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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: patal@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 ($\lambda = 0.71073 \text{ \AA}$) 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 undertaken 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 F² 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

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X-ray Crystallographic data

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

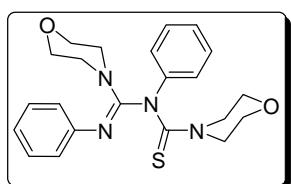
	3d	15'a
Formula	C ₂₈ H ₃₈ N ₄ S	C ₁₁ H ₁₁ BrN ₂ OS
CCDC number	894067	894068
Formula weight	462.69	299.19
T (K)	296(2)	296(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	Monoclinic	Orthorhombic
Space group	P 21 / c	P-1
<i>a</i> (Å)	9.5021(13)	10.01289(3)
<i>b</i> (Å)	11.2799(14)	11.2225(3)
<i>c</i> (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
<i>θ</i> _{min} , <i>θ</i> _{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
<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 , wR ₂ ^b (<i>I</i> ≥ 2σ(<i>I</i>))	0.0570, 0.1242	0.0851, 0.0836
R1 ^a , wR ₂ ^b (all data)	0.1134, 0.1421	0.0851, 0.0866

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Spectral Data

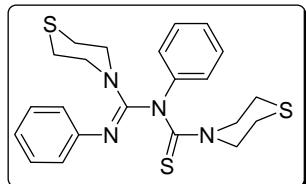
N-((E)-Morpholino(phenylimino)methyl)-N-phenylmorpholine-4-carbothioamide

(1a):



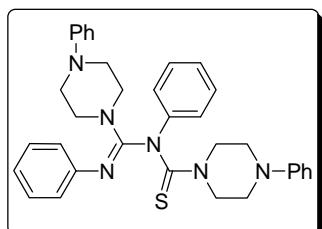
White solid; M.p. 163–165 °C; ^1H NMR (400 MHz, CDCl_3): δ 2.90–3.52 (m, 16H), 6.95 (d, 2H, J = 8.0 Hz), 6.98 (d, 2H, J = 7.6 Hz), 7.09 (t, 2H, J = 7.6 Hz), 7.17 (t, 2H, J = 8.0 Hz), 7.30 (d, 2H, J = 7.6 Hz); ^{13}C NMR (100 MHz, CDCl_3) δ 46.8, 50.6, 65.4, 66.2, 121.2, 122.1, 122.8, 122.9, 124.7, 128.8,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

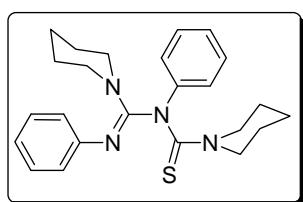
N,4-Diphenyl-N-((E)-(phenylimino)(4-phenylpiperazin-1-yl)methyl)piperazine-1-carbothioamide (1c):



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^+).

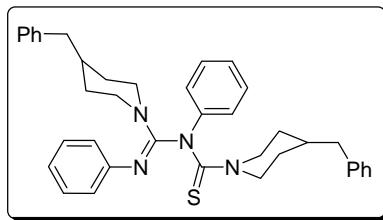
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N-Phenyl-N-((E)-(phenylimino)(piperidin-1-yl)methyl)piperidine-1-carbothioamide (1d):



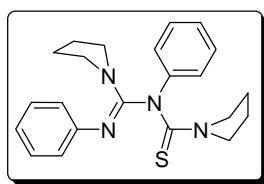
White solid; M.p. 183–184 °C; ^1H NMR (400 MHz, CDCl_3): δ 0.84–1.67 (m, 12H), 2.63–3.82 (m, 8H), 6.90 (t, 2H, J = 7.6 Hz), 7.02–7.12 (m, 3H), 7.16 (t, 2H, J = 8.4 Hz), 7.26–7.40 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 23.6, 24.5, 24.6, 24.9, 47.4, 51.4, 122.1, 122.3, 124.1, 128.4, 129.2, 143.7, 149.7, 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):

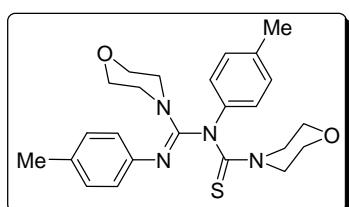


White solid; M.p. 153–155 °C; ^1H NMR (400 MHz, CDCl_3): δ 1.05–2.50 (m, 12H), 3.37–3.90 (m, 4H), 6.82 (m, 1H), 6.89 (t, 1H, J = 7.2 Hz), 6.96 (m, 1H), 7.04 (t, 1H, J = 7.6 Hz), 7.09 (d, 2H, J = 7.6 Hz), 7.15 (m, 2H), 7.19–7.36 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 24.3, 25.1, 25.8, 26.2, 47.2, 48.4, 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^+).

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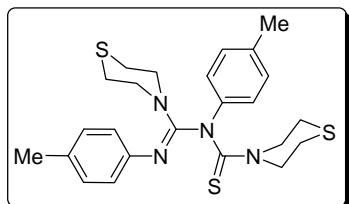
N-((E)-(p-Tolylimino)(morpholino)methyl)-N-p-tolylmorpholine-4-carbothioamide

(2a):



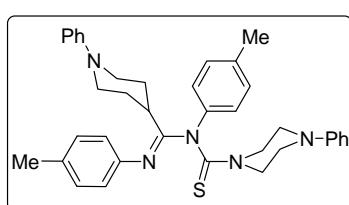
White solid; M.p. 140–141 °C; ^1H NMR (400 MHz, CDCl_3): δ 2.17 (s, 3H), 2.25 (s, 3H), 2.82–3.47 (m, 16H), 6.84 (d, 4H, J = 8.0 Hz), 6.92 (d, 4H, J = 7.2 Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 20.7, 20.8, 46.6, 50.5, 65.2, 66.1, 121.0, 121.8, 129.1, 130.1, 131.6, 134.3, 140.1, 146.6, 149.3, 185.1; IR (KBr): 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 °C; ^1H 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 $\text{C}_{24}\text{H}_{30}\text{N}_4\text{S}_3$: 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.

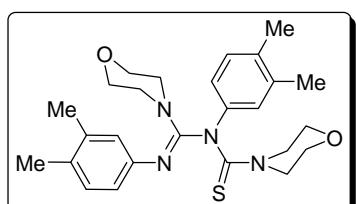
N-((E)-(p-Tolylimino)(1-phenylpiperidin-4-yl)methyl)-4-phenyl-tolylpiperazine-1-carbothioamide (2c):



White solid; M.p. 215–216 °C; ^1H 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^+).

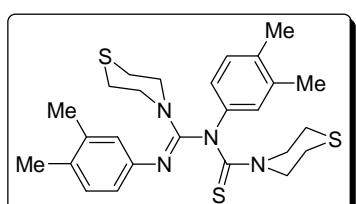
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N-((E)-(3,4-Dimethylphenylimino)(morpholino)methyl)-N-(3,4-dimethylphenyl) morpholine-4-carbothioamide (3a):



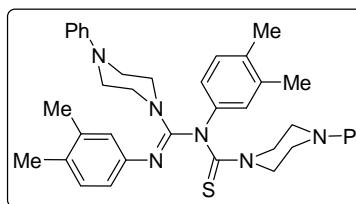
Gummy; ^1H NMR (400 MHz, CDCl_3): δ 2.10 (s, 3H), 2.11 (s, 3H), 2.18 (s, 6H), 2.85–3.76 (m, 16H), 6.69 (d, 2H, J = 7.6 Hz), 6.77 (s, 2H), 6.89 (d, 2H, J = 8.0 Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 19.0, 19.2, 19.8, 20.1, 46.6, 50.6, 65.4, 66.2, 119.1, 123.3, 129.7, 130.4, 133.0, 136.4, 137.9, 140.4, 147.0, 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 °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^+).

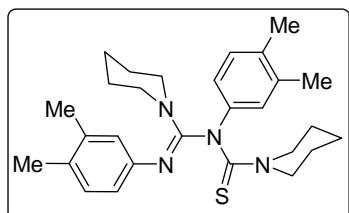
N-((E)-(3,4-Dimethylphenylimino)(4-phenylpiperazin-1-yl)methyl)-N-(3,4-dimethylphenyl)-4-phenylpiperazine-1-carbothioamide (3c):



White solid; M.p. 190–191 °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^+).

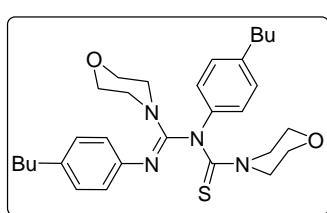
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N-((E)-(3,4-Dimethylphenylimino)(piperidin-1-yl)methyl)-N-(3,4-dimethylphenyl)piperidine-1-carbothioamide (3d):



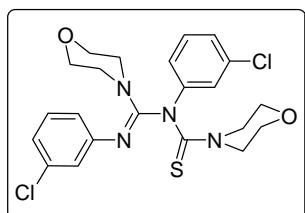
White solid; M.p. 188–189 °C; ^1H NMR (400 MHz, CDCl_3): δ 0.69–1.80 (m, 12H), 2.09 (s, 6H), 2.17 (s, 6H), 2.87–3.73 (m, 8H), 6.14–7.03 (m, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 18.9, 19.1, 19.7, 19.9, 47.3, 51.5, 119.5, 121.5, 123.5, 125.2, 129.5, 129.7, 130.1, 132.3, 136.0, 137.3, 141.4, 147.4, 150.3, 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; ^1H 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^+).

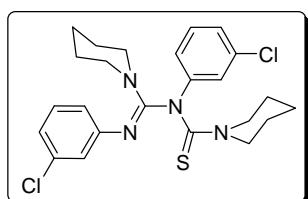
N-((E)-(3-Chlorophenylimino)(morpholino)methyl)-N-(3-chlorophenyl)morpholine-4-carbothioamide (5a):



White solid; M.p. 172–173 °C; ^1H 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^+).

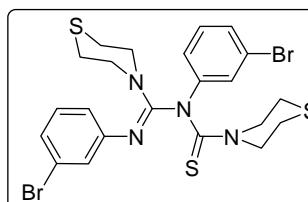
-S9 -

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



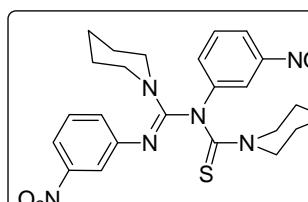
White solid; M.p. 123–125 °C; ^1H NMR (400 MHz, CDCl_3): δ 1.23–1.71 (m, 16H), 3.11–3.51 (m, 4H), 6.87 (t, 4H, J = 4.8 Hz), 6.98 (s, 1H), 7.05 (d, 2H, J = 7.2 Hz), 7.24 (d, 1H, J = 3.2 Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 23.7, 24.5, 24.8, 25.1, 47.7, 51.9, 119.9, 121.0, 122.4, 124.5, 129.6, 130.4, 134.0, 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^+).

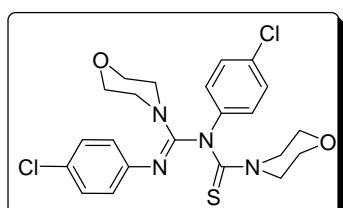
N-((E)-(3-nitrophenylimino)(piperidin-1-yl)methyl)-N-(3-nitrophenyl)piperidine-1-carbothioamide (7d):



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^+).

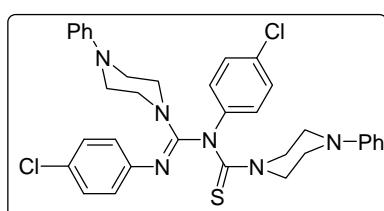
-S10 -

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



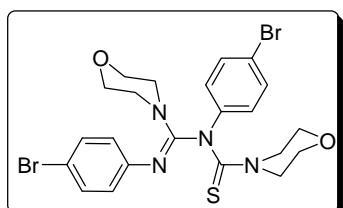
White solid; M.p. 162–164 °C; ^1H NMR (400 MHz, CDCl_3): δ 2.81–3.92 (m, 16H), 6.74 (m, 2H), 6.93 (d, 2H, J = 8.0 Hz), 7.17 (d, 2H, J = 8.0 Hz), 7.33 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 46.9, 50.9, 65.5, 66.3, 122.3, 123.5, 128.3, 128.9, 130.1, 130.5, 141.2, 147.7, 149.5, 184.9; IR (KBr): 2963, 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 $\text{C}_{22}\text{H}_{24}\text{Cl}_2\text{N}_4\text{O}_2\text{S}$: 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)-(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, 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^+).

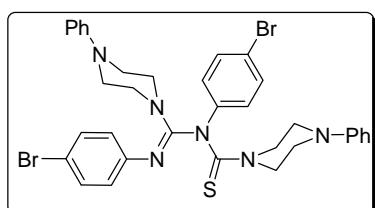
N-((E)-(4-bromophenylimino)(morpholino)methyl)-N-(4-bromophenyl)morpholine-4-carbothioamide (9a):



White solid; M.p. 174–175 °C; ^1H NMR (400 MHz, CDCl_3): 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); ^{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 $\text{C}_{22}\text{H}_{24}\text{Br}_2\text{N}_4\text{O}_2\text{S}$: 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.

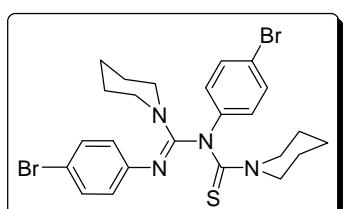
-S11 -

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^+).

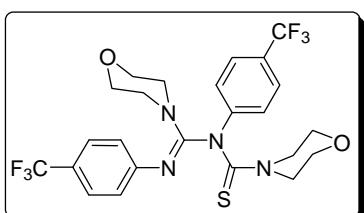
N-((E)-(4-bromophenylimino)(piperidin-1-yl)methyl)-N-(4-bromophenyl)piperidine-1-carbothioamide (9d):



White solid; M.p. 177–179 °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.

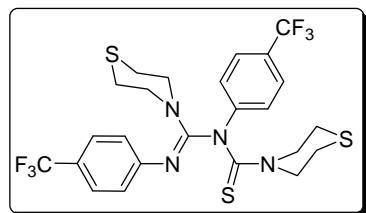
-S12 -

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



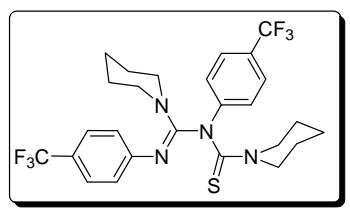
White solid; M.p. 148–149 °C; ^1H NMR (400 MHz, CDCl_3): δ 2.92–3.95 (m, 16H), 6.90 (brs, 2H), 7.07 (d, 2H, J = 8.0 Hz), 7.47 (d, 2H, J = 8.0 Hz), 7.62 (brs, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 46.9, 51.0, 65.4, 66.2, 120.5, 121.1, 122.3, 122.4, 124.9, 125.2, 125.3, 125.9, 126.1, 126.5, 126.8, 127.2, 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. 170–1471 °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^+).

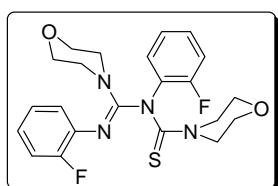
N-((E)-(4-(trifluoromethyl)phenylimino)(piperidin-1-yl)methyl)-N-(4-(trifluoromethyl)phenyl)piperidine-1-carbothioamide (10d):



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.

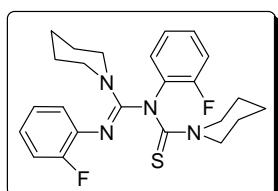
-S13 -

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



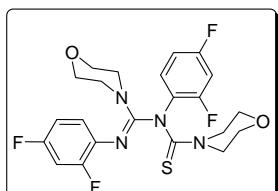
White solid; M.p. 123–125 °C; ^1H NMR (400 MHz, CDCl_3): δ 2.68–3.74 (m, 16H), 6.87–7.33 (m, 8H); ^{13}C NMR (100 MHz, CDCl_3): δ 44.2, 50.5, 66.1, 66.4, 114.6, 114.8, 11.1, 115.3, 116.7, 116.9, 121.9, 123.4, 123.5, 124.0, 124.5, 124.9, 125.3, 125.7, 126.2, 127.3, 130.4, 136.4, 150.6, 154.5, 186.3; IR (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 °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^+).

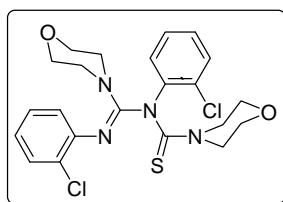
N-((E)-(2,4-(Difluorophenylimino)(morpholino)-N-(2,4-(difluorophenyl)morpholine-4-carbothioamide (12a):



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^+).

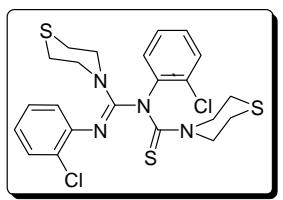
-S14 -

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



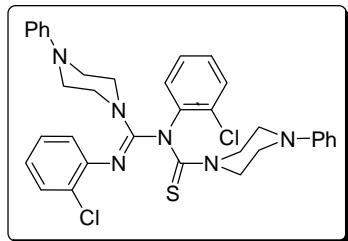
Mp 154–155 °C; ^1H NMR (400 MHz, CDCl_3): δ 2.50–4.60 (m 16H), 6.39–7.68 (m, 8H); ^{13}C NMR (100 MHz, CDCl_3): δ 44.1, 47.0, 50.9, 66.0, 121.5, 122.8, 123.4, 126.2, 126.4, 127.3, 128.0, 129.1, 131.0, 139.6, 145.7, 148.5, 187.2; IR (KBr): 3057, 2950, 2894, 2849, 1632, 1580, 1470, 1427, 1401, 1363, 1303, 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^+).

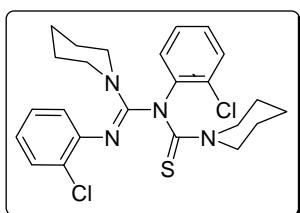
N-((E)-(2-Chlorophenylimino)(4-phenylpiperazin-1-yl)methyl)-N-(2-chlorophenyl)-4-phenylpiperazine-1-carbothioamide (13c):



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.

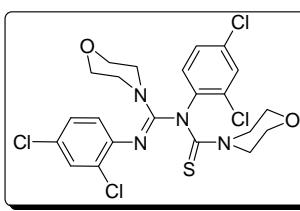
-S15 -

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



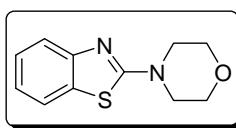
Gummy; ^1H NMR (400 MHz, CDCl_3): δ 0.83-2.01 (m, 16H), 3.68 (m, 4H), 6.62-7.39 (m, 8H); ^{13}C NMR (100 MHz, CDCl_3): δ 24.0, 24.7, 25.1, 25.7, 48.3, 51.9, 121.5, 122.2, 122.9, 123.7, 126.4, 126.9, 127.7, 128.9, 130.7, 140.5, 142.0, 147.5, 187.7; IR (KBr): 3448, 2935, 2853, 1620, 1580, 1475, 1440, 1297, 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^+).

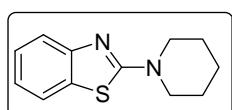
2-Morpholinobenzo[d]thiazole (11'a):



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.

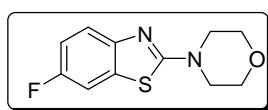
-S16 -

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



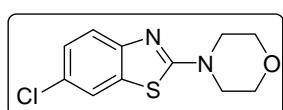
White solid; M.p. 96–97 °C; ^1H NMR (400 MHz, CDCl_3): δ 1.67 (s, 6H), 3.58 (s, 4H), 7.03 (t, 1H, J = 8.0 Hz), 7.26 (t, 1H, J = 8.0 Hz), 7.55 (dd, 2H, J_1 = 8.0 Hz, J_2 = 5.2 Hz); ^{13}C NMR (100 MHz, CDCl_3): δ 24.3, 25.4, 49.7, 118.9, 120.7, 121.1, 126.0, 130.8, 153.1, 169.0; IR (KBr): 2934, 2922, 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):



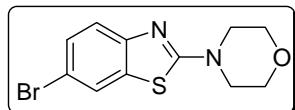
White solid; M.p. 157–158 °C; ^1H NMR (400 MHz, CDCl_3): δ 3.51 (t, 4H, J = 4.8 Hz), 3.75 (t, 4H, J = 4.4 Hz), 6.97 (m, 1H), 7.25 (m, 1H), 7.44 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 48.4, 66.1, 107.4, 107.6, 113.6, 113.9, 119.7, 119.8, 131.2, 131.4, 148.9, 157.0, 159.4, 168.5; IR (KBr): 2982, 2901, 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):

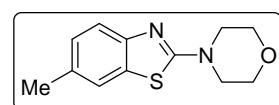


White solid; M.p. 165–167 °C; ^1H NMR (400 MHz, CDCl_3): δ 3.57 (t, 4H, J = 4.8 Hz), 3.80 (t, 4H, J = 4.8 Hz), 7.37 (s, 2H), 7.68 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 48.5, 66.3, 114.0,

-S17 -

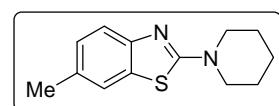
120.5, 123.3, 129.4, 132.4, 151.6, 169.1; IR (KBr): 2918, 2857, 1591, 1535, 1443, 1372, 1280, 1258, 1229, 1110, 1026, 940, 863, 813 cm⁻¹; Anal. Calcd for C₁₁H₁₁N₂OSBr: C 44.16, H 3.71, N 9.36, S 10.72; found C 44.23, H 3.76, N 9.28, S 10.64.

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



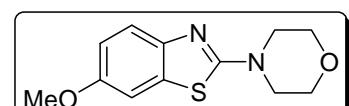
White solid; M.P. 134–136 °C; ¹H NMR (400 MHz, CDCl₃): δ 2.37 (s, 3H), 3.56 (t, 4H, *J* = 4.8 Hz), 3.79 (t, 4H, *J* = 4.8 Hz), 7.09 (d, 1H, *J* = 8.0 Hz), 7.39 (s, 1H), 7.44 (d, 1H, *J* = 8.0 Hz); ¹³C NMR (100 MHz, CDCl₃): δ 21.3, 48.6, 66.3, 119.0, 120.9, 127.4, 130.7, 131.6, 150.4, 168.6; IR (KBr): 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, CDCl₃): 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); ¹³C NMR (100 MHz, CDCl₃): 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⁺).

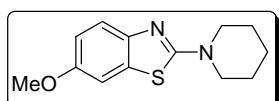
6-Methoxy-2-morpholinobenzo[d]thiazole (19'a):



White solid; M.p. 130–132 °C; ¹H NMR (400 MHz, CDCl₃): 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); ¹³C NMR (100 MHz, CDCl₃): 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⁺).

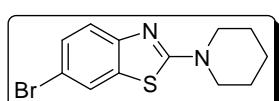
-S18 -

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^+).

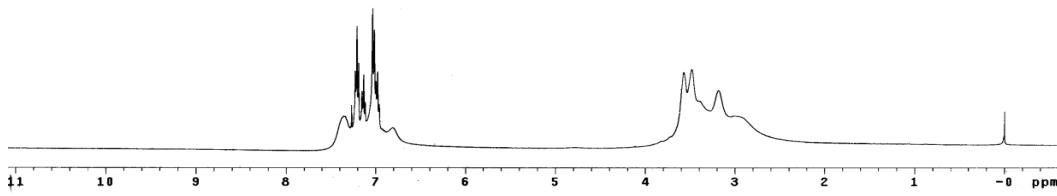
-S19 -

Spectra

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

(1a). ^1H NMR (400 MHz, CDCl_3):

