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Supporting Information

Copper-Catalyzed One-Pot Synthesis of *N*-Substituted Benzo[*d*]isothiazol-3(2*H*)-ones via *C-S/N-S* Bond Formation

Rajesh Paul and Tharmalingam Punniyamurthy*

Department of Chemistry, Indian Institute of Technology Guwahati, Guwahati-781039, India.

tpunni@iitg.ernet.in

General Information. CuCl (98%) and sulfur powder (97%) were purchased from Rankem and used without further purification. $Cu(OAc)_2 \cdot 1H_2O$ (98%)_was purchased from Merck and used without further purification. 2-Iodobenzoic acid (98%), 2-bromobenzoic acid (97%) and anilines were purchased from Aldrich. Column chromatography was performed with Rankem silica gel (60-120 mesh). The substituted 2-halobenzamides were prepared according to the reported procedures.[11] NMR (^{1}H and ^{13}C) spectra were recorded with a Varian 400 spectrometer. Melting points were determined with a Büchi B-545 apparatus and are uncorrected. Elemental analyses were recorded using PerkinElmer CHNS analyzer. X-Ray data were collected on a Bruker SMART APEX equipped with a CCD area detector using Mo Kα radiation. The structure was solved by direct method using *SHELLX-97* (Göttingen, Germany).

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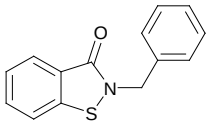
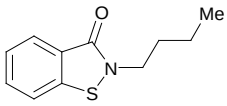
General Procedure for Preparation of *N*-Substituted Benzo[*d*]isothiazol-3(2*H*)-ones. An oven dried round bottom flask (10 mL) was charged with *N*-substituted 2-halobenzamide (0.5 mmol), CuCl (10 mol %), sulfur powder (1.5 mmol) and K_2CO_3 or Cs_2CO_3 (1.5 mmol) in DMF (1 mL) under nitrogen atmosphere. The resultant mixture was stirred at 75-135 °C under nitrogen balloon for the appropriate time. The progress of the reaction was monitored by TLC using ethyl acetate and hexane as eluent. The reaction mixture was then cooled to room temperature and diluted with ethyl acetate (10 mL). The organic layer was separated and washed with water (3 x 5 mL) and brine (1 x 5 mL). Drying (Na_2SO_4) and evaporation of the solvent gave a residue that was purified on silica gel column chromatography using hexane and ethyl acetate as eluent.

Characterization Data of 2-Substituted Benzo[*d*]isothiazol-3(2*H*)-ones



***N*-Benzylbenzo[*d*]isothiazol-3(2*H*)-one[2] (table 1, entry 1).** Colorless solid; 88% yield; mp = 88-89 °C (lit. mp[3] 89 °C); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.99 (d, *J* = 7.6 Hz, 1H), 7.49 (t, *J* = 7.2 Hz, 1H), 7.41 (d, *J* = 8.4 Hz, 1H), 7.33-7.23 (m, 6H), 4.96 (s, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 165.5, 140.5, 136.3, 131.9, 128.9, 128.5, 128.4, 126.9, 125.6, 124.5, 120.5, 47.6; FT-IR (KBr): 3078, 3022, 2962, 2923, `667, 1592, 1445, 1336, 1261, 1243, 1184, 1064, 1029 cm^{-1}. Elemental analysis calcd (%) for $C_{14}H_{11}NOS$: C, 69.68; H, 4.59; N, 5.80; S, 13.29, found: C, 69.64; H, 4.56; N, 5.83; S, 13.31.



***N*-Butylbenzo[*d*]isothiazol-3(2*H*)-one[4] (table 2, entry 1).** Yellow oil; 93% yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.01 (d, *J* = 8.0 Hz, 1H), 7.58-7.50 (m, 2H), 7.36 (t, *J* = 7.2 Hz, 1H), 3.88 (t, *J* = 7.2 Hz, 2H), 1.75 (t, *J* = 7.2 Hz, 2H), 1.71-1.33 (m, 2H), 0.95 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 165.5, 140.3, 131.7, 126.8, 125.6, 125.2, 120.4, 43.8, 31.7, 19.9, 13.8. FT-IR (neat): 2962, 2857, 1682, 1490, 1449, 1261, 1091 cm^{-1}. Elemental analysis calcd

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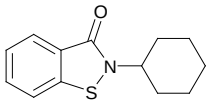
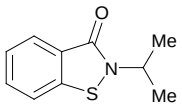
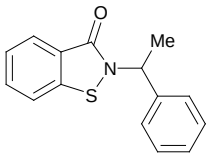
(%) for $C_{11}H_{13}NOS$: C, 63.74; H, 6.32; N, 6.76; S, 15.47, found: C, 63.71; H, 6.35; N, 6.73; S, 15.50.



***N*-Cyclohexylbenzo[*d*]isothiazol-3(2*H*)-one[3] (table 2, entry 2).** Colorless solid; 95% yield; mp = 86-87 °C (lit.[3] mp 87-88 °C); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.01 (d, *J* = 8.0 Hz, 1H), 7.54-7.50 (m, 1H), 7.36-7.31 (m, 2H), 4.59-4.53 (m, 1H), 2.01 (d, *J* = 10.4 Hz, 1H), 1.85 (d, *J* = 12.8 Hz, 2H), 1.71-1.67 (m, 1H), 1.55-1.38 (m, 5H), 1.21-1.12 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 164.9, 140.4, 131.5, 126.6, 125.6, 125.4, 120.5, 53.3, 33.06, 25.7, 25.4; FT-IR (KBr): 2929, 2854, 1651, 1448, 1332, 1305, 1262, 1240, 1210, 1191, 1149, 1062 cm^{-1}. Elemental analysis calcd (%) $C_{13}H_{15}NOS$: C, 66.92; H, 6.48; N, 6.00; S, 13.74, found: C, 66.95; H, 6.46; N, 6.03; S, 13.76.



***N*-Isopropylbenzo[*d*]isothiazol-3(2*H*)-one[6] (table 2, entry 3).** Yellow oil; 93% yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.01 (d, *J* = 7.6 Hz, 1H), 7.57-7.54 (m, 1H), 7.36 (t, *J* = 6.4 Hz, 2H), 5.01-4.95 (m,1H), 1.40 (d, *J* = 6.4 Hz, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 164.9, 140.1, 131.5, 126.4, 125.5, 125.4, 120.5, 46.1, 22.2. FT-IR (neat): 2935, 2851, 1641, 1447,1332, 1239, 1192, 1034 cm^{-1}. Elemental analysis calcd (%) for $C_{10}H_{11}NOS$: C, 62.15; H, 5.74; N, 7.25; S, 16.59, found: C, 62.18; H, 5.76; N, 7.24; S, 16.57.



***N*-(1-Phenylethyl)benzo[*d*]isothiazol-3(2*H*)-one (table 2, entry 4).** Yellow oil; 87%, yield; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.83-7.81 (m, 1H), 7.40-7.25 (m, 7H), 7.14-7.05 (m, 1H), 5.33-5.26 (m, 1H), 1.63 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 165.1, 140.6, 131.7, 128.8, 128.6, 128.3, 127.4, 126.7, 125.5, 120.5, 52.3, 19.3. FT-IR (neat): 2935, 2851, 1640, 1440, 1331,

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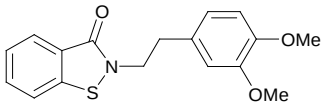
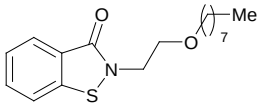
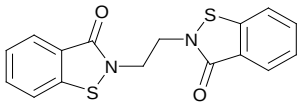
1229, 1192, 1092, 1034 cm^{-1}. Elemental analysis calcd (%) for $C_{15}H_{13}NOS$: C, 70.56; H, 5.13; N, 5.49; S, 12.56, found: C, 70.53; H, 5.15; N, 5.53; S, 12.52.



***N*-(3,4-Dimethoxyphenethyl)benzo[*d*]isothiazol-3(2*H*)-one (table 2, entry 5).** Yellow solid; 83% yield; mp 105-107 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.95 (d, *J* = 7.6 Hz, 1H), 7.51-7.47 (m, 1H), 7.43 (d, *J* = 8.0 Hz, 1H), 7.31 (t, *J* = 7.2 Hz, 1H), 6.71-6.65 (m, 3H), 4.04 (t, *J* = 6.8 Hz, 2H), 3.75 (s, 3H), 3.70 (s, 3H), 2.94 (t, *J* = 6.8 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 165.4, 149.1, 147.9, 140.3, 131.8, 130.3, 126.7, 125.5, 124.6, 120.9, 120.2, 112.1, 111.4, 55.9, 55.8, 45.2, 35.2. FT-IR (KBr): 2935, 2067, 1639, 1518, 1446, 1337, 1263, 1230, 1185, 1143, 1026 cm^{-1}. Elemental analysis calcd (%) for $C_{17}H_{17}NO_3S$: C, 67.74; H, 5.43; N, 4.44; S, 10.17, found: C, C, 67.71; H, 5.45; N, 4.46; S, 10.15.



***N*-(2-(Octyloxy)ethyl)benzo[*d*]isothiazol-3(2*H*)-one (table 2, entry 6).** Yellow oil; 90% yield ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.97 (d, *J* = 8.0 Hz, 1H), 7.52(t, *J* = 8.0 Hz, 1H), 7.34-7.30 (m, 1H), 7.03(t, *J* = 7.6 Hz, 1H), 4.03 (t, *J* = 5.2 Hz, 2H), 3.65 (t, *J* = 4.8 Hz, 2H), 3.43-3.39 (m, 2H), 1.57-1.49 (m, 2H), 1.28-1.19 (m, 10H), 0.83(t, *J* = 6.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 165.7, 140.0, 131.9, 126.7, 125.4, 124.3, 120.3, 71.6, 69.4, 44.2, 31.9, 29.8, 29.6, 26.4, 26.3, 22.8, 14.3. FT-IR (neat): 2935, 2851, 1641, 1467, 1331, 1192, 1034 cm^{-1}. Elemental analysis calcd (%) for $C_{17}H_{25}NO_2S$: C, 66.13; H, 7.79; N, 4.33; S, 9.91, found: C, 66.17; H, 7.76; N, 4.34; S, 9.87.



***N*,*N*'-(Ethane-1,2-diyl)dibenzo[*d*]isothiazol-3(2*H*)-one (table 2, entry 7).** Colorless solid; 81% yield; mp 165-167 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.01 (d, *J* = 8.0 Hz, 2H), 7.58 (t, *J* = 7.2 Hz, 2H), 7.46 (d, *J* = 8.0 Hz, 2H), 7.38 (t, *J* = 7.2 Hz, 2H), 4.21 (s, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 165.8, 140.9, 132.2, 126.9, 126.8, 125.8, 120.6, 43.1. FT-IR (KBr): 2964, 2924, 2853,

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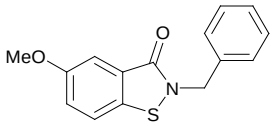
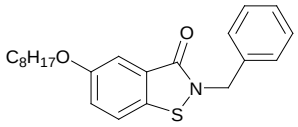
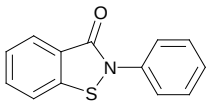
1644, 1505, 1447, 1330, 1304, 1261, 1097, 1065, 1019 cm^{-1}. Elemental analysis calcd (%) for $C_{16}H_{12}N_2O_2S$: C, 58.52; H, 3.68; N, 8.53; S, 19.53, found: C, 58.55; H, 3.64; N, 8.50; S, 19.54.



***N*-Benzyl-5-methoxybenzo[*d*]isothiazol-3(2*H*)-one (table 2, entry 8).** Colorless solid, 67% yield; m.p. 134-135 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (s, 1H), 7.83-7.81(m, 1H), 7.33-7.31 (m, 5H), 7.24-7.21 (m, 1H), 5.01 (s, 2H), 3.8 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.9, 140.5, 139.9, 136.0, 135.8, 129.1, 128.6, 126.6, 122.2, 55.7, 47.9. FT-IR (KBr): 2917, 2840, 1651, 1591, 1576, 1408, 1266 cm^{-1}. Elemental analysis calcd (%) for $C_{15}H_{13}NO_2S$: C, 66.40; H, 4.83; N, 5.16; 11.82, found C, 66.44; H, 4.78; N, 5.19, S, 11.83.



***N*-Benzyl-5-(octyloxy)benzo[*d*]isothiazol-3(2*H*)-one (table 2, entry 9).** Yellow liquid; 72% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (s, 1H), 7.83-7.81(m, 1H), 7.33-7.31 (m, 5H), 7.24-7.21 (m, 1H), 5.01 (s, 2H), 4.03 (t, J = 5.2 Hz, 2H), 1.57-1.49 (m, 3H), 1.28-1.19 (m, 10H), 0.83(t, J = 6.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.9, 140.5, 139.9, 136.0, 135.8, 129.1, 128.6, 126.6, 122.2, 69.4, 55.7, 47.9, 31.9, 29.8, 29.6, 26.4, 26.3, 22.8, 14.3. FT-IR (KBr): 2917, 2840, 1651, 1591, 1576, 1408, 1376, 1299, 1266, 1021 cm^{-1}. Elemental analysis calcd (%) for $C_{22}H_{27}NO_2S$: C, 71.51; H, 7.36; N, 3.79; S, 8.68, found C, 71.54; H,7.33; N, 3.81; S, 8.71.



***N*-Phenylbenzo[*d*]isothiazol-3(2*H*)-one[6] (table 3, entry 1).** Colorless solid; 90% yield; mp 140-142 °C (lit.[7] mp 141.5-142.5 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, J = 8.0 Hz, 1H), 7.72-7.65 (m, 2H), 7.59 (d, J = 8.0 Hz, 2H), 7.49-7.42 (m, 2H), 7.34 (t, J = 7.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.3, 139.8, 136.0, 132.8, 132.7, 129.7, 127.5, 126.2, 125.8, 120.4. FT-IR (KBr): 2963, 2923, 2840, 1633, 1412, 1261, 1095, 1022 cm^{-1}. Elemental analysis calcd (%) for $C_{13}H_9NOS$: C, 68.70; H, 3.99; N, 6.16; S, 14.11, found C, 68.72; H, 3.97; N, 6.18; S, 14.14.

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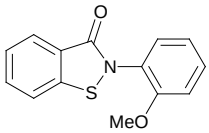
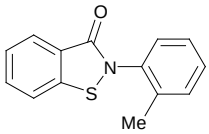
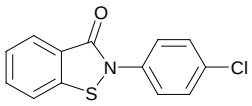


***N*-(2-Methoxyphenyl)benzo[*d*]isothiazol-3(2*H*)-one (table 3, entry 2).** Colorless solid; 84% yield; mp 105-107 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.09 (d, *J* = 8.0 Hz, 1H), 7.61 (d, *J* = 6.8 Hz, 1H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.42-7.37 (m, 3H), 7.03 (t, *J* = 8.0 Hz, 2H), 3.81 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 165.1, 156.9, 141.6, 132.1, 130.7, 130.3, 127.2, 125.4, 124.6, 123.9, 120.9, 112.5, 56.0; FT-IR (KBr): 2923, 2923, 2851, 1663, 1593, 1497, 1445, 1333, 1261, 1094, 1021 cm^{-1}. Elemental analysis calcd (%) for $C_{14}H_{11}NO_2S$: C, 65.35; H, 4.31; N, 5.44; S, 12.46, found: C, 65.38; H, 4.29; N, 5.47; S, 12.44.



***N*-(2-Methylphenyl)benzo[*d*]isothiazol-3(2*H*)-one (table 3, entry 3).** Colorless solid; mp 122-124 °C (lit. mp[2] 122-123 °C); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.07 (d, *J* = 8.0 Hz, 1H), 7.63 (t, *J* = 8.0 Hz, 1H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.49 (s, 1H), 7.46-7.38 (m, 2H), 7.34 (t, *J* = 8.0 Hz, 1H), 7.11 (d, *J* = 7.6 Hz, 1H), 2.38 (s, 3H); ^{13}C NMR ($CDCl_3$, 100MHz) δ 164.4, 140.2, 139.6, 137.3, 132.5, 129.4, 128.2, 127.4, 125.9, 125.6, 125.1, 121.9, 120.3, 21.6. FT-IR (KBr): 2963, 2917, 1644, 1504, 1331, 1016 cm^{-1}. Elemental analysis calcd (%) for $C_{14}H_{11}NOS$: C, 69.68; H, 4.59; N, 5.80; S, 13.29, found: C, 69.64; H, 4.61; N, 5.78; S, 13.27.



***N*-(4-Chlorophenyl)benzo[*d*]isothiazol-3(2*H*)-one[7] (table 3, entry 5).** Colorless solid; 85% yield; m.p. 127-128 °C (lit.[7] mp 128-129 °C); ^{1}H NMR ($CDCl_3$, 400MHz) δ; 8.08 (d, *J* = 8.0 Hz, 1H), 7.65-7.63 (m, 2H), 7.57 (d, *J* = 8.0 Hz, 2H), 7.43-7.39 (m, 3H); ^{13}C NMR ($CDCl_3$, 400MHz) δ 163.1, 138.6, 134.8, 131.6, 128.5, 128.1, 126.2, 124.9, 124.6, 123.6, 119.1; FT-IR (KBr): 2962, 2926, 2851, 1661,1591, 1490, 1444, 1325, 1303, 1261, 1122, 1028 cm^{-1}. Elemental analysis calcd (%) for $C_{13}H_8ClNOS$: C, 59.66; H, 3.08; N, 5.35; S, 12.25, found C, 59.64; H, 3.10; N, 5.33; S, 12.27.

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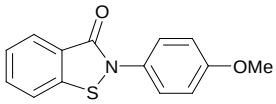
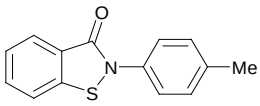
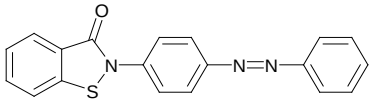


***N*-(4-Methoxyphenyl)benzo[*d*]isothiazol-3(2*H*)-one[7] (table 3, entry 6):** Colorless solid; 89% yield; m.p. 146-147 °C (lit.[7] mp 147-149 °C); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.08 (d, *J* = 8.0 Hz, 1H), 7.62 (t, *J* =6.8 Hz, 1H), 7.55-7.51 (m, 3H), 7.41 (t, *J* = 7.6 Hz, 1H), 6.96 (d, *J* =6.8 Hz, 2H), 3.8 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 164.5, 158.9, 140.2, 132.3, 129.8, 127.3, 127.0, 125.9, 124.8, 120.2, 114.7, 55.7. FT-IR (KBr): 2923, 2854, 1663, 1591, 1490, 1445, 1331, 1267, 1095 cm^{-1}. Elemental analysis calcd (%) for $C_{14}H_{11}NO_2S$: C, 65.35; H, 4.31; N, 5.44; S, 12.40, found C, 65.36; H, 4.33; N, 5.46; S, 12.42.



***N*-p-Tolylbenzo[*d*]isothiazol-3(2*H*)-one[7] (table 3, entry 7).** Colorless solid; 93% yield; mp 135-136 °C (lit.[7] mp 136-137 °C); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.02 (d, *J* = 8.0 Hz, 1H), 7.56-7.54 (m, 1H), 7.47 (d, *J* = 6.4 Hz, 4H), 7.36 (t, *J* = 8.0 Hz, 1H), 7.18 (d, *J* = 7.6 Hz, 1H), 2.29 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 164.4, 140.1, 137.4, 134.7, 132.4, 130.1, 127.3, 125.9, 124.9, 120.2, 21.3. FT-IR (KBr): 2923, 2917, 2851, 1644, 1504, 1446, 1331, 1261, 1096, 1019 cm^{-1}. Elemental analysis calcd (%) for $C_{14}H_{11}NOS$: C, 69.68; H, 4.59; N, 5.80; S, 13.29, found 69.65; H, 4.56; N, 5.77; S, 13.25.



***N*-(4-(Phenyldiazenyl)phenyl)benzo[*d*]isothiazol-3(2*H*)-one (table 3, entry 9).** Orange solid; 63% yield; mp 147-149 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.10 (d, *J* = 8.0 Hz, 1H), 7.65-7.61 (m, 1H), 7.56 (d, *J* = 8.0 Hz, 1H), 7.45-7.36 (m, 8H), 7.22 (d, *J* = 8.0 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 164.4, 152.8, 150.6, 139.8, 132.8, 131.4, 129.3, 127.5, 127.3, 126.2, 124.3, 124.2, 124.1, 123.1, 120.4. FT-IR (KBr): 3066, 2961, 2924, 2854, 2852, 1653, 1594, 1526, 1497, 1446, 1327, 1261, 1101, 1018 cm^{-1}. Elemental analysis calcd (%) for $C_{19}H_{13}N_3OS$: C, 68.86; H, 3.95; N, 12.68; S, 9.68, found .C, 68.84; H, 3.96; N, 12.64 S, 9.71.

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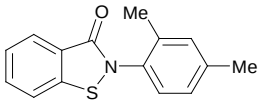
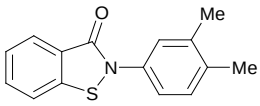
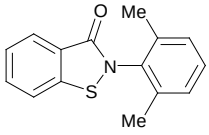


***N*-(2,4-Dimethylphenyl)benzo[*d*]isothiazol-3(2*H*)-one (table 3, entry 10).** Colorless solid; 92% yield; mp 114-115 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.00 (d, *J* = 8.0 Hz, 1H), 7.55 (t, *J* =7.2 Hz, 1H), 7.47 (d, *J* = 8.4 Hz, 1H), 7.30 (t, *J* = 8.4 Hz, 1H), 7.12 (d, *J* = 7.6 Hz, 1H), 7.04 (s,1H), 6.98 (d, *J* = 8.0 Hz, 1H), 2.26 (s, 3H), 2.15 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 164.7, 141.3, 139.7, 137.4, 132.2, 132.0, 131.3, 128.8, 127.7, 127.2, 125.7, 124.1, 120.4, 21.3, 17.9. FT-IR (KBr): 2923, 2854, 1659, 1593, 1500, 1446, 1329, 1309, 1262, 1104, 1017 cm^{-1}. Elemental analysis calcd (%) for $C_{15}H_{13}NOS$: C, 73.56; H, 5.13; N, 5.49; S, 12.56, found C, 73.54; H, 5.16; N, 5.47; S, 12.54.



***N*-(3,4-Dimethylphenyl)benzo[*d*]isothiazol-3(2*H*)-one (table 3, entry 11).** Colorless solid; 91% yield; mp 114-116 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.07 (d, *J* = 8.0 Hz, 1H), 7.61 (t, *J* = 7.6 Hz, 1H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.43-7.34 (m, 3H), 7.19 (d, *J* = 8.0 Hz, 1H), 2.28 (s, 3H), 2.26 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 164.3, 140.2, 137.9, 136.2, 134.8, 132.3, 130.5, 127.2, 126.2, 125.8, 124.9,122.5, 120.2, 20.0, 19.5. FT-IR (KBr): 2920, 2849, 2920, 1637, 1467, 1350, 1307, 1261, 1101, 1021 cm^{-1}. Elemental analysis calcd (%) for $C_{15}H_{13}NOS$: C, 70.56; H, 5.13; N, 5.49; S, 12.56, found C, 70.59; H, 5.11; N, 5.51; S, 12.54.



