

Supporting Informations

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

Santosh K. Sahoo, Nilufa Khatun, Anupal Gogoi, Arghya Deb and Bhisma K. Patel*

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

Email id: patel@iitg.ernet.in

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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 F₂₅₄ (0.25mm). NMR spectra were recorded in CDCl₃, 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-K α 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-

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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 für Anorganische Chemie der Universität: 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

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X-ray Crystallographic data

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

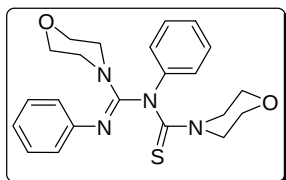
	3d	15'a
Formula	C ₂₈ H ₃₈ N ₄ S	C ₁₁ H ₁₁ BrN ₂ OS
CCDC number	894067	894068
Formula weight	462.69	299.19
T (K)	296(2)	296(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	Monoclinic	Orthorhombic
Space group	P 21 / c	P-1
<i>a</i> (Å)	9.5021(13)	10.01289(3)
<i>b</i> (Å)	11.2799(14)	11.2225(3)
<i>c</i> (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)
<i>V</i> (Å ³)	2641.0(6)	1151.66(7)
<i>Z</i>	4	4
$\theta_{min}, \theta_{max}$	2.12, 26.56	2.13, 30.00
<i>D</i> _{calcd} (g m ⁻³)	1.164	1.726
μ (mm ⁻¹)	0.145	3.729
<i>F</i> (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 , wR2 ^b (<i>I</i> ≥ 2σ(<i>I</i>))	0.0570, 0.1242	0.0851, 0.0836
R1 ^a , wR2 ^b (all data)	0.1134, 0.1421	0.0851, 0.0866

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Spectral Data

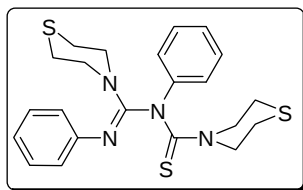
N-((*E*)-Morpholino(phenylimino)methyl)-*N*-phenylmorpholine-4-carbothioamide

(1a):



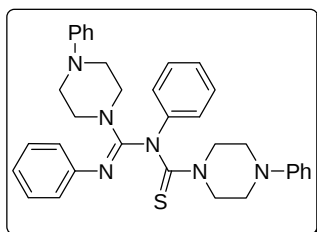
White solid; M.p. 163–165 °C; ^1H NMR (400 MHz, CDCl_3): δ 2.90–3.52 (m, 16H), 6.95 (d, 2H, J = 8.0 Hz), 6.98 (d, 2H, J = 7.6 Hz), 7.09 (t, 2H, J = 7.6 Hz), 7.17 (t, 2H, J = 8.0 Hz), 7.30 (d, 2H, J = 7.6 Hz); ^{13}C NMR (100 MHz, CDCl_3) δ 46.8, 50.6, 65.4, 66.2, 121.2, 122.1, 122.8, 122.9, 124.7, 128.8, 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 °C; ^1H 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^+).

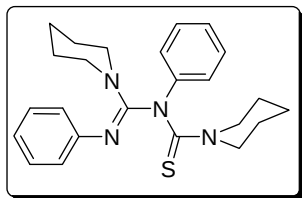
N,4-Diphenyl-*N*-((*E*)-(phenylimino)(4-phenylpiperazin-1-yl)methyl)piperazine-1-carbothioamide (1c):



White solid; M.p. 200–201 °C; ^1H 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^+).

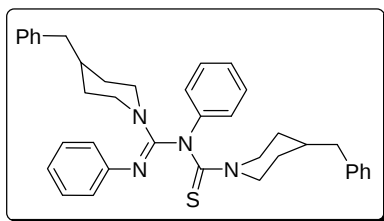
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***N*-Phenyl-*N*-((*E*)-(phenylimino)(piperidin-1-yl)methyl)piperidine-1-carbothioamide (1d):**



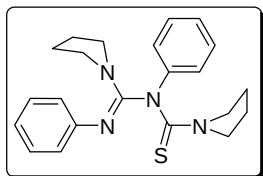
White solid; M.p. 183–184 °C; ^1H NMR (400 MHz, CDCl_3): δ 0.84–1.67 (m, 12H), 2.63–3.82 (m, 8H), 6.90 (t, 2H, $J = 7.6$ Hz), 7.02–7.12 (m, 3H), 7.16 (t, 2H, $J = 8.4$ Hz), 7.26–7.40 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 23.6, 24.5, 24.6, 24.9, 47.4, 51.4, 122.1, 122.3, 124.1, 128.4, 129.2, 143.7, 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 °C; ^1H 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^+).

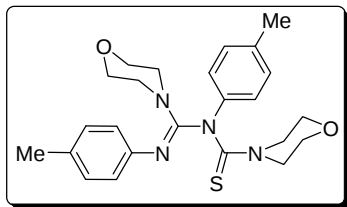
***N*-phenyl-*N*-((*E*)-(phenylimino)(pyrrolidin-1-yl)methyl)pyrrolidine-1-carbothioamide (1f):**



White solid; M.p. 153–155 °C; ^1H 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^+).

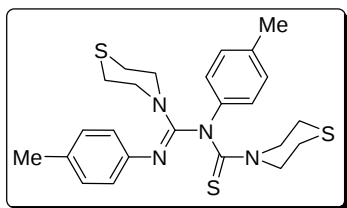
-S6 -

***N*-((*E*)-(p-Tolylimino)(morpholino)methyl)-*N*-p-tolylmorpholine-4-carbothioamide (2a):**



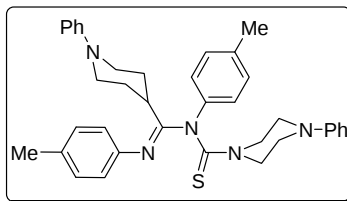
White solid; M.p. 140–141 °C; ¹H NMR (400 MHz, CDCl₃): δ 2.17 (s, 3H), 2.25 (s, 3H), 2.82–3.47 (m, 16H), 6.84 (d, 4H, *J* = 8.0 Hz), 6.92 (d, 4H, *J* = 7.2 Hz); ¹³C NMR (100 MHz, CDCl₃): δ 20.7, 20.8, 46.6, 50.5, 65.2, 66.1, 121.0, 121.8, 129.1, 130.1, 131.6, 134.3, 140.1, 146.6, 149.3, 185.1; IR (KBr): 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 °C; ¹H NMR (400 MHz, CDCl₃): 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); ¹³C NMR (100 MHz, CDCl₃): 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 C₂₄H₃₀N₄S₃: 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.

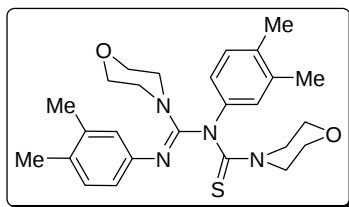
***N*-((*E*)-(p-Tolylimino)(1-phenylpiperidin-4-yl)methyl)-4-phenyl-tolylpiperazine-1-carbothioamide (2c):**



White solid; M.p. 215–216 °C; ¹H NMR (400 MHz, CDCl₃): 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); ¹³C NMR (100 MHz, CDCl₃): 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⁺).

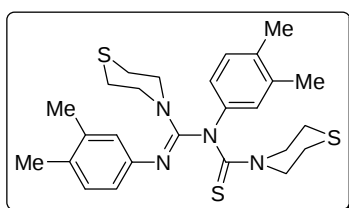
-S7 -

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



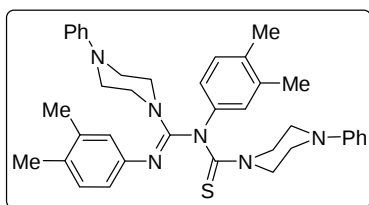
Gummy; ^1H NMR (400 MHz, CDCl_3): δ 2.10 (s, 3H), 2.11 (s, 3H), 2.18 (s, 6H), 2.85–3.76 (m, 16H), 6.69 (d, 2H, $J = 7.6$ Hz), 6.77 (s, 2H), 6.89 (d, 2H, $J = 8.0$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 19.0, 19.2, 19.8, 20.1, 46.6, 50.6, 65.4, 66.2, 119.1, 123.3, 129.7, 130.4, 133.0, 136.4, 137.9, 140.4, 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 $\text{C}_{26}\text{H}_{34}\text{N}_4\text{O}_2\text{S}$: 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 $^{\circ}\text{C}$; ^1H 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^+).

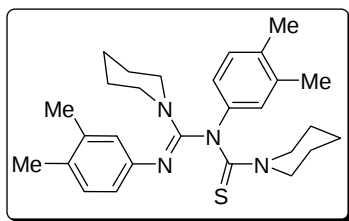
***N*-((*E*)-(3,4-Dimethylphenylimino)(4-phenylpiperazin-1-yl)methyl)-*N*-(3,4-dimethylphenyl)-4-phenylpiperazine-1-carbothioamide (3c):**



White solid; M.p. 190–191 $^{\circ}\text{C}$ ^1H 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^+).

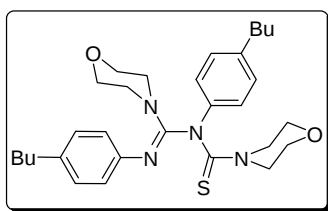
-S8 -

***N*-((*E*)-(3,4-Dimethylphenylimino)(piperidin-1-yl)methyl)-*N*-(3,4-dimethylphenyl)piperidine-1-carbothioamide (3d):**



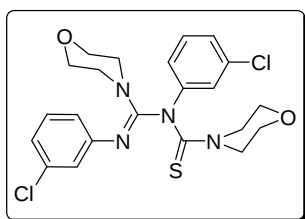
White solid; M.p. 188–189 °C; ¹H NMR (400 MHz, CDCl₃): δ 0.69–1.80 (m, 12H), 2.09 (s, 6H), 2.17 (s, 6H), 2.87–3.73 (m, 8H), 6.14–7.03 (m, 6H); ¹³C NMR (100 MHz, CDCl₃): δ 18.9, 19.1, 19.7, 19.9, 47.3, 51.5, 119.5, 121.5, 123.5, 125.2, 129.5, 129.7, 130.1, 132.3, 136.0, 137.3, 141.4, 147.4, 150.3, 184.9; 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; ¹H NMR (400 MHz, CDCl₃): 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); ¹³C NMR (100 MHz, CDCl₃): 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⁺).

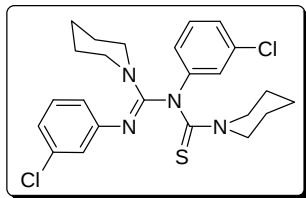
***N*-((*E*)-(3-Chlorophenylimino)(morpholino)methyl)-*N*-(3-chlorophenyl)morpholine-4-carbothioamide (5a):**



White solid; M.p. 172–173 °C; ¹H NMR (400 MHz, CDCl₃): 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); ¹³C NMR (100 MHz, CDCl₃): 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⁺).

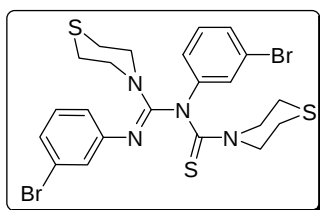
-S9 -

***N*-((*E*)-(3-chlorophenylimino)(piperidin-1-yl)methyl)-*N*-(3-chlorophenyl)piperidine-1-carbothioamide (5d):**



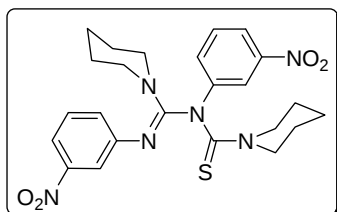
White solid; M.p. 123–125 °C; ^1H NMR (400 MHz, CDCl_3): δ 1.23–1.71 (m, 16H), 3.11–3.51 (m, 4H), 6.87 (t, 4H, $J = 4.8$ Hz), 6.98 (s, 1H), 7.05 (d, 2H, $J = 7.2$ Hz), 7.24 (d, 1H, $J = 3.2$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 23.7, 24.5, 24.8, 25.1, 47.7, 51.9, 119.9, 121.0, 122.4, 124.5, 129.6, 130.4, 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 $\text{C}_{24}\text{H}_{28}\text{Cl}_2\text{N}_4\text{S}$: 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; ^1H 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^+).

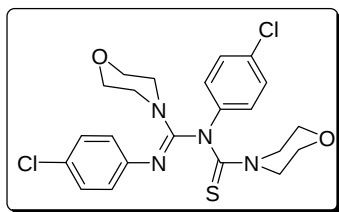
***N*-((*E*)-(3-nitrophenylimino)(piperidin-1-yl)methyl)-*N*-(3-nitrophenyl)piperidine-1-carbothioamide (7d):**



Yellow solid; M.p. 178–180 °C; ^1H 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^+).

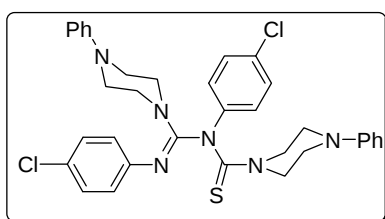
-S10 -

***N*-((*E*)-(4-Chlorophenylimino)(morpholino)methyl)-*N*-(4-chlorophenyl)morpholine-4-carbothioamide (8a):**



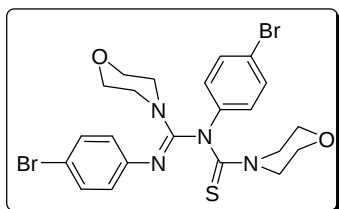
White solid; M.p. 162–164 °C; ¹H NMR (400 MHz, CDCl₃): δ 2.81–3.92 (m, 16H), 6.74 (m, 2H), 6.93 (d, 2H, *J* = 8.0 Hz), 7.17 (d, 2H, *J* = 8.0 Hz), 7.33 (m, 2H); ¹³C NMR (100 MHz, CDCl₃): δ 46.9, 50.9, 65.5, 66.3, 122.3, 123.5, 128.3, 128.9, 130.1, 130.5, 141.2, 147.7, 149.5, 184.9; IR (KBr): 2963, 2889, 2845, 1637, 1584, 1487, 1461, 1416, 1360, 1297, 1273, 1258, 1232, 1207, 1159, 1112, 1094, 1074, 1010, 997, 825 cm⁻¹; Anal. Calcd for C₂₂H₂₄Cl₂N₄O₂S: 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 °C; ¹H NMR (400 MHz, CDCl₃): 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); ¹³C NMR (100 MHz, CDCl₃): 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⁺).

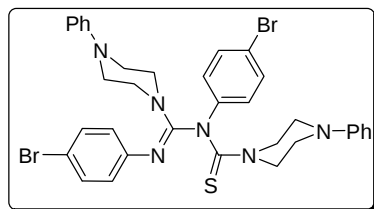
***N*-((*E*)-(4-bromophenylimino)(morpholino)methyl)-*N*-(4-bromophenyl)morpholine-4-carbothioamide (9a):**



White solid; M.p. 174–175 °C; ¹H NMR (400 MHz, CDCl₃): δ 2.60–3.81 (m, 16H), 6.85 (brs, 2H), 6.87 (d, 2H, *J* = 8.4 Hz), 7.31 (d, 2H, *J* = 8.4 Hz), 7.49 (brs, 2H); ¹³C NMR (100 MHz, CDCl₃): 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 C₂₂H₂₄Br₂N₄O₂S: 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.

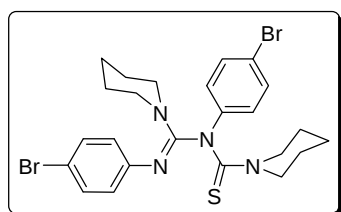
-S11 -

***N*-((*E*)-(4-bromophenylimino)(4-phenylpiperazin-1-yl)methyl)-*N*-(4-bromophenyl)-4-phenylpiperazine-1-carbothioamide (9c):**



Gummy; ^1H 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^+).

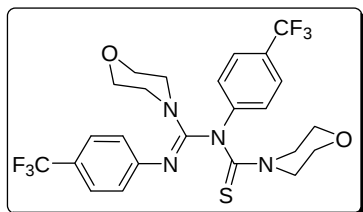
***N*-((*E*)-(4-bromophenylimino)(piperidin-1-yl)methyl)-*N*-(4-bromophenyl)piperidine-1-carbothioamide (9d):**



White solid; M.p. 177–179 $^{\circ}\text{C}$; ^1H 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, $J = 4.4$ Hz); ^{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 $\text{C}_{24}\text{H}_{28}\text{Br}_2\text{N}_4\text{S}$: 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.

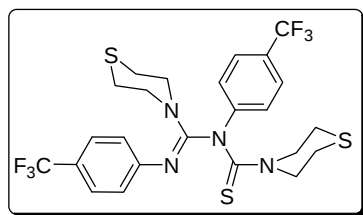
-S12 -

***N*-((*E*)-(4-(Trifluoromethyl)phenylimino)(morpholino)methyl)-*N*-(4-(trifluoromethyl)phenyl)morpholine-4-carbothioamide (10a):**



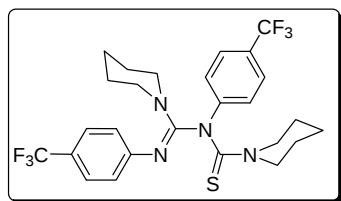
White solid; M.p. 148–149 °C; ^1H NMR (400 MHz, CDCl_3): δ 2.92–3.95 (m, 16H), 6.90 (brs, 2H), 7.07 (d, 2H, $J = 8.0$ Hz), 7.47 (d, 2H, $J = 8.0$ Hz), 7.62 (brs, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 46.9, 51.0, 65.4, 66.2, 120.5, 121.1, 122.3, 122.4, 124.9, 125.2, 125.3, 125.9, 126.1, 126.5, 126.8, 127.2, 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 $\text{C}_{24}\text{H}_{24}\text{F}_6\text{N}_4\text{O}_2\text{S}$: 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-(trifluoromethyl)phenyl)thiomorpholine-4-carbothioamide (10b):**



White solid; M.p. 170–171 °C; ^1H 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^+).

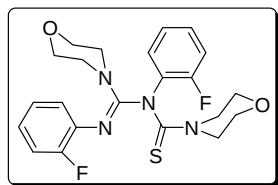
***N*-((*E*)-(4-(trifluoromethyl)phenylimino)(piperidin-1-yl)methyl)-*N*-(4-(trifluoromethyl)phenyl)piperidine-1-carbothioamide (10d):**



White solid; M.p. 138–140 °C; ^1H 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 $\text{C}_{26}\text{H}_{28}\text{F}_6\text{N}_4\text{S}$: 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.

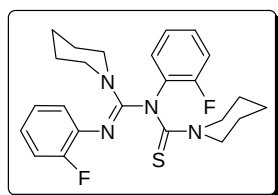
-S13 -

***N*-((*E*)-(2-Fluorophenylimino)(morpholino)methyl)-*N*-(2-fluorophenyl)morpholine-4-carbothioamide (11a):**



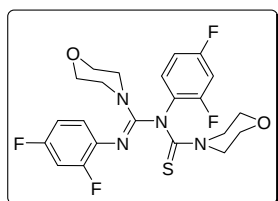
White solid; M.p. 123–125 °C; ^1H NMR (400 MHz, CDCl_3): δ 2.68–3.74 (m, 16H), 6.87–7.33 (m, 8H); ^{13}C NMR (100 MHz, CDCl_3): δ 44.2, 50.5, 66.1, 66.4, 114.6, 114.8, 111.1, 115.3, 116.7, 116.9, 121.9, 123.4, 123.5, 124.0, 124.5, 124.9, 125.3, 125.7, 126.2, 127.3, 130.4, 136.4, 150.6, 154.5, 186.3; 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 °C; ^1H 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^+).

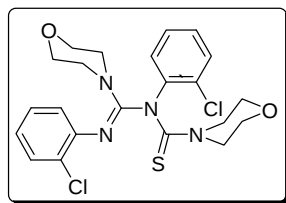
***N*-((*E*)-(2,4-Difluorophenylimino)(morpholino)-*N*-(2,4-(difluorophenyl)morpholine-4-carbothioamide (12a):**



White solid; M.p. 138–140 °C; ^1H 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^+).

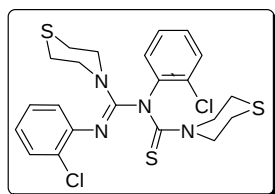
-S14 -

***N*-((*E*)-(2-chlorophenylimino)(morpholino)methyl)-*N*-(2-chlorophenyl)morpholine-4-carbothioamide (13a):**



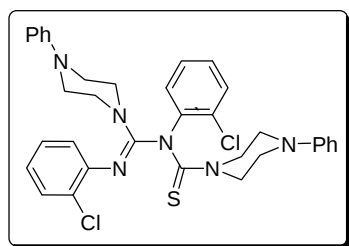
Mp 154–155 °C; ^1H NMR (400 MHz, CDCl_3): δ 2.50–4.60 (m 16H), 6.39–7.68 (m, 8H); ^{13}C NMR (100 MHz, CDCl_3): δ 44.1, 47.0, 50.9, 66.0, 121.5, 122.8, 123.4, 126.2, 126.4, 127.3, 128.0, 129.1, 131.0, 139.6, 145.7, 148.5, 187.2; IR (KBr): 3057, 2950, 2894, 2849, 1632, 1580, 1470, 1427, 1401, 1363, 1303, 1272, 1237, 1219, 1206, 1159, 1150, 1119, 1109, 1051, 1031, 999, 953, 876, 757. cm^{-1} . Anal. Calcd for $\text{C}_{22}\text{H}_{24}\text{Cl}_2\text{N}_4\text{O}_2\text{S}$: 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; ^1H 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^+).

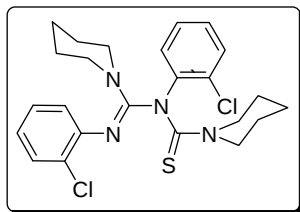
***N*-((*E*)-(2-Chlorophenylimino)(4-phenylpiperazin-1-yl)methyl)-*N*-(2-chlorophenyl)-4-phenylpiperazine-1-carbothioamide (13c):**



Mp 207–208 °C; ^1H 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 $\text{C}_{34}\text{H}_{34}\text{Cl}_2\text{N}_6\text{S}$: 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.

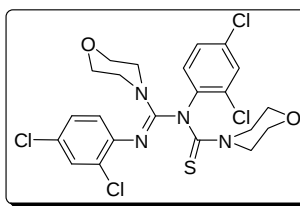
-S15 -

***N*-((*E*)-(2-chlorophenylimino)(piperidin-1-yl)methyl)-*N*-(2-chlorophenyl)piperidine-1-carbothioamide (13d):**



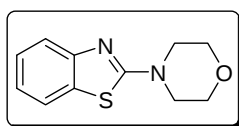
Gummy; ^1H NMR (400 MHz, CDCl_3): δ 0.83-2.01 (m, 16H), 3.68 (m, 4H), 6.62-7.39 (m, 8H); ^{13}C NMR (100 MHz, CDCl_3): δ 24.0, 24.7, 25.1, 25.7, 48.3, 51.9, 121.5, 122.2, 122.9, 123.7, 126.4, 126.9, 127.7, 128.9, 130.7, 140.5, 142.0, 147.5, 187.7; IR (KBr): 3448, 2935, 2853, 1620, 1580, 1475, 1440, 1297, 1234, 1207, 1176, 1031, 755 cm^{-1} ; Anal. Calcd for $\text{C}_{24}\text{H}_{28}\text{Cl}_2\text{N}_4\text{S}$: 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; ^1H 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^+).

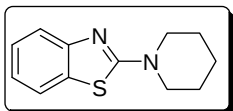
2-Morpholinobenzo[d]thiazole (11'a):



White solid; M.p. 120–122 $^{\circ}\text{C}$; ^1H 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 $\text{C}_{11}\text{H}_{12}\text{N}_2\text{OS}$: 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.

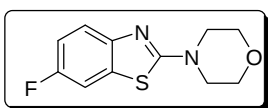
-S16 -

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



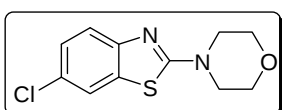
White solid; M.p. 96–97 °C; ^1H NMR (400 MHz, CDCl_3): δ 1.67 (s, 6H), 3.58 (s, 4H), 7.03 (t, 1H, $J = 8.0$ Hz), 7.26 (t, 1H, $J = 8.0$ Hz), 7.55 (dd, 2H, $J_1 = 8.0$ Hz, $J_2 = 5.2$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 24.3, 25.4, 49.7, 118.9, 120.7, 121.1, 126.0, 130.8, 153.1, 169.0; IR (KBr): 2934, 2922, 2849, 1588, 1534, 1440, 1382, 1332, 1257, 1234, 1209, 1120, 1006, 760 cm^{-1} ; Anal. Calcd for $\text{C}_{12}\text{H}_{14}\text{N}_2\text{S}$: 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):



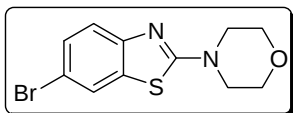
White solid; M.p. 157–158 °C; ^1H NMR (400 MHz, CDCl_3): δ 3.51 (t, 4H, $J = 4.8$ Hz), 3.75 (t, 4H, $J = 4.4$ Hz), 6.97 (m, 1H), 7.25 (m, 1H), 7.44 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 48.4, 66.1, 107.4, 107.6, 113.6, 113.9, 119.7, 119.8, 131.2, 131.4, 148.9, 157.0, 159.4, 168.5; IR (KBr): 2982, 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 °C; ^1H 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):

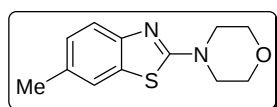


White solid; M.p. 165–167 °C; ^1H NMR (400 MHz, CDCl_3): δ 3.57 (t, 4H, $J = 4.8$ Hz), 3.80 (t, 4H, $J = 4.8$ Hz), 7.37 (s, 2H), 7.68 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 48.5, 66.3, 114.0,

-S17-

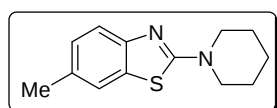
120.5, 123.3, 129.4, 132.4, 151.6, 169.1; IR (KBr): 2918, 2857, 1591, 1535, 1443, 1372, 1280, 1258, 1229, 1110, 1026, 940, 863, 813 cm^{-1} ; Anal. Calcd for $\text{C}_{11}\text{H}_{11}\text{N}_2\text{OSBr}$: C 44.16, H 3.71, N 9.36, S 10.72; found C 44.23, H 3.76, N 9.28, S 10.64.

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



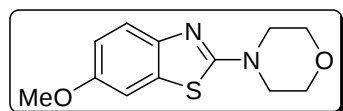
White solid; M.P. 134–136 °C; ^1H NMR (400 MHz, CDCl_3): δ 2.37 (s, 3H), 3.56 (t, 4H, $J = 4.8$ Hz), 3.79 (t, 4H, $J = 4.8$ Hz), 7.09 (d, 1H, $J = 8.0$ Hz), 7.39 (s, 1H), 7.44 (d, 1H, $J = 8.0$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 21.3, 48.6, 66.3, 119.0, 120.9, 127.4, 130.7, 131.6, 150.4, 168.6; IR (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 °C; ^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^+).

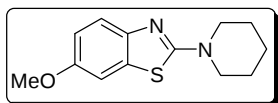
6-Methoxy-2-morpholinobenzo[d]thiazole (19'a):



White solid; M.p. 130–132 °C; ^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, $J = 8.8$ Hz, $J = 2.4$ 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^+).

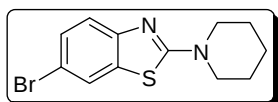
-S18 -

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



White solid; M.p. 108–110°C; ^1H 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):

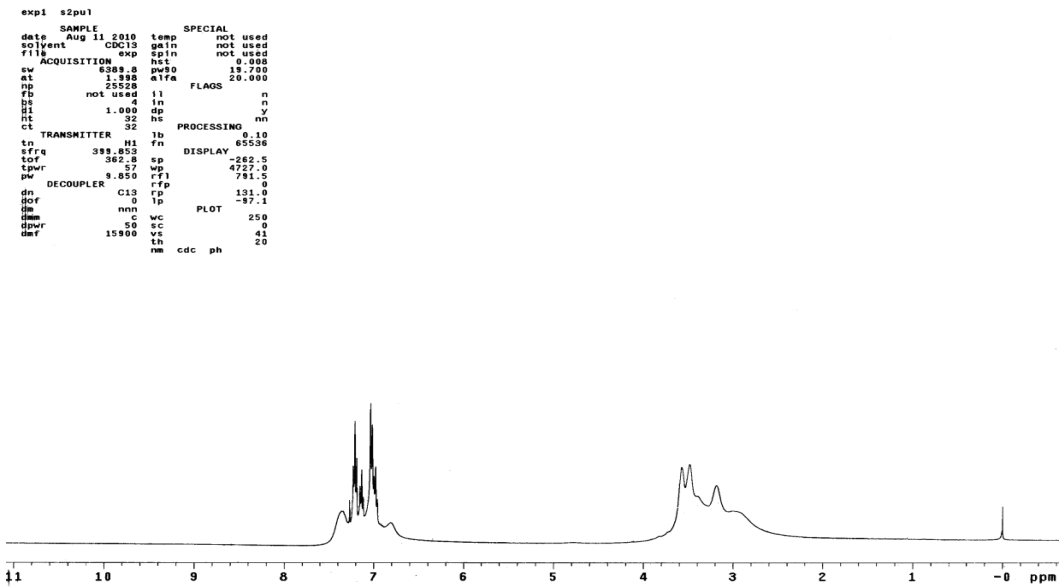


White solid; M.p. 118–120 °C; ^1H NMR (400 MHz, CDCl_3): δ 1.68 (s, 6H), 3.58 (s, 4H), 7.35 (s, 2H), 7.67 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 24.3, 25.4, 49.8, 113.3, 120.0, 123.2, 129.2, 132.5, 152.2, 169.0; IR (KBr): 3445, 2927, 2852, 1629, 1594, 1536, 1442, 1380, 1334, 1255, 1208, 1124, 1004,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

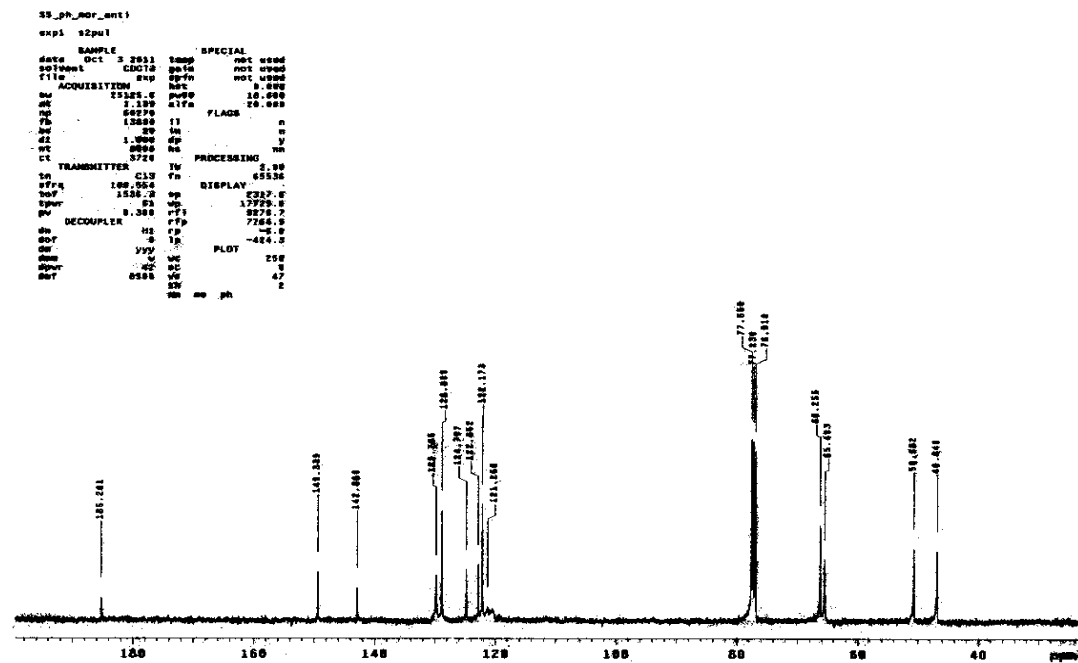
-S19 -

Spectra

N-((*E*)-Morpholino(phenylimino)methyl)-*N*-phenylmorpholine-4-carbothioamide
(1a). ¹H NMR (400 MHz, CDCl₃):

