Supporting Informations

Cu(II) Catalysed chemoselective oxidative transformation of thiourea to thioamidoguanidine / 2-aminobenzothiazole

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General information. All the reagents were commercial grade and purified according to the established procedures. Organic extracts were dried over anhydrous sodium sulphate. Solvents were removed in a rotary evaporator under reduced pressure. Silica gel (60-120 mesh size) was used for the column chromatography. Reactions were monitored by TLC on silica gel 60 F_{254} (0.25mm). NMR spectra were recorded in $CDCl_3$, ESI-MS were recorded using ESI mode. IR spectra were recorded in KBr or neat.

General procedures for X-ray structure determination: The crystals were mounted on a glass fiber and the intensity data were collected using a Bruker SMART APEX II CCD diffractometer, equipped with a fine focus 1.75 kW sealed tube Mo−Kα radiation (λ = 0.71073 Å) at 298(2) K, with increasing ω (width of 0.3° per frame) at a scan speed of 3 s per frame. The SMART software was used for data acquisition. Data integration and reduction were under taken with SAINT and XPREP[a] software. Multi-scan empirical absorption corrections were applied to the data using the program SADABS.[b] Structures were solved by direct methods using SHELXS-97[c] and were refined by full-matrix least-

squares on F^2 using SHELXL-97[d] program package. In all the three, non-hydrogen atoms were refined anisotropically. Hydrogen atoms attached to all carbon atoms are geometrically fixed. Structural illustrations have been generated using ORTEP-3[e] and MERCURY1.3[f] for Windows. The molecular structures of compound **3d**, **15'a** were determined and the crystallographic and refinement parameters are listed in Table S1.

(a) Saint, Smart XPREP; Siemens Analytical X-ray Instruments Inc.: Madison, Wisconsin, USA, 1995.

(b) Sheldrick, G. M. SADABS: Software for Empirical Absorption Correction; University of Göttingen, Institute fur Anorganische Chemieder Universitat: Göttingen, Germany, 1999−2003.

(c) Sheldrick, G. M. SHELXS-97; University of Göttingen: Germany, 1997.

(d) Sheldrick, G. M. SHELXL-97, Program for Crystal Structure Refinement; University of Göttingen: Germany, 1997.

(e) Farrugia, L. J. *J. Appl. Crystallogr.* 1997, **30**, 565.

(f) Mercury 1.3 Supplied with Cambridge Structural Database; CCDC: Cambridge, U.K., 2003−2004.

Crystallographic data can be obtained free of charge from the Cambridge crystallographic Data Centre via www.ccdc.cam.ac.uk/datarequest/cif

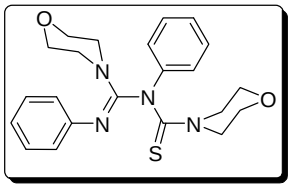
X-ray Crystallographic data

Table S1: Crystallographic data and refinement parameters for compound 3d and 15'a.

	3d	**15'a**
Formula	$C_{28}H_{38}N_4S$	$C_{11}H_{11}BrN_2OS$
CCDC number	894067	894068
Formula weight	462.69	299.19
T (K)	296(2)	296(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	Monoclinic	Orthorhombic
Space group	P 21 / c	P-1
a (Å)	9.5021(13)	10.01289(3)
b (Å)	11.2799(14)	11.2225(3)
c (Å)	24.739(3)	11.7532(4)
α (°)	90.00	94.059(2)
β (°)	95.125(8)	112.599(2)
γ (°)	90.00	107.266(2)
V (Å^3)	2641.0(6)	1151.66(7)
Z	4	4
θ_{min}, θ_{max}	2.12, 26.56	2.13, 30.00
D_{calcd} (g m^{-3})	1.164	1.726
μ(mm^{-1})	0.145	3.729
F(0 0 0)	1000.0	600.0
Reflection collected	2737	3592
Unique reflections	29006	18708
Goodness of fit (GOF)[a]	1.045	1.383
R1[a], wR_2[b] ($I \geq 2\sigma(I)$)	0.0570, 0.1242	0.0851, 0.0836
R1[a], wR_2[b] (all data)	0.1134, 0.1421	0.0851, 0.0866

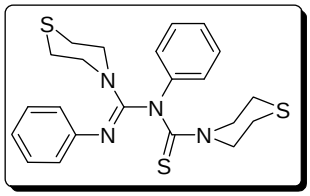
Spectral Data

_N_-((_E_)-Morpholino(phenylimino)methyl)-_N_-phenylmorpholine-4-carbothioamide (1a):



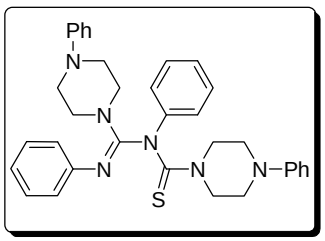
White solid; M.p. 163–165 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.90-3.52 (m, 16H), 6.95 (d, 2H, J = 8.0 Hz), 6.98 (d, 2H, J = 7.6 Hz), 7.09 (t, 2H, J = 7.6 Hz), 7.17 (t, 2H, J = 8.0 Hz), 7.30 (d, 2H, J = 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 46.8, 50.6, 65.4, 66.2, 121.2, 122.1, 122.8, 122.9, 124.7, 128.8, 129.7, 142.8, 149.3, 185.2; IR (KBr): 2963, 2920, 2856, 1637, 1587, 1485, 1421, 1302, 1277, 1239, 1109, 1062, 994, 765, 753, 691 cm^{-1}; MS (ESI): 411.2045 (MH^+).

_N_-((_E_)-Thiomorpholino(phenylimino)methyl)-_N_-phenylthiomorpholine-4-carbothioamide (1b):



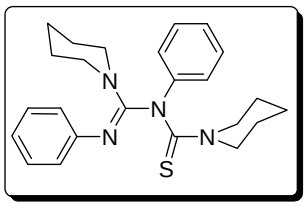
White solid; M.p. 188–190 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.42–3.53 (m, 16H), 6.87–6.92 (m, 4H), 7.06 (t, 2H, J = 7.2 Hz), 7.13 (t, 4H, J = 8.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 26.5, 26.6, 48.9, 53.0, 121.0, 122.1, 122.8, 125.1, 128.8, 129.8, 143.2, 149.2, 149.5, 186.4; IR (KBr): 3446, 2919, 2855, 1630, 1586, 1474, 1416, 1358, 1295, 1274, 1223, 1019, 945, 751 cm^{-1}; MS (ESI): 443.1050 (MH^+).

_N_,4-Diphenyl-_N_-((_E_)-(phenylimino)(4-phenylpiperazin-1-yl)methyl)piperazine-1-carbothioamide (1c):



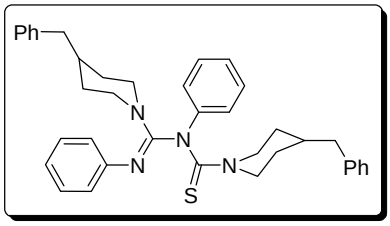
White solid; M.p. 200–201 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.61–3.66 (m, 16H), 6.62 (d, 2H, J = 8.8 Hz), 6.74 (d, 4H, J = 6.8 Hz), 6.88 (t, 2H, J = 7.2 Hz), 7.00 (t, 4H, J = 7.2 Hz), 7.08–7.26 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 46.3, 47.8, 48.6, 50.0, 115.5, 116.1, 116.3, 120.0, 120.3, 122.3, 122.9, 124.8, 128.9, 129.2, 129.3, 129.7, 143.1, 149.3, 149.7, 150.3, 151.2, 185.3 ; IR (KBr): 3431, 2904, 2819, 1638, 1591, 1479, 1413, 1305, 1252, 1224, 1152, 1048, 1024, 993, 918, 758, 691 cm^{-1}; MS (ESI): 561.2363 (MH^+).

_N_-Phenyl-_N_-((_E_)-(phenylimino)(piperidin-1-yl)methyl)piperidine-1-carbothioamide (1d):



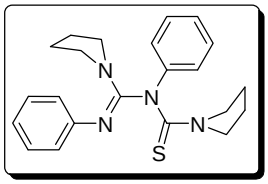
White solid; M.p. 183–184 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.84–1.67 (m, 12H), 2.63–3.82 (m, 8H), 6.90 (t, 2H, J = 7.6 Hz), 7.02–7.12 (m, 3H), 7.16 (t, 2H, J = 8.4 Hz), 7.26–7.40 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 23.6, 24.5, 24.6, 24.9, 47.4, 51.4, 122.1, 122.3, 124.1, 128.4, 129.2, 143.7, 149.7, 150.0, 184.9; IR (KBr): 2936, 2854, 1632, 1588, 1481, 1454, 1295, 1240, 1028, 989, 749 cm^{-1}; MS (ESI): 407.2261 (MH^+).

_N_-Benzyl-_N_-((_E_)-(4-benzylpiperidin-1-yl)(phenylimino)methyl)-_N_-phenylpiperidine-1-carbothioamide (1e):



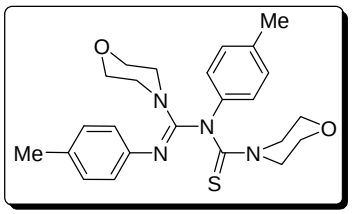
White solid; M.p. 151–152 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.84–4.12 (m, 22H), 7.00 (m, 5H), 7.15 (t, 2H, J = 7.2 Hz), 7.23 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 30.8, 37.4, 38.0, 42.5, 43.0, 46.8, 50.9, 122.4, 123.0, 124.2, 125.9, 126.1, 128.2, 128.3, 128.6, 129.1, 129.2, 129.3, 139.9, 140.3, 143.8, 149.8, 184.9; IR (KBr): 3428, 2989, 3024, 2921, 2848, 1651, 1589, 1493, 1396, 1296, 1236, 1221, 1142, 1056, 963, 746, 697 cm^{-1}; MS (ESI): 587.2807 (MH^+).

_N_-phenyl-_N_-((_E_)-(phenylimino)(pyrrolidin-1-yl)methyl)pyrrolidine-1-carbothioamide (1f):



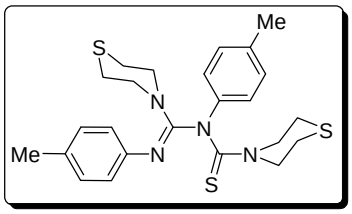
White solid; M.p. 153–155 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.05–2.50 (m, 12H), 3.37–3.90 (m, 4H), 6.82 (m, 1H), 6.89 (t, 1H, J = 7.2 Hz), 6.96 (m, 1H), 7.04 (t, 1H, J = 7.6 Hz), 7.09 (d, 2H, J = 7.6 Hz), 7.15 (m, 2H), 7.19–7.36 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 24.3, 25.1, 25.8, 26.2, 47.2, 48.4, 51.9, 53.7, 120.9, 122.2, 123.2, 123.9, 128.4, 129.3, 129.8, 141.8, 150.0, 181.0; IR (KBr): 2962, 2863, 1587, 1488, 1438, 1415, 1330, 1288, 1260, 1175, 906, 859, 770 cm^{-1}; MS (ESI): 379.1642 (MH^+).

_N_-((_E_)-(p-Tolylimino)(morpholino)methyl)-_N_-p-tolylmorpholine-4-carbothioamide (2a):



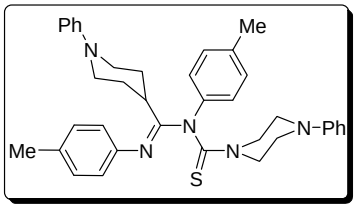
White solid; M.p. 140–141 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.17 (s, 3H), 2.25 (s, 3H), 2.82–3.47 (m, 16H), 6.84 (d, 4H, J = 8.0 Hz), 6.92 (d, 4H, J = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 20.7, 20.8, 46.6, 50.5, 65.2, 66.1, 121.0, 121.8, 129.1, 130.1, 131.6, 134.3, 140.1, 146.6, 149.3, 185.1; IR (KBr): 3436, 3021, 2959, 2920, 2855, 1630, 1605, 1505, 1472, 1438, 1288, 1232, 1158, 1115, 1068, 1000, 855, 828 cm^{-1}; MS (ESI): 439.1779 (MH^+).

_N_-((_E_)-(_p_-Tolylimino)(thiomorpholino)methyl)-_N_-_p_-tolylmorpholine-4-carbothioamide (2b):



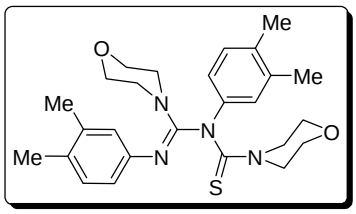
White solid; M.p. 161–162 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.25 (s, 3H), 2.33(s, 3H), 2.50–3.62 (m, 16H), 6.90 (d, 2H, J = 8.0 Hz), 7.02 (d, 2H, J = 8.0 Hz), 7.17 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 20.8, 20.9, 26.4, 26.6, 48.8, 52.9, 121.9, 129.3, 130.3, 131.9, 134.8, 140.7, 146.6, 149.6, 186.4; IR (KBr): 2911, 2851, 1633, 1605, 1505, 1473, 1414, 1358, 1306, 1278, 1224, 1135, 1018, 946, 891, 832 cm^{-1}; Anal. Calcd for $C_{24}H_{30}N_4S_3$: C 61.24, H 6.42, N 11.90, S 20.44; found C 61.29, H 6.45, N 11.86, S 20.49.

_N_-((_E_)-(p-Tolylimino)(1-phenylpiperidin-4-yl)methyl)-4-phenyl-tolylpiperazine-1-carbothioamide (2c):



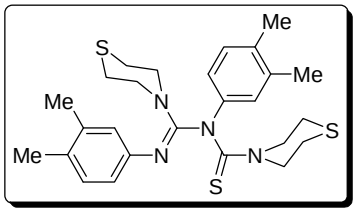
White solid; M.p. 215–216 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.15 (s, 3H), 2.27 (s, 3H), 2.70–3.52 (m, 16H), 6.68 (d, 2H, J = 8.0 Hz), 6.83 (m, 5H), 6.94 (m, 6H), 7.20 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 20.8, 20.9, 46.2, 47.8, 48.5, 50.0, 115.9, 116.2, 119.9, 120.2, 122.0, 129.3, 129.4, 130.2, 131.8, 134.4, 140.7, 146.9, 150.4, 151.3, 185.3; IR (KBr): 3430, 2919, 1633, 1598, 1505, 1486, 1412, 1305, 1230,. 1193, 1102, 998, 891, 792, 756 cm^{-1}; MS (ESI): 589.2782 (MH^+).

_N_-((_E_)-(3,4-Dimethylphenylimino)(morpholino)methyl)-_N_-(3,4-dimethylphenyl) morpholine-4-carbothioamide (3a):



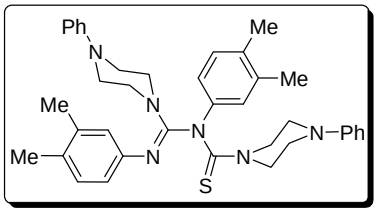
Gummy; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.10 (s, 3H), 2.11 (s, 3H), 2.18 (s, 6H), 2.85–3.76 (m, 16H), 6.69 (d, 2H, J = 7.6 Hz), 6.77 (s, 2H), 6.89 (d, 2H, J = 8.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 19.0, 19.2, 19.8, 20.1, 46.6, 50.6, 65.4, 66.2, 119.1, 123.3, 129.7, 130.4, 133.0, 136.4, 137.9, 140.4, 147.0, 149.3, 185.1; IR (Neat): 3444, 2962, 2919, 2856, 1633, 1448, 1423, 1303, 1236, 1114, 1065, 1020, 992, 860, 818, 734 cm^{-1}; Anal. Calcd for $C_{26}H_{34}N_4O_2S$: C 66.92, H 7.34, N 12.01, S 6.87; found C 66.97, H 7.37, N 11.98, S 6.92.

_N_-((_E_)-(3,4-Dimethylphenylimino)(thiomorpholino)methyl)-_N_-(3,4-dimethylphenyl) thiomorpholine-4-carbothioamide (3b):



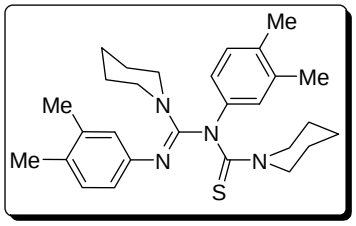
White solid; M.p. 188–189 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.10 (s, 3H), 2.12 (s, 3H), 2.14 (s, 3H), 2.17 (s, 3H), 2.19–3.72 (m, 16H), 6.34-7.01 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 18.9, 19.1, 19.7, 20.0, 26.2, 26.5, 26.8, 48.7, 52.8, 119.0, 123.2, 129.6, 129.9, 130.2, 130.5, 133.2, 136.4, 137.9, 140.7, 146.9, 149.3, 186.1; IR (Neat): 3426, 3005, 2911, 2857, 1633, 1497, 1448, 1416, 1341, 1296, 1216, 1190, 1166, 1021, 952, 841 cm^{-1}; MS (ESI): 499.2154 (MH^+).

_N_-((_E_)-(3,4-Dimethylphenylimino)(4-phenylpiperazin-1-yl)methyl)-_N_-(3,4-dimethylphe-nyl)-4-phenylpiperazine-1-carbothioamide (3c):



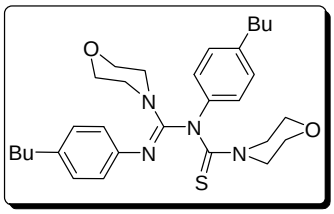
White solid; M.p. 190–191 ^{o}C ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.10 (s, 3H), 2.11 (s, 3H), 2.18 (s, 6H), 2.85–3.76 (m, 16H), 6.69 (d, 2H, J = 7.6 Hz), 6.77 (s, 2H), 6.89 (d, 2H, J = 8.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 19.0, 19.2, 19.9, 20.2, 46.2, 47.9, 48.6, 50.0, 116.0, 116.2, 119.3, 119.8, 120.3, 123.7, 129.2, 129.3, 129.9, 130.5, 133.0, 136.6, 138.1, 140.8, 147.0, 150.4, 151.2, 185.1; IR (Neat): 3432, 2913, 2846, 2824, 1632, 1598, 1497, 1448, 1388, 1305, 1281, 1227, 1153, 991, 924, 908, 812, 762 cm^{-1}; MS (ESI): 617.3067 (MH^+).

_N_-((_E_)-(3,4-Dimethylphenylimino)(piperidin-1-yl)methyl)-_N_-(3,4-dimethylphenyl) piperidine-1-carbothioamide (3d):



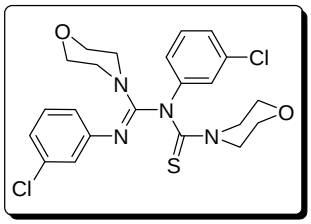
White solid; M.p. 188–189 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.69-1.80 (m, 12H), 2.09 (s, 6H), 2.17 (s, 6H), 2.87–3.73 (m, 8H), 6.14-7.03 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 18.9, 19.1, 19.7, 19.9, 47.3, 51.5, 119.5, 121.5, 123.5, 125.2, 129.5, 129.7, 130.1, 132.3, 136.0, 137.3, 141.4, 147.4, 150.3, 184.9; IR (Neat): 3447, 3014, 2929, 2856, 1628, 1601, 1473, 1416, 1300, 1270, 1239, 1117, 999, 822 cm^{-1}; MS (ESI): 463.2850 (MH^+).

_N_-((_E_)-(4-Butylphenylimino)(morpholino)methyl)-_N_-(4-butylphenyl)morpholine-4-carbothioamide (4a):



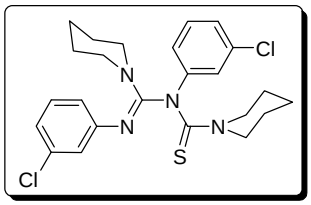
Gummy; ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.86 (m, 6H), 1.29 (m, 4H), 1.49 (m, 4H), 2.47 (m, 4H), 2.88–3.48 (m, 16H), 6.87 (d, 2H, J = 8.0 Hz), 6.96 (d, 2H, J = 8.0 Hz, 7.07 (M, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.9, 22.2, 22.4, 33.4, 33.8, 34.9, 35.0, 46.7, 50.5, 65.4, 66.1, 121.8, 128.6, 129.5, 136.9, 139.5, 140.5, 146.8, 149.4, 185.3; IR (Neat): 3464, 2957, 2927, 2856, 2634, 1604, 1505, 1467, 1416, 1359, 1297, 1234, 1160, 1115, 1066, 1017, 998, 941, 838 cm^{-1}; MS (ESI): 523.2705 (MH^+).

_N_-((_E_)-(3-Chlorophenylimino)(morpholino)methyl)-_N_-(3-chlorophenyl)morpholine-4-carbothioamide (5a):



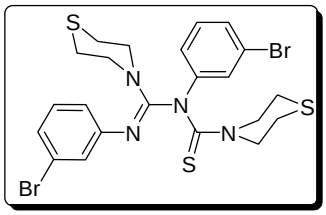
White solid; M.p. 172–173 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.25–3.78 (m, 16H), 6.83 (d, 2H, J = 8.0 Hz), 6.94 (d, 2H, J = 8.4 Hz), 6.96 (d, 2H, J = 4.8 Hz), 7.11 (t, 2H, J = 8.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 46.9, 50.8, 65.5, 66.2, 119.1, 120.6, 122.2, 122.9, 125.1, 129.9, 130.8, 134.3, 135.6, 143.7, 149.2, 150.5, 184.5; IR (KBr): 3054, 2978, 2895, 2850, 1639, 1583, 1474, 1297, 1239, 1160, 1111, 1064, 938, 861, 776.cm^{-1}; MS (ESI): 479.0717 (MH^+).

_N_-((_E_)-(3-chlorophenylimino)(piperidin-1-yl)methyl)-_N_-(3-chlorophenyl)piperidine-1-carbothioamide (5d):



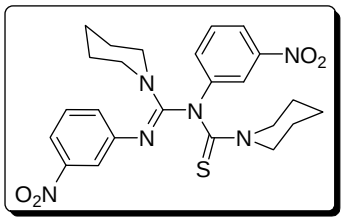
White solid; M.p. 123–125 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.23–1.71 (m, 16H), 3.11–3.51 (m, 4H), 6.87 (t, 4H, J = 4.8 Hz), 6.98 (s, 1H), 7.05 (d, 2H, J = 7.2 Hz), 7.24 (d, 1H, J = 3.2 Hz).; ^{13}C NMR (100 MHz, $CDCl_3$): δ 23.7, 24.5, 24.8, 25.1, 47.7, 51.9, 119.9, 121.0, 122.4, 124.5, 129.6, 130.4, 134.0, 135.0, 144.6, 150.1, 150.9, 184.3; IR (KBr): 3446, 2929, 2851, 1637, 1584, 1474, 1420, 1364, 1294, 1233, 1204, 1183, 1026, 989, 853, 768, 747, 694 cm^{-1}; Anal. Calcd for $C_{24}H_{28}Cl_2N_4S$: C 60.62, H 5.94, N 11.78, S 6.74; found C 60.67, H 5.99, N 11.72, S 6.78.

_N_-((_E_)-(3-Bromophenylimino)(thiomorpholino)methyl)-_N_-(3-bromophenyl) thiomorpholine-4-carbothioamide (6b):



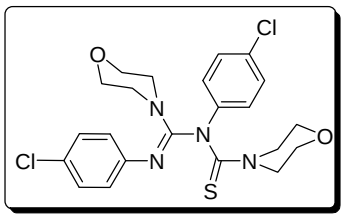
Gummy; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.96-3.53 (m, 16H), 6.82 (m, 2H), 7.03 (m, 4H), 7.21 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 26.4, 48.8, 53.0, 120.9, 122.2, 123.1, 124.2, 124.7, 125.5, 128.0, 128.6, 130.0, 130.3, 130.6, 130.9, 143.8, 150.3, 185.1; IR (KBr): 3403, 3058, 2960, 2914, 2851, 1735, 1621, 1580, 1470, 1437, 1418, 1291, 1223, 1197, 1127, 1052, 1032, 951, 910, 806, 755 cm^{-1}; MS (ESI): 600.9188 (MH^+).

_N_-((_E_)-(3-nitrophenylimino)(piperidin-1-yl)methyl)-_N_-(3-nitrophenyl)piperidine-1-carbothioamide (7d):



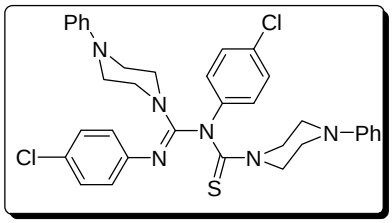
Yellow solid; M.p. 178–180 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.91–1.92(m, 12H), 3.35 (m, 8H), 7.14–7.41 (m, 3H), 7.50 (t, 1H, J = 7.6 Hz), 7.63–7.86 (m, 3H), 7.93 (d, 1H, J = 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 23.6, 24.3, 25.0, 47.9, 52.2, 116.8, 117.1, 119.53, 127.4, 129.3, 130.4, 144.4, 148.9, 150.5, 184.1; IR (KBr): 3080, 2942, 2925, 2851, 1637, 1606, 1522, 1479, 1444, 1352, 1299, 1280, 1244, 1206, 1182, 1027, 901, 739 cm^{-1}; MS (ESI): 497.1540 (MH^+).

_N_-((_E_)-(4-Chlorophenylimino)(morpholino)methyl)-_N_-(4-chlorophenyl)morpholine-4-carbothioamide (8a):



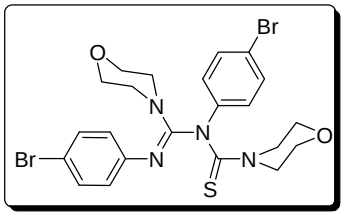
White solid; M.p. 162–164 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.81–3.92 (m, 16H), 6.74 (m, 2H), 6.93 (d, 2H, J = 8.0 Hz), 7.17 (d, 2H, J = 8.0 Hz), 7.33 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 46.9, 50.9, 65.5, 66.3, 122.3, 123.5, 128.3, 128.9, 130.1, 130.5, 141.2, 147.7, 149.5, 184.9; IR (KBr): 2963, 2889, 2845, 1637, 1584, 1487, 1461, 1416, 1360, 1297, 1273, 1258, 1232, 1207, 1159, 1112, 1094, 1074, 1010, 997, 825 cm^{-1}; Anal. Calcd for $C_{22}H_{24}Cl_2N_4O_2S$: C 55.12, H 5.05, N 11.69, S 6.69; found C 55.17, H 5.09, N 11.63, S 6.73.

_N_-((_E_)-(4-Chlorophenylimino)(4-phenylpiperazin-1-yl)methyl)-_N_-(4-chlorophenyl)-4-phenylpiperazine-1-carbothioamide (8c):



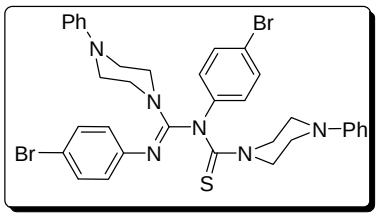
White solid; M.p. 159–160 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.80–3.67 (m, 16H), 6.77 (d, 2H, J = 8.0 Hz), 6.87 (m, 5H), 6.96 (d, 2H, J = 8.4 Hz), 7.17 (d, 2H, J = 8.4 Hz), 7.24 (m, 5H), 7.30 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 46.3, 48.0, 48.6, 50.3, 116.3, 116.4, 120.1, 120.6, 123.5, 128.0, 128.8, 129.2, 129.3, 129.9, 130.2, 141.4, 147.9, 150.2, 151.0, 184 .8; IR (KBr): 3433, 2910, 2840, 1633, 1600, 1487, 1422, 1299, 1226, 1157, 1092, 998, 890, 833, 761 cm^{-1}; MS (ESI): 629.2162 (MH^+).

_N_-((_E_)-(4-bromophenylimino)(morpholino)methyl)-_N_-(4-bromophenyl)morpholine-4-carbothioamide (9a):



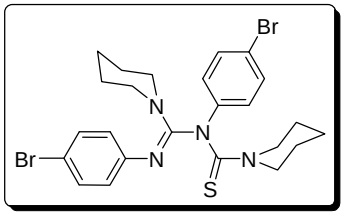
White solid; M.p. 174–175 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.60–3.81 (m, 16H), 6.85 (brs, 2H), 6.87 (d, 2H, J = 8.4Hz), 7.31 (d, 2H, J = 8.4 Hz), 7.49 (brs, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 46.9, 50.9, 65.5, 66.3, 115.8, 118.0, 121.9, 123.9, 131.8, 132.9, 141.7, 148.3, 148.7, 149.3, 184.8; IR (KBr): 3046, 2964, 2921, 2853, 1633, 1578, 1485, 1417, 1359, 1296, 1274, 1235, 1156, 1113, 1067, 999, 854, 831, 785 cm^{-1}; Anal. Calcd for $C_{22}H_{24}Br_2N_4O_2S$: C 46.49, H 4.26, N 9.86, S 5.64; found C 46.43, H 4.30, N 9.81, S 5.68.

_N_-((_E_)-(4-bromophenylimino)(4-phenylpiperazin-1-yl)methyl)-_N_-(4-bromophenyl)-4-phenylpiperazine-1-carbothioamide (9c):



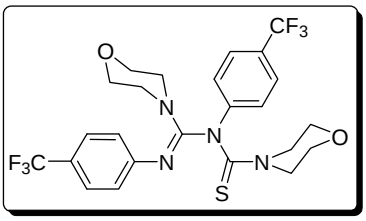
Gummy; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.79–3.63 (m, 16H), 6.76 (d, 2H, J = 8.0 Hz), 6.84 (t, 5H, J = 7.6 Hz), 6.90 (d, 2H, J = 9.2 Hz), 7.22 (t, 5H, J = 7.2 Hz), 7.30 (d, 2H, J = 8.4 Hz), 7.43 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 46.2, 48.0, 48.5, 50.3, 115.6, 116.3, 117.8, 120.1, 120.5, 124.0, 129.2, 129.3, 131.7, 132.8, 141.8, 148.3, 149.2, 150.1, 151.0, 184.5; IR (KBr): 3433, 2894, 2846, 1632, 1599, 1484, 1427, 1386, 1300, 1224, 1168, 1067, 999, 891, 828, 761 cm^{-1}; MS (ESI): 719.1096 (MH^+).

_N_-((_E_)-(4-bromophenylimino)(piperidin-1-yl)methyl)-_N_-(4-bromophenyl)piperidine-1-carbothioamide (9d):



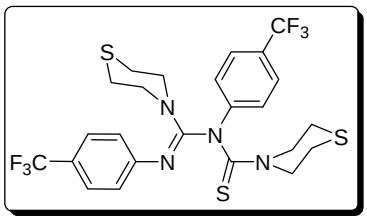
White solid; M.p. 177–179 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.01–1.85 (m, 12H), 2.81–3.87 (m, 8H), 6.77 (m, 2H), 6.88 (d, 2H, J = 8.4 Hz), 7.26 (d, 2H, J = 8.4 Hz), 7.42 (d, 2H, J = 4.4Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 23.8, 24.5, 24.9, 25.1, 47.7, 51.9, 115.2, 117.4, 123.1, 124.2, 131.5, 132.5, 142.8, 148.8, 150.1, 184.7; IR (KBr): 3006, 2936, 2917, 2851, 1630, 1578, 1483, 1423, 1362, 1297, 1270, 1240, 1205, 1185, 1066, 1051, 1026, 1005, 987, 891, 851, 822, 776 cm^{-1}; Anal. Calcd for $C_{24}H_{28}Br_2N_4S$: C 51.08, H 5.00, N 9.93, S 5.68; found C 51.14, H 5.03, N 9.87, S 5.72.

_N_-((_E_)-(4-(Trifluoromethyl)phenylimino)(morpholino)methyl)-_N_-(4-(trifluoro methyl)phenyl)morpholine-4-carbothioamide (10a):



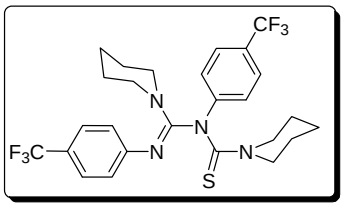
White solid; M.p. 148–149 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.92–3.95 (m, 16H), 6.90 (brs, 2H), 7.07 (d, 2H, J = 8.0 Hz), 7.47 (d, 2H, J = 8.0 Hz), 7.62 (brs, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 46.9, 51.0, 65.4, 66.2, 120.5, 121.1, 122.3, 122.4, 124.9, 125.2, 125.3, 125.9, 126.1, 126.5, 126.8, 127.2, 145.4, 148.9, 152.5, 184.5; IR (KBr): 2965, 2920, 2857, 1640, 1602, 1514, 1475, 1424, 1324, 1292, 1261, 1235, 1159, 1113, 1064, 1035, 1013, 998, 942, 844 cm^{-1}; Anal calcd for $C_{24}H_{24}F_6N_4O_2S$: C, 52.74; H, 4.43; N, 10.25; S, 5.87; found: C, 52.77; H, 4.39; N, 10.28; S, 5.80.

_N_-((_E_)-(4-(Trifluoromethyl)phenylimino)(thiomorpholino)methyl)-_N_-(4-(trifluorometh-yl)phenyl)thiomorpholine-4-carbothioamide (10b):



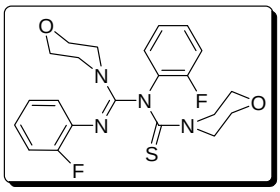
White solid; M.p. 170–1471 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 187-3.75 (m, 16H), 7.01 (d, 2H, J = 8.4 Hz), 7.43 (d, 2H, J = 8.0 Hz), 7.57 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 26.5, 46.8, 49.0, 53.3, 122.2, 123.1, 125.0, 126.0, 127.1, 145.6, 148.9, 152.3, 185.4; IR (KBr): 3060, 2917, 1634, 1601, 1469, 1416, 1321, 1200, 1176, 1125, 1064, 1012, 951, 845 cm^{-1}; MS (ESI): 579.1278 (MH^+).

_N_-((_E_)-(4-(trifluoromethyl)phenylimino)(piperidin-1-yl)methyl)-_N_-(4-(trifluoromethyl)phenyl)piperidine-1-carbothioamide (10d):



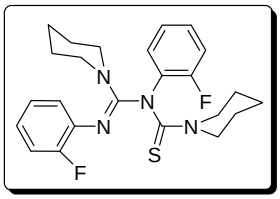
White solid; M.p. 138–140 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.22–1.76 (m 16H), 3.06–3.26 (m, 4H) 6.95 (s, 2H), 7.04 (d, 2H, J = 8.0 Hz), 7.38 (d, 2H, J = 8.0 Hz), 7.53 (d, 2H, J = 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 23.6, 24.4, 24.9, 25.0, 47.8, 52.0, 121.5, 122.5, 123.4, 124.3, 124.6, 125.3, 125.8, 126.7, 146.4, 149.8, 153.0, 184.2.; IR (KBr): 3065, 2936, 2854, 1635, 1597, 1479, 1432, 1327, 1302, 1239, 1163, 1118, 1100, 1064, 891, 840 cm^{-1}; Anal calcd for $C_{26}H_{28}F_6N_4S$: C 57.55, H 5.20, N 10.33, S 5.91; found C 57.59, H 5.24, N 10.29, S 5.96.

_N_-((_E_)-(2-Fluorophenylimino)(morpholino)methyl)-_N_-(2-fluorophenyl)morpholine-4-carbothioamide (11a):



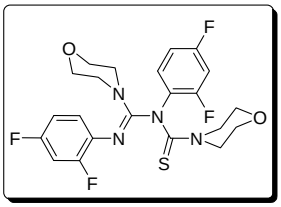
White solid; M.p. 123–125 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.68–3.74 (m, 16H), 6.87–7.33 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 44.2, 50.5, 66.1, 66.4, 114.6114.8, 11.1, 115.3, 116.7, 116.9, 121.9, 123.4, 123.5, 124.0, 124.5, 124.9, 125.3, 125.7, 126.2, 127.3, 130.4, 136.4, 150.6, 154.5, 186.3; IR (KBr): 3368, 2954, 2905, 2849, 1629, 1603, 1496, 1455, 1276, 1235, 1156, 1111, 1064, 1009, 938, 856, 755 cm^{-1}; MS (ESI): 447.1290 (MH^+).

_N_-((_E_)-(2-Fluorophenylimino)(piperidin-1-yl)methyl)-_N_-(2-fluorophenyl)piperidine-1-carbothioamide (11d):



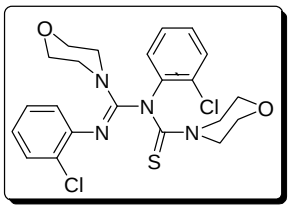
White solid; M.p. 104–106 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.25–1.83 (m, 12H), 3.38-3.46 (m, 8H), 6.61–7.27 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 24.2, 24.9, 25.5, 45.1, 47.5, 48.0, 114.3 114.5, 115.0, 116.3, 116.5, 121.7, 122.6, 122.7, 123.5, 124.3, 124.6, 126.0, 126.7, 127.6, 127.7, 151.5, 153.9, 154.3, 186.0; IR (KBr): 3240, 3170, 3098, 3052, 1661, 1588, 1537, 1492, 1423, 1311, 1005, 831, 755 cm^{-1}; MS (ESI): 443.2314 (MH^+).

_N_-((_E_)-(2,4-(Difluorophenylimino)(morpholino)-_N_-(2,4-(difluorophenyl)morpholine-4-carbothioamide (12a):



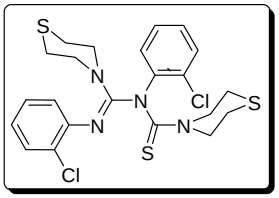
White solid; M.p. 138–140 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.36 (t, 4H, J = 4.4 Hz), 3.62-3.67 (m, 8H), 3.81 (t, 4H, J = 4.4 Hz), 6.73-6.81 (m, 4H), 7.30-7.36 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 44.2, 48.7, 66.1, 66.4, 103.3, 103.6, 103.8, 104.1, 104.3, 104.4, 104.6, 111.0, 111.1, 111.2, 111.3, 123.7, 124.0, 129.2, 129.3, 154.8, 157.7, 159.4, 161.9, 162.0, 183.1 ppm; IR (KBr): 2956, 2923, 2859, 1625, 1513, 1433, 1333, 1253, 1117, 1028, 969, 852, 800, 727 cm^{-1}; MS (ESI): 483.1043 (MH^+).

_N_-((_E_)-(2-chlorophenylimino)(morpholino)methyl)-_N_-(2-chlorophenyl)morpholine-4-carbothioamide (13a):



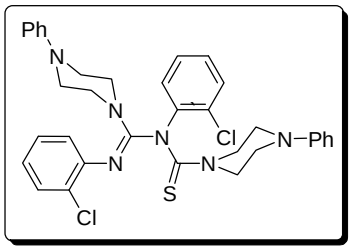
Mp 154–155 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.50–4.60 (m 16H), 6.39–7.68 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 44.1, 47.0, 50.9, 66.0, 121.5, 122.8, 123.4, 126.2, 126.4, 127.3, 128.0, 129.1, 131.0, 139.6, 145.7, 148.5, 187.2; IR (KBr): 3057, 2950, 2894, 2849, 1632, 1580, 1470, 1427, 1401, 1363, 1303, 1272, 1237, 1219, 1206, 1159, 1150, 1119, 1109, 1051, 1031, 999, 953, 876, 757.cm^{-1}. Anal. Calcd for $C_{22}H_{24}Cl_2N_4O_2S$: C 55.12, H 5.05, N 11.69, S 6.69; found C 55.17, H 5.09, N 11.63, S 6.73.

_N_-((_E_)-(2-Chlorophenylimino)(thiomorpholino)methyl)-_N_-(2-chlorophenyl) thiomorpho-line-4-carbothioamide (13b):



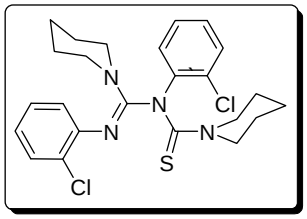
Gummy; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.84–3.78 (m 16H), 6.87 (m, 2H), 7.08 (m, 4H), 7.22 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 26.5, 48.9, 53.1, 121.0, 122.3, 123.2, 124.8, 125.6, 128.1, 130.1, 131.0, 144.0, 149.2, 150.4, 185.3; IR (KBr): 3443, 2950, 2889, 2851, 1634, 1581, 1465, 1426, 1410, 1299, 1223, 1179, 1135, 1061, 947, 901, 836, 784, 772 cm^{-1}; MS (ESI): 511.0250 (MH^+).

_N_-((_E_)-(2-Chlorophenylimino)(4-phenylpiperazin-1-yl)methyl)-_N_-(2-chlorophenyl)-4-phenylpiperazine-1-carbothioamide (13c):



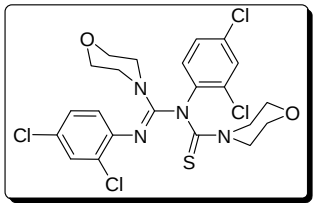
Mp 207–208 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.83–3.64 (m 16H), 6.76 (d, 2H, J = 8.8 Hz), 6.85 (m, 5H), 6.95 (m, 1H), 7.08 (m, 2H), 7.24(m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 46.4, 48.1, 48.7, 50.3, 116.5, 120.2, 120.7, 121.3, 122.4, 123.3, 123.7, 125.0, 125.8, 127.9, 129.3, 129.4, 130.2, 131.0, 144.1, 149.3, 150.2, 150.7, 151.1, 184.4; IR (KBr): 3431, 2901, 2826, 1635, 1599, 1580, 1470, 1424, 1385, 1307, 1223, 1152, 1001, 907, 757, 693 cm^{-1}; Anal. Calcd for $C_{34}H_{34}Cl_2N_6S$: C 64.86, H 5.44, N 13.35, S 5.09; found C 64.91, H 5.49, N 13.31, S 5.13.

_N_-((_E_)-(2-chlorophenylimino)(piperidin-1-yl)methyl)-_N_-(2-chlorophenyl)piperidine-1-carbothioamide (13d):



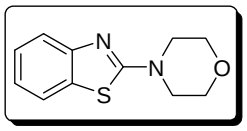
Gummy; ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.83-2.01 (m, 16H), 3.68 (m, 4H), 6.62-7.39 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 24.0, 24.7, 25.1, 25.7, 48.3, 51.9, 121.5, 122.2, 122.9, 123.7, 126.4, 126.9, 127.7, 128.9, 130.7, 140.5, 142.0, 147.5, 187.7; IR (KBr): 3448, 2935, 2853, 1620, 1580, 1475, 1440, 1297, 1234, 1207, 1176, 1031, 755 cm^{-1}; Anal. Calcd for $C_{24}H_{28}Cl_2N_4S$: C 60.62, H 5.94, N 11.78, S 6.74; found C 60.67, H 5.99, N 11.72, S 6.78.