***N*-(2,6-Dimethylphenyl)benzo[*d*]isothiazol-3(2*H*)-one (table 3, entry 12).** Colorless solid; 86% yield; mp 116-117 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) 8.04 (d, *J* = 8.4 Hz, 1H), 7.57 (d, *J* = 7.2 Hz, 1H), 7.51(d, *J* = 7.6 Hz, 1H), 7.36-7.34 (m, 1H), 7.12-7.07 (m, 3H), 2.26 (s, 3H), 2.12 (s, 3H); ^{13}C NMR ($CDCl_3$, 400MHz) δ 164.7, 141.4, 136.9, 134.6, 134.5, 132.3, 131.2, 130.5, 129.6, 127.3, 125.8, 124.1, 120.4, 20.9, 17.6. FT-IR(KBr): 2920, 2849, 2920, 1637, 1470, 1307, 1265, 1111, 1021 cm^{-1}. Elemental analysis calcd (%) for $C_{15}H_{13}NOS$: C, 70.56; H, 5.13; N, 5.49; S, 12.56, found C, 70.58; H, 5.15; N, 5.52; S, 12.54.

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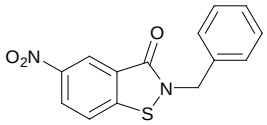
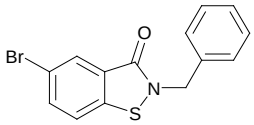
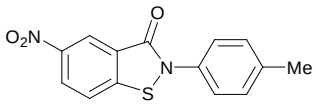


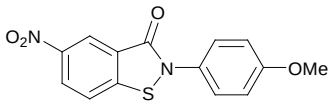
***N*-Benzyl-5-nitrobenzo[*d*]isothiazol-3(2*H*)-one (table 4, entry 2).** Yellow solid; 35% yield; mp 178-180 °C; ^{1}H NMR 8.33-8.31 (m, 1H), 7.36-7.35 (m, 1H), 6.93-6.90 (m, 1H), 6.46-6.34 (m, 5H), 5.02 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) 165.1, 146.7, 139.3, 138.3, 137.8, 132.0, 129.1, 128.0, 127.7, 126.1, 124.3, 55.6. FT-IR (KBr): 3399, 2962, 2977, 2857, 1651, 1591, 1513, 1408, 1340, 1299, 1261, 1094, 1021 cm^{-1}. Elemental analysis calcd (%) for $C_{14}H_{10}N_2O_3S$: C, 58.73; H, 3.52; N, 9.78; S, 11.20, found C, 58.76; H, 3.50; N, 9.75; S, 11.23.



***N*-Benzyl-5-bromobenzo[*d*]isothiazol-3(2*H*)-one (table 4, entry 3).** Colorless solid; 90% yield; m.p. 139-140 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.177-8.172 (m, 1H), 7.67 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.36-7.30 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.0, 138.8, 133.5, 131.7, 131.4, 131.3, 130.6, 129.9, 128.3, 126.9, 125.9, 42.5. FT-IR (KBr): 2930, 1627, 1331, 1356, 1252, 1075, 1041 cm^{-1}. Elemental analysis calcd (%) for $C_{14}H_{10}BrNOS$: C, 52.51; H, 3.15; N, 4.37; S, 10.01, found C, 52.48; H, 3.16; N, 4.35; S, 10.08.



5-Nitro-*N*-p-tolylbenzo[*d*]isothiazol-3(2*H*)-one (table 4, entry 6). Yellow solid; 35% yield; m.p. 111-112 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.77-8.71 (m, 1H), 8.43-8.39 (m, 1H), 7.67(d, *J* = 8.4 Hz, 2H), 7.60 (d, J = 8.4 Hz, 1H), 7.18 (d, *J* = 8.4 Hz, 2H); 2.28 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 163.7, 148.4, 137.0, 134.7, 133.8, 130.8, 129.9, 129.8, 126.7, 123.0, 121.3, 21.2. FT-IR(KBr): 2930, 2923, 2256, 1651, 1048, 1025 cm^{-1}. Elemental analysis calcd (%) for $C_{14}H_{10}NO_3S$: C, 58.73; H, 3.52; N, 9.78; S, 11.20, found C, 58.76; H, 3.55; N, 9.75; S, 11.18.



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***N*-(4-Methoxyphenyl)-5-nitrobenzo[*d*]isothiazol-3(2*H*)-one (table 5, entry 4).** Yellow solid; 45% yield; 114-115 °C (DMSO); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.68-8.67 (m, 1H), 7.61 (d, *J* = 8.0 Hz, 2H), 7.24 (d, *J* = 8.4 Hz, 1H), 7.00 (d, *J* = 8.4 Hz, 3H), 3.73 (s, 3H); ^{13}C NMR ($CDCl_3$, 100MHz) δ 162.4, 156.0, 146.2, 137.9, 137.2, 131.6, 131.4, 125.6, 123.9, 121.5, 114.0, 55.3. FT-IR(KBr): 2255, 2128, 1651, 1510, 1246, 1048, 1025, 1002 cm^{-1}. Elemental analysis calcd (%) for $C_{14}H_{10}NO_4S$: C, 55.62; H, 3.33; N, 9.27, S, 10.61, found C, 55.66; H, 3.31; N, 9.30, S, 10.63.

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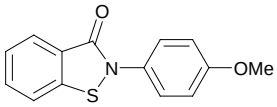
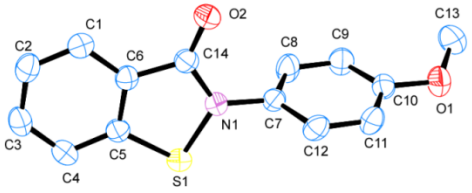
Crystal Structure of N-(4-methoxyphenyl)benzo[*d*]isothiazol-3(2*H*)-one





Crystal number: Summary of Data CCDC 876574 Thermal ellipsoids are drawn at a 40% probability level. Hydrogen atoms have been omitted for clarity.

Formula: C_{14} H_{11} N O_2 S

Unit cell parameters: a 10.5093(14) b 13.6166(17) c 9.1287(12) beta 114.028(6) space group P 21/c

Datablock:

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	alpha=90	beta=114.028(6)	gamma=90
Temperature:	296 K		
	Calculated		Reported
Volume	1193.1(3)		1193.1(3)
Space group	P 21/c		P2(1)/c
Hall group	-P 2ybc		?
Moiety formula	C14 H11 N O2 S		?
Sum formula	C14 H11 N O2 S		C14 H11 N O2 S
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Dx,g cm-3	1.433		1.432
Z	4		4
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F000'	536.72		
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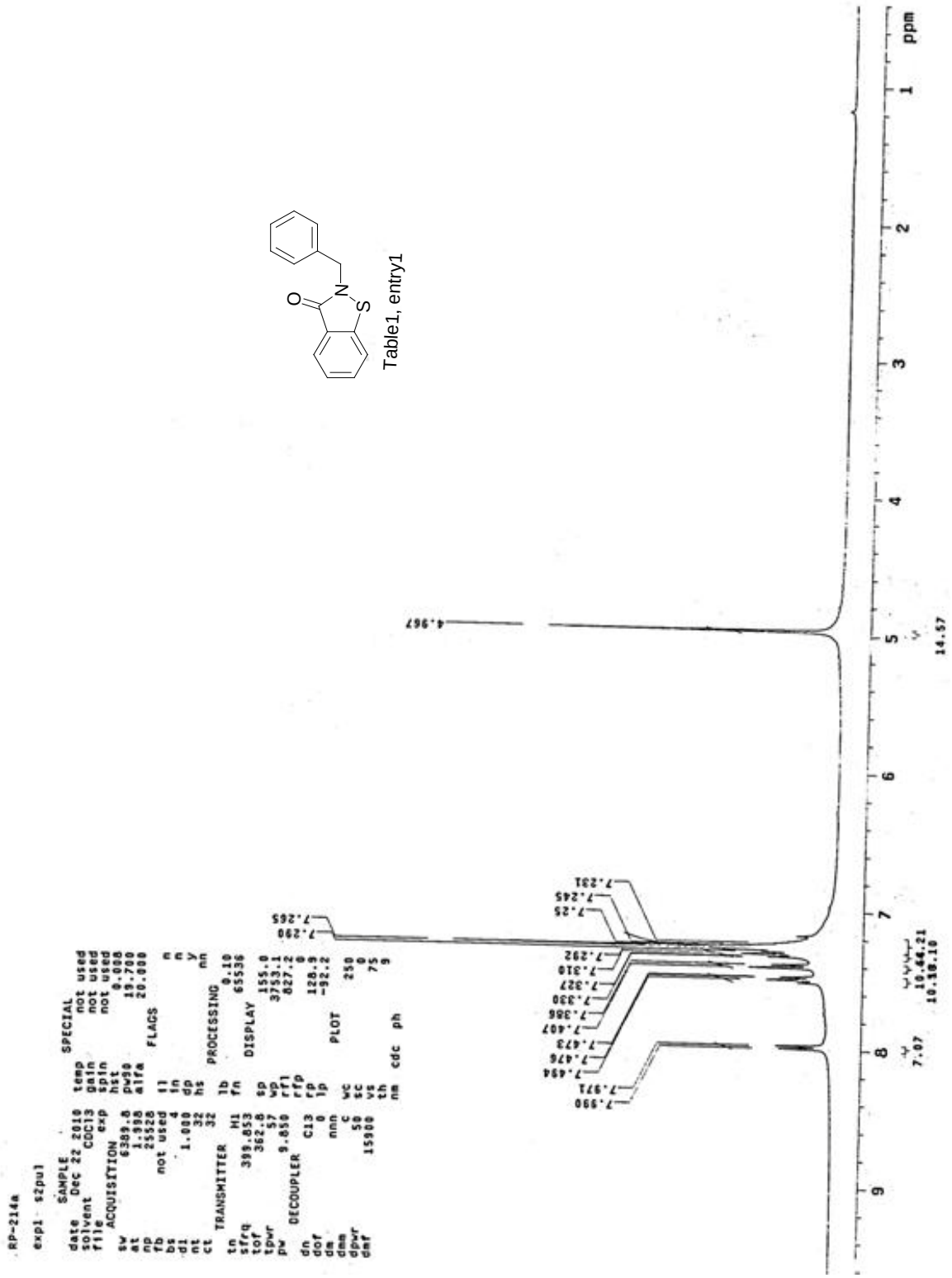
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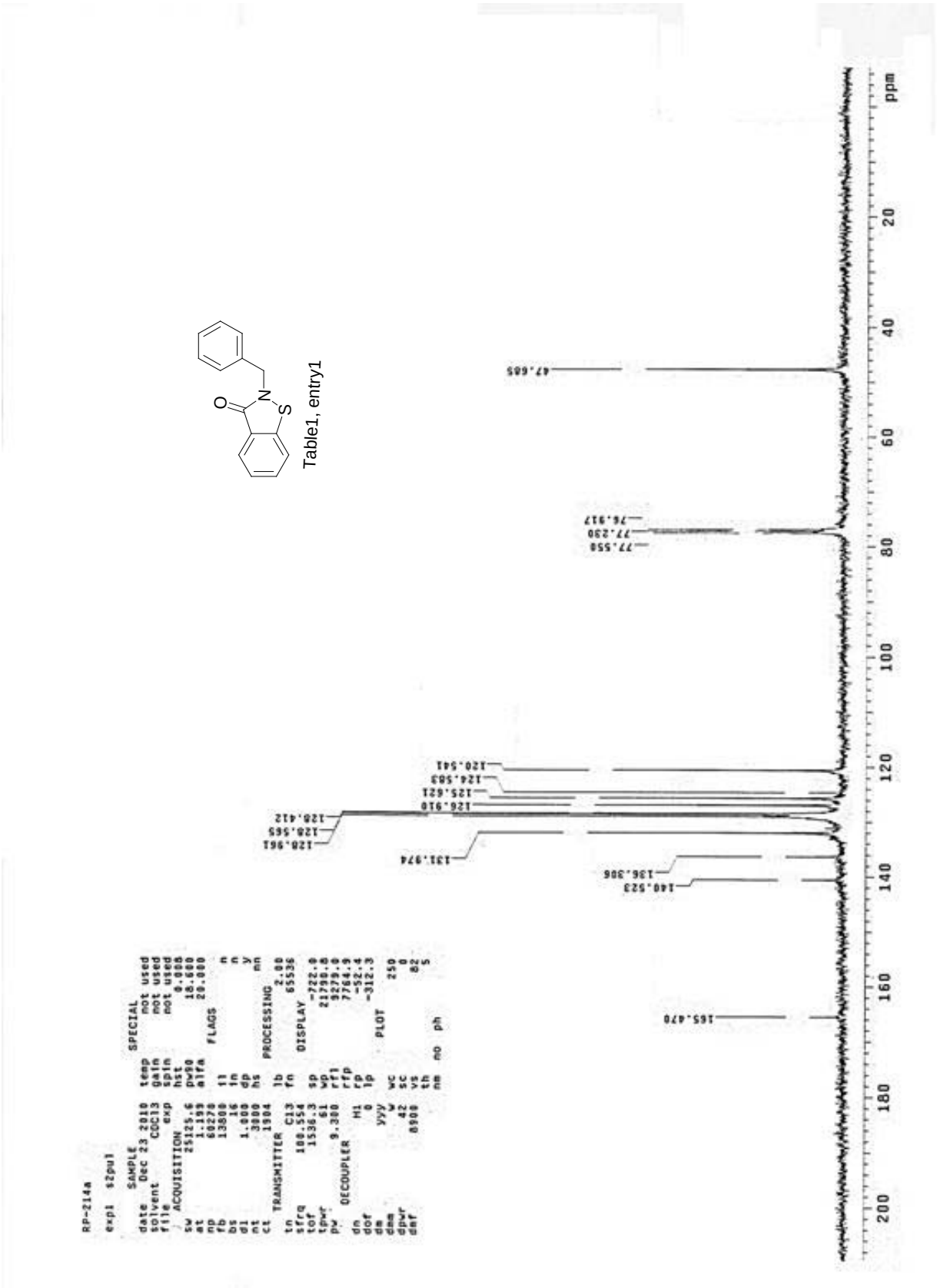
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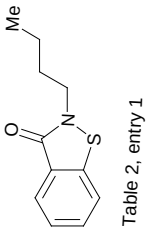

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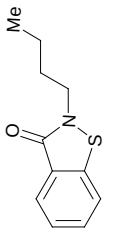

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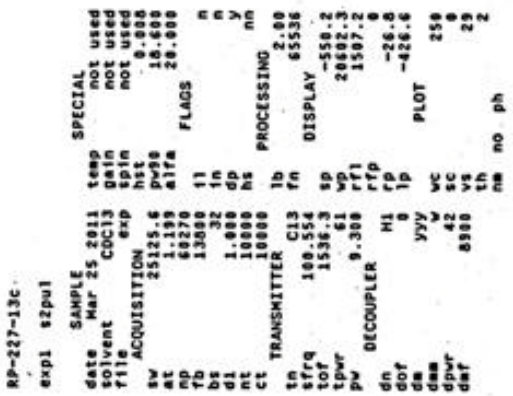

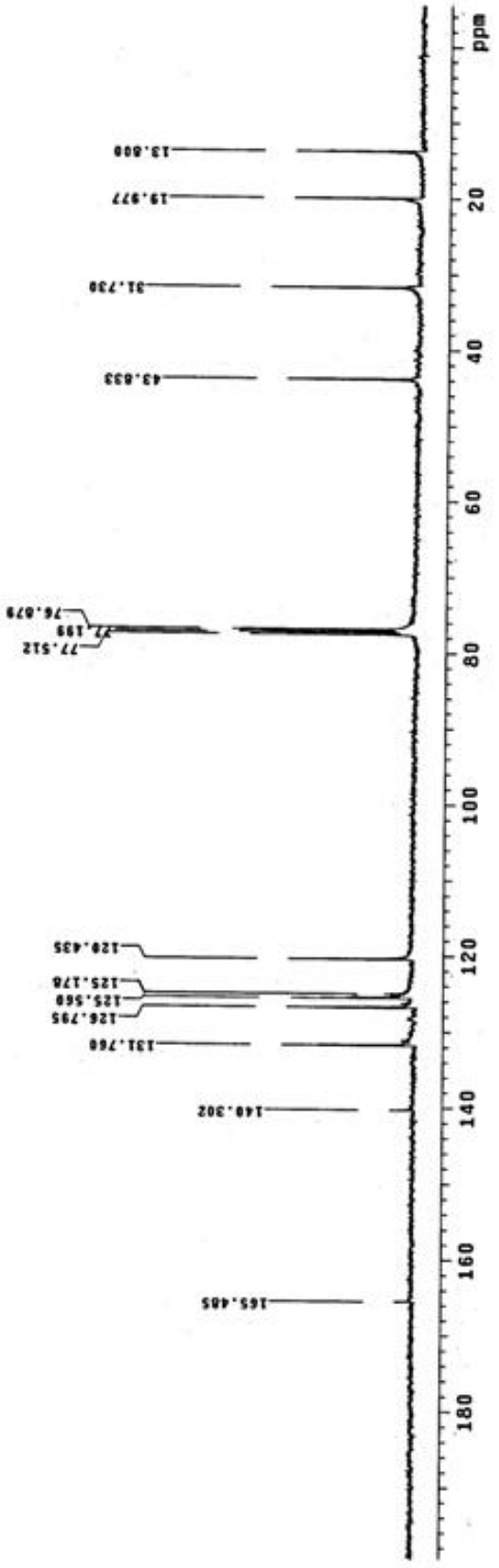

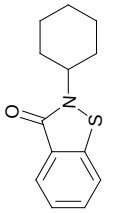

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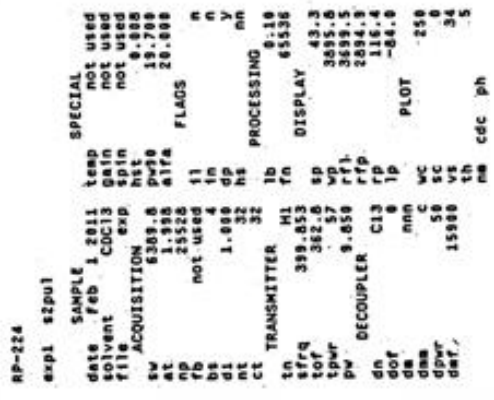

