13C
P1               10.50 usec
PLW1        95.00000000 W

======== CHANNEL f2 ========
SFO2        600.1724007 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            70.00 usec
PLW2        21.00000000 W
PLW12        0.61714000 W
PLW13        0.30239999 W

F2 - Processing parameters
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SF          150.9128375 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
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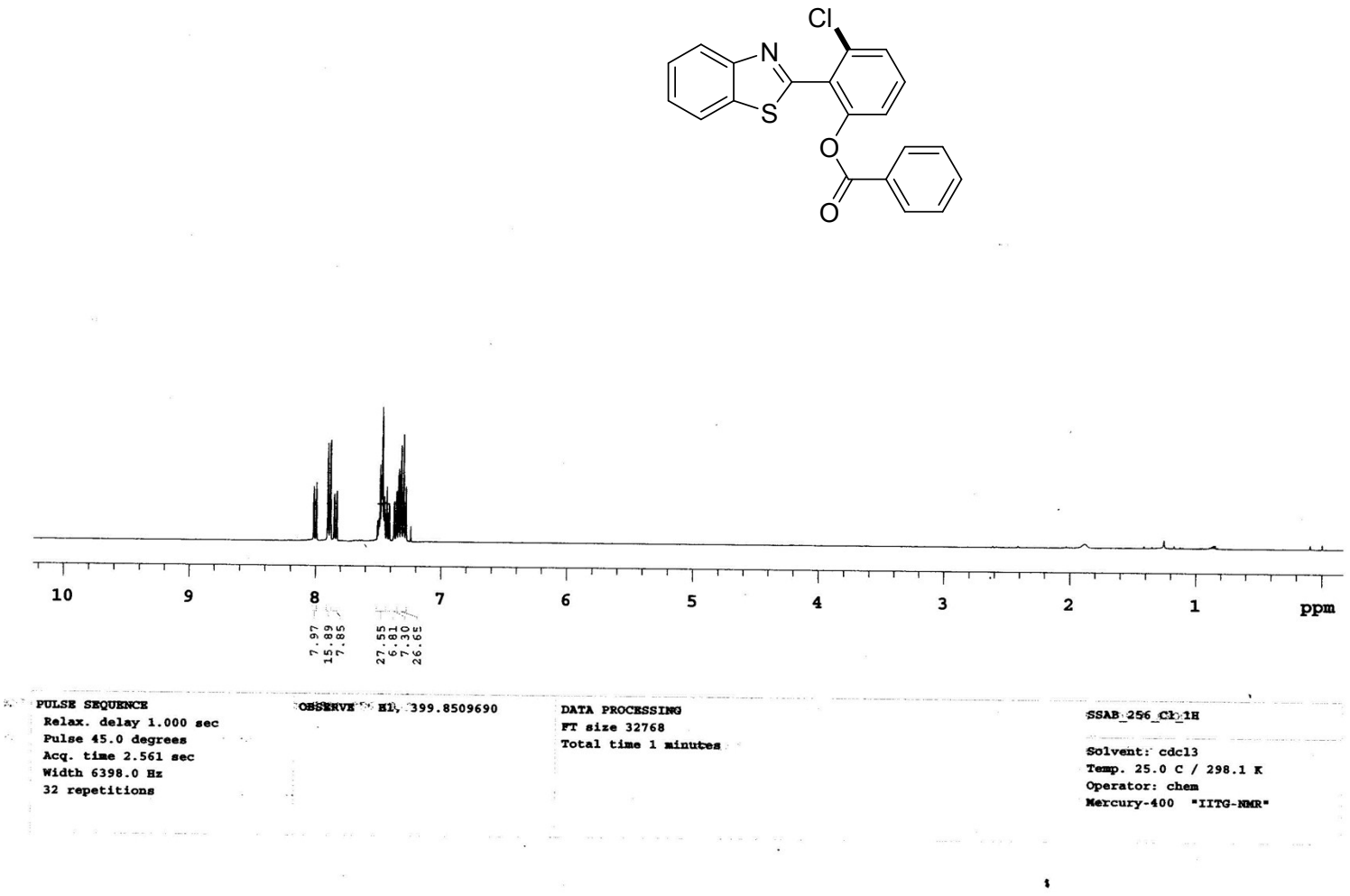
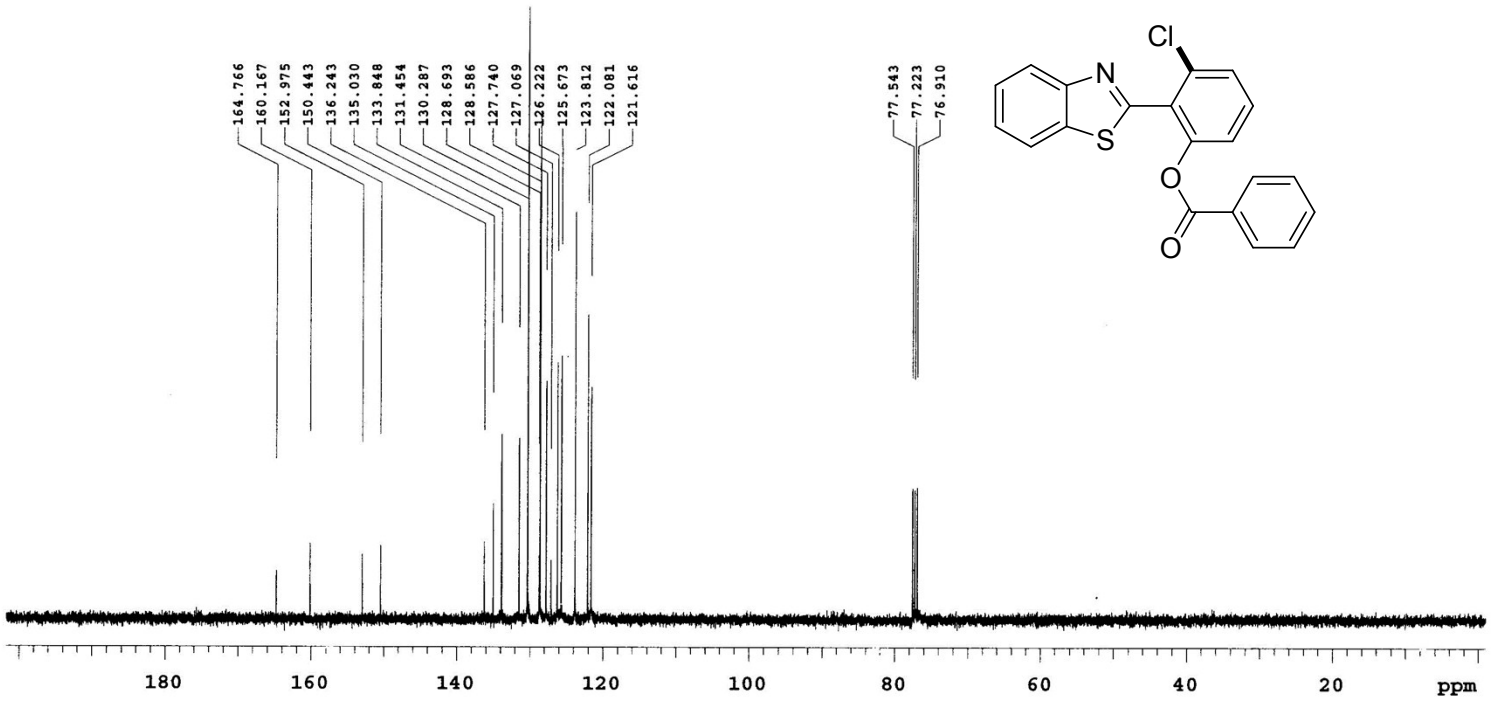
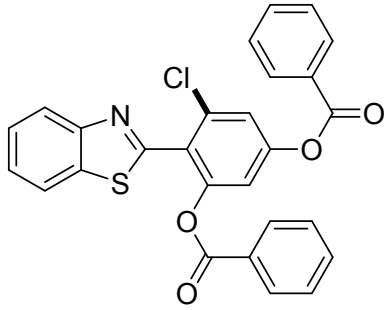
2-(Benzo[*d*]thiazol-2-yl)-3-chlorophenyl benzoate (1b): ^{1}H NMR ($CDCl_3$, 400 MHz)

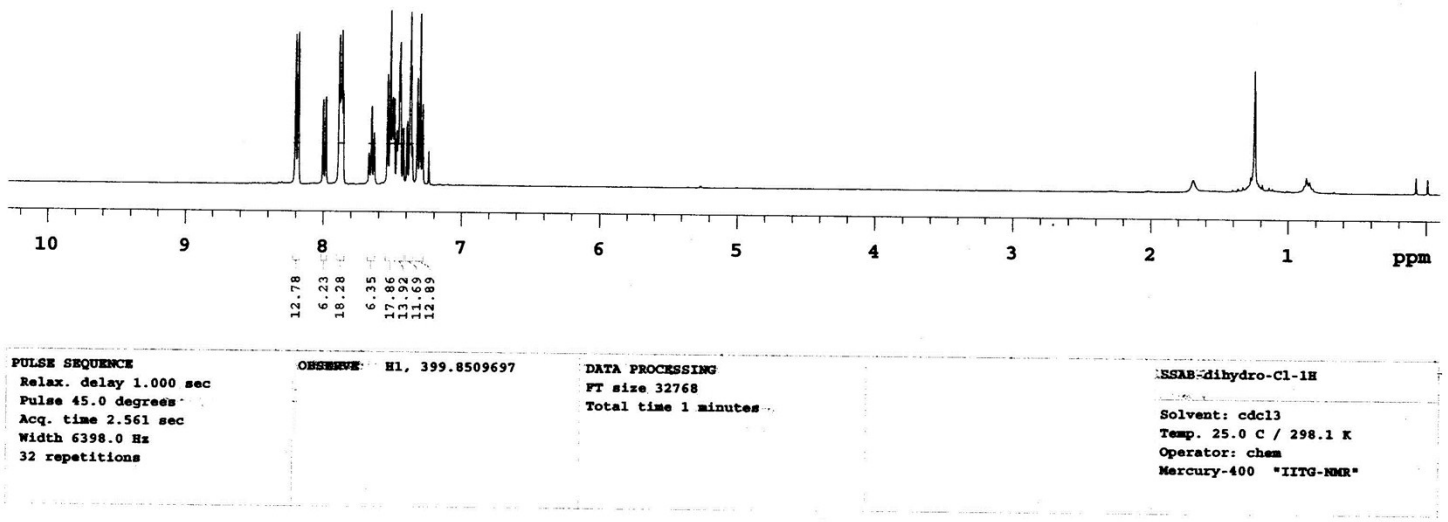


2-(Benzo[*d*]thiazol-2-yl)-3-chlorophenyl benzoate (1b): ^{13}C NMR ($CDCl_3$, 100 MHz)

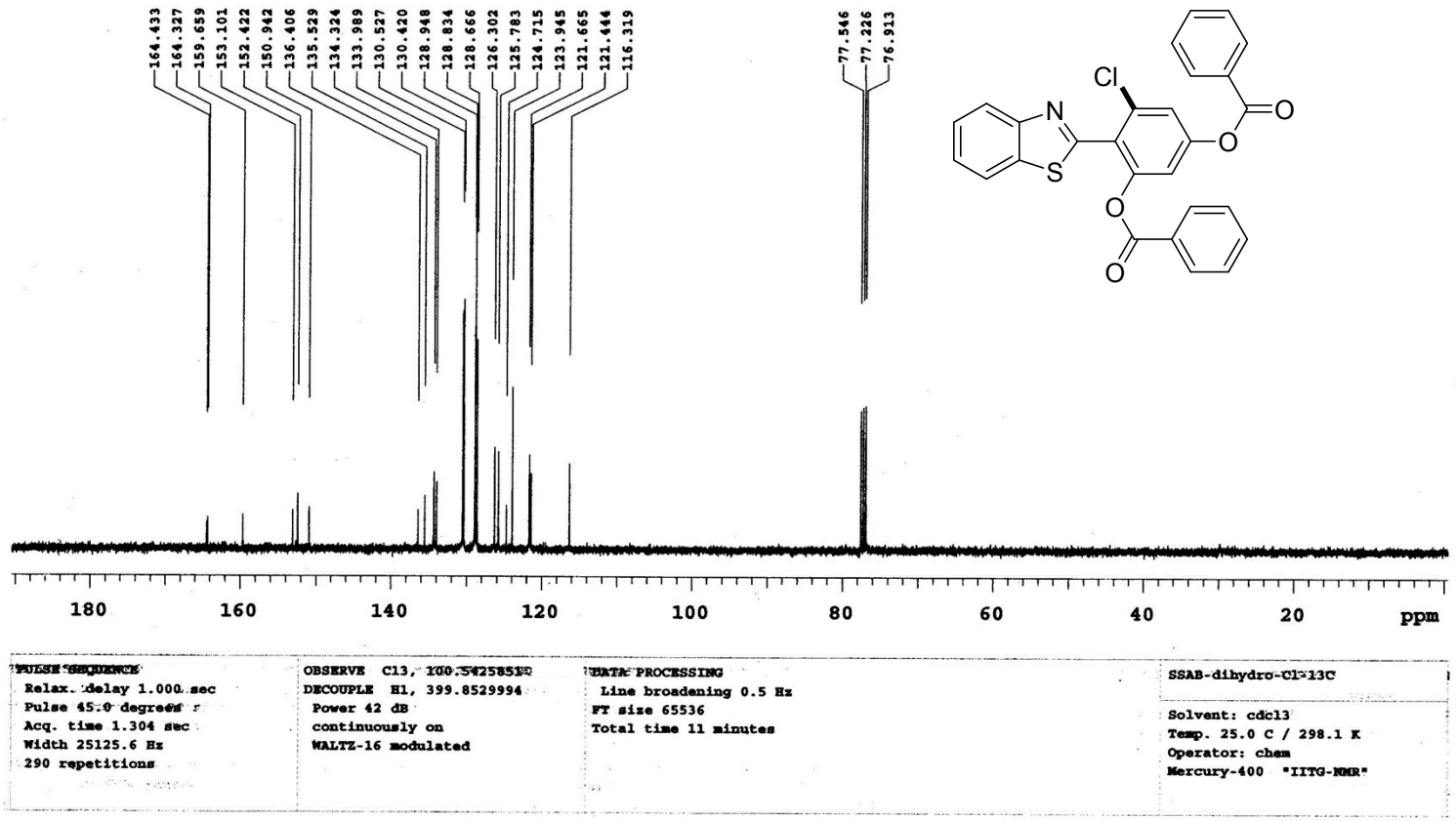


4-(Benzo[*d*]thiazol-2-yl)-5-chloro-1,3-phenylene dibenzoate (5b): ^{1}H NMR ($CDCl_3$, 400 MHz)

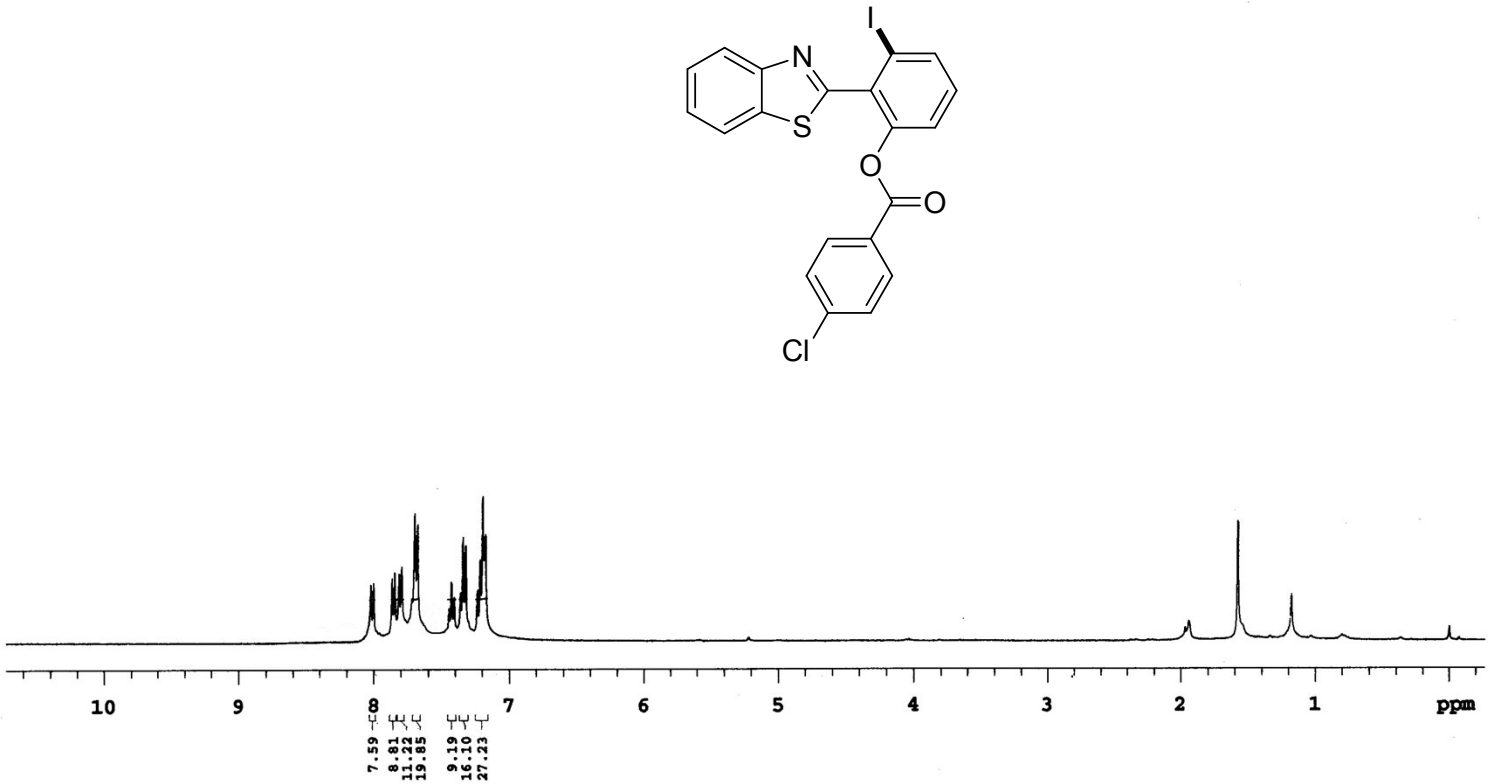




4-(Benzo[*d*]thiazol-2-yl)-5-chloro-1,3-phenylene dibenzoate (5b): ^{13}C NMR ($CDCl_3$, 100 MHz)

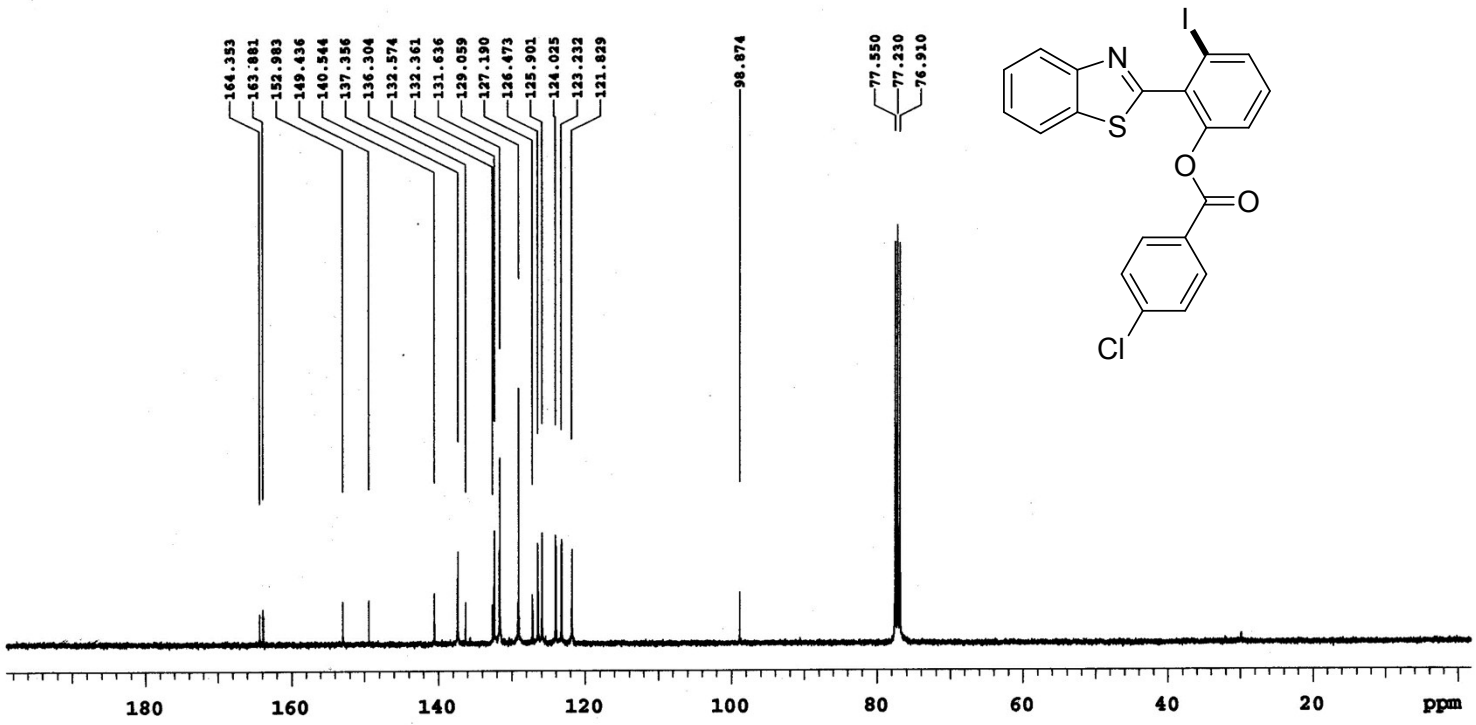


2-(Benzo[*d*]thiazol-2-yl)-3-iodophenyl 4-chlorobenzoate (9c): ^{1}H NMR ($CDCl_3$, 400 MHz)



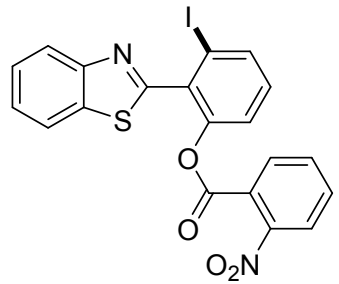
PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	OBSERVE H1, 399.8509926	DATA PROCESSING FT size 32768 Total time 1 minutes		SSAB-PClE-I-1H Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem File: SSAB-PClE-I-1H Mercury-400 "IITG-NMR"

2-(Benzo[*d*]thiazol-2-yl)-3-iodophenyl 4-chlorobenzoate (9c): ^{13}C NMR ($CDCl_3$, 100 MHz)



PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 14430 repetitions	OBSERVE C13, 100.5425824 DECOUPLE H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 5.2 hours		SSAB_PC1E_13C Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem File: SSAB_PC1E_13C Mercury-400 "IITG-NMR"

2-(Benzo[*d*]thiazol-2-yl)-3-iodophenyl 2-nitrobenzoate (10c): ^{1}H NMR ($CDCl_3$, 600 MHz)

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Current Data Parameters
NAME          SSAB-100-1H
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20141009
Time                10.21
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             12019.230 Hz
FIDRES          0.366798 Hz
AQ              1.3631488 sec
RG                   113
DW                41.600 usec
DE                 6.50 usec
TE                298.3 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          600.1737063 MHz
NUC1                  1H
P1                 12.00 usec
PLW1          21.00000000 W