_N_-((_E_)-(2,4-(Dichlorophenylimino)(morpholino)-_N_-(2,4-(dichlorophenyl)morpholine-4-carbothioamide (14a):



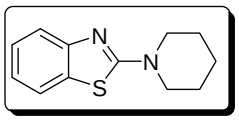
Gummy; ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.40-3.67 (m, 16H), 6.89 (m, 3H), 7.25 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 44.2, 51.0, 65.9, 66.4, 121.8, 122.8, 126.5, 127.2, 127.7, 127.9, 128.4, 128.6, 130.7, 132.6, 134.4, 144.6, 153.9, 186.7; IR (KBr): 2961, 2921, 2856, 1633, 1471, 1423, 1358, 1294, 1235, 1145, 1114, 1034, 999, 820, 737 cm^{-1}; MS (ESI): 548.9885 (MH^+).

2-Morpholinobenzo[_d_]thiazole (11'a):



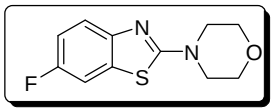
White solid; M.p. 120–122 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.59 (t, 4H, J = 4.4 Hz), 3.80 (t, 4H., J = 4.4 Hz), 7.07 (t, 1H, J = 7.6 Hz), 7.28 (t, 1H, J = 8.0 Hz), 7.57 (dd, 1H, J_1 = 6.4 Hz, J_2 = 4.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 48.5, 66.2, 119.4,120.8, 121.7, 126.1, 130.6, 152.5, 169.0 IR (KBr): 2918, 2854, 1591, 1537, 1441, 1377, 1289, 1229, 1113, 1067, 1032, 945, 859, 756 cm^{-1}; Anal. Calcd for $C_{11}H_{12}N_2OS$: C 59.97, H 5.49, N 12.72, S 14.56; found C 60.07, H 5.55, N 12.62, S 14.48.

2-(Piperidin-1-yl)benzo[*d*]thiazole (11'd):



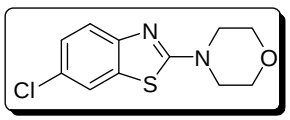
White solid; M.p. 96–97 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.67 (s, 6H), 3.58 (s, 4H), 7.03 (t, 1H, J = 8.0 Hz), 7.26 (t, 1H, J = 8.0 Hz), 7.55 (dd, 2H, J_1 = 8.0 Hz, J_2 = 5.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 24.3, 25.4, 49.7, 118.9, 120.7, 121.1, 126.0, 130.8, 153.1, 169.0; IR (KBr): 2934, 2922, 2849, 1588, 1534, 1440, 1382, 1332, 1257, 1234, 1209, 1120, 1006, 760 cm^{-1}; Anal. Calcd for $C_{12}H_{14}N_2S$: C 66.02, H 6.46, N 12.83, S 14.69; found C 66.08, H 6.50, N 12.76, S 14.55.

6-Fluoro-2-morpholinobenzo[*d*]thiazole (12'a):



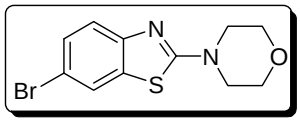
White solid; M.p. 157–158 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.51 (t, 4H, J = 4.8 Hz), 3.75 (t, 4H, J = 4.4 Hz), 6.97 (m, 1H), 7.25 (m, 1H), 7.44 (m, 1H); ^{13}CNMR (100 MHz, $CDCl_3$): δ 48.4, 66.1, 107.4, 107.6, 113.6, 113.9, 119.7, 119.8, 131.2, 131.4, 148.9, 157. 0, 159.4, 168.5; IR (KBr): 2982, 2901, 2863, 1673, 1597, 1538, 1459, 1376, 1343, 1287, 1234, 1181, 1111, 1073, 1029, 948, 920, 844 cm^{-1}; MS (ESI): 239.0662 (MH^+).

6-Chloro-2-morpholinobenzo[*d*]thiazole (14'a):



White solid; M.p. 144–145 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.61 (t, 4H, J = 4.8 Hz), 3.81 (t, 4H, J = 5.2 Hz), 7.19 (dd, 1H, J_1 = 8.4 Hz, J_2 = 2.0 Hz), 7.39 (d, 1H, J = 8.8 Hz), 7.49 (d, 1H, J = 2.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 48.4, 66.1, 119.9, 120.4, 126.5, 126.7, 131.8, 151.2, 169.0; IR (KBr): 2943, 2919, 2859, 1594, 1537, 1447, 1330, 1279, 1233, 1110, 1027, 940, 814 cm^{-1}; MS (ESI): 255.0448 (MH^+).

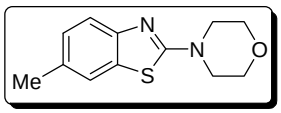
6-Bromo-2-morpholinobenzo[*d*]thiazole (15'a):



White solid; M.p. 165–167 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.57 (t, 4H, J = 4.8 Hz), 3.80 (t, 4H, J = 4.8 Hz), 7.37 (s, 2H), 7.68 (s, 1H); ^{13}CNMR (100 MHz, $CDCl_3$): δ 48.5, 66.3, 114.0,

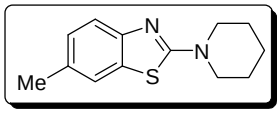
120.5, 123.3, 129.4, 132.4, 151.6, 169.1; IR (KBr): 2918, 2857, 1591, 1535, 1443, 1372, 1280, 1258, 1229, 1110, 1026, 940, 863, 813 cm^{-1}; Anal. Calcd for $C_{11}H_{11}N_2OSBr$: C 44.16, H 3.71, N 9.36, S 10.72; found C 44.23, H 3.76, N 9.28, S 10.64.

6-Methyl-2-morpholinobenzo[*d*]thiazole (18'a):



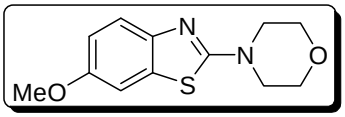
White solid; M.P. 134–136 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 2.37 (s, 3H), 3.56 (t, 4H, J = 4.8 Hz), 3.79 (t, 4H, J = 4.8 Hz), 7.09 (d, 1H, J = 8.0 Hz), 7.39 (s, 1H), 7.44 (d, 1H, J = 8.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.3, 48. 6, 66.3, 119.0, 120.9, 127.4, 130.7, 131.6, 150.4, 168.6; IR (KBr): 2963, 2912, 2856, 1599, 1575, 1544, 1464, 1434, 1352, 1281, 1235, 1113, 1026, 943, 811 cm^{-1}; MS (ESI): 235.1035 (MH^+).

6-Methyl-2-(piperidin-1-yl)benzo[*d*]thiazole (18'd):



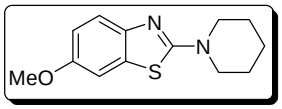
White solid; M.p. 105–107 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 1.66 (s, 6H), 2.35 (s, 3H), 3.55 (s, 4H), 7.06 (d, 1H, J = 8.0 Hz), 7.36 (s, 1H), 7.44 (d, 1H, J = 8.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.4, 24.4, 25.5, 49.8, 118.6, 120.8, 127.2, 130.9, 150.9, 168.6; IR (KBr): 3434, 2924, 2852, 1569, 1537, 1459, 1440, 1382, 1336, 1264, 1240, 1121, 1006, 810, 626 cm^{-1}; MS (ESI): 233.1284 (MH^+).

6-Methoxy-2-morpholinobenzo[*d*]thiazole (19'a):



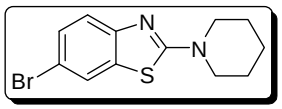
White solid; M.p. 130–132 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 3.53 (t, 4H, J = 4.4 Hz), 3.77 (t, 4H, J = 4.4 Hz), 3.78 (s, 3H), 6.89 (dd, 1H, J = 8.8Hz, J = 2.4 Hz), 7.12 (d, 1H, J = 2.8 Hz), 7.45 (d, 1H, J = 8.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 48.6, 56.0, 66.3, 105.3, 113.9, 119.9, 131.7, 146.8, 155.4, 167.8; IR (KBr): 3447, 2925, 2850, 1599, 1547, 1474, 1437, 1371, 1289, 1264, 1235, 1179, 1111, 1026, 946, 802, 652 cm^{-1}; MS (ESI): 251.1026 (MH^+).

6-Methoxy-2-(piperidin-1-yl)benzo[*d*]thiazole (19'd):



White solid; M.p. 108–110^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.66 (s, 6H), 3.53 (s, 4H), 3.79 (s 3H), 6.86 (dd, 1H, J = 8.0 Hz, J = 2.8 Hz), 7.11 (d, 1H, J = 2.4 Hz), 7.42 (d, 1H, J = 8.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 24.4, 25.4, 49.8, 56.1, 105.4, 113.6, 119.3, 131.6, 147.1, 155.0, 167.8; IR (KBr): 3245, 2923, 2852, 1631, 1603, 1490, 1407, 1389, 1232, 1216, 1035, 986, 797 cm^{-1}; MS (ESI): 249.1063 (MH^+).

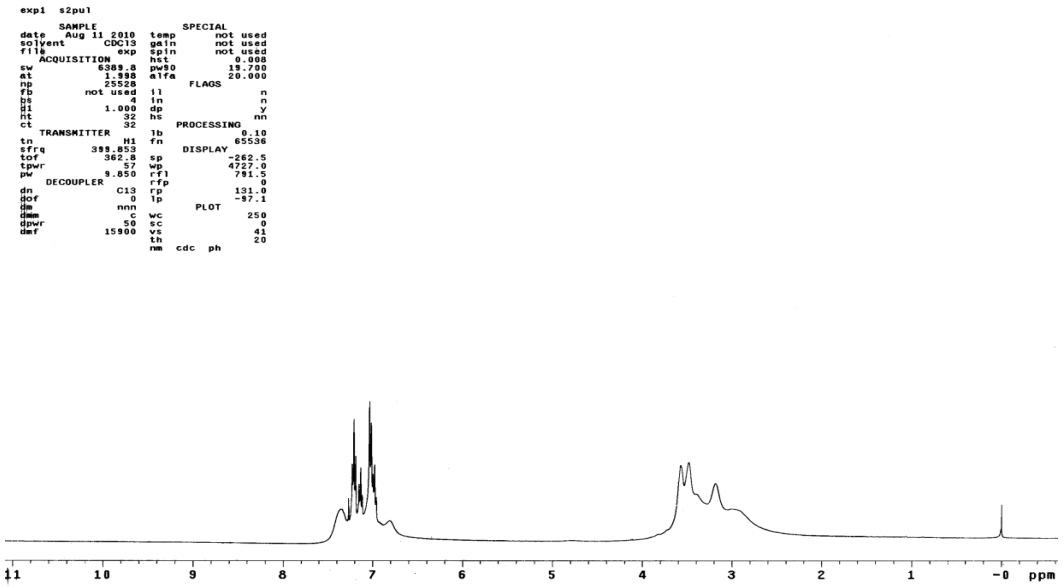
6-Bromo-2-(piperidin-1-yl)benzo[*d*]thiazole (20'd):



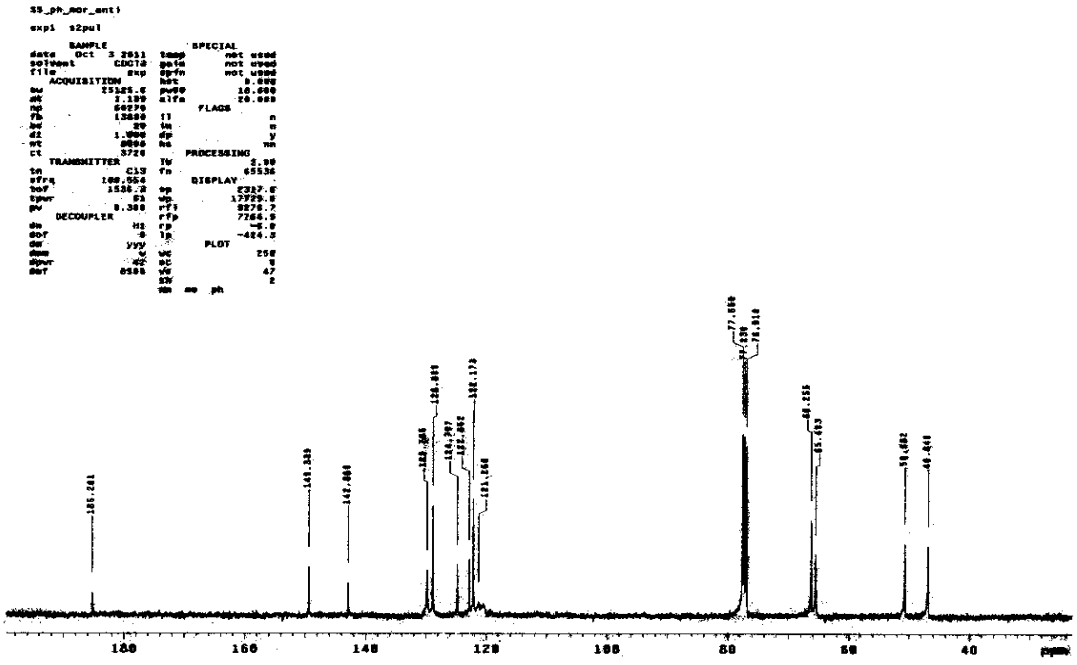
White solid; M.p. 118–120 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.68 (s, 6H), 3.58 (s, 4H), 7.35 (s, 2H), 7.67 (s, 1H); ^{13}CNMR (100 MHz, $CDCl_3$): δ 24.3, 25.4, 49.8, 113.3, 120.0, 123.2, 129.2, 132.5, 152.2, 169.0; IR (KBr): 3445, 2927, 2852, 1629, 1594, 1536, 1442, 1380, 1334, 1255, 1208, 1124, 1004, 812 cm^{-1}; MS (ESI): 297.0067 (MH^+).

Spectra

_N_-((_E_)-Morpholino(phenylimino)methyl)-_N_-phenylmorpholine-4-carbothioamide (1a). ^{1}H NMR (400 MHz, $CDCl_3$):

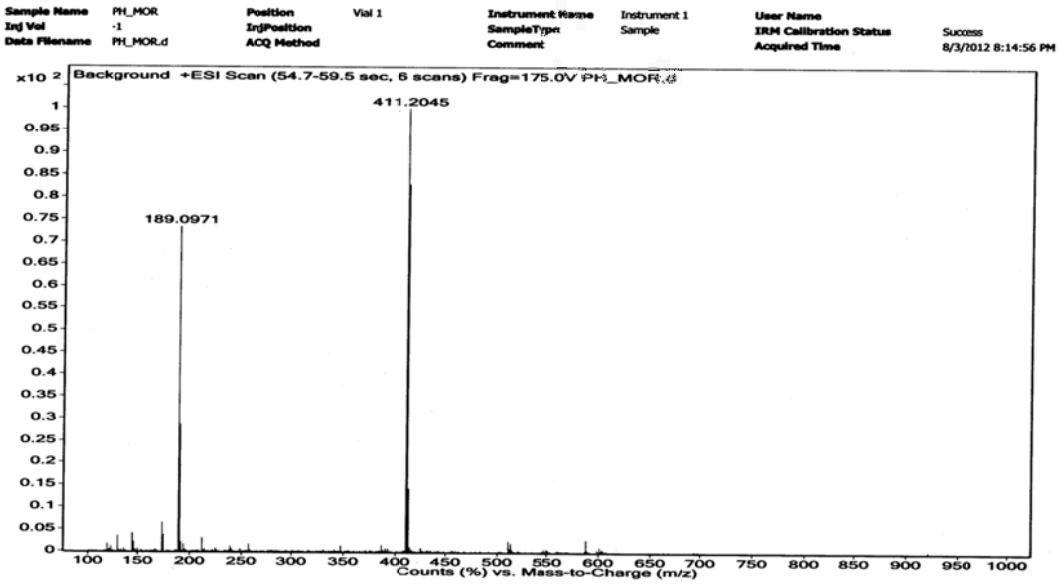


_N_-((_E_)-Morpholino(phenylimino)methyl)-_N_-phenylmorpholine-4-carbothioamide (1a). ^{13}C NMR (100 MHz, $CDCl_3$):

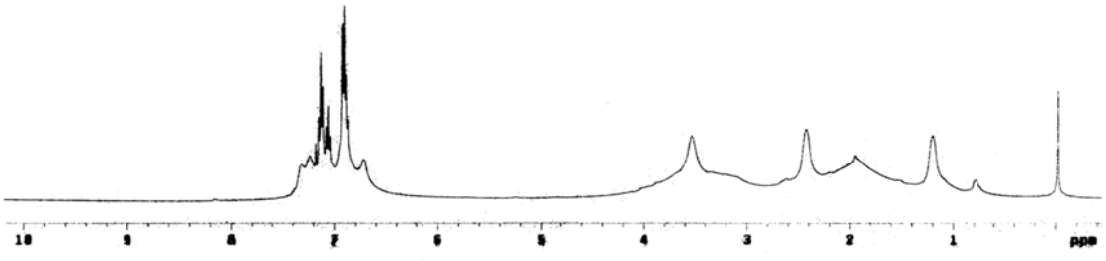


_N_-((_E_)-Morpholino(phenylimino)methyl)-_N_-phenylmorpholine-4-carbothioamide (1a).

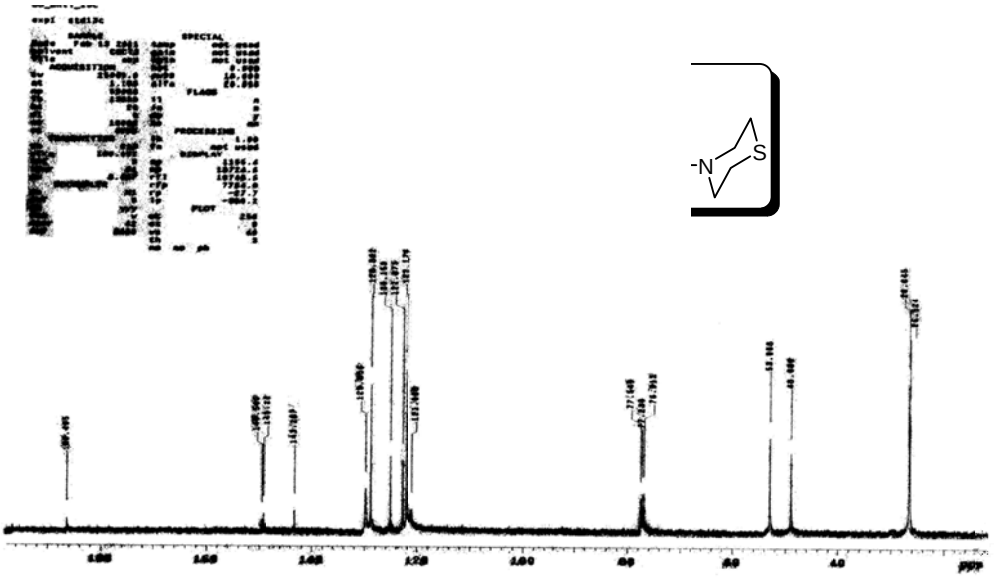
MASS SPECTRA:



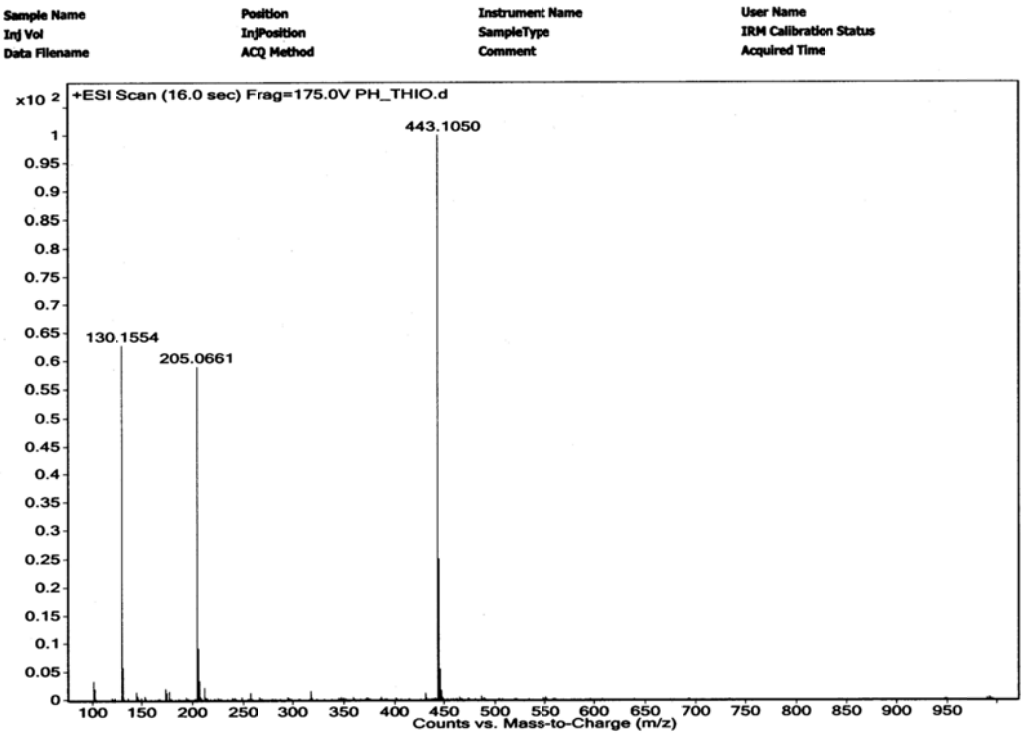
_N_-Phenyl-_N_-((_E_)-(phenylimino)(thiomorholino)methyl)thiomorpholine-4-carbothioamide (1b). ^{1}H NMR (400 MHz, $CDCl_3$):



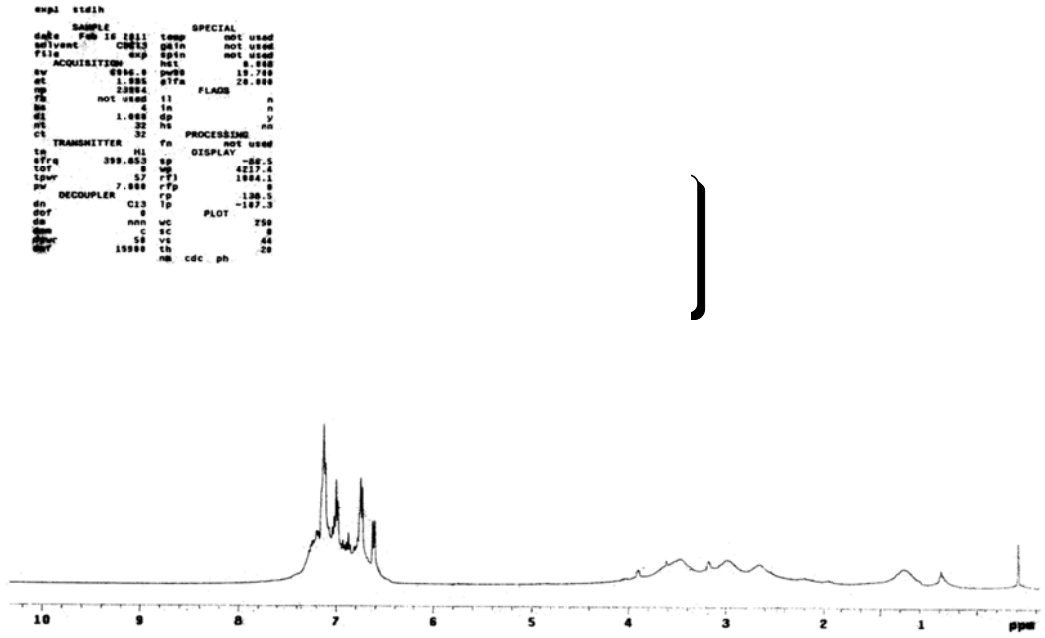
_N_-Phenyl-_N_-((_E_)-(phenylimino)(thiomorholino)methyl)thiomorpholine-4-carbothioamide (1b). ^{13}C NMR (100 MHz, $CDCl_3$):



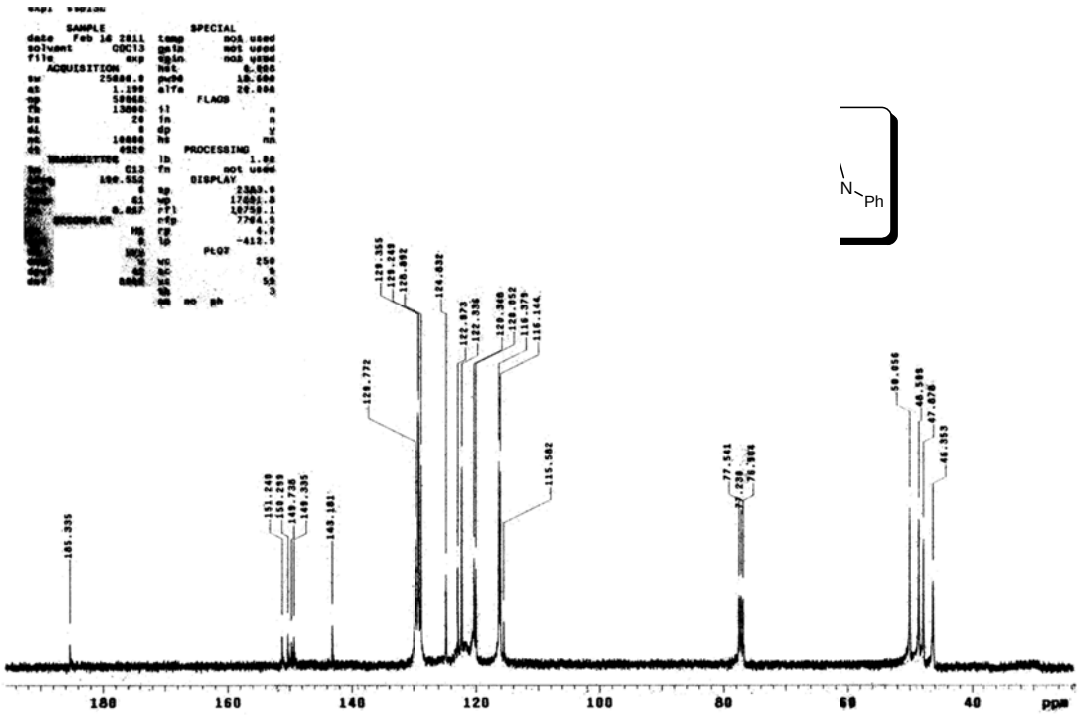
_N_-Phenyl-_N_-((_E_)-(phenylimino)(thiomorholino)methyl)thiomorpholine-4-carbothioamide (1b). MASS SPECTRA:



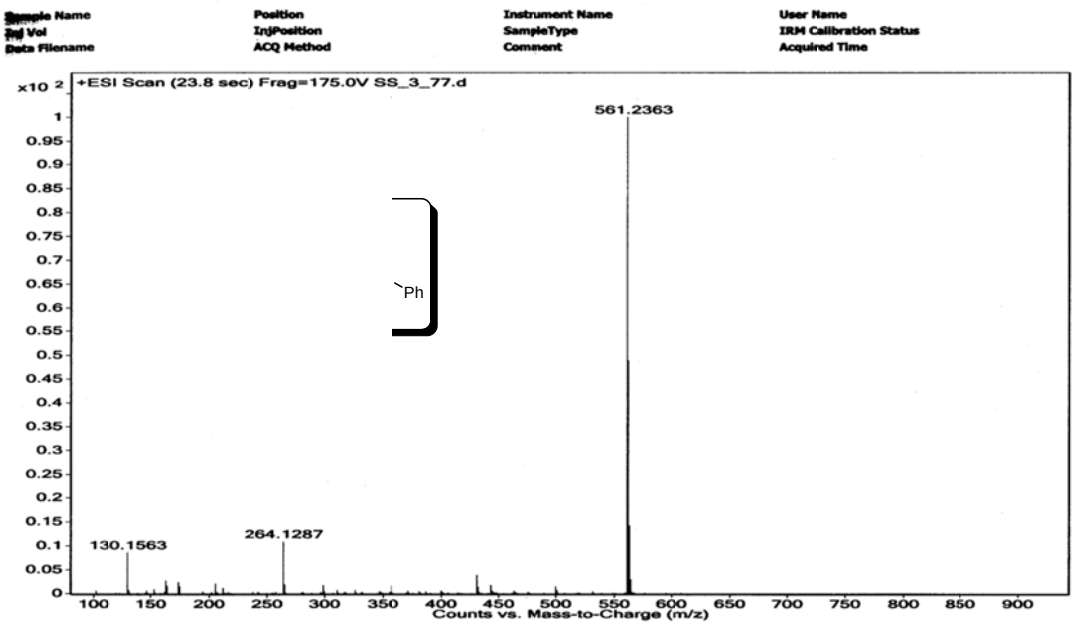
_N_,4-Diphenyl-_N_-((_E_)-(phenylimino)(4-phenylpiperazine-1-yl)methyl)piperazine-1-carbothioamide (1c). ^{1}H NMR (400 MHz, $CDCl_3$):



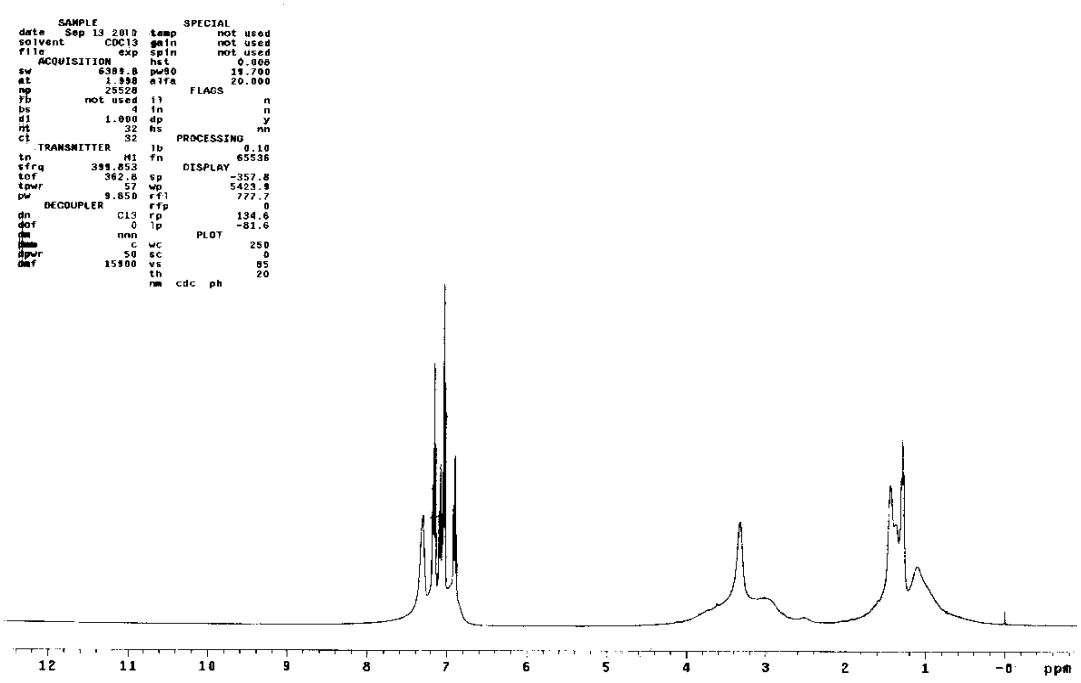
_N_,4-Diphenyl-_N_-((_E_)-(phenylimino)(4-phenylpiperazine-1-yl)methyl)piperazine-1-carbothioamide (1c). ^{13}C NMR (100 MHz, $CDCl_3$):



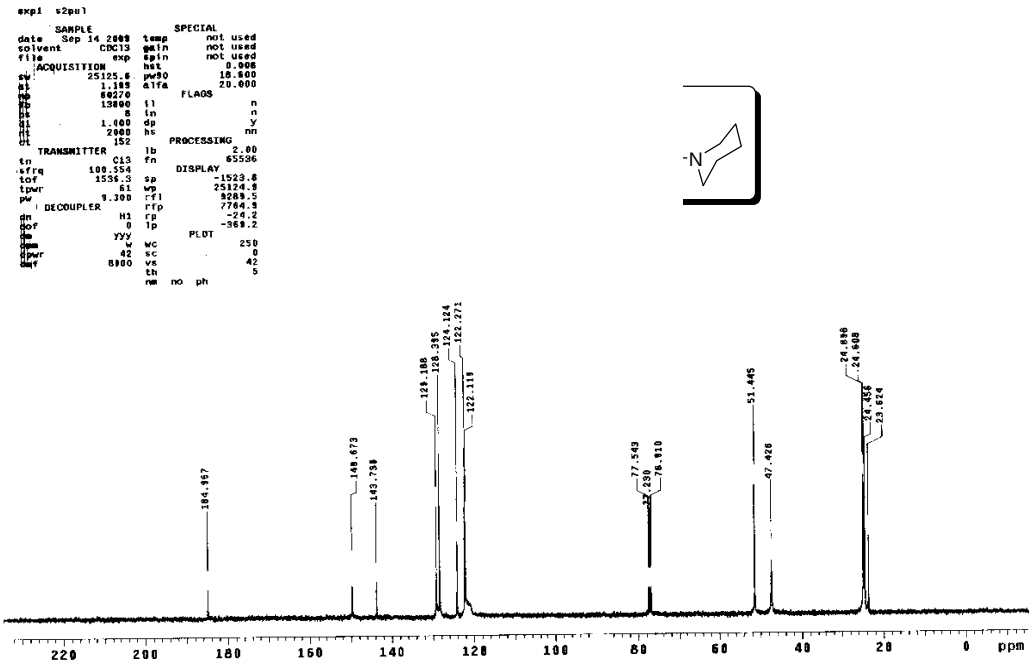
_N_,4-Diphenyl-_N_-((_E_)-(phenylimino)(4-phenylpiperazine-1-yl)methyl)piperazine-1-carbothioamide (1c). MASS SPECTRA:



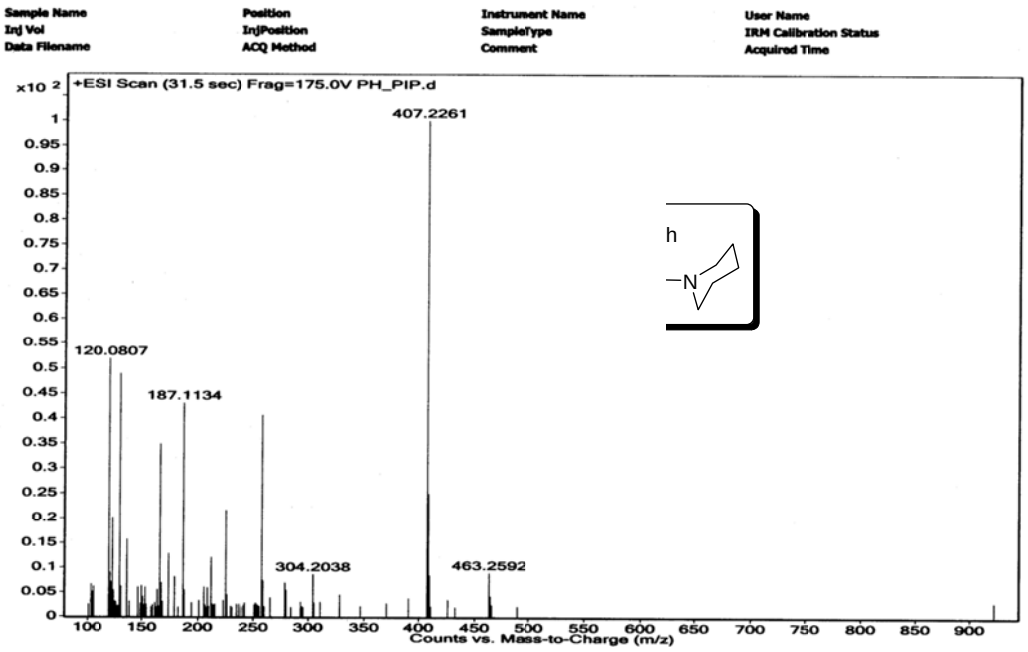
_N_-Phenyl-_N_-((_E_)-(phenylimino)(piperidin-1-yl)methyl)piperidine-1-carbothioamide (1d). ^{1}H NMR (400 MHz, $CDCl_3$):



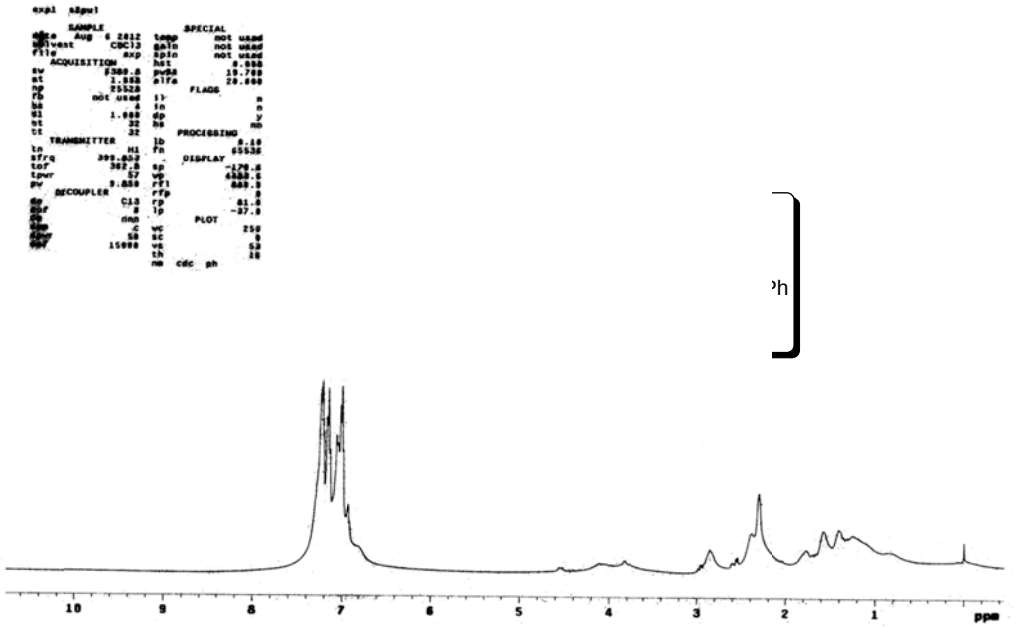
_N_-Phenyl-_N_-((_E_)-(phenylimino)(piperidin-1-yl)methyl)piperidine-1-carbothioamide (1d). ^{13}C NMR (100 MHz, $CDCl_3$):



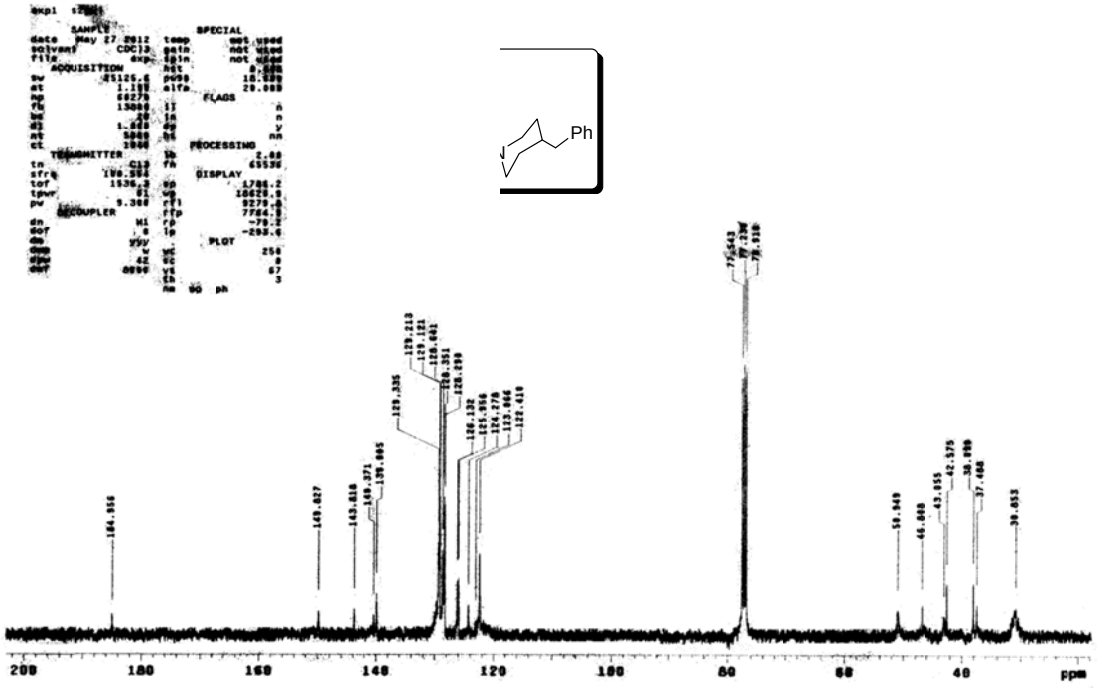
_N_-Phenyl-_N_-((_E_)-(phenylimino)(piperidin-1-yl)methyl)piperidine-1-carbothioamide (1d). MASS SPECTRA:



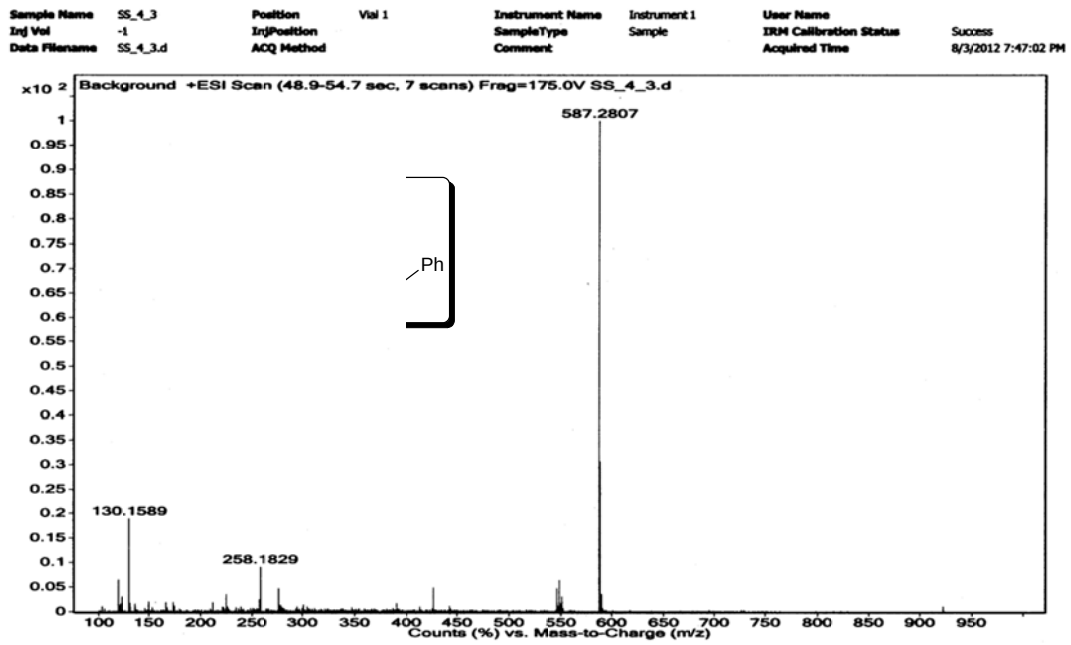
4-Benzyl-*N*-((*E*)-(4-benzylpiperidin-1-yl)(phenylimino)methyl)-*N*-phenylpiperidine-1-carbothioamide (1e). ^{1}H NMR (400 MHz, $CDCl_3$):