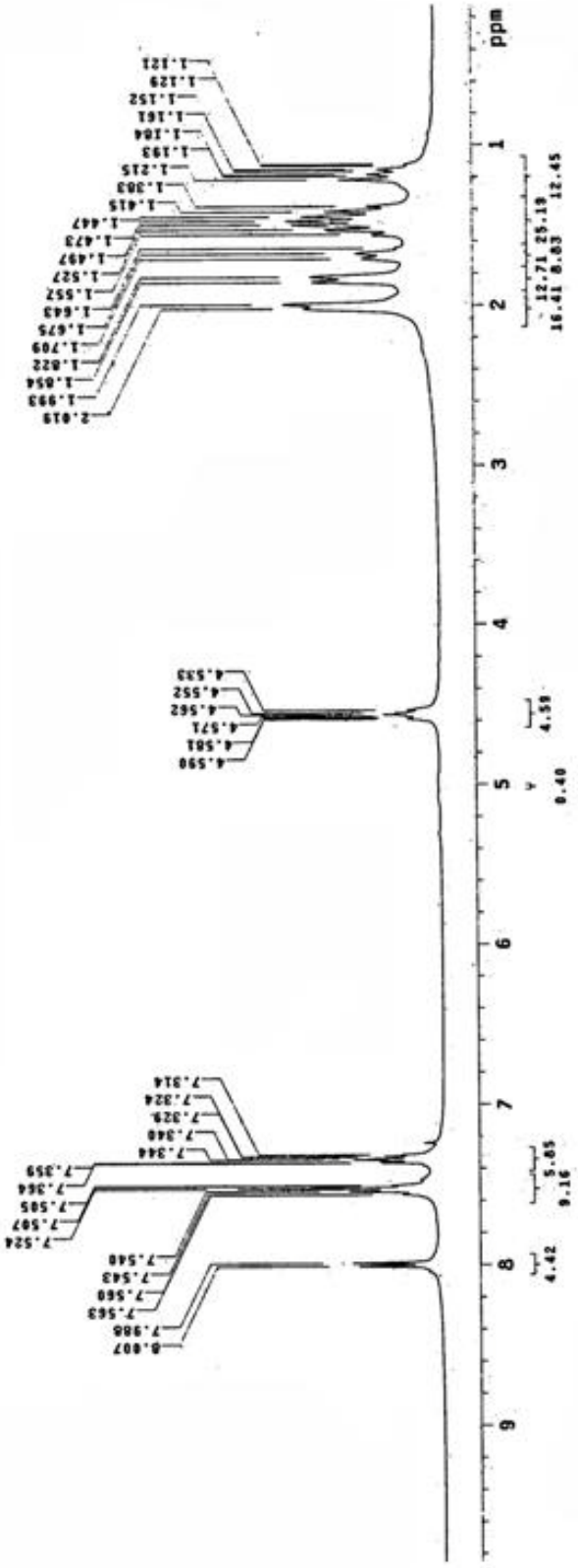

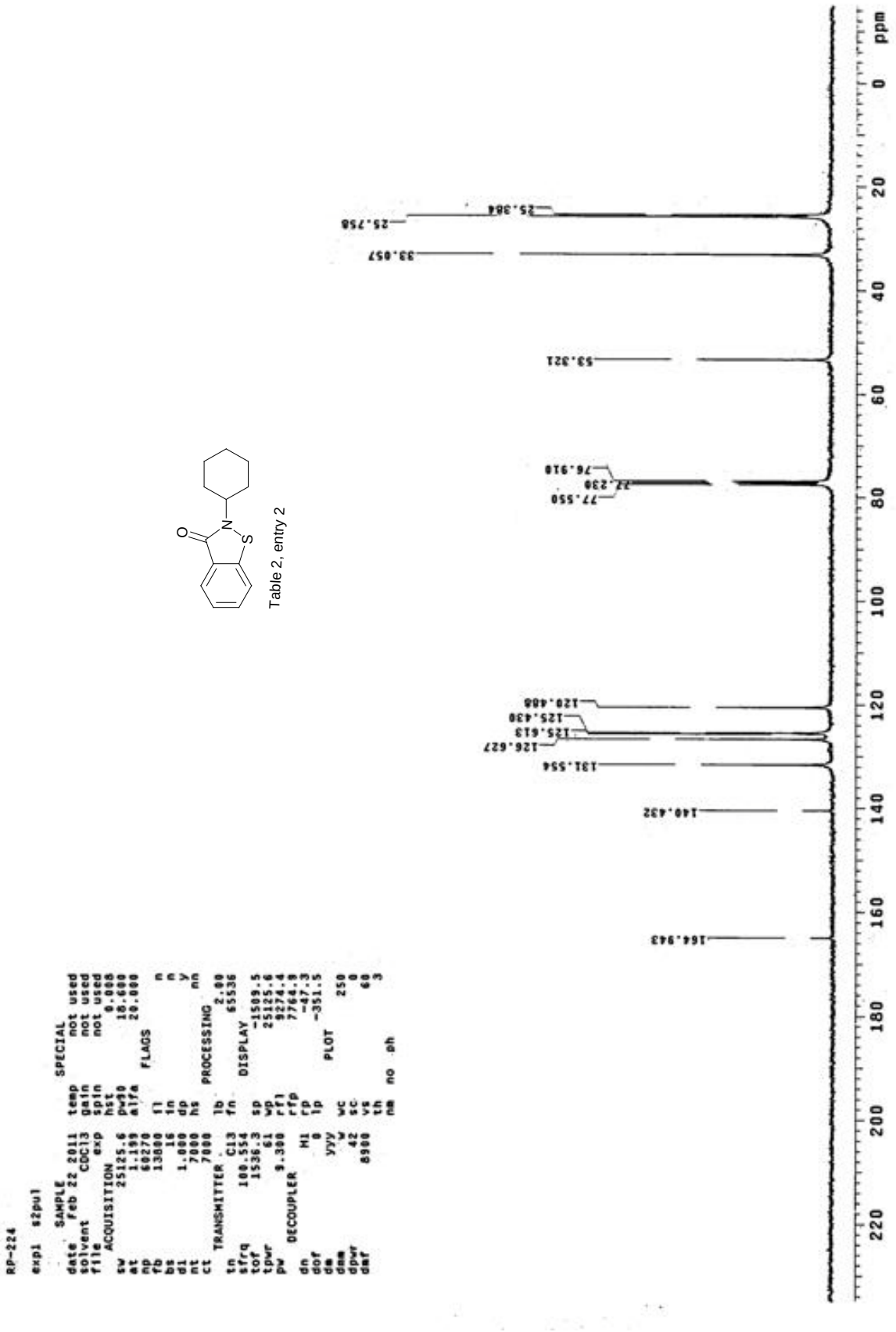
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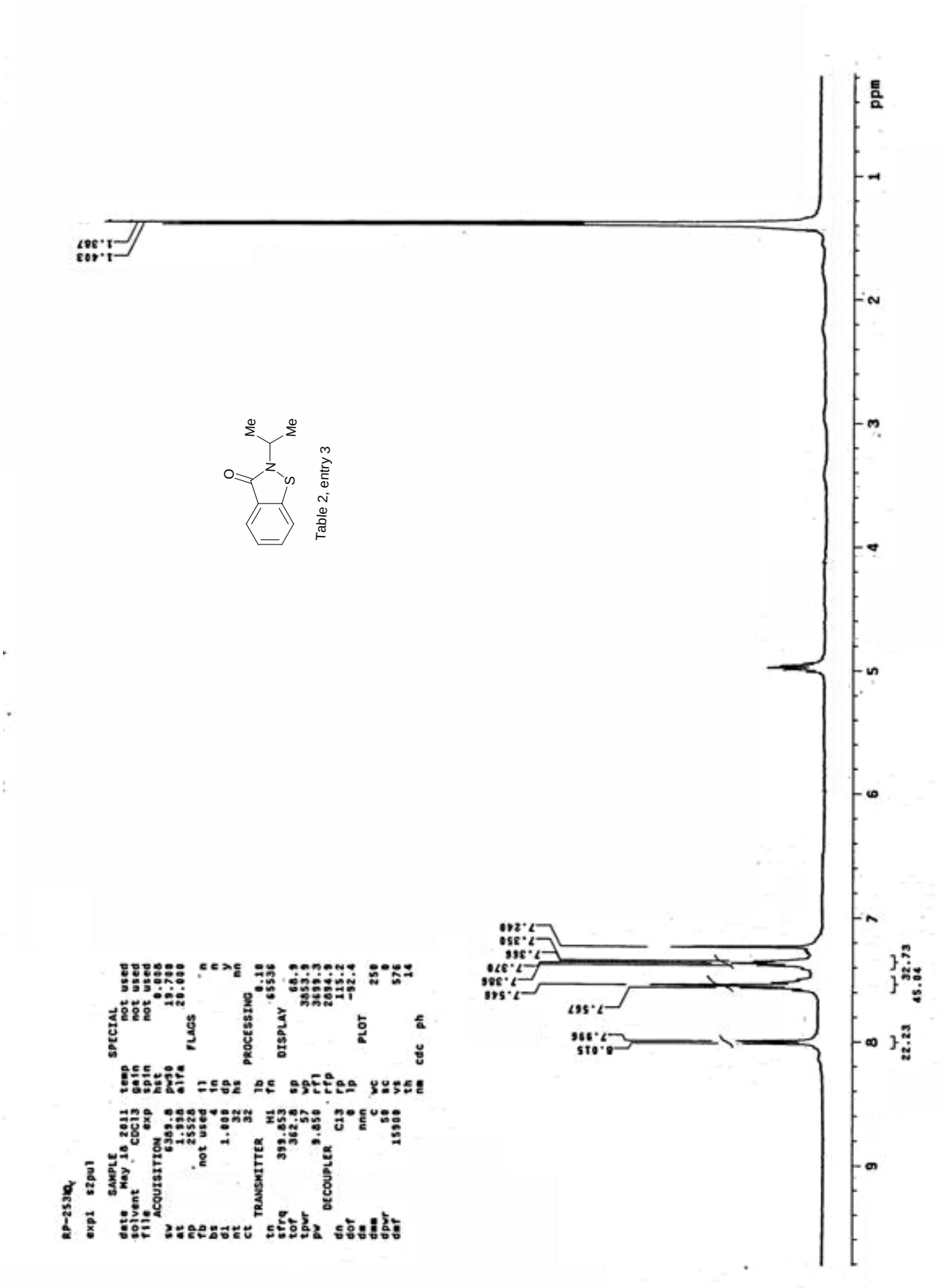
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7.996
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ppm
1
2
3
4
5
6
7
8
9
22.23
32.73
45.84

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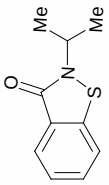
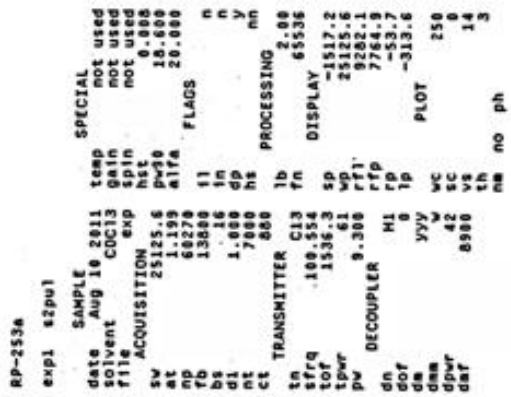
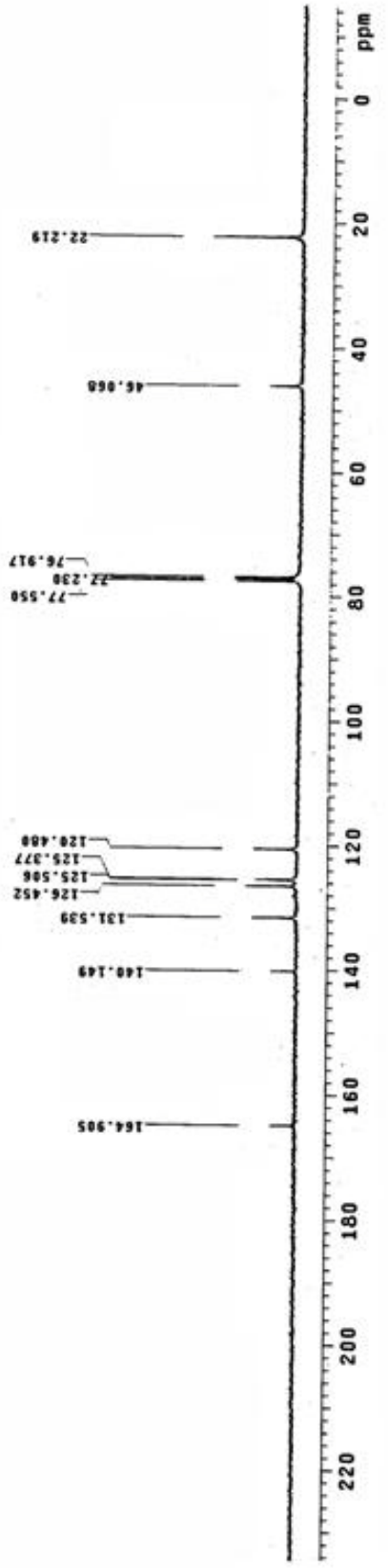
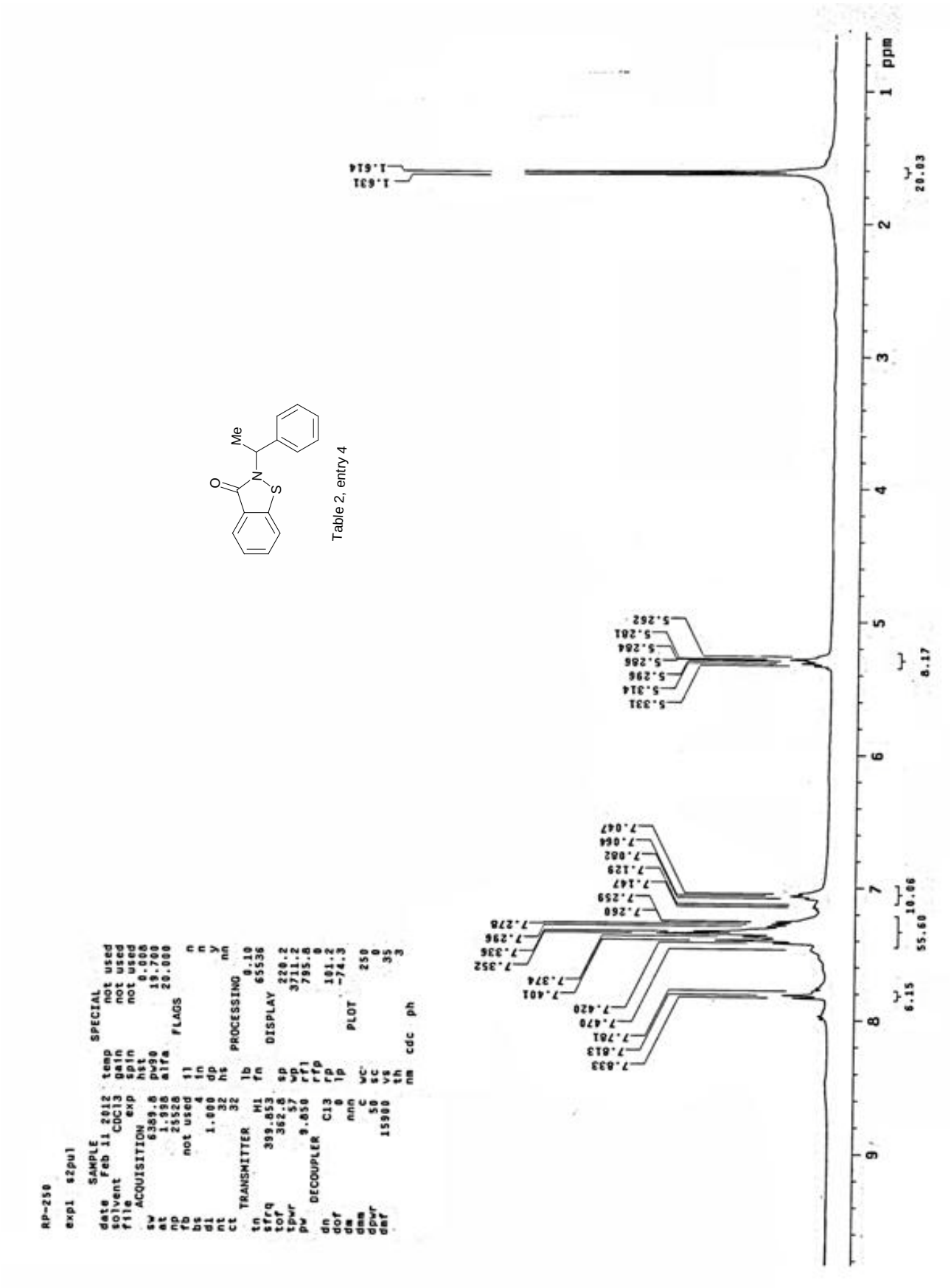
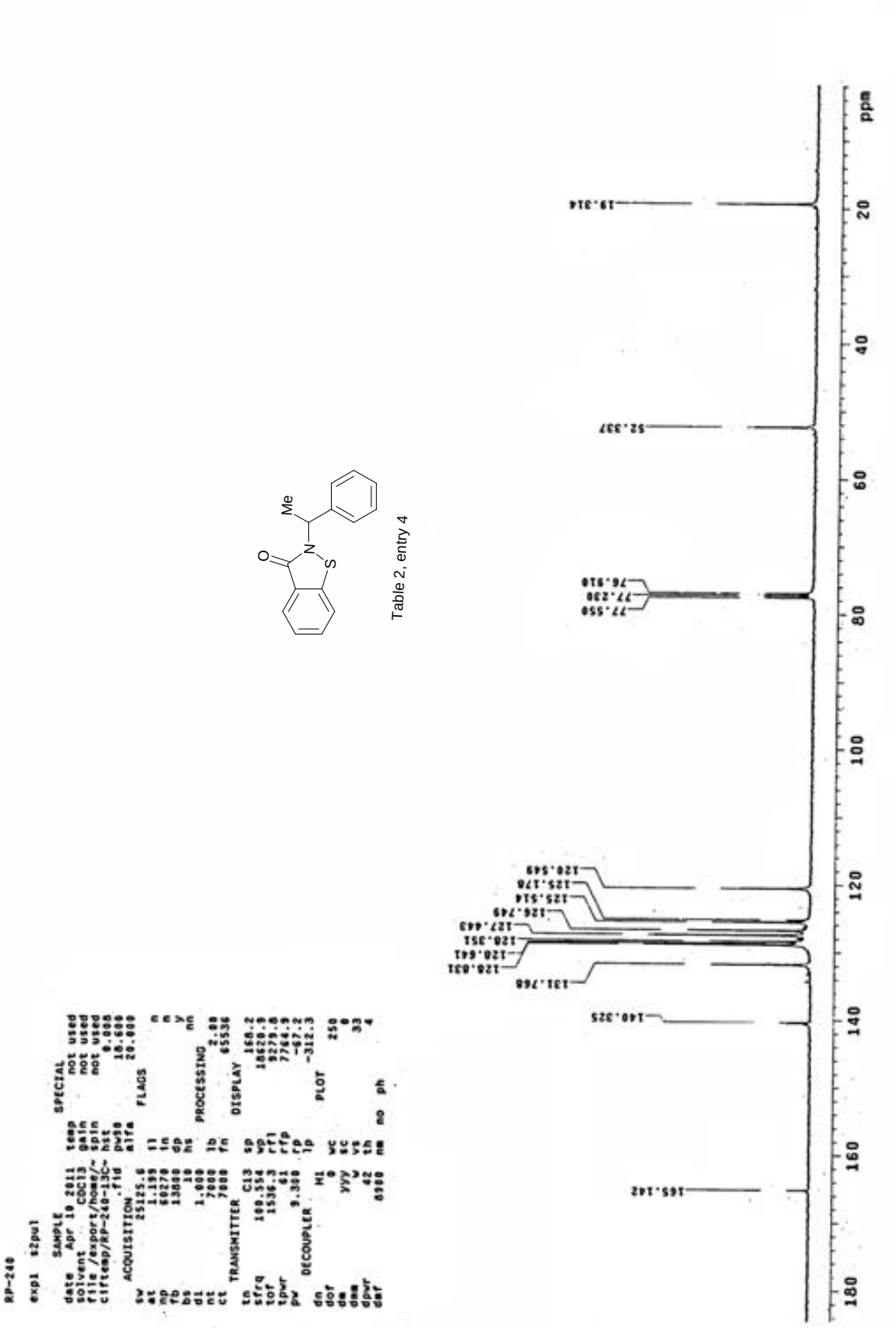


Table 2, entry 3






Me
N
O
S
Table 2, entry 4
1.631
1.614
5.331
5.314
5.296
5.286
5.264
5.261
5.262
7.033
7.613
7.781
7.470
7.420
7.401
7.374
7.352
7.336
7.296
7.278
7.260
7.259
7.147
7.129
7.082
7.064
7.047
1 ppm
20.03
8.17
10.06
55.60
6.15


Me
N
O
S
Table 2, entry 4
ppm
19.314
52.337
76.918
77.238
77.550
120.549
125.176
125.514
126.749
127.443
128.351
128.641
128.631
131.768
140.325
165.142

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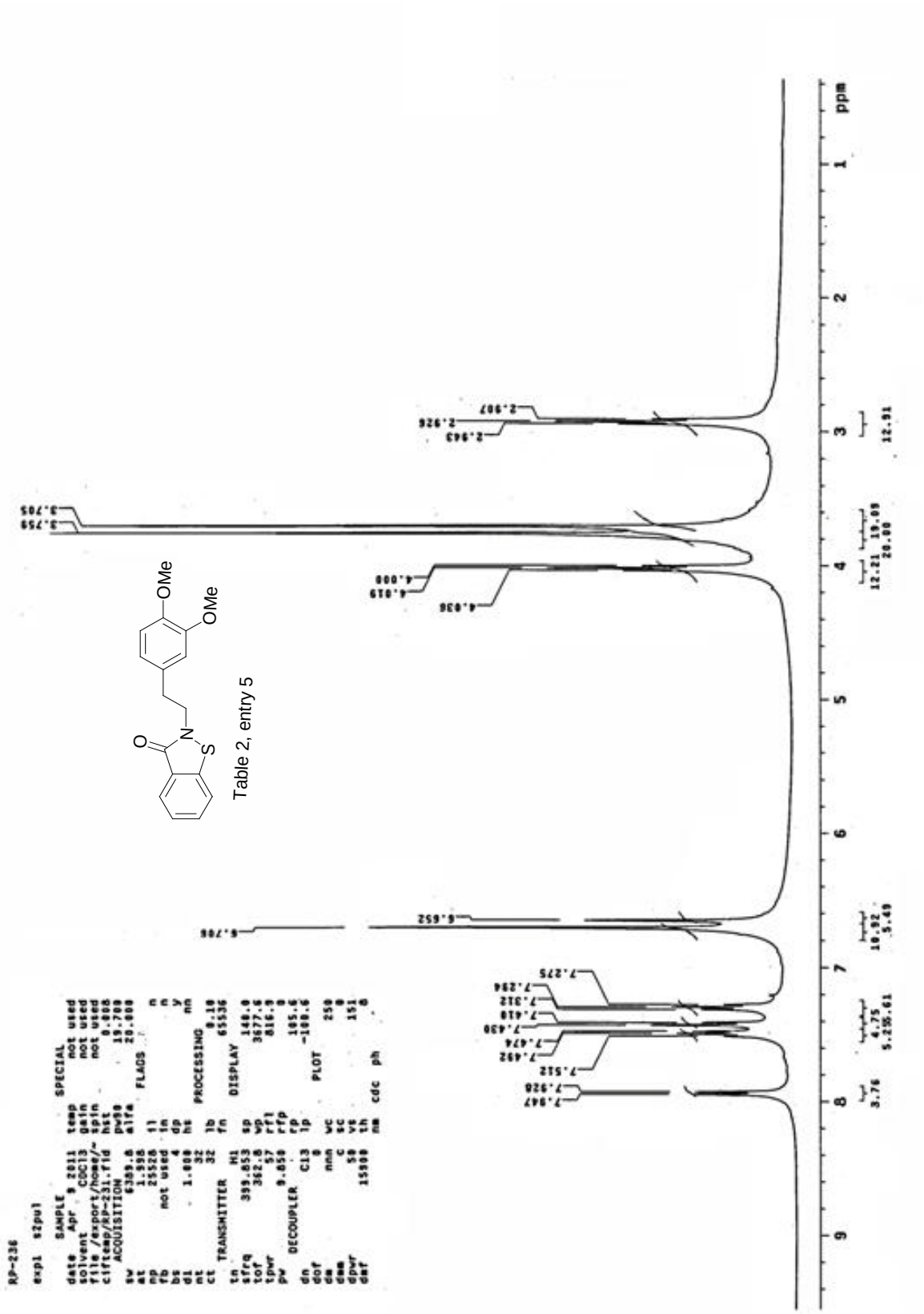


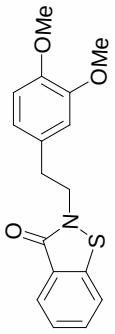
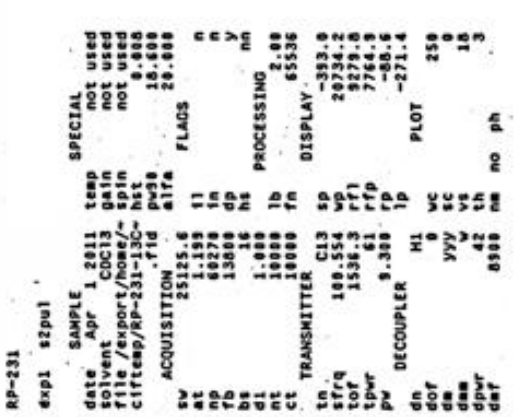
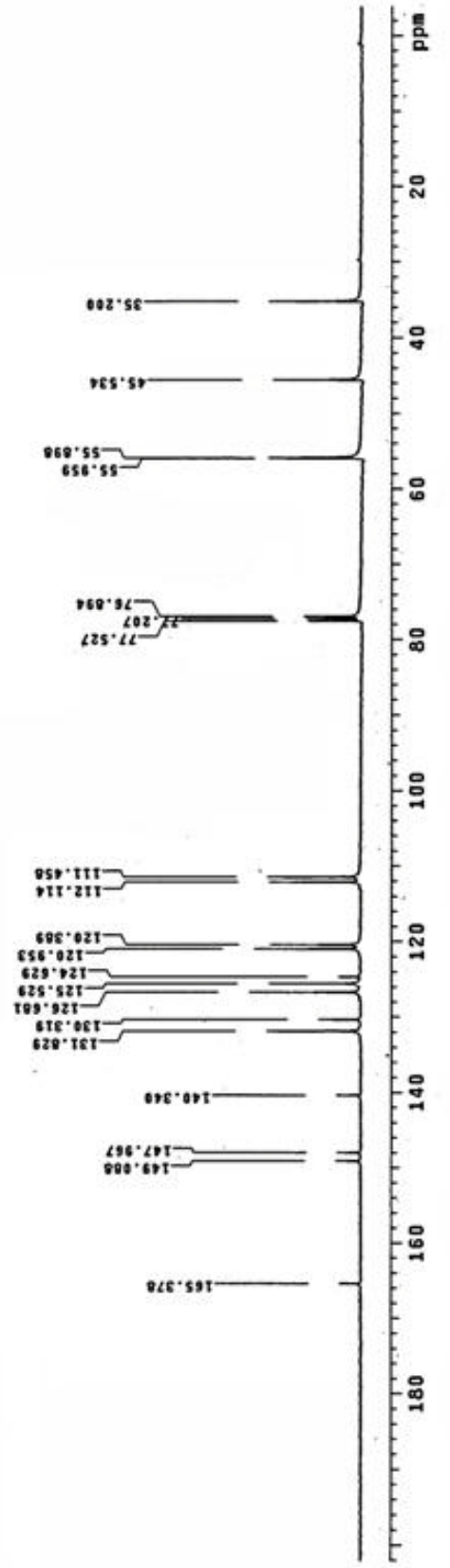


