Supporting Information

Domino assembly of dithiocarbamates *via* Cu-catalyzed denitrogenative thiolation of iodotriazole-based diazo precursors

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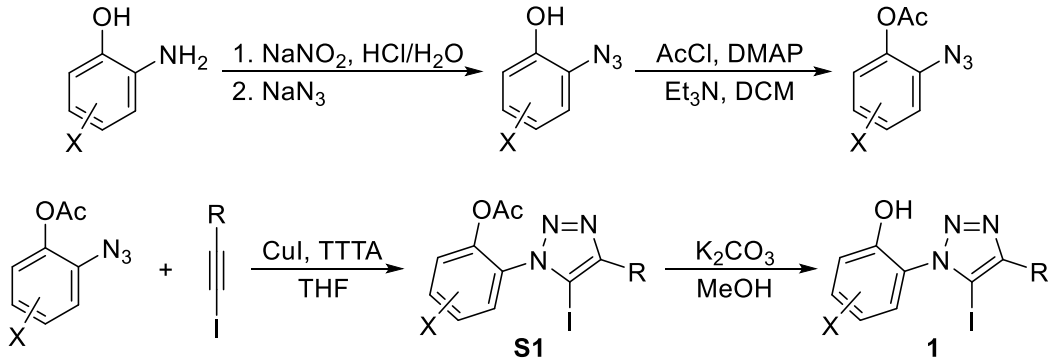
General information

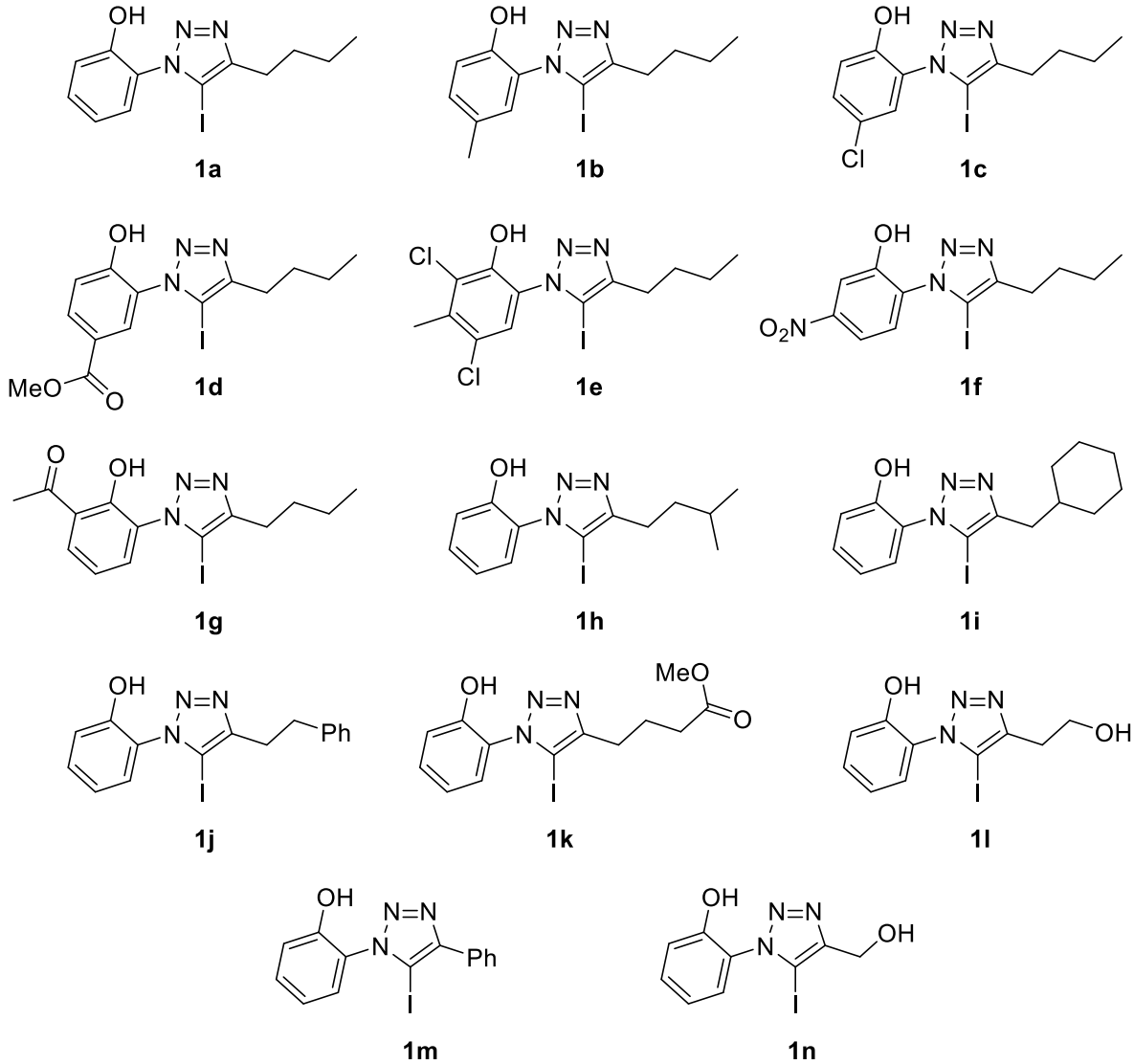
NMR spectra were recorded with Bruker Avance 400, Agilent 400MR (^{1}H 400 MHz, ^{13}C 100 MHz), and Bruker Avance 600 (^{1}H 600 MHz, ^{13}C 151 MHz) spectrometers at ambient temperature. Chemical shifts are presented in ppm (δ scale) and referenced to hexamethyldisiloxane (δ = 0.05 ppm) or tetramethylsilane (δ = 0 ppm) in the ^{1}H NMR spectra and to the solvent signal in the ^{13}C NMR spectra. IR spectra (cm^{-1}) were registered on Thermo Scientific Nicolet iS5 FT-IR spectrometer using iD3 Attenuated Total Reflectance (ATR) accessory. IR bands in 2365–2340 cm^{-1} range belong to atmospheric CO_2. MALDI-TOF spectra were recorded with a Bruker Daltonics UltraFlex instrument in a dithranol matrix using PEG 300, PEG 400 or PEG 600 as the internal standard. ESI mass spectra were obtained from Thermo Scientific LTQ Orbitrap and Sciex TripleTOF 5600+ spectrometers. Column chromatography was carried out on Macherey–Nagel silica gel 60 (0.040–0.063 mm).

Experimental procedures and characterization data for compounds

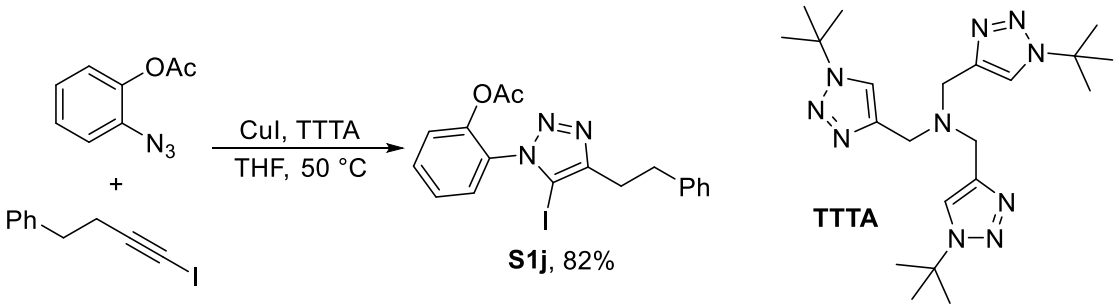
General scheme for the synthesis of 2-(5-iodotriazolyl)phenols 1



Iodotriazoles **1a-d**,**f**,**l**,**n**,[1] **1e**,**g**,**k**[2] and **1h**,**i**,**m**[3] were previously reported.

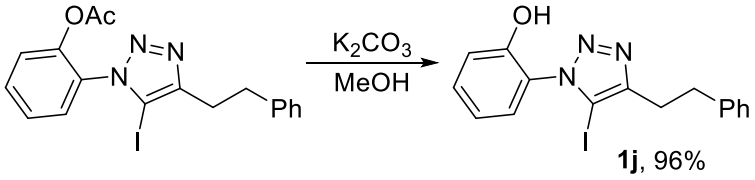


2-[5-Iodo-4-(2-phenylethyl)-1*H*-1,2,3-triazol-1-yl]phenyl acetate (S1j)



2-Azidophenyl acetate[1] (354.3 mg, 2.00 mmol), (4-iodobut-3-yn-1-yl)benzene[4] (563.4 mg, 2.20 mmol), CuI (19.1 mg, 0.100 mmol, 5 mol %), and tris[(1-*tert*-butyl-1*H*-1,2,3-triazol-4-yl)methyl]amine (TTTA) (42.8 mg, 0.100 mmol, 5 mol %) were mixed under an Ar atmosphere in THF (4 mL). The reaction mixture was stirred at 50 °C for 48 h (TLC control), then diluted with CH_2Cl_2 (50 mL), washed with EDTA solution (50 mL) and water (50 mL). The organic layer was dried with anhydrous Na_2SO_4, and the solvents were evaporated *in vacuo*. The residue was purified by column chromatography (eluent: hexanes–EtOAc = 4:1). Yield 710 mg (82%). Yellowish solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (m, 1H), 7.44–7.36 (m, 3H), 7.32–7.27 (m, 2H), 7.25–7.18 (m, 3H), 3.12–3.02 (m, 4H, CH_2CH_2), 2.04 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.9 (C=O), 151.0 (quat.), 145.7 (quat.), 140.8 (quat.), 131.4, 129.2 (quat.), 128.6, 128.5 [2C, CH(Ph)], 128.4 [2C, CH(Ph)], 126.3, 126.2, 123.9, 81.3 (CI), 35.1, 28.1, 20.6.

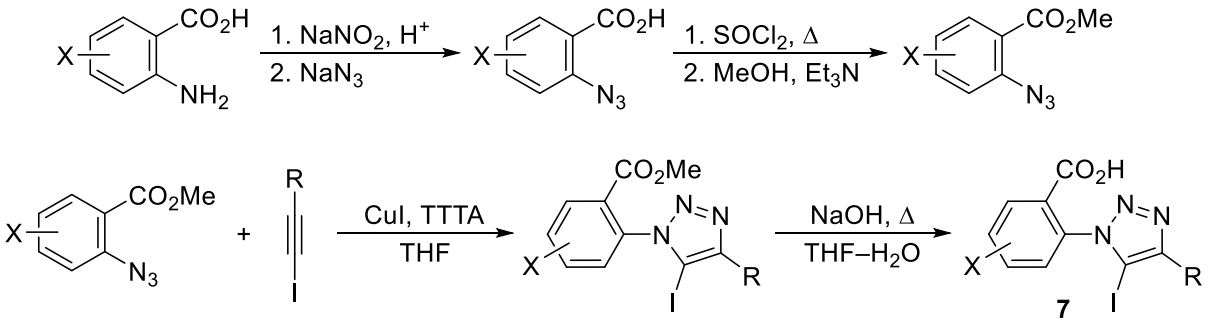
2-[5-Iodo-4-(2-phenylethyl)-1*H*-1,2,3-triazol-1-yl]phenol (1j)



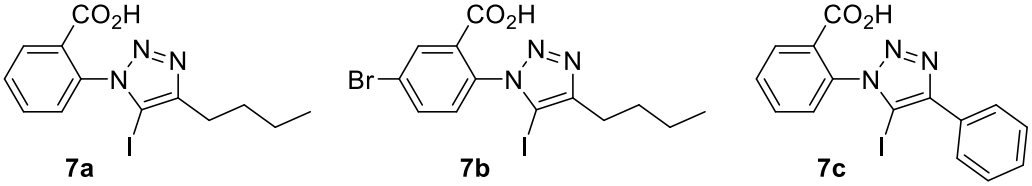
K_2CO_3 (440 mg, 3.18 mmol, 2 equiv) was added to a solution of 2-(5-iodo-1*H*-1,2,3-triazol-1-yl)phenyl acetate **S1j** (689 mg, 1.59 mmol) in MeOH (13.7 mL). The obtained suspension was stirred at ambient temperature for 30 min (TLC control), then diluted with 10 % HCl (40 mL) and extracted with CH_2Cl_2 (3 × 25 mL). Combined organic extracts were dried with anhydrous Na_2SO_4, and the solvents were evaporated *in vacuo*. The residue was purified by column chromatography (eluent: CH_2Cl_2–MeOH = 30:1). Yield 598 mg (96%). White solid; mp 172–173 °C; ^{1}H NMR (400 MHz, $CDCl_3$–CD_3OD) δ 7.38 [ddd, J = 8.3, 7.3, 1.6 Hz, 1H, 4-CH(Ar)], 7.32–7.26 [m, 2H, 3,5-CH(Ph)], 7.24–7.18 (m, 4H), 7.06 [dd, J = 8.3, 1.3 Hz, 1H, 6-CH(Ar)], 6.98 [m, 1H, 4-CH(Ar)], 3.10–2.99 (m, 4H, CH_2CH_2); ^{13}C NMR (100 MHz, $CDCl_3$–CD_3OD) δ 152.3 (quat.), 150.7 (quat.), 140.7 (quat.), 131.7, 128.4 [2C, CH(Ph)], 128.3 [2C, CH(Ph)], 128.1, 126.0, 124.2 (quat.), 119.5, 117.0, 82.7 (CI), 35.1, 28.2; IR (neat, cm^{-1}) ν 3061, 3027,

2957, 2924, 2856, 1602, 1516, 1497, 1464, 1420, 1375, 1303, 1279, 1228, 1002, 834, 753, 700; HRMS (MALDI-TOF) calcd for $C_{16}H_{15}IN_3O$ $[M+H]^+$ 392.0254; found 392.0247.

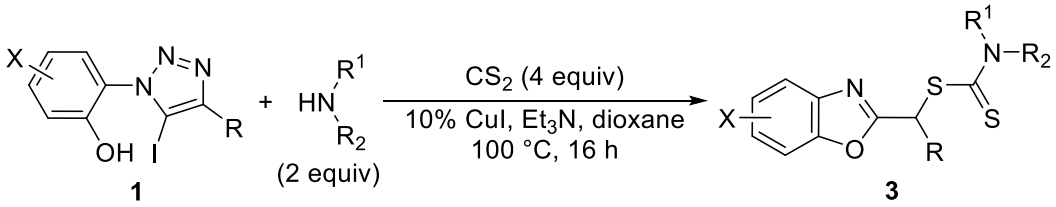
General scheme for the synthesis of 2-(5-iodotriazolyl)benzoic acids 7



Iodotriazoles **7a-c**[5] were previously reported.

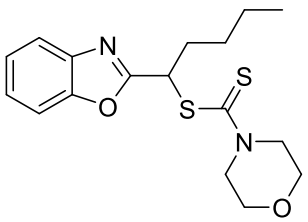


Synthesis of 1-(1,3-benzoxazol-2-yl)alkyl dithiocarbamates 3



General procedure. In a vial with a screw cap iodotriazole **1** (0.25 mmol), secondary amine (0.50 mmol, 2 equiv), CuI (4.8 mg, 0.025 mmol, 10 mol %), CS_2 (60.3 μL, 1.00 mmol, 4 equiv), and Et_3N (70 μL, 0.50 mmol, 2 equiv) were mixed under an Ar atmosphere in dioxane (2.5 mL). The reaction mixture was stirred at 100 °C for 16 h, then diluted with CH_2Cl_2 (20 mL), and washed with water (20 mL). The organic layer was dried with anhydrous Na_2SO_4, and the solvents were evaporated *in vacuo*. The residue was purified by column chromatography.

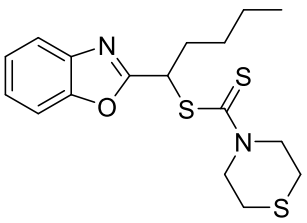
1-(1,3-Benzoxazol-2-yl)pentyl morpholine-4-carbodithioate (3a):



Prepared from iodotriazole **1a** (68.6 mg, 0.20 mmol) and morpholine (36.0 μL, 0.40 mmol) according to the general procedure; eluent: hexanes–EtOAc = 4:1. Yield 52.8 mg (75%). Yellow oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.69 [m, 1H, 4-CH(Ar)], 7.50 [m, 1H, 7-CH(Ar)],

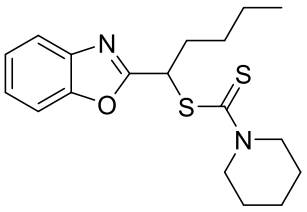
7.33–7.27 [m, 2H, 5,6-CH(Ar)], 5.66 (dd, *J* = 8.2, 6.7 Hz, 1H, CHS), 4.27 (br s, 2H, CH_2N), 3.98 (br s, 2H, CH_2N), 3.76–3.70 (m, 4H, CH_2O), 2.27 (m, 1H, C*H*$_2$Pr), 2.18 (m, 1H, C*H*$_2$Pr), 1.52–1.33 (m, 4H, C*H*$_2$C*H*$_2$Me), 0.87 (t, *J* = 7.2 Hz, 3H, CH_3); ^{13}C NMR (151 MHz, $CDCl_3$) δ 194.9 (C=S), 165.7 [2-C(Ar)], 150.8 [7a-C(Ar)], 141.2 [3a-C(Ar)], 125.1 [5- or 6-CH(Ar)], 124.4 [5- or 6-CH(Ar)], 120.1 [4-CH(Ar)], 110.7 [7-CH(Ar)], 66.2 (br, 2C, CH_2O), 51.1 (br, 2C, CH_2N), 49.1 (CHS), 33.5, 29.3, 22.3, 13.8 (CH_3); IR (neat, cm^{-1}) *ν* 2957, 2924, 2856, 1610, 1563, 1455, 1421, 1268, 1230, 1215, 1115, 1030, 996, 762, 748; HRMS (MALDI-TOF) calcd for $C_{17}H_{22}N_2NaO_2S_2$ $[M+Na]^+$ 373.1015; found 373.1022.

1-(1,3-Benzoxazol-2-yl)pentyl thiomorpholine-4-carbodithioate (3b):



Prepared from iodotriazole **1a** (85.8 mg, 0.25 mmol) and thiomorpholine (50.3 μL, 0.50 mmol) according to the general procedure; eluent: hexanes–EtOAc = 8:1. Yield 46 mg (50%). Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 [m, 1H, 4-CH(Ar)], 7.50 [m, 1H, 7-CH(Ar)], 7.34–7.27 [m, 2H, 5,6-CH(Ar)], 5.62 (dd, *J* = 8.1, 6.8 Hz, 1H, CHS), 4.55 (br s, 2H, CH_2N), 4.25 (br s, 2H, CH_2N), 2.76–2.68 (m, 4H, CH_2S), 2.31–2.11 (m, 2H, C*H*$_2$Pr), 1.53–1.31 (m, 4H, C*H*$_2$C*H*$_2$Me), 0.87 (t, *J* = 7.0 Hz, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.0 (C=S), 165.7 [2-C(Ar)], 150.6 [7a-C(Ar)], 141.1 [3a-C(Ar)], 125.0 [5- or 6-CH(Ar)], 124.3 [5- or 6-CH(Ar)], 120.1 [4-CH(Ar)], 110.6 [7-CH(Ar)], 54.6 (br, CH_2N), 53.3 (br, CH_2N), 49.2 (CHS), 33.5, 29.3, 27.2 (br, 2C, CH_2S), 22.2, 13.8 (CH_3); IR (neat, cm^{-1}) *ν* 2956, 2925, 2870, 2858, 1611, 1564, 1467, 1454, 1435, 1414, 1356, 1282, 1243, 1214, 1191, 1143, 1031, 1003, 949, 935, 762, 747; HRMS (MALDI-TOF) calcd for $C_{17}H_{23}N_2OS_3$ $[M+H]^+$ 367.0967; found 367.0969.

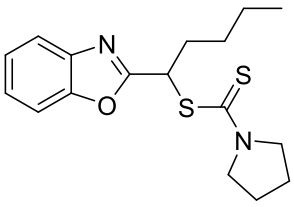
1-(1,3-Benzoxazol-2-yl)pentyl piperidine-4-carbodithioate (3c):



Prepared from iodotriazole **1a** (85.8 mg, 0.25 mmol) and piperidine (49.4 μL, 0.50 mmol) according to the general procedure; eluent: hexanes–EtOAc = 10:1. Yield 56.5 mg (65%). Brownish solid; mp 75–77 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 [m, 1H, 4-CH(Ar)], 7.50 [m, 1H, 7-CH(Ar)], 7.33–7.26 [m, 2H, 5,6-CH(Ar)], 5.67 (dd, *J* = 8.2, 6.7 Hz, 1H, CHS), 4.38–4.14 (m, 2H, CH_2N), 3.87 (br s, 2H, CH_2N), 2.32–2.12 (m, 2H, C*H*$_2$Pr), 1.73–1.59 [m, 6H, 3,4,5-CH_2(piperidine)], 1.53–1.32 (m, 4H, C*H*$_2$C*H*$_2$Me), 0.87 (t, *J* = 7.1 Hz, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.8 (C=S), 166.1 [2-C(Ar)], 150.6 [7a-C(Ar)], 141.1 [3a-C(Ar)], 124.9 [5- or 6-CH(Ar)], 124.2 [5- or 6-CH(Ar)], 120.0 [4-CH(Ar)], 110.6 [7-CH(Ar)], 53.3 (br, CH_2N), 51.5 (br, CH_2N), 49.2 (CHS), 33.6, 29.3, 26.0 (br, *C*H_2CH_2N), 25.4 (br, *C*H_2CH_2N), 24.2, 22.3, 13.8 (CH_3); IR (neat, cm^{-1}) *ν* 2935, 2857, 1611, 1564, 1475, 1454, 1429, 1280, 1242, 1227, 1134,

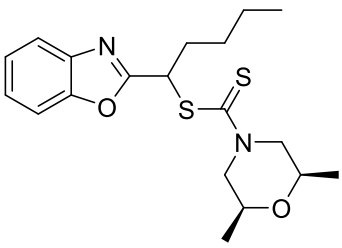
1113, 1004, 976, 763, 747; HRMS (MALDI-TOF) calcd for $C_{18}H_{24}N_2NaOS_2$ $[M+Na]^+$ 371.1222; found 371.1221.

1-(1,3-Benzoxazol-2-yl)pentyl pyrrolidine-4-carbodithioate (3d):



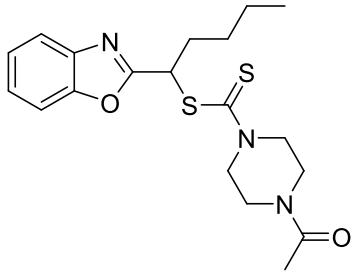
Prepared from iodotriazole **1a** (85.8 mg, 0.25 mmol) and pyrrolidine (41.7 μL, 0.50 mmol) according to the general procedure; eluent: hexanes–EtOAc = 10:1. Yield 42.8 mg (51%). Brownish solid; mp 66–68 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.72 [m, 1H, 4-CH(Ar)], 7.52 [m, 1H, 7-CH(Ar)], 7.34–7.30 [m, 2H, 5,6-CH(Ar)], 5.70 (dd, J = 7.9, 7.0 Hz, 1H, CHS), 3.97–3.90 (m, 2H, CH_2N), 3.71–3.64 (m, 2H, CH_2N), 2.29 (m, 1H, CH_2Pr), 2.20 (m, 1H, CH_2Pr), 2.11–2.03 (m, 2H, CH_2CH_2N), 2.01–1.93 (m, 2H, CH_2CH_2N), 1.50 (m, 1H, CH_2Et), 1.43 (m, 1H, CH_2Et), 1.39 (m, 2H, CH_2Me), 0.90 (t, J = 7.1 Hz, 3H, CH_3); ^{13}C NMR (151 MHz, $CDCl_3$) δ 189.9 (C=S), 165.9 [2-C(Ar)], 150.6 [7a-C(Ar)], 141.0 [3a-C(Ar)], 124.9 [6-CH(Ar)], 124.2 [5-CH(Ar)], 119.9 [4-CH(Ar)], 110.6 [7-CH(Ar)], 55.3 (CH_2N), 50.5 (CH_2N), 48.3 (CHS), 33.4 (CH_2Pr), 29.1 (CH_2Et), 26.0 (CH_2CH_2N), 24.1 (CH_2CH_2N), 22.2 (CH_2Me), 13.8 (CH_3); IR (neat, cm^{-1}) ν 2956, 2928, 2871, 1611, 1564, 1501, 1454, 1434, 1338, 1242, 1183, 1160, 1104, 1006, 957, 763, 747; HRMS (MALDI-TOF) calcd for $C_{17}H_{23}N_2OS_2$ $[M+H]^+$ 335.1246; found 335.1249.

1-(1,3-Benzoxazol-2-yl)pentyl (2*R*,6*S*)-2,6-dimethylmorpholine-4-carbodithioate (3e):



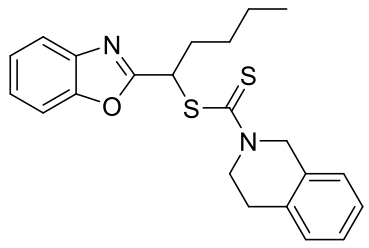
Prepared from iodotriazole **1a** (85.8 mg, 0.25 mmol) and *cis*-2,6-dimethylmorpholine (61.6 μL, 0.50 mmol) according to the general procedure; eluent: hexanes–EtOAc = 8:1. Yield 45.7 mg (48%). Yellow oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.72 [m, 1H, 4-CH(Ar)], 7.52 [m, 1H, 7-CH(Ar)], 7.35–7.30 [m, 2H, 5,6-CH(Ar)], 5.69 (dd, J = 8.0, 6.8 Hz, 1H, CHS), 5.42 (m, 1H), 4.45 (m, 1H), 3.74–3.57 (m, 2H, CHO), 2.89 (m, 1H), 2.76 (m, 1H), 2.28 (m, 1H, CH_2Pr), 2.21 (m, 1H, CH_2Pr), 1.54–1.35 (m, 4H, CH_2CH_2Me), 1.23 (d, J = 6.2 Hz, 3H, CHCH_3), 1.22 (br s, 3H, CHCH_3), 0.89 (t, J = 7.1 Hz, 3H, CH_2CH_3); ^{13}C NMR (151 MHz, $CDCl_3$) δ 194.2 (C=S), 165.8 [2-C(Ar)], 150.7 [7a-C(Ar)], 141.1 [3a-C(Ar)], 125.0 [5- or 6-CH(Ar)], 124.3 [5- or 6-CH(Ar)], 120.1 [4-CH(Ar)], 110.6 [7-CH(Ar)], 71.3 (br, 2C, CHO), 56.5 (br, CH_2N), 55.3 (br, CH_2N), 48.9 (CHS), 33.6, 29.3, 22.3, 18.5 (2C, CHCH_3), 13.8 (CH_2CH_3); IR (neat, cm^{-1}) ν 2957, 2930, 2859, 1611, 1564, 1455, 1422, 1376, 1323, 1231, 1172, 1138, 1097, 1082, 1001, 965, 948, 929, 839, 762, 747; HRMS (MALDI-TOF) calcd for $C_{19}H_{27}N_2O_2S_2$ $[M+H]^+$ 379.1508; found 379.1511.

1-(1,3-Benzoxazol-2-yl)pentyl 4-acetylpiperazine-1-carbodithioate (3f):



Prepared from iodotriazole **1a** (85.8 mg, 0.25 mmol) and *N*-acetylpiperazine (75.7 mg, 0.59 mmol) according to the general procedure; eluent: EtOAc. Yield 54 mg (55%). Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 [m, 1H, 4-CH(Ar)], 7.53 [m, 1H, 7-CH(Ar)], 7.37–7.29 [m, 2H, 5,6-CH(Ar)], 5.64 (dd, J = 8.2, 6.7 Hz, 1H, CHS), 4.32 (br s, 2H, CH_2NCS_2), 4.02 (br s, 2H, CH_2NCS_2), 3.77–3.71 (m, 2H, CH_2NAc), 3.63–3.57 (m, 2H, CH_2NAc), 2.35–2.15 (m, 2H, CH_2Pr), 2.13 (s, 3H, Ac), 1.56–1.33 (m, 4H, CH_2CH_2Me), 0.90 (t, J = 7.1 Hz, 3H, CH_2CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.9 (C=S), 169.2 (C=O), 165.5 [2-C(Ar)], 150.6 [7a-C(Ar)], 140.9 [3a-C(Ar)], 125.0 [5- or 6-CH(Ar)], 124.3 [5- or 6-CH(Ar)], 120.0 [4-CH(Ar)], 110.6 [7-CH(Ar)], 50.6 (br, CH_2NCS_2), 49.5 (br, CH_2NCS_2), 49.2 (CHS), 45.0 (CH_2NAc), 40.4 (CH_2NAc), 33.3, 29.2, 22.2, 21.2 [CH_3C(O)], 13.7 (CH_2CH_3); IR (neat, cm^{-1}) ν 2956, 2927, 2870, 2859, 1652 (C=O), 1612, 1564, 1455, 1419, 1360, 1282, 1241, 1223, 1161, 1104, 1032, 987, 963, 923, 837, 763, 749; HRMS (MALDI-TOF) calcd for $C_{19}H_{26}N_3O_2S_2$ $[M+H]^+$ 392.1461; found 392.1462.

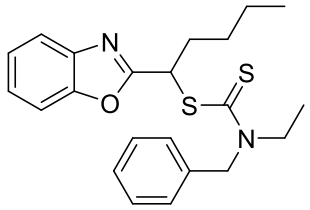
1-(1,3-Benzoxazol-2-yl)pentyl 3,4-dihydroisoquinoline-2(1*H*)-carbodithioate (3g):



Prepared from iodotriazole **1a** (85.8 mg, 0.25 mmol) and 1,2,3,4-tetrahydroisoquinoline (62.6 μL, 0.50 mmol) according to the general procedure; eluent: hexanes–EtOAc = 10:1. Yield 62.5 mg (63%). Yellowish oil; mixture of two rotamers (58:42) in $CDCl_3$; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 [m, 1H, 4-CH(benzoxazole)], 7.52 [m, 1H, 7-CH(benzoxazole)], 7.35–7.28 [m, 2H, 5,6-CH(benzoxazole)], 7.25–7.08 (m, 4H), 5.76 (dd, J = 8.1, 6.9 Hz, 1H, CHS), 5.36 [d, J = 17.2 Hz, 1H, 1-CH_2(isoquinoline), major], 5.27 [d, J = 17.2 Hz, 1H, 1-CH_2(isoquinoline), major], 5.01 [br s, 2H, 1-CH_2(isoquinoline), minor], 4.50–4.36 [m, 2H, 3-CH_2(isoquinoline), minor], 4.12–4.03 [m, 2H, 3-CH_2(isoquinoline), major], 2.98 [br t, J = 6.0 Hz, 2H, 4-CH_2(isoquinoline)], 2.36–2.17 (m, 2H, CH_2Pr), 1.58–1.34 (m, 4H, CH_2CH_2Me), 0.90 (t, J = 7.1 Hz, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.7 [2×C, C=S], 165.8 [2×2-C(benzoxazole)], 150.7 [2×7a-C(benzoxazole)], 141.1 [2×3a-C(benzoxazole)], 135.0 (quat.), 134.2 (quat.), 132.6 (quat.), 131.3 (quat.), 128.2, 127.6, 127.4, 127.2, 126.9, 126.7, 126.6, 126.2, 125.0 [2×C, 5- or 6-CH(benzoxazole)], 124.3 [2×C, 5- or 6-CH(benzoxazole)], 120.0 [2×C, 4-CH(benzoxazole)], 110.7 [2×C, 7-CH(benzoxazole)], 54.2, 51.3, 50.3, 48.9, 48.7, 48.0, 33.5 (2×C), 29.3 (2×C), 29.0 (CH_2CH_2N), 28.5 (CH_2CH_2N), 22.3 (2×C), 13.8 (2×CH_3); IR (neat, cm^{-1}) ν 2955, 2925, 2869, 2857, 1610, 1562, 1453, 1421, 1402, 1341, 1278, 1241, 1220,

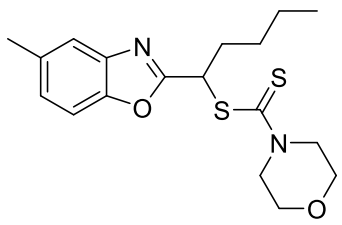
1186, 1153, 1109, 1002, 955, 926, 837, 762, 746; HRMS (MALDI-TOF) calcd for $C_{22}H_{25}N_2OS_2$ $[M+H]^+$ 397.1403; found 397.1404.

1-(1,3-Benzoxazol-2-yl)pentyl benzyl(ethyl)dithiocarbamate (3h):



Prepared from iodotriazole **1a** (85.8 mg, 0.25 mmol) and benzyl(ethyl)amine (74.4 μL, 0.50 mmol) according to the general procedure; eluent: hexanes–EtOAc = 10:1. Yield 62.6 mg (63%). Yellow oil; mixture of two rotamers (58:42) in $CDCl_3$; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76–7.69 [m, 1H, 4-CH(Ar)], 7.56–7.49 [m, 1H, 7-CH(Ar)], 7.36–7.18 [m, 7H, 2H 5,6-CH(Ar) + 5H CH(Ph)], 5.73–5.67 (m, 1H, CHS), 5.38 (d, J = 14.9 Hz, 1H, CH_2Ph, major), 5.29 (d, J = 14.9 Hz, 1H, CH_2Ph, major), 5.03 (d, J = 16.4 Hz, 1H, CH_2Ph, minor), 4.89 (d, J = 16.4 Hz, 1H, CH_2Ph, minor), 4.10 (m, 1H, NCH_2CH$_3$, minor), 3.94 (m, 1H, NCH_2CH$_3$, minor), 3.83–3.63 (m, 2H, NCH_2CH$_3$, major), 2.38–2.13 (m, 2H, CH_2Pr), 1.57–1.33 (m, 4H, CH_2CH_2Me), 1.28–1.20 (m, 3H, NCH$_2$CH_3), 0.94–0.85 (m, 3H, CH$_2$CH$_2$CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.0 (C=S), 194.1 (C=S), 165.5 [2×2-C(Ar)], 150.3 [2×7a-C(Ar)], 140.8 [2×3a-C(Ar)], 135.2 [1-C(Ph), major], 134.2 [1-C(Ph), minor], 128.5 [2C, CH(Ph), minor], 128.3 [2C, CH(Ph), major], 127.6 [4-CH(Ph), minor], 127.4 [2×2C, CH(Ph)], 126.6 [4-CH(Ph), major], 124.6 [2×C, 5- or 6-CH(Ar)], 123.9 [2×C, 5- or 6-CH(Ar)], 119.7 [2×C, 4-CH(Ar)], 110.3 [2×C, 7-CH(Ar)], 56.7 (*C*H$_2$Ph, major), 54.6 (*C*H$_2$Ph, minor), 49.6 (N*C*H$_2$Me, minor), 49.3 (2×CHS), 46.0 (N*C*H$_2$Me, major), 33.4 (major), 33.2 (minor), 29.0 (2×C), 21.9 (2×C), 13.5 (2×C, CH$_2$CH$_2$*C*H$_3$), 11.9 (NCH$_2$*C*H$_3$, major), 10.8 (NCH$_2$*C*H$_3$, minor); IR (neat, cm^{-1}) ν 2957, 2928, 2870, 2858, 1610, 1561, 1496, 1479, 1466, 1453, 1438, 1414, 1378, 1353, 1290, 1241, 1192, 1171, 1114, 1103, 1077, 1002, 951, 837, 762, 746, 697; HRMS (MALDI-TOF) calcd for $C_{22}H_{27}N_2OS_2$ $[M+H]^+$ 399.1559; found 399.1540.

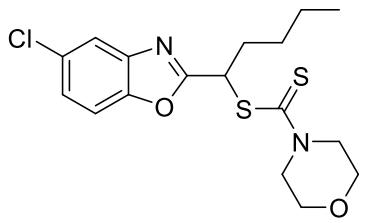
1-(5-Methyl-1,3-benzoxazol-2-yl)pentyl morpholine-4-carbodithioate (3l):



Prepared from iodotriazole **1b** (89.3 mg, 0.25 mmol) and morpholine (45.0 μL, 0.50 mmol) according to the general procedure; eluent: hexanes–EtOAc = 4:1. Yield 59.1 mg (65%). Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 [br s, 1H, 4-CH(Ar)], 7.39 [d, J = 8.3 Hz, 1H, 7-CH(Ar)], 7.13 [br d, J = 8.3 Hz, 1H, 6-CH(Ar)], 5.64 (dd, J = 8.2, 6.7 Hz, 1H, CHS), 4.31 (br s, 2H, CH$_2$N), 3.95 (br s, 2H, CH$_2$N), 3.79–3.71 (m, 4H, CH$_2$O), 2.45 [s, 3H, CH_3C(Ar)], 2.34–2.12 (m, 2H, CH_2Pr), 1.53–1.33 (m, 4H, CH_2CH_2Me), 0.89 (t, J = 6.9 Hz, 3H, CH$_2$CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.7 (C=S), 165.6 [2-C(Ar)], 148.8 [7a-C(Ar)], 141.2 [3a-C(Ar)], 134.1 [5-C(Ar)], 126.1 [6-CH(Ar)], 119.9 [4-CH(Ar)], 110.0 [7-CH(Ar)], 66.1 (br, 2C, CH$_2$O), 51.6 (br, CH$_2$N), 50.5 (br,

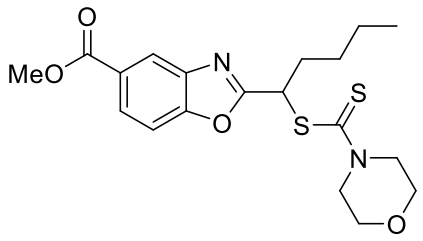
CH_2N), 49.0 (CHS), 33.5, 29.2, 22.2, 21.4 [*C*H_3C(Ar)], 13.8 (CH_2*C*H_3); IR (neat, cm^{-1}) *v* 2957, 2925, 2857, 1564, 1460, 1420, 1267, 1228, 1214, 1179, 1113, 1029, 995, 868, 842, 800; HRMS (ESI-TOF) calcd for $C_{18}H_{25}N_2O_2S_2$ $[M+H]^+$ 365.1352; found 365.1355.

1-(5-Chloro-1,3-benzoxazol-2-yl)pentyl morpholine-4-carbodithioate (3m):



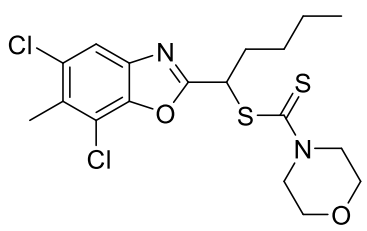
Prepared from iodotriazole **1c** (94.2 mg, 0.25 mmol) and morpholine (45.0 μL, 0.50 mmol) according to the general procedure; eluent: hexanes–EtOAc = 6:1. Yield 61.0 mg (63%). Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 [d, *J* = 1.9 Hz, 1H, 4-CH(Ar)], 7.45 [d, *J* = 8.7 Hz, 1H, 7-CH(Ar)], 7.30 [dd, *J* = 8.7, 1.9 Hz, 1H, 6-CH(Ar)], 5.64 (dd, *J* = 8.1, 6.8 Hz, 1H, CHS), 4.31 (br s, 2H, CH_2N), 3.96 (br s, 2H, CH_2N), 3.81–3.71 (m, 4H, CH_2O), 2.32–2.12 (m, 2H, C*H*$_2$Pr), 1.54–1.33 (m, 4H, C*H*$_2$C*H*$_2$Me), 0.90 (t, *J* = 7.1 Hz, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.4 (C=S), 167.3 [2-C(Ar)], 149.2 [7a-C(Ar)], 142.2 [3a-C(Ar)], 129.8 [5-C(Ar)], 125.3 [6-CH(Ar)], 120.0 [4-CH(Ar)], 111.4 [7-CH(Ar)], 66.1 (br, 2C, CH_2O), 51.6 (br, CH_2N), 50.6 (br, CH_2N), 48.9 (CHS), 33.2, 29.2, 22.2, 13.8 (CH_3); IR (neat, cm^{-1}) *v* 2958, 2925, 2857, 1560, 1451, 1420, 1268, 1257, 1229, 1214, 1189, 1113, 1054, 1029, 995, 919, 865, 842, 804, 703; HRMS (MALDI-TOF) calcd for $C_{17}H_{22}ClN_2O_2S_2$ $[M+H]^+$ 385.0806; found 385.0792.

Methyl 2-{1-[(morpholin-4-ylcarbonothioyl)thio]pentyl}-1,3-benzoxazole-5-carboxylate (3n):



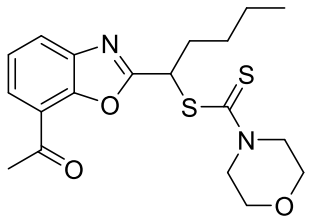
Prepared from iodotriazole **1d** (100.3 mg, 0.25 mmol) and morpholine (45.0 μL, 0.50 mmol) according to the general procedure; eluent: PhH–MeCN = 20:1. Yield 59.5 mg (58%). Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 [br d, *J* = 1.5 Hz, 1H, 4-CH(Ar)], 8.09 [dd, *J* = 8.6, 1.5 Hz, 1H, 6-CH(Ar)], 7.56 [d, *J* = 8.6 Hz, 1H, 7-CH(Ar)], 5.68 (dd, *J* = 8.1, 6.9 Hz, 1H, CHS), 4.32 (br s, 2H, CH_2N), 3.96 (br s, 2H, CH_2N), 3.95 (s, 3H, CH_3O), 3.81–3.73 (m, 4H, CH_2O), 2.35–2.14 (m, 2H, C*H*$_2$Pr), 1.57–1.34 (m, 4H, C*H*$_2$C*H*$_2$Me), 0.90 (t, *J* = 7.1 Hz, 3H, CH_2C*H*$_3$); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.4 (C=S), 167.2 (quat.), 166.5 (quat.), 153.5 [7a-C(Ar)], 141.1 [3a-C(Ar)], 127.0 [6-CH(Ar)], 126.8 [5-C(Ar)], 122.0 [4-CH(Ar)], 110.4 [7-CH(Ar)], 66.1 (br, 2C, CH_2O), 52.3 (CH_3O), 51.5 (br, CH_2N), 50.5 (br, CH_2N), 48.9 (CHS), 33.2, 29.2, 22.2, 13.8 (CH_2*C*H_3); IR (neat, cm^{-1}) *v* 2956, 2926, 2857, 1722 (C=O), 1620, 1566, 1464, 1435, 1422, 1296, 1285, 1267, 1229, 1215, 1113, 1082, 1030, 994, 908, 866, 843, 814, 768, 751; HRMS (MALDI-TOF) calcd for $C_{19}H_{25}N_2O_4S_2$ $[M+H]^+$ 409.1250; found 409.1261.

1-(5,7-Dichloro-6-methyl-1,3-benzoxazol-2-yl)pentyl morpholine-4-carbodithioate (3o):



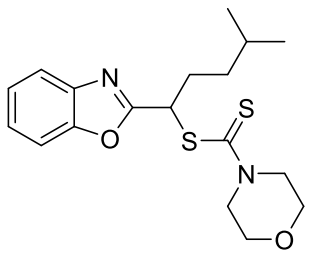
Prepared from iodotriazole **1e** (106.5 mg, 0.25 mmol) and morpholine (45.0 μL, 0.50 mmol) according to the general procedure; eluent: hexanes–EtOAc = 7:1. Yield 43.9 mg (41%). Beige solid; mp 105–108 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 [s, 1H, 4-CH(Ar)], 5.62 (dd, J = 8.0, 6.9 Hz, 1H, CHS), 4.31 (br s, 2H, CH_2N), 3.96 (br s, 2H, CH_2N), 3.83–3.71 (m, 4H, CH_2O), 2.55 [s, 3H, CH_3C(Ar)], 2.31–2.13 (m, 2H, CH_2Pr), 1.54–1.33 (m, 4H, CH_2CH_2Me), 0.90 (t, J = 7.0 Hz, 3H, CH_2CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.3 (C=S), 166.9 [2-C(Ar)], 146.8 [7a-C(Ar)], 139.7 [3a-C(Ar)], 131.4 (quat.), 130.9 (quat.), 118.6 [4-CH(Ar)], 116.5 (quat.), 66.1 (br, 2C, CH_2O), 51.5 (br, CH_2N), 50.5 (br, CH_2N), 48.9 (CHS), 33.3, 29.2, 22.2, 17.1 [CH_3C(Ar)], 13.8 (CH_2CH_3); IR (neat, cm^{-1}) ν 2958, 2925, 2858, 1561, 1463, 1421, 1384, 1300, 1268, 1229, 1214, 1188, 1114, 1030, 996, 951, 920, 863, 814, 774, 737; HRMS (MALDI-TOF) calcd for $C_{18}H_{23}Cl_2N_2O_2S_2$ $[M+H]^+$ 433.0573; found 433.0566.

1-(7-Acetyl-1,3-benzoxazol-2-yl)pentyl morpholine-4-carbodithioate (3q):



Prepared from iodotriazole **1g** (96.3 mg, 0.25 mmol) and morpholine (45.0 μL, 0.50 mmol) according to the general procedure; eluent: hexanes–EtOAc = 3:1. Yield 47.8 mg (49%). Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 [dd, J = 7.8, 1.2 Hz, 1H, 4- or 6-CH(Ar)], 7.92 [dd, J = 7.8, 1.2 Hz, 1H, 4- or 6-CH(Ar)], 7.42 [t, J = 7.8 Hz, 1H, 5-CH(Ar)], 5.73 (dd, J = 8.0, 7.0 Hz, 1H, CHS), 4.32 (br s, 2H, CH_2N), 3.96 (br s, 2H, CH_2N), 3.81–3.73 (m, 4H, CH_2O), 2.84 (s, 3H, Ac), 2.38–2.18 (m, 2H, CH_2Pr), 1.61–1.35 (m, 4H, CH_2CH_2Me), 0.92 (t, J = 7.1 Hz, 3H, CH_2CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.7 (quat.), 194.3 (quat.), 166.5 [2-C(Ar)], 149.3 [7a-C(Ar)], 142.2 [3a-C(Ar)], 125.5, 125.1, 124.4, 121.8 [7-C(Ar)], 66.0 (br, 2C, CH_2O), 51.5 (br, CH_2N), 50.5 (br, CH_2N), 48.8 (CHS), 33.1, 30.5 [CH_3C(O)], 29.2, 22.2, 13.8 (CH_2CH_3); IR (neat, cm^{-1}) ν 2957, 2925, 2856, 1687 (C=O), 1647, 1616, 1566, 1458, 1419, 1361, 1268, 1229, 1215, 1189, 1114, 1056, 1029, 994, 957, 863, 801, 748; HRMS (ESI-TOF) calcd for $C_{19}H_{25}N_2O_3S_2$ $[M+H]^+$ 393.1301; found 393.1306.

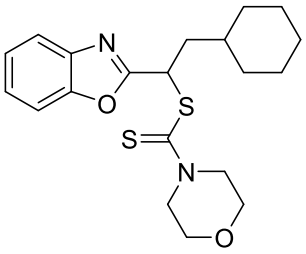
1-(1,3-Benzoxazol-2-yl)-4-methylpentyl morpholine-4-carbodithioate (3r):



Prepared from iodotriazole **1h** (89.3 mg, 0.25 mmol) and morpholine (45.0 μL, 0.50 mmol) according to the general procedure; eluent: hexanes–EtOAc = 3:1. Yield 49 mg (54%). White solid; mp 84–86 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 [m, 1H, 4-CH(Ar)], 7.53 [m, 1H, 7-CH(Ar)], 7.36–7.29 [m, 2H, 5,6-CH(Ar)], 5.65 (dd, J = 8.1, 6.8 Hz,

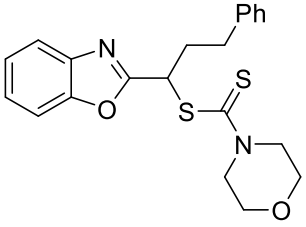
1H, CHS), 4.31 (br s, 2H, CH_2N), 3.96 (br s, 2H, CH_2N), 3.82–3.71 (m, 4H, CH_2O), 2.36–2.14 (m, 2H, CH_2*i*-Bu), 1.62 (nonet, *J* = 6.6 Hz, 1H, C*H*Me$_2$), 1.42 (m, 1H, CH_2*i*-Pr), 1.30 (m, 1H, CH_2*i*-Pr), 0.89 (d, *J* = 6.6 Hz, 3H, $2CH_3$); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.7 (C=S), 165.7 [2-C(Ar)], 150.6 [7a-C(Ar)], 141.0 [3a-C(Ar)], 125.0 [5- or 6-CH(Ar)], 124.3 [5- or 6-CH(Ar)], 120.1 [4-CH(Ar)], 110.6 [7-CH(Ar)], 66.1 (br, 2C, CH_2O), 51.5 (br, CH_2N), 50.5 (br, CH_2N), 49.2 (CHS), 36.1, 31.7, 27.8, 22.4 ($2CH_3$); IR (neat, cm^{-1}) *ν* 2957, 2924, 2854, 1610, 1560, 1454, 1419, 1267, 1227, 1214, 1112, 1029, 994, 763, 749; HRMS (MALDI-TOF) calcd for $C_{18}H_{25}N_2O_2S_2$ $[M+H]^+$ 365.1352; found 365.1339.

1-(1,3-Benzoxazol-2-yl)-2-cyclohexylethyl morpholine-4-carbodithioate (3s):



Prepared from iodotriazole **1i** (95.8 mg, 0.25 mmol) and morpholine (45.0 μL, 0.50 mmol) according to the general procedure; eluent: hexanes–EtOAc = 4:1. Yield 54.7 mg (56%). White solid; mp 86–88 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 [m, 1H, 4-CH(Ar)], 7.53 [m, 1H, 7-CH(Ar)], 7.37–7.29 [m, 2H, 5,6-CH(Ar)], 5.77 (dd, *J* = 8.9, 7.2 Hz, 1H, CHS), 4.31 (br s, 2H, CH_2N), 3.95 (br s, 2H, CH_2N), 3.82–3.68 (m, 4H, CH_2O), 2.21 (ddd, *J* = 13.8, 8.9, 6.4 Hz, 1H, CH_2Cy), 2.04 (dt, *J* = 13.8, 7.2 Hz, 1H, CH_2Cy), 1.92 (m, 1H), 1.81–1.57 (m, 4H), 1.39 (m, 1H), 1.29–1.11 (m, 3H), 1.09–0.92 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.6 (C=S), 166.0 [2-C(Ar)], 150.6 [7a-C(Ar)], 141.1 [3a-C(Ar)], 125.0 [5- or 6-CH(Ar)], 124.3 [5- or 6-CH(Ar)], 120.1 [4-CH(Ar)], 110.7 [7-CH(Ar)], 66.0 (br, 2C, CH_2O), 51.5 (br, CH_2N), 50.4 (br, CH_2N), 46.9 (CHS), 41.1, 35.4, 33.2, 32.6, 26.3, 25.9 (2C); IR (neat, cm^{-1}) *ν* 2922, 2851, 1610, 1563, 1454, 1420, 1267, 1229, 1215, 1115, 1030, 996, 762, 747; HRMS (MALDI-TOF) calcd for $C_{20}H_{27}N_2O_2S_2$ $[M+H]^+$ 391.1508; found 391.1497.

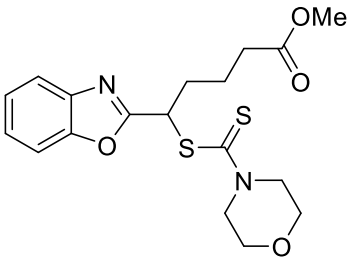
1-(1,3-Benzoxazol-2-yl)-3-phenylpropyl morpholine-4-carbodithioate (3t):



Prepared from iodotriazole **1j** (97.8 mg, 0.25 mmol) and morpholine (45.0 μL, 0.50 mmol) according to the general procedure; eluent: PhH–MeCN = 20:1. Yield 65.7 mg (66%). Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 [m, 1H, 4-CH(Ar)], 7.52 [m, 1H, 7-CH(Ar)], 7.37–7.29 [m, 2H, 5,6-CH(Ar)], 7.25 [m, 2H, 3,5-CH(Ph)], 7.19 [m, 2H, 2,6-CH(Ph)], 7.16 [m, 1H, 4-CH(Ph)], 5.75 (dd, *J* = 8.1, 6.7 Hz, 1H, CHS), 4.31 (br s, 2H, CH_2N), 3.94 (br s, 2H, CH_2N), 3.82–3.68 (m, 4H, CH_2O), 2.91–2.73 (m, 2H), 2.68–2.46 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.2 (C=S), 165.1 [2-C(Ar)], 150.6 [7a-C(Ar)], 141.0 (quat.), 140.4 (quat.), 128.4 [2C, CH(Ph)], 128.3 [2C, CH(Ph)], 126.1, 125.1, 124.4, 120.1 [4-CH(Ar)], 110.6 [7-CH(Ar)], 66.1 (br, 2C, CH_2O), 51.5 (br, CH_2N), 50.4 (br, CH_2N), 48.7 (CHS), 35.4, 33.4; IR (neat, cm^{-1}) *ν* 2964, 2923, 2856, 1610, 1563, 1496, 1455, 1421, 1300, 1268, 1231, 1215, 1115,

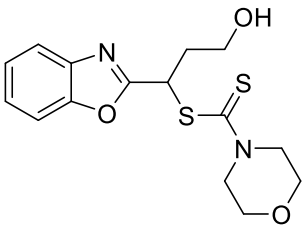
1030, 995, 933, 909, 865, 835, 749, 701; HRMS (MALDI-TOF) calcd for $C_{21}H_{23}N_2O_2S_2$ $[M+H]^+$ 399.1195; found 399.1189.