4-Benzyl-*N*-((*E*)-(4-benzylpiperidin-1-yl)(phenylimino)methyl)-*N*-phenylpiperidine-1-carbothioamide (1e). ^{13}C NMR (100 MHz, $CDCl_3$):

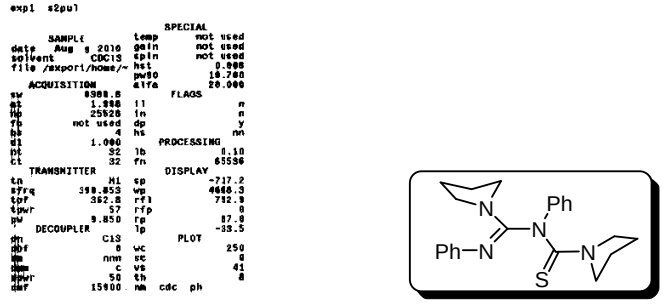


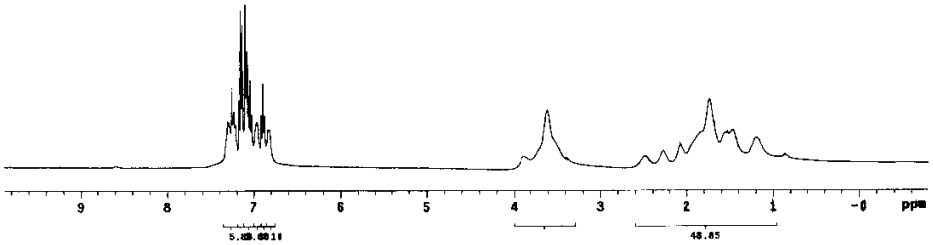
4-Benzyl-*N*-((*E*)-(4-benzylpiperidin-1-yl)(phenylimino)methyl)-*N*-phenylpiperidine-1-carbothioamide (1e). MASS SPECTRA:



***N*-Phenyl-*N*-((*E*)-(phenylimino)(pyrrolidin-1-yl)methyl)pyrrolidine-1-carbothioamide (1f).**

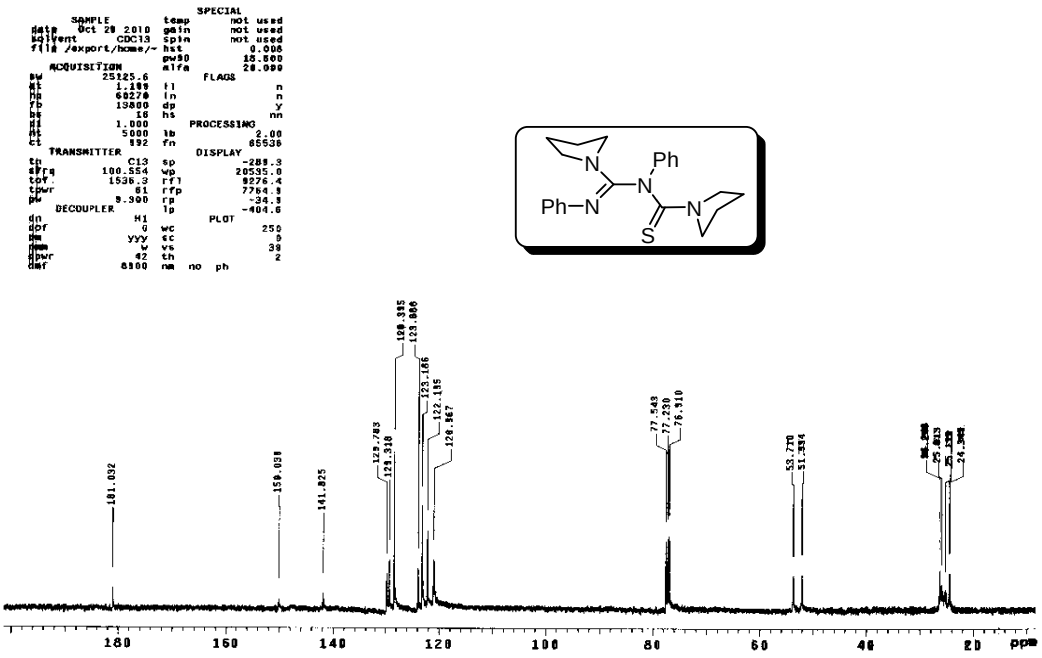
^{1}H NMR (400 MHz, $CDCl_3$):





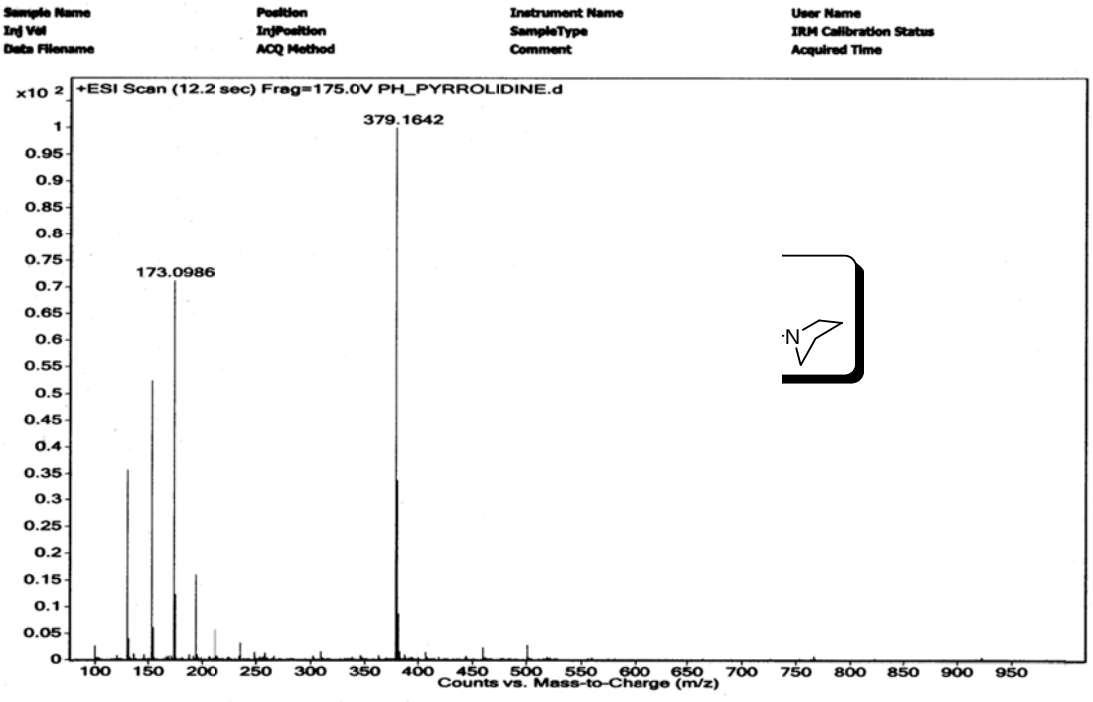
_N_-Phenyl-_N_-((_E_)-(phenylimino)(pyrrolidin-1-yl)methyl)pyrrolidine-1-carbothioa- mide (1f).

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

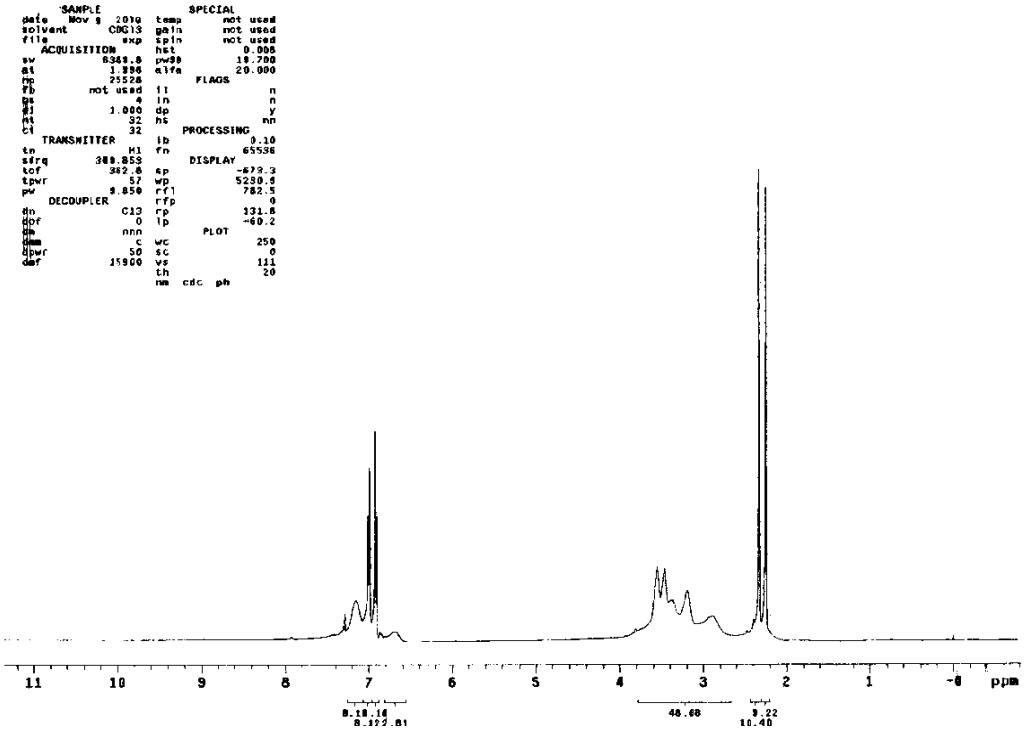


_N_-Phenyl-_N_-((_E_)-(phenylimino)(pyrrolidin-1-yl)methyl)pyrrolidine-1-carbothioamide (1f).

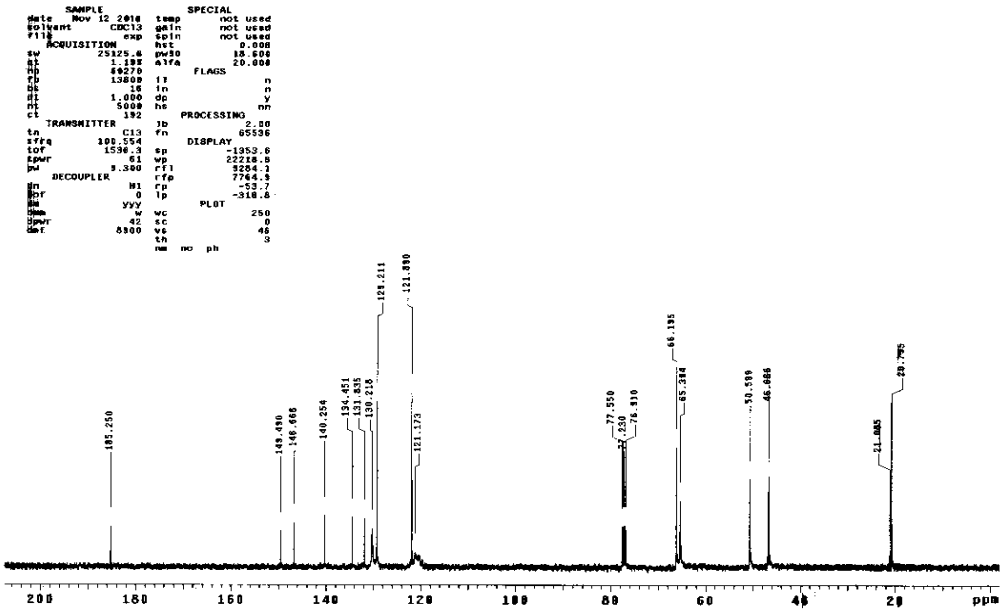
MASS SPECTRA:



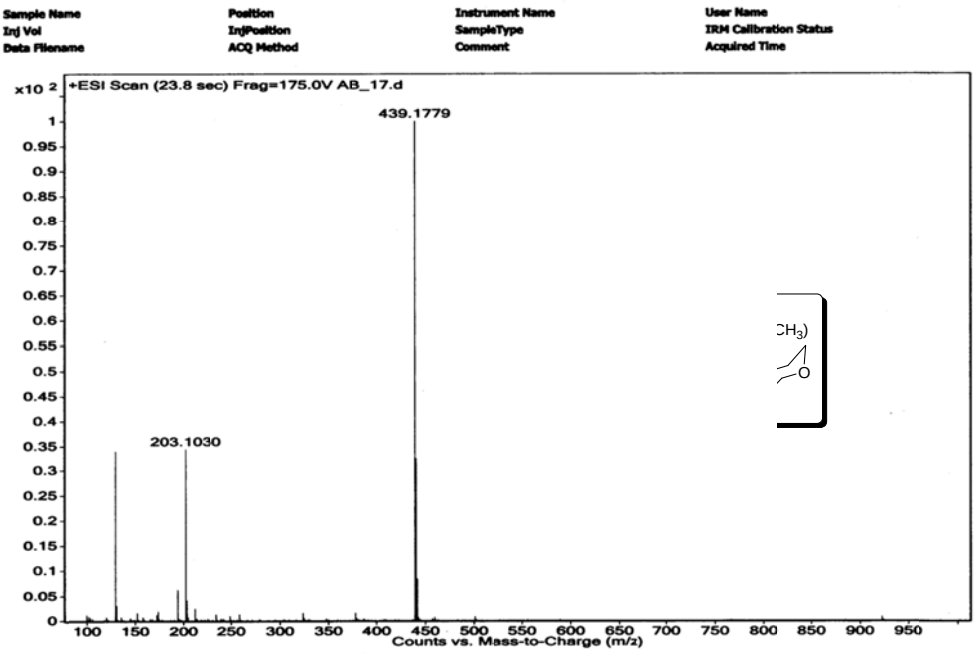
_N_-((_E_)-(_p_-Tolylimino)(morpholino)methyl)-_N_-_p_-tolylmorpholine-4-carbothioamide (2a). ^{1}H NMR (400 MHz, $CDCl_3$):



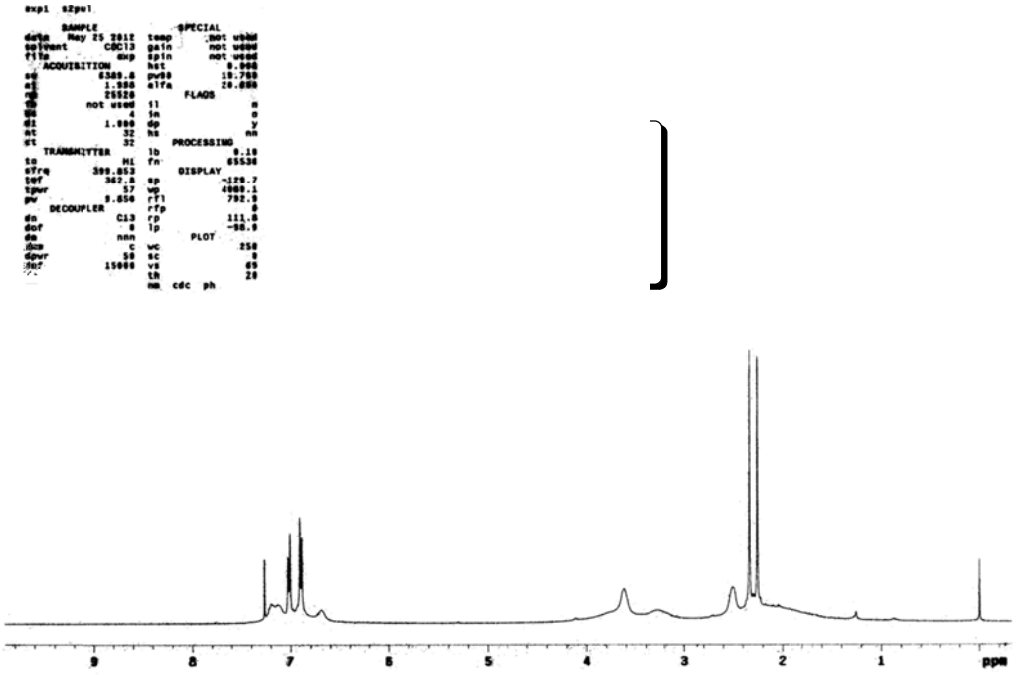
_N_-((_E_)-(_p_-Tolylimino)(morpholino)methyl)-_N_-_p_-tolylmorpholine-4-carbothioamide (2a). ^{13}C NMR (100 MHz, $CDCl_3$):



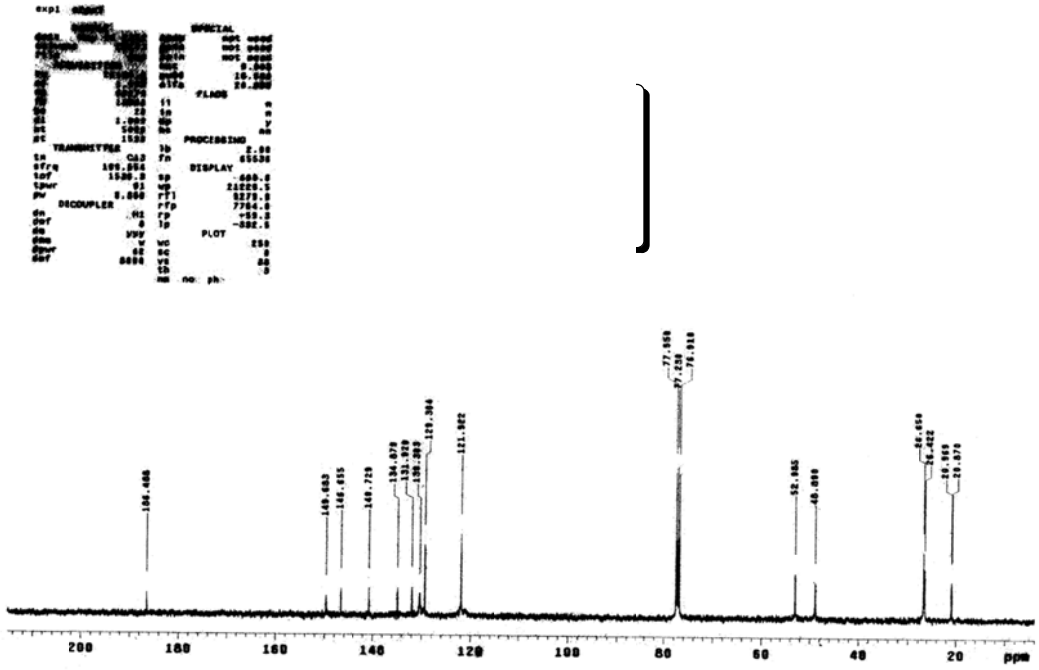
_N_-((_E_)-(_p_-Tolylimino)(morpholino)methyl)-_N_-_p_-tolylmorpholine-4-carbothioamide (3a). MASS SPECTRA:



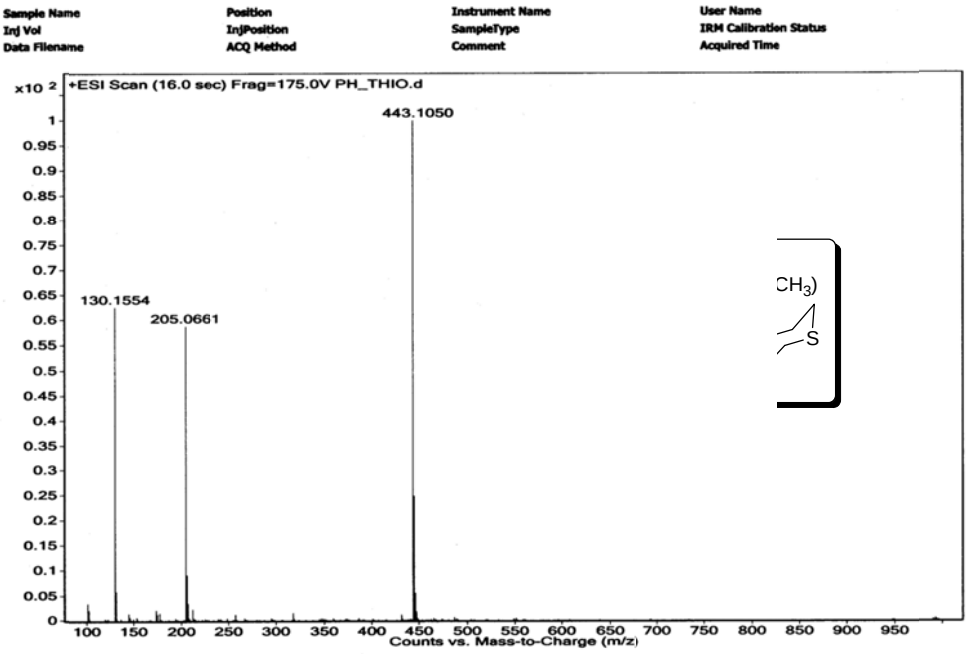
_N_-((_E_)-(_p_-Tolylimino)(thiomorpholino)methyl)-_N_-_p_-tolylthiomorpholine-4-carbothioamide (2b). ^{1}H NMR (400 MHz, $CDCl_3$):



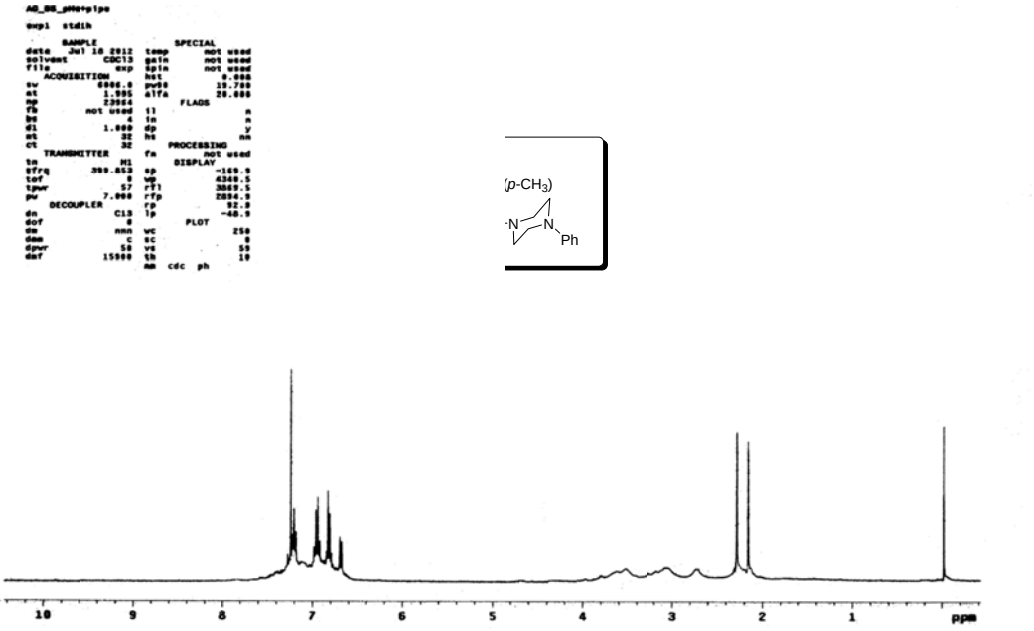
_N_-((_E_)-(_p_-Tolylimino)(thiomorpholino)methyl)-_N_-_p_-tolylthiomorpholine-4-carbothioamide (2b). ^{13}C NMR (100 MHz, $CDCl_3$):



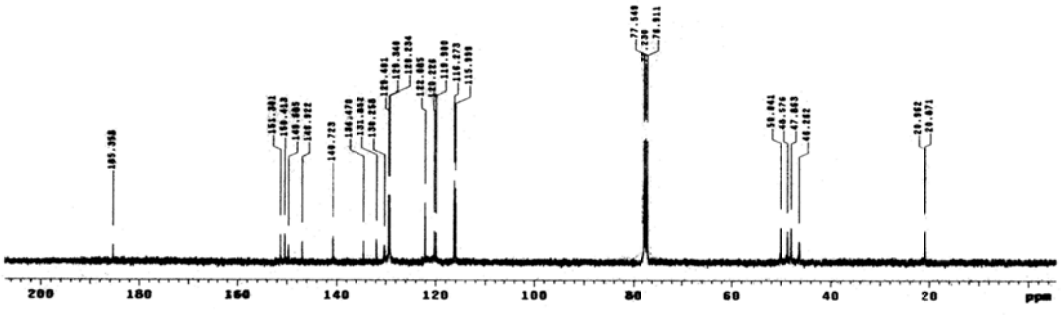
_N_-((_E_)-(_p_-Tolylimino)(thiomorpholino)methyl)-_N_-_p_-tolylthiomorpholine-4-carbothioamide (2b). MASS SPECTRA:



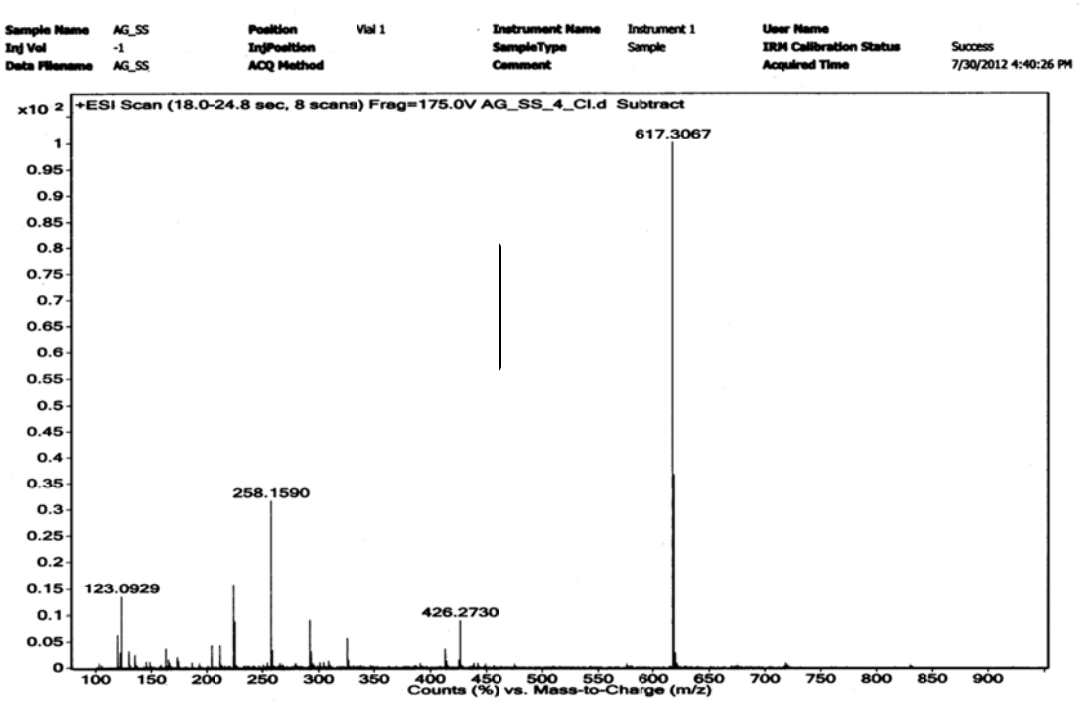
_N_-((_E_)-(_p_-Tolylimino)(4-phenylpiperzin-1-yl)methyl)-4-phenyl-_N_-_p_-tolylpiperazine-1-carbothioamide (2c). ^{1}H NMR (400 MHz, $CDCl_3$):



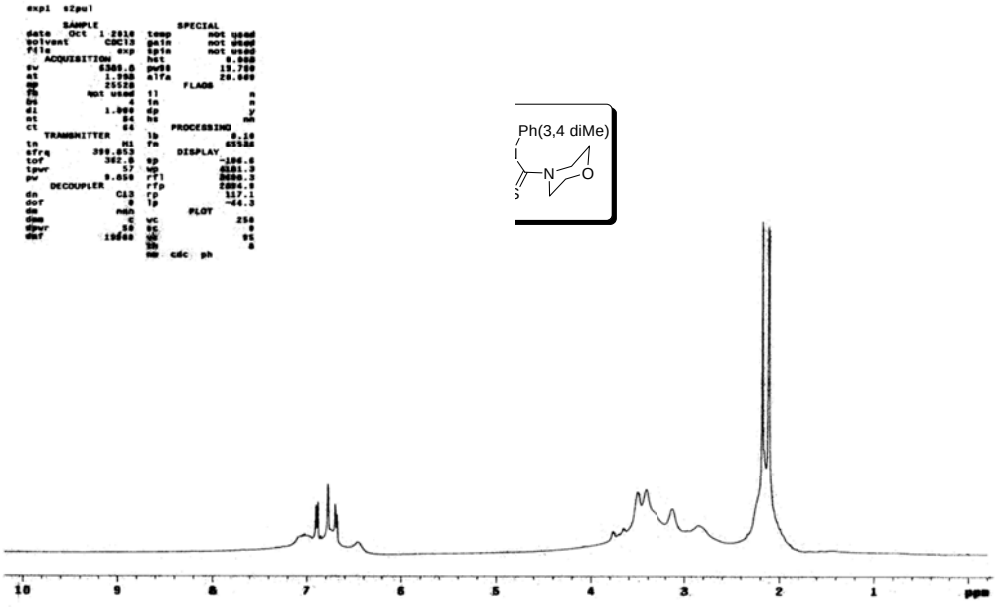
_N_-((_E_)-(_p_-Tolylimino)(4-phenylpiperzin-1-yl)methyl)-4-phenyl-_N_-_p_-tolylpiperazine-1-carbothioamide (2c). ^{13}C NMR (100 MHz, $CDCl_3$):



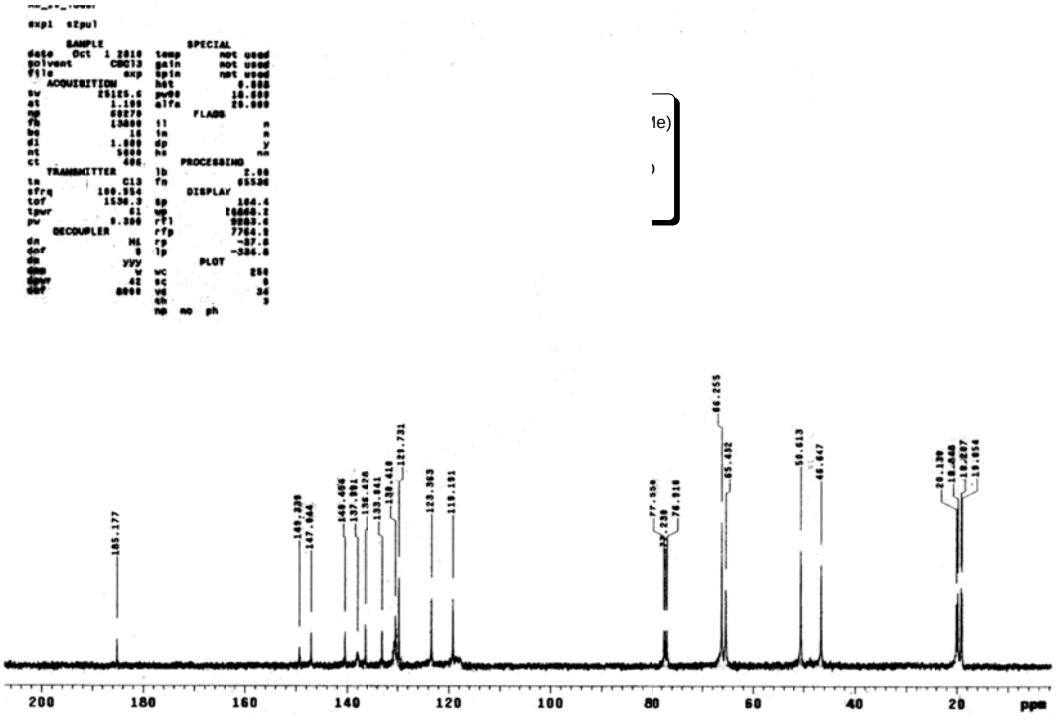
_N_-((_E_)-(_p_-Tolylimino)(4-phenylpiperzin-1-yl)methyl)-4-phenyl-_N_-_p_-tolylpiperazine-1-carbothioamide (2c). MASS SPECTRA:



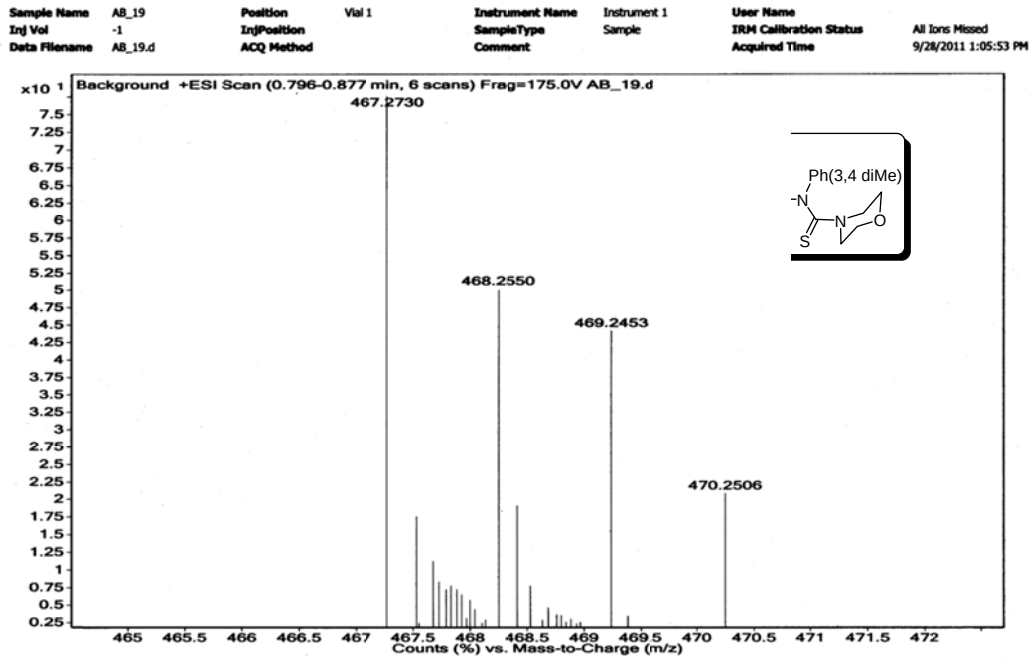
_N_-((_E_)-(3,4-Dimethylphenylimino)(morpholino)methyl)-_N_-(3,4-dimethylphenyl) morpholine-4-carbothioamide (3a). ^{1}H NMR (400 MHz, $CDCl_3$):



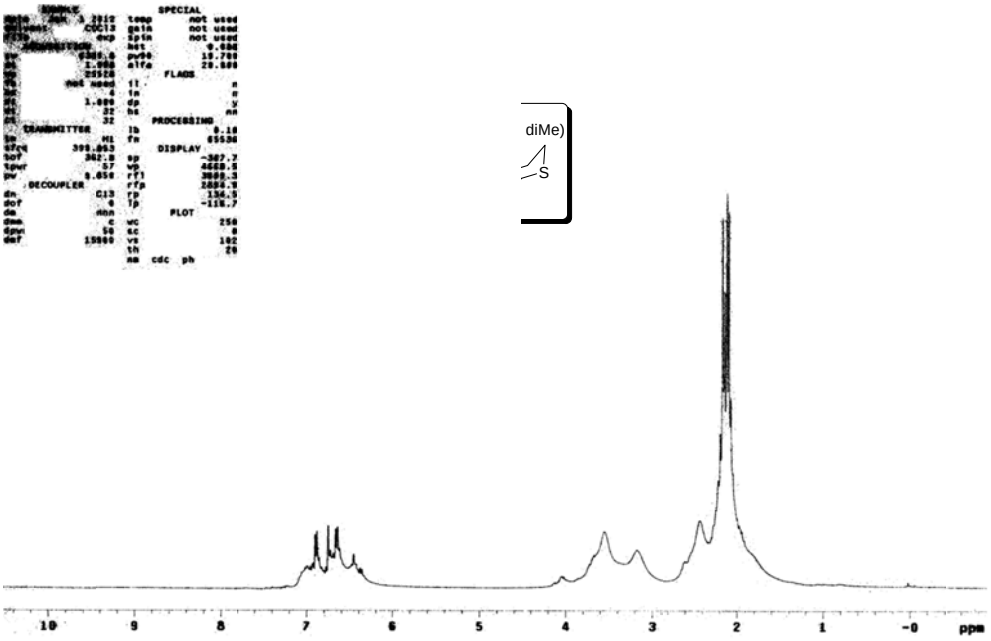
***N*-((*E*)-(3,4-Dimethylphenylimino)(morpholino)methyl)-*N*-(3,4-dimethylphenyl) morpholine-4-carbothioamide (3a). ^{13}C NMR (100 MHz, $CDCl_3$):**



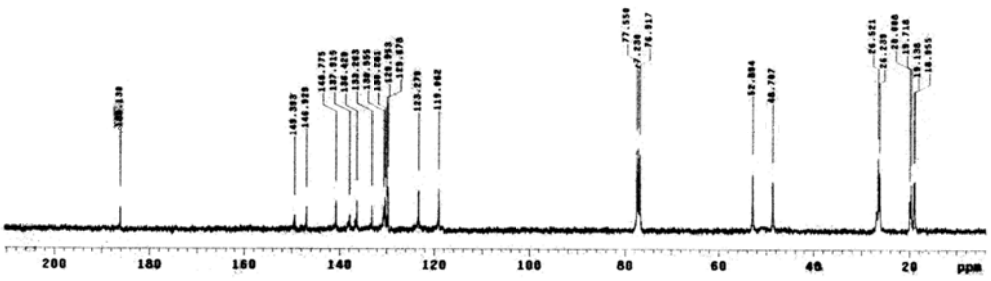
***N*-((*E*)-(3,4-Dimethylphenylimino)(morpholino)methyl)-*N*-(*3,4*-dimethylphenyl) morpholine-4-carbothioamide (3a). MASS SPECTRA:**



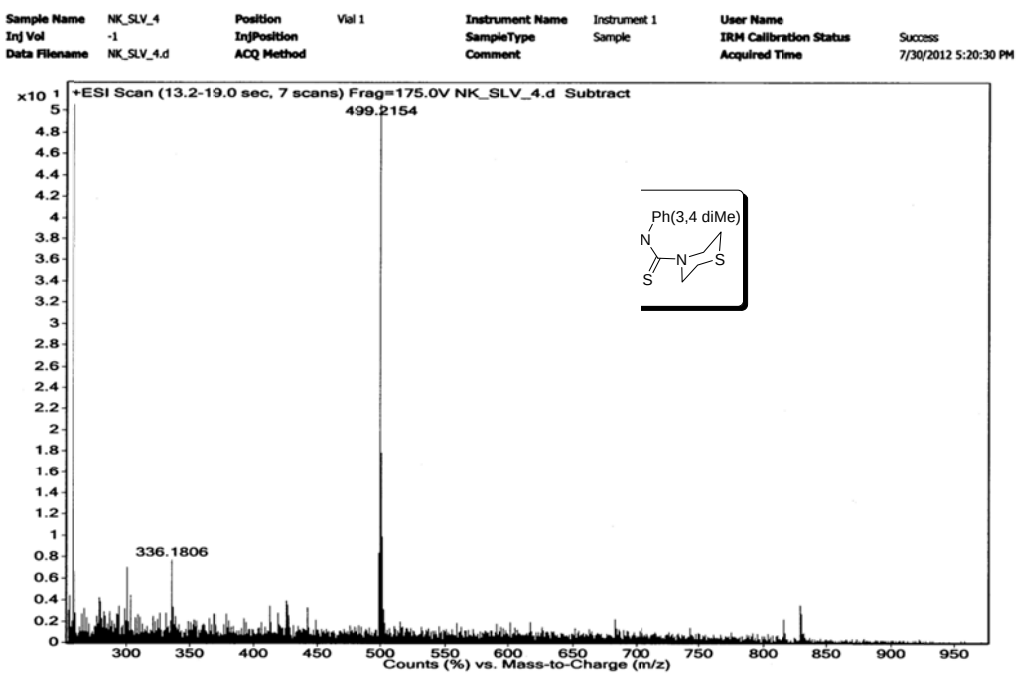
***N*-((*E*)-(3,4-Dimethylphenylimino)(thiomorpholino)methyl)-*N*-(3,4-dimethylphenyl) thiomorpholine-4-carbothioamide (3b). ^{1}H NMR (400 MHz, $CDCl_3$):**



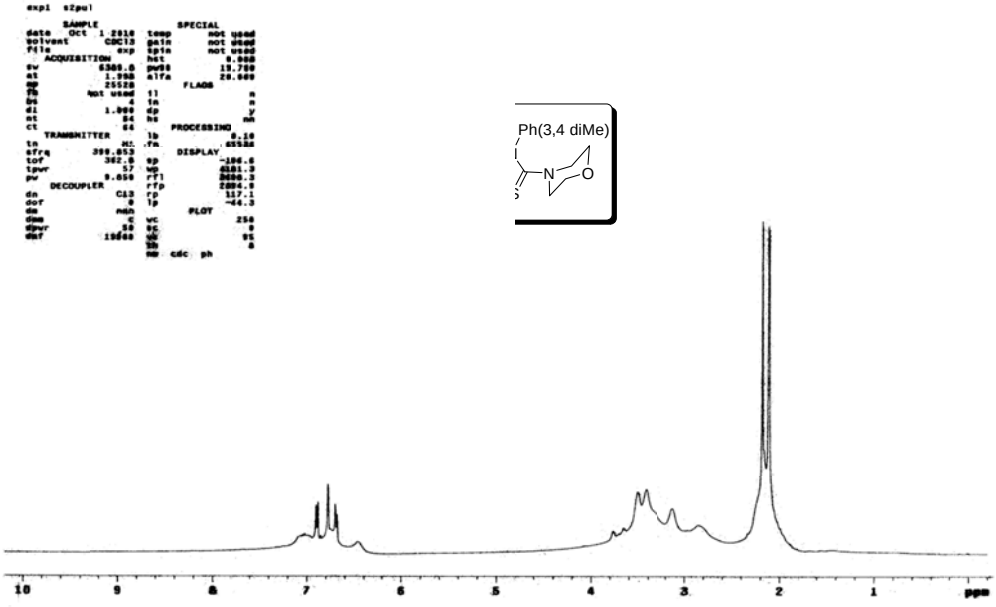
***N*-((*E*)-(3,4-Dimethylphenylimino)(thiomorpholino)methyl)-*N*-(*3,4*-dimethylphenyl) thiomorpholine-4-carbothioamide (3b). ^{13}C NMR (100 MHz, $CDCl_3$):**