F2 - Processing parameters
SI                 16384
SF            600.1700152 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz ,
GB        0
PC                 1.00
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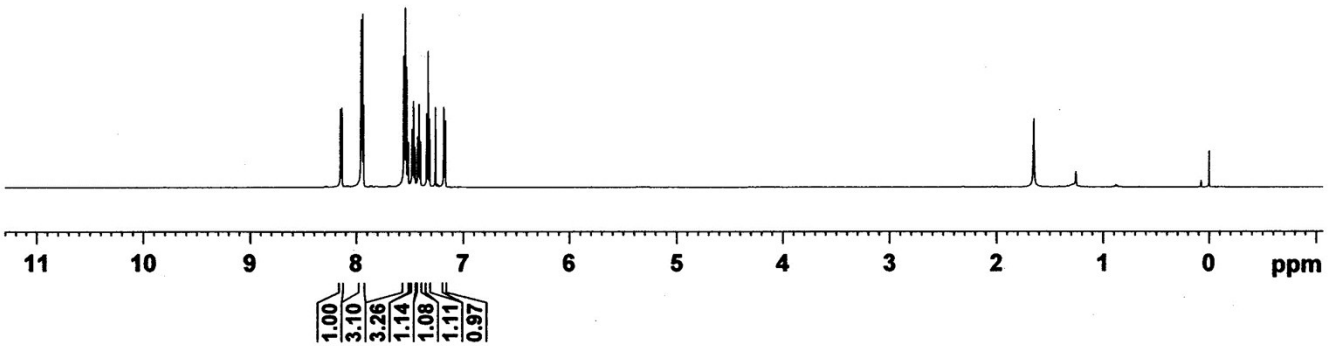
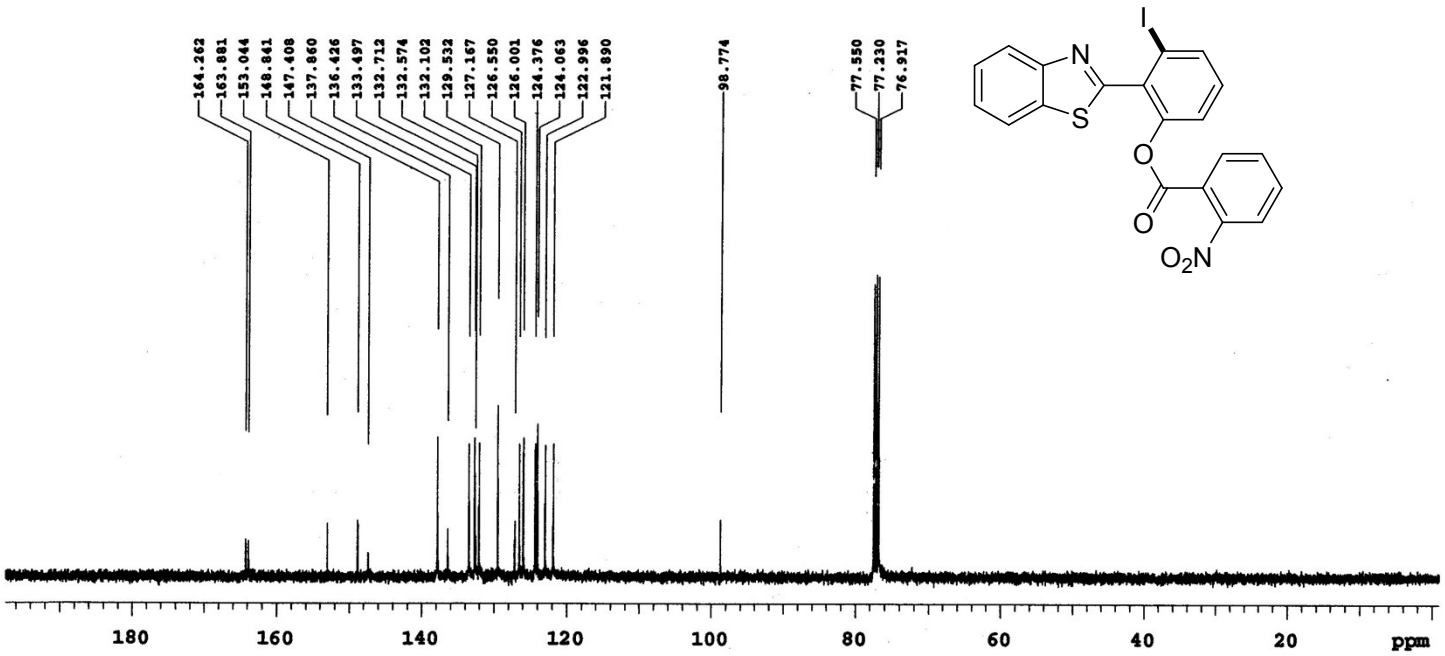
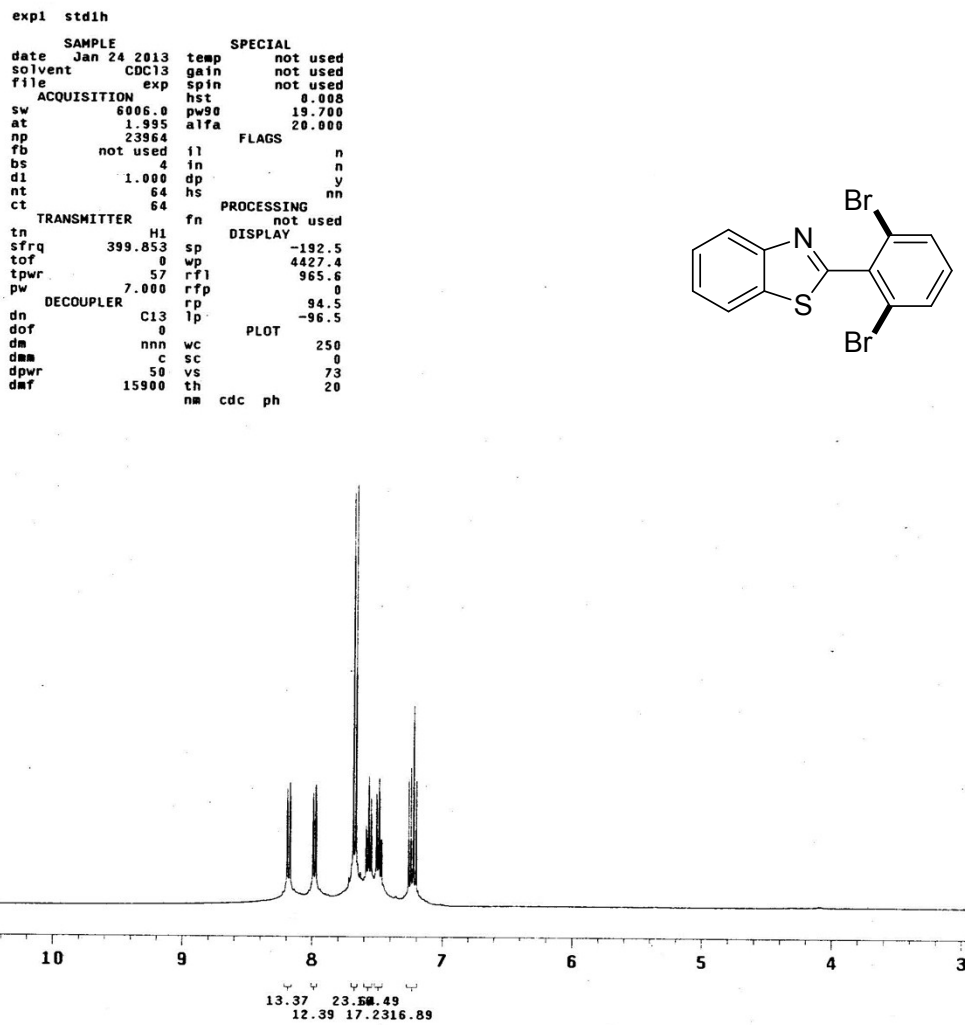


2-(Benzo[*d*]thiazol-2-yl)-3-iodophenyl 2-nitrobenzoate (10c): ^{13}C NMR ($CDCl_3$, 100 MHz)

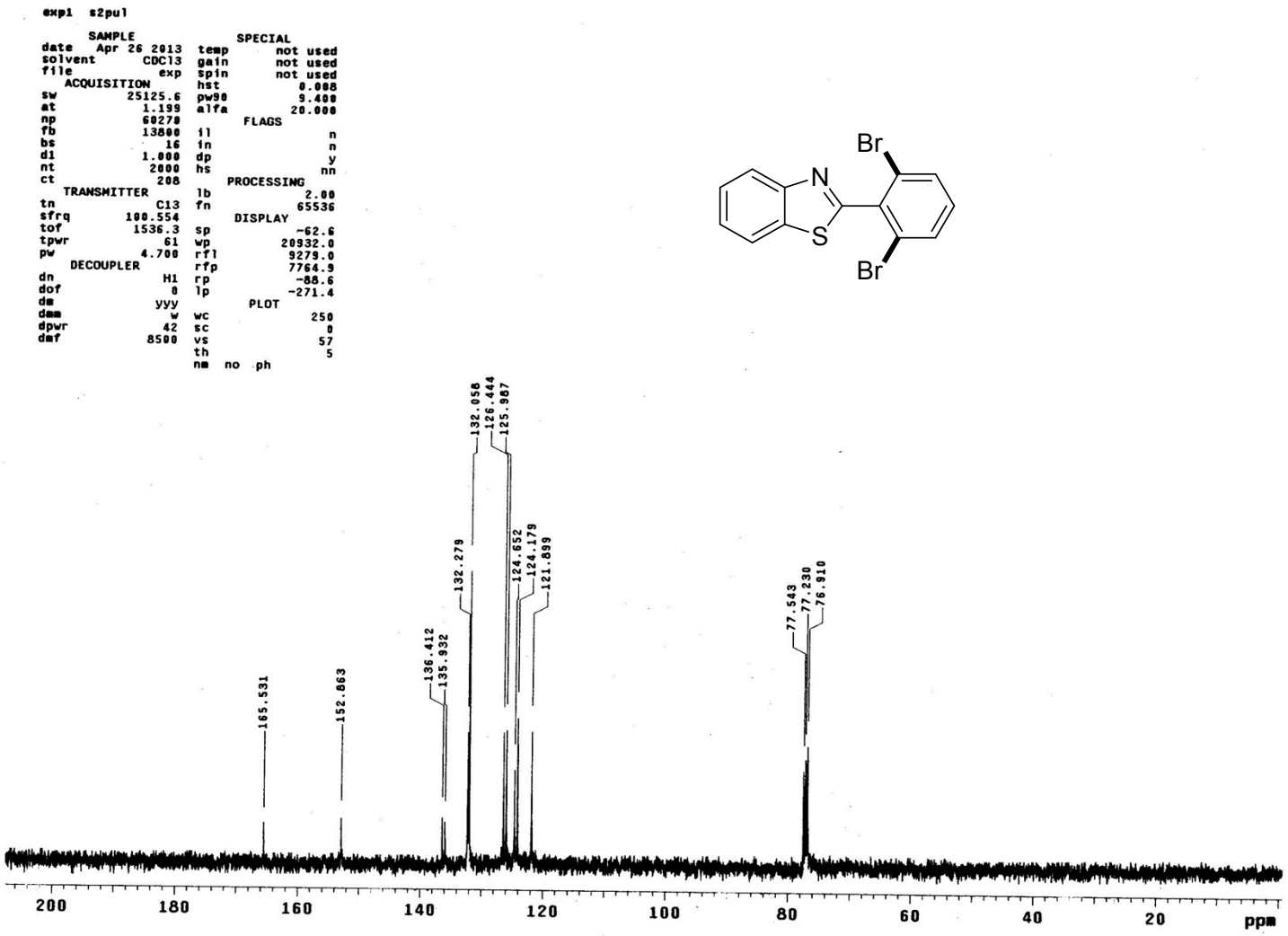


PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 1700 repetitions	OBSERVE C13, 100.5425840 DECOUPLE H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 65 minutes		SSAB_100_2NO2I_13C Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 "IITG-NMR"

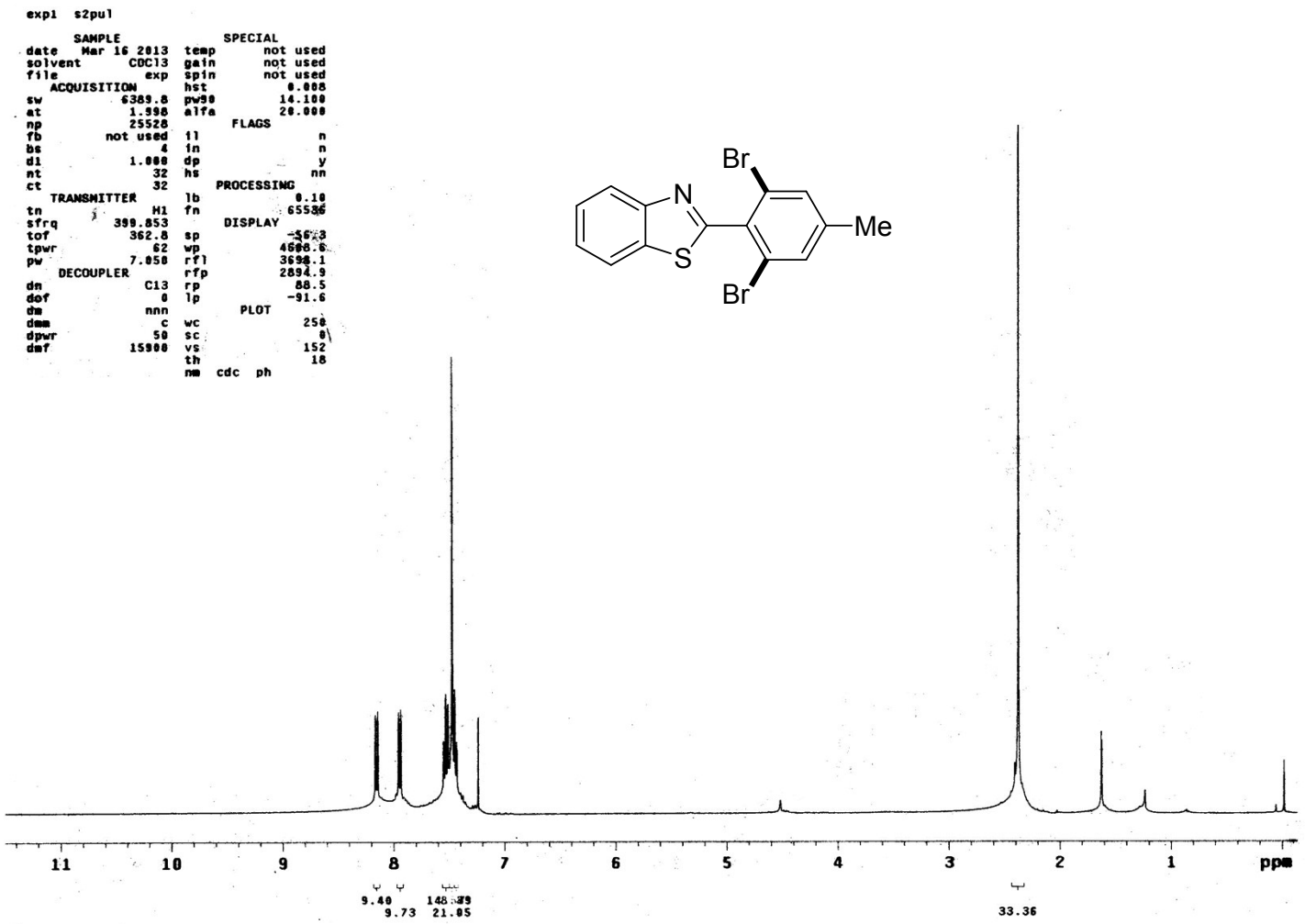
2-(2,6-Dibromophenyl)benzo[*d*]thiazole (11a): ^{1}H NMR ($CDCl_3$, 400 MHz)



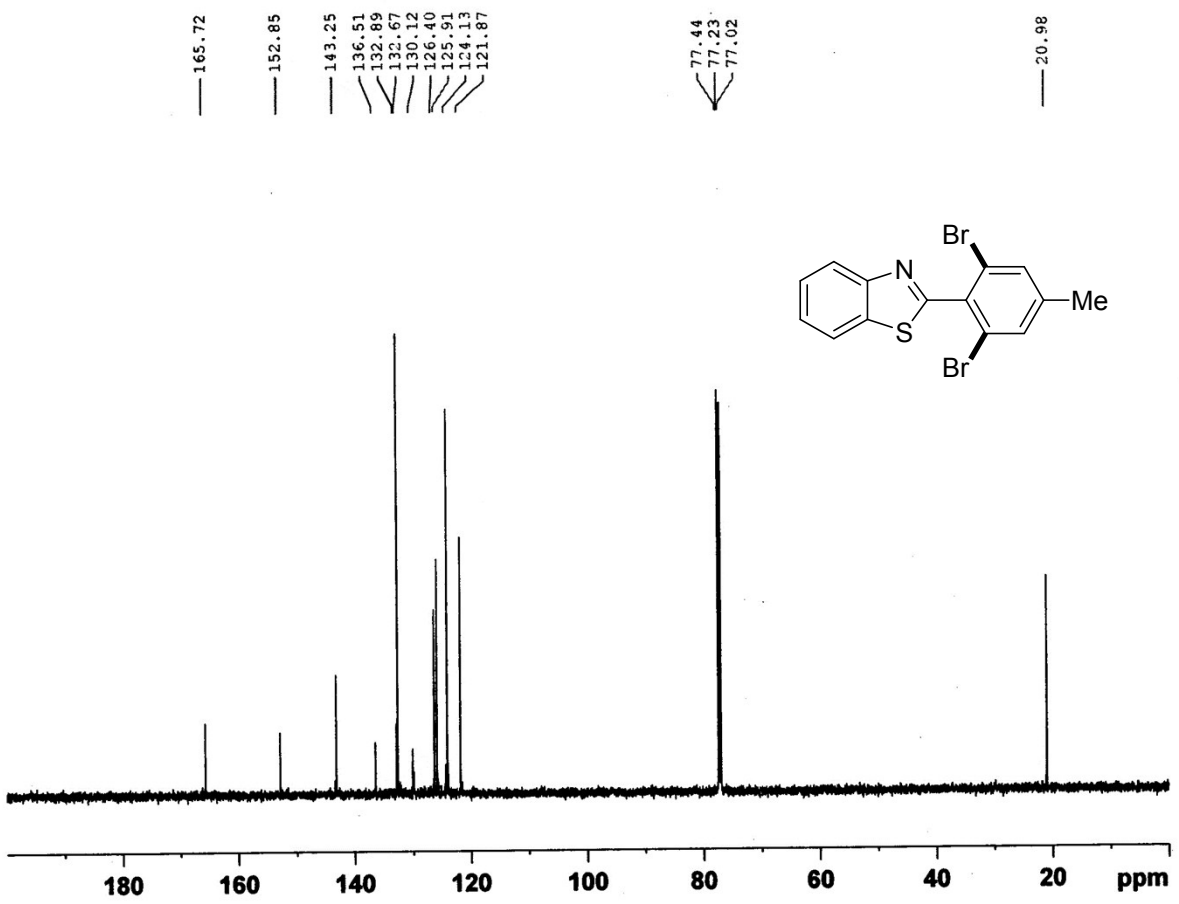
2-(2,6-Dibromophenyl)benzo[*d*]thiazole (11a): ^{13}C NMR ($CDCl_3$, 100 MHz)



2-(2,6-Dibromo-4-methylphenyl)benzo[*d*]thiazole (12a): ^{1}H NMR ($CDCl_3$, 400 MHz)



2-(2,6-Dibromo-4-methylphenyl)benzo[*d*]thiazole (12a): ^{13}C NMR ($CDCl_3$, 150 MHz)

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Current Data Parameters
NAME          SSAB-93-13C
EXPNO                   1
PROCNO                  1

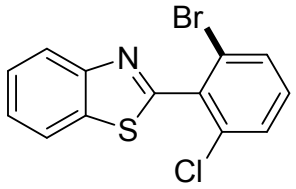
F2 - Acquisition Parameters
Date_              20140603
Time                 11.05
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                   177
DS                     2
SWH            36057.691 Hz
FIDRES          1.100393 Hz
AQ             0.4543829 sec
RG                 65.24
DW                13.867 usec
DE                 6.50 usec
TE                299.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

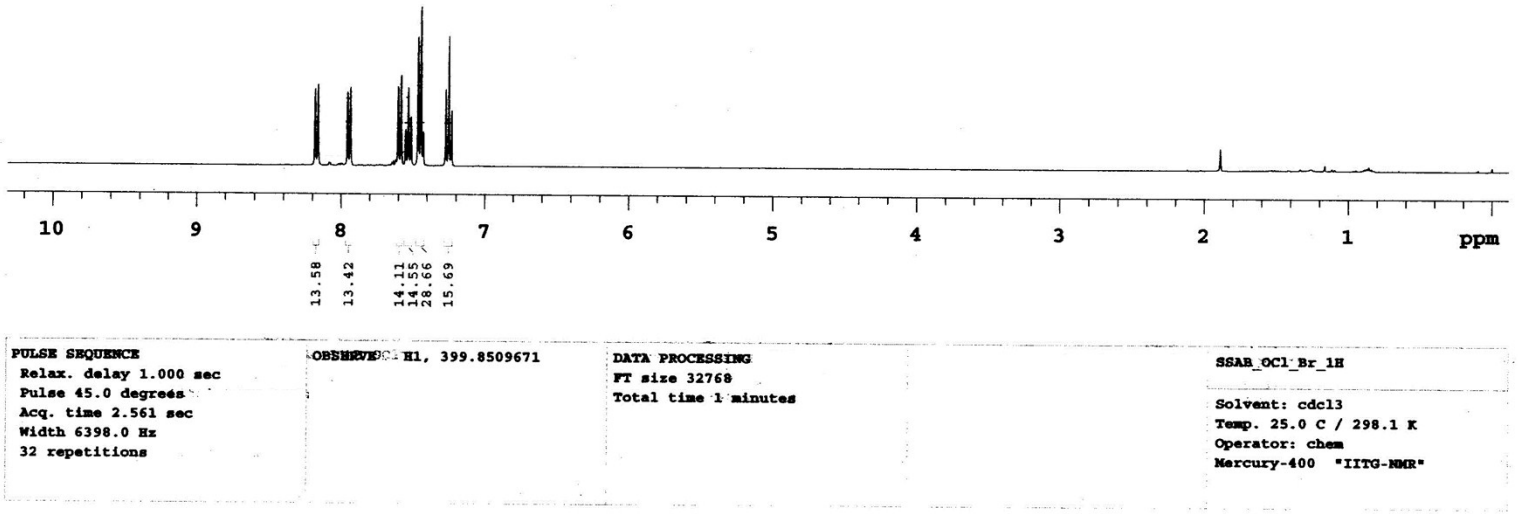
======== CHANNEL f1 ========
SFO1          150.9279571 MHz
NUC1                 13C
P1                10.50 usec
PLW1          95.00000000 W

======== CHANNEL f2 ========
SFO2          600.1724007 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             70.00 usec
PLW2          21.00000000 W
PLW12          0.61714000 W
PLW13          0.30239999 W