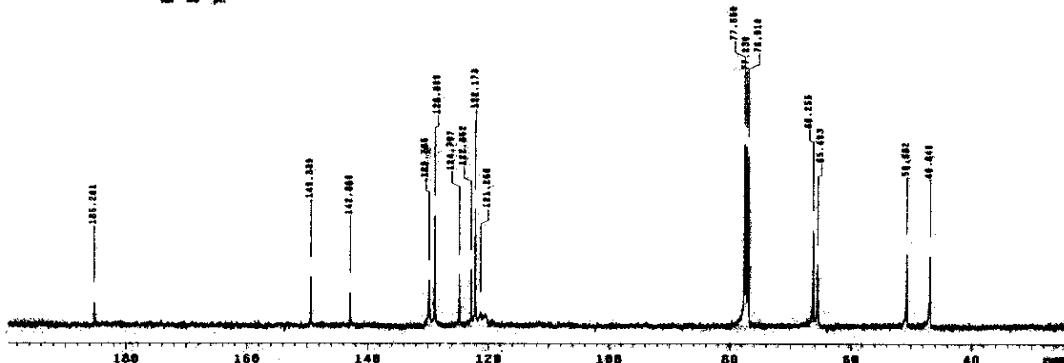
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exp1 s2pul
SAMPLE          SPECIAL
date  Aug 11 2010 temp    not used
solvent   CDCl3  gain   not used
filler    H2O    ntau   not used
ACQUISITION      ntau   0.008
tw       1.0000  p1ta   20.000
at       1.0000  p1ta   20.000
np       25528   flags
rf      399.875  n
ps       4      in
dt      1.0000  nc
nt      32      nc
ct      32      PROCESSING
tn     TRANSMITTER H1  fn      0.10
tr     399.875  DISPLAY 65536
sfrq   399.875
tof    362.8   sp      -262.5
tpowr  9.850   rfi    479.5
pw     9.850   rfi    781.5
DECOUPLER        rfp    0
dn     C13   131.0
dof    0      1p    -97.1
dm     nm
dim    c      wc    250
dpowr 15900   sc    0
dmtf    45      th    20
nm   cdc  ph
```



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

(1a). ^{13}C NMR (100 MHz, CDCl_3):

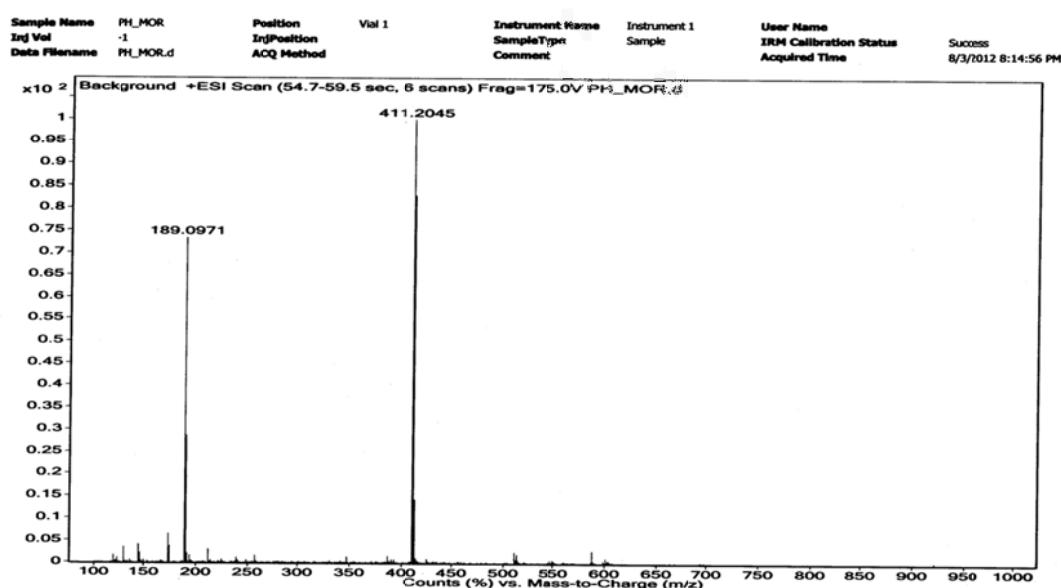
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ss_ph_mor_ant
exp1 s2pul
SAMPLE          SPECIAL
date  Oct  3 2011 temp    not used
solvent   CDCl3  gain   not used
filler    H2O    ntau   not used
ACQUISITION      ntau   0.008
tw       1.0000  p1ta   20.000
at       1.0000  p1ta   20.000
np       60270   flags
rf      138.664  DISPLAY 65536
ps       5      in
dt      20      nc
nt      1.0000  dp
ct      3726   PROCESSING
tn     TRANSMITTER C13  fm      2.99
tr     138.664
sfrq   138.664
tof    138.664  sp      -327.6
tpowr  8.380   rfi    5278.2
pw     8.380   rfi    7764.0
DECOUPLER        rfp    0
dn     H1   45336
dof    0      1p    -484.5
dm     nm
dim    c      wc    250
dpowr 65536   sc    0
dmtf    45      th    20
nm   mp  ph
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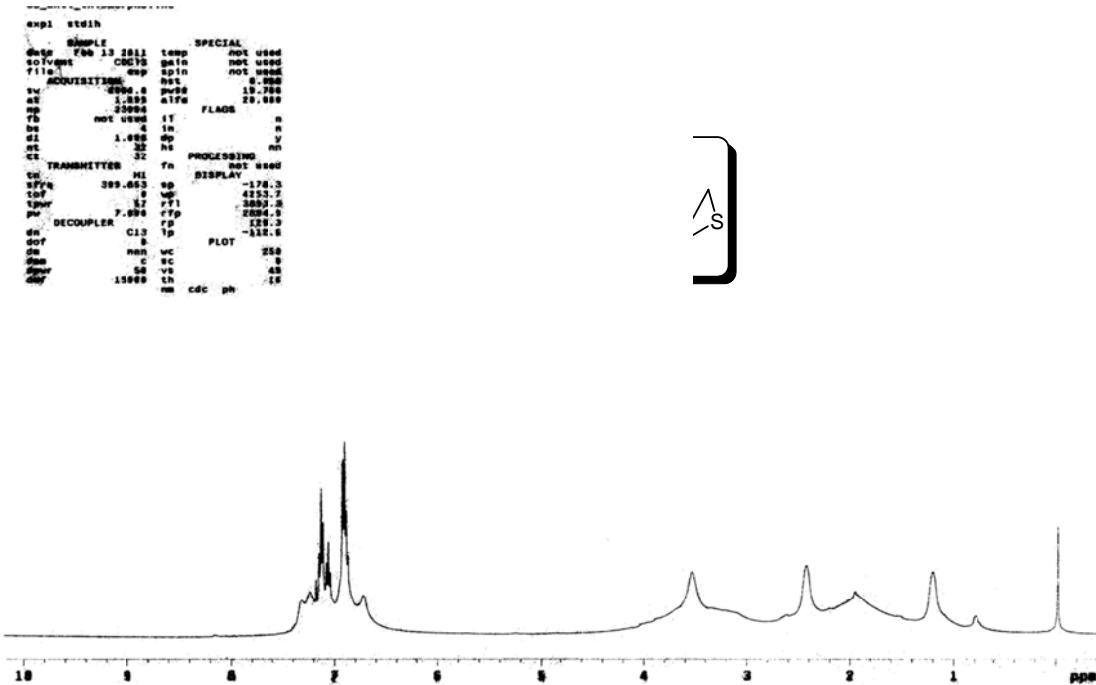
-S20 -

N-((E)-Morpholino(phenylimino)methyl)-N-phenylmorpholine-4-carbothioamide (1a).

MASS SPECTRA:

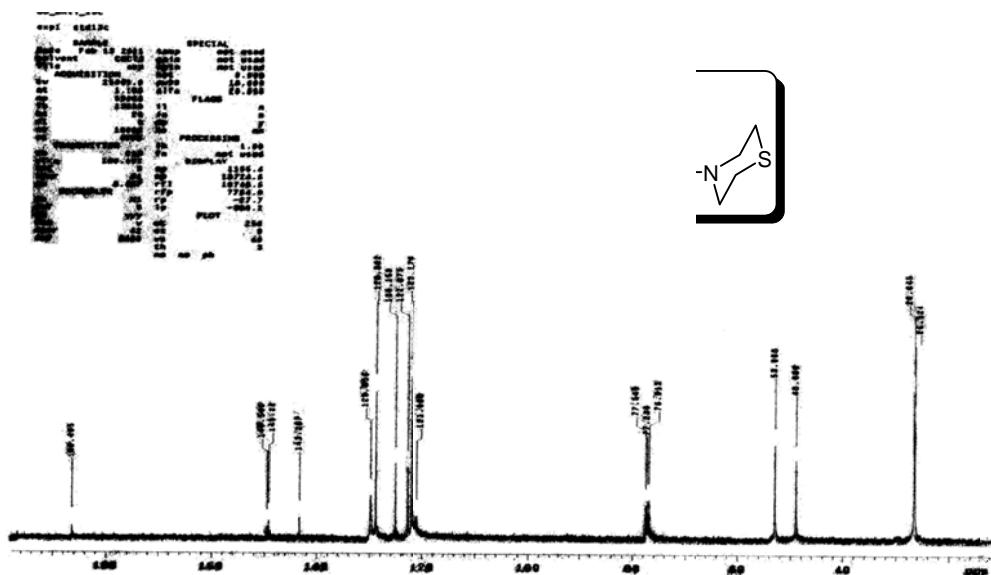


N-Phenyl-N-((E)-(phenylimino)(thiomorholino)methyl)thiomorpholine-4-carbothioamide (1b). ^1H NMR (400 MHz, CDCl_3):

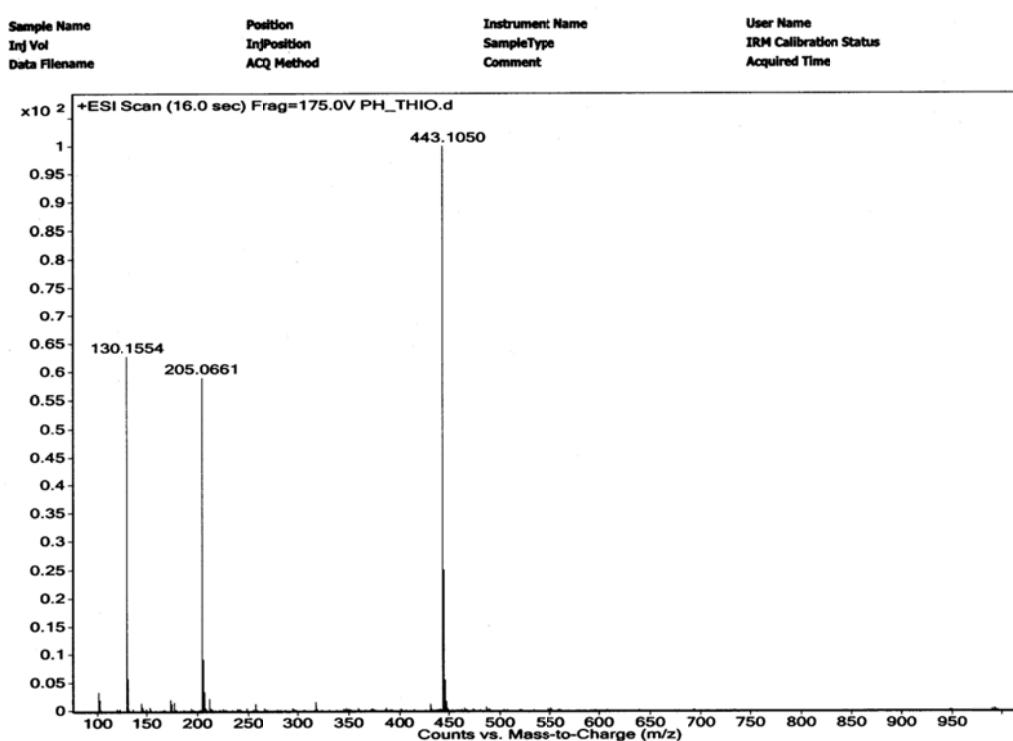


-S21 -

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



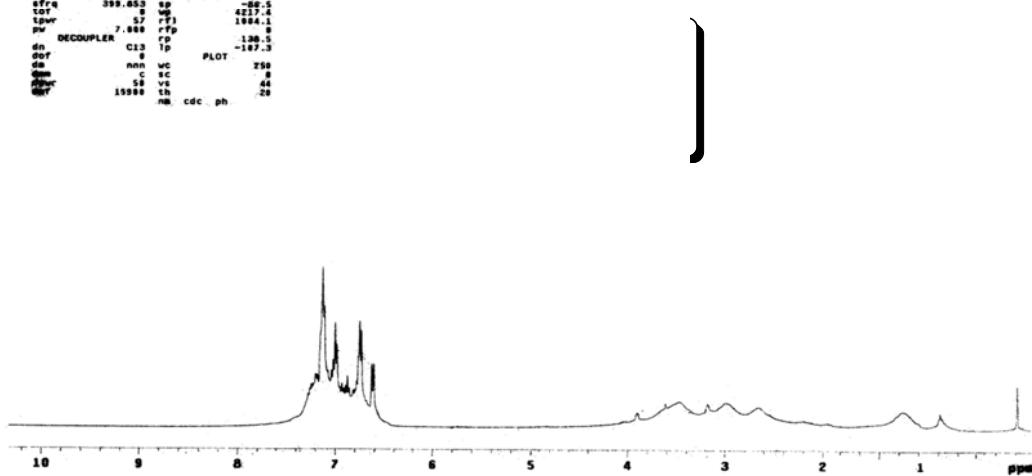
N-Phenyl-N-((E)-(phenylimino)(thiomorholino)methyl)thiomorpholine-4-carbothioamide (1b). MASS SPECTRA:



-S22 -

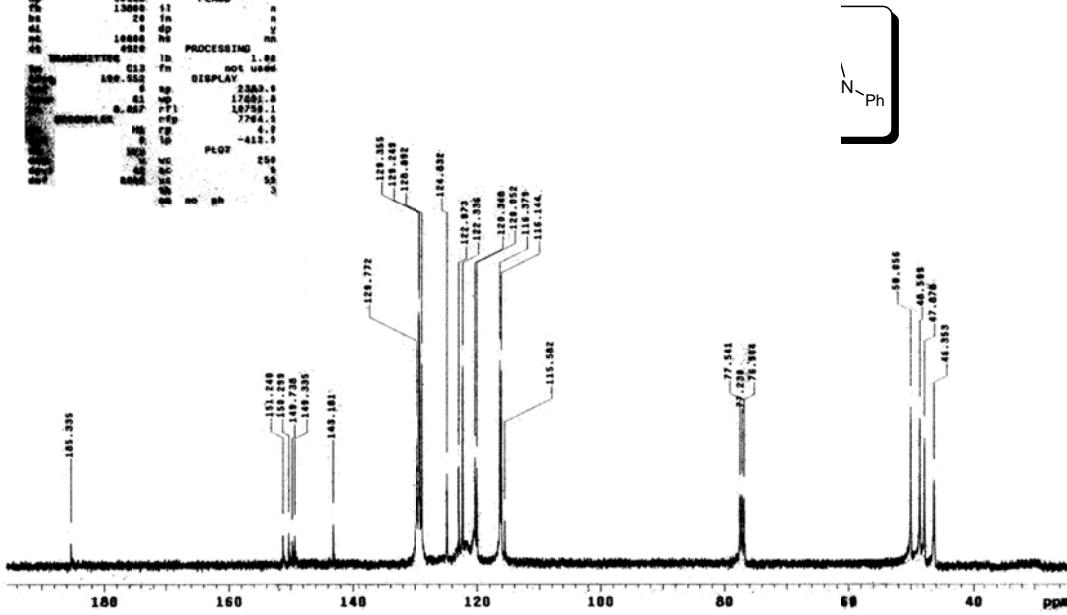
N,4-Diphenyl-N-((E)-(phenylimino)(4-phenylpiperazine-1-yl)methyl)piperazine-1-carbothioamide (1c). ^1H NMR (400 MHz, CDCl_3):

WINDI 5.0101
SAMPLE: Feb 16 2011
TEMP: not used
PULPROG: QCPD3
TD: 65536
ACQTIME: 1.000
SW: 4000.0 Hz
ET: 1.2500
NP: 256000
TD0: not used
DS: 11
SF: 1.0000
DW: 100.000
RG: 32
CT: 32
TRANSMITTER: Td: not used
TE: 399.452 s
ETR: 200.000
TPWR: 57 rF1
PW: 7.888 rFp
DECOPULER: C13 IP: 130.0
D1: C13 IP: -187.3
D2: nnn xc PLOT: ZSI
D3: nnn xc
D4: c xc
D5: z xc
D6: g xc
D7: 46
D8: 26
D9: 19988 TH: cdc_ph



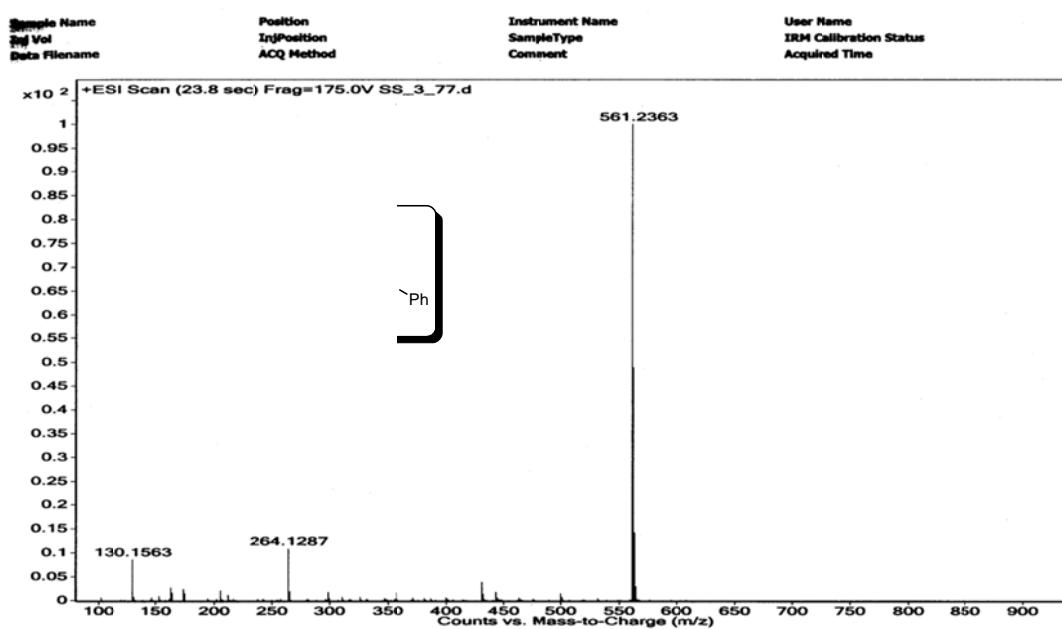
N,4-Diphenyl-N-((E)-(phenylimino)(4-phenylpiperazine-1-yl)methyl)piperazine-1-carbothioamide (1c). ^{13}C NMR (100 MHz, CDCl_3):

WINDI 5.0101
SAMPLE: Feb 16 2011
TEMP: not used
PULPROG: QCPD3
TD: 65536
ACQTIME: 1.000
SW: 10000.0 Hz
ET: 1.2500
NP: 256000
TD0: not used
DS: 11
SF: 1.0000
DW: 100.000
RG: 4096
CT: 4096
TRANSMITTER: Td: not used
TE: 100.552 s
ETR: 200.000
TPWR: 61 rF1
PW: 1.67981 rFp
DECOPULER: MS: 412.0
D1: MS: 250
D2: PLOT: ZSI
D3: NO ph

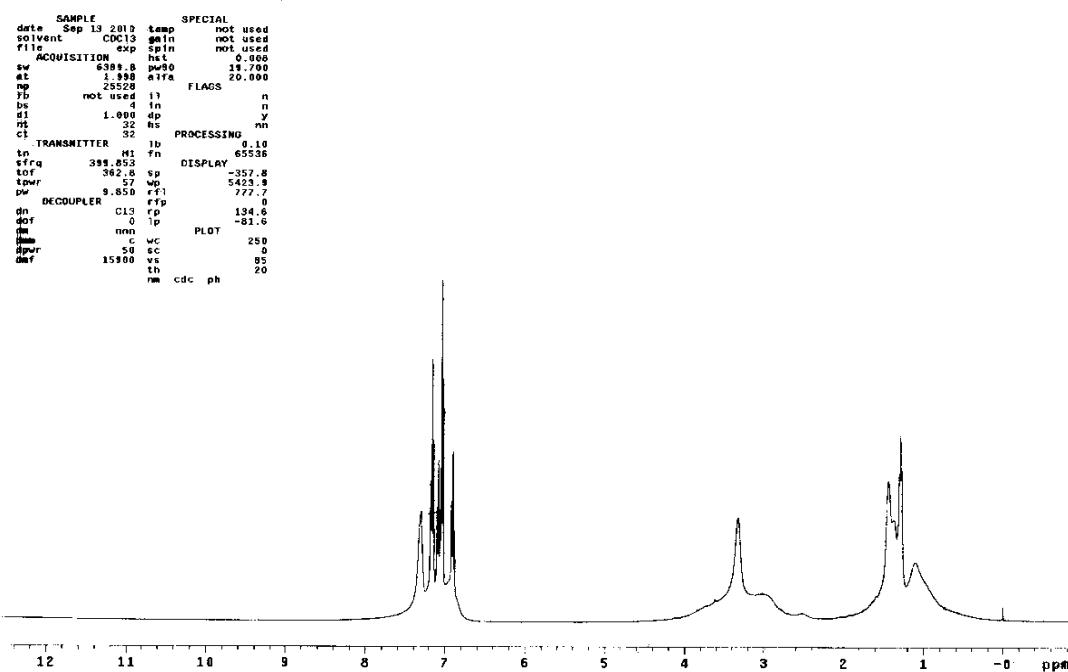


-S23 -

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

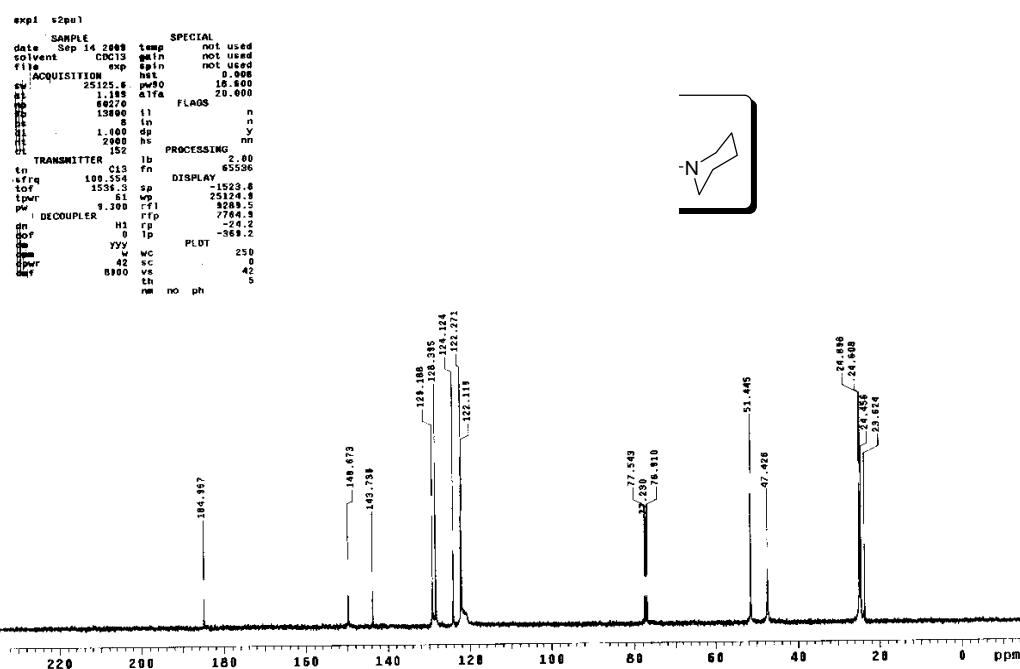


N-Phenyl-N-((E)-(phenylimino)(piperidin-1-yl)methyl)piperidine-1-carbothioamide (1d). ^1H NMR (400 MHz, CDCl_3):

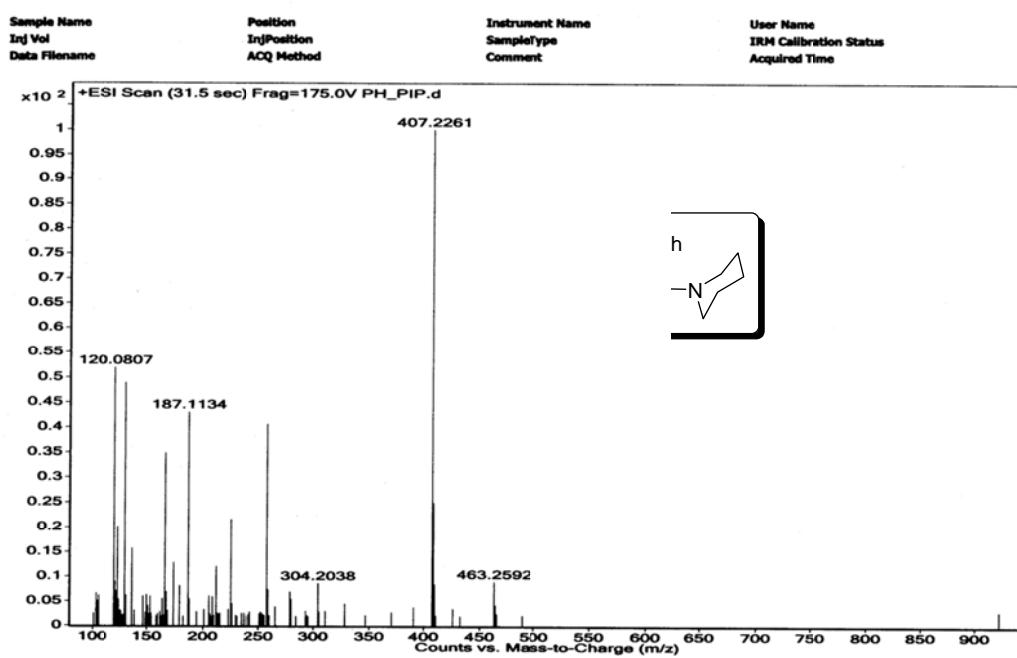


-S24 -

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

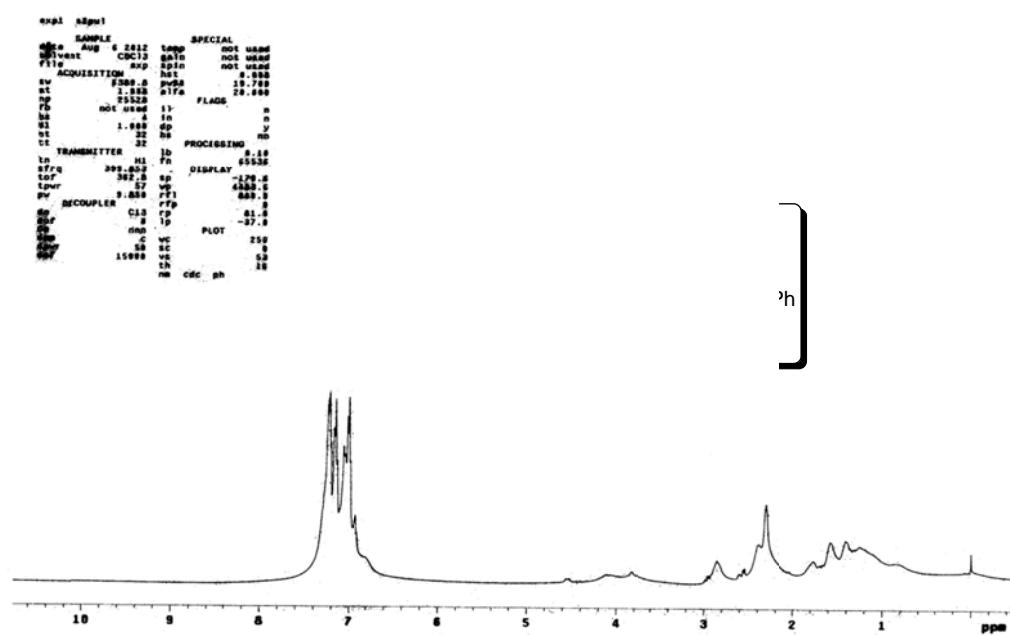


N-Phenyl-N-((E)-(phenylimino)(piperidin-1-yl)methyl)piperidine-1-carbothioamide (1d). MASS SPECTRA:

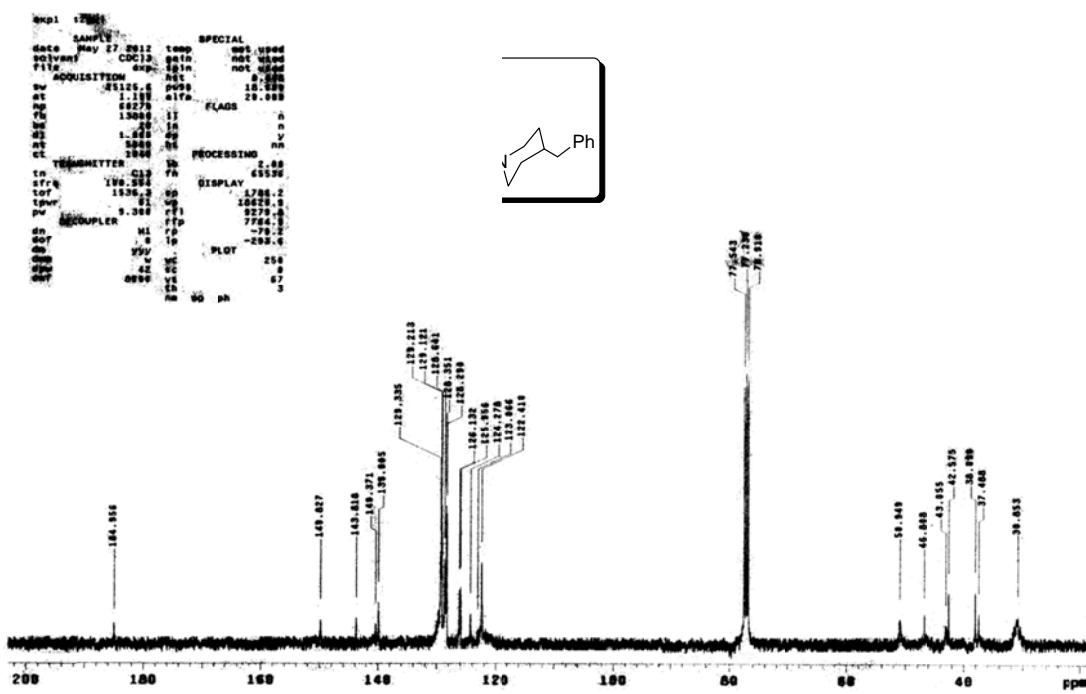


-S25 -

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

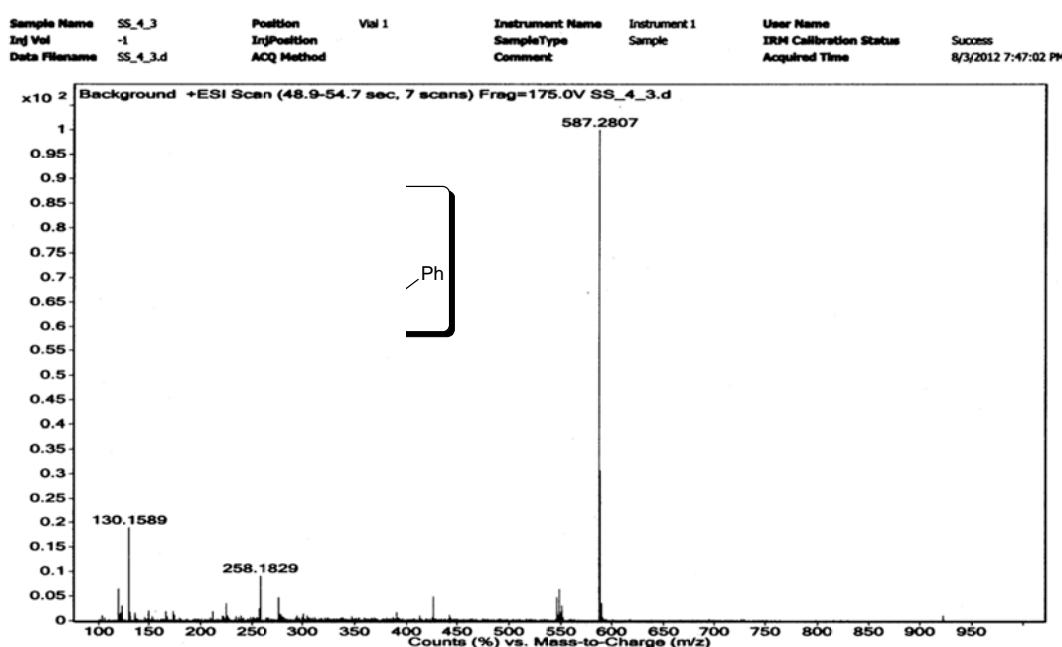


4-Benzyl-N-((E)-(4-benzylpiperidin-1-yl)(phenylimino)methyl)-N-phenylpiperidine-1-carbothioamide (1e). ^{13}C NMR (100 MHz, CDCl_3):



-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):

exp1_s2pu1

SPECIAL

SAMPLE temp not used
date Aug 8 2010 gain not used
solvent CDCl₃ spin not used
file /export/home/... ps60 1.988
ps60 19.700
ACQUISITION a17a 20.000

sw 3000.0 flags

rt 1.980 11 n

dp 25928 in n

dt not used dp y

hs 4 ns mn

di 1.060 processing mn

nc 32 tb 0.10

ct 32 rh 65596

transmitter DISPLAY

tnq 398.8 H1 sp -217.2

tnrq 398.853 qp 466.3

tpf 382.8 rf1 712.9

tpfr 37 712.9

ppm 9.850 rp 87.9

DECOPPLER C13 ip -35.5

RTF C13 PLOT

RTF mm ec 250

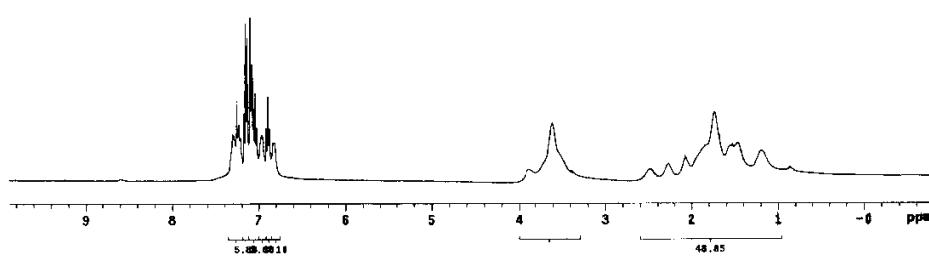
RTF c vs 41

RTF s sh 4

RTF 15000 nm cdc ph

Ph

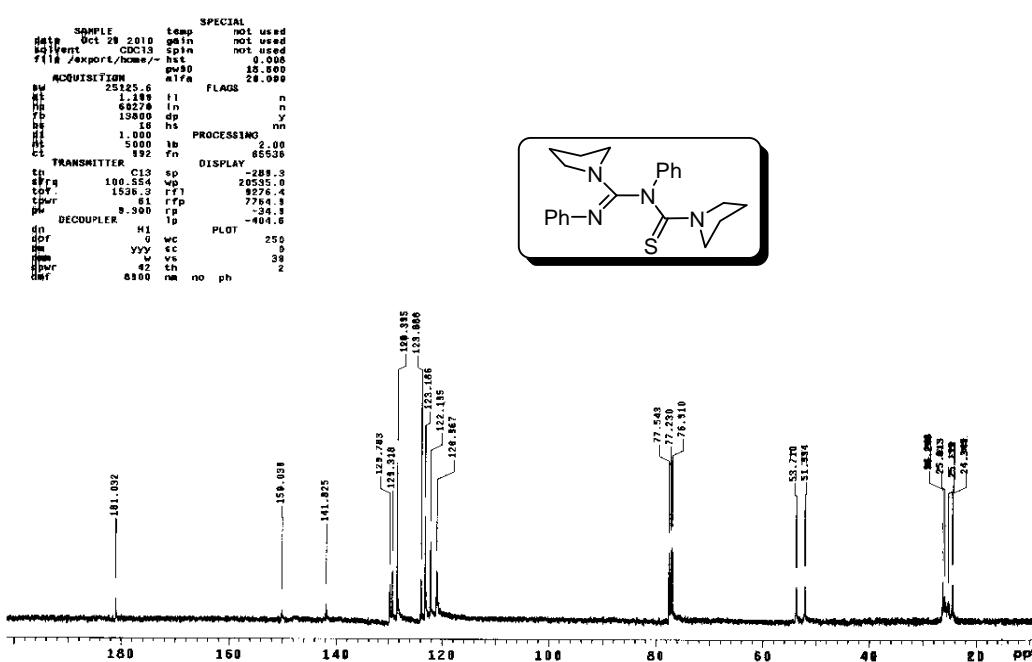
Ph-N=C-N(C(=S)Ph)-C₂H₅



-S27 -

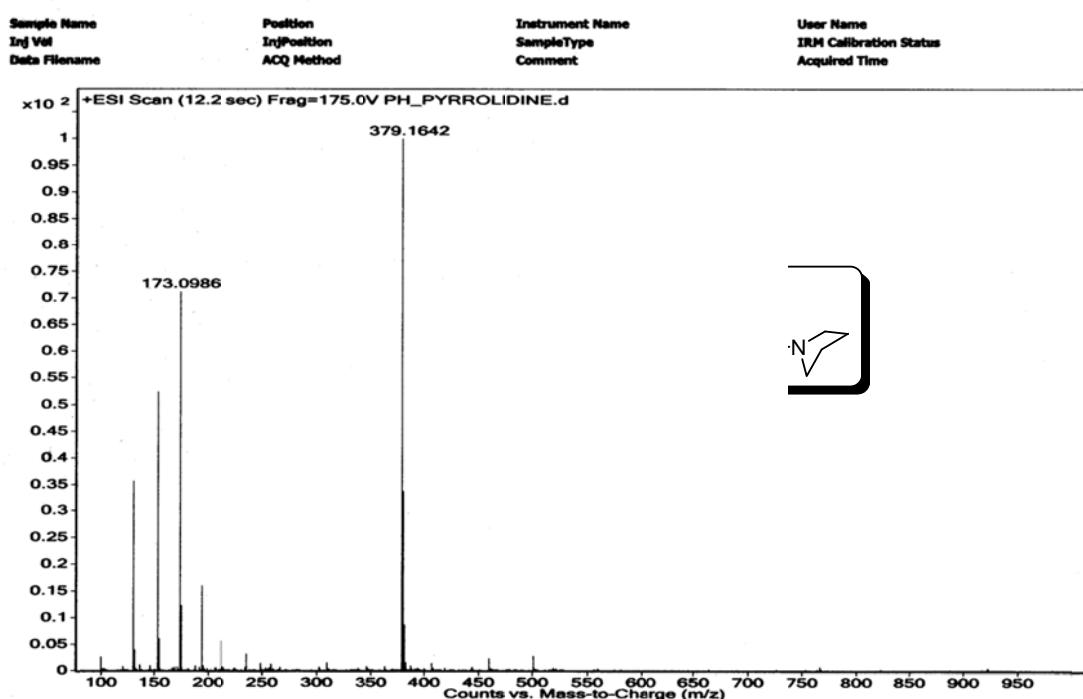
N-Phenyl-N-((E)-(phenylimino)(pyrrolidin-1-yl)methyl)pyrrolidine-1-carbothioa-mide (1f).

¹³C NMR (100 MHz, CDCl₃):



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

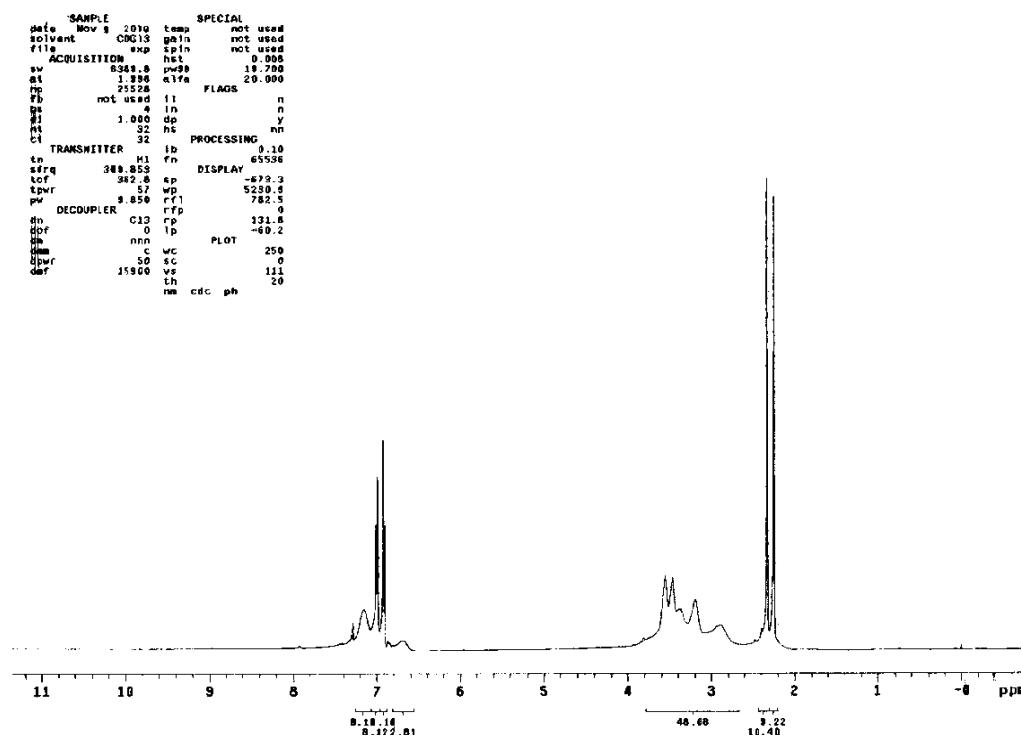
MASS SPECTRA:



-S28 -

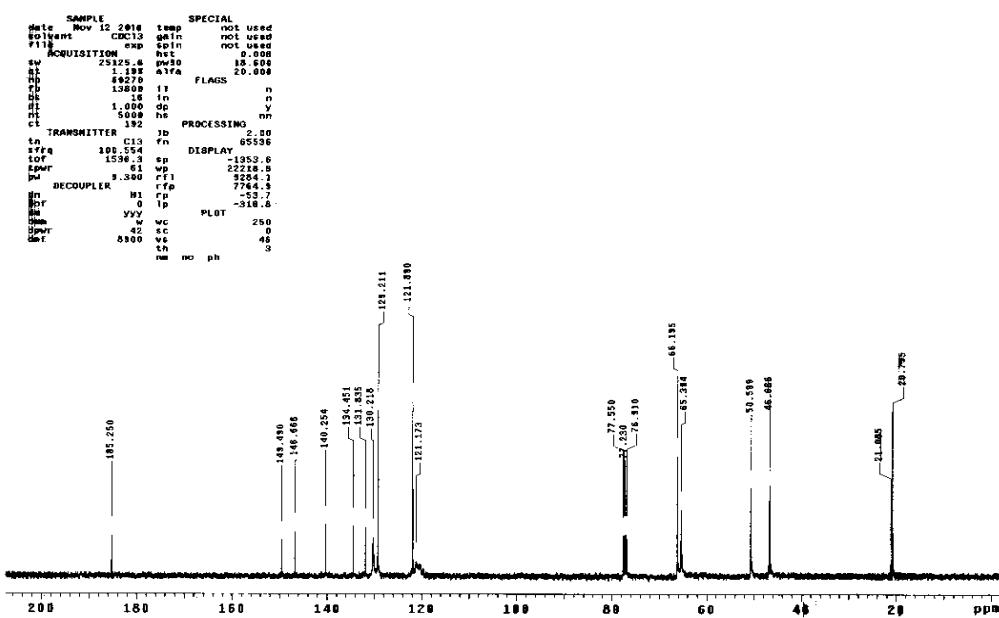
N-((E)-(p-Tolylimino)(morpholino)methyl)-N-p-tolylmorpholine-4-carbothioamide

(2a). ^1H NMR (400 MHz, CDCl_3):



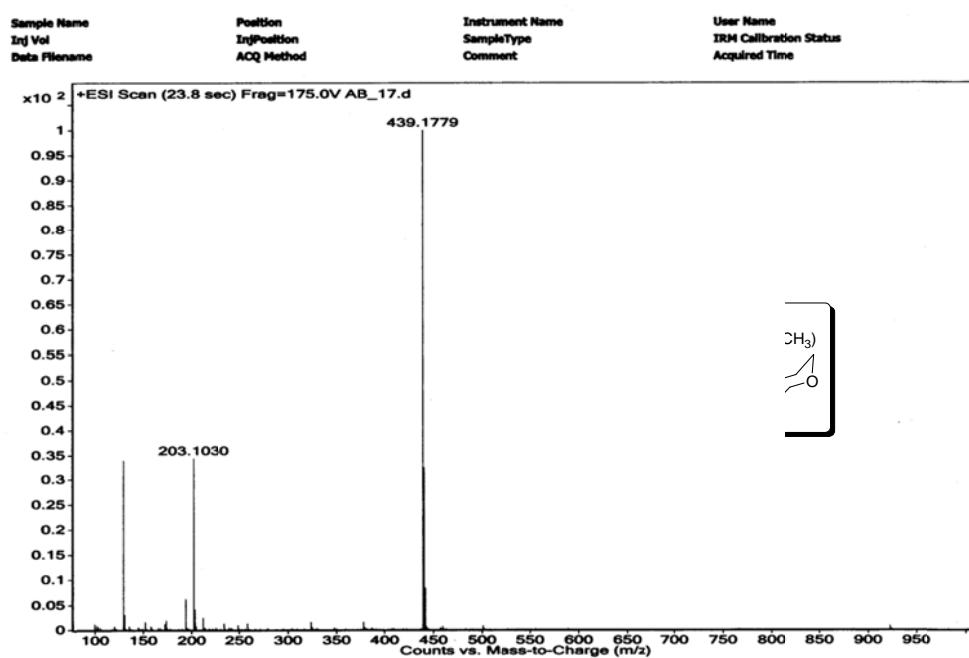
N-((E)-(p-Tolylimino)(morpholino)methyl)-N-p-tolylmorpholine-4-carbothioamide

(2a). ^{13}C NMR (100 MHz, CDCl_3):



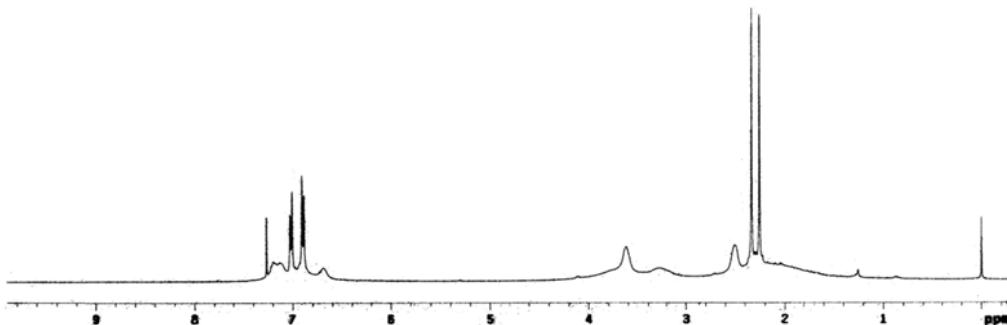
-S29 -

N-((E)-(p-Tolylimino)(morpholino)methyl)-N-p-tolylmorpholine-4-carbothioamide (3a). MASS SPECTRA:



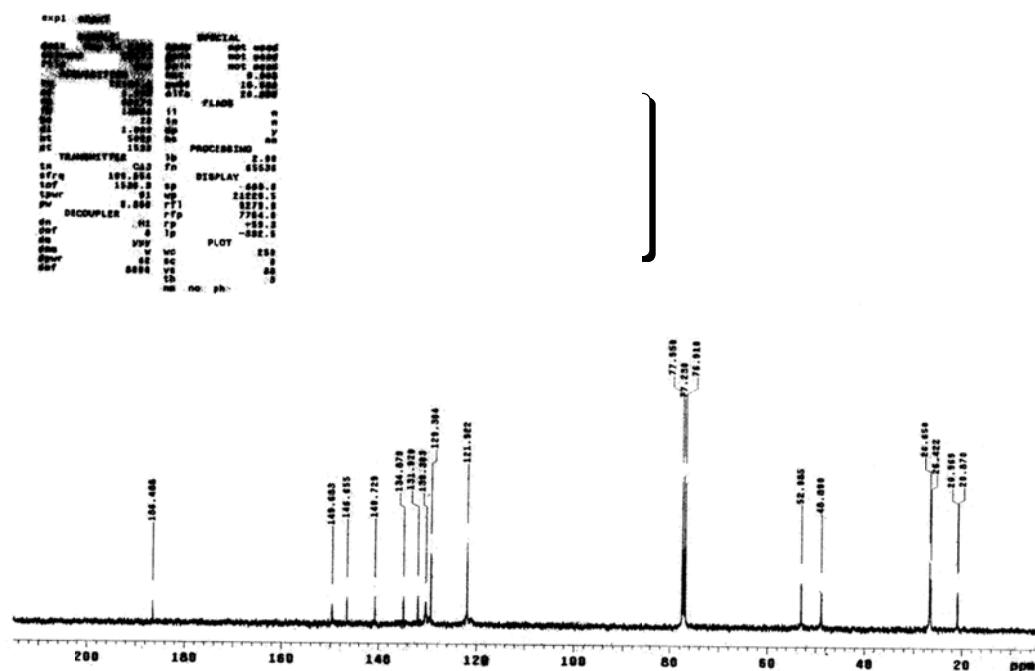
N-((E)-(p-Tolylimino)(thiomorpholino)methyl)-N-p-tolylthiomorpholine-4-carbothioamide (2b). ¹H NMR (400 MHz, CDCl₃):