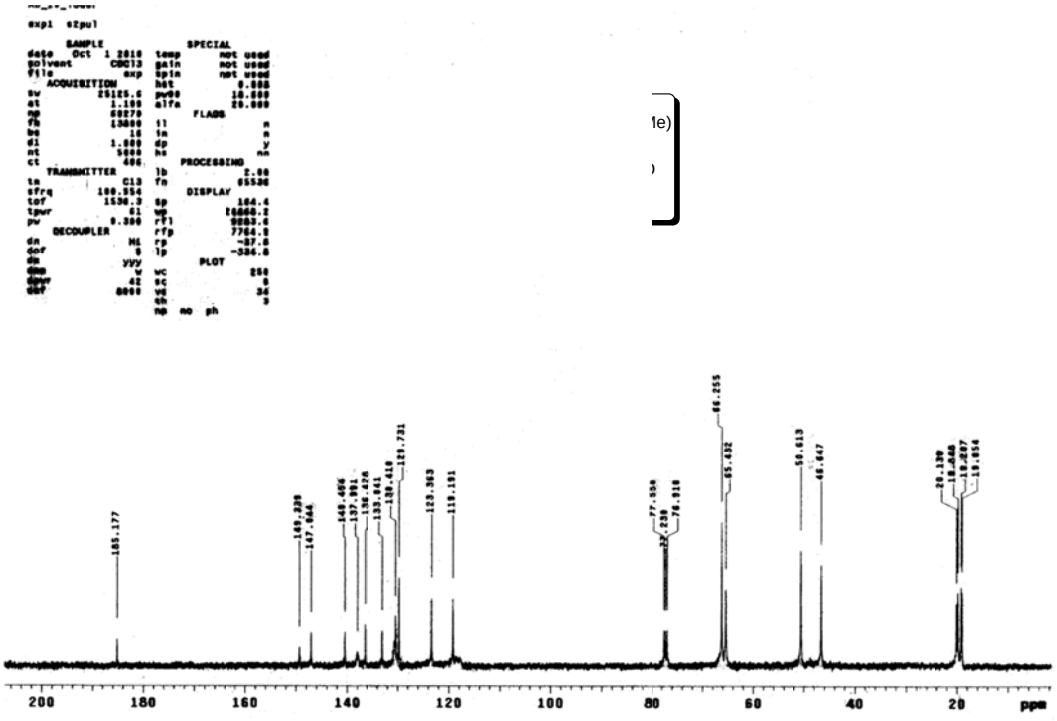
_N_-((_E_)-(3,4-Dimethylphenylimino)(thiomorpholino)methyl)-_N_-(_3,4_-dimethylphenyl) thiomorpholine-4-carbothioamide (3b). MASS SPECTRA:



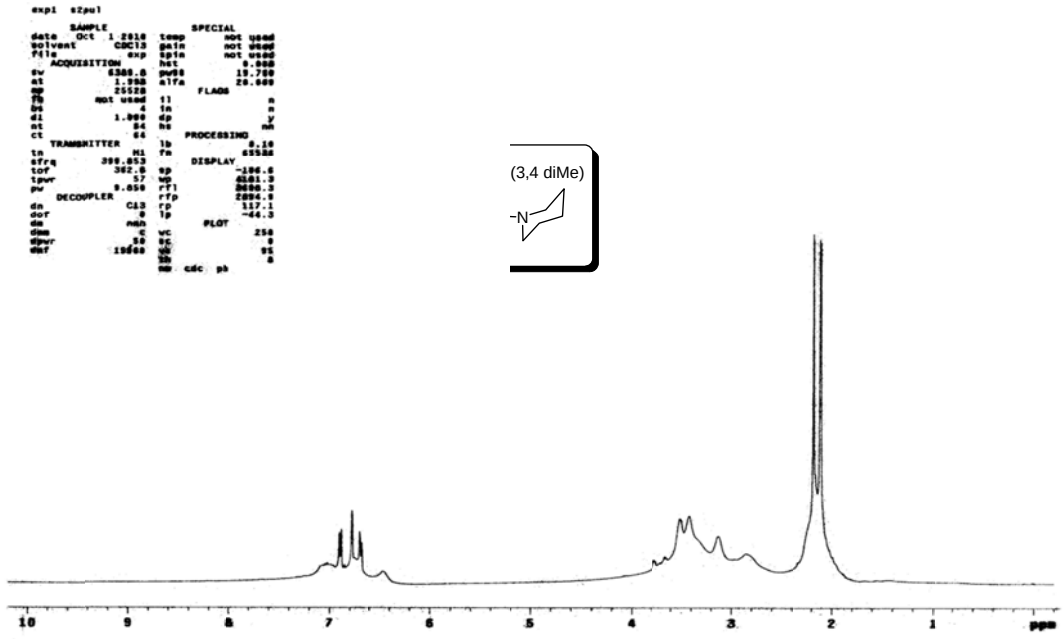
_N_-((_E_)-(3,4-Dimethylphenylimino)(morpholino)methyl)-_N_-(_3,4_-dimethylphenyl) morpholine-4-carbothioamide (4'a). ^{1}H NMR (400 MHz, $CDCl_3$):



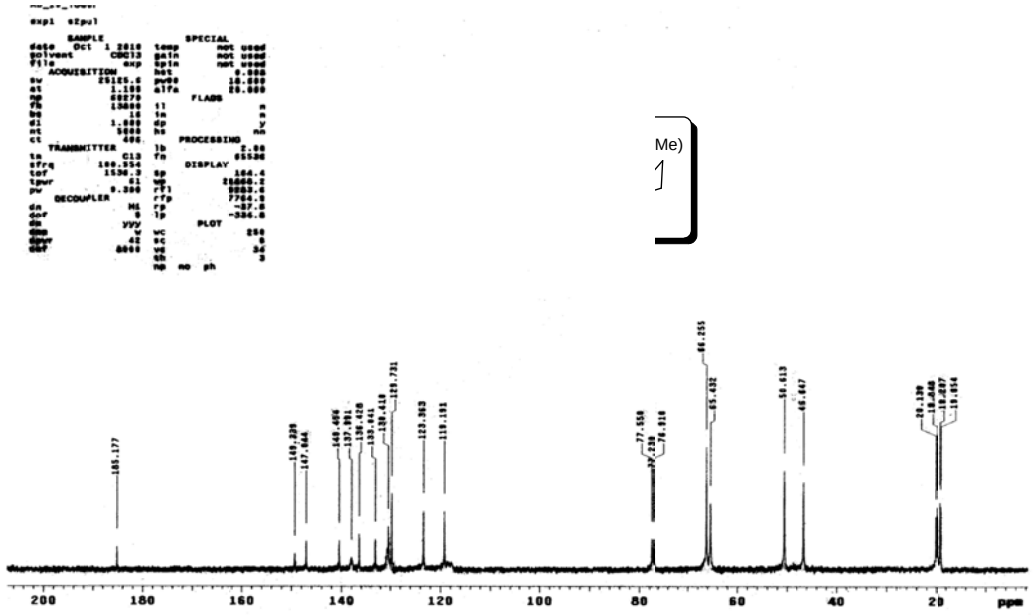
***N*-((*E*)-(3,4-Dimethylphenylimino)(morpholino)methyl)-*N*-(*3,4*-dimethylphenyl) morpholine-4-carbothioamide (8a). ^{13}C NMR (100 MHz, $CDCl_3$):**



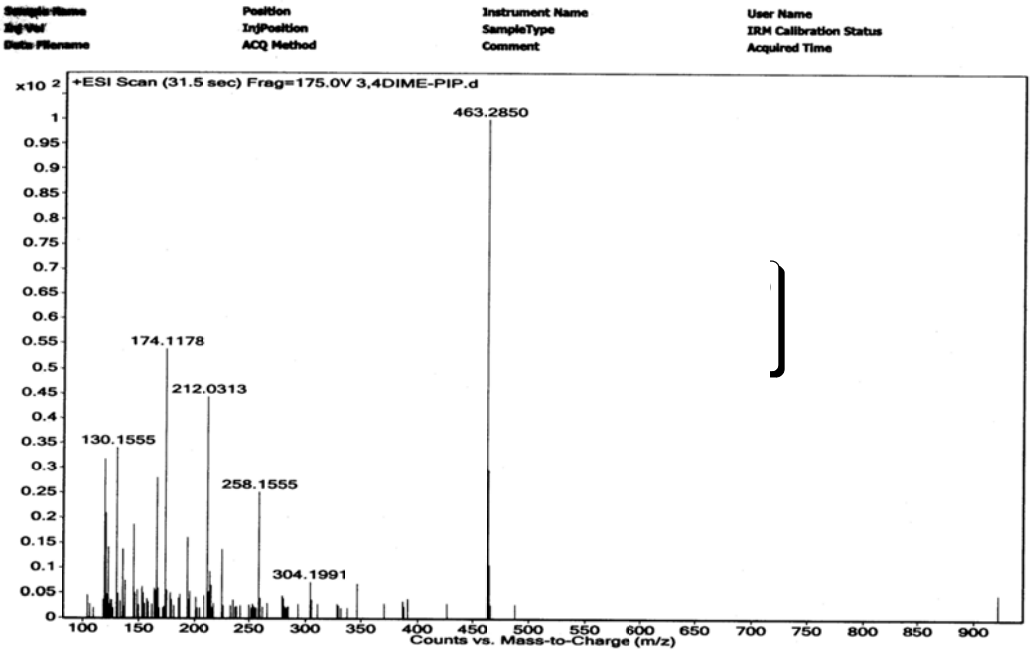
***N*-((*E*)-(3,4-Dimethylphenylimino)(pi[peridin-1-yl)methyl)-*N*-(3,4-dimethylphenyl) piperidine-1-carbothioamide (3d) ^{1}H NMR (400 MHz, $CDCl_3$):**



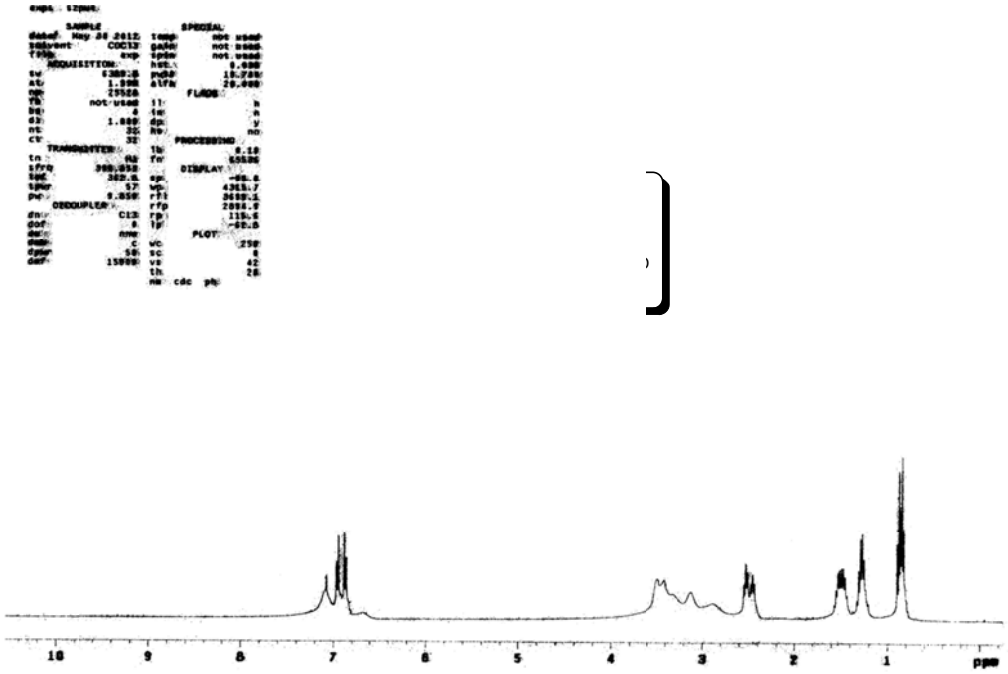
_N_-((_E_)-(3,4-Dimethylphenylimino)(piperidin-1-yl)methyl)-_N_-(3,4-dimethylphenyl) piperidine-1-carbothioamide (3d). ^{1}H NMR (400 MHz, $CDCl_3$):



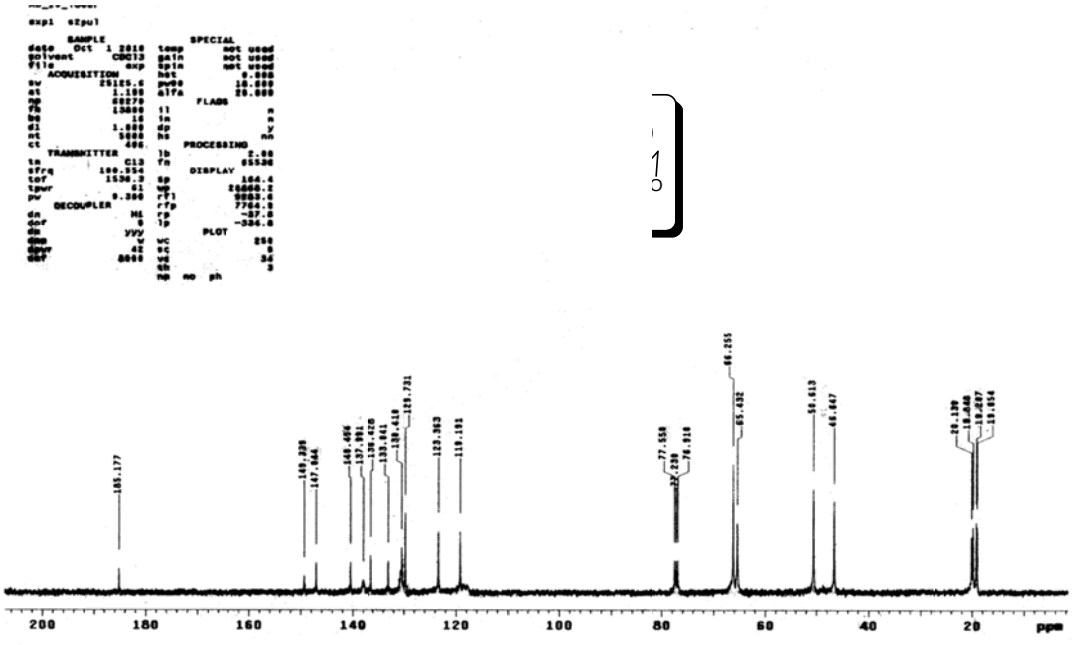
_N_-((_E_)-(3,4-Dimethylphenylimino)(morpholino)methyl)-_N_-(3,4-dimethylphenyl) morpholine-4-carbothioamide (3d). MASS SPECTRA:



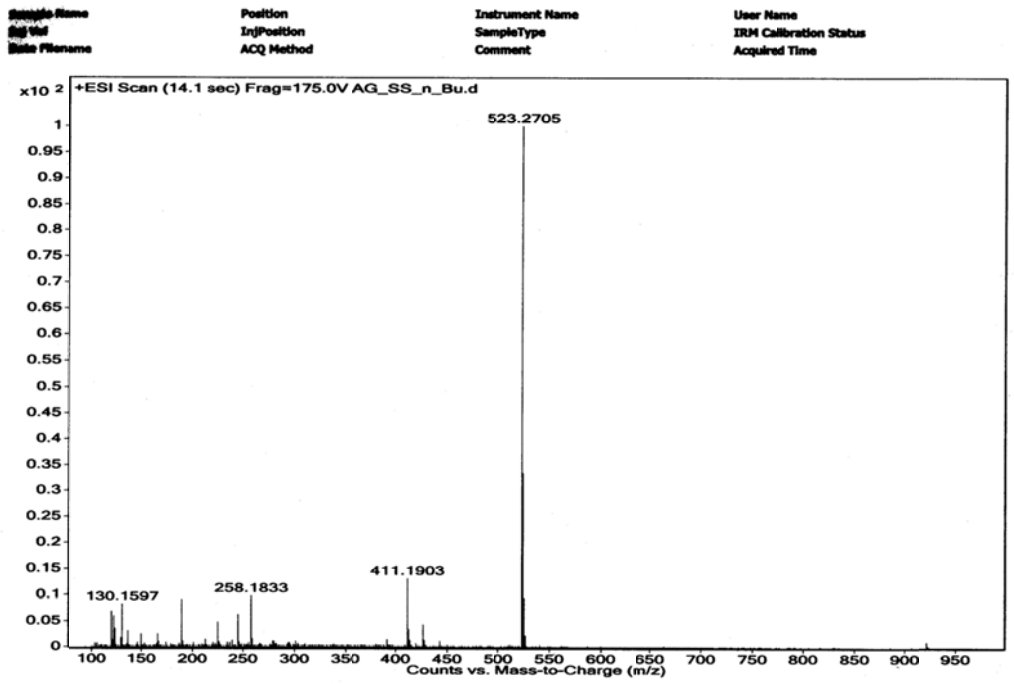
_N_-((_E_)-(4-Butylphenylimino)(morpholino)methyl)-_N_-(4-butylylphenyl)morpholine-4-carbothioamide (4a) ^{1}H NMR (400 MHz, $CDCl_3$):



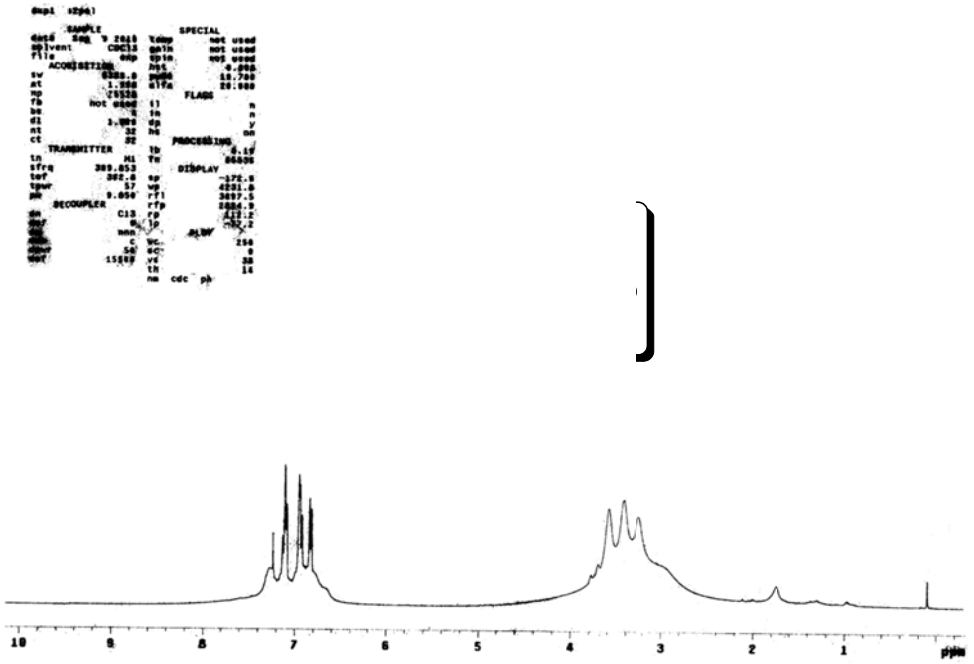
_N_-((_E_)-(4-Butylphenylimino)(morpholino)methyl)-_N_-(4-butylylphenyl)morpholine-4-carbothioamide (4a) ^{13}C NMR (100 MHz, $CDCl_3$):



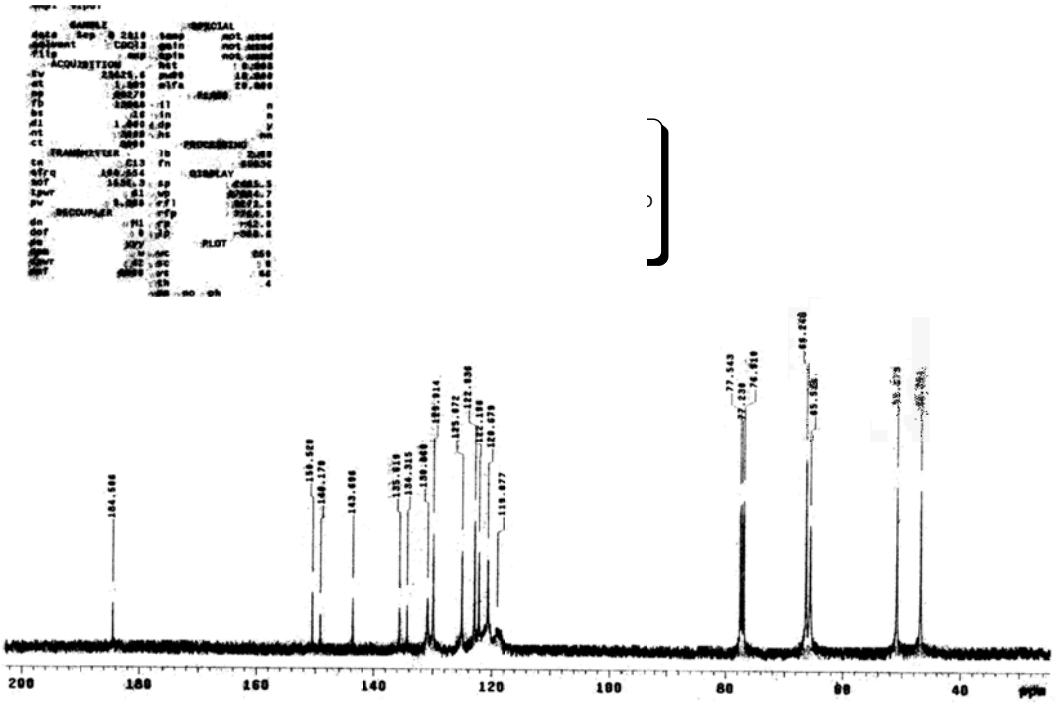
_N_-((_E_)-(4-Butylphenylimino)(morpholino)methyl)-_N_-(4-butylylphenyl)morpholine-4-carbothioamide (4a) MASS SPECTRA:



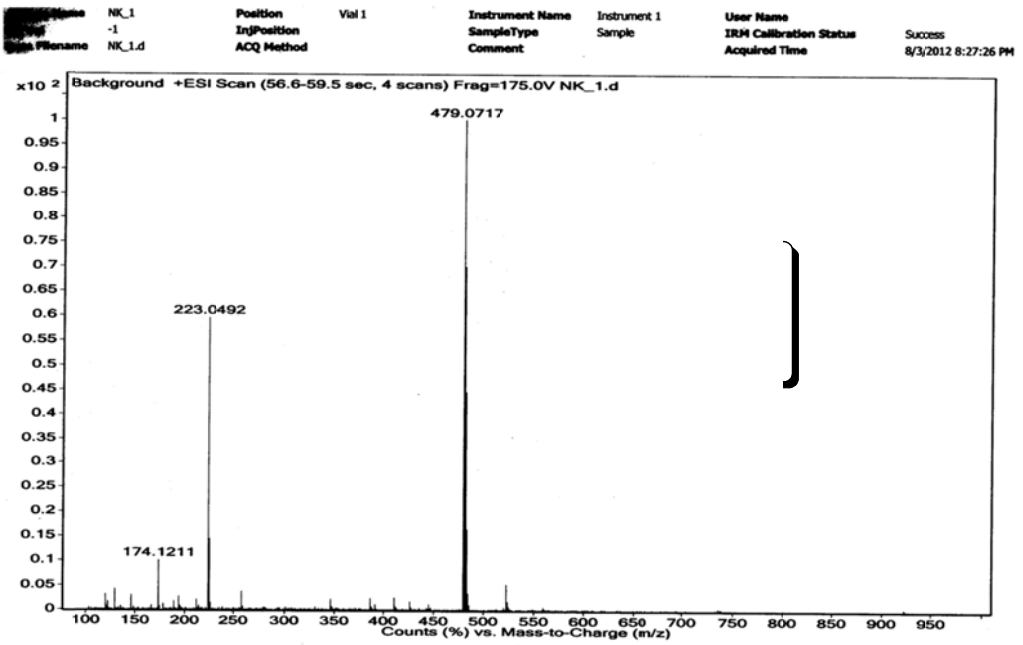
_N_-((_E_)-(3-Chlorophenylimino)(morpholino)methyl)-_N_-(3-Chlorophenyl)morpholine-4-carbothioamide (5a).^{1}H NMR (400 MHz, $CDCl_3$):



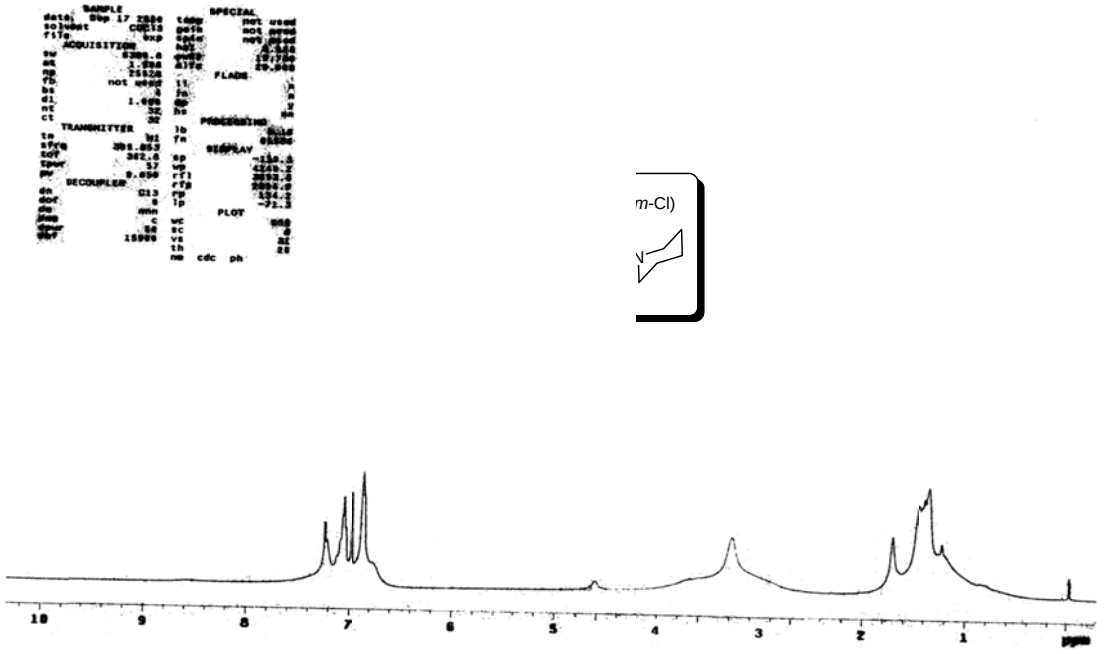
_N_-((_E_)-(3-Chlorophenylimino)(morpholino)methyl)-_N_-(3-Chlorophenyl)morpholine-4-carbothioamide (5a).^{13}C NMR (100 MHz, $CDCl_3$):



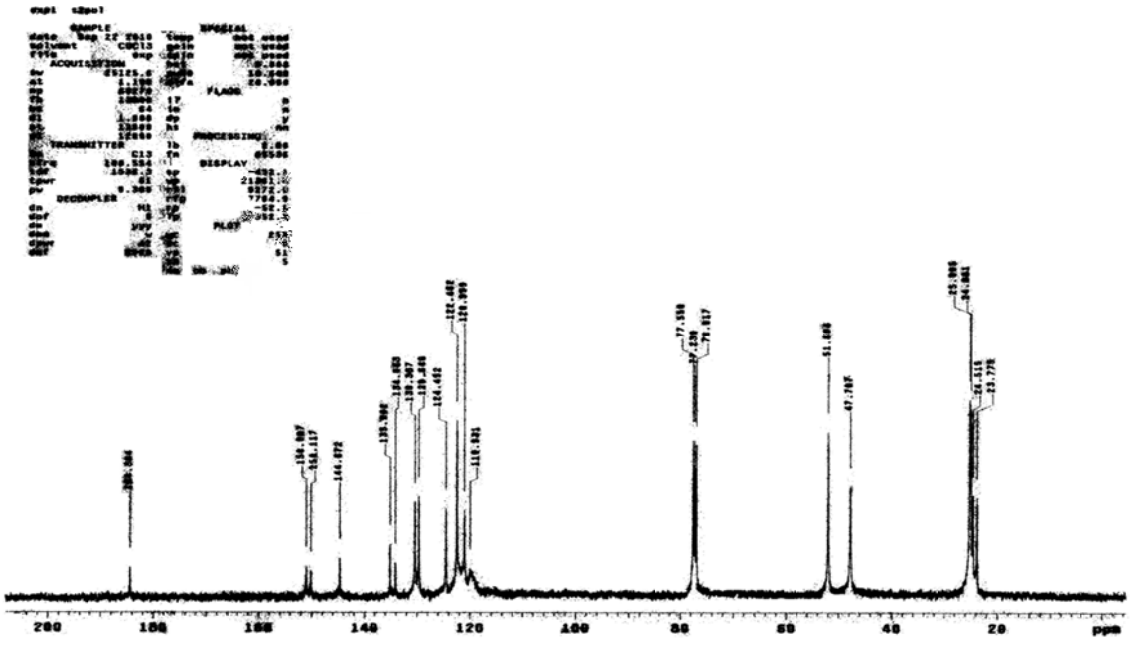
_N_-((_E_)-(3-Chlorophenylimino)(morpholino)methyl)-_N_-(3-Chlorophenyl)morpholine-4-carbothioamide (5a). MASS SPECTRA:



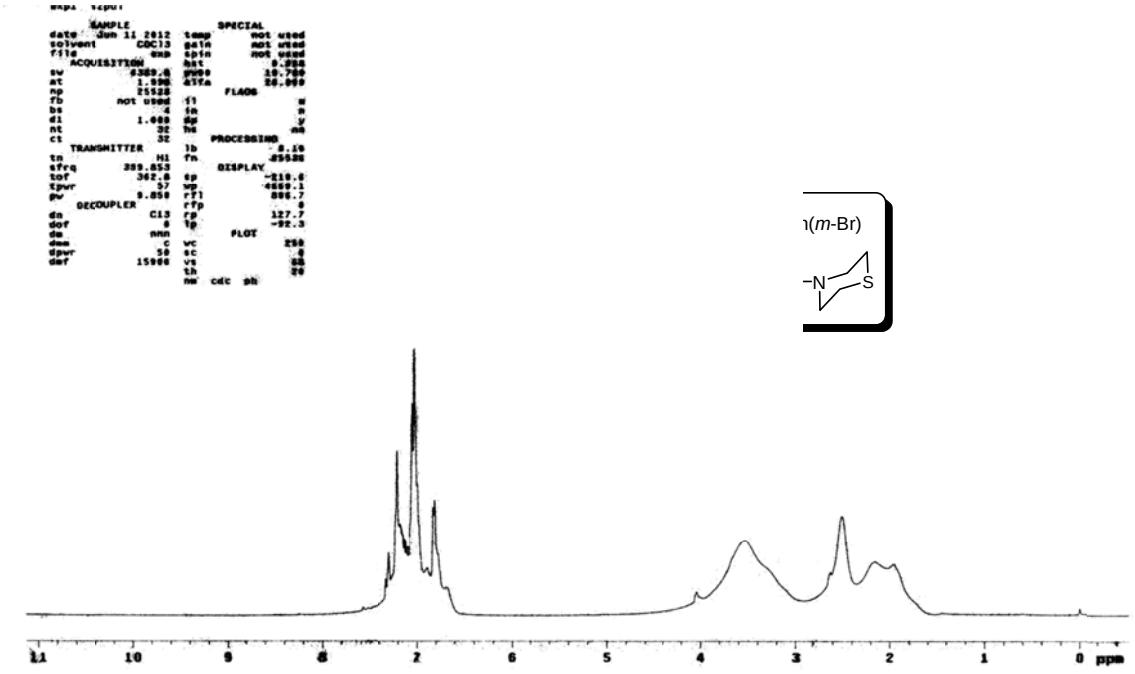
_N_-((_E_)-(3-Chlorophenylimino)(piperidin-1-yl)methyl)-_N_-(3-chlorophenyl)piperidine-1-carbothioamide (5d): ^{1}H NMR (400 MHz, $CDCl_3$):



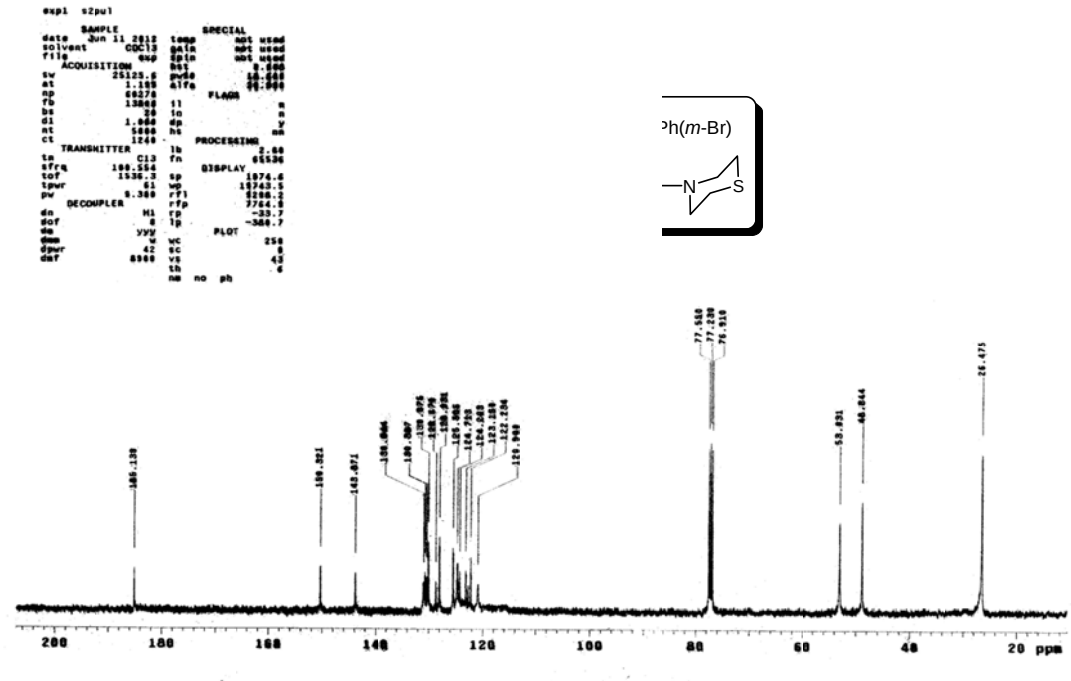
_N_-((_E_)-(3-Chlorophenylimino)(piperidin-1-yl)methyl)-_N_-(3-chlorophenyl)piperidine-1-carbothioamide (5d). ^{13}CNMR (100 MHz, $CDCl_3$):



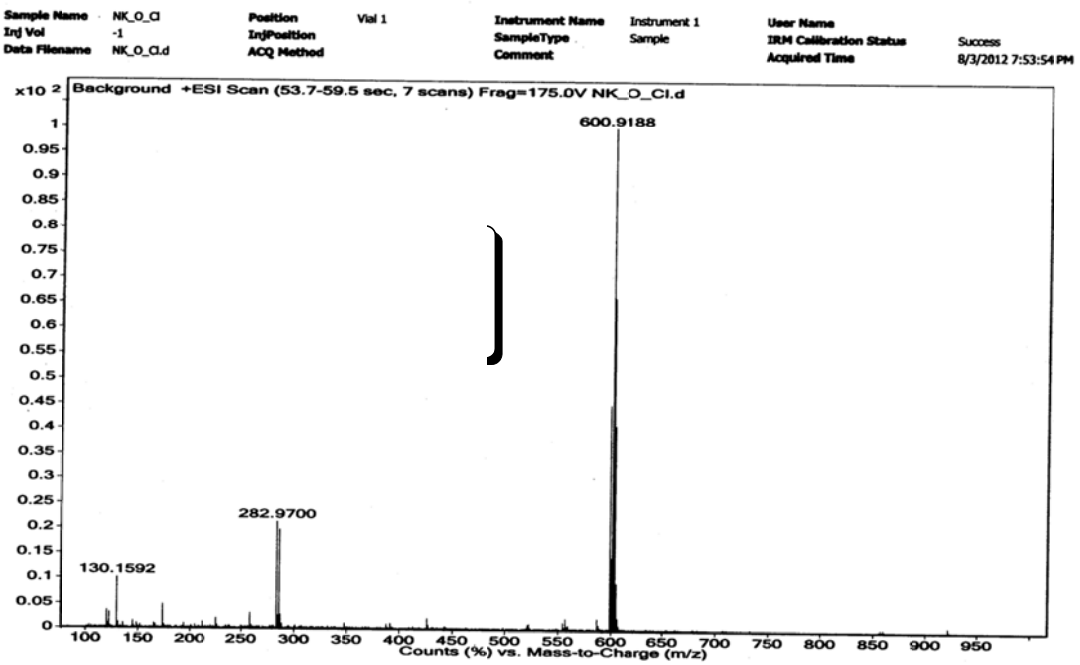
_N_-((_E_)-(3-Bromophenylimino)(thiomorpholino)methyl)-_N_-(3-bromophenyl)thiomorpholine-4-carbothioamide (6b).^{1}H NMR (400 MHz, $CDCl_3$):



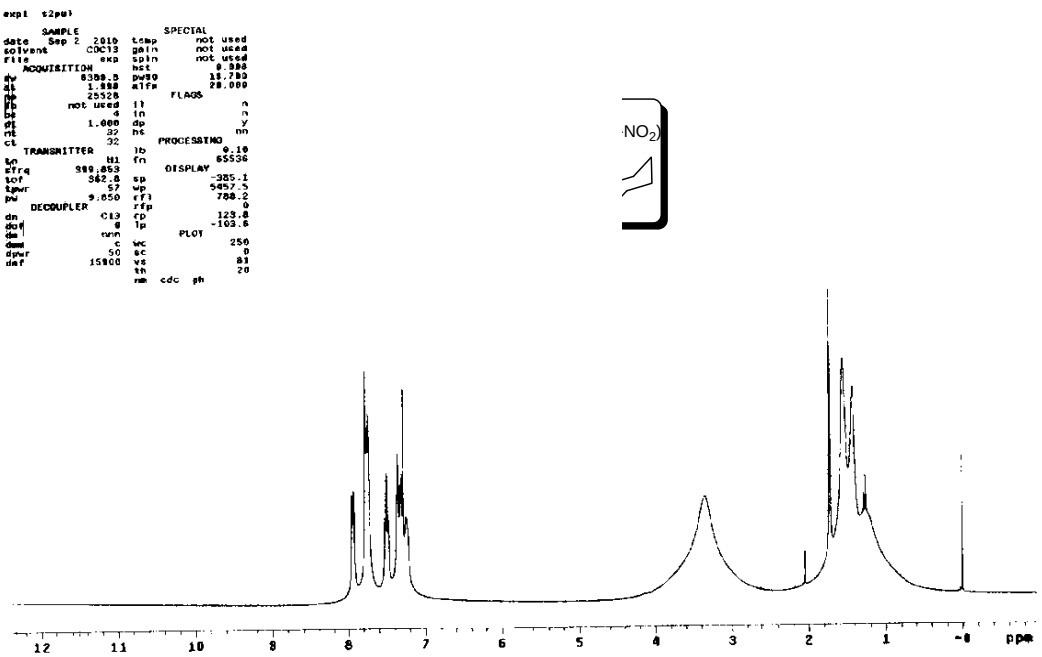
_N_-((_E_)-(3-Bromophenylimino)(thiomorpholino)methyl)-_N_-(3-bromophenyl)thiomorpholine-4-carbothioamide (6b). ^{13}C NMR (100 MHz, $CDCl_3$):



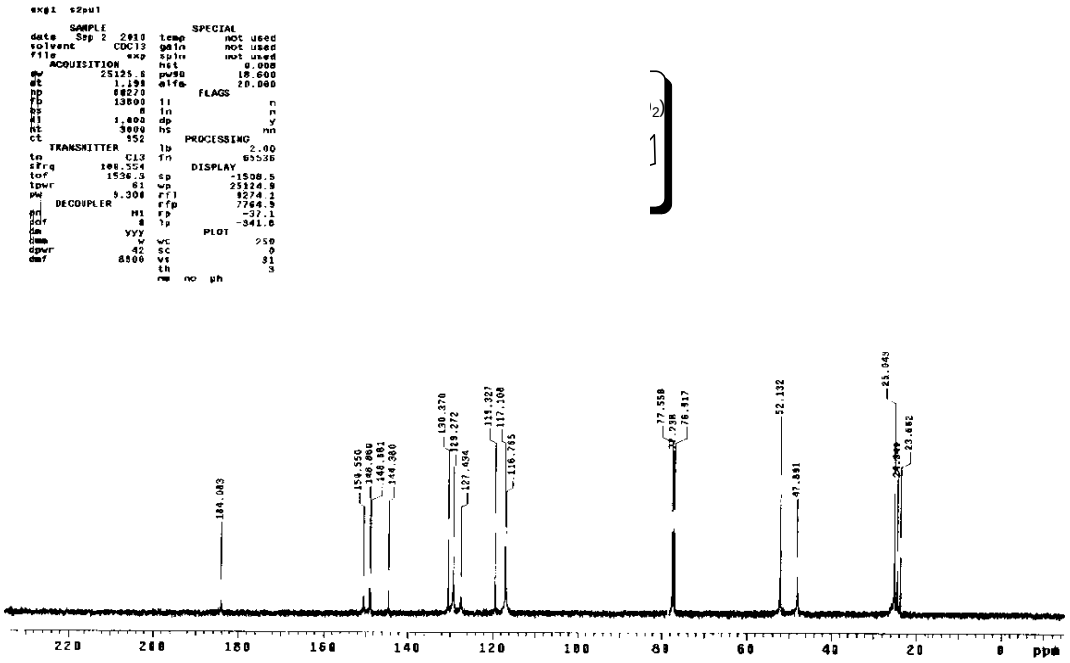
_N_-((_E_)-(3-Bromophenylimino)(thiomorpholino)methyl)-_N_-(3-bromophenyl)thiomorpholine-4-carbothioamide (6b). MASS SPECTRA:



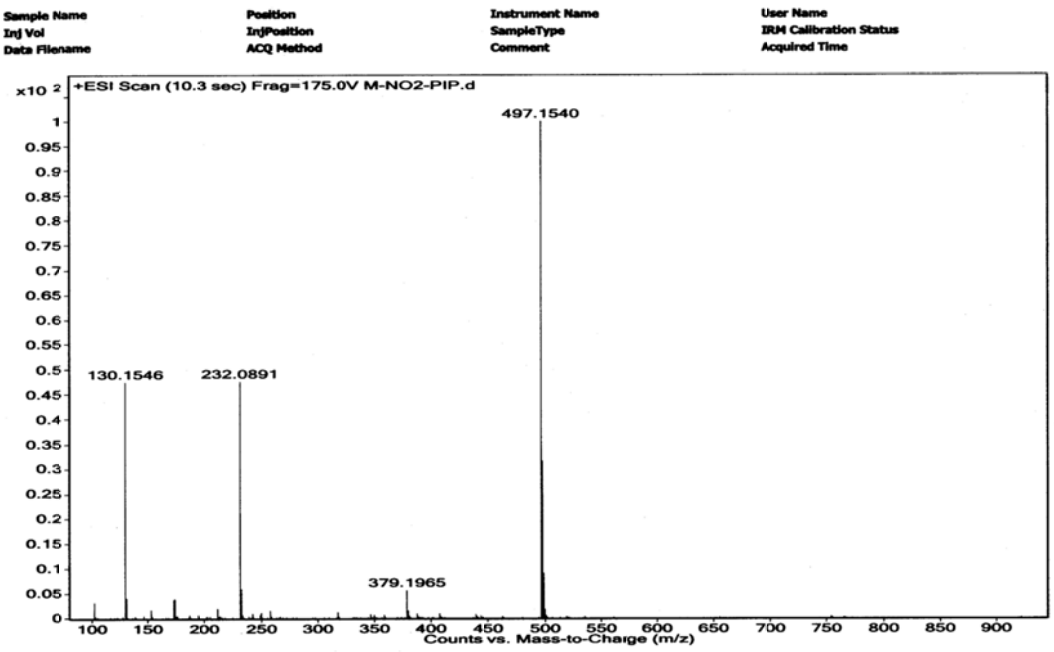
_N_-((_E_)-(3-Nitrophenylimino)(piperidin-1-yl)methyl)-_N_-(3-nitrophenyl)piperidine-1-carbothioamide (7d).^{1}H NMR (400 MHz, $CDCl_3$):