Methyl 5-(1,3-benzoxazol-2-yl)-5-[(morpholin-4-ylcarbonothioyl)thio]pentanoate (3u):



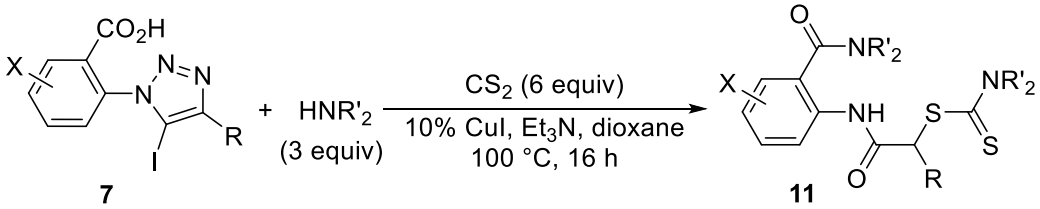
Prepared from iodotriazole **1k** (96.8 mg, 0.25 mmol) and morpholine (45.0 μL, 0.50 mmol) according to the general procedure; eluent: hexanes–EtOAc = 3:1. Yield 52.7 mg (53%). Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 [m, 1H, 4-CH(Ar)], 7.52 [m, 1H, 7-CH(Ar)], 7.37–7.30 [m, 2H, 5,6-CH(Ar)], 5.74 (dd, J = 8.0, 6.8 Hz, 1H, CHS), 4.33 (br s, 2H, CH_2N), 3.95 (br s, 2H, CH_2N), 3.82–3.71 (m, 4H, CH_2O), 3.65 (s, 3H, CH_3O), 2.42 [t, J = 7.5 Hz, 2H, $CH_2C(O)$], 2.39–2.20 (m, 2H, CH_2CHS), 1.94–1.75 [m, 2H, CH_2CH$_2$C(O)]; ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.3 (C=S), 173.3 (C=O), 165.0 [2-C(Ar)], 150.7 [7a-C(Ar)], 140.9 [3a-C(Ar)], 125.2 [5- or 6-CH(Ar)], 124.4 [5- or 6-CH(Ar)], 120.0 [4-CH(Ar)], 110.7 [7-CH(Ar)], 66.2 (br, 2C, CH_2O), 51.8 (br, CH_2N), 51.5 (CH_3O), 50.6 (br, CH_2N), 48.5 (CHS), 33.3, 33.0, 22.3; IR (neat, cm^{-1}) ν 2950, 2923, 2854, 1735 (C=O), 1610, 1563, 1455, 1422, 1268, 1231, 1215, 1195, 1174, 1145, 1114, 1029, 995, 763, 750; HRMS (MALDI-TOF) calcd for $C_{18}H_{23}N_2O_4S_2$ $[M+H]^+$ 395.1094; found 395.1100.

1-(1,3-Benzoxazol-2-yl)-3-hydroxypropyl morpholine-4-carbodithioate (3v):



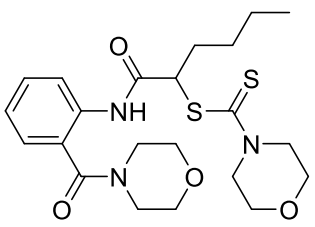
Prepared from iodotriazole **1l** (66.2 mg, 0.20 mmol) and morpholine (36.0 μL, 0.50 mmol) according to the general procedure; eluent: hexanes–EtOAc = 1:1. Yield 55.0 mg (81%). Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 [m, 1H, 4-CH(Ar)], 7.52 [m, 1H, 7-CH(Ar)], 7.38–7.30 [m, 2H, 5,6-CH(Ar)], 6.00 (dd, J = 7.8, 6.7 Hz, 1H, CHS), 4.35 (br s, 2H, CH_2N), 3.96 (br s, 2H, CH_2N), 3.92–3.68 (m, 6H, 3×CH_2O), 3.08 (br s, 1H, OH), 2.60 (m, 1H, CH_2CHS), 2.42 (m, 1H, CH_2CHS); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.6 (C=S), 165.2 [2-C(Ar)], 150.6 [7a-C(Ar)], 140.7 [3a-C(Ar)], 125.3 [5- or 6-CH(Ar)], 124.5 [5- or 6-CH(Ar)], 119.9 [4-CH(Ar)], 110.7 [7-CH(Ar)], 66.3 (br, OCH$_2$CH$_2$N), 65.9 (br, OCH$_2$CH$_2$N), 59.2 (CH_2OH), 52.1 (br, CH_2N), 50.6 (br, CH_2N), 46.6 (CHS), 36.2 (CH$_2$CHS); IR (neat, cm^{-1}) ν 3401 (O–H), 2958, 2922, 2854, 1610, 1561, 1455, 1421, 1267, 1229, 1215, 1112, 1063, 1028, 993, 867, 763, 748; HRMS (MALDI-TOF) calcd for $C_{15}H_{19}N_2O_3S_2$ $[M+H]^+$ 339.0832; found 339.0829.

Synthesis of thiolated anthranilamides 11



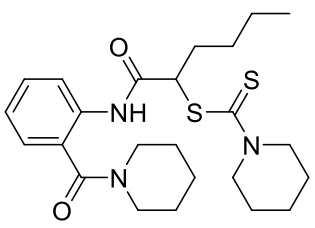
General procedure. In a vial with a screw cap iodotriazole **7** (0.25 mmol), secondary amine (0.75 mmol, 3 equiv), CuI (4.8 mg, 0.025 mmol, 10 mol %), CS_2 (90.5 μL, 1.50 mmol, 6 equiv), and Et_3N (70 μL, 0.50 mmol, 2 equiv) were mixed under an Ar atmosphere in dioxane (2.5 mL). The reaction mixture was stirred at 100 °C for 16 h, then diluted with CH_2Cl_2 (20 mL), and washed with water (20 mL). The organic layer was dried with anhydrous Na_2SO_4, and the solvents were evaporated *in vacuo*. The residue was purified by column chromatography.

1-({[2-(Morpholin-4-ylcarbonyl)phenyl]amino}carbonyl)pentyl morpholine-4-carbodithioate (11a):



Prepared from iodotriazole **7a** (92.8 mg, 0.25 mmol) and morpholine (67.5 μL, 0.75 mmol) according to the general procedure; eluent: hexanes–EtOAc = 1:1. Yield 90.1 mg (77%). Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.27 (br s, 1H, NH), 8.19 [br d, J = 8.1 Hz, 1H, 6-CH(Ar)], 7.39 [m, 1H, 5-CH(Ar)], 7.18 [br d, J = 7.3 Hz, 1H, 3-CH(Ar)], 7.11 [m, 1H, 4-CH(Ar)], 4.77 (t, J = 7.2 Hz, 1H, CHS), 4.30 (br s, 2H), 3.97 (br s, 2H), 3.88–3.33 (m, 12H), 2.17 (m, 1H, CH_2Pr), 1.93 (m, 1H, CH_2Pr), 1.57–1.32 (m, 4H, CH_2CH_2Me), 0.92 (t, J = 7.1 Hz, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.6 (C=S), 169.7 (C=O), 168.5 (C=O), 135.8 [1-C(Ar)], 130.5, 127.0, 125.2 [2-C(Ar)], 123.7, 122.9, 66.7 (br, 2C, CH_2O), 66.3 (br, CH_2O), 66.0 (br, CH_2O), 55.1 (CHS), 51.6 (br, CH_2N), 50.6 (br, CH_2N), 48.3 (br, CH_2N), 42.3 (br, CH_2N), 30.4, 29.4, 22.4, 13.8 (CH_3); IR (neat, cm^{-1}) ν 3304 (N–H), 2958, 2925, 2856, 1691 (C=O), 1629, 1599, 1585, 1518, 1460, 1444, 1424, 1300, 1268, 1230, 1114, 1020, 996, 760; HRMS (MALDI-TOF) calcd for $C_{22}H_{31}N_3NaO_4S_2$ $[M+Na]^+$ 488.1648; found 488.1650.

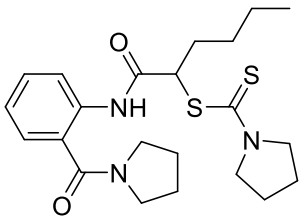
1-({[2-(Piperidin-4-ylcarbonyl)phenyl]amino}carbonyl)pentyl piperidine-4-carbodithioate (11b):



Prepared from iodotriazole **7a** (92.8 mg, 0.25 mmol) and piperidine (74.1 μL, 0.75 mmol) according to the general procedure; eluent: hexanes–EtOAc = 3:1. Yield 87.3 mg (76%). Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.22 (br s, 1H, NH), 8.22 [br d, J = 8.1 Hz, 1H, 6-CH(Ar)], 7.35 [m, 1H, 5-CH(Ar)], 7.18 [br d, J = 7.2 Hz, 1H, 3-

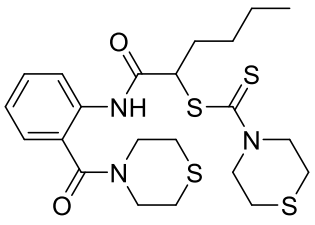
CH(Ar)], 7.08 [m, 1H, 4-CH(Ar)], 4.80 (t, *J* = 7.2 Hz, 1H, CHS), 4.34 (m, 1H), 4.16 (m, 1H), 3.95 (m, 1H), 3.86 (m, 1H), 3.72 (br s, 2H), 3.31 (br s, 2H), 2.15 (m, 1H, C*H*$_2$Pr), 1.92 (m, 1H, C*H*$_2$Pr), 1.77–1.61 (m, 10H), 1.56–1.32 (m, 6H), 0.91 (t, *J* = 7.1 Hz, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.3 (C=S), 169.8 (C=O), 168.0 (C=O), 135.2 [1-C(Ar)], 129.7, 126.6, 126.4 [2-C(Ar)], 123.4, 122.4, 55.1 (CHS), 53.1 (br, CH_2N), 51.4 (br, CH_2N), 48.5 (br, CH_2N), 42.8 (br, CH_2N), 30.4, 29.2, 26.3 (br), 25.7 (br), 25.3 (br), 25.2 (br), 24.3, 23.9, 22.2, 13.6 (CH_3); IR (neat, cm^{-1}) *v* 3299 (N–H), 2935, 2856, 1692 (C=O), 1627, 1597, 1585, 1519, 1477, 1430, 1351, 1272, 1259, 1242, 1228, 1163, 1129, 1113, 1002, 977, 890, 853, 759; HRMS (MALDI-TOF) calcd for $C_{24}H_{35}KN_3O_2S_2$ $[M+K]^+$ 500.1802; found 500.1811.

1-({[2-(Pyrrolidin-4-ylcarbonyl)phenyl]amino}carbonyl)pentyl pyrrolidine-4-carbodithioate (11c):



Prepared from iodotriazole **7a** (92.8 mg, 0.25 mmol) and pyrrolidine (62.6 μL, 0.75 mmol) according to the general procedure; eluent: hexanes–EtOAc = 1:1. Yield 93.6 mg (86%). Brown oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.61 (br s, 1H, NH), 8.24 [br d, *J* = 8.2 Hz, 1H, 6-CH(Ar)], 7.36 [m, 1H, 5-CH(Ar)], 7.28 [br d, *J* = 7.3 Hz, 1H, 3-CH(Ar)], 7.09 [m, 1H, 4-CH(Ar)], 4.75 (t, *J* = 7.1 Hz, 1H, CHS), 3.97–3.58 (m, 6H, 4H CH_2NCS + 2H CH_2NCO), 3.40–3.31 (m, 2H, CH_2NCO), 2.18–2.04 (m, 3H), 2.02–1.83 (m, 7H), 1.55–1.32 (m, 4H, C*H*$_2$C*H*$_2$Me), 0.91 (t, *J* = 7.1 Hz, 3H, CH_3); ^{13}C NMR (151 MHz, $CDCl_3$) δ 190.4 (br, C=S), 169.7 [C(O)NH], 167.8 [*C*(O)C(Ar)], 135.1 [1-C(Ar)], 129.9 [5-CH(Ar)], 126.8 [2-C(Ar)], 126.6 [3-CH(Ar)], 123.2 [4-CH(Ar)], 122.0 [6-CH(Ar)], 54.9 (br, *C*H_2NCS), 54.5 (CHS), 50.5 (br, *C*H_2NCS), 49.2 (*C*H_2NCO), 45.7 (*C*H_2NCO), 30.2 (*C*H_2Pr), 29.1 (*C*H_2Et), 25.9, 25.8, 24.2, 23.9, 22.1 (*C*H_2Me), 13.6 (CH_3); IR (neat, cm^{-1}) *v* 3282 (N–H), 2955, 2928, 2872, 1690 (C=O), 1624, 1595, 1519, 1462, 1435, 1338, 1295, 1251, 1182, 1160, 1006, 956, 759, 733; HRMS (ESI-TOF) calcd for $C_{22}H_{32}N_3O_2S_2$ $[M+H]^+$ 434.1930; found 434.1934.

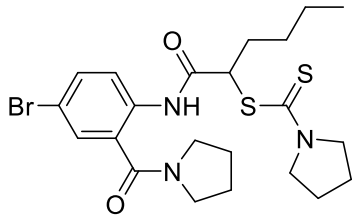
1-({[2-(Thiomorpholin-4-ylcarbonyl)phenyl]amino}carbonyl)pentyl thiomorpholine-4-carbodithioate (11d):



Prepared from iodotriazole **7a** (92.8 mg, 0.25 mmol) and thiomorpholine (75.5 μL, 0.75 mmol) according to the general procedure; eluent: hexanes–EtOAc = 2:1. Yield 96.2 mg (77%). Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.16 (br s, 1H, NH), 8.19 [br d, *J* = 8.2 Hz, 1H, 6-CH(Ar)], 7.39 [m, 1H, 5-CH(Ar)], 7.16 [br d, *J* = 7.5 Hz, 1H, 3-CH(Ar)], 7.11 [m, 1H, 4-CH(Ar)], 4.76 (t, *J* = 7.4 Hz, 1H, CHS), 4.74 (br s, 1H), 4.52–4.30 (m, 2H), 4.19 (br s, 1H), 4.11–3.87 (m, 2H), 3.65 (br s, 2H), 2.88–2.45 (m, 8H,

4×CH_2S), 2.16 (m, 1H, C*H*$_2$Pr), 1.94 (m, 1H, C*H*$_2$Pr), 1.56–1.33 (m, 4H, C*H*$_2$C*H*$_2$Me), 0.92 (t, *J* = 7.1 Hz, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.7 (C=S), 169.6 (C=O), 168.8 (C=O), 135.5 [1-C(Ar)], 130.3, 126.7, 125.7 [2-C(Ar)], 123.8, 123.0, 55.2 (CHS), 54.8 (br, CH_2N), 53.4 (br, CH_2N), 50.1 (br, CH_2N), 44.4 (br, CH_2N), 30.4, 29.3, 27.9 (br, CH_2S), 27.2 (3C, br, CH_2S), 22.3, 13.7 (CH_3); IR (neat, cm^{-1}) *v* 3305 (N–H), 2954, 2921, 2858, 1690 (C=O), 1628, 1598, 1584, 1517, 1467, 1443, 1418, 1356, 1283, 1259, 1247, 1215, 1191, 1162, 1142, 1027, 1005, 951, 936, 758, 733; HRMS (MALDI-TOF) calcd for $C_{22}H_{31}N_3NaO_2S_4$ $[M+Na]^+$ 520.1191; found 520.1184.

1-({[4-Bromo-2-(pyrrolidin-1-ylcarbonyl)phenyl]amino}carbonyl)pentyl pyrrolidine-1-carbodithioate (11e):

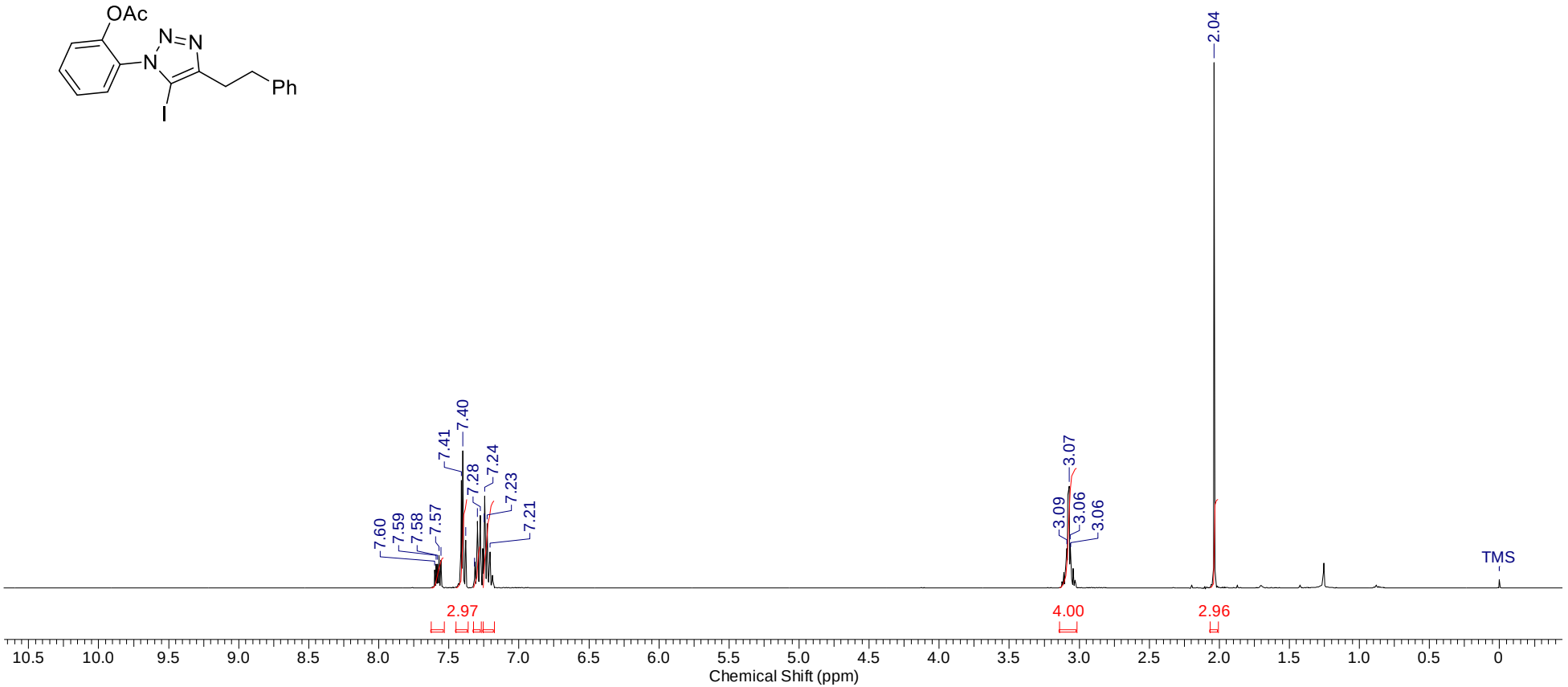


Prepared from iodotriazole **7b** (112.5 mg, 0.25 mmol) and pyrrolidine (62.6 μL, 0.75 mmol) according to the general procedure; eluent: hexanes–EtOAc = 2:1. Yield 100.8 mg (79%). Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.53 (br s, 1H, NH), 8.18 [d, *J* = 8.8 Hz, 1H, 6-CH(Ar)], 7.46 [dd, *J* = 8.8, 2.1 Hz, 1H, 5-CH(Ar)], 7.41 [d, *J* = 2.1 Hz, 1H, 3-CH(Ar)], 4.74 (t, *J* = 7.4 Hz, 1H, CHS), 3.95–3.82 (m, 2H), 3.78–3.57 (m, 4H), 3.41–3.3 (m, 2H), 2.19–1.84 (m, 10H), 1.55–1.31 (m, 4H, C*H*$_2$C*H*$_2$Me), 0.90 (t, *J* = 7.1 Hz, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.7 (C=S), 170.0 (C=O), 166.3 (C=O), 134.5 [1-C(Ar)], 132.8, 129.5, 128.7 [2-C(Ar)], 123.8, 115.9 (CBr), 55.2, 54.5, 50.7, 49.3, 46.0, 30.2, 29.2, 26.0, 25.9, 24.3, 24.1, 22.3, 13.7 (CH_3); IR (neat, cm^{-1}) *v* 3272 (N–H), 2955, 2926, 2872, 1692 (C=O), 1626, 1592, 1576, 1507, 1462, 1436, 1385, 1338, 1291, 1250, 1183, 1160, 1006, 956, 825, 733; HRMS (MALDI-TOF) calcd for $C_{22}H_{30}BrKN_3O_2S_2$ $[M+K]^+$ 550.0594; found 550.0599.

Copies of NMR spectra

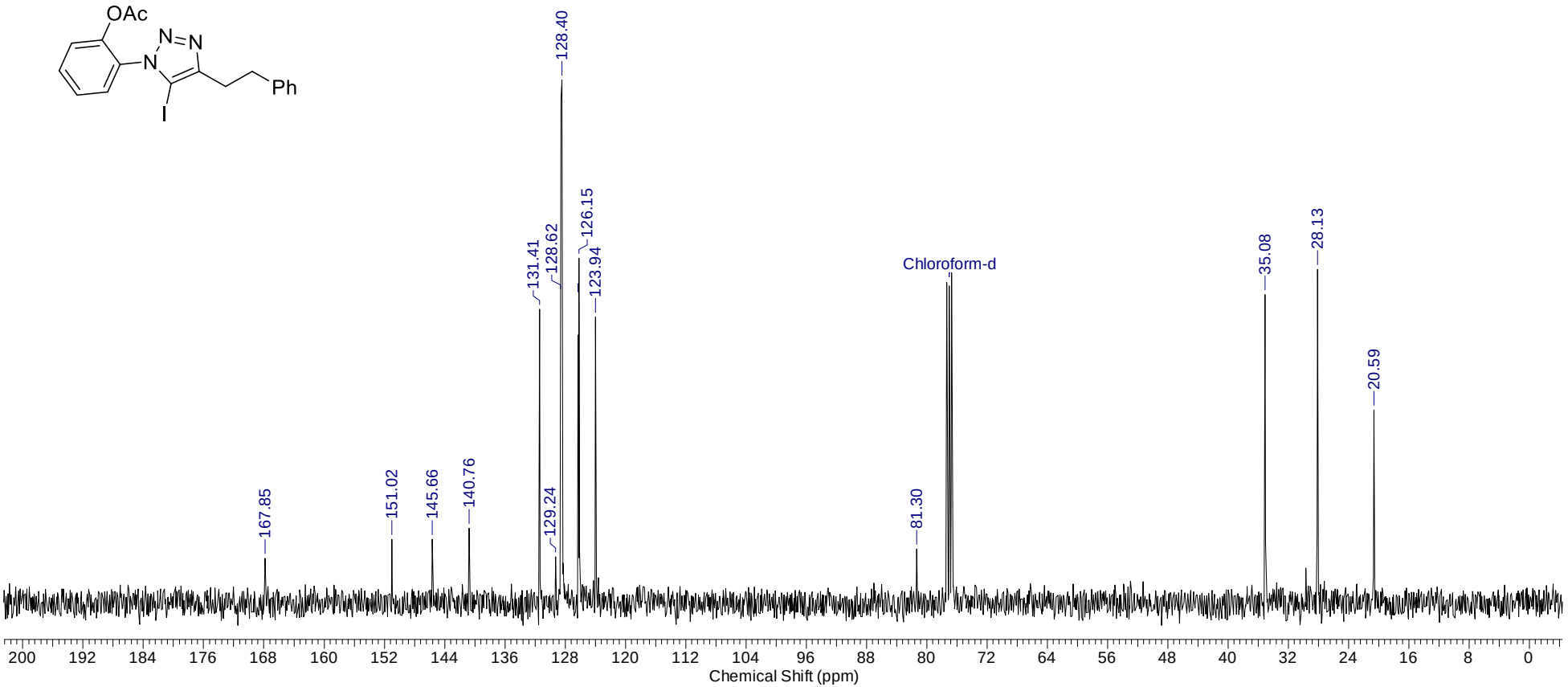
2-[5-Iodo-4-(2-phenylethyl)-1*H*-1,2,3-triazol-1-yl]phenyl acetate (S1j)

^{1}H NMR (400 MHz, $CDCl_3$)



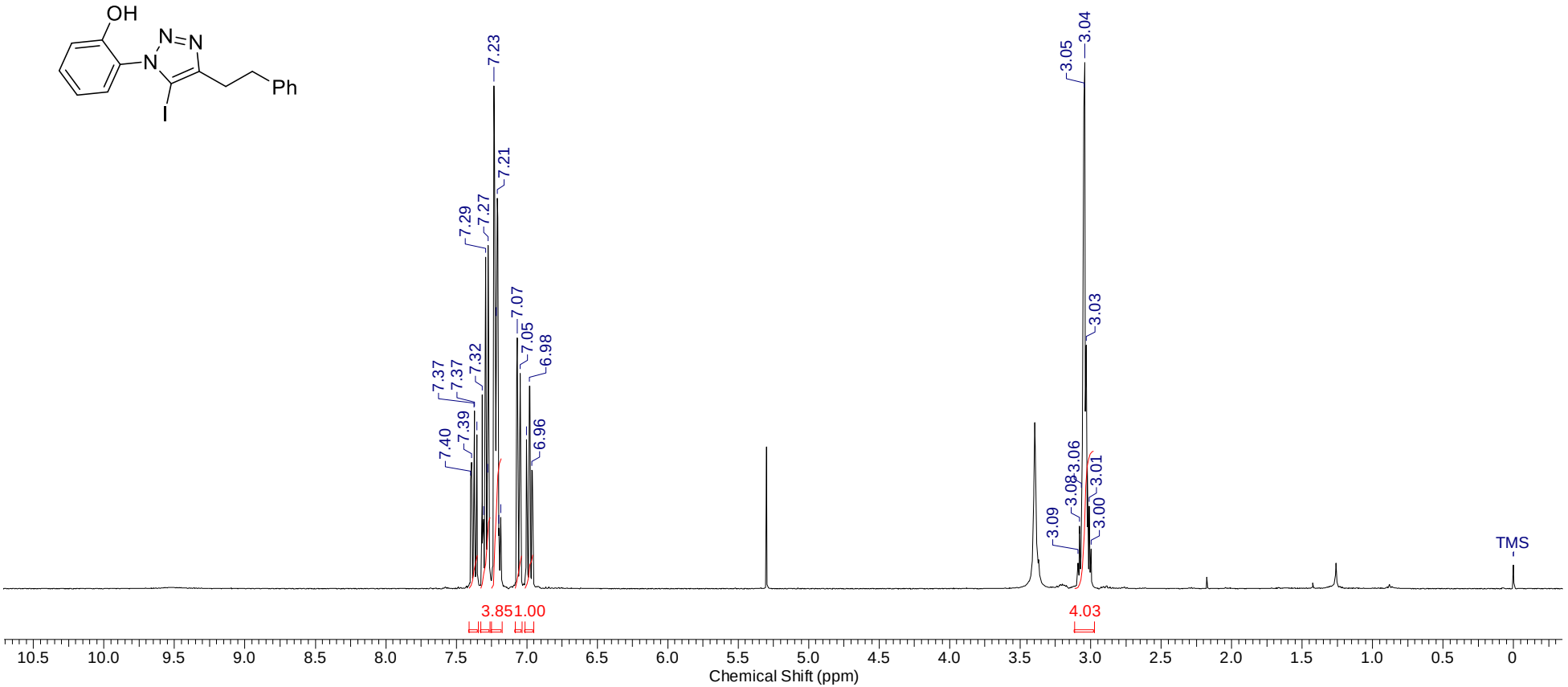
2-[5-Iodo-4-(2-phenylethyl)-1*H*-1,2,3-triazol-1-yl]phenyl acetate (S1j)

^{13}C NMR (100 MHz, $CDCl_3$)



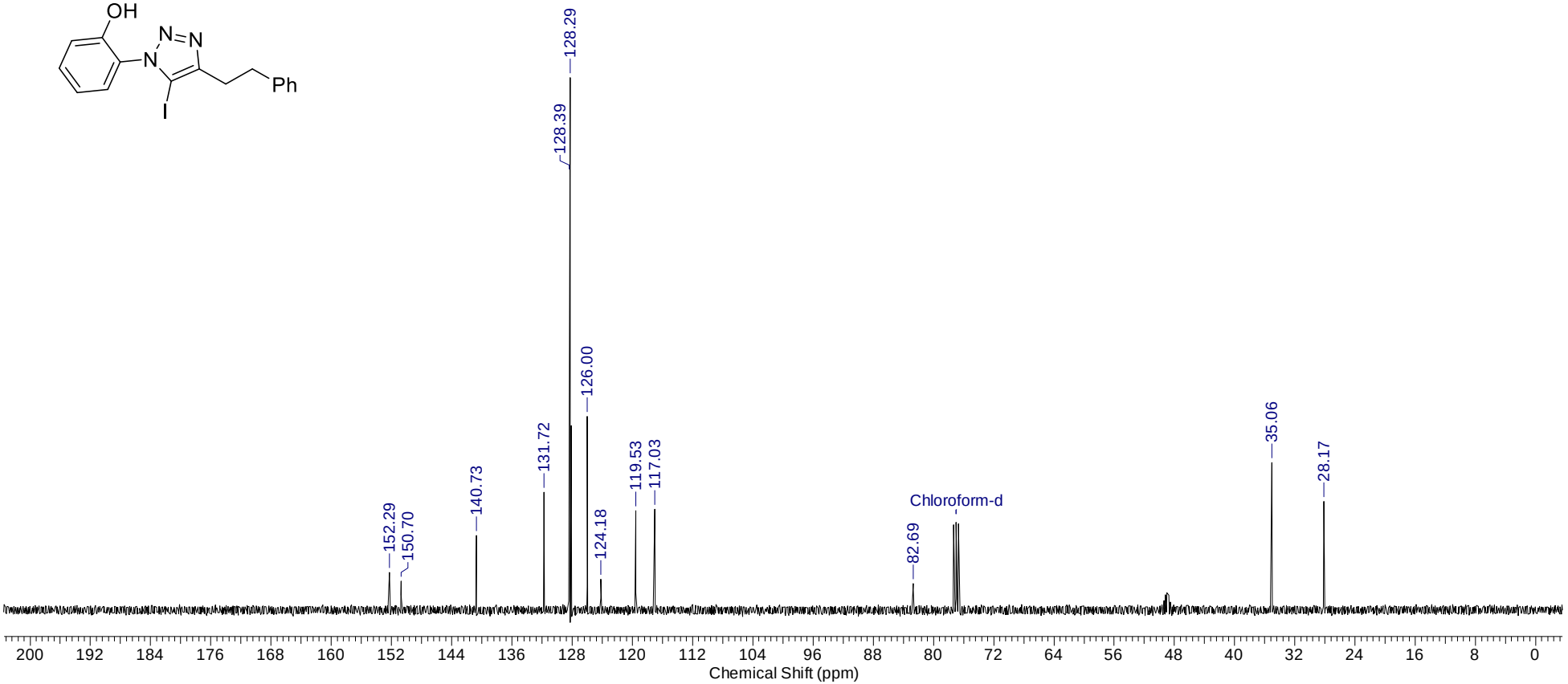
2-[5-Iodo-4-(2-phenylethyl)-1*H*-1,2,3-triazol-1-yl]phenol (1j)

^{1}H NMR (400 MHz, $CDCl_3$–CD_3OD)



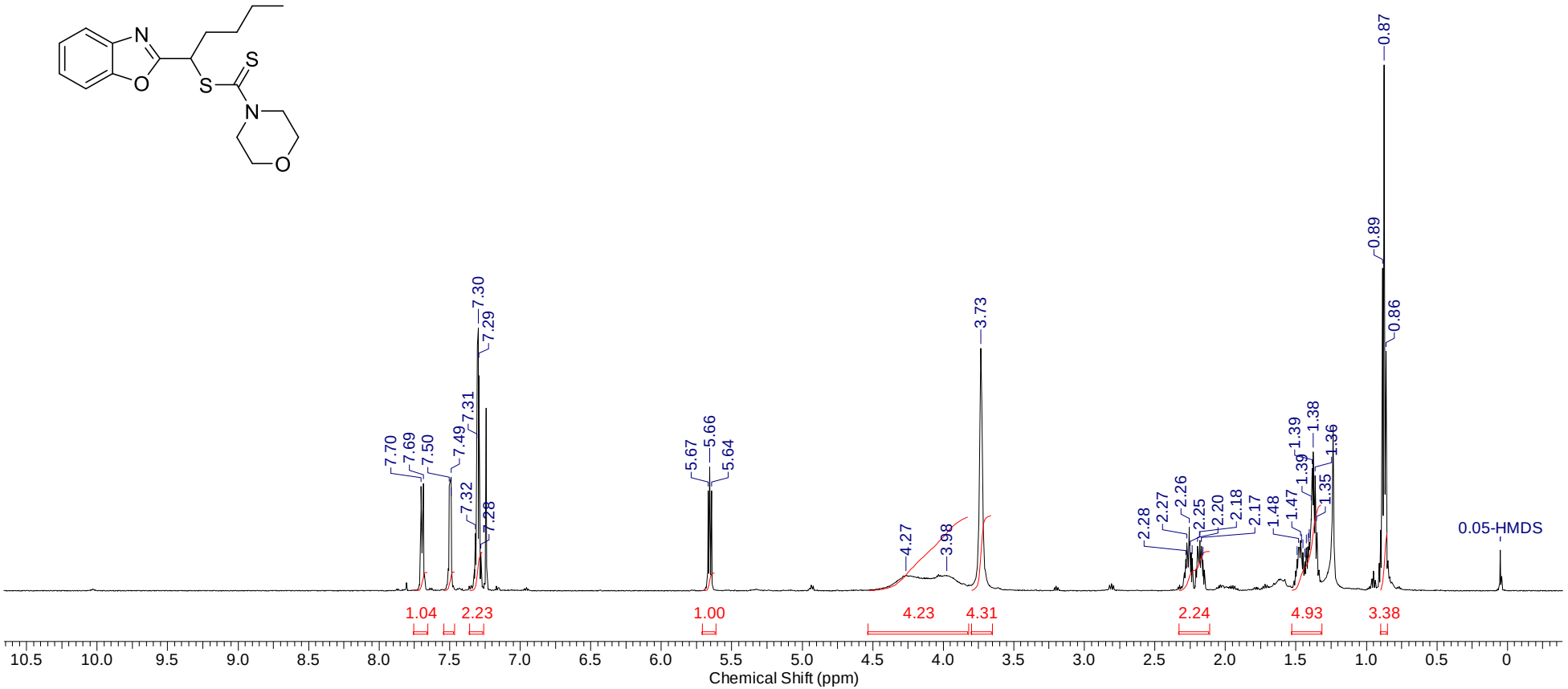
2-[5-Iodo-4-(2-phenylethyl)-1*H*-1,2,3-triazol-1-yl]phenol (1j)

^{13}C NMR (100 MHz, $CDCl_3$–CD_3OD)



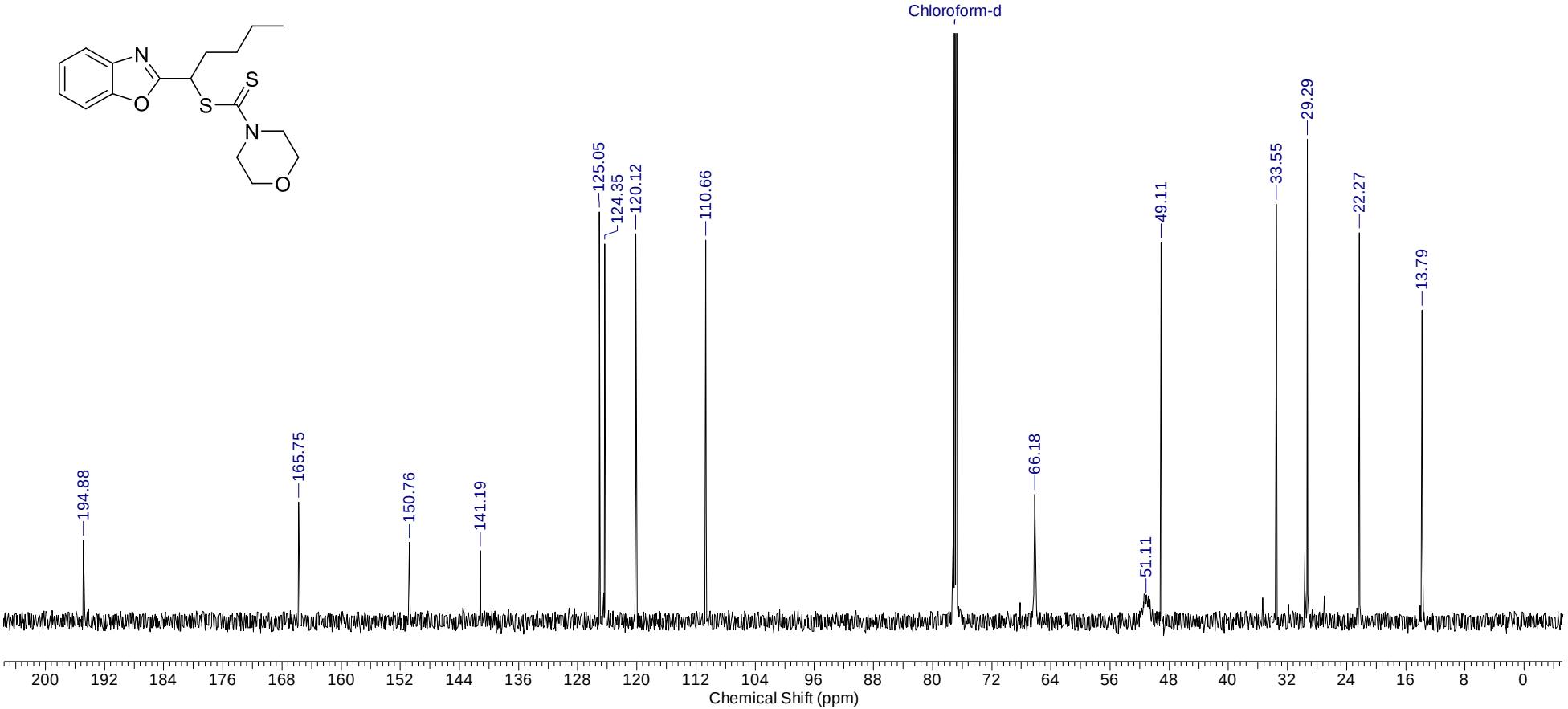
1-(1,3-Benzoxazol-2-yl)pentyl morpholine-4-carbodithioate (3a)

^{1}H NMR (600 MHz, $CDCl_3$)



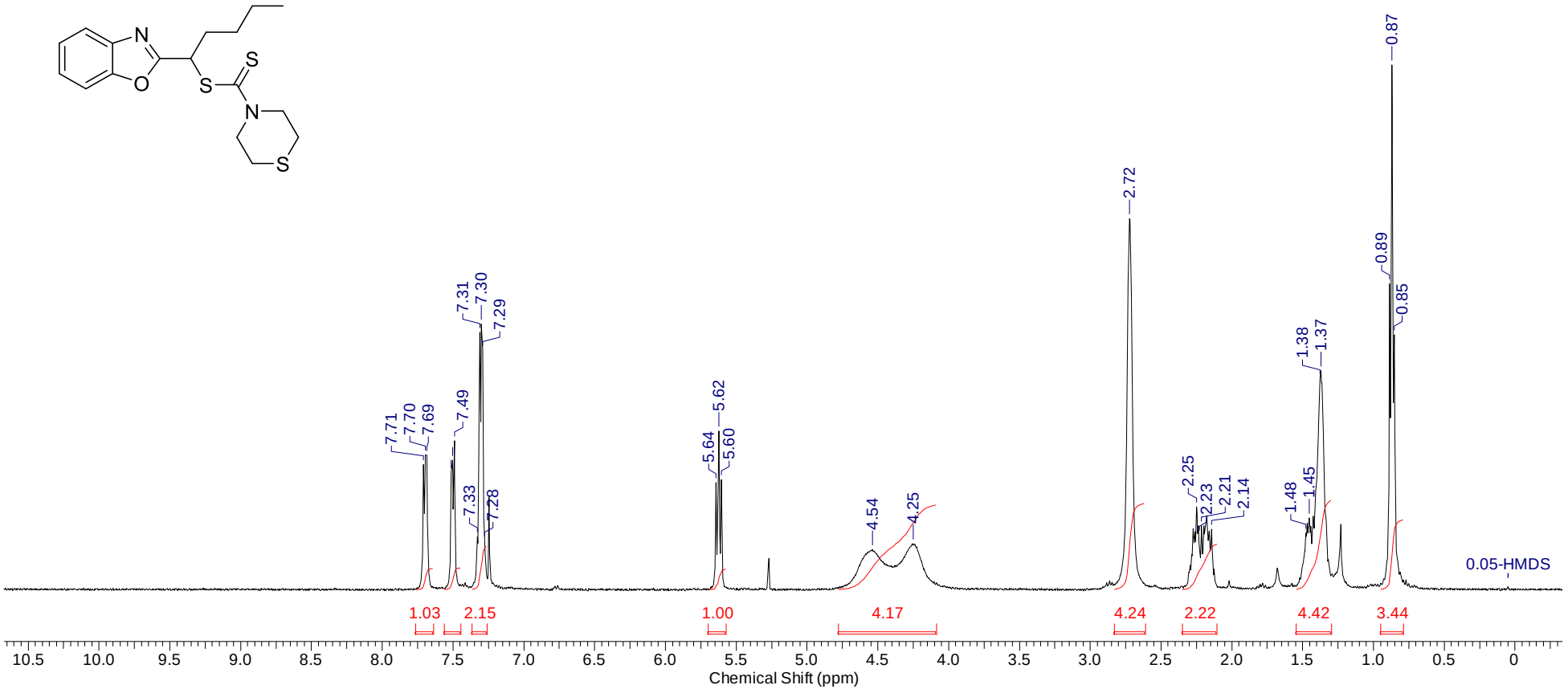
1-(1,3-Benzoxazol-2-yl)pentyl morpholine-4-carbodithioate (3a)

^{13}C NMR (151 MHz, $CDCl_3$)



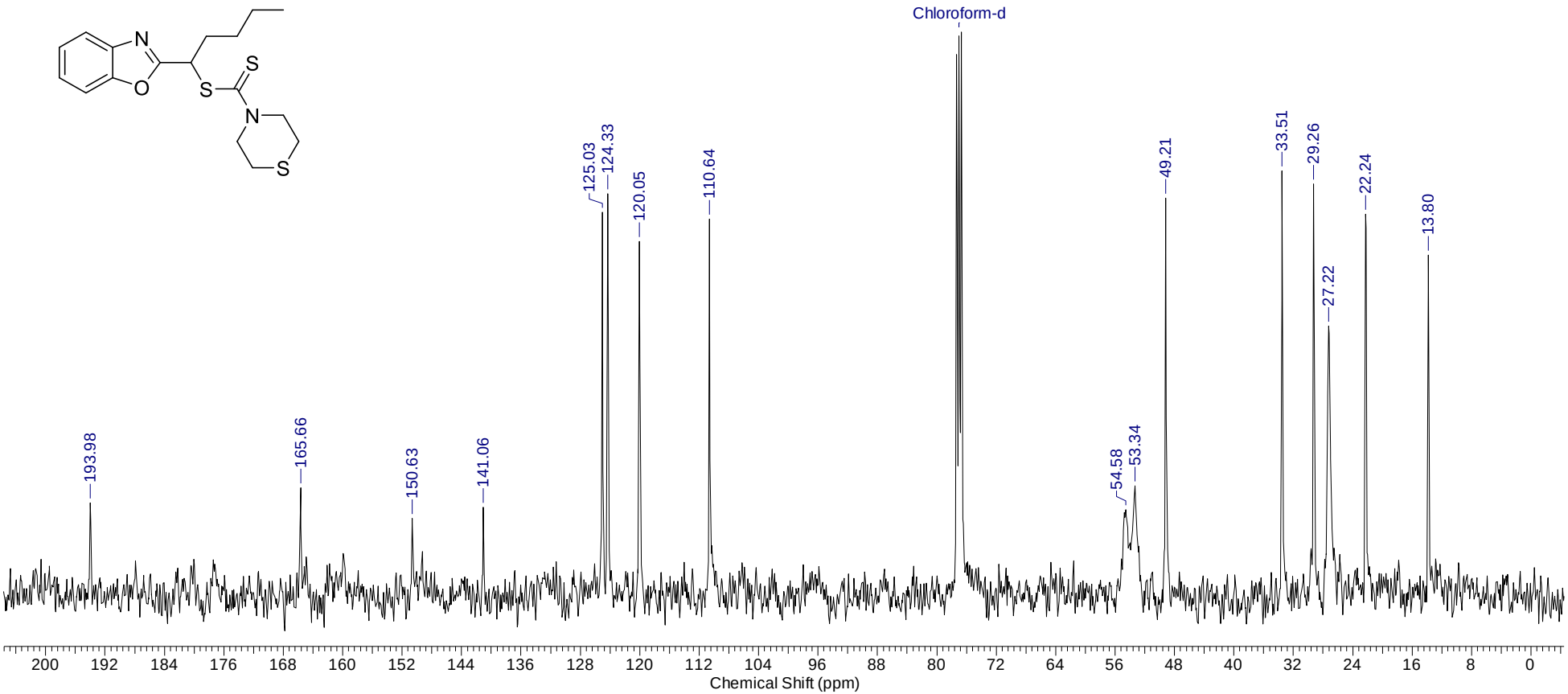
1-(1,3-Benzoxazol-2-yl)pentyl thiomorpholine-4-carbodithioate (3b)

^{1}H NMR (400 MHz, $CDCl_3$)



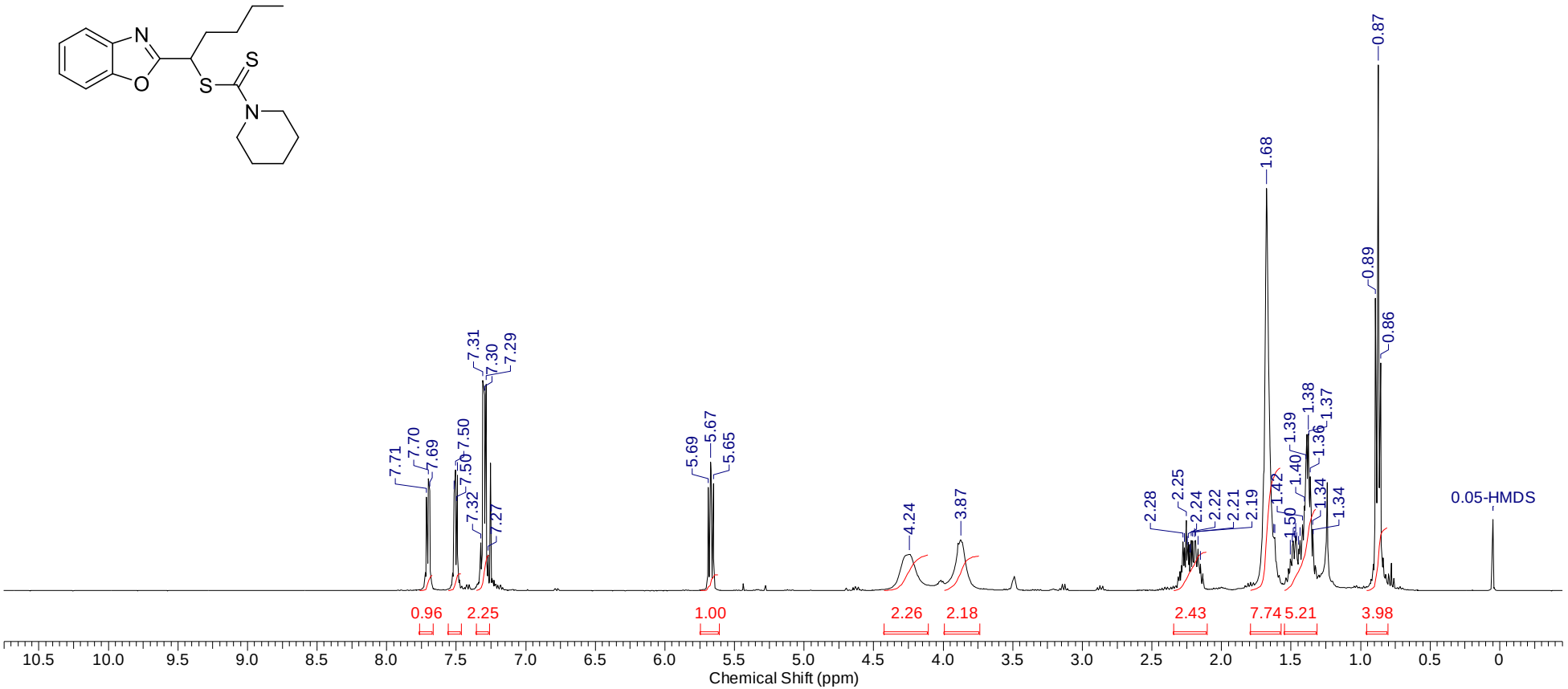
1-(1,3-Benzoxazol-2-yl)pentyl thiomorpholine-4-carbodithioate (3b)

^{13}C NMR (100 MHz, $CDCl_3$)



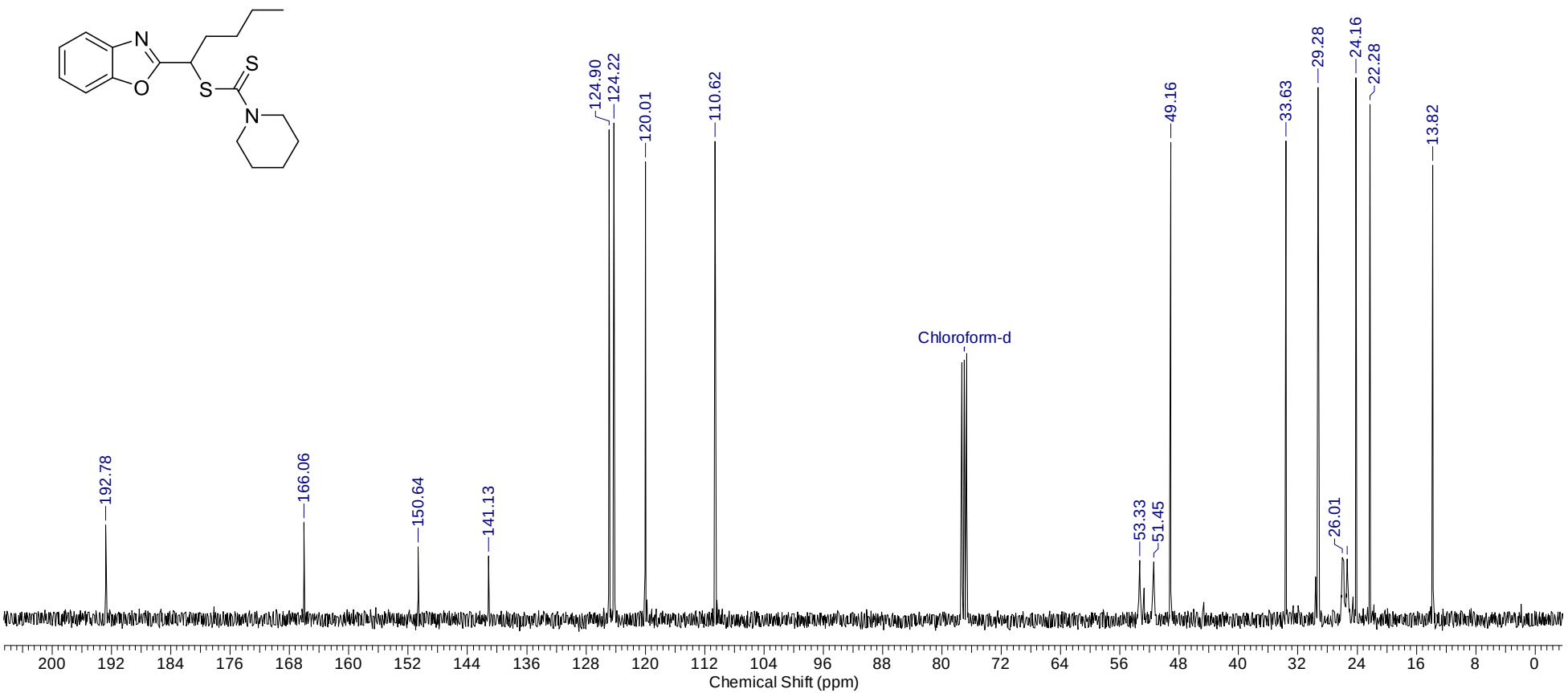
1-(1,3-Benzoxazol-2-yl)pentyl piperidine-4-carbodithioate (3c)

^{1}H NMR (400 MHz, $CDCl_3$)