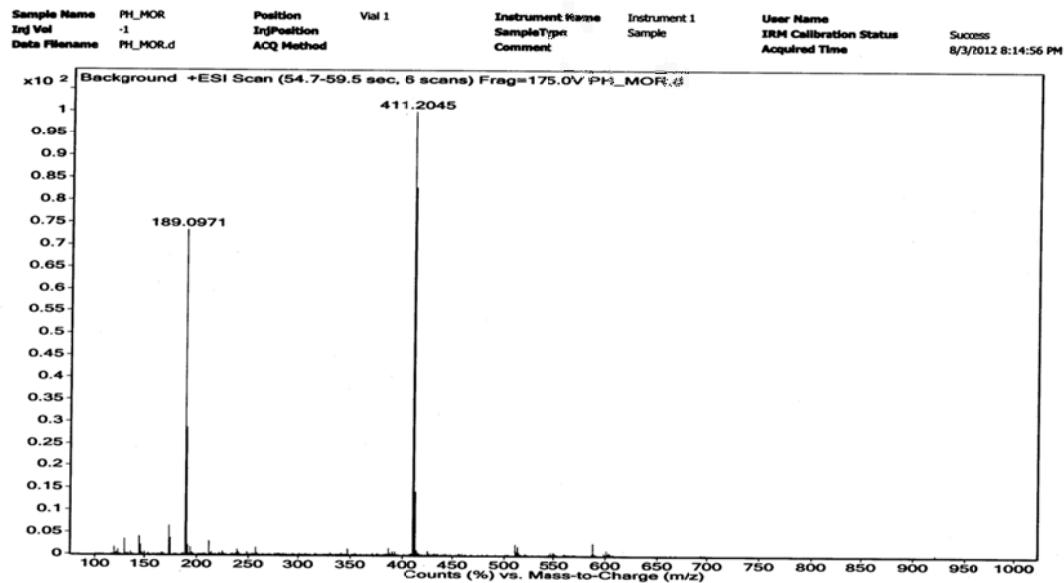


N-((*E*)-Morpholino(phenylimino)methyl)-*N*-phenylmorpholine-4-carbothioamide
(1a). ¹³C NMR (100 MHz, CDCl₃):



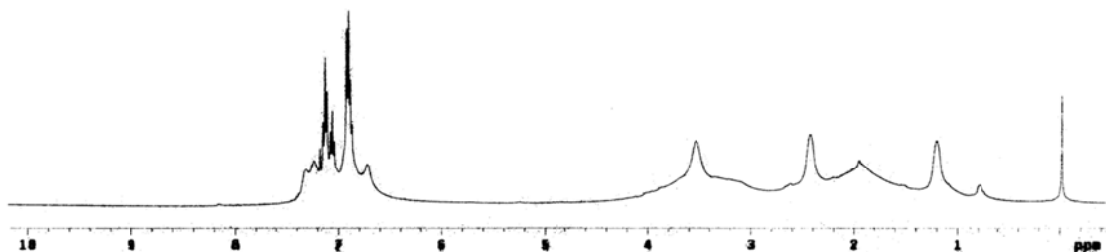
-S20 -

N-((*E*)-Morpholino(phenylimino)methyl)-*N*-phenylmorpholine-4-carbothioamide (1a).
MASS SPECTRA:



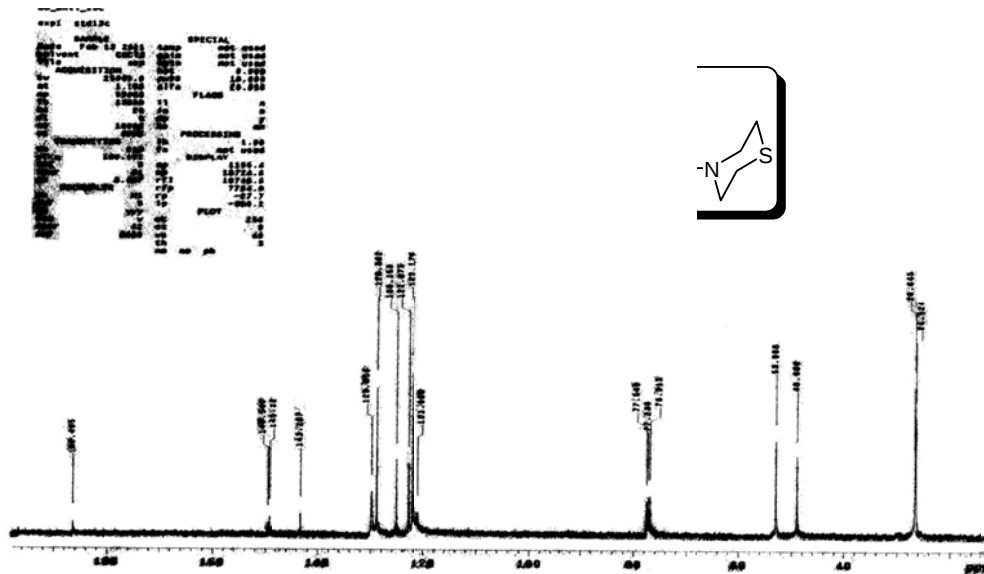
N-Phenyl-*N*-((*E*)-(phenylimino)(thiomorpholino)methyl)thiomorpholine-4-carbothioamide (1b). ¹H NMR (400 MHz, CDCl₃):

```
expl st01h
=====
NAME      SAMPLE
Date      F06 13 2012
Software  CMC70
File       exp
ACQUISITION
sv         0.000.0
at         1.000
ap         20000
rs         not used
ds         5
dl         1.000
nl         32
cl         32
=====
TRANSMITTER
ql         399.653
vffq      399.653
tof        5
spwr       5.7
pw         7.000
deCOUPLER C13
dc         5
dot        8
dm         non
dpr        C
dof        50
dof        15000
=====
SPECIAL
temp       not used
gain       not used
spin       not used
het        0.000
nuc        13.000
atm        20.000
=====
FLAGS
n          n
n          n
y          y
nn         nn
=====
Tn         not used
=====
DISPLAY
-178.3
4253.7
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2884.9
118.3
-112.6
=====
PLOT
250
0
45
15
=====
nm cdc ph
```



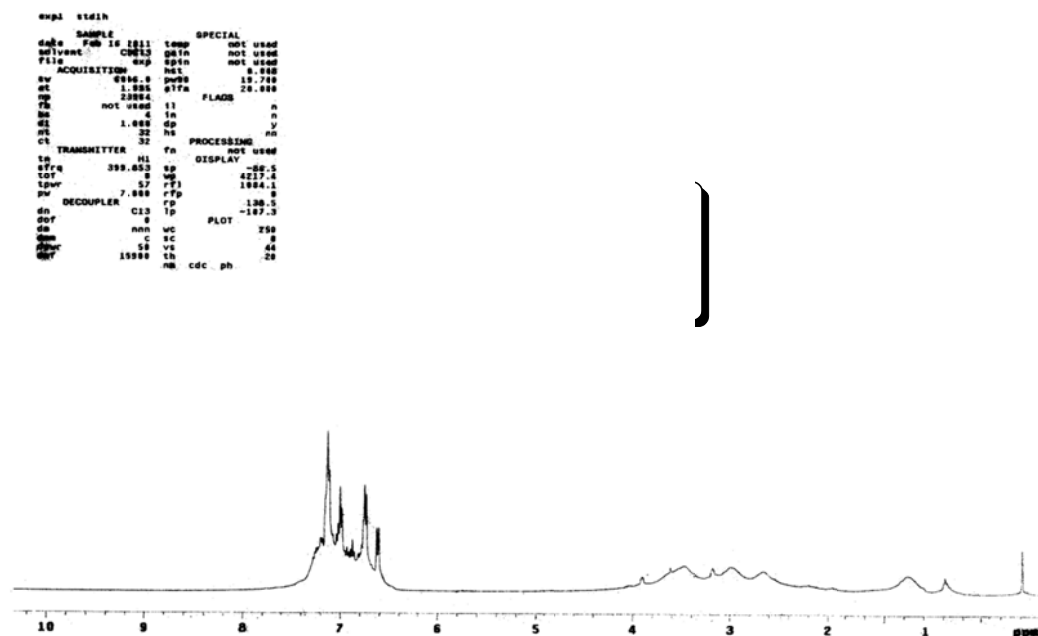
-S21 -

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

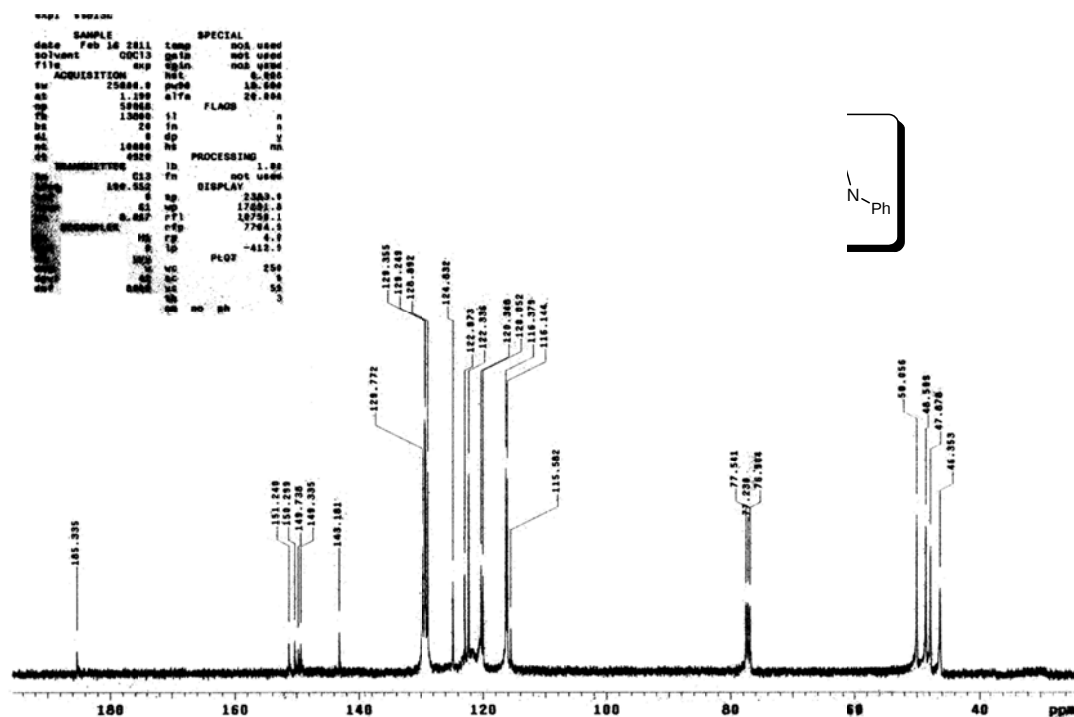


-S22 -

N,4-Diphenyl-*N*-((*E*)-(phenylimino)(4-phenylpiperazine-1-yl)methyl)piperazine-1-carbothioamide (1c). ^1H NMR (400 MHz, CDCl_3):

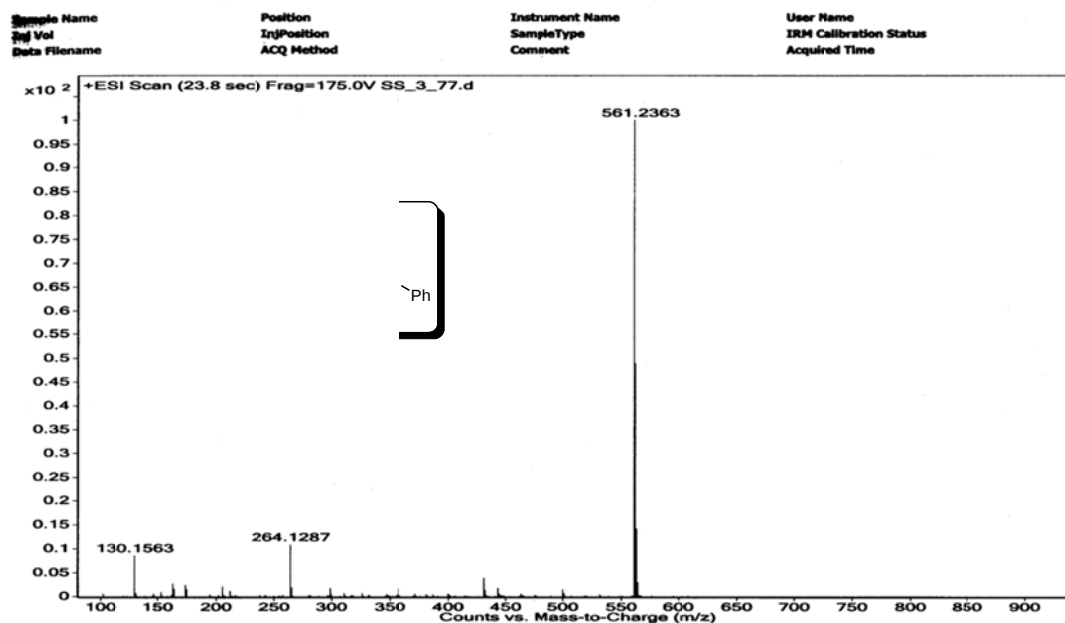


N,4-Diphenyl-*N*-((*E*)-(phenylimino)(4-phenylpiperazine-1-yl)methyl)piperazine-1-carbothioamide (1c). ^{13}C NMR (100 MHz, CDCl_3):

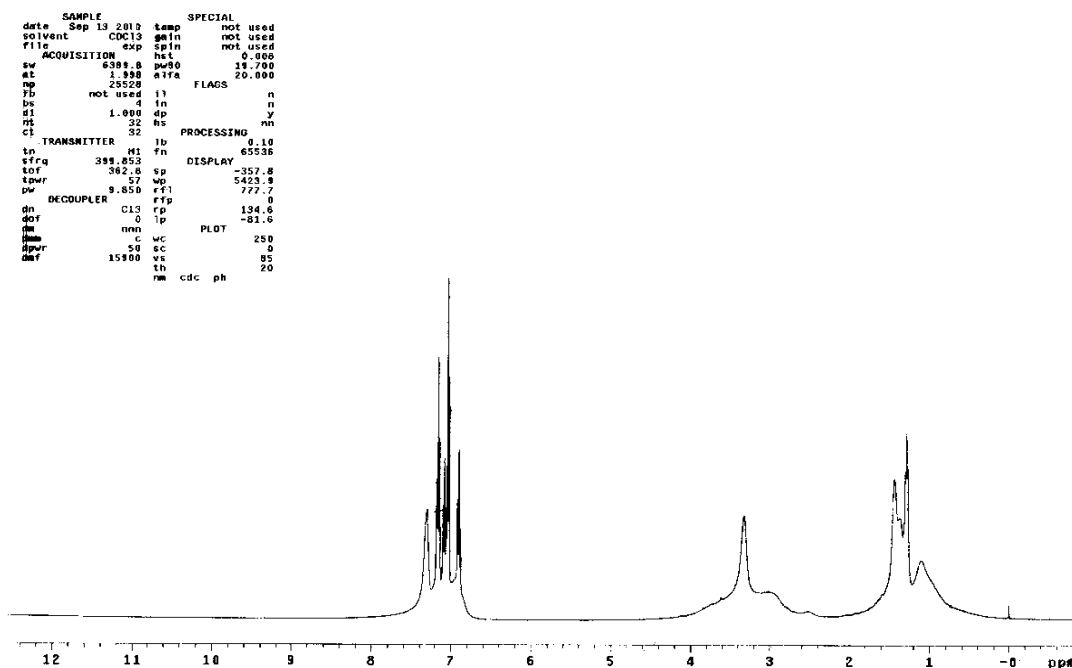


-S23 -

***N*,4-Diphenyl-*N*-((*E*)-(phenylimino)(4-phenylpiperazine-1-yl)methyl)piperazine-1-carbothioamide (1c). MASS SPECTRA:**

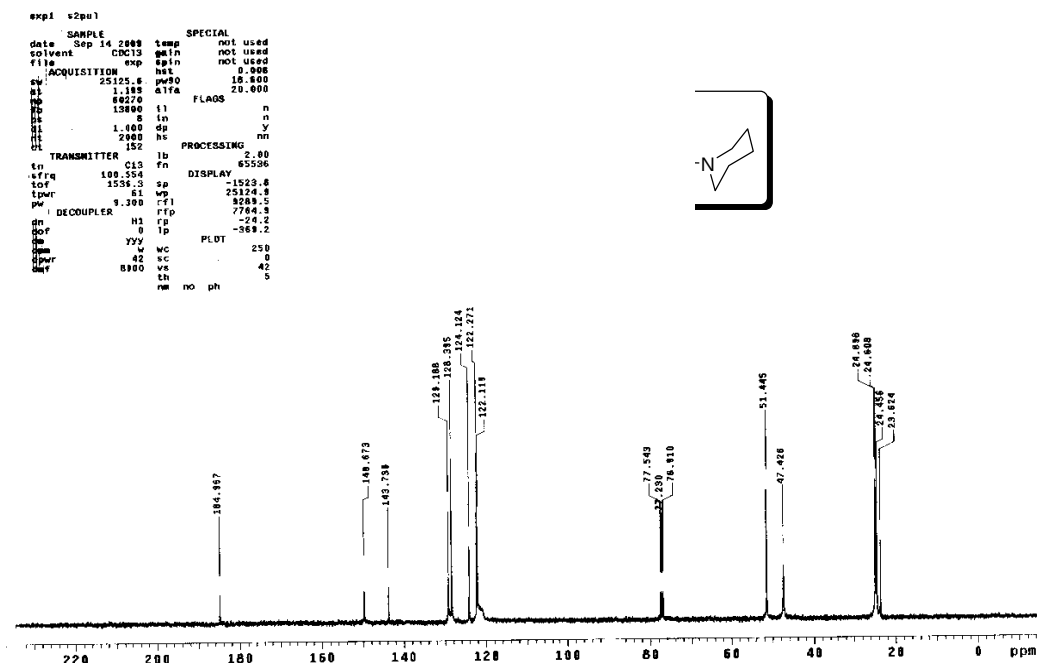


***N*-Phenyl-*N*-((*E*)-(phenylimino)(piperidin-1-yl)methyl)piperidine-1-carbothioamide (1d). ¹H NMR (400 MHz, CDCl₃):**

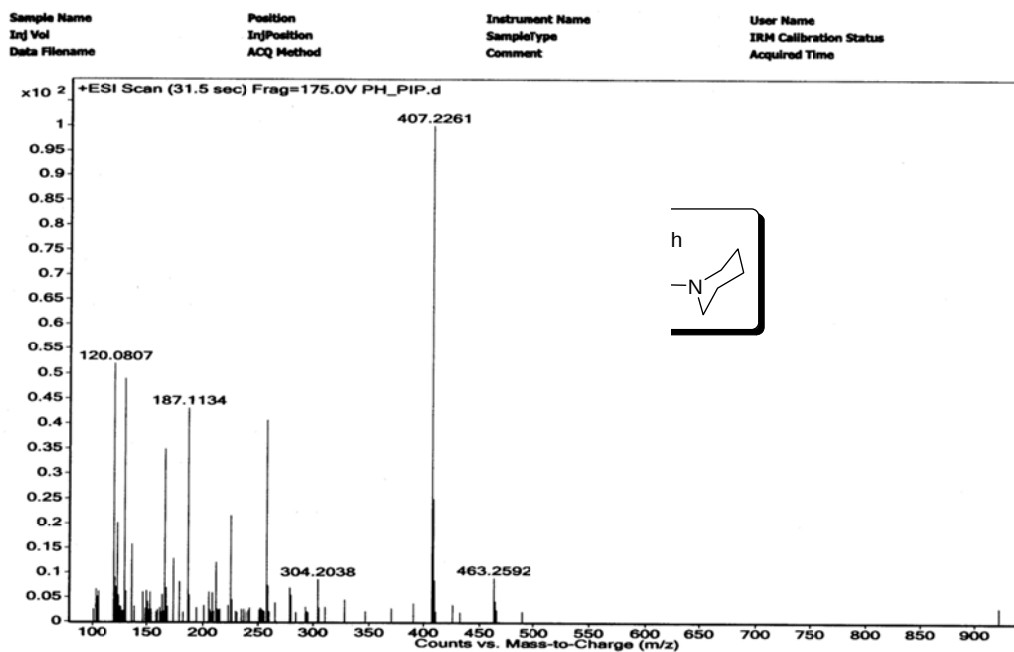


-S24 -

***N*-Phenyl-*N*-((*E*)-(phenylimino)(piperidin-1-yl)methyl)piperidine-1-carbothioamide (1d). ¹³C NMR (100 MHz, CDCl₃):**

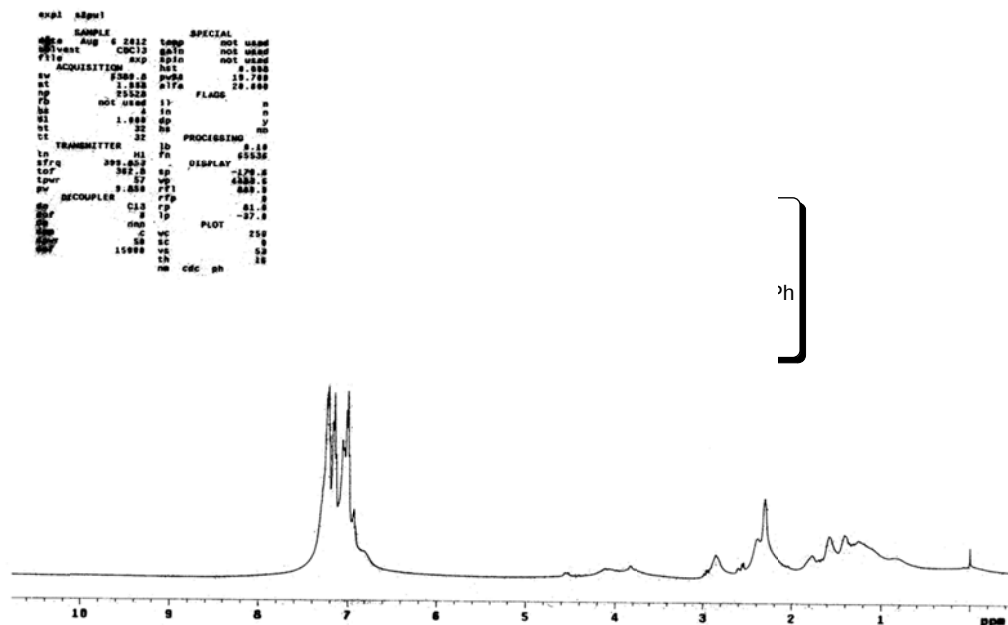


***N*-Phenyl-*N*-((*E*)-(phenylimino)(piperidin-1-yl)methyl)piperidine-1-carbothioamide (1d). MASS SPECTRA:**

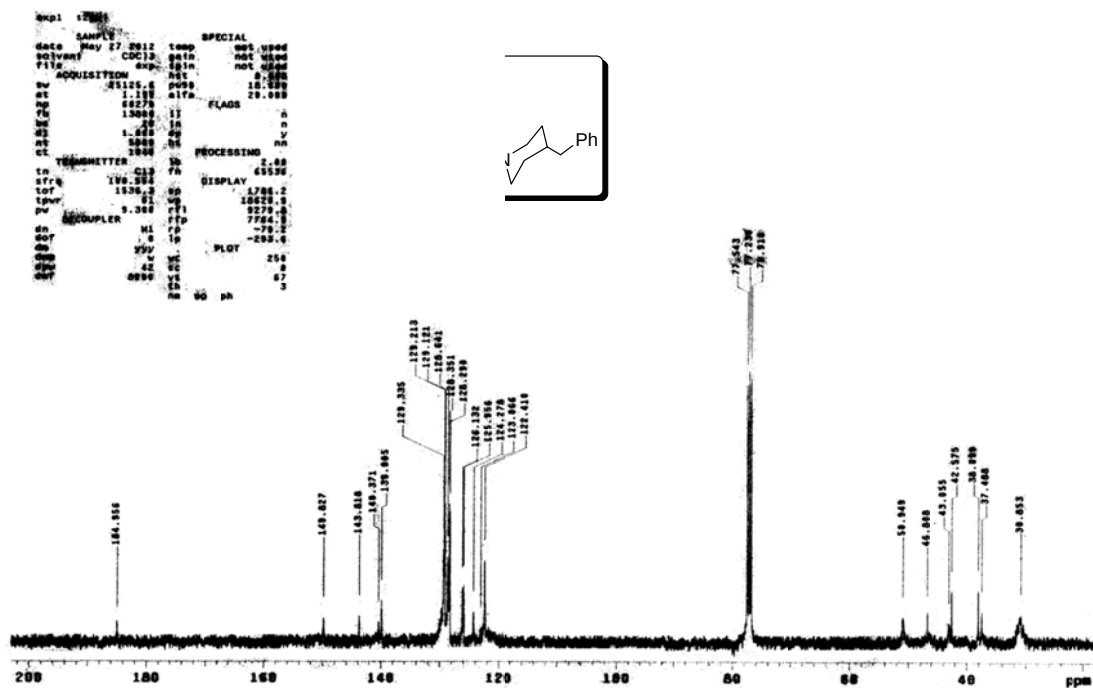


-S25 -

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

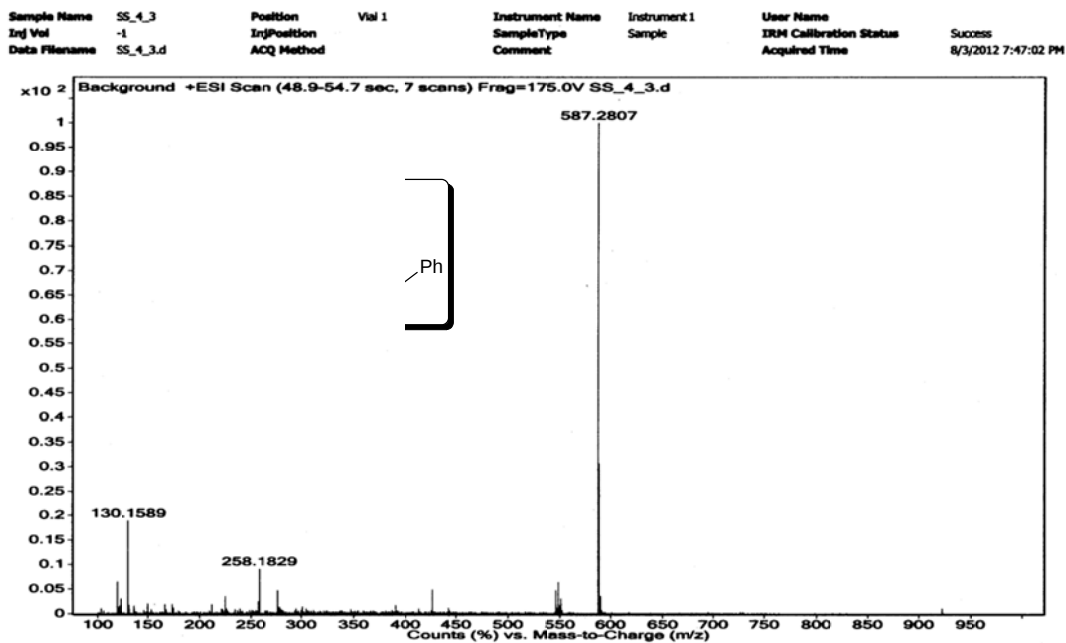


4-Benzyl-*N*-((*E*)-(4-benzylpiperidin-1-yl)(phenylimino)methyl)-*N*-phenylpiperidine-1-carbothioamide (1e). ^{13}C NMR (100 MHz, CDCl_3):



-S26 -

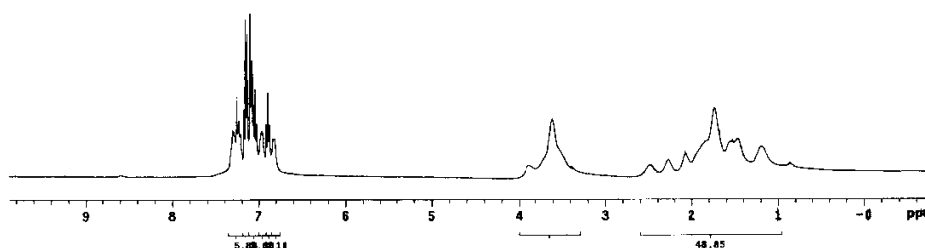
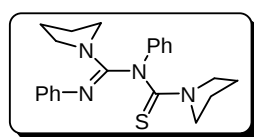
4-Benzyl-*N*-((*E*)-(4-benzylpiperidin-1-yl)(phenylimino)methyl)-*N*-phenylpiperidine-1-carbothioamide (1e). MASS SPECTRA:



***N*-Phenyl-*N*-((*E*)-(phenylimino)(pyrrolidin-1-yl)methyl)pyrrolidine-1-carbothioamide (1f).
¹H NMR (400 MHz, CDCl₃):**

```

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=====
SAMPLE      Temp      SPECIAL
date Aug 3 2010 gain not used
solvent CDCl3 spin not used
file /export/home/~ hst 0.000
           pw10 10.700
           d1to 20.000
=====
ACQUISITION
sv 898.8 11 FLAGS n
st 1.886 in n
tp 25528 in n
fb not used dp y
hs 4 hs nn
dt 1.000 PROCESSING 8.10
DE 32 fb 65536
CL 32 fn
=====
TRANSMITTER H1 sp DISPLAY ~717.2
rfreq 399.853 wp 4080.3
sfr 382.3 rfi 755.3
tpwr 57 rfp 0
nm 9.850 tp 87.9
DECOUPLER C13 PL0T -33.5
          0 uc 250
          nm ec 0
          c vo 41
          spwr 50 th 0
          dcf 15900 nm cdc ph
  
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-S27-

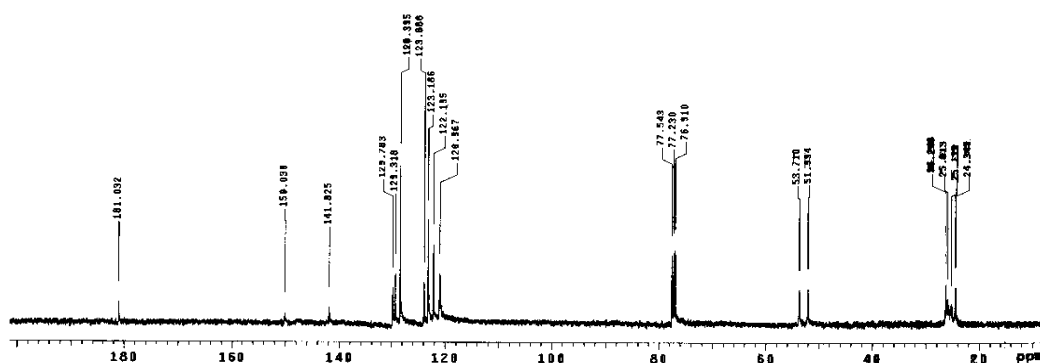
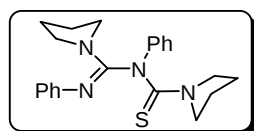
N-Phenyl-*N*-((*E*)-(phenylimino)(pyrrolidin-1-yl)methyl)pyrrolidine-1-carbothioamide (1f).

¹³C NMR (100 MHz, CDCl₃):