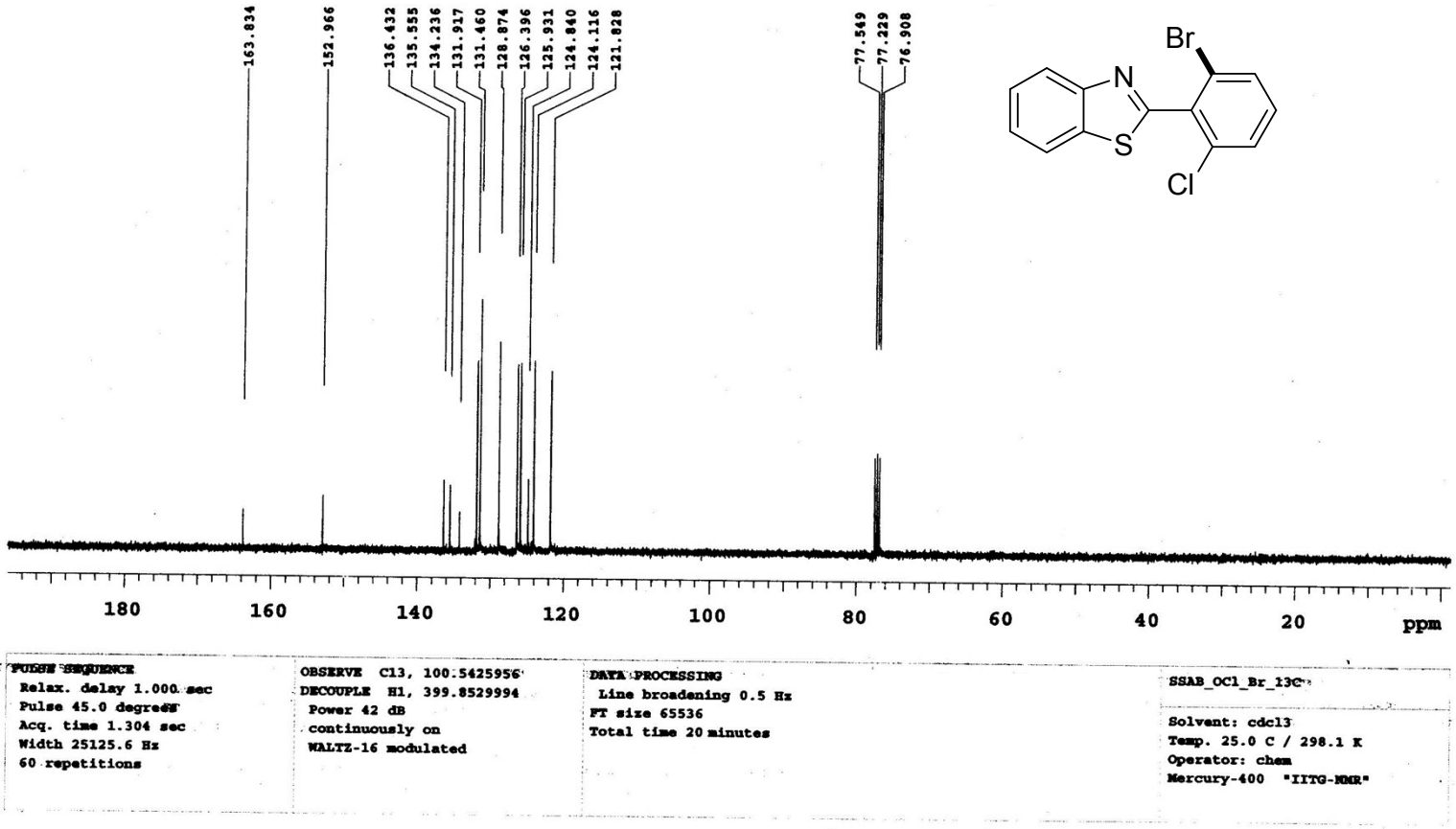
F2 - Processing parameters
SI                 16384
SF            150.9128457 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

2-(2-Bromo-6-chlorophenyl)benzo[*d*]thiazole (13a):^{1}H NMR ($CDCl_3$, 400 MHz)

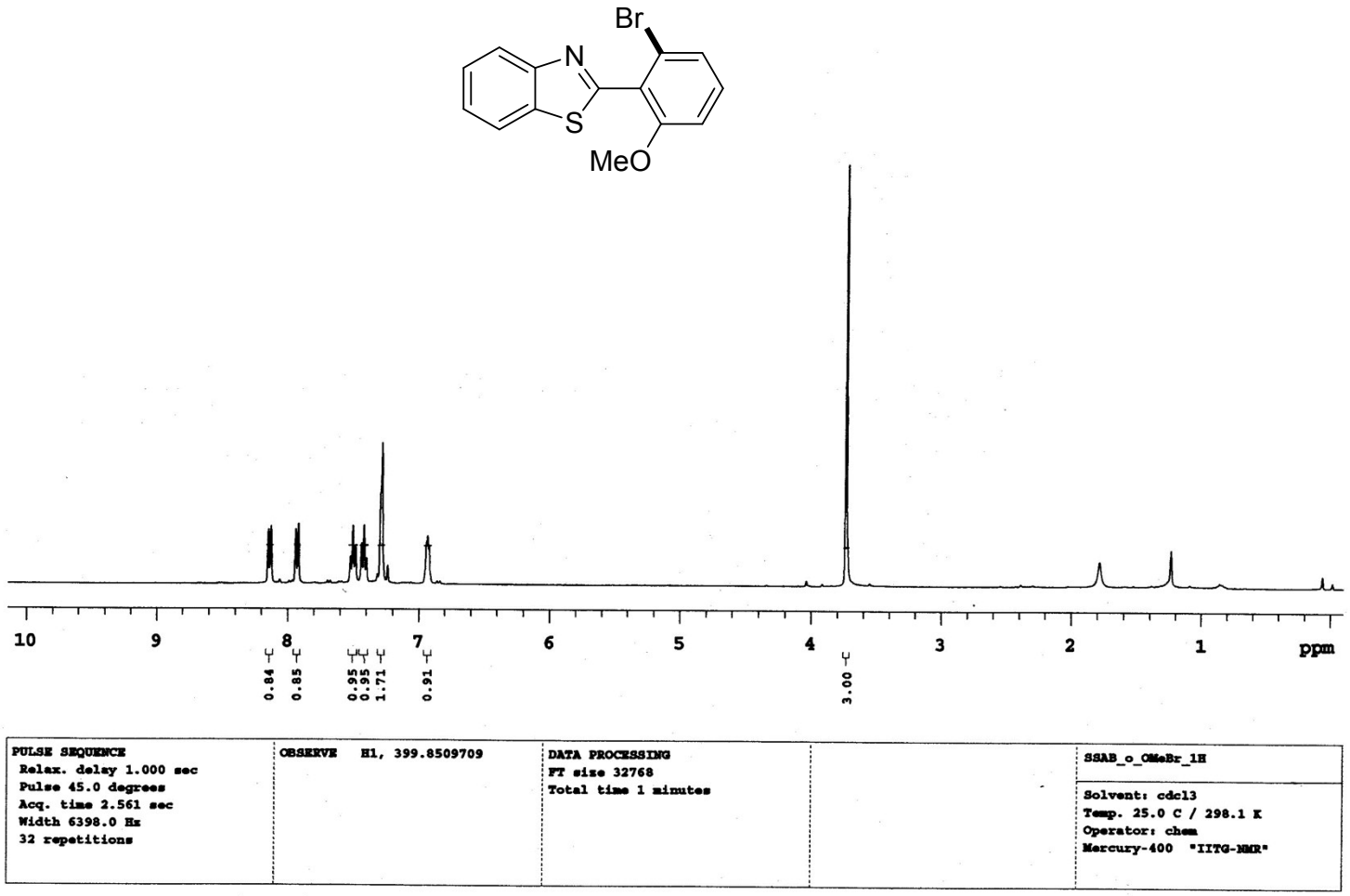




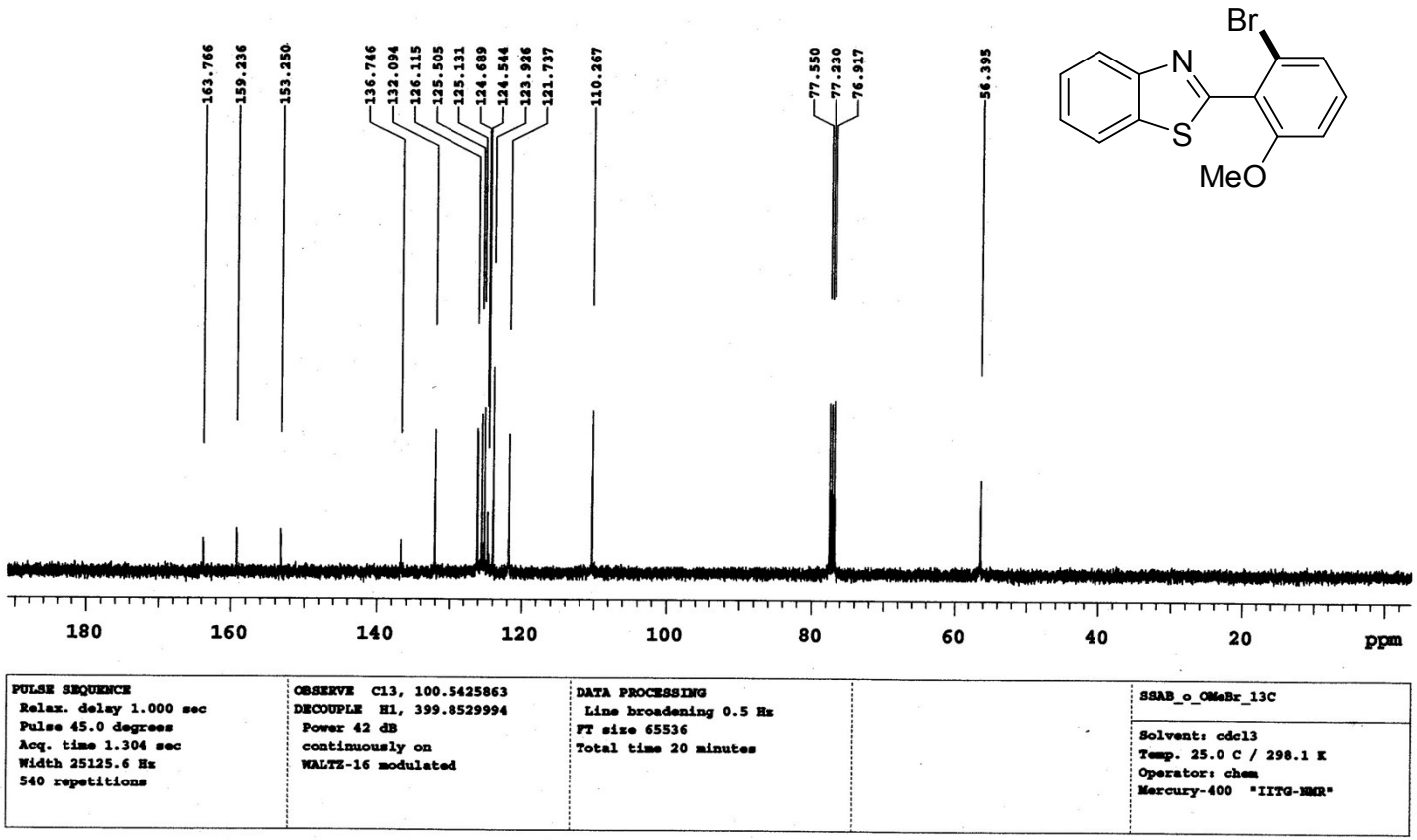
2-(2-Bromo-6-chlorophenyl)benzo[*d*]thiazole (13a):^{13}C NMR ($CDCl_3$, 100 MHz)



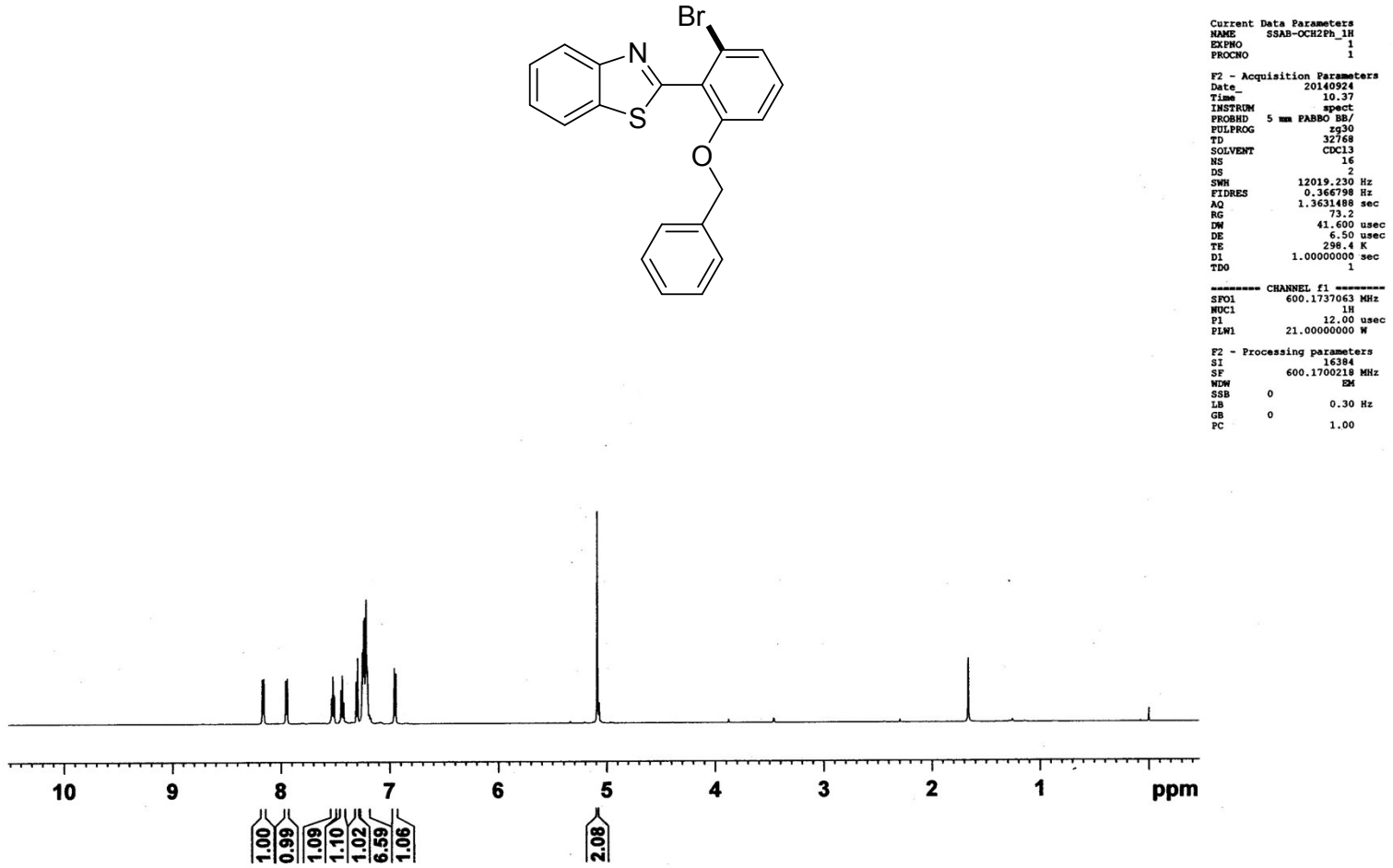
2-(2-Bromo-6-methoxyphenyl)benzo[*d*]thiazole (14a): ^{1}H NMR ($CDCl_3$, 400 MHz)



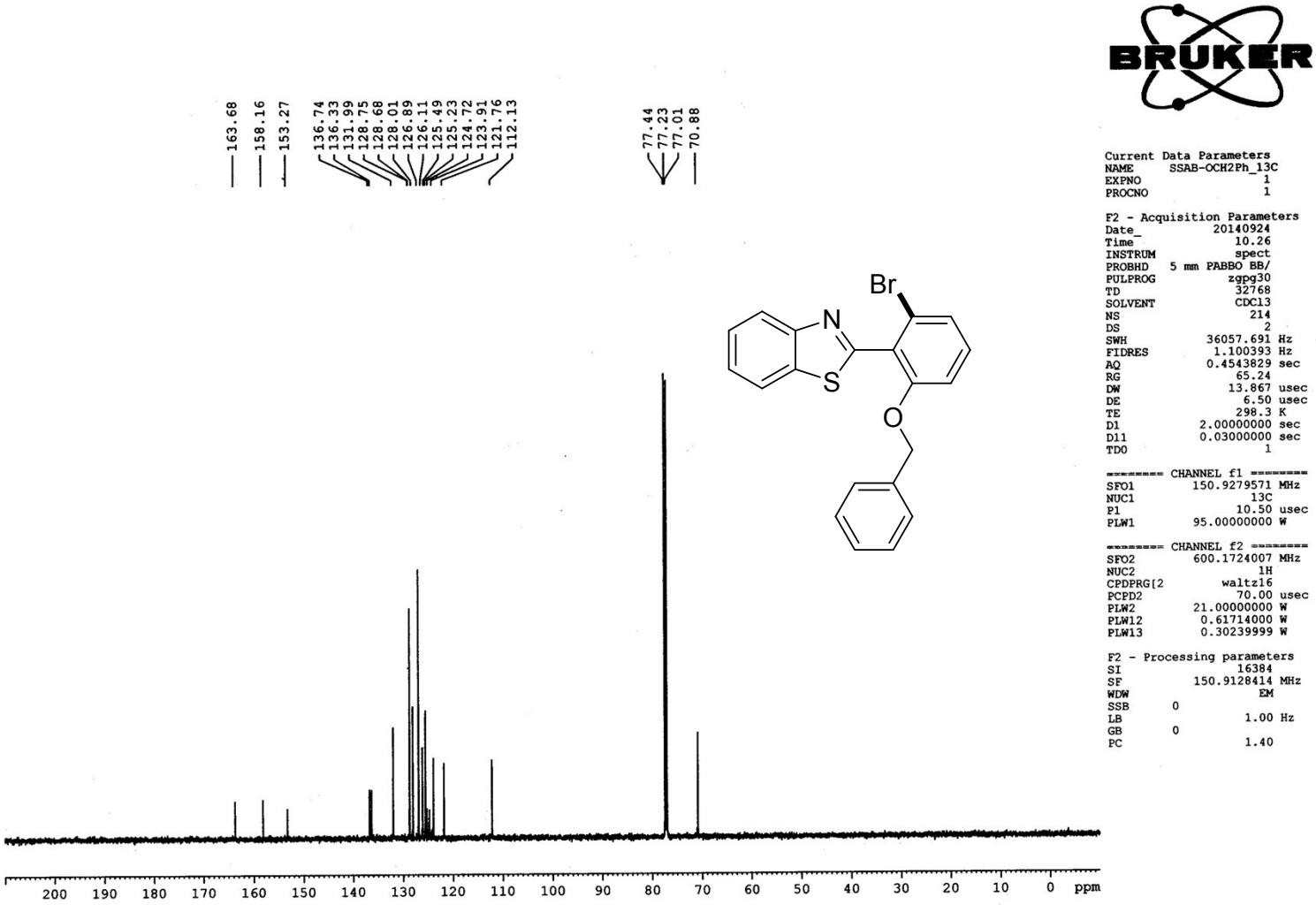
2-(2-Bromo-6-methoxyphenyl)benzo[*d*]thiazole (14a): ^{13}C NMR ($CDCl_3$, 100 MHz)



2-(2-(Benzyloxy)-6-bromophenyl)benzo[*d*]thiazole (15a): ^{1}H NMR ($CDCl_3$, 600 MHz)



2-(2-(Benzyloxy)-6-bromophenyl)benzo[*d*]thiazole (15a): ^{13}C NMR ($CDCl_3$, 150 MHz)

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Current Data Parameters
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EXPNO                   1
PROCNO                  1

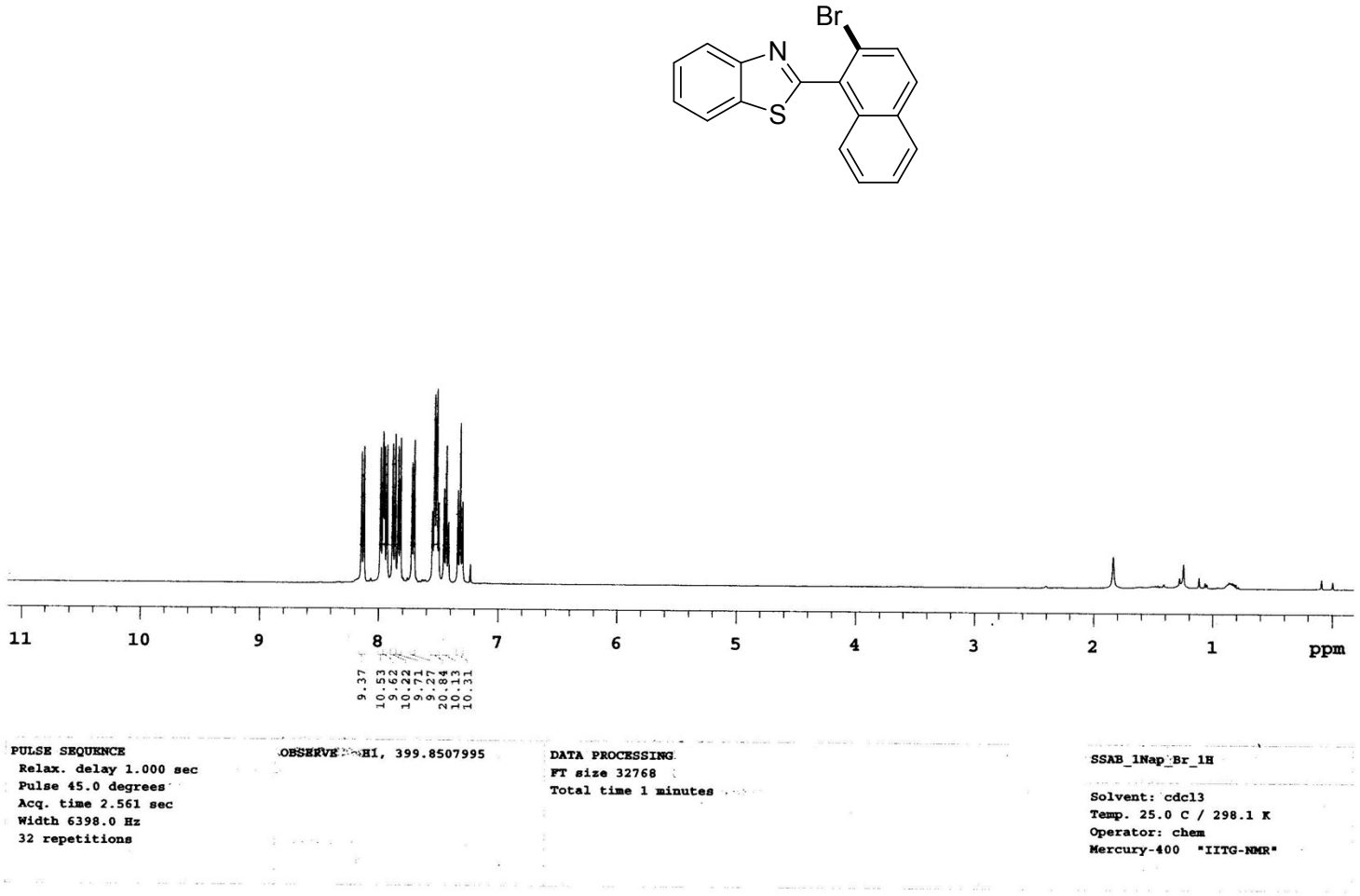
F2 - Acquisition Parameters
Date_            20140924
Time                10.26
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 32768
SOLVENT             CDCl3
NS                    214
DS                      2
SWH           36057.691 Hz
FIDRES         1.100393 Hz
AQ            0.4543829 sec
RG                 65.24
DW                13.867 usec
DE                 6.50 usec
TE                298.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1        150.9279571 MHz
NUC1                13C
P1                10.50 usec
PLW1        95.00000000 W