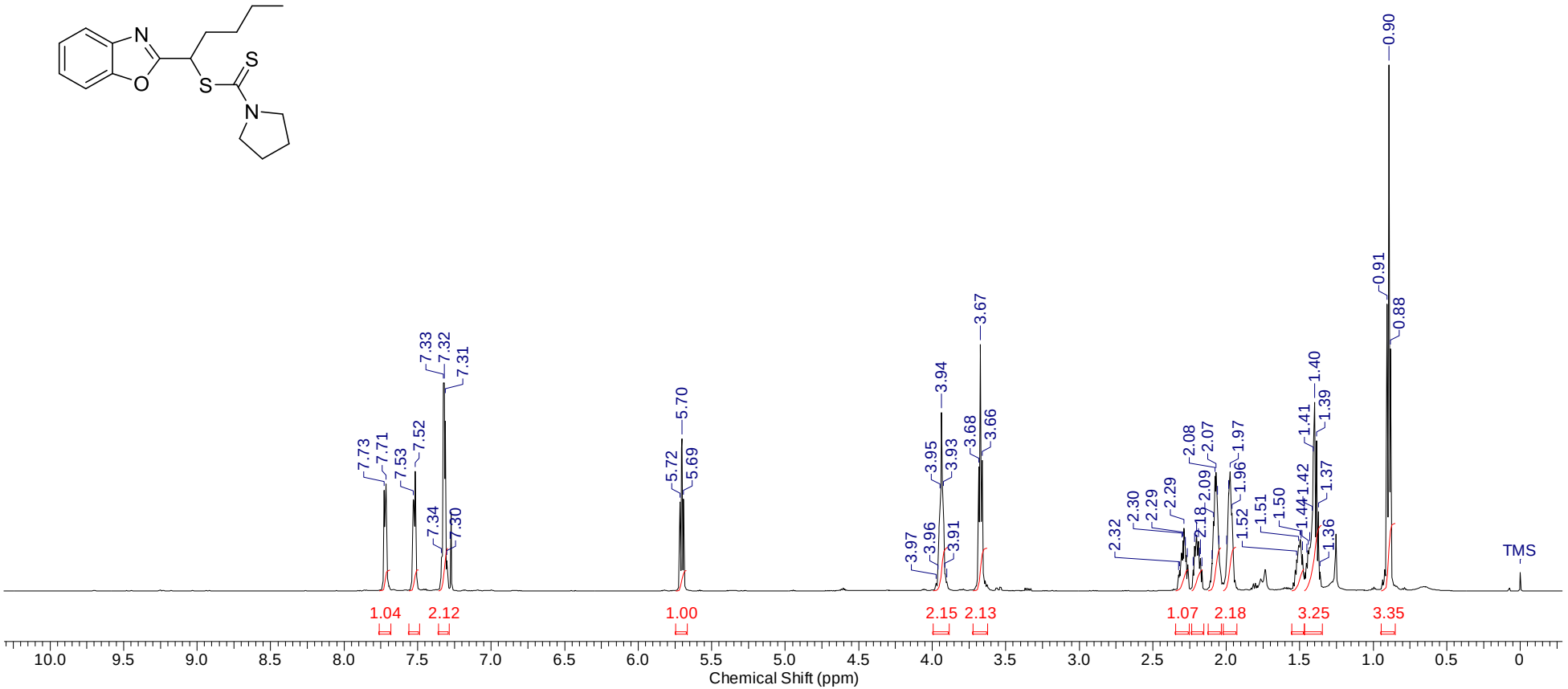
1-(1,3-Benzoxazol-2-yl)pentyl piperidine-4-carbodithioate (3c)

^{13}C NMR (100 MHz, $CDCl_3$)



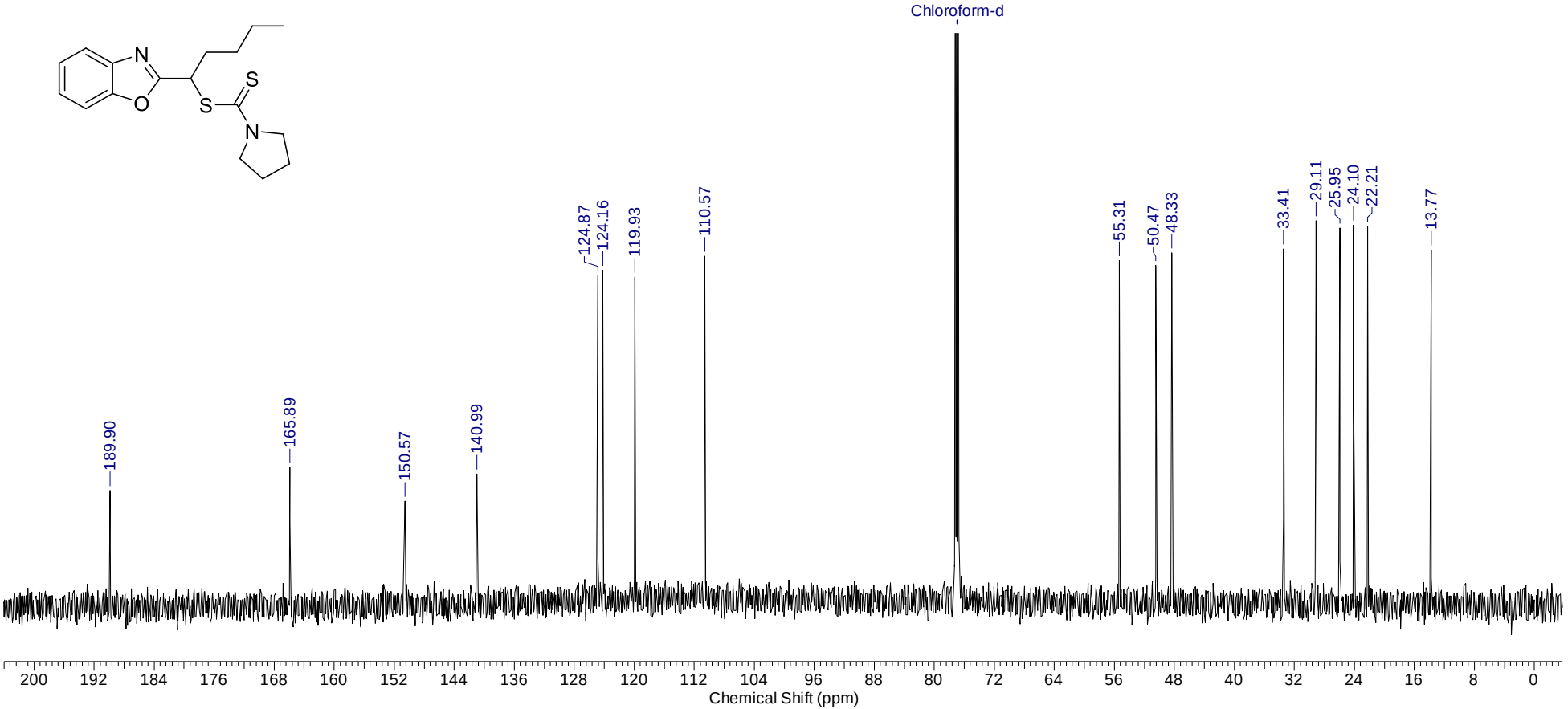
1-(1,3-Benzoxazol-2-yl)pentyl pyrrolidine-4-carbodithioate (3d)

^{1}H NMR (600 MHz, $CDCl_3$)



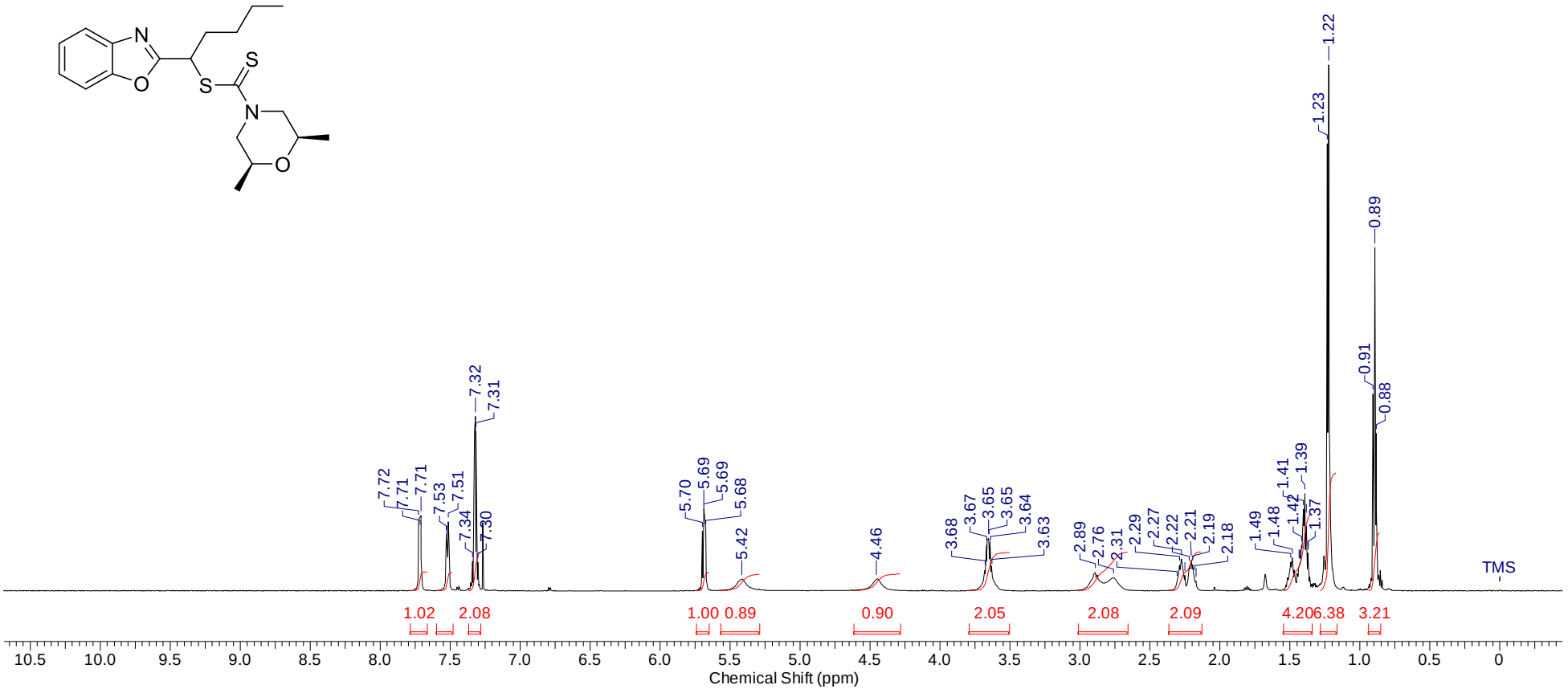
1-(1,3-Benzoxazol-2-yl)pentyl pyrrolidine-4-carbodithioate (3d)

^{13}C NMR (151 MHz, $CDCl_3$)



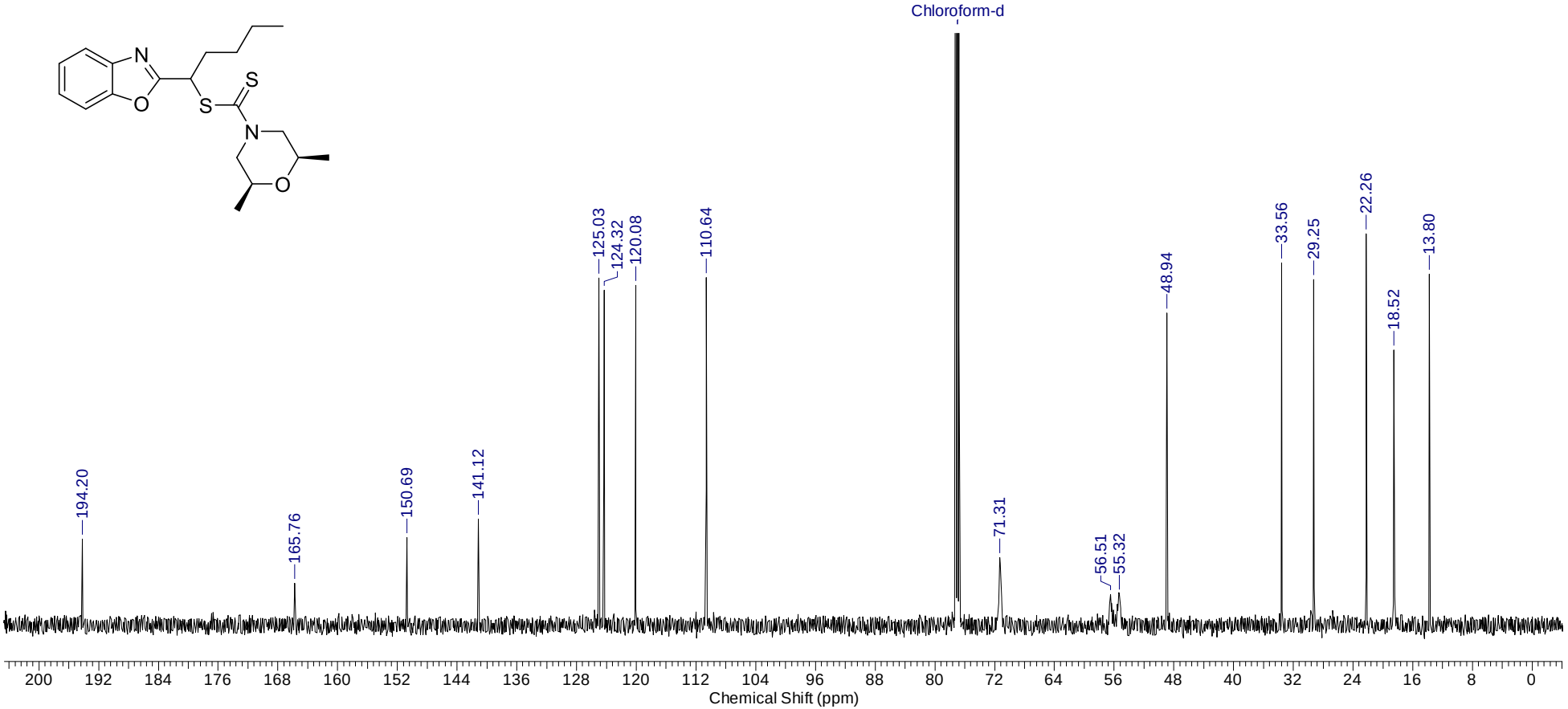
1-(1,3-Benzoxazol-2-yl)pentyl (2*R*,6*S*)-2,6-dimethylmorpholine-4-carbodithioate (3e)

^{1}H NMR (600 MHz, $CDCl_3$)



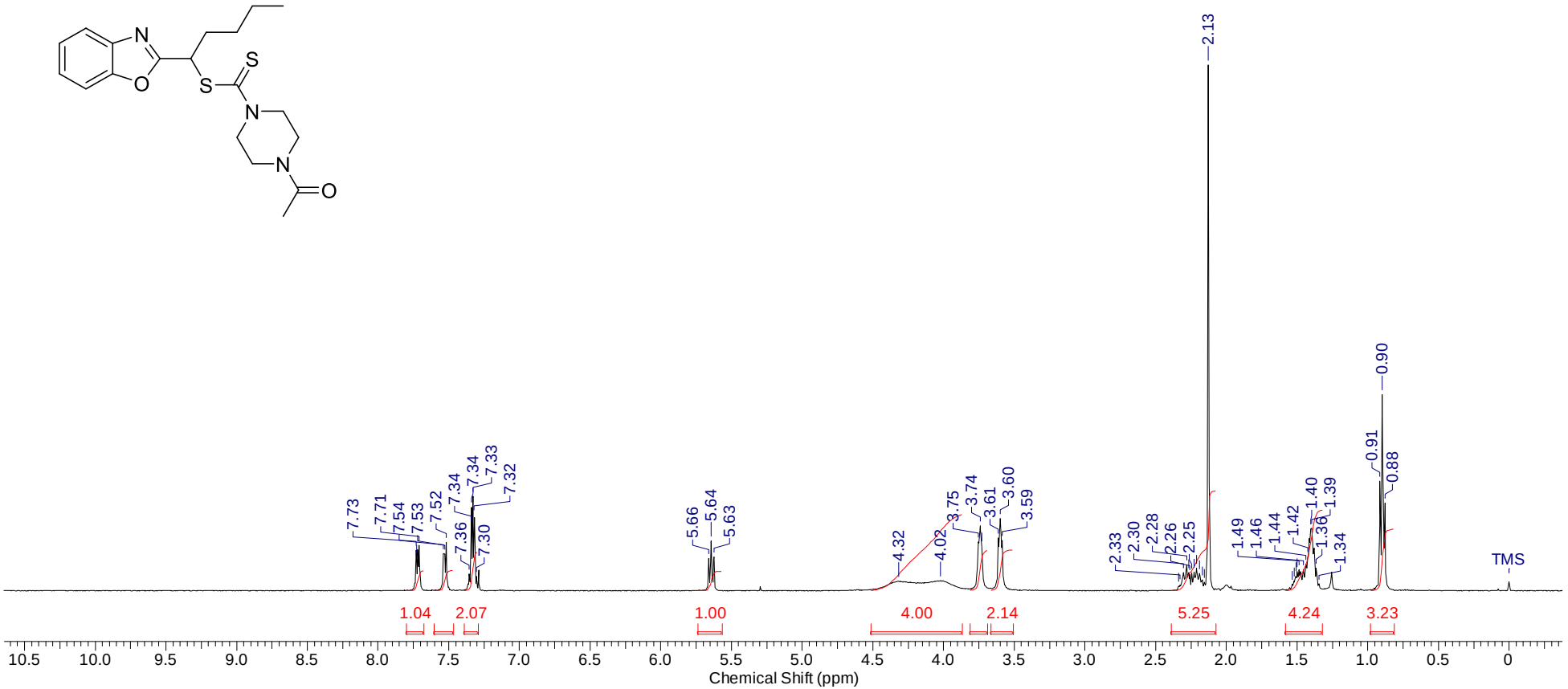
1-(1,3-Benzoxazol-2-yl)pentyl (2*R*,6*S*)-2,6-dimethylmorpholine-4-carbodithioate (3e)

^{13}C NMR (151 MHz, $CDCl_3$)



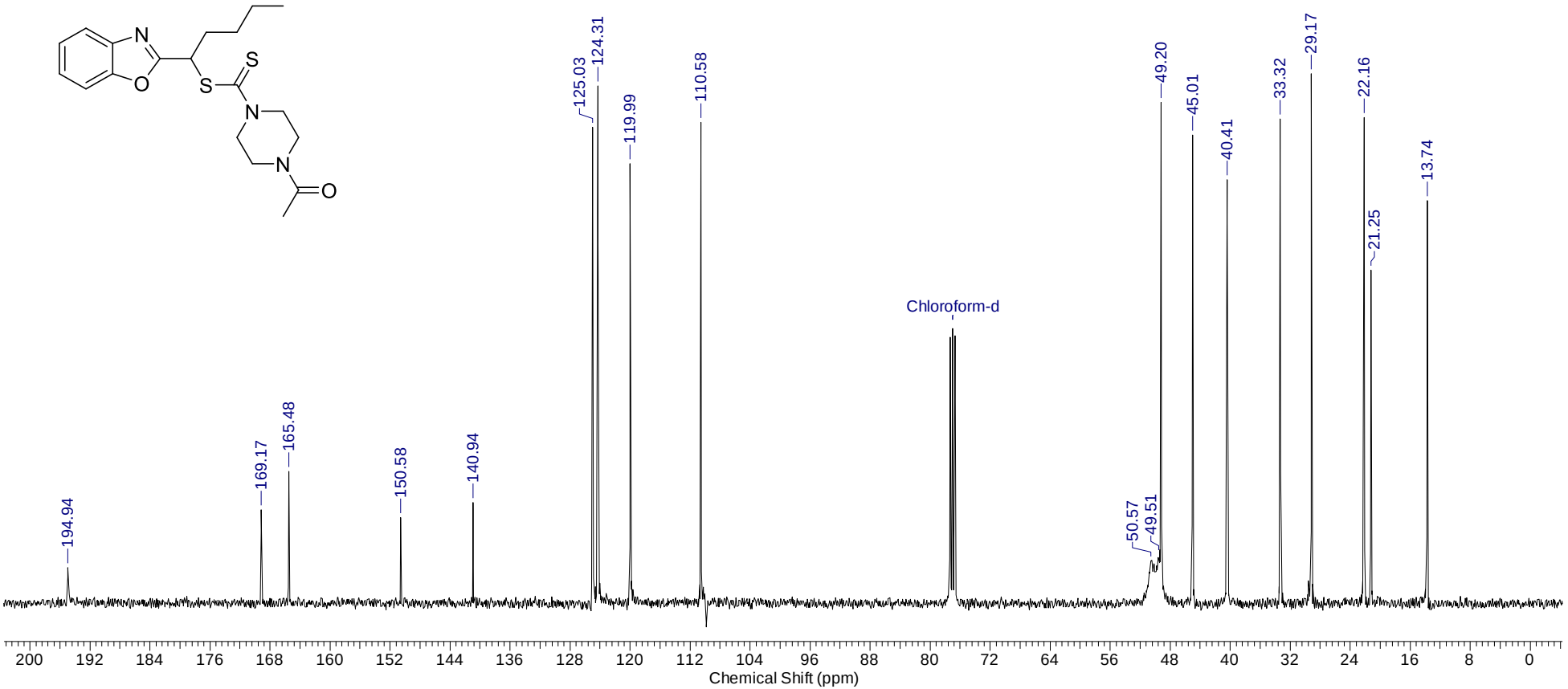
1-(1,3-Benzoxazol-2-yl)pentyl 4-acetylpiperazine-1-carbodithioate (3f)

^{1}H NMR (400 MHz, $CDCl_3$)



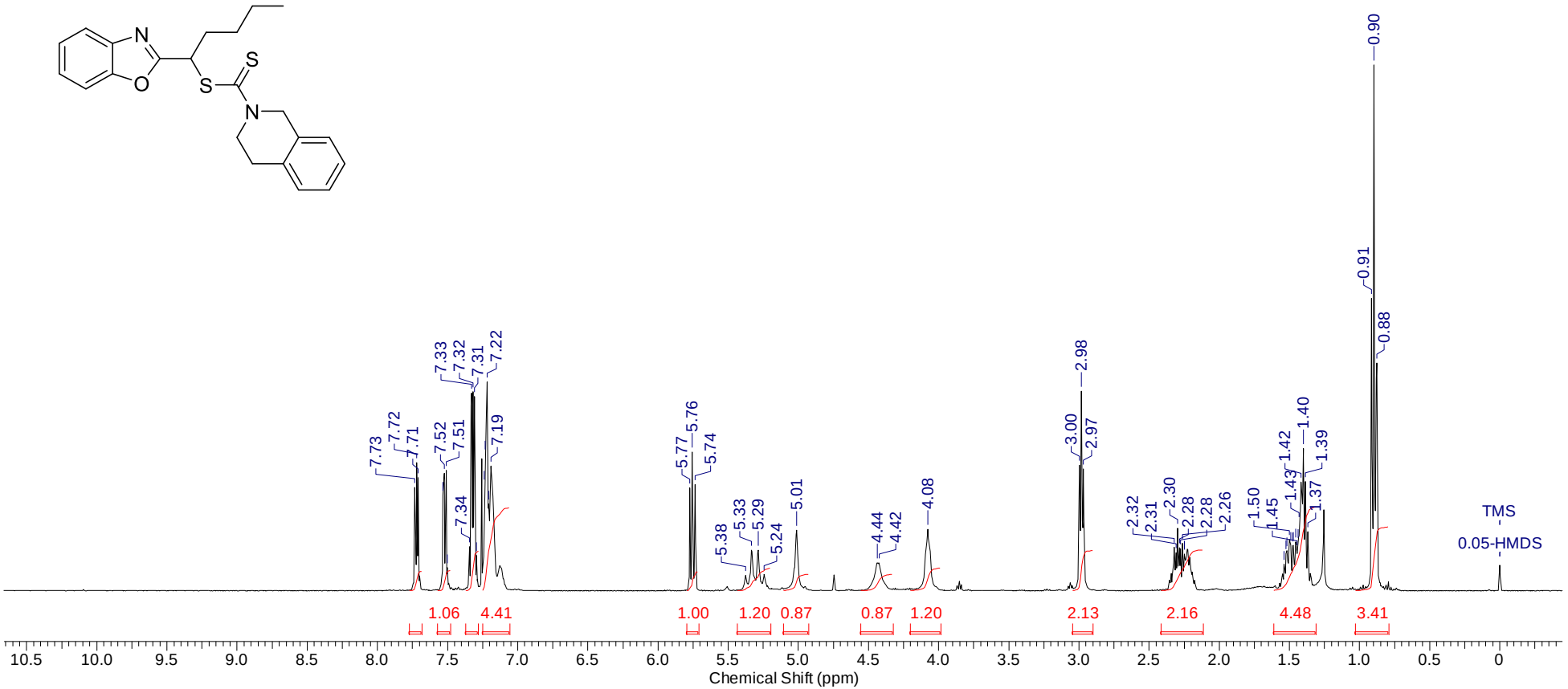
1-(1,3-Benzoxazol-2-yl)pentyl 4-acetylpiperazine-1-carbodithioate (3f)

^{13}C NMR (100 MHz, $CDCl_3$)



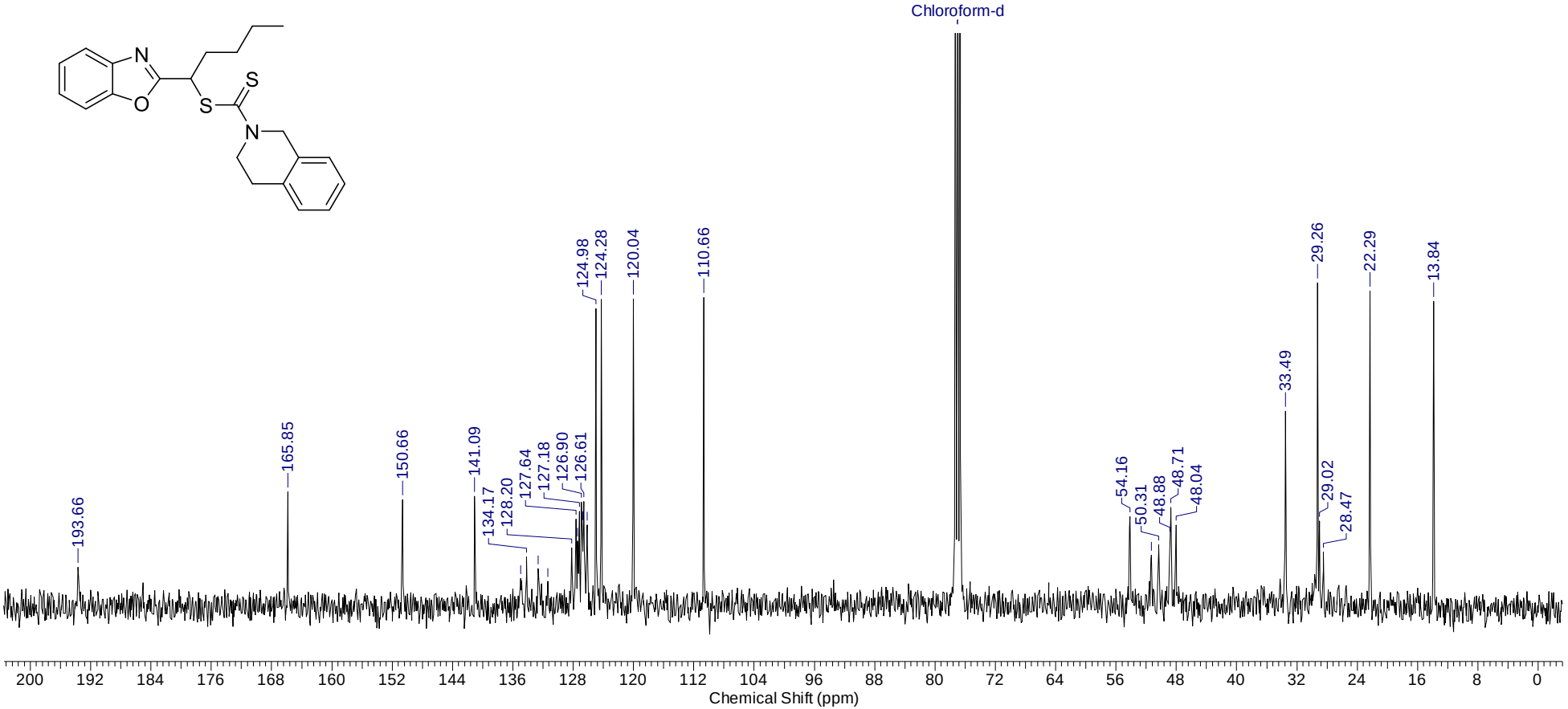
1-(1,3-Benzoxazol-2-yl)pentyl 3,4-dihydroisoquinoline-2(1*H*)-carbodithioate (3g)

^{1}H NMR (400 MHz, $CDCl_3$)



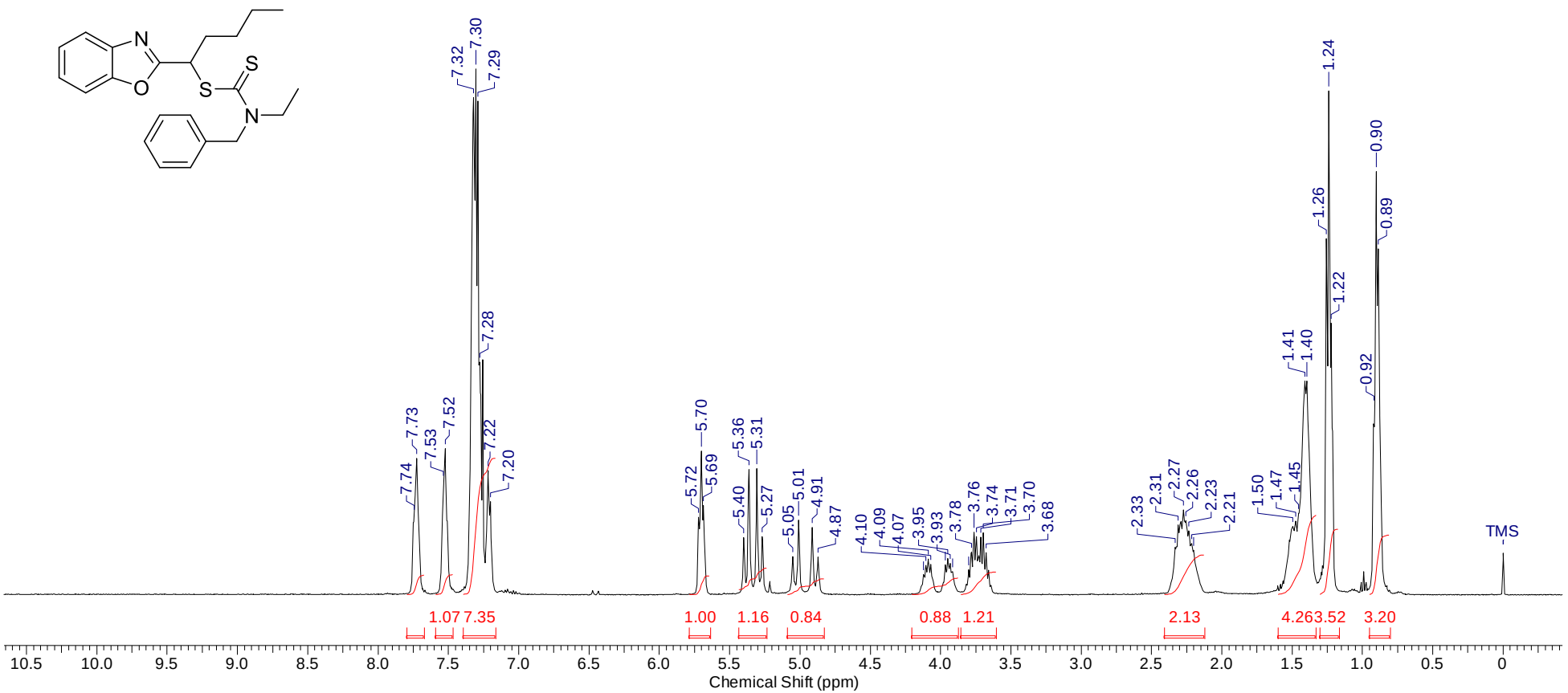
1-(1,3-Benzoxazol-2-yl)pentyl 3,4-dihydroisoquinoline-2(1*H*)-carbodithioate (3g)

^{13}C NMR (100 MHz, $CDCl_3$)



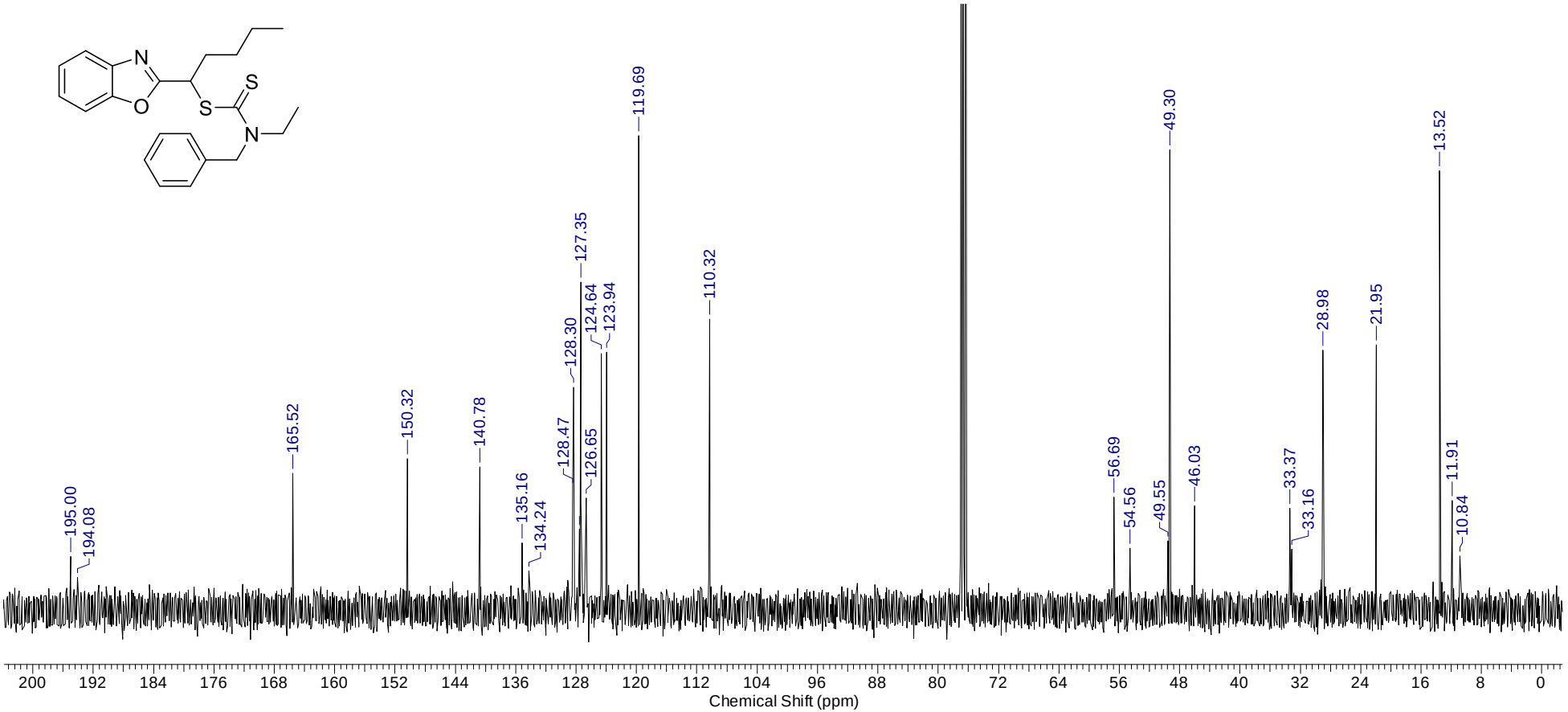
1-(1,3-Benzoxazol-2-yl)pentyl benzyl(ethyl)dithiocarbamate (3h)

^{1}H NMR (400 MHz, $CDCl_3$)



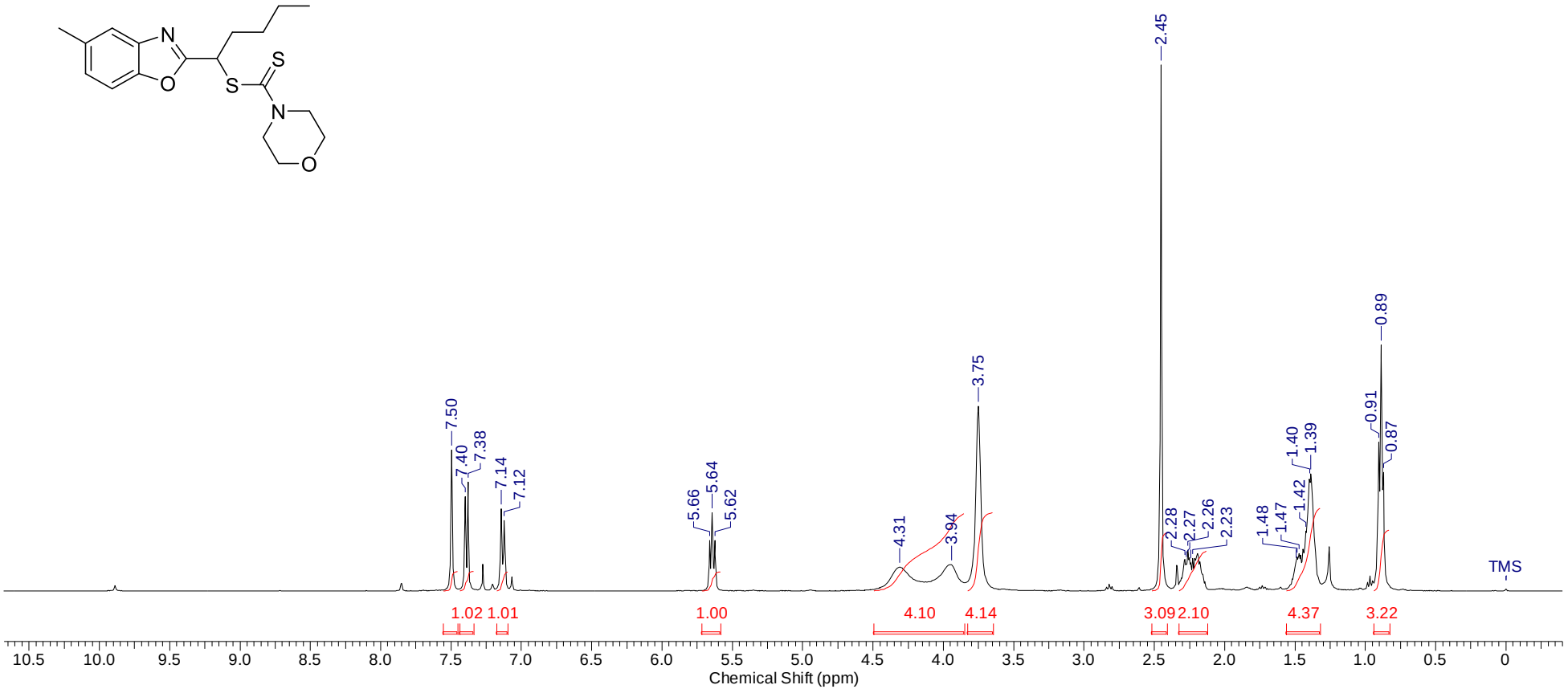
1-(1,3-Benzoxazol-2-yl)pentyl benzyl(ethyl)dithiocarbamate (3h)

^{13}C NMR (100 MHz, $CDCl_3$)



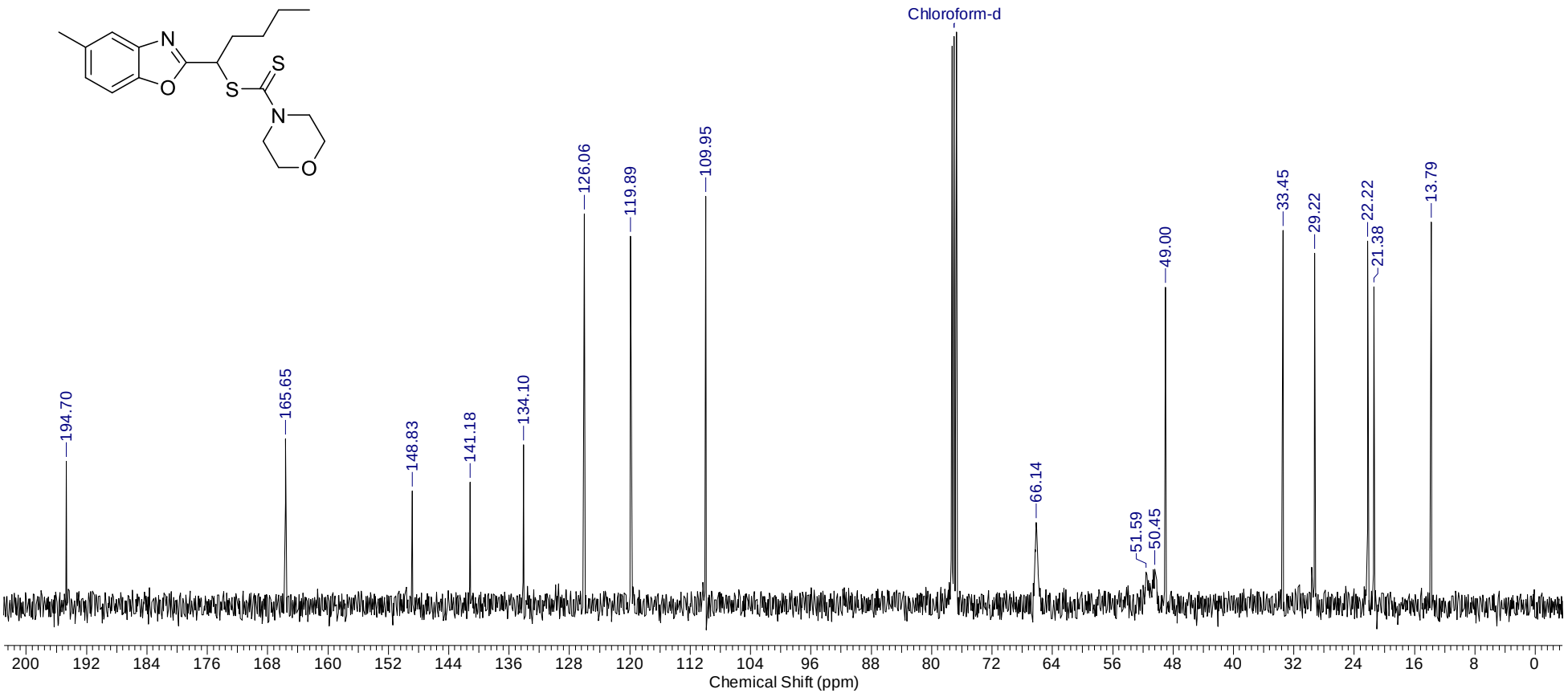
1-(5-Methyl-1,3-benzoxazol-2-yl)pentyl morpholine-4-carbodithioate (3l)

^{1}H NMR (400 MHz, $CDCl_3$)



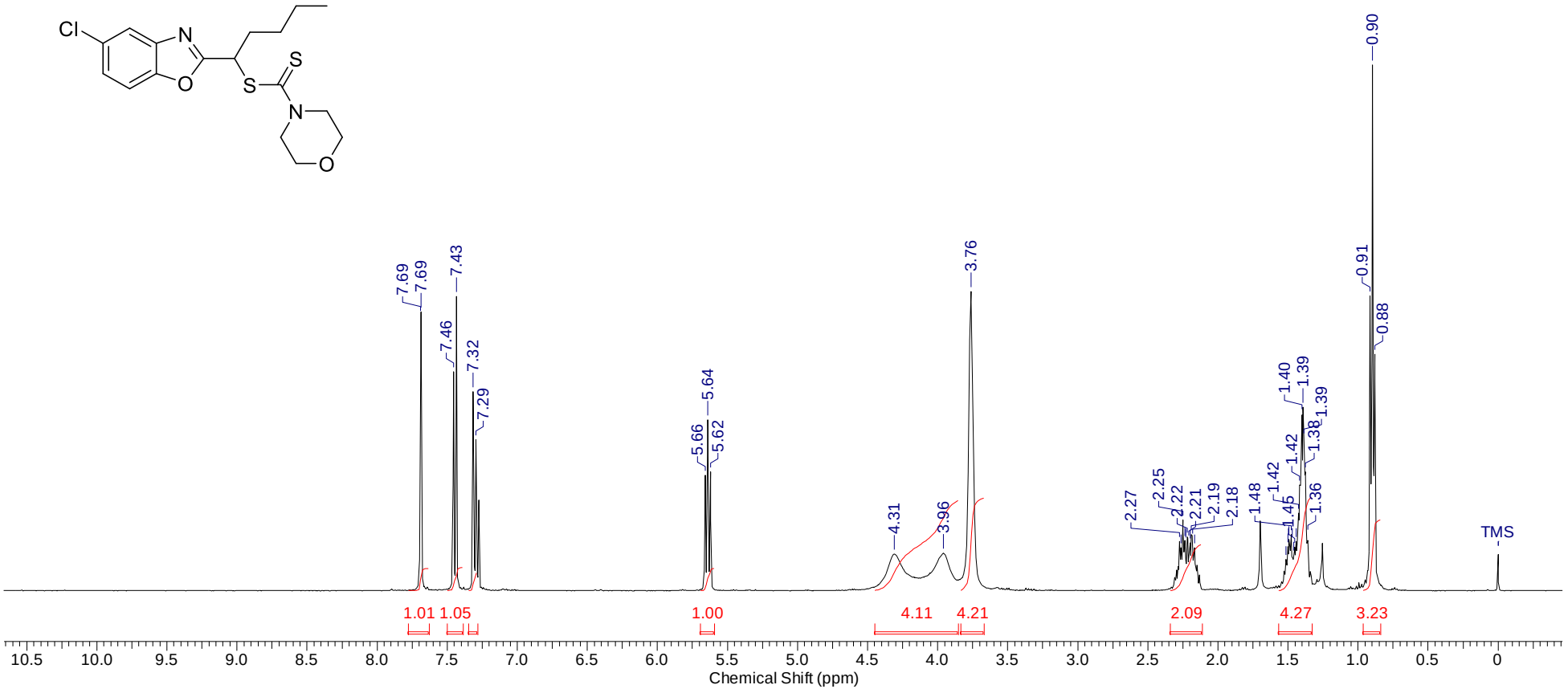
1-(5-Methyl-1,3-benzoxazol-2-yl)pentyl morpholine-4-carbodithioate (3l)

^{13}C NMR (100 MHz, $CDCl_3$)



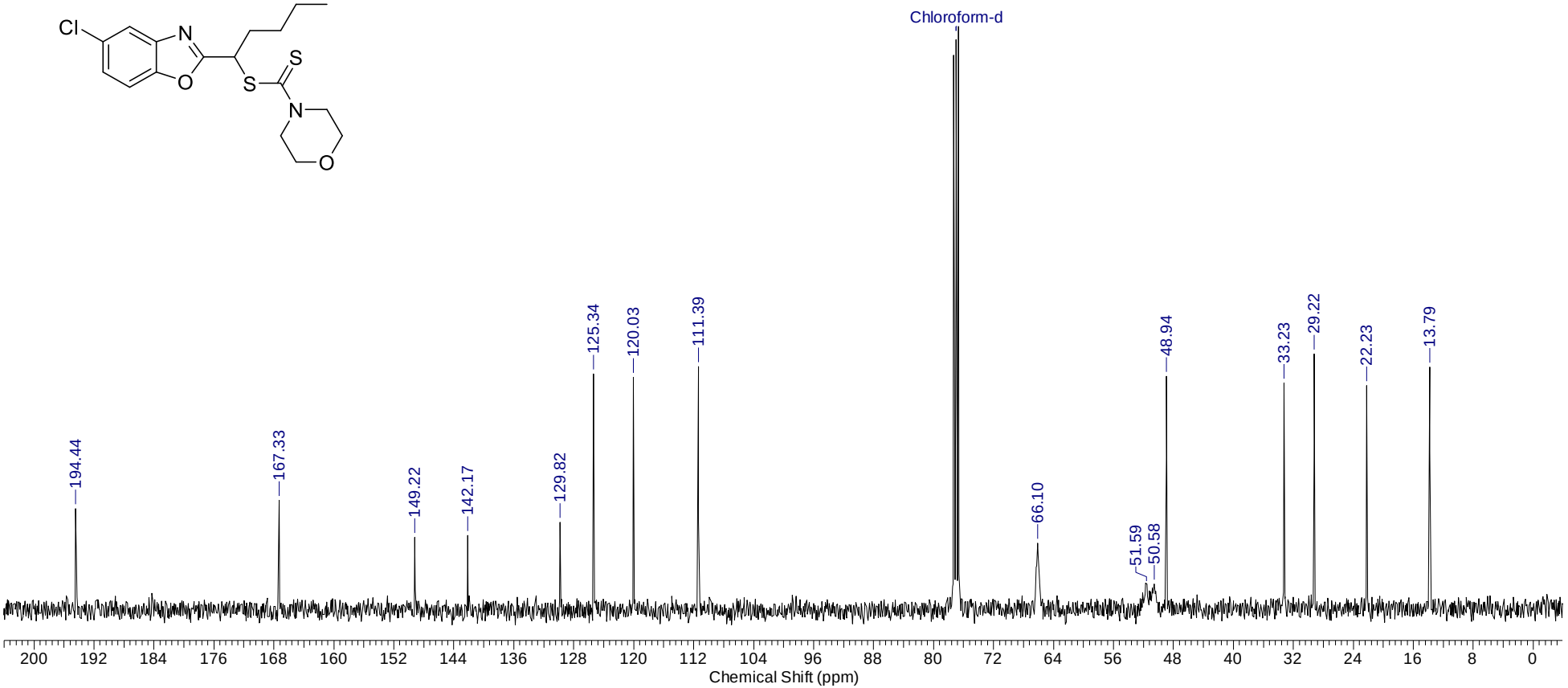
1-(5-Chloro-1,3-benzoxazol-2-yl)pentyl morpholine-4-carbodithioate (3m)

^{1}H NMR (400 MHz, $CDCl_3$)



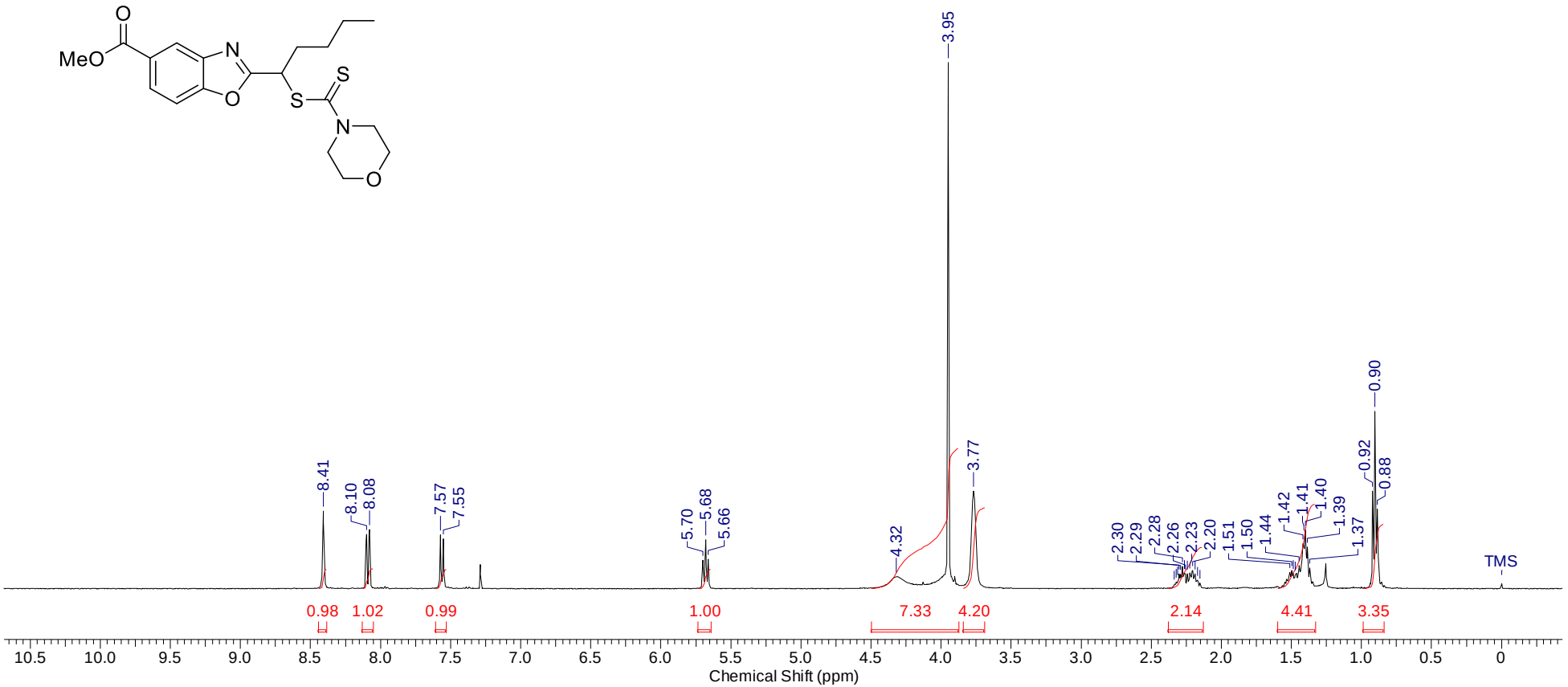
1-(5-Chloro-1,3-benzoxazol-2-yl)pentyl morpholine-4-carbodithioate (3m)