```

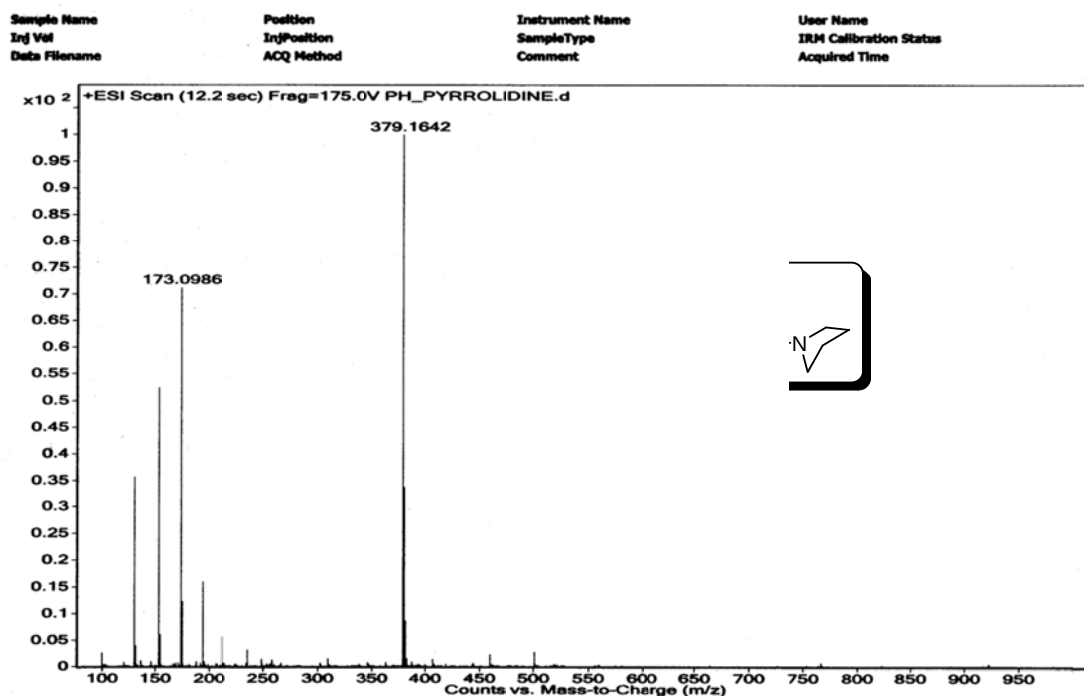
SAMPLE          temp      SPECIAL
Date            Oct 28 2010 gain      not used
Acqvent         CDC13  spin      not used
File            /export/home/... hst      0.000
                                pvs90    10.000
                                mifa     20.000
ACQUISITION
pw             25125.6        FLAGS      n
ns             1.189         in         n
fb             6827.0         in         n
ls             15000         dp         y
hs             18           hs         nn
f1             1.000         PROCESSING 2.00
f2             5000         fn         65536
ct             892          DISPLAY -289.3
TRANSMITTER    C13          sp         20535.0
tp             100.554       wp         8976.4
cp             1538.3       rfp        7764.8
pwr            81          rf         -34.3
ph             9.900        tp         -404.6
DECOUPLER      H1          PLOT       250
dn             0            wc         0
sm             yyy         vc         0
nm             42          th         38
hpr            8100         rm         no ph
dnt

```



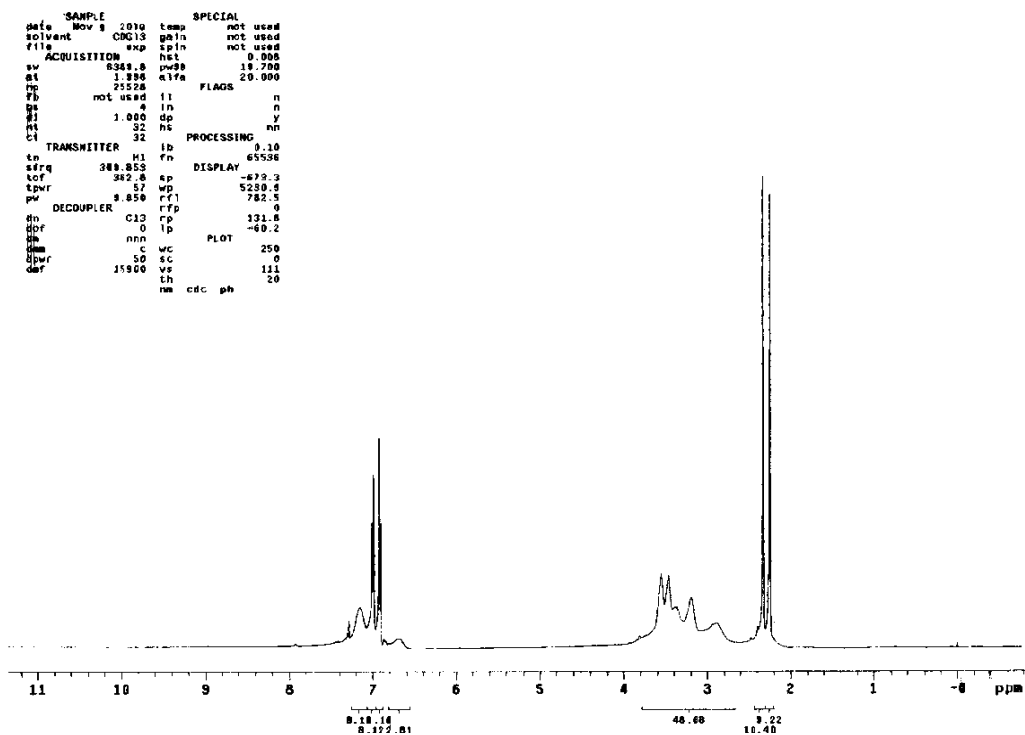
N-Phenyl-*N*-((*E*)-(phenylimino)(pyrrolidin-1-yl)methyl)pyrrolidine-1-carbothioamide (1f).

MASS SPECTRA:

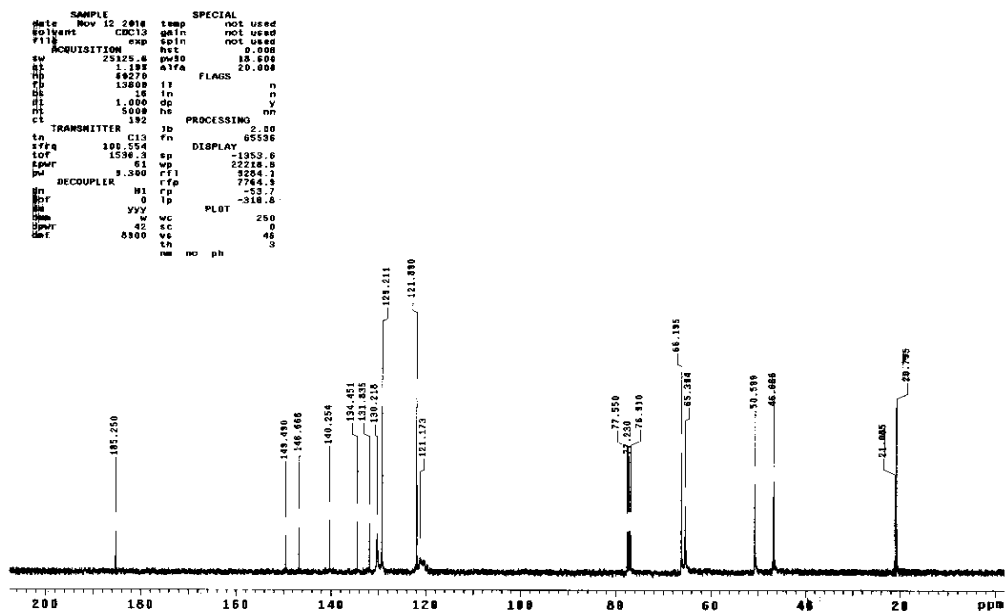


-S28 -

N-((*E*)-(*p*-Tolylimino)(morpholino)methyl)-*N*-*p*-tolylmorpholine-4-carbothioamide
(2a). ^1H NMR (400 MHz, CDCl_3):

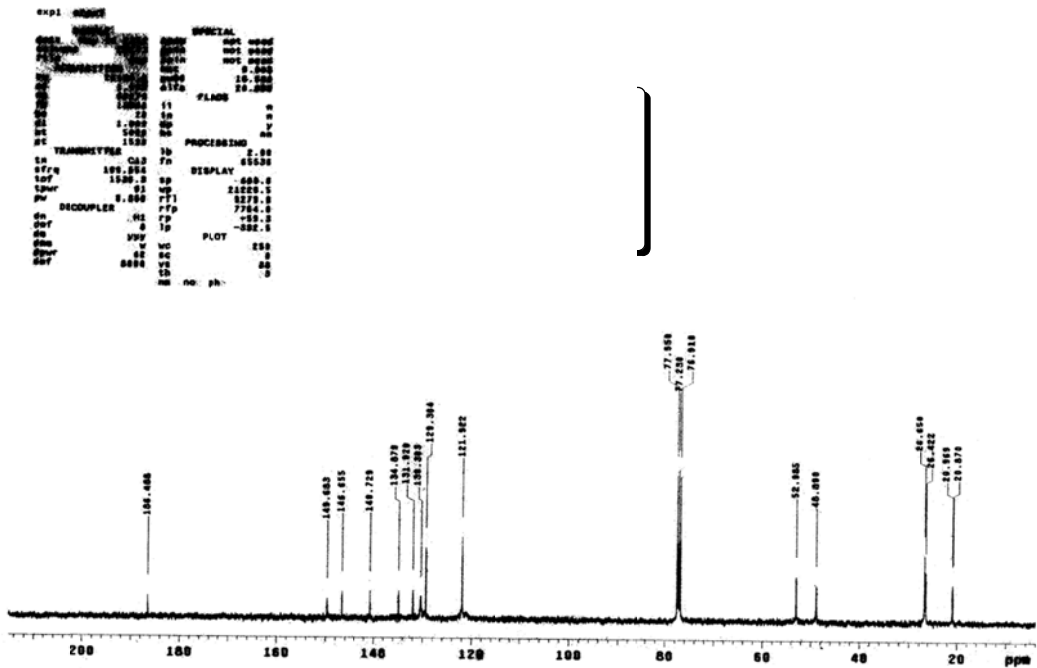


N-((*E*)-(*p*-Tolylimino)(morpholino)methyl)-*N*-*p*-tolylmorpholine-4-carbothioamide
(2a). ^{13}C NMR (100 MHz, CDCl_3):

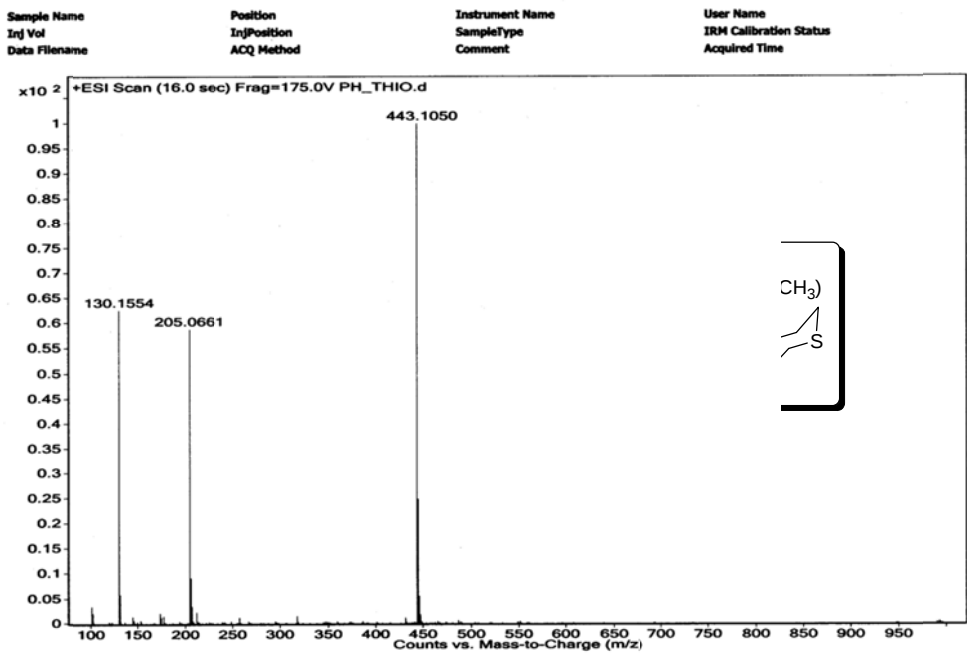


-S30 -

N-((*E*)-(p-Tolylimino)(thiomorpholino)methyl)-*N*-p-tolylthiomorpholine-4-carbothioamide (2b). ¹³C NMR (100 MHz, CDCl₃):

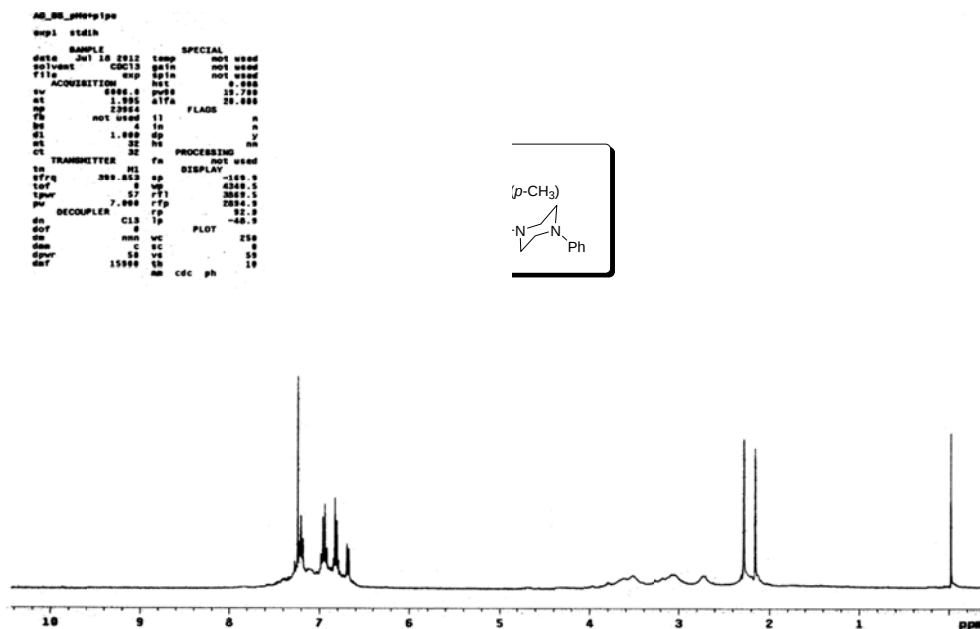


N-((*E*)-(p-Tolylimino)(thiomorpholino)methyl)-*N*-p-tolylthiomorpholine-4-carbothioamide (2b).
MASS SPECTRA:

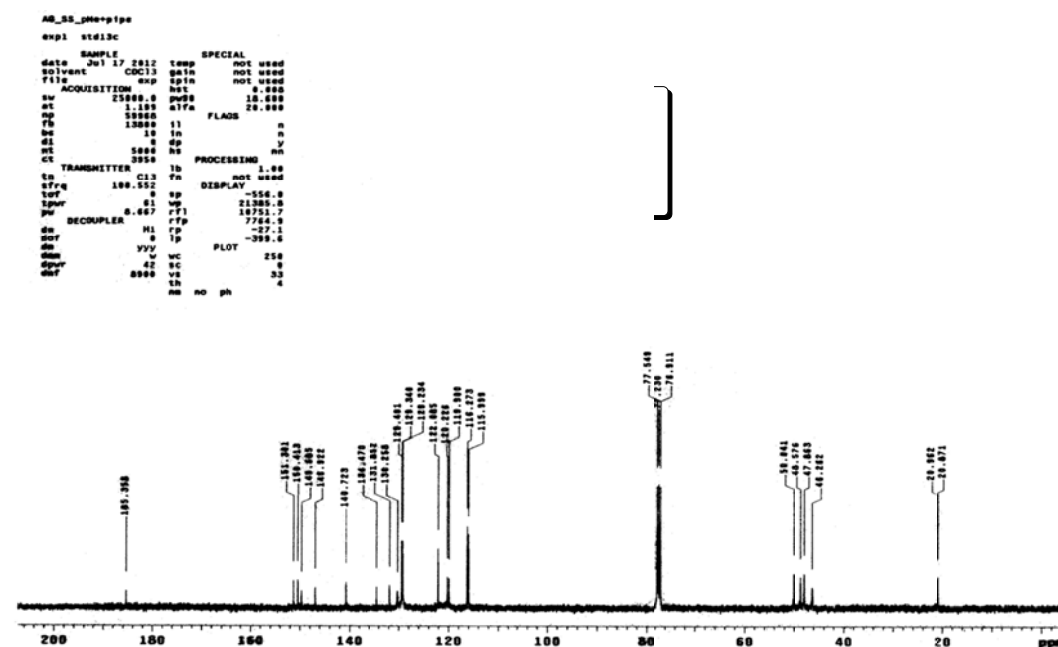


-S31 -

N-((*E*)-(p-Tolylimino)(4-phenylpiperzin-1-yl)methyl)-4-phenyl-*N*-p-tolylpiperazine-1-carbothioamide (2c). ^1H NMR (400 MHz, CDCl_3):

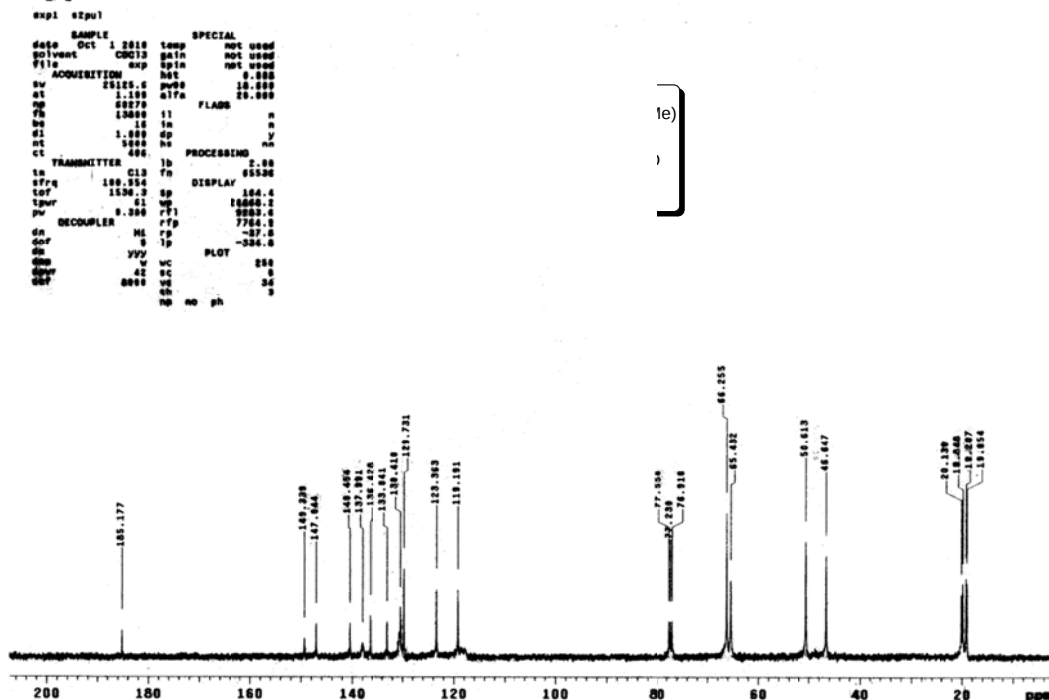


N-((*E*)-(p-Tolylimino)(4-phenylpiperzin-1-yl)methyl)-4-phenyl-*N*-p-tolylpiperazine-1-carbothioamide (2c). ^{13}C NMR (100 MHz, CDCl_3):

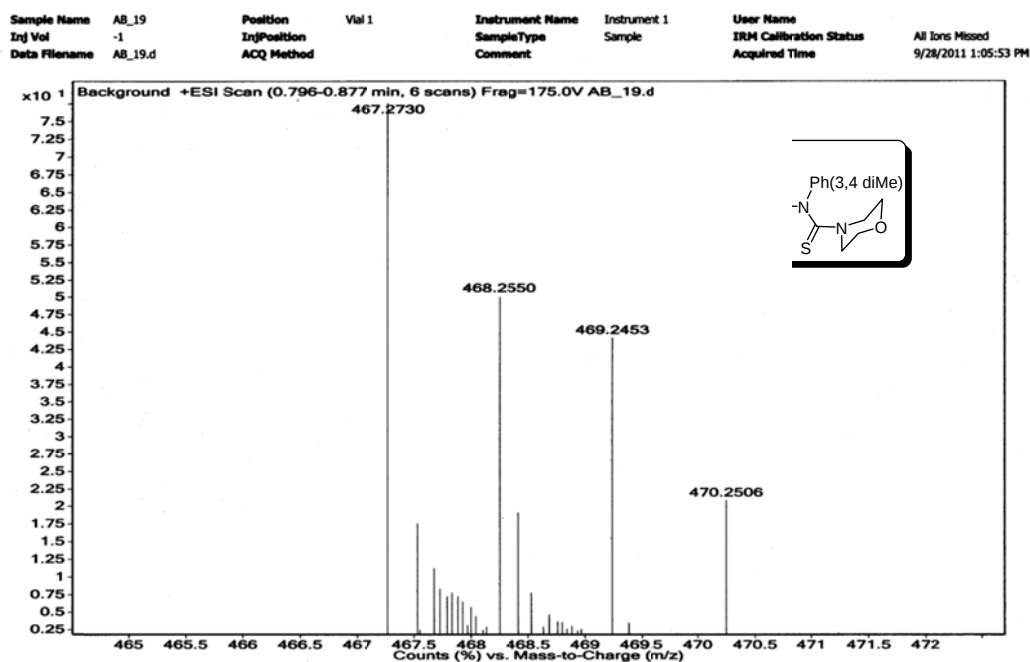


-S33 -

N-((*E*)-(3,4-Dimethylphenylimino)(morpholino)methyl)-*N*-(3,4-dimethylphenyl) morpholine-4-carbothioamide (3a). ¹³C NMR (100 MHz, CDCl₃):

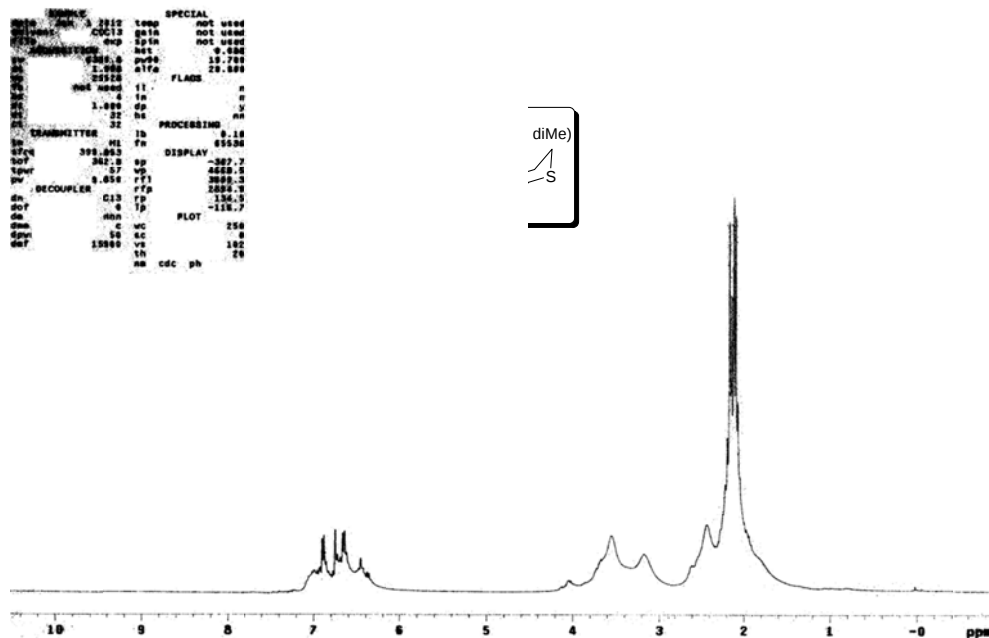


N-((*E*)-(3,4-Dimethylphenylimino)(morpholino)methyl)-*N*-(3,4-dimethylphenyl) morpholine-4-carbothioamide (3a). MASS SPECTRA:

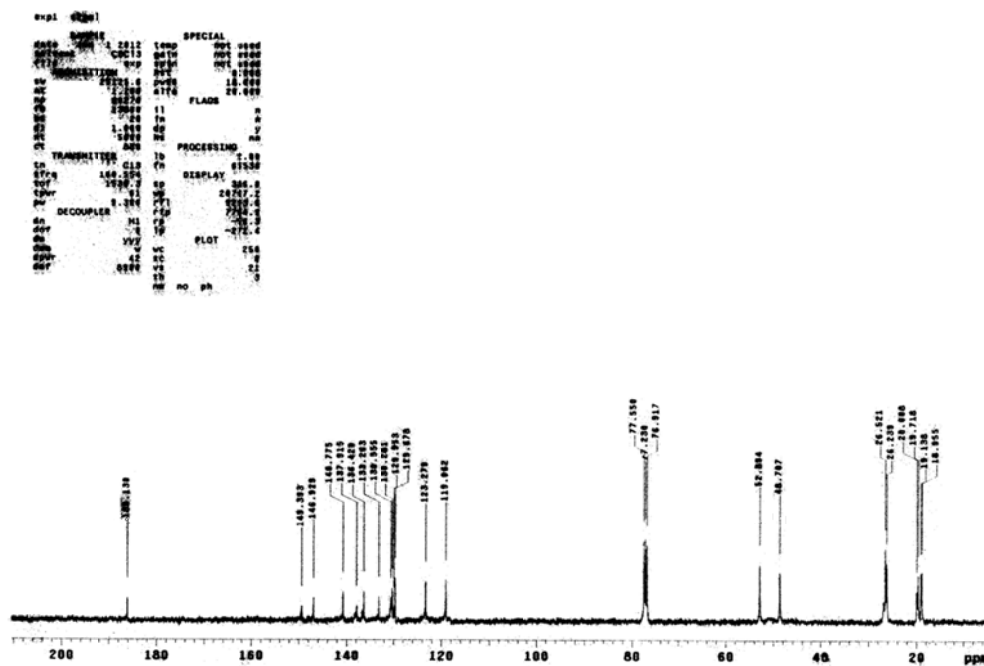


-S34 -

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

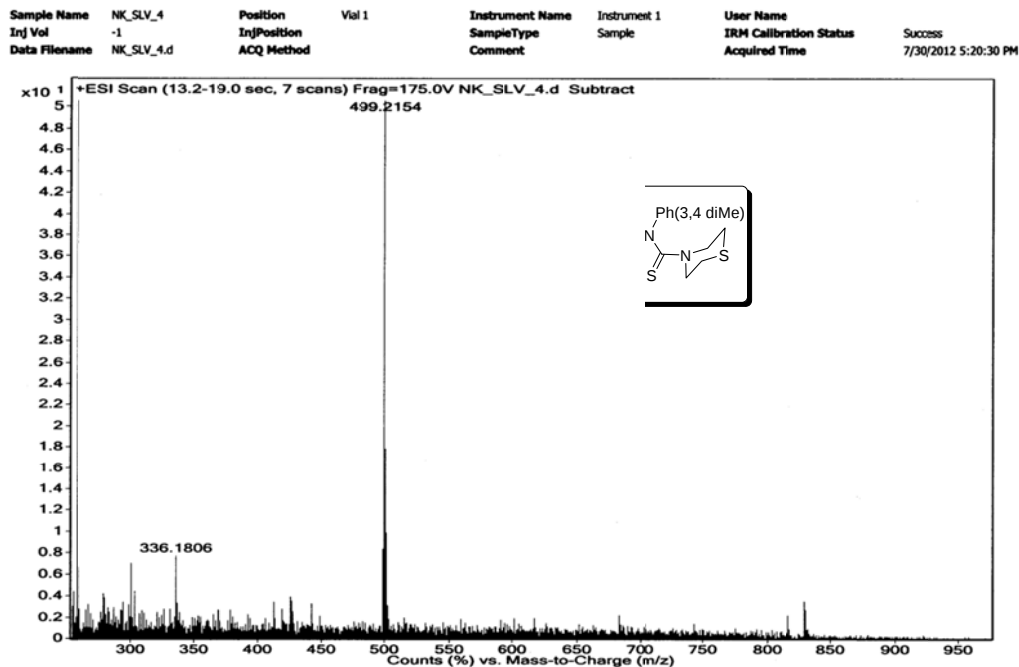


N-((*E*)-(3,4-Dimethylphenylimino)(thiomorpholino)methyl)-*N*-(3,4-dimethylphenyl)thiomorpholine-4-carbothioamide (3b). ^{13}C NMR (100 MHz, CDCl_3):

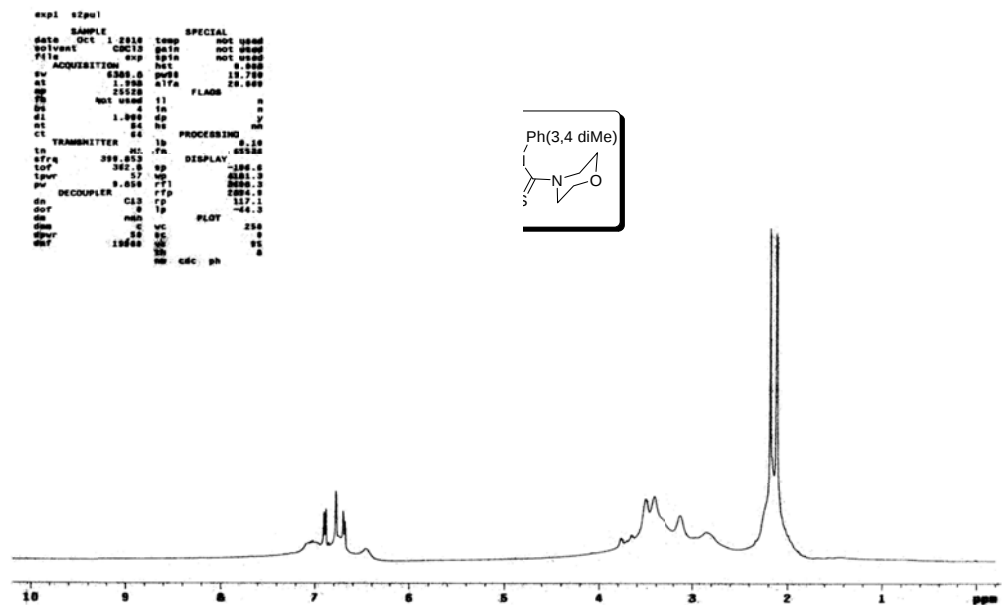


-S35 -

N-((*E*)-(3,4-Dimethylphenylimino)(thiomorpholino)methyl)-*N*-(3,4-dimethylphenyl)thiomorpholine-4-carbothioamide (3b). MASS SPECTRA:

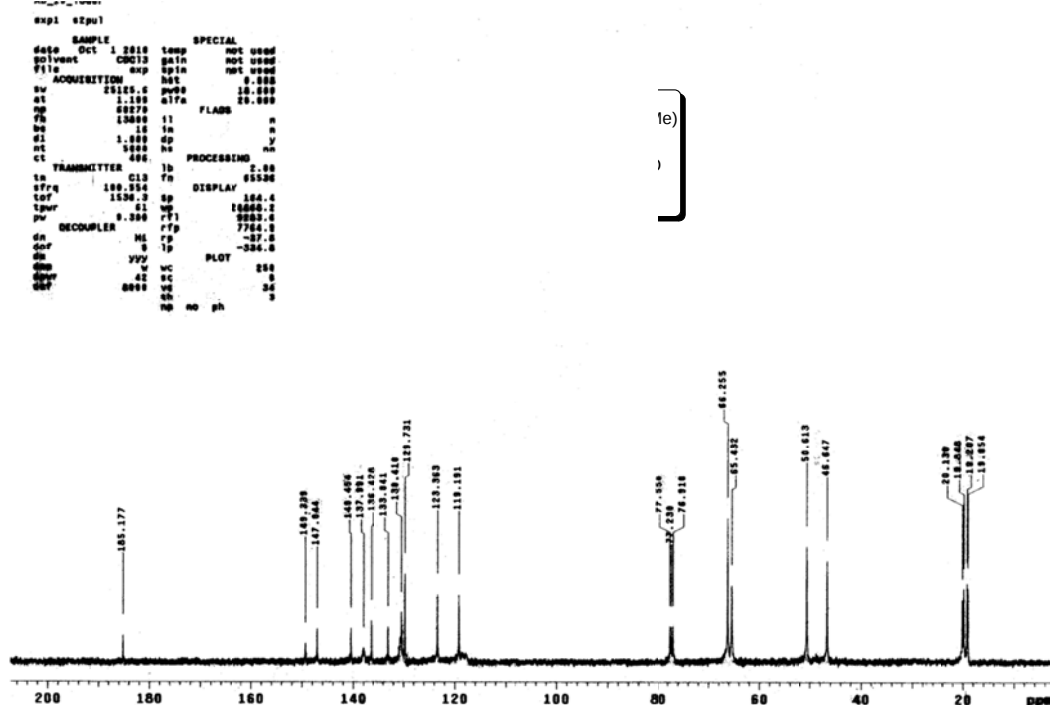


N-((*E*)-(3,4-Dimethylphenylimino)(morpholino)methyl)-*N*-(3,4-dimethylphenyl)morpholine-4-carbothioamide (4'a). ¹H NMR (400 MHz, CDCl₃):

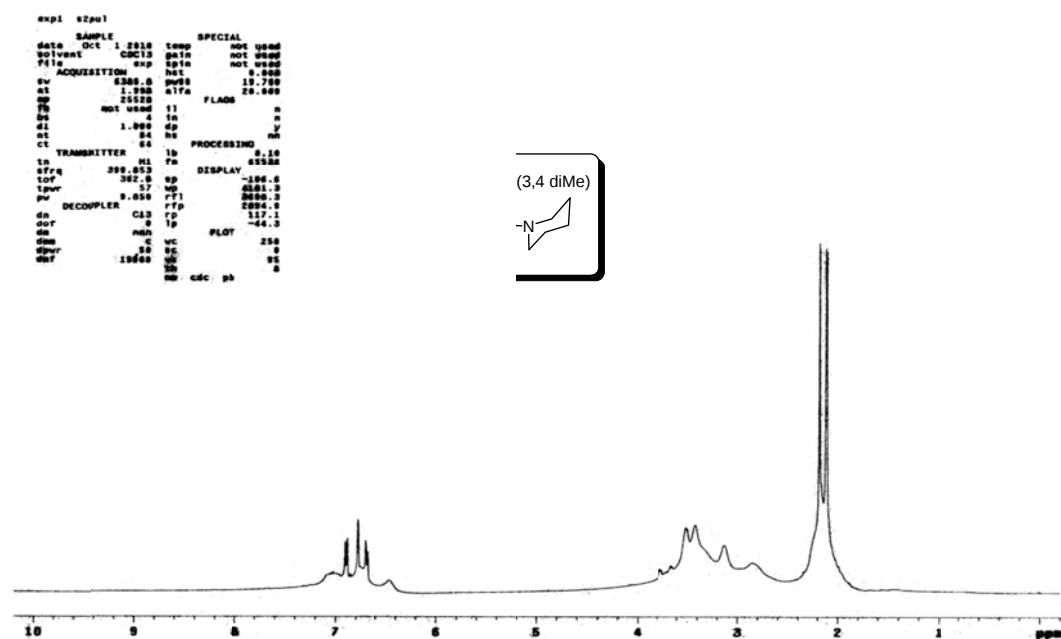


-S36-

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

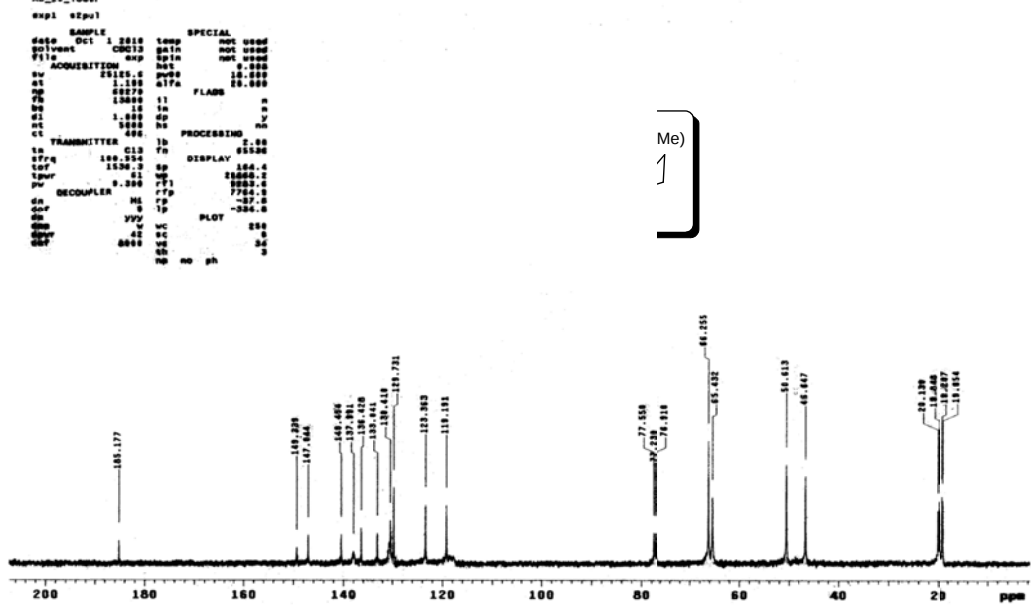


N-((*E*)-(3,4-Dimethylphenylimino)(piperidin-1-yl)methyl)-*N*-(3,4-dimethylphenyl) piperidine-1-carbothioamide (3d) ^1H NMR (400 MHz, CDCl_3):

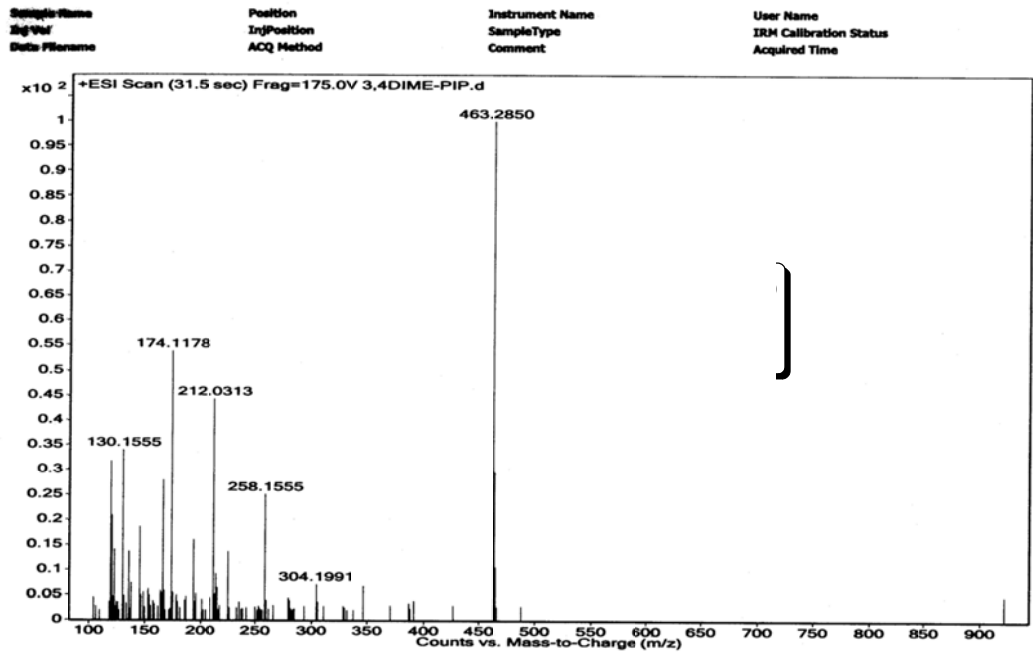


-S37 -

N-((*E*)-(3,4-Dimethylphenylimino)(piperidin-1-yl)methyl)-*N*-(3,4-dimethylphenyl) piperidine-1-carbothioamide (3d). ¹H NMR (400 MHz, CDCl₃):

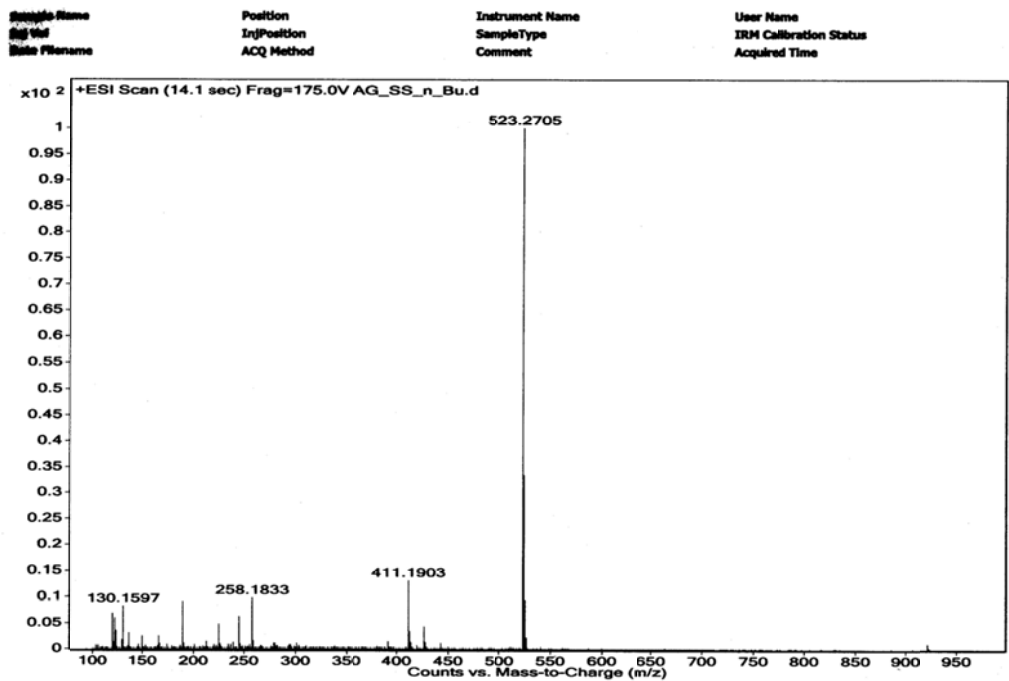


N-((*E*)-(3,4-Dimethylphenylimino)(morpholino)methyl)-*N*-(3,4-dimethylphenyl) morpholine-4-carbothioamide (3d). MASS SPECTRA:

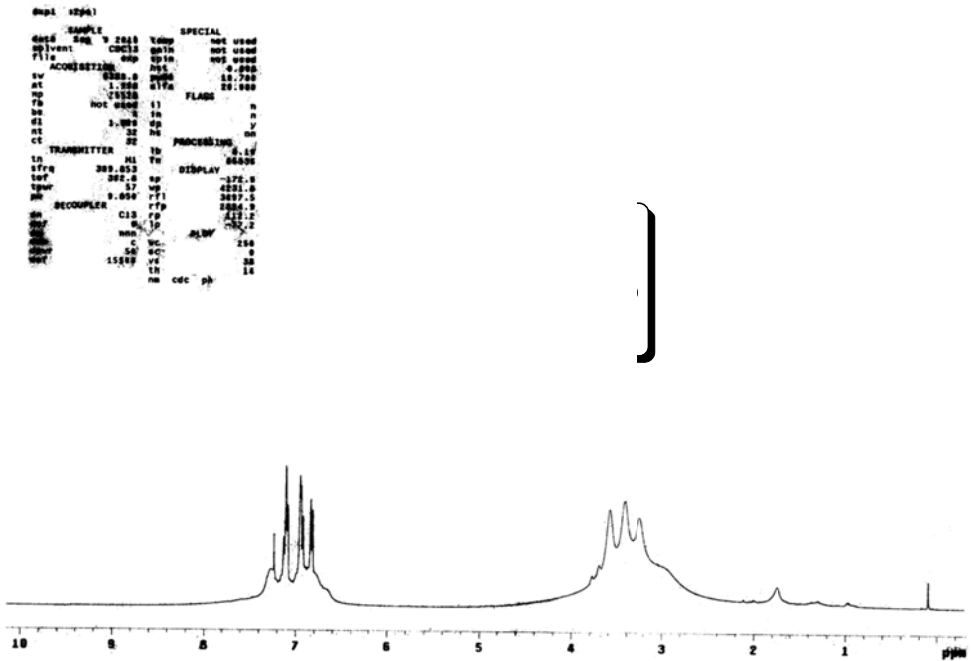


-S39 -

N-((*E*)-(4-Butylphenylimino)(morpholino)methyl)-*N*-(4-butylphenyl)morpholine-4-carbothioamide (4a) MASS SPECTRA:

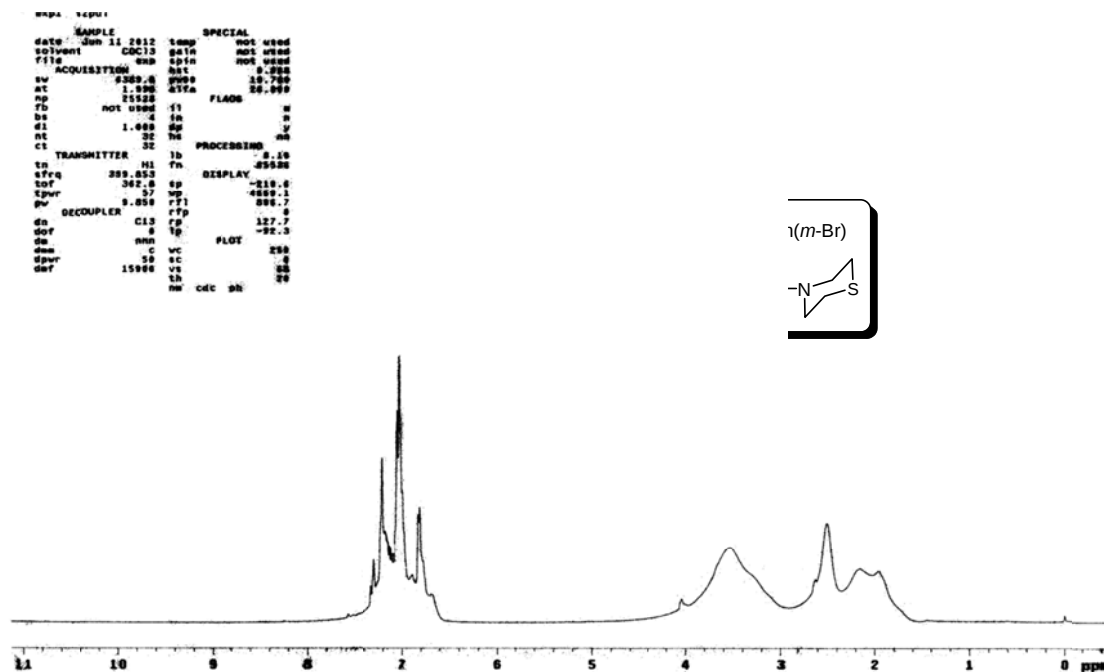


N-((*E*)-(3-Chlorophenylimino)(morpholino)methyl)-*N*-(3-Chlorophenyl)morpholine-4-carbothioamide (5a).¹H NMR (400 MHz, CDCl₃):

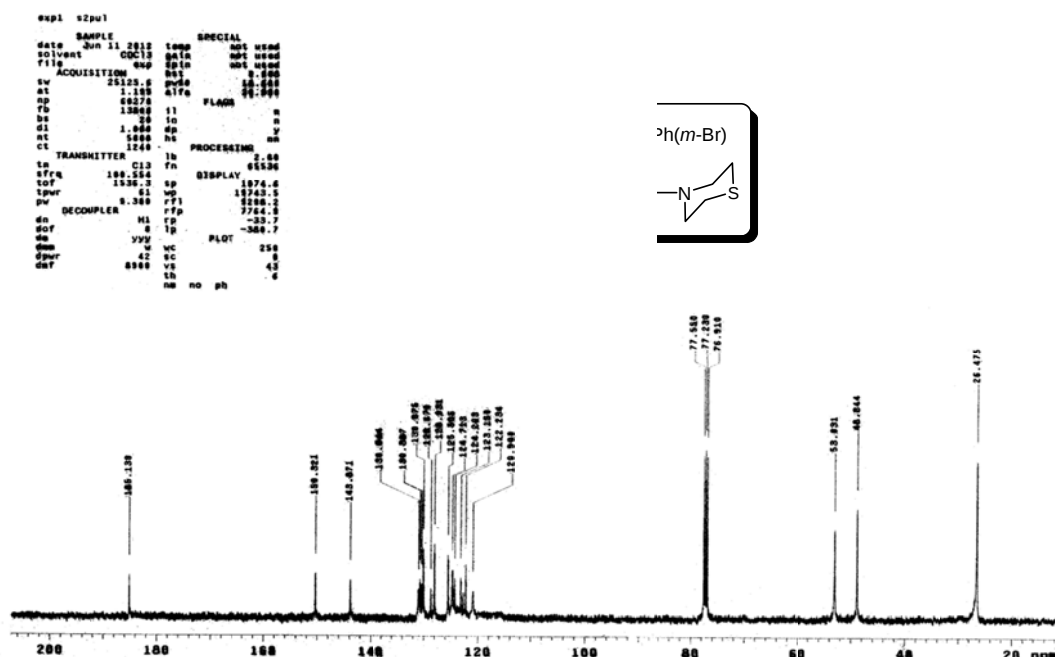


-S42-

N-((*E*)-(3-Bromophenylimino)(thiomorpholino)methyl)-*N*-(3-bromophenyl)thiomorpholine-4-carbothioamide (6b). ^1H NMR (400 MHz, CDCl_3):

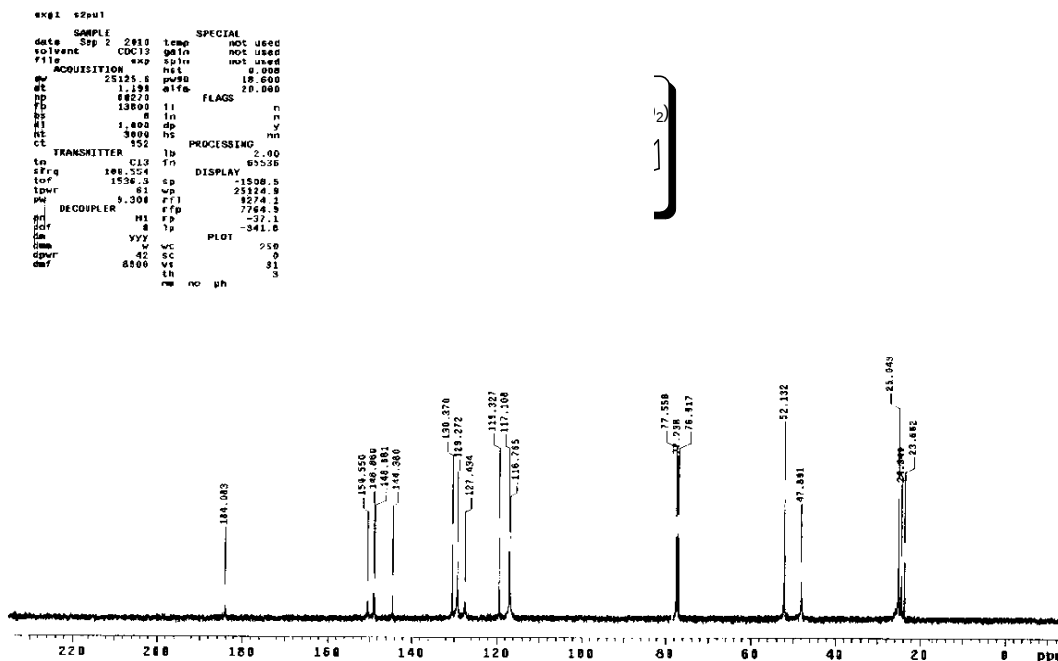


N-((*E*)-(3-Bromophenylimino)(thiomorpholino)methyl)-*N*-(3-bromophenyl)thiomorpholine-4-carbothioamide (6b). ^{13}C NMR (100 MHz, CDCl_3):

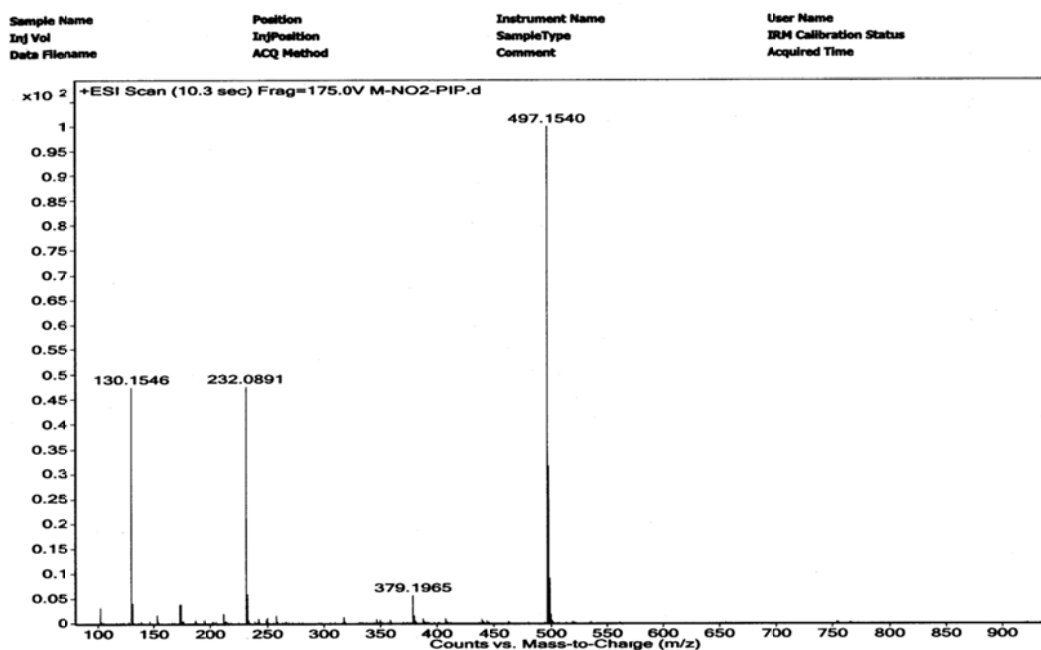


-S44 -

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:



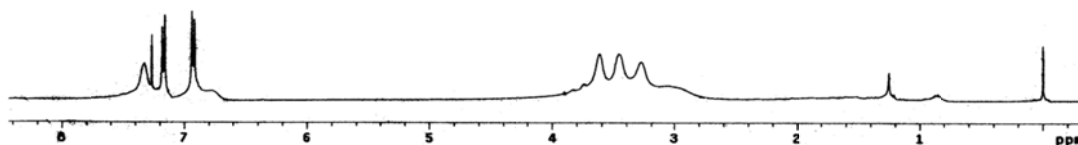
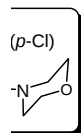
-S45 -

N-((*E*)-(4-Chlorophenylimino)(morpholino)methyl)-*N*-(4-chlorophenyl)morpholine-4-carbothioamide (**8a**). ^1H NMR (400 MHz, CDCl_3):