```
expt s2p1
SAMPLE          SPECTRAL
date  May 25 2012  temp    .not used
solvent   CDCl3  gain    .not used
time    .000000  disp    .not used
ACQUISITION      freq    400.000
            w1f9  19.765
            w1f10 26.000
            w1f26 25.226
            flags
            not used 11  n
            1.000  n
            1.000  v
            32  ns  nh
            32  ps  nh
            32  PROCESSING  nh
TRANSMITTER      1b  9.18
to      H1  fm  65536
trate  399.812  ap  DISPLAY
tref  342.57  ap  -129.7
tppr  57  vp  4668.1
pw  3.656  rt1  792.1
DECOUPLER        C13  rfp  111.8
d1  nan  ip  -99.9
dof  nan  PLOT
dppf  C  wc  256
dppr  50  sc  1
dpsr  154000  tr  65
        28
nr  cdc  ph
```

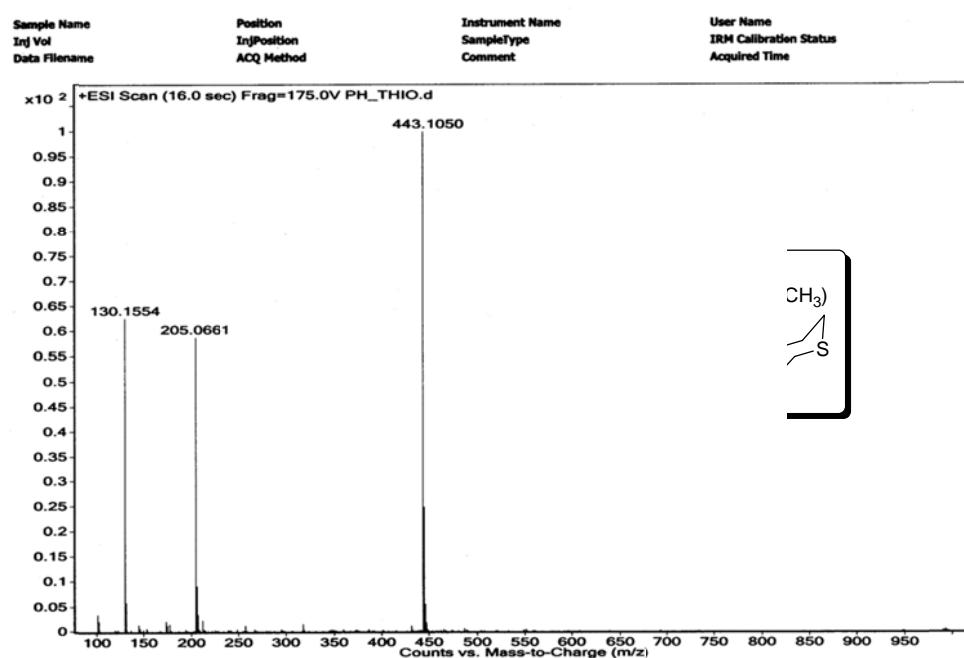


-S30 -

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

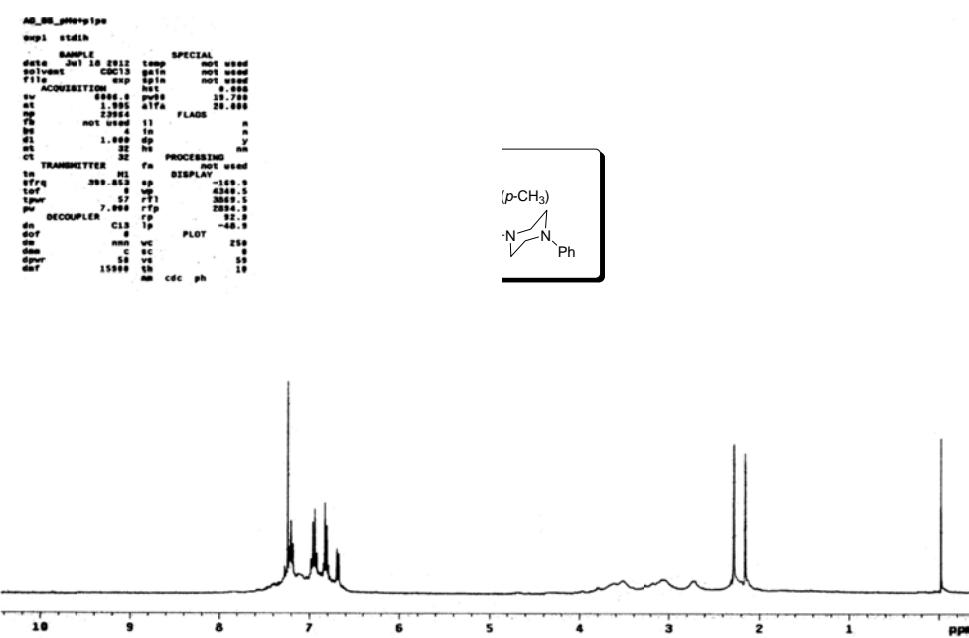


N-((E)-(p-Tolylimino)(thiomorpholino)methyl)-N-p-tolylthiomorpholine-4-carbothioamide (2b). MASS SPECTRA:

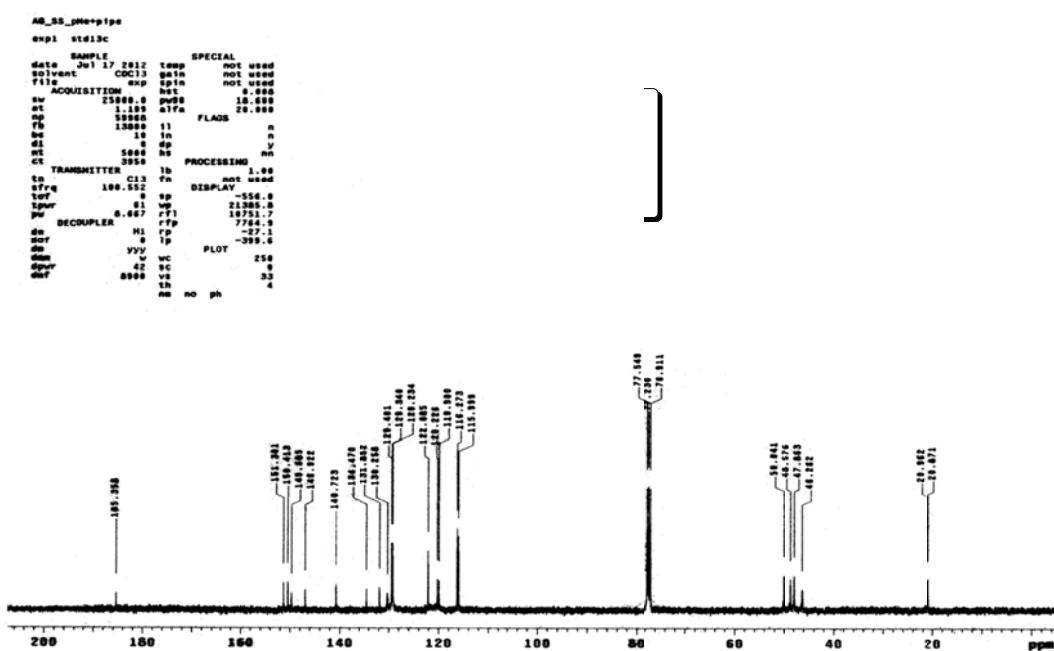


-S31 -

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

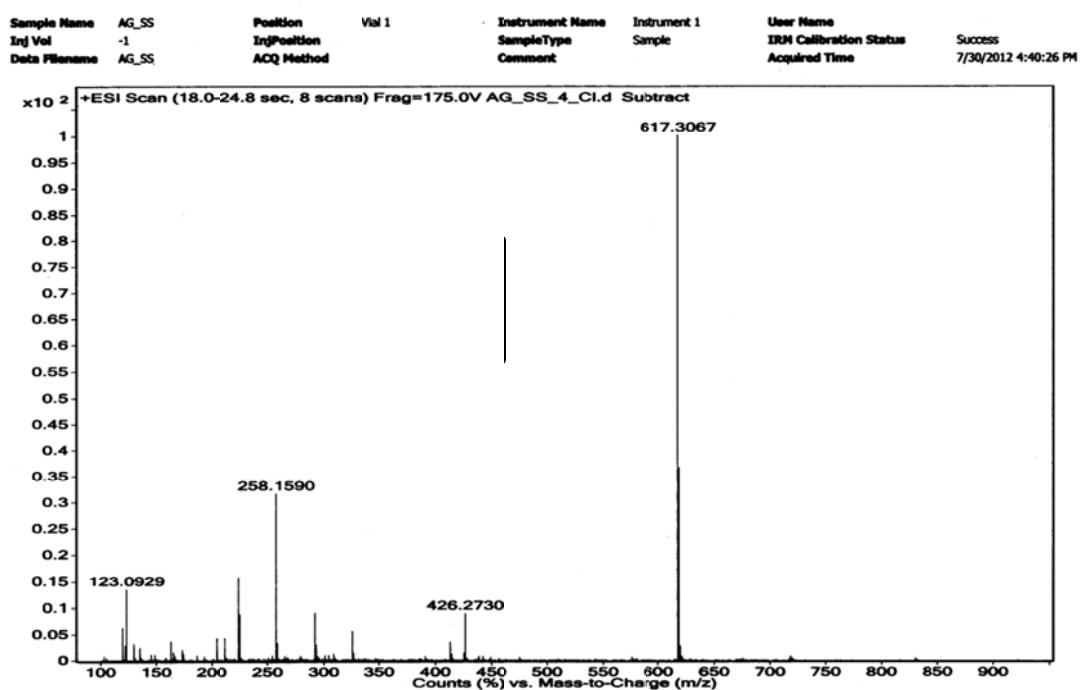


N-((E)-(p-Tolylimino)(4-phenylpiperzin-1-yl)methyl)-4-phenyl-N-p-tolylpiperazine-1-carbothioamide (2c). ^{13}C NMR (100 MHz, CDCl_3):

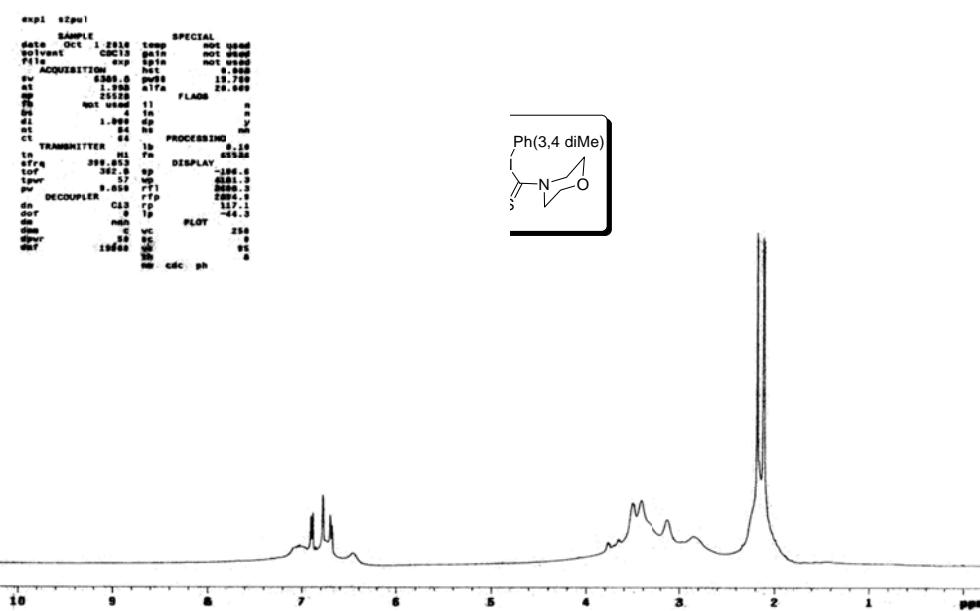


-S32 -

N-((E)-(p-Tolylimino)(4-phenylpiperzin-1-yl)methyl)-4-phenyl-N-p-tolylpiperazine-1-carbothioamide (2c). MASS SPECTRA:

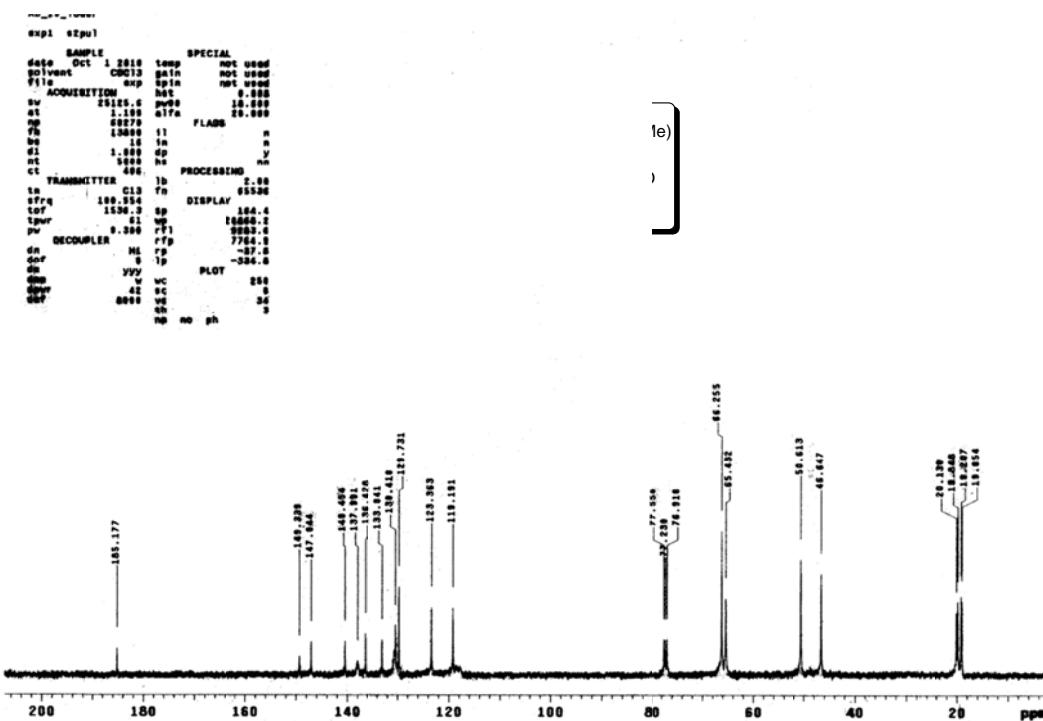


N-((E)-(3,4-Dimethylphenylimino)(morpholino)methyl)-N-(3,4-dimethylphenyl) morpholine-4-carbothioamide (3a). ¹H NMR (400 MHz, CDCl₃):

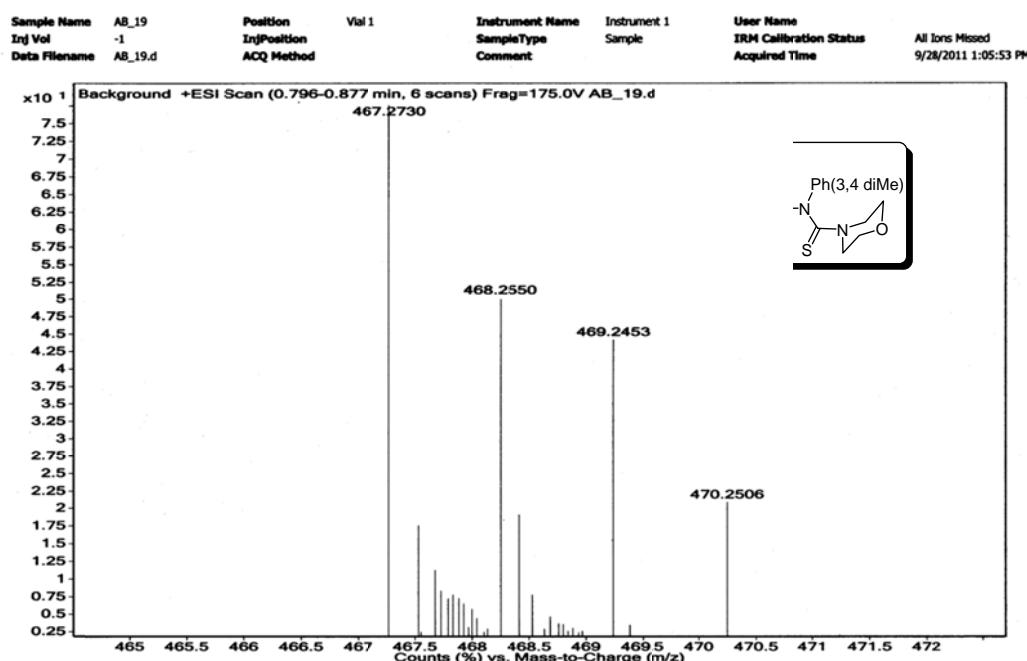


-S33 -

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

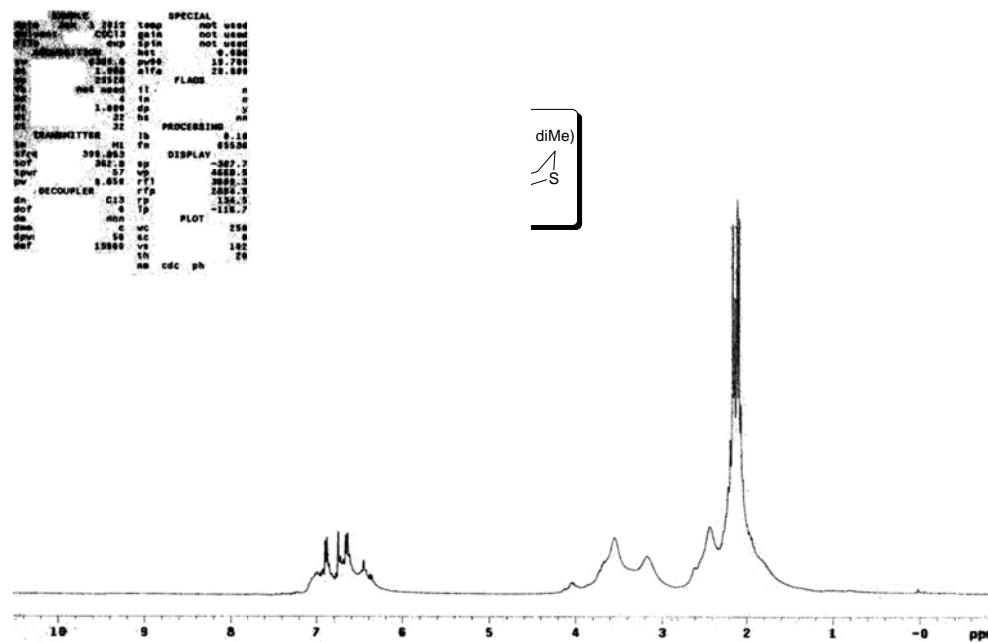


N-((E)-(3,4-Dimethylphenylimino)(morpholino)methyl)-N-(3,4-dimethylphenyl) carbothioamide (3a). MASS SPECTRA: morpholine-4-

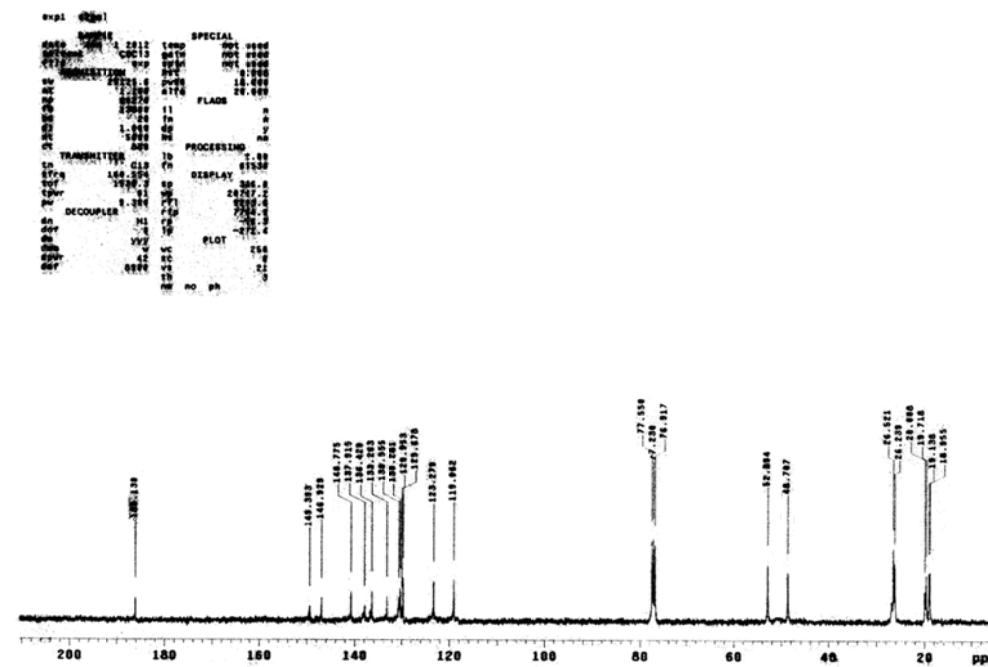


-S34 -

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

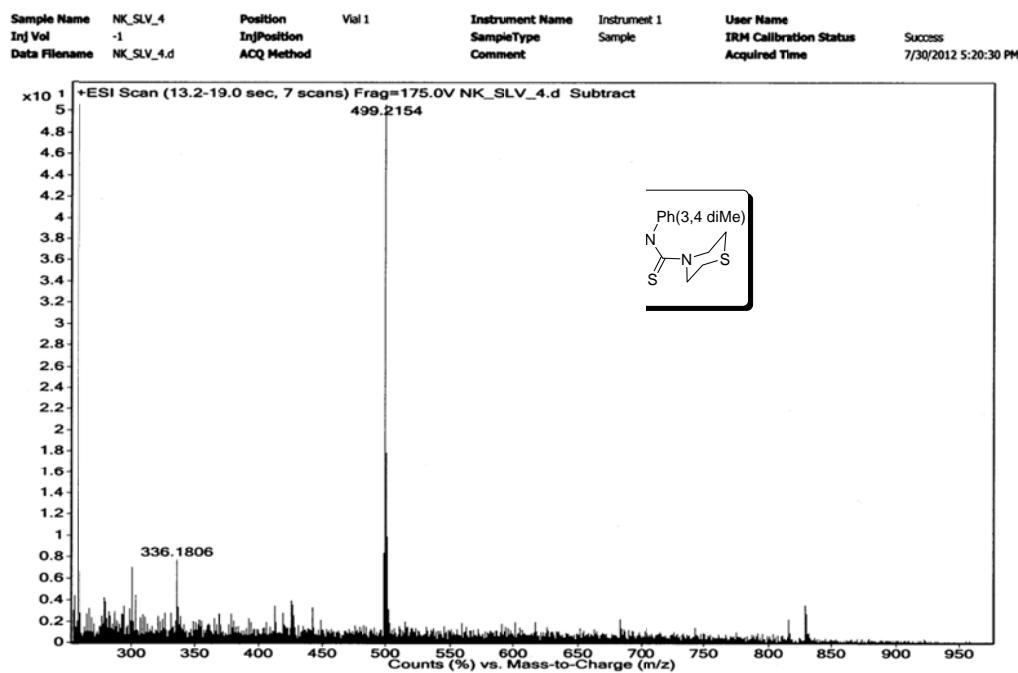


N-((E)-(3,4-Dimethylphenylimino)(thiomorpholino)methyl)-N-(3,4-dimethylphenyl) thiomorpholine-4-carbothioamide (3b). ^{13}C NMR (100 MHz, CDCl_3):

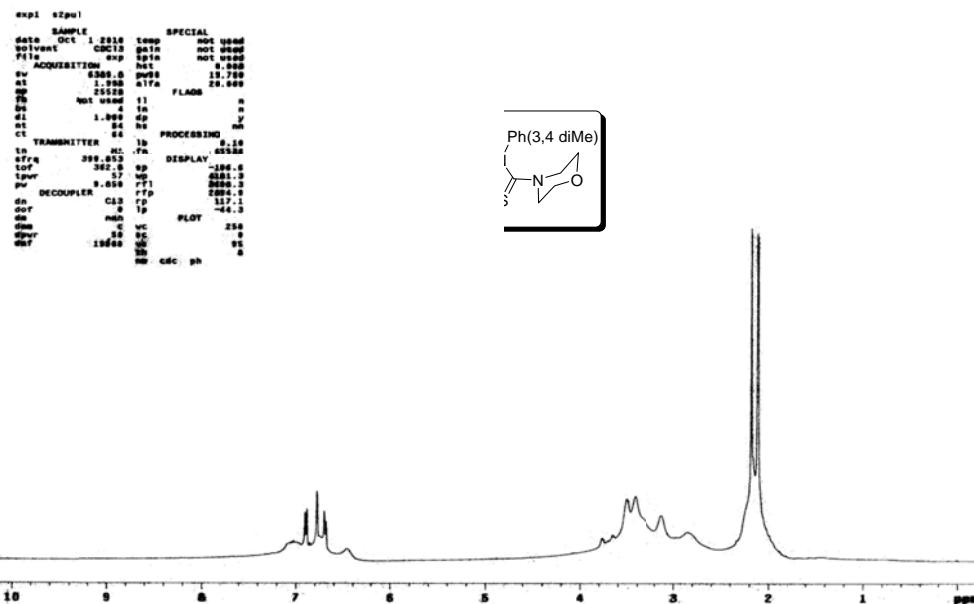


-S35 -

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

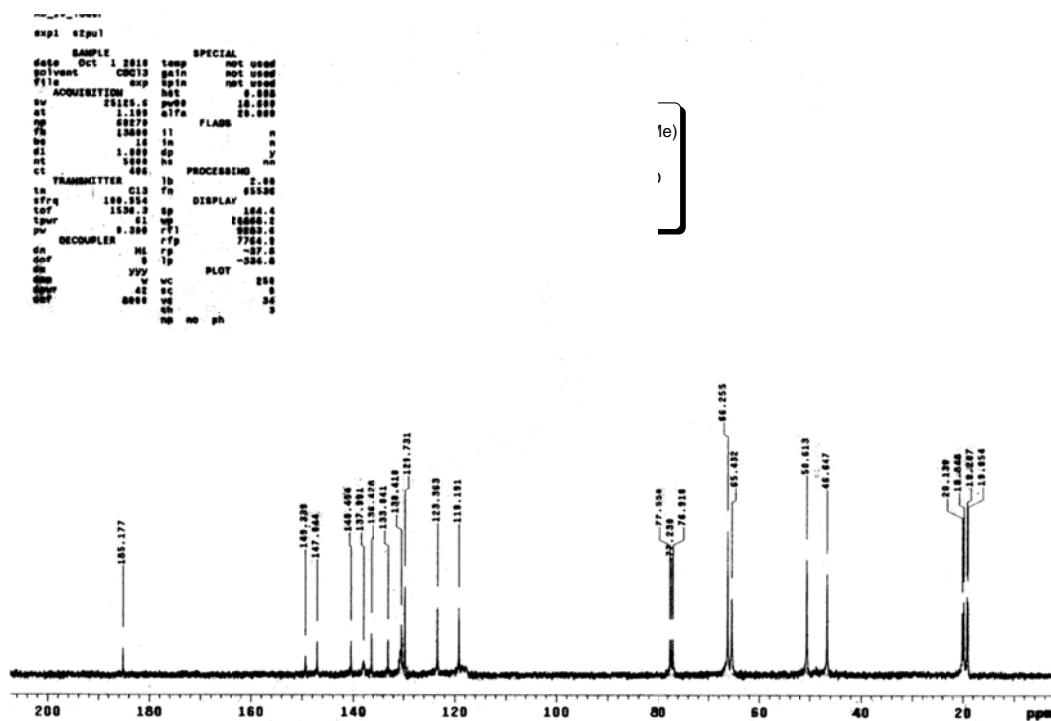


N-((E)-(3,4-Dimethylphenylimino)(morpholino)methyl)-N-(3,4-dimethylphenyl)carbothioamide (4'a). ^1H NMR (400 MHz, CDCl_3):

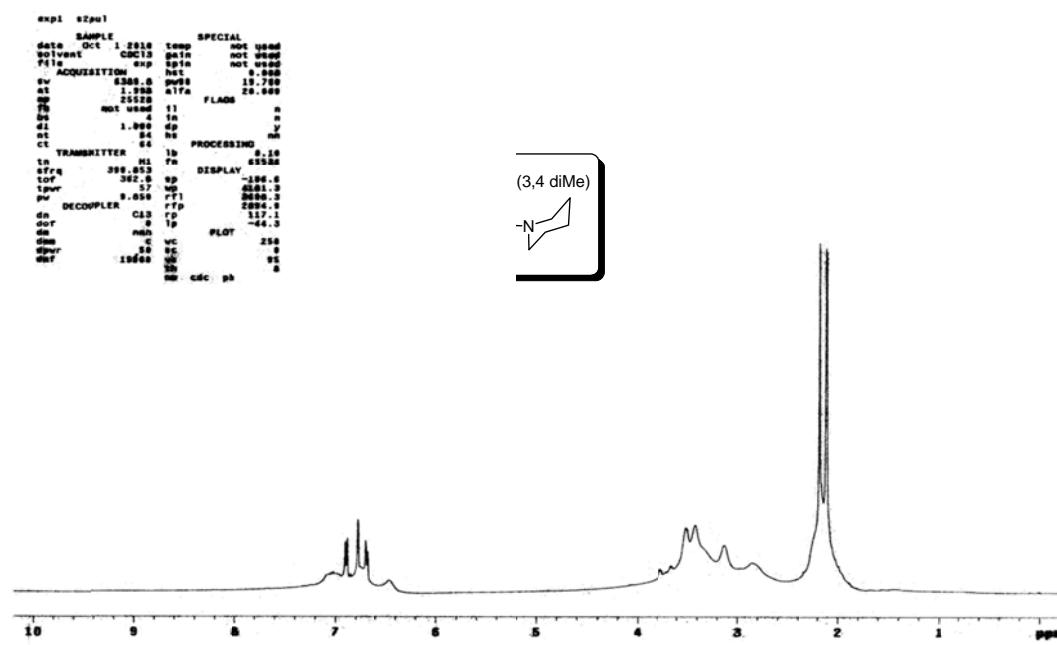


-S36 -

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

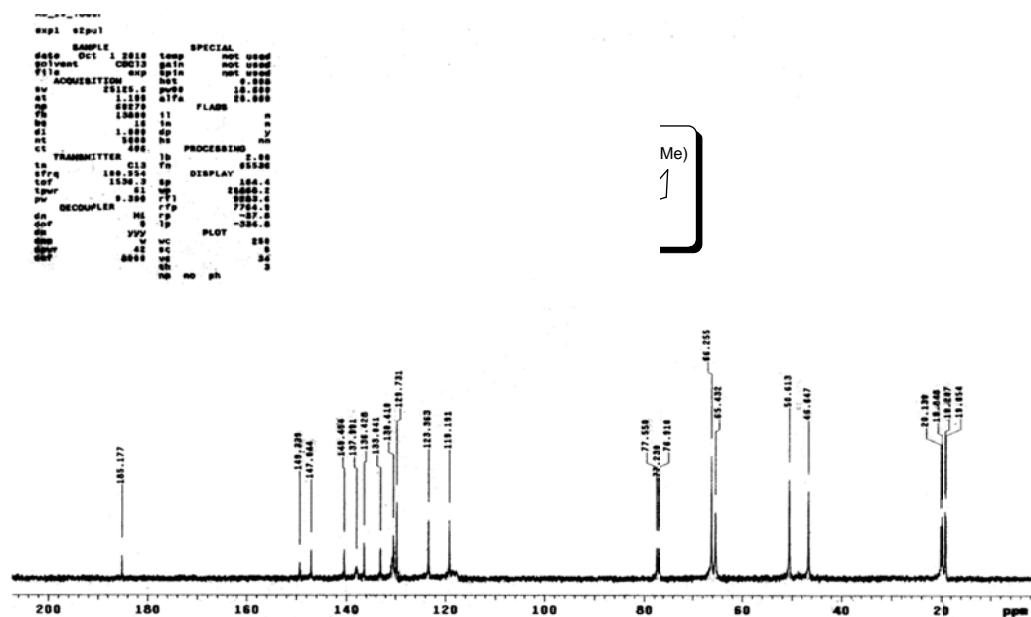


N-((E)-(3,4-Dimethylphenylimino)(pi[peridin-1-yl]methyl)-N-(3,4-dimethylphenyl) piperidine-1-carbothioamide (3d). ^1H NMR (400 MHz, CDCl_3):

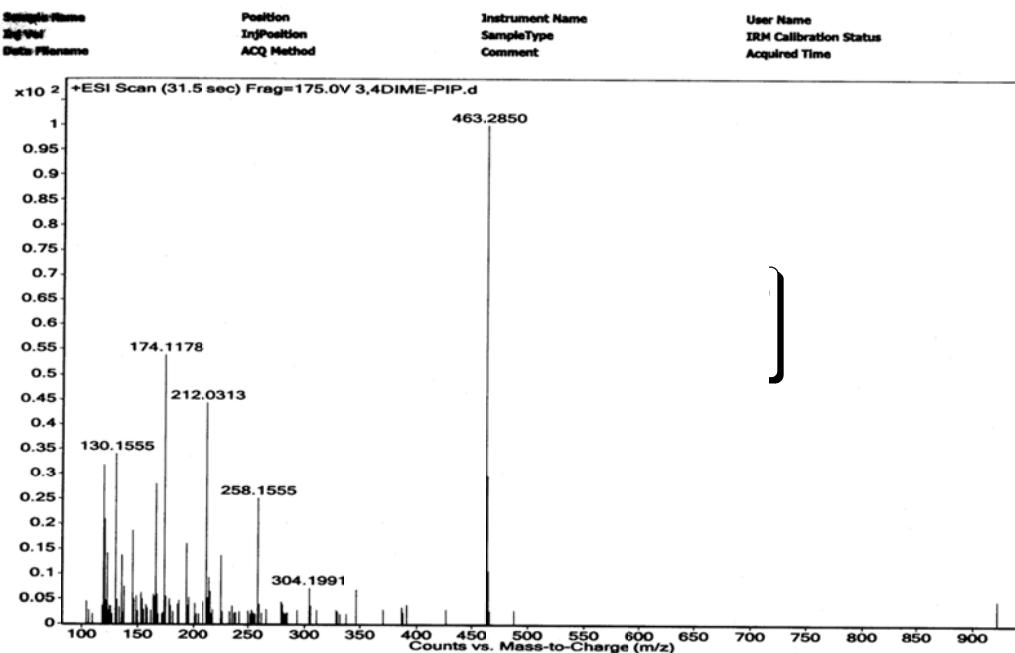


-S37 -

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

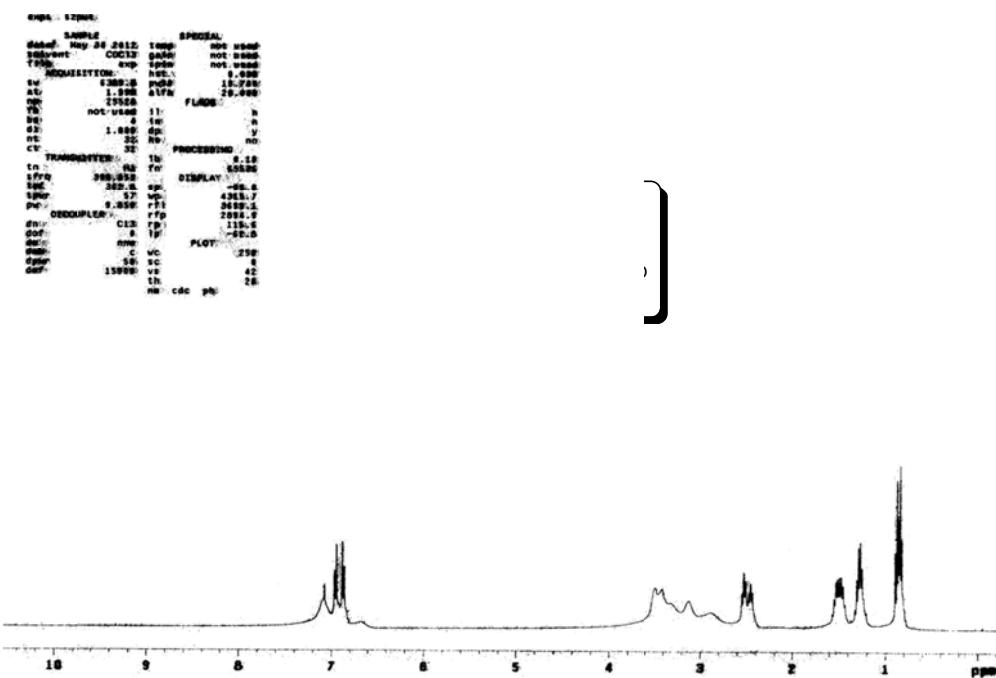


N-((E)-(3,4-Dimethylphenylimino)(morpholino)methyl)-N-(3,4-dimethylphenyl) morpholine-4-carbothioamide (3d). MASS SPECTRA:

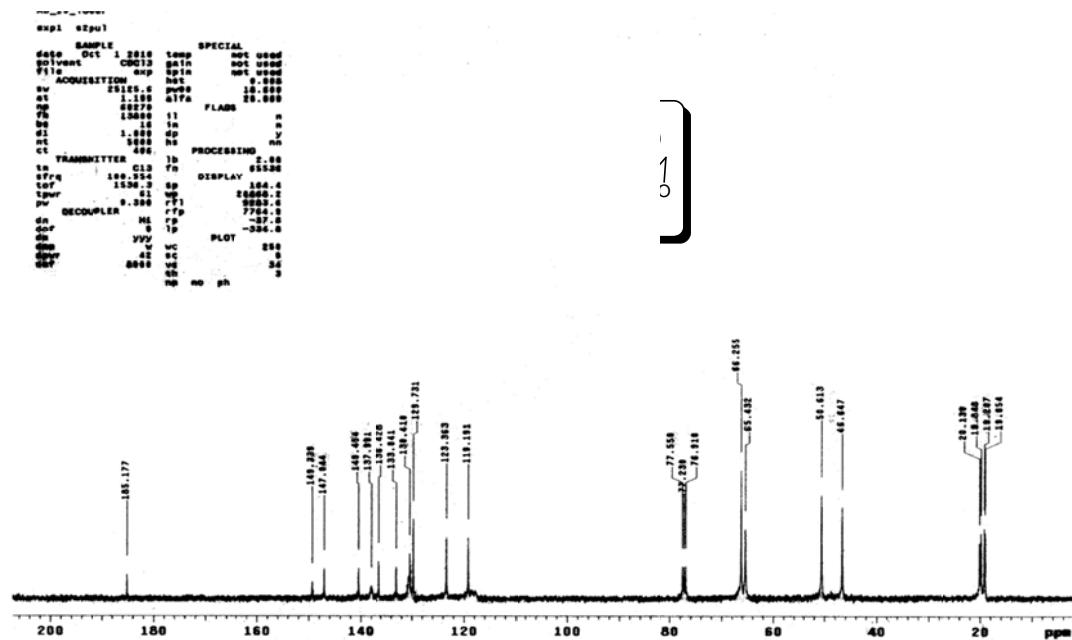


-S38 -

N-((E)-(4-Butylphenylimino)(morpholino)methyl)-N-(4-butylphenyl)morpholine-4-carbothioamide (4a) ^1H NMR (400 MHz, CDCl_3):

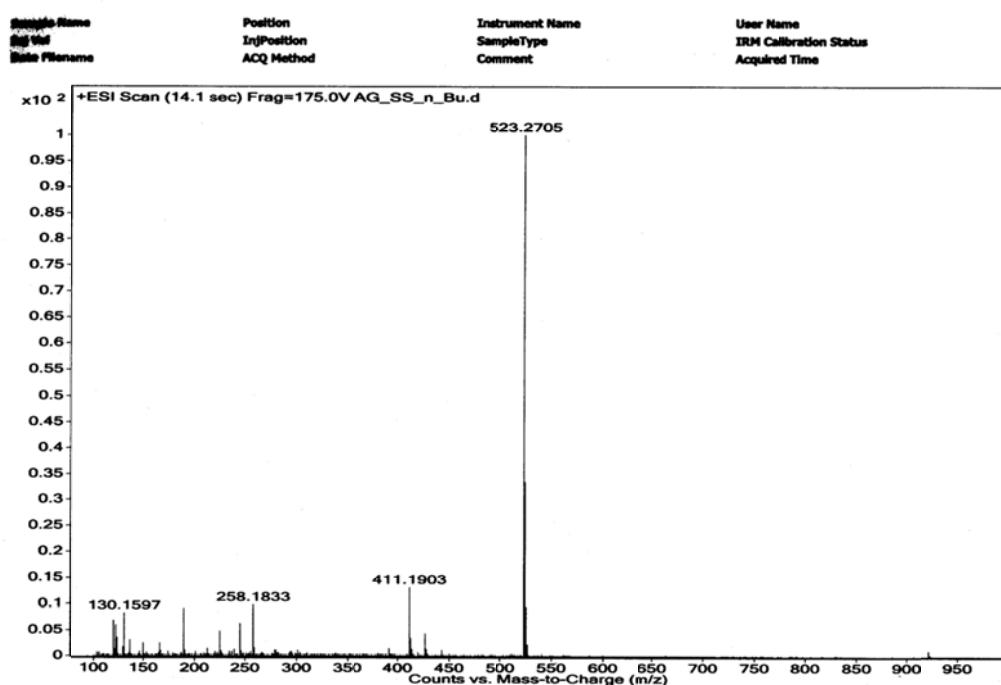


N-((E)-(4-Butylphenylimino)(morpholino)methyl)-N-(4-butylphenyl)morpholine-4-carbothioamide (4a) ^{13}C NMR (100 MHz, CDCl_3):

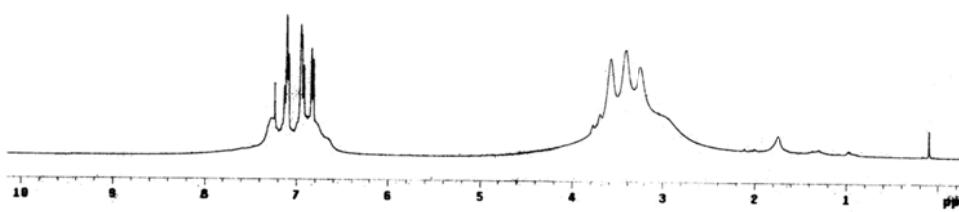
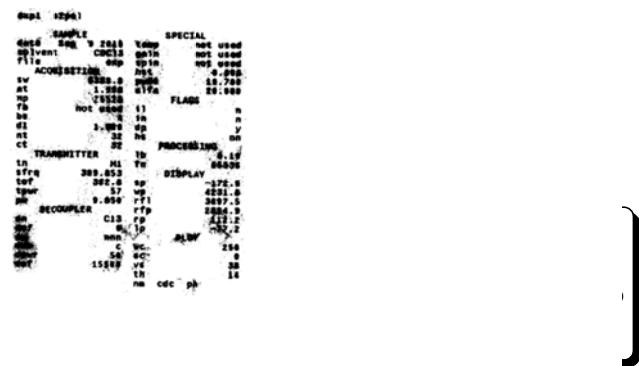


-S39 -

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

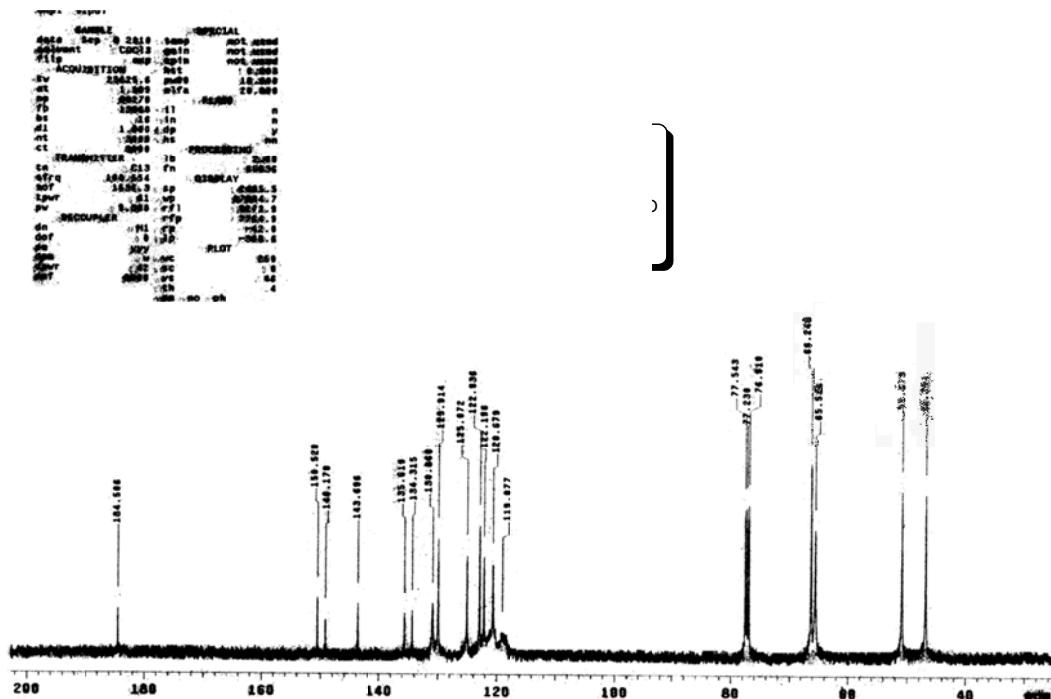


N-((E)-(3-Chlorophenylimino)(morpholino)methyl)-N-(3-Chlorophenyl)morpholine-4-carbothioamide (5a).¹H NMR (400 MHz, CDCl₃):

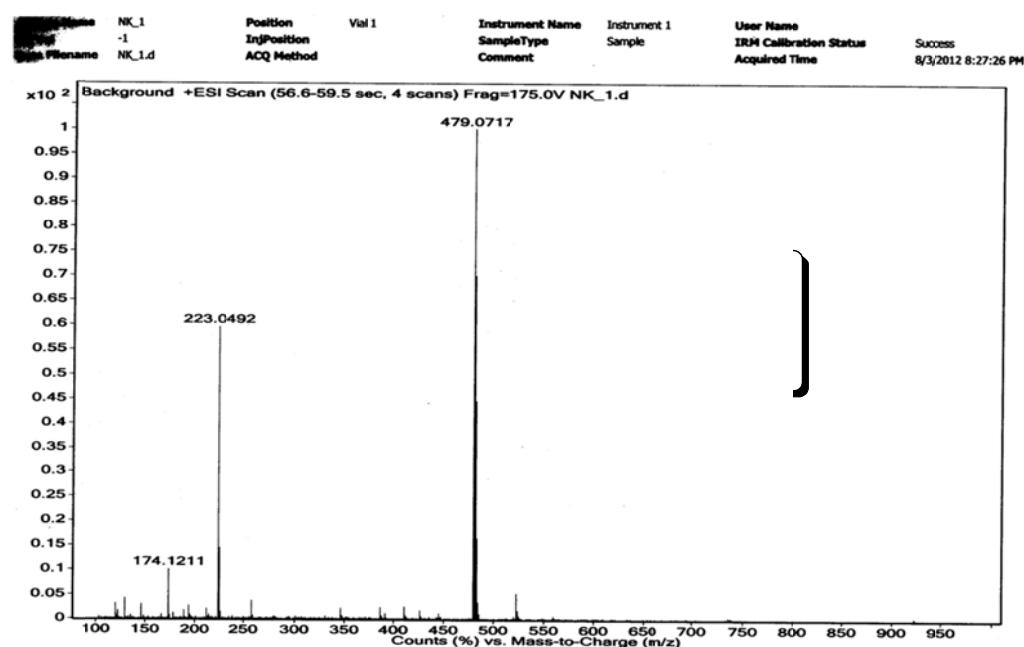


-S40 -

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

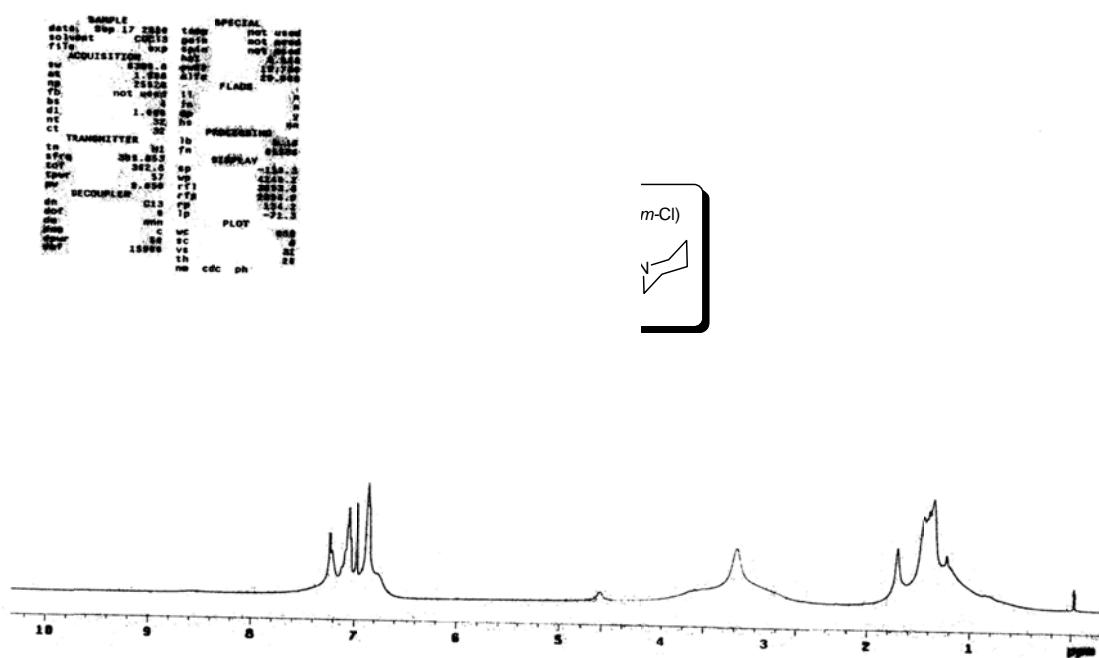


N-((E)-(3-Chlorophenylimino)(morpholino)methyl)-N-(3-Chlorophenyl)morpholine-4-carbothioamide (5a). MASS SPECTRA:

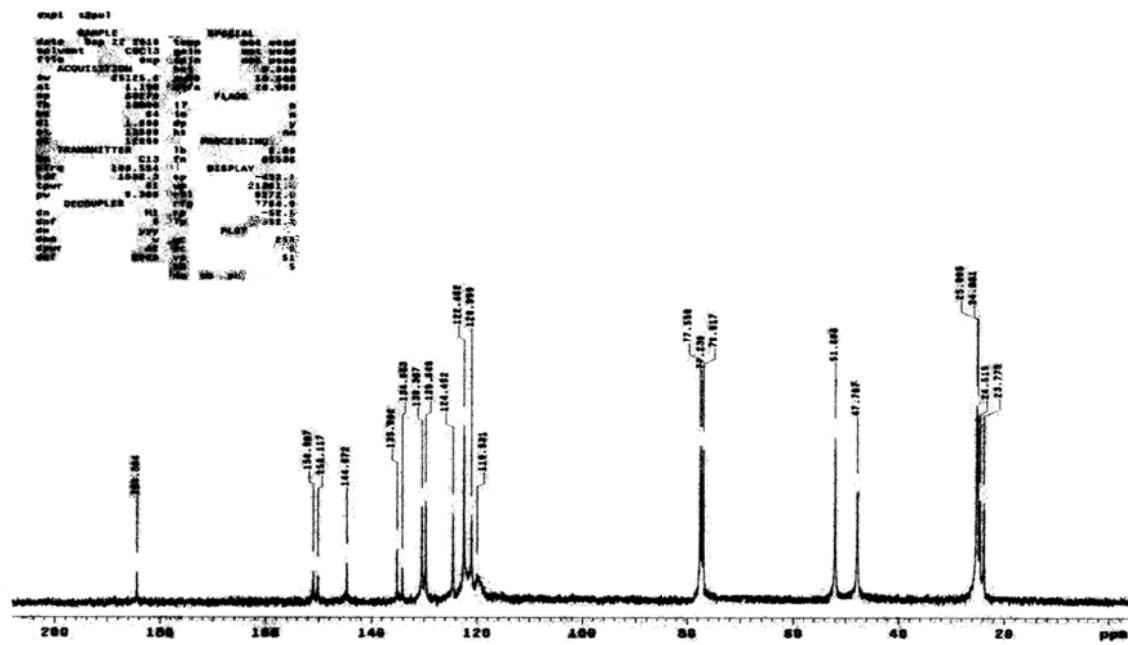


-S41 -

N-((E)-(3-Chlorophenylimino)(piperidin-1-yl)methyl)-N-(3-chlorophenyl)piperidine-1-carbothioamide (5d): ^1H NMR (400 MHz, CDCl_3):

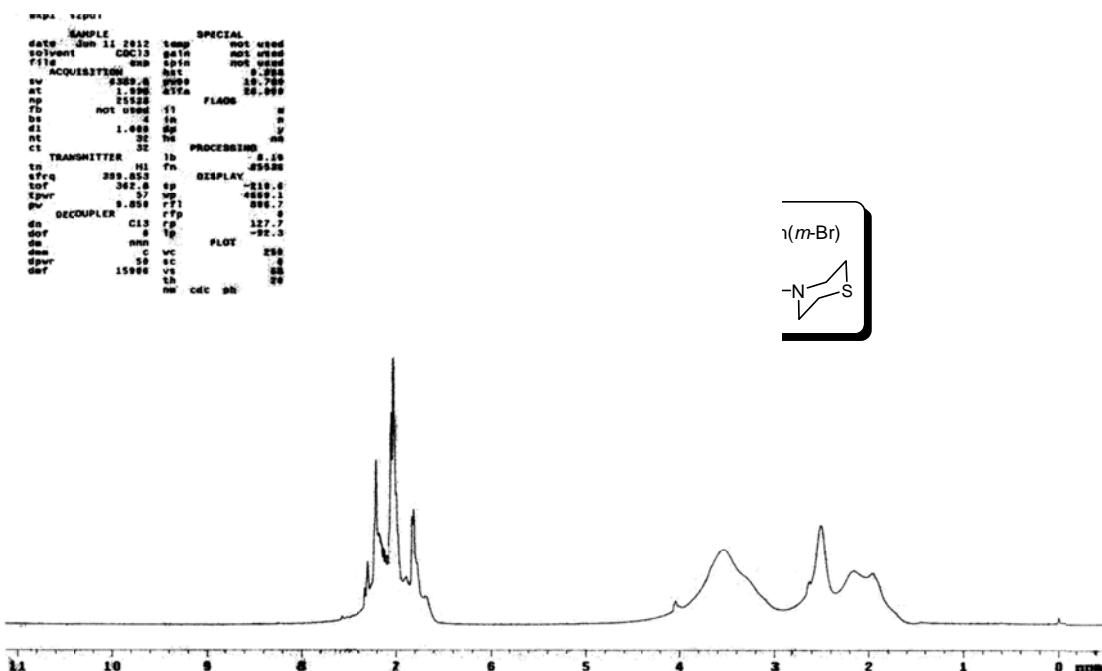


N-((E)-(3-Chlorophenylimino)(piperidin-1-yl)methyl)-N-(3-chlorophenyl)piperidine-1-carbothioamide (5d). ^{13}C NMR (100 MHz, CDCl_3):

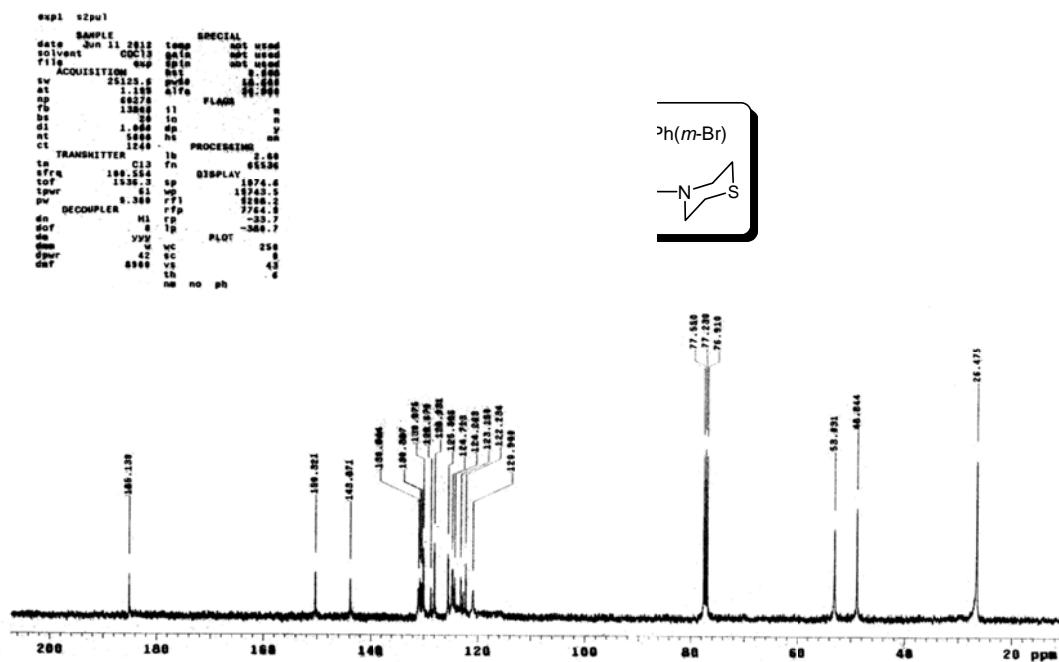


-S42 -

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

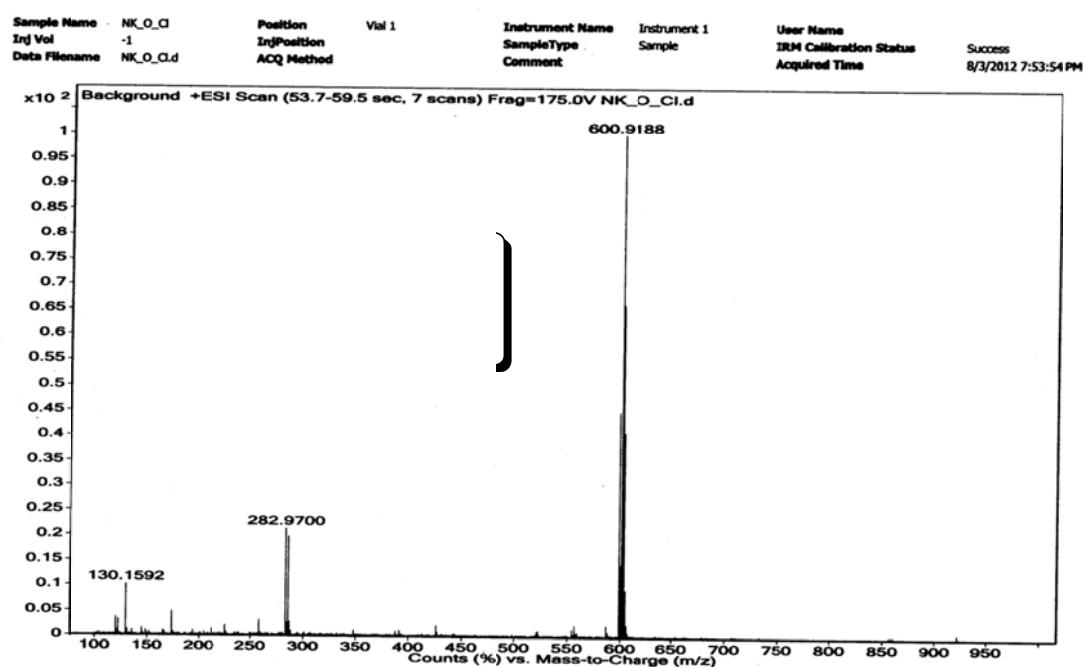


N-((E)-(3-Bromophenylimino)(thiomorpholino)methyl)-N-(3-bromophenyl)thiomorpholine-4-carbothioamide (6b). ^{13}C NMR (100 MHz, CDCl_3):

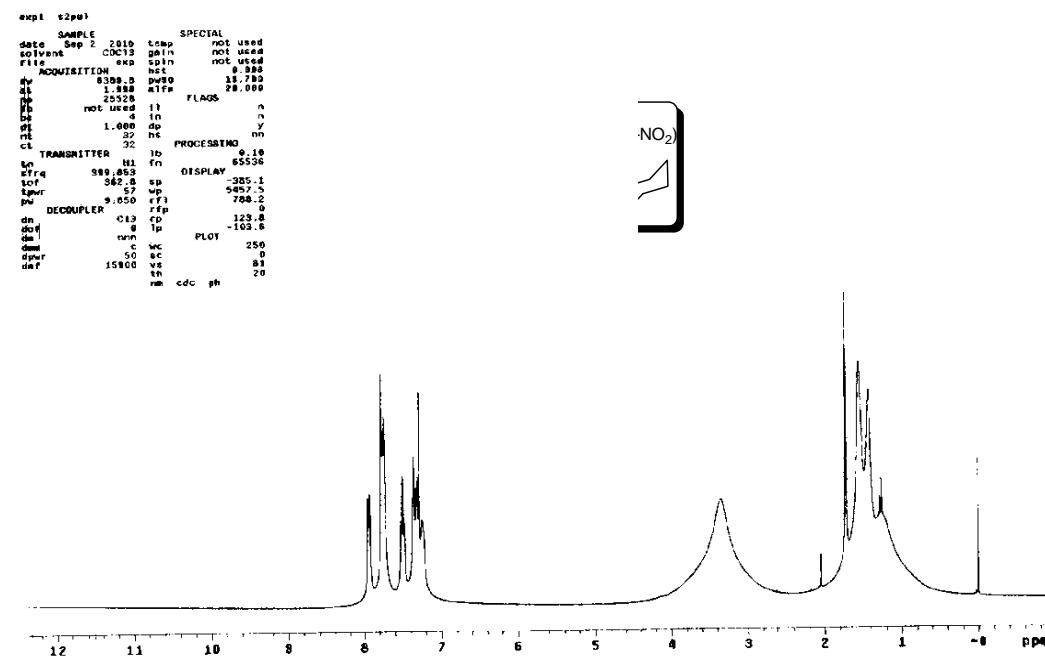


-S43 -

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

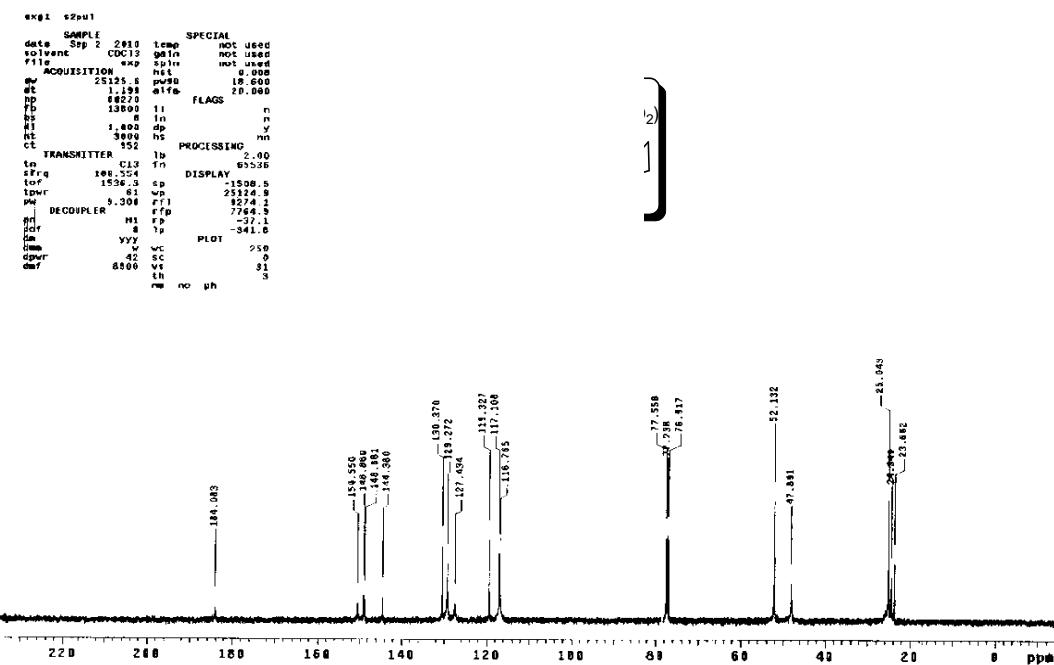


N-((E)-(3-Nitrophenylimino)(piperidin-1-yl)methyl)-N-(3-nitrophenyl)piperidine-1-carbothioamide (7d). ^1H NMR (400 MHz, CDCl_3):

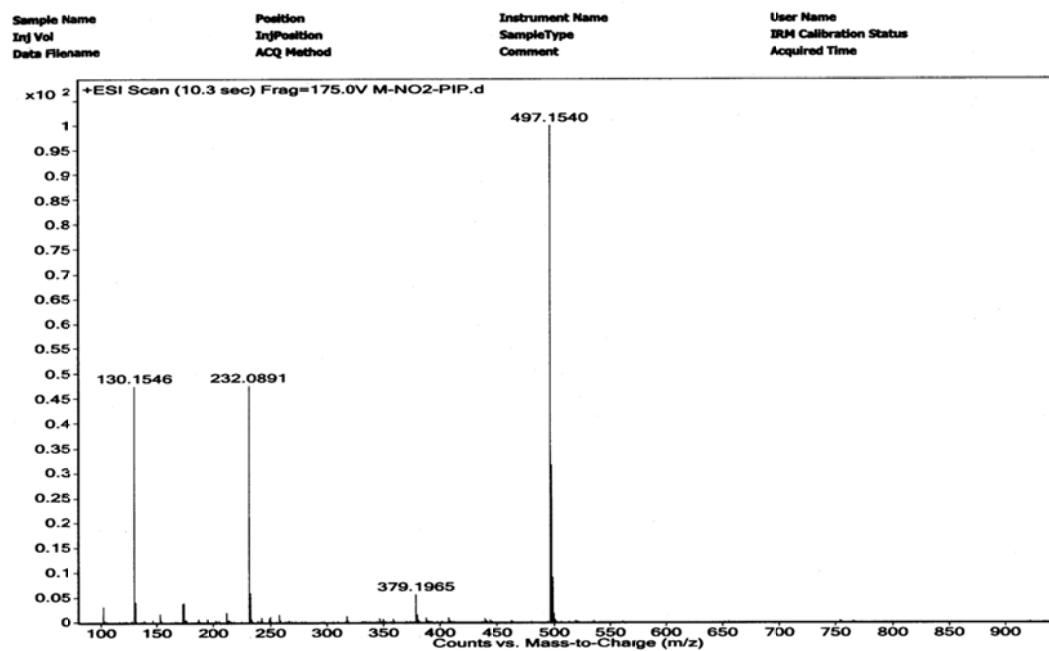


-S44 -

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

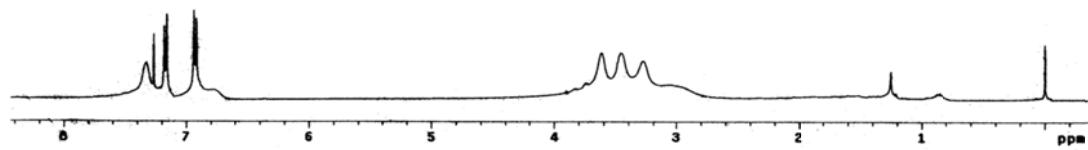


N-((E)-(3-Nitrophenylimino)(piperidin-1-yl)methyl)-N-(3-nitrophenyl)piperidine-1-carbothioamide (7d). MASS SPECTRA:

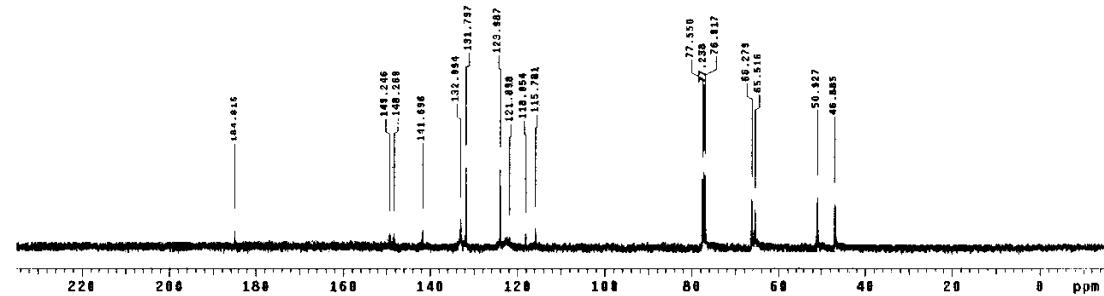
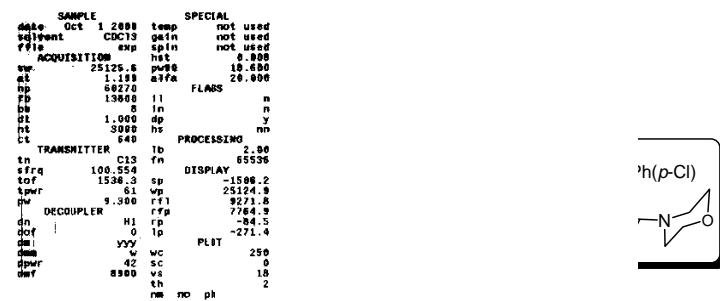


-S45 -

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



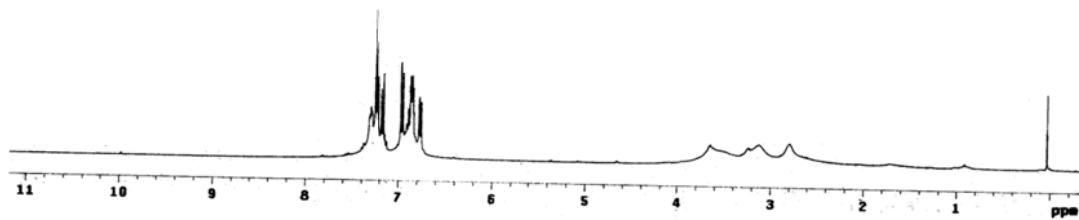
N-((E)-(4-Chlorophenylimino)(morpholino)methyl)-N-(4-chlorophenyl)morpholine-4-carbothioamide (8a). ^{13}C NMR (100 MHz, CDCl_3):



-S46 -

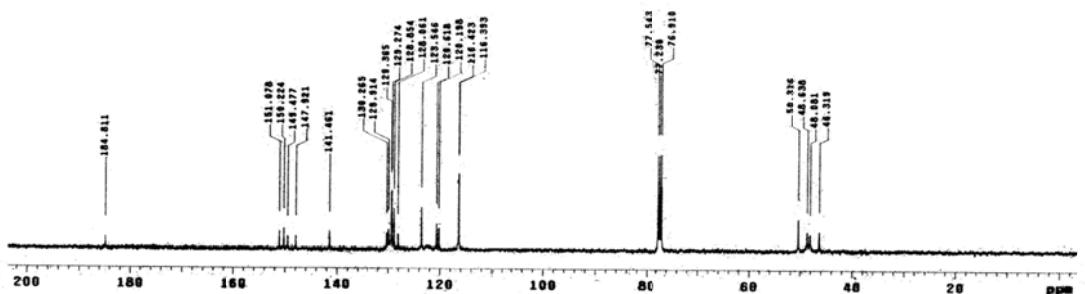
N-((E)-(4-Chlorophenylimino)(4-phenylpiperazine-1-yl)methyl)-N-(4-chlorophenyl)-4-phenylpiperazine-1-carbothioamide (8c).¹H NMR (100 MHz, CDCl₃):