^{13}C NMR (100 MHz, $CDCl_3$)



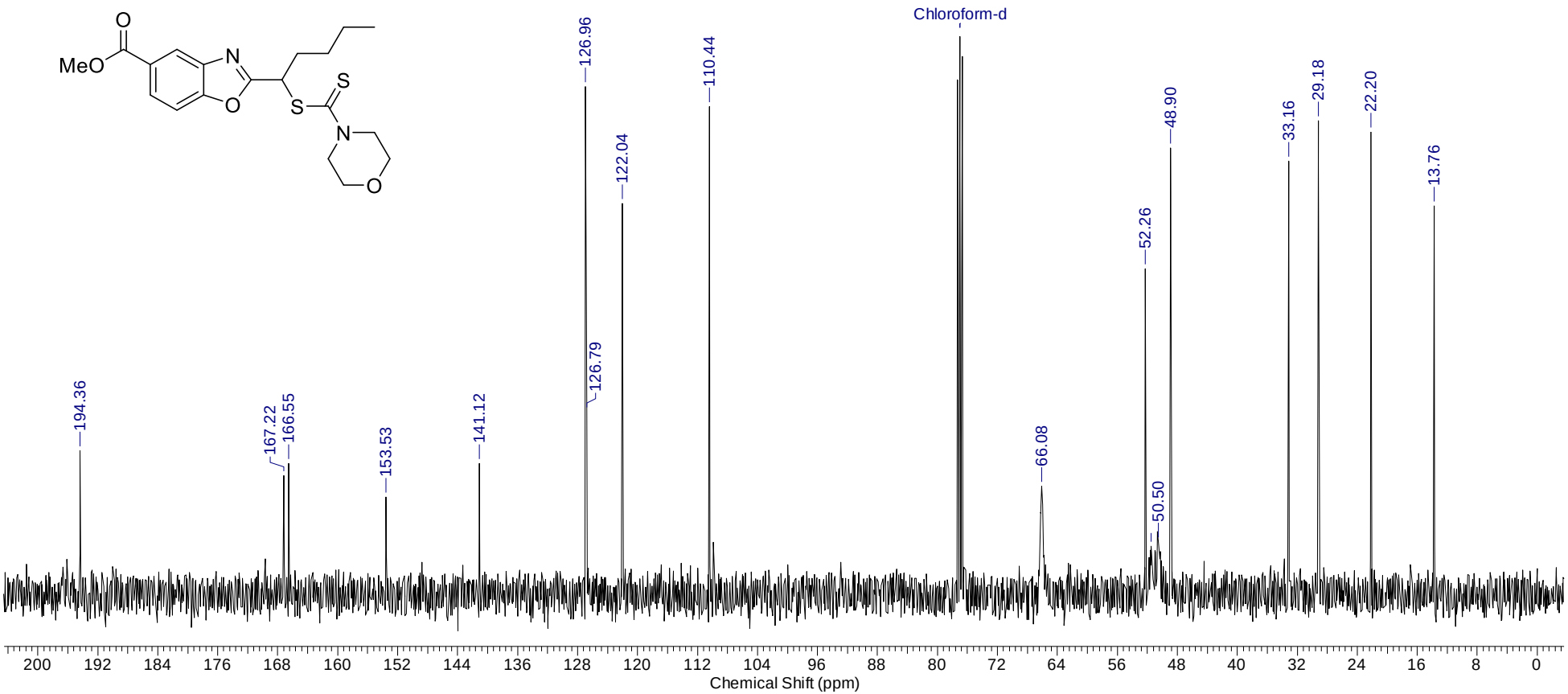
Methyl 2-{1-[(morpholin-4-ylcarbonothioyl)thio]pentyl}-1,3-benzoxazole-5-carboxylate (3n)

^{1}H NMR (400 MHz, $CDCl_3$)



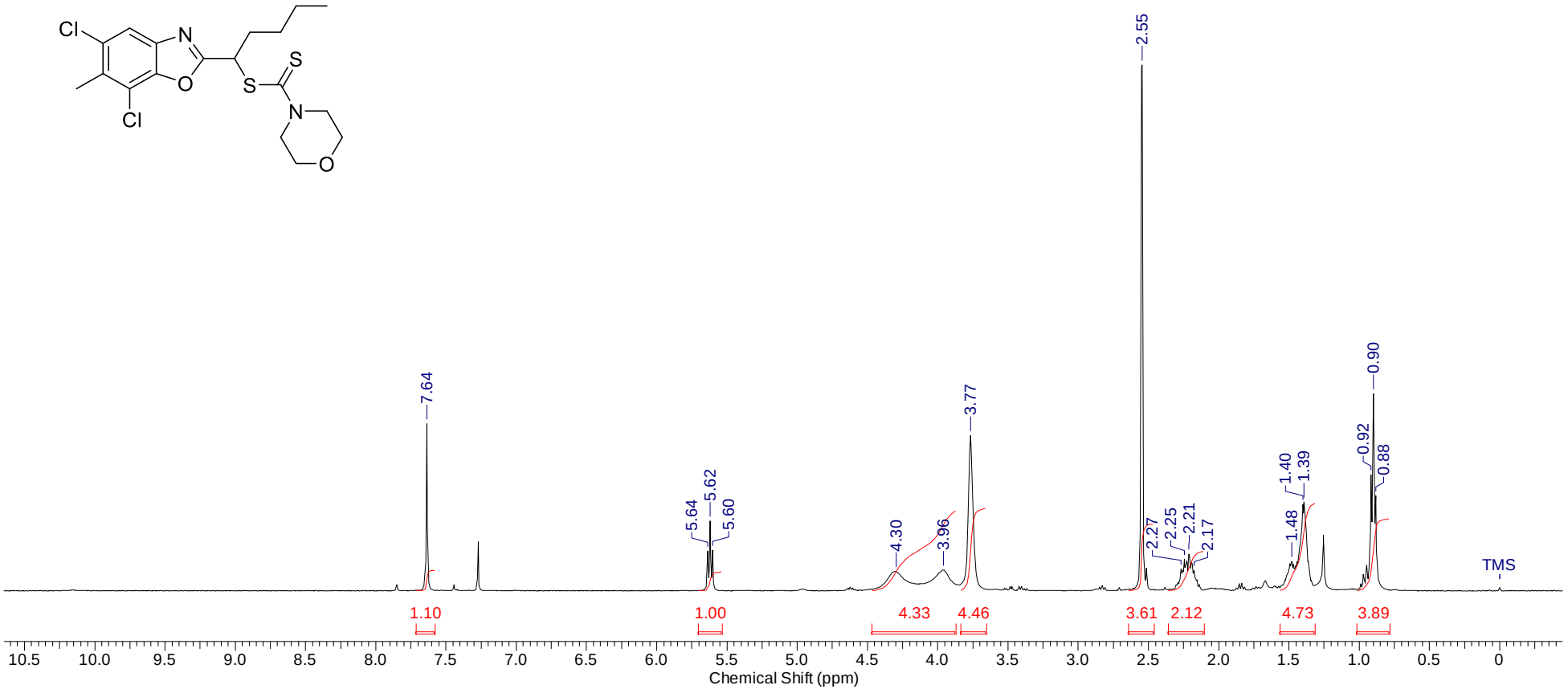
Methyl 2-{1-[(morpholin-4-ylcarbonothioyl)thio]pentyl}-1,3-benzoxazole-5-carboxylate (3n)

^{13}C NMR (100 MHz, $CDCl_3$)



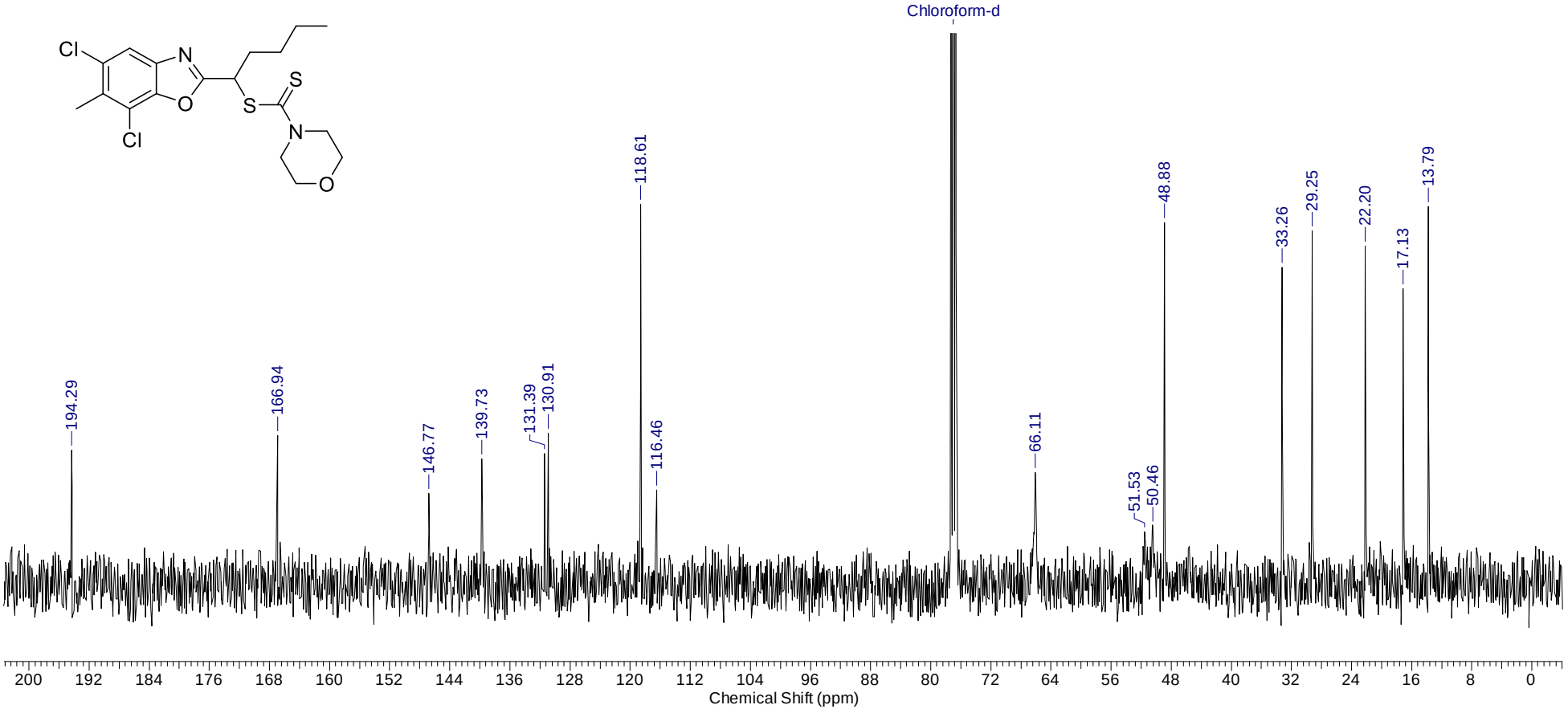
1-(5,7-Dichloro-6-methyl-1,3-benzoxazol-2-yl)pentyl morpholine-4-carbodithioate (3o)

^{1}H NMR (400 MHz, $CDCl_3$)



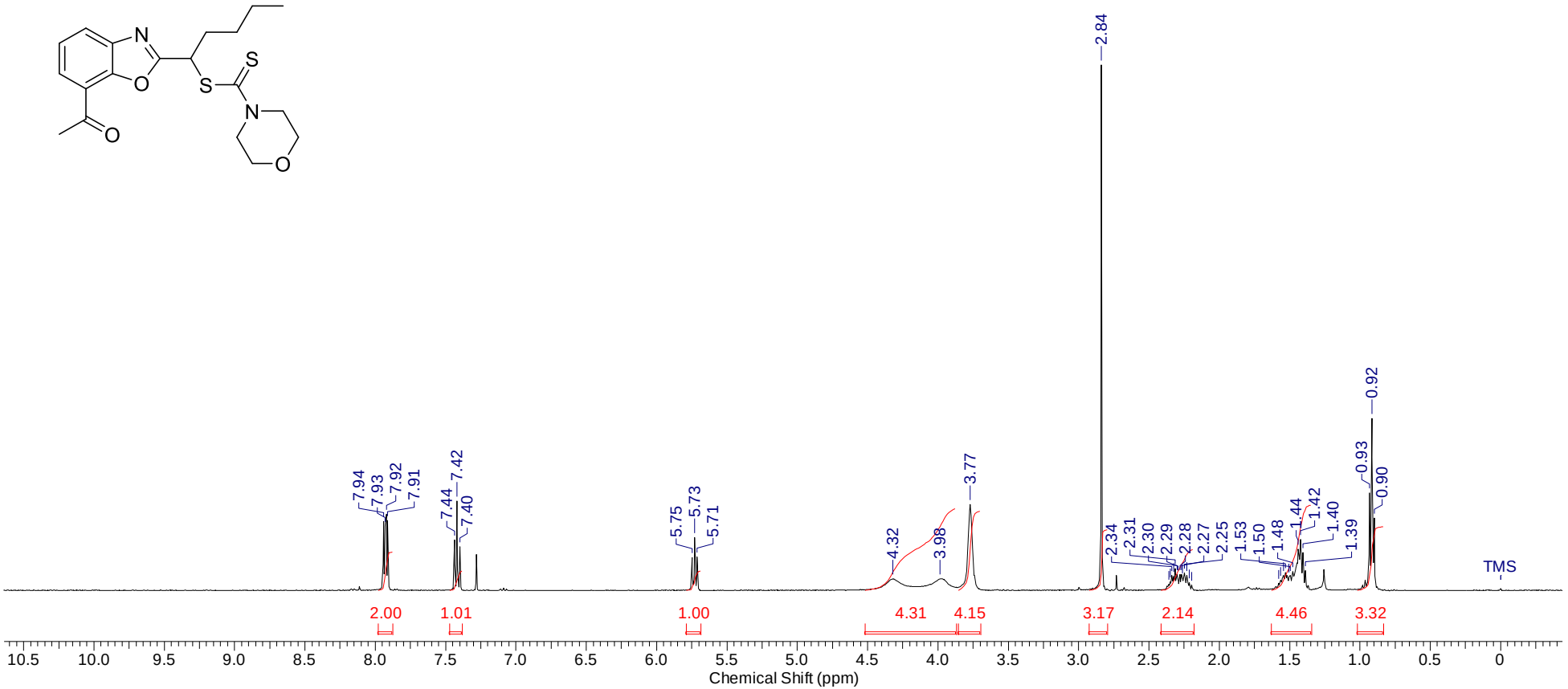
1-(5,7-Dichloro-6-methyl-1,3-benzoxazol-2-yl)pentyl morpholine-4-carbodithioate (3o)

^{13}C NMR (100 MHz, $CDCl_3$)



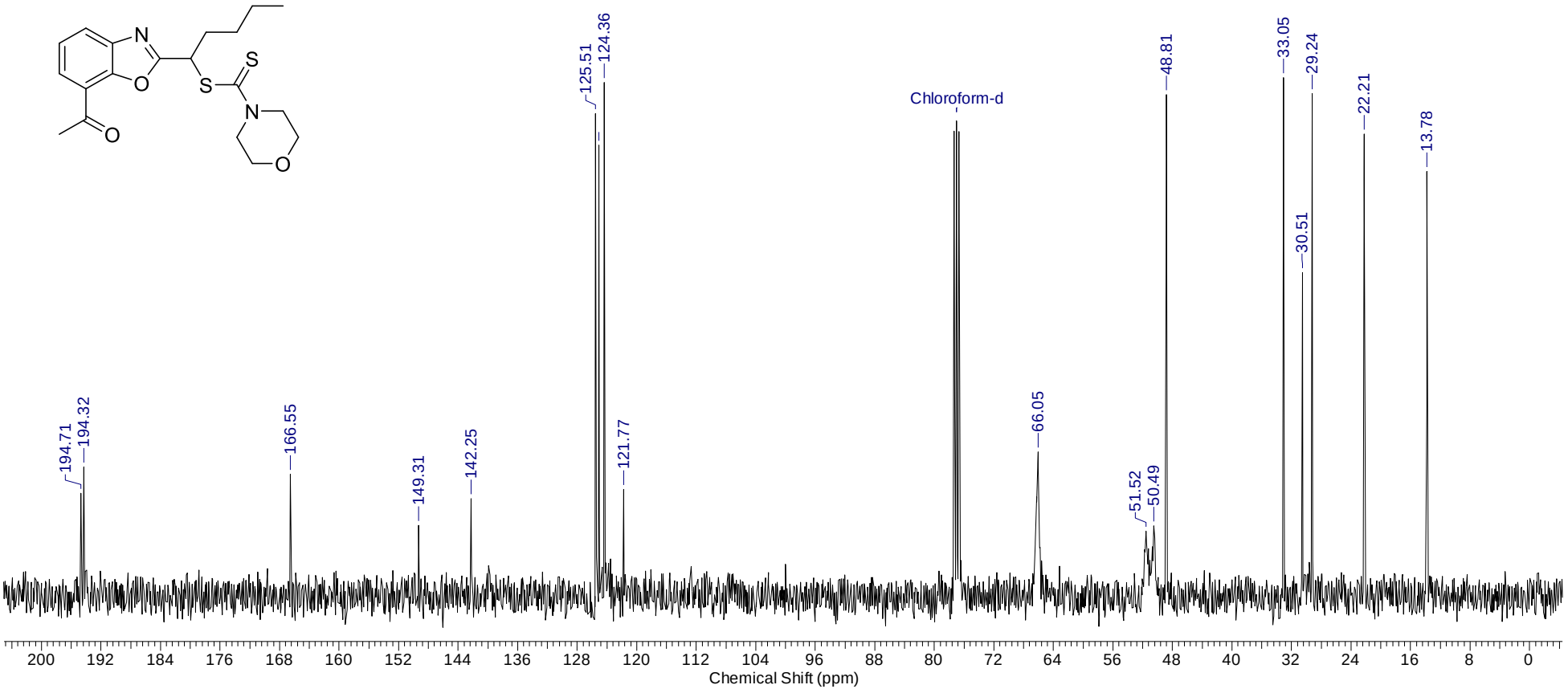
1-(7-Acetyl-1,3-benzoxazol-2-yl)pentyl morpholine-4-carbodithioate (3q)

^{1}H NMR (400 MHz, $CDCl_3$)



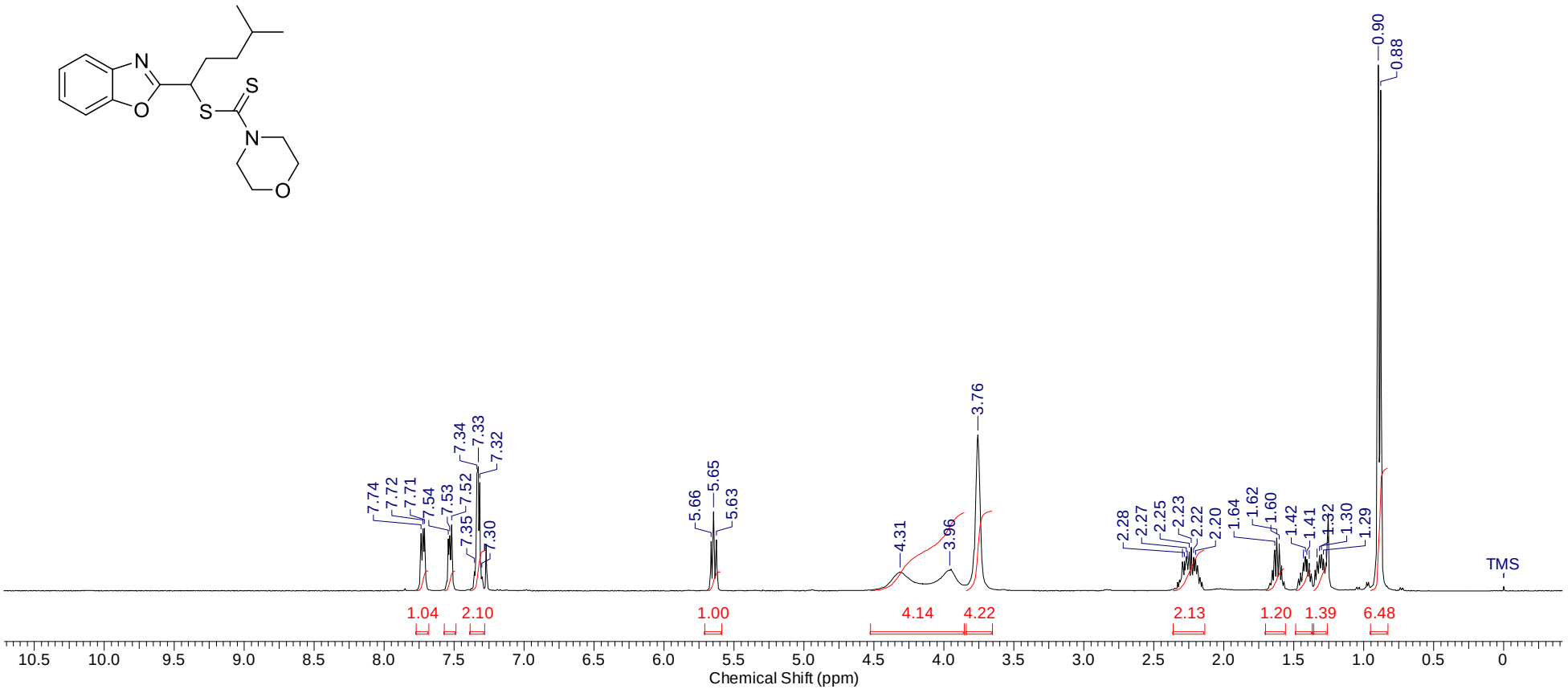
1-(7-Acetyl-1,3-benzoxazol-2-yl)pentyl morpholine-4-carbodithioate (3q)

^{13}C NMR (100 MHz, $CDCl_3$)



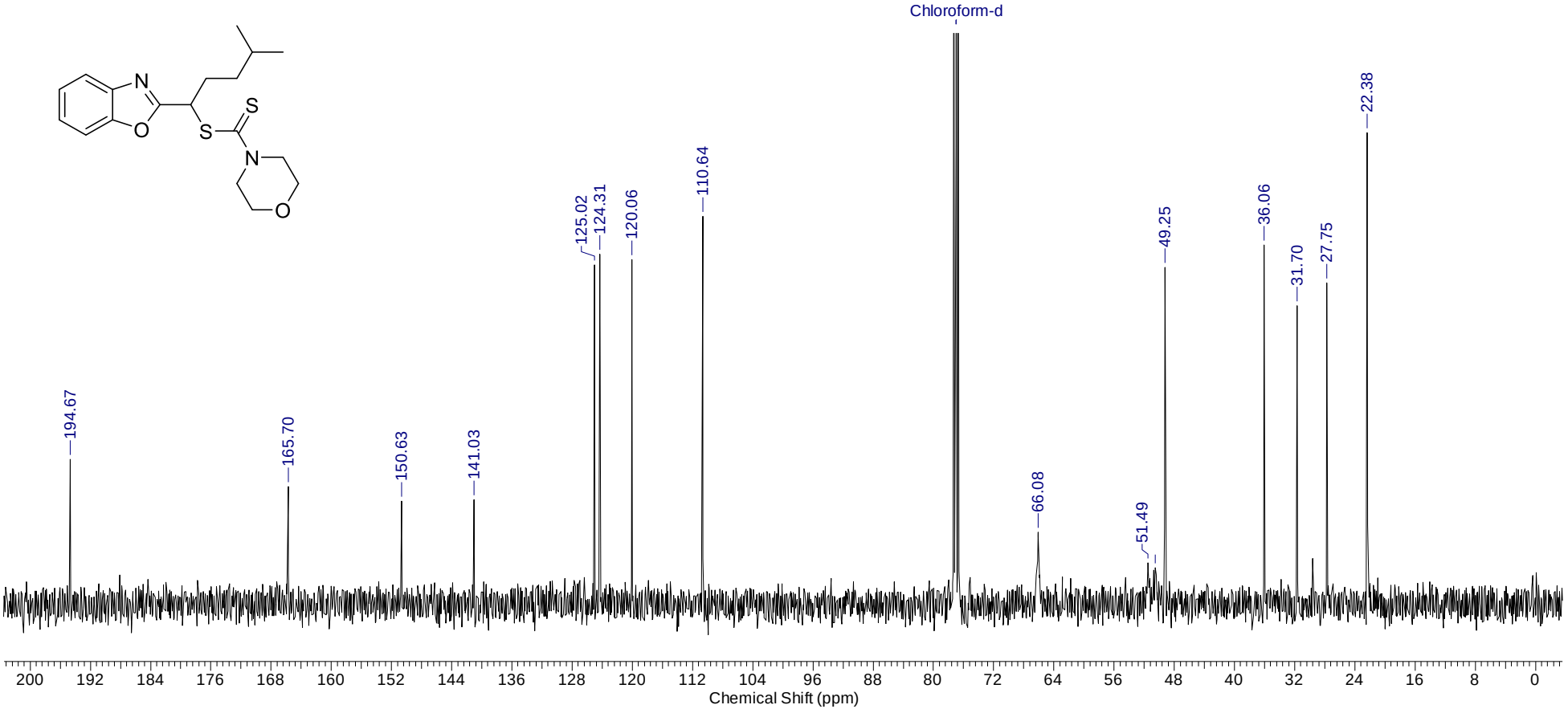
1-(1,3-Benzoxazol-2-yl)-4-methylpentyl morpholine-4-carbodithioate (3r)

^{1}H NMR (400 MHz, $CDCl_3$)



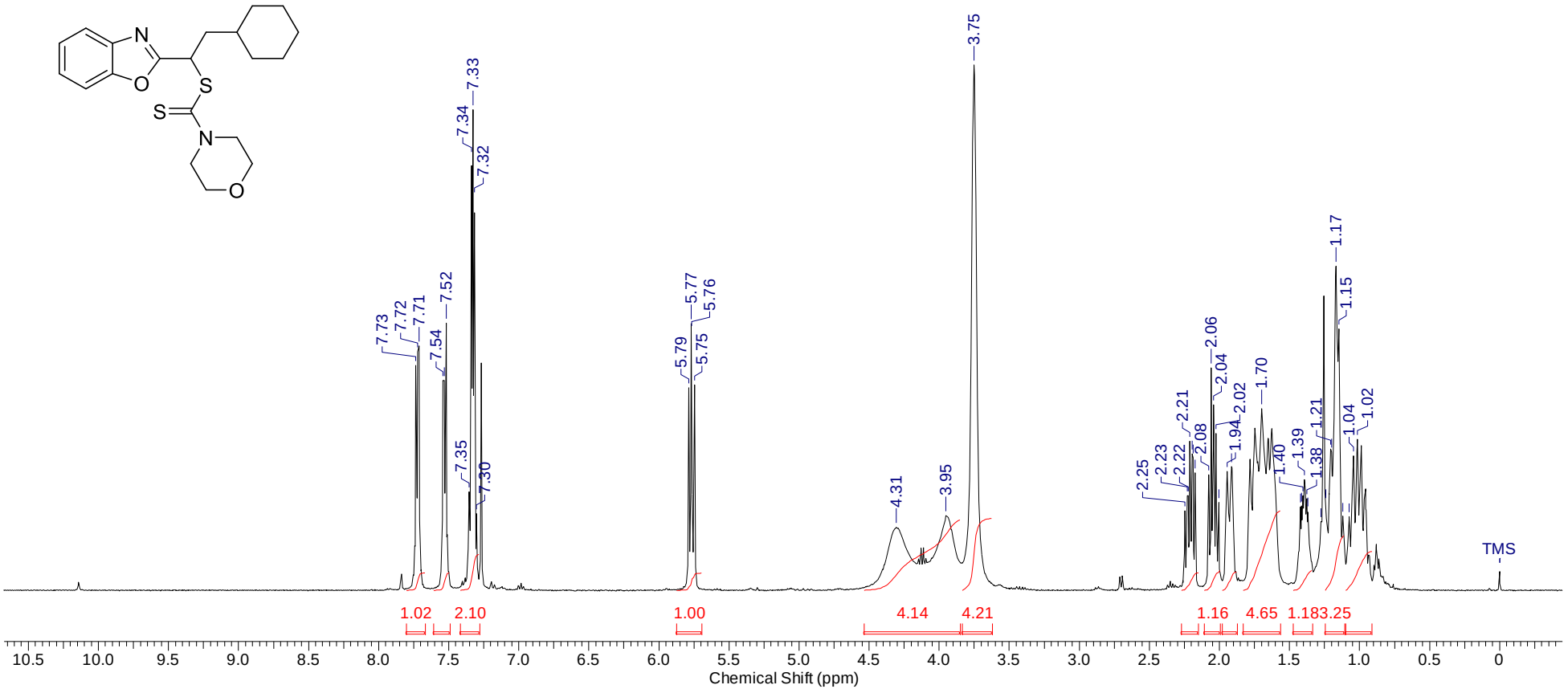
1-(1,3-Benzoxazol-2-yl)-4-methylpentyl morpholine-4-carbodithioate (3r)

^{13}C NMR (100 MHz, $CDCl_3$)



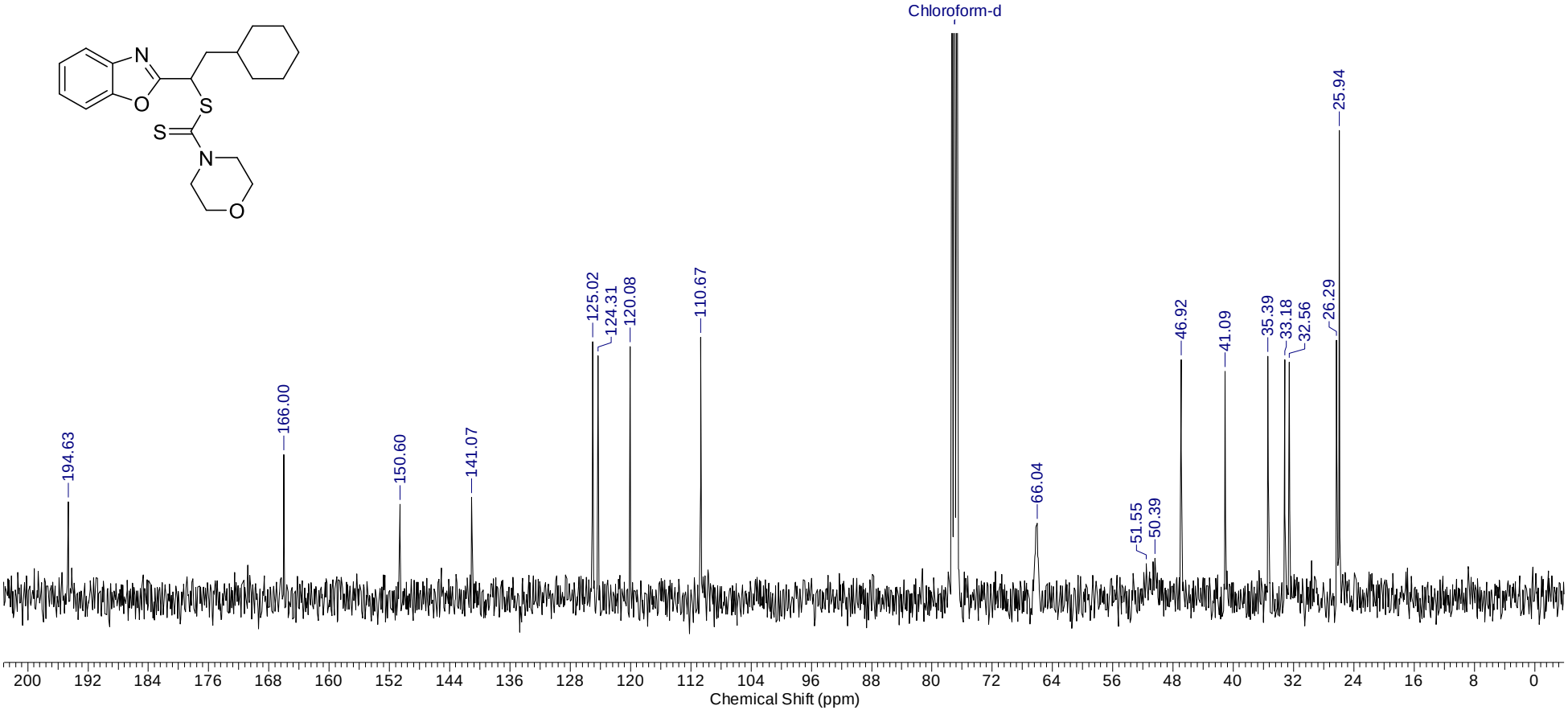
1-(1,3-Benzoxazol-2-yl)-2-cyclohexylethyl morpholine-4-carbodithioate (3s)

^{1}H NMR (400 MHz, $CDCl_3$)



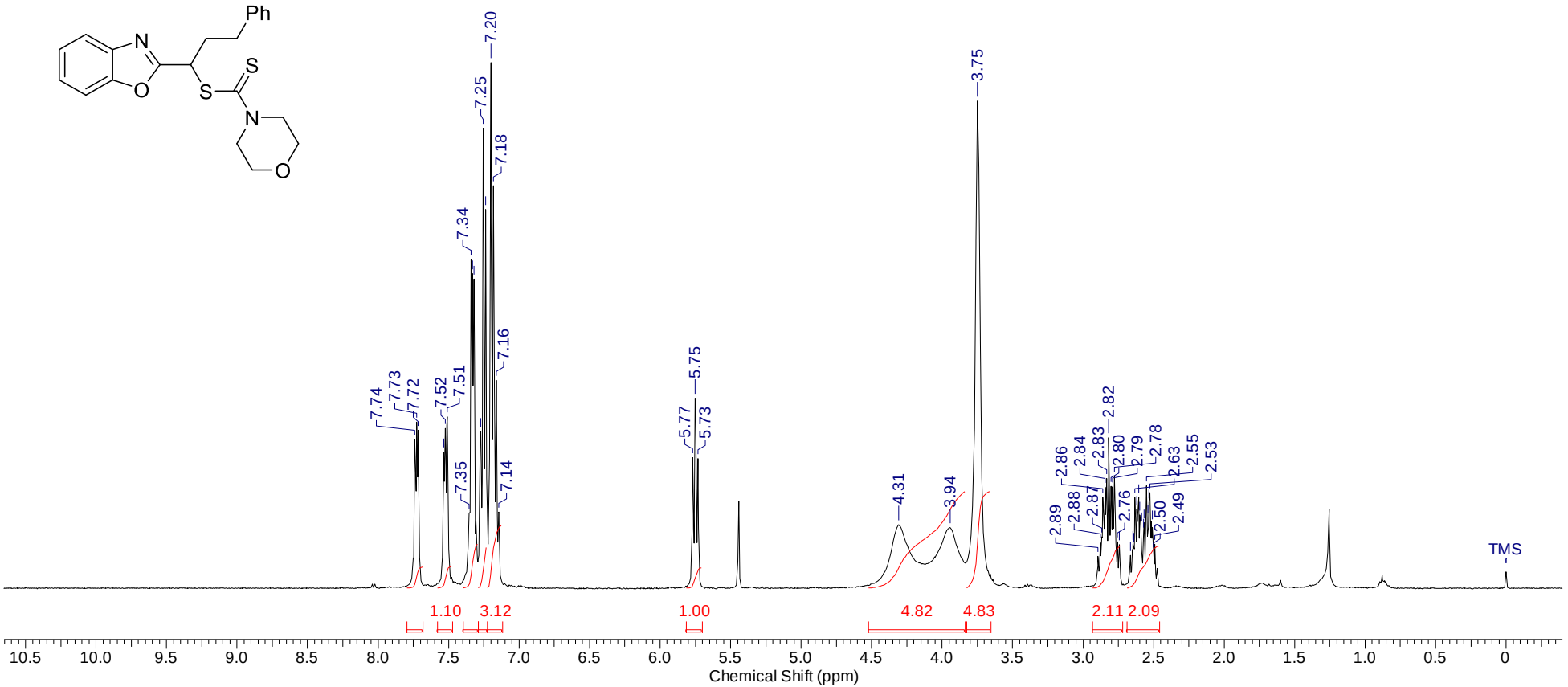
1-(1,3-Benzoxazol-2-yl)-2-cyclohexylethyl morpholine-4-carbodithioate (3s)

^{13}C NMR (100 MHz, $CDCl_3$)



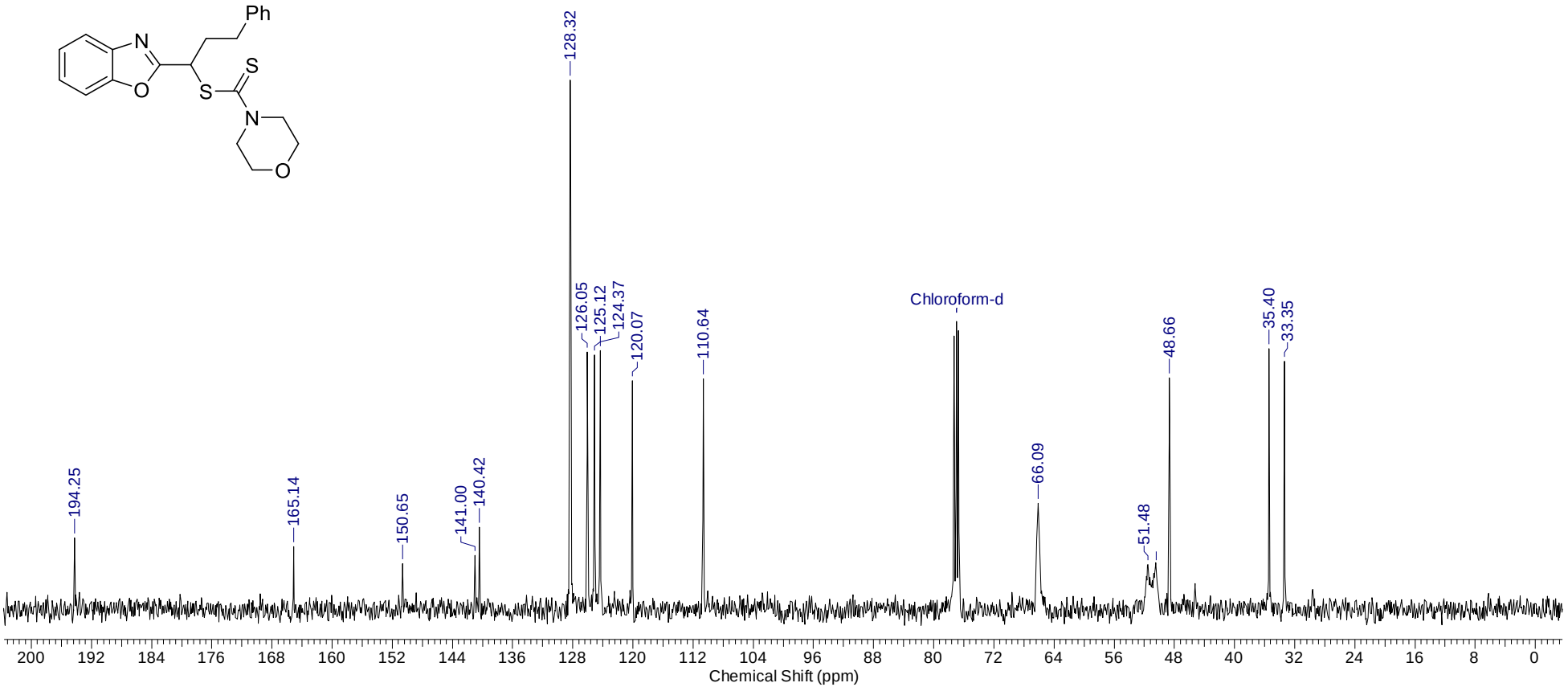
1-(1,3-Benzoxazol-2-yl)-3-phenylpropyl morpholine-4-carbodithioate (3t)

^{1}H NMR (400 MHz, $CDCl_3$)



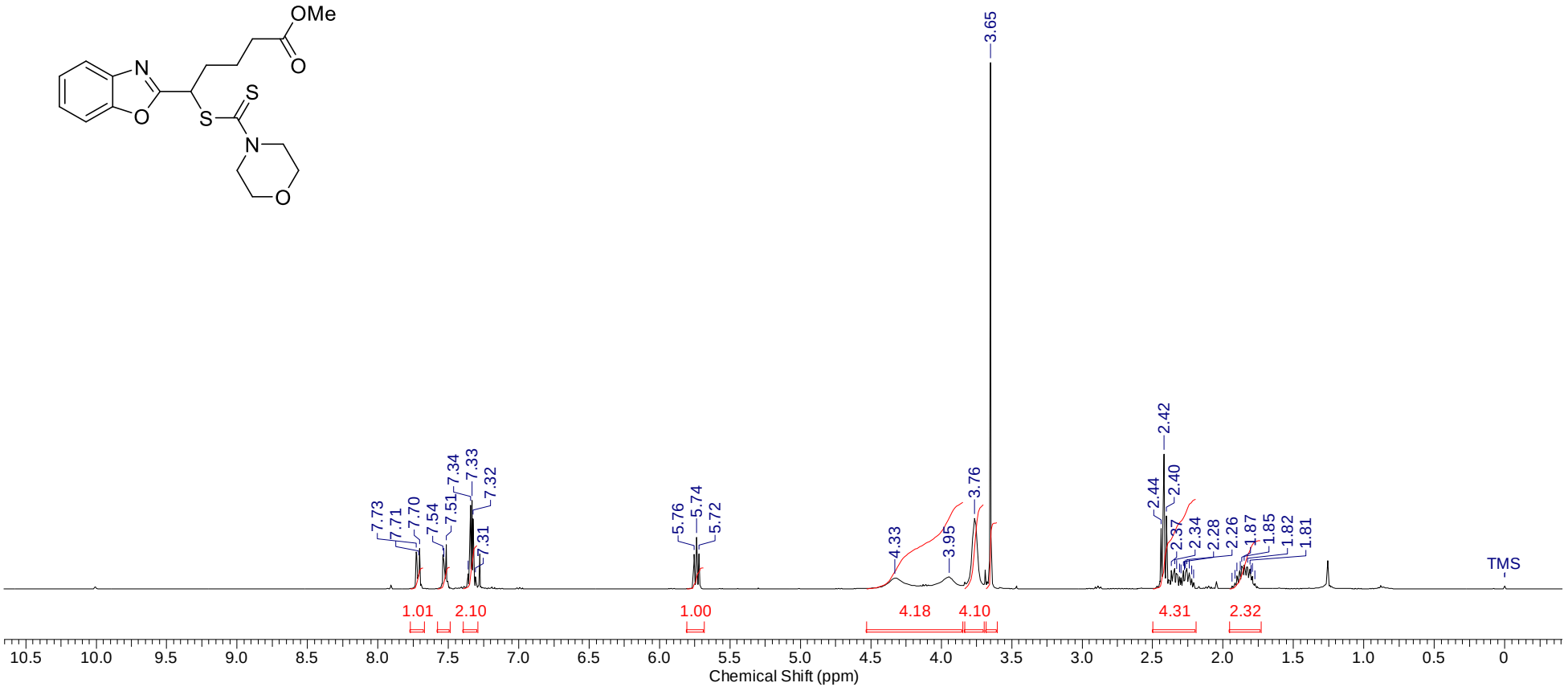
1-(1,3-Benzoxazol-2-yl)-3-phenylpropyl morpholine-4-carbodithioate (3t)

^{13}C NMR (100 MHz, $CDCl_3$)



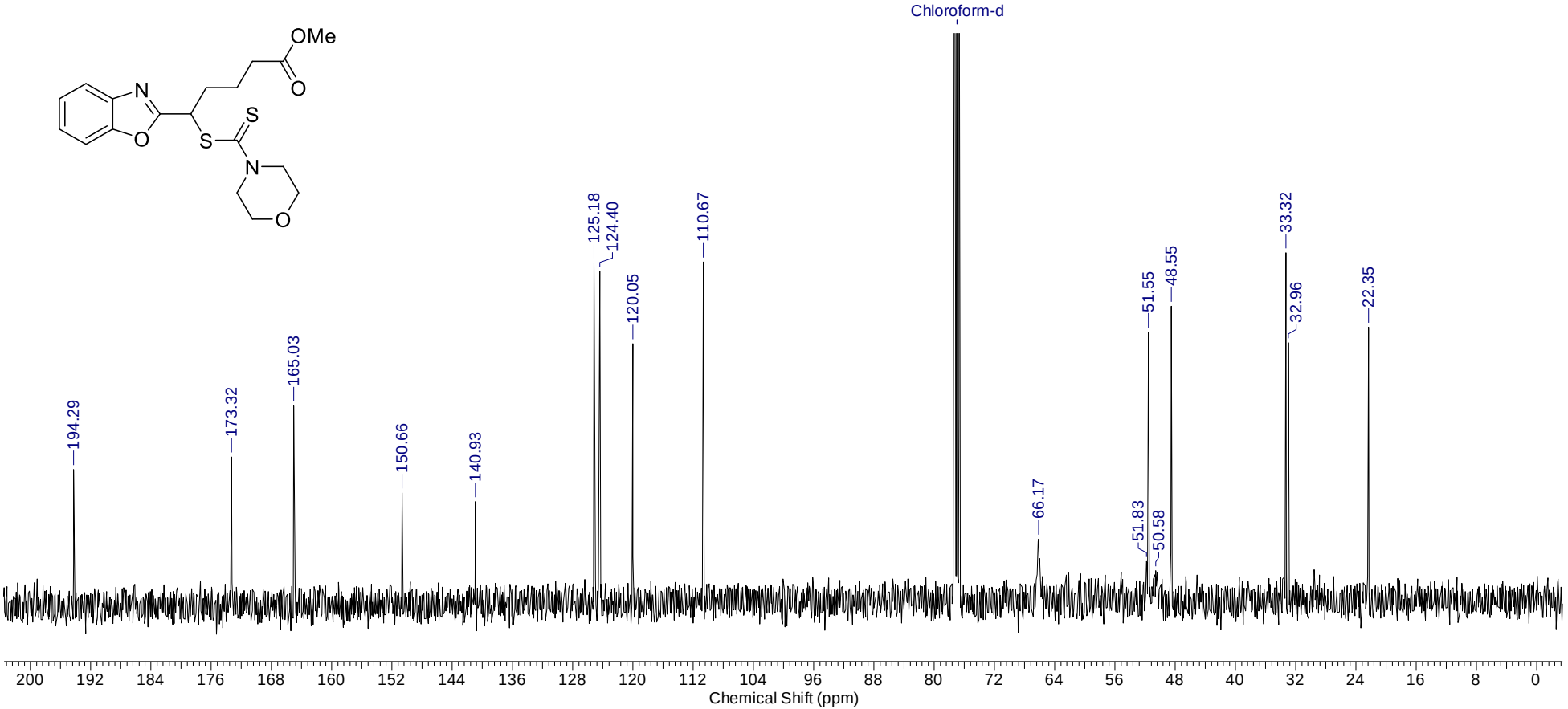
Methyl 5-(1,3-benzoxazol-2-yl)-5-[(morpholin-4-ylcarbonothioyl)thio]pentanoate (3u)

^{1}H NMR (400 MHz, $CDCl_3$)



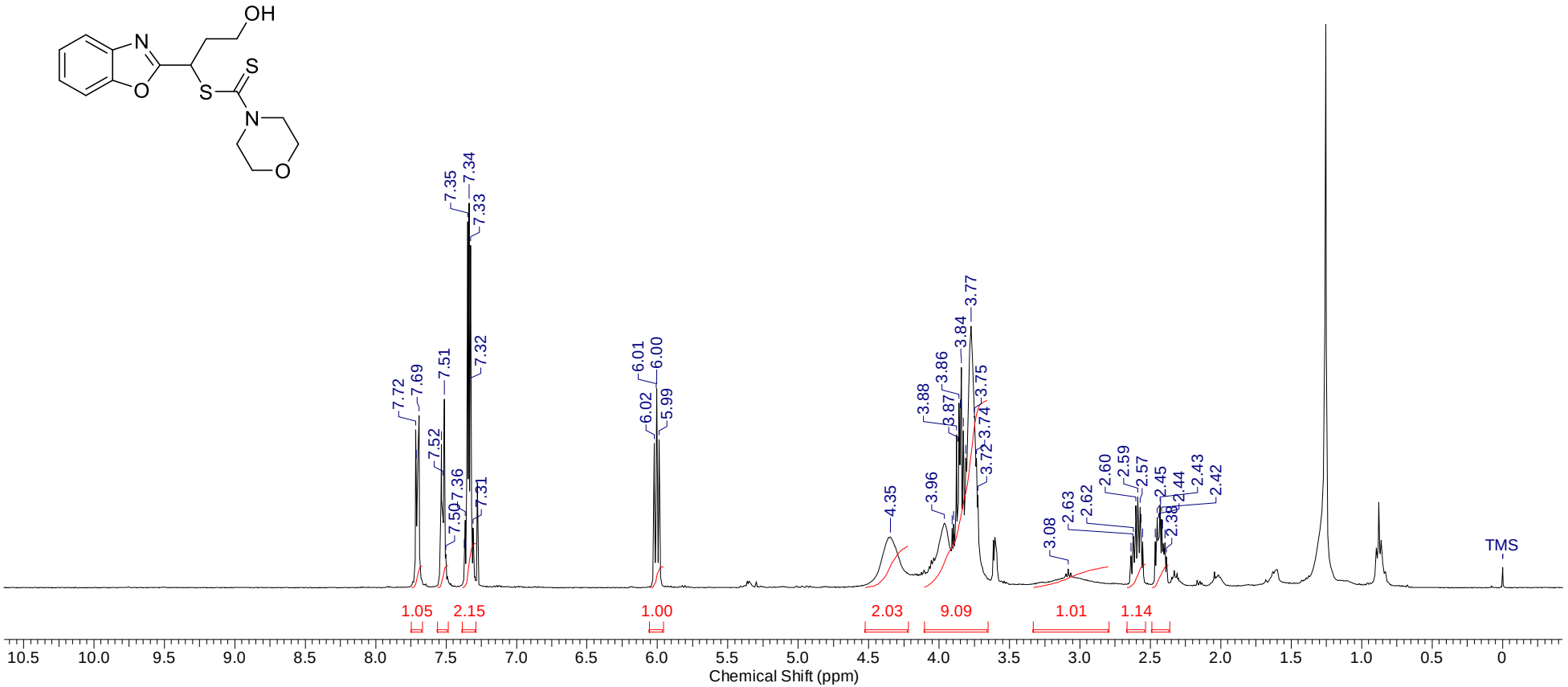
Methyl 5-(1,3-benzoxazol-2-yl)-5-[(morpholin-4-ylcarbonothioyl)thio]pentanoate (3u)

^{13}C NMR (100 MHz, $CDCl_3$)



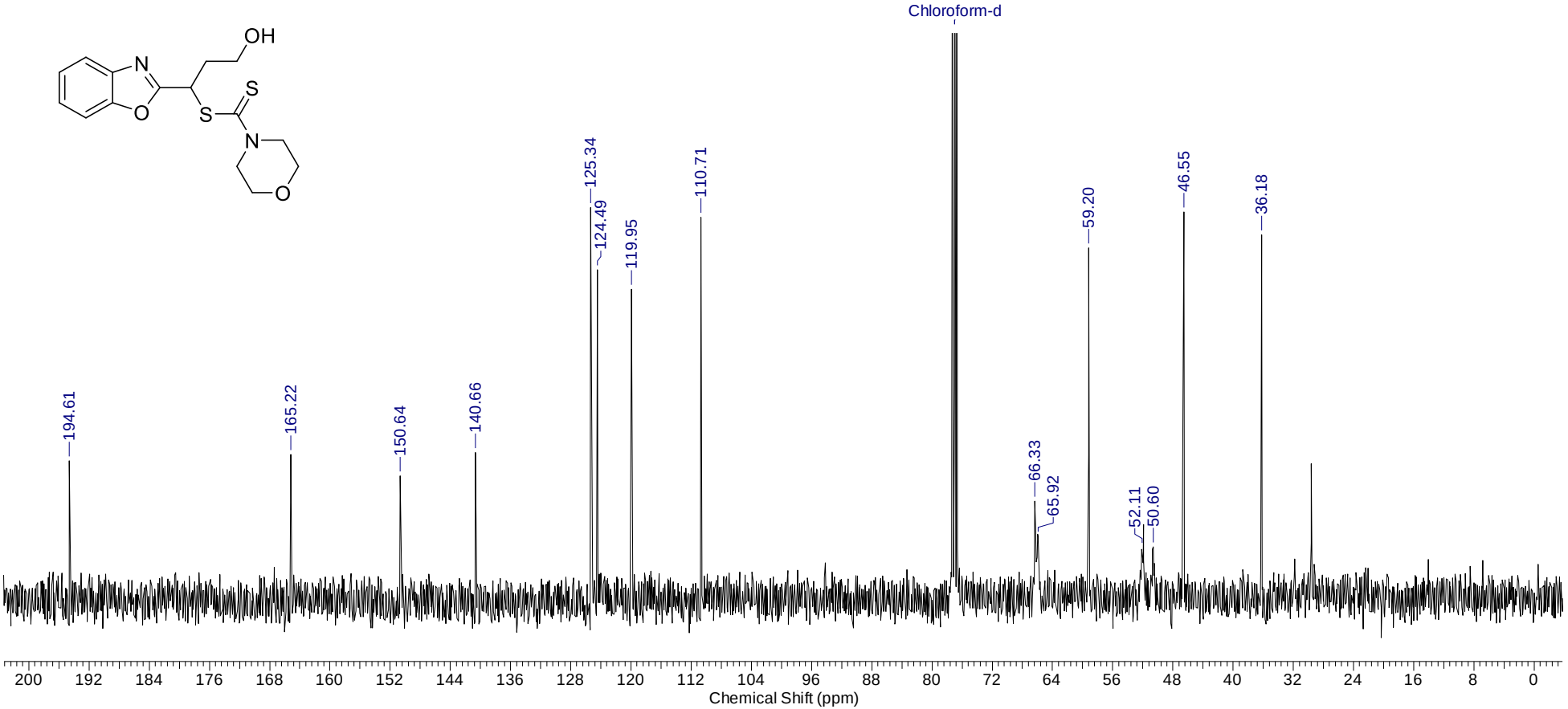
1-(1,3-Benzoxazol-2-yl)-3-hydroxypropyl morpholine-4-carbodithioate (3v)