```

expt1 szpul
=====
date   SAMPLE  temp  SPECIAL
solvent CDC13  gain  not used
file   exp    spin  not used
=====
ACQUISITION
nu      8389.8  hst    0.000
at      1.988  aTfA   20.000
ap      25528
=====
f2      not used  f1      n
b2      4        in      n
d1      1.000    dp      y
nt      32      hs      nm
ct      32
=====
TRANSMITTER  t1  b1  PROCESSING  8.10
tn           C13  f1n  DISPLAY      65536
sfrq        389.803  sp      -148.0
tof         57      hp      25124.9
tpwr        9.850  rf1      764.9
pw          C13  rf2      137.5
=====
dn          9      rp      -84.5
dof         0      tp      -271.4
=====
dml         yyy  PL0T      250
dms         w   wc      9
dpr         42   sc      1.8
dwt         8900  vs      2.4
=====
nm          cdc  ph      10

```

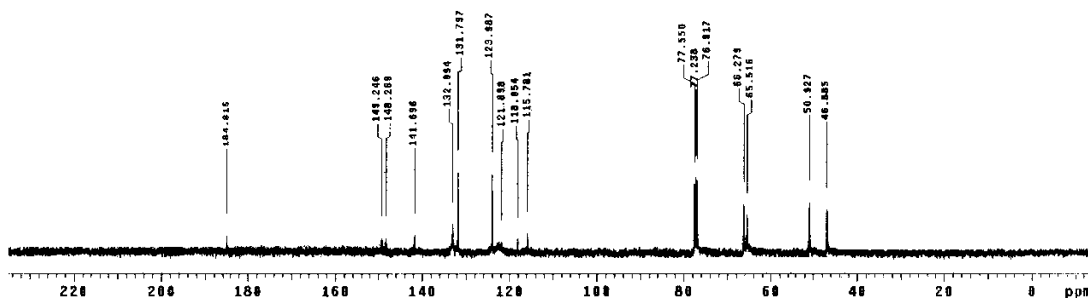
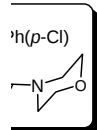


N-((*E*)-(4-Chlorophenylimino)(morpholino)methyl)-*N*-(4-chlorophenyl)morpholine-4-carbothioamide (**8a**). ^{13}C NMR (100 MHz, CDCl_3):

```

=====
date   SAMPLE  temp  SPECIAL
solvent CDC13  gain  not used
file   exp    spin  not used
=====
ACQUISITION
nu      25125.6  hst    0.000
at      1.198  aTfA   20.000
ap      60270
=====
f2      13800  f1      n
b2      8      in      n
d1      1.000    dp      y
nt      3000   hs      nm
ct      640
=====
TRANSMITTER  t1  b1  PROCESSING  2.00
tn           C13  f1n  DISPLAY      65536
sfrq        100.625  sp      -1588.2
tof         1538.5  hp      25124.9
tpwr        9.300  rf1      9271.8
pw          C13  rf2      764.9
=====
dn          0      rp      -84.5
dof         0      tp      -271.4
=====
dml         yyy  PL0T      250
dms         w   wc      9
dpr         42   sc      1.8
dwt         8900  vs      2.4
=====
nm          cdc  ph      2

```



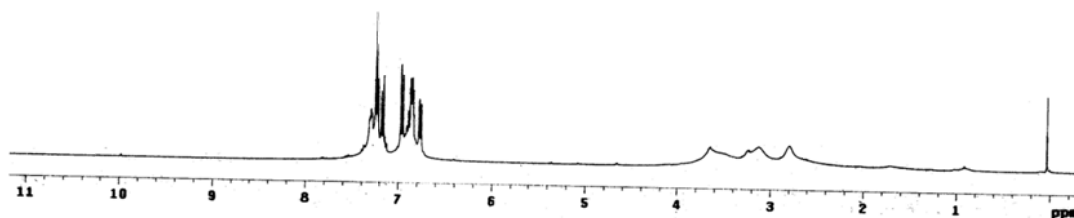
-S46-

N-((*E*)-(4-Chlorophenylimino)(4-phenylpiperazine-1-yl)methyl)-*N*-(4-chlorophenyl)-4-phenylpiperazine-1-carbothioamide (8c). ¹H NMR (100 MHz, CDCl₃):

```

SAMPLE
date Jun 19 2012
solvent CDCl3
file
ACQUISITION
sv 6389.8
at 1.998
np 15528
fb not used
di 1.988
nt 32
ct 32
TRANSMITTER
tr 1b
sfreq 399.653
tqf 362.8
tpwr 57
pw 9.658
deCOUPLER
dn C13
dof 8
dne 8
dpr 15908
dat 15908
SPECIAL
temp not used
gain not used
spin not used
nucl 0.008
puls 19.788
a1fa 20.089
FLABS
n
n
y
nn
PROCESSING
f2 0.10
f3 65536
DISPLAY
-141.4
4882.4
798.2
192.0
-80.4
PLOT
250
8
37
20
na cdc ph

```

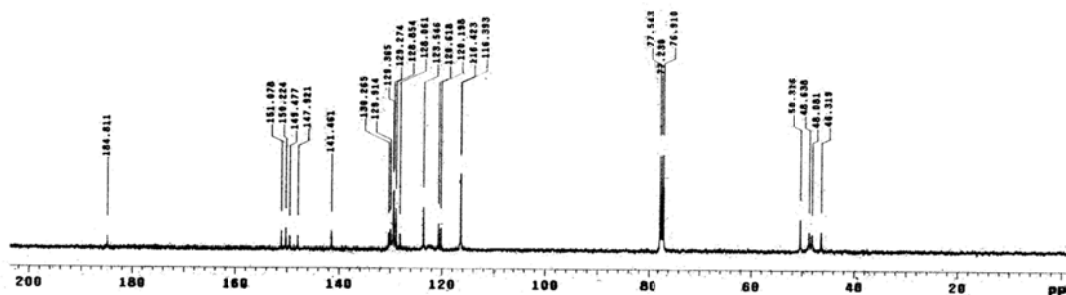


N-((*E*)-(4-Chlorophenylimino)(4-phenylpiperazine-1-yl)methyl)-*N*-(4-chlorophenyl)-4-phenylpiperazine-1-carbothioamide (8c). ¹³C NMR (400 MHz, CDCl₃):

```

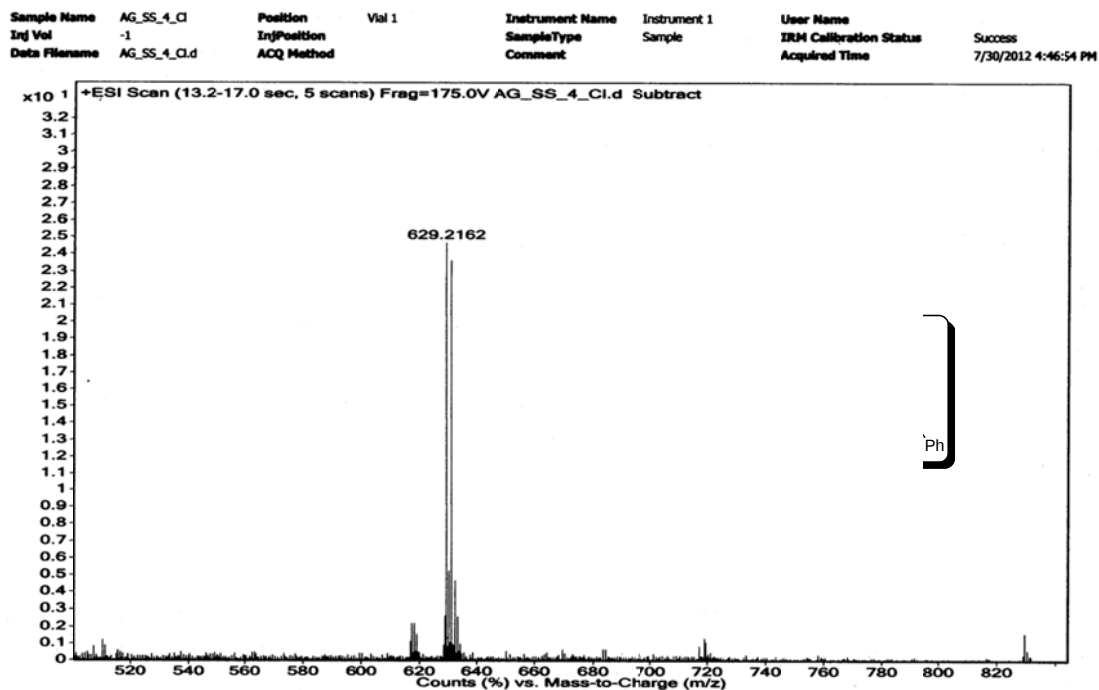
expl szpu1
SAMPLE
date Jun 19 2012
solvent CDCl3
file
ACQUISITION
sv 25125.6
at 1.998
np 89278
fb 13889
di 1.988
nt 32
ct 32
TRANSMITTER
tr C13
sfreq 100.625
tqf 1536.5
tpwr 61
pw 9.368
deCOUPLER
dn H1
dof 8
dne 8
dpr 8939
dat 8939
SPECIAL
temp not used
gain not used
spin not used
nucl 0.008
puls 19.788
a1fa 20.089
FLABS
n
n
y
nn
PROCESSING
f2 0.10
f3 65536
DISPLAY
-241.4
28833.1
7764.9
-51.4
-543.3
PLOT
250
8
37
20
na cdc ph

```

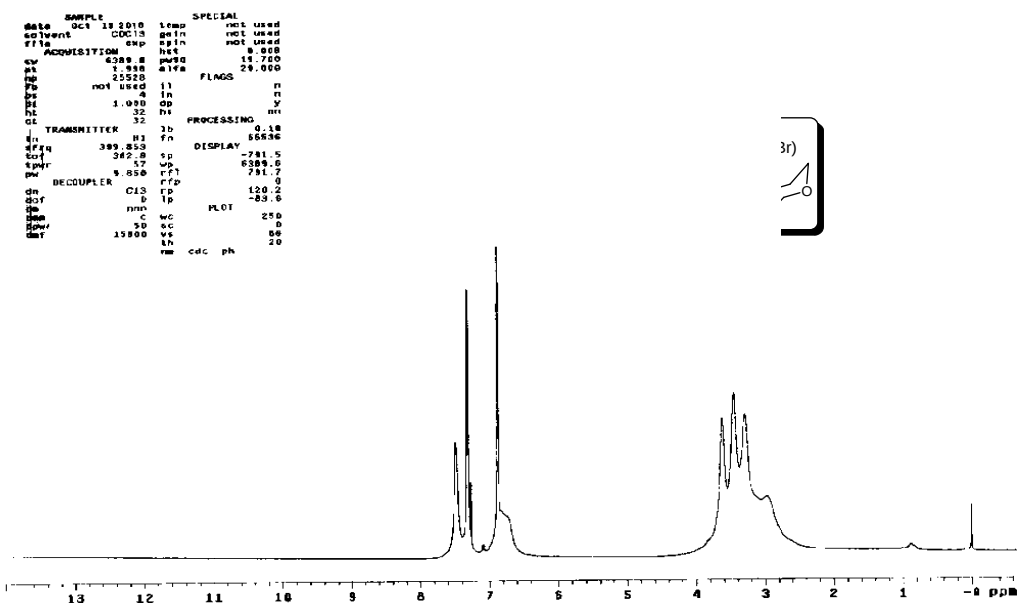


-S47 -

***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). ¹H NMR (400 MHz, CDCl₃):**



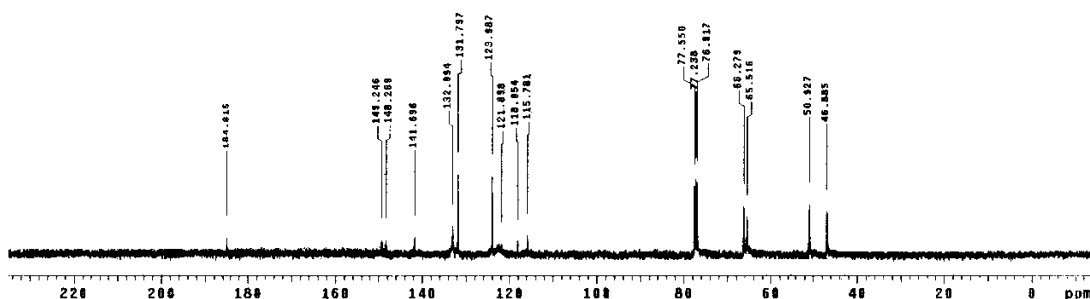
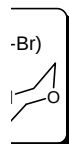
-S48 -

N-((*E*)-(4-Bromoophenylimino)(morpholino)methyl)-*N*-(4-bromophenyl)morpholine-4-carbothioamide (9a). ¹³C NMR (100 MHz, CDCl₃):