```
SAMPLE          SPECIAL
date Jun 18 2012 temp not used
solvent CDCl3 gain not used
file      exp spin not used
ACQUISITION hz16
sw       6388.0 pw90 15.786
sp       12828 alfa 26.000
np       25228 flags
t0      not used t1      n
dt      1.04 dpp  n
d1      32.00 dpp  y
n1      32 hs    nn
ct      32      PROCESSING
tn      H1 fn   8.18
sfrq   399.853 f1   65536
tfrq   382.000 sp   DISPLAY
tpwr   57.000 rfp  778.2
pv      8.059 rfi  778.2
DECOUPLER C13 rfp  182.0
dn      C13 rfp  182.0
dof     8    1P   -66.4
dme    nnn vc    256
dpwrt  50.000 sc   0
dpwrf  15998 vs   37
d1f    15998 ph   20
nm cdcl3 ph
```



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

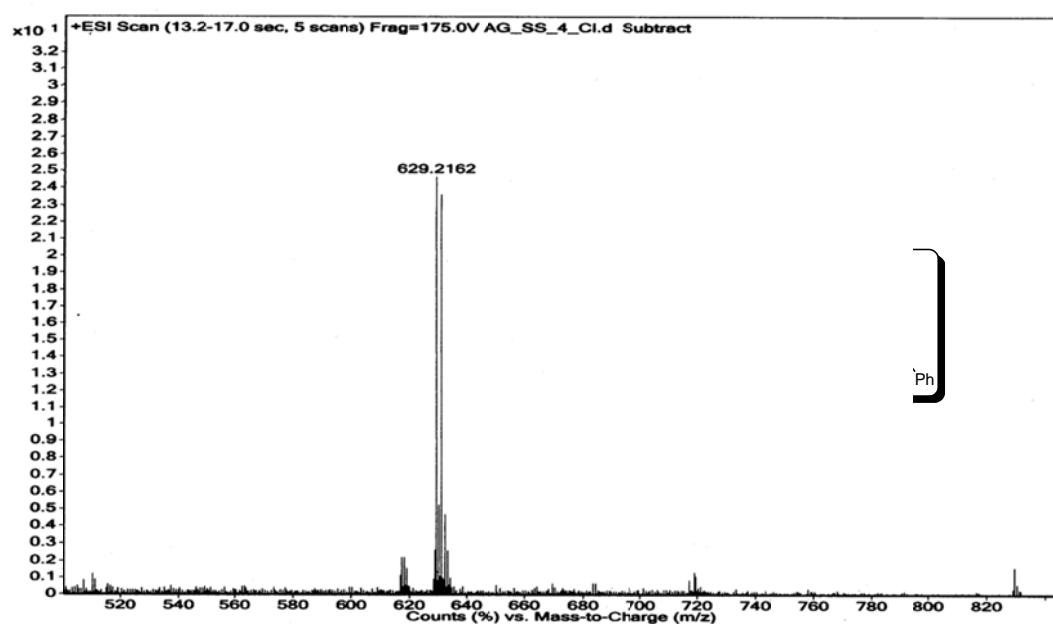
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exp1 s2pu1
SAMPLE          SPECIAL
date Jun 13 2012 temp not used
solvent CDCl3 gain not used
file      exp spin not used
ACQUISITION hz16
sw       25125.4 pw90 15.786
sp       12828 flags
np       25228 t1      n
t0      not used t1      n
dt      1.000 dpp  n
d1      1.000 dpp  y
n1      1.000 hs    nn
ct      15998 PROCESSING
tn      C13 fn   2.00
sfrq   100.554 f1   65536
tfrq   159.000 sp   DISPLAY
tpwr   57.000 rfp  2882.1
pv      8.000 rfi  2882.1
DECOUPLER C13 rfp  7784.3
dn      H1 rfp  7784.3
dof     8    1P   -343.3
dme    vvv vc    256
dpwrt  42.000 sc   0
dpwrf  65998 vs   24
d1f    65998 ph   20
nm cdcl3 ph
```