^{1}H NMR (400 MHz, $CDCl_3$)



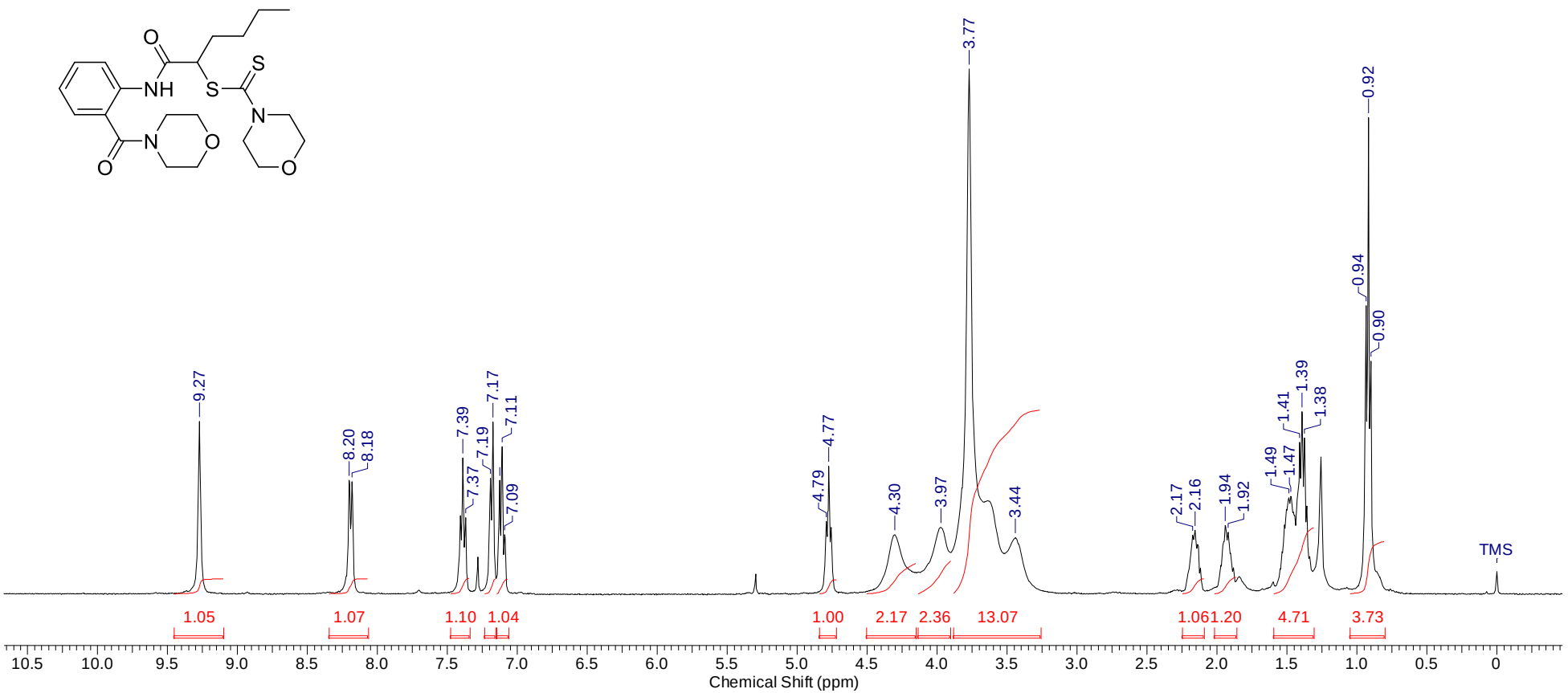
1-(1,3-Benzoxazol-2-yl)-3-hydroxypropyl morpholine-4-carbodithioate (3v)

^{13}C NMR (100 MHz, $CDCl_3$)



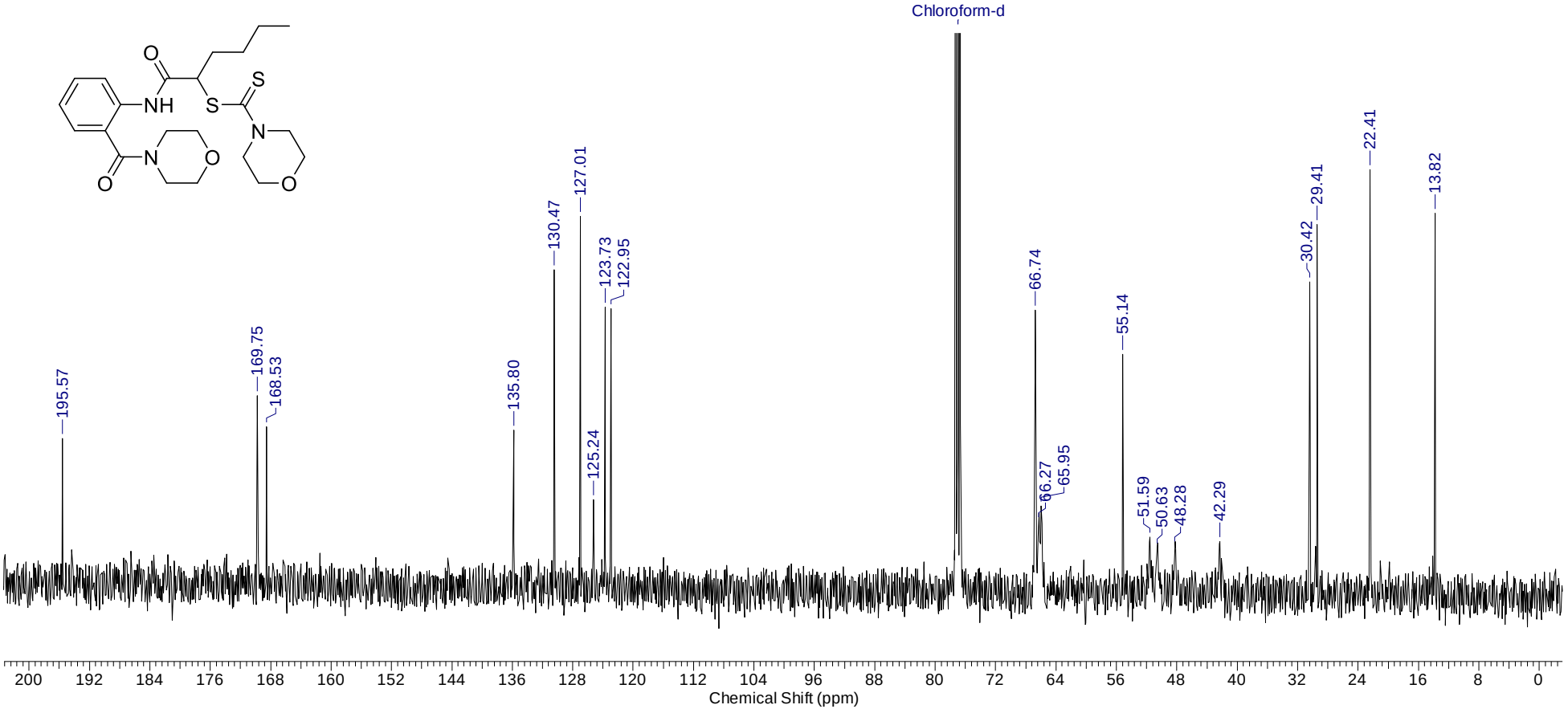
1-({[2-(Morpholin-4-ylcarbonyl)phenyl]amino}carbonyl)pentyl morpholine-4-carbodithioate (11a)

^{1}H NMR (400 MHz, $CDCl_3$)



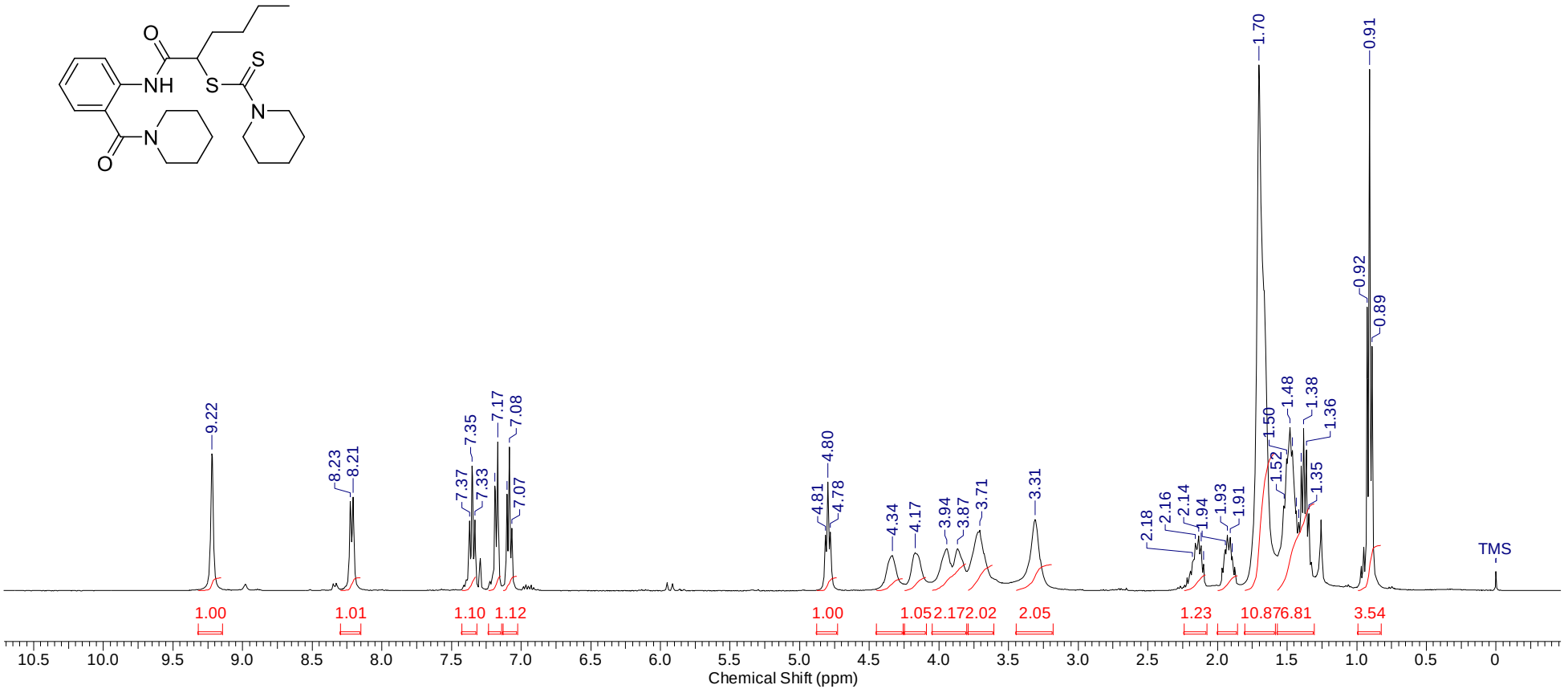
1-({[2-(Morpholin-4-ylcarbonyl)phenyl]amino}carbonyl)pentyl morpholine-4-carbodithioate (11a)

^{13}C NMR (100 MHz, $CDCl_3$)



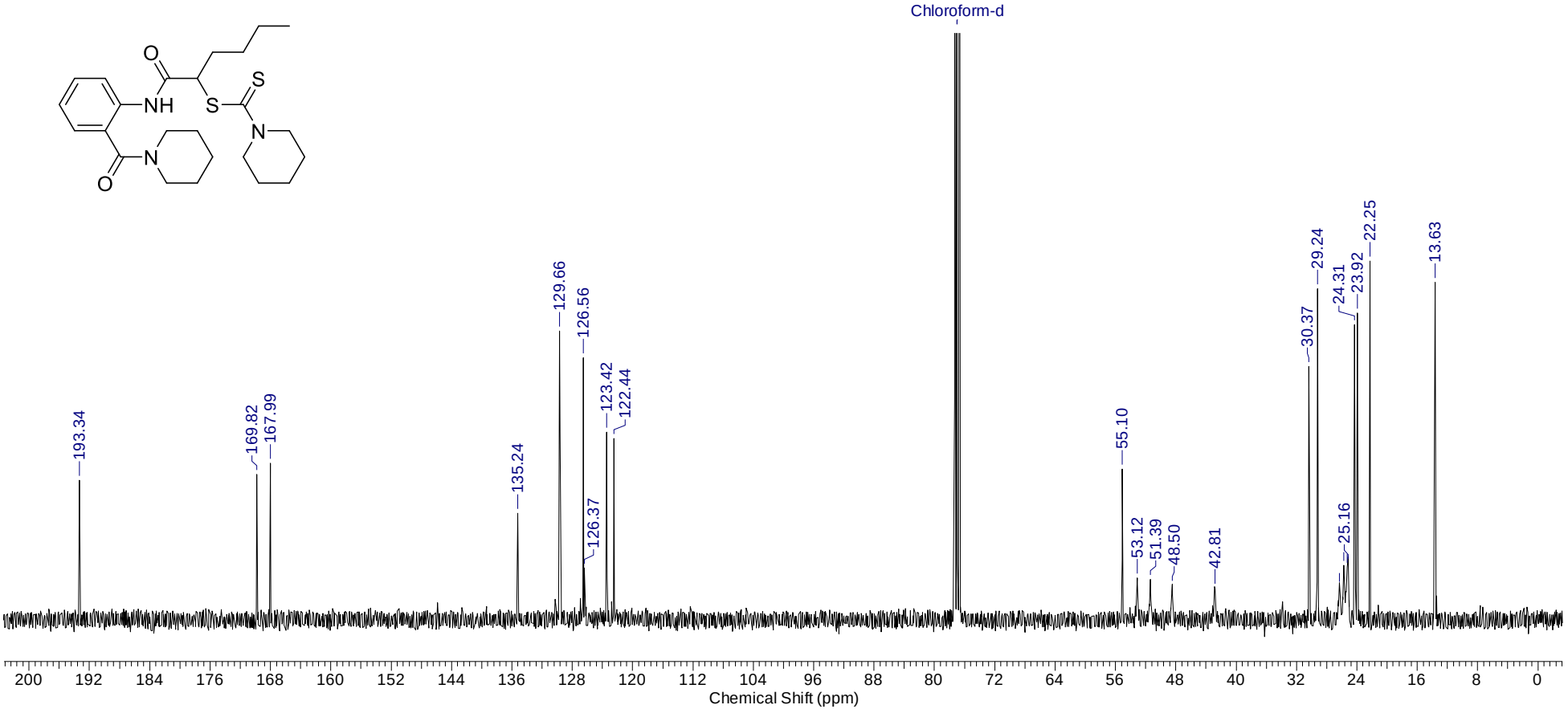
1-({[2-(Piperidin-4-ylcarbonyl)phenyl]amino}carbonyl)pentyl piperidine-4-carbodithioate (11b)

^{1}H NMR (400 MHz, $CDCl_3$)



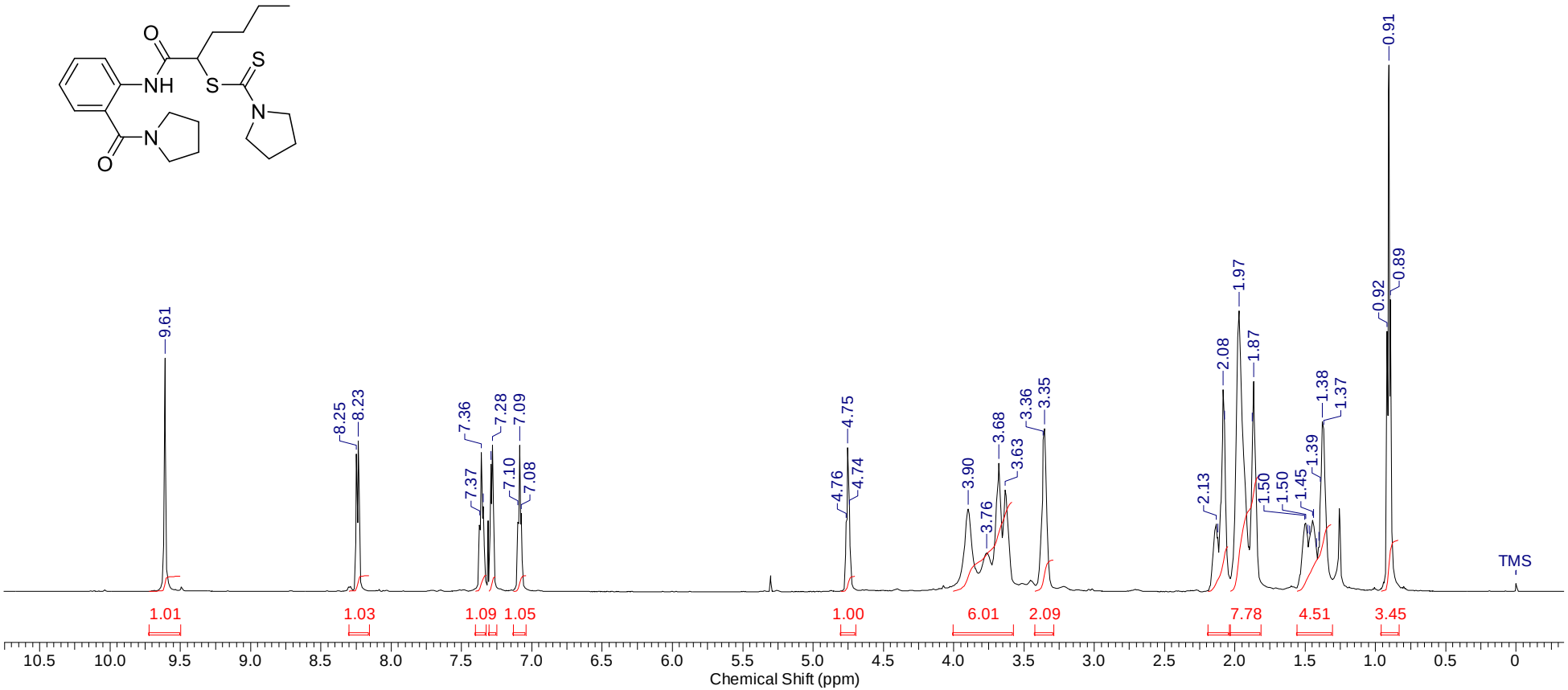
1-({[2-(Piperidin-4-ylcarbonyl)phenyl]amino}carbonyl)pentyl piperidine-4-carbodithioate (11b)

^{13}C NMR (100 MHz, $CDCl_3$)



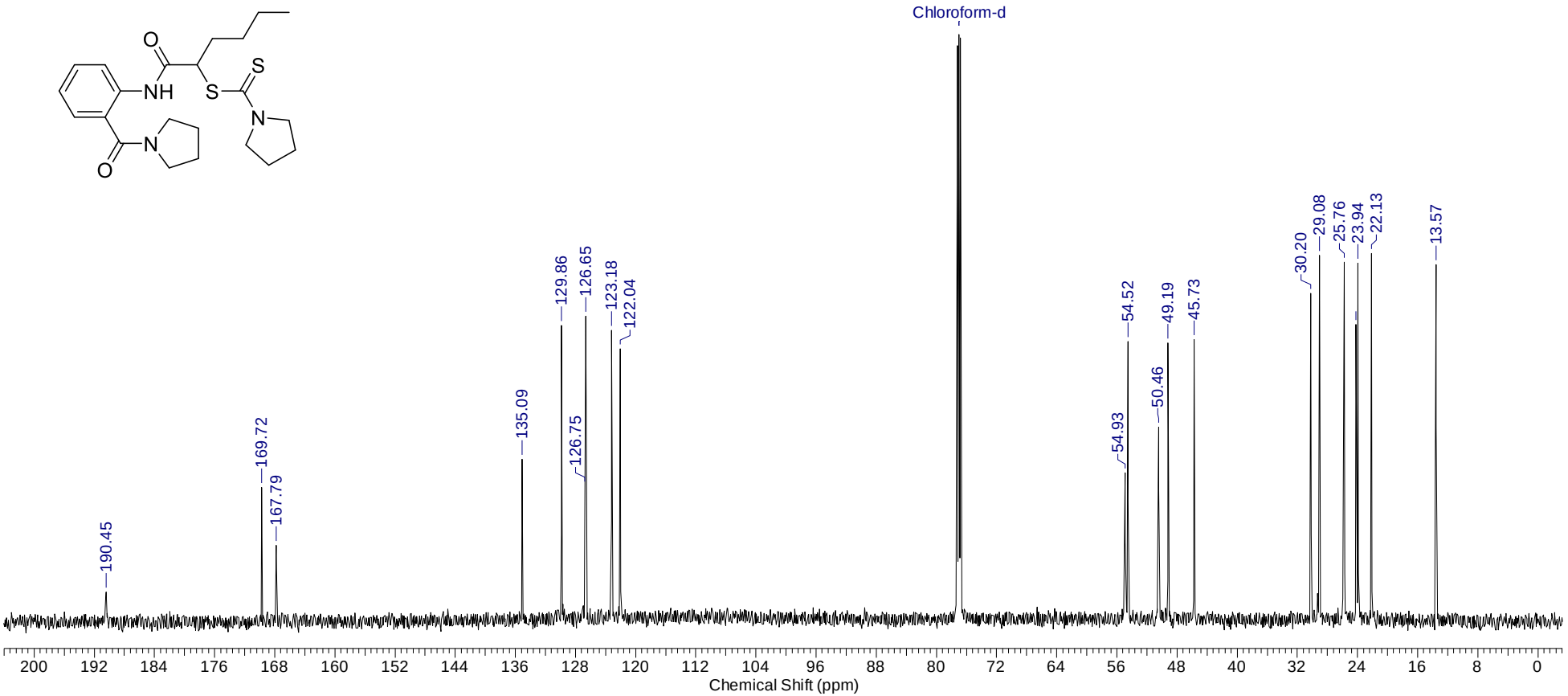
1-({[2-(Pyrrolidin-4-ylcarbonyl)phenyl]amino}carbonyl)pentyl pyrrolidine-4-carbodithioate (11c)

^{1}H NMR (600 MHz, $CDCl_3$)



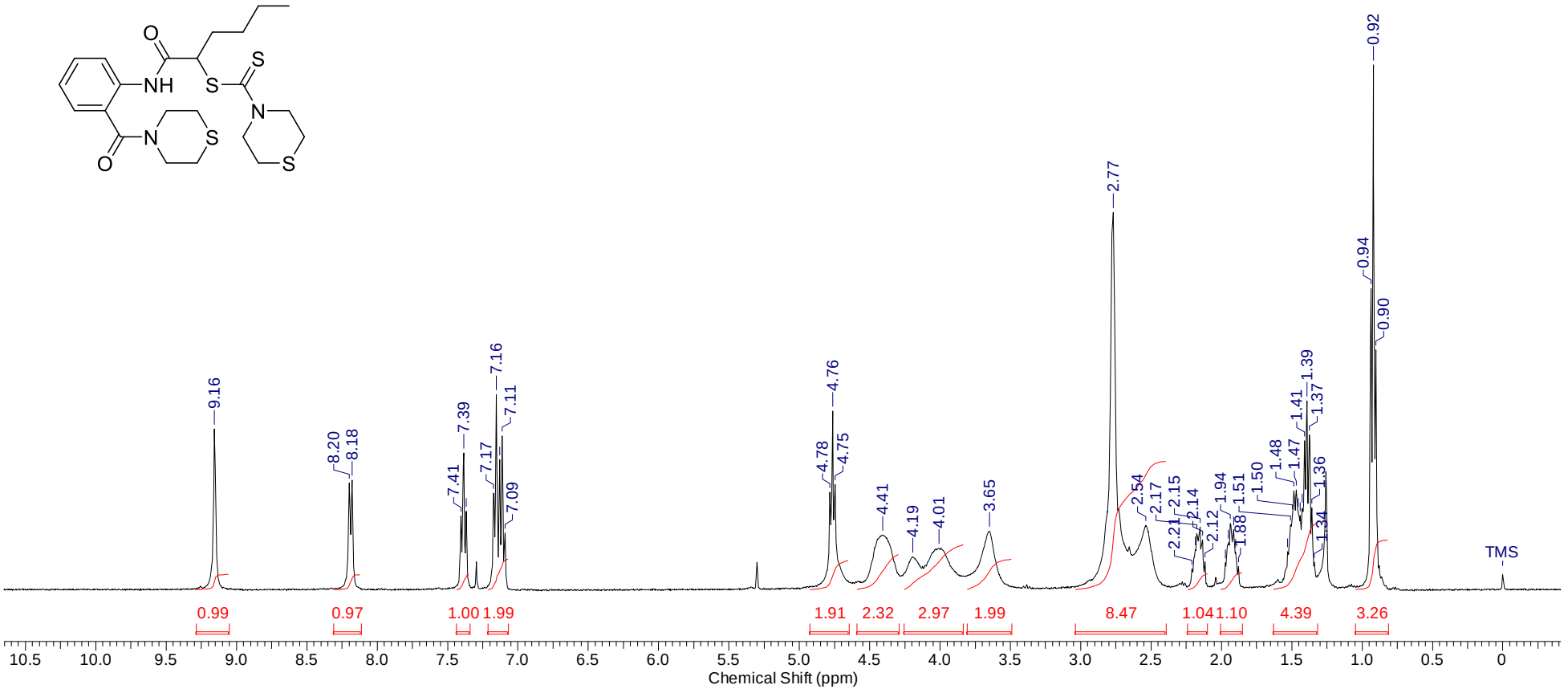
1-({[2-(Pyrrolidin-4-ylcarbonyl)phenyl]amino}carbonyl)pentyl pyrrolidine-4-carbodithioate (11c)

^{13}C NMR (151 MHz, $CDCl_3$)



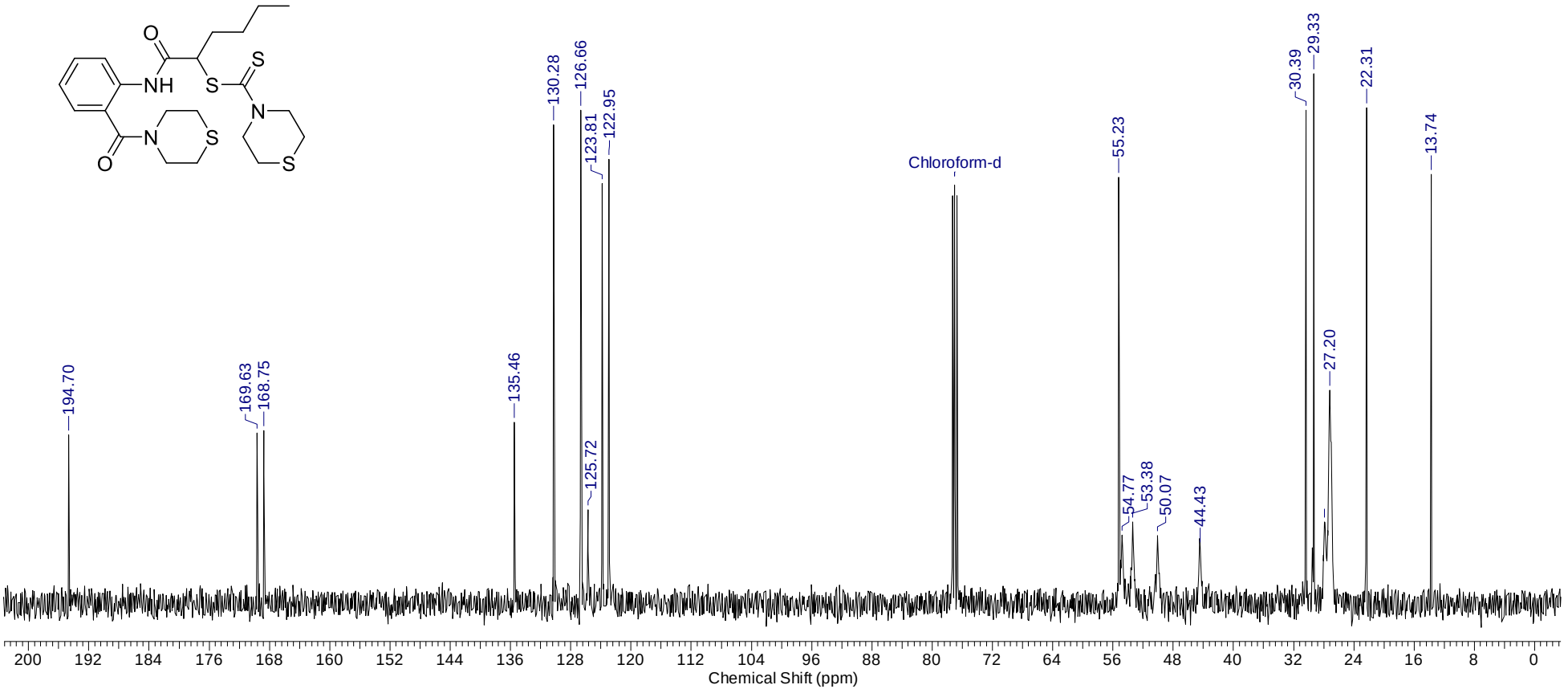
1-({[2-(Thiomorpholin-4-ylcarbonyl)phenyl]amino}carbonyl)pentyl thiomorpholine-4-carbodithioate (11d)

^{1}H NMR (400 MHz, $CDCl_3$)



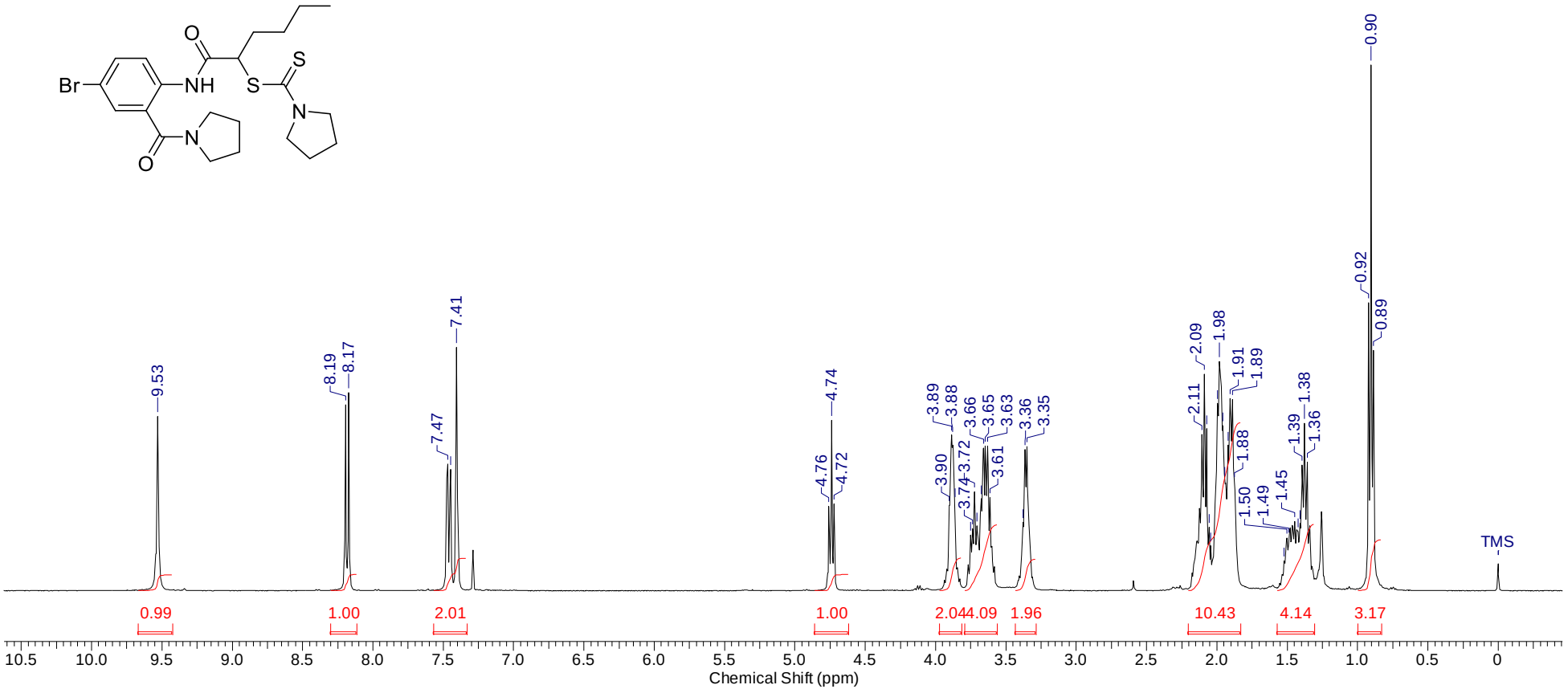
1-({[2-(Thiomorpholin-4-ylcarbonyl)phenyl]amino}carbonyl)pentyl thiomorpholine-4-carbodithioate (11d)

^{13}C NMR (100 MHz, $CDCl_3$)



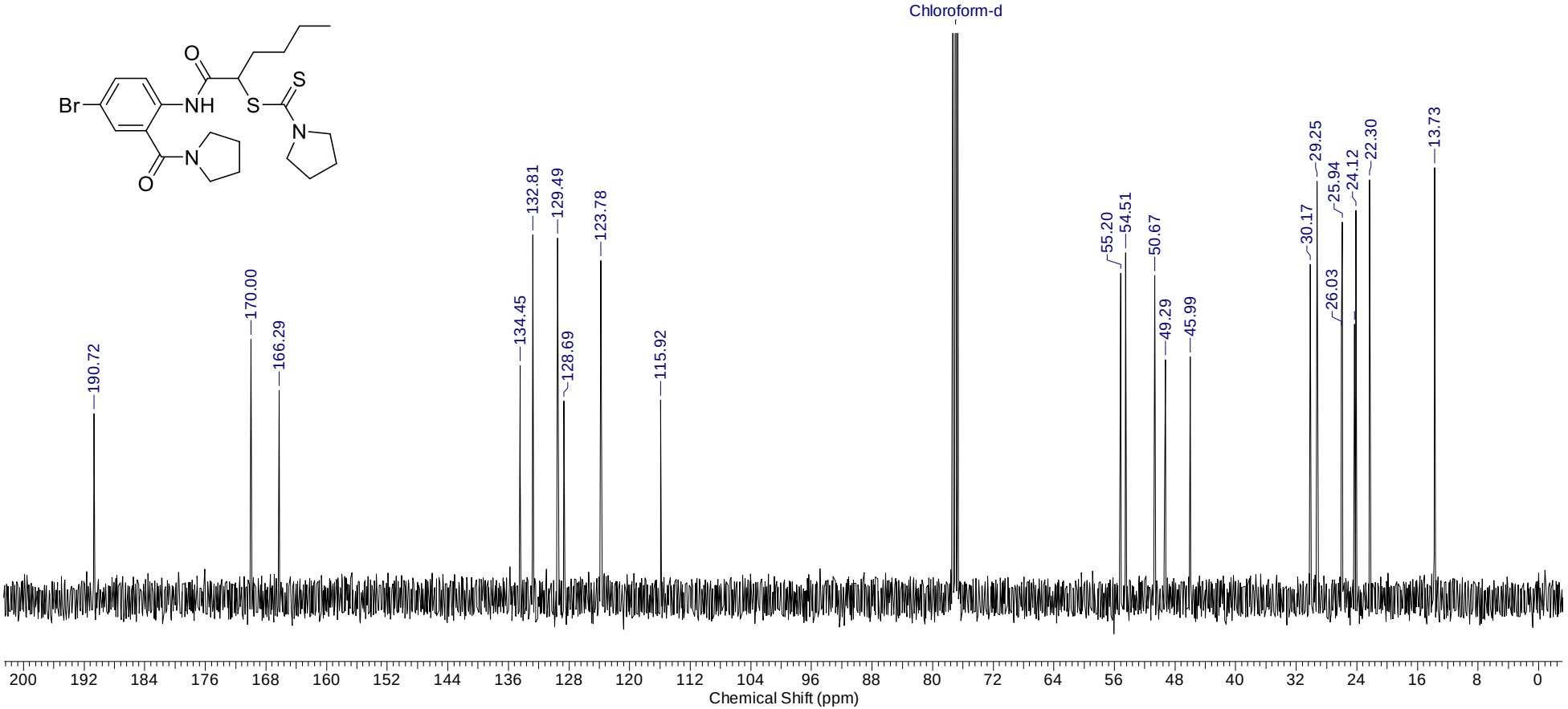
1-({[4-Bromo-2-(pyrrolidin-1-ylcarbonyl)phenyl]amino}carbonyl)pentyl pyrrolidine-1-carbodithioate (11e)

^{1}H NMR (400 MHz, $CDCl_3$)



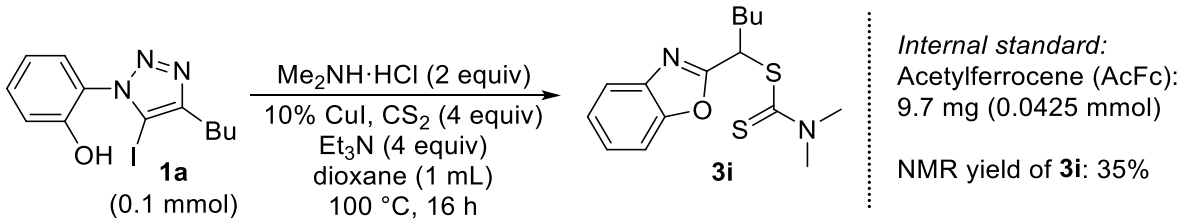
1-({[4-Bromo-2-(pyrrolidin-1-ylcarbonyl)phenyl]amino}carbonyl)pentyl pyrrolidine-1-carbodithioate (11e)

^{13}C NMR (100 MHz, $CDCl_3$)



Analysis of crude reaction mixtures

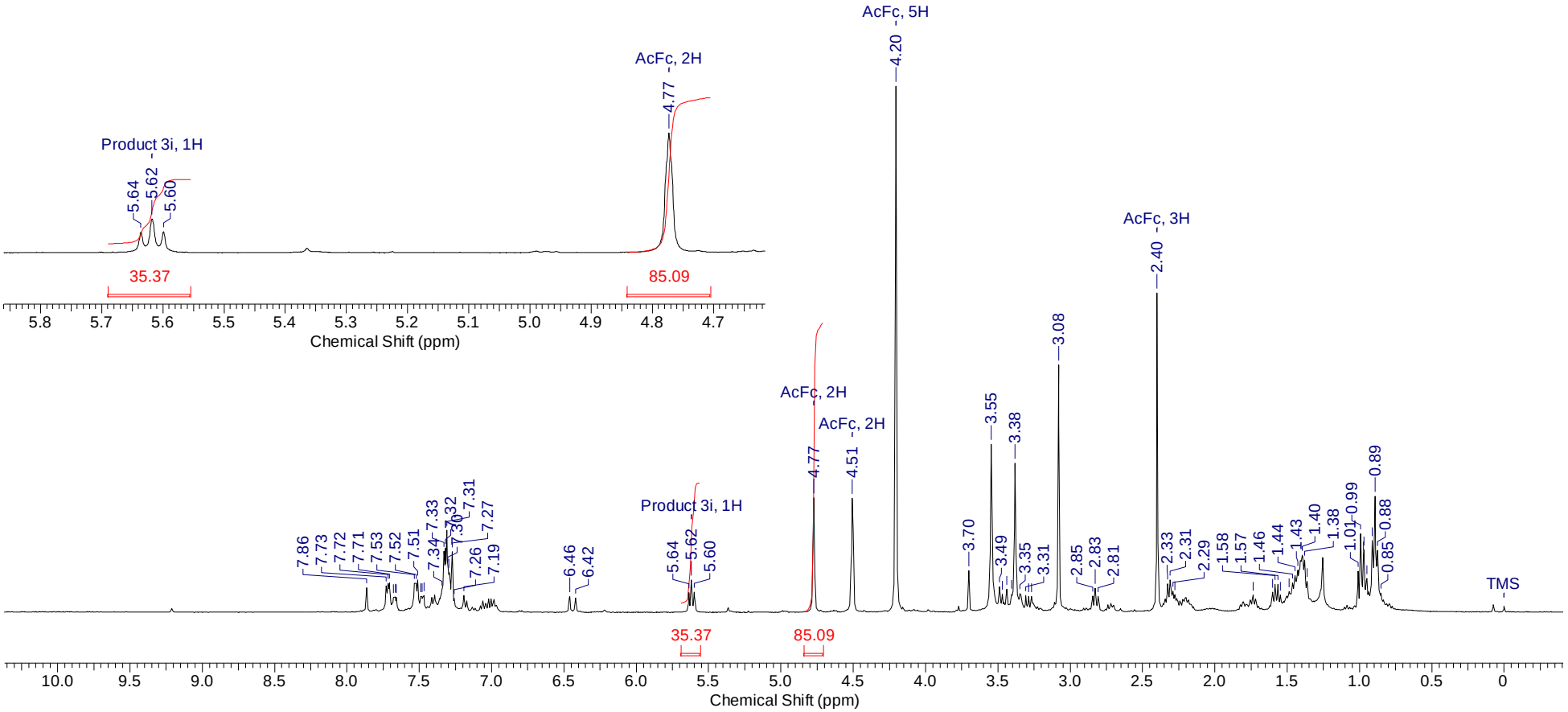
1-(1,3-Benzoxazol-2-yl)pentyl dimethyldithiocarbamate (3i)



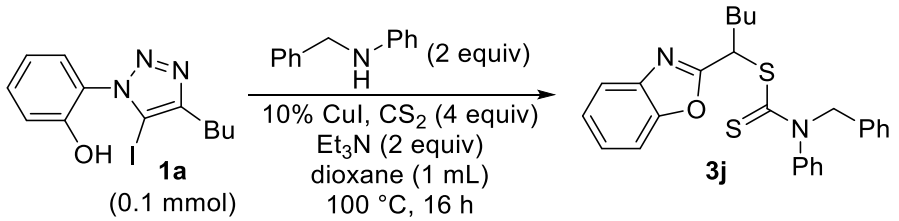
Internal standard:
Acetylferrocene (AcFc):
9.7 mg (0.0425 mmol)

NMR yield of **3i**: 35%

^{1}H NMR (400 MHz, $CDCl_3$)



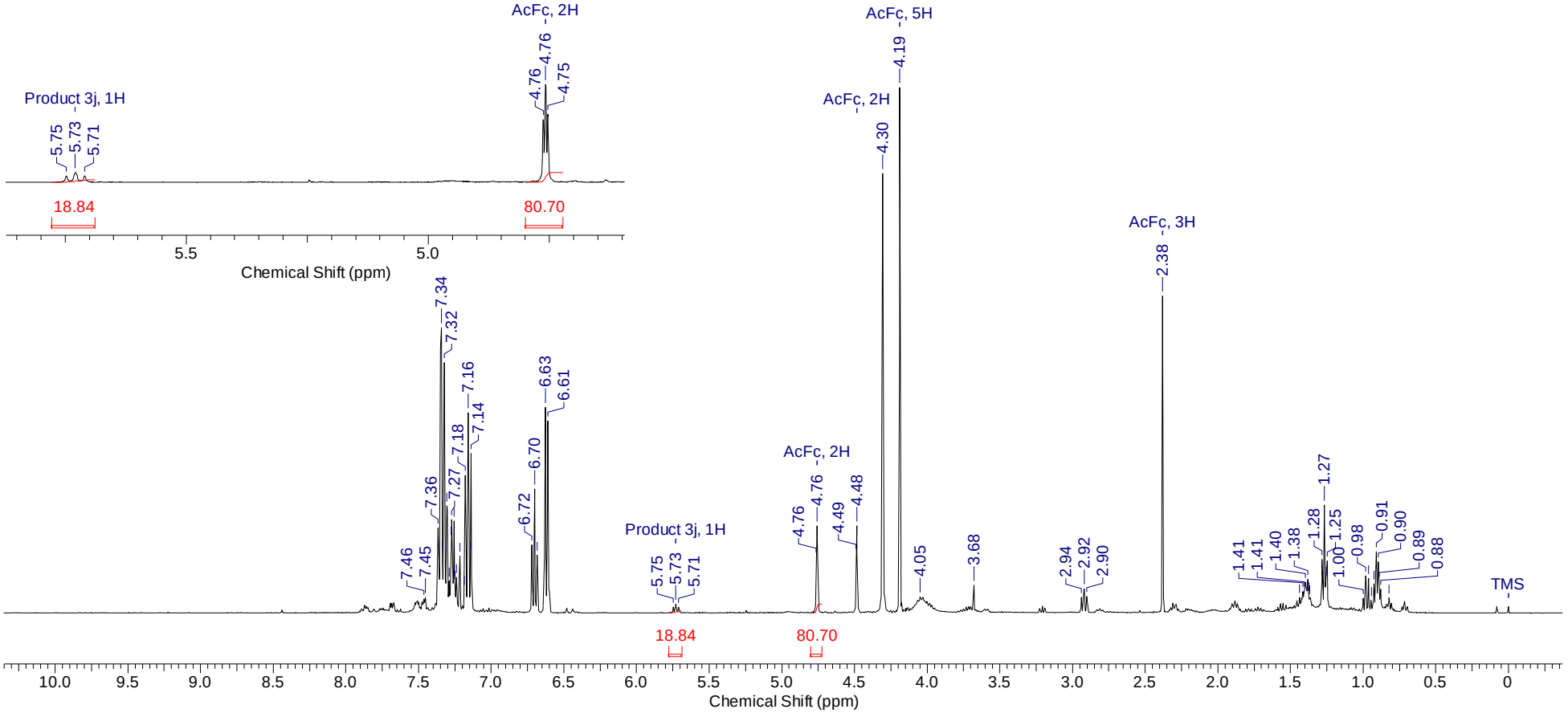
1-(1,3-Benzoxazol-2-yl)pentyl benzyl(phenyl)dithiocarbamate (3j)



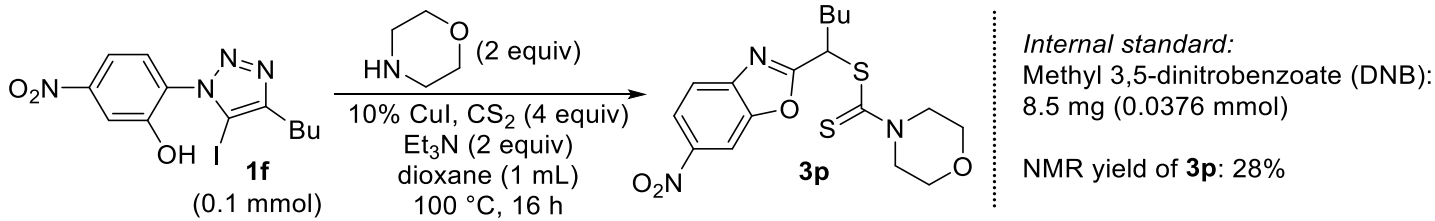
Internal standard:
Acetylferrocene (AcFc):
9.2 mg (0.0404 mmol)

NMR yield of **3j**: 19%

^{1}H NMR (400 MHz, $CDCl_3$)



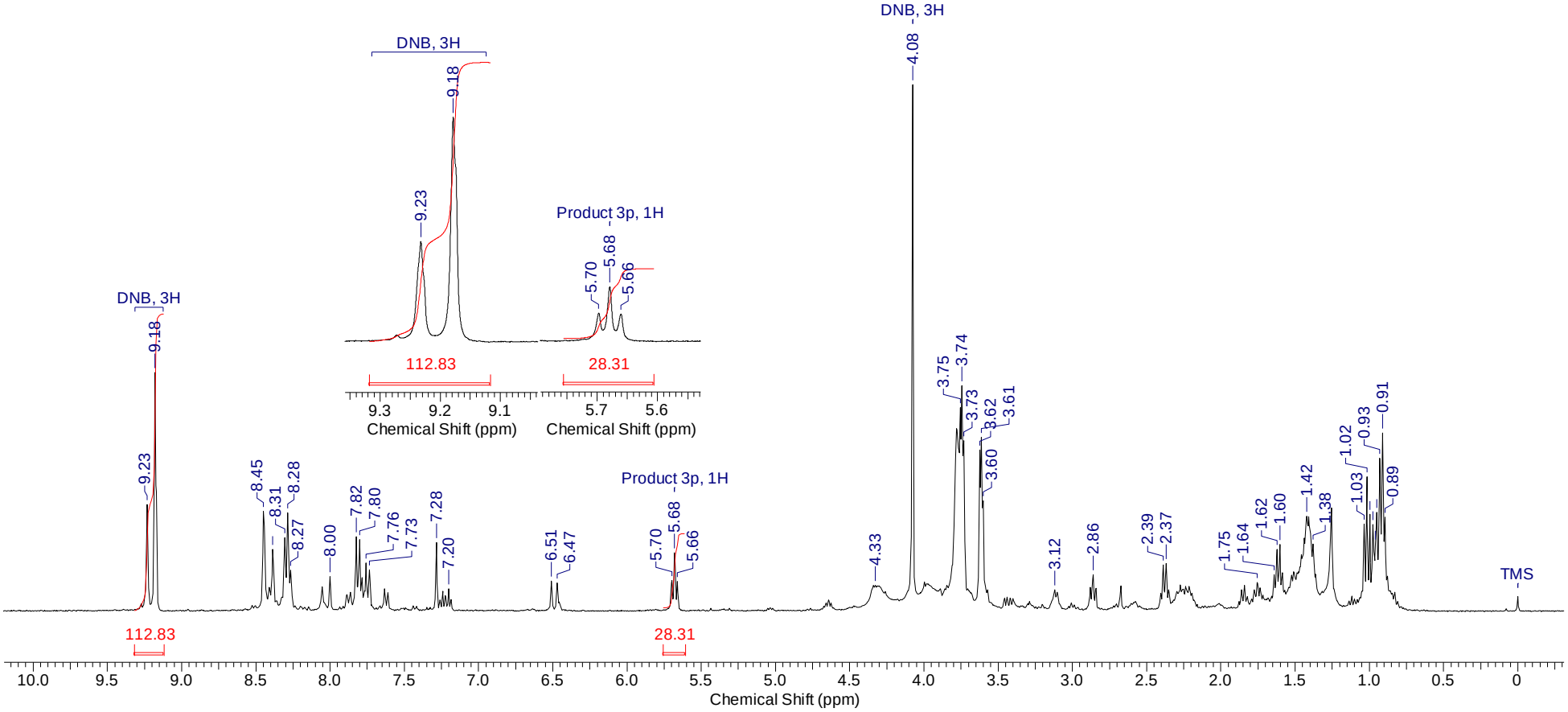
1-(6-Nitro-1,3-benzoxazol-2-yl)pentyl morpholine-4-carbodithioate (3p)



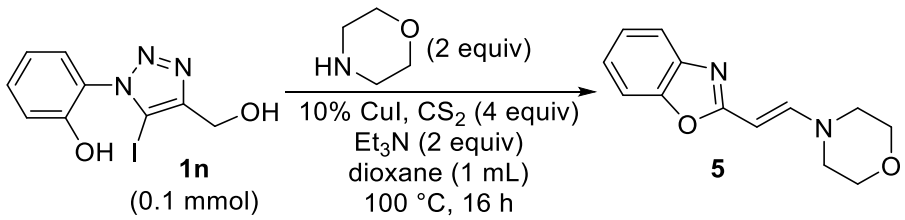
Internal standard:
Methyl 3,5-dinitrobenzoate (DNB):
8.5 mg (0.0376 mmol)

NMR yield of **3p**: 28%

^{1}H NMR (400 MHz, $CDCl_3$)