```

SAMPLE
date Oct 1 2009 temp SPECIAL
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION hst 0.000
sw 25125.6 ppg 10.000
at 1.198 atfa 20.000
np 60270
fp 13600 il FLAS n
bs 8 in n
d1 1.000 dp y
nt 3000 hs nn
ct 840
TRANSMITTER lb 2.00
tn C13 fn 65536
sfrq 100.554 DISPLAY
tof 1536.3 sp -1500.2
tpr 61 vp 25124.9
pw 9.300 rti 9271.8
DECOUPLER rfp 7764.9
dn H1 rp -84.5
dof 0 lp -271.4
dml yyy PLOT
dms w wc 250
dpr 42 sc 0
dnt 8900 vs 10
th 2
ne no ph

```

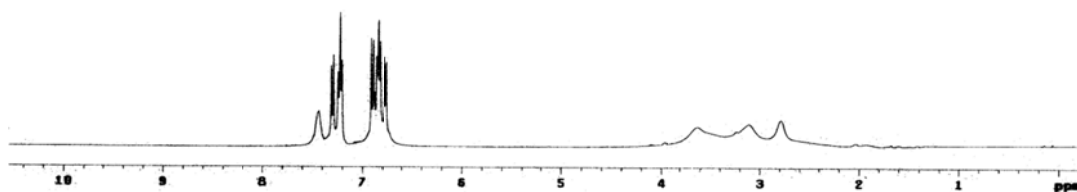
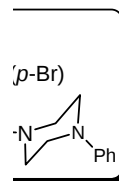


N-((*E*)-(4-Bromoophenylimino)(4-phenylpiperazin-1-yl)methyl)-*N*-(4-bromophenyl)phenylpiperazine-4-carbothioamide (9c). ¹H NMR (400 MHz, CDCl₃):

```

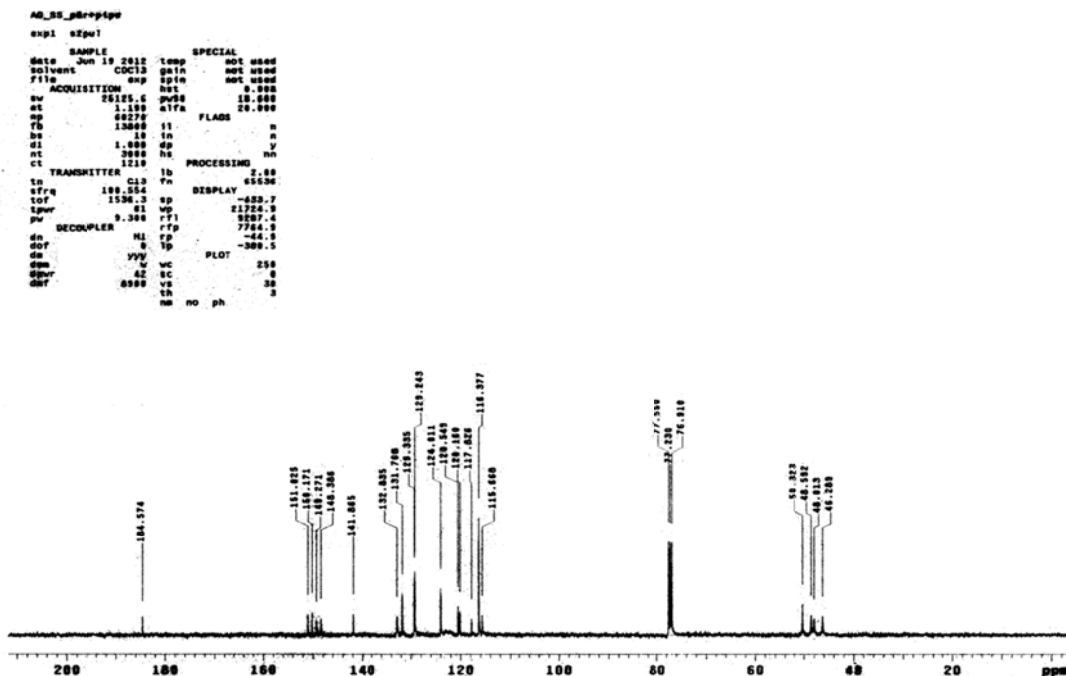
SAMPLE
date Jun 19 2012 temp SPECIAL
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION hst 0.000
sw 60000.0 ppg 10.000
at 1.998 atfa 20.000
np 25520
fb not used il FLAS n
bs 8 in n
d1 1.000 dp y
nt 32 hs nn
ct 32
TRANSMITTER lb 9.18
tn H1 fn 65506
sfrq 399.652 DISPLAY
tof 362.8 sp -110.8
tpr 87 vp 4332.5
pw 9.050 rti 812.6
DECOUPLER rfp 120.2
dn C13 rp -84.5
dof 8 lp
dml nm PLOT
dms c wc 250
dpr 50 sc 0
dnt 15000 vs 20
th 28
ne cdc ph

```

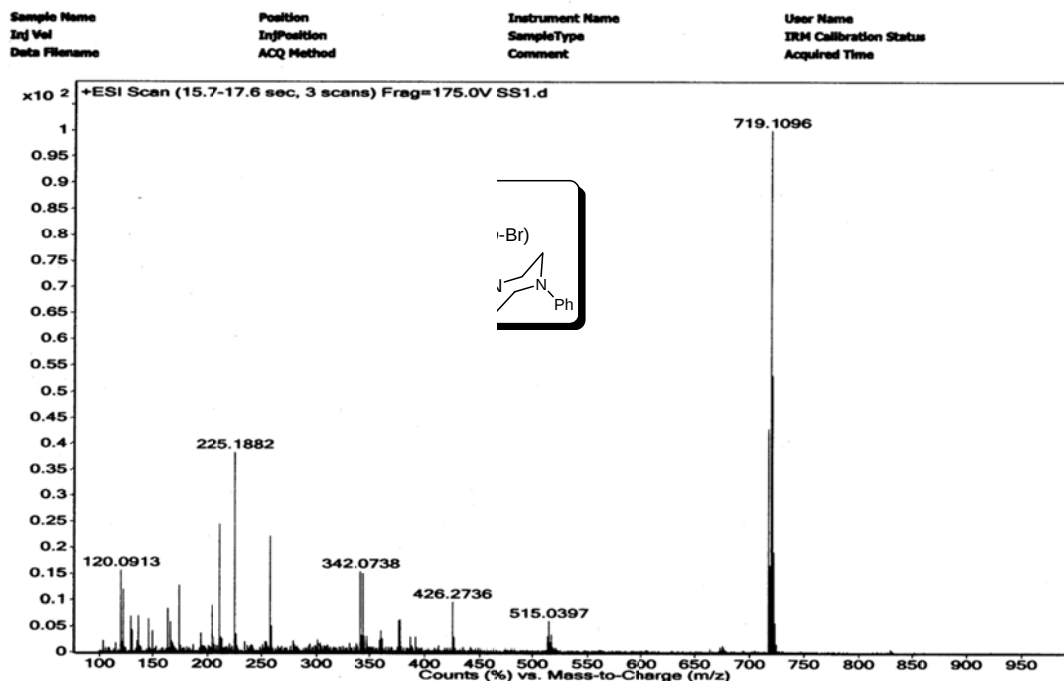


-S49 -

N-((*E*)-(4-Bromoophenylimino)(4-phenylpiperazin-1-yl)methyl)-*N*-(4-bromophenyl) phenylpiperazine-4-carbothioamide (9c). ¹³CNMR (100 MHz, CDCl₃):

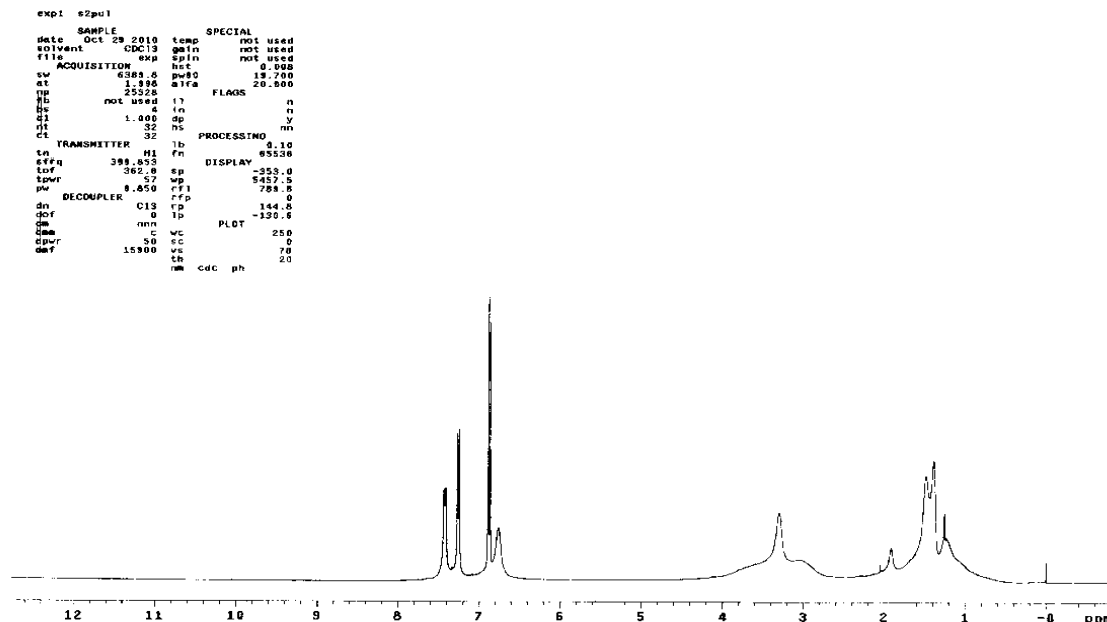


N-((*E*)-(4-Bromoophenylimino)(4-phenylpiperazin-1-yl)methyl)-*N*-(4-bromophenyl) phenylpiperazine-4-carbothioamide (9c). MASS SPECTRA:

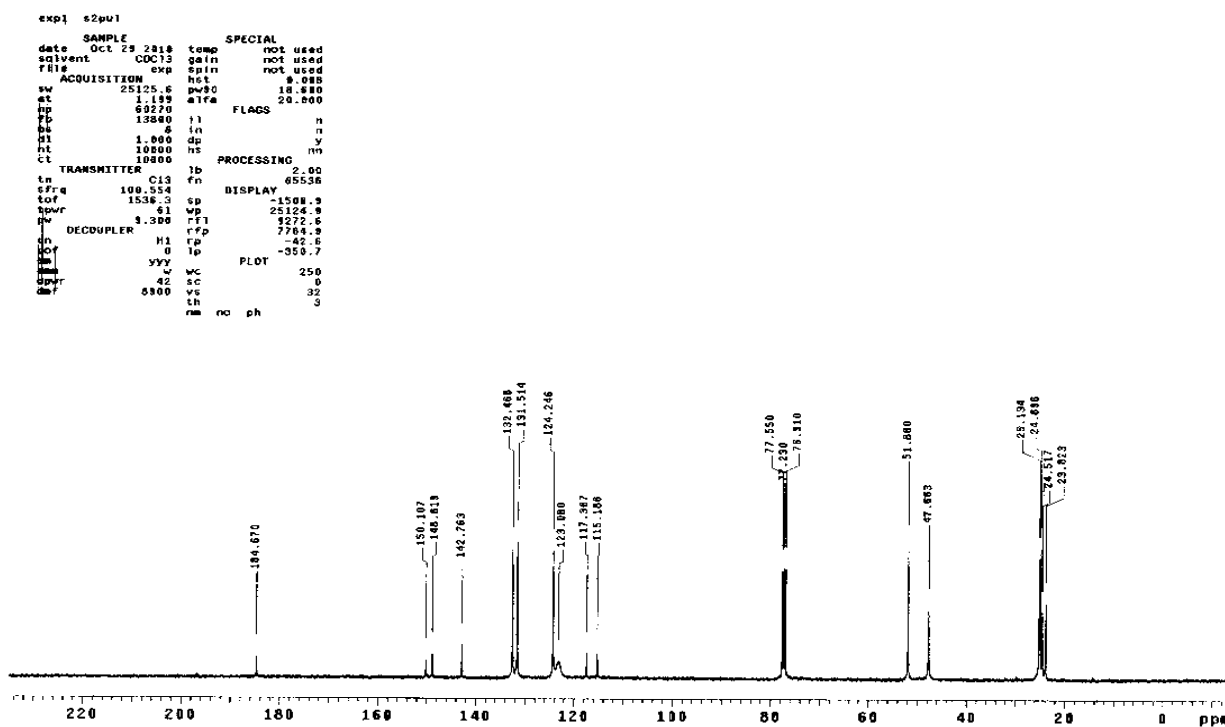


-S50-

N-((*E*)-(4-Bromoophenylimino)(piperidin-1-yl)methyl)-*N*-(2-bromophenyl)piperidine-1-carbothioamide (9d). ^1H 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):

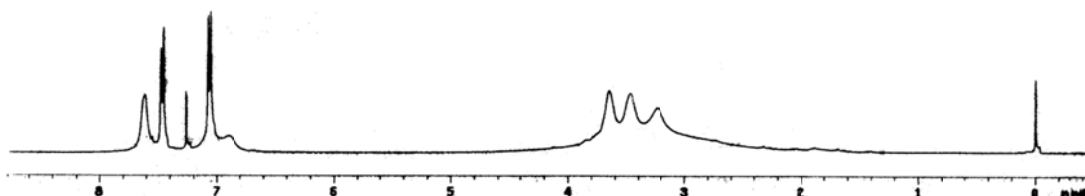
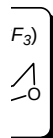


-S51 -

N-((*E*)-(4-Trifluoromethyl)phenylimino(morpholino)methyl)-*N*-(4-trifluorophenyl)
morpholine-4-carbothioamide (10a). ¹H NMR (400 MHz, CDCl₃):

```

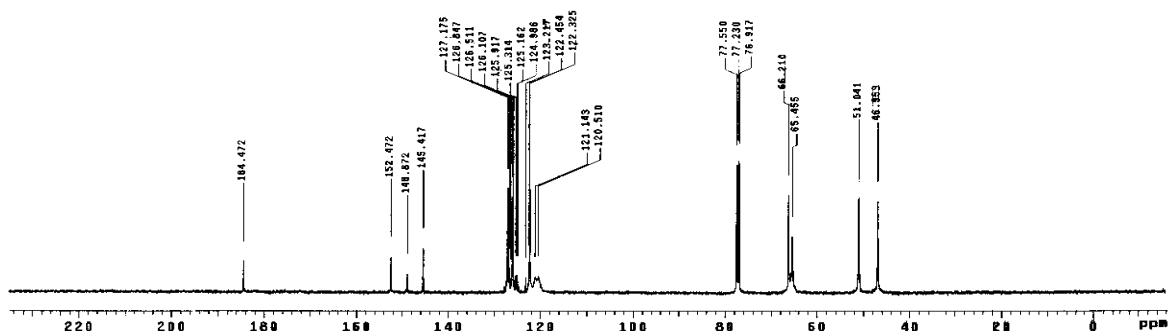
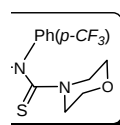
RV_2_280
exp1 szpuY
SAMPLE
date Aug 2 2010 temp not used
solvent CDCl3 gain not used
file /export/home/n spin not used
path /RV_2_280-rla hst 0.000
ACQUISITION pw90 10.700
          atfa 20.000
sv 5359.8
st 1.198
sp 25520
dp 11
f2 not used
f3 4
f4 1.000
f5 32
f6 32
f7 32
f8 32
f9 32
f10 32
TRANSMITTER C13
ct 32
tn H1
f1 399.853
f2 362.8
f3 377.3
f4 3.850
f5 3.850
f6 3.850
f7 3.850
f8 3.850
f9 3.850
f10 3.850
DECOUPLER C13
dn 0
dp 0
f1 0
f2 0
f3 0
f4 0
f5 0
f6 0
f7 0
f8 0
f9 0
f10 0
PLOT 250
nm cdc ph
  
```



N-((*E*)-(4-Trifluoromethyl)phenylimino(morpholino)methyl)-*N*-(4-trifluorophenyl)
morpholine-4-carbothioamide (10a). ¹³C NMR (400 MHz, CDCl₃):

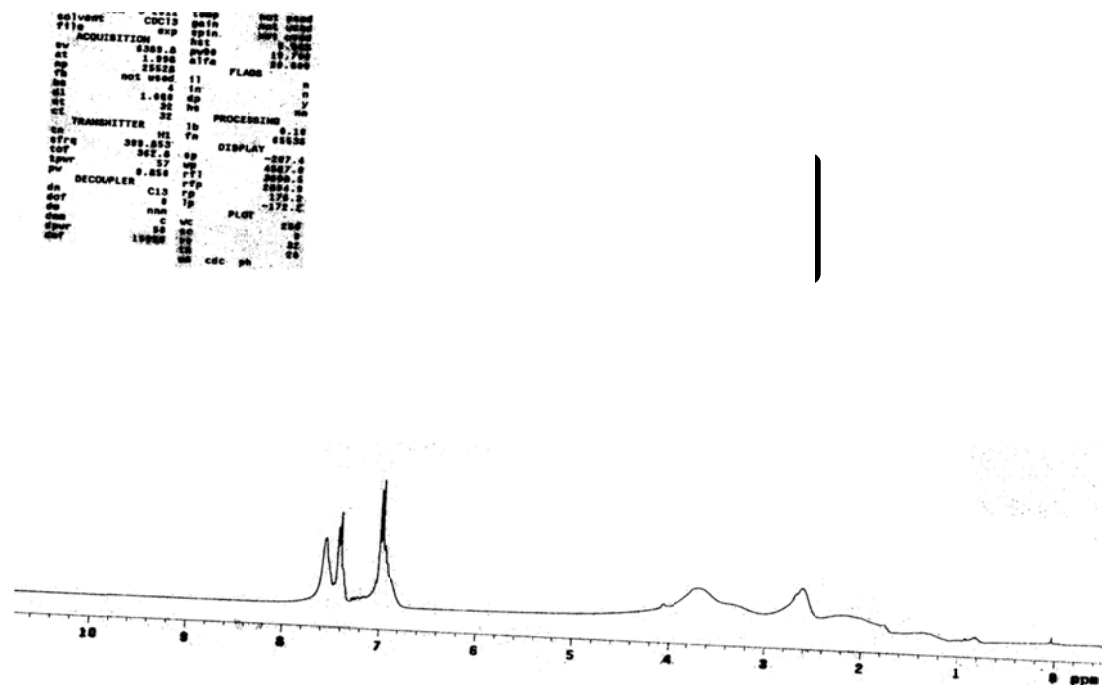
```

SAMPLE
date Aug 2 2010 temp not used
solvent CDCl3 gain not used
file /export/home/n spin not used
path /RV_2_280-rla hst 0.000
ACQUISITION pw90 10.700
          atfa 20.000
sv 25125.6
st 1.198
sp 25520
dp 11
f2 not used
f3 4
f4 1.000
f5 32
f6 32
f7 32
f8 32
f9 32
f10 32
TRANSMITTER C13
ct 32
tn H1
f1 399.853
f2 362.8
f3 377.3
f4 3.850
f5 3.850
f6 3.850
f7 3.850
f8 3.850
f9 3.850
f10 3.850
DECOUPLER C13
dn 0
dp 0
f1 0
f2 0
f3 0
f4 0
f5 0
f6 0
f7 0
f8 0
f9 0
f10 0
PLOT 250
nm cdc ph
  
```

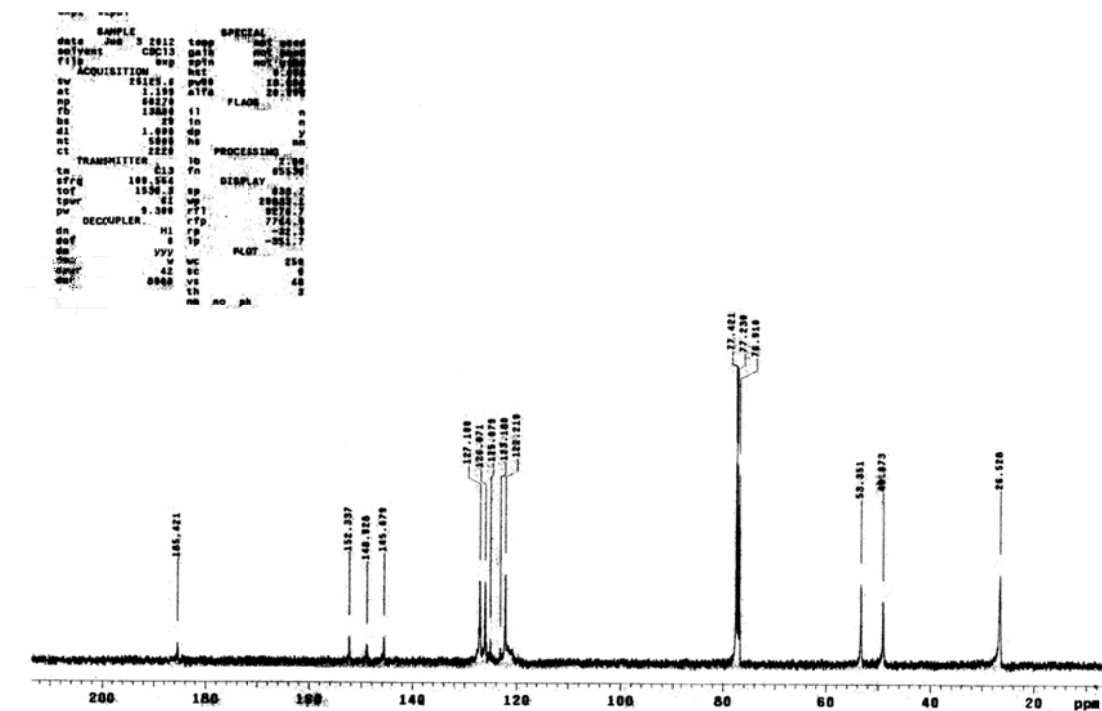


-S52-

N-((*E*)-(4-Trifluoromethyl)phenylimino(thiomorpholino)methyl)-*N*-(4-trifluorophenyl)thiomorpholine-4-carbothioamide (10b). ^1H NMR (400 MHz, CDCl_3):

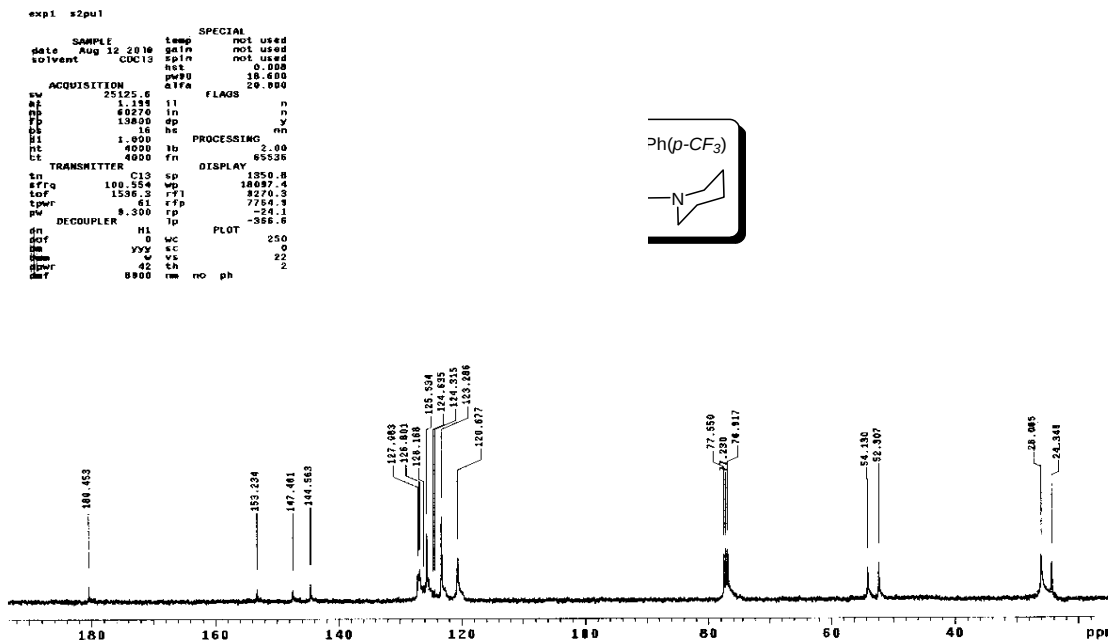


N-((*E*)-(4-Trifluoromethyl)phenylimino(thiomorpholino)methyl)-*N*-(4-trifluorophenyl)thiomorpholine-4-carbothioamide (10b). ^{13}C NMR (100 MHz, CDCl_3):

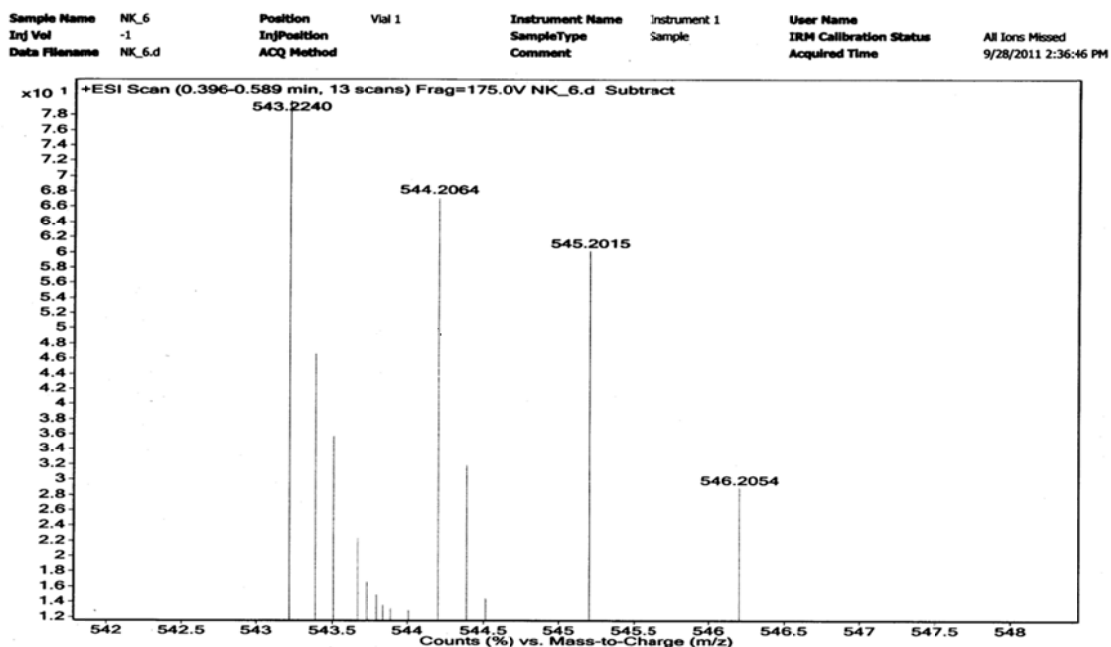


-S54 -

N-((*E*)-(4-Trifluoromethyl)(phenylimino)(piperidin-1-yl)methyl)-*N*-(4-bromophenyl)morpholine-1-carbothioamide (10d). ¹³C NMR (100 MHz, CDCl₃):



N-((*E*)-(4-Trifluoromethyl)(phenylimino)(piperidin-1-yl)methyl)-*N*-(4-bromophenyl)morpholine-1-carbothioamide (10d). MASS SPECTRA:



-S55 -

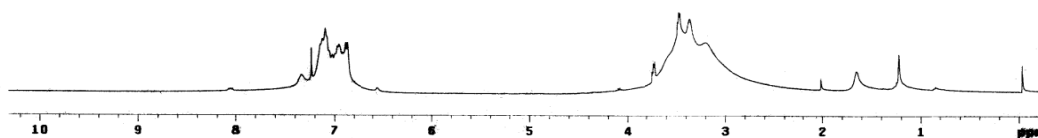
N-((*E*)-(2-Fluorophenylimino)(morpholino)methyl)-*N*-(2-fluorophenyl)morpholine-4-carbothioamide (11a). ^1H NMR (400 MHz, CDCl_3):

```

exp1 s2pu1
=====
date  Oct 11 2010   temp  not used
solvent  CDCl3      gain  not used
file     exp       spin  not used
=====
ACQUISITION  hst      8.000
sv  6389.8  pw99      18.000
at  1.980  a1fa      20.000
np  25520
rb  not used  11      n
bs  4        1n      n
d1  1.000    dp      y
nt  64      hs      nn
ct  64
=====
TRANSMITTER  1b  PROCESSING  2.00
to  s1f1      fn  65536
sfreq  100.554  sp  2542.3
tof  1536.3  sp  17894.7
tpr  61      r1  8283.6
pw  9.000    r1p  7764.8
=====
DECOUPLER  H1  r2  -37.8
dn  0        1p  -353.5
dof  0
ds  y/v      WC  250
dm  42      SC  8
dpr  8900   VS  65
det  8900   th  4
nm  no ph

```

1

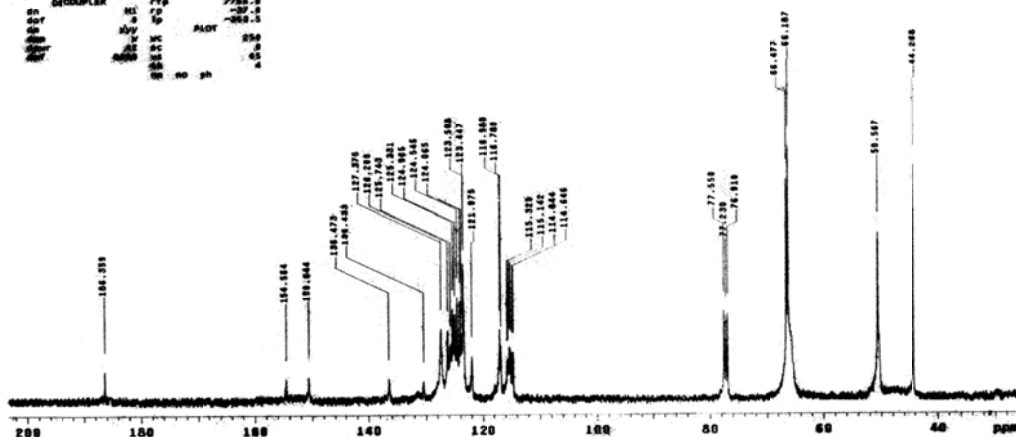


N-((*E*)-(2-Fluorophenylimino)(morpholino)methyl)-*N*-(2-fluorophenyl)morpholine-4-carbothioamide (11a). ^{13}C NMR (100 MHz, CDCl_3):