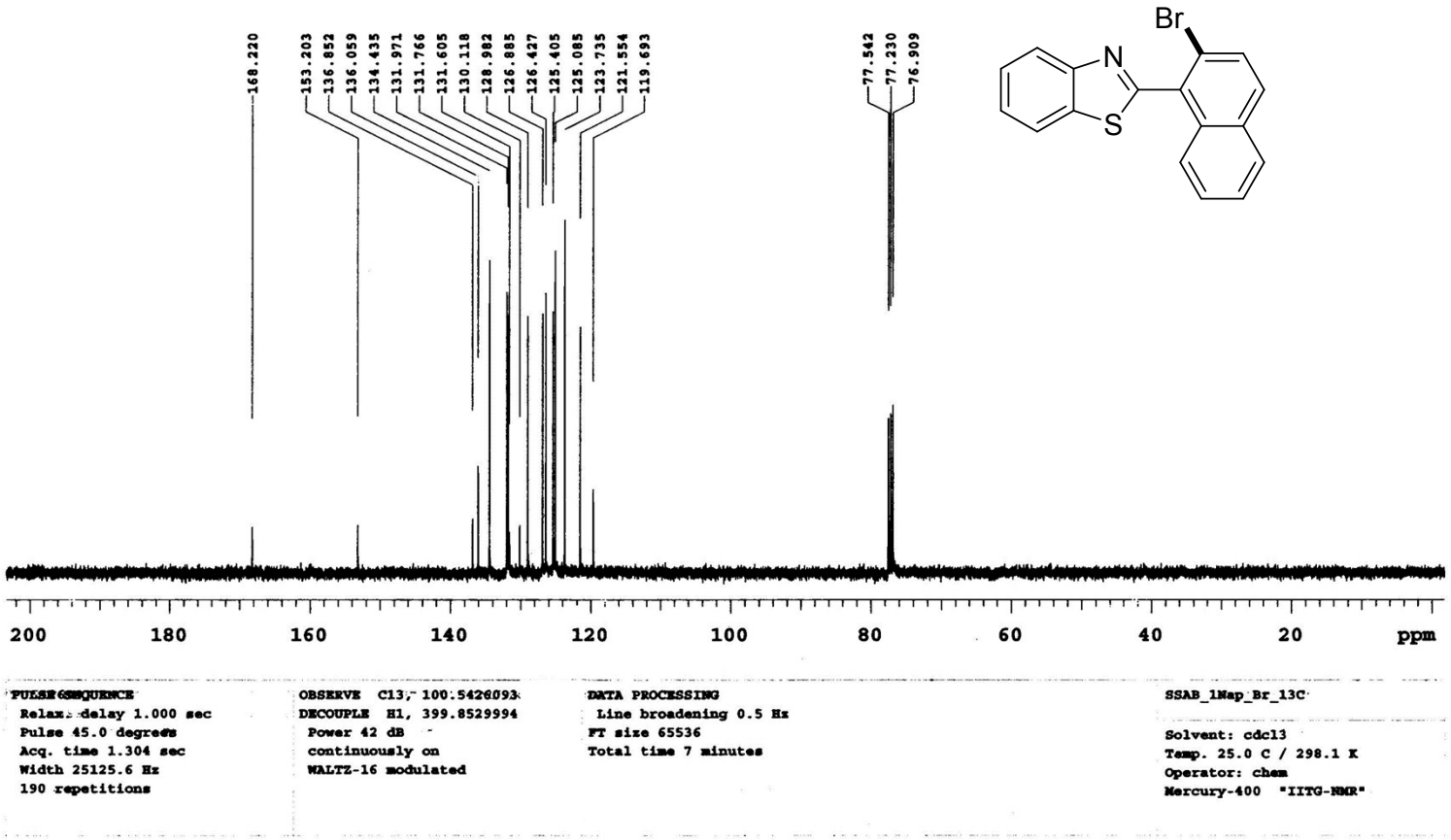
======== CHANNEL f2 ========
SFO2        600.1724007 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             70.00 usec
PLW2        21.00000000 W
PLW12        0.61714000 W
PLW13        0.30239999 W

F2 - Processing parameters
SI                  16384
SF          150.9128414 MHz
WDW                    EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

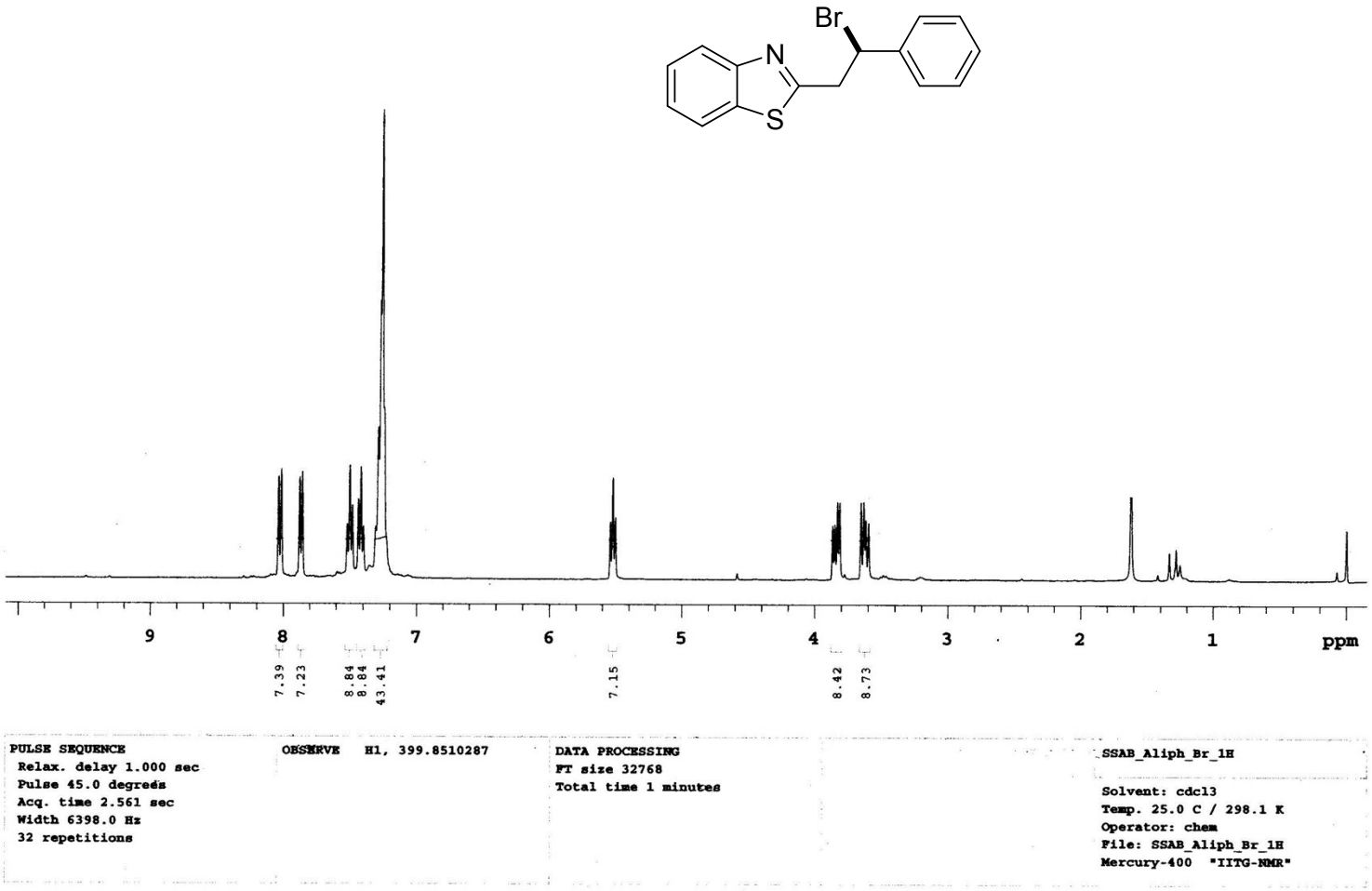
2-(2-Bromonaphthalen-1-yl)benzo[*d*]thiazole (16a): ^{1}H NMR ($CDCl_3$, 400 MHz)



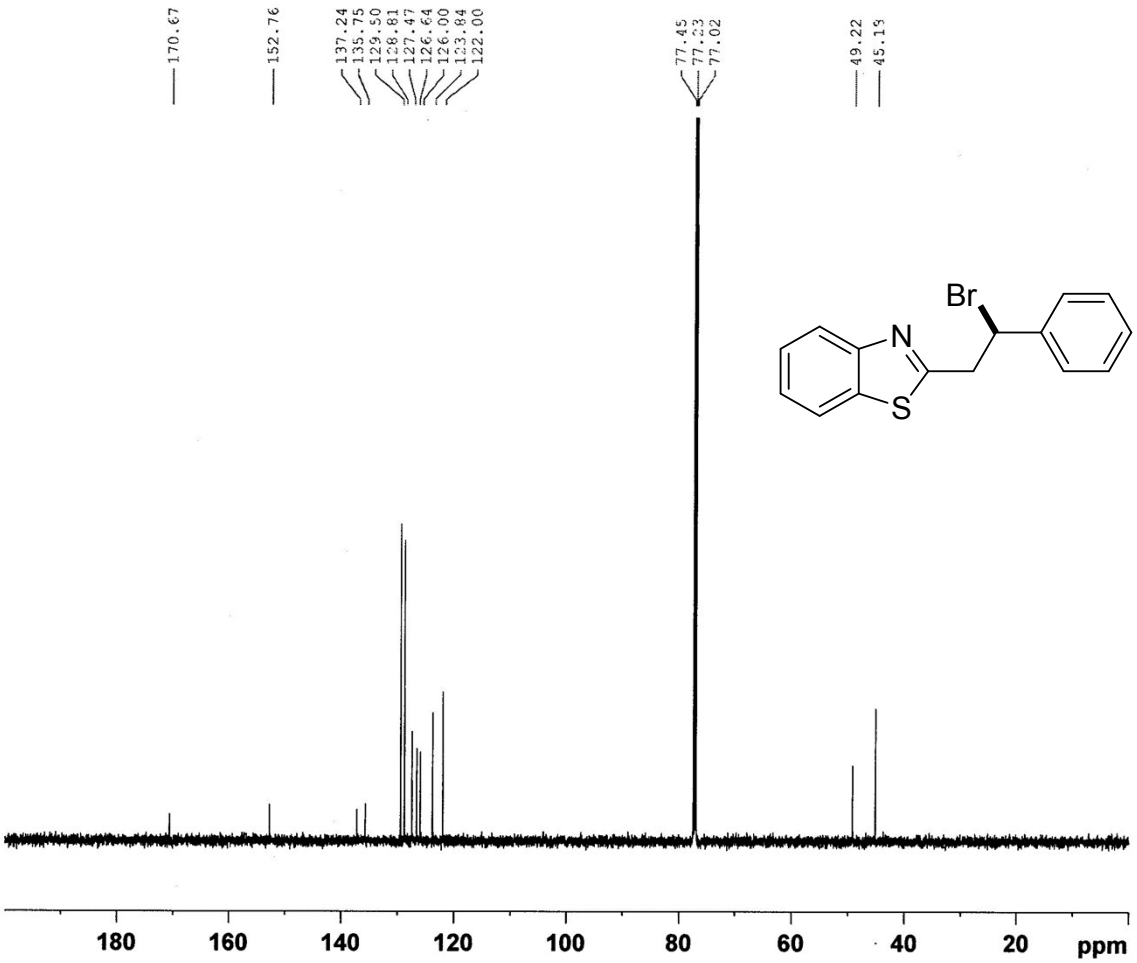
2-(2-Bromonaphthalen-1-yl)benzo[*d*]thiazole (16a): ^{13}C NMR ($CDCl_3$, 100 MHz)



2-(2-Bromo-2-phenylethyl)benzo[*d*]thiazole (17a): ^{1}H NMR ($CDCl_3$, 400 MHz)



2-(2-Bromo-2-phenylethyl)benzo[*d*]thiazole (17a): ^{13}C NMR ($CDCl_3$, 150 MHz)