Table 2, entry 5





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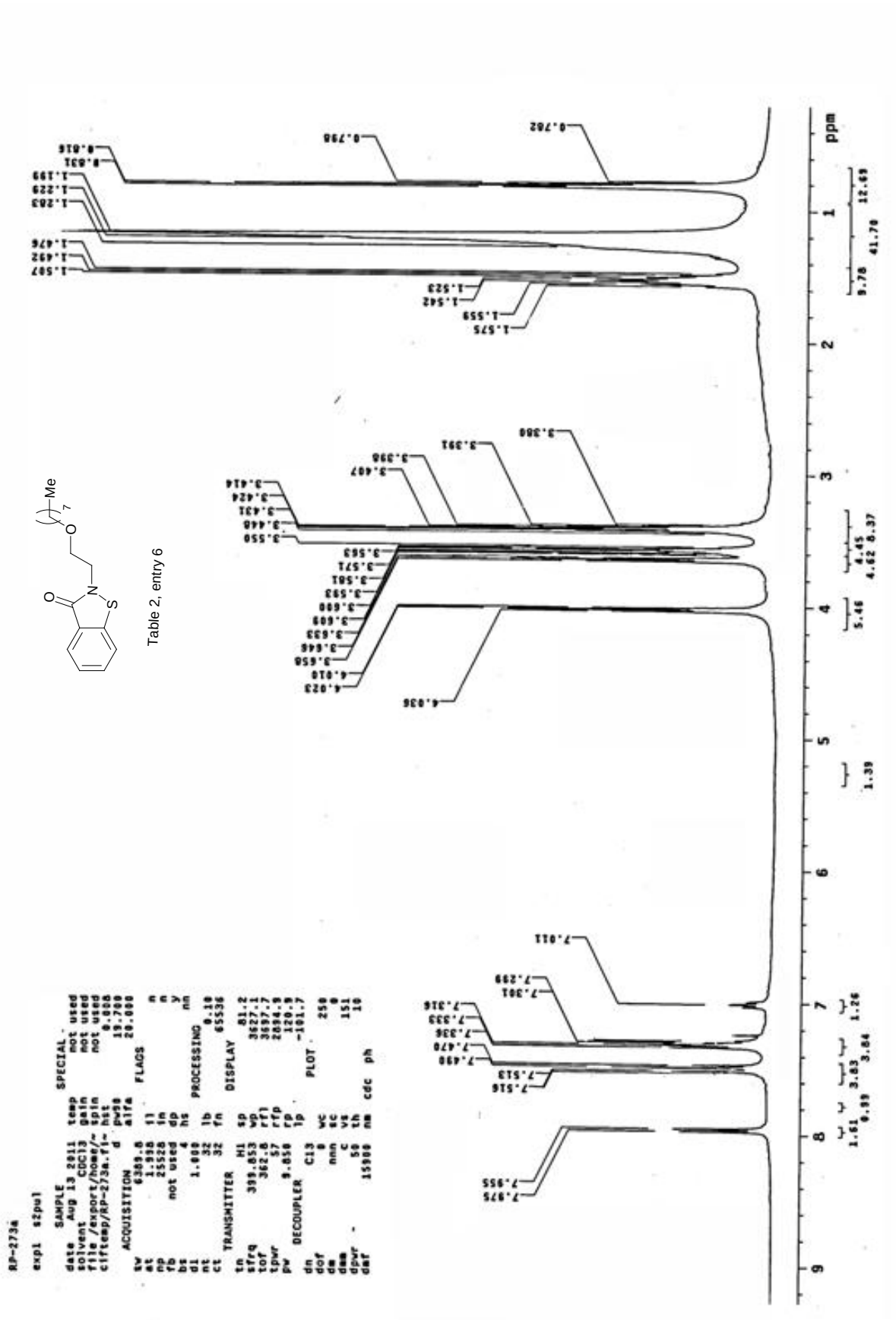

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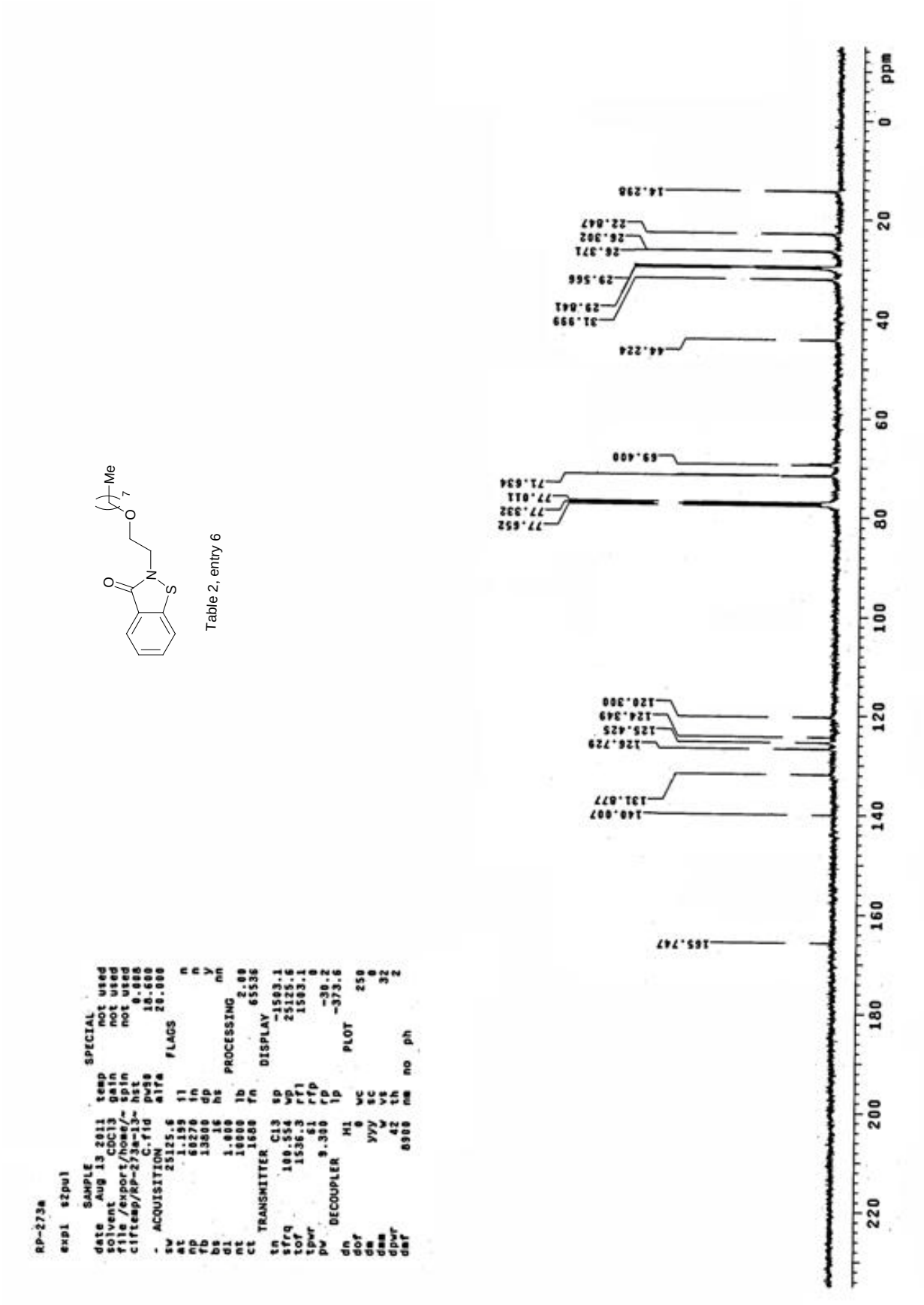

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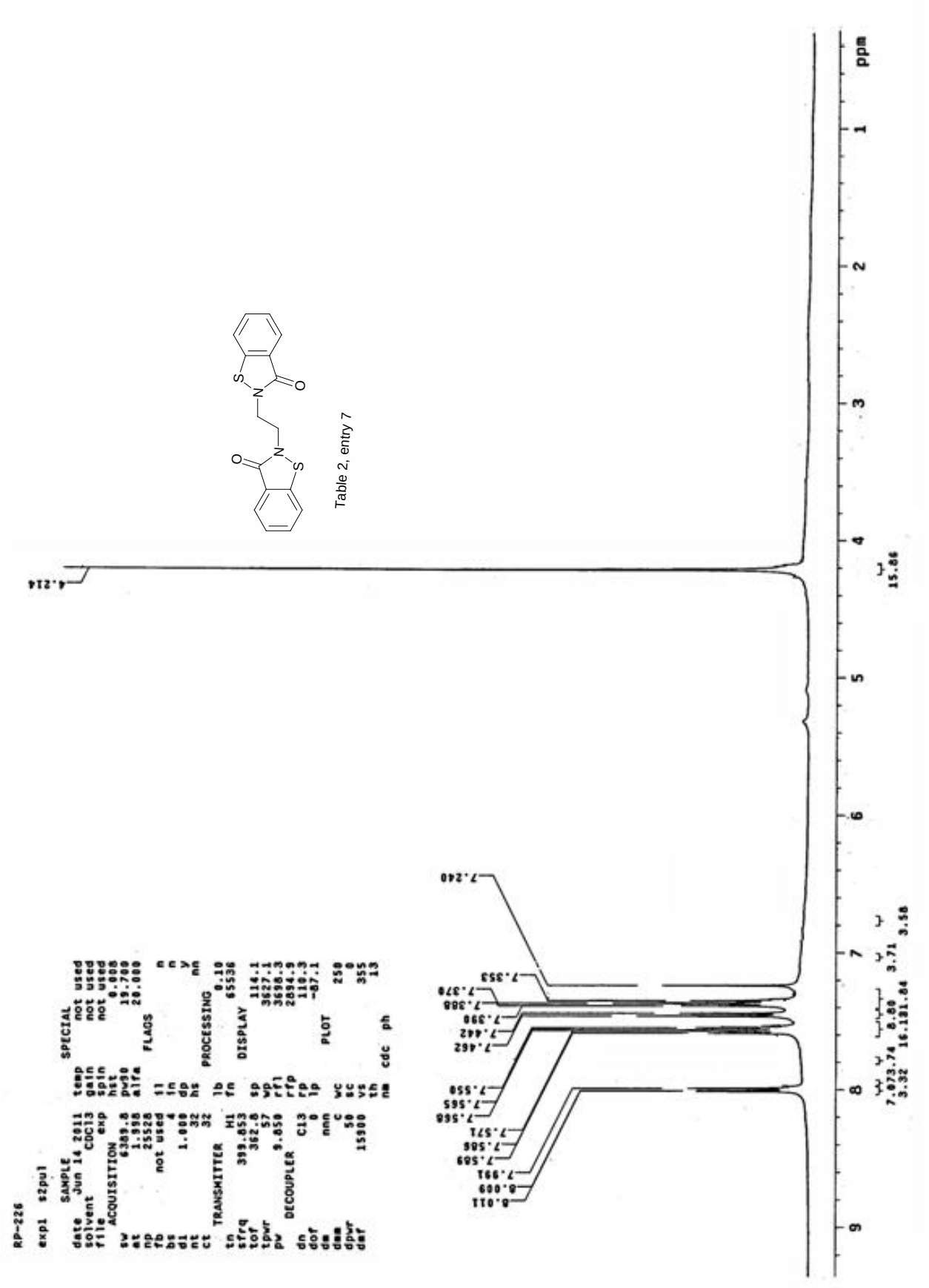

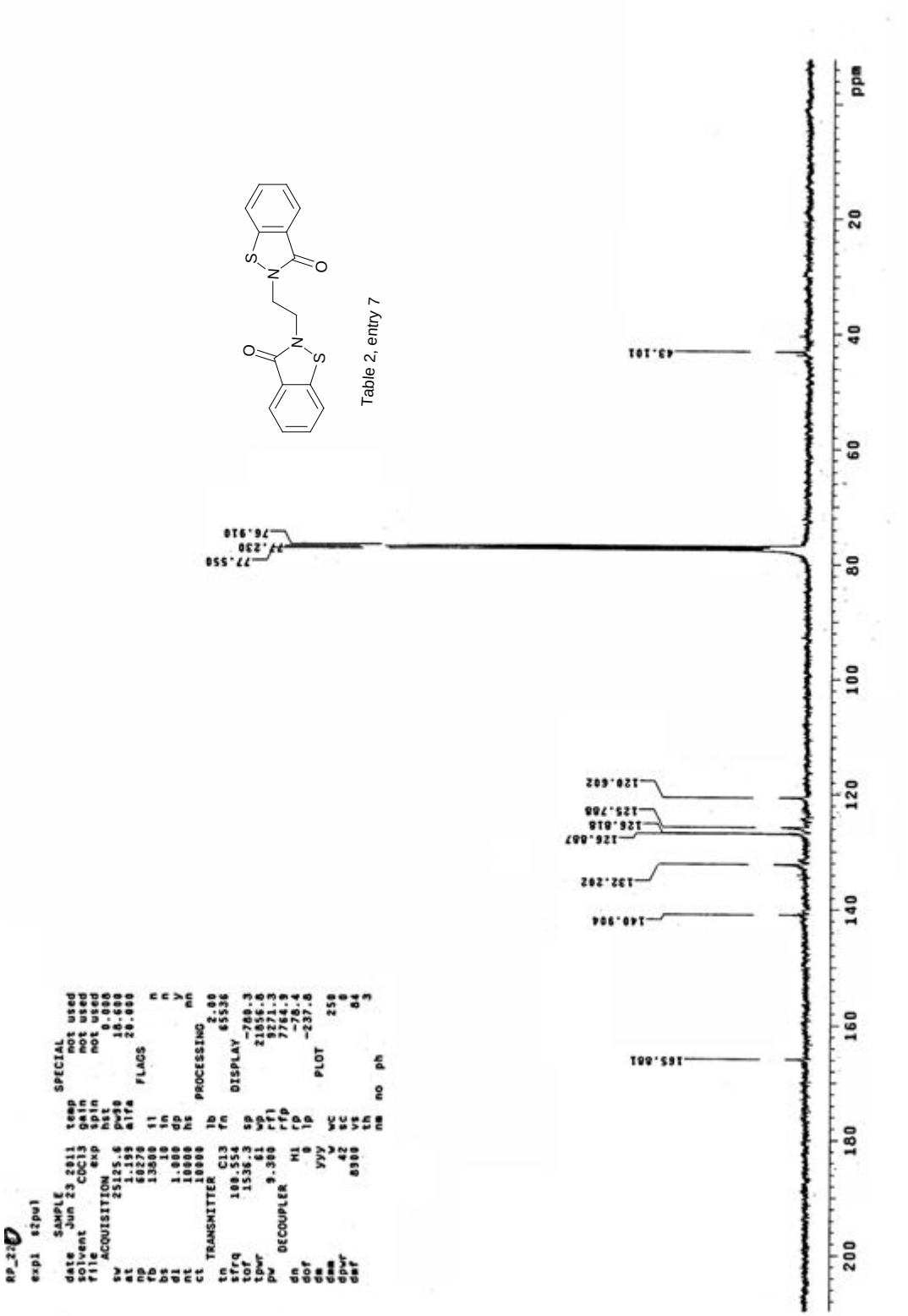
Table 2, entry 7
77.550
77.230
76.910
43.101
165.861
140.904
132.282
126.067
126.816
125.766
120.602
ppm

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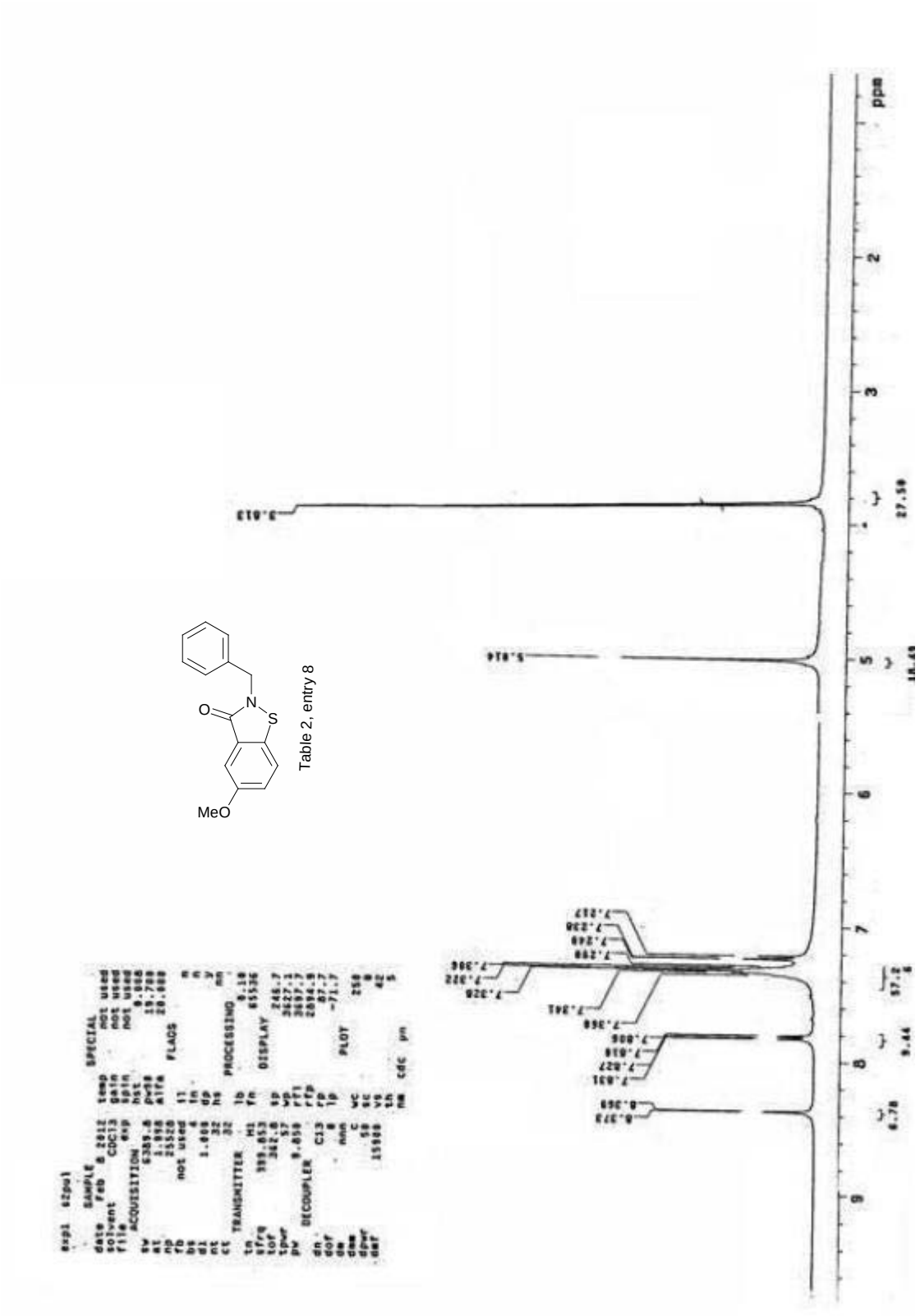

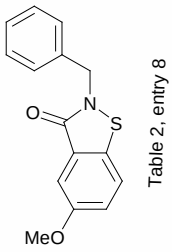

Table 2, entry 8

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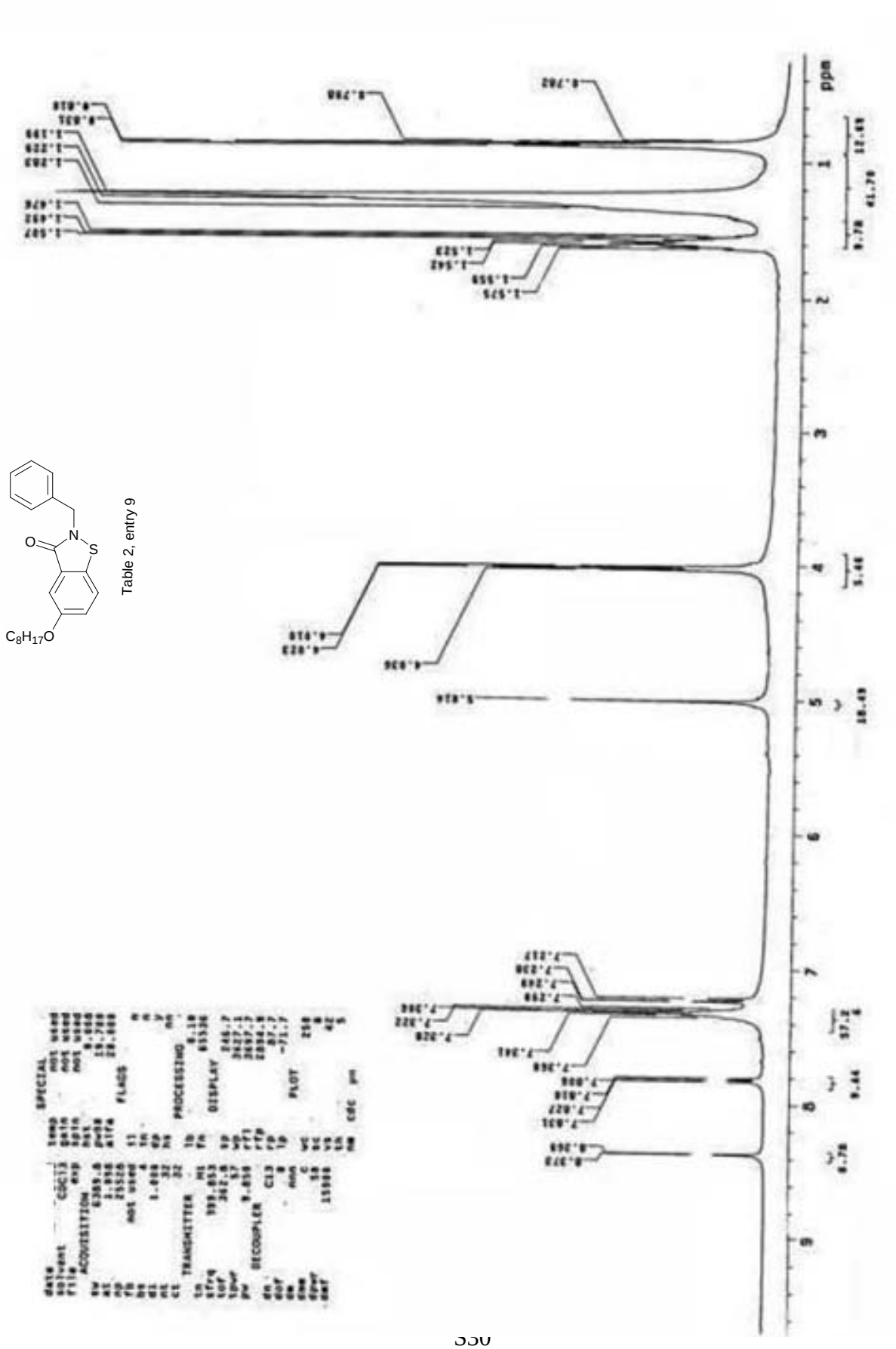