```

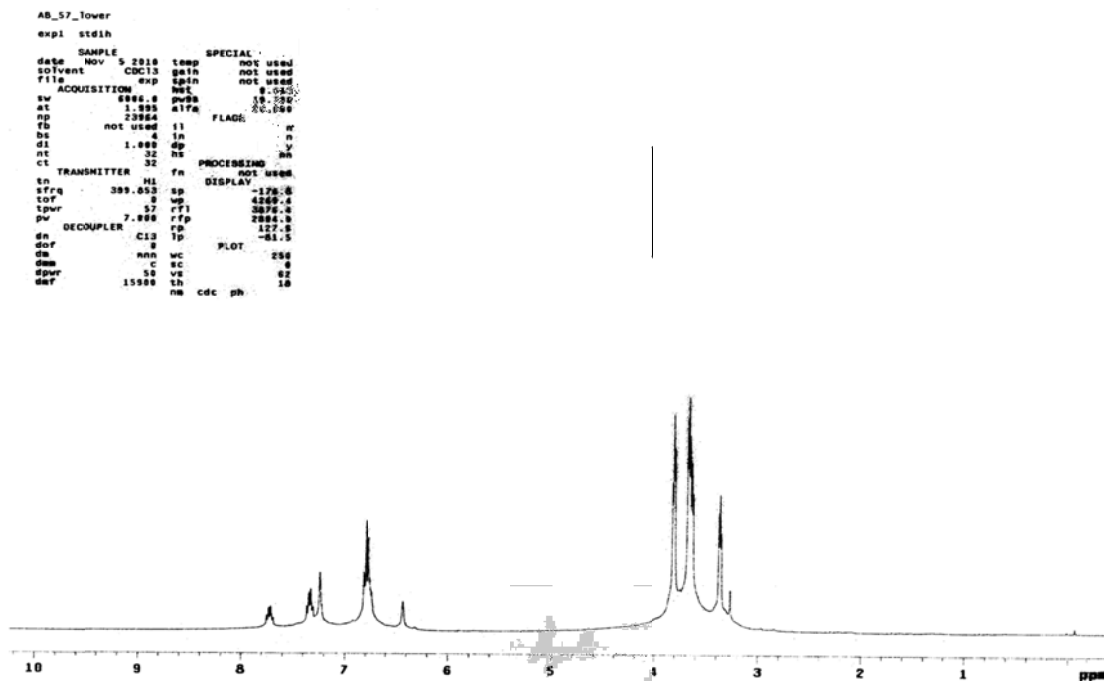
exp1 s2pu1
=====
date  Oct 11 2010   temp  not used
solvent  CDCl3      gain  not used
file     exp       spin  not used
=====
ACQUISITION  hst      8.000
sv  6389.8  pw99      18.000
at  1.980  a1fa      20.000
np  25520
rb  not used  11      n
bs  4        1n      n
d1  1.000    dp      y
nt  64      hs      nn
ct  64
=====
TRANSMITTER  1b  PROCESSING  2.00
to  s1f1      fn  65536
sfreq  100.554  sp  2542.3
tof  1536.3  sp  17894.7
tpr  61      r1  8283.6
pw  9.000    r1p  7764.8
=====
DECOUPLER  H1  r2  -37.8
dn  0        1p  -353.5
dof  0
ds  y/v      WC  250
dm  42      SC  8
dpr  8900   VS  65
det  8900   th  4
nm  no ph

```

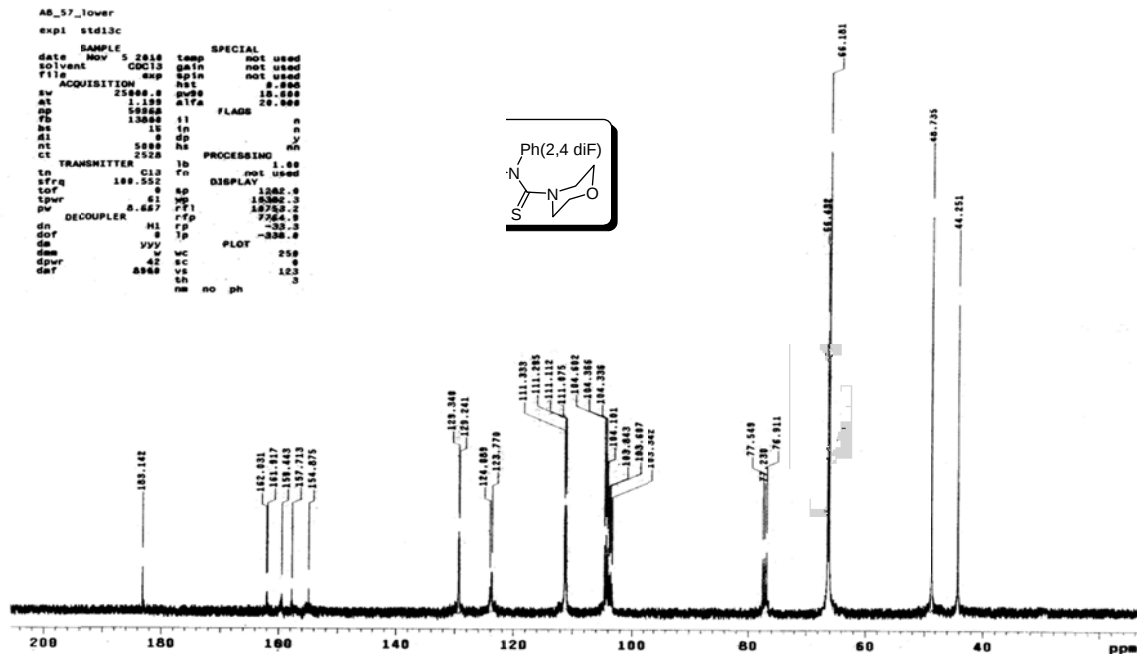


-S58-

N-((*E*)-(2,4-Difluorophenylimino)(morpholino)methyl)-*N*-(2,4-difluorophenyl)morpholine-4-carbothioamide (12a). ^1H NMR (400 MHz, CDCl_3):

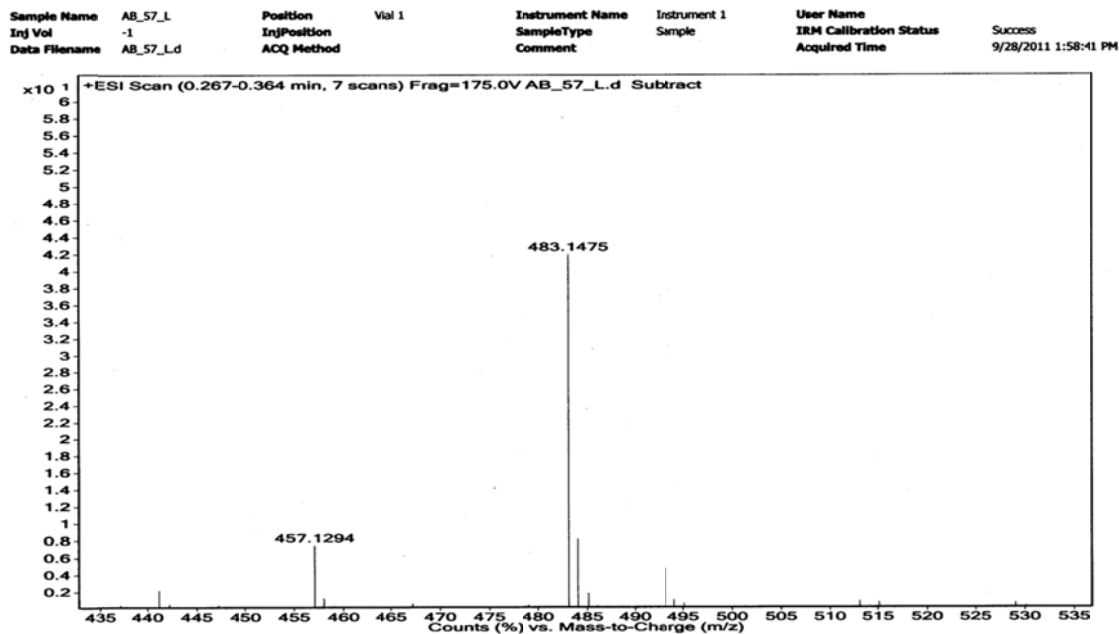


N-((*E*)-(2,4-Difluorophenylimino)(morpholino)methyl)-*N*-(2,4-difluorophenyl)morpholine-4-carbothioamide (12a). ^{13}C NMR (100 MHz, CDCl_3):

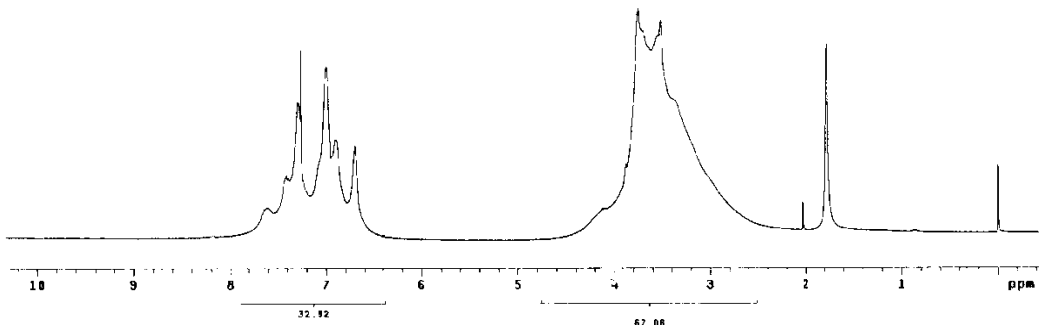
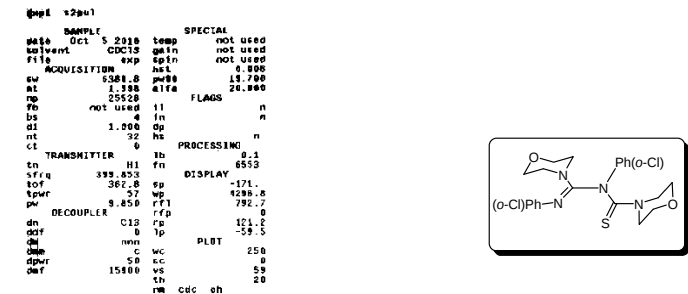


-S59 -

N-((*E*)-(2,4-Difluorophenylimino)(morpholino)methyl)-*N*-(2,4-difluorophenyl)morpholine-4-carbothioamide (12a). MASS SPECTRA:

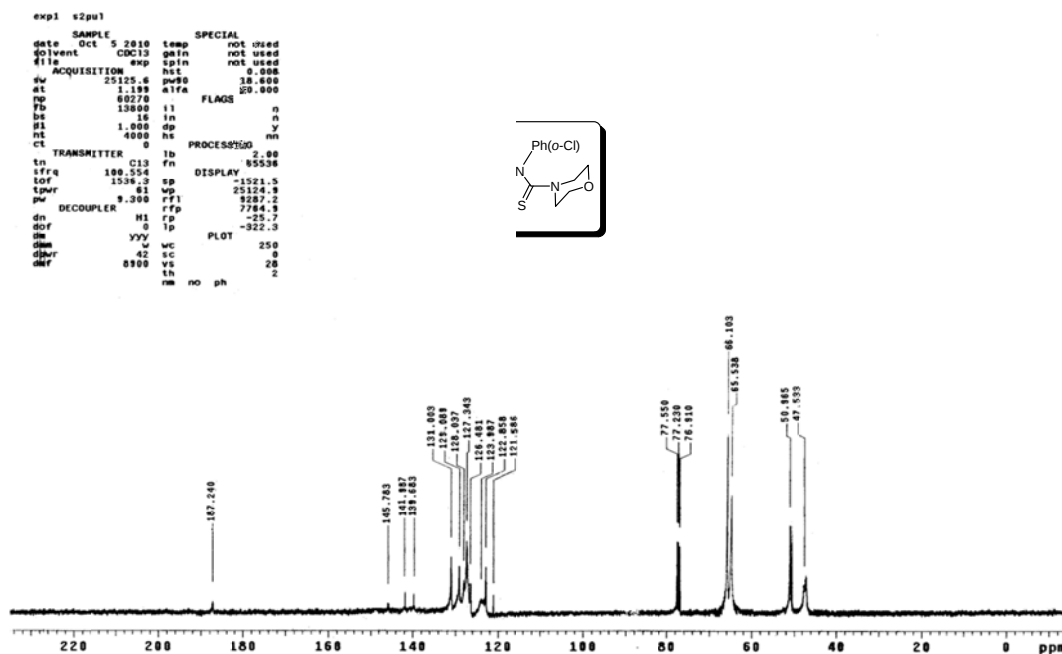


N-((*E*)-(2-Chlorophenylimino)(morpholino)methyl)-*N*-(2-chlorophenyl)morpholine-4-carbothioamide (13a). ¹H NMR (400 MHz, CDCl₃):

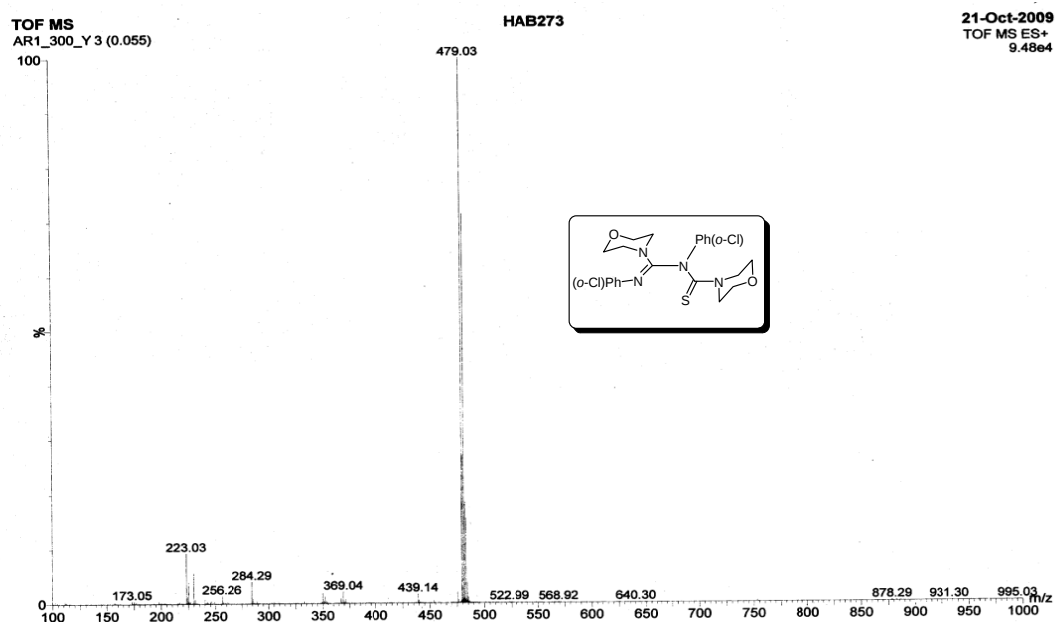


-S60-

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

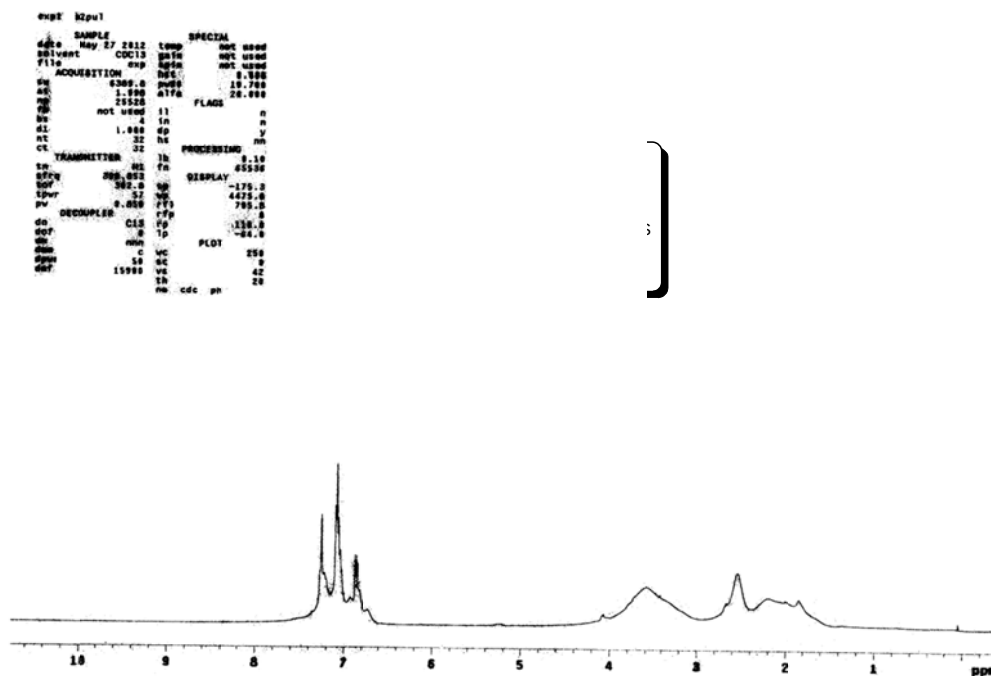


N-((*E*)-(2-Chlorophenylimino)(morpholino)methyl)-*N*-(2-chlorophenyl)morpholine-4-carbothioamide (13a): Mass Spectra

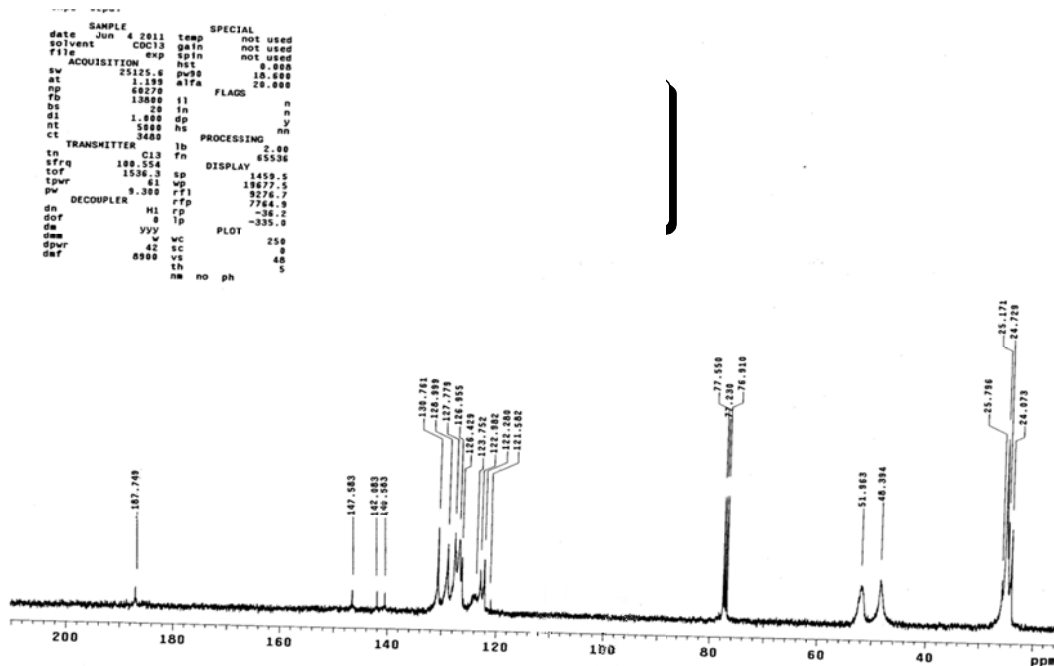


-S61 -

N-((*E*)-(2-Chlorophenylimino)(thiomorpholino)methyl)-*N*-(2-chlorophenyl) thiomorholine-1-carbothioamide (13b). ^1H NMR (400 MHz, CDCl_3):

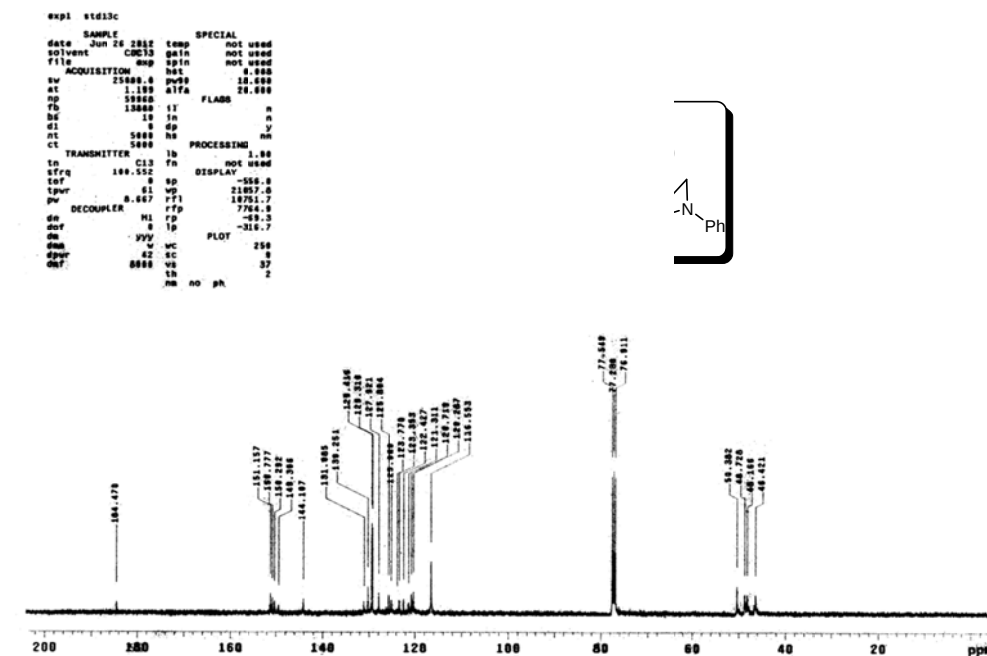


N-((*E*)-(2-Chlorophenylimino)(thiomorpholino)methyl)-*N*-(2-chlorophenyl) thiomorholine-1-carbothioamide (13b). ^{13}C NMR (100 MHz, CDCl_3):

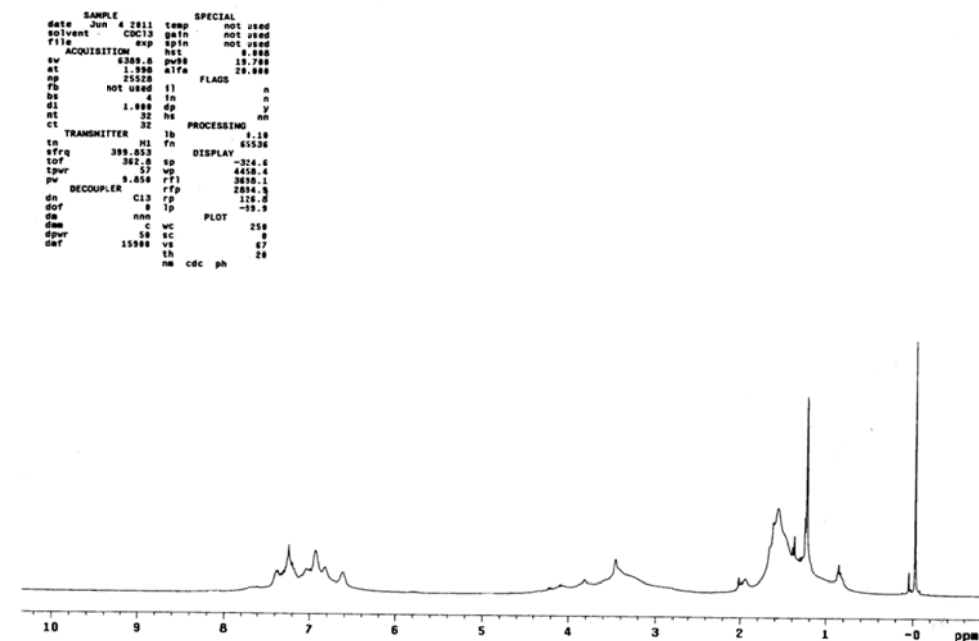


-S63 -

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

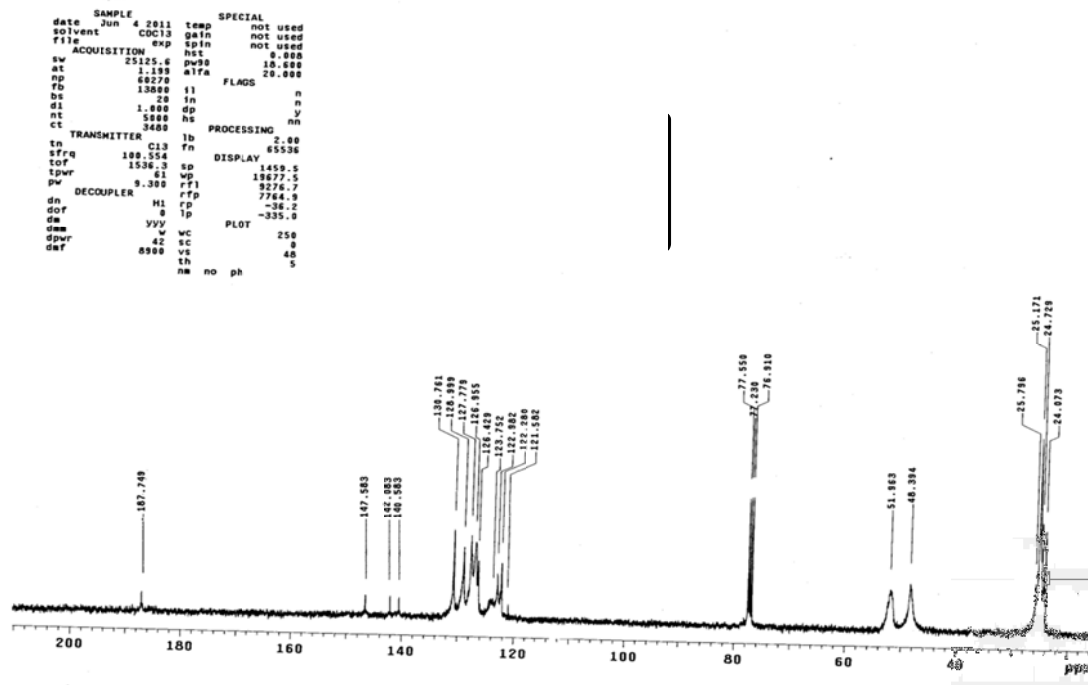


N-((*E*)-(2-Chlorophenylimino)(piperidin-1-yl)methyl)-*N*-(2-chlorophenyl)piperidine-1-carbothioamide (13d). ^1H NMR (400 MHz, CDCl_3):

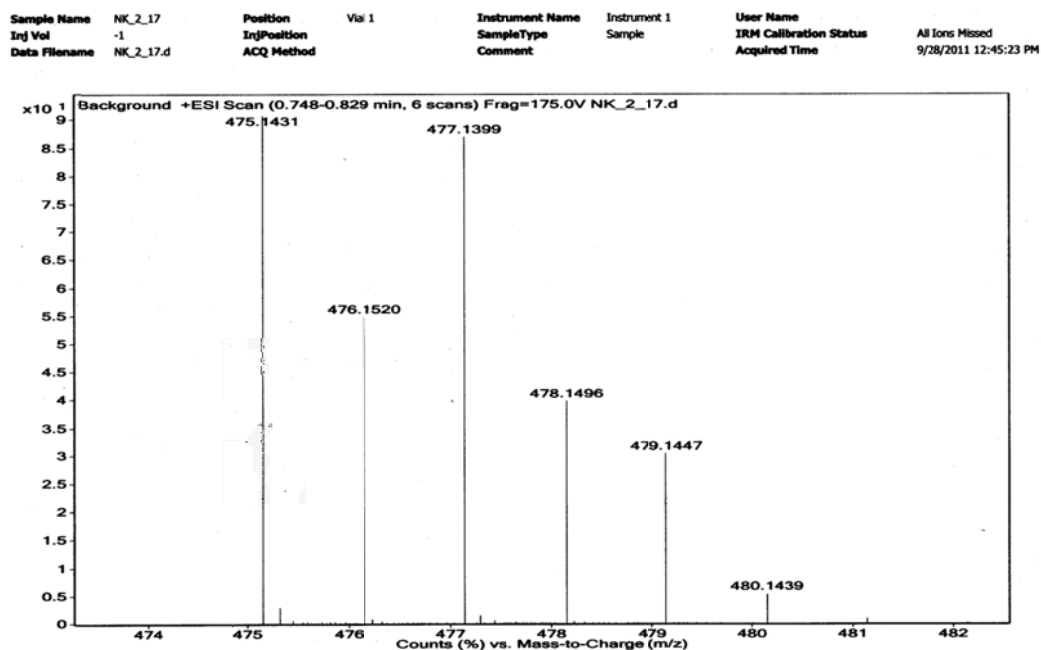


-S64 -

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

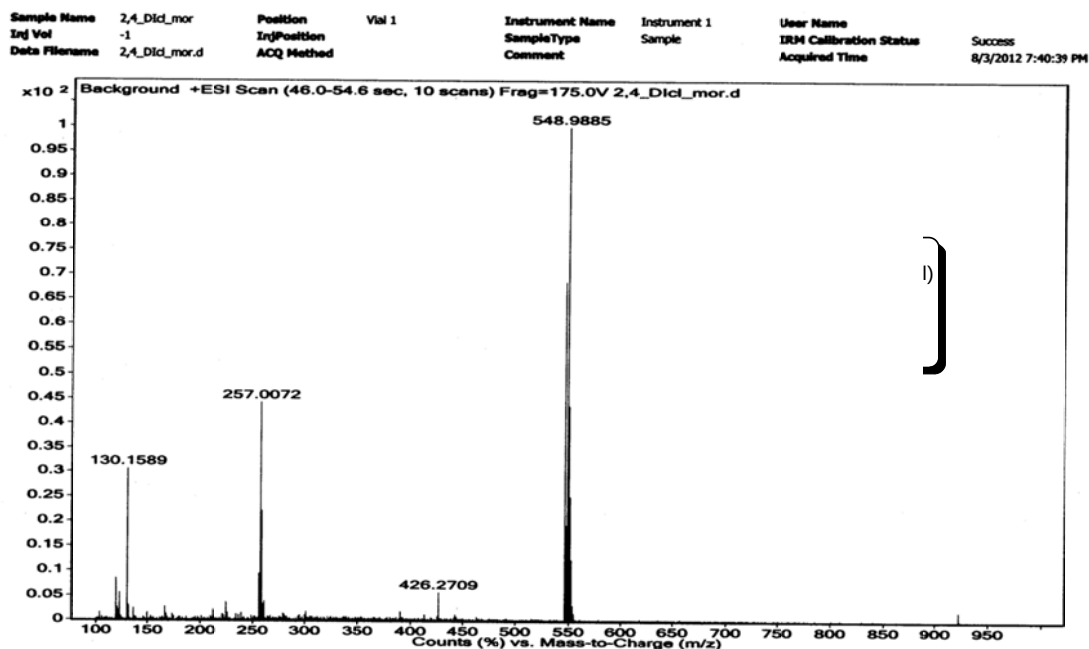


N-((*E*)-(2-Chlorophenylimino)(piperidin-1-yl)methyl)-*N*-(2-chlorophenyl)piperidine-1-carbothioamide (13d). MASS SPECTRA:



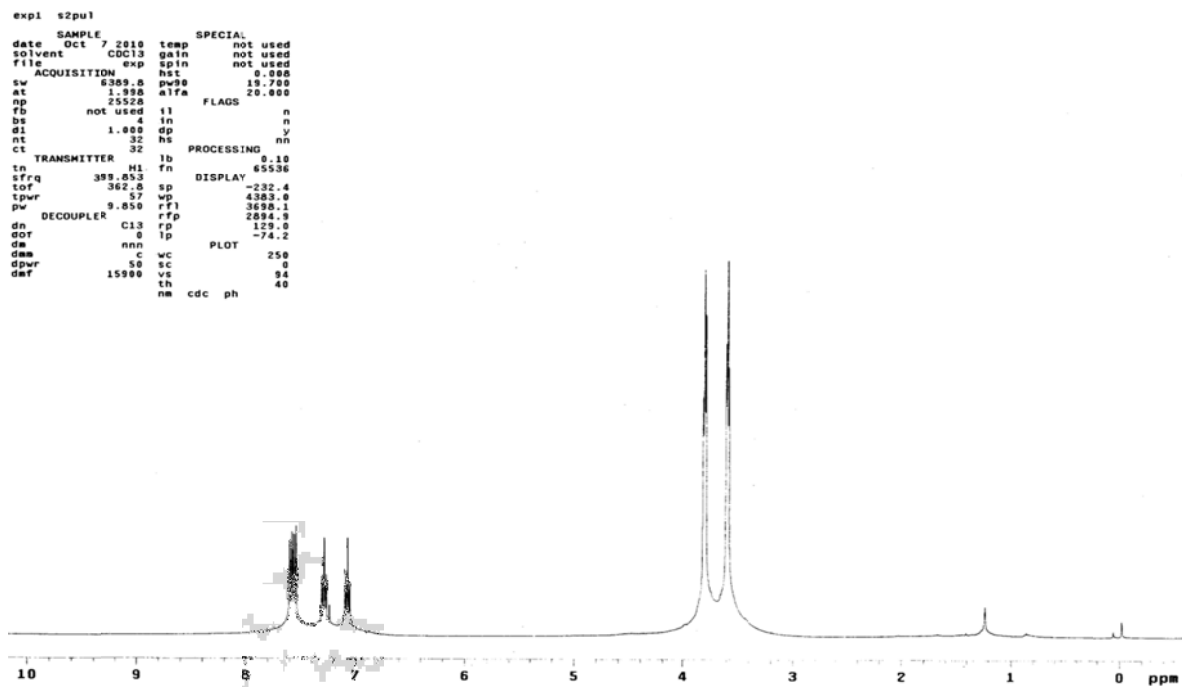
-S66-

N-((*E*)-(2,4-Dichlorophenylimino)(morpholino)methyl)-*N*-(2,4-dichlorophenyl)morpholine-4-carbothioamide (14a). MASS SPECTRA:



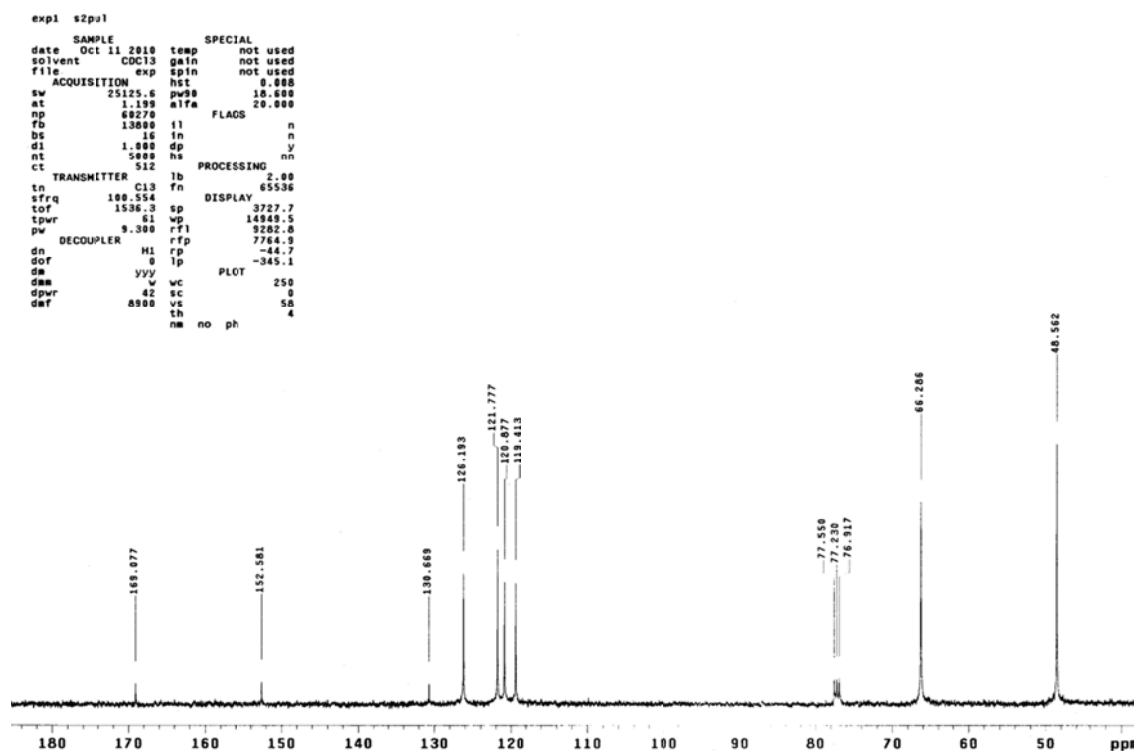
Benzothiazole

2-morpholinobenzo[d]thiazole (11'a): ^1H NMR (400 MHz, CDCl_3):

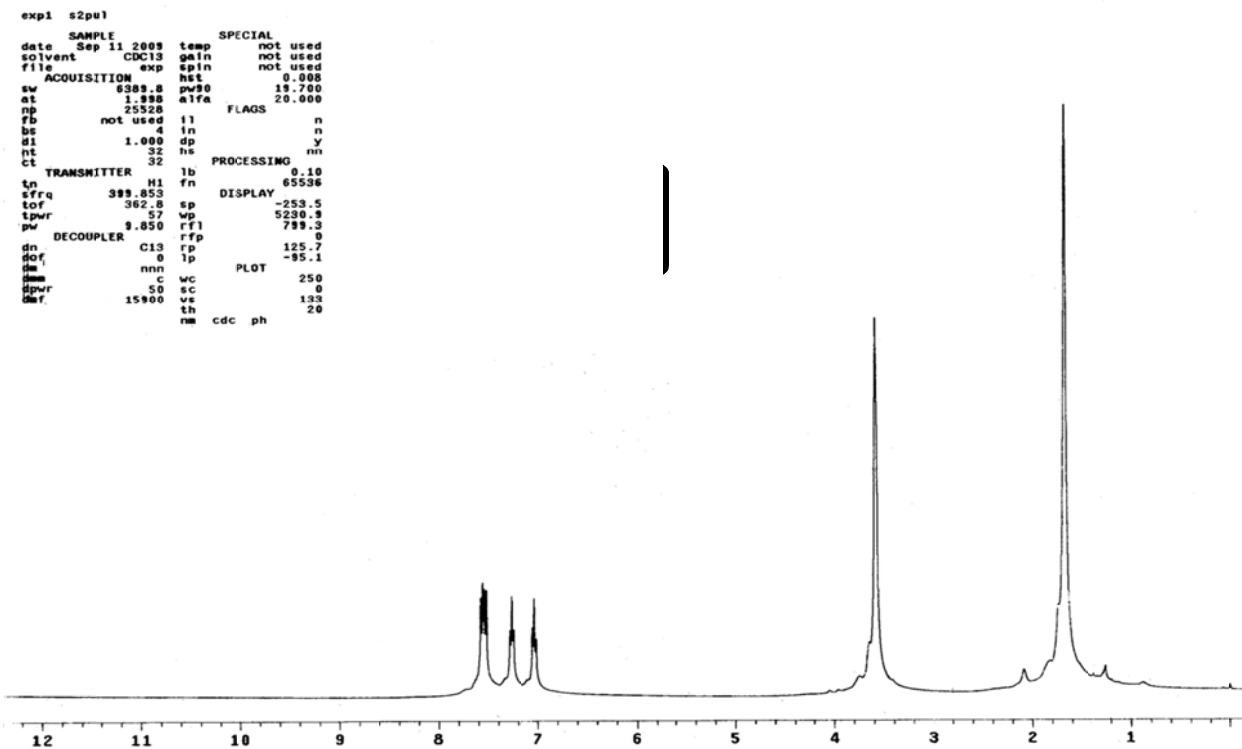


-S67-

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

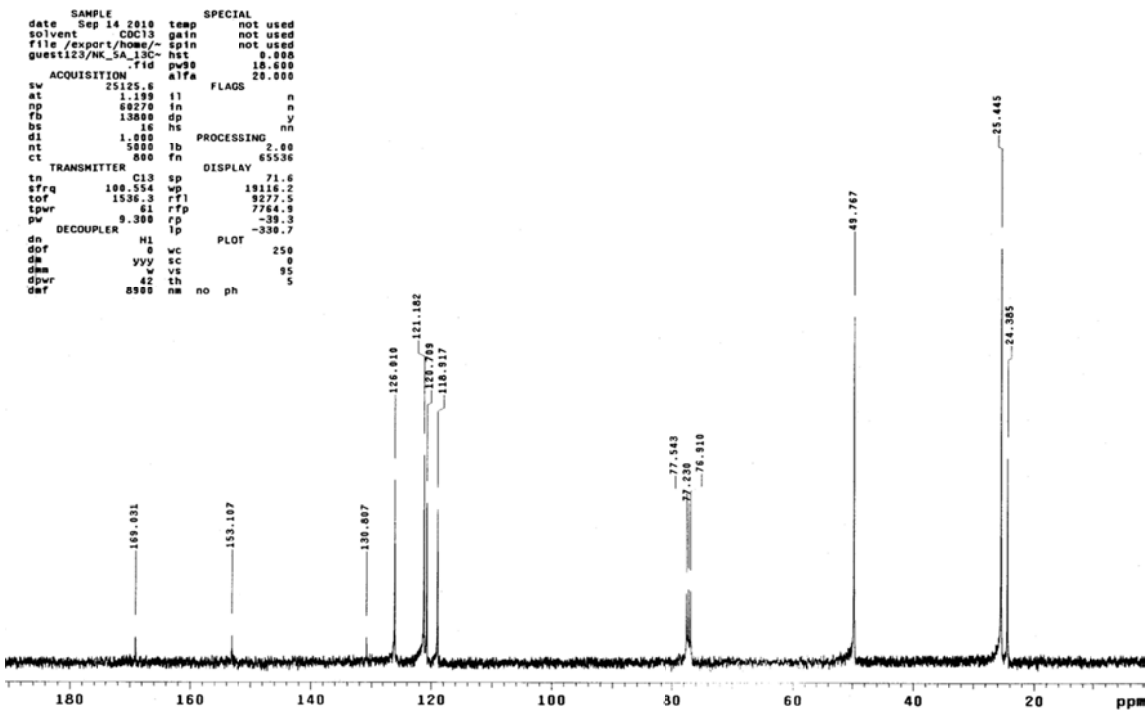


2-(Piperidin-1-yl)benzo[d]thiazole (11'd): ^1H NMR (400 MHz, CDCl_3):



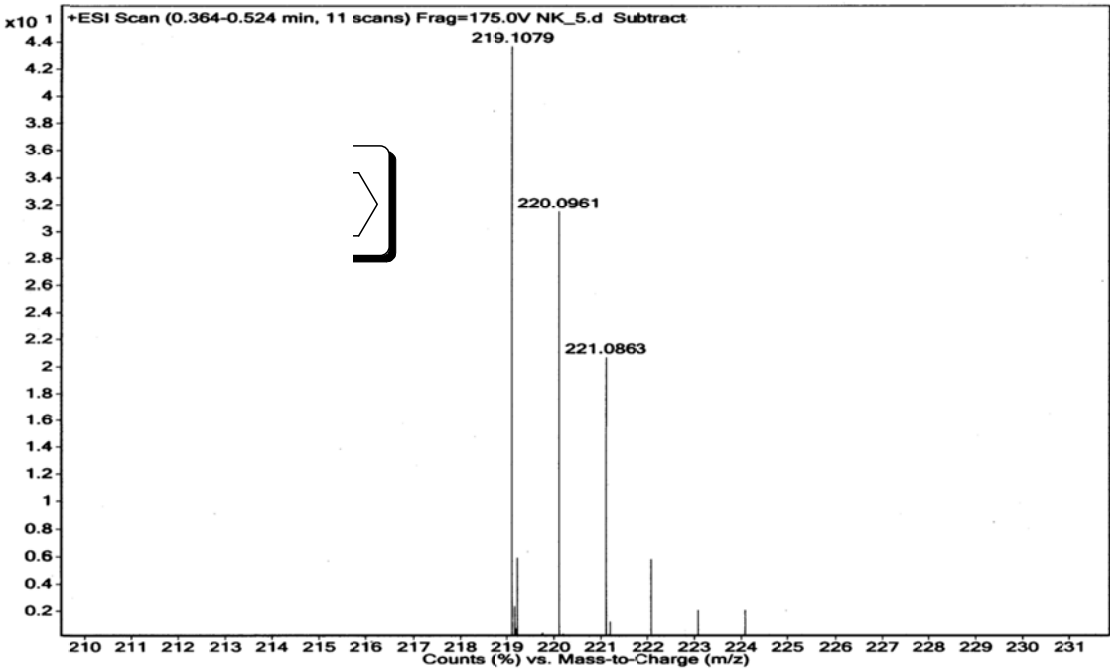
-S68 -

2-(Piperidin-1-yl)benzo[d]thiazole (11'd): ¹³CNMR (100 MHz, CDCl₃):



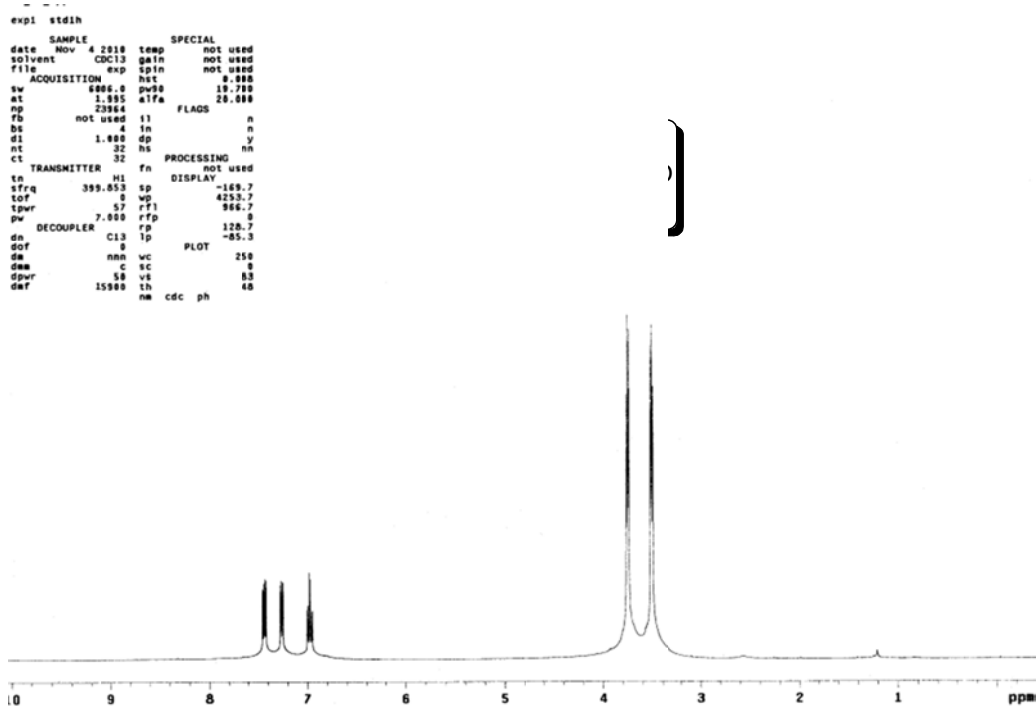
2-(Piperidin-1-yl)benzo[d]thiazole (11'd): IR (KBr or Neat):

Sample Name	NK_5	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	All Ions Missed
Data Filename	NK_5.d	ACQ Method		Comment		Acquired Time	9/28/2011 12:52:00 PM

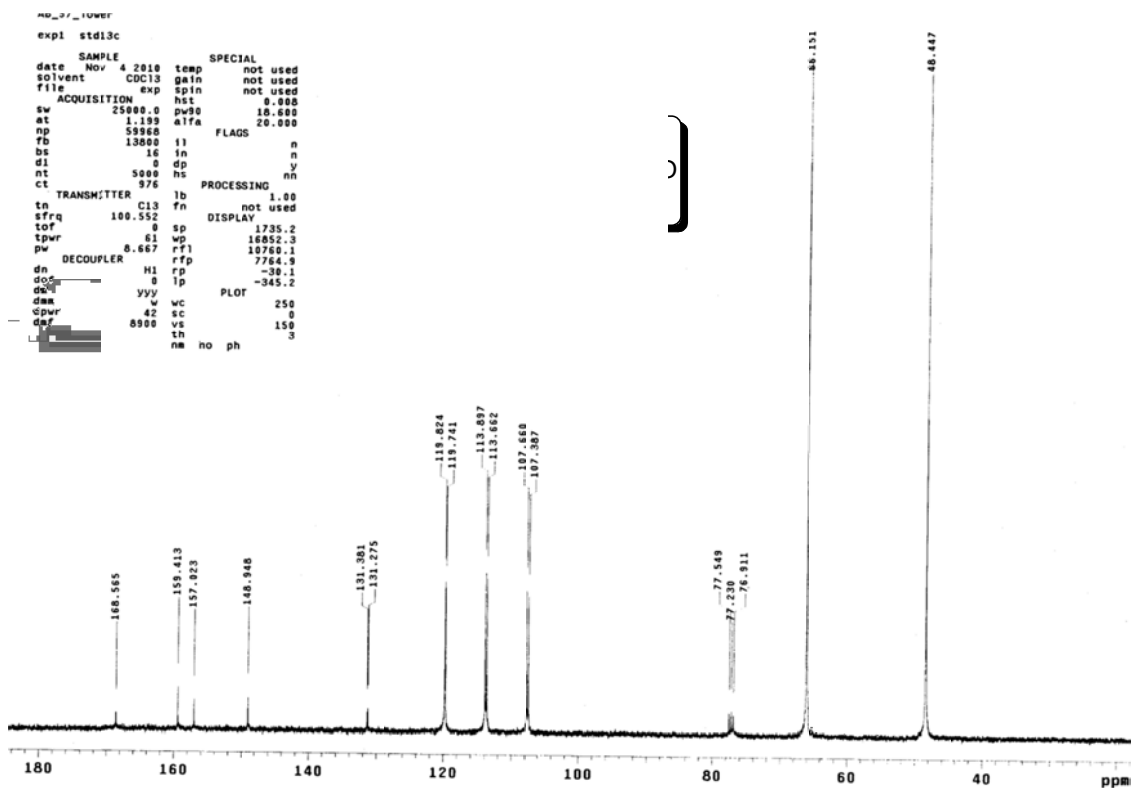


-S69 -

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



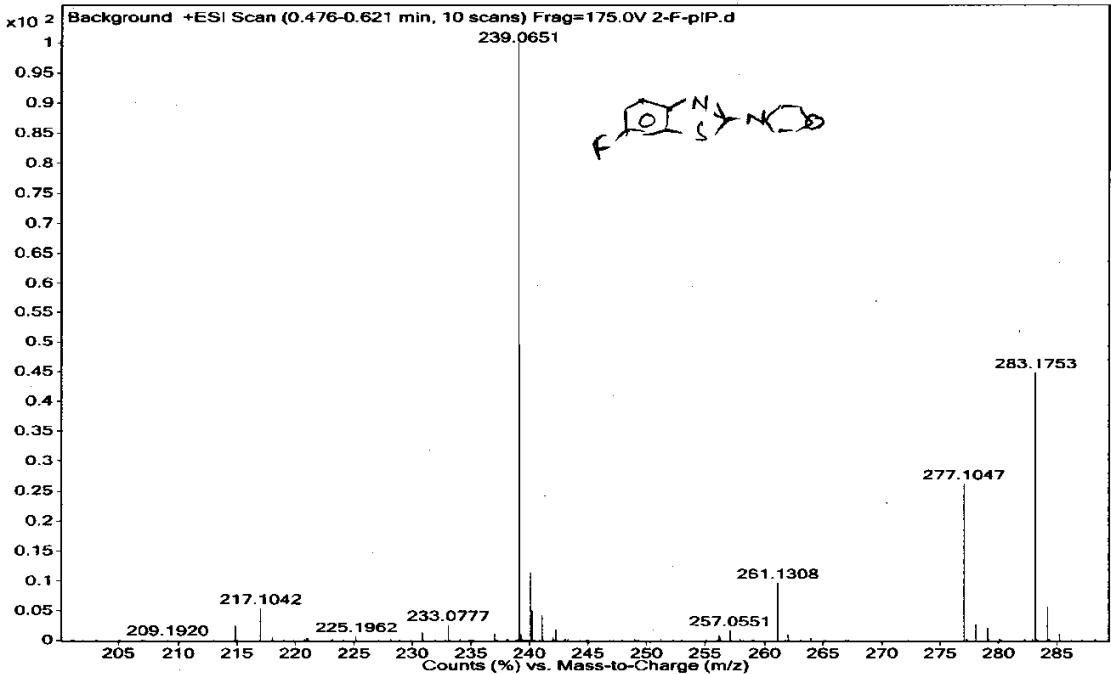
6-Fluoro-2-morpholinobenzo[d]thiazole (12'a): ^{13}C NMR (100 MHz, CDCl_3):



-S70 -

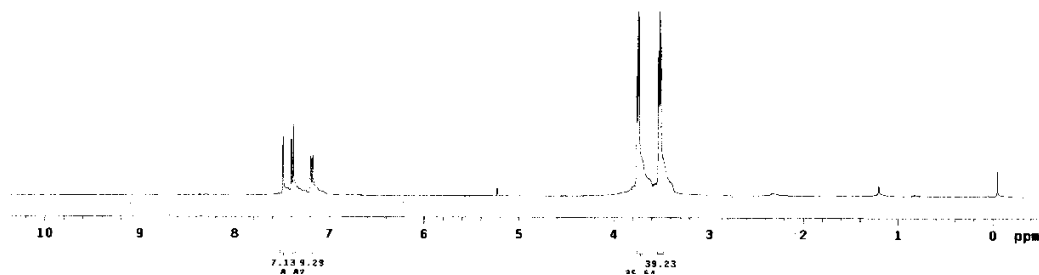
6-Fluoro-2-morpholinobenzo[d]thiazole (12'a): MASS SPECTRA:

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	ADQ Method		Comment		Acquired Time	5/4/2011 11:20:13 AM



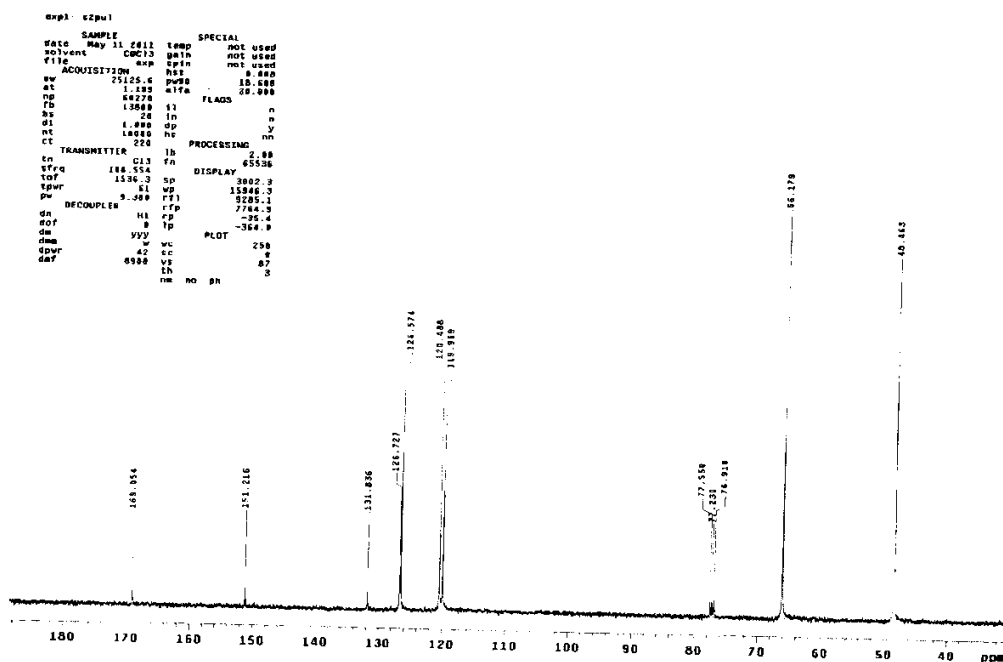
6-Chloro-2-morpholinobenzo[d]thiazole (14'a): ¹HNMR (400 MHz, CDCl₃):