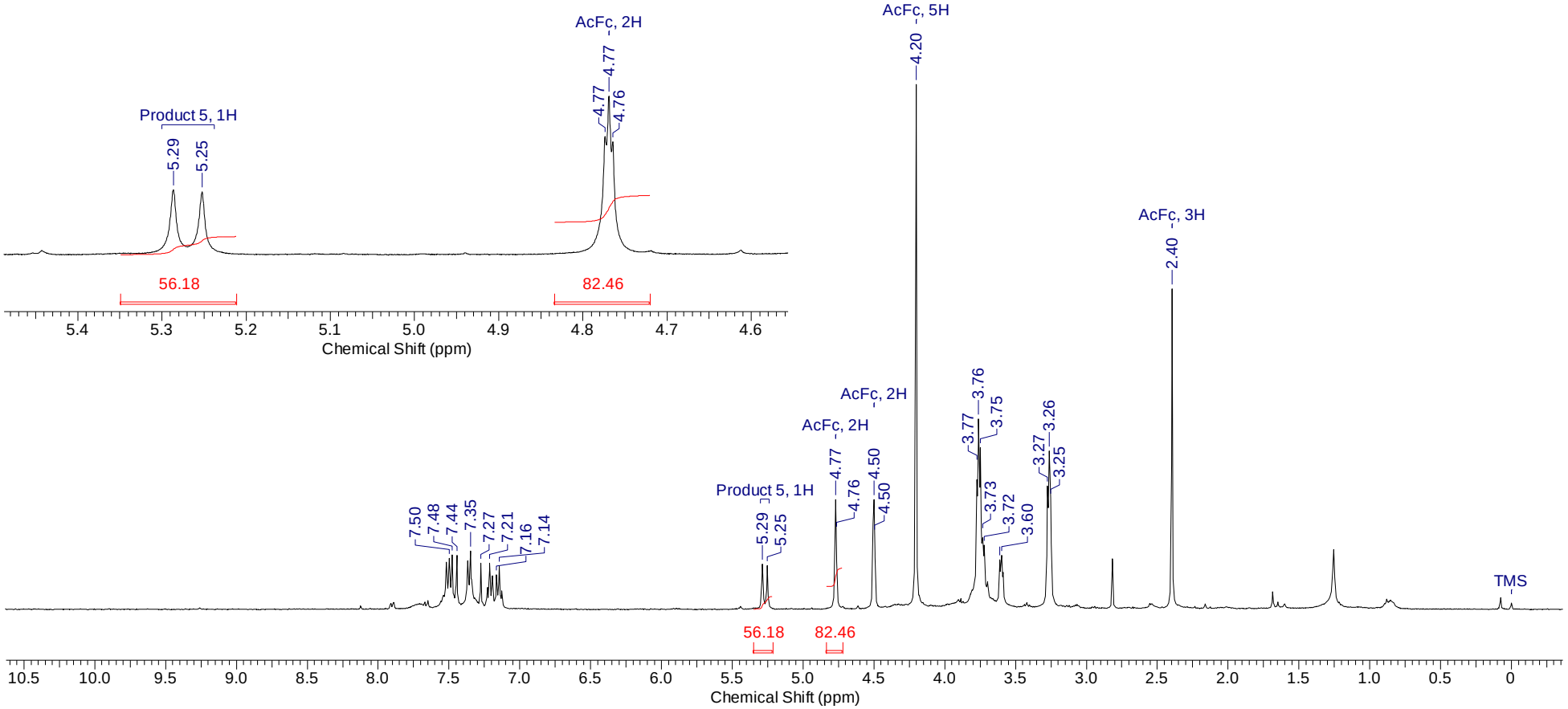
2-[(*E*)-2-Morpholin-4-ylvinyl]-1,3-benzoxazole (5)



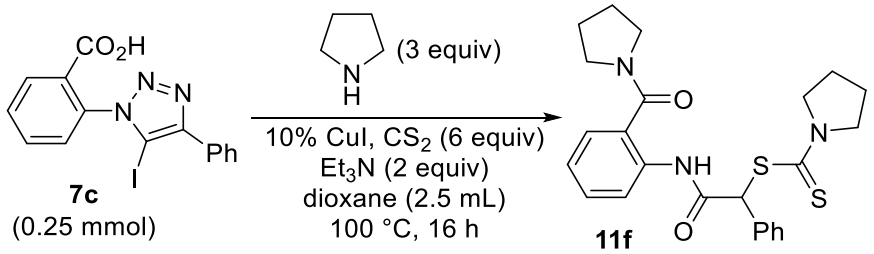
Internal standard:
Acetylferrocene (AcFc):
9.4 mg (0.0412 mmol)

NMR yield of **5**: 56%

^{1}H NMR (400 MHz, $CDCl_3$)



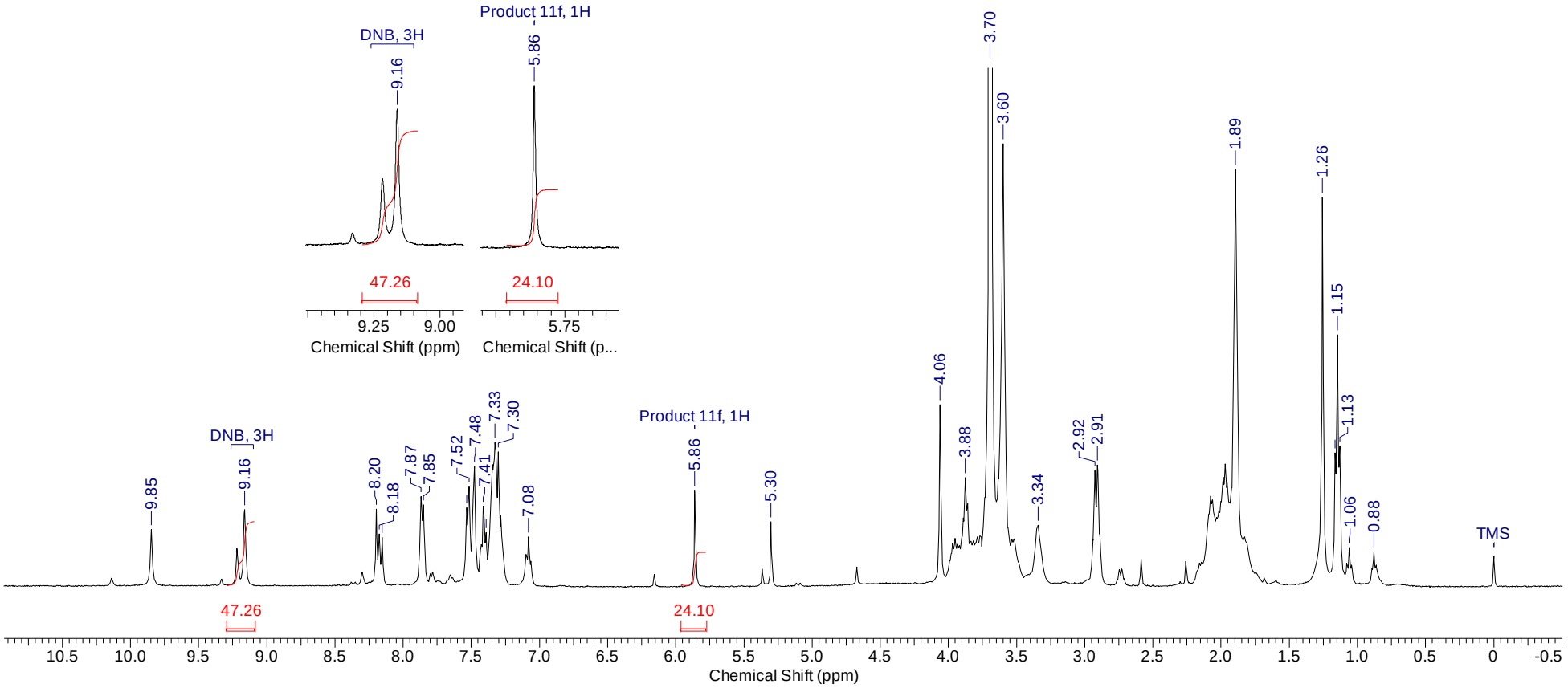
2-Oxo-1-phenyl-2-{[2-(pyrrolidin-1-ylcarbonyl)phenyl]amino}ethyl pyrrolidine-1-carbodithioate (11f)



Internal standard:
Methyl 3,5-dinitrobenzoate (DNB):
8.9 mg (0.0394 mmol)

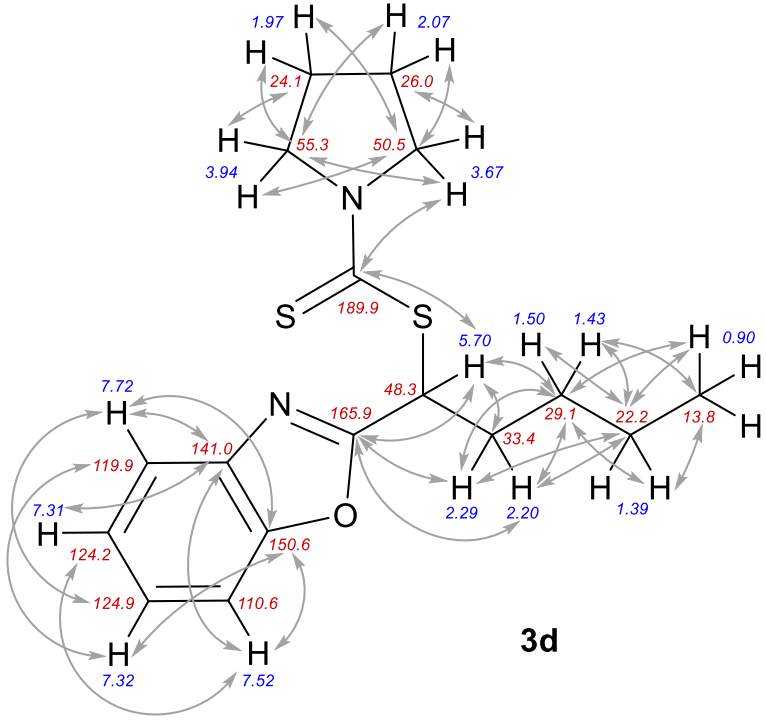
NMR yield of **11f**: 24%

^{1}H NMR (400 MHz, $CDCl_3$)

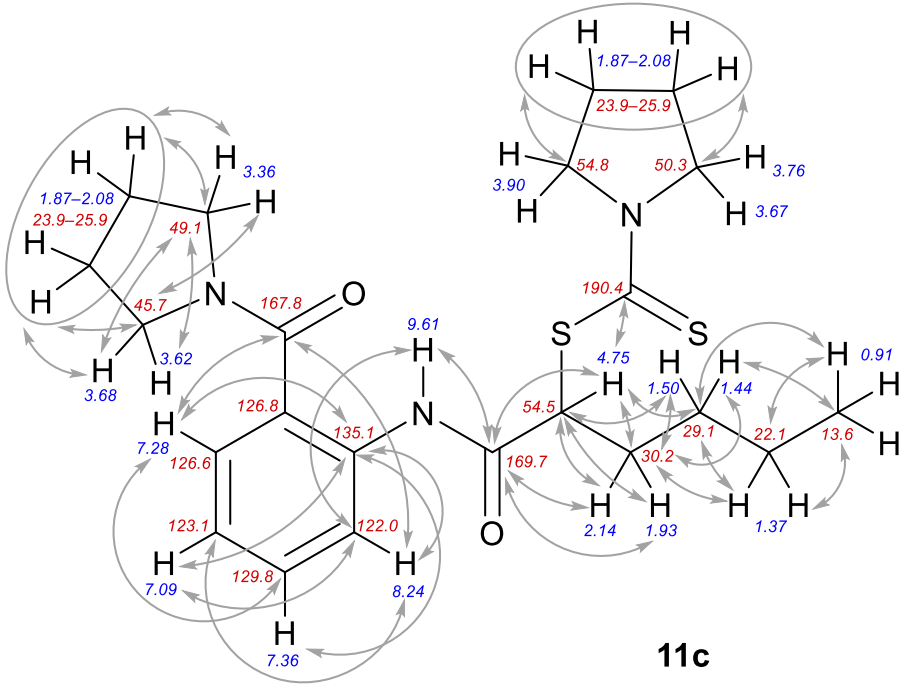


2D NMR of 3d and 11c

Assigned signals and ^{1}H-^{13}C HMBC correlations in **3d** and **11c**

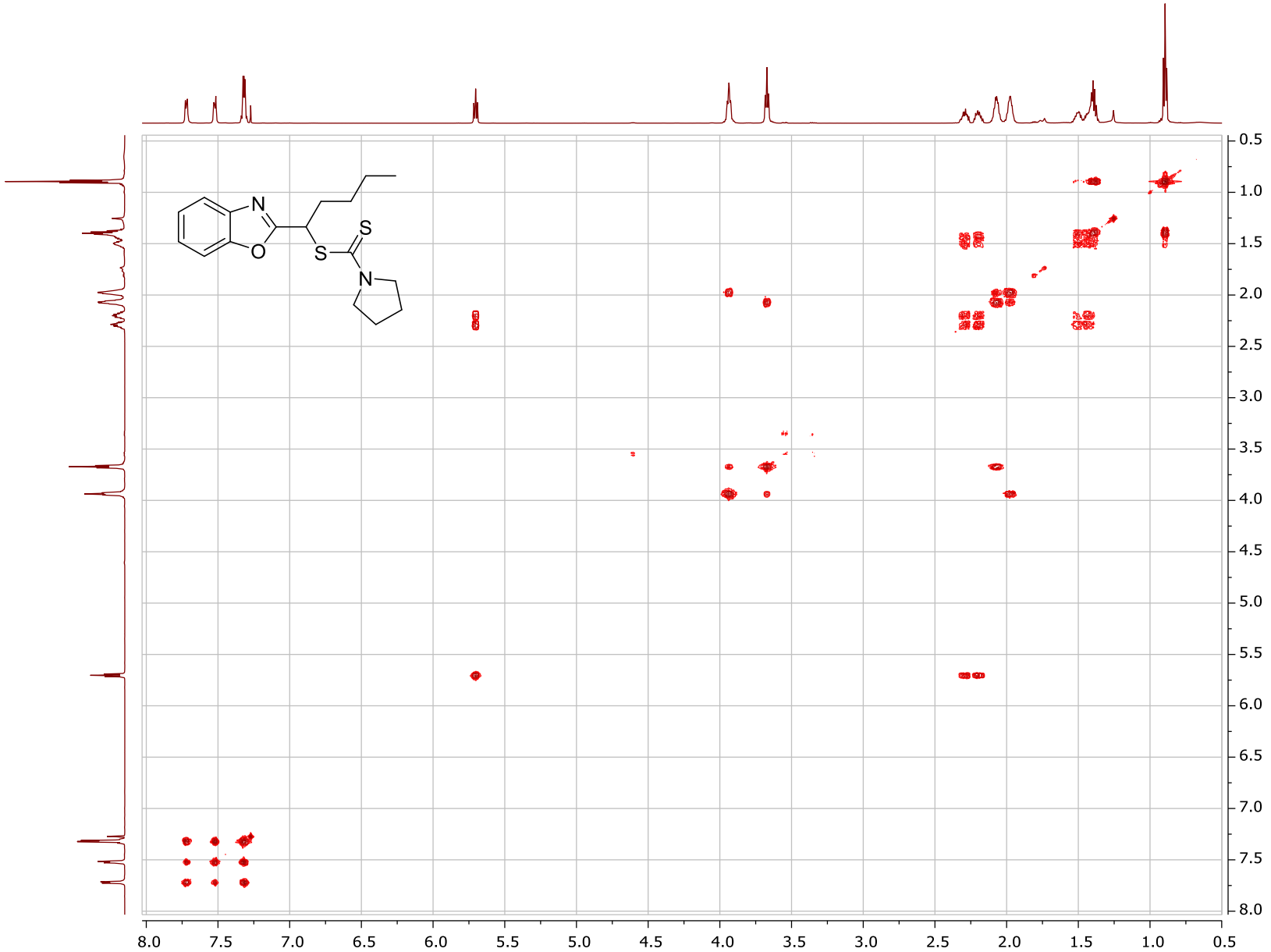


3d

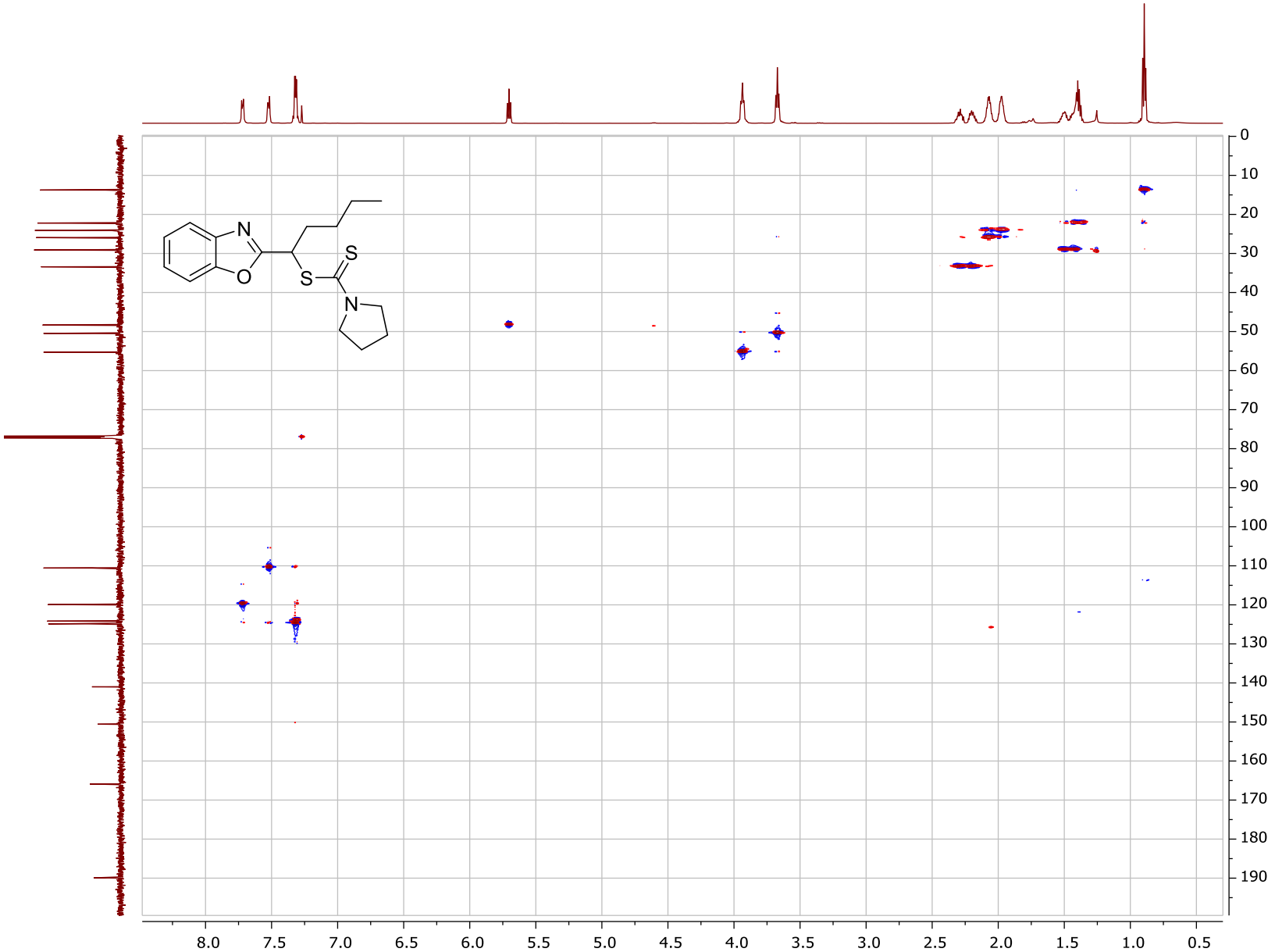


11c

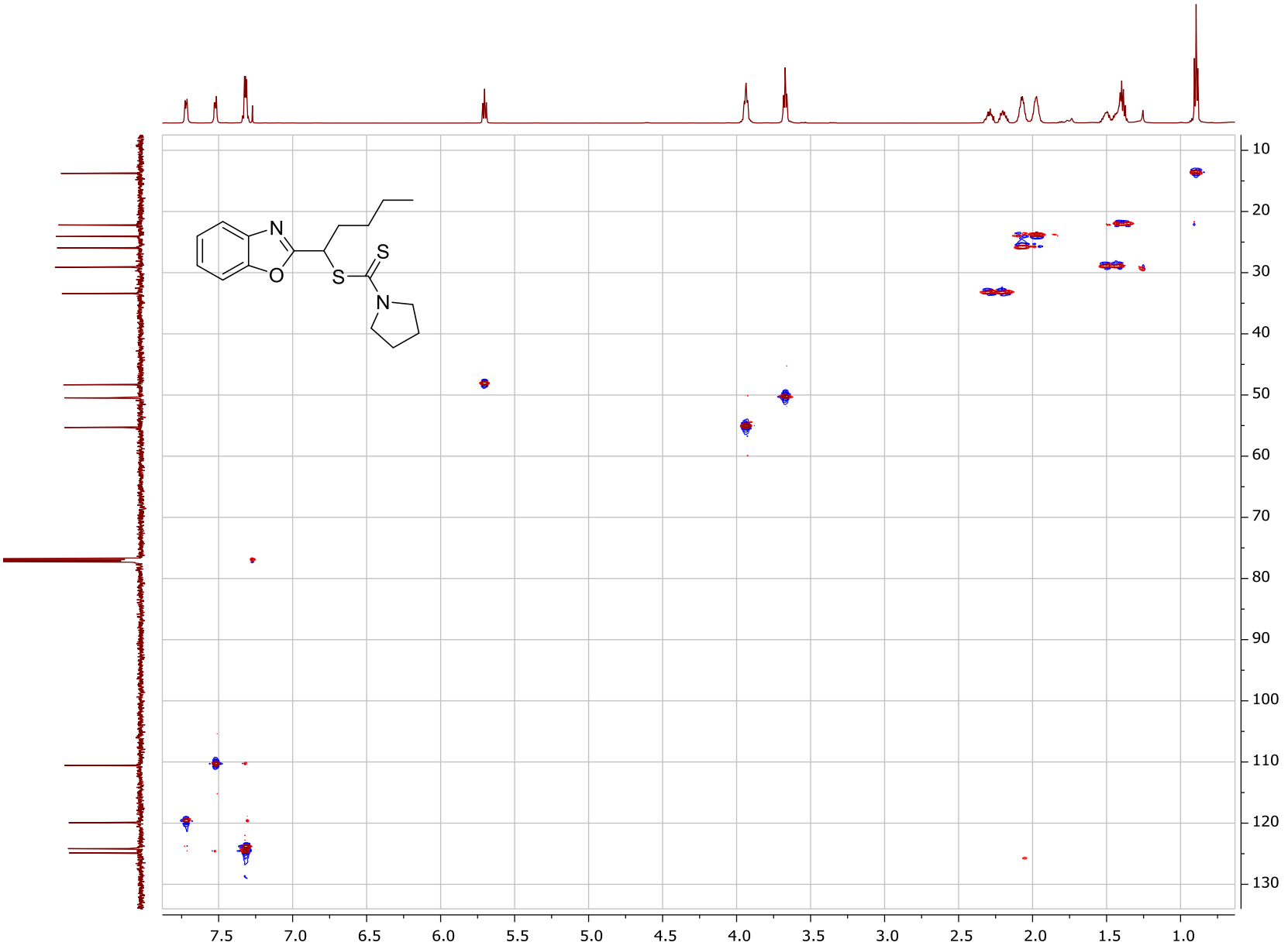
1-(1,3-Benzoxazol-2-yl)pentyl pyrrolidine-4-carbodithioate (3d) ^{1}H-^{1}H COSY



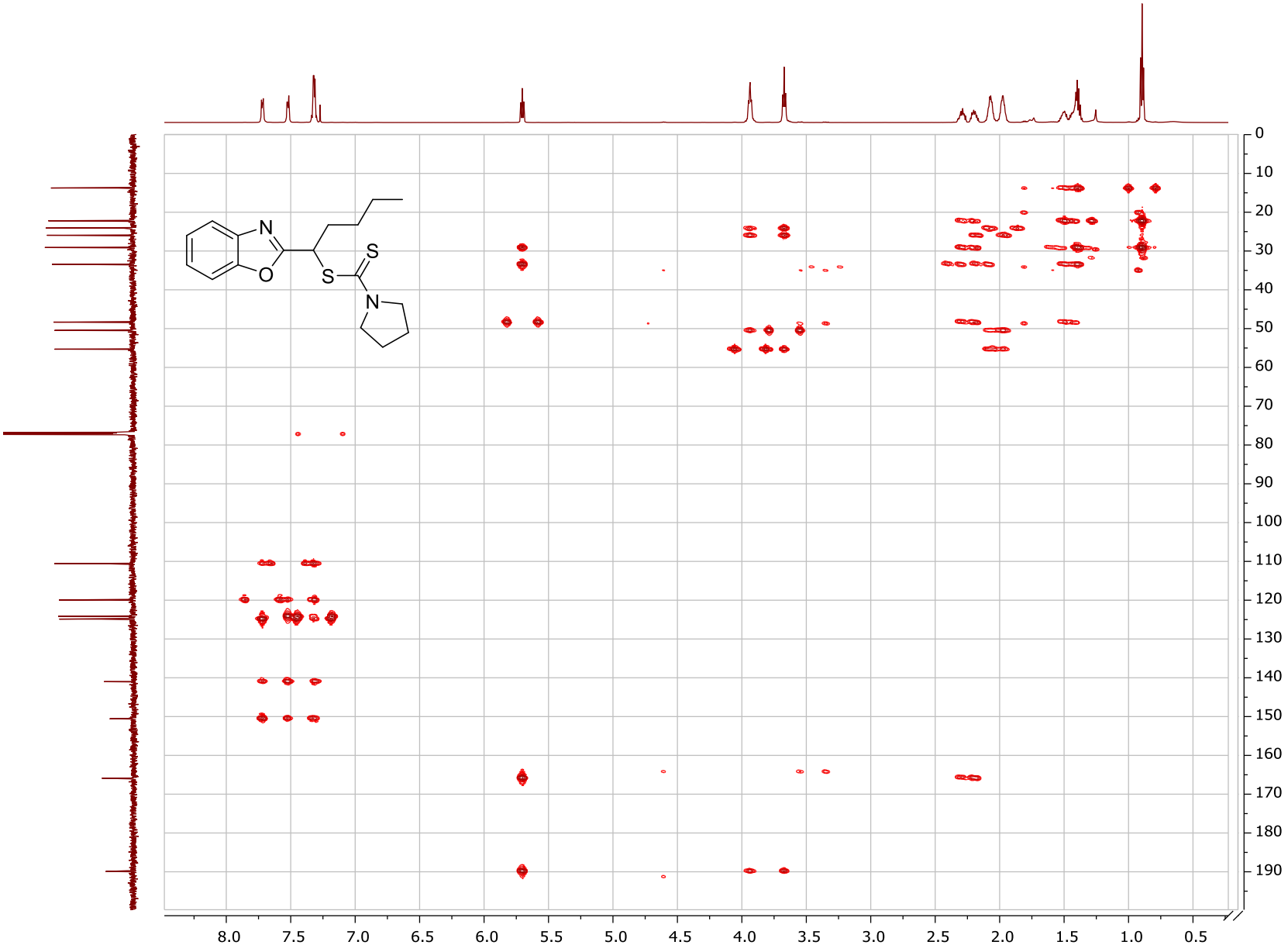
1-(1,3-Benzoxazol-2-yl)pentyl pyrrolidine-4-carbodithioate (3d) ^{1}H-^{13}C HSQC



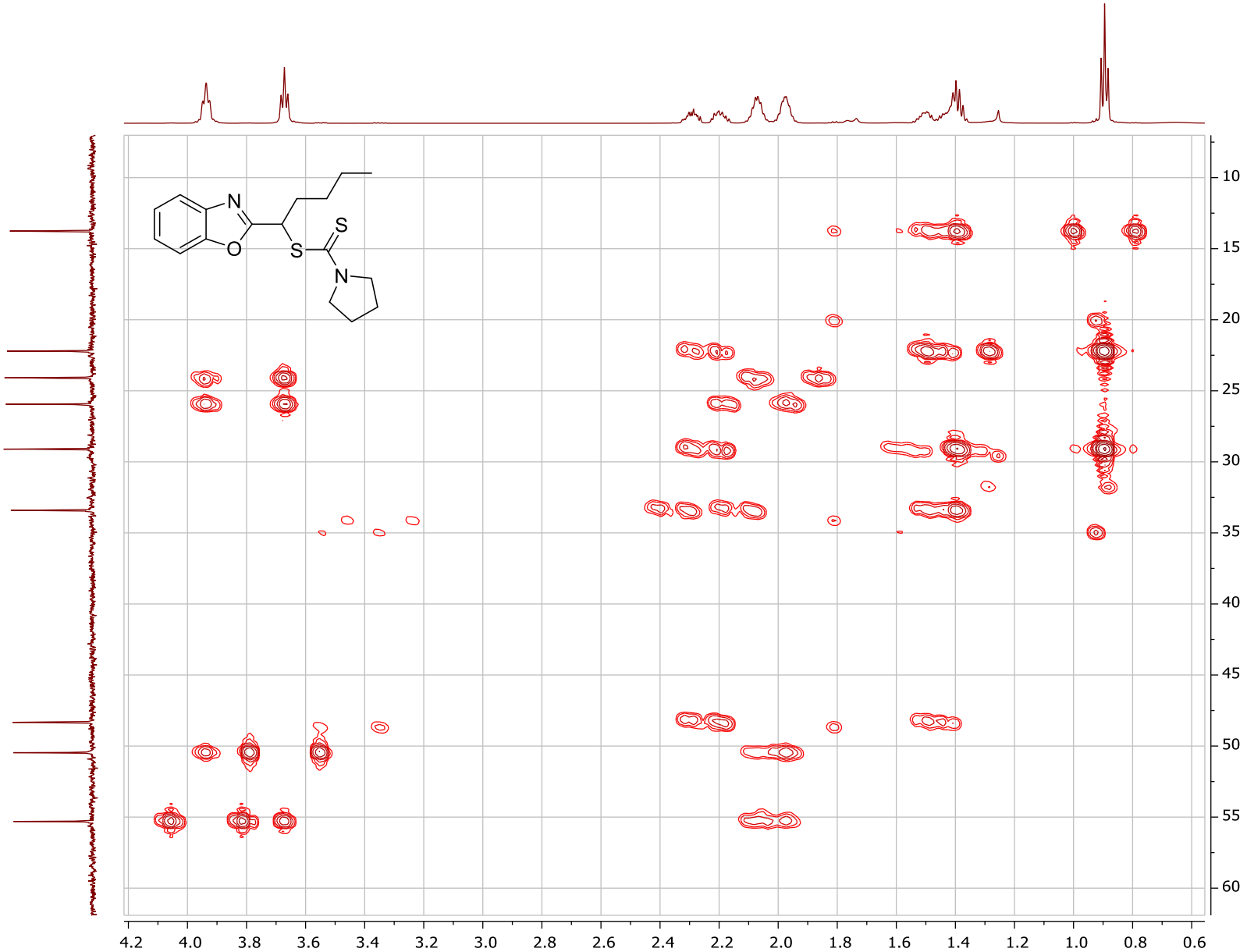
1-(1,3-Benzoxazol-2-yl)pentyl pyrrolidine-4-carbodithioate (3d) ^{1}H-^{13}C HSQC



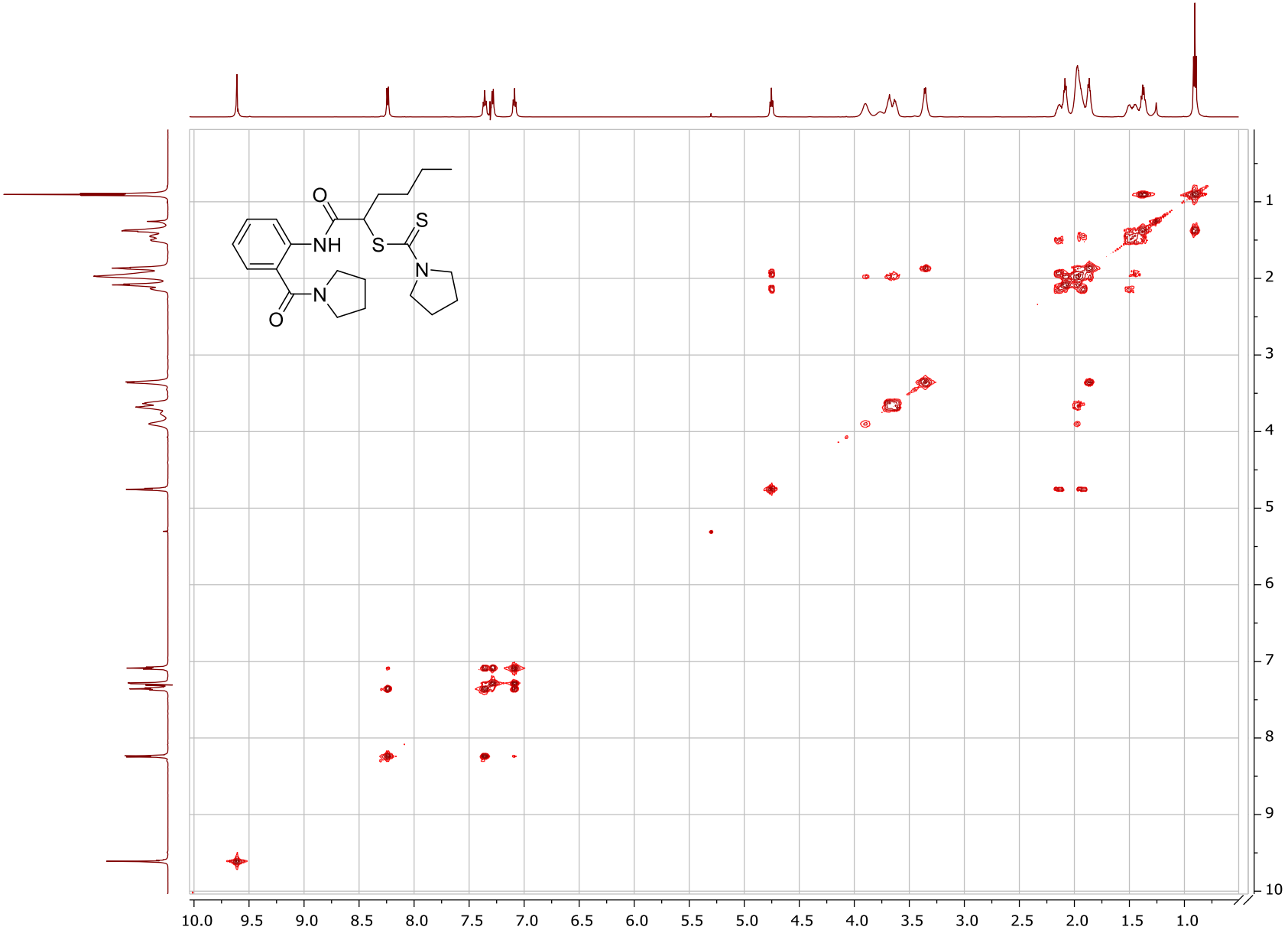
1-(1,3-Benzoxazol-2-yl)pentyl pyrrolidine-4-carbodithioate (3d) ^{1}H-^{13}C HMBC



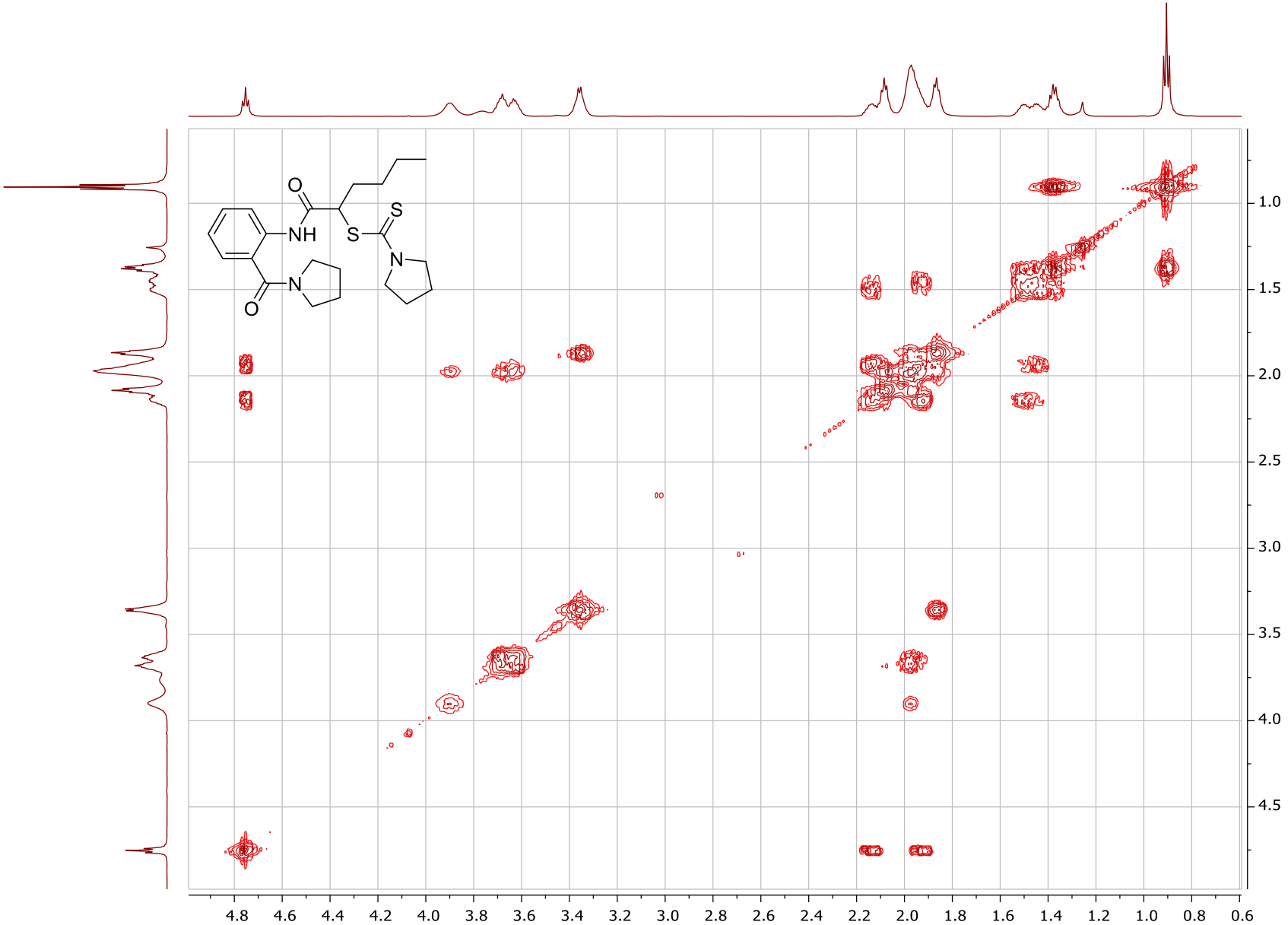
1-(1,3-Benzoxazol-2-yl)pentyl pyrrolidine-4-carbodithioate (3d) ^{1}H-^{13}C HMBC



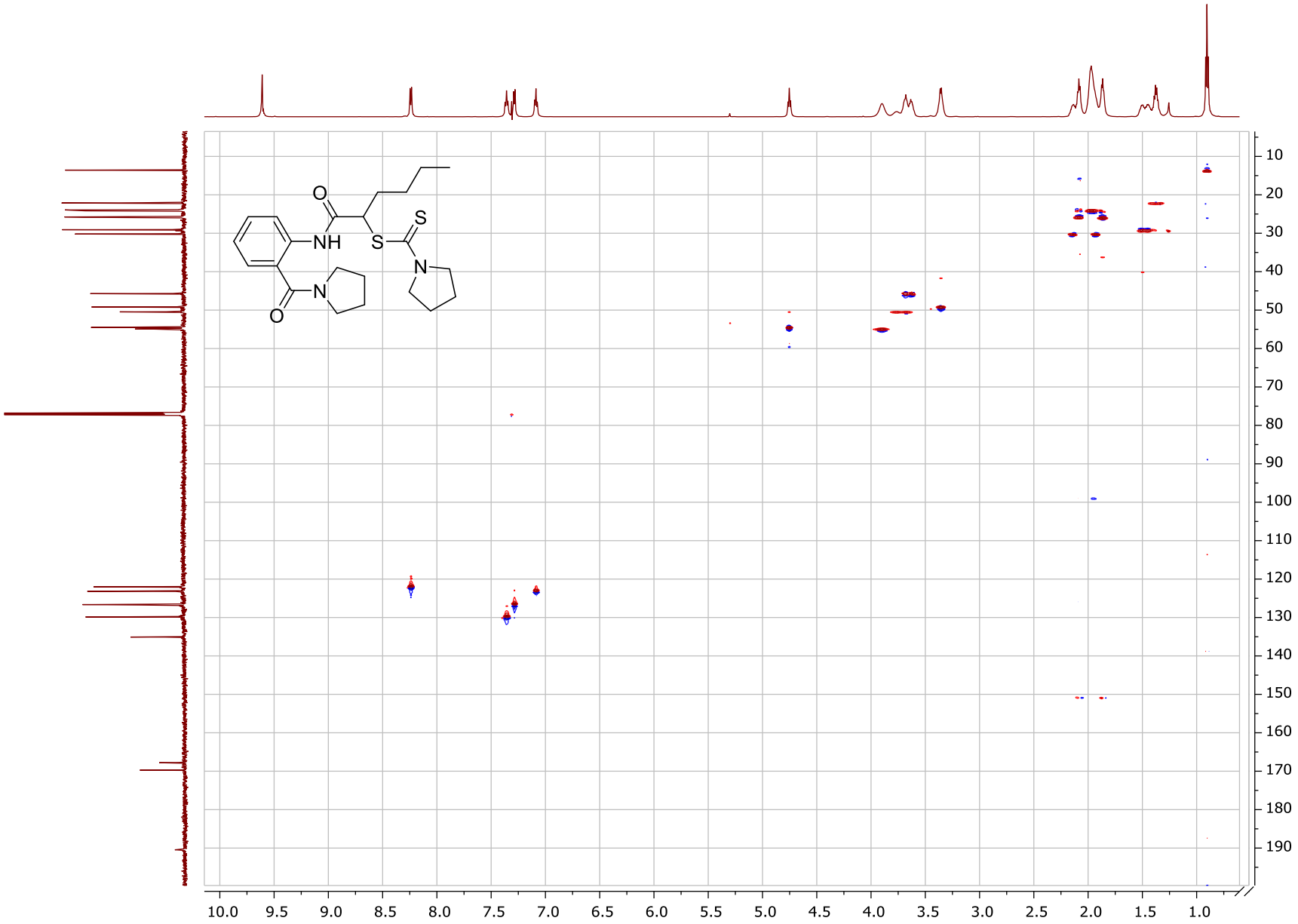
1-({[2-(Pyrrolidin-4-ylcarbonyl)phenyl]amino}carbonyl)pentyl pyrrolidine-4-carbodithioate (11c) ^{1}H-^{1}H COSY



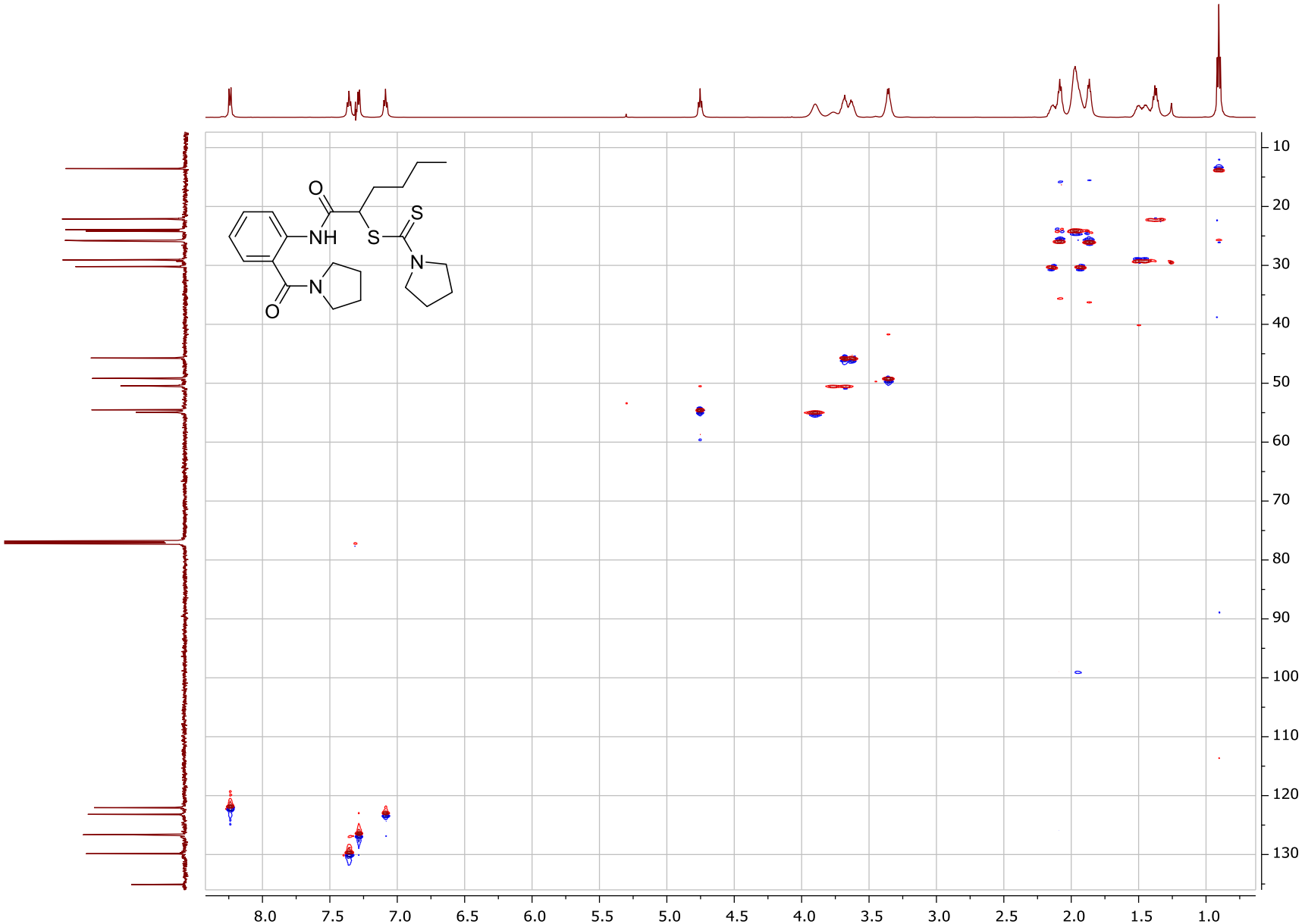
1-({[2-(Pyrrolidin-4-ylcarbonyl)phenyl]amino}carbonyl)pentyl pyrrolidine-4-carbodithioate (11c) ^{1}H-^{1}H COSY



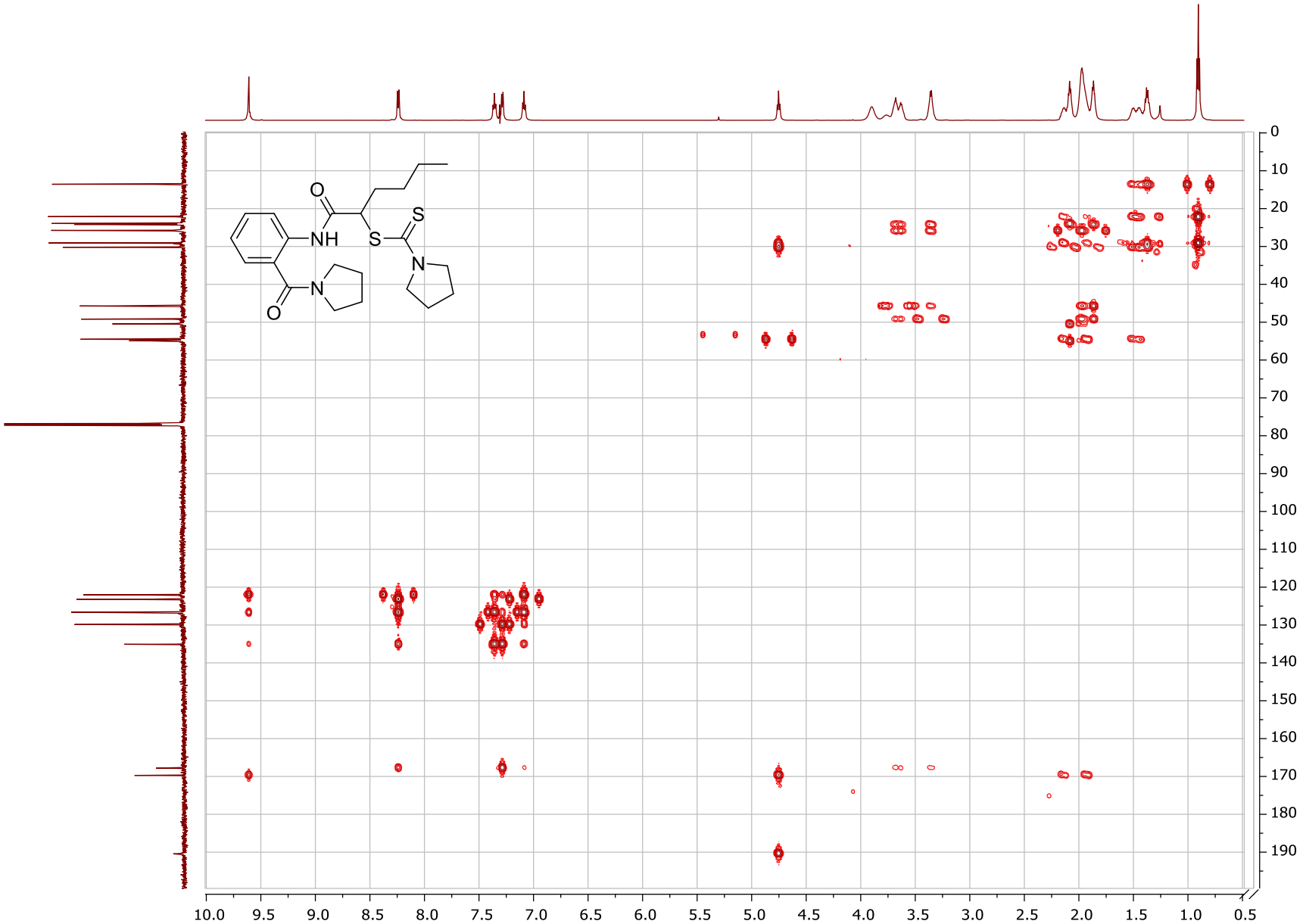
1-({[2-(Pyrrolidin-4-ylcarbonyl)phenyl]amino}carbonyl)pentyl pyrrolidine-4-carbodithioate (11c) ^{1}H-^{13}C HSQC



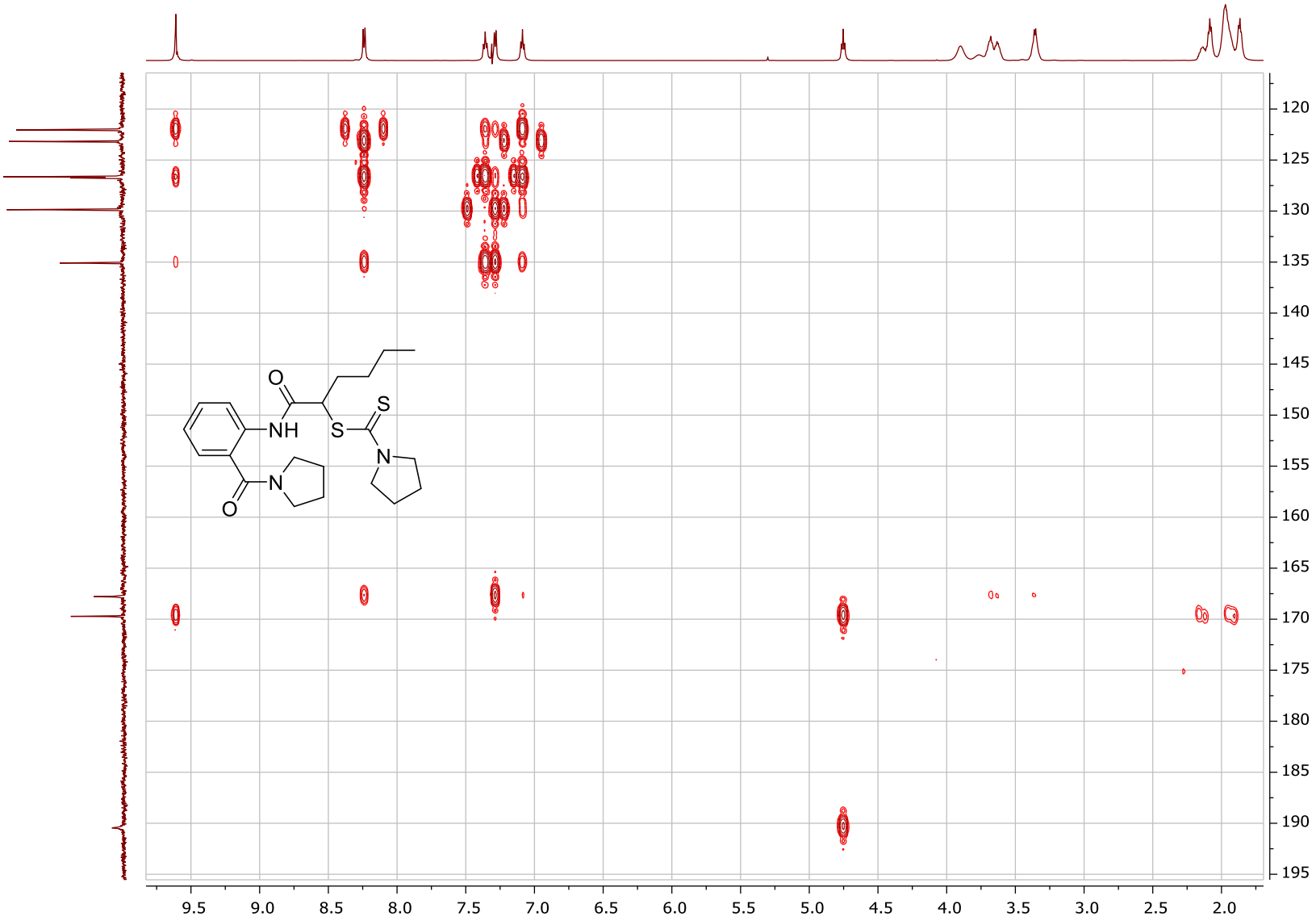
1-({[2-(Pyrrolidin-4-ylcarbonyl)phenyl]amino}carbonyl)pentyl pyrrolidine-4-carbodithioate (11c) ^{1}H-^{13}C HSQC