-S47 -

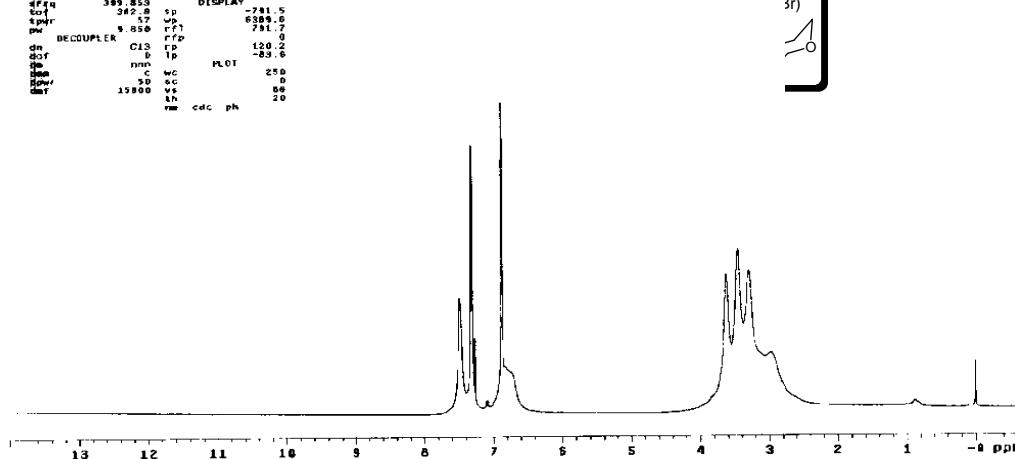
N-((E)-(4-Chlorophenylimino)(4-phenylpiperazine-1-yl)methyl)-N-(4-chlorophenyl)-4-phenylpiperazine-1-carbothioamide (8c). MASS SPECTRA:

Sample Name	AG_SS_4_Cl	Position	Vial 1	Instrument Name	Instrument 1	User Name	IRM Calibration Status	Acquired Time	Success
Inj Vol	-1	InjPosition		SampleType	Sample	Comment			
Data Filename	AG_SS_4_Cl.d	ACQ Method							7/30/2012 4:46:54 PM



N-((E)-(4-Bromoophenylimino)(morpholino)methyl)-N-(4-bromophenyl)morpholine-4-carbothioamide (9a). ^1H NMR (400 MHz, CDCl_3):

```
SAMPLE          SPECIAL
date Oct 19 2010 temp not used
solvent CDCl3 pres not used
rf1w1 300.0 sec not used
rf1w2 300.0 sec not used
ACQUISITION time 8.000
dt 1.000 a1vs 25.000
sc 25528
sp not 1024.4 11 n
ps 1.050 00 v
RE 1.050 00 nmt
D1 32.000 00
GT 32.000 PROCESSING
    TRANSMITTER 3b 0.18
    H1      f1 56536
    TFFQ 389.853 sp DISPLAY
    T1 389.853 t1 -781.5
    T2P1 6389.6
    T2P1 731.7
    PWR 9.856 rfp 0
    DECOUPLER C13 rfp 120.2
    QM 13C   rfp 0.5
    QCPMG 13C   PLOT
    QCPMG 13C   250
    QCPMG 13C   0
    QCPMG 13C   50
    QCPMG 13C   20
    QCPMG 13C   cdc ph
```



-S48 -

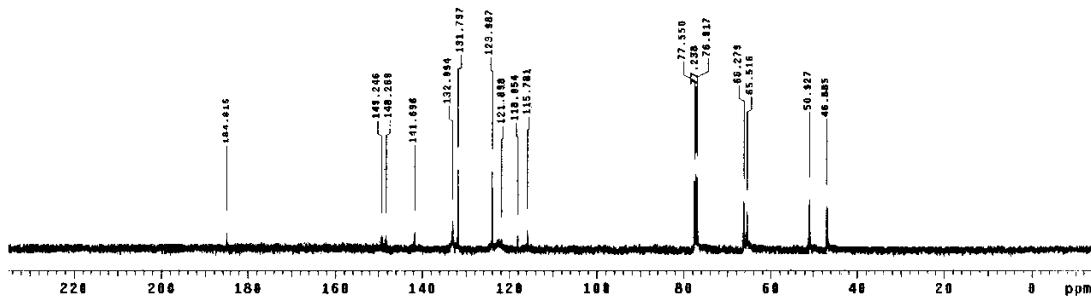
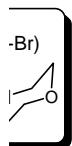
N-((E)-(4-Bromoophenylimino)(morpholino)methyl)-N-(4-bromophenyl)morpholine-4-carbothioamide (9a). ^{13}C NMR (100 MHz, CDCl_3):

```

SAMPLE          SPECIAL
date Oct 1 2009 temp not used
solvent CDCl3 gain not used
title          exp spin not used
ACQUISITION    pres 10.000
sw 25125.6 pw88 10.000
et 1.158 a1fa 20.000
dt 66276 11 FLANS
dp 13800 11 n
bb 8 in n
dt 1,000 dp y
nt 3000 hs nn
ct 640

TRANSMITTER   1b PROCESSING 2.00
th C13 tn 65536
trq 100.000 DISPLAY
tot 1536.3 sp -1500.2
tppw 61 vp 25124.9
pw 9.300 r11 9271.8
dec 7.300 r11 7271.8
DECOUPLER     H1 rfp -84.5
dn 0 lp -271.4
dof 1
dpp 42 sc 0
dpr 8500 vs 18
dft 11 th 2
rd no ph

```

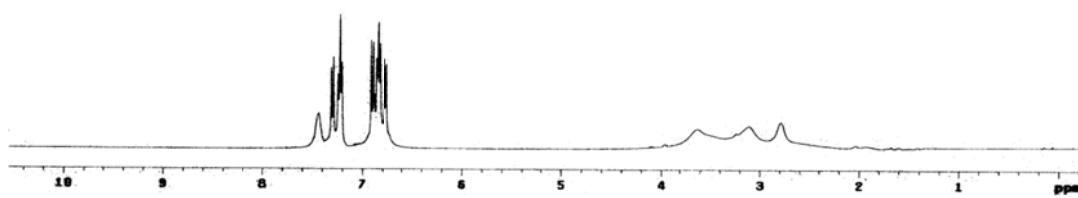
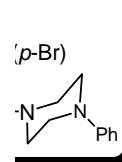


N-((E)-(4-Bromoophenylimino)(4-phenylpiperazin-1-yl)methyl)-N-(4-bromophenyl)phenylpiperazine-4-carbothioamide (9c). ^1H NMR (400 MHz, CDCl_3):

```

SAMPLE          SPECIAL
date Jun 19 2012 temp not used
solvent CDCl3 gain not used
title          exp spin not used
ACQUISITION    pres 10.000
sw 6388.8 pw88 10.700
et 1.000 a1fa 20.000
dt 65526 11 FLANS
dpb not used 11 n
bb 32 in n
dt 1.000 dp y
nt 32 hs nn
ct 32 PROCESSING 8.18
th H1 tn 65536
trq 389.000 DISPLAY
tot 362.0 sp -115.0
tppw 9.854 r11 481.8
pw 9.854 r11 812.8
dec 9.854 r11 812.8
DECOUPLER     C13 rfp 128.0
dn C13 td 128.0
dpp 0 ec 0
dpr 15000 vs 38
dft 11 th 24
rd cdc ph

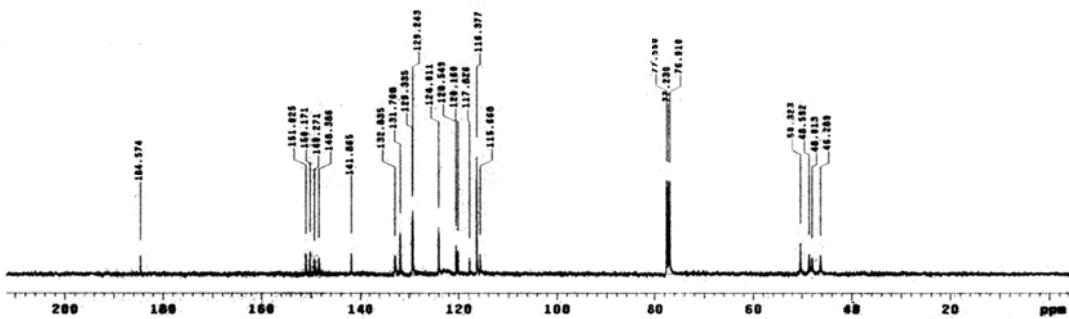
```



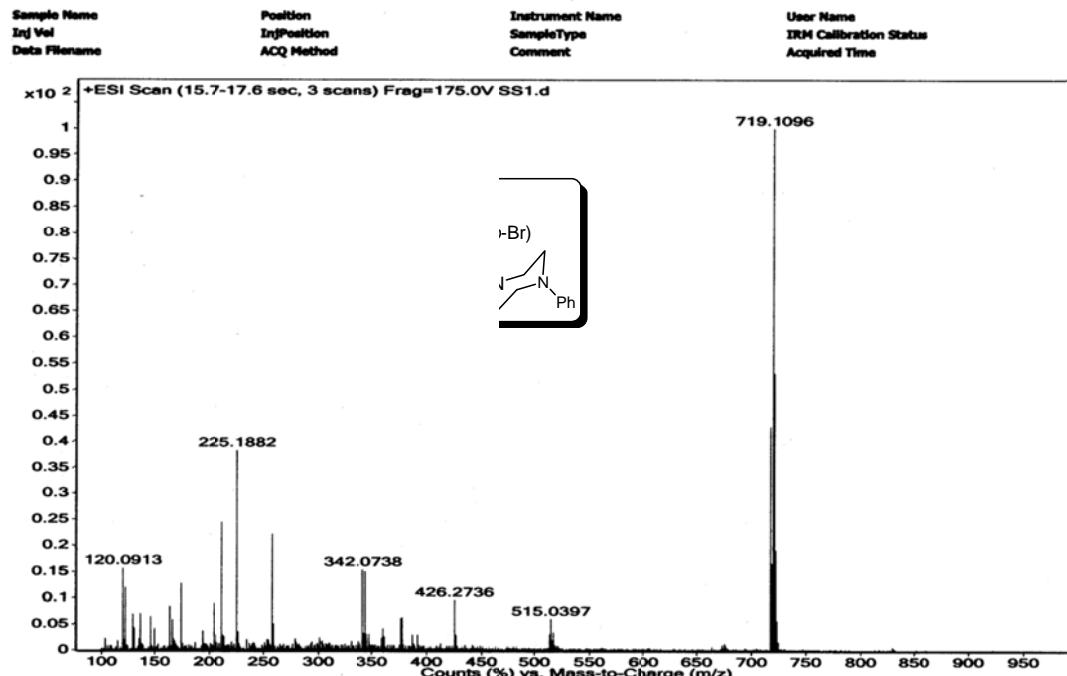
-S49 -

N-((E)-(4-Bromoophenylimino)(4-phenylpiperazin-1-yl)methyl)-N-(4-bromophenyl) phenylpiperazine-4-carbothioamide (9c). ^{13}C NMR (100 MHz, CDCl_3):

AD_9c_pbcptpp
expt: xspw1
SAMPLE: SPECIAL
date: Jun 19 2012 temp: not used
solvent: CDCl₃ gain: not used
f1label: spw1 nmt: not used
ACQUISITION: nmt: not used
sw: 26105.6 Hz: 10.000
spw1: 40000 t1: 25.000
np: 64272 flags:
tb: 138000 t1i:
di: 1.000 dp:
nt: 30000 ns:
ct: 1225 processing: nn
TRANSMITTER: 1b: 2.00
tn: C13: Tn: 655.30
tr: 188.50 DISPLAY: 655.30
t0f: 1536.3 sP: -655.7
tpw: 9.301 vtp: 255.7
pw: 9.301 rtp: 775.1
DECOUPLER: 11: -300.5
dn: 6: Tp: -300.5
da: vpp: PLOT
dm: 42: vc: 251
dpr: 6500 vs:
dpf: 6500 ts:
no: ph:



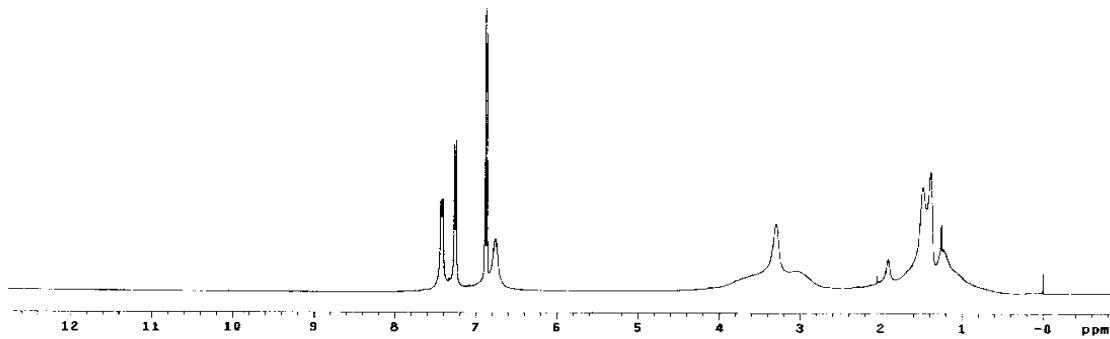
N-((E)-(4-Bromoophenylimino)(4-phenylpiperazin-1-yl)methyl)-N-(4-bromophenyl) phenylpiperazine-4-carbothioamide (9c). MASS SPECTRA:



-S50 -

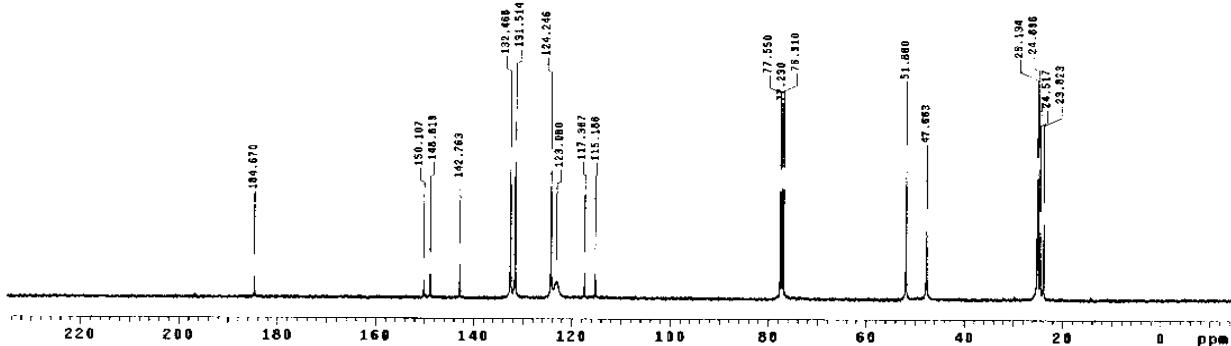
N-((E)-(4-Bromoophenylimino)(piperidin-1-yl)methyl)-N-(2-bromophenyl)piperidine-1-carbothioamide (9d).¹H NMR (400 MHz, CDCl₃):

```
exp1 s2pul
SAMPLE          SPECIAL
date Oct 29 2010 temp not used
solvent   CDCl3  gain not used
f1flip      exp spin not used
f1width    0.098
sw        6383.6 pws9
et        25528
tp        25528
ns       10000
dt        1.000
sc        1.000
ct        32    PROCESSING
transmitter 1b
tn        H1  f1  0.10
tr        388.853 DISPLAY
td        382.5 sp
tppr     542.5
tpwr    0.850 rrf1
decoupler C13 rrp
dn        0 1p  144.0
dof       0 1p  -130.6
dp        min 250
dpcv     50  vc  250
dcvr    15300  tc  70
scf      20
rm        CDCl3 ph
```



N-((E)-(4-Bromoophenylimino)(piperidin-1-yl)methyl)-N-(2-bromophenyl)piperidine-1-carbothioamide (9d).¹³C NMR (100 MHz, CDCl₃):

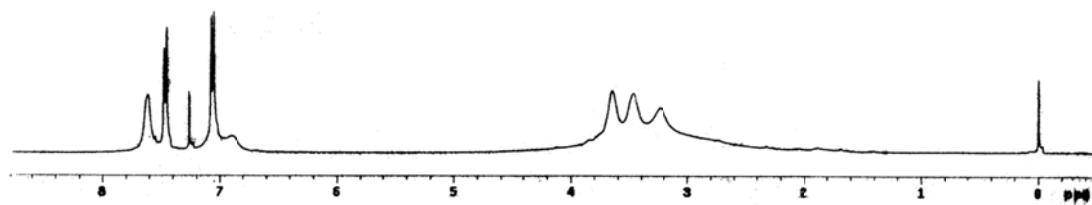
```
exp1 s2pul
SAMPLE          SPECIAL
date Oct 29 2010 temp not used
solvent   CDCl3  gain not used
f1flip      exp spin not used
f1width    0.098
sw        25125.6 pws9
et        20000
tp        60270
ns       10000
dt        10000
ht        10000
ct        32    PROCESSING
transmitter 1b
tn        C13  f1  2.00
tr        100.554 DISPLAY
td        153k3 sp  -1508.9
tppr     61  wp  25124.9
tpwr    5.300 rrf1
decoupler C13 rrp
dn        H1  rrp  77.9
dof       0 1p  -42.6
dp        min 250
dpcv     42  vc  0
dcvr    8900  tc  32
scf      30
rm        CDCl3 ph
```



-S51 -

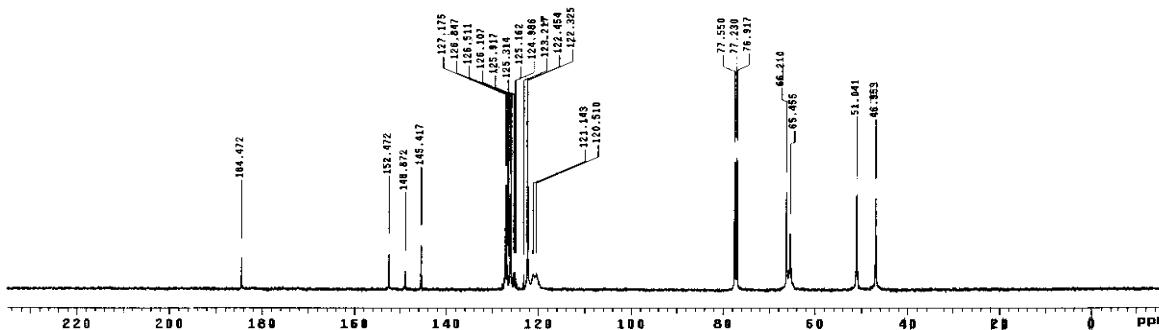
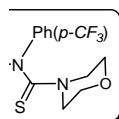
***N*-(*E*)-(4-Trifluoromethyl)phenylimino(morpholino)methyl-*N*-(4-trifluorophenyl)morpholine-4-carbothioamide (10a). ^1H NMR (400 MHz, CDCl_3):**

```
RV_2_280
exp1 42puY
SAMPLE      SPECIAL
date Aug 17 2009 temp not used
solvent   CDCl3 gain not used
files /export/home/nan/10a/10a_400
p1/RT 100.000 spin not used
ACQUISITION mode 17.700
SW 1580.000 apts 20.000
TD 25528 n1 11
TE 225.000 n2 n
NOT USED IN n3 v
DW 1.000 n4 nm
TE 32.000 n5 nm
CT 32.000 n6 nm
TRANSMITTER 1b TA 90.000
tn H1 SP -107.7
tdf 399.250 ap 3702.7
tpr 57.000 r11 795.0
pw 9.650 rfp 130.0
dec DECOUPLER C13 10 130.0
dt 0.000 10 -90.2
dpf 10.000 PLOT
dppm 256
dpph 50
dpc 36
dpcr 36
dpcp 26
dpcph 26
```



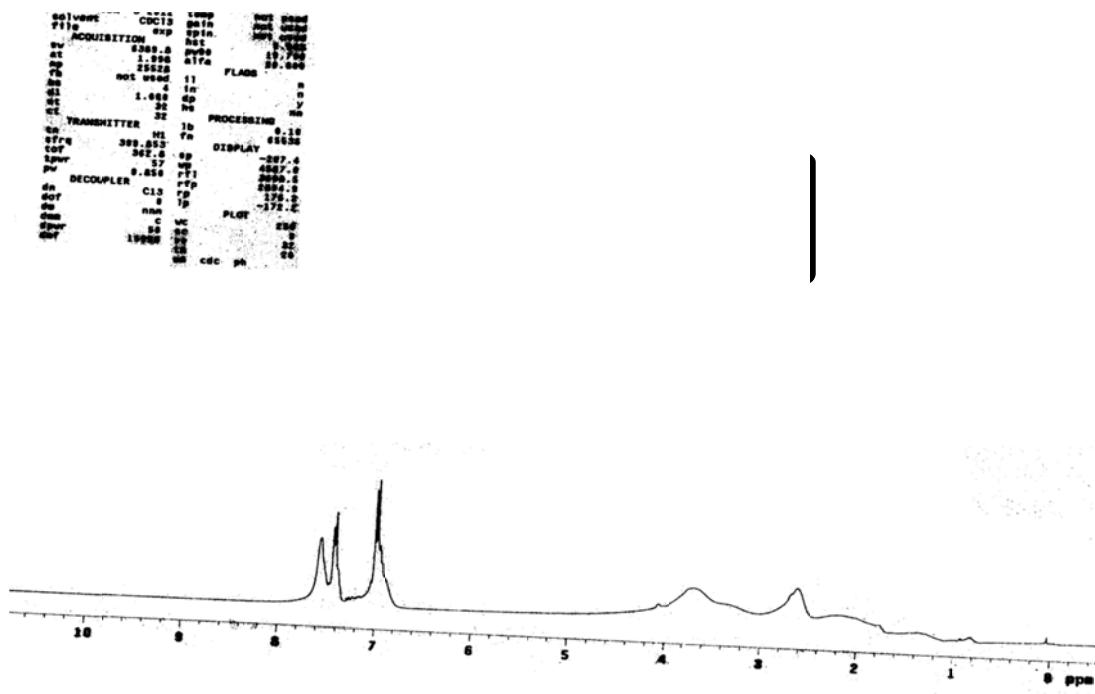
***N*-(*E*)-(4-Trifluoromethyl)phenylimino(morpholino)methyl-*N*(4-trifluorophenyl)morpholine-4-carbothioamide (10a). ^1H NMR (400 MHz, CDCl_3):**

```
SAMPLE      SPECIAL
date Aug 2 2010 temp not used
solvent   CDCl3 gain not used
files /export/home/nan/10a/10a_400
p1/RT 100.000 spin not used
ACQUISITION mode 18.000
SW 25125.6 apts 20.000
TD 158000 n1 11
TE 225.000 n2 n
DW 1.000 n3 v
CT 158000 n4 nm
CH 158000 1b 2.00
C14 14048 rn 65558
TRANSMITTER C13 SP -1503.1
tn H1 SP -1503.1
tdf 100.554 w1 25124.9
tpr 100.554 r11 1904.4
tpr 100.554 rfp 9
pw 9.300 rfp -27.8
dec DECOUPLER C13 10 -355.4
dt 0.000 PLOT
dppm 256
dpph 50
dpc 36
dpcr 42
dpcp 33
dpcph 33
```

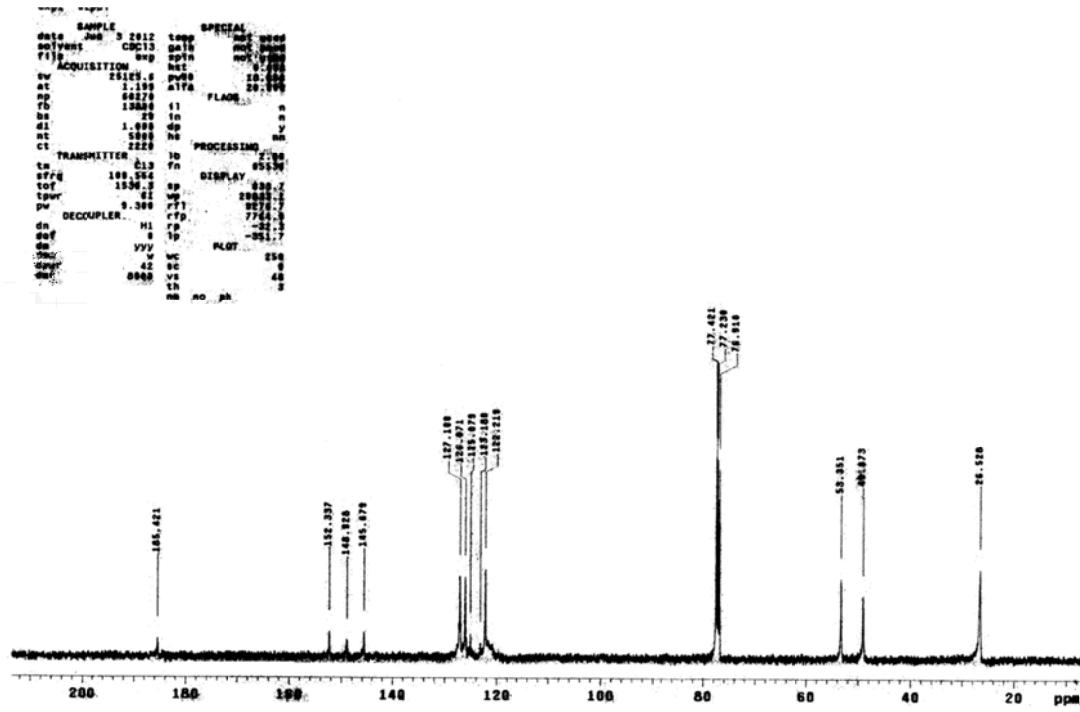


-S52 -

N-((E)-(4-Trifluoromethyl)phenylimino(thiomorpholino)methyl)-N(4-trifluorophenyl) thiomorpholine-4-carbothioamide (10b).¹H NMR (400 MHz, CDCl₃):