BRUKER

```
Current Data Parameters
NAME      SSAB-aliph-br-13C
EXPNO                     1
PROCNO                    1

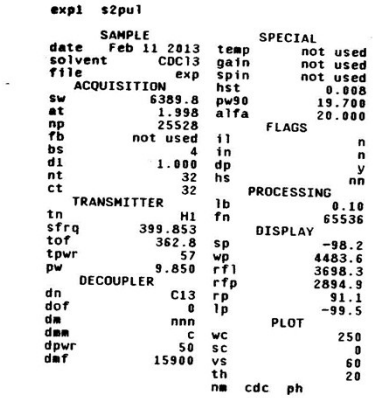
F2 - Acquisition Parameters
Date_           20140312
Time               13.53
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  118
DS                    2
SWH           36057.691 Hz
FIDRES         1.100393 Hz
AQ             0.4543829 sec
RG                65.24
DW               13.867 usec
DE                6.50 usec
TE                301.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        150.9279571 MHz
NUC1                13C
P1                10.50 usec
PLW1        95.00000000 W

======== CHANNEL f2 ========
SFO2        600.1724007 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             70.00 usec
PLW2         21.00000000 W
PLW12         0.61714000 W
PLW13         0.30239999 W

F2 - Processing parameters
SI                16384
SF          150.9128347 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

2-(2,6-Dichlorophenyl)benzo[*d*]thiazole (11b): ^{1}H NMR ($CDCl_3$, 400 MHz)



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expl  s2pul

      SAMPLE                    SPECIAL
date    Feb 11 2013   temp          not used
solvent       CDCl3   gain          not used
file            exp   spin          not used
   ACQUISITION        hst             0.008
sw            6389.8  pw90           19.700
at             1.998  alfa           20.000
np               25528          FLAGS
fb           not used  il                  n
bs                  4  in                  n
di              1.000  dp                  y
nt                 32  hs                 nn
ct                 32       PROCESSING
   TRANSMITTER         lb              0.10
tn                 H1  fn             65536
sfrq          399.853        DISPLAY
tof             362.8  sp             -98.2
tpwr               57  wp            4483.6
pw              9.850  rfl           3698.3
    DECOUPLER          rfp           2894.9
dn                 C13  rp             91.1
dof                  0  lp            -99.5
dm                 nnn       PLOT
dmm                  c  wc               250
dpwr                50  sc                 0
dmf              15900  vs                60
                        th                20
                        nm  cdc  ph
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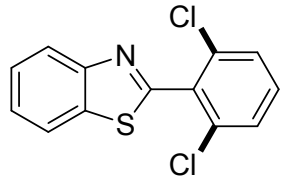
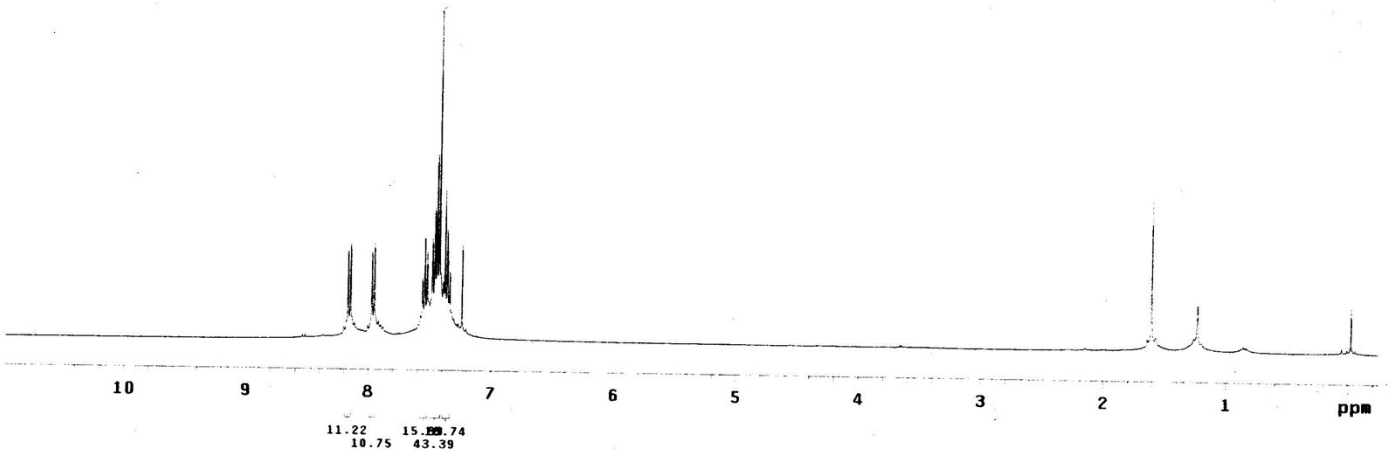
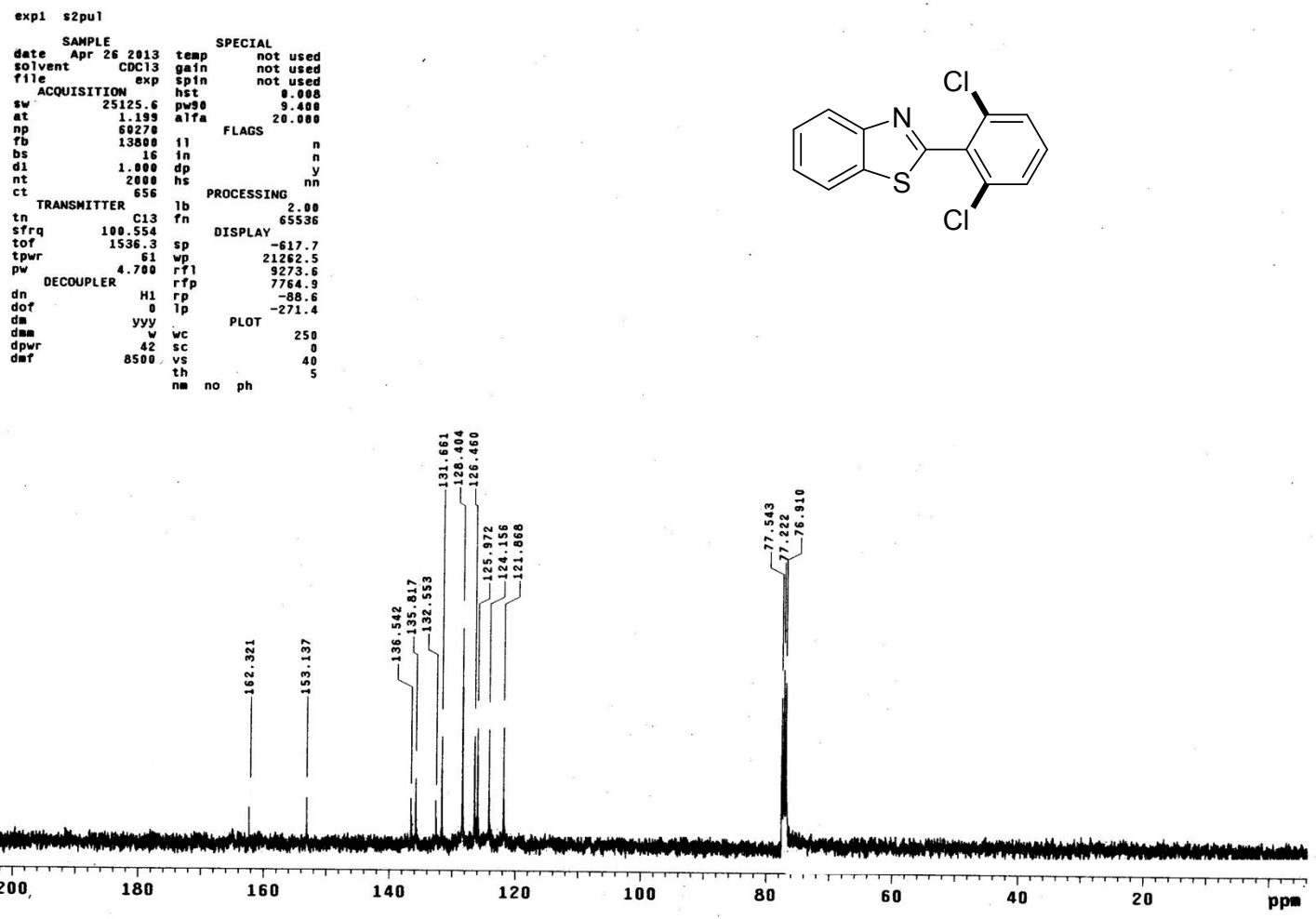
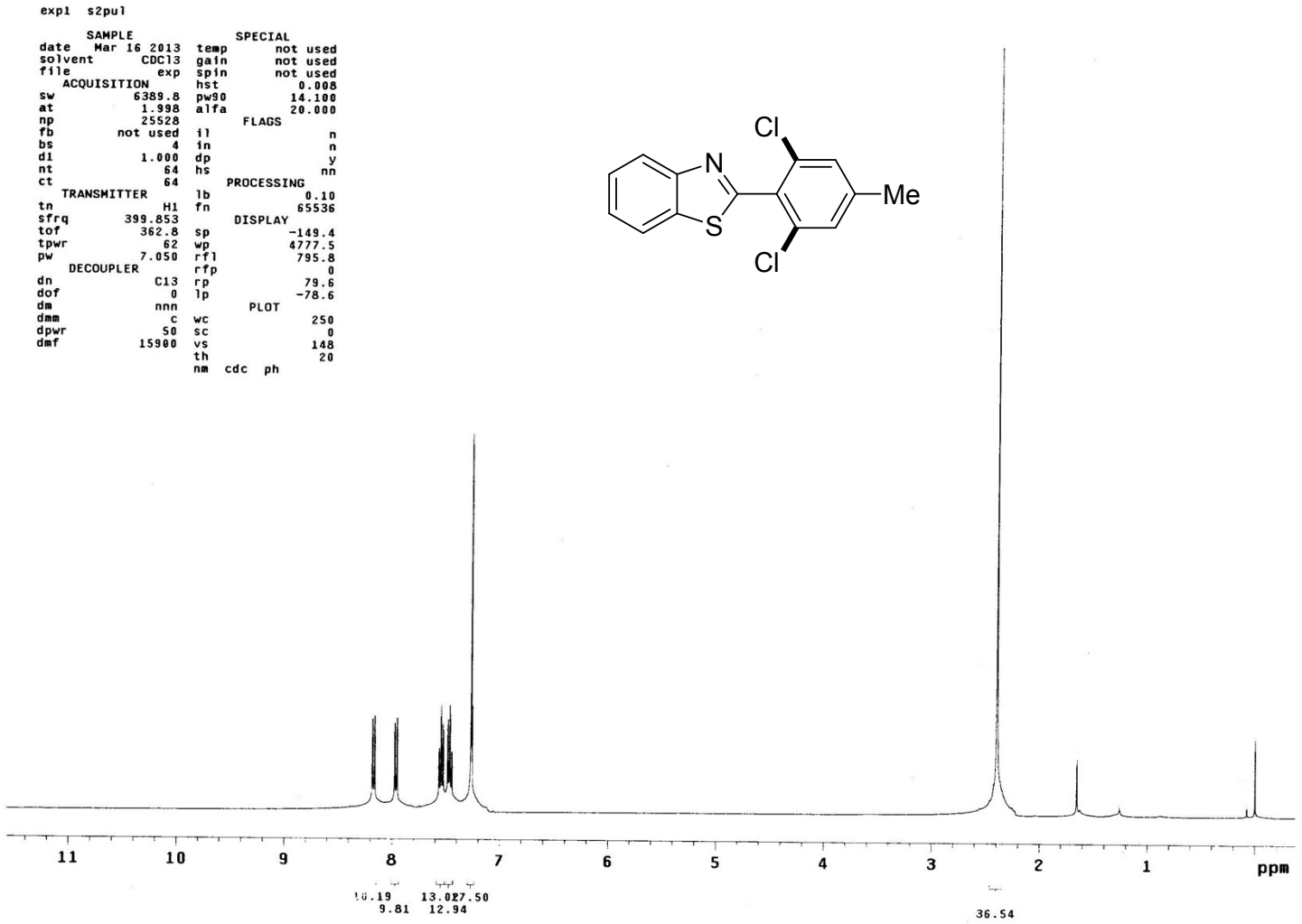




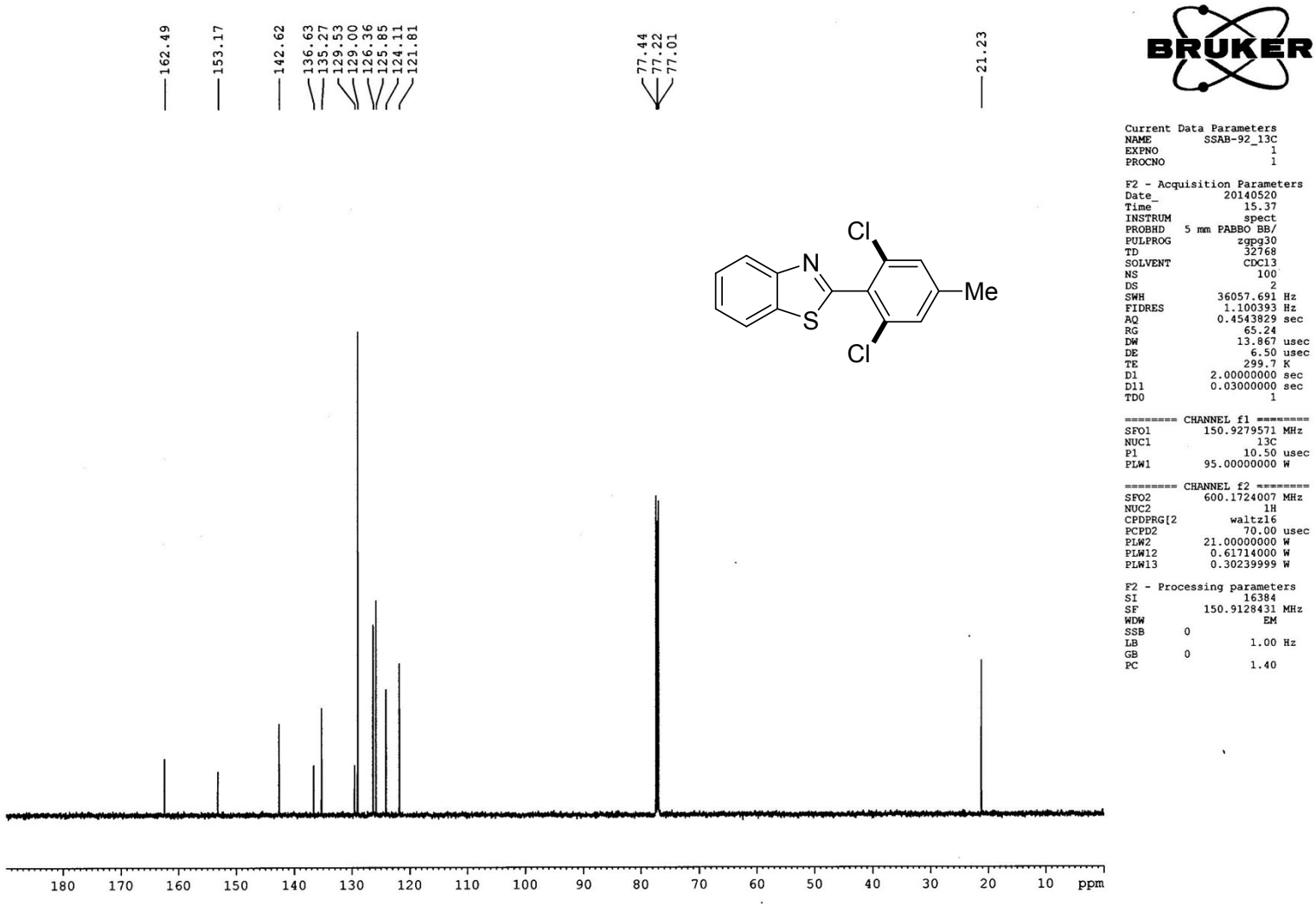
2-(2,6-Dichlorophenyl)benzo[*d*]thiazole (11b): ^{13}C NMR ($CDCl_3$, 100 MHz)



2-(2,6-Dichloro-4-methylphenyl)benzo[*d*]thiazole (12b): ^{1}H NMR ($CDCl_3$, 400 MHz)



2-(2,6-Dichloro-4-methylphenyl)benzo[*d*]thiazole (12b): ^{13}C NMR ($CDCl_3$, 150 MHz)

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Current Data Parameters
NAME          SSAB-92_13C
EXPNO                   1
PROCNO                  1

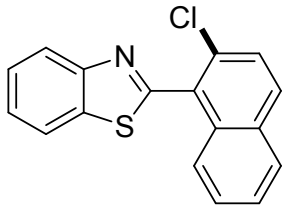
F2 - Acquisition Parameters
Date_              20140520
Time                 15.37
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   32768
SOLVENT              CDCl3
NS                     100
DS                       2
SWH              36057.691 Hz
FIDRES            1.100393 Hz
AQ                0.4543829 sec
RG                    65.24
DW                   13.867 usec
DE                    6.50 usec
TE                   299.7 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

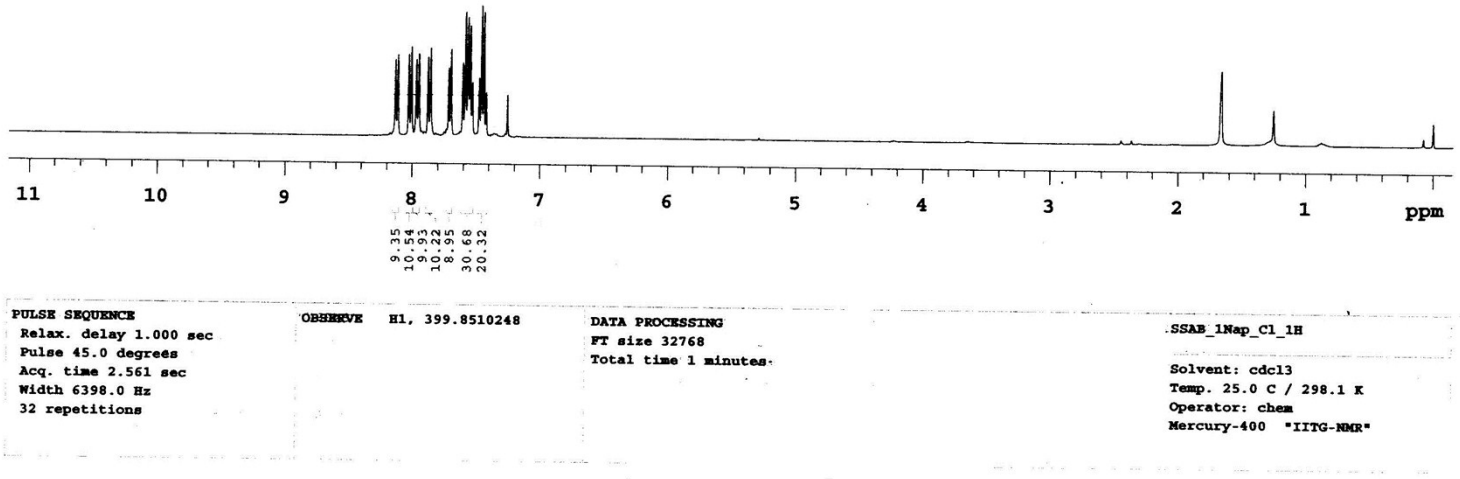
======== CHANNEL f1 ========
SFO1          150.9279571 MHz
NUC1                   13C
P1                   10.50 usec
PLW1          95.00000000 W

======== CHANNEL f2 ========
SFO2          600.1724007 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2                70.00 usec
PLW2          21.00000000 W
PLW12          0.61714000 W
PLW13          0.30239999 W

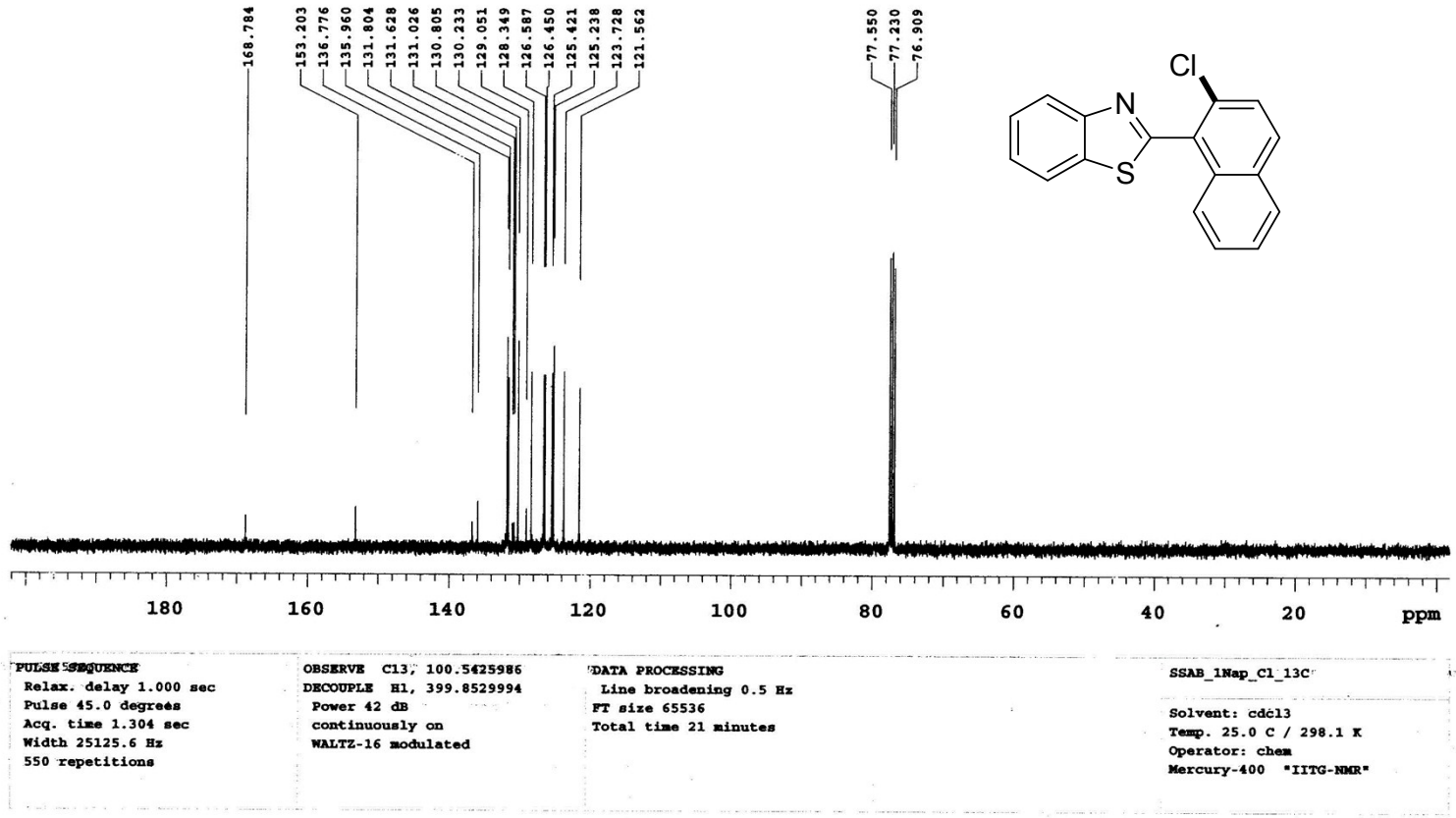
F2 - Processing parameters
SI                   16384
SF            150.9128431 MHz
WDW                     EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

2-(2-Chloronaphthalen-1-yl)benzo[*d*]thiazole (16b): ^{1}H NMR ($CDCl_3$, 400 MHz)

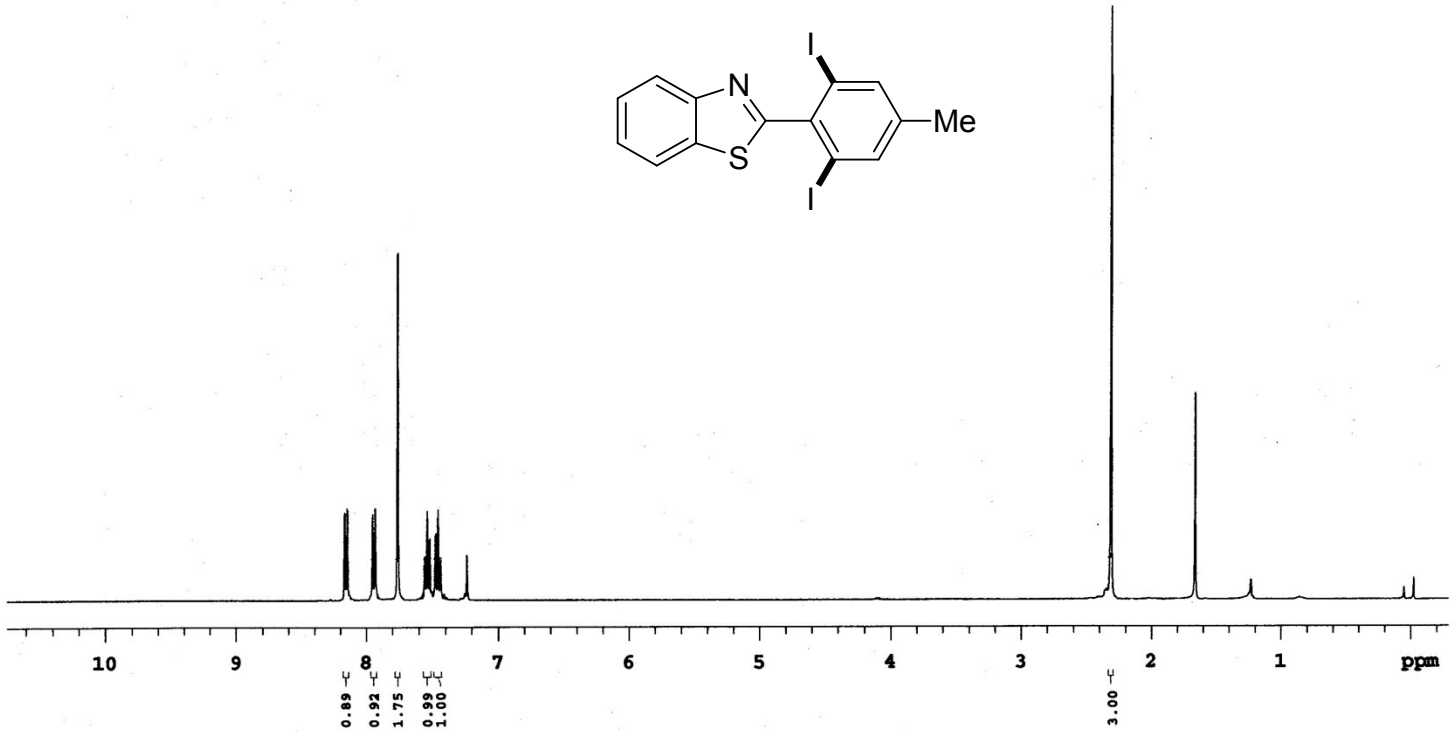




2-(2-Chloronaphthalen-1-yl)benzo[*d*]thiazole (16b): ^{13}C NMR ($CDCl_3$, 100 MHz)

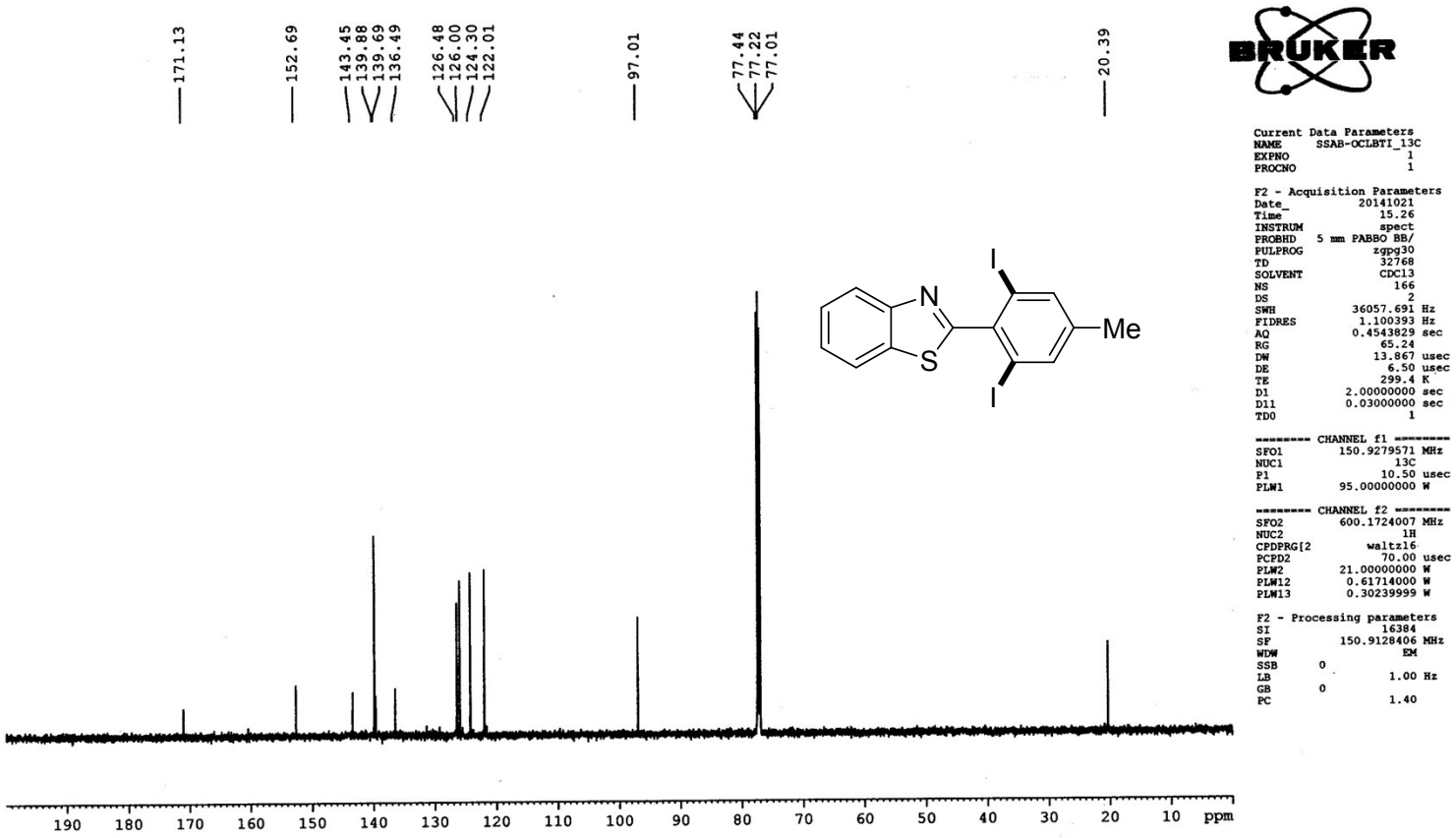


2-(2,6-Diiodo-4-methylphenyl)benzo[*d*]thiazole (12c): ^{1}H NMR ($CDCl_3$, 400 MHz)



PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	OBSERVE H1, 399.8509721	DATA PROCESSING FT size 32768 Total time 1 minutes		SSAB_PMeBT_I_1H Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 "IITG-NMR"

2-(2,6-Diiodo-4-methylphenyl)benzo[*d*]thiazole (12c): ^{13}C NMR ($CDCl_3$, 150 MHz)

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Current Data Parameters
NAME      SSAB-OCLBTI_13C
EXPNO                   1
PROCNO                  1

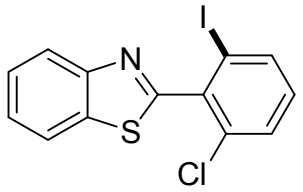
F2 - Acquisition Parameters
Date_            20141021
Time                15.26
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 32768
SOLVENT             CDCl3
NS                    166
DS                      2
SWH             36057.691 Hz
FIDRES          1.100393 Hz
AQ              0.4543829 sec
RG                  65.24
DW                 13.867 usec
DE                  6.50 usec
TE                 299.4 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

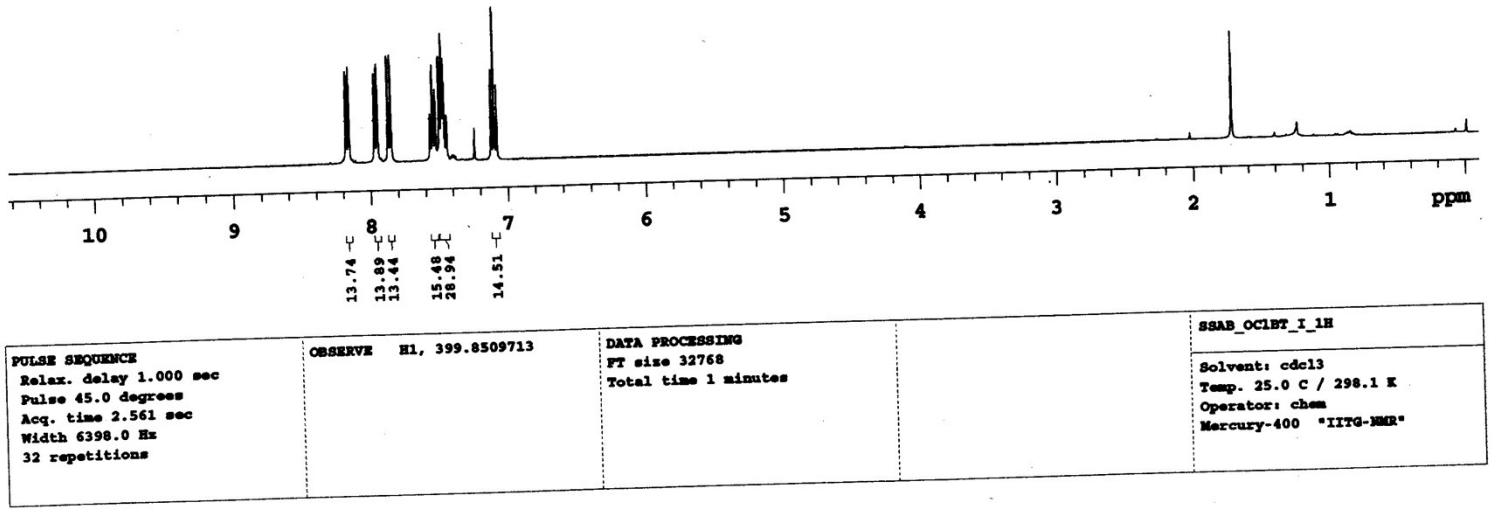
======== CHANNEL f1 ========
SFO1          150.9279571 MHz
NUC1                  13C
P1                  10.50 usec
PLW1          95.00000000 W

======== CHANNEL f2 ========
SFO2          600.1724007 MHz
NUC2                  1H
CPDPRG[2           waltz16
PCPD2               70.00 usec
PLW2          21.00000000 W
PLW12          0.61714000 W
PLW13          0.30239999 W

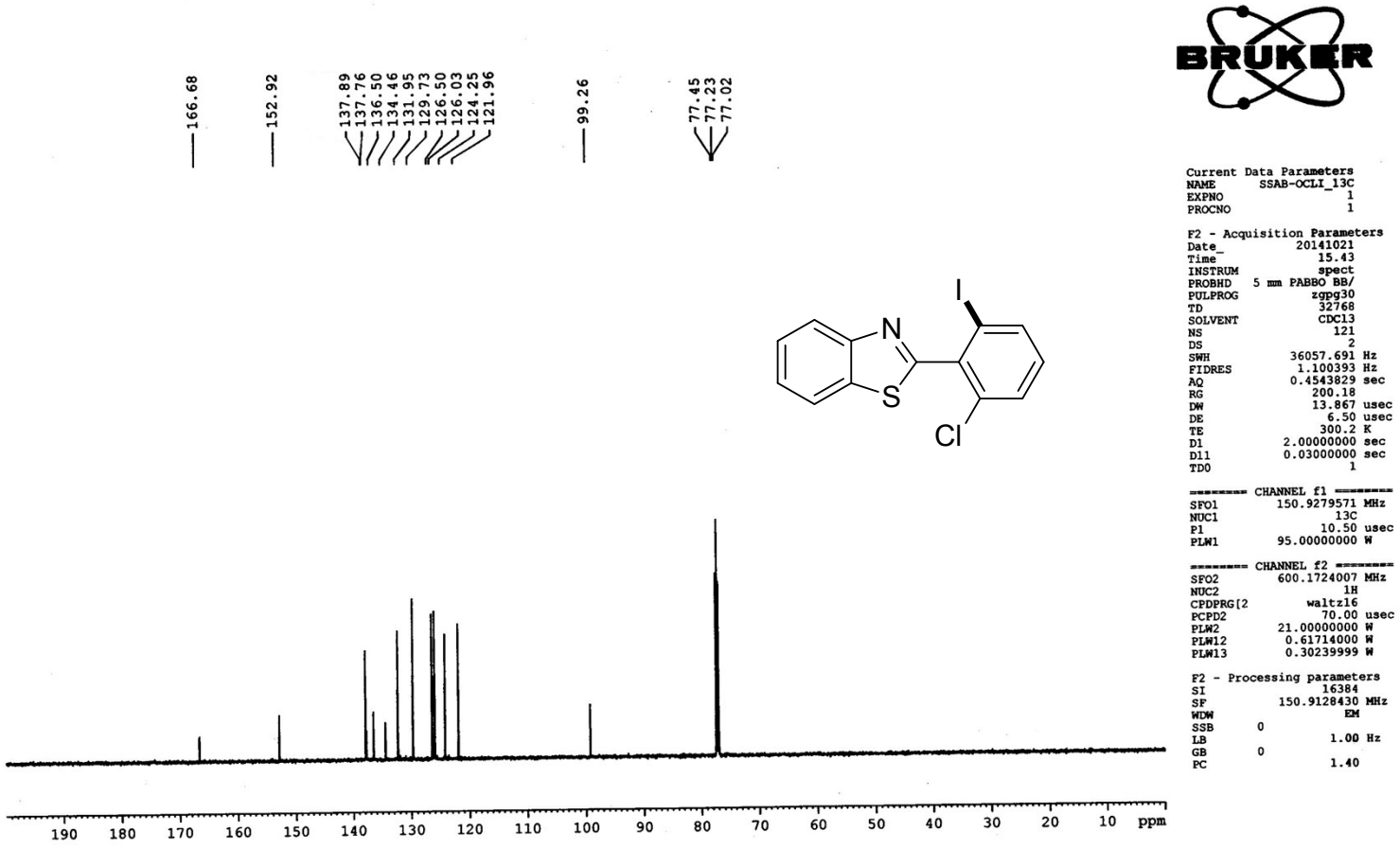
F2 - Processing parameters
SI                    16384
SF            150.9128406 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

2-(2-Chloro-6-iodophenyl)benzo[*d*]thiazole (13c): ^{1}H NMR (400 MHz, $CDCl_3$):





2-(2-Chloro-6-iodophenyl)benzo[*d*]thiazole (13c): ^{13}C NMR (150 MHz, $CDCl_3$):

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PROCNO                1

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PULPROG        zgpg30
TD              32768
SOLVENT         CDCl3
NS                121
DS                  2
SWH         36057.691 Hz
FIDRES       1.100393 Hz
AQ           0.4543829 sec
RG              200.18
DW             13.867 usec
DE              6.50 usec
TE             300.2 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                 1

======== CHANNEL f1 ========
SFO1       150.9279571 MHz
NUC1              13C
P1              10.50 usec
PLW1       95.00000000 W

======== CHANNEL f2 ========
SFO2       600.1724007 MHz
NUC2              1H
CPDPRG[2       waltz16
PCPD2           70.00 usec
PLW2       21.00000000 W
PLW12       0.61714000 W
PLW13       0.30239999 W

F2 - Processing parameters
SI                16384
SF         150.9128430 MHz
WDW                EM
SSB       0
LB              1.00 Hz
GB        0
PC              1.40
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2-(2-Bromophenyl)-3-phenylquinoxaline (20a): ^{1}H NMR (400 MHz, $CDCl_3$):