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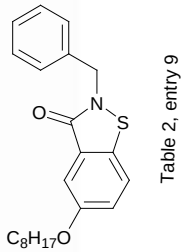
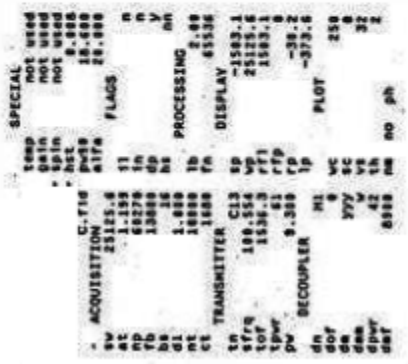
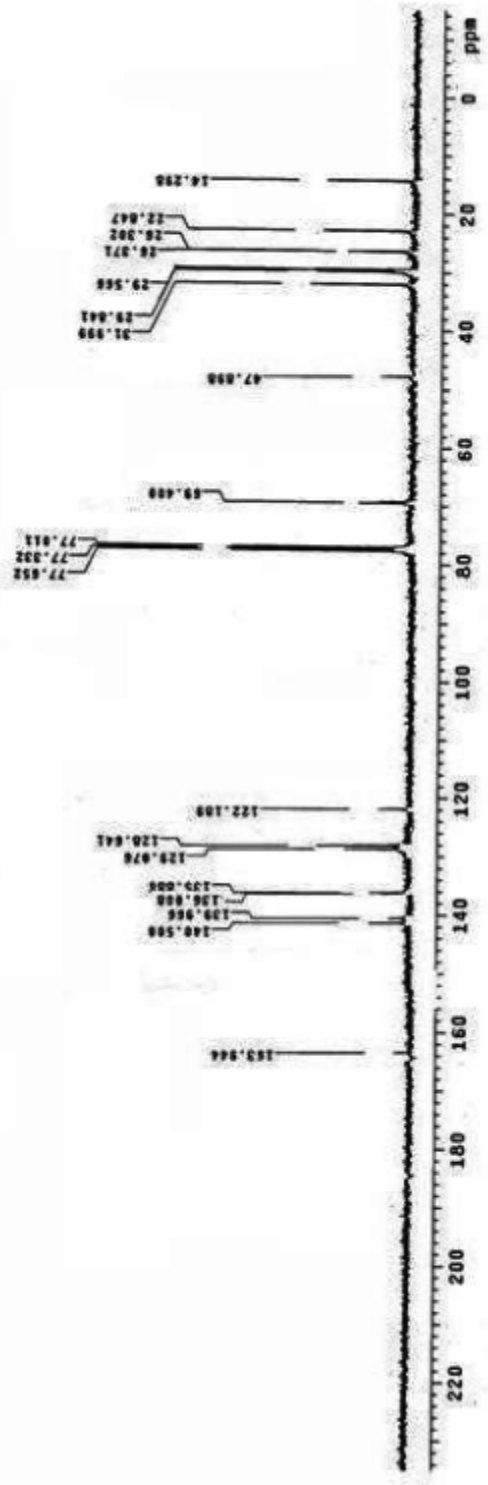


Table 2, entry 9





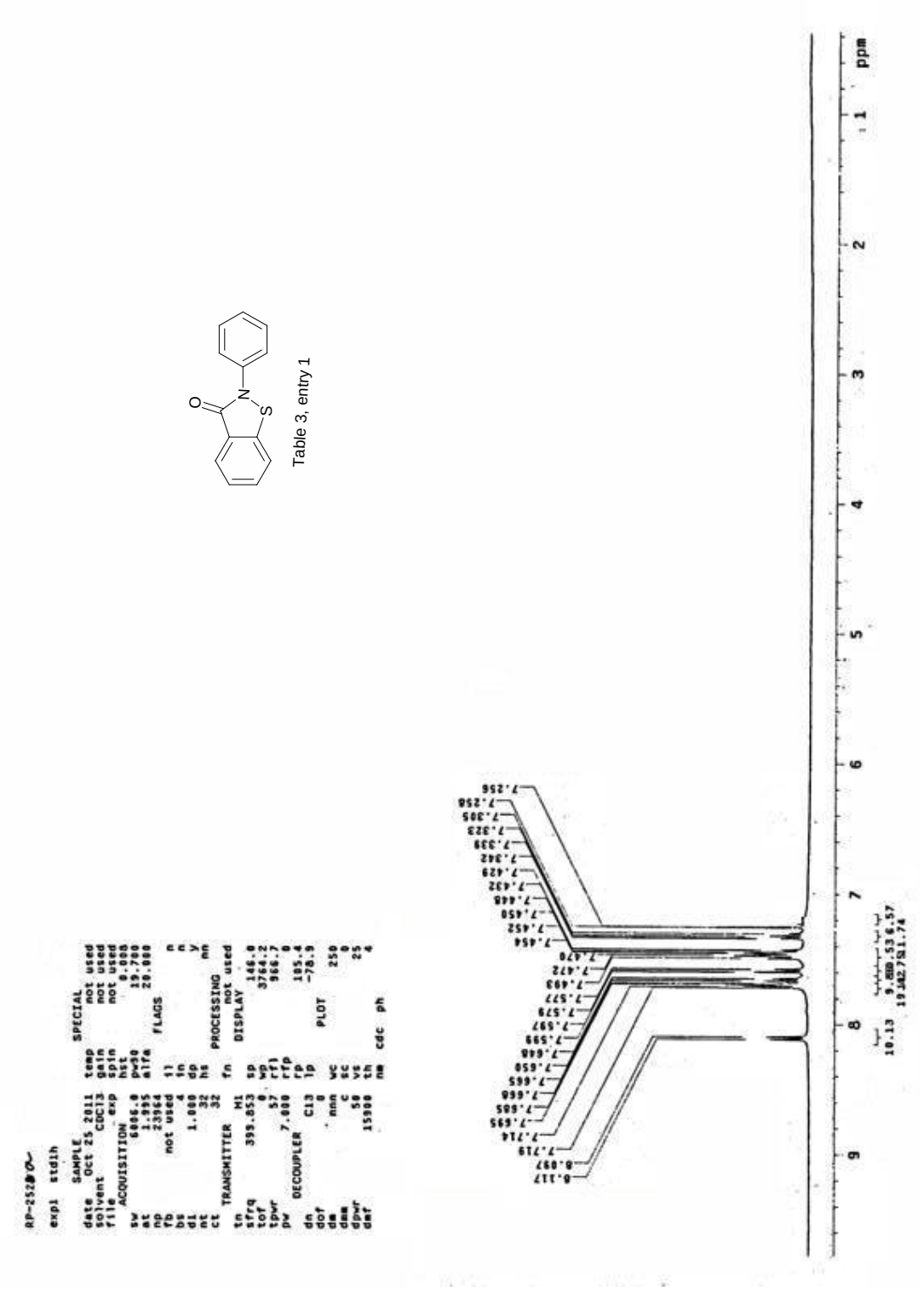


Table 3, entry 1

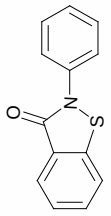
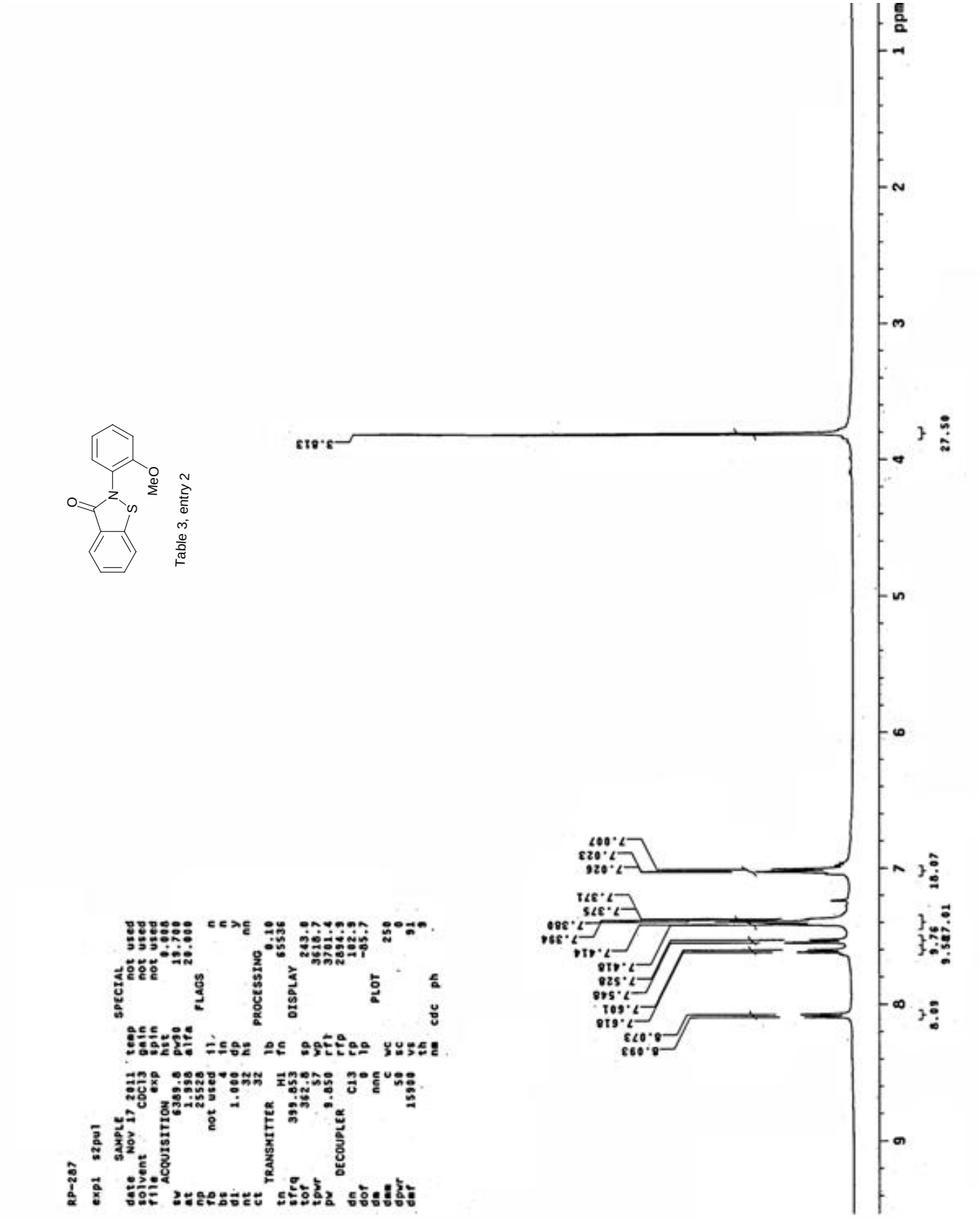


Table 3, entry 1


MeO
O
N
S
Table 3, entry 2
3.813
8.093
8.073
7.618
7.601
7.548
7.528
7.418
7.414
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7.375
7.371
7.026
7.023
7.007
1 ppm

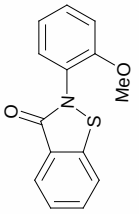
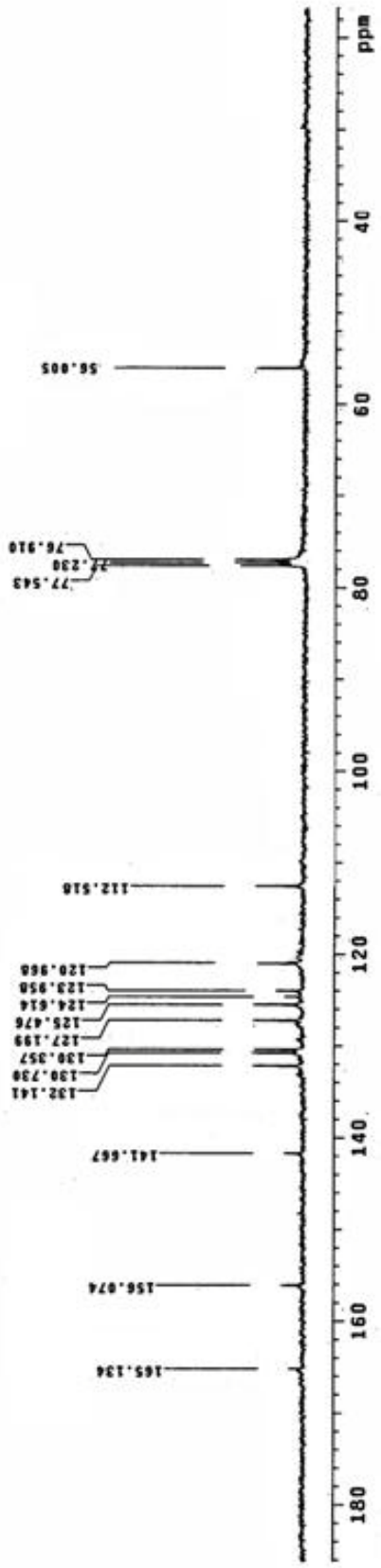
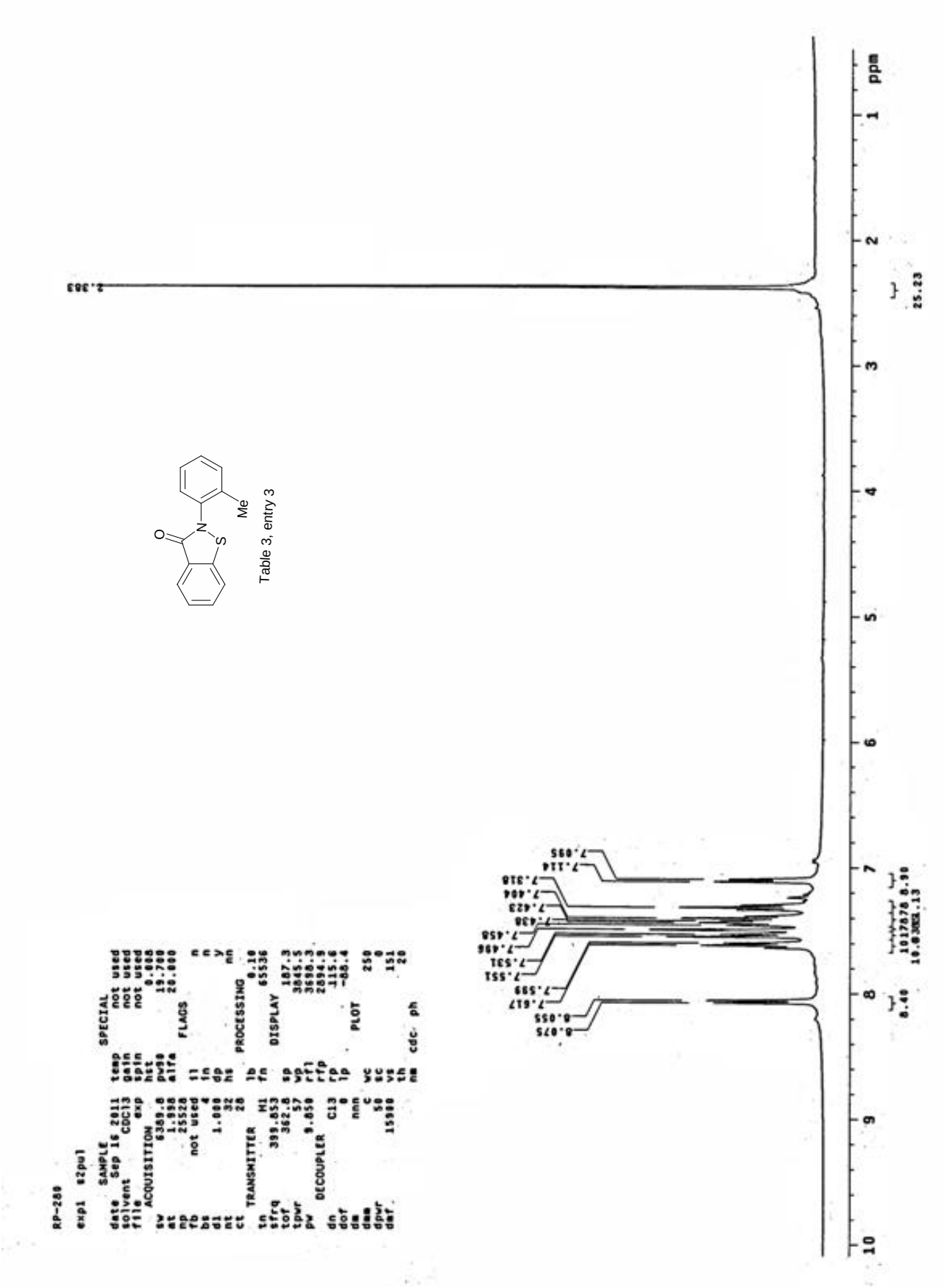


Table 3, entry 2




Me
O
N
S
Table 3, entry 3
ppm
8.075
8.055
7.617
7.599
7.551
7.531
7.498
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7.438
7.423
7.404
7.318
7.114
7.095
2.383

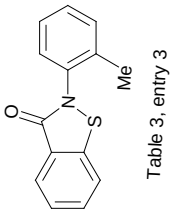
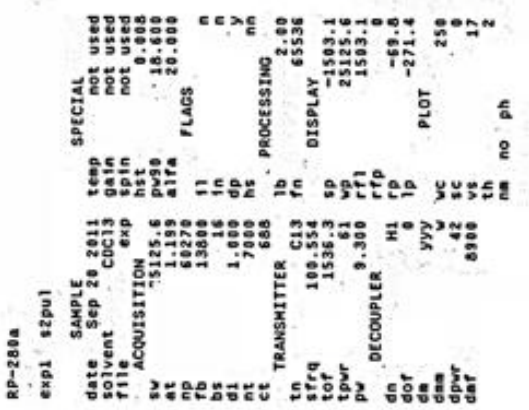
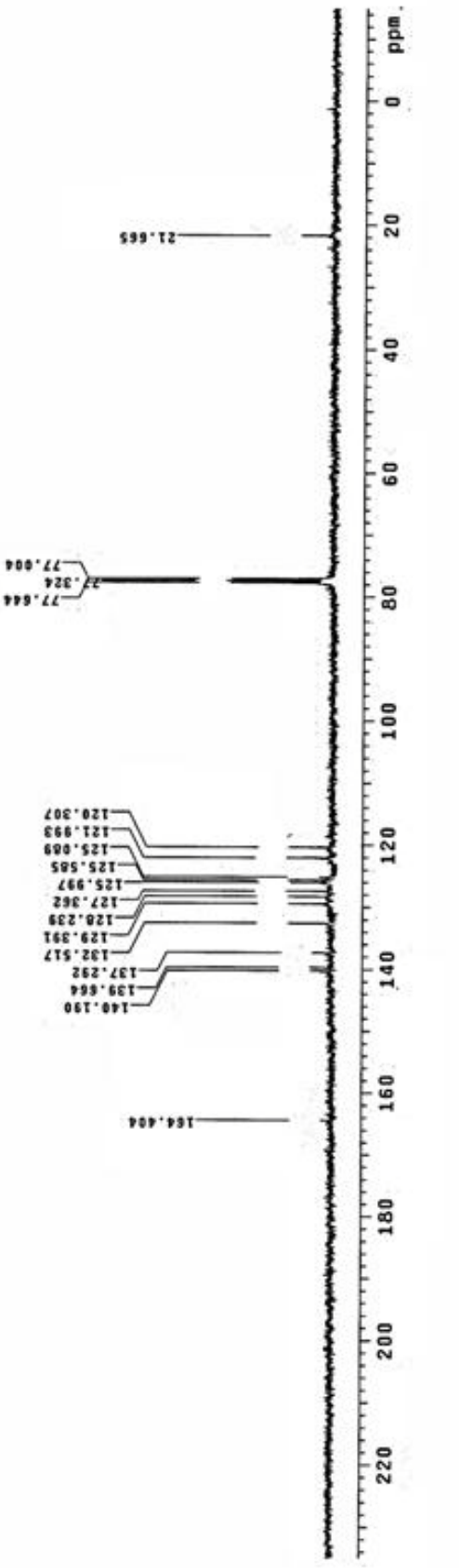


Table 3, entry 3





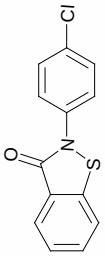
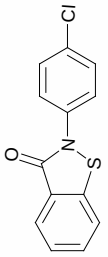