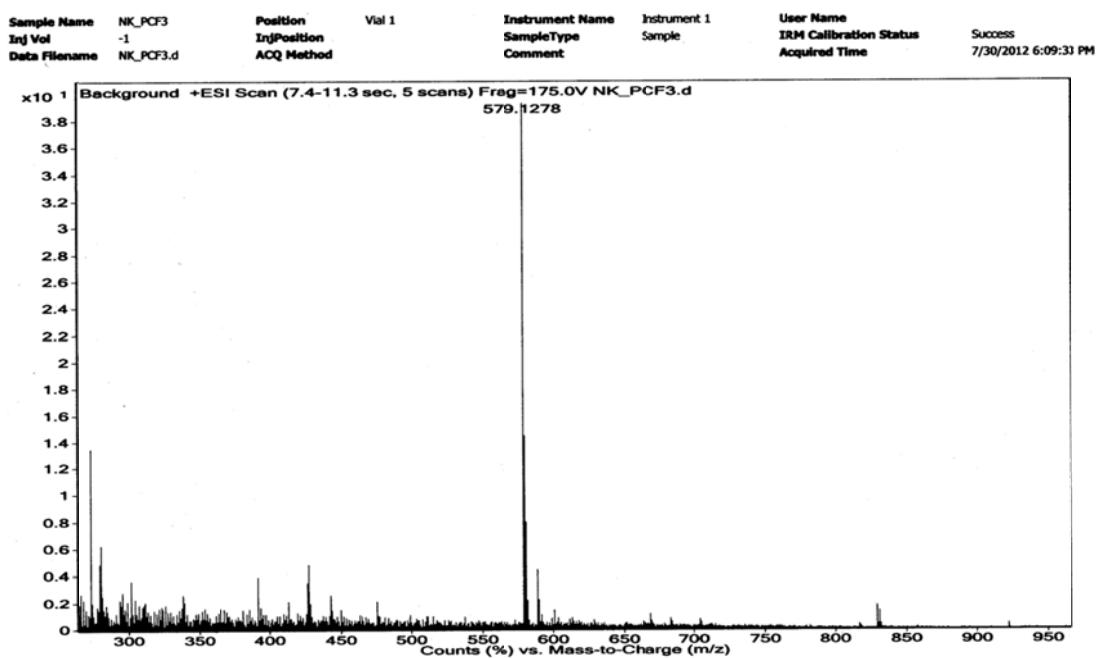


N-((E)-(4-Trifluoromethyl)phenylimino(thiomorpholino)methyl)-N(4-trifluorophenyl) thiomorpholine-4-carbothioamide (10b).¹³C NMR (100 MHz, CDCl₃):



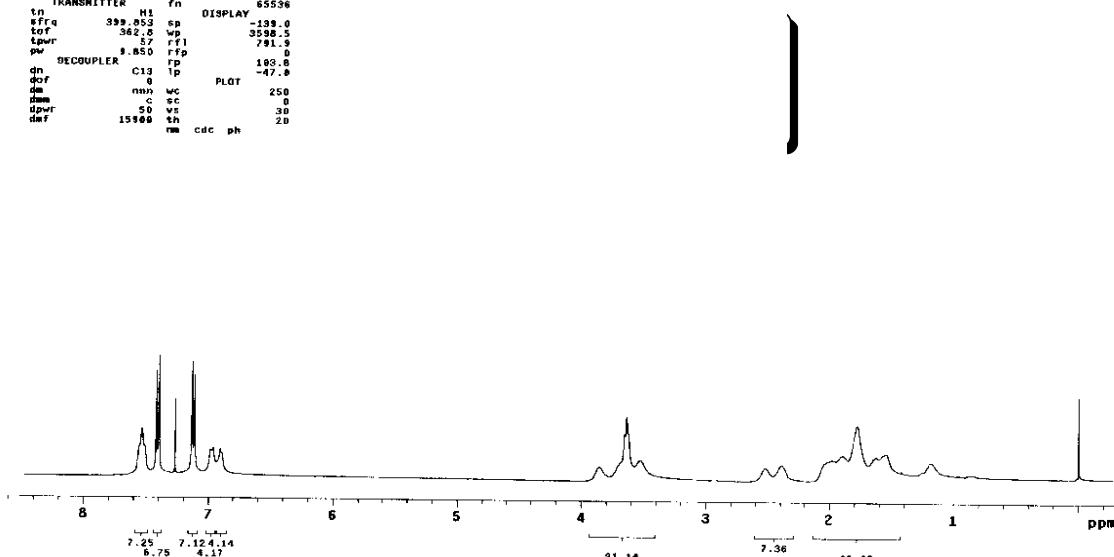
-S53 -

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



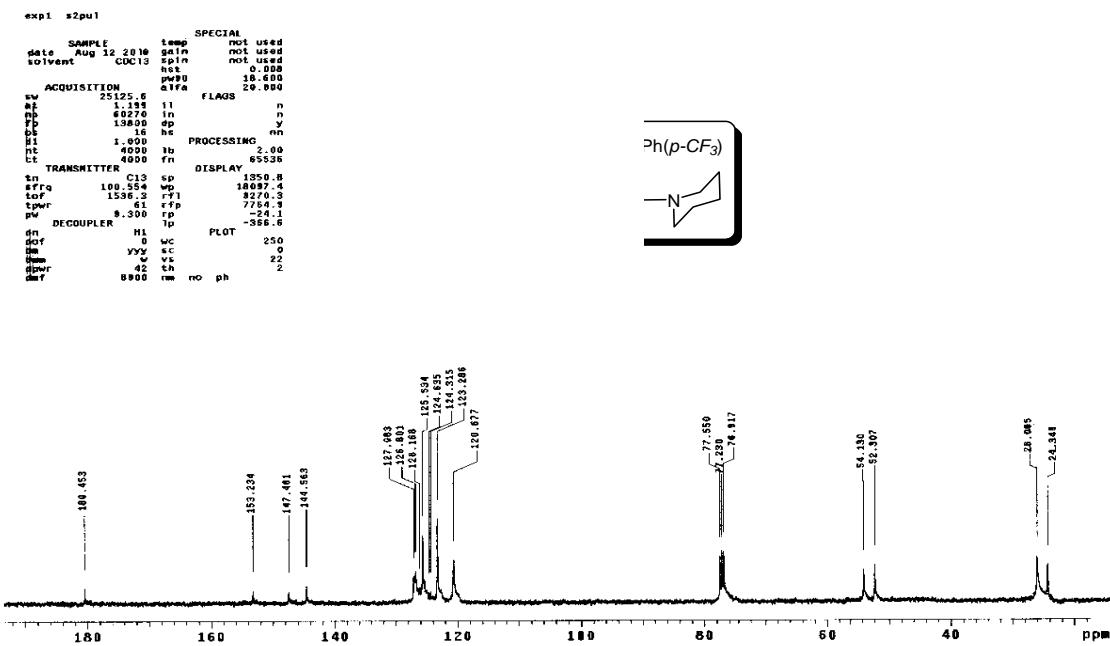
N-((E)-(4-Trifluoromethyl)(phenylimino)(piperidin-1-yl)methyl)-N-(4-bromophenyl) morpholine-1-carbothioamide (10d).¹H NMR (400 MHz, CDCl₃):

```
exp: 62pu1
      SPECIAL
date   SAMPLE    temp    not used
solvent        gain    not used
          CDCl3    ref    not used
          net     0.008
av    639.8    pw80    19.700
nt    1        alfa   20.000
np    25528    flags
fb    not used  11    n
bb    not used  1    n
p1    1.000    dp    v
nt    .32      hs    m
ct    26      PROCESSING  m
      1b    0.10
      fn    65536
      TRANSMITTER
      t1n    H1    DISPLAY
      kffq   399.853  sp   -139.0
      t0f    362.8  wp   3598.5
      t0r    5.57   rfi  791.9
      pwr    9.850  fp    0
      DECOUPLER
      C13  fp   103.8
      d1f    C13  fp   -47.8
      d1c    mmn  wc   250
      d1m    c   sc    0
      d1p    s   th   30
      d1r    5.60  th   20
      15960  nm  cdc  ph
      nm  cdc  ph
```

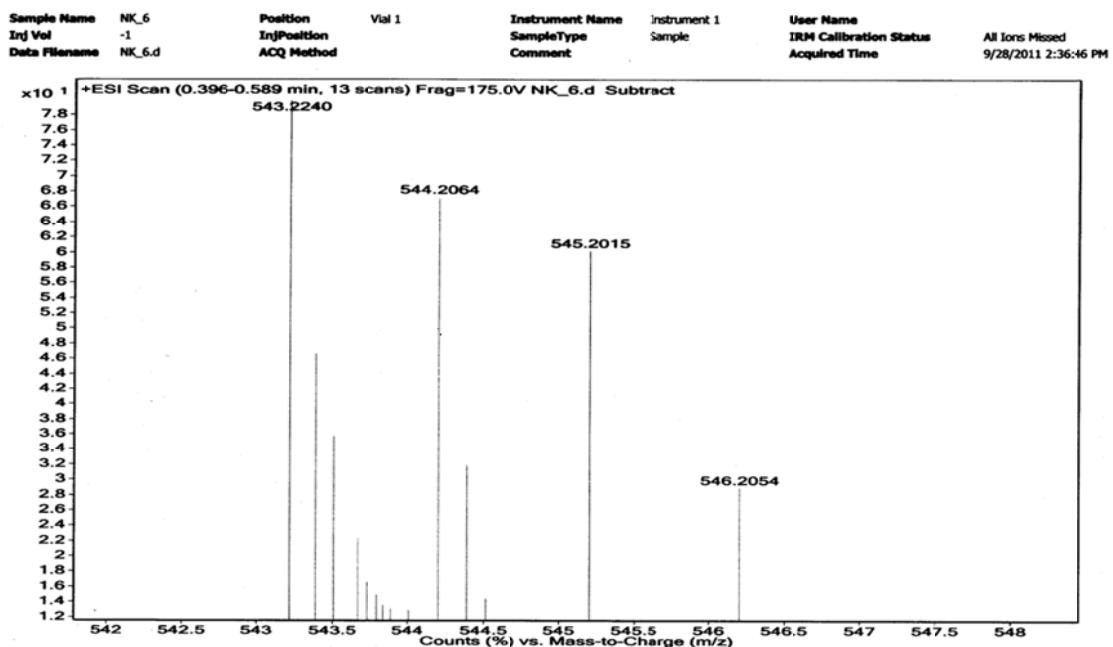


-S54 -

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:

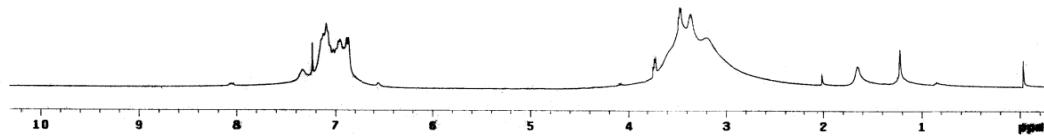


-S55 -

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

```
expt1 s2pu1
SAMPLE          SPECIAL
data Oct 11 2012  temp    not used
solvent      CDCl3  gain    not used
file          exp  spin    not used
time          0.00  pres    10.000
sv       6369.0  pw08   20.000
av        256    d1ta   20.000
dp       2568    flags
rd      not used  t1    n
b1      1.000    n
d1      64      dp    n
nt      64      nh   nn
ct      64      PROCESSING 2.00
TRANSMITTER   1b   tn   65536
trfrq     199.94  HI   DISPLAY 65536
trf      1536.3  sp   2542.3
tpfr      1536.3  sp   1536.3
pwr      9.399  w1   8263.7
DECOUPLER    HI   rrp   7764.9
dn      0      tp   -353.5
dnf      0      tp   -353.5
ds      vvv   PLOT  250
dse      vc    250
dppr      42    sc    0
dmt      8999  vs    65
rm      no   ph

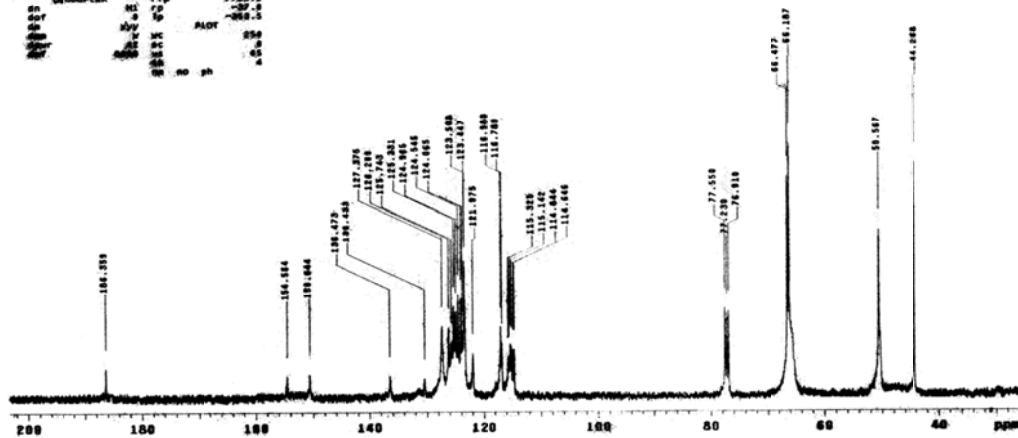
```



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

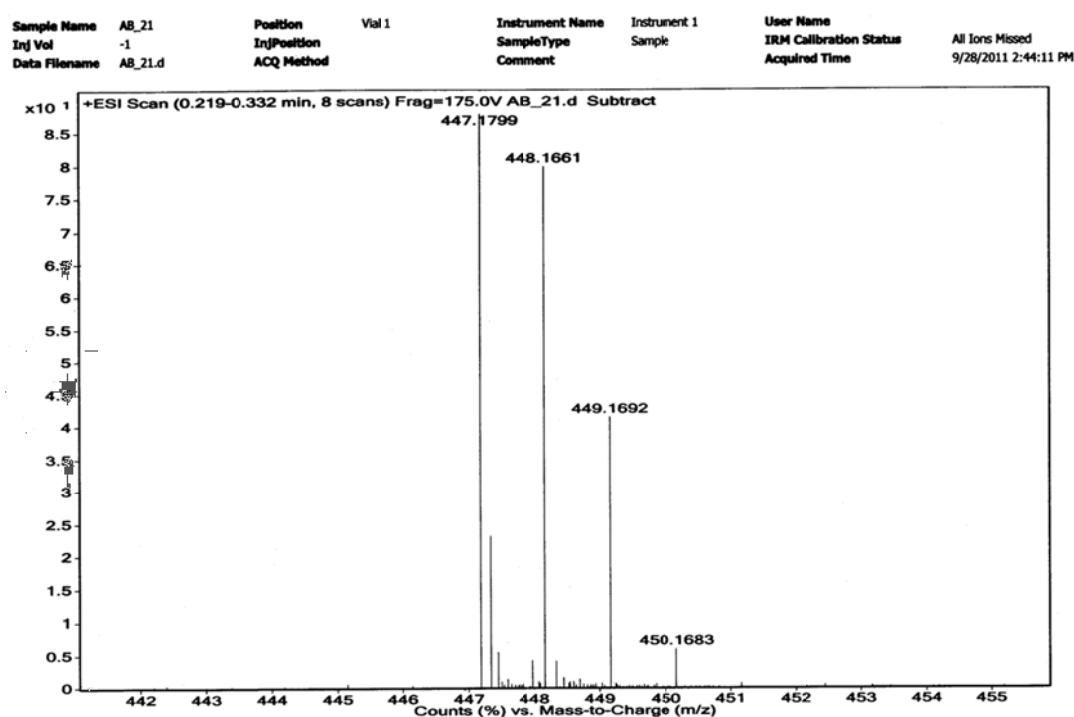
```
expt1 s2pu1
SAMPLE          SPECIAL
data Oct 11 2012  temp    not used
solvent      CDCl3  gain    not used
file          exp  spin    not used
time          0.00  pres    10.000
sv       6369.0  pw08   20.000
av        256    d1ta   20.000
dp       2568    flags
rd      not used  t1    n
b1      1.000    n
d1      64      dp    n
nt      64      nh   nn
ct      64      PROCESSING 2.00
TRANSMITTER   1b   tn   65536
trfrq     199.94  HI   DISPLAY 65536
trf      1536.3  sp   2542.3
tpfr      1536.3  sp   1536.3
pwr      9.399  w1   8263.7
DECOUPLER    HI   rrp   7764.9
dn      0      tp   -353.5
dnf      0      tp   -353.5
ds      vvv   PLOT  250
dse      vc    250
dppr      42    sc    0
dmt      8999  vs    65
rm      no   ph

```



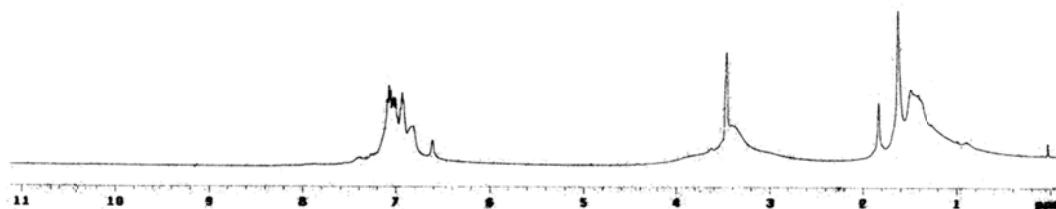
-S56 -

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



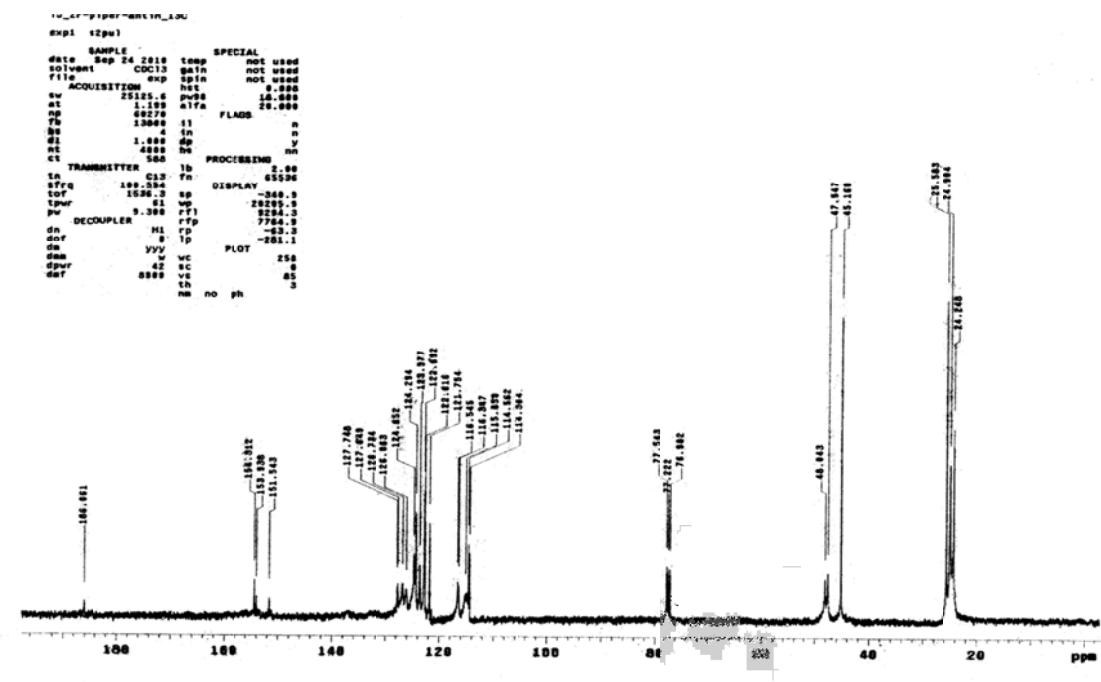
N-((E)-(2-Fluorophenylimino)(piperidin-1-yl)methyl)-N-(2-fluorophenyl)piperidine-1-carbothioamide (11d). ^1H NMR (400 MHz, CDCl_3):

expt 12pu1
SAMPLE: Sdp 24 2818
SPECIAL:
date: 2011-09-01
time: 10:16:16
comment: not used
ACQUISITION:
date: 2011-09-01
at: 10:16:16
sw: 1000.0 Hz
et: 204800
npw: 21.750 ms
dp: 90°
ns: 1
sc: 1.0000
ds: 1
rt: 0.0000
ct: 0.0000
transmitter: 1b
processing:
ta: 1000.0000
t1frc: 300.0000
tot: 1000.0000
tpwr: 50.0000
pw: 9.854
decoupling: 100.0000
dm: C13
dof: 1024
dpp: 1000.0000
dppr: 1000.0000
dppf: 1000.0000
plot: 1000.0000
ppm: 11.0000
ppm: 10.0000
ppm: 9.0000
ppm: 8.0000
ppm: 7.0000
ppm: 6.0000
ppm: 5.0000
ppm: 4.0000
ppm: 3.0000
ppm: 2.0000
ppm: 1.0000
ppm: 0.0000



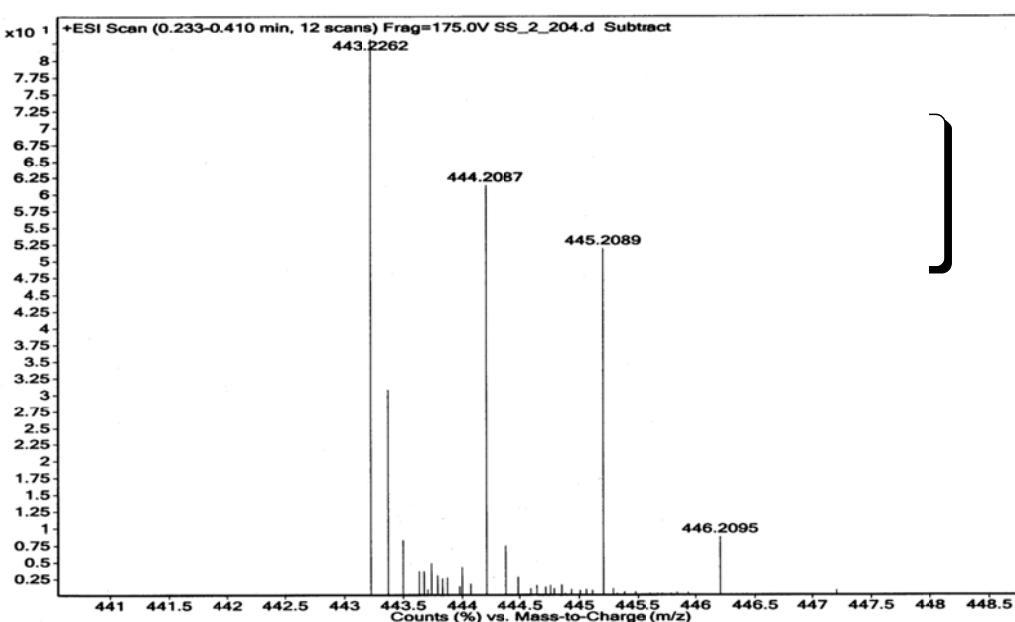
-S57 -

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):

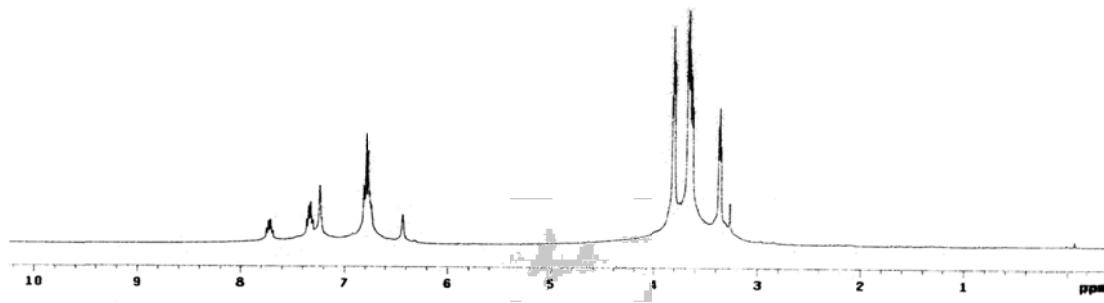
Sample Name	SS_2_204	Position	Vial 1	Instrument Name	Instrument 1	User Name	IRM Calibration Status	Acquired Time
Inj Vol	-1	InjPosition		SampleType	Sample	All Ions Missed		
Data Filename	SS_2_204.d	ACQ Method		Comment				9/28/2011 2:10:32 PM



-S58 -

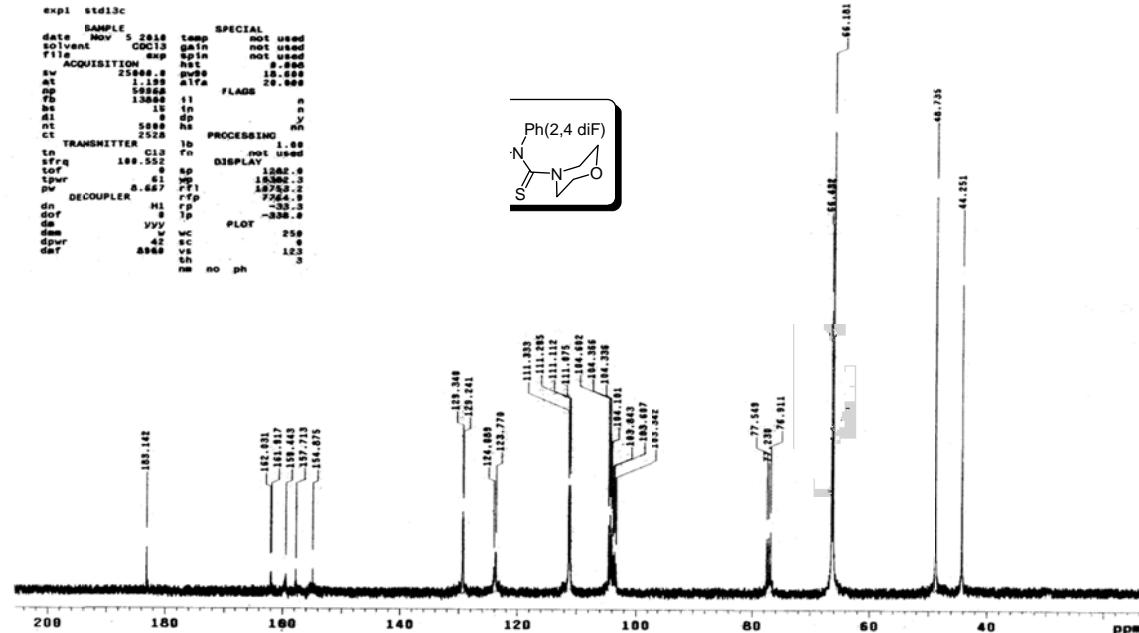
N-((E)-(2,4-Difluorophenylimino)(morpholino)methyl)-N-(2,4-difluorophenyl)morpholine-4-carbothioamide (12a).¹H NMR (400 MHz, CDCl₃):

AB_57_Lower
expt std1H
SAMPLE SPECIAL
date Nov 5 2010 temp not used
solvent CDCl₃ gain not used
file exp spin not used
ACQUISITION dec rate not used
av 6500 psize 16.668
at 23984 flags 32.000
nt 1.000 n1 1
dt 1.000 dp 1
ct 32 PROCESSING
TRANSMITTER HI fm not used
trfq 399.053 sp DISPLAY -176.6
tot 8 s w1 4266.4
tper 1 s r1 2884.5
pw 7.800 rfp 2884.5
DECOUPLER RP 127.5
dn C13 tp -61.5
dof 256
db 256 wc 256
dppr 50 vc 0
dmt 15384 th cdc ph 10



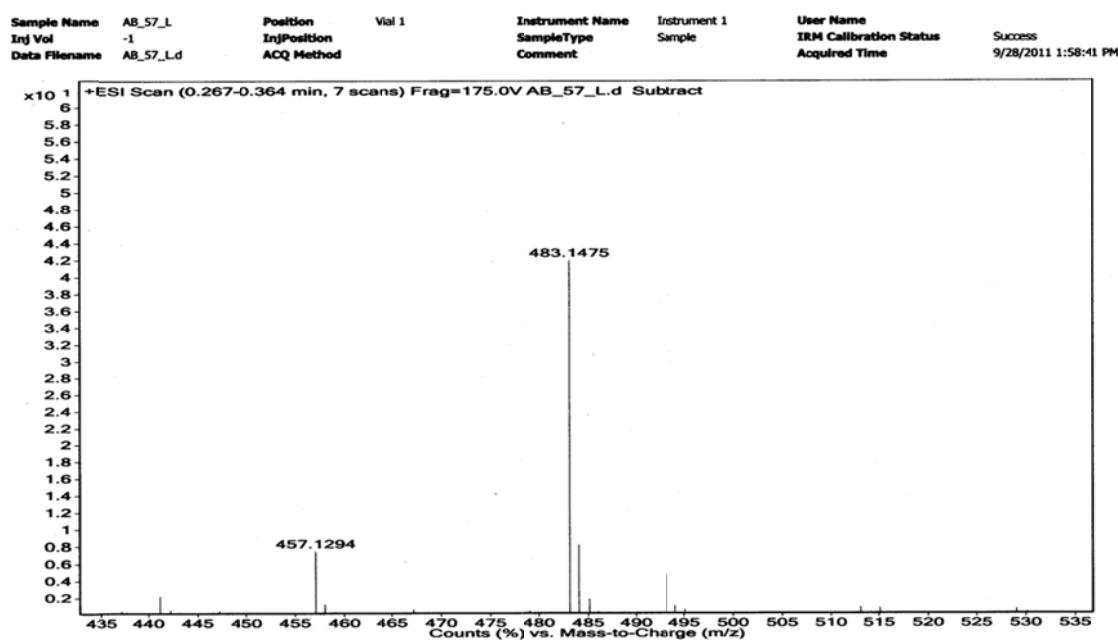
N-((E)-(2,4-Difluorophenylimino)(morpholino)methyl)-N-(2,4-difluorophenyl)morpholine-4-carbothioamide (12a).¹³C NMR (100 MHz, CDCl₃):

AB_57_Lower
expt std13C
SAMPLE SPECIAL
date Nov 5 2010 temp not used
solvent CDCl₃ gain not used
file exp spin not used
ACQUISITION dec rate not used
av 25000 psize 16.668
at 1.158 alta 20.000
nt 1.000 flags 32.000
dt 1.000 dp 1
ct 2528 PROCESSING
TRANSMITTER HI fm 1.00
trfq 188.532 sp not used
tot 8 s w1 1082.0
tper 1 s r1 1075.5
pw 8.657 rfp 1075.5
DECOUPLER RP 7264.9
dn C13 tp -338.0
dof 256
db 256 wc 256
dppr 42 vc 0
dmt 8500 th 12.3
nm no ph

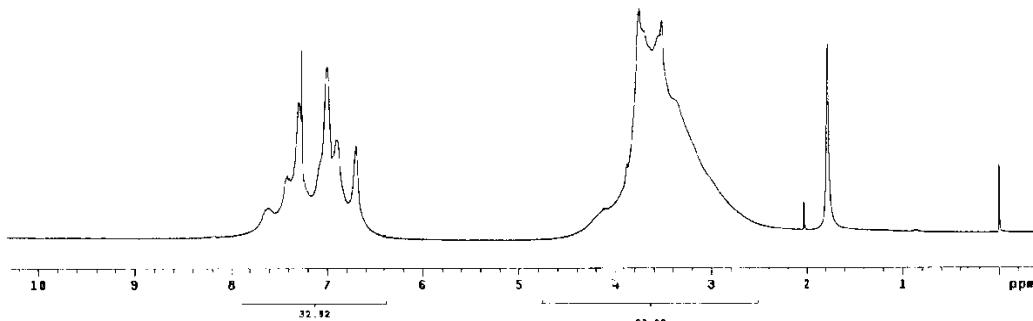
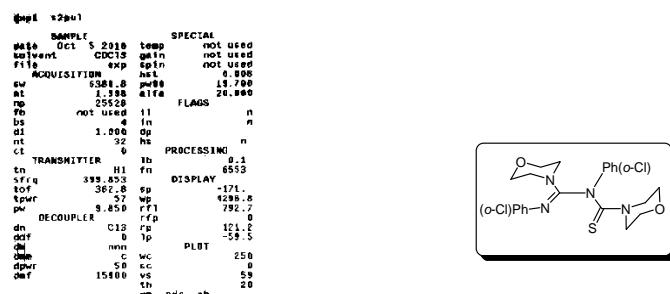


-S59 -

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



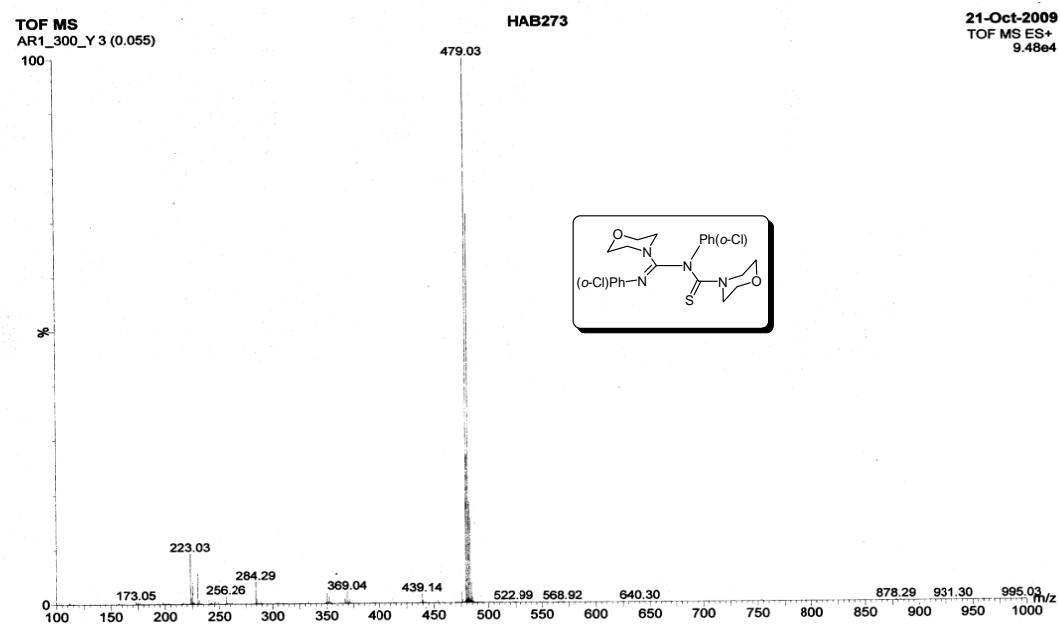
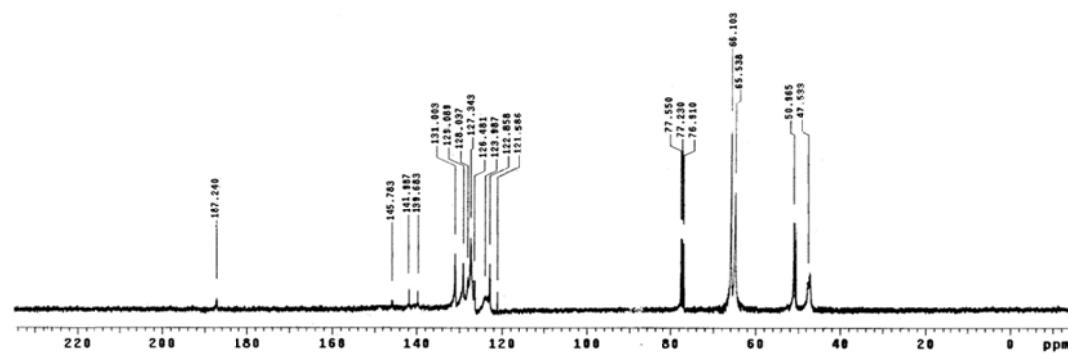
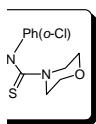
N-((E)-(2-Chlorophenylimino)(morpholino)methyl)-N-(2-chlorophenyl)morpholine-4-carbothioamide (13a). ^1H NMR (400 MHz, CDCl_3):