```
expl  s2pul

      SAMPLE              SPECIAL
date   Jun  6 2012  temp       not used
solvent      CDCl3  gain       not used
file           exp  spin       not used
   ACQUISITION       hst          0.008
sw          6389.8  pw90        19.700
at           1.998  alfa        20.000
np           25528        FLAGS
fb       not used  il               n
bs              4  in               n
d1          1.000  dp               y
nt             32  hs              nn
ct             32      PROCESSING
   TRANSMITTER     lb           0.10
tn             H1  fn          65536
sfrq       399.853       DISPLAY
tof          362.8  sp         -795.0
tpwr            57  wp         6389.8
pw           9.850  rfl         795.0
    DECOUPLER      rfp            0
dn             C13  rp          113.3
dof              0  lp          -93.2
dm             nnn         PLOT
dmm              c  wc           250
dpwr            50  sc             0
dmf          15900  vs            53
                    th            11
                    nm  cdc  ph
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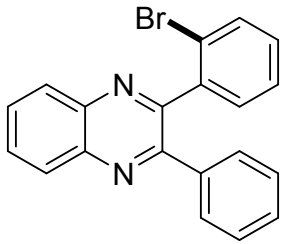
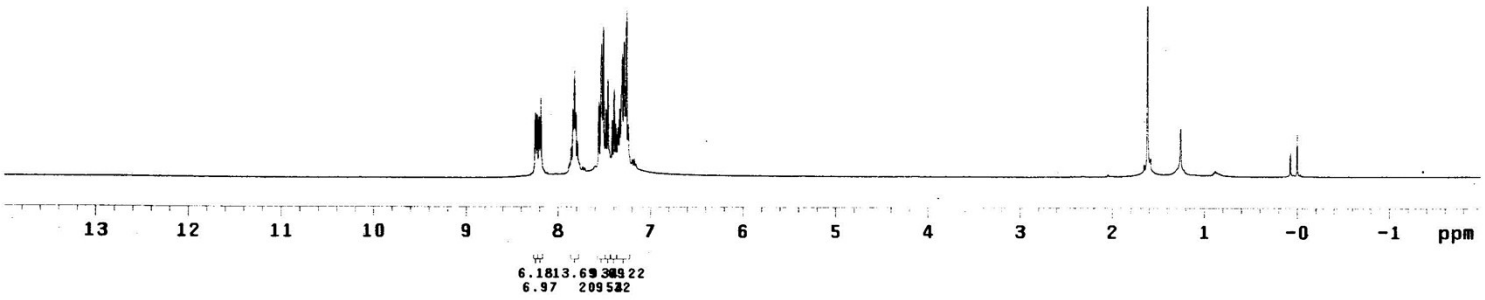
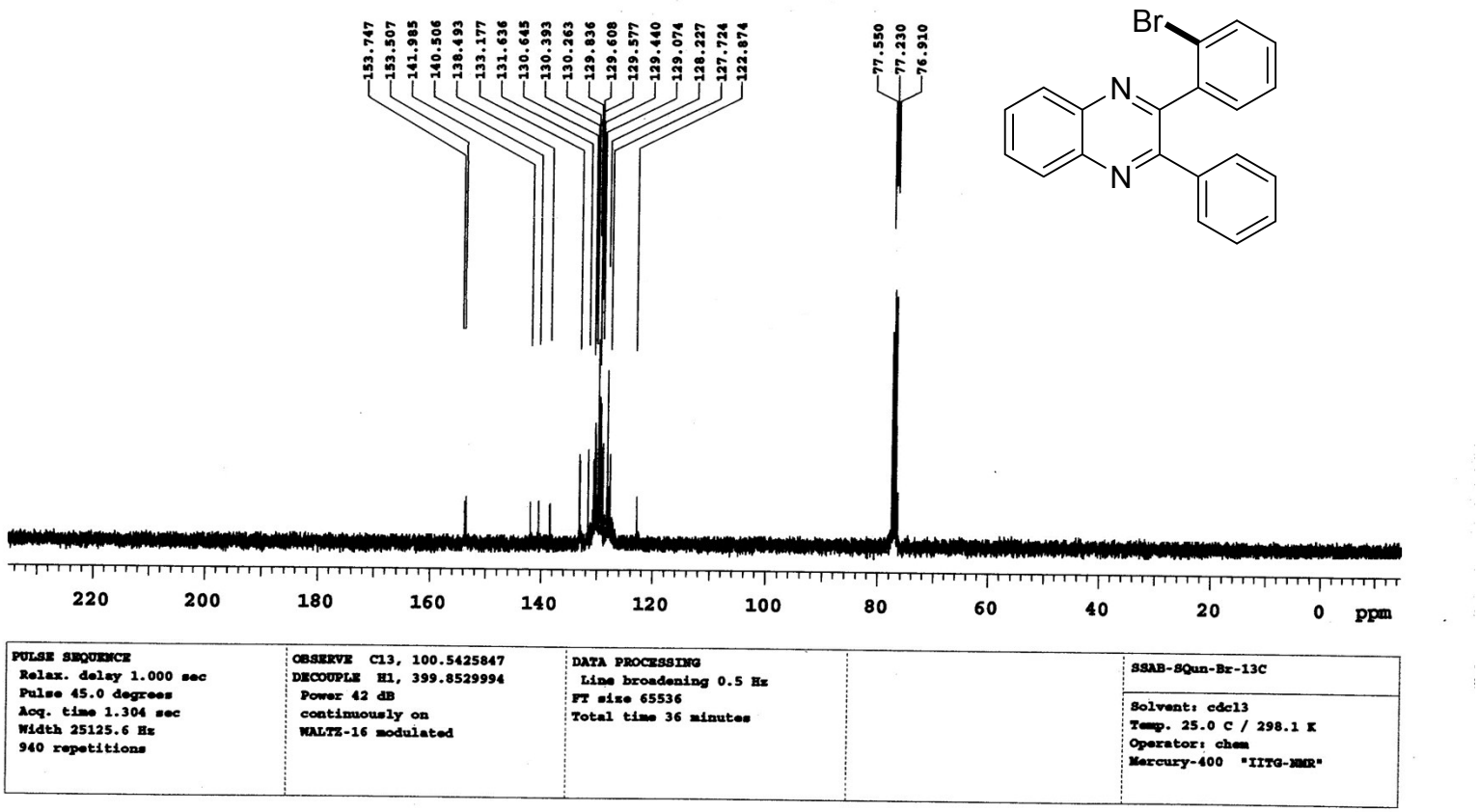
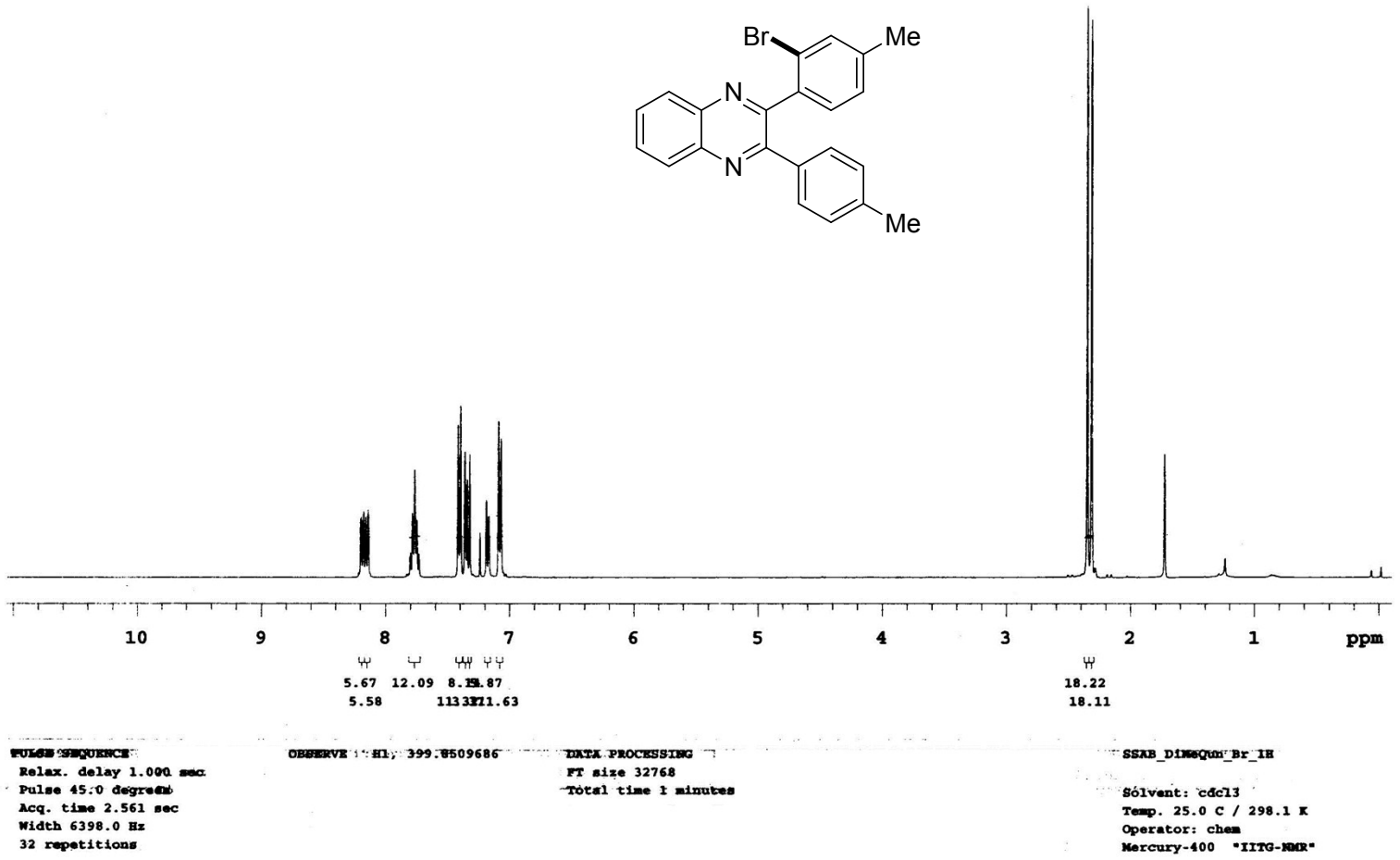




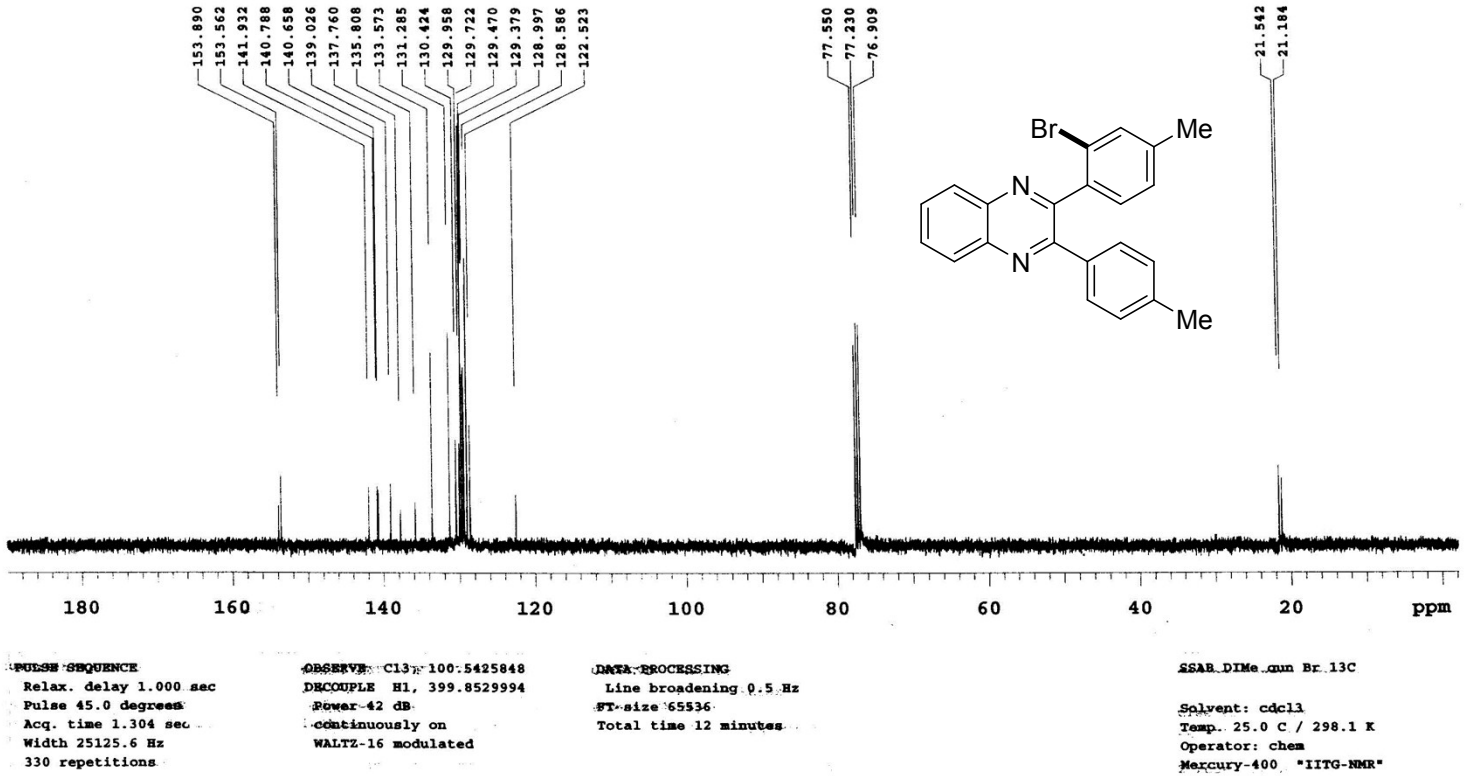
2-(2-Bromophenyl)-3-phenylquinoxaline (20a): ^{13}C NMR (100 MHz, $CDCl_3$):



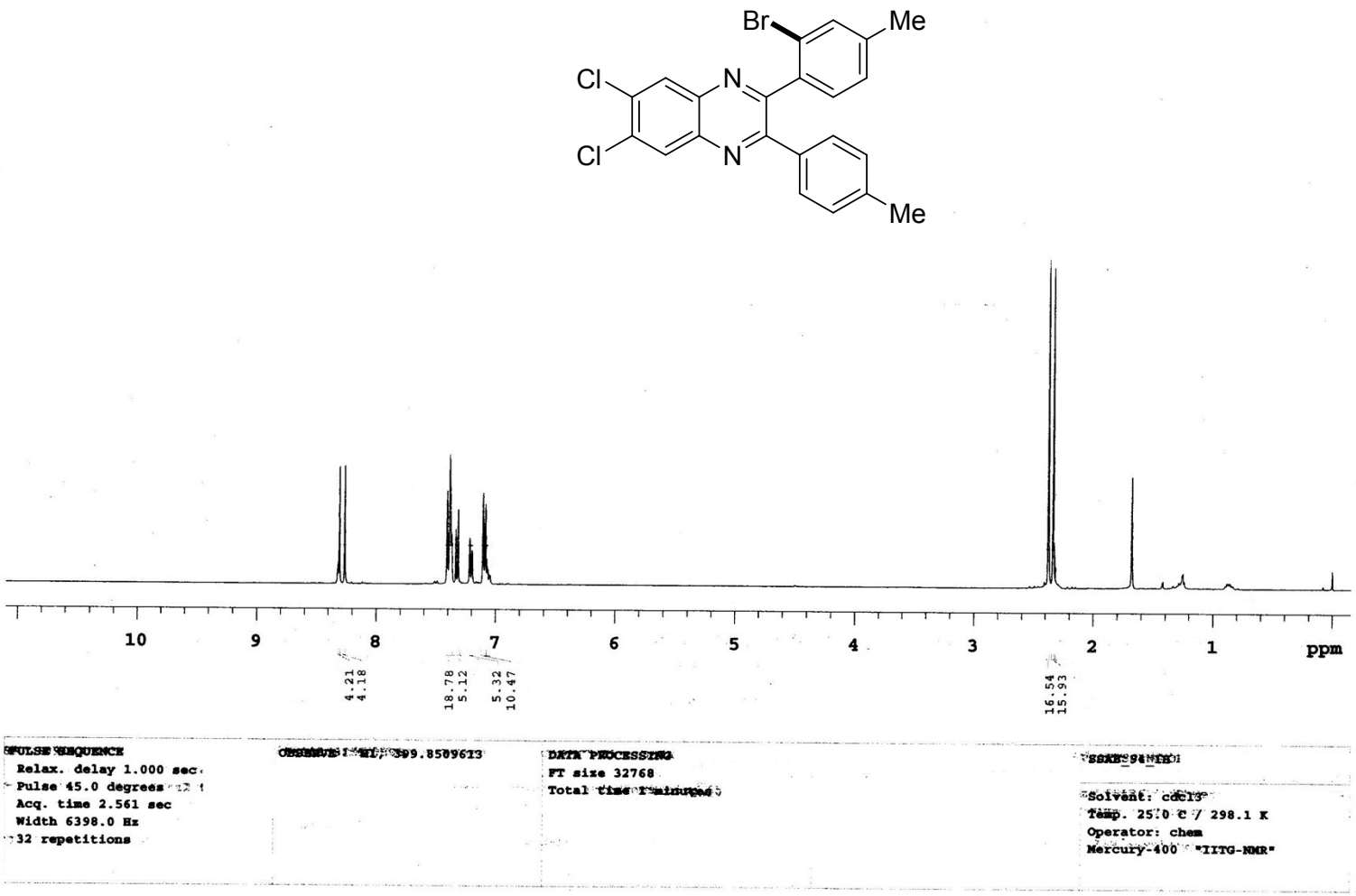
2-(2-Bromo-4-methylphenyl)-3-(p-tolyl)quinoxaline (21a): ^{1}H NMR (400 MHz, $CDCl_3$):