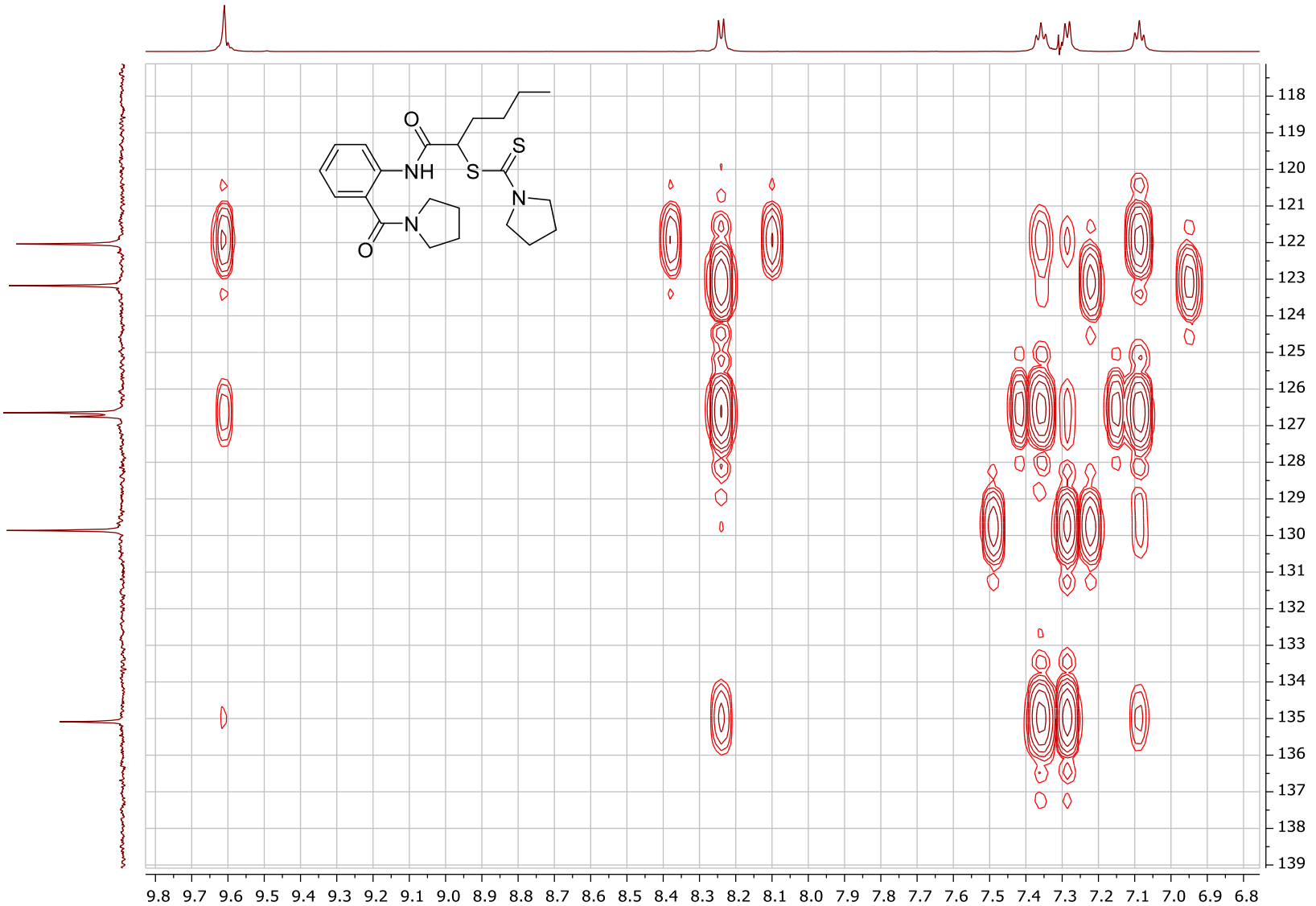
1-({[2-(Pyrrolidin-4-ylcarbonyl)phenyl]amino}carbonyl)pentyl pyrrolidine-4-carbodithioate (11c) ^{1}H-^{13}C HMBC



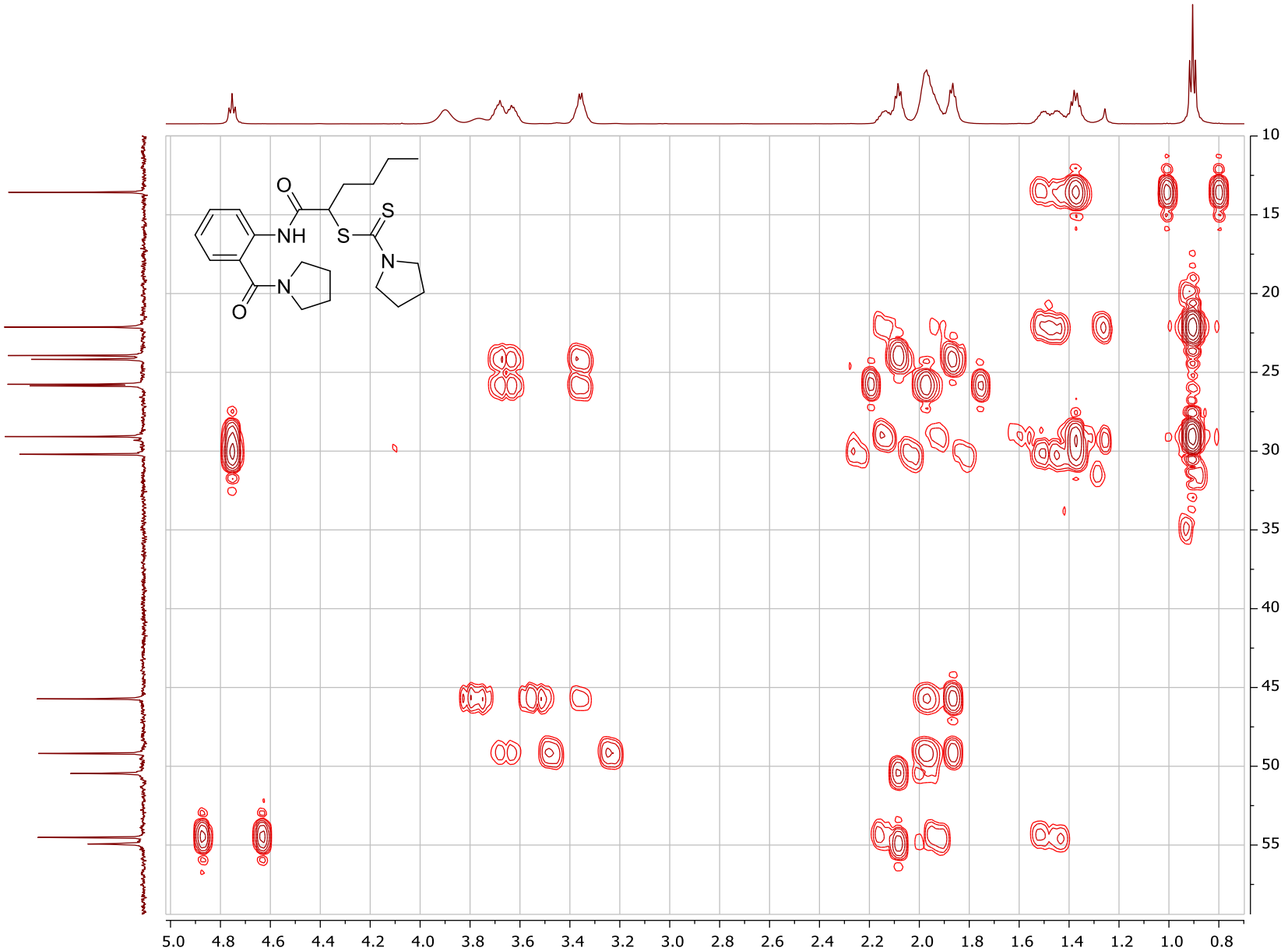
1-({[2-(Pyrrolidin-4-ylcarbonyl)phenyl]amino}carbonyl)pentyl pyrrolidine-4-carbodithioate (11c) ^{1}H-^{13}C HMBC



1-({[2-(Pyrrolidin-4-ylcarbonyl)phenyl]amino}carbonyl)pentyl pyrrolidine-4-carbodithioate (11c) ^{1}H-^{13}C HMBC



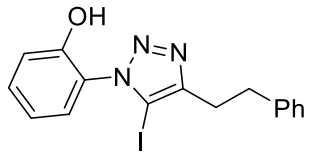
1-({[2-(Pyrrolidin-4-ylcarbonyl)phenyl]amino}carbonyl)pentyl pyrrolidine-4-carbodithioate (11c) ^{1}H-^{13}C HMBC

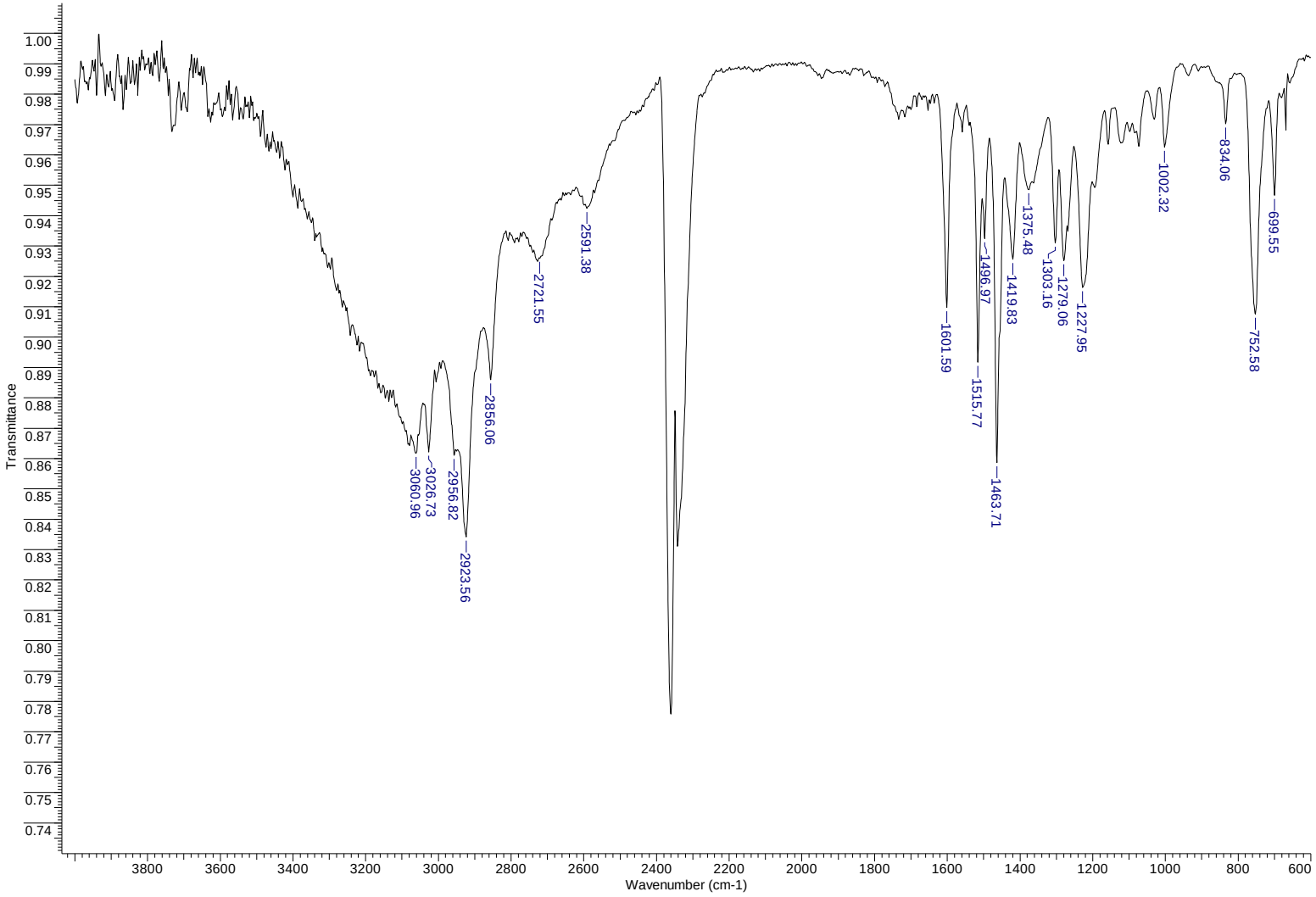


Copies of IR spectra

2-[5-Iodo-4-(2-phenylethyl)-1*H*-1,2,3-triazol-1-yl]phenol (1j)

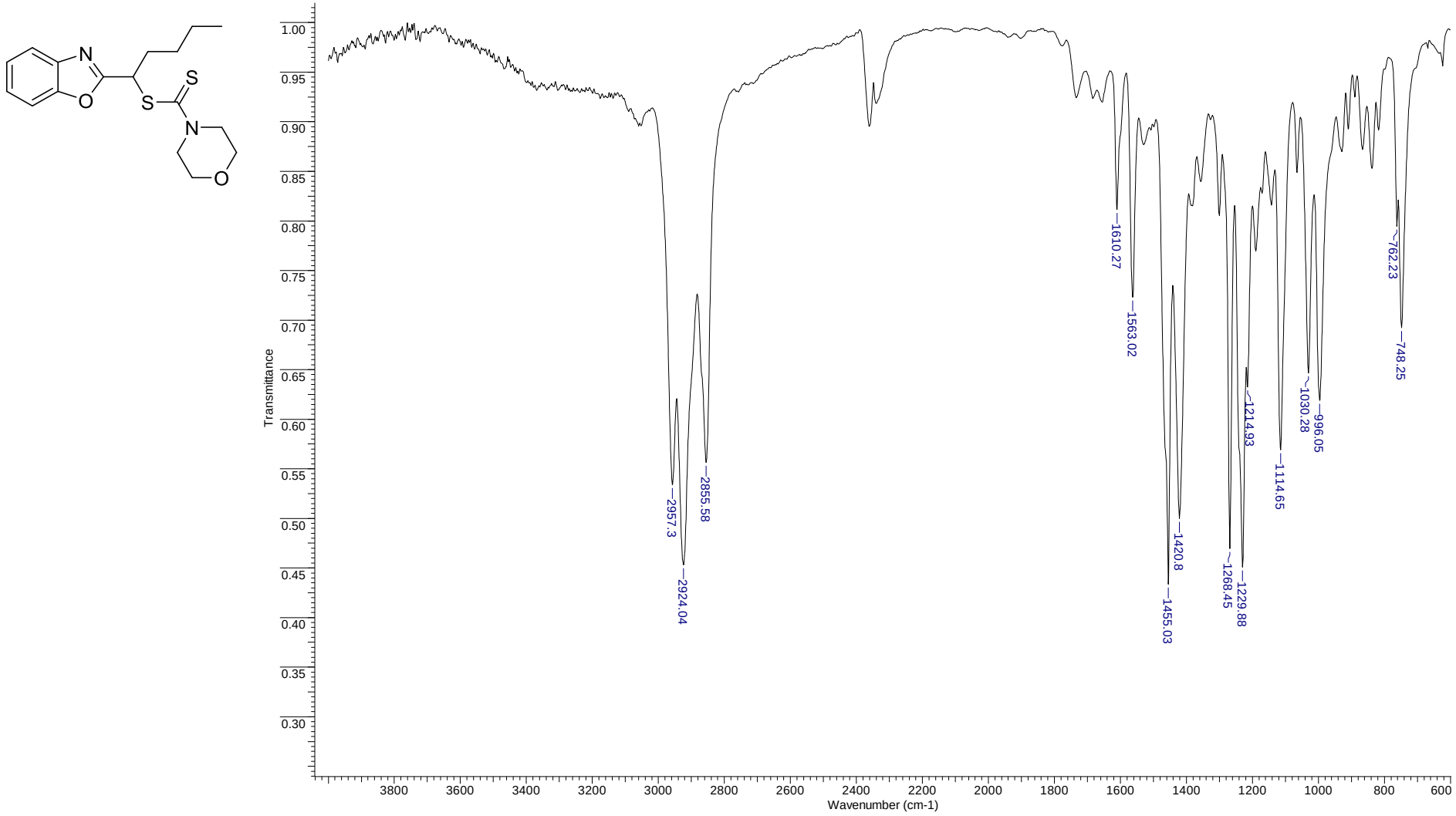
IR (neat)





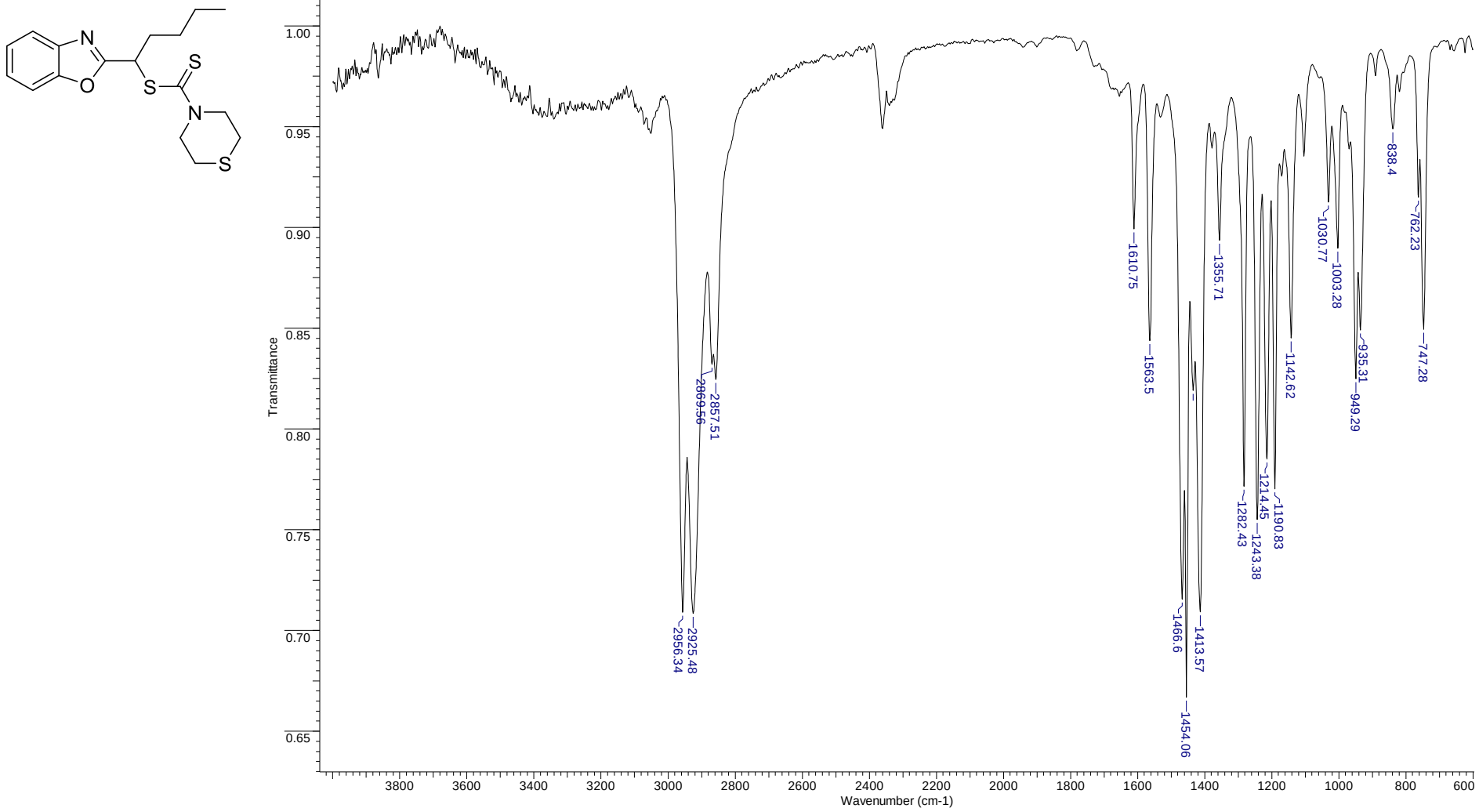
1-(1,3-Benzoxazol-2-yl)pentyl morpholine-4-carbodithioate (3a)

IR (neat)



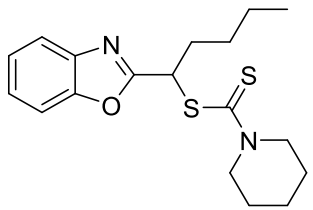
1-(1,3-Benzoxazol-2-yl)pentyl thiomorpholine-4-carbodithioate (3b)

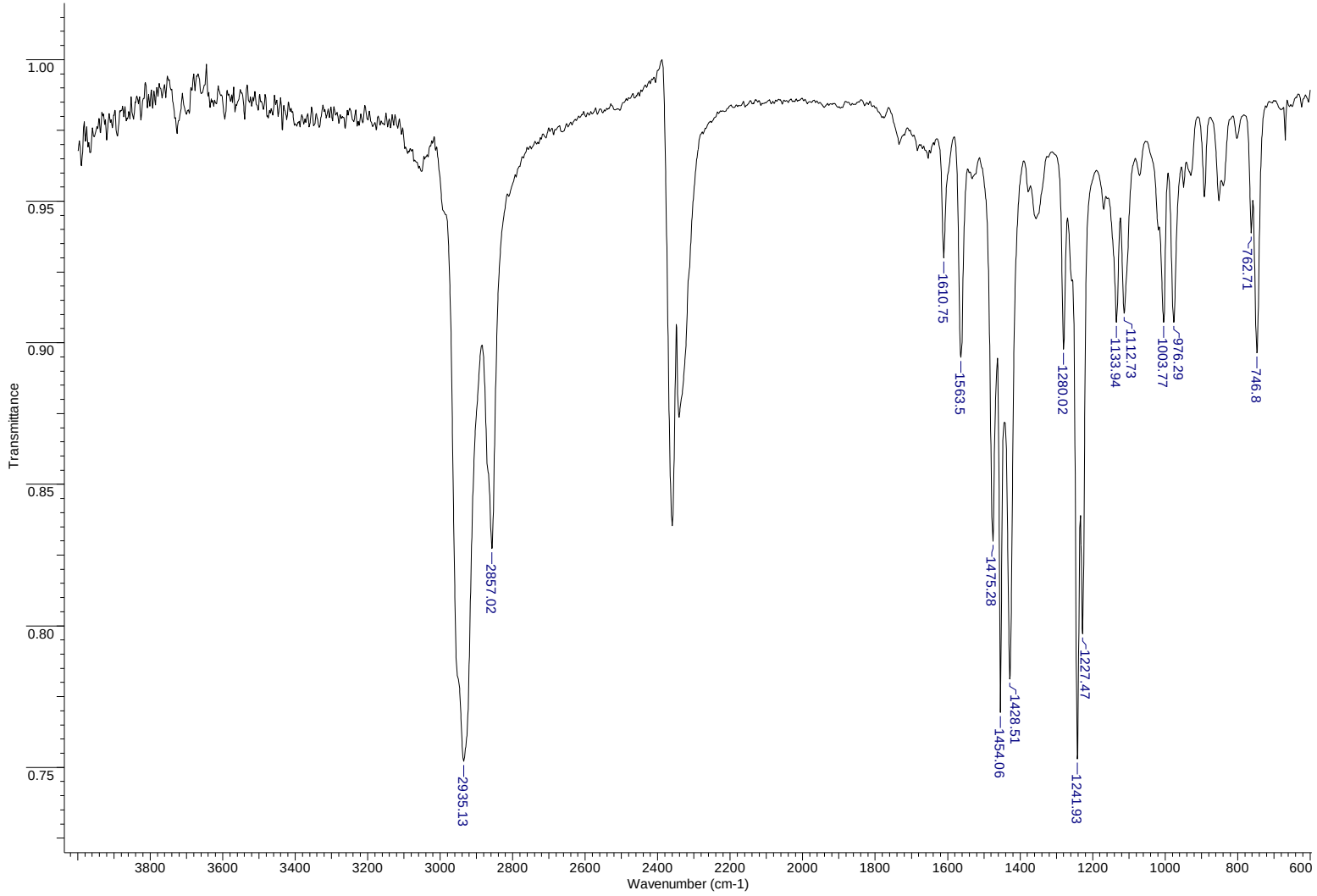
IR (neat)



1-(1,3-Benzoxazol-2-yl)pentyl piperidine-4-carbodithioate (3c)

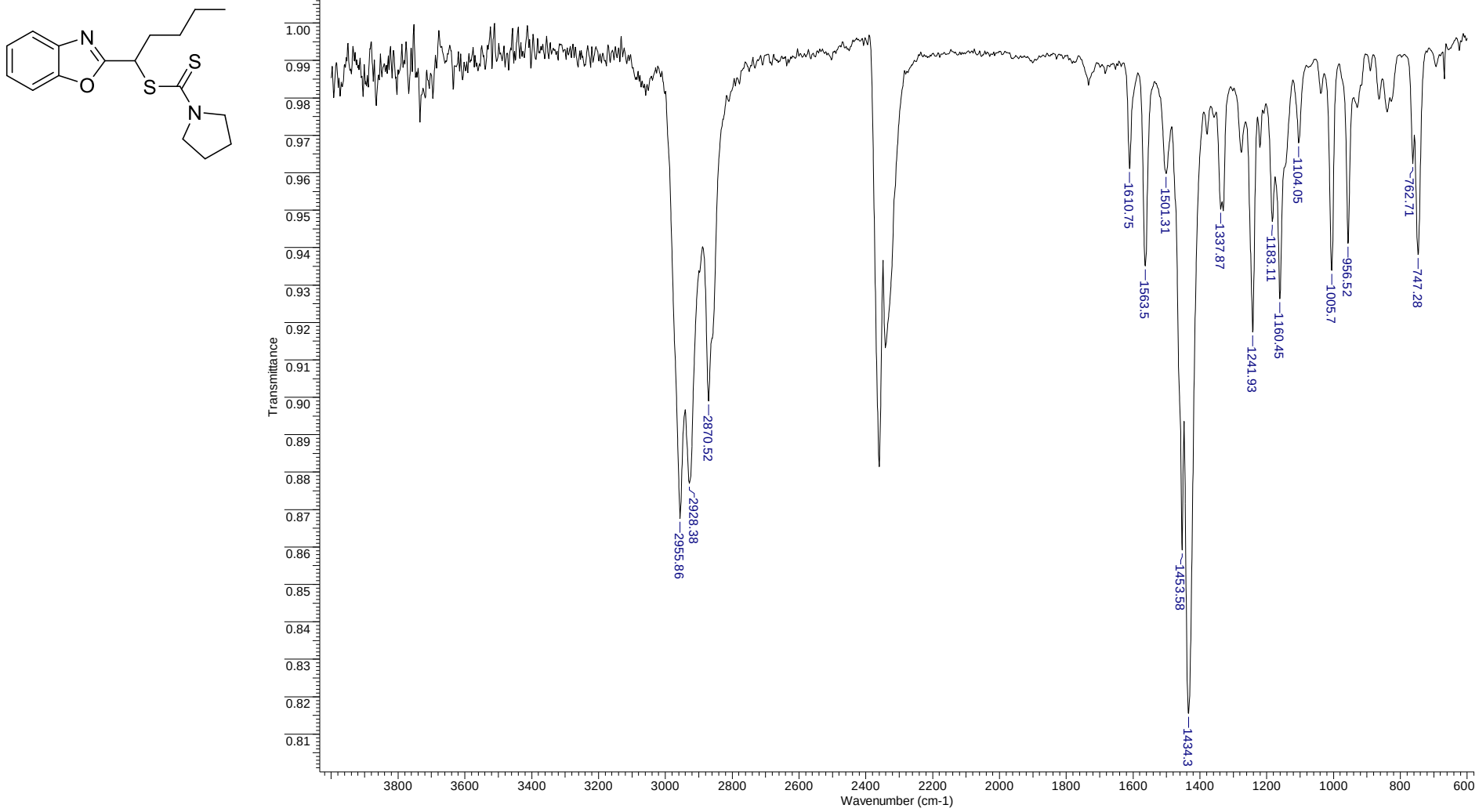
IR (neat)





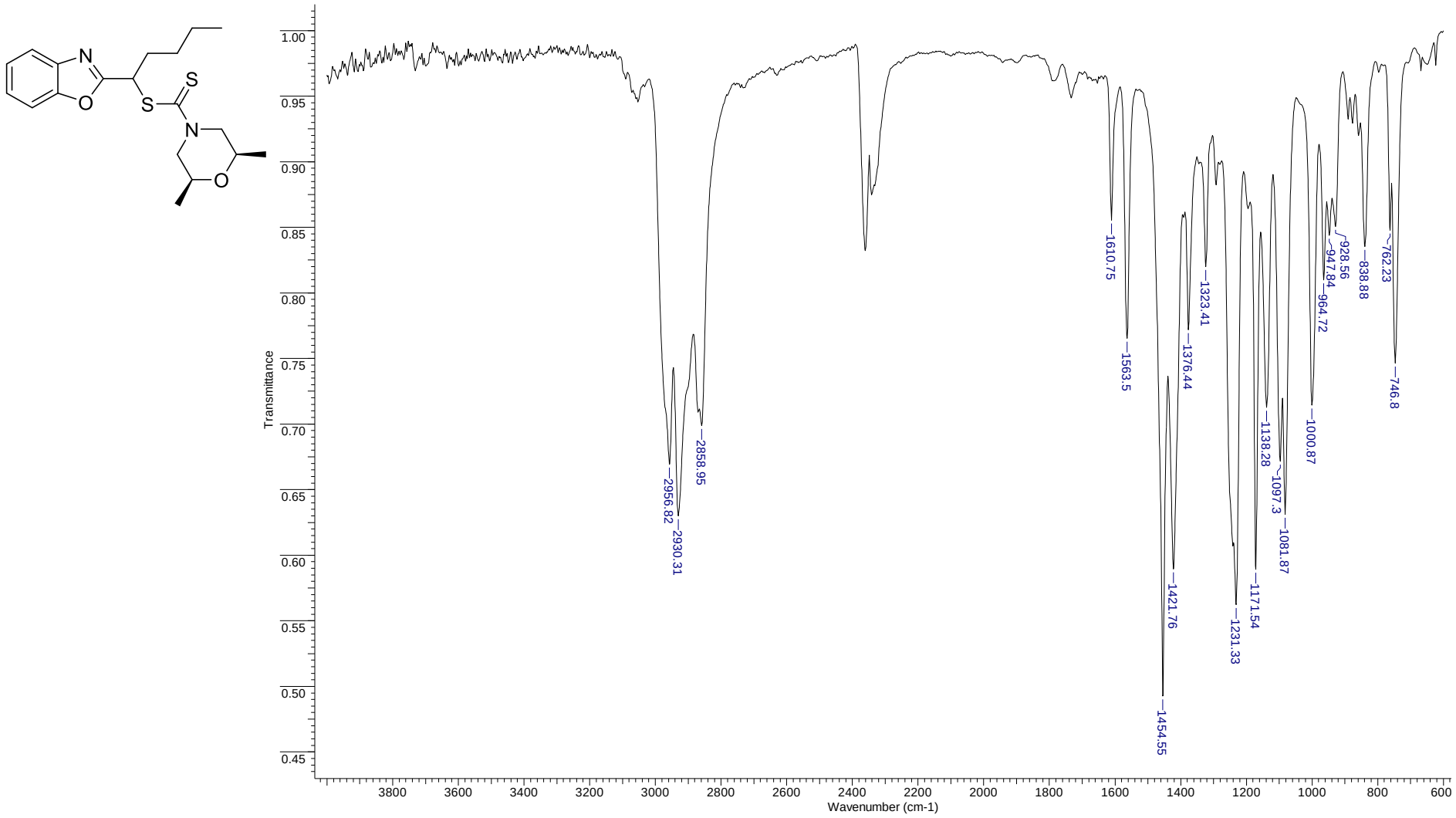
1-(1,3-Benzoxazol-2-yl)pentyl pyrrolidine-4-carbodithioate (3d)

IR (neat)



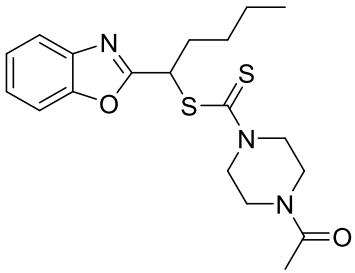
1-(1,3-Benzoxazol-2-yl)pentyl (2*R*,6*S*)-2,6-dimethylmorpholine-4-carbodithioate (3e)

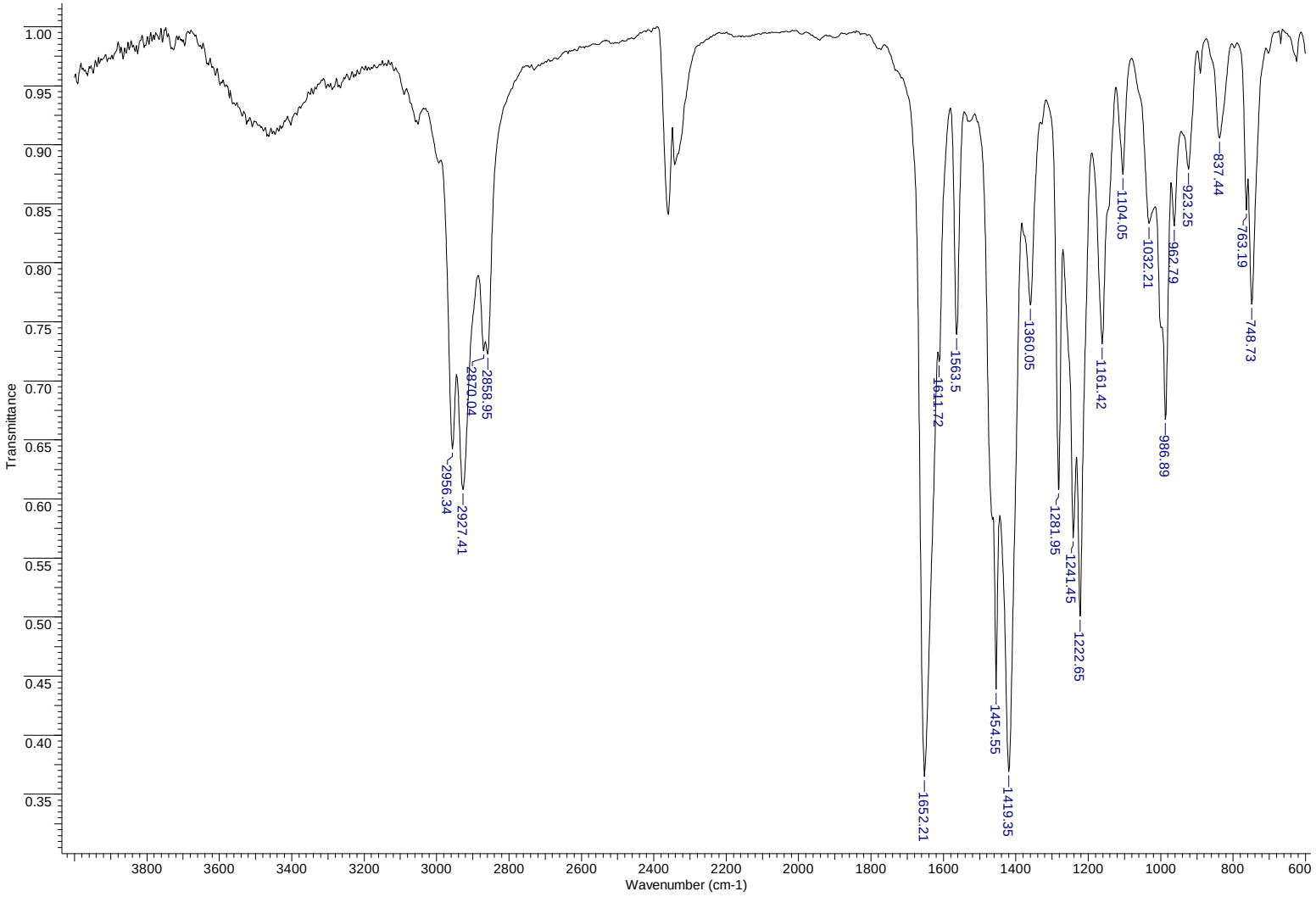
IR (neat)



1-(1,3-Benzoxazol-2-yl)pentyl 4-acetylpiperazine-1-carbodithioate (3f)

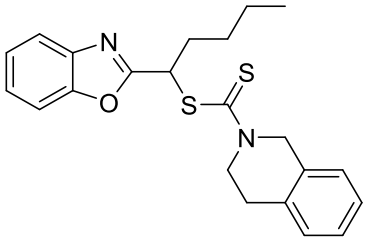
IR (neat)

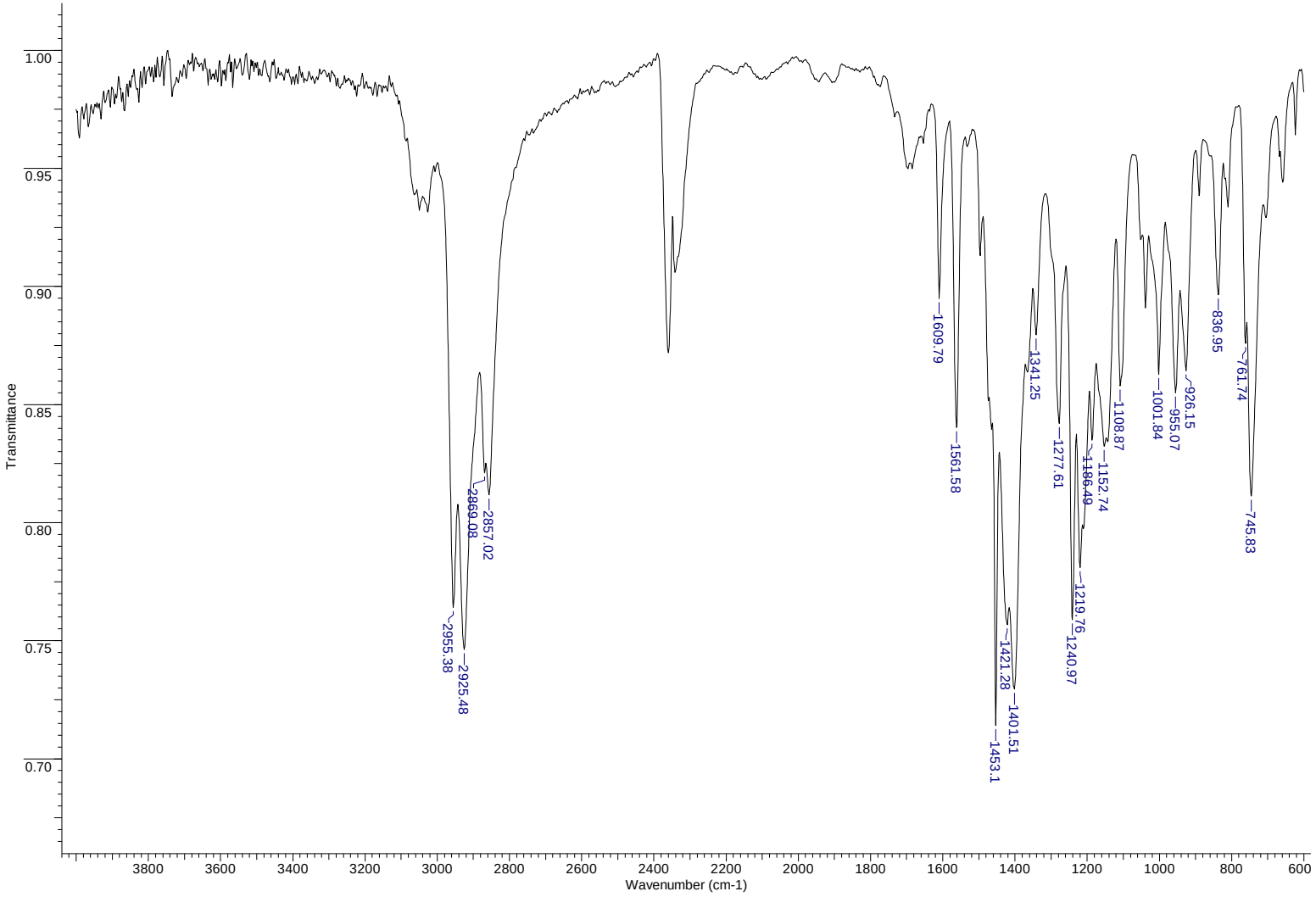




1-(1,3-Benzoxazol-2-yl)pentyl 3,4-dihydroisoquinoline-2(1*H*)-carbodithioate (3g)

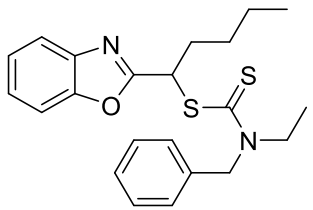
IR (neat)

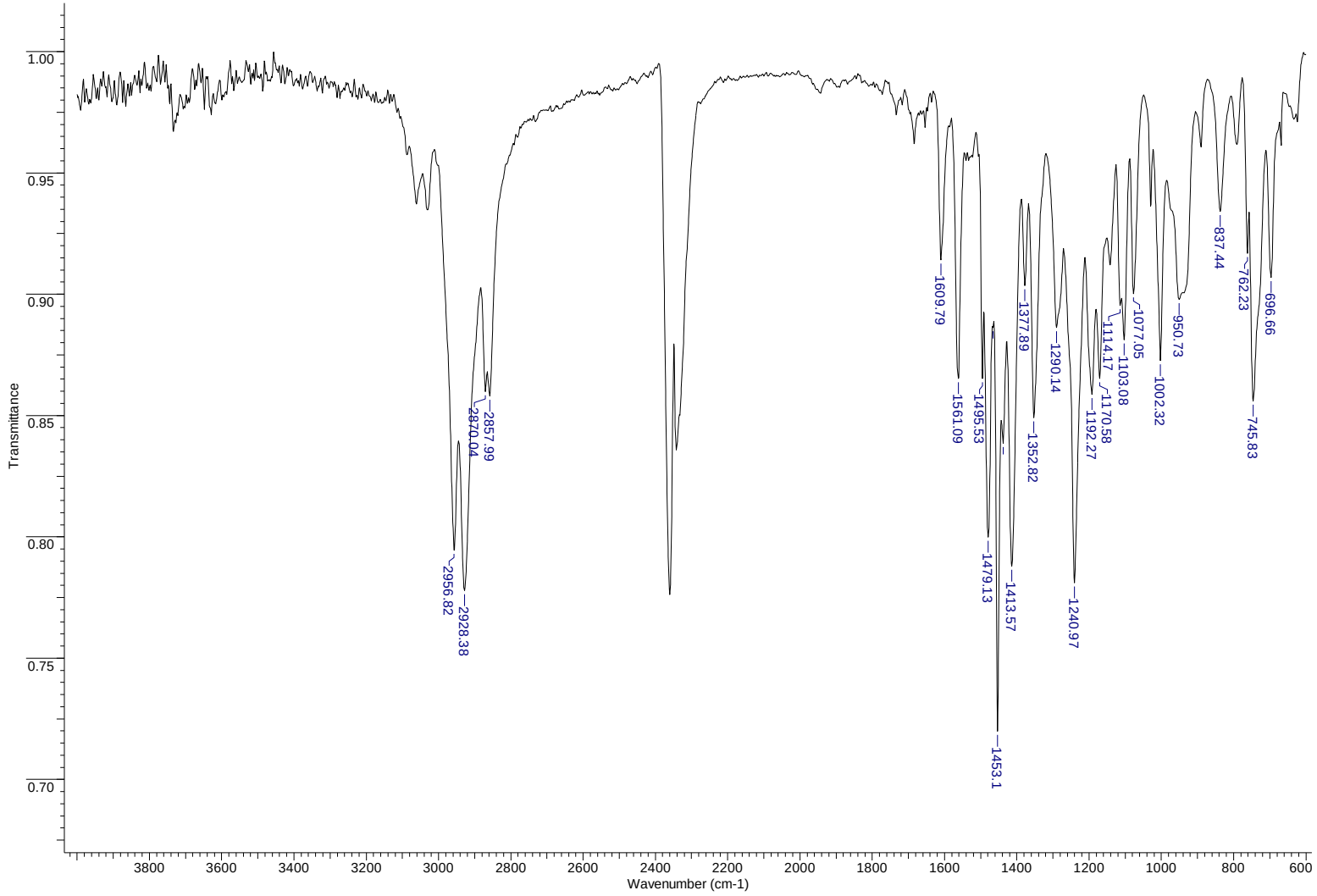




1-(1,3-Benzoxazol-2-yl)pentyl benzyl(ethyl)dithiocarbamate (3h)

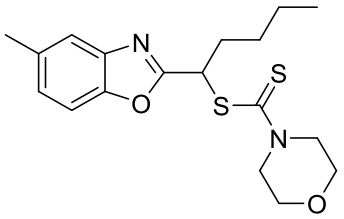
IR (neat)

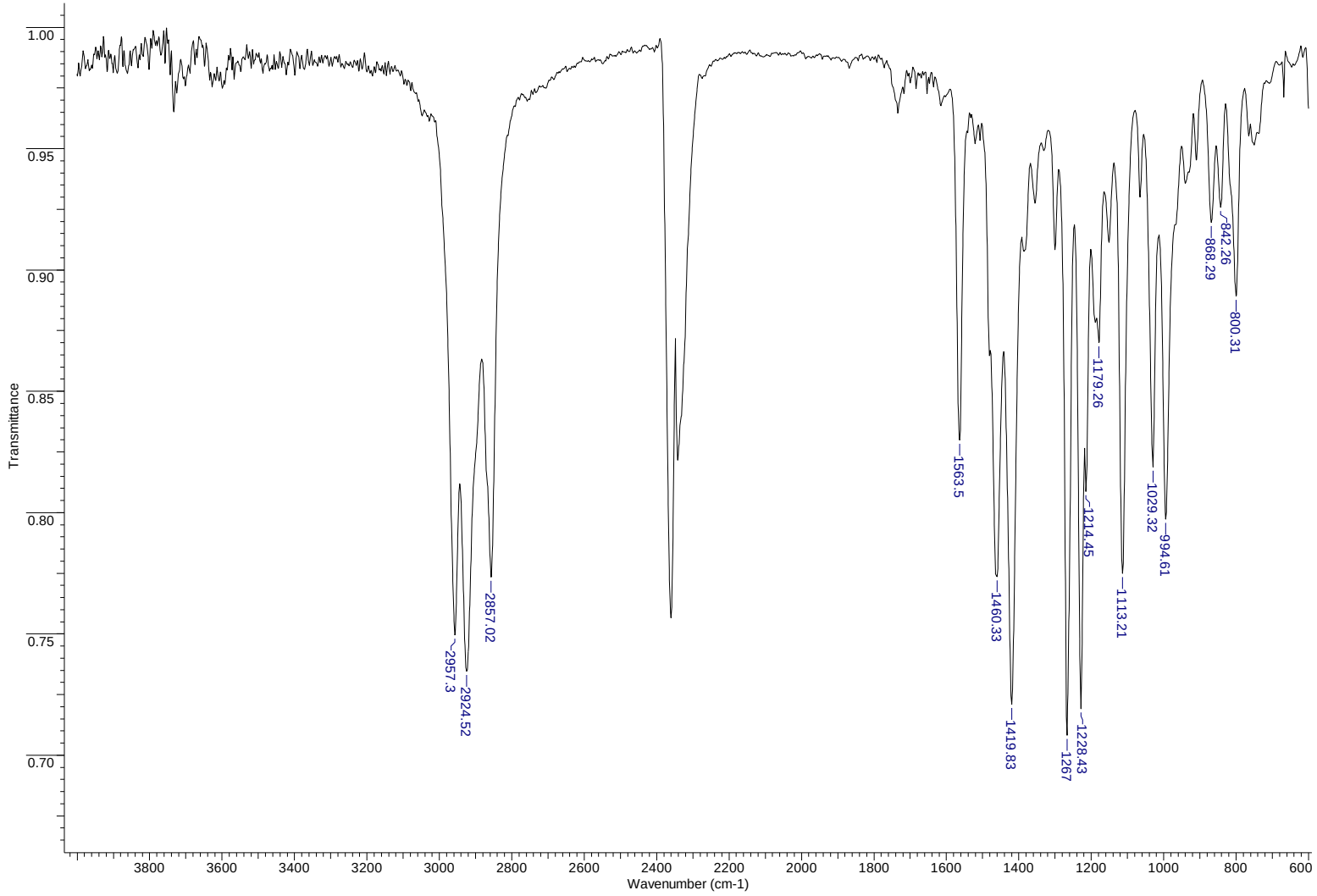




1-(5-Methyl-1,3-benzoxazol-2-yl)pentyl morpholine-4-carbodithioate (3l)

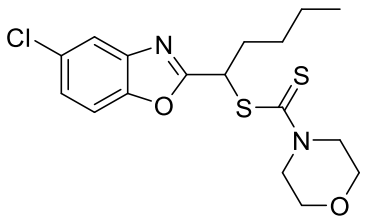
IR (neat)

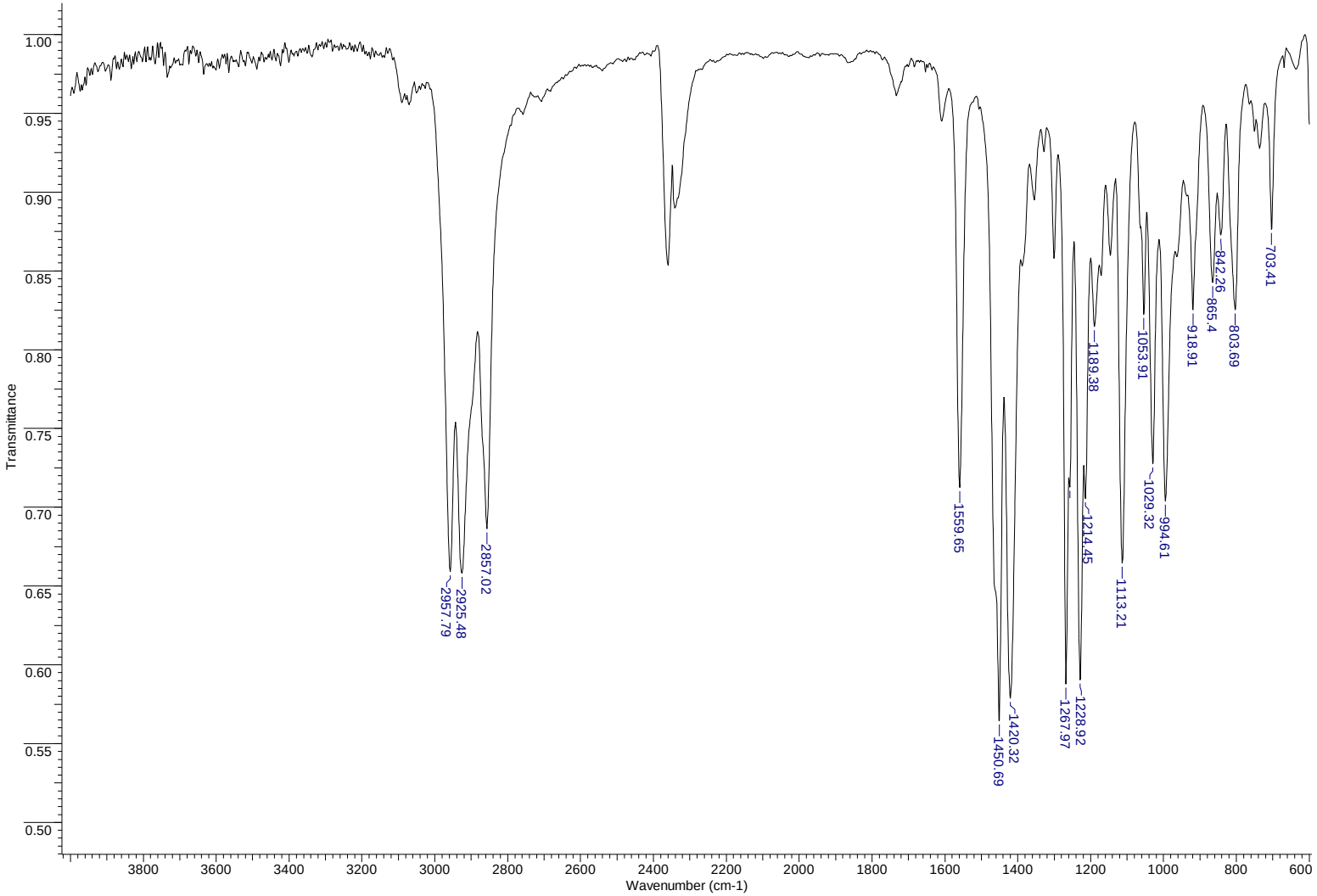




1-(5-Chloro-1,3-benzoxazol-2-yl)pentyl morpholine-4-carbodithioate (3m)