-S60 -

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

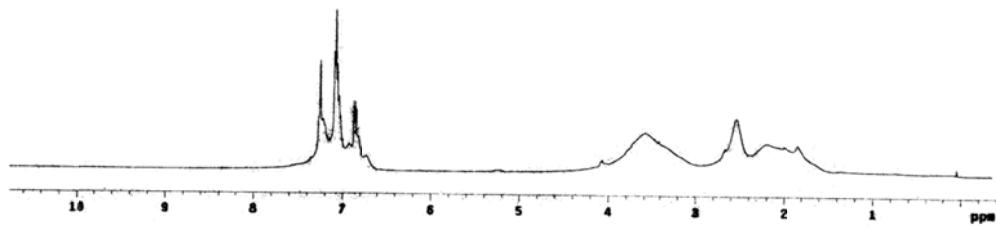
```
exp1 s2pul
SAMPLE C13
SPECIAL
date Oct 5 2010
temp not used
solvent CDCl3
gain not used
d1 1s
exp 1
spin not used
sw 25125.6
pw0 1.600
at 8.000
rt 20.000
dt 0.0270
fb 13800
l1 11
f1 11
nt 1
sc 1.000
ppm
nc 4000
ct 0
c1 TRANSMITTER
lb 0.00
fn 85536
tn C13
DISPLAY 85536
tr 100.000
t0f 1534.2
sp 71521.5
tpw 61
vp 25124.9
pw 9.390
rf1 7744.9
DECOUPLER H1
rfp 7744.9
dn 25.7
dmf 322.3
dme 250
dmc 40
dmr 8
dmr 5900
v1 28
rm no ph
```



-S61 -

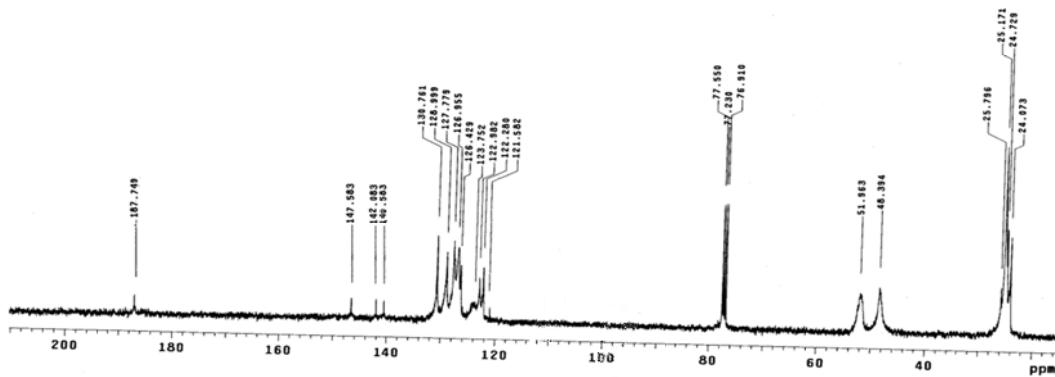
N-((E)-(2-Chlorophenylimino)(thiomorpholino)methyl)-N-(2-chlorophenyl) thiomorholine-1-carbothioamide (13b). ^1H NMR (400 MHz, CDCl_3):

```
expt 129ul
SAMPLE      May 27 2012
solvent      CDCl3
temp        not used
file        exp
ACQUISITION exp
spin        not used
sw          6300.0
spw         1000
n1          256
t1          1.000
d1          1.000
f1          1.000
not used   11
nt          32
sc          32
ct          22
PROCESSING 3.10
tr          1b
td          653.0
tdw        175.0
display    4473.0
tpw        795.0
p1          7.000
DECOUPLER   C13
dp          100.0
dof         128
dm          VV
plot       256
nm          42
dav        15932
th          40
no         cdc
ph          20
```



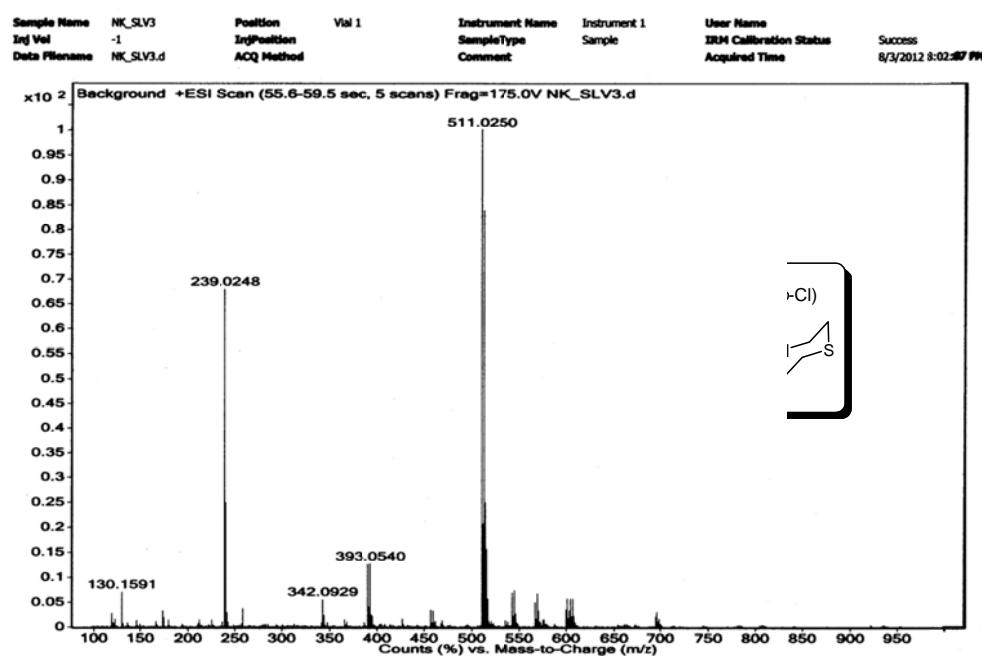
N-((E)-(2-Chlorophenylimino)(thiomorpholino)methyl)-N-(2-chlorophenyl) thiomorholine-1-carbothioamide (13b). ^{13}C NMR (100 MHz, CDCl_3):

```
expt 129ul
SAMPLE      SPECIAL
date Jun 4 2012 temp not used
solvent      CDCl3 gain not used
file        exp spin not used
ACQUISITION exp
temp        not used
sw          25125.6
spw         1000
n1          656
t1          1.193
f1          1.000
np          656
rb          136000
d1          11
rt          28
di          1.000
nt          5000
sc          256
ct          3400
PROCESSING 2.00
tr          C13 fn
td          653.0
tdw        1459.5
display    19677.5
tpw        61
p1          9.388
r1          9276.7
DECOUPLER   H1 rfp
dp          77.9
dof         36
dm          VV
plot       256
nm          42
dav        8992
th          40
no         cdc
ph          5
```



-S62 -

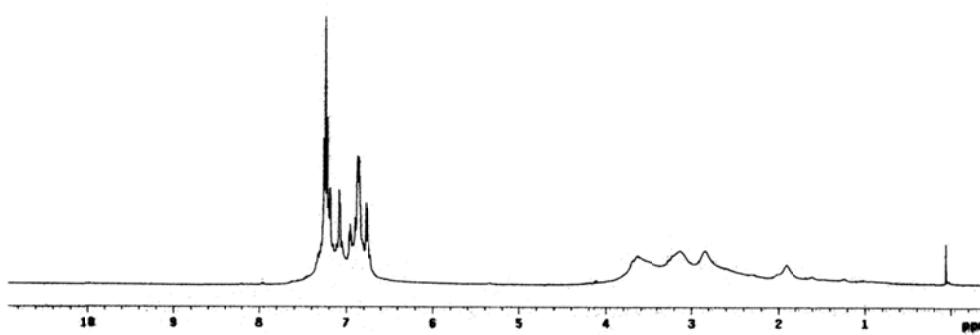
N-((E)-(2-Chlorophenylimino)(thiomorpholino)methyl)-N-(2-chlorophenyl) thiomorholine-1-carbothioamide (13b). MASS SPECTRA:



N-((E)-(2-Chlorophenylimino)(4-piperazin-1-yl)methyl)-N-(2-chlorophenyl) piperazine-1-carbothioamide (13c). ¹H NMR (400 MHz, CDCl₃):

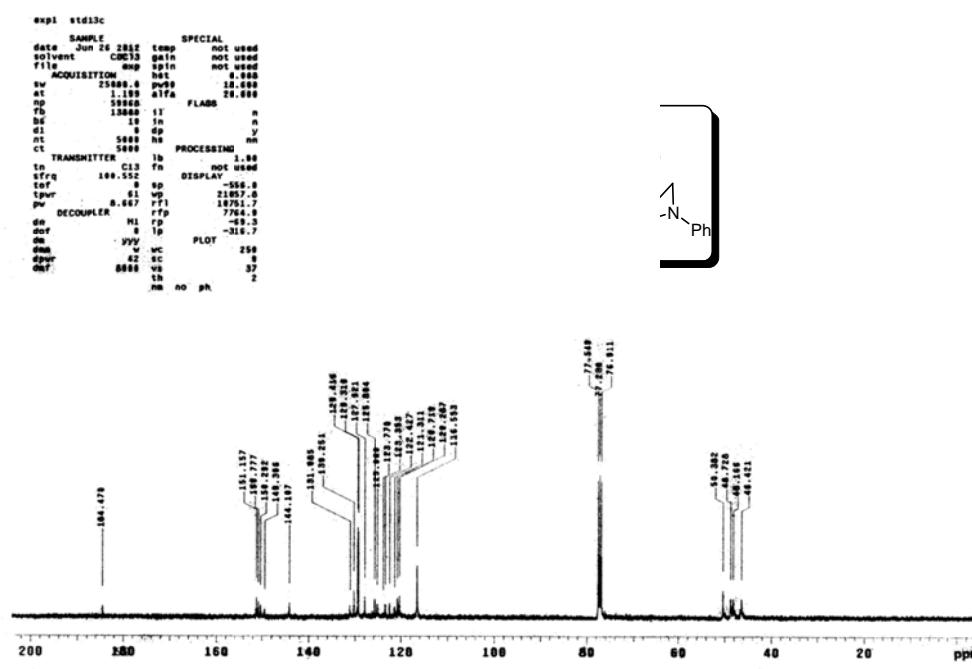
exp1.vsmpl

SAMPLE	SPECIAL
date Jul 18 2012	temp not used
parent CDCl ₃	path not used
title	not used
ACQUISITION	not used
st	600.000
et	1.999
sc	32768
dp	20000
dpw	not used
bs	1.000
ds	1.000
cs	32
TRANSMITTER	fm not used
tr	HI
trfreq	399.653
trif	sp
trifreq	-182.6
trp	0
trppr	4545.8
trppr2	971.1
trppr3	7.499
DECOUPLER	rp
dpr	92.6
da	C13
def	8
dpf	PLOT
dm	mmv
dc	vc
dppr	256
df	50
dfpr	10
dfppr	15999
dfp	mm
dcfc	cde
ph	10

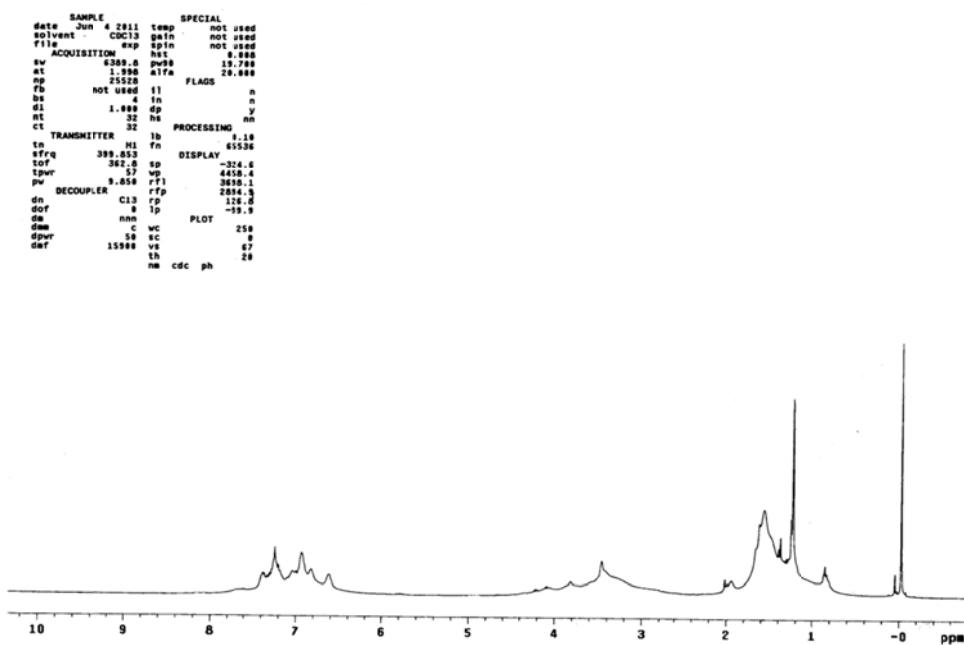


-S63 -

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

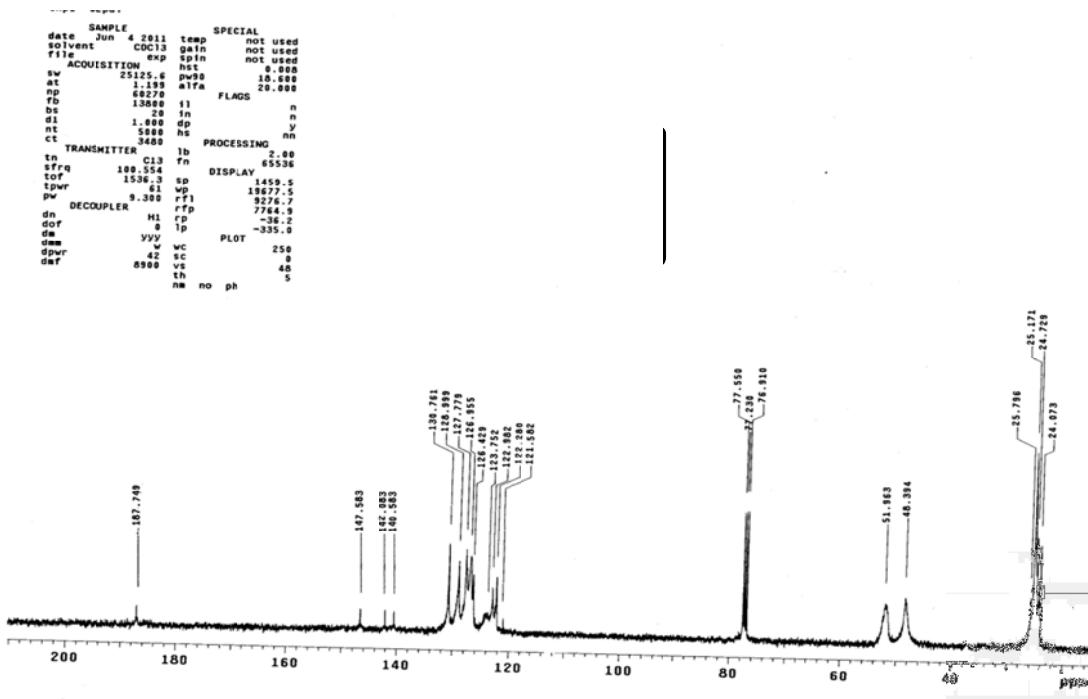


N-((E)-(2-Chlorophenylimino)(piperidin-1-yl)methyl)-N-(2-chlorophenyl)piperidine-1-carbothioamide (13d). ^1H NMR (400 MHz, CDCl_3):



-S64 -

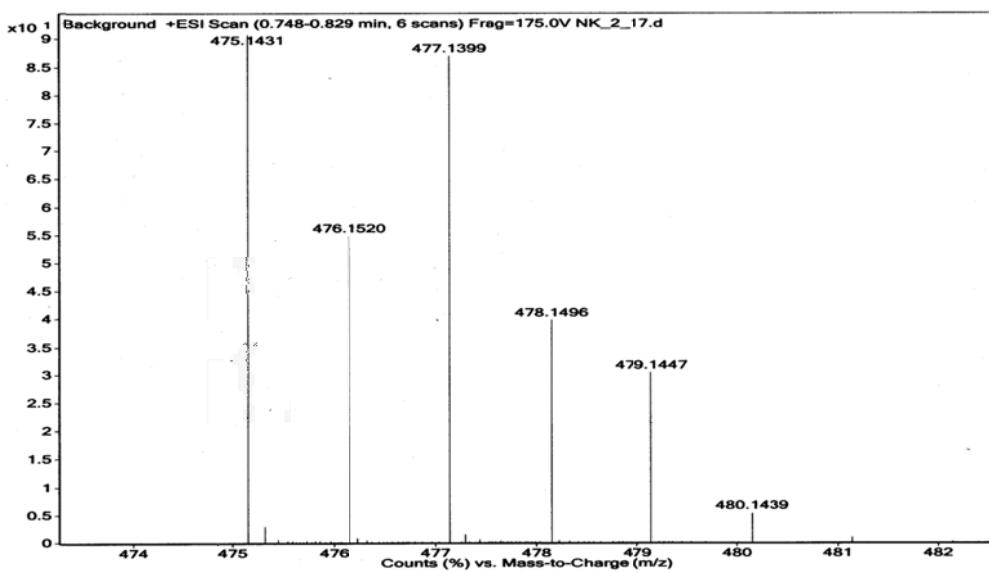
N-((E)-(2-Chlorophenylimino)(piperidin-1-yl)methyl)-N-(2-chlorophenyl)piperidine-1-carbothioamide (13d). ¹³C NMR (100 MHz, CDCl₃):



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

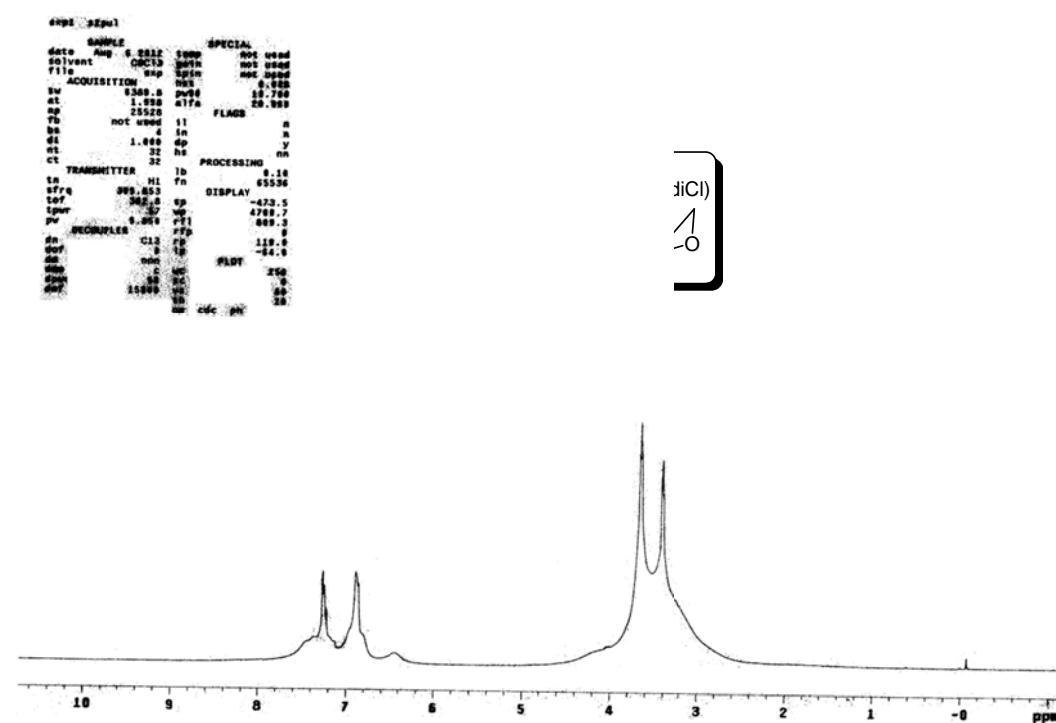
Sample Name	NK_2_17	Position	Vial 1	Instrument Name	Instrument 1	User Name
Inj Vol	-1	InjPosition	1	SampleType	Sample	IRM Calibration Status
Data Filename	NK_2_17.d	ACQ Method		Comment		Acquired Time

All Ions Missed
9/28/2011 12:45:23 PM

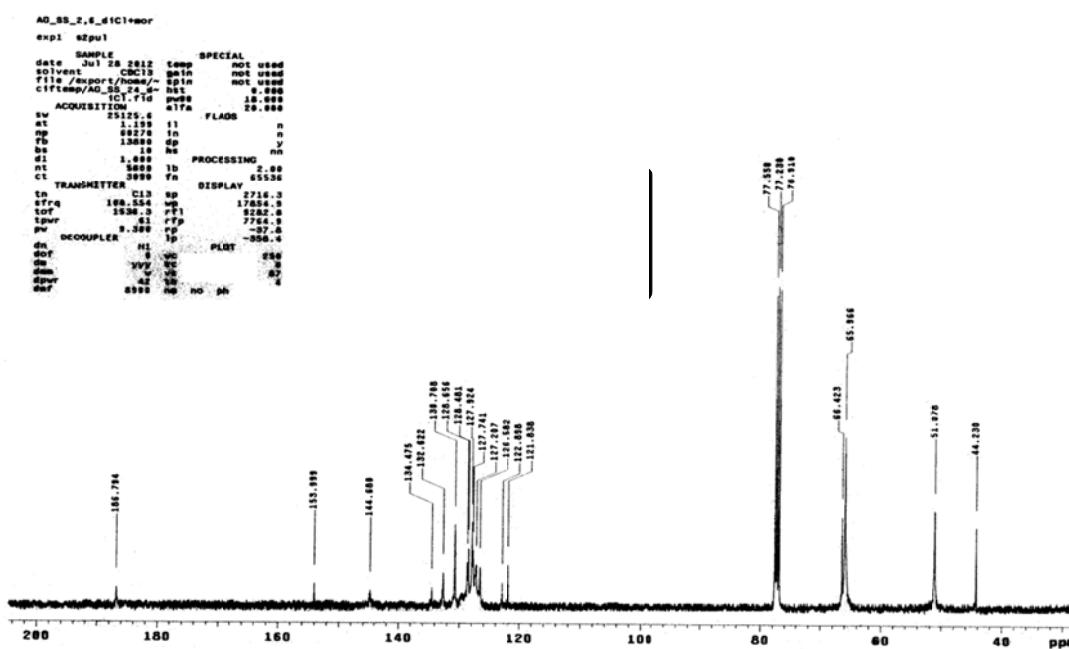


-S65 -

N-((E)-(2,4-Dichlorophenylimino)(morpholino)methyl)-N-(2,4-dichlorophenyl)morpholine-4-carbothioamide (14a).¹H NMR (400 MHz, CDCl₃):

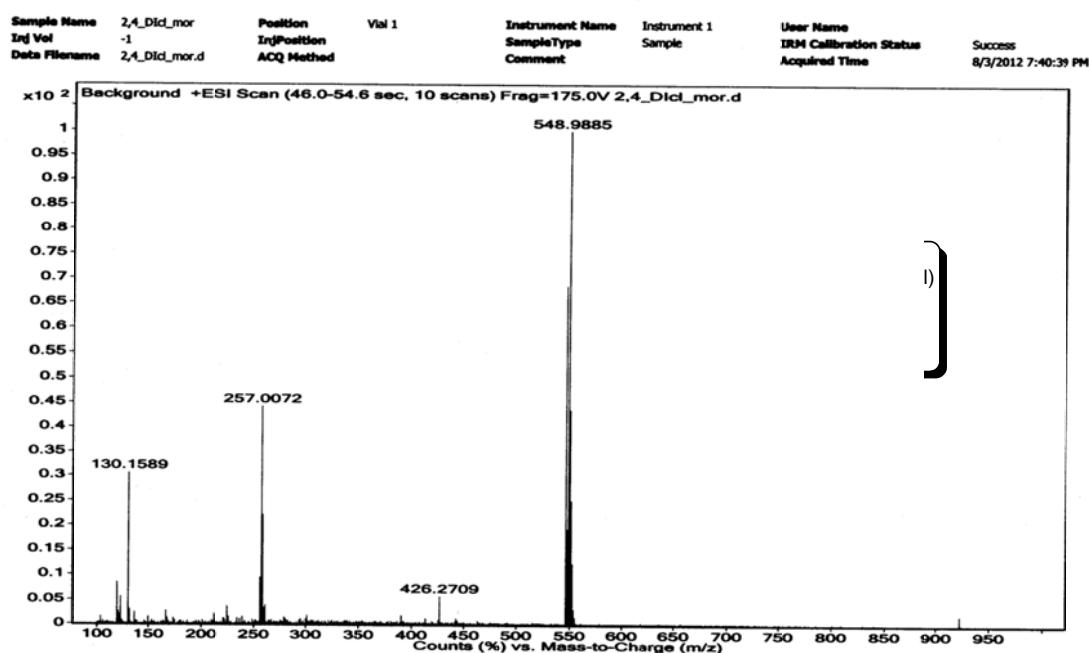


N-((E)-(2,4-Dichlorophenylimino)(morpholino)methyl)-N-(2,4-dichlorophenyl)morpholine-4-carbothioamide (14a).¹³C NMR (100 MHz, CDCl₃):



-S66 -

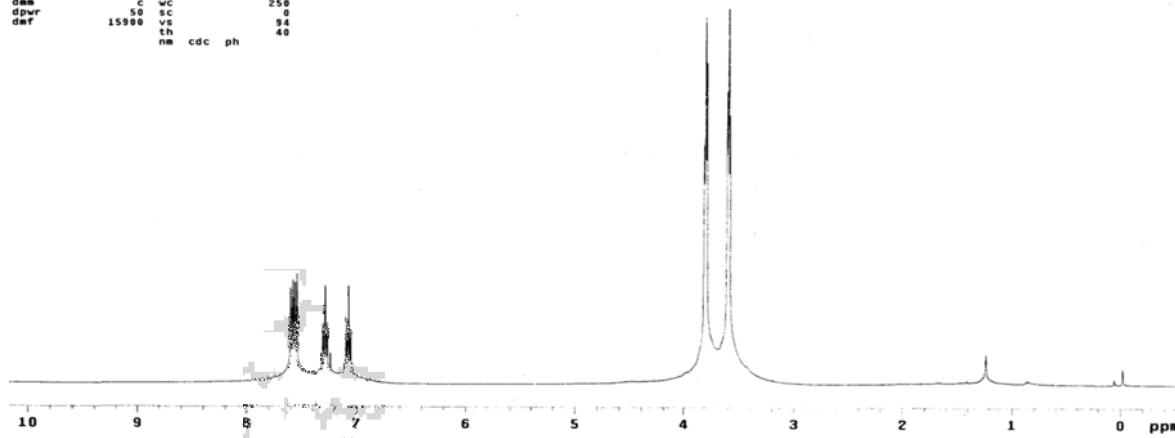
N-((E)-(2,4-Dichlorophenylimino)(morpholino)methyl)-N-(2,4-dichlorophenyl)morpholine-4-carbothioamide (14a). MASS SPECTRA:



Benzothiazole

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

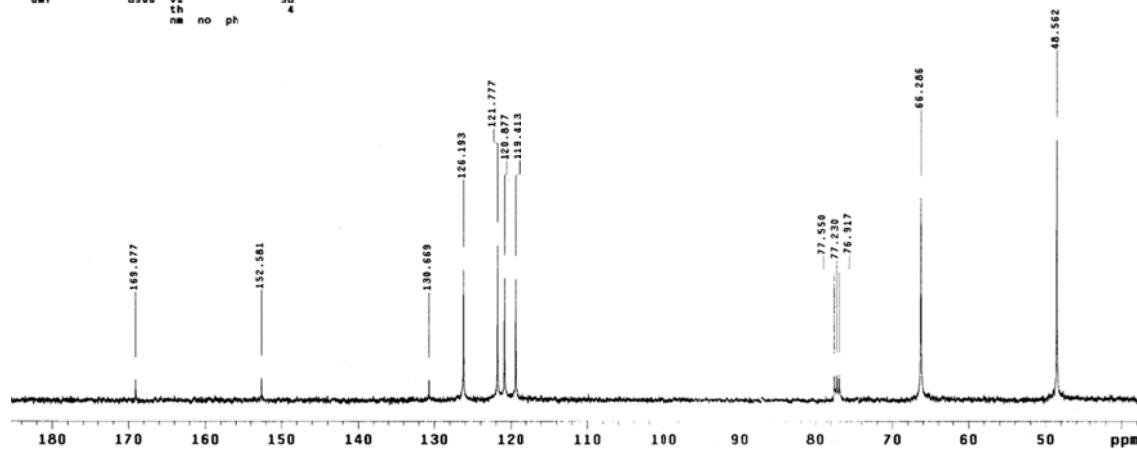
```
expt s2pul
SAMPLE          SPECIAL
date Oct 7 2010 temp not used
solvent   CDCl3 gain not used
file      exp spin not used
ACQUISITION hst g 0.008
sw       6389.8   1000 1000
at       1.398   61fa 20.000
np       25528   flags
tb       not used 11 n
bs       4        in n
d1      1.000   dp     y
nt      32        nn
ct      32        PROCESSING 0.10
tn      TRANSMITTER 1b
rf      HI fn 65536
sfrq    399.853   DISPLAY
tof      362.8   sp -232.4
tpwr    5        wp 423.0
pw      9.850   rfp 2854.1
dec    DECOUPLER C13 rfp 2854.9
dn      C13 rp 129.0
dot    0        tp -74.2
dm      nnn PLOT
dme    c wc 250
dpwr    50
dmr    15999 vs 94
nm      cdc ph 40
```



-S67 -

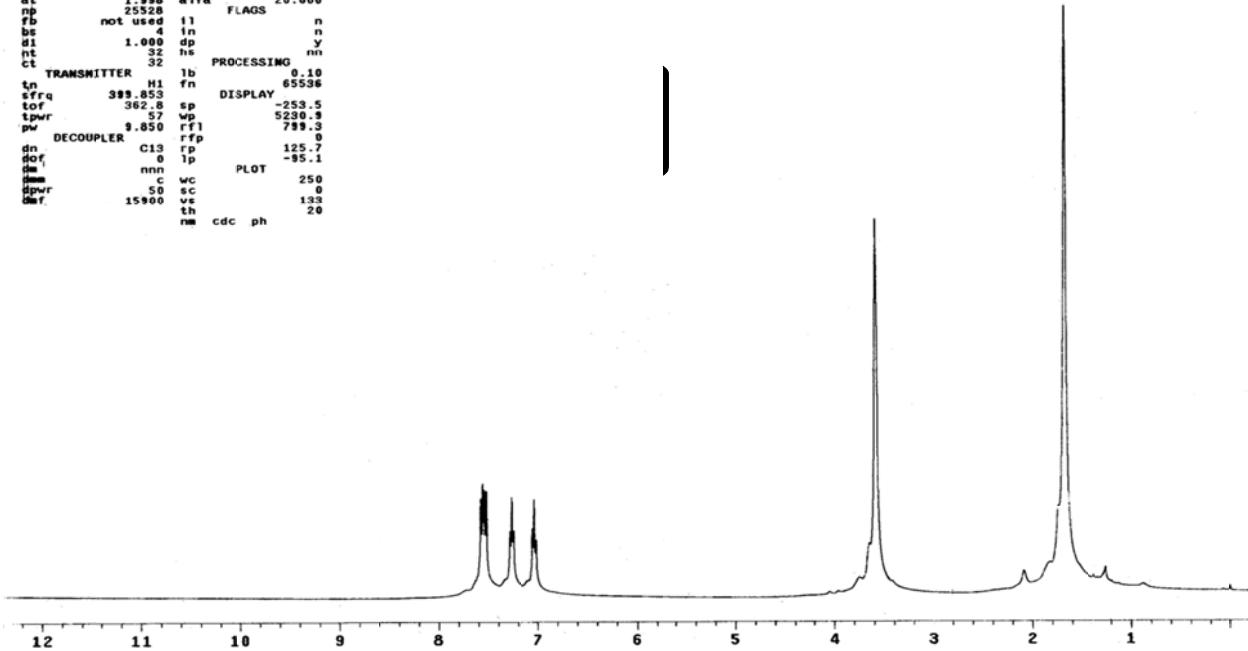
2-morpholinobenzo[*d*]thiazole (11'a): ^{13}C NMR (100 MHz, CDCl_3):

```
expt1 s2pu1
SAMPLE          SPECIAL
date  Oct 11 2010 temp   not used
solvent    CDCl3 gain    not used
file      exp spin   not used
ACQUISITION hst      0.008
sw       25125.6 pw90   15.600
at        1.000 alfa   20.000
np        68270   FLAG0
fb        13800   11      n
bs        1.000   1p      n
di        1.000   1p      y
nt        5000   hs      nn
ct        512    PROCESSING
TRANSMITTER 1b      2.00
tn       C13   fn      65536
sfrq    100.554   DISPLAY
t0f     1536.3   sp      3727.7
tpwr    9.300   wp      1400.5
pw       9.300   rfp     7764.9
DECOUPLER   H1   rfp     7764.9
d1       0      1p      -44.7
dof      0      1p      -345.1
dss      250    PLOT
dpwv    42     sc      0
dpwr    8500   vc      58
dmf      4      th      4
nm      no      ph
```