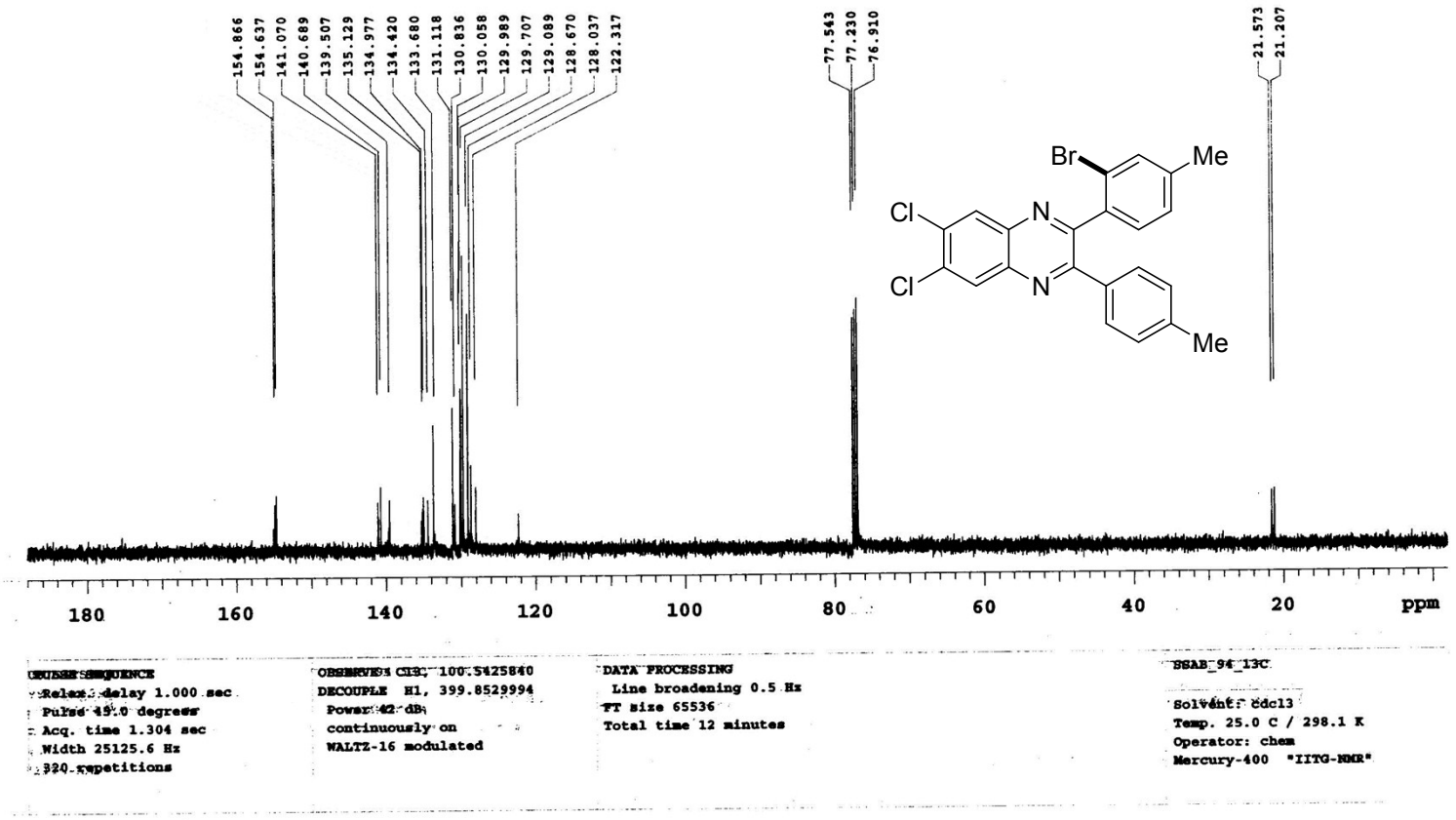
2-(2-Bromo-4-methylphenyl)-3-(p-tolyl)quinoxaline (21a): ^{13}C NMR (100 MHz, $CDCl_3$):



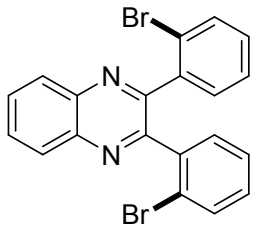
2-(2-Bromo-4-methylphenyl)-6,7-dichloro-3-(p-tolyl)quinoxaline (22a): ^{1}H NMR (400 MHz, $CDCl_3$):

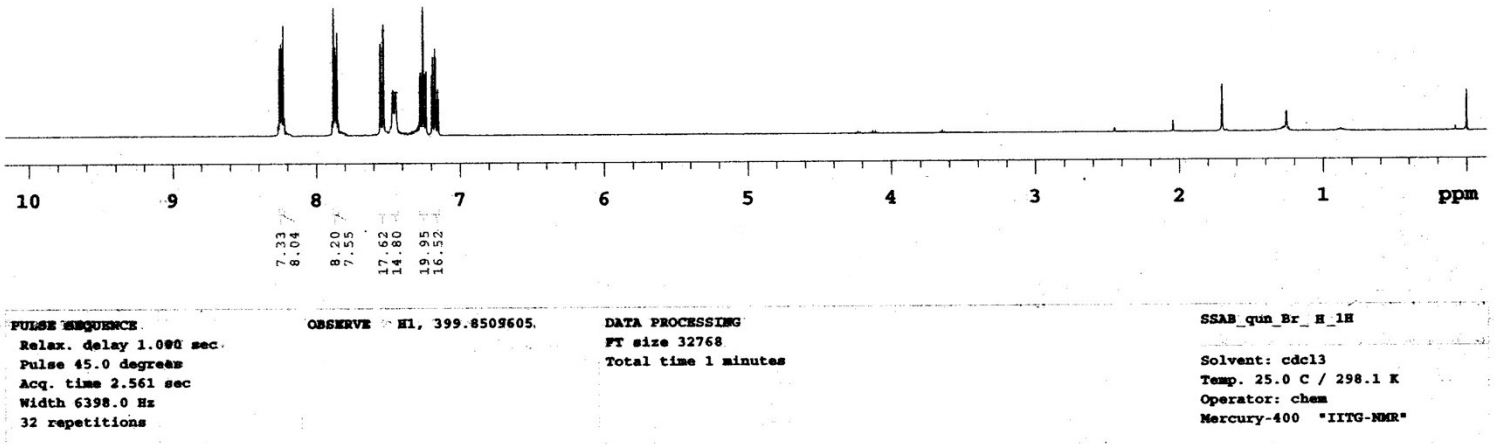


2-(2-Bromo-4-methylphenyl)-6,7-dichloro-3-(p-tolyl)quinoxaline (22a): ^{13}C NMR (100 MHz, $CDCl_3$):

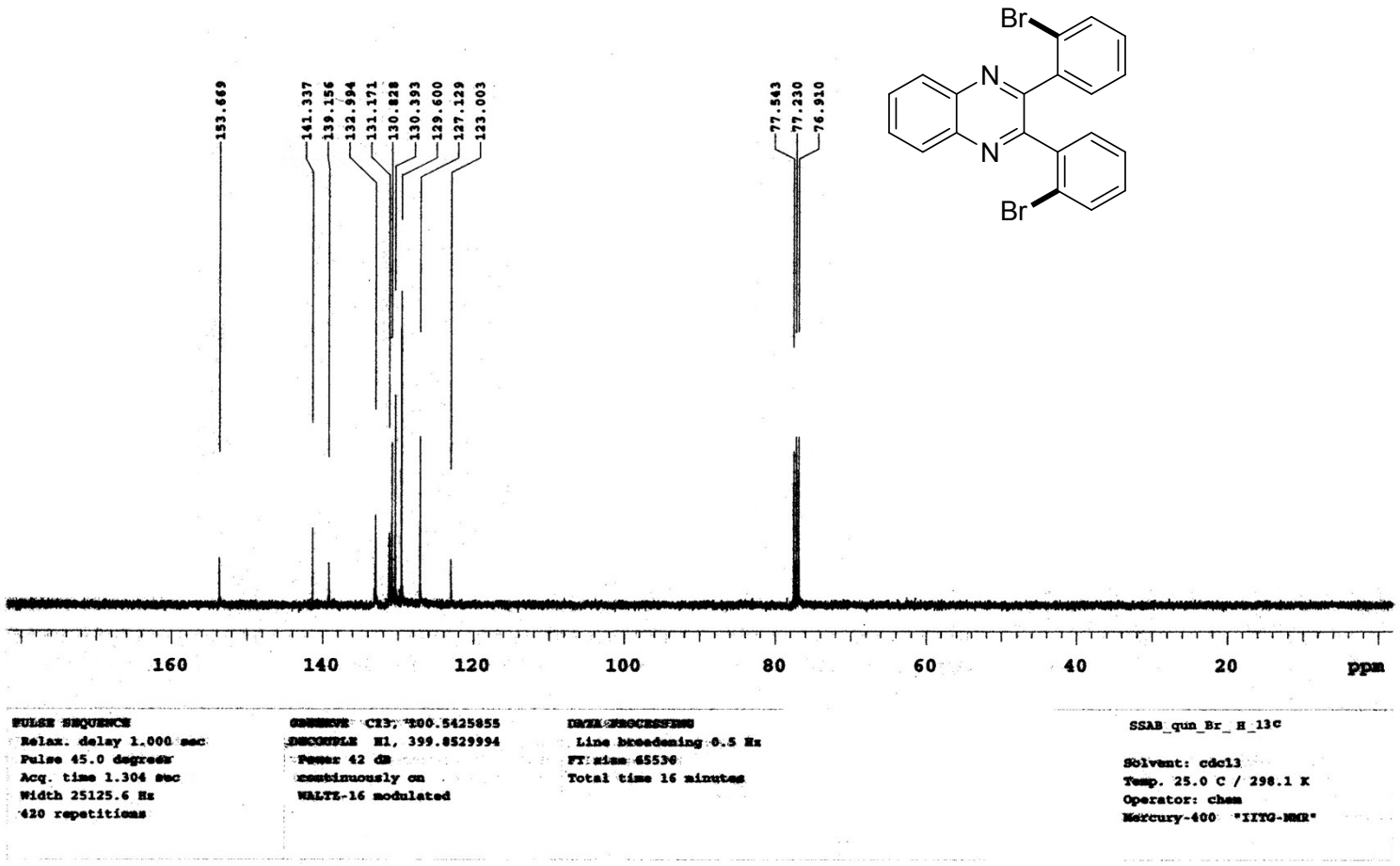


2,3-Bis(2-bromophenyl)quinoxaline (20aa): ^{1}H NMR (400 MHz, $CDCl_3$):

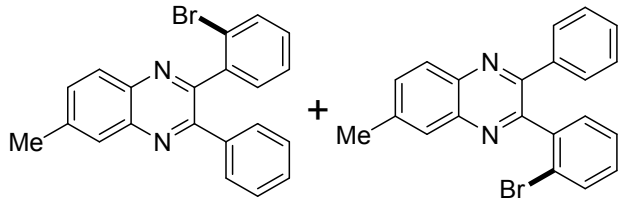


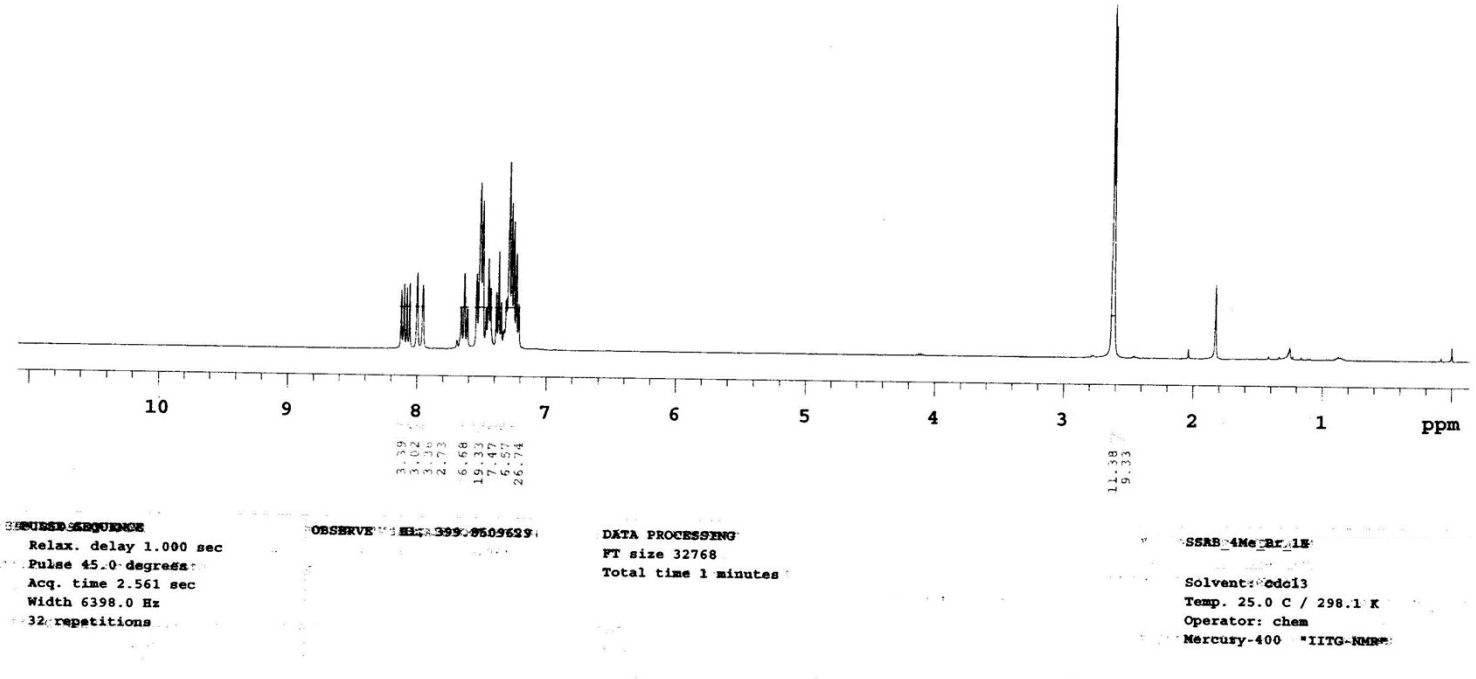


2,3-Bis(2-bromophenyl)quinoxaline (20aa): ^{13}C NMR (100 MHz, $CDCl_3$):

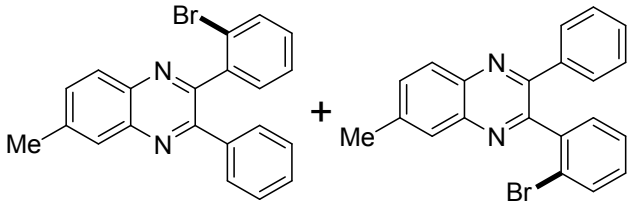


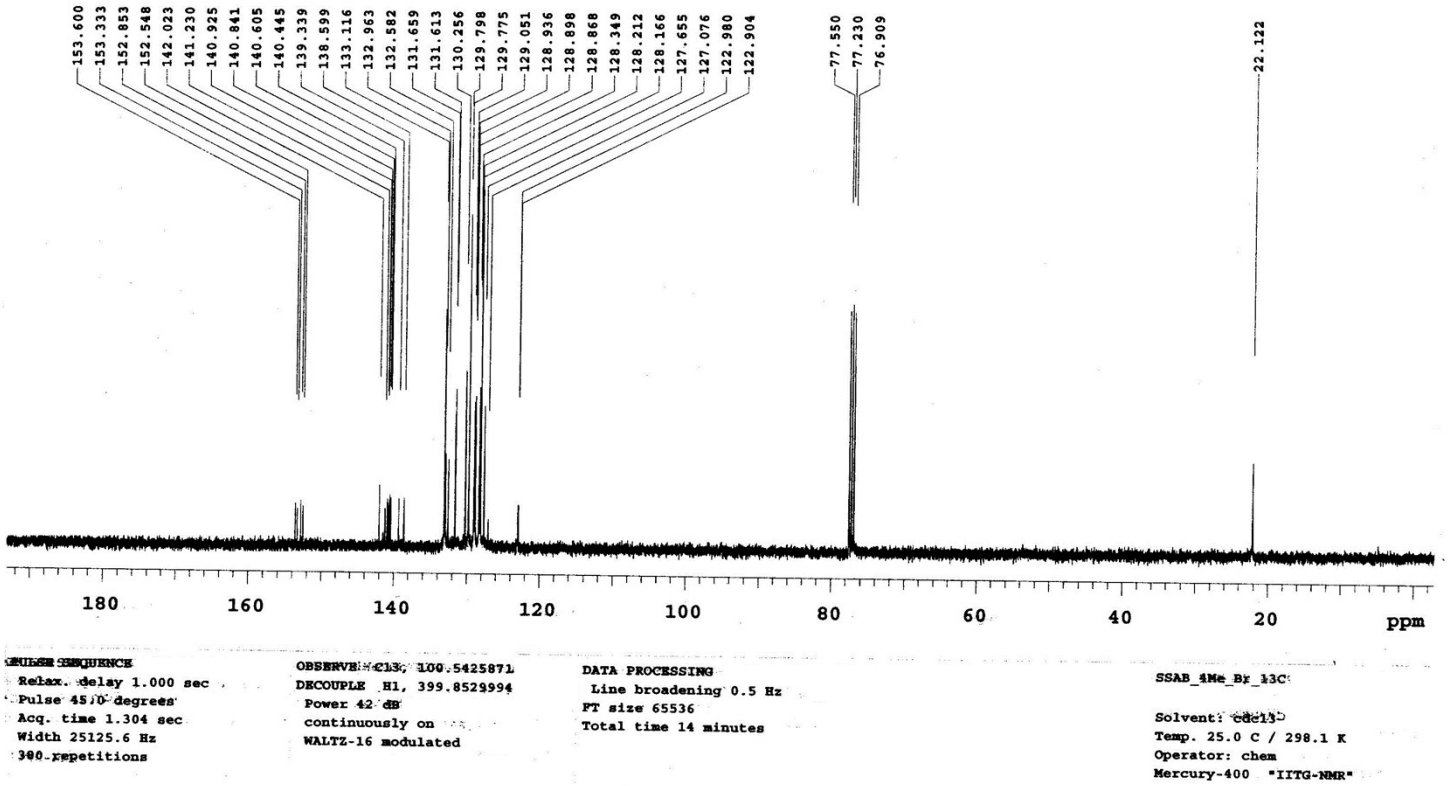
2-(2-Bromophenyl)-6-methyl-3-phenylquinoxaline compound and 3-(2-Bromophenyl)-6-methyl-2-phenylquinoxaline (23a and 23a´): ^{1}H NMR (400 MHz, $CDCl_3$):



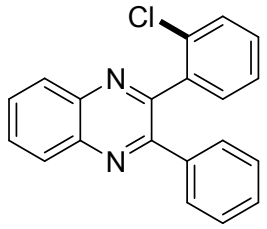


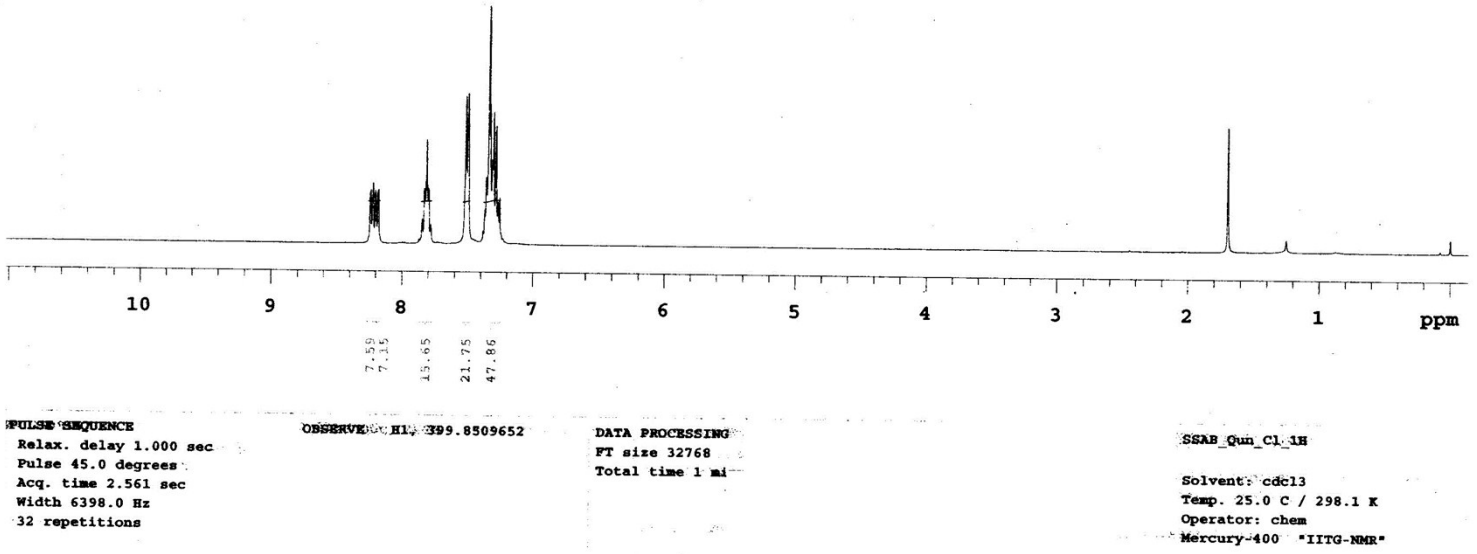
2-(2-Bromophenyl)-6-methyl-3-phenylquinoxaline compound and 3-(2-Bromophenyl)-6-methyl-2-phenylquinoxaline (23a and 23a′): ^{13}C NMR (100 MHz, $CDCl_3$):