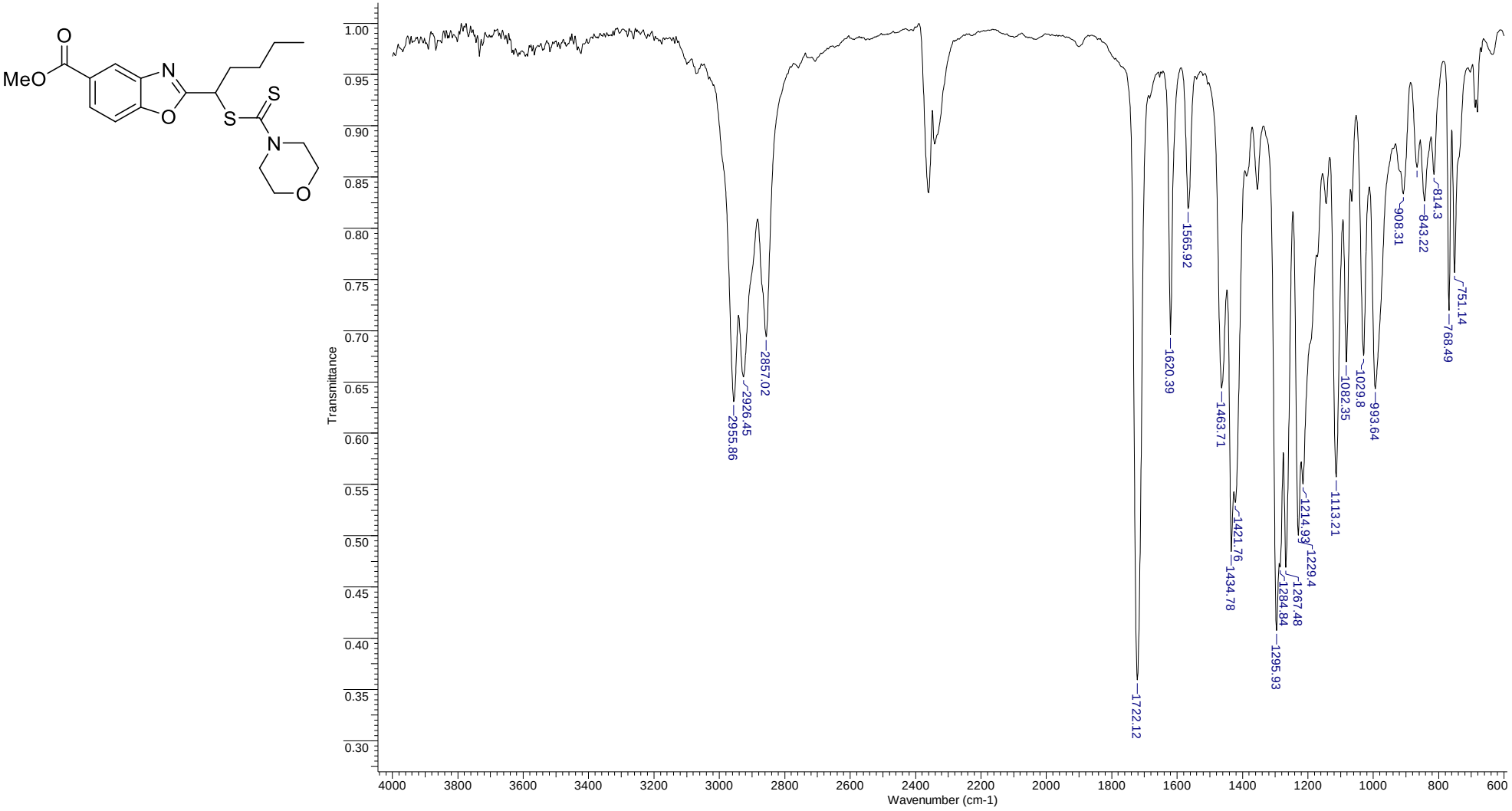
IR (neat)





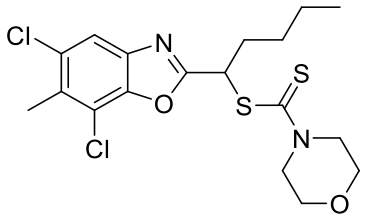
Methyl 2-{1-[(morpholin-4-ylcarbonothioyl)thio]pentyl}-1,3-benzoxazole-5-carboxylate (3n)

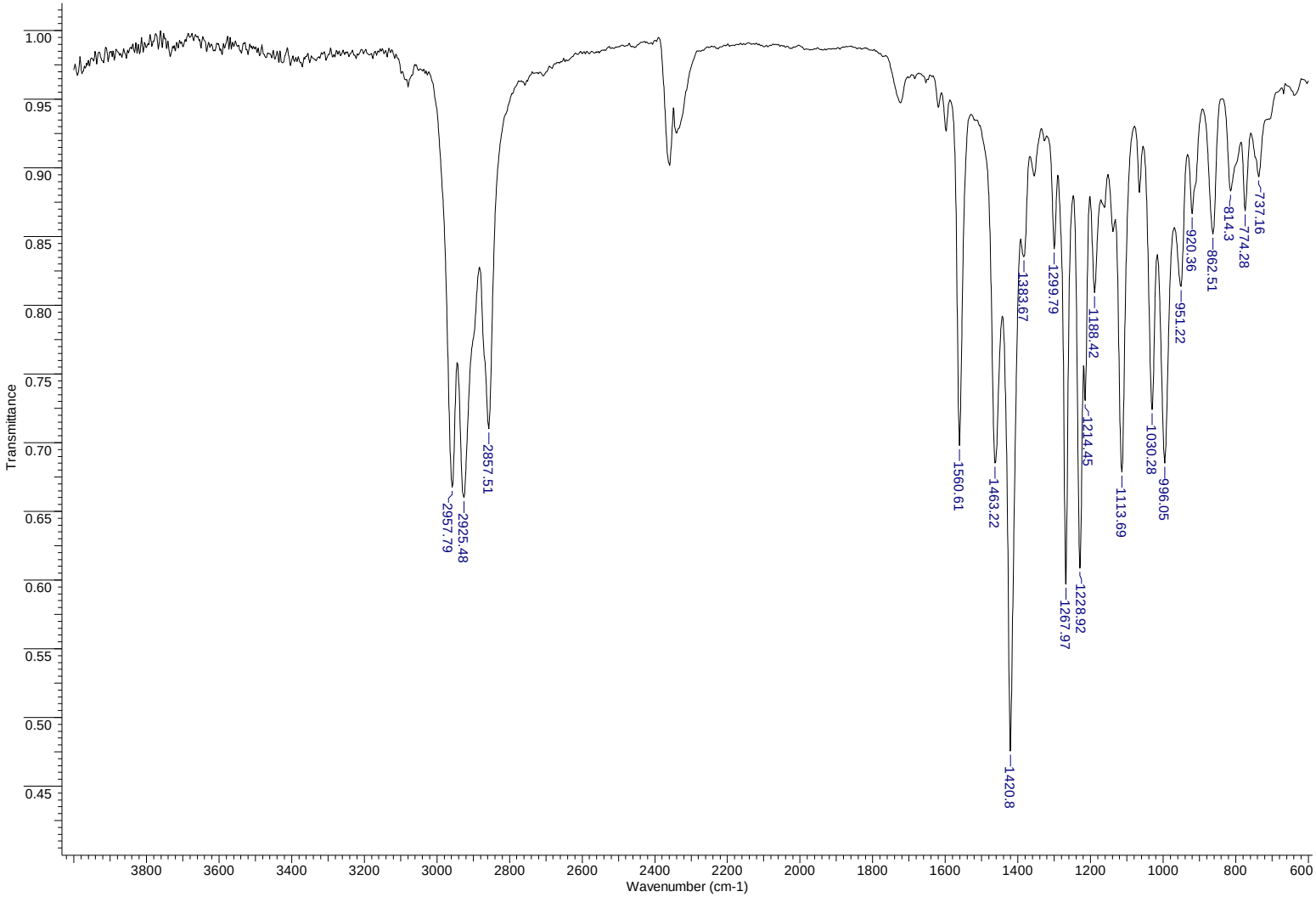
IR (neat)



1-(5,7-Dichloro-6-methyl-1,3-benzoxazol-2-yl)pentyl morpholine-4-carbodithioate (3o)

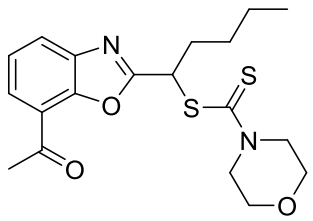
IR (neat)

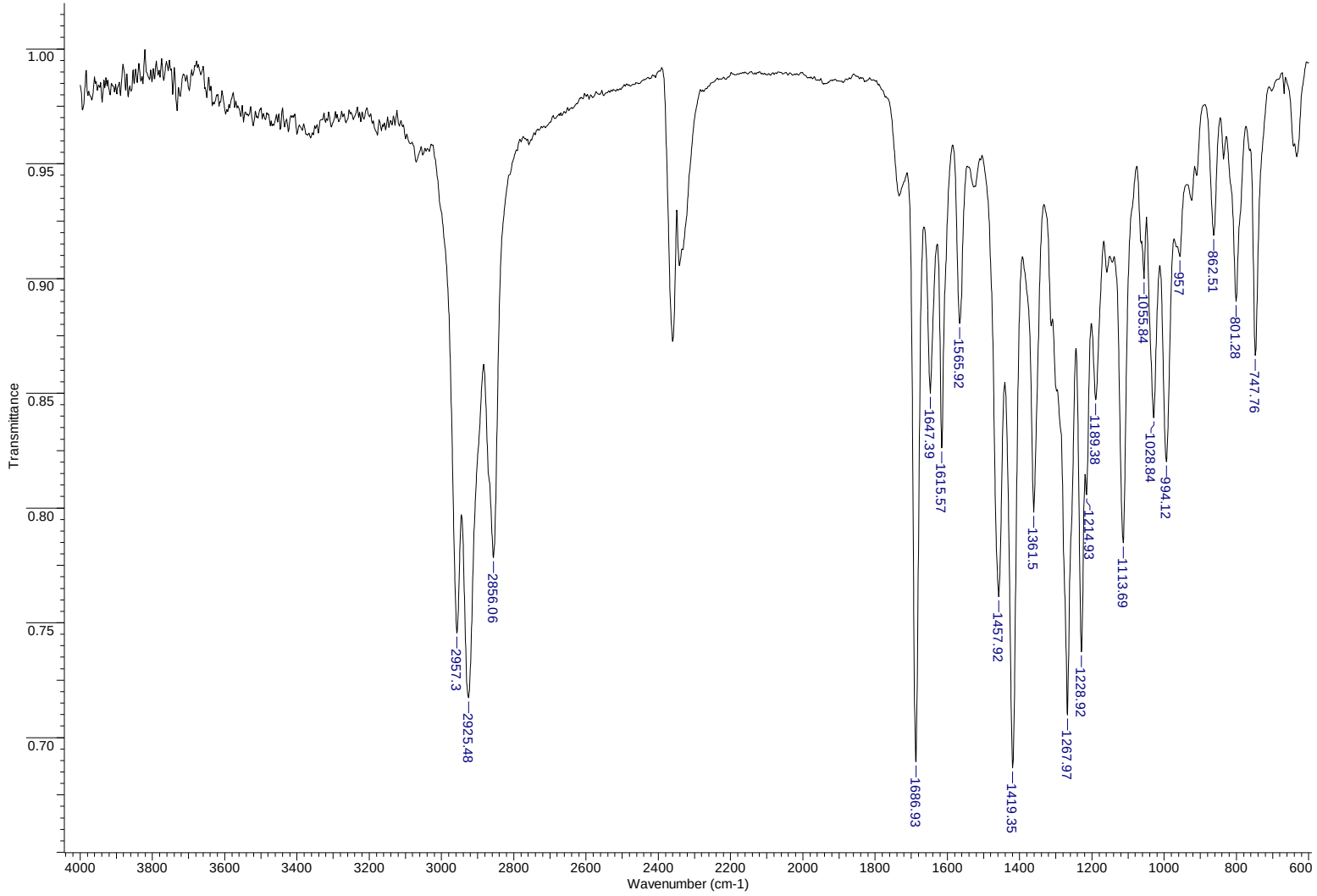




1-(7-Acetyl-1,3-benzoxazol-2-yl)pentyl morpholine-4-carbodithioate (3q)

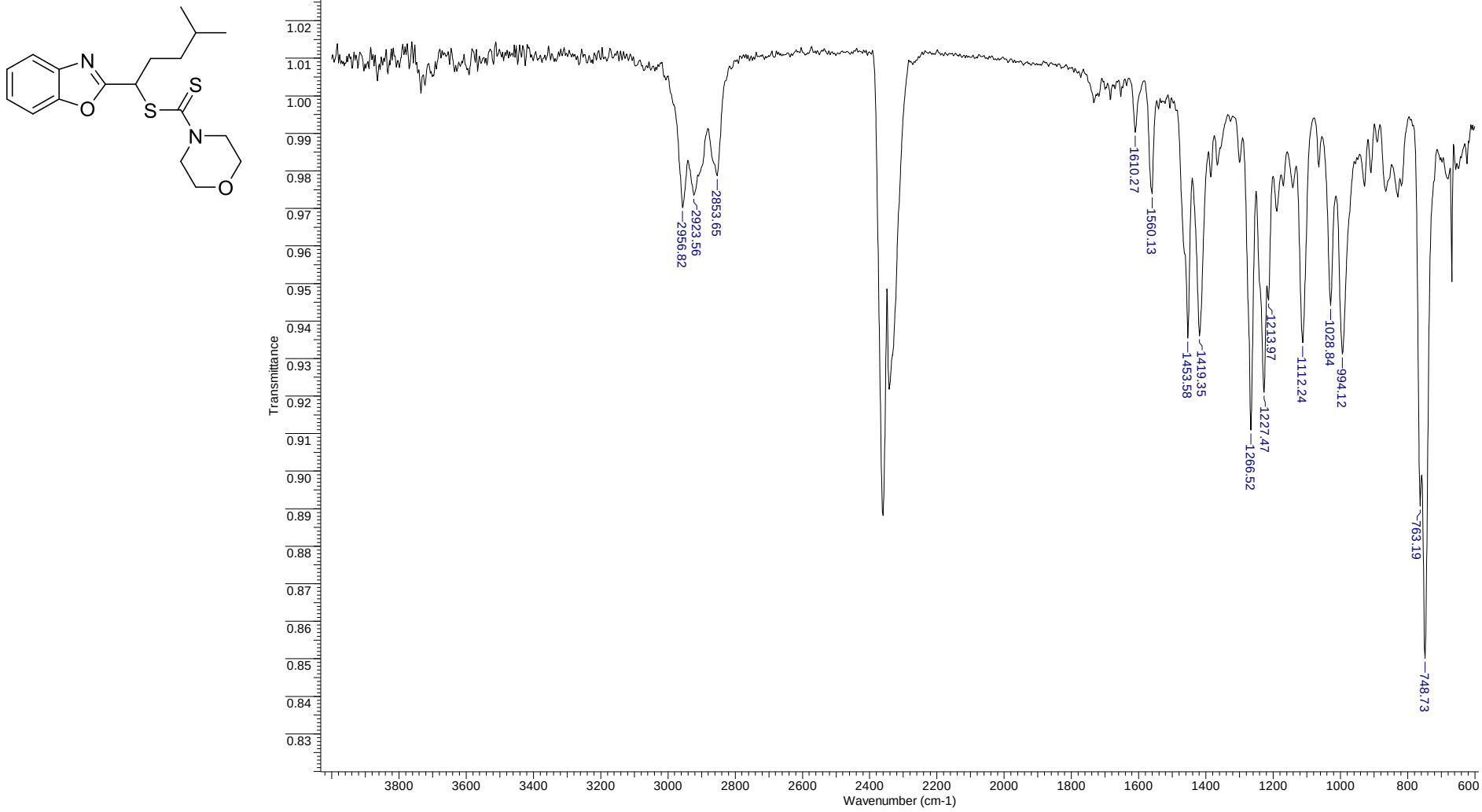
IR (neat)





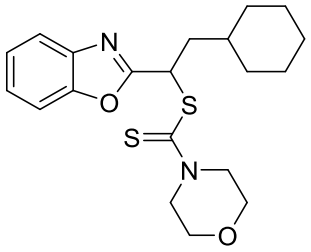
1-(1,3-Benzoxazol-2-yl)-4-methylpentyl morpholine-4-carbodithioate (3r)

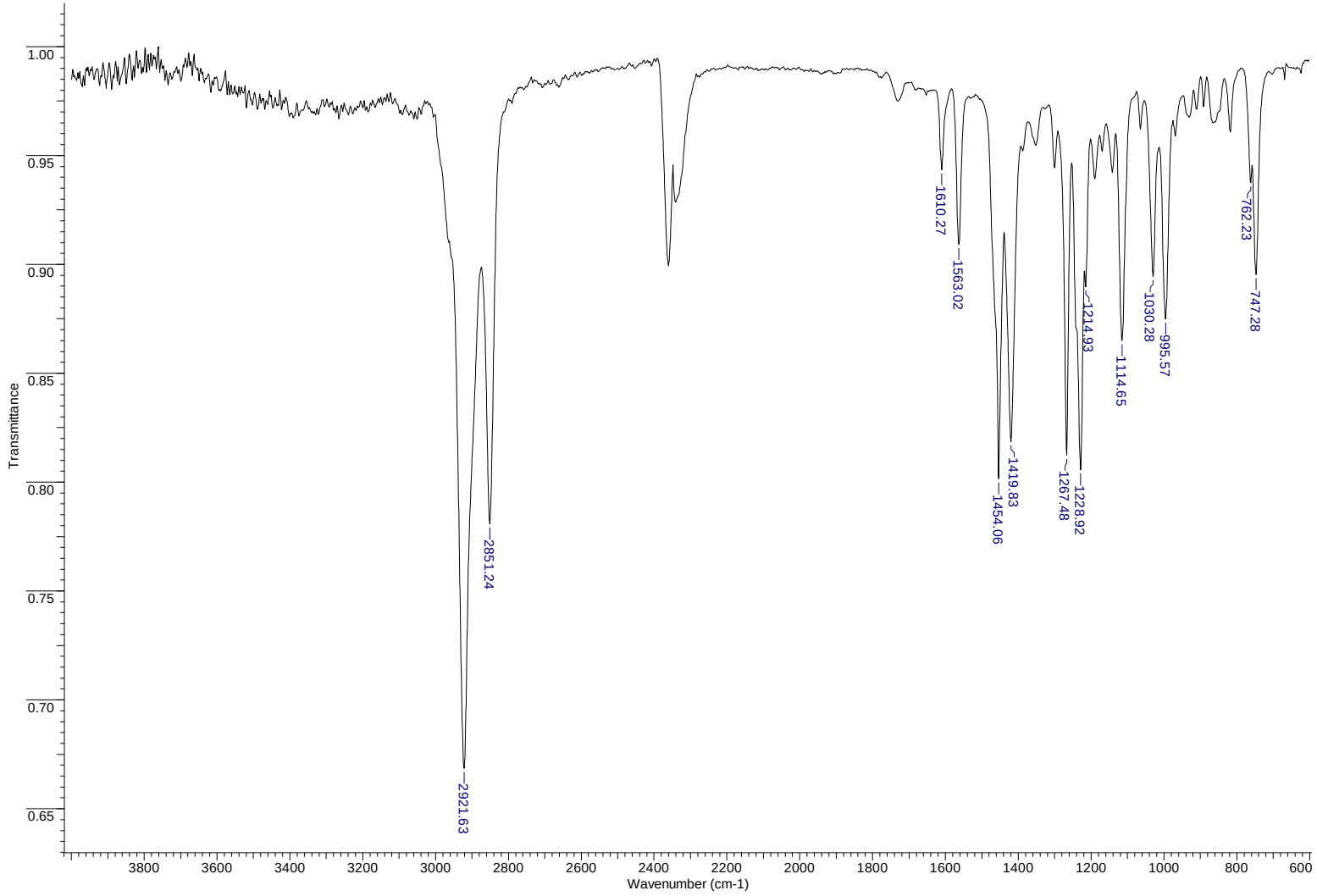
IR (neat)



1-(1,3-Benzoxazol-2-yl)-2-cyclohexylethyl morpholine-4-carbodithioate (3s)

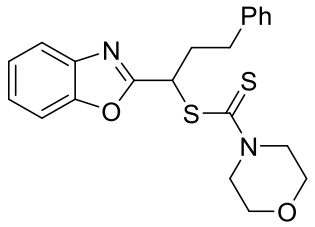
IR (neat)

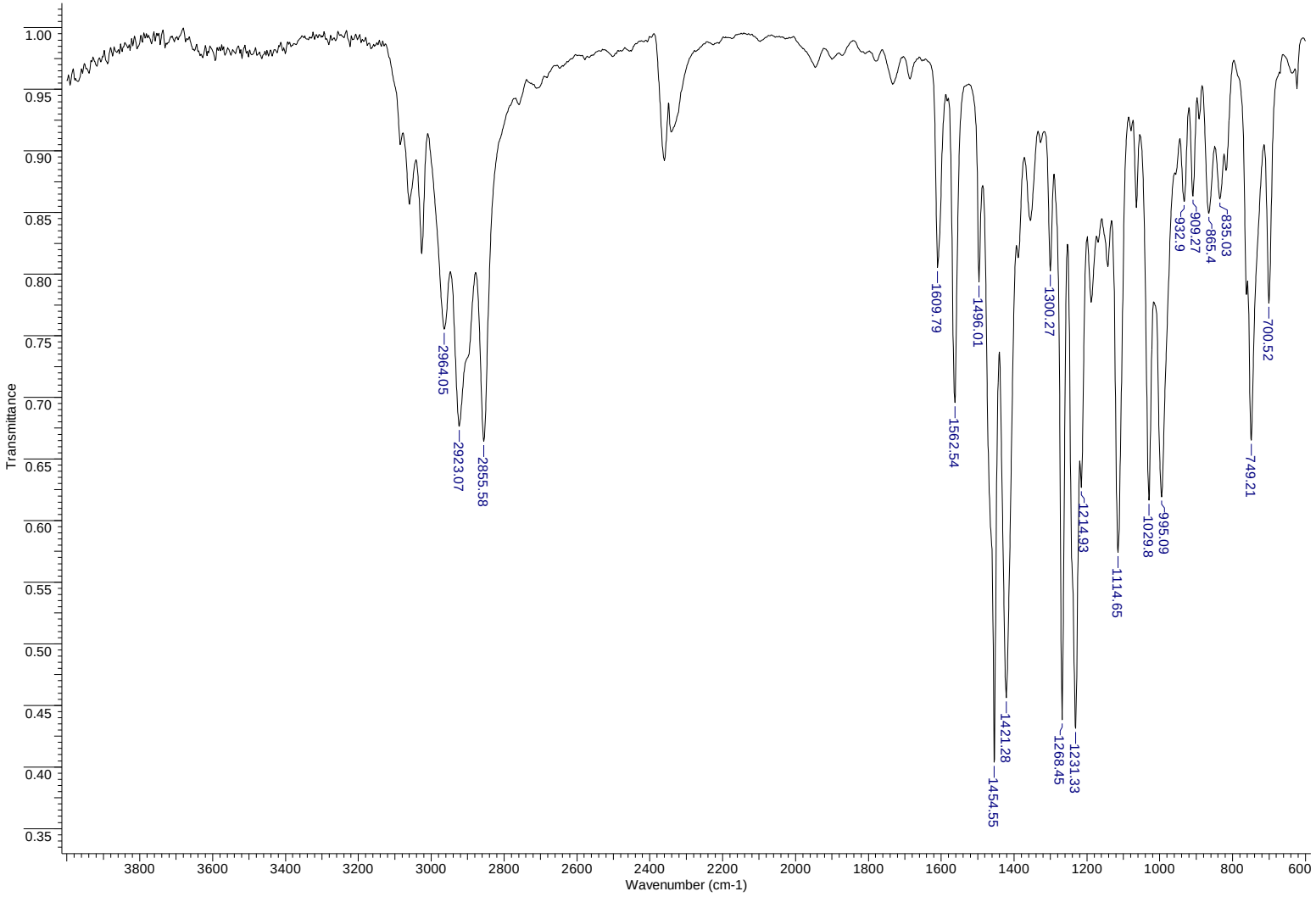




1-(1,3-Benzoxazol-2-yl)-3-phenylpropyl morpholine-4-carbodithioate (3t)

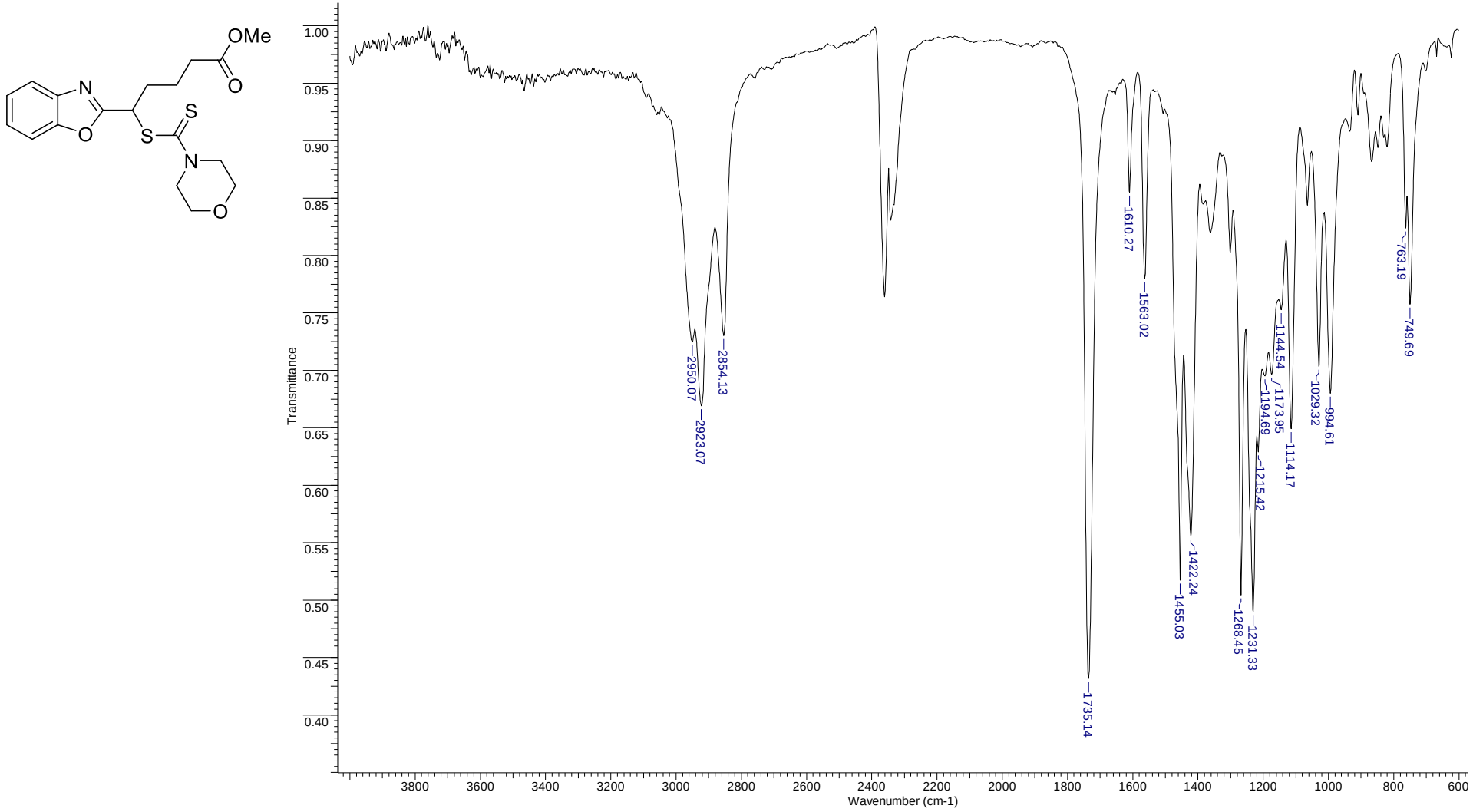
IR (neat)





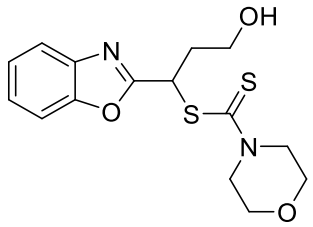
Methyl 5-(1,3-benzoxazol-2-yl)-5-[(morpholin-4-ylcarbonothioyl)thio]pentanoate (3u)

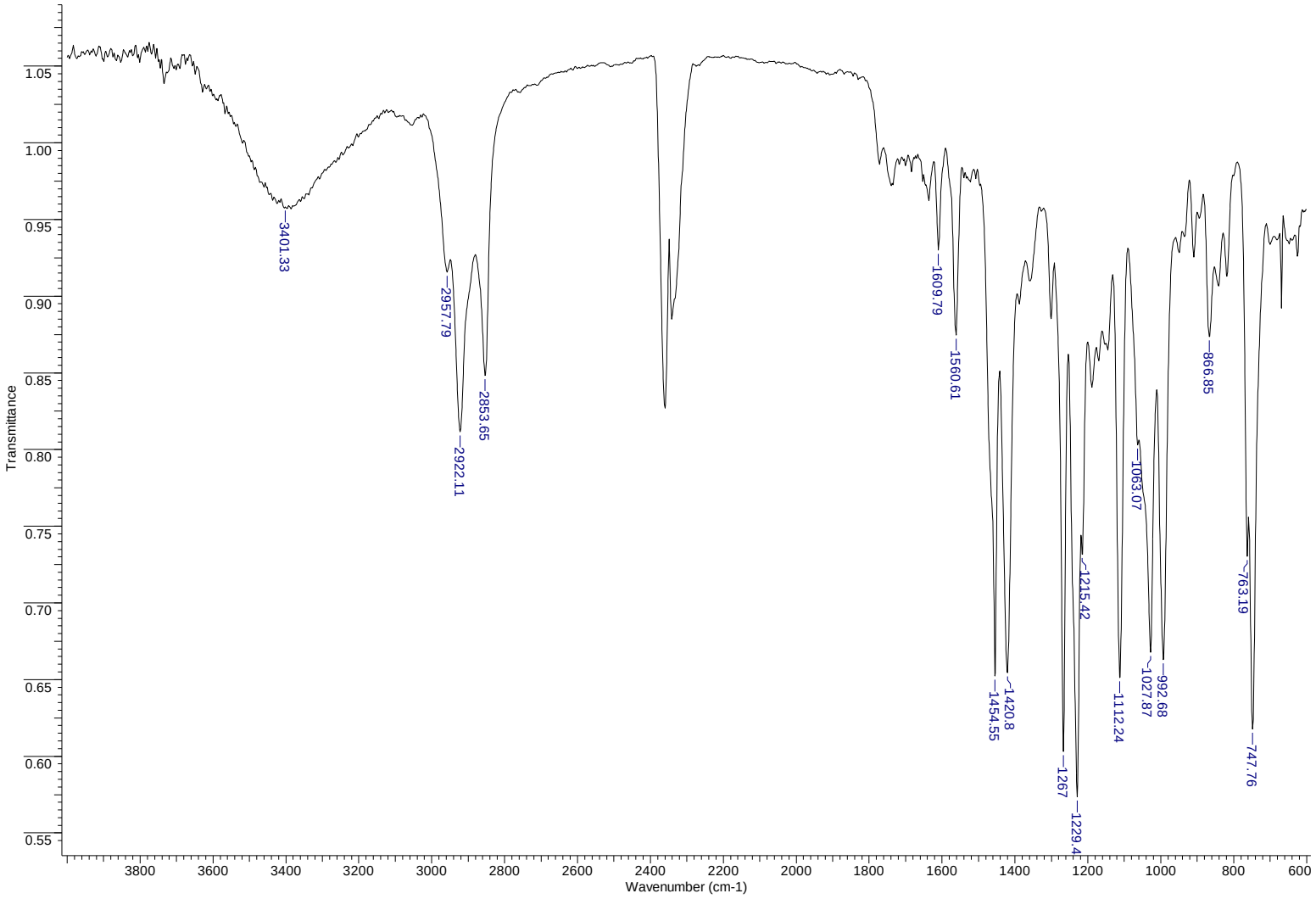
IR (neat)



1-(1,3-Benzoxazol-2-yl)-3-hydroxypropyl morpholine-4-carbodithioate (3v)

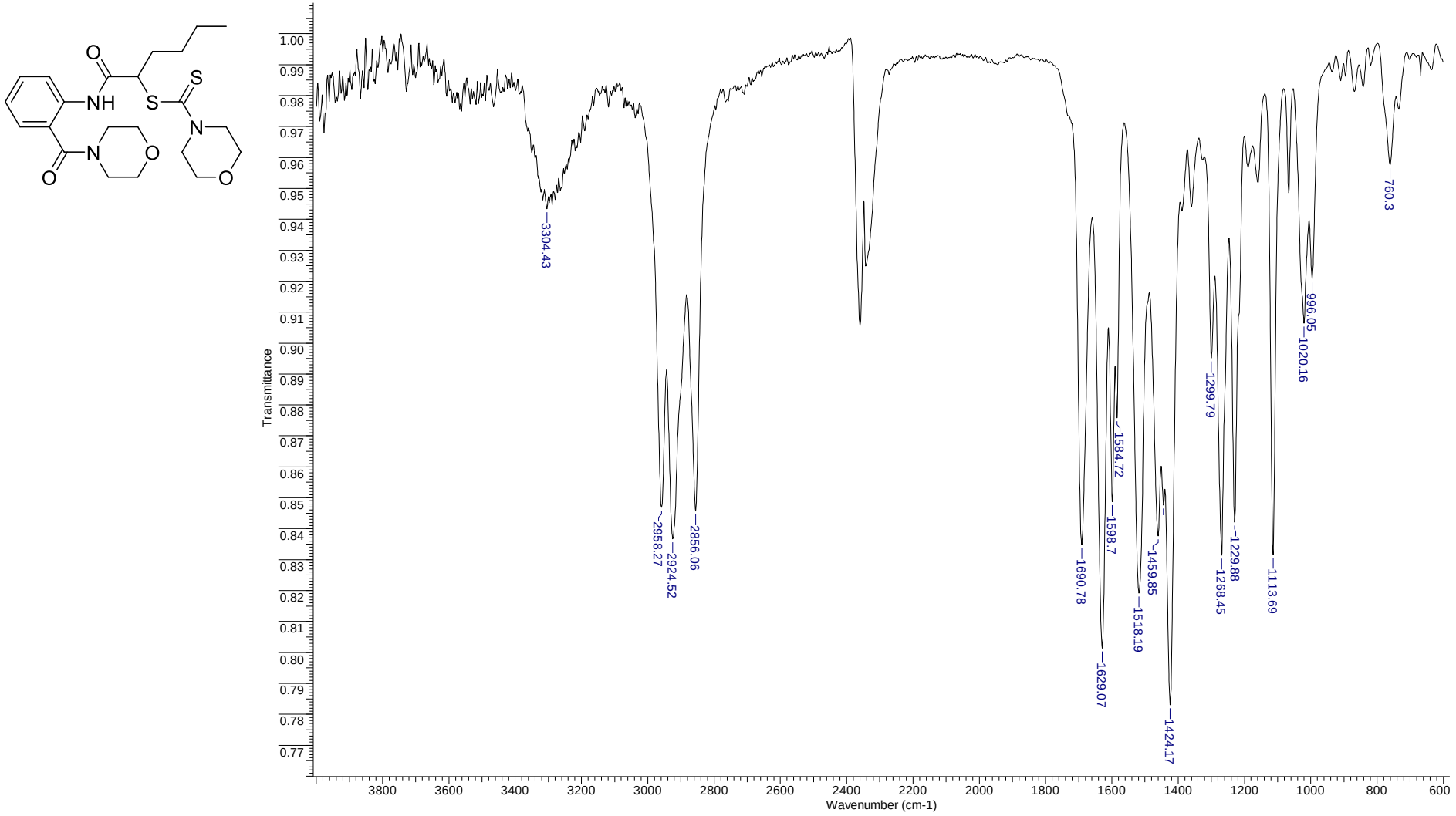
IR (neat)





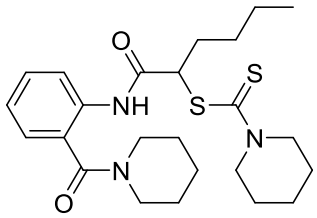
1-({[2-(Morpholin-4-ylcarbonyl)phenyl]amino}carbonyl)pentyl morpholine-4-carbodithioate (11a)

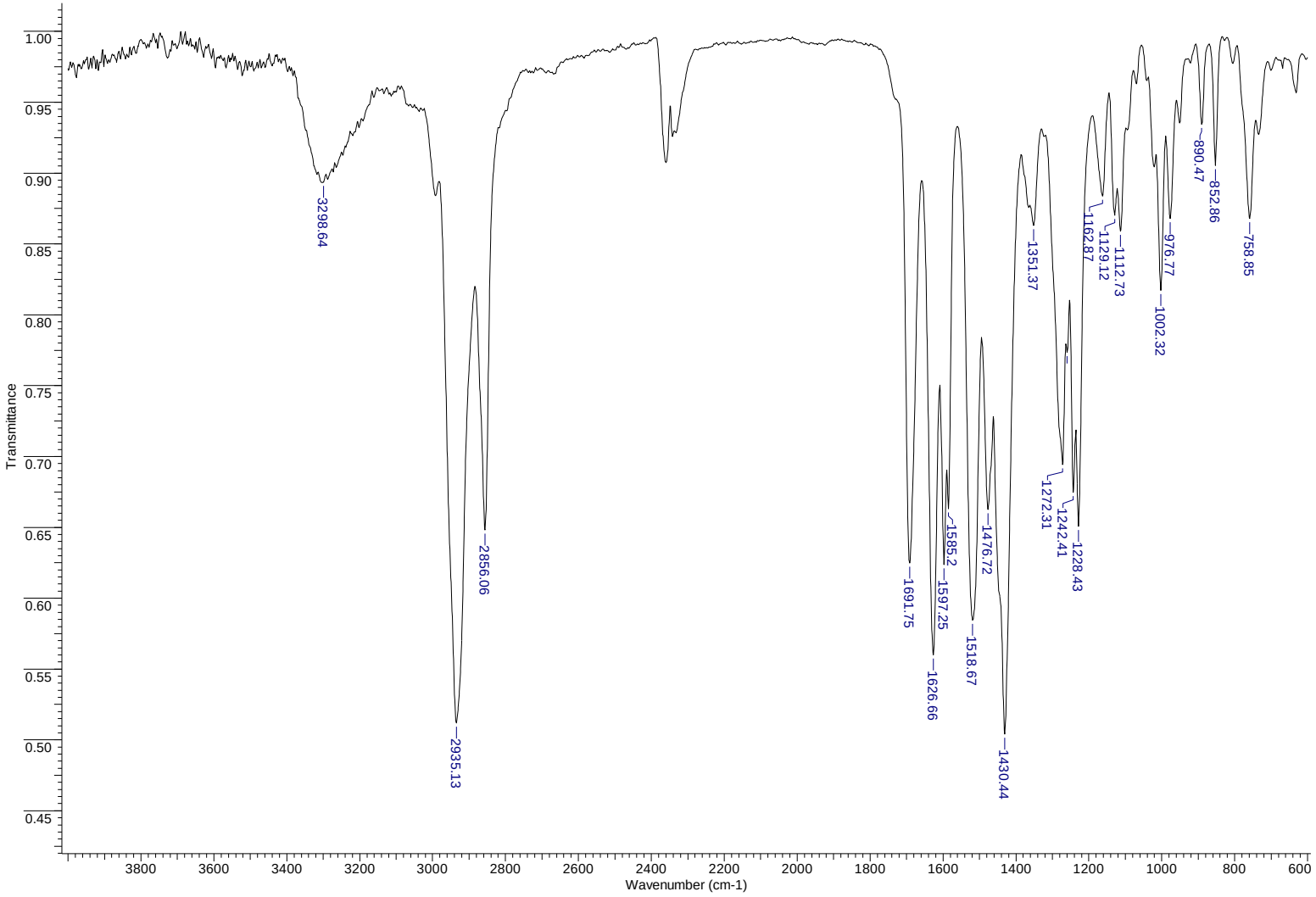
IR (neat)



1-({[2-(Piperidin-4-ylcarbonyl)phenyl]amino}carbonyl)pentyl piperidine-4-carbodithioate (11b)

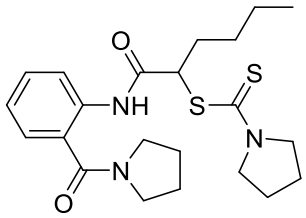
IR (neat)

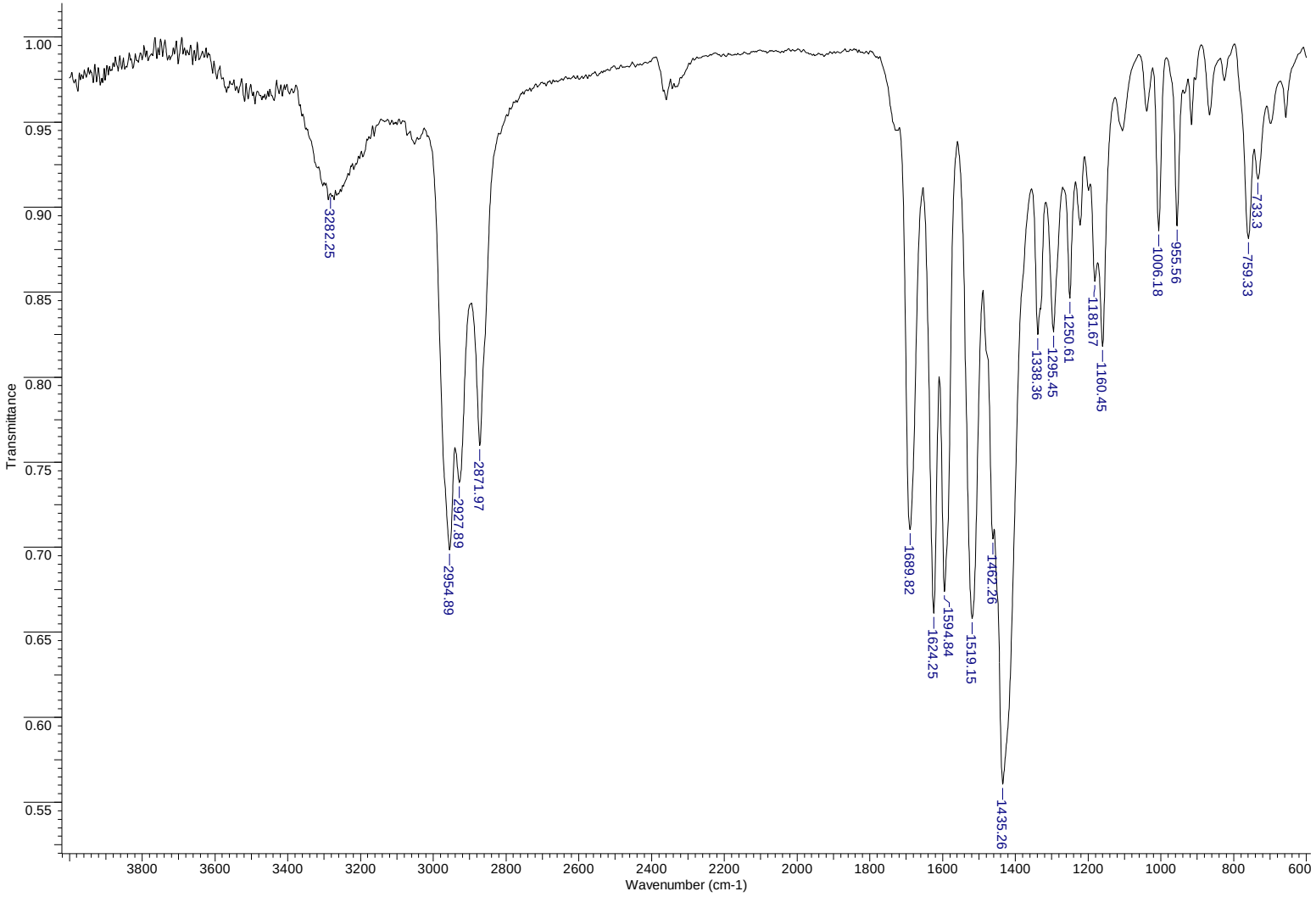




1-({[2-(Pyrrolidin-4-ylcarbonyl)phenyl]amino}carbonyl)pentyl pyrrolidine-4-carbodithioate (11c)

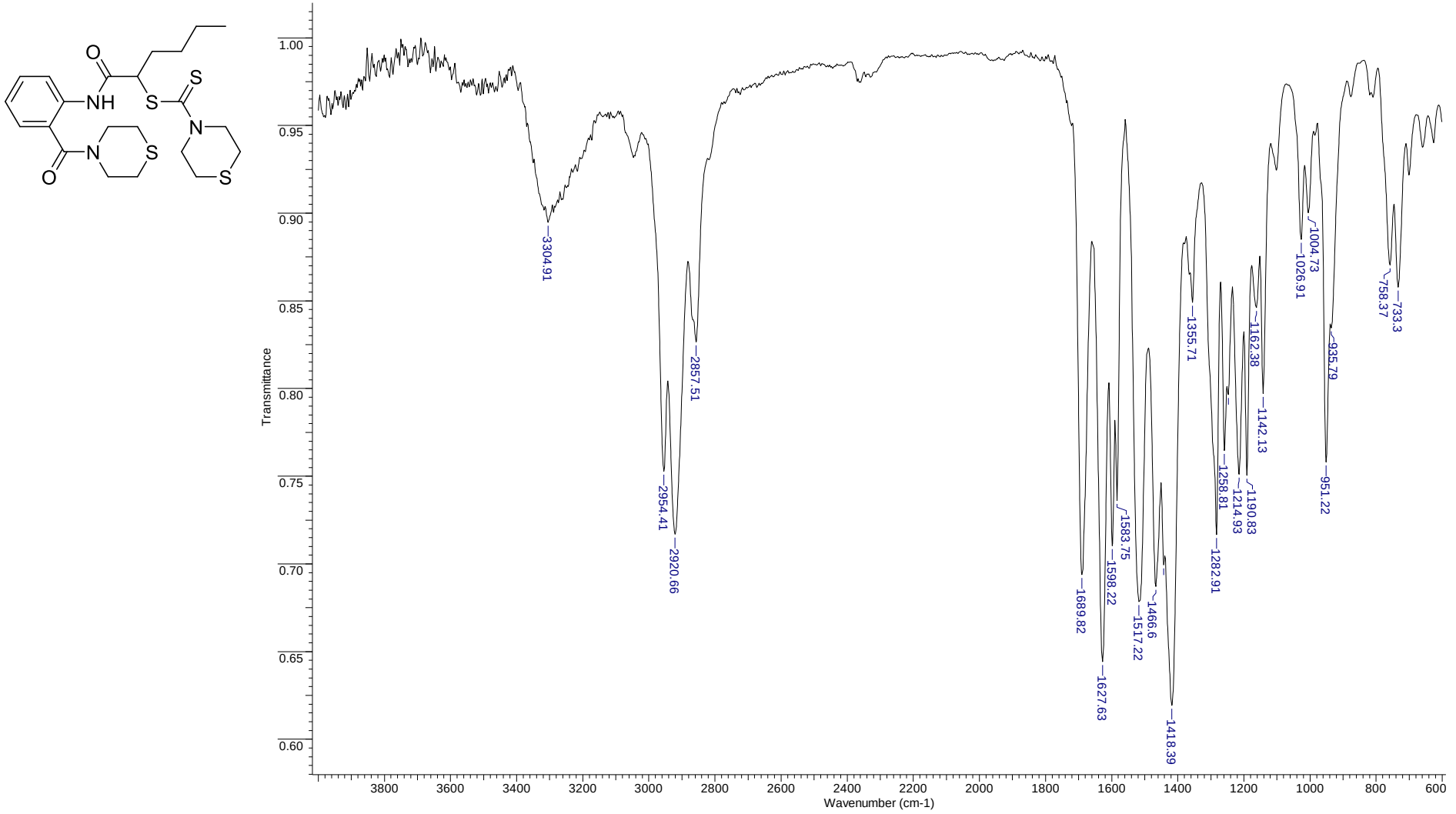
IR (neat)





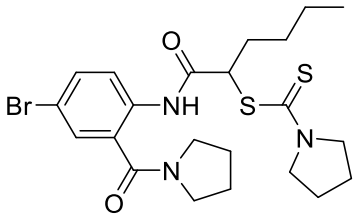
1-({[2-(Thiomorpholin-4-ylcarbonyl)phenyl]amino}carbonyl)pentyl thiomorpholine-4-carbodithioate (11d)

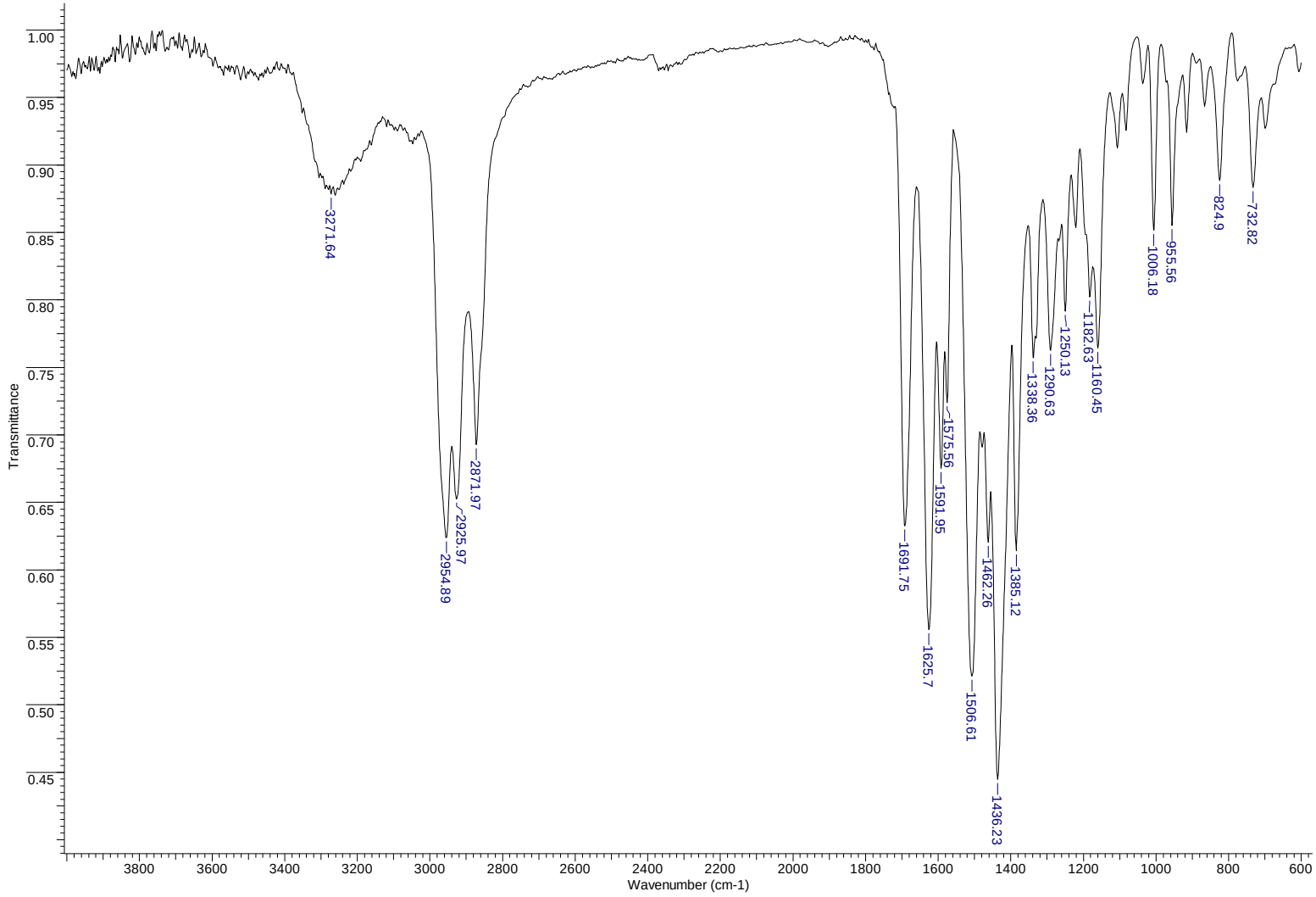
IR (neat)



1-({[4-Bromo-2-(pyrrolidin-1-ylcarbonyl)phenyl]amino}carbonyl)pentyl pyrrolidine-1-carbodithioate (11e)

IR (neat)





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