```
AMPL 82001
=====
date May 11 2011 temp not used
solvent CDCl3 gain not used
file exp spin not used
=====
ACQUISITION
sc 6380.0 pv99 19.700
et 1.990 afra 20.000
ap 25528
fb not used li
bs 4 in e
dl 1.000 dp y
nl 32 hs nn
ct 32
=====
TRANSMITTER lb 0.10
tl Tn 655.36
=====
sfrq 399.853
tof 362.0 sp -213.0
tpwr 57 wp 4386.2
pw 9.050 rfi 3688.3
=====
RECOUPLER rfp 2894.9
dn Cl3 rfp 126.9
dof 0 fp -191.7
da nnn
=====
PLOT
dsw C wc 250
dpr 50 sc 8
def 15990 vs 44
th 36
na cdc ph
```



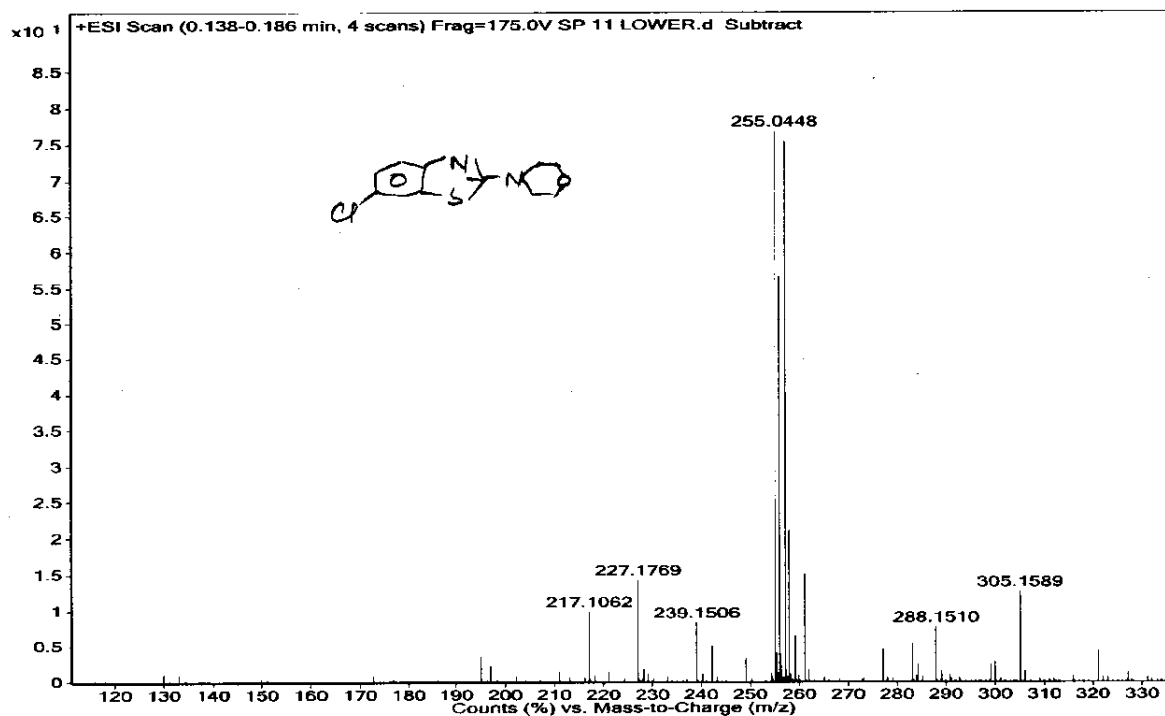
-S71-

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



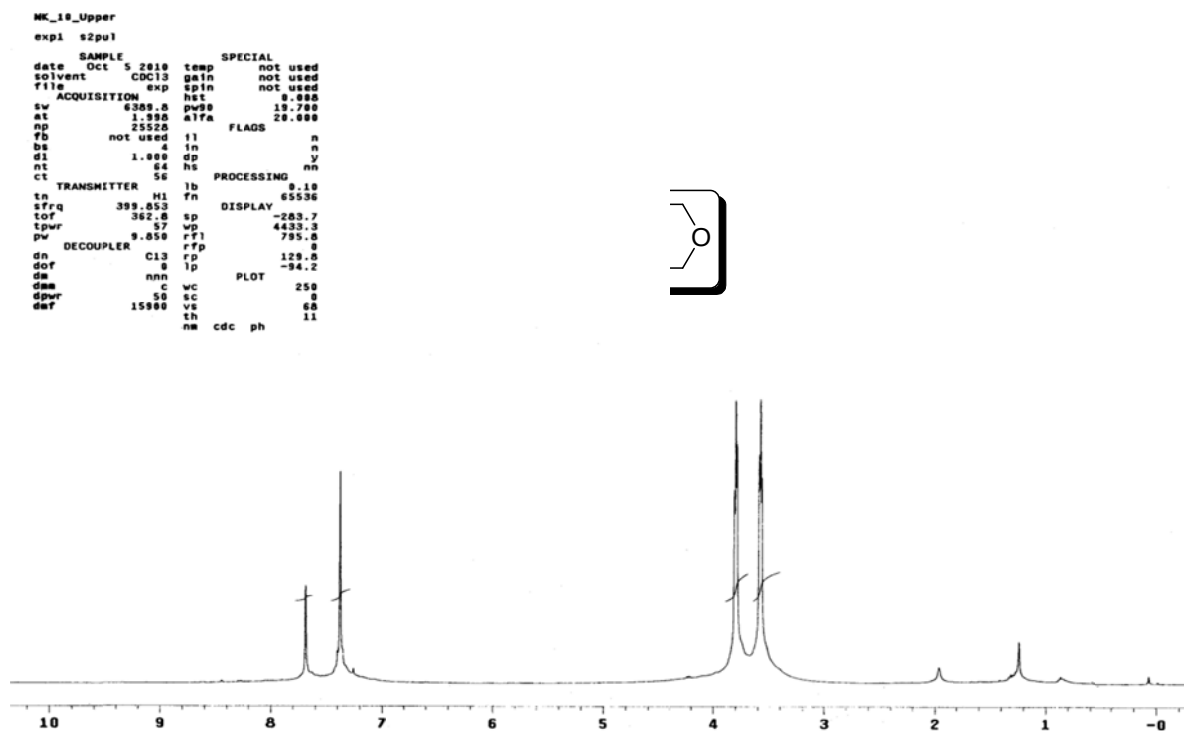
6-Chloro-2-morpholinobenzo[d]thiazole (14'a): MASS SPECTRA:

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

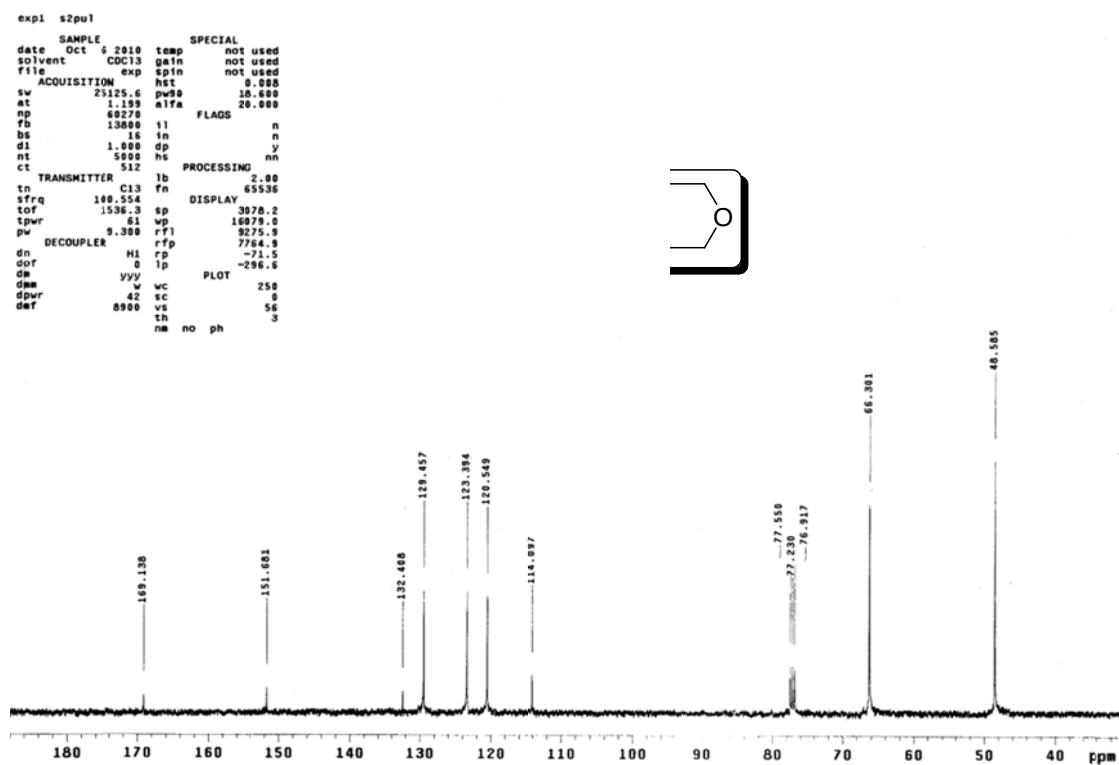


-S72 -

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



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

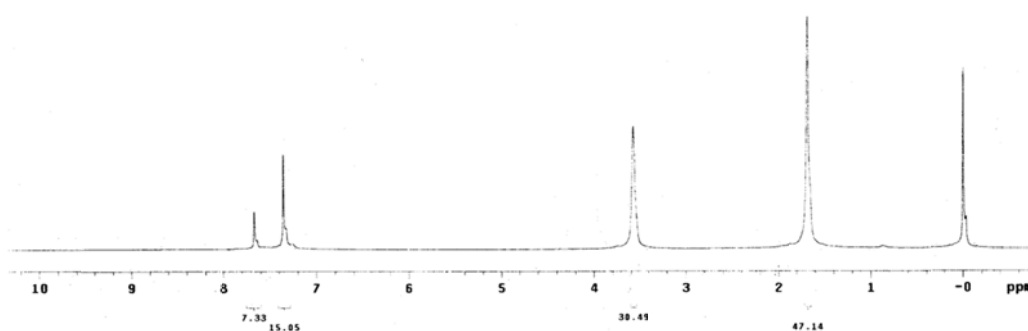


-S73 -

6-Bromo-2-(piperidin-1-yl)[d]thiazole (20'd): ¹H NMR (400 MHz, CDCl₃):