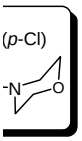
_N_-((_E_)-(3-Nitrophenylimino)(piperidin-1-yl)methyl)-_N_-(3-nitrophenyl)piperidine-1-carbothioamide (7d). ^{13}C NMR (100 MHz, $CDCl_3$):

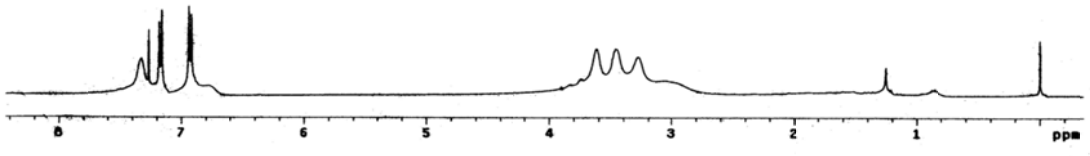


_N_-((_E_)-(3-Nitrophenylimino)(piperidin-1-yl)methyl)-_N_-(3-nitrophenyl)piperidine-1-carbothioamide (7d). MASS SPECTRA:

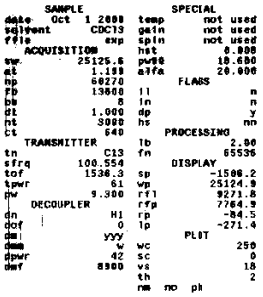


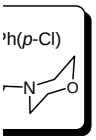
_N_-((_E_)-(4-Chlorophenylimino)(morpholino)methyl)-_N_-(4-chlorophenyl)morpholine-4-carbothioamide (8a).^{1}H NMR (400 MHz, $CDCl_3$):

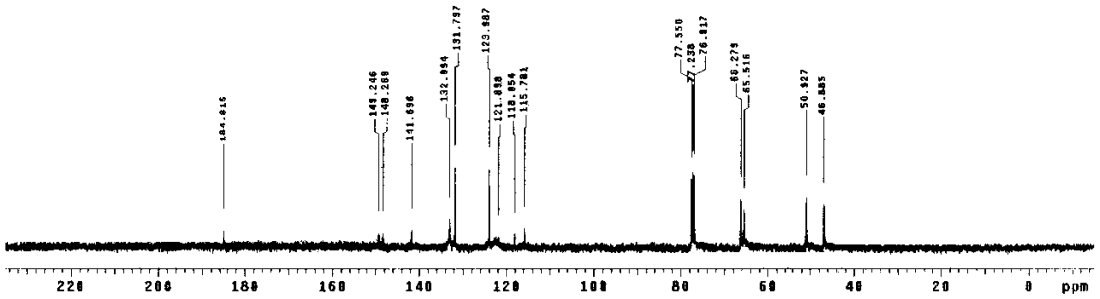




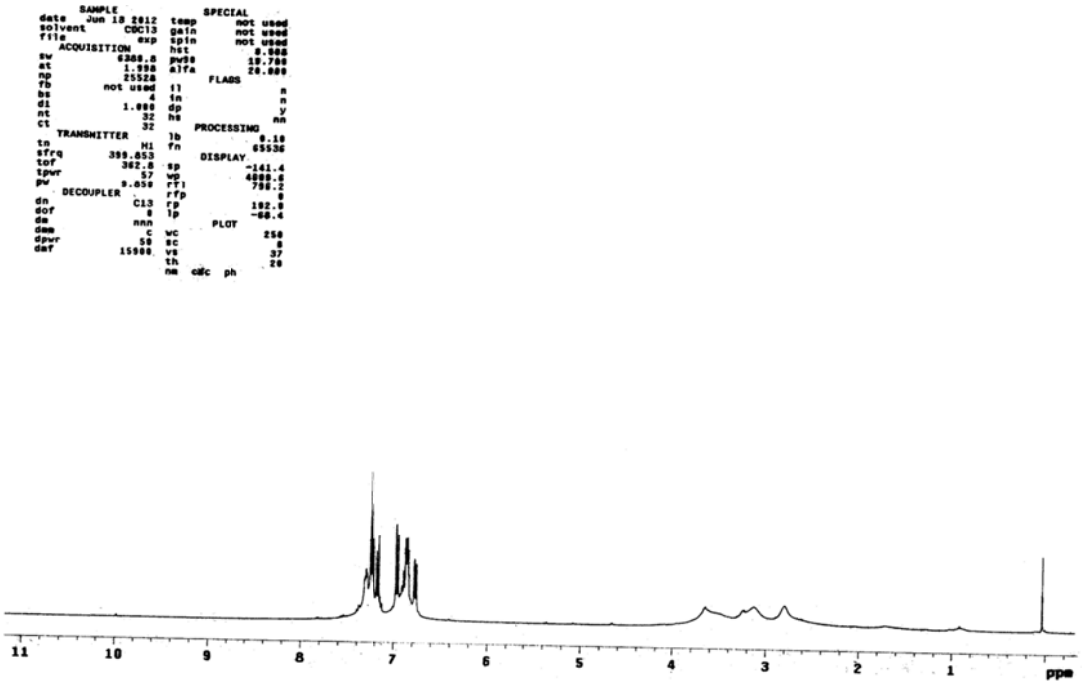
_N_-((_E_)-(4-Chlorophenylimino)(morpholino)methyl)-_N_-(4-chlorophenyl)morpholine-4-carbothioamide (8a).^{13}CNMR (100 MHz, $CDCl_3$):



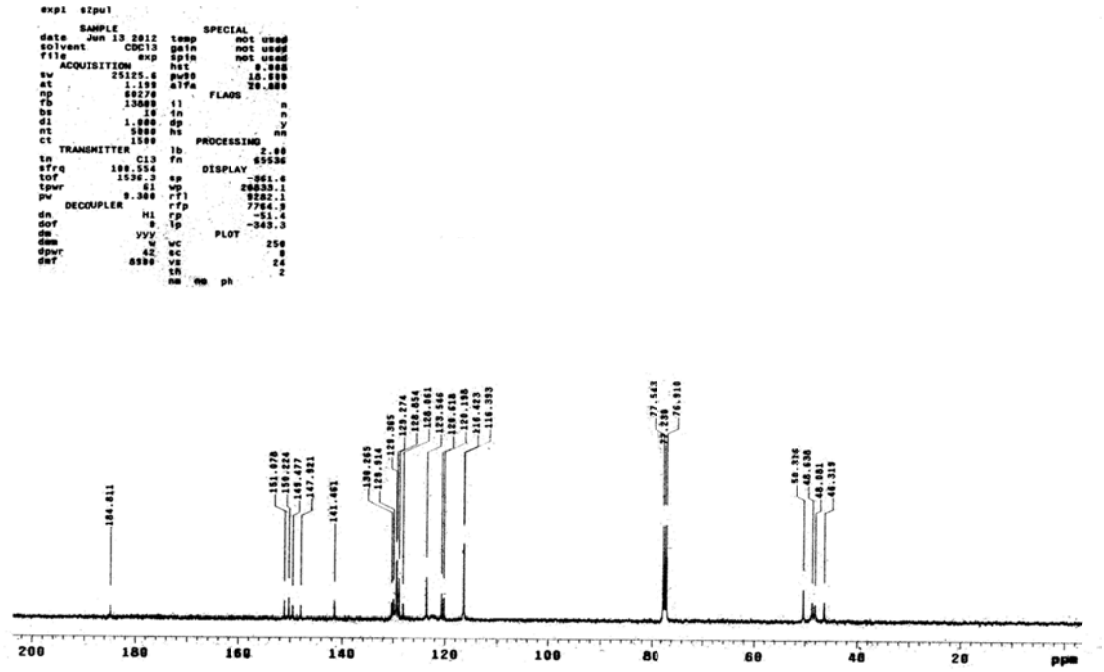




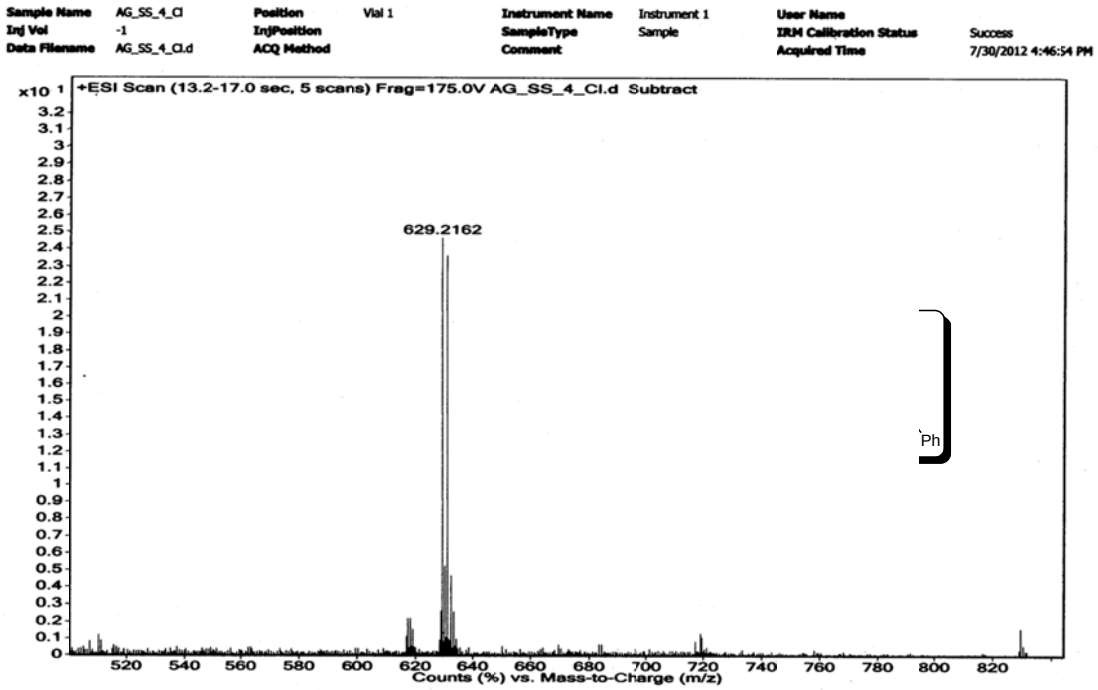
_N_-((_E_)-(4-Chlorophenylimino)(4-phenylpiperazine-1-yl)methyl)-_N_-(4-chlorophenyl)-4-phenylpiperazine-1-carbothioamide (8c).^{1}H NMR (100 MHz, $CDCl_3$):



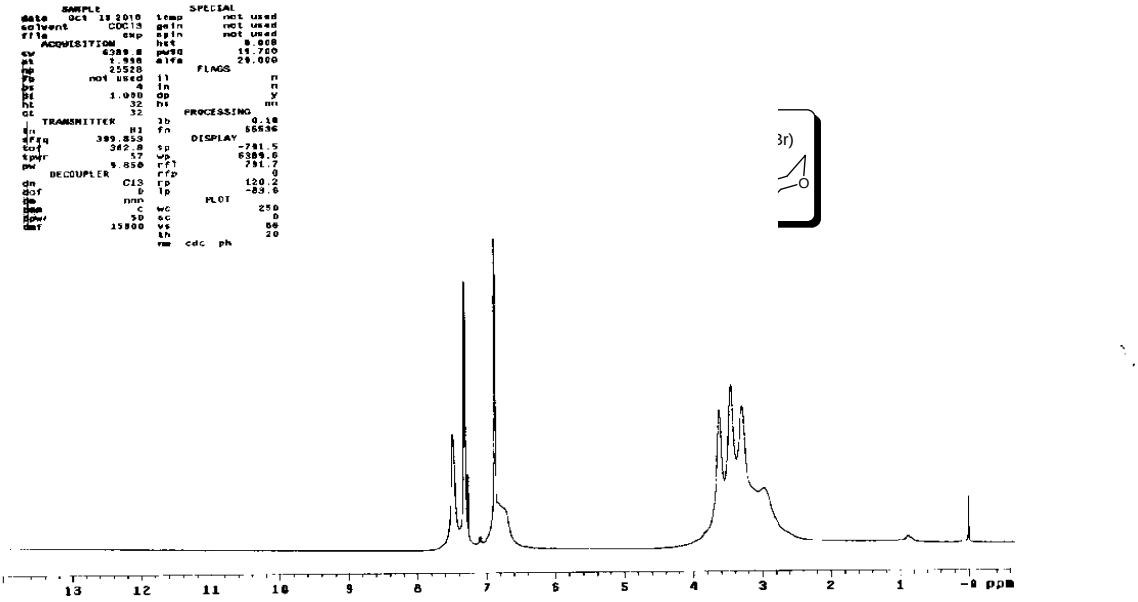
_N_-((_E_)-(4-Chlorophenylimino)(4-phenylpiperazine-1-yl)methyl)-_N_-(4-chlorophenyl)-4-phenylpiperazine-1-carbothioamide (8c).^{13}C NMR (400 MHz, $CDCl_3$):



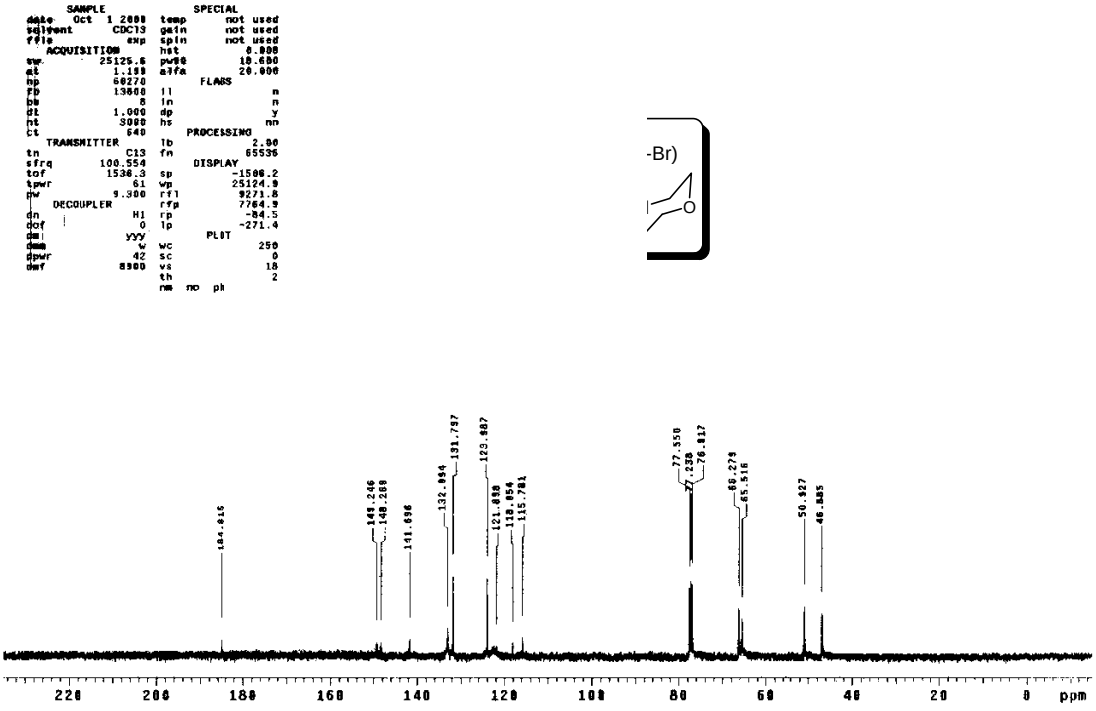
_N_-((_E_)-(4-Chlorophenylimino)(4-phenylpiperazine-1-yl)methyl)-_N_-(4-chlorophenyl)-4-phenylpiperazine-1-carbothioamide (8c). MASS SPECTRA:



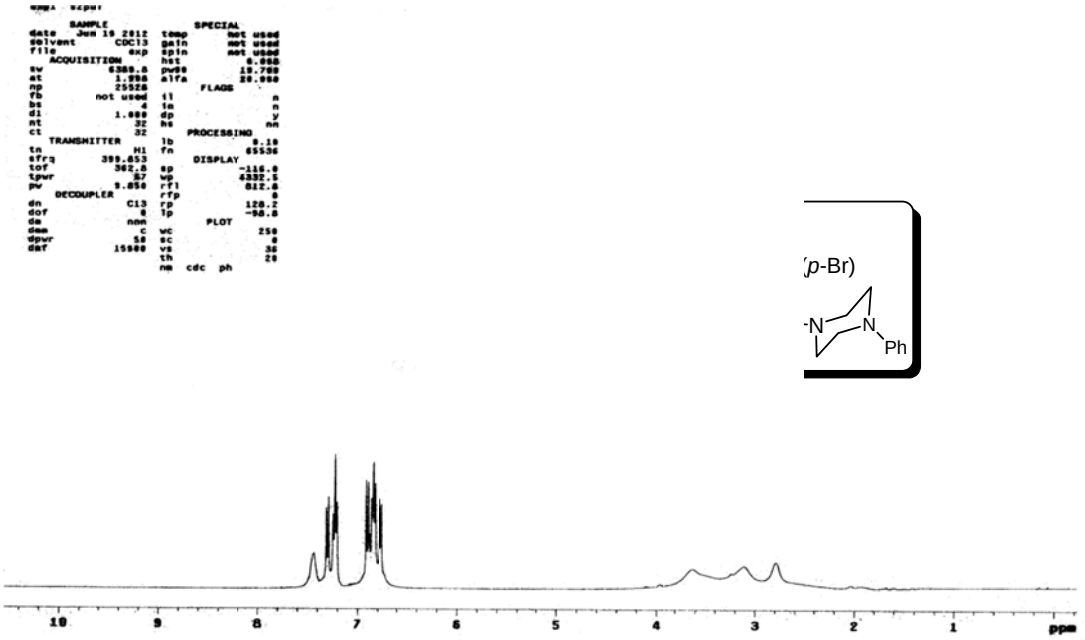
_N_-((_E_)-(4-Bromoophenylimino)(morpholino)methyl)-_N_-(4-bromophenyl)morpholine-4-carbothioamide (9a).^{1}H NMR (400 MHz, $CDCl_3$):



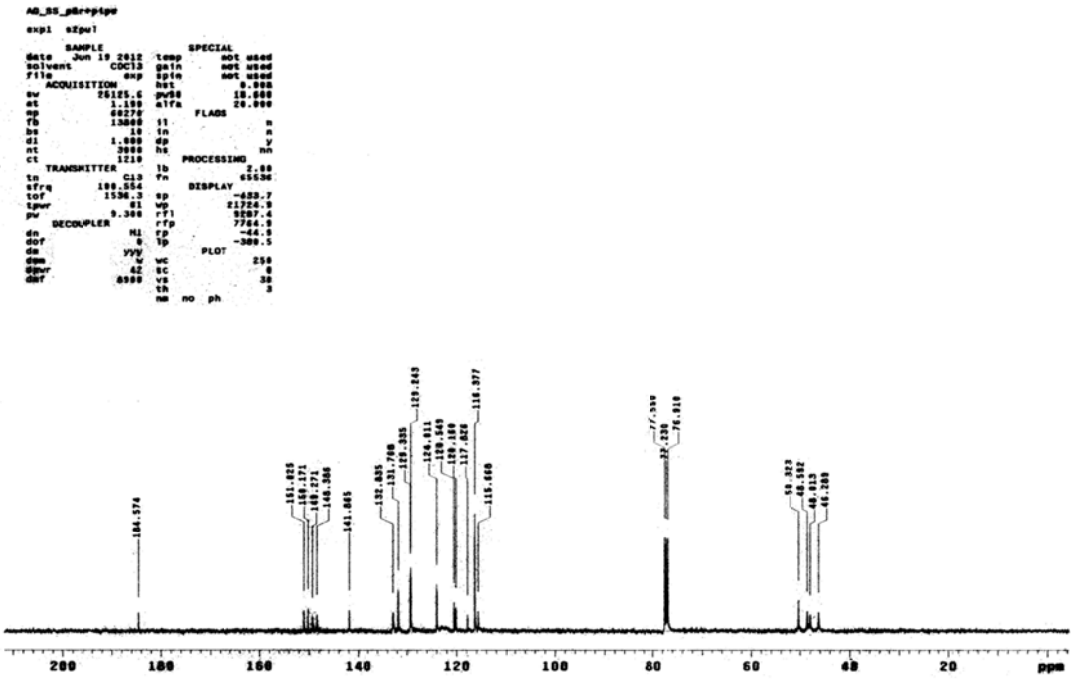
_N_-((_E_)-(4-Bromoophenylimino)(morpholino)methyl)-_N_-(4-bromophenyl)morpholine-4-carbothioamide (9a).^{13}CNMR (100 MHz, $CDCl_3$):



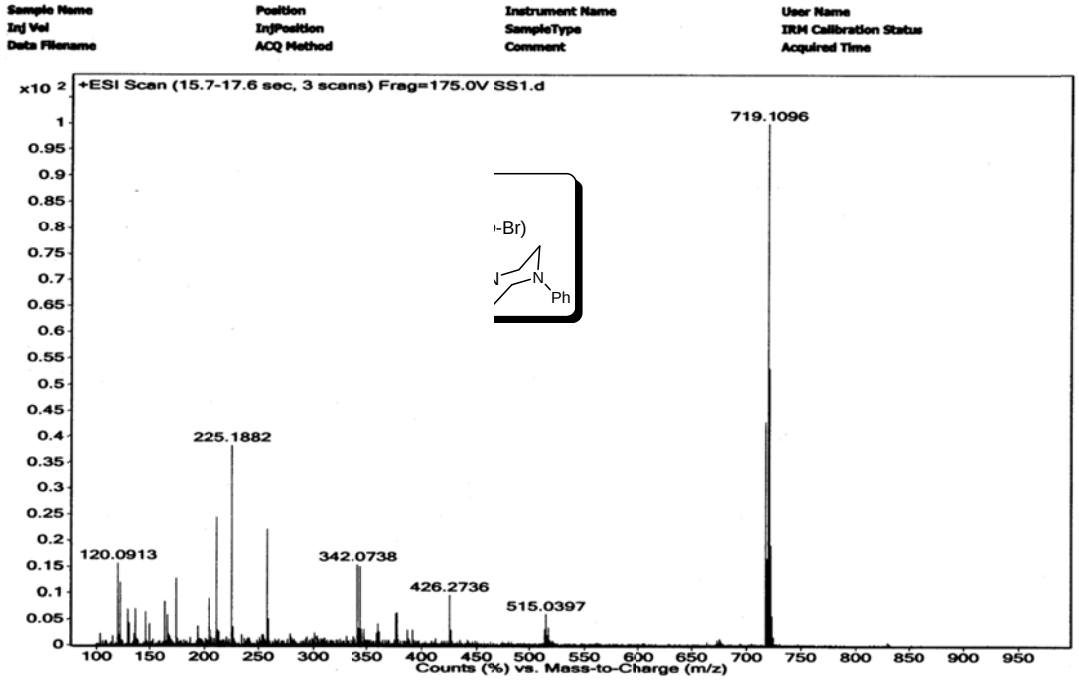
_N_-((_E_)-(4-Bromoophenylimino)(4-phenylpiperazin-1-yl)methyl)-_N_-(4-bromophenyl) phenylpiperazine-4-carbothioamide (9c).^{1}H NMR (400 MHz, $CDCl_3$):



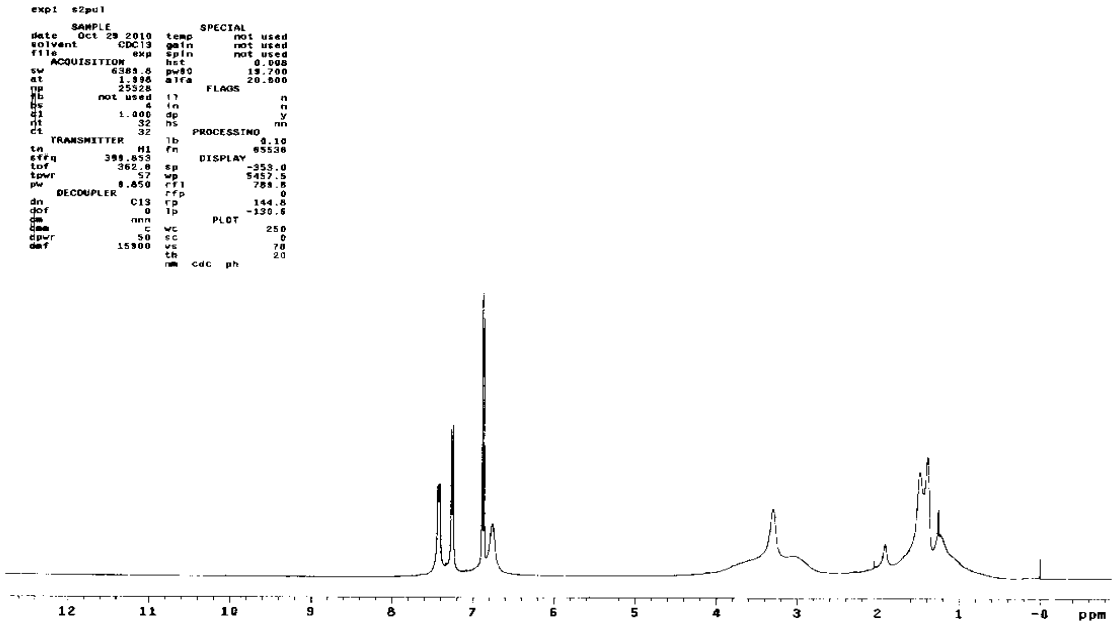
_N_-((_E_)-(4-Bromoophenylimino)(4-phenylpiperazin-1-yl)methyl)-_N_-(4-bromophenyl) phenylpiperazine-4-carbothioamide (9c).^{13}CNMR (100 MHz, $CDCl_3$):



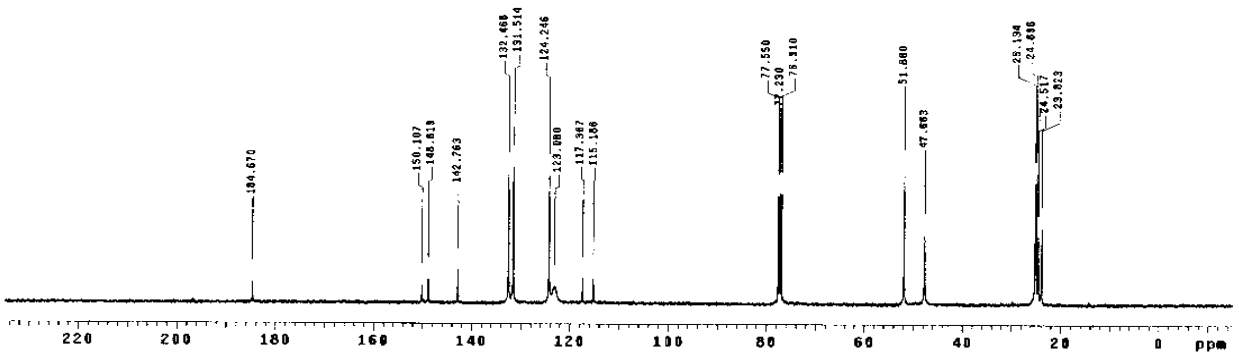
_N_-((_E_)-(4-Bromoophenylimino)(4-phenylpiperazin-1-yl)methyl)-_N_-(4-bromophenyl) phenylpiperazine-4-carbothioamide (9c). MASS SPECTRA:



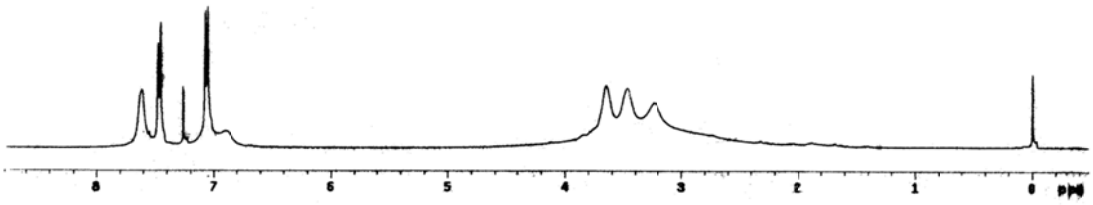
_N_-((_E_)-(4-Bromoophenylimino)(piperidin-1-yl)methyl)-_N_-(2-bromophenyl)piperidine-1-carbothioamide (9d).^{1}H NMR (400 MHz, $CDCl_3$):



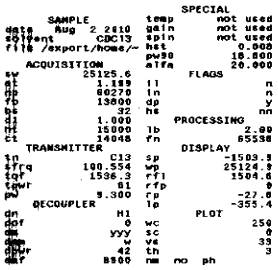
_N_-((_E_)-(4-Bromoophenylimino)(piperidin-1-yl)methyl)-_N_-(2-bromophenyl)piperidine-1-carbothioamide (9d).^{13}C NMR (100 MHz, $CDCl_3$):

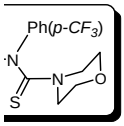


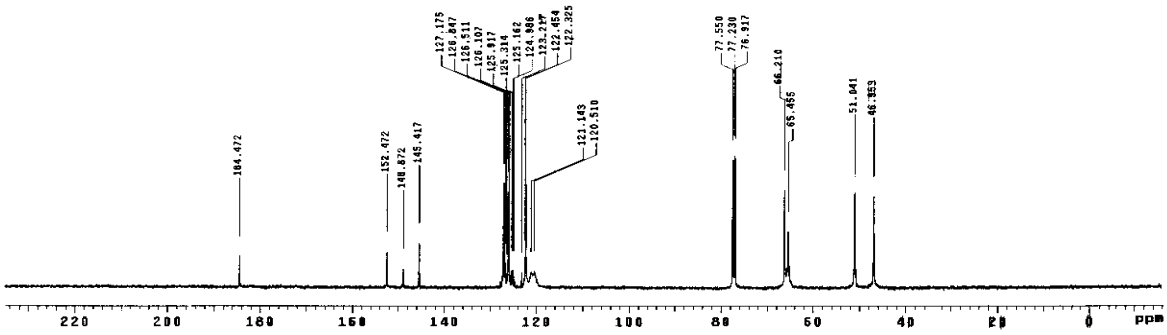
_N_-((_E_)-(4-Trifluoromethyl)phenylimino(morpholino)methyl)-_N_-(4-trifluorophenyl) morpholine-4-carbothioamide (10a).^{1}H NMR (400 MHz, $CDCl_3$):



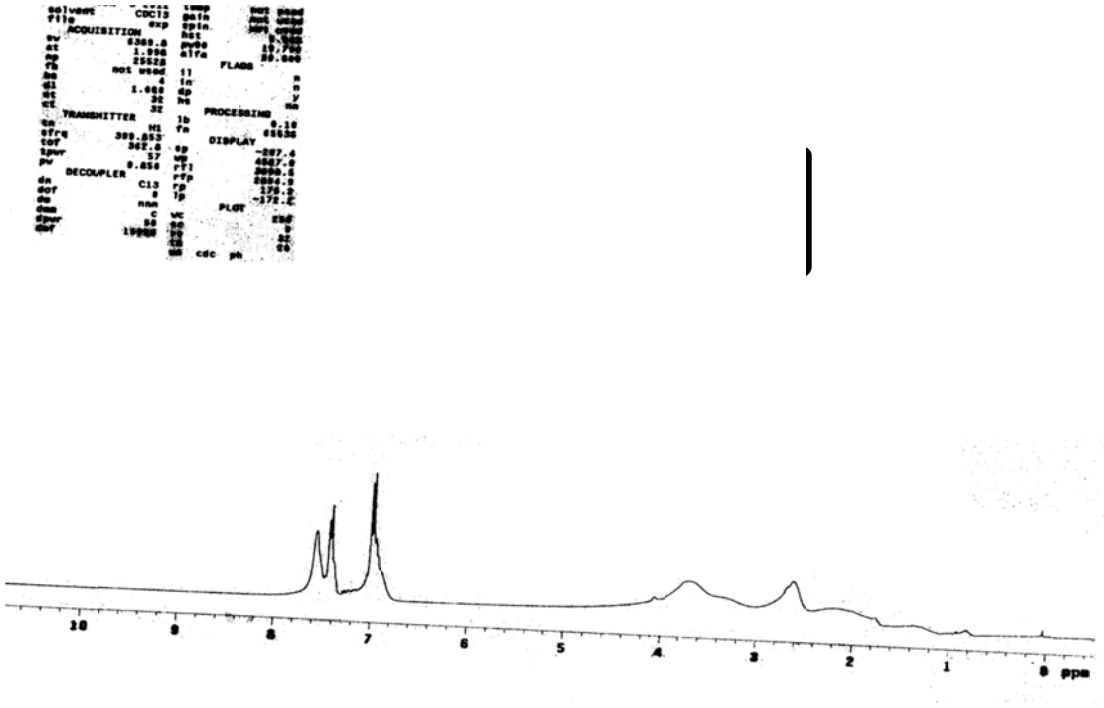
_N_-((_E_)-(4-Trifluoromethyl)phenylimino(morpholino)methyl)-_N_(4-trifluorophenyl) morpholi-ne-4-carbothioamide (10a).^{1}H NMR (400 MHz, $CDCl_3$):



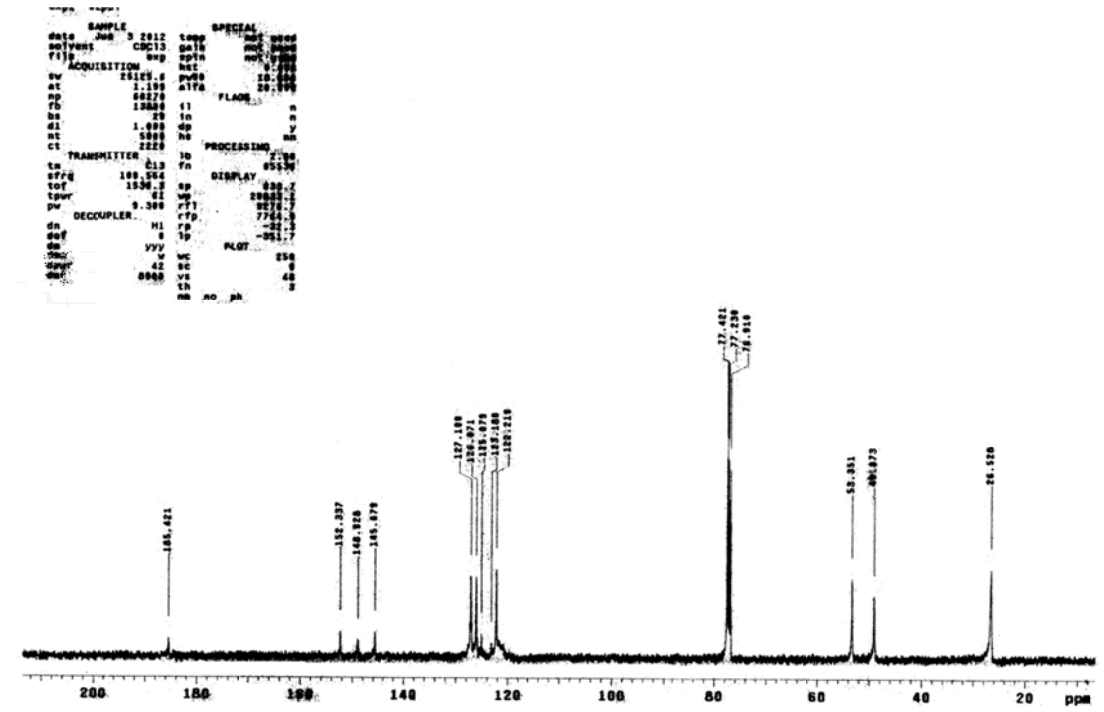




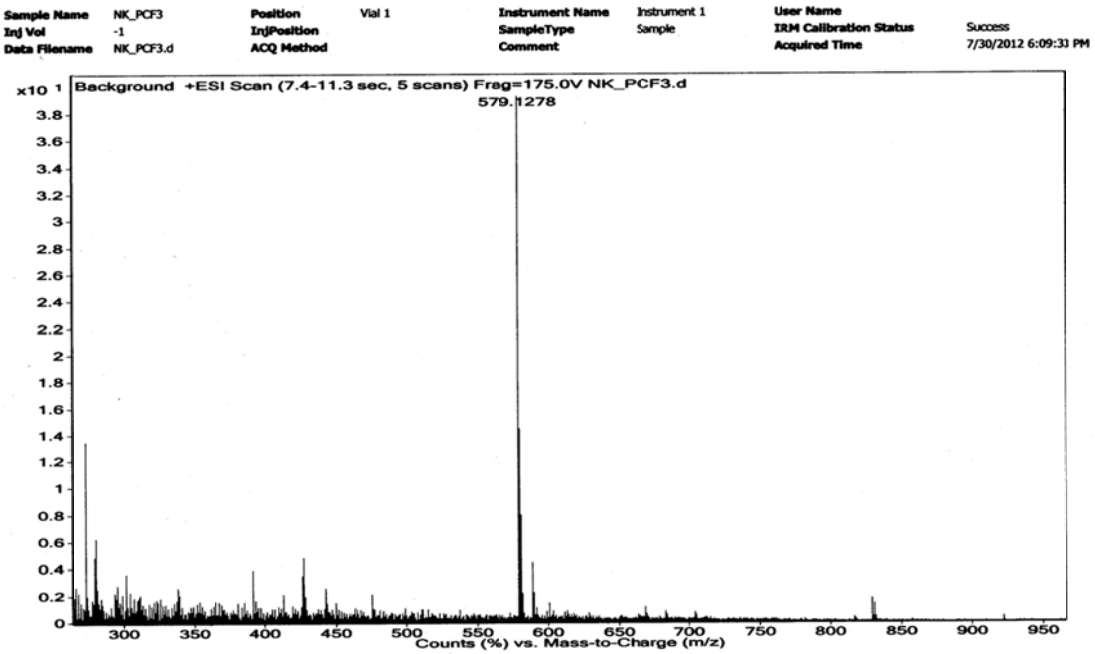
_N_-((_E_)-(4-Trifluoromethyl)phenylimino(thiomorpholino)methyl)-_N_(4-trifluorophenyl) thiomorpholine-4-carbothioamide (10b).^{1}H NMR (400 MHz, $CDCl_3$):



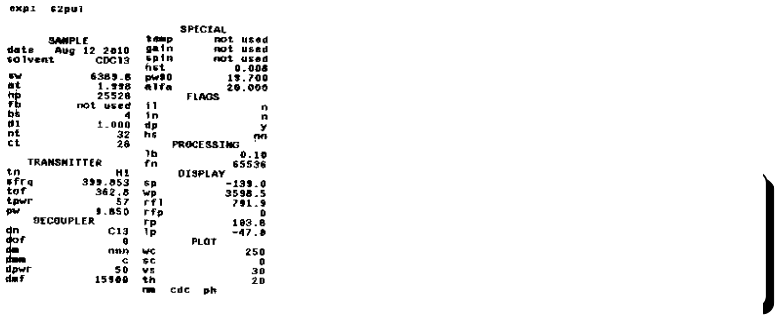
_N_-((_E_)-(4-Trifluoromethyl)phenylimino(thiomorpholino)methyl)-_N_(4-trifluorophenyl) thiomorpholine-4-carbothioamide (10b).^{13}C NMR (100 MHz, $CDCl_3$):

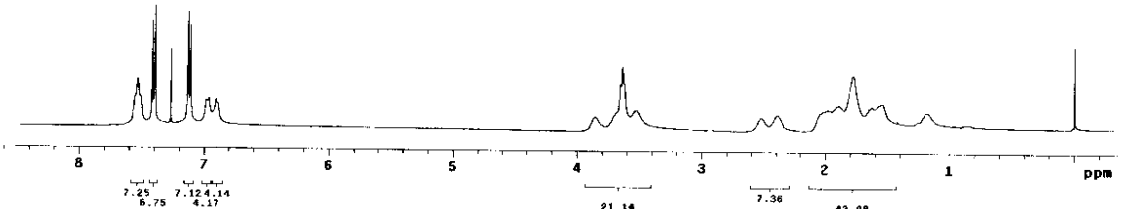


_N_-((_E_)-(4-Trifluoromethyl)phenylimino(thiomorpholino)methyl)-_N_(4-trifluorophenyl) thiomorpholine-4-carbothioamide (10b).MASS SPECTRA:

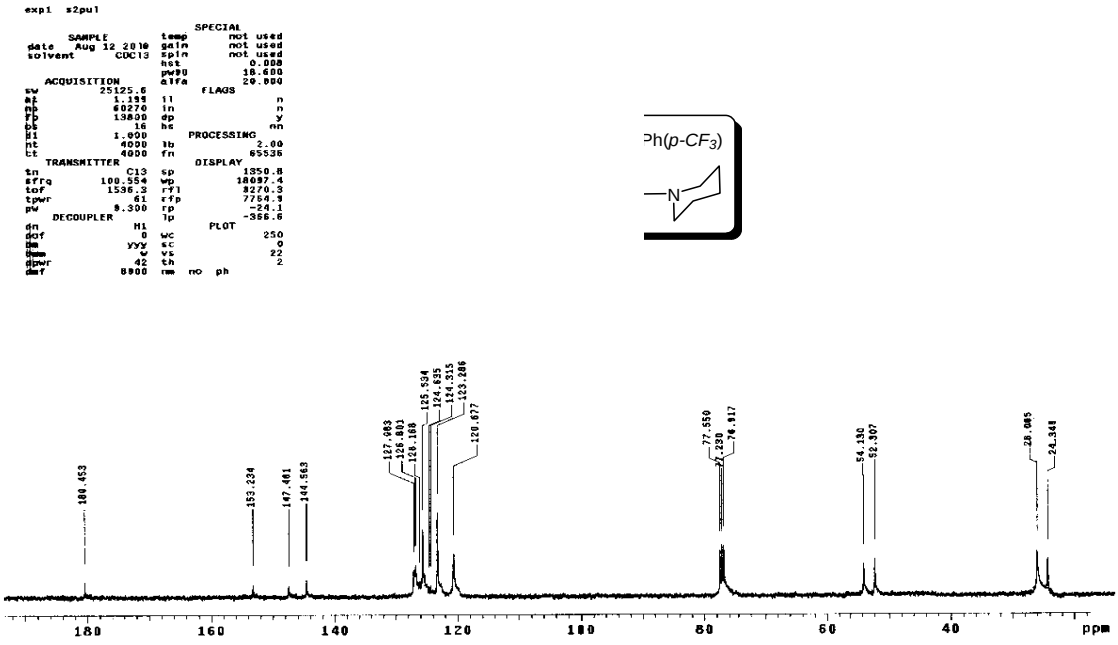


_N_-((_E_)-(4-Trifluoromethyl)(phenylimino)(piperidin-1-yl)methyl)-_N_-(4-bromophenyl) morpholine-1-carbothioamide (10d).^{1}H NMR (400 MHz, $CDCl_3$):