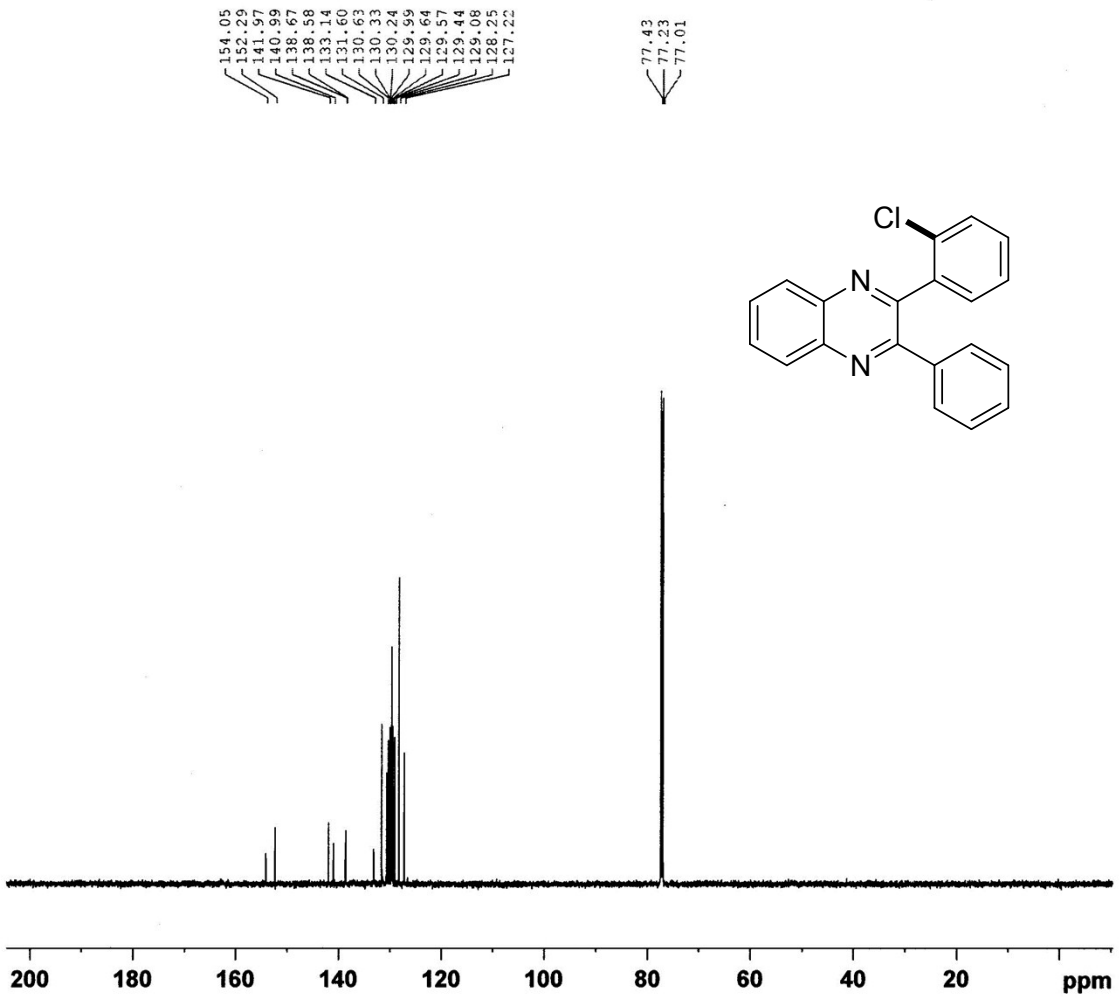


2-(2-Chlorophenyl)-3-phenylquinoxaline (20b): ^{1}H NMR (400 MHz, $CDCl_3$):





2-(2-Chlorophenyl)-3-phenylquinoxaline (20b): ^{13}C NMR (150 MHz, $CDCl_3$):



BRUKER

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Current Data Parameters
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EXPNO                   1
PROCNO                  1

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PULPROG         zgpg30
TD                32768
SOLVENT           CDCl3
NS                  161
DS                    2
SWH           36057.691 Hz
FIDRES         1.100393 Hz
AQ            0.4543829 sec
RG                65.24
DW               13.867 usec
DE                6.50 usec
TE                300.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        150.9279571 MHz
NUC1                13C
P1                10.50 usec
PLW1        95.00000000 W

======== CHANNEL f2 ========
SFO2        600.1724007 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             70.00 usec
PLW2        21.00000000 W
PLW12        0.61714000 W
PLW13        0.30239999 W

F2 - Processing pàrameters
SI                16384
SF          150.9128391 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
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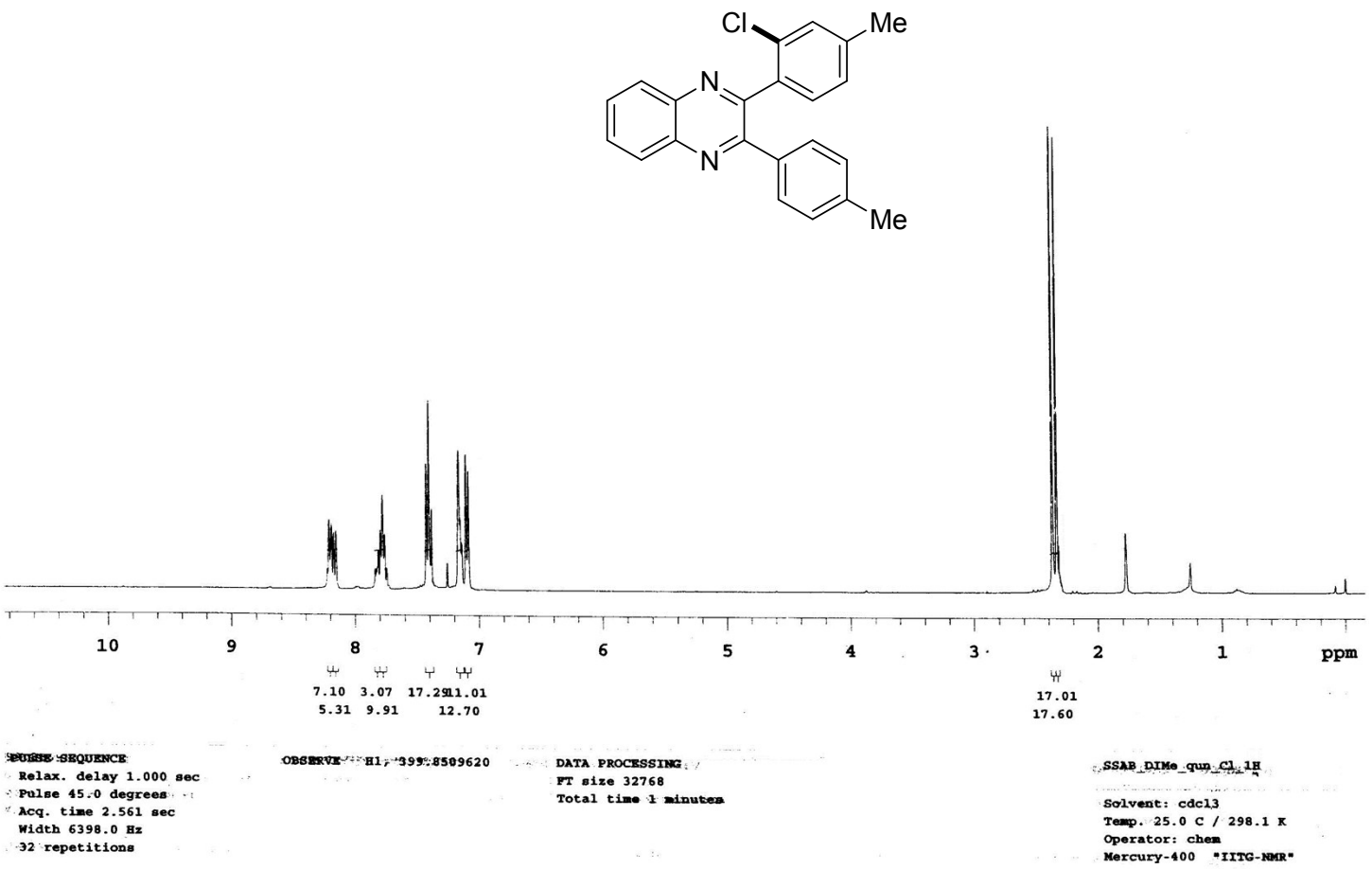
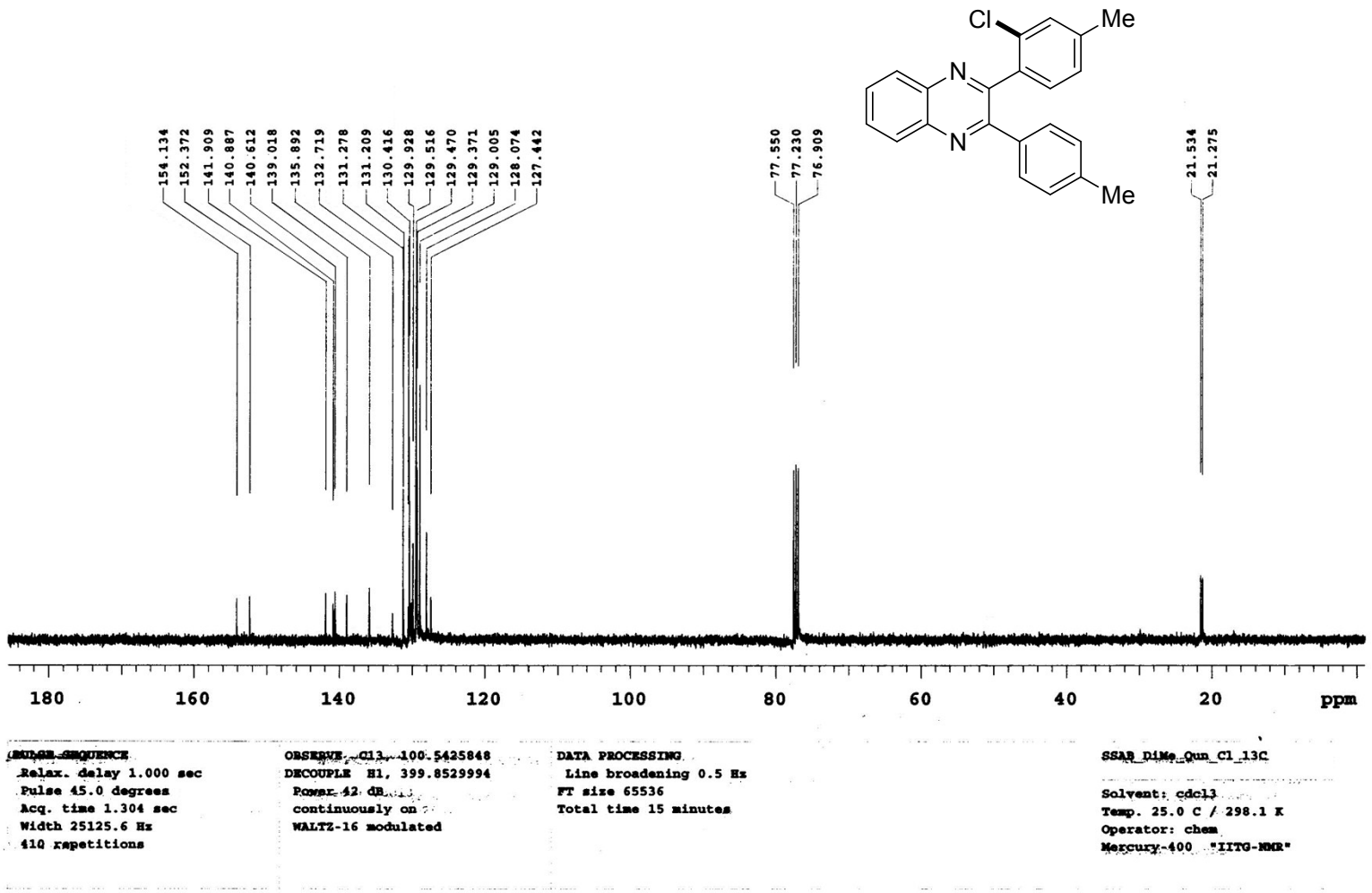
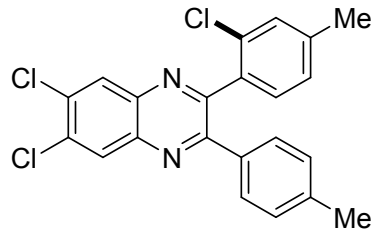
2-(2-Chloro-4-methylphenyl)-3-(p-tolyl)quinoxaline (21b): ^{1}H NMR (400 MHz, $CDCl_3$):

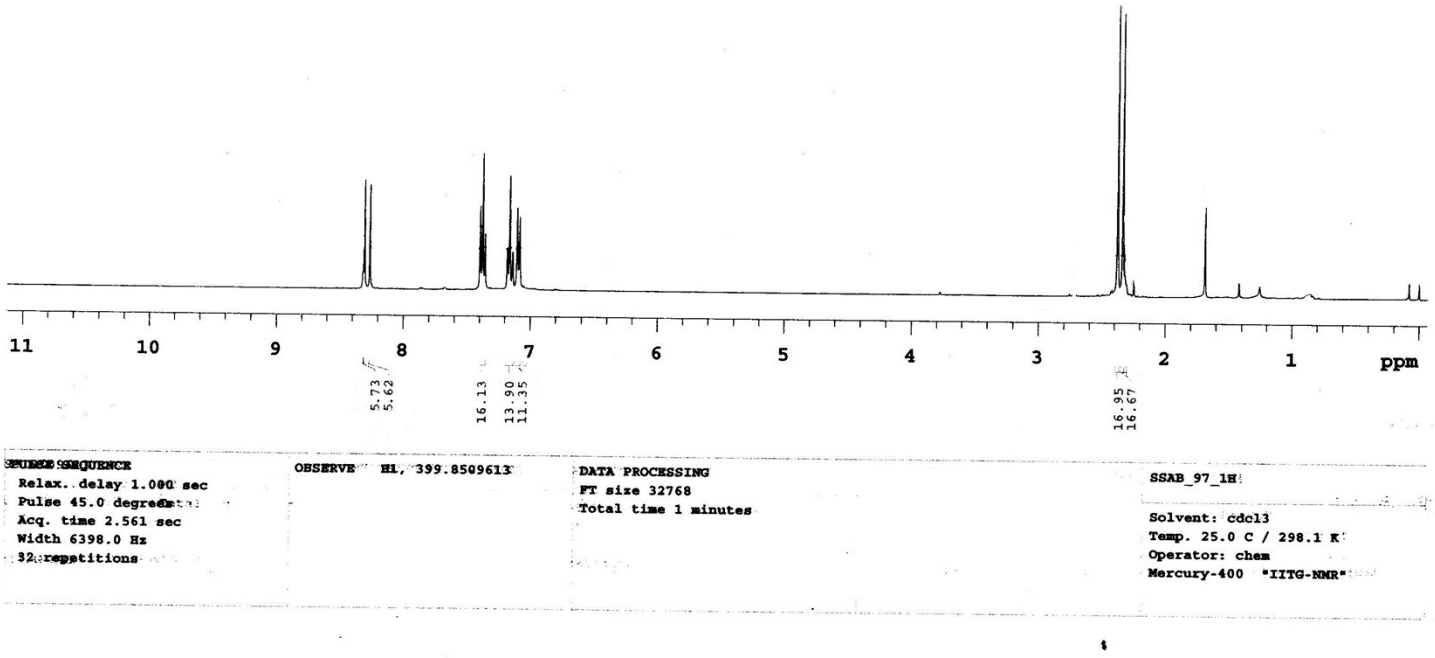


2-(2-Chloro-4-methylphenyl)-3-(p-tolyl)quinoxaline (21b): ^{13}C NMR (100 MHz, $CDCl_3$):

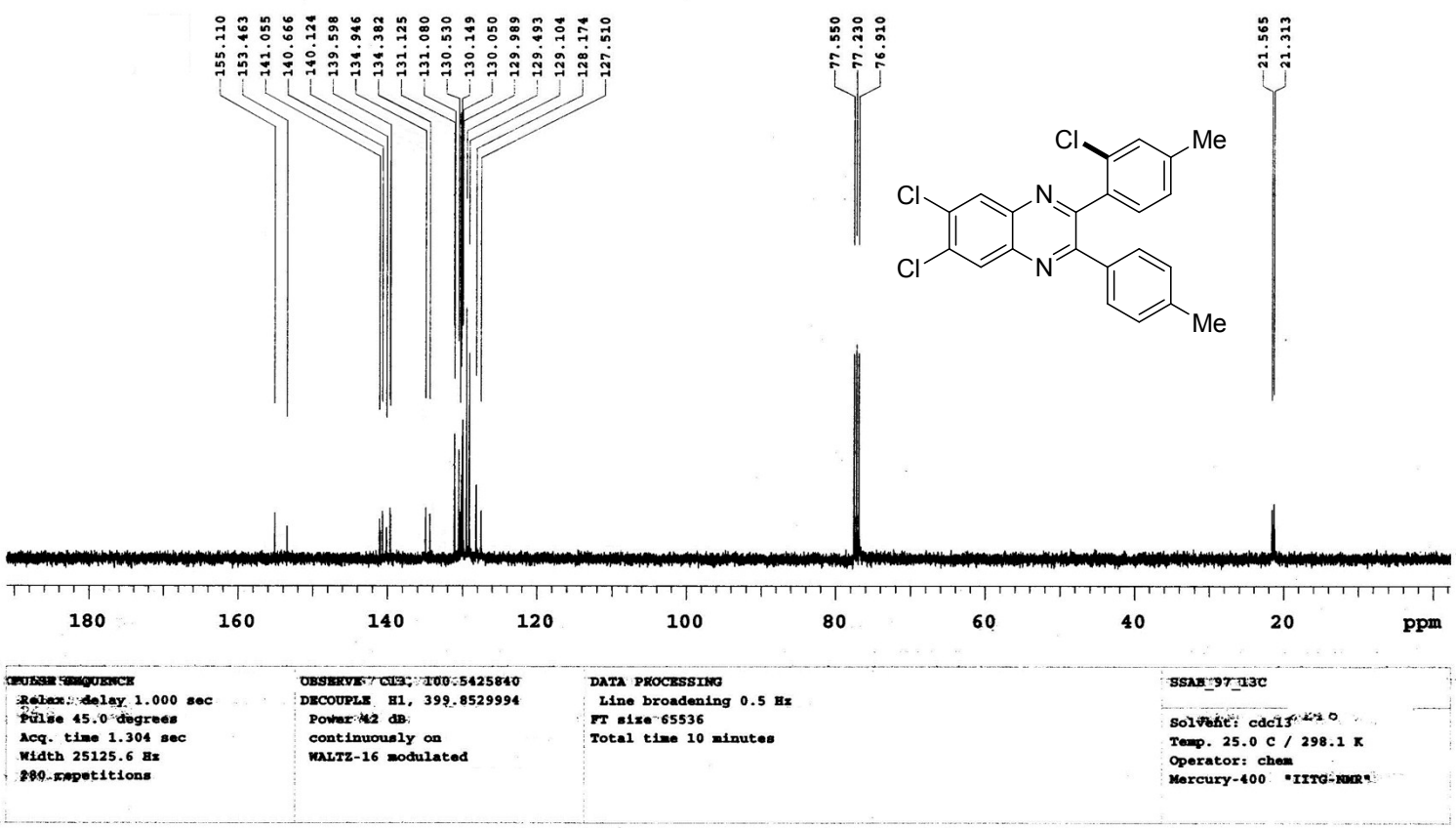


6,7-Dichloro-2-(2-chloro-4-methylphenyl)-3-(p-tolyl)quinoxaline (22b):^{1}H NMR (400 MHz, $CDCl_3$):

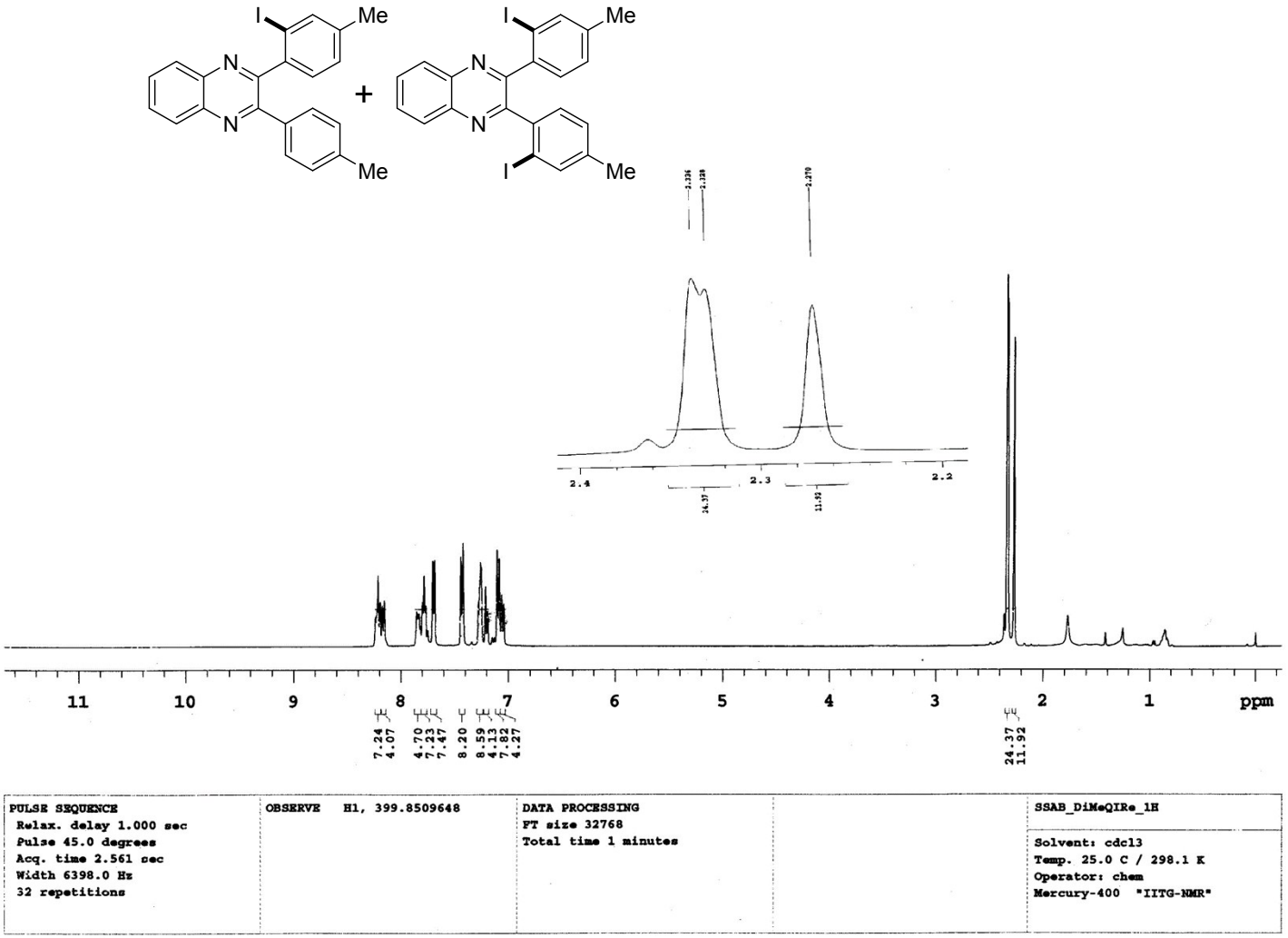




6,7-Dichloro-2-(2-chloro-4-methylphenyl)-3-(p-tolyl)quinoxaline (22b):^{13}C NMR (100 MHz, $CDCl_3$):



2,3-Bis(2-iodo-4-methylphenyl)quinoxaline compound and 2-(2-Iodo-4-methylphenyl)-3-(p-tolyl)quinoxaline (21c and 21cc): ^{1}H NMR (400 MHz, $CDCl_3$):



PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	OBSERVE H1, 399.8509648	DATA PROCESSING FT size 32768 Total time 1 minutes		SSAB_DiMeQIRe_1H Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 "IITG-NMR"

2,3-Bis(2-iodo-4-methylphenyl)quinoxaline compound and 2-(2-Iodo-4-methylphenyl)-3-(*p*-tolyl)quinoxaline (21c and 21cc): ^{13}C NMR (100 MHz, $CDCl_3$):