```

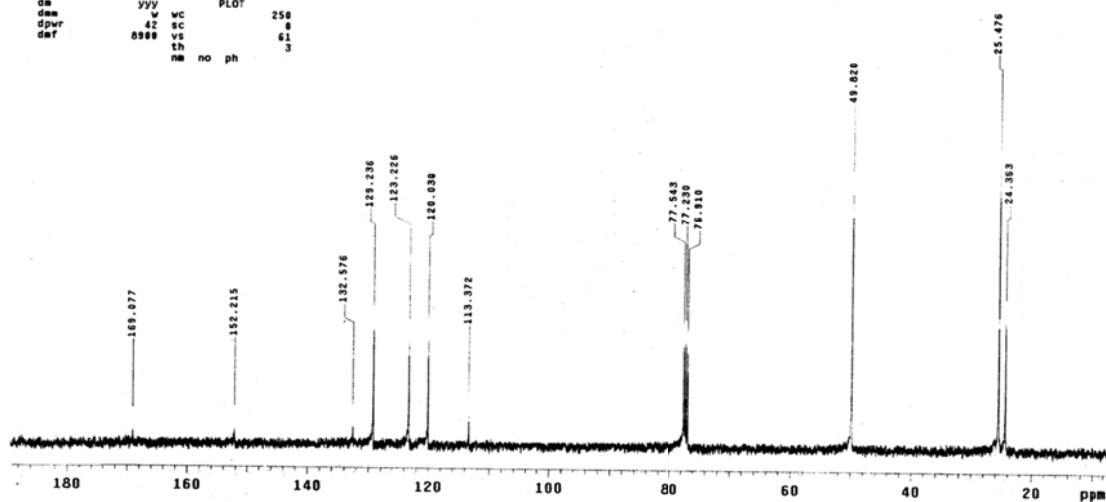
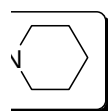
expt s2pul
SAMPLE
date Apr 27 2011 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION hst 0.000
sv 6389.8 pw90 19.700
at 1.990 alfa 20.000
np 25520
fb not used il n
bs 4 in n
dl 1.000 dp y
nt 32 hs nn
ct 32
TRANSMITTER lb 0.10
tn H1 fn 65536
sfrq 399.853 DISPLAY
tof 362.0 sp -316.3
tpwr 57 vp 4450.0
pw 9.050 rfp 794.0
DECOUPLER C13 rp 122.2
dn 0 lp -96.6
dof nnn PLOT
dm c 250
dpr 50 sc 0
dat -15900 vs 56
th 20
nm cdc ph
  
```



6-Bromo-2-(piperidin-1-yl)[d]thiazole (20'd): ¹³C NMR (100 MHz, CDCl₃):

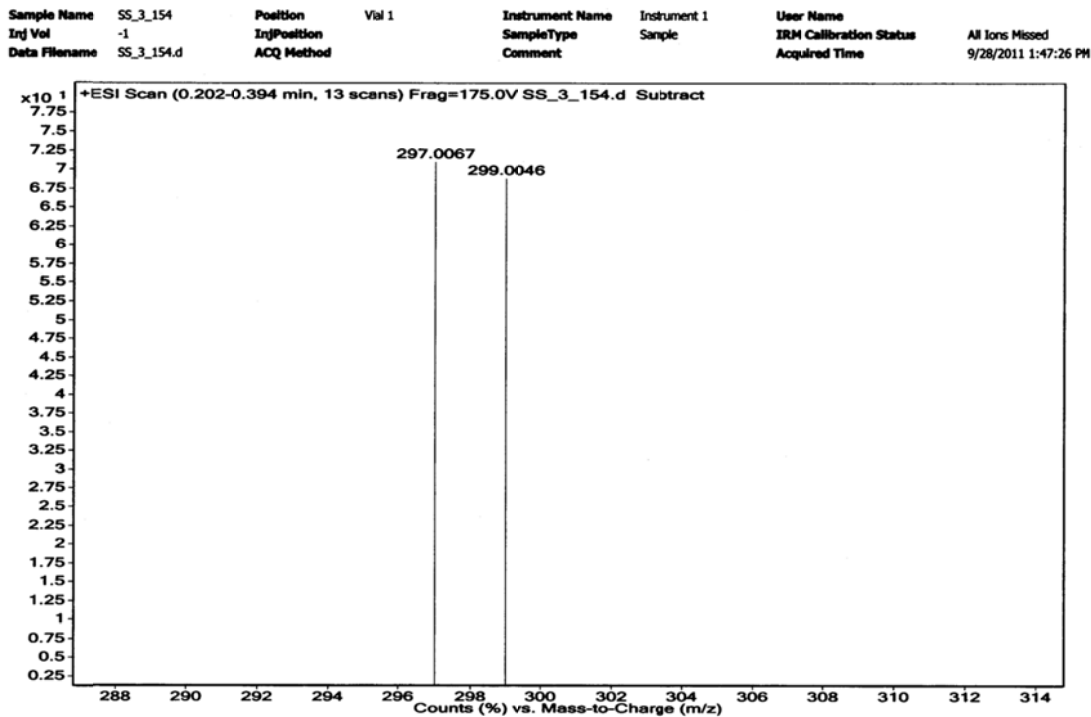
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date Apr 27 2011 temp not used
solvent CDCl3 gain not used
file exp spin not used
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at 1.100 alfa 20.000
np 60270
fb 13000 il n
bs 20 in n
dl 1.000 dp y
nt 5000 hs nn
ct 1040
TRANSMITTER lb 0.00
tn C13 fn 65536
sfrq 100.554 DISPLAY
tof 1536.3 sp 678.5
tpwr 61 vp 10357.1
pw 9.300 rfp 9272.9
DECOUPLER H1 rp 7764.9
dn 0 lp -43.6
dof yyy PLOT
dm v 250
dpr 42 sc 0
dat 8900 vs 61
th no ph 3
  
```

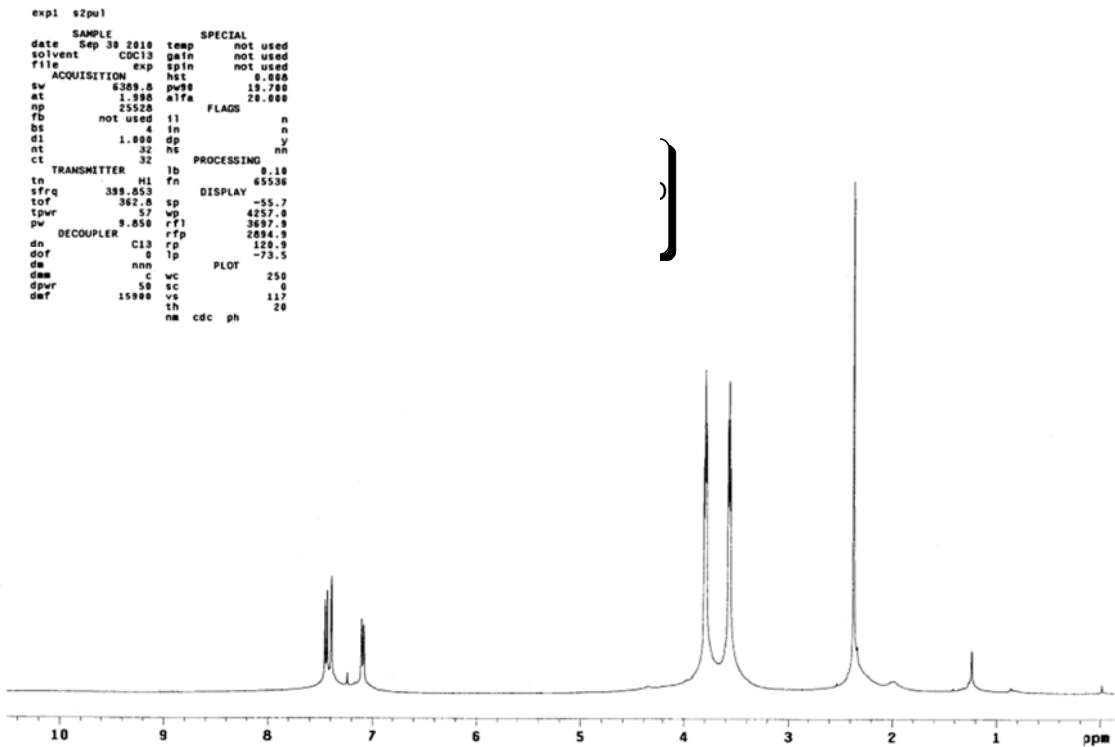


-S74 -

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

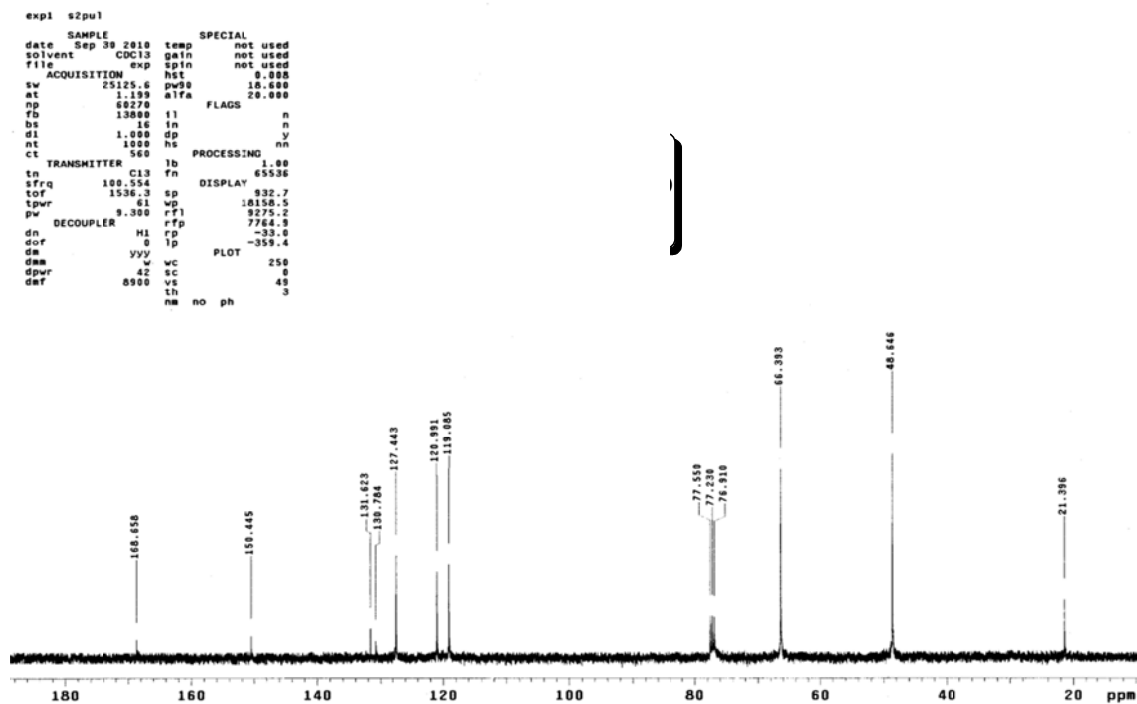


6-methyl-2-morholinobenzo[d]thiazole (18'a): ¹H NMR (400 MHz, CDCl₃):

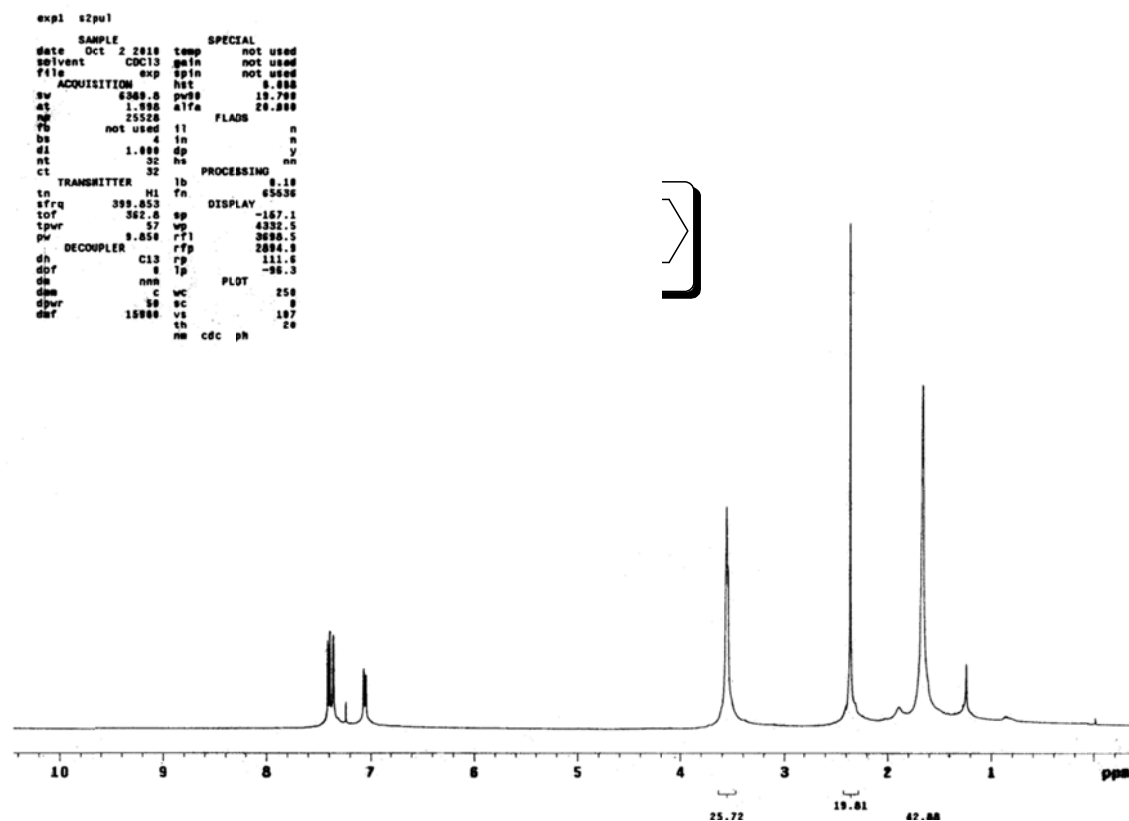


-S75 -

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

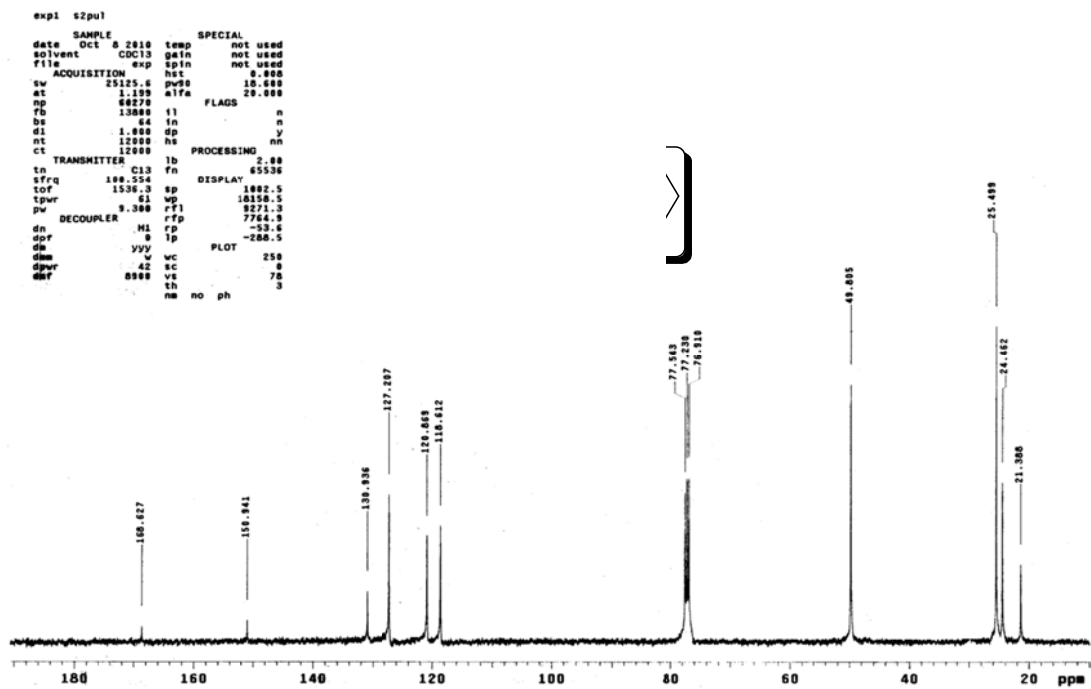


6-methyl-2-(Piperidin-1-yl)benzo[d]thiazole (18'd): ^1H NMR (400 MHz, CDCl_3):



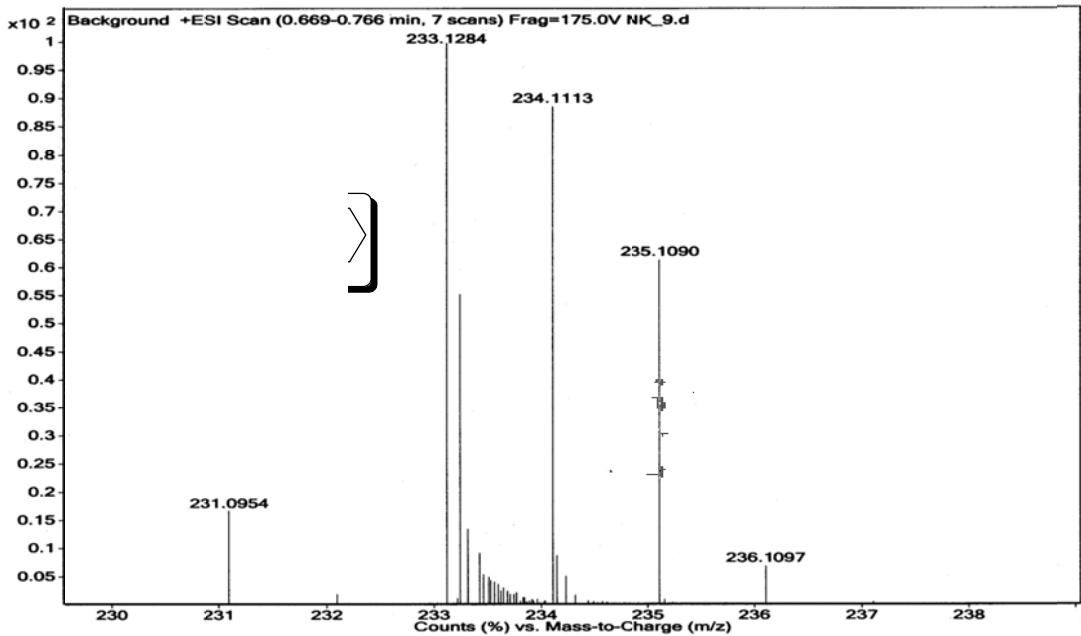
-S76 -

6-methyl-2-(Piperidin-1-yl)benzo[d]thiazole (18'd): ¹³CNMR (100 MHz, CDCl₃):



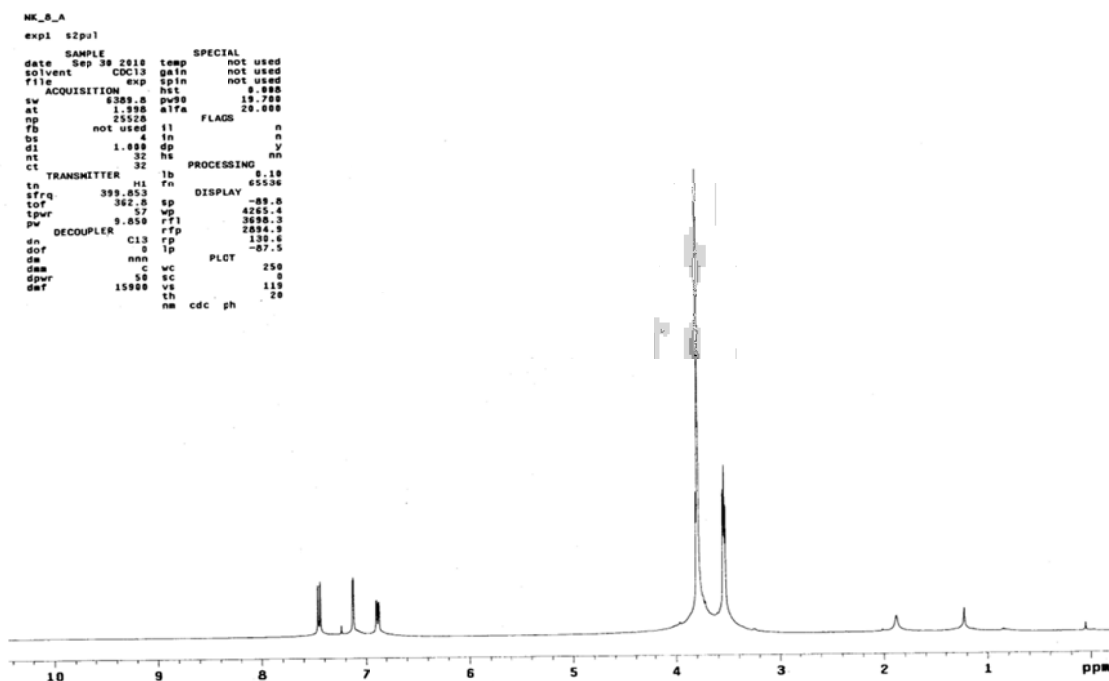
6-methyl-2-(Piperidin-1-yl)benzo[d]thiazole (18'd): MASS SPECTRA:

Sample Name	NK_9	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inf Vol	-1	IntPosition		SampleType	Sample	IRM Calibration Status	All Ions Missed
Data Filename	NK_9.d	ACQ Method		Comment		Acquired Time	9/28/2011 12:31:23 PM

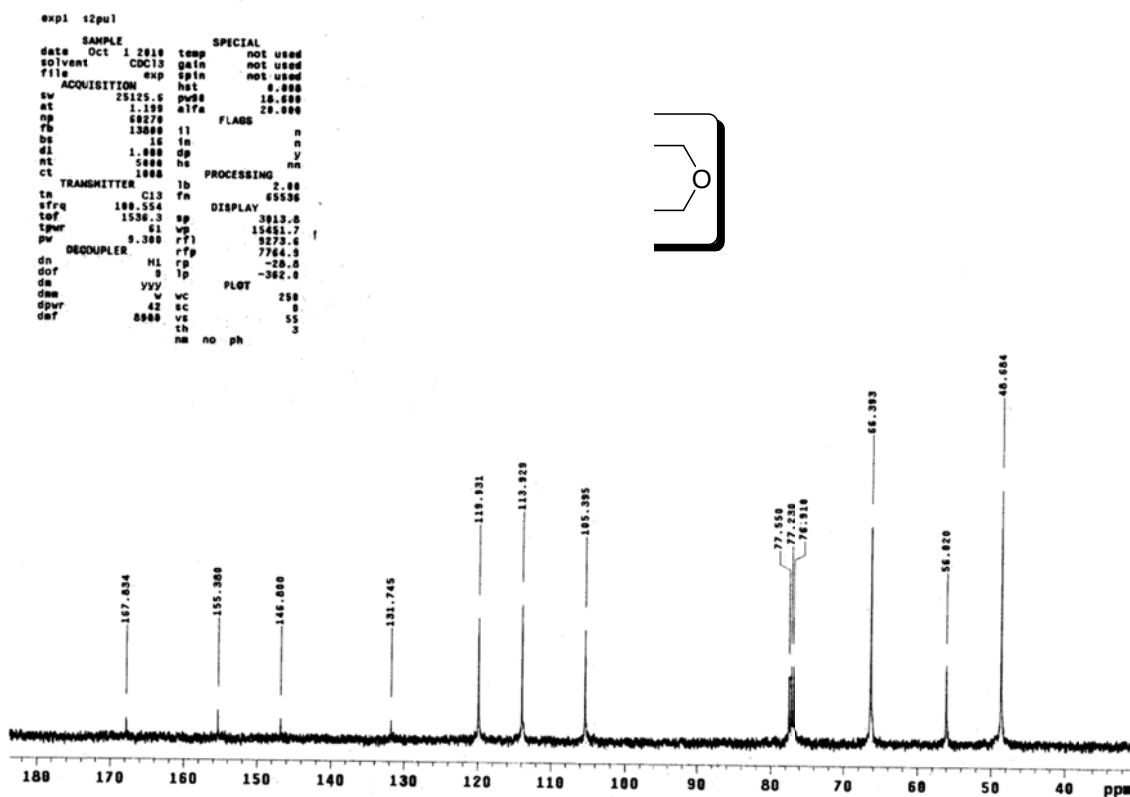


-S77-

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

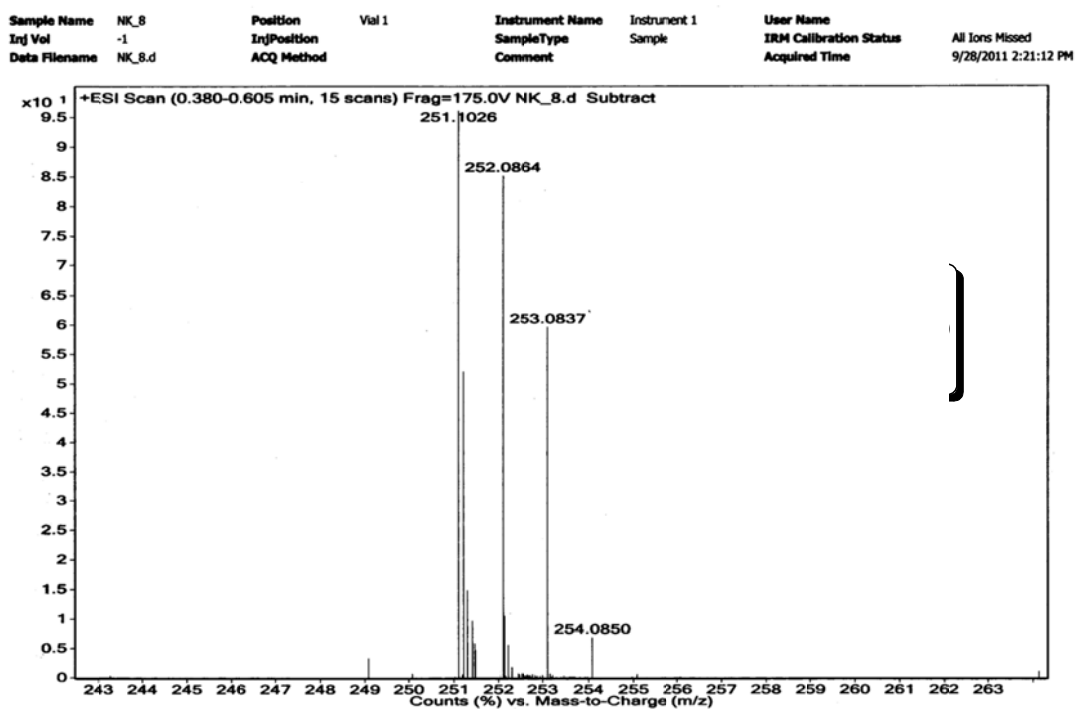


6-methoxy-2-morpholino[d]thiazole (19'a): ^{13}C NMR (100 MHz, CDCl_3):

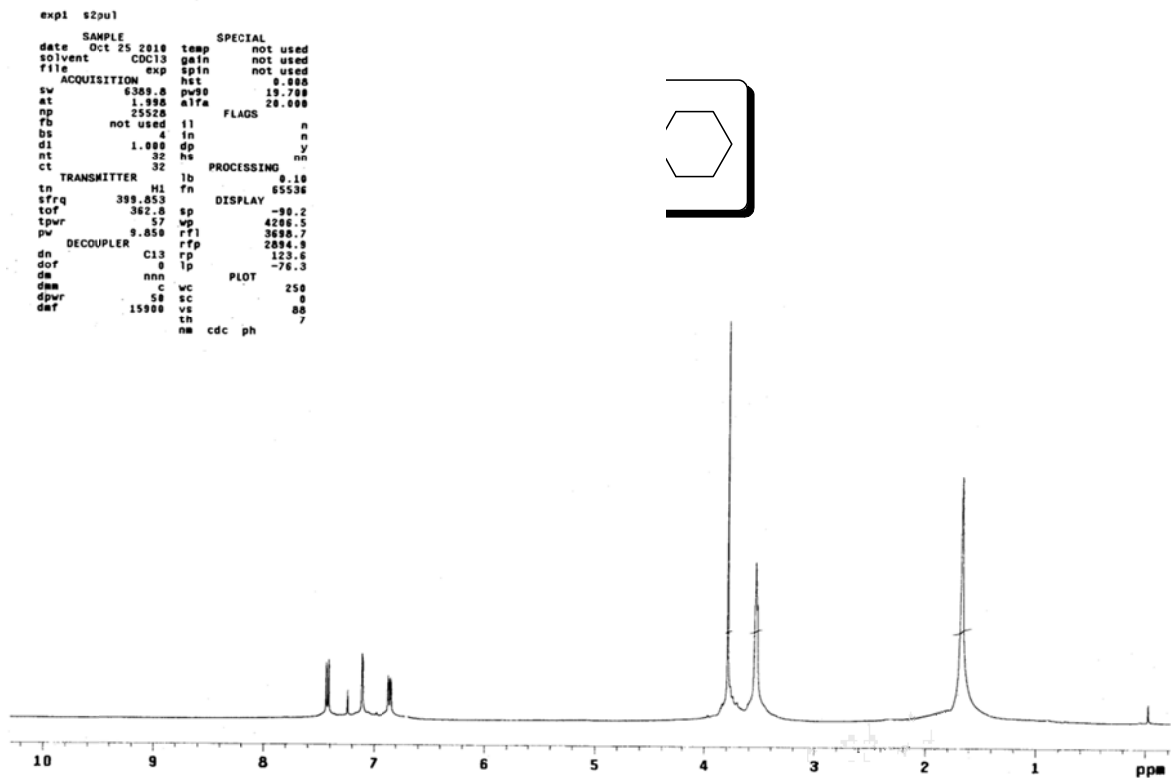


-S78 -

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

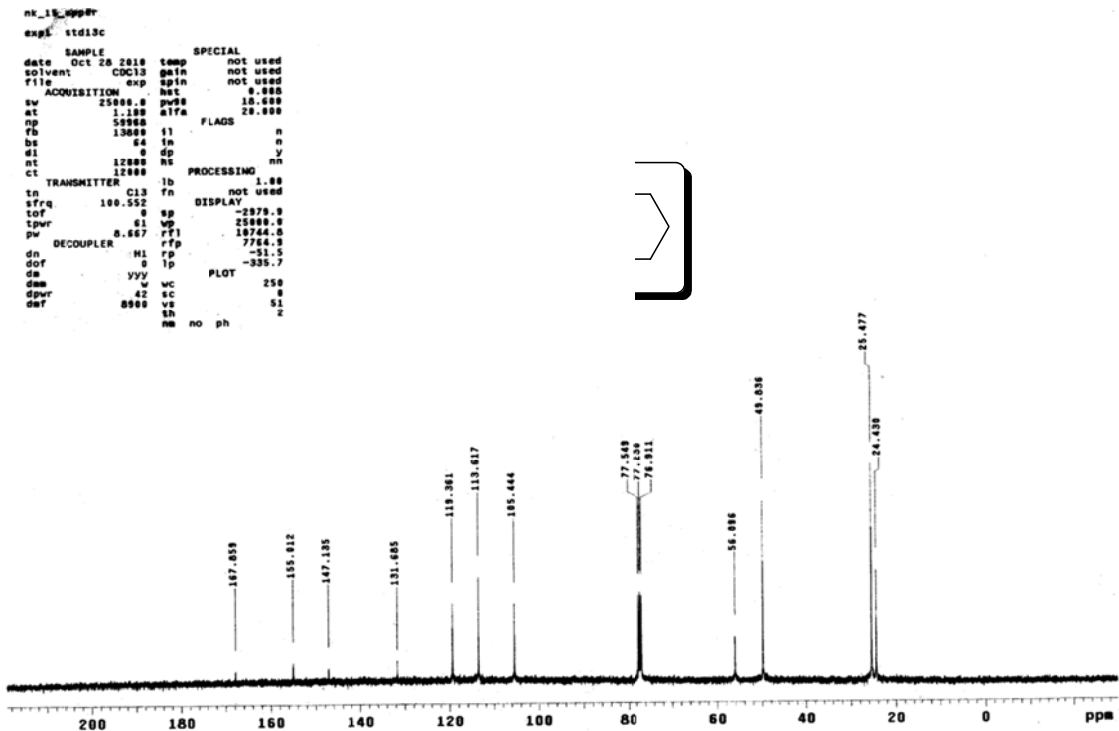


6-methoxy-2-(piperidin-1-yl)benzo[d]thiazole (19'd): ¹H NMR (400 MHz, CDCl₃):



-S79 -

6-methoxy-2-(piperidin-1-yl)[d]thiazole (19'd): ¹³C NMR (100 MHz, CDCl₃):



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

Sample Name	NK_15	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	All Ions Missed
Data Filename	NK_15.d	ACQ Method		Comment		Acquired Time	9/28/2011 12:24:31 PM