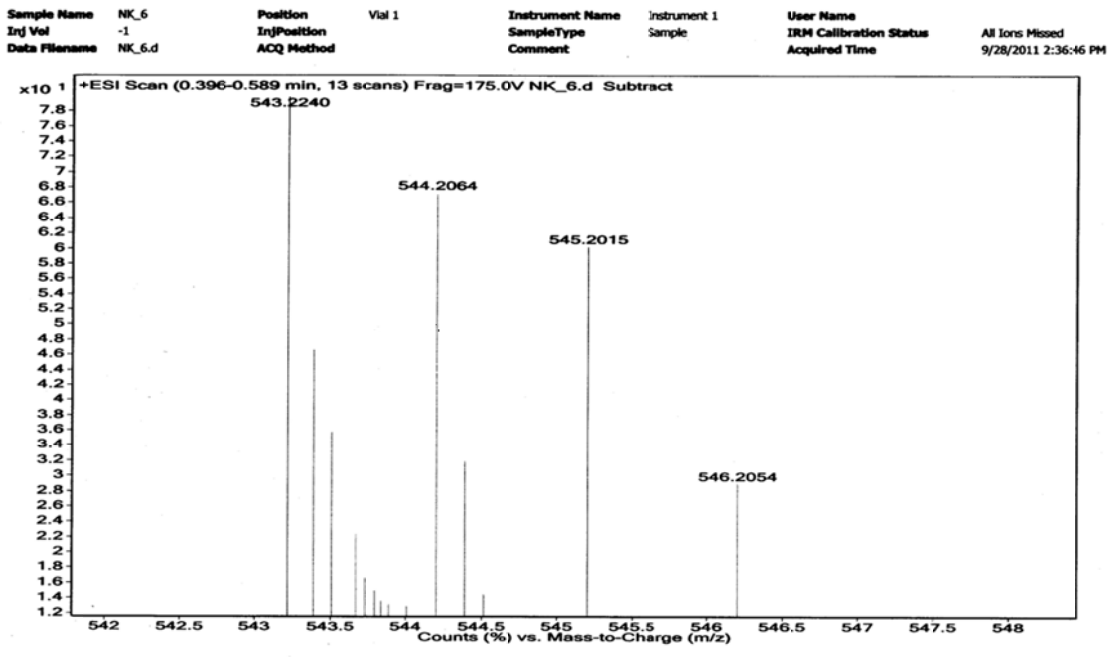




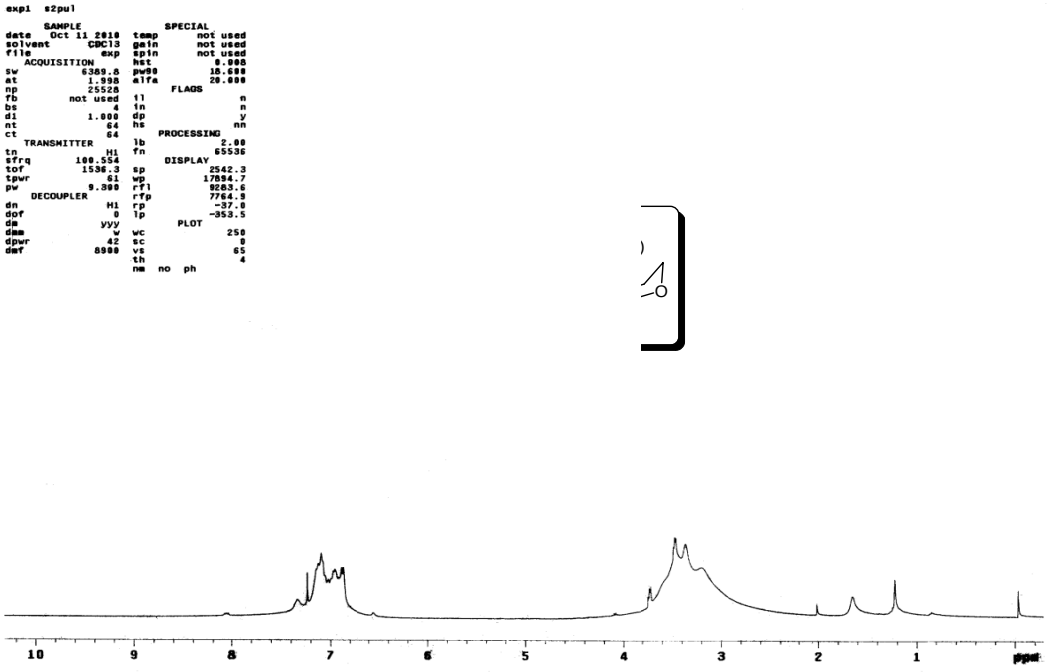
_N_-((_E_)-(4-Trifluoromethyl)(phenylimino)(piperidin-1-yl)methyl)-_N_-(4-bromophenyl) morpholine-1-carbothioamide (10d).^{13}C NMR (100 MHz, $CDCl_3$):



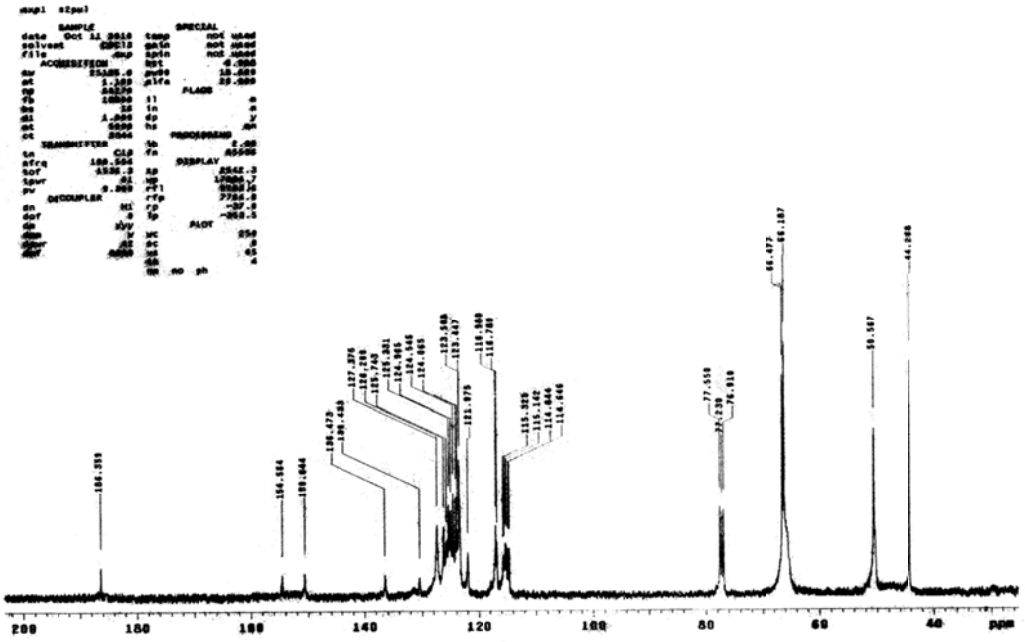
_N_-((_E_)-(4-Trifluoromethyl)(phenylimino)(piperidin-1-yl)methyl)-_N_-(4-bromophenyl) morpholine-1-carbothioamide (10d). MASS SPECTRA:



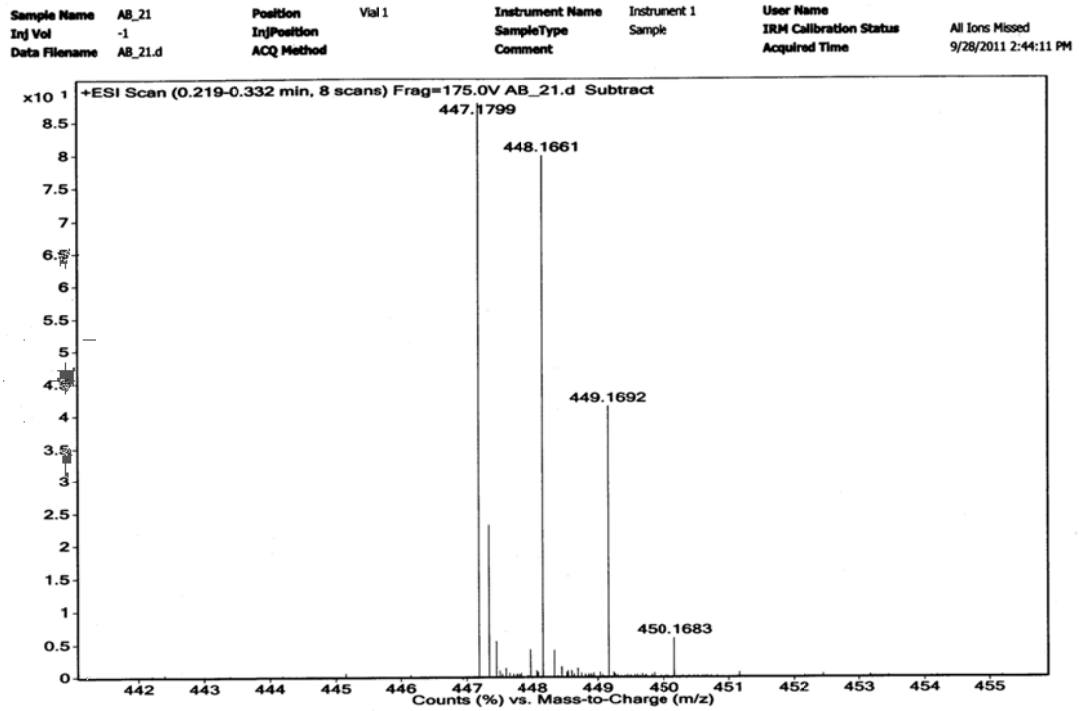
_N_-((_E_)-(2-Fluorophenylimino)(morpholino)methyl)-_N_-(2-fluorophenyl)morpholine-4-carbothioamide (11a). ^{1}H NMR (400 MHz, $CDCl_3$):



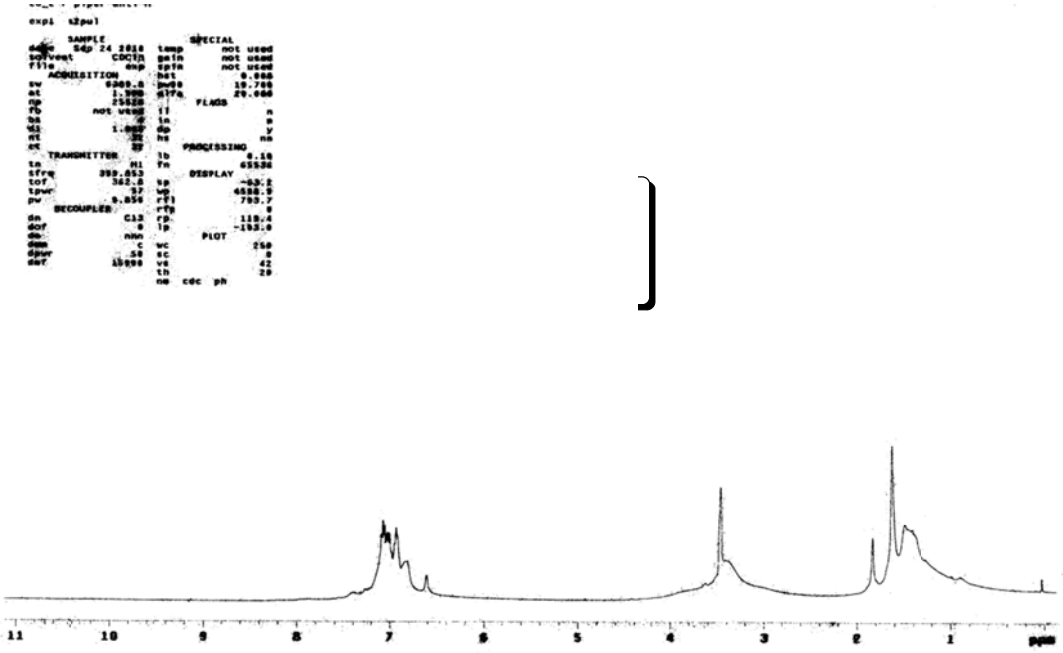
_N_-((_E_)-(2-Fluorophenylimino)(morpholino)methyl)-_N_-(2-fluorophenyl)morpholine-4-carbothioamide (11a). ^{13}C NMR (100 MHz, $CDCl_3$):



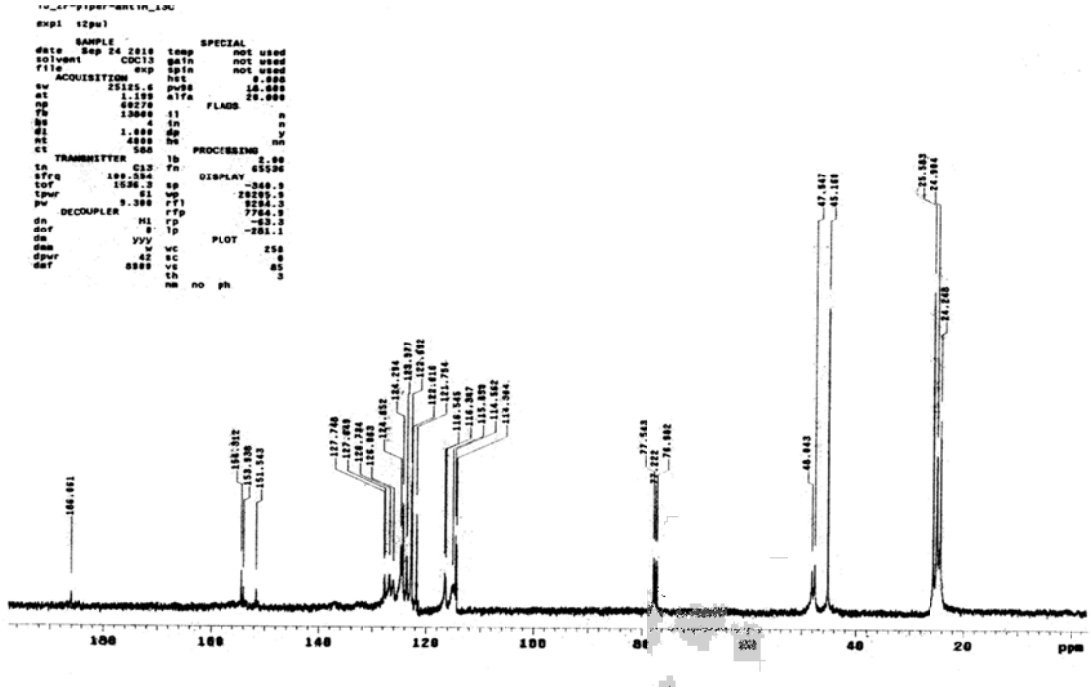
_N_-((_E_)-(2-Fluorophenylimino)(morpholino)methyl)-_N_-(2-fluorophenyl)morpholine-4-carbothioamide (11a). MASS SPECTRA:



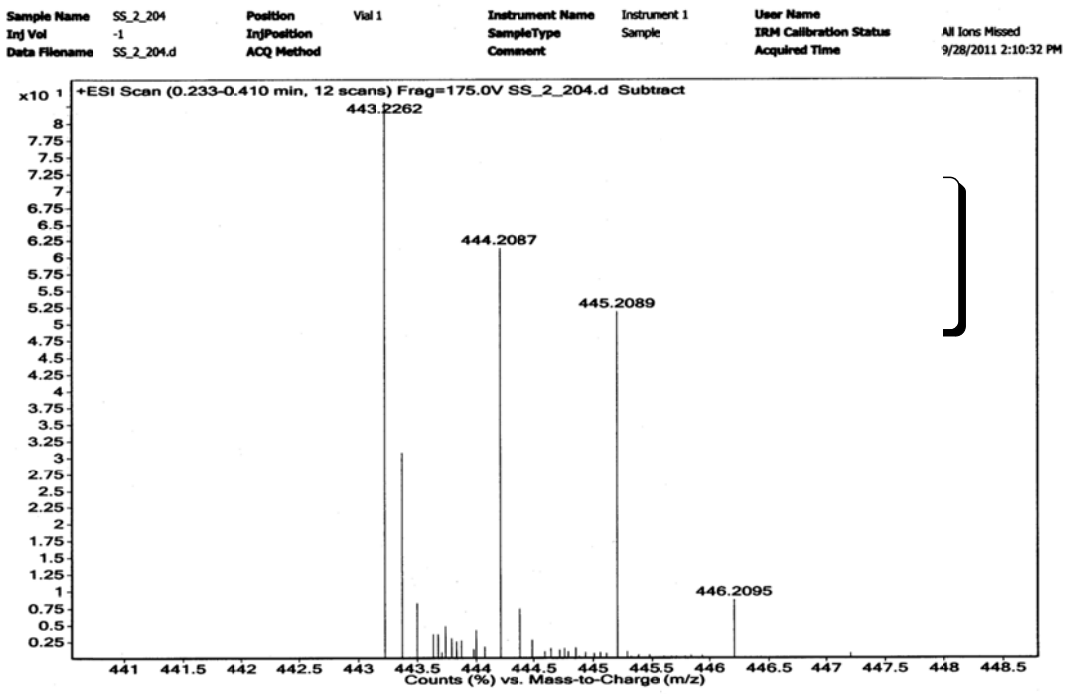
_N_-((_E_)-(2-Fluorophenylimino)(piperidin-1-yl)methyl)-_N_-(2-fluorophenyl)piperidine-1-carbothioamide (11d). ^{1}H NMR (400 MHz, $CDCl_3$):



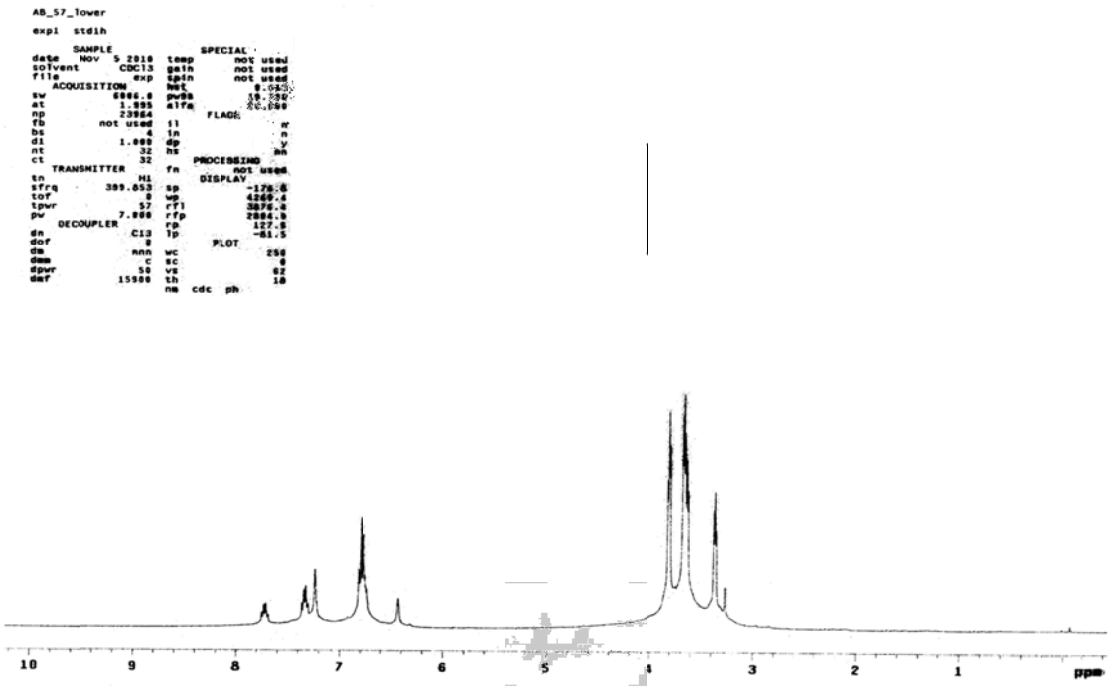
_N_-((_E_)-(2-Fluorophenylimino)(piperidin-1-yl)methyl)-_N_-(2-fluorophenyl)piperidine-1-carbothioamide (11d). ^{13}C NMR (100 MHz, $CDCl_3$):



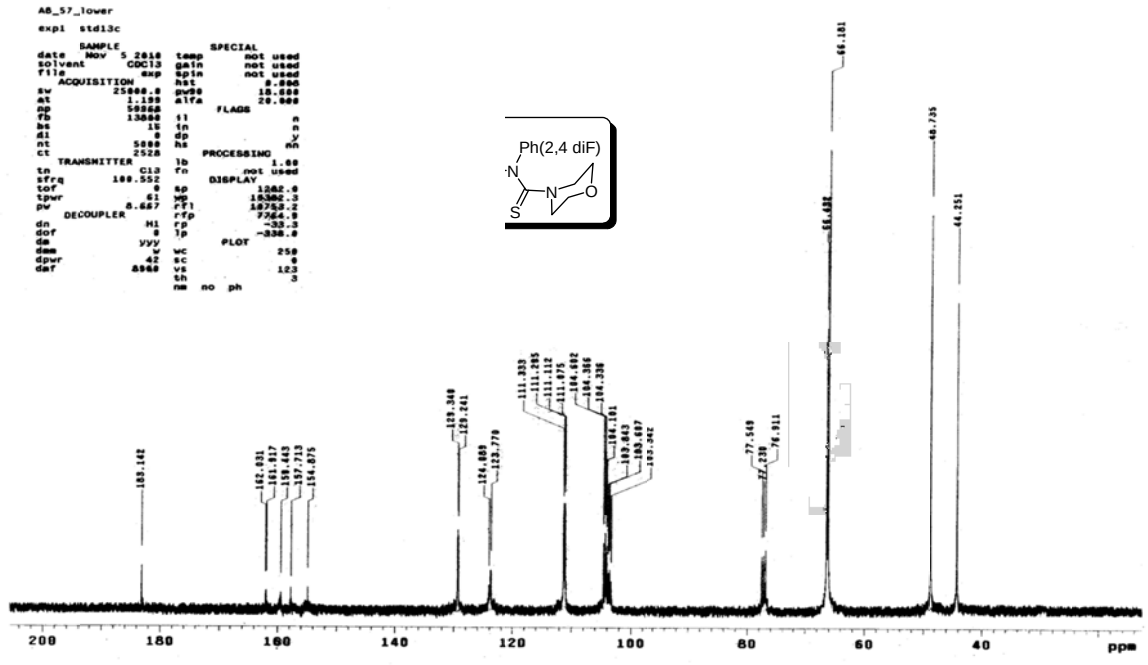
_N_-((_E_)-(2-Fluorophenylimino)(piperidin-1-yl)methyl)-_N_-(2-fluorophenyl)piperidine-1-carbothioamide (11d). ^{13}C NMR (100 MHz, $CDCl_3$):



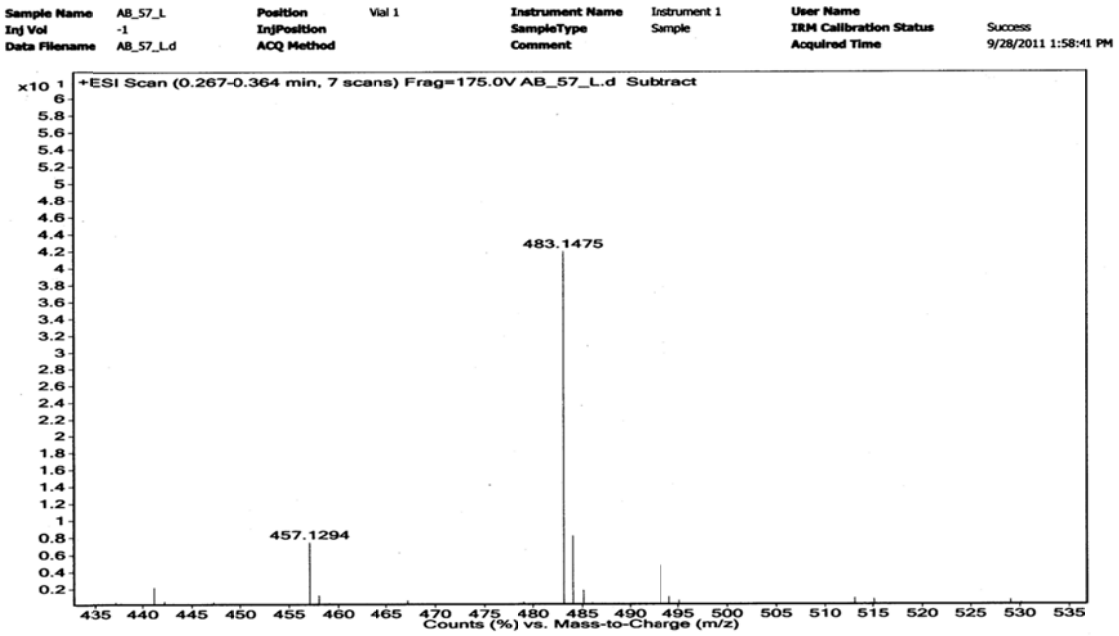
_N_-((_E_)-(2,4-Difluorophenylimino)(morpholino)methyl)-_N_-(2,4-difluorophenyl)morpholine-4-carbothioamide (12a).^{1}H NMR (400 MHz, $CDCl_3$):



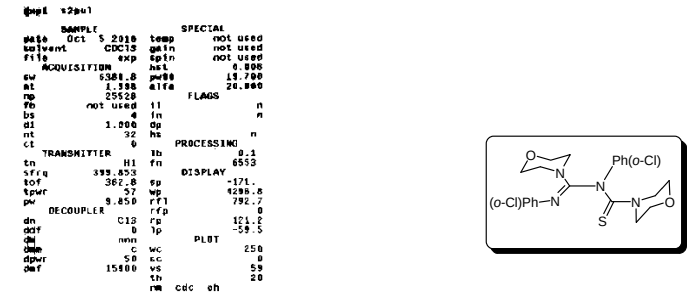
_N_-((_E_)-(2,4-Difluorophenylimino)(morpholino)methyl)-_N_-(2,4-difluorophenyl)morpholine-4-carbothioamide (12a).^{13}C NMR (100 MHz, $CDCl_3$):

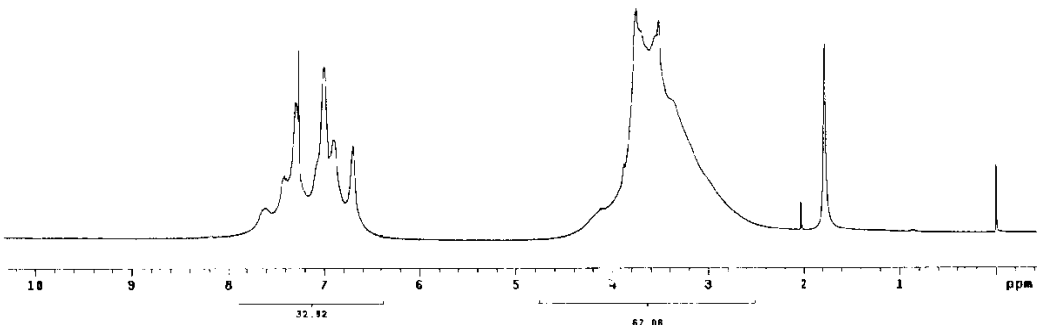


_N_-((_E_)-(2,4-Difluorophenylimino)(morpholino)methyl)-_N_-(2,4-difluorophenyl)morpholine-4-carbothioamide (12a). MASS SPECTRA:

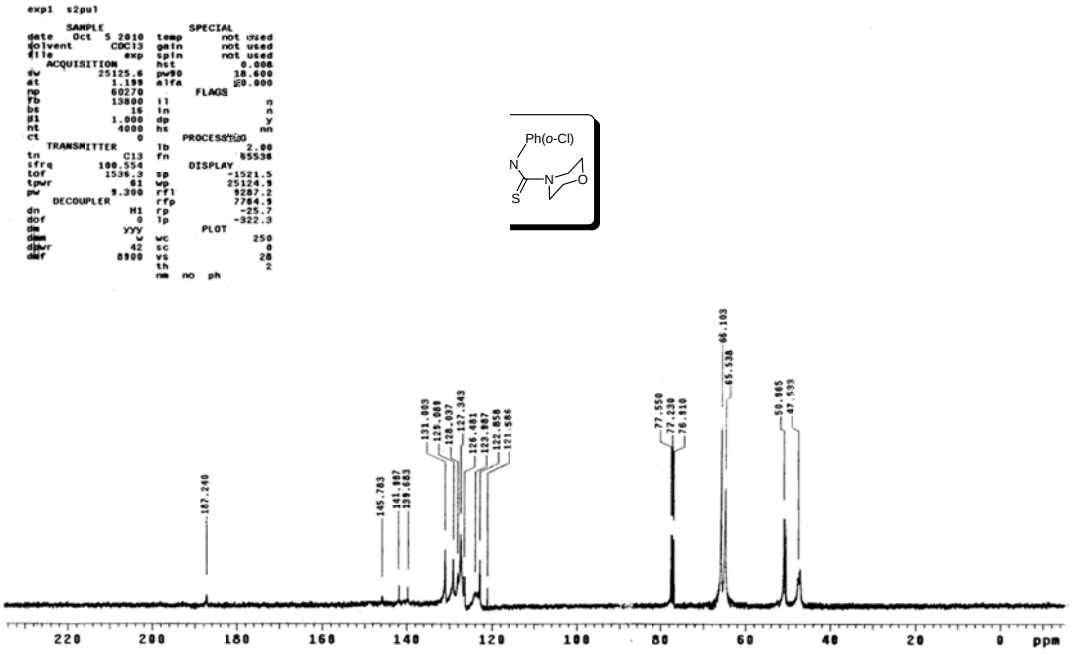


_N_-((_E_)-(2-Chlorophenylimino)(morpholino)methyl)-_N_-(2-chlorophenyl)morpholine-4-carbothioamide (13a). ^{1}H NMR (400 MHz, $CDCl_3$):

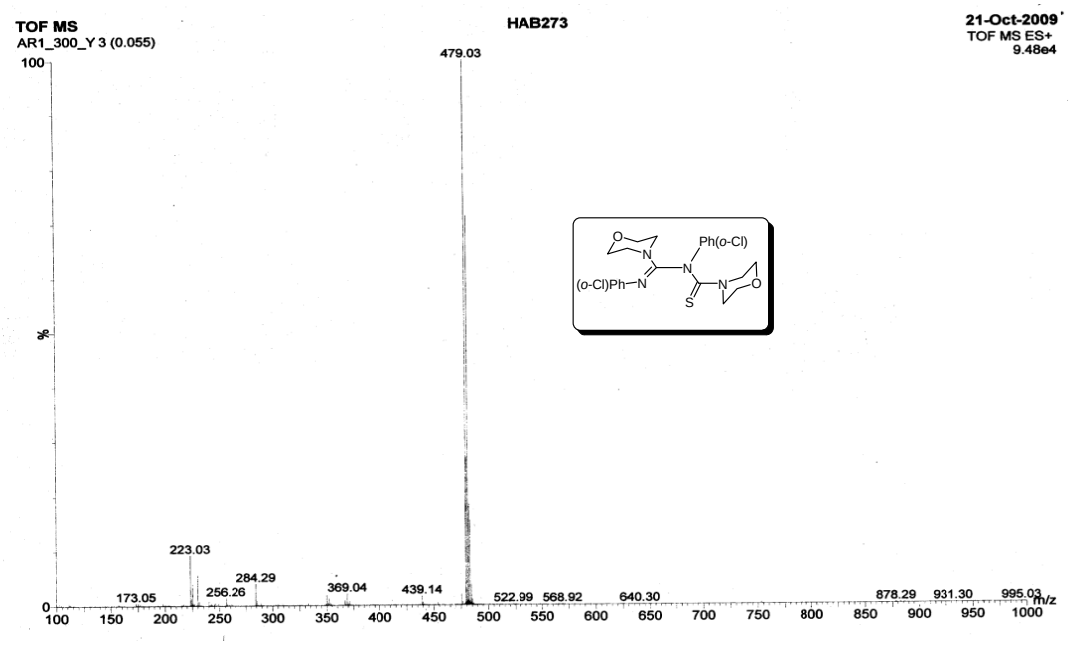




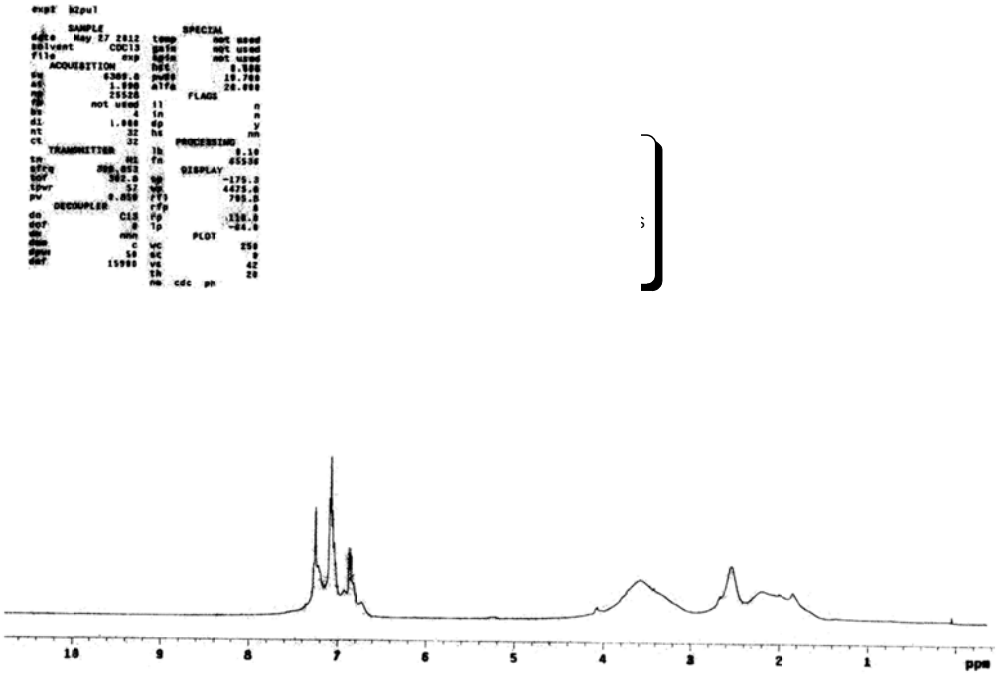
_N_-((_E_)-(2-Chlorophenylimino)(morpholino)methyl)-_N_-(2-chlorophenyl)morpholine-4-carbothioamide (13a). ^{13}C NMR (100 MHz, $CDCl_3$):



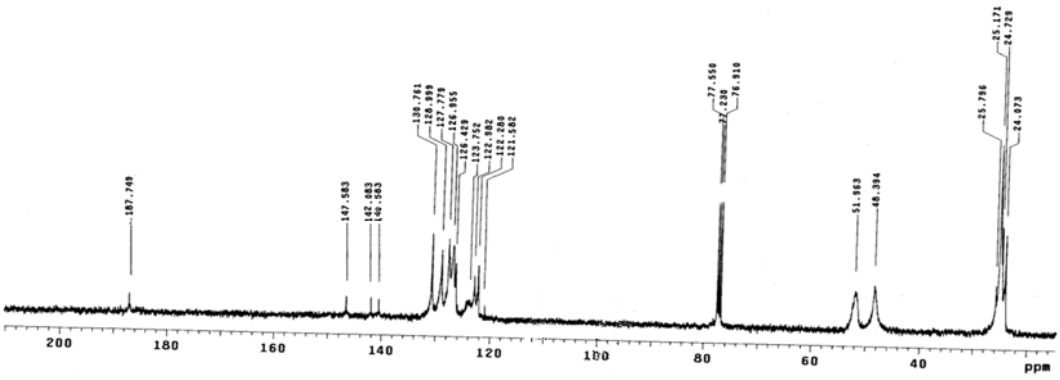
_N_-((_E_)-(2-Chlorophenylimino)(morpholino)methyl)-_N_-(2-chlorophenyl)morpholine-4-carbothioamide (13a): Mass Spectra



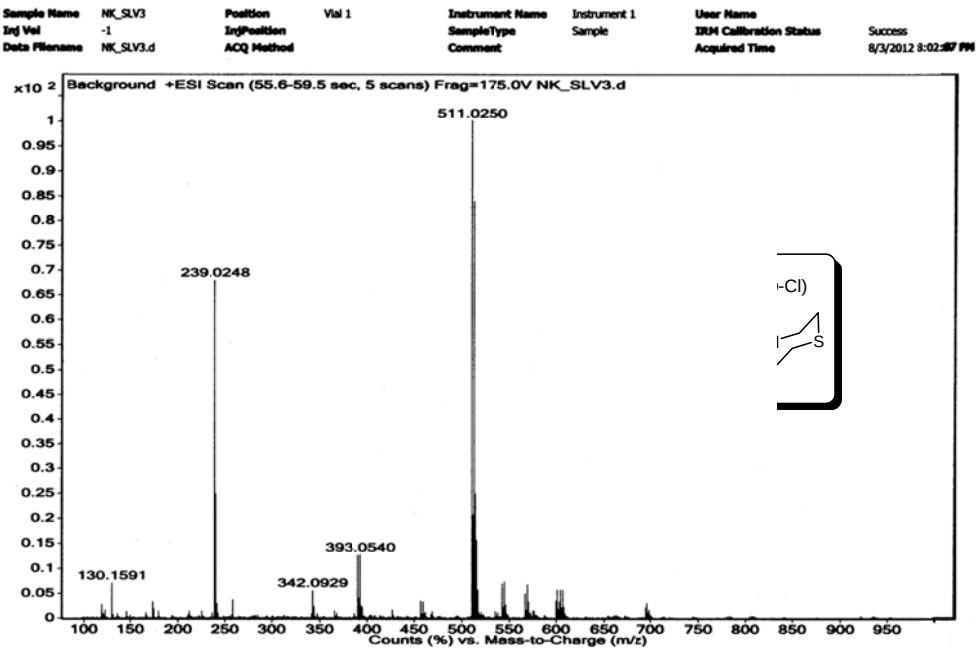
_N_-((_E_)-(2-Chlorophenylimino)(thiomorpholino)methyl)-_N_-(2-chlorophenyl) thiomorholine-1-carbothioamide (13b). ^{1}H NMR (400 MHz, $CDCl_3$):



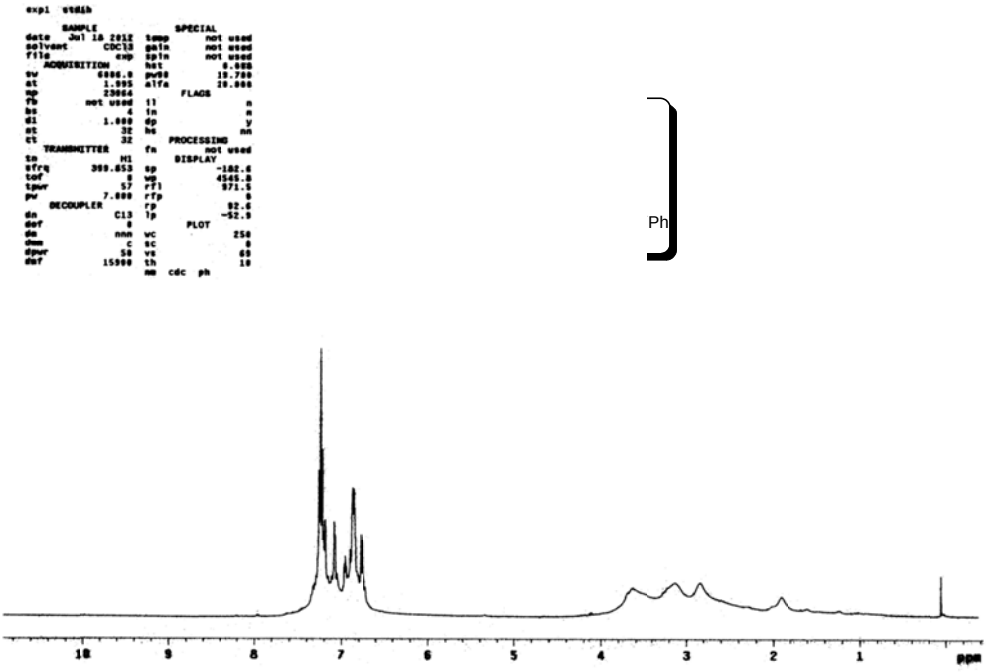
_N_-((_E_)-(2-Chlorophenylimino)(thiomorpholino)methyl)-_N_-(2-chlorophenyl) thiomorholine-1-carbothioamide (13b). ^{13}C NMR (100 MHz, $CDCl_3$):



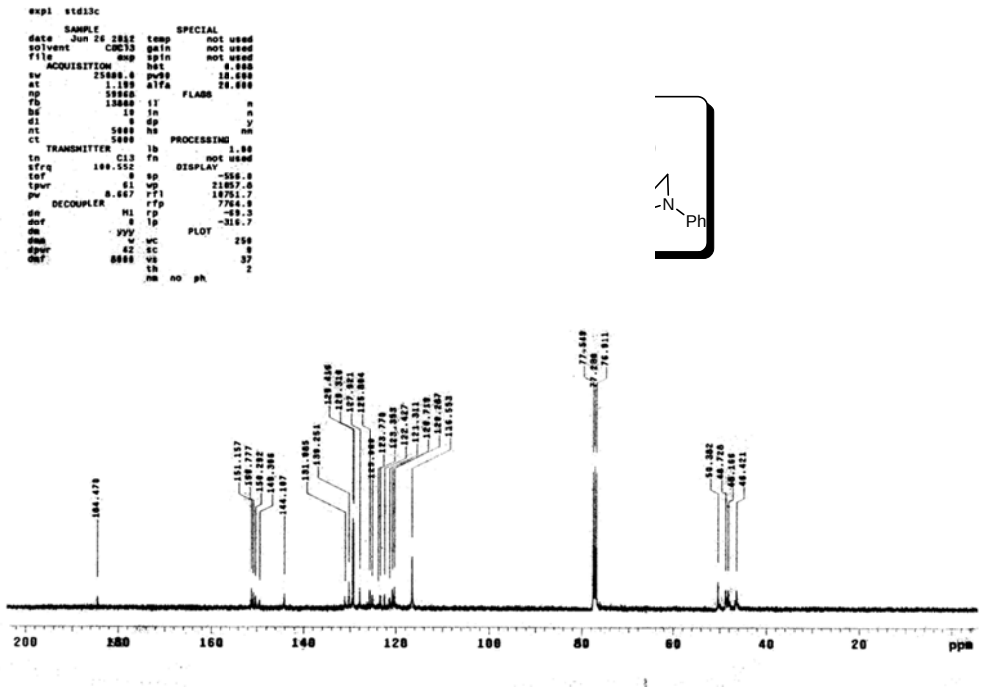
_N_-((_E_)-(2-Chlorophenylimino)(thiomorpholino)methyl)-_N_-(2-chlorophenyl) thiomorholine-1-carbothioamide (13b). MASS SPECTRA:



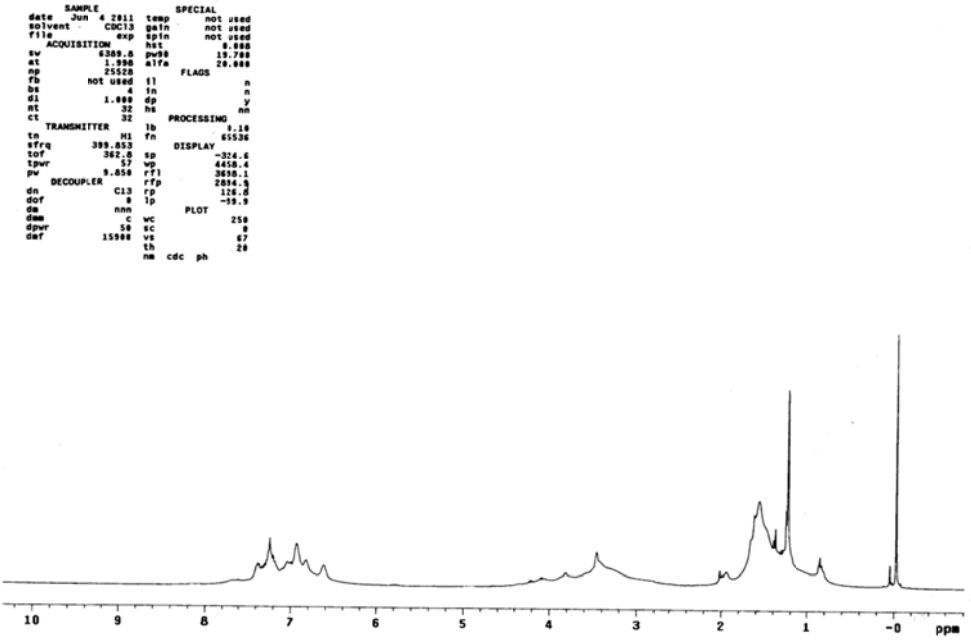
_N_-((_E_)-(2-Chlorophenylimino)(4-piperazin-1-yl)methyl)-_N_-(2-chlorophenyl) piperazine-1-carbothioamide (13c). ^{1}H NMR (400 MHz, $CDCl_3$):



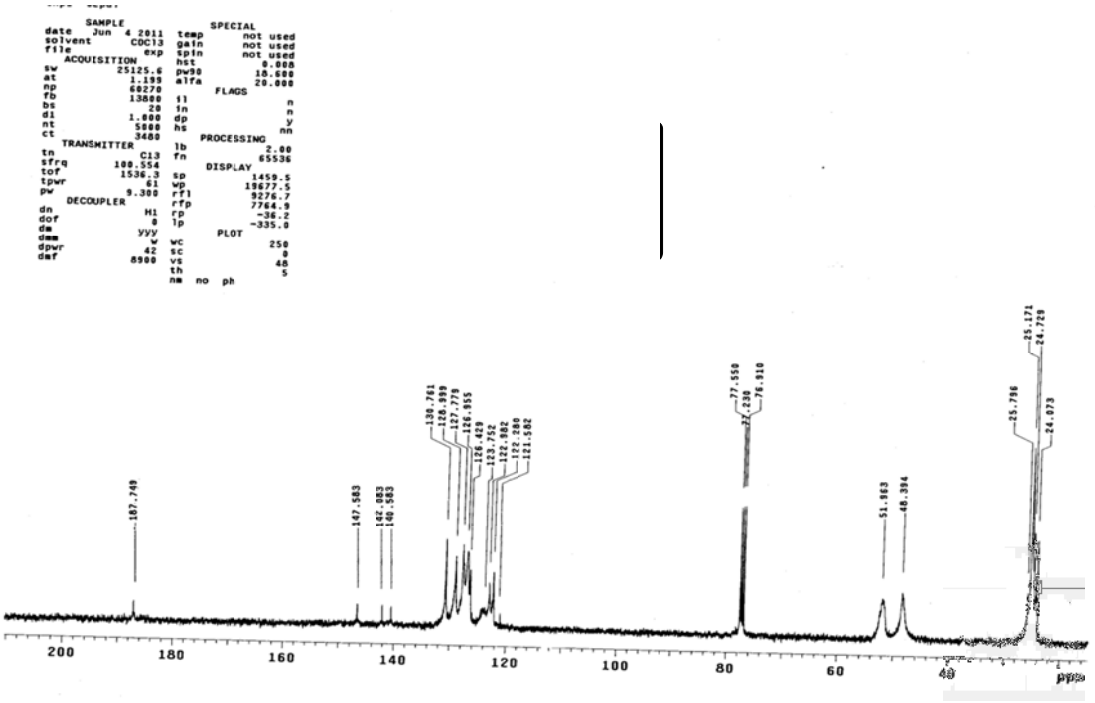
_N_-((_E_)-(2-Chlorophenylimino)(4-piperazin-1-yl)methyl)-_N_-(2-chlorophenyl) piperazine-1-carbothioamide (13c). ^{13}C NMR (100 MHz, $CDCl_3$):



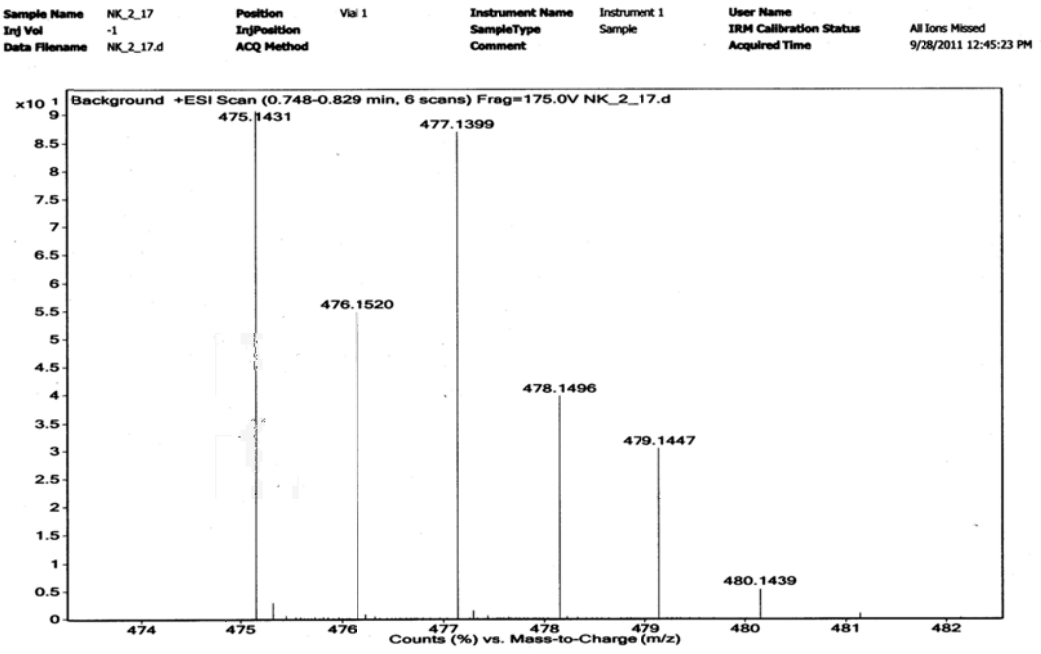
_N_-((_E_)-(2-Chlorophenylimino)(piperidin-1-yl)methyl)-_N_-(2-chlorophenyl)piperidine-1-carbothioamide (13d). ^{1}H NMR (400 MHz, $CDCl_3$):



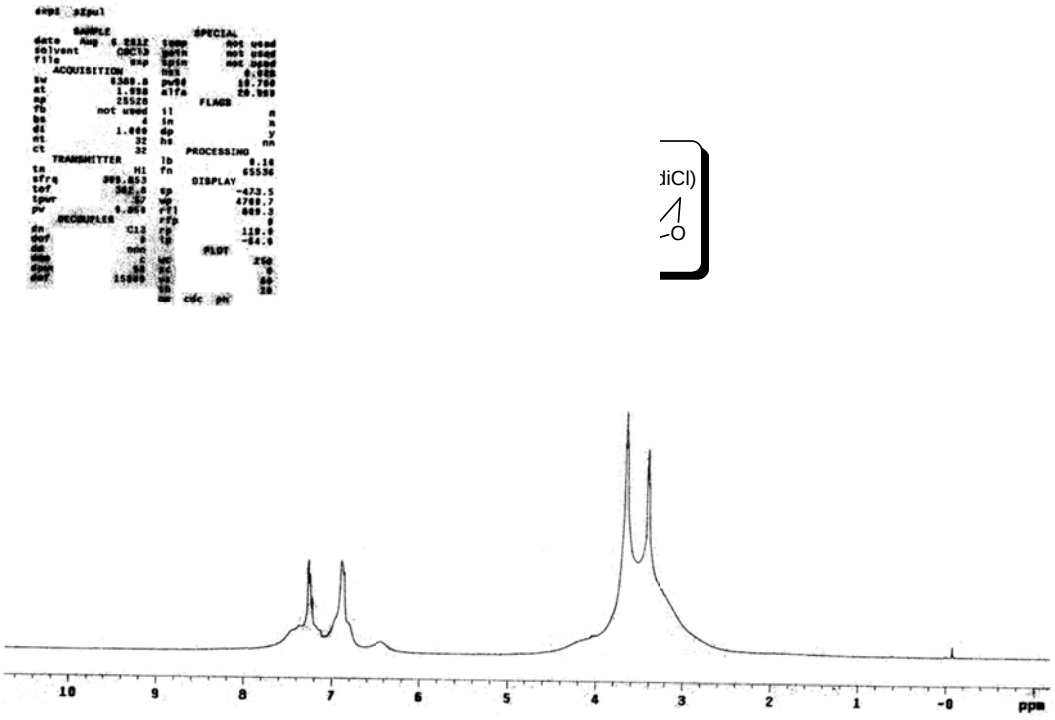
_N_-((_E_)-(2-Chlorophenylimino)(piperidin-1-yl)methyl)-_N_-(2-chlorophenyl)piperidine-1-carbothioamide (13d). ^{13}C NMR (100 MHz, $CDCl_3$):



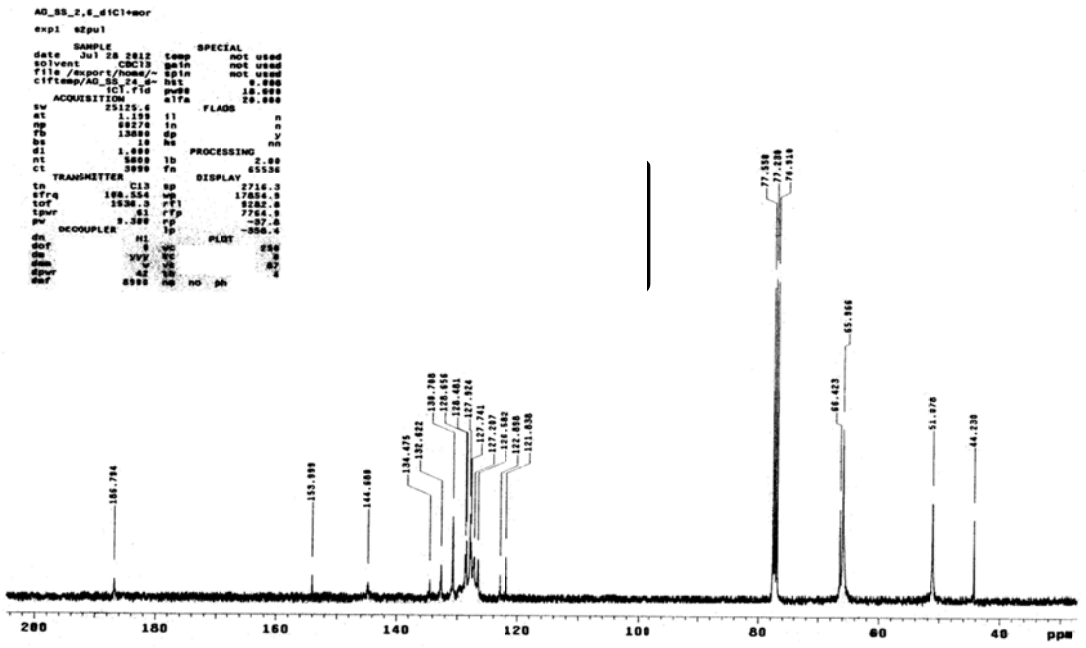
_N_-((_E_)-(2-Chlorophenylimino)(piperidin-1-yl)methyl)-_N_-(2-chlorophenyl)piperidine-1-carbothioamide (13d). MASS SPECTRA:



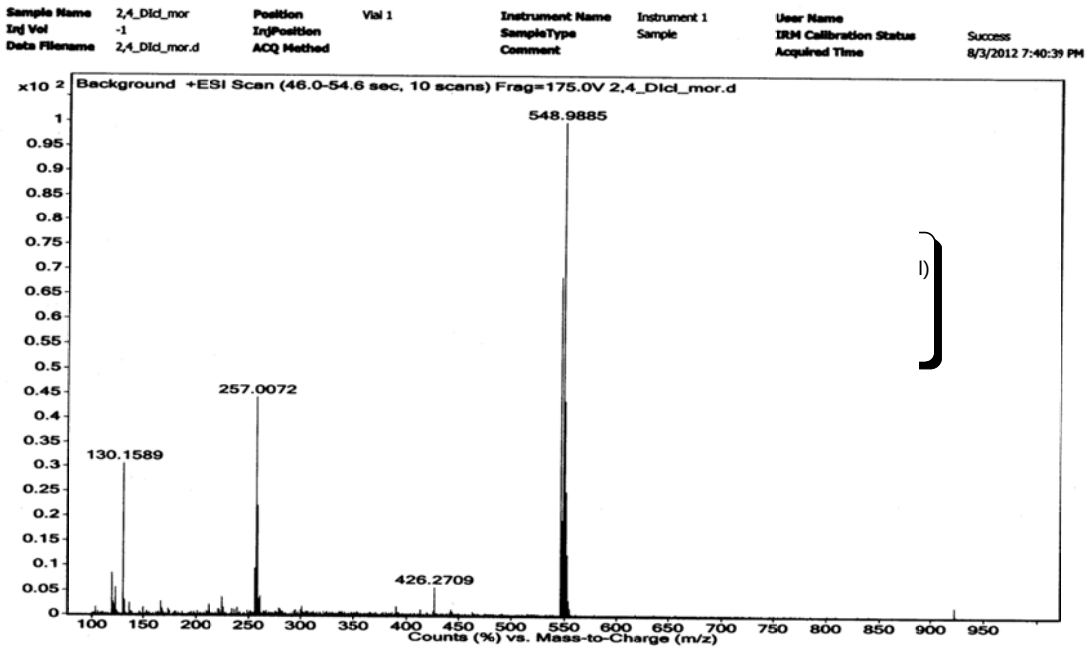
_N_-((_E_)-(2,4-Dichlorophenylimino)(morpholino)methyl)-_N_-(2,4-dichlorophenyl)morpholine-4-carbothioamide (14a).^{1}H NMR (400 MHz, $CDCl_3$):



_N_-((_E_)-(2,4-Dichloorophenylimino)(morpholino)methyl)-_N_-(2,4-dichlorophenyl) morpholine-4-carbothioamide (14a).^{13}C NMR (100 MHz, $CDCl_3$):

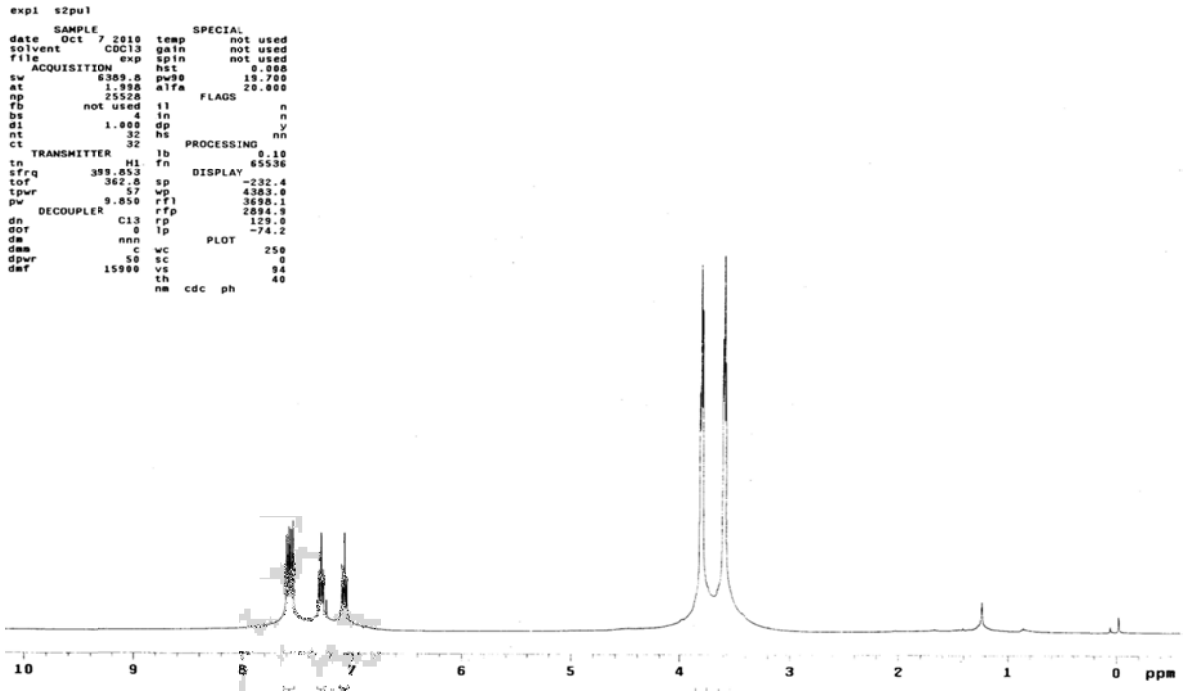


_N_-((_E_)-(2,4-Dichlorophenylimino)(morpholino)methyl)-_N_-(2,4-dichlorophenyl)morpholine-4-carbothioamide (14a). MASS SPECTRA:

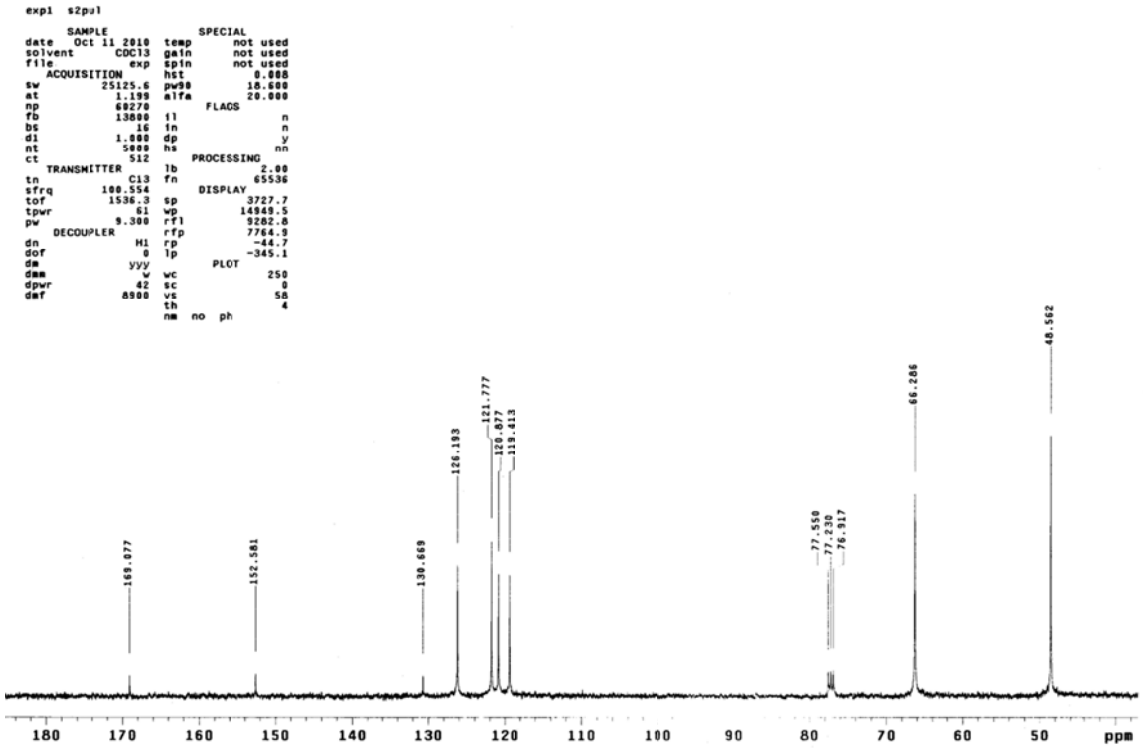


Benzothiazole

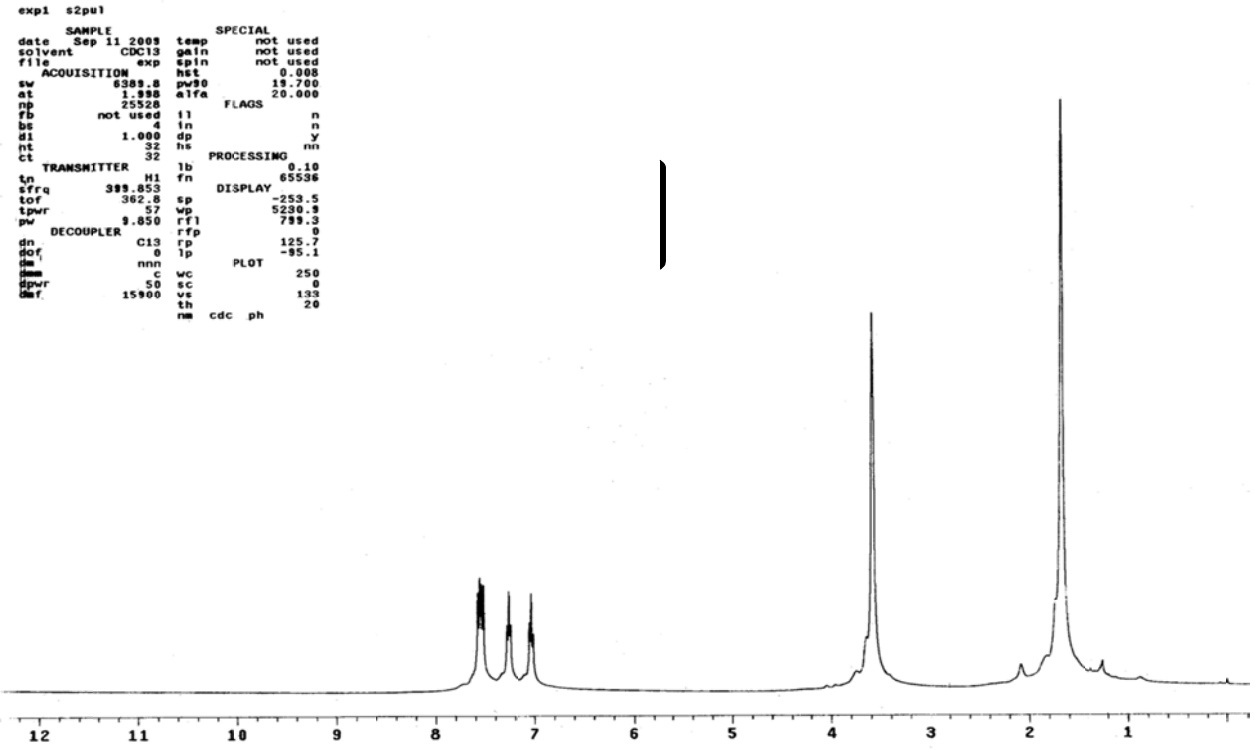
2-morholinobenzo[*d*]thiazole (11'a): **^{1}H NMR (400 MHz, $CDCl_3$):**



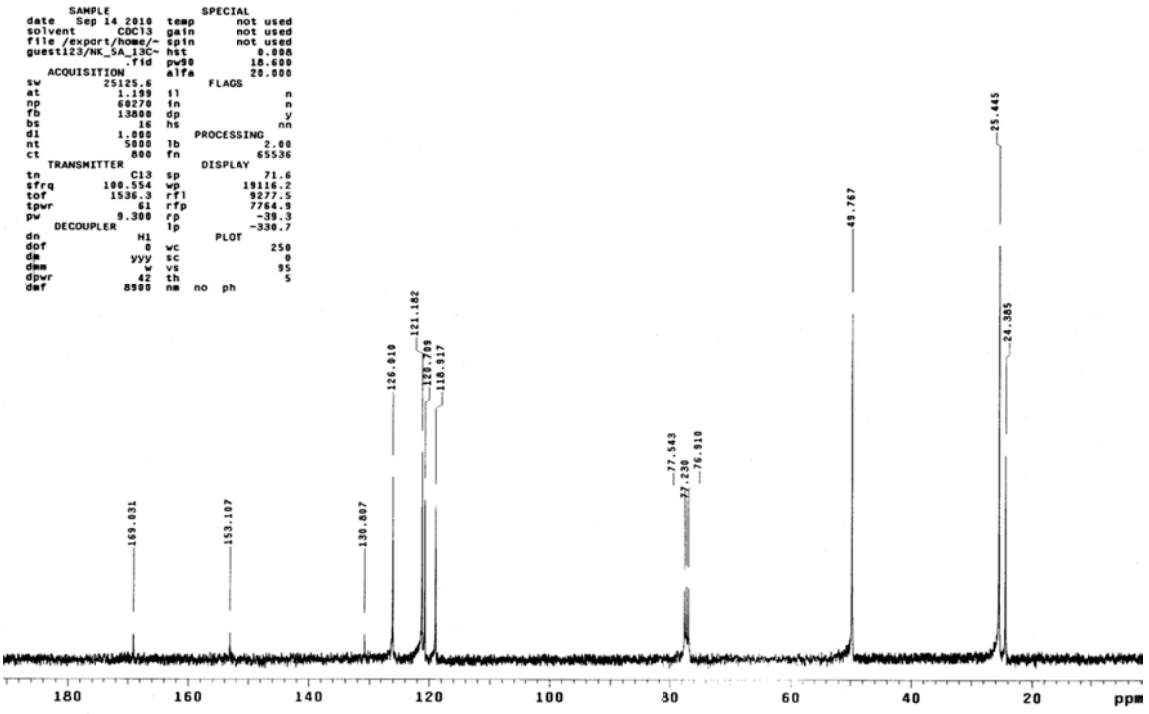
2-morholinobenzo[*d*]thiazole (11'a): **^{13}C NMR (100 MHz, $CDCl_3$):**



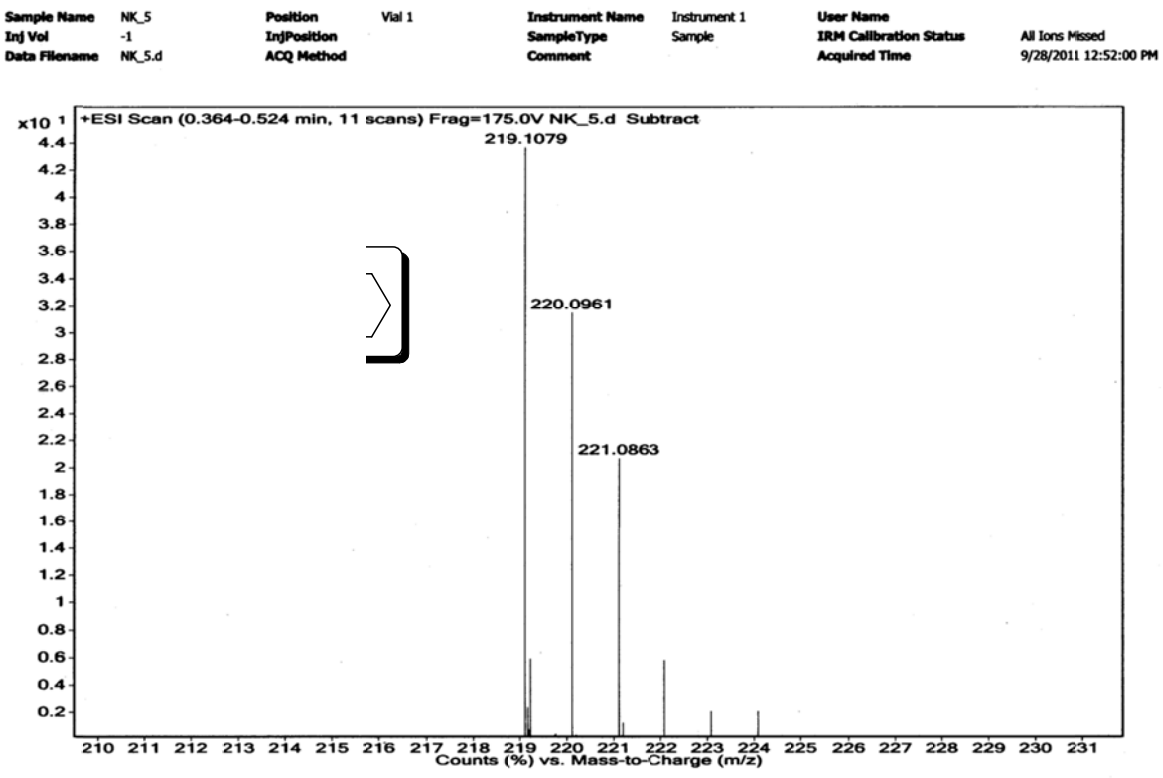
2-(Piperidin-1-yl)benzo[*d*]thiazole (11'd): **^{1}H NMR (400 MHz, $CDCl_3$):**



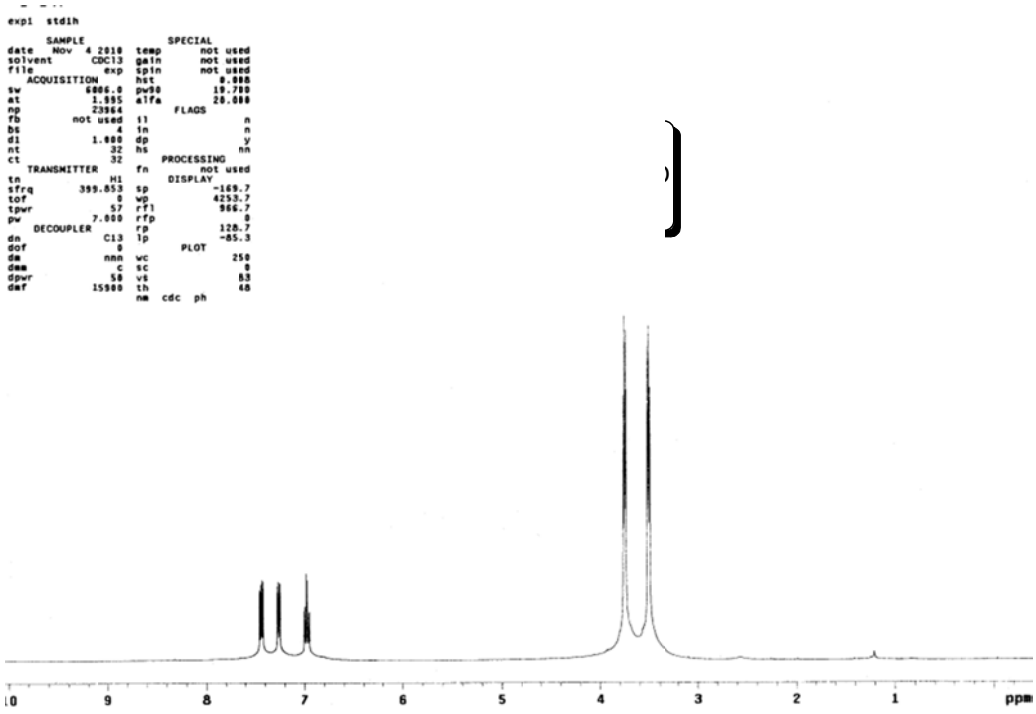
2-(Piperidin-1-yl)benzo[*d*]thiazole (11'd): **^{13}CNMR (100 MHz, $CDCl_3$):**



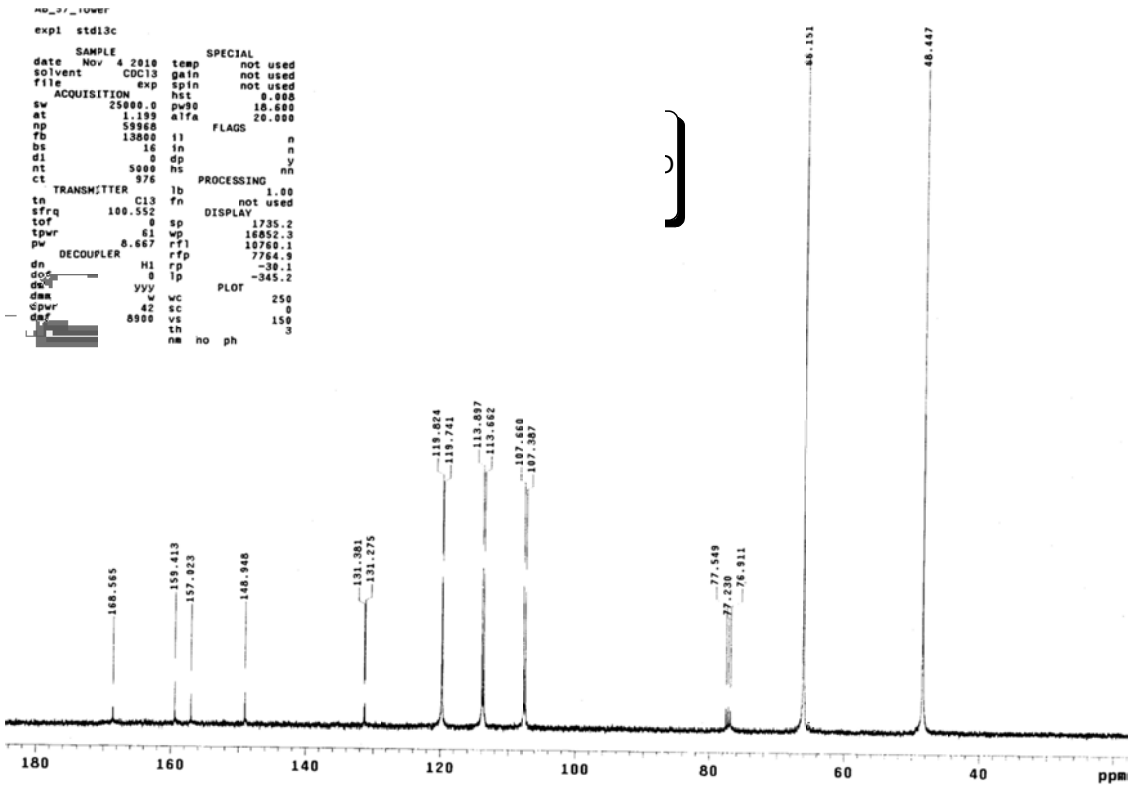
2-(Piperidin-1-yl)benzo[*d*]thiazole (11'd): **IR (KBr or Neat):**



6-Fluoro-2-morpholinobenzo[*d*]thiazole (12'a):^{1}H NMR (400 MHz, $CDCl_3$):

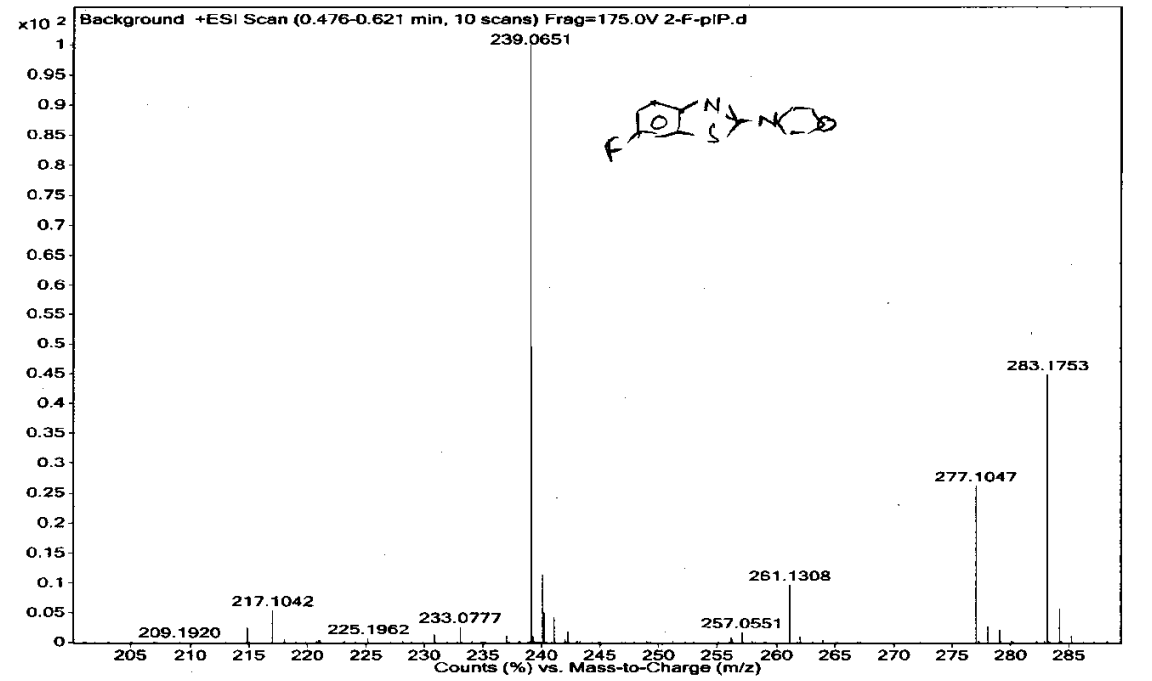


6-Fluoro-2-morpholinobenzo[*d*]thiazole (12'a):^{13}C NMR (100 MHz, $CDCl_3$):

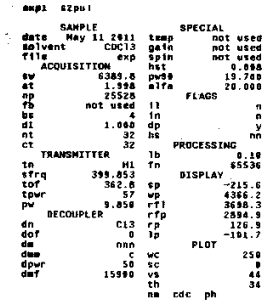


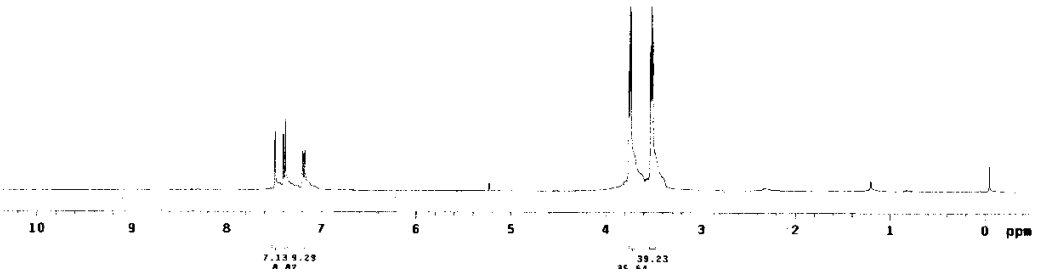
6-Fluoro-2-morpholinobenzo[*d*]thiazole (12'a): MASS SPECTRA:

Sample Name	2-F-pIP	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	2-F-pIP.d	**ACQ Method**		**Comment**		**Acquired Time**	5/4/2011 11:20:13 AM

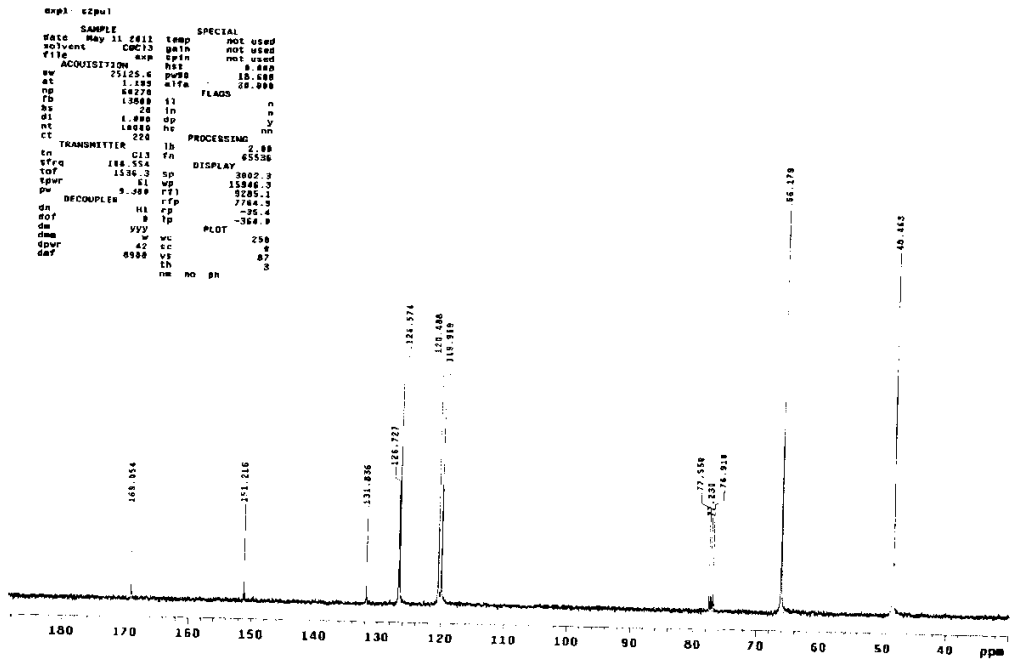


6-Chloro-2-morpholinobenzo[*d*]thiazole (14'a): ^{1}HNMR (400 MHz, $CDCl_3$):



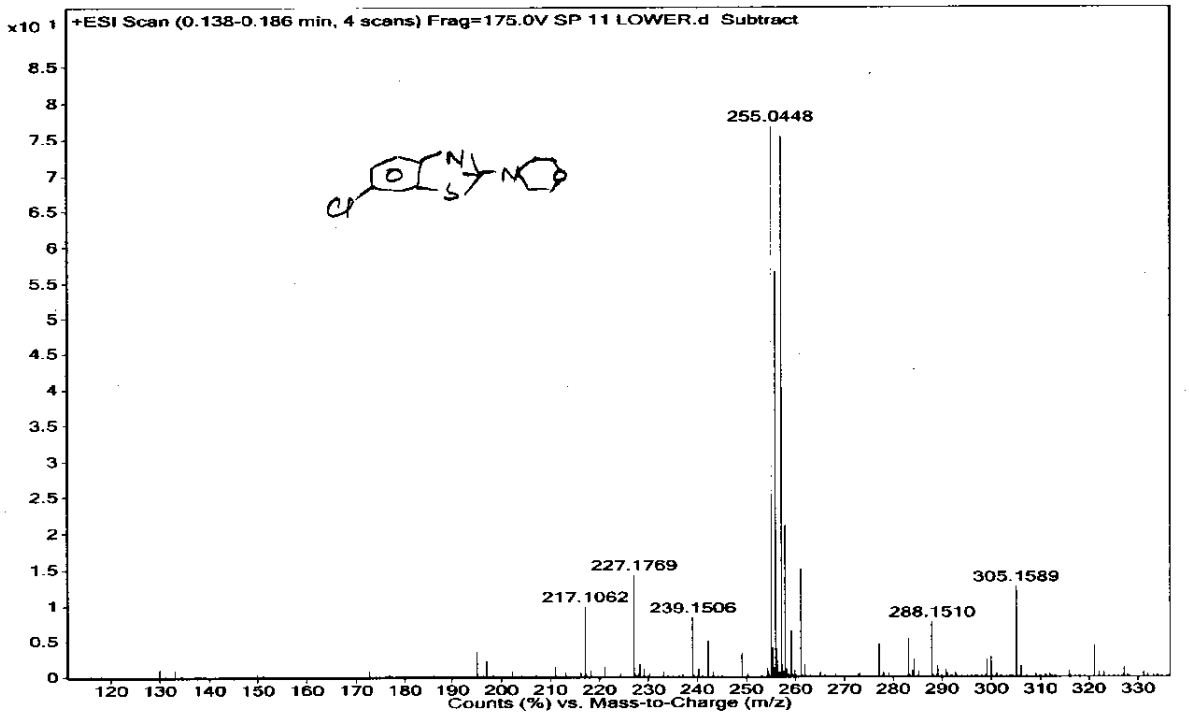


6-Chloro-2-morpholinobenzo[*d*]thiazole (14'a): ^{13}CNMR (100 MHz, $CDCl_3$):