Table 3, entry 5



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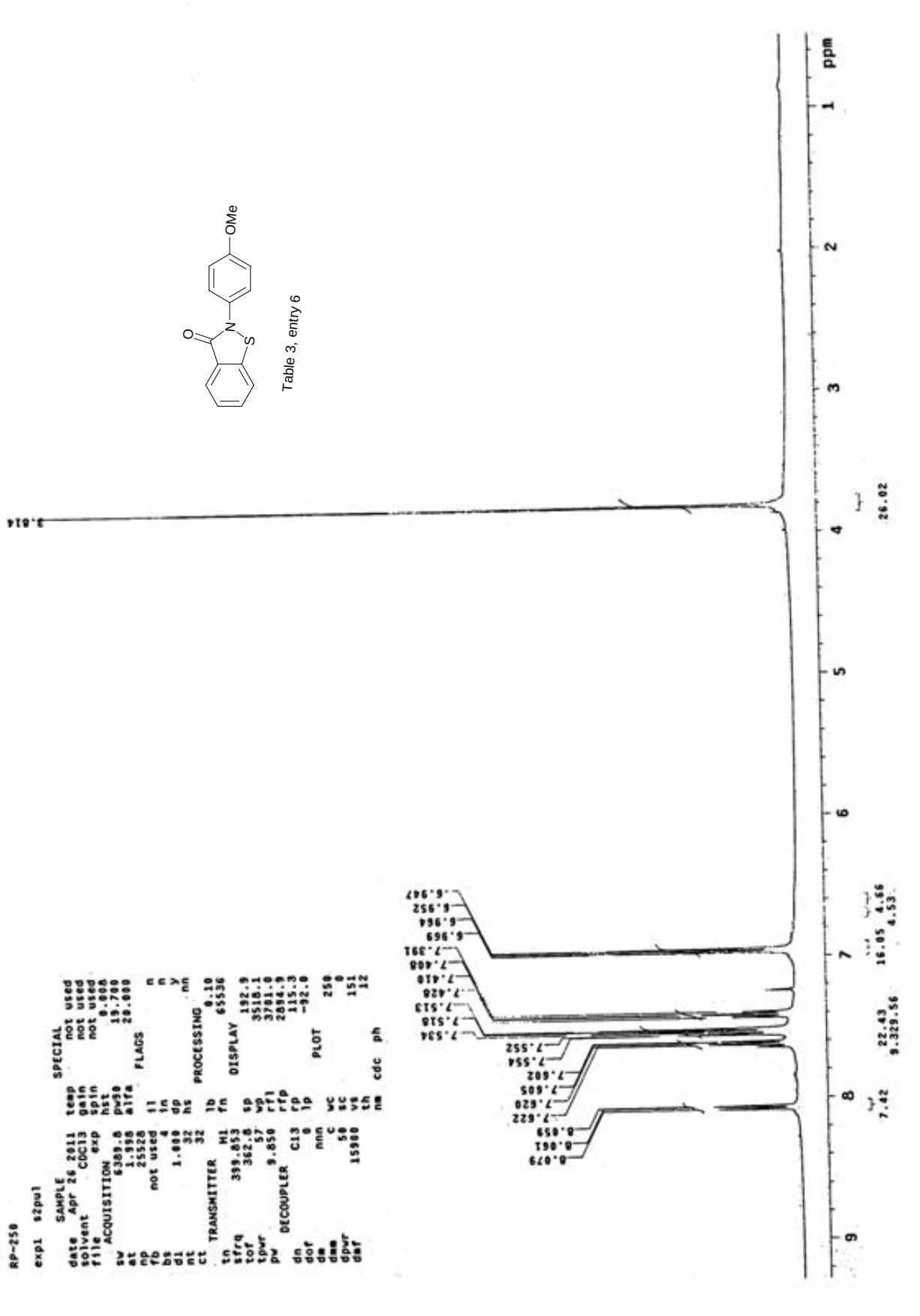
OMe
N
S
O
Table 3, entry 6
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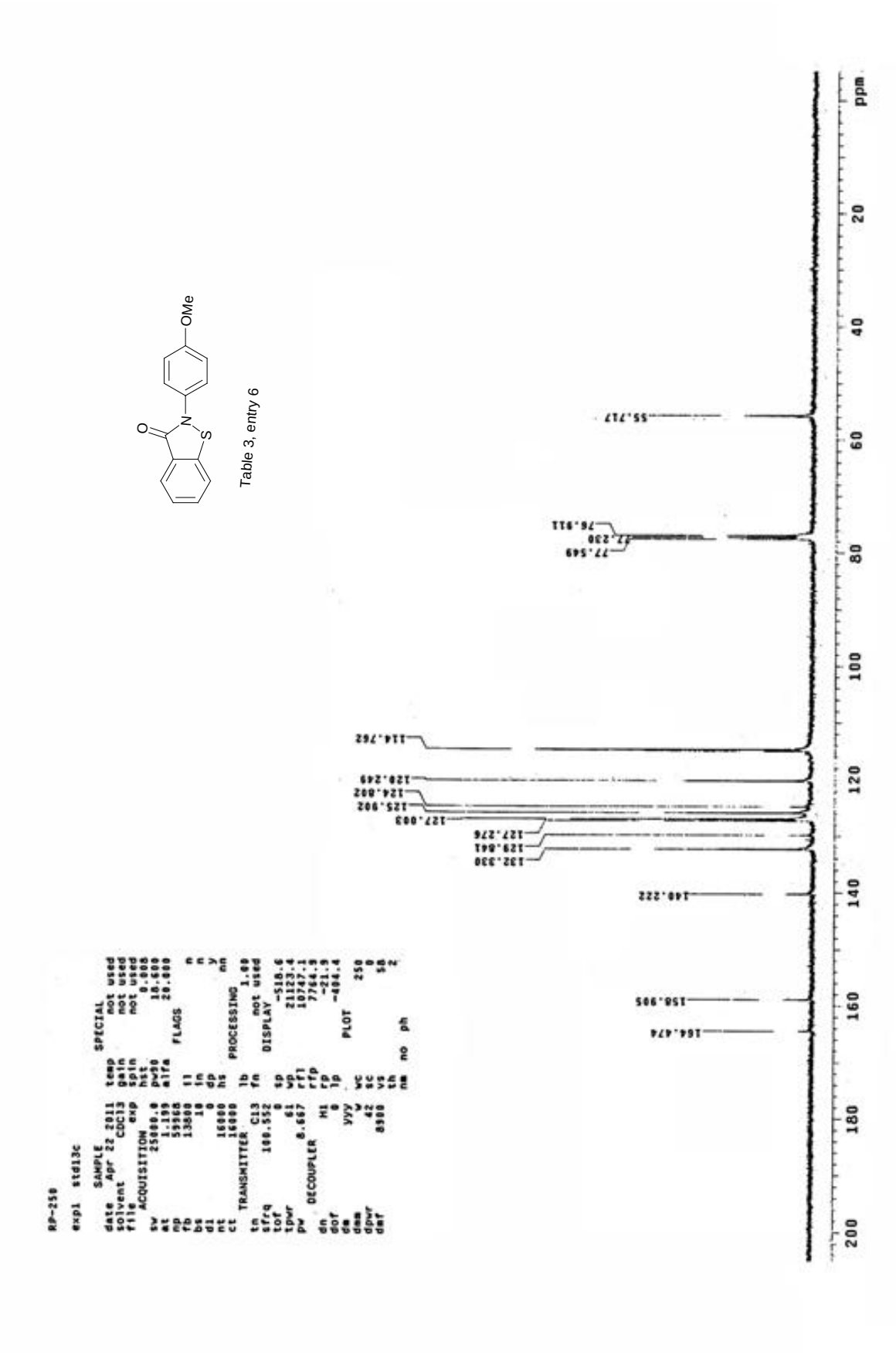
6.947
6.952
6.964
6.969
7.391
7.408
7.418
7.426
7.513
7.518
7.534
7.552
7.554
7.602
7.605
7.620
7.622
8.059
8.061
8.079
ppm
1
2
3
4
5
6
7
8
9
7.42
22.43
9.329.56
16.05
4.66
4.53
26.02


OMe
O
N
S
Table 3, entry 6
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77.230
77.549
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120.249
124.802
125.902
127.003
127.276
129.641
132.330
148.222
158.985
164.474
ppm
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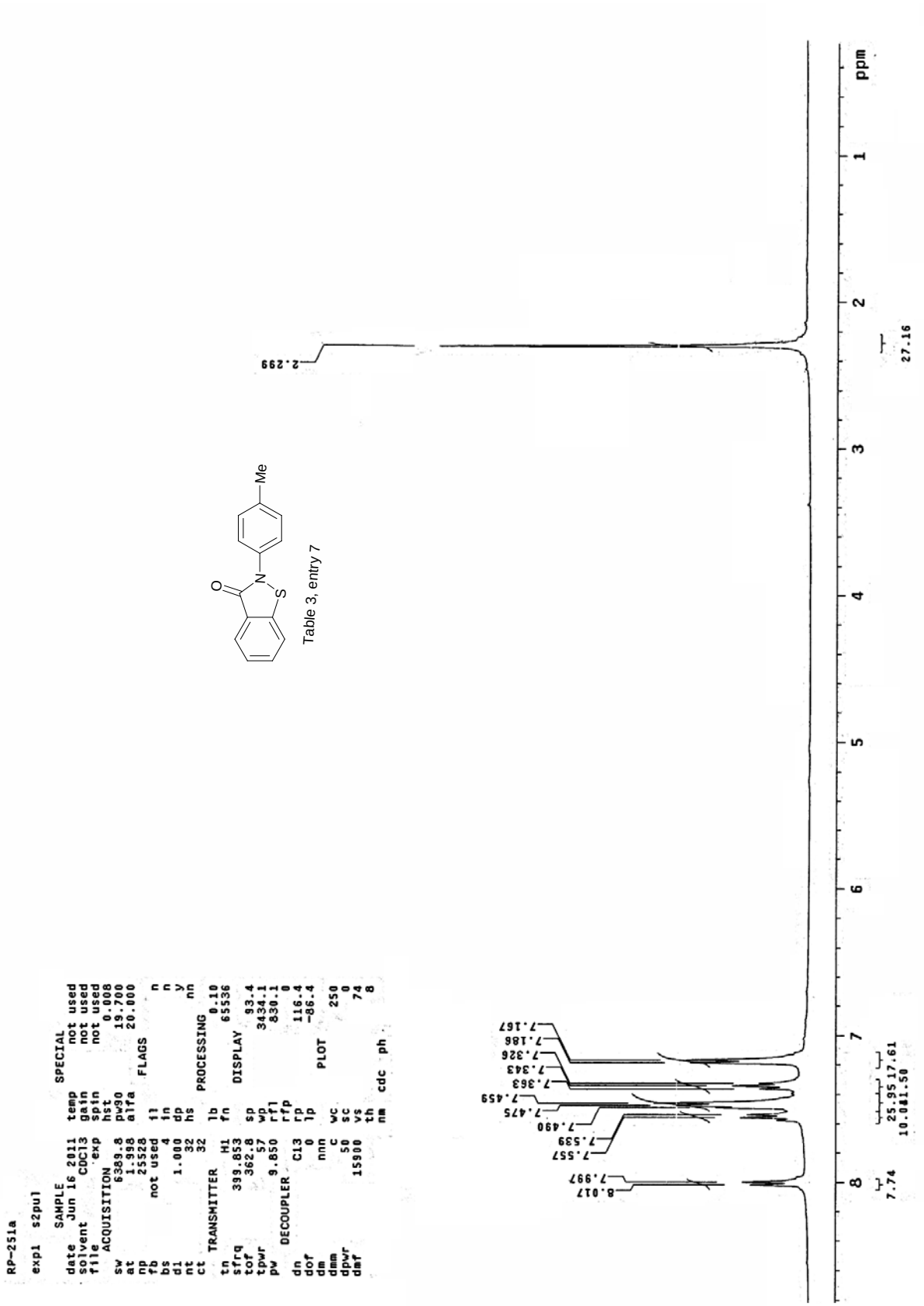
40
60
80
100
120
140
160
180
200


RP-251a
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SAMPLE
date Jun 16 2011
solvent CDCl3
file exp
ACQUISITION
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at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dof 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 19.700
alfa 20.000
FLAGS
fl n
fn n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp 93.4
wp 3434.1
rfl 830.1
rfp 0
rp 116.4
lp -86.4
PLOT
wc 250
sc 0
vs 74
th 8
nm cdc ph
Me
O
N
S
Table 3, entry 7
2.299
8.017
7.997
7.557
7.539
7.490
7.475
7.459
7.363
7.343
7.326
7.186
7.167
ppm
27.16
7.74
25.95 17.61
10.041.50

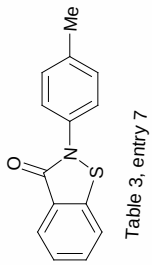
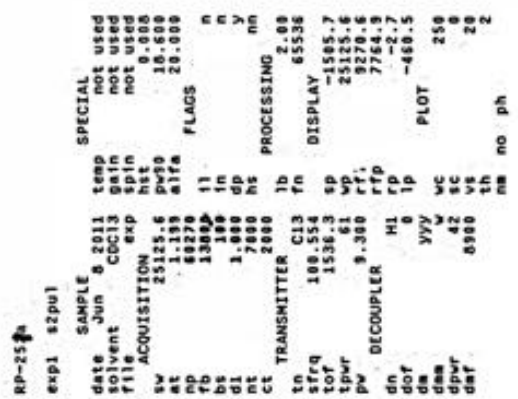
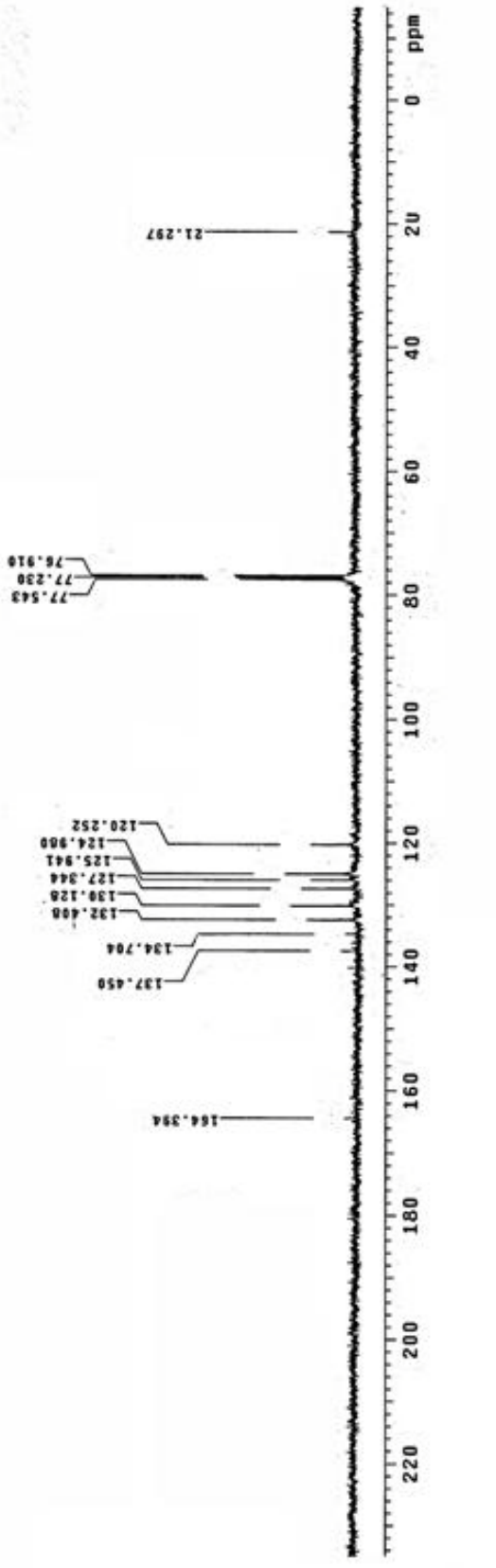


Table 3, entry 7





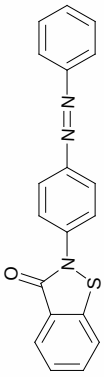


Table 3, entry 9

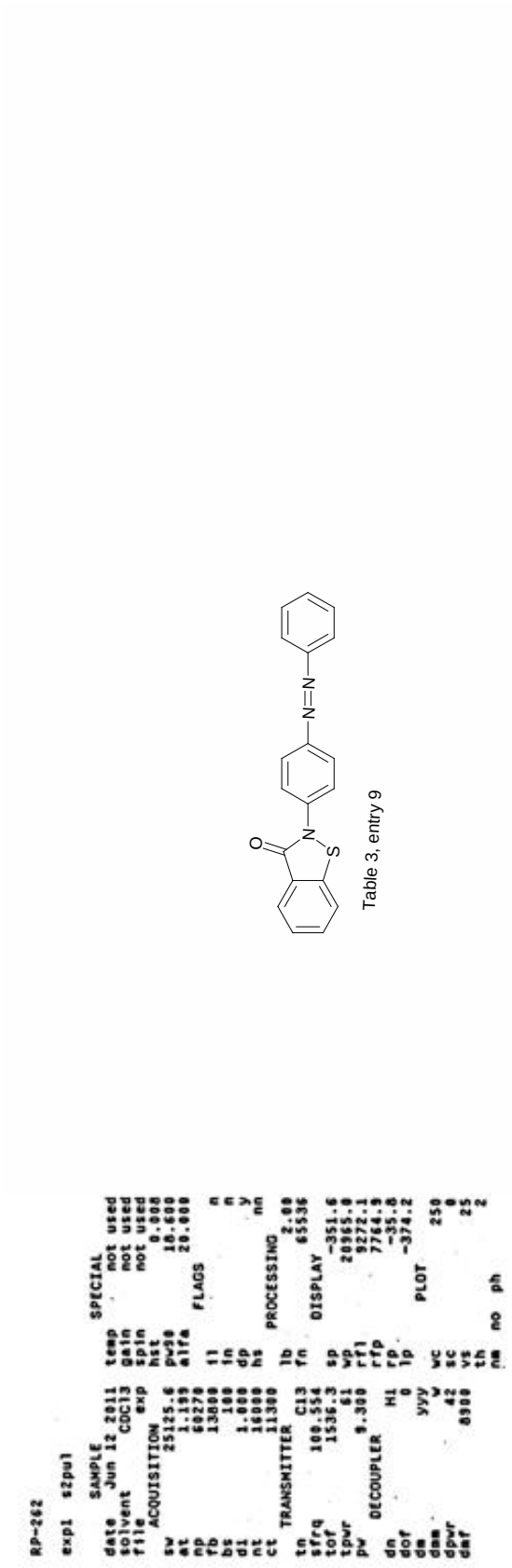
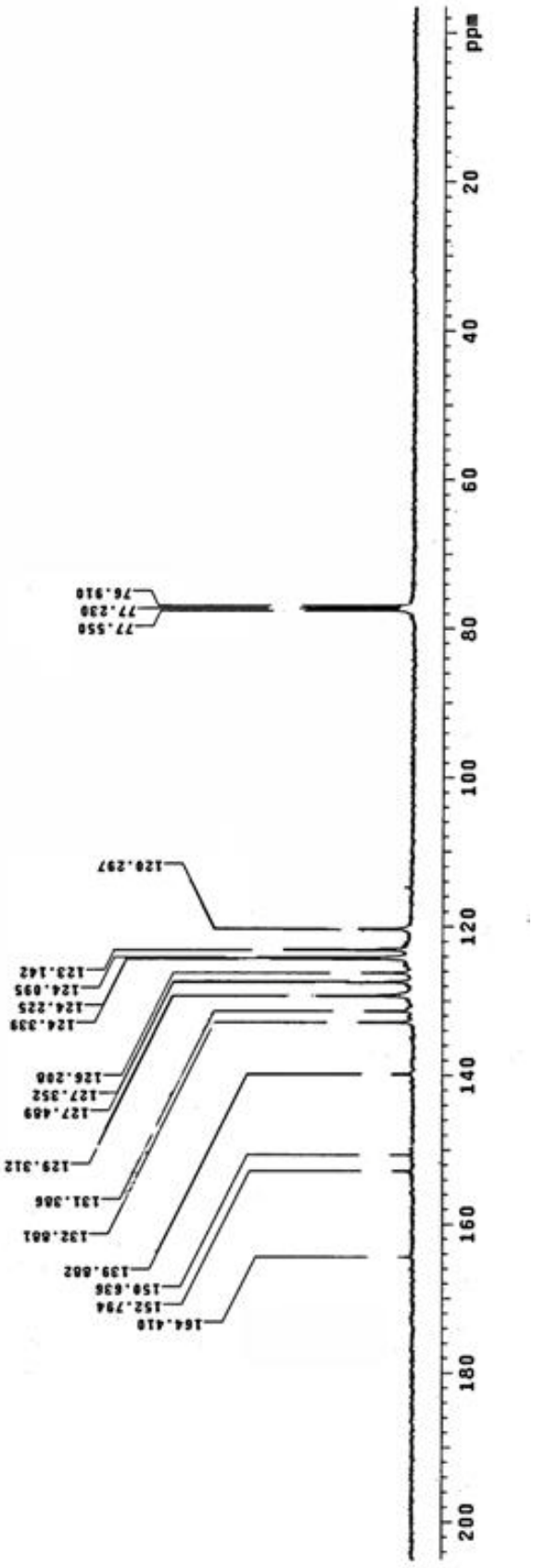
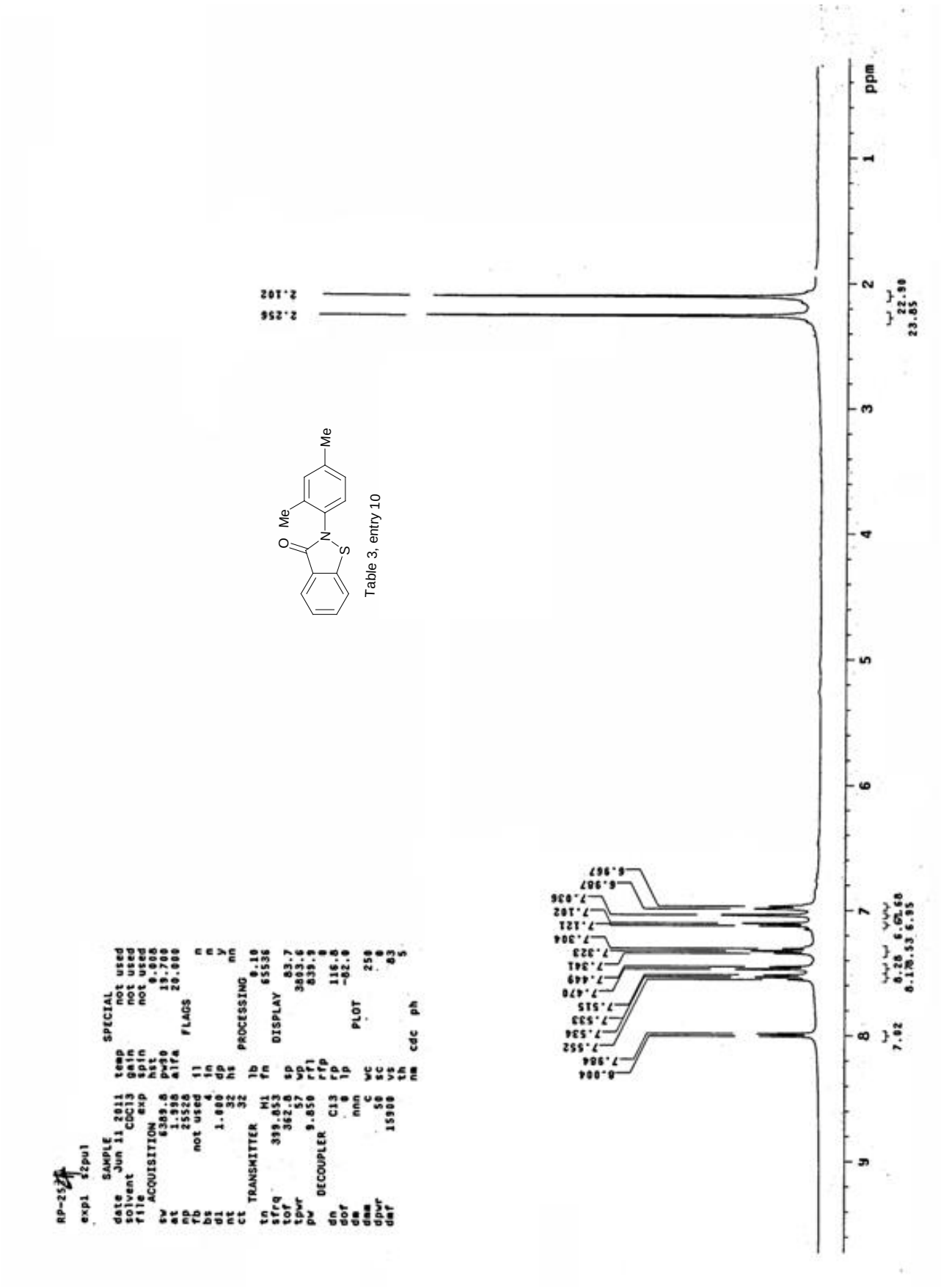


Table 3, entry 9




Me
Me
O
N
S
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ppm
1
2
3
4
5
6
7
8
9
22.90
23.85
7.82
8.28
6.00
6.68
6.170.53
6.95
8.084
7.984
7.552
7.534
7.533
7.515
7.470
7.449
7.341
7.323
7.304
7.121
7.102
7.036
6.987
6.987
RP-25
exp1 d2pul
SAMPLE
date Jun 11 2011
solvent CDCl3
file exp
ACQUISITION
sw 6389.8
at 1.398
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.006
pw90 19.700
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp 83.7
wp 3803.6
rfl 839.9
rfp 0
rp 116.8
lp -82.9
PLOT
wc 250
sc 0
vs 83
th 5
cdc ph

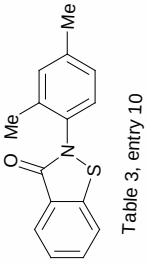
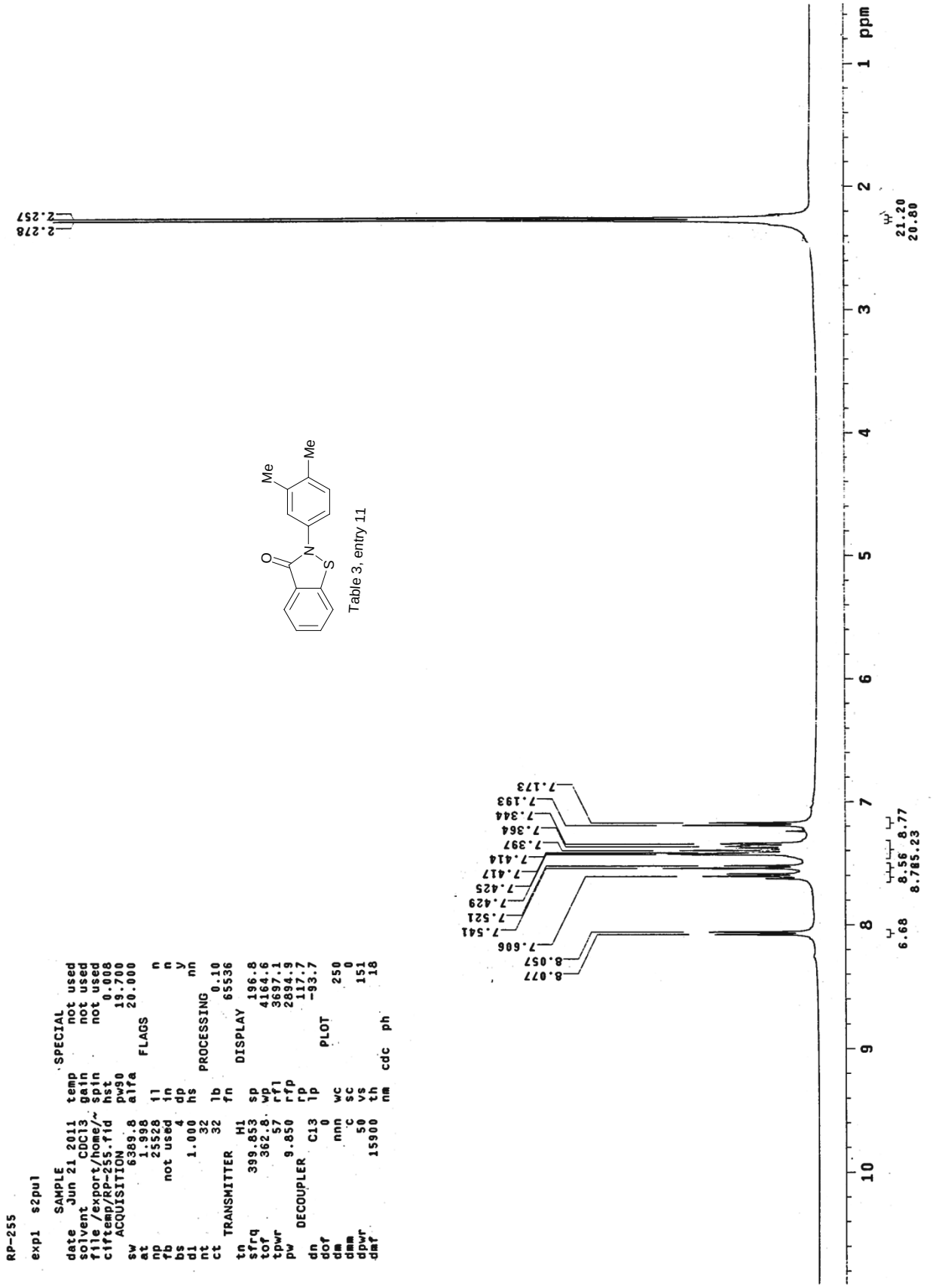


Table 3, entry 10


RP-255
exp1 s2pul
SAMPLE
date Jun 21 2011
solvent CDCl3
file /export/home/~
ciftemp/RP-255.fid
ACQUISITION
sw 6389.8
at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin
hst 0.008
pw90 19.700
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp 196.8
wp 4164.6
rfl 3697.1
rfp 2894.9
rp 117.7
lp -93.7
PLOT
wc 250
sc 0
vs 151
th 18
nm cdc ph
Me
Me
O
N
S
Table 3, entry 11
2.278
2.257
8.077
8.057
7.606
7.541
7.521
7.429
7.425
7.417
7.414
7.397
7.364
7.344
7.193
7.173
6.68
8.56
8.785
8.77
23
21.20
20.80
ppm

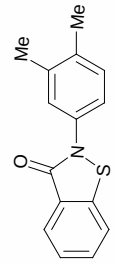
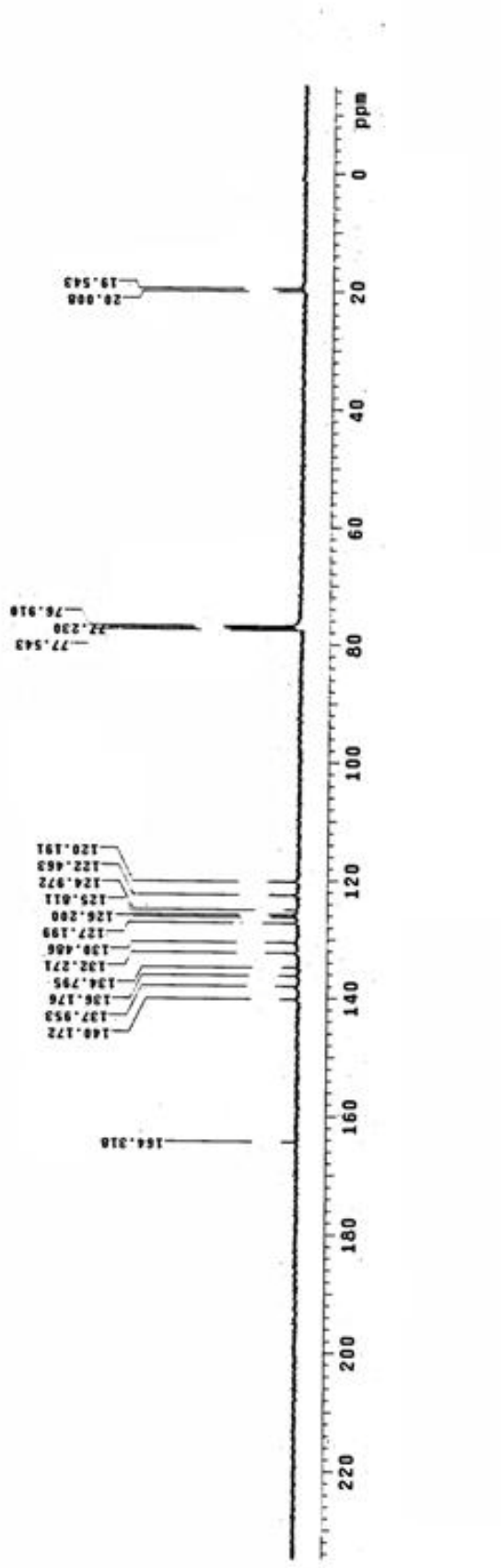


Table 3, entry 11



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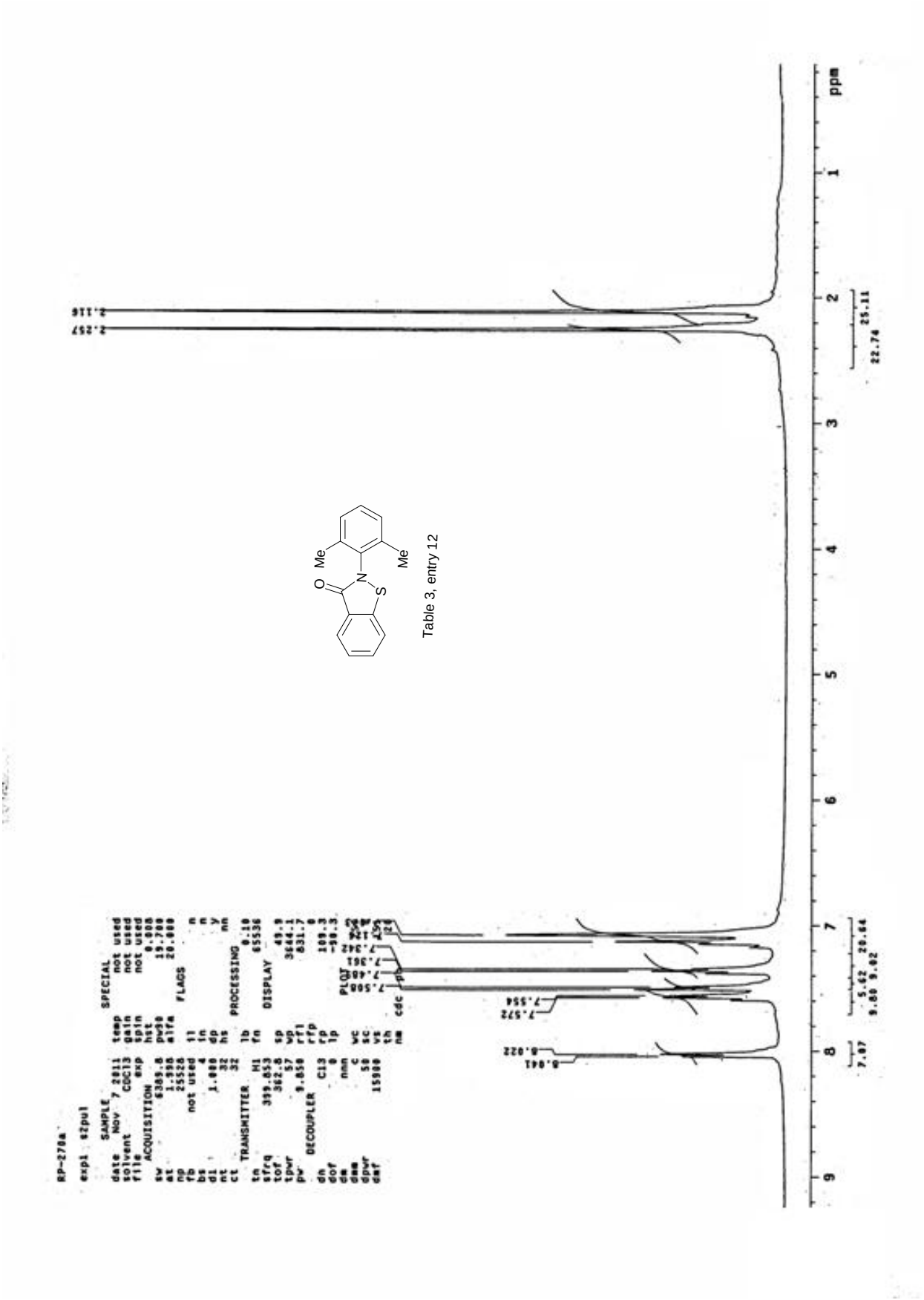


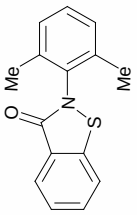
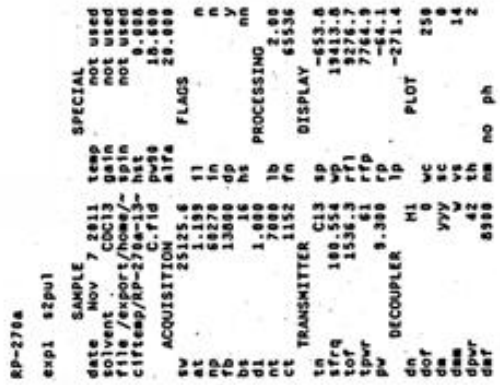
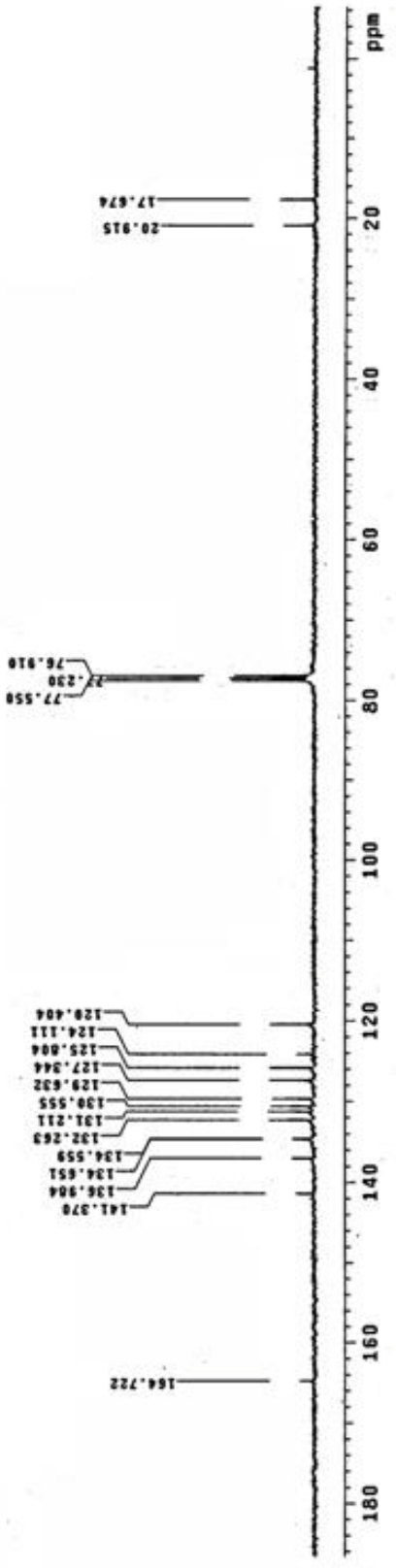


Table 3, entry 12





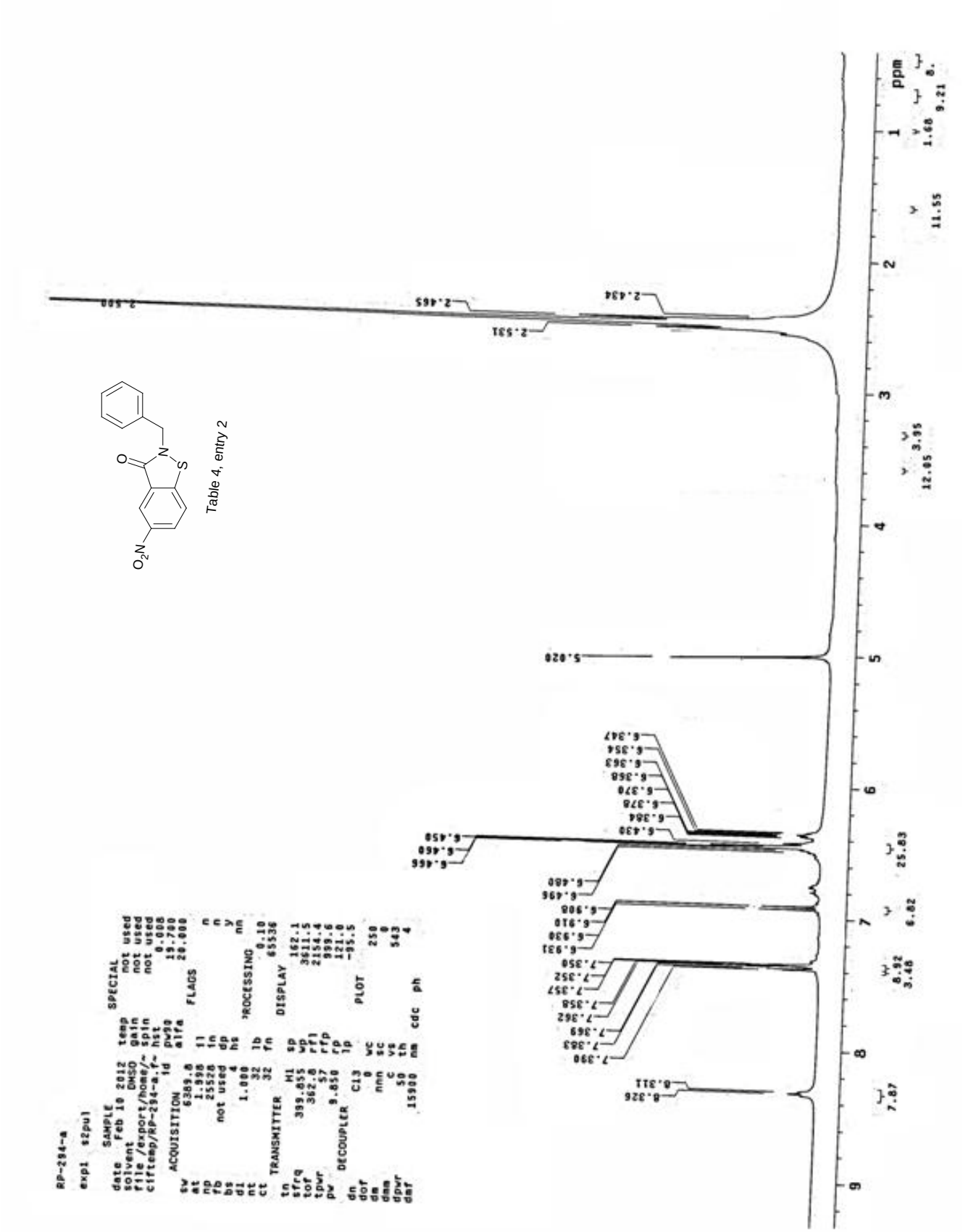
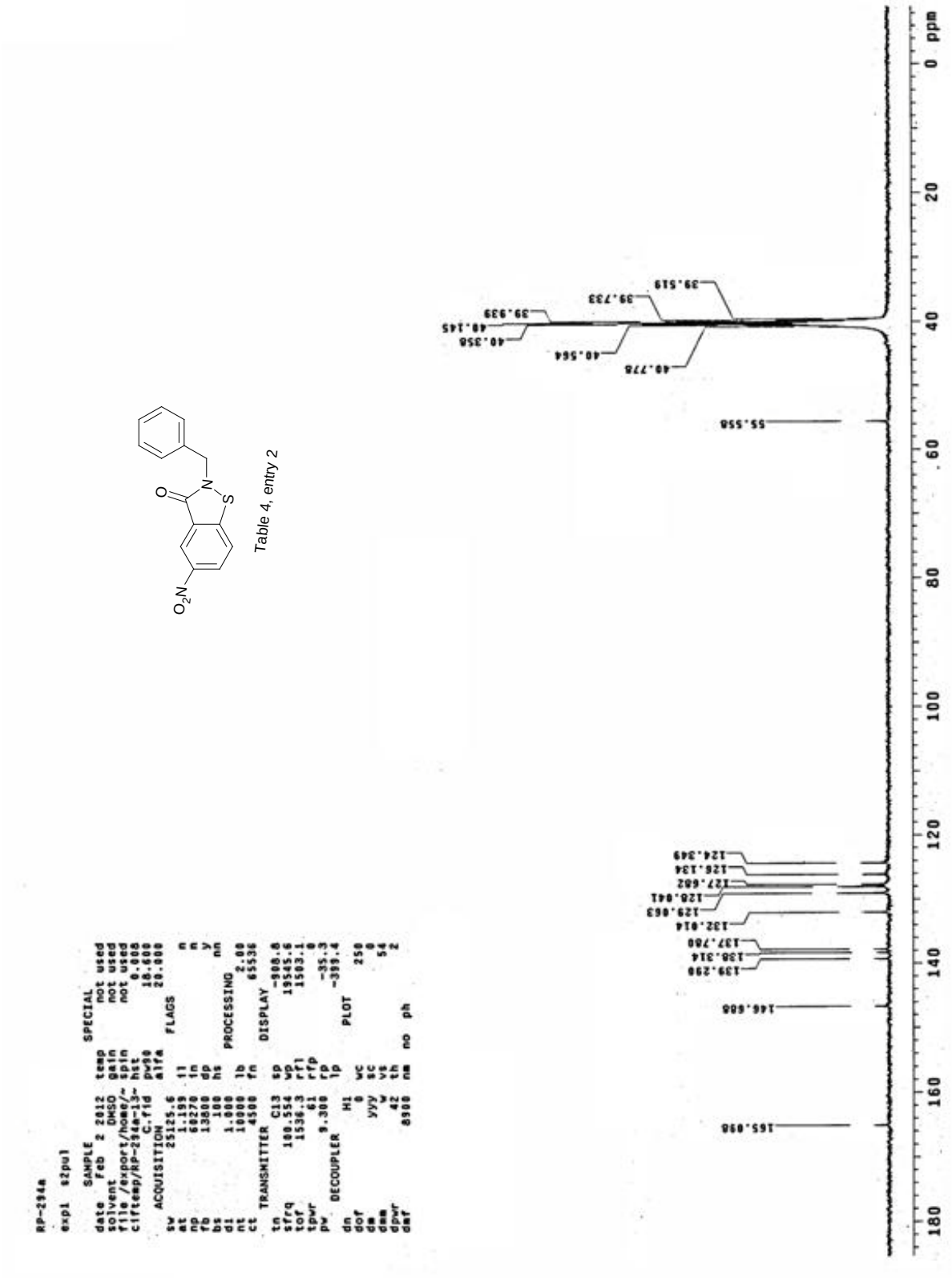


Table 4, entry 2
O
N
S
O_2N
RP-294-a
expl s2pul
SAMPLE
date Feb 10 2012
solvent DMSO
file /export/home/~
ciftemp/RP-294-a.f~
ACQUISITION
sw 6389.8
at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.855
tof 362.8
tpur 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pwlg 19.780
alfa 20.000
FLAGS
PROCESSING
DISPLAY
PLOT
2.580
2.465
2.434
2.531
5.828
6.347
6.354
6.363
6.368
6.378
6.384
6.438
6.458
6.466
6.480
6.496
6.908
6.918
6.930
6.931
7.350
7.352
7.357
7.358
7.362
7.369
7.383
7.390
8.311
8.326
ppm


RP-294a
expl s2pul
SAMPLE
date Feb 2 2012
solvent DMSO
file /export/home/~
cliftemp/RP-294a-13~
C.fid
ACQUISITION
sw 25125.6
at 1.199
np 68270
fb 13800
bs 100
bs 1.000
nt 10000
ct 4500
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 9.300
DECOUPLER
tn H1
dn
dof 0
da yyy
dm y
dmm 42
dpwr 8900
dmf
SPECIAL
temp not used
gain not used
spin not used
hst 0.000
pw90 18.600
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -900.6
wp 15545.6
rfl 1503.1
rfp 0
rp -35.3
lp -399.4
PLOT
wc 250
sc 0
vs 54
th 2
nm
no ph
O
N
S
O_2N
Table 4, entry 2
39.519
39.733
39.939
40.145
40.358
40.564
40.778
55.558
124.349
126.134
127.602
128.041
129.063
132.014
137.760
138.314
139.298
146.606
165.098
0 ppm
20
40
60
80
100
120
140
160
180