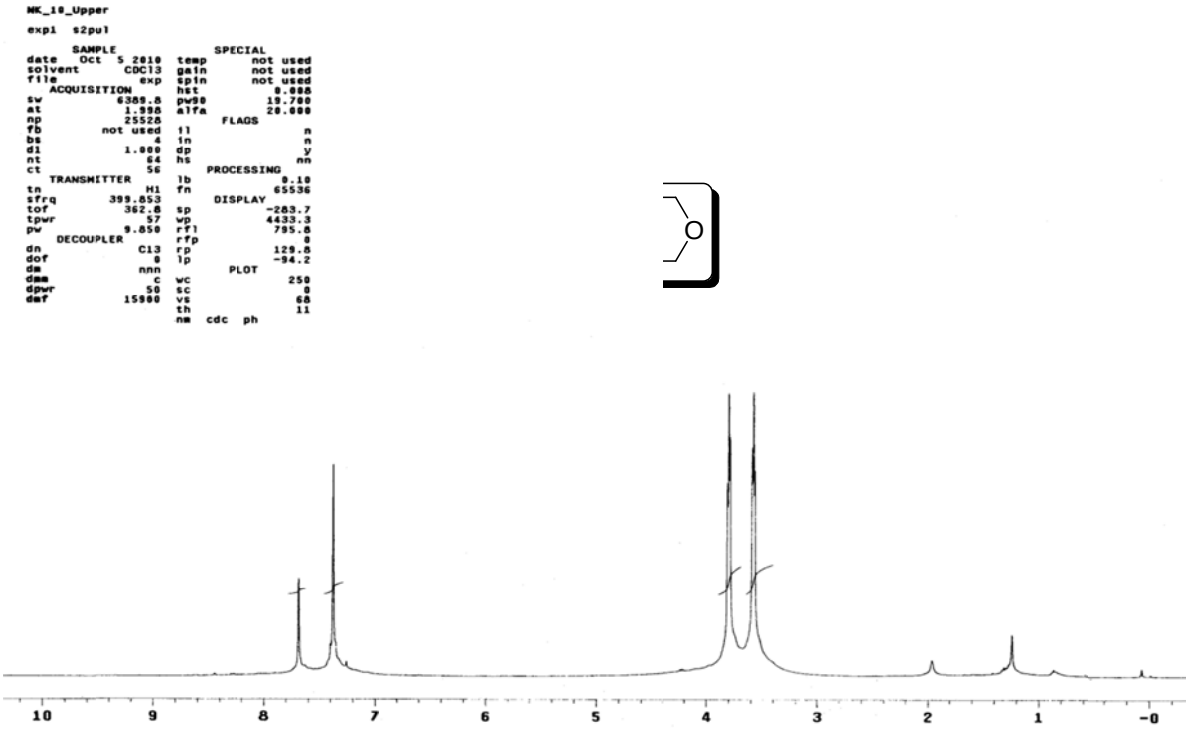


6-Chloro-2-morpholinobenzo[*d*]thiazole (14'a): MASS SPECTRA:

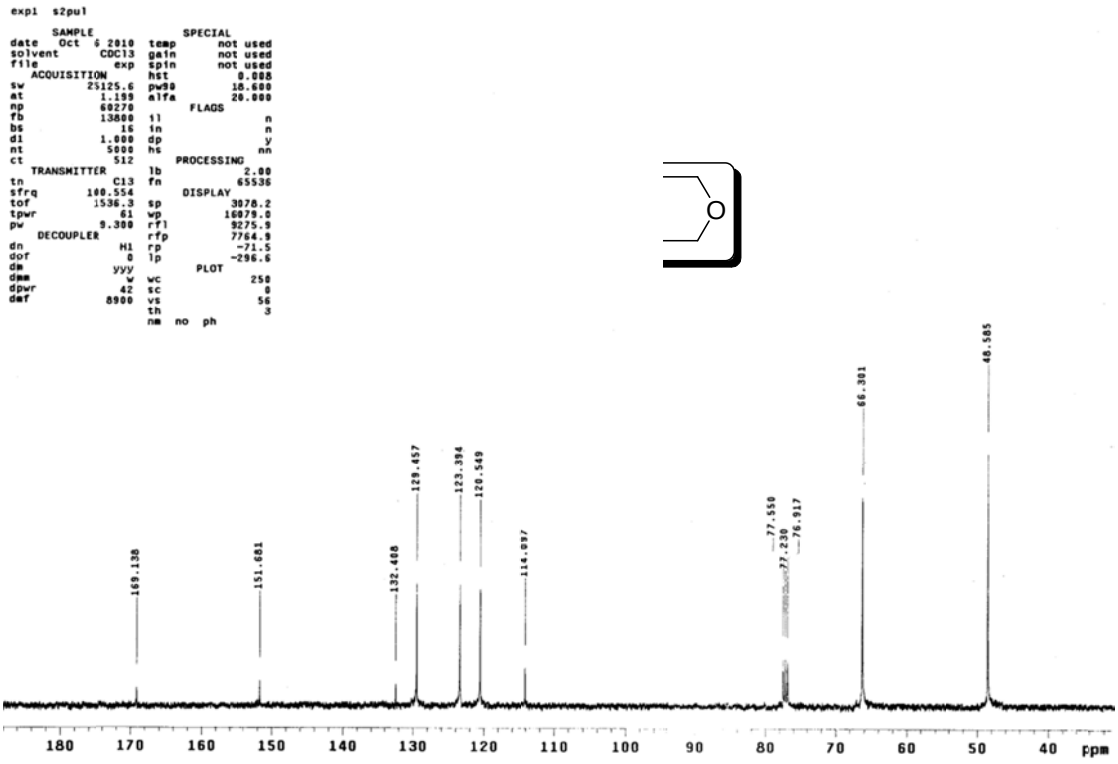
Sample Name	SP11 LOWER	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	SP 11 LOWER.d	**ACQ Method**		**Comment**		**Acquired Time**	5/12/2011 10:42:31 AM



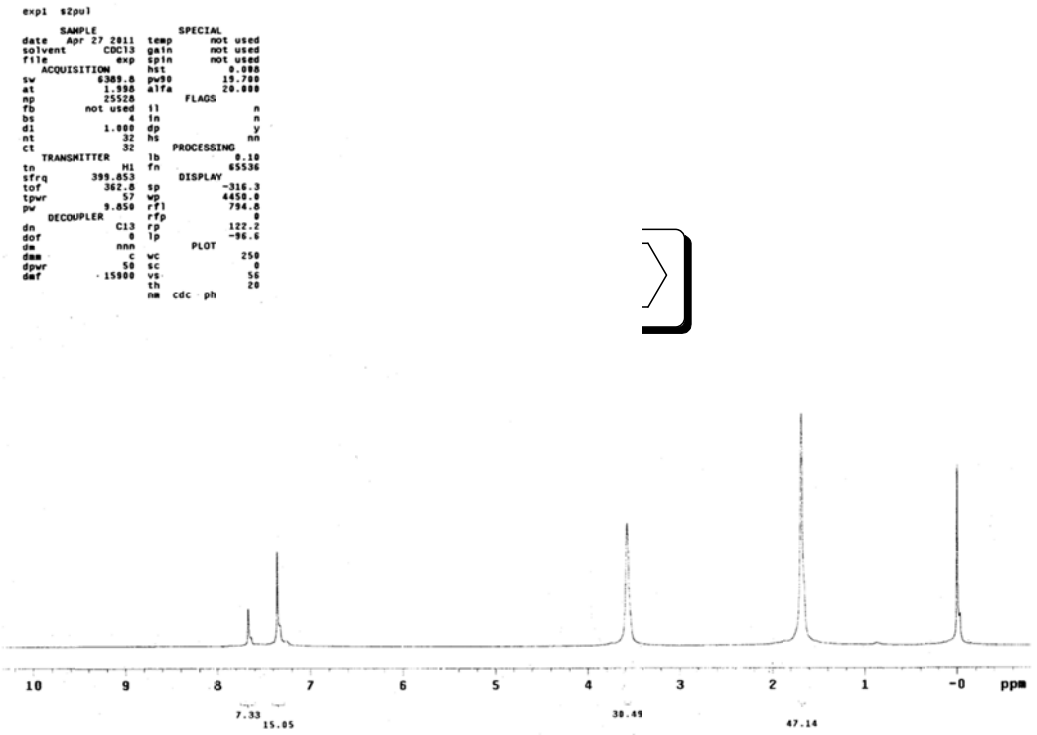
6-Bromo-2-morpholino[*d*]thiazole (15'a): **^{1}H NMR (400 MHz, $CDCl_3$):**



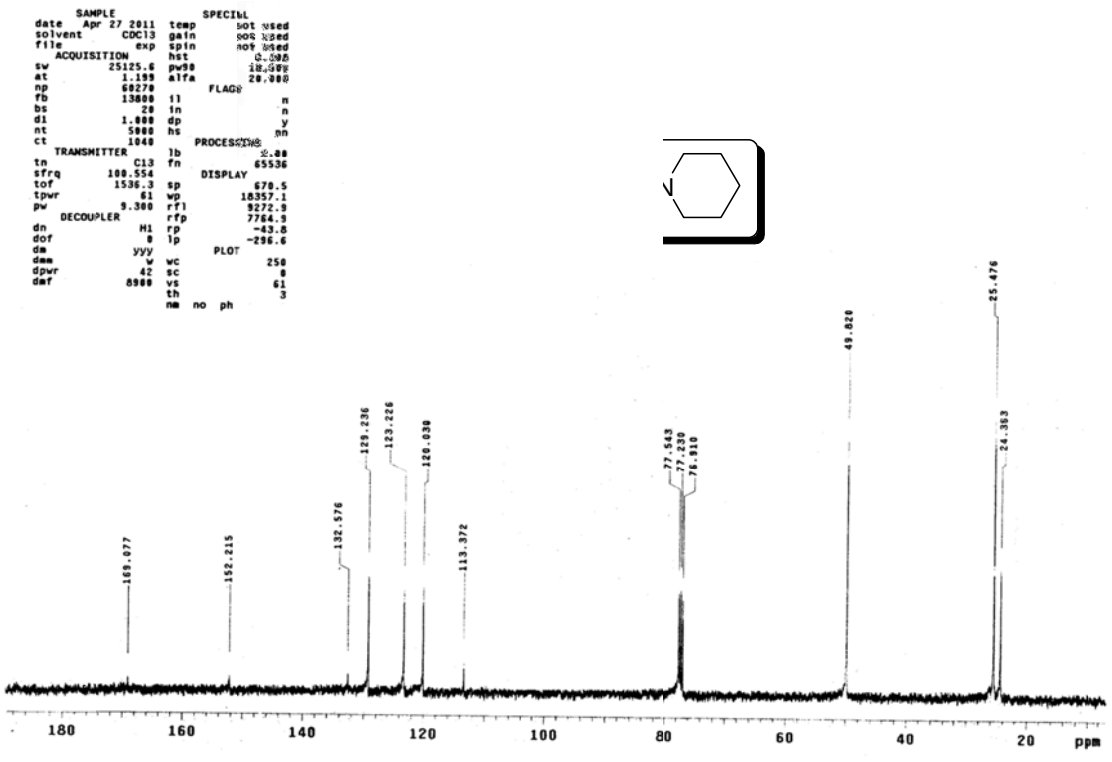
6-Bromo-2-morpholino[*d*]thiazole (15'a): **^{13}C NMR (100 MHz, $CDCl_3$):**



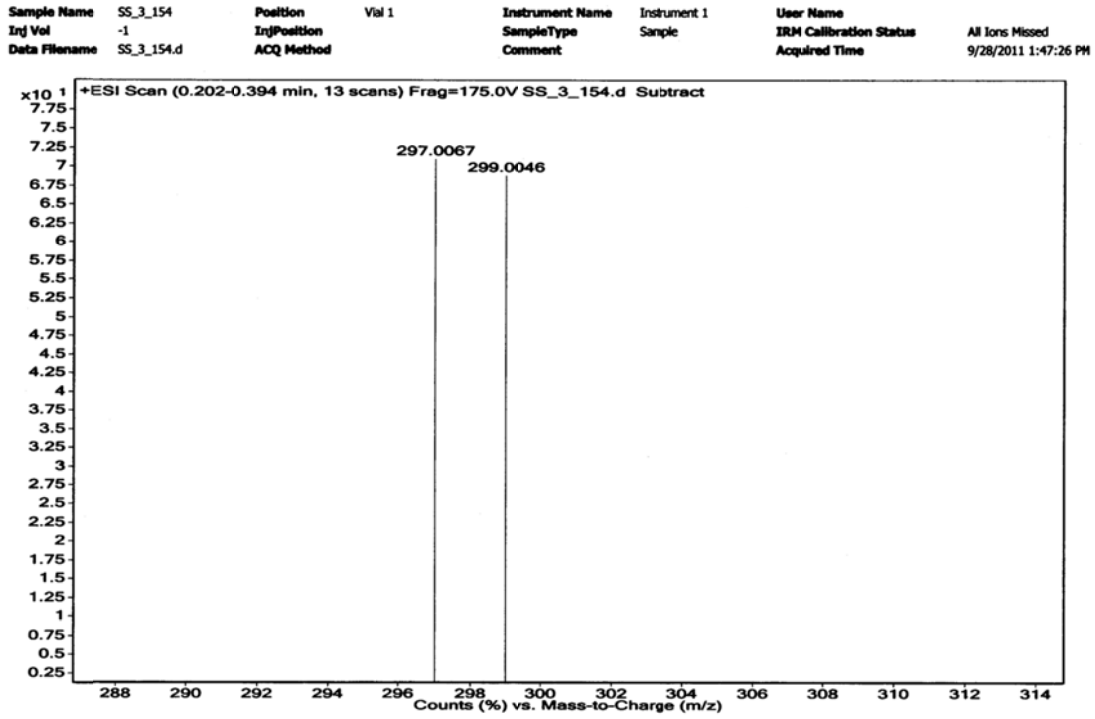
6-Bromo-2-(piperidin-1-yl)[*d*]thiazole (2 0'd): **^{1}H NMR (400 MHz, $CDCl_3$):**



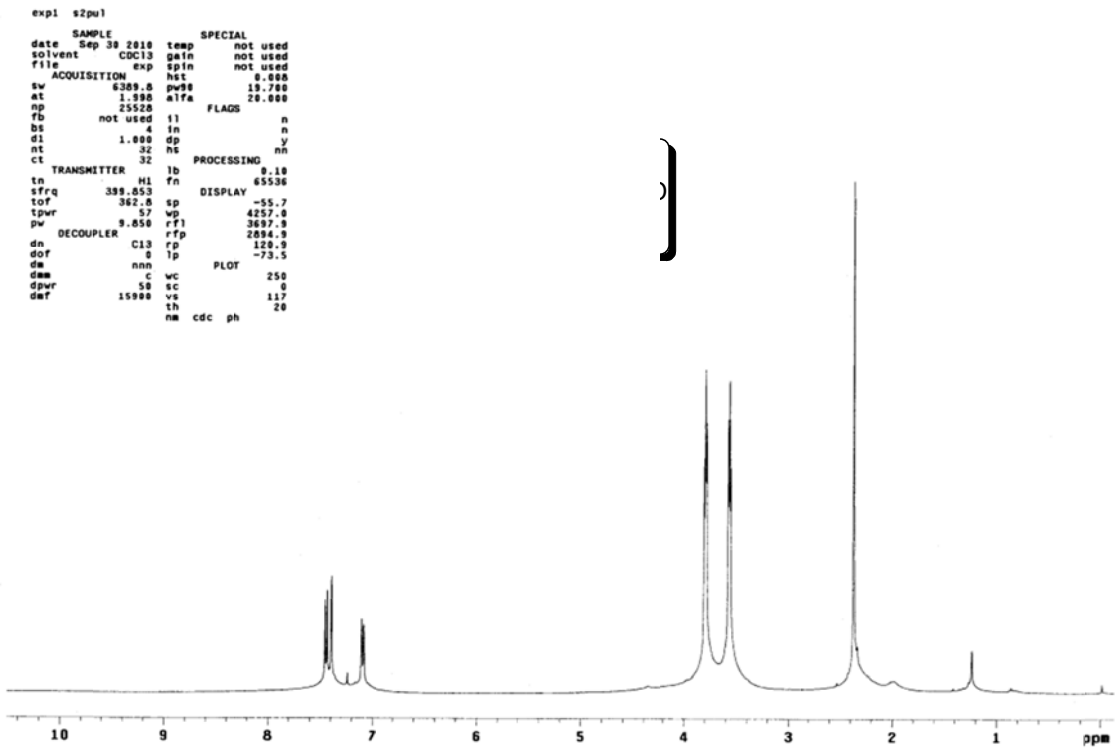
6-Bromo-2-(piperidin-1-yl)[*d*]thiazole (20'd): **^{13}C NMR (100 MHz, $CDCl_3$):**



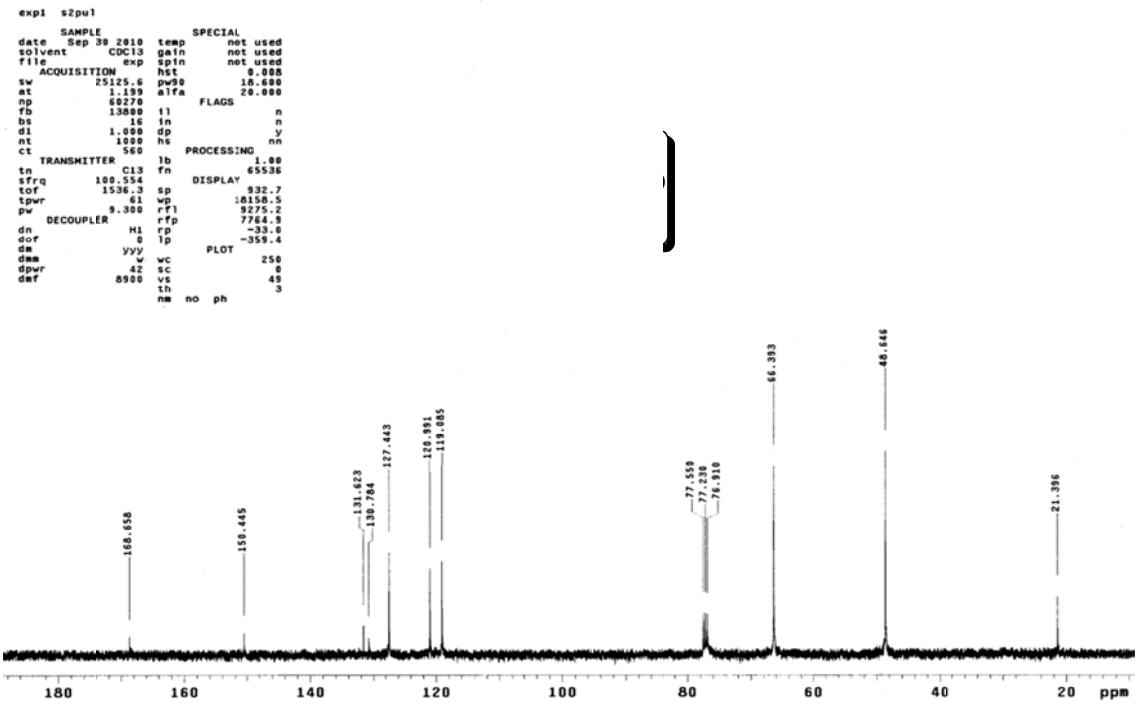
6-Bromo-2-(piperidin-1-yl)[*d*]thiazole (20'd): MASS SPECTRA:



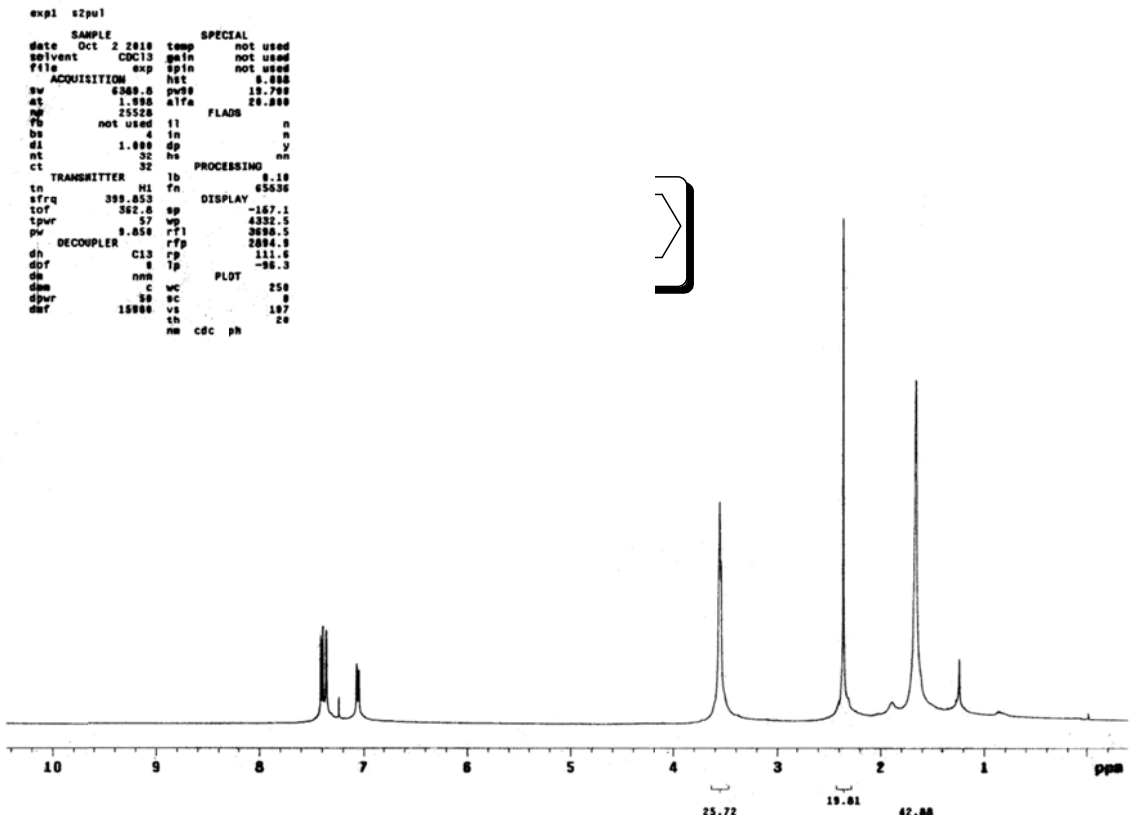
6-methyl-2-morholinobenzo[*d*]thiazole (18'a): ^{1}H NMR (400 MHz, $CDCl_3$):



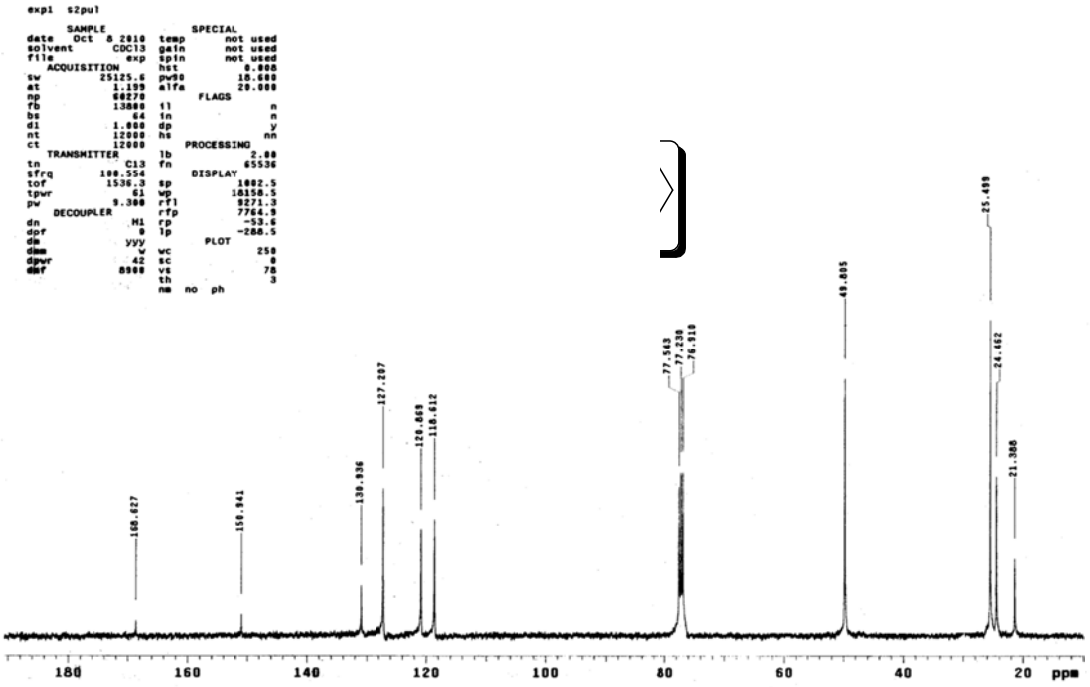
6-methyl-2-morholinobenzo[*d*]thiazole (18'a): **^{13}C NMR (100 MHz, $CDCl_3$):**



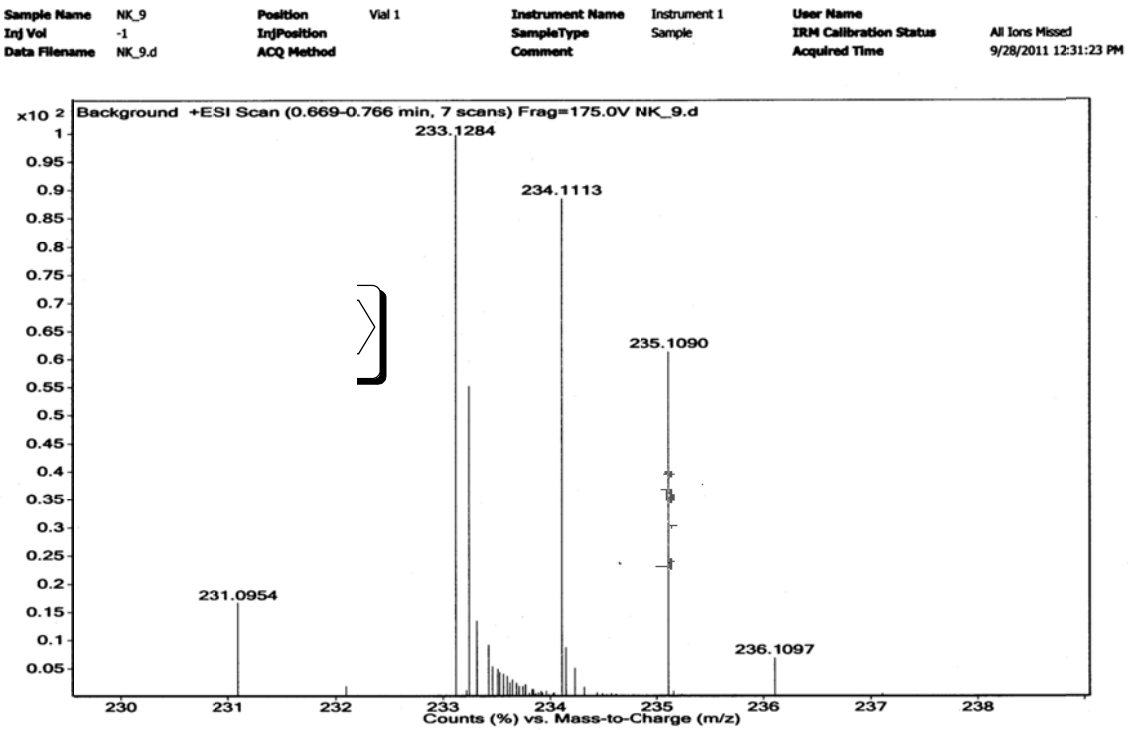
6-methyl-2-(Piperidin-1-yl)benzo[*d*]thiazole (18'd): **^{1}HNMR (400 MHz, $CDCl_3$):**



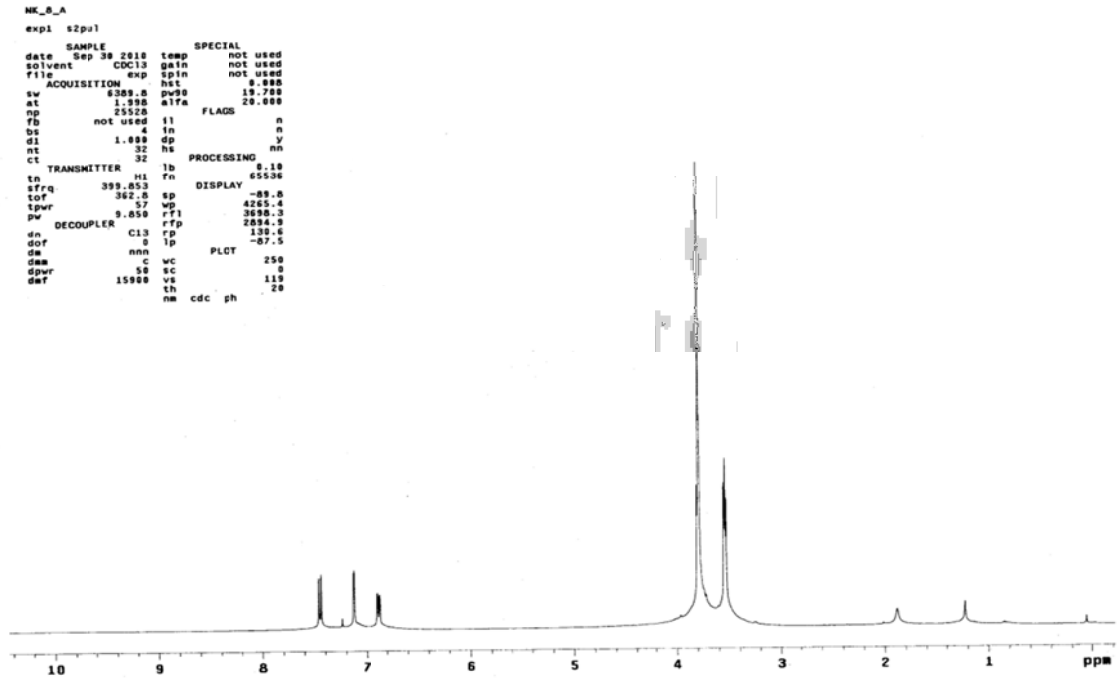
6-methyl-2-(Piperidin-1-yl)benzo[*d*]thiazole (18'd): **^{13}CNMR (100 MHz, $CDCl_3$):**



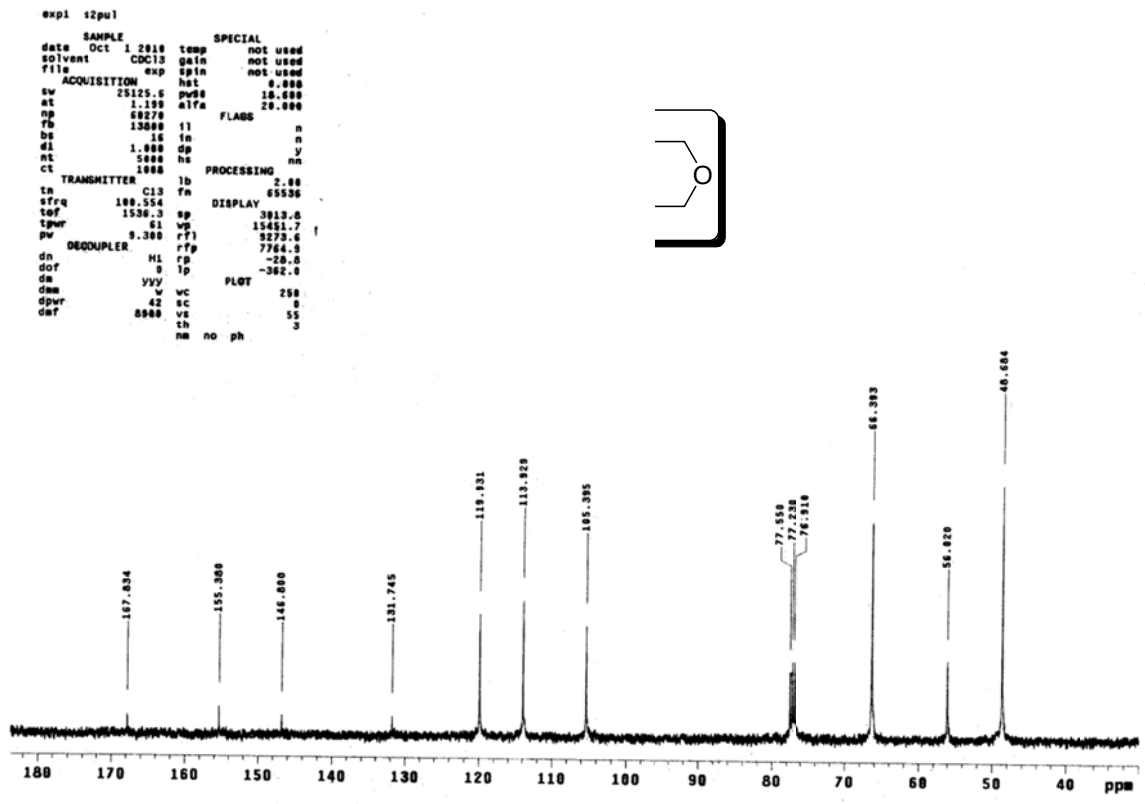
6-methyl-2-(Piperidin-1-yl)benzo[*d*]thiazole (18'd): **MASS SPECTRA:**



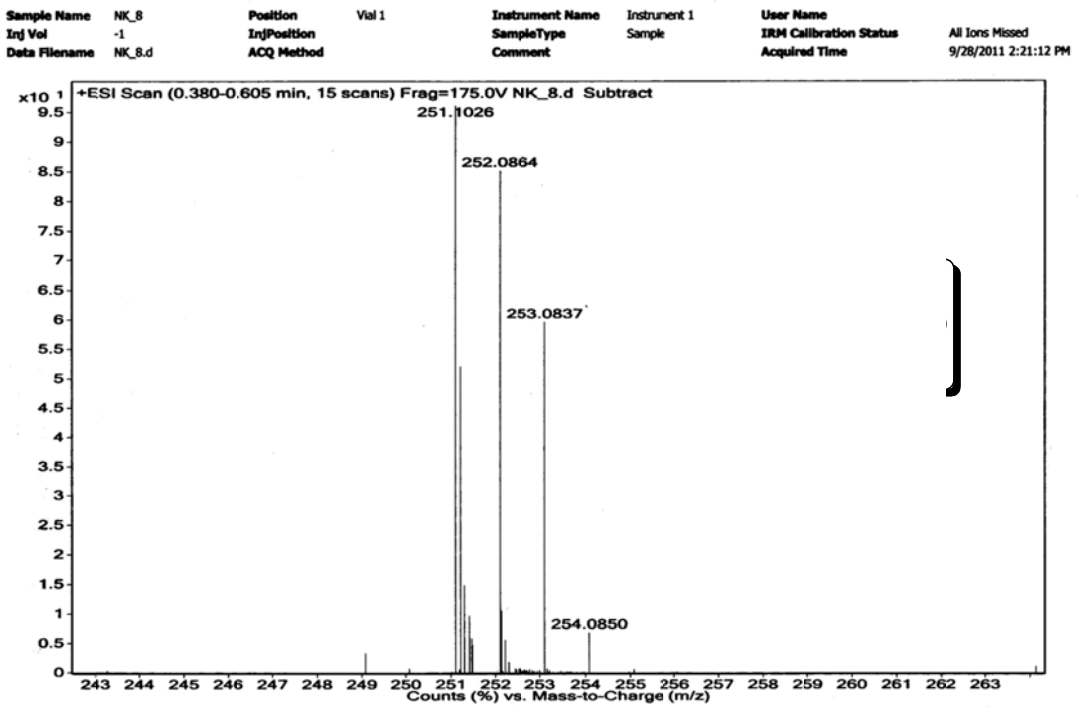
6-methoxy-2-morpholino[*d*]thiazole (19'a): **^{1}H NMR (400 MHz, $CDCl_3$):**



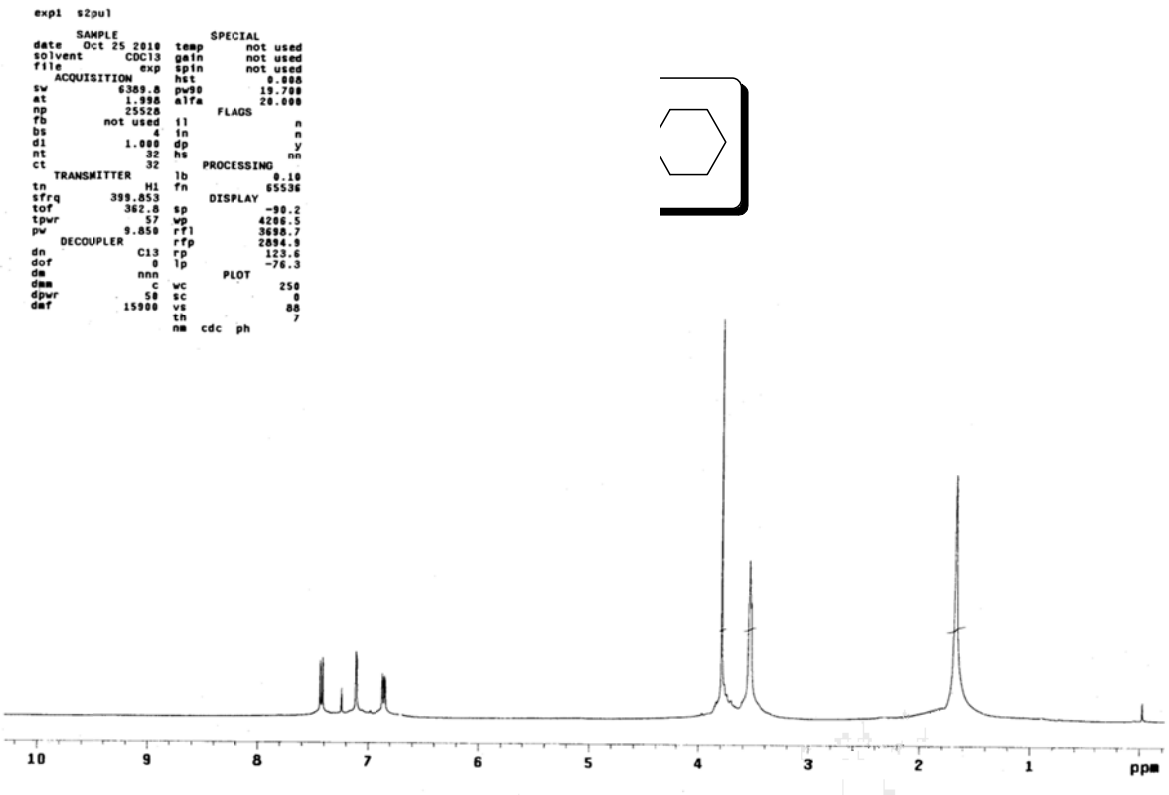
6-methoxy-2-morpholino[*d*]thiazole (19'a): **^{13}C NMR (100 MHz, $CDCl_3$):**



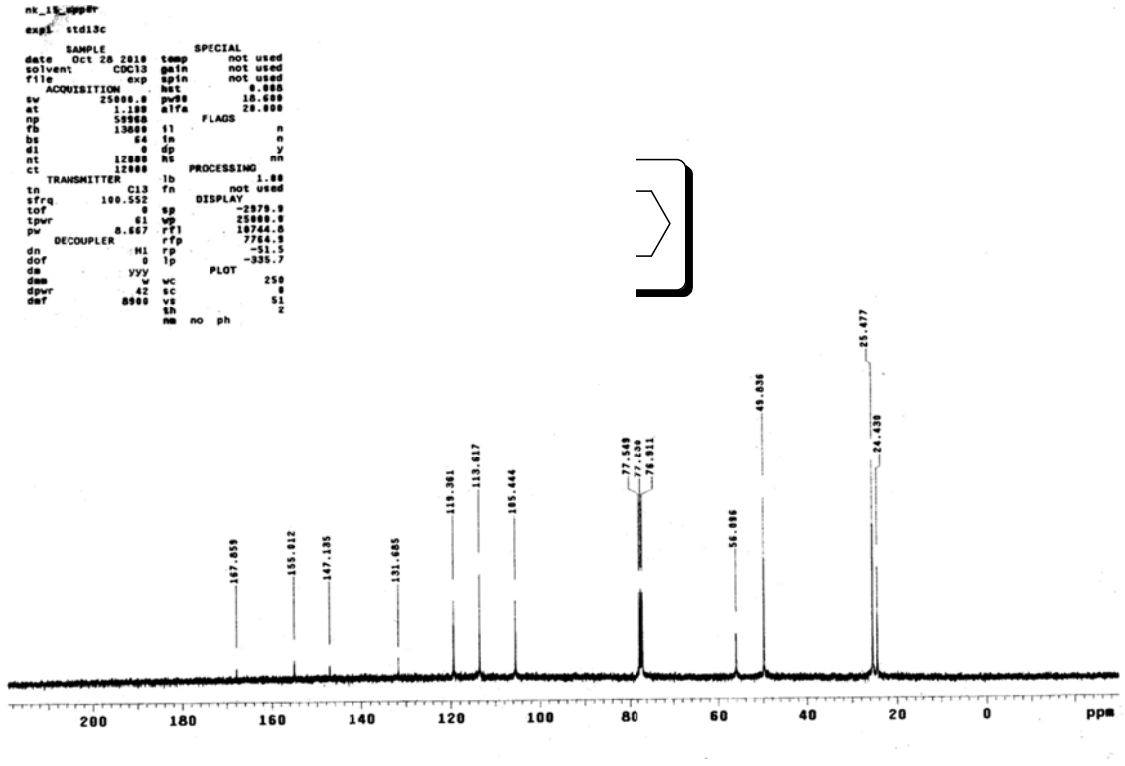
6-methoxy-2-morpholino[*d*]thiazole (19'a): MASS SPECTRA:



6-methoxy-2-(piperidin-1-yl)benzo[*d*]thiazole (19'd): ^{1}H NMR (400 MHz, $CDCl_3$):



6-methoxy-2-(piperidin-1-yl)[*d*]thiazole (19'd): **^{13}C NMR (100 MHz, $CDCl_3$):**



6-methoxy-2-(piperidin-1-yl)benzo[*d*]thiazole (19'd): **MASS SPECTRA:**