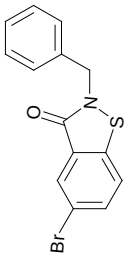
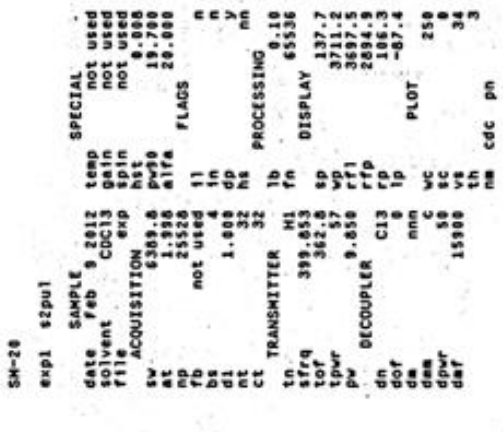
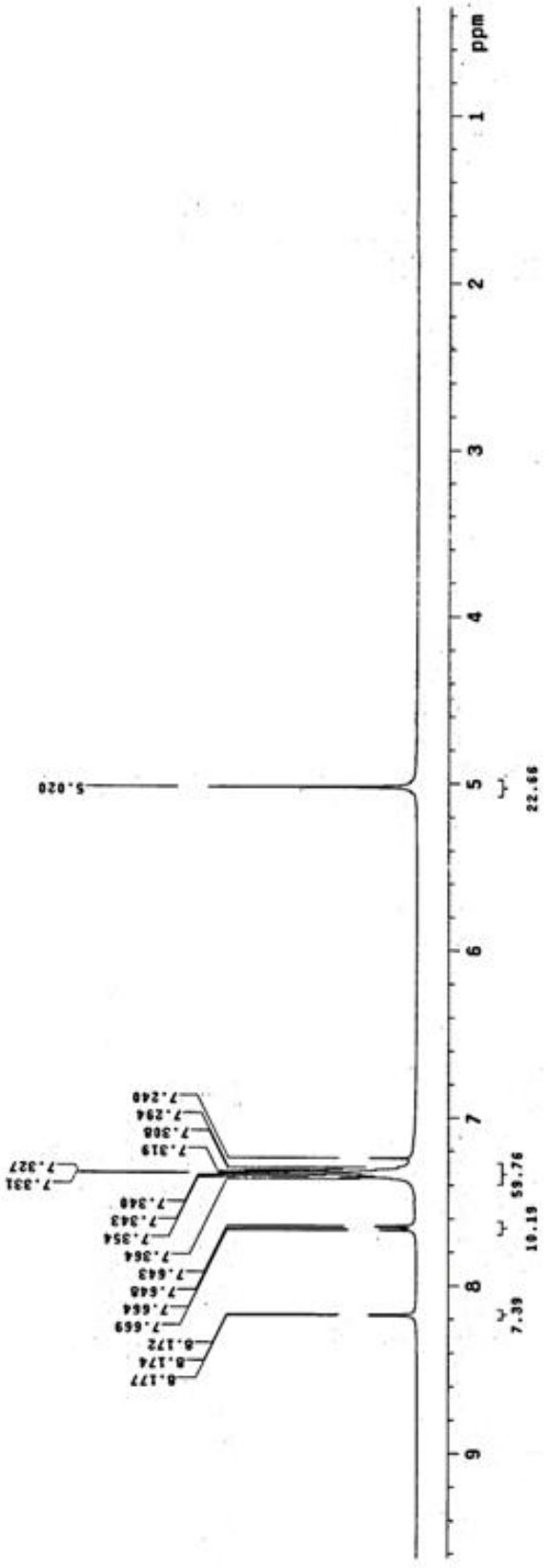


Table 4, entry 3





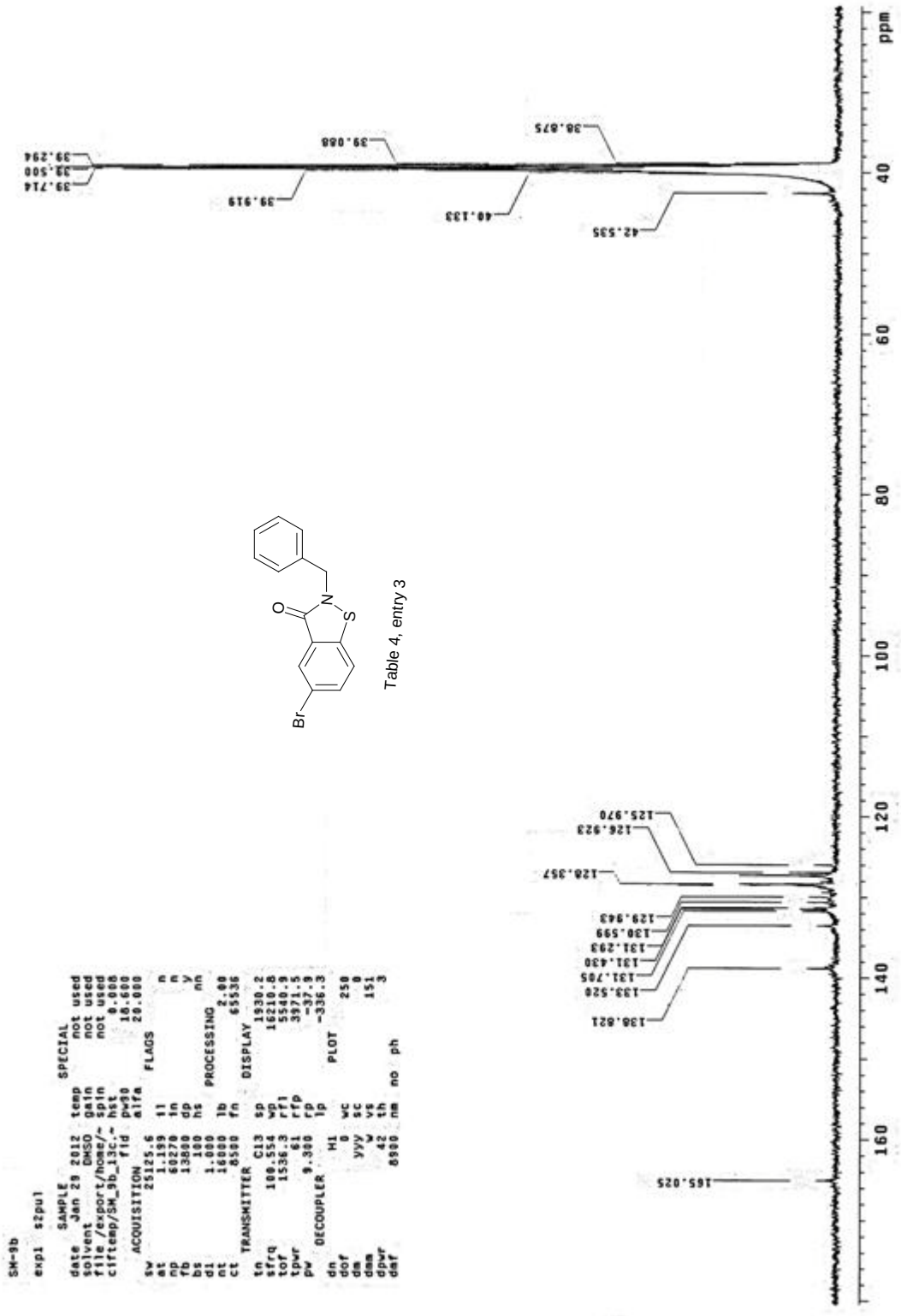


Table 4, entry 3

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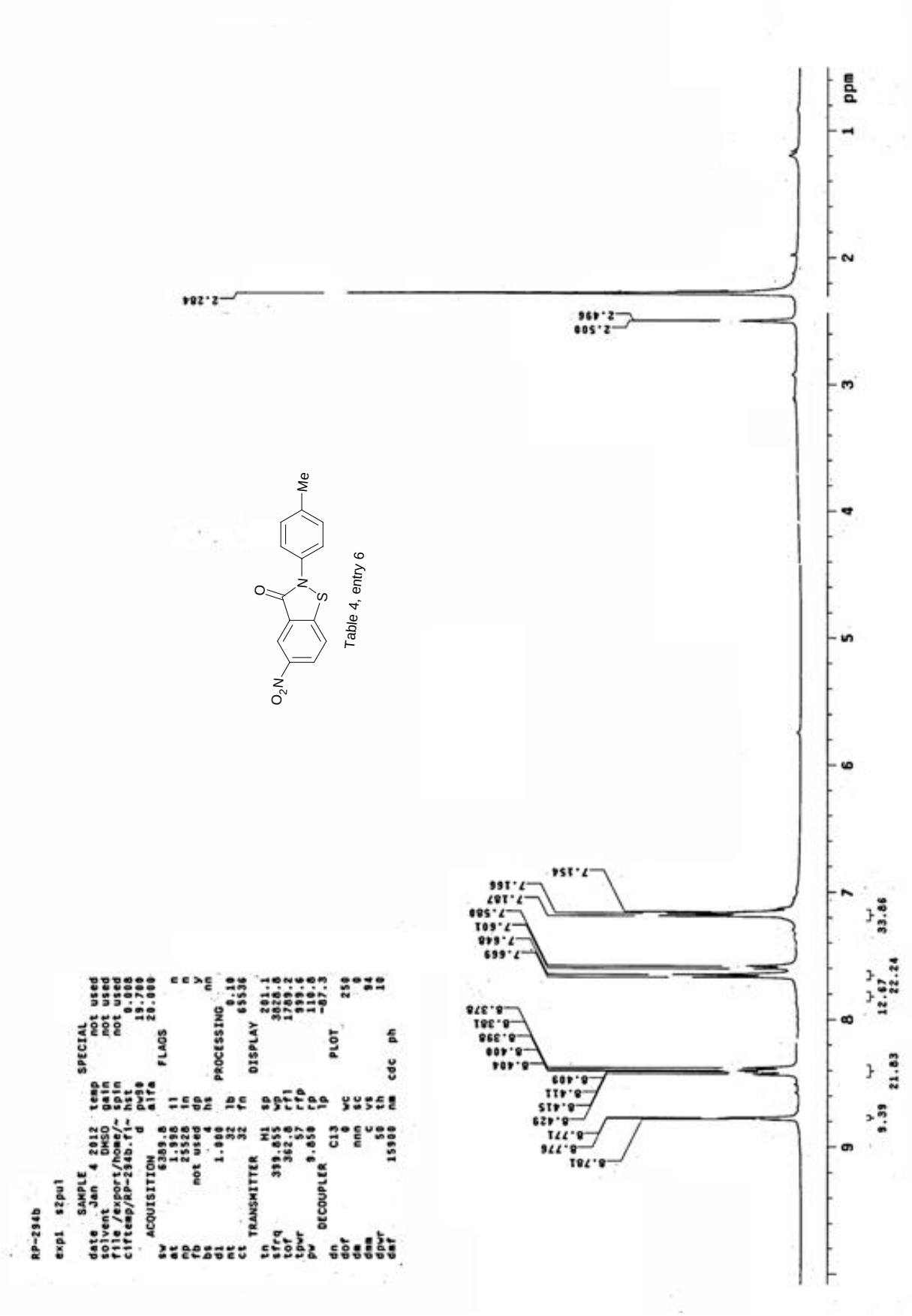
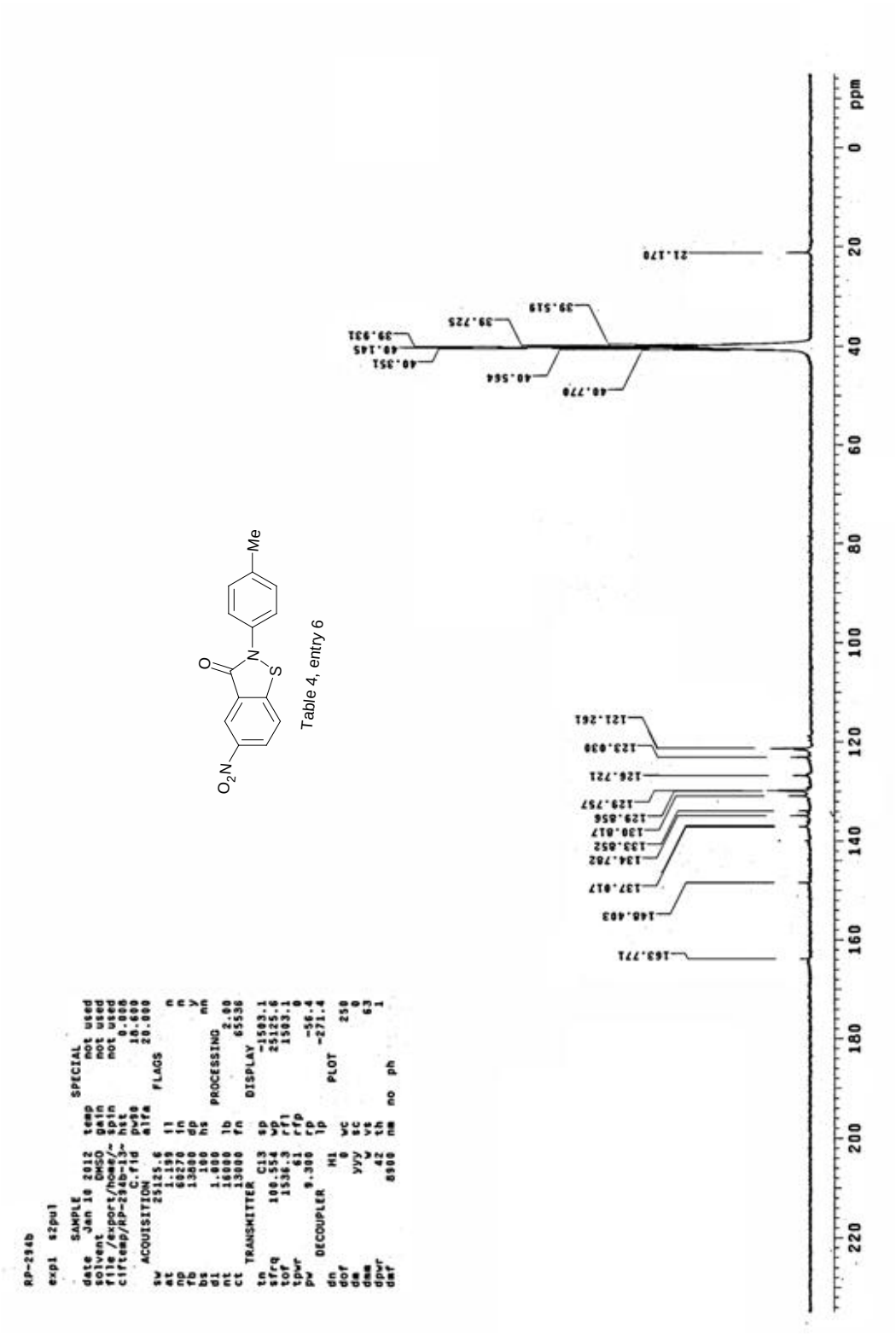
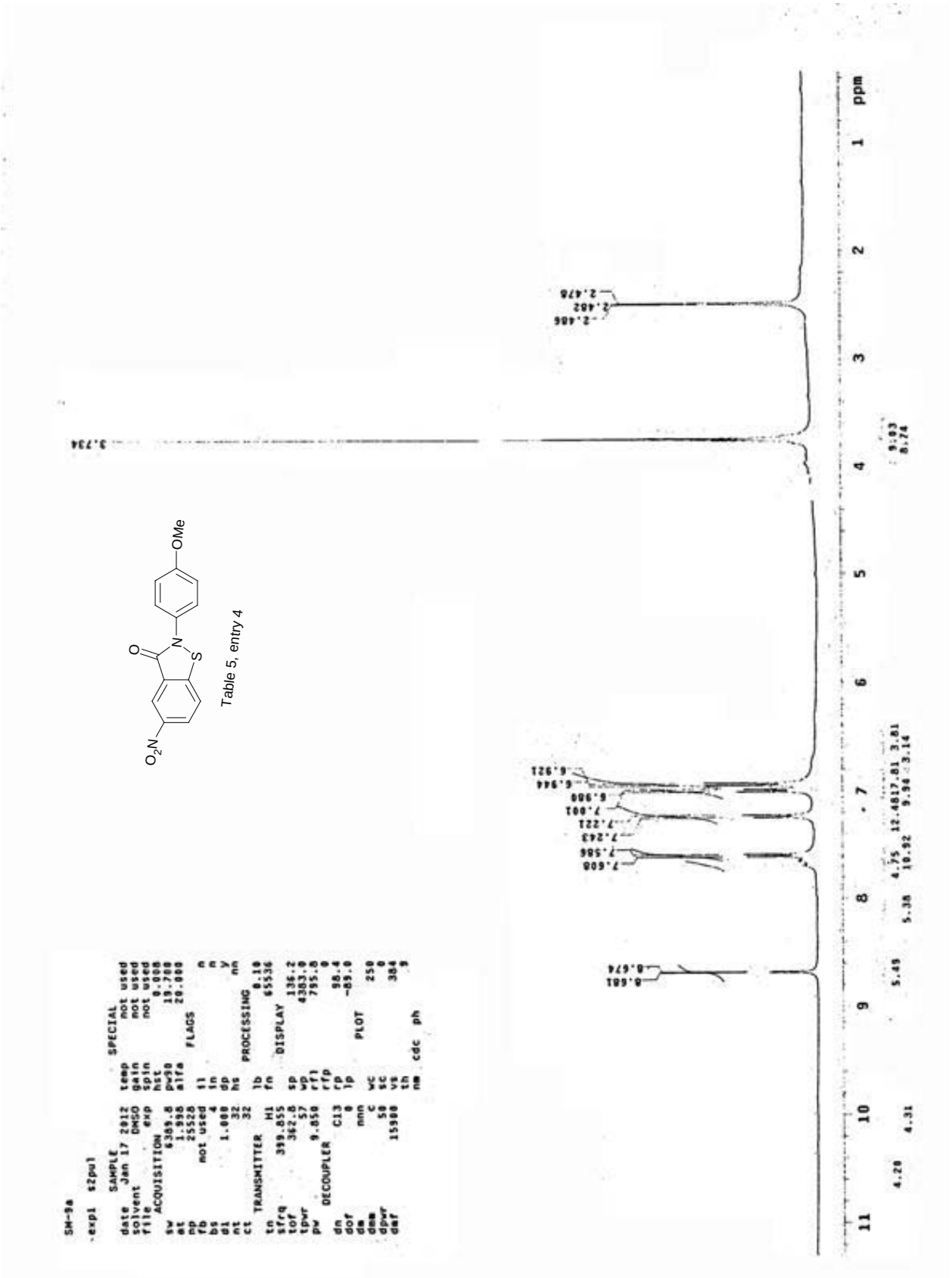
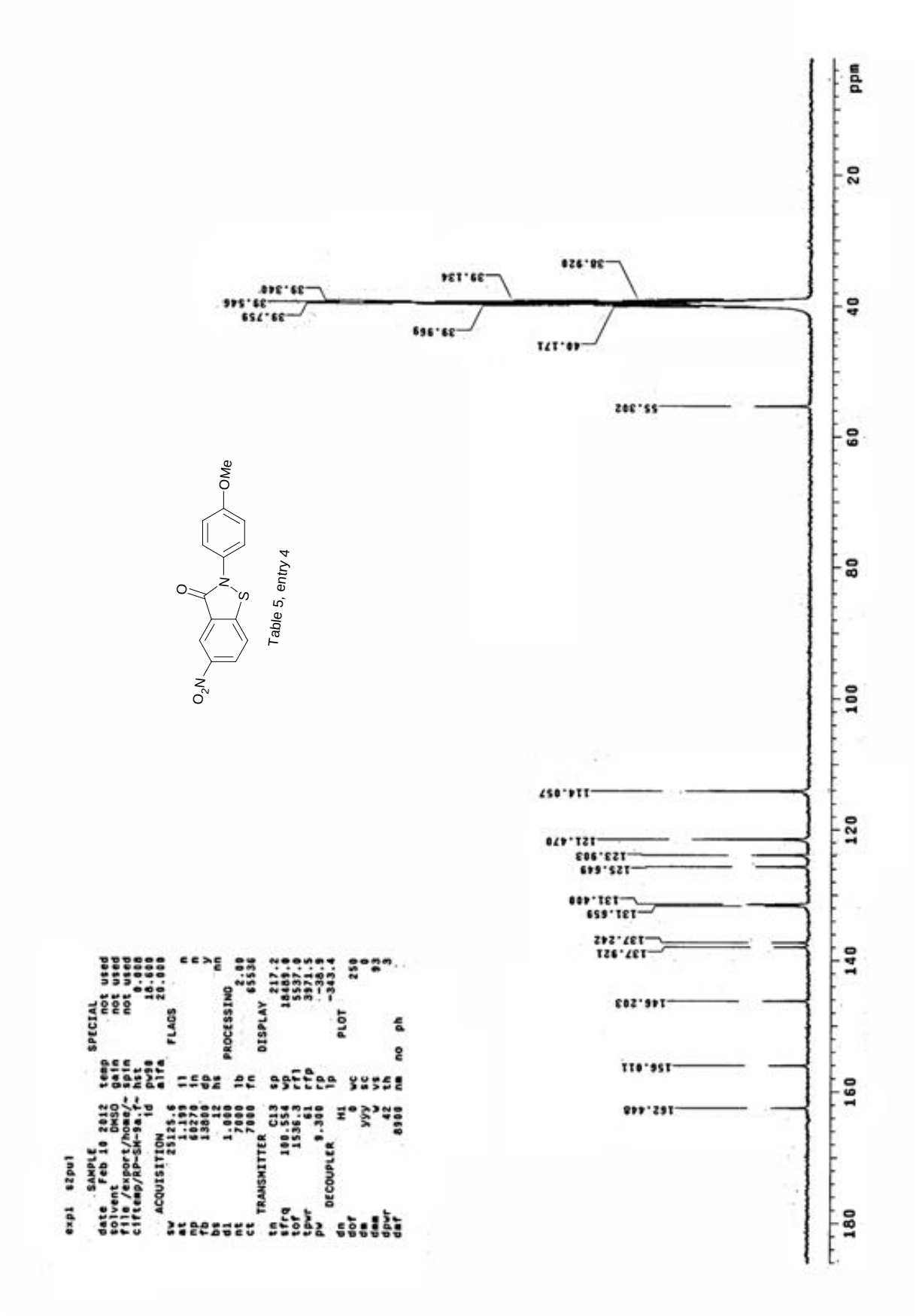


Table 4, entry 6


Me
O
N
S
O2N
Table 4, entry 6
21.170
39.519
39.725
39.931
40.145
40.351
40.564
40.770
121.261
123.038
126.721
129.757
129.856
130.017
133.052
134.762
137.017
140.403
163.771
ppm
0
20
40
60
80
100
120
140
160
180
200
220


OMe
O
N
S
O_2N
Table 5, entry 4
3.734
2.478
2.462
2.446
8.681
8.674
7.608
7.586
7.243
7.221
7.001
6.988
6.944
6.921
ppm


OMe
O
N
S
O_2N
Table 5, entry 4
ppm
20
40
60
80
100
120
140
160
180
55.382
114.057
121.470
123.903
125.649
131.488
131.659
137.242
137.921
146.203
156.011
162.448