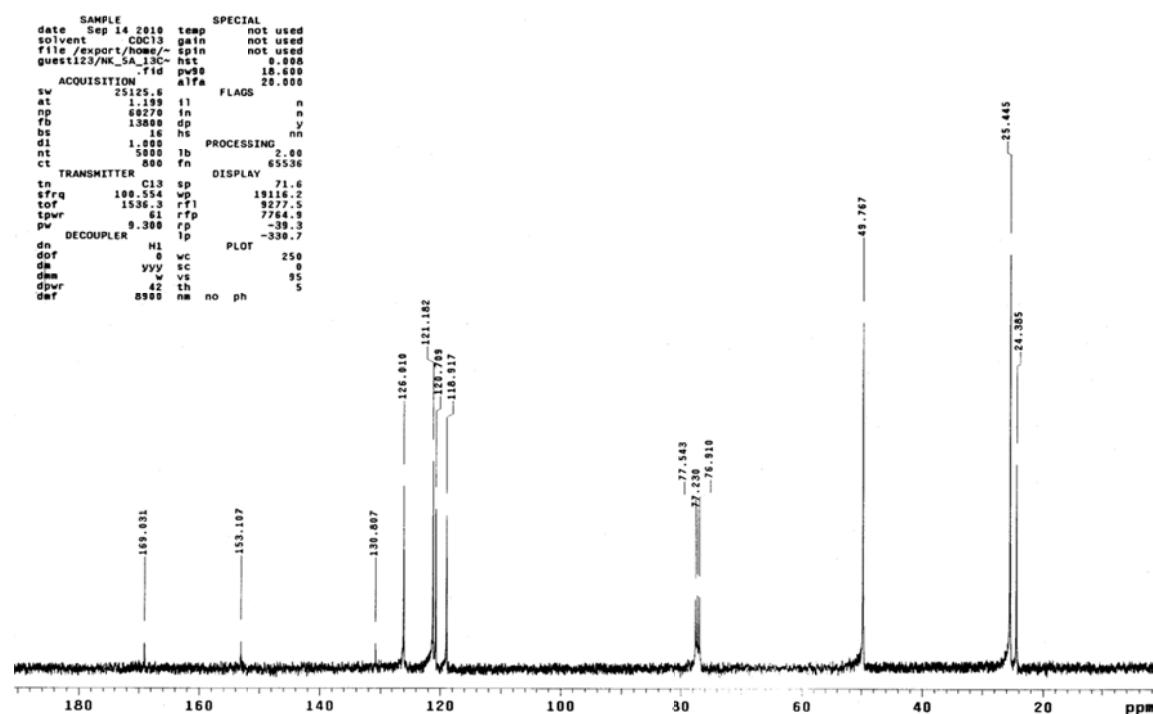
2-(Piperidin-1-yl)benzo[*d*]thiazole (11'd): ^1H NMR (400 MHz, CDCl_3):

```
expt1 s2pu1
SAMPLE          SPECIAL
date  Sep 11 2009 temp   not used
solvent    CDCl3 gain    not used
file      exp spin   not used
ACQUISITION hst      0.008
sw       6381.5 pw90   15.700
at        1.000 alfa   20.000
np        25528   FLAG0
fb        not used  11      n
bs        1.000   1p      n
di        1.000   1p      y
nt        32    hs      nn
ct        32    PROCESSING
TRANSMITTER 1b      0.10
tn       H1   fn      65536
sfrq    399.853   DISPLAY
t0f     362.8   sp      -253.5
tpwr    9.850   wp      5230.9
pw       9.850   rfp     793.3
DECOUPLER   H1   rfp     0
d1       C13   rfp     125.7
dof      0      1p      -95.1
dss      250    PLOT
dpwv    50     sc      0
dpwr    15900   vc      133
dmf      20     th      20
nm      cdc      ph
```

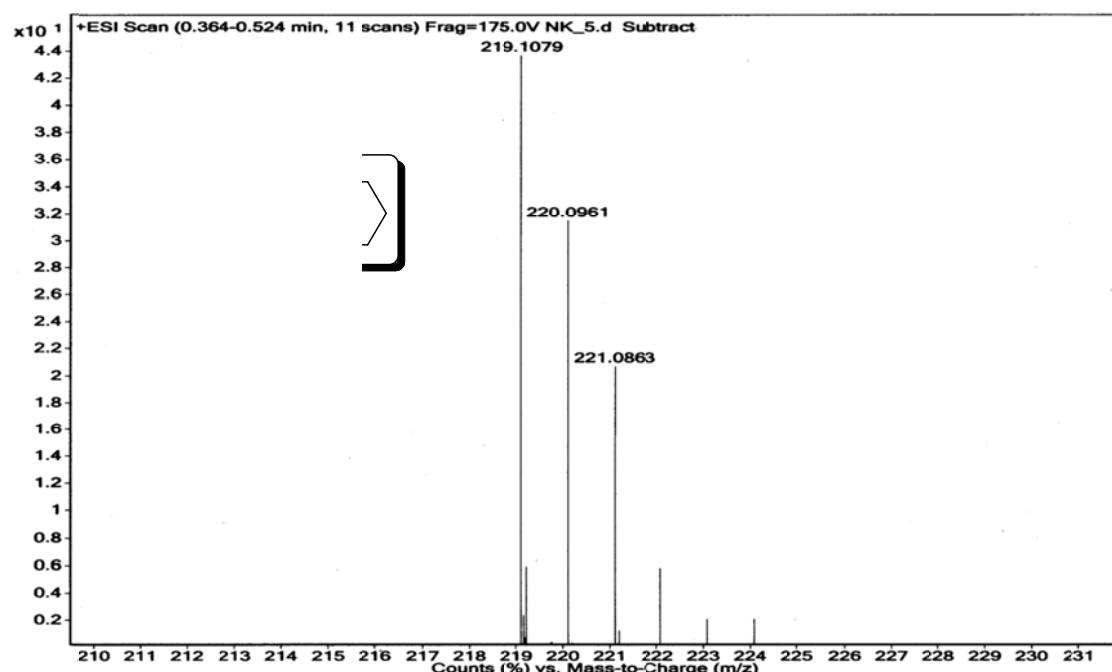


-S68 -

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

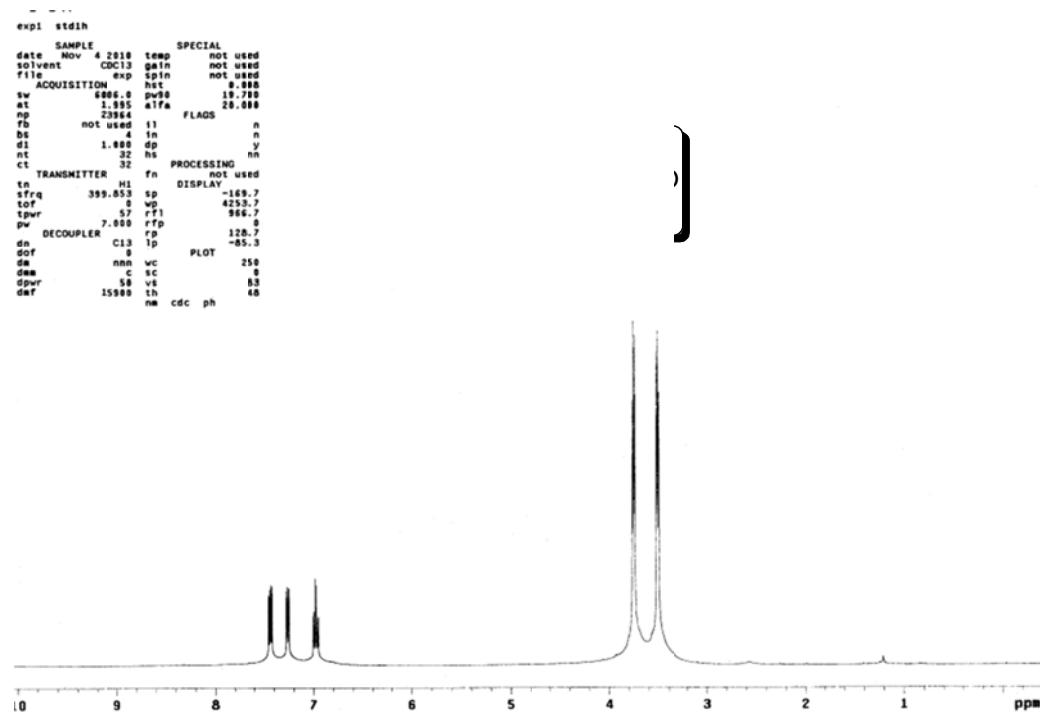


Sample Name	NK_5	Position	Vial 1	Instrument Name	Instrument 1	User Name
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status
Data Filename	NK_5.d	ACQ Method		Comment		Acquired Time

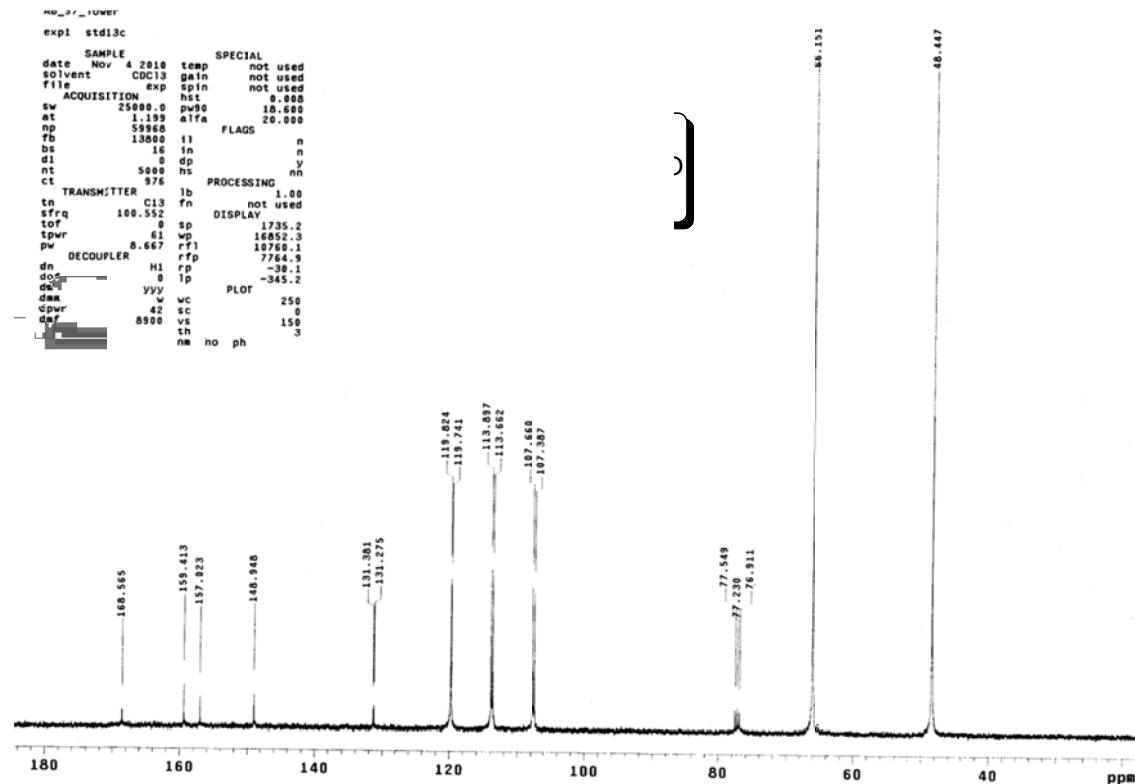


-S69 -

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



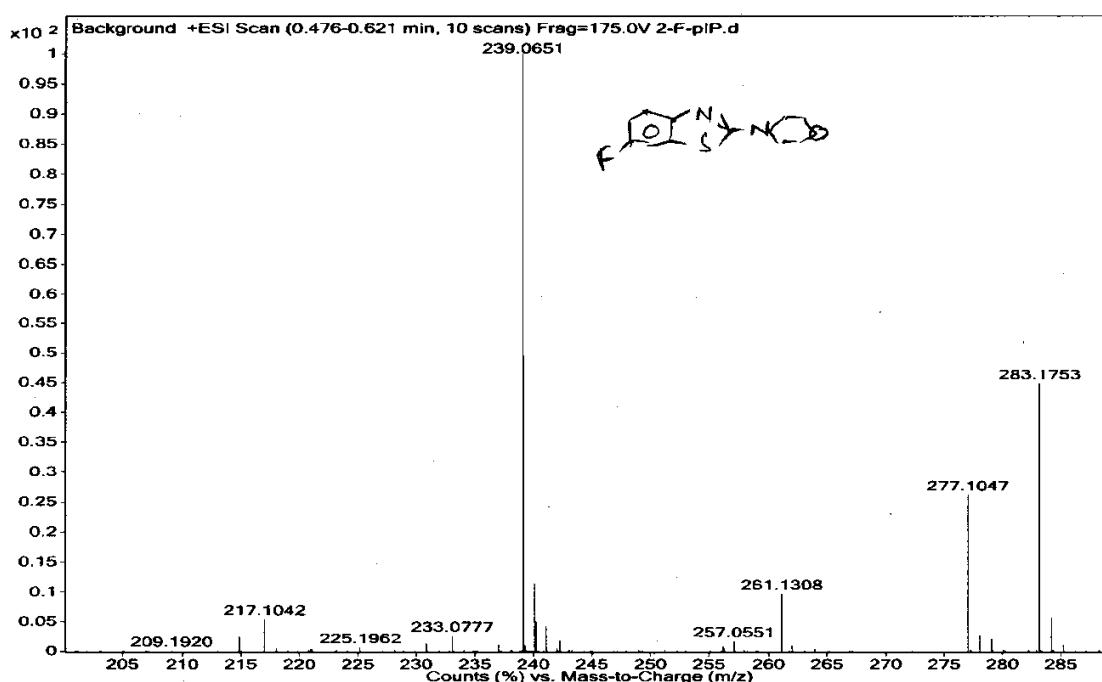
6-Fluoro-2-morpholinobenzo[*d*]thiazole (12'a): ^{13}C NMR (100 MHz, CDCl_3):



-S70 -

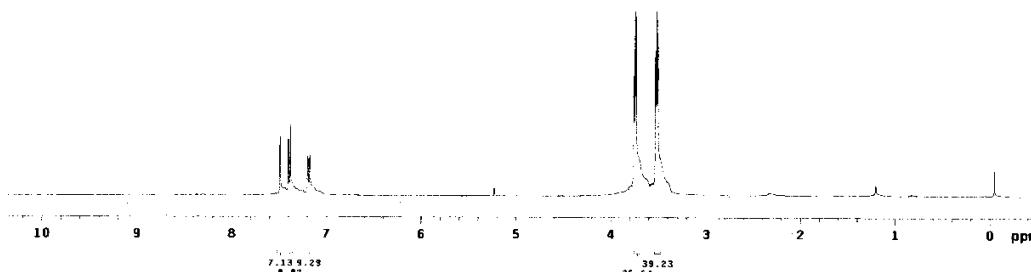
6-Fluoro-2-morpholinobenzo[d]thiazole (12'a): MASS SPECTRA:

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



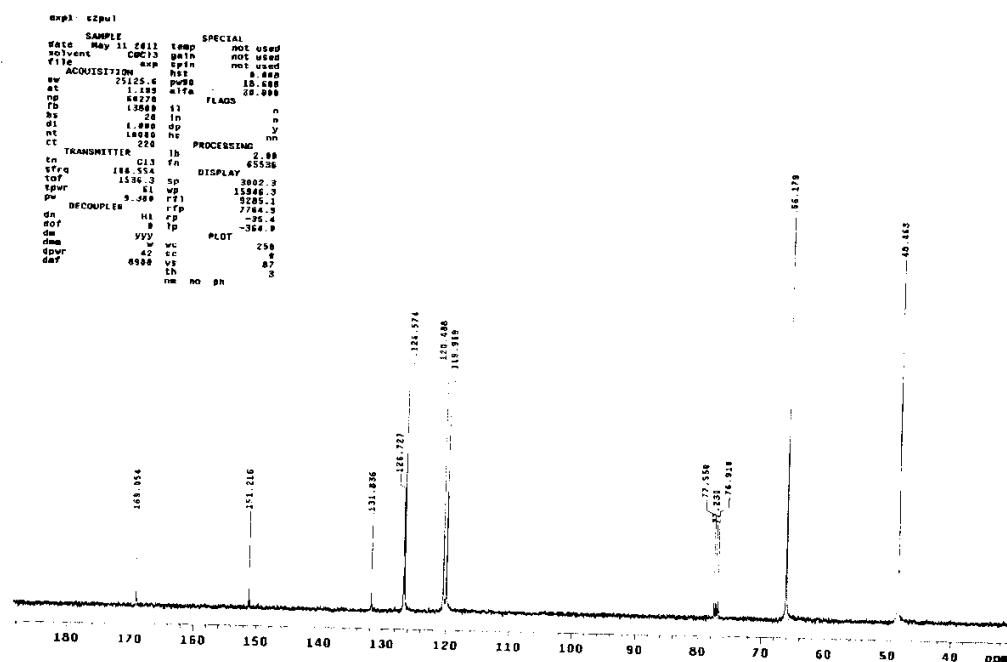
6-Chloro-2-morpholinobenzo[d]thiazole (14'a): ^1H NMR (400 MHz, CDCl_3):

```
smpl 62pu1
SAMPLE          SPECIAL
date  May 11 2011 temp      not used
solvent   CDCl3 gain      not used
file    exp  spin      not used
        1       0      0
ACQUISITION      0.0000
        6389.6 pw09     19.700
        1.998 alra    20.000
        2552.0 fwhm    10.000
        2552.0 flags
        not used 1t      n
        4      1p      n
        1.000 dp      y
        32      hs      nn
        32      PROCESSING
        1b      0.19
TRANSMITTER      1b      0.19
        1n      H1      65536
        399.853 DISPLAY
        362.6 SP      -215.6
        t0f      362.6 t0      435.2
        t0r      362.6 r0      3658.3
        p0      9.811 rrf0    2894.9
        DECOUPLER      rfp      2894.9
        d1      CLS rfp    -126.9
        d1f      0 1p    -191.7
        dm      nnn PLOT
        dw      c wc    250
        dpr      50
        dmt      15990 vs      44
        nm      th      34
        nm      cdc ph
```



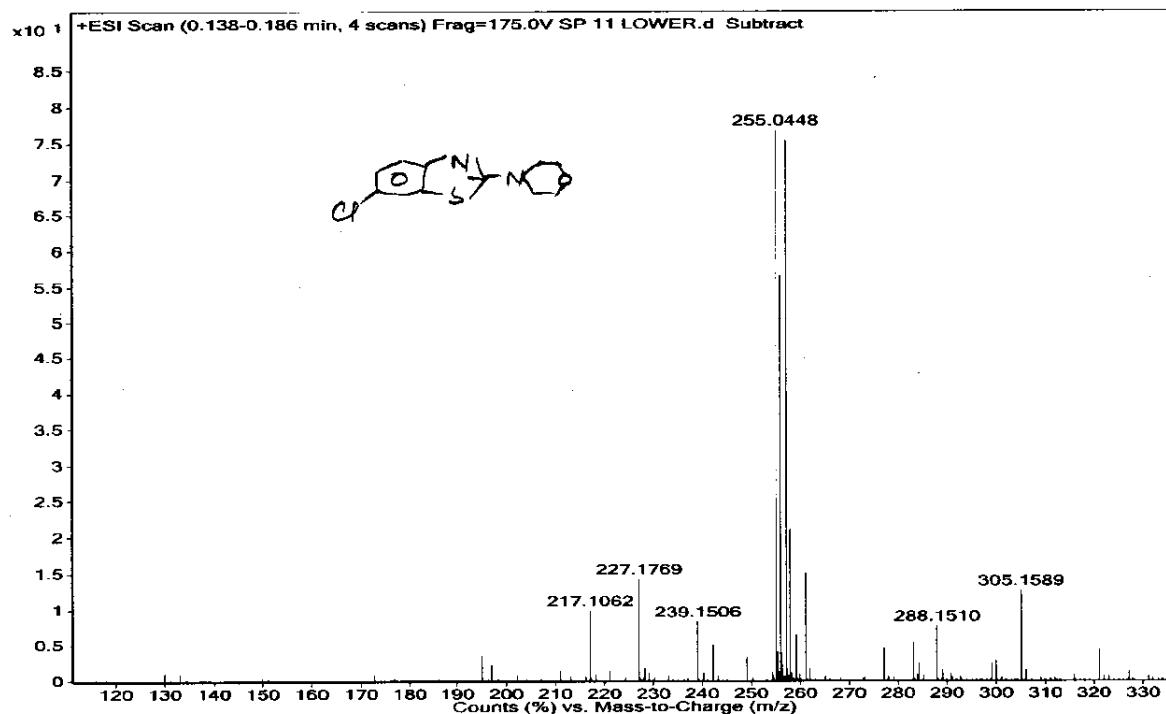
-S71 -

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



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

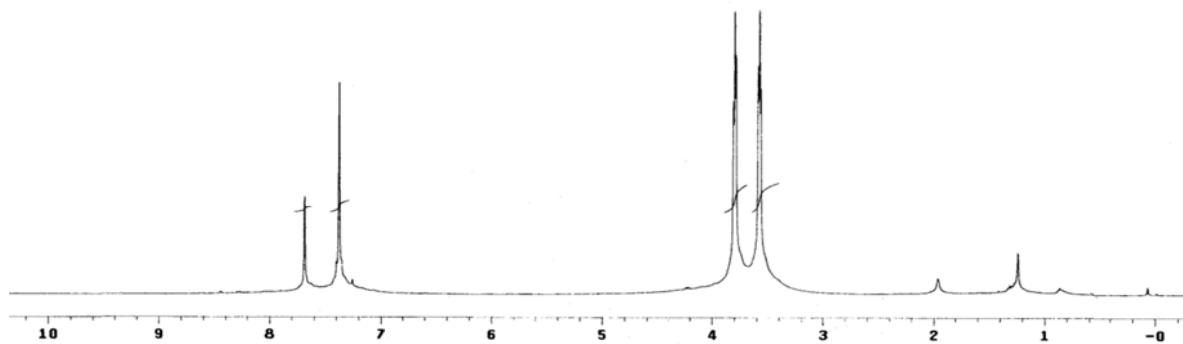
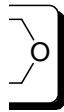
Sample Name	SP11 LOWER	Position	Vial 1	Instrument Name	Instrument 1	User Name	IRM Calibration Status	Success
Inj Vol	-1	InjPosition		SampleType	Sample	Comment		
Data Filename	SP 11 LOWER.d	ACQ Method				Acquired Time		



-S72 -

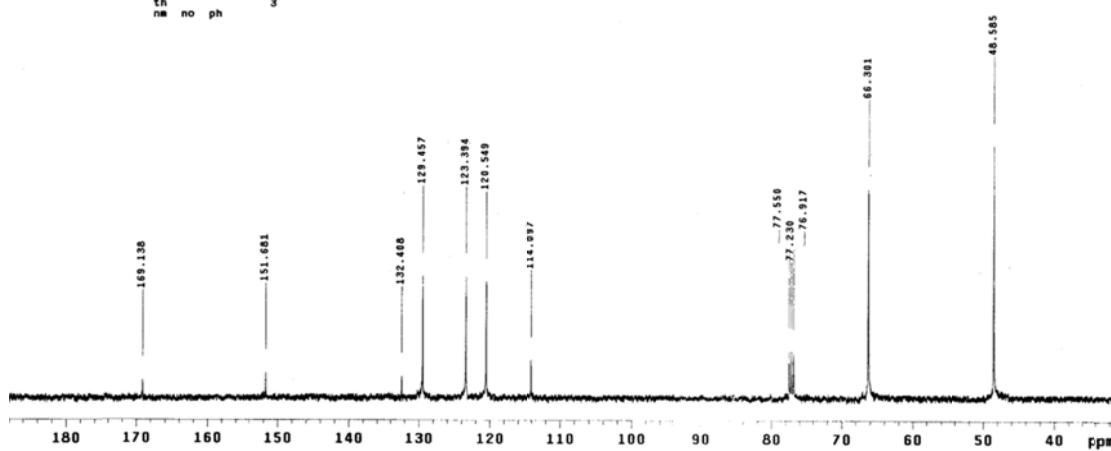
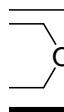
6-Bromo-2-morpholino[*d*]thiazole (15'a): ^1H NMR (400 MHz, CDCl_3):

```
ME_1B_Upper
exp1 s2pul
SAMPLE          SPECIAL
date Oct 5 2010 temp not used
solvent  CDCl3 gain  not used
file    exp spin  not used
ACQUISITION hst  9.000
sw    6369.8 pw90  18.000
at    1.999 alfa  20.000
np    25528   FLAGS
fb    not used t1  n
bs    4      in  n
di    1.000 dp  y
nt    56      hs  nn
ct    54      PROCESSING
tn    HI fn  0.10
sfreq 399.853 DISPLAY
t0f   362.8 sp  -283.7
tpwr  57 wp  4433.3
pw    9.858 rfp  0
DECOUPLER C13 rfp  129.8
dof   8 ip  -94.2
dm   nm PLOT
dme   c wc  250
dpwr 50 sc  0
dfr   15900 vt  68
      th  11
nm cdc ph
```



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

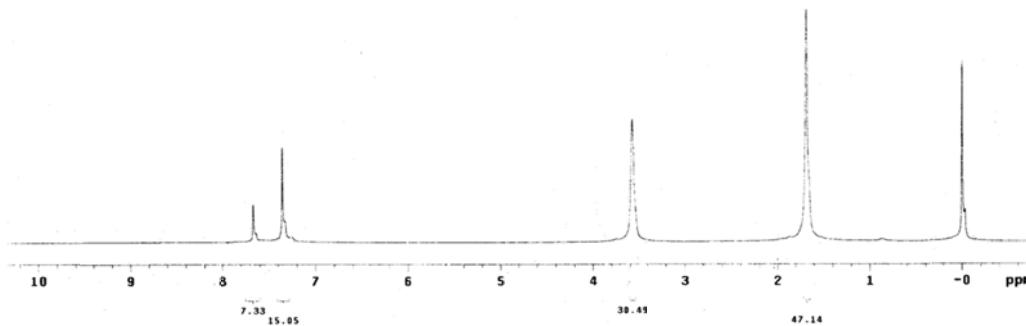
```
exp1 s2pul
SAMPLE          SPECIAL
date Oct 6 2010 temp not used
solvent  CDCl3 gain  not used
file    exp spin  not used
ACQUISITION hst  9.000
sw    25125.6 pw90  10.000
at    1.199 alfa  20.000
np    60256   FLAGS
fb    13600 t1  n
bs    16      in  n
di    1.000 dp  y
nt    5000 hs  nn
ct    512      PROCESSING
tn    HI fn  2.00
sfreq 180.554 DISPLAY
t0f   15900 sp  3978.2
tpwr  61 wp  16979.0
pw    9.300 rfp  9275.9
DECOUPLER C13 rfp  7764.9
dof   0 ip  -71.5
dm   yyy PLOT
dme   w wc  250
dpwr 42 tc  0
dfr   8900 vt  56
      th  3
nm no ph
```



-S73 -

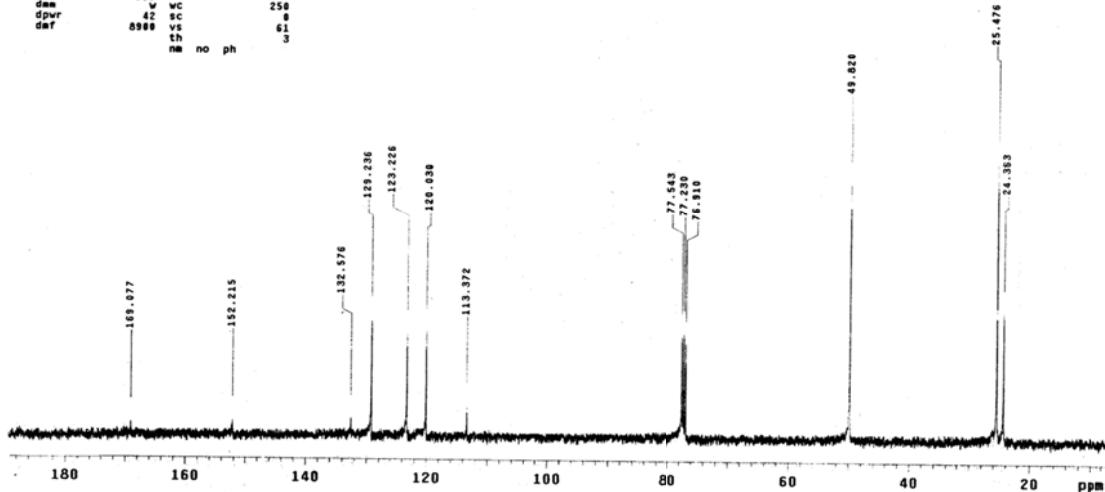
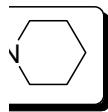
6-Bromo-2-(piperidin-1-yl)[d]thiazole (20'd): ^1H NMR (400 MHz, CDCl_3):

```
expt #2pu1
SAMPLE          SPECIAL
date Apr 27 2011 temp not used
solvent CDCl3 gain 900.000
file      exp spin not used
ACQUISITION hz 100.000
sw       6389.8 pw90 15.700
spw     25528 alfa 20.000
np        1.000 flags
fb      not used 11 n
bs        1.000 dp n
dt        32 hs y
nt        32 nn
ct        32 PROCESSING
TRANSMITTER 1b 0.10
tn      H1 fn 65536
sfrq   399.853 DISPLAY
tr      362.27 sp -316.3
tpwr    6.47 vp 4450.0
pw      9.858 rfp 794.8
DECOUPLER 9.858 rfp 9
dn      C13 rp 122.2
dof      0 1p -96.6
dm      nnn PLOT
swave  vc 250
dpwr    50 sc 0
dmtf   -15900 vs 56
            th 20
            nm cdc ph
```



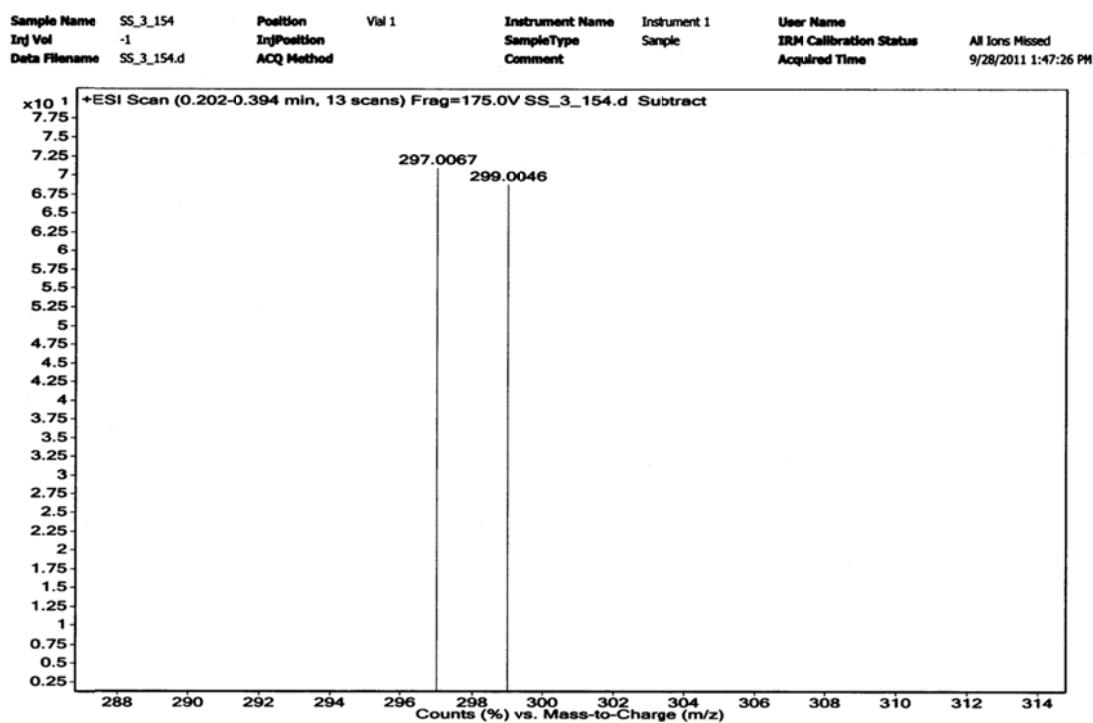
6-Bromo-2-(piperidin-1-yl)[d]thiazole (20'd): ^{13}C NMR (100 MHz, CDCl_3):

```
SAMPLE          SPECIAL
date Apr 27 2011 temp not used
solvent CDCl3 gain 900.000
file      exp spin not used
ACQUISITION hz 100.000
sw       25125.6 pw90 15.700
at        1.195 alfa 20.000
np        68278 flags
fb      1530.0 11 0.000
bs        28 in n
dt        1.000 dp y
nt        5000 hs nn
ct        1040 PROCESSING
TRANSMITTER 1b 0.00
tn      C13 fn 65536
sfrq   100.554 DISPLAY
tr      1530.0 sp 478.5
tpwr    6.41 vp 1851.1
pw      9.300 rfp 9272.9
DECOUPLER 9.300 rfp 7764.9
dn      H1 rp -43.8
dof      0 1p -296.6
dm      vyy PLOT
swave  vc 250
dpwr    42 sc 0
dmtf   8900 vs 61
            th 3
            nm no ph
```



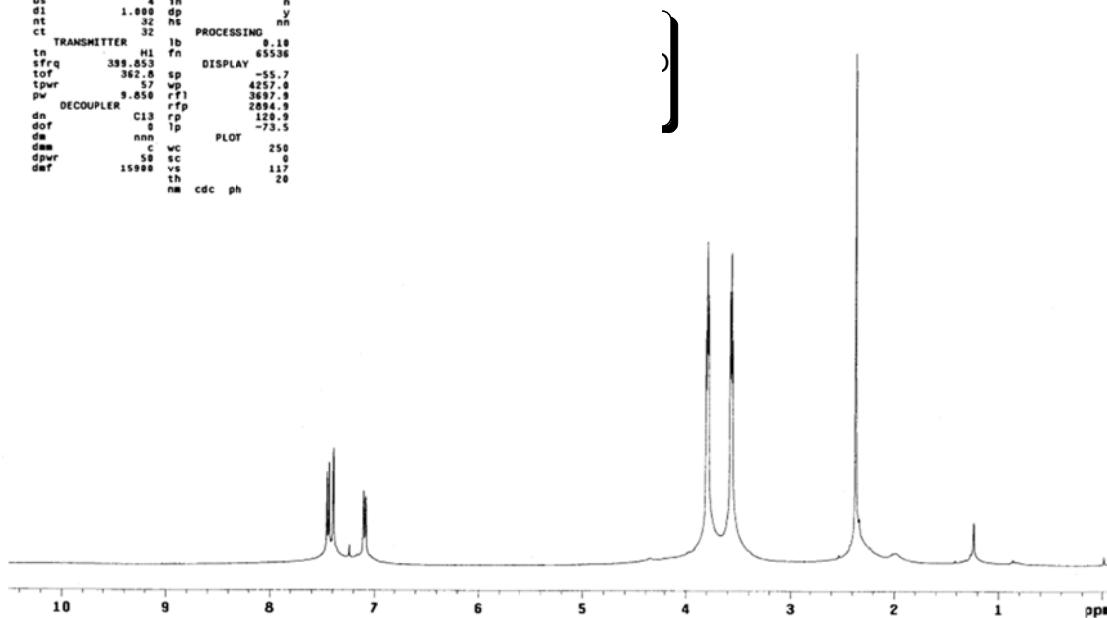
-S74 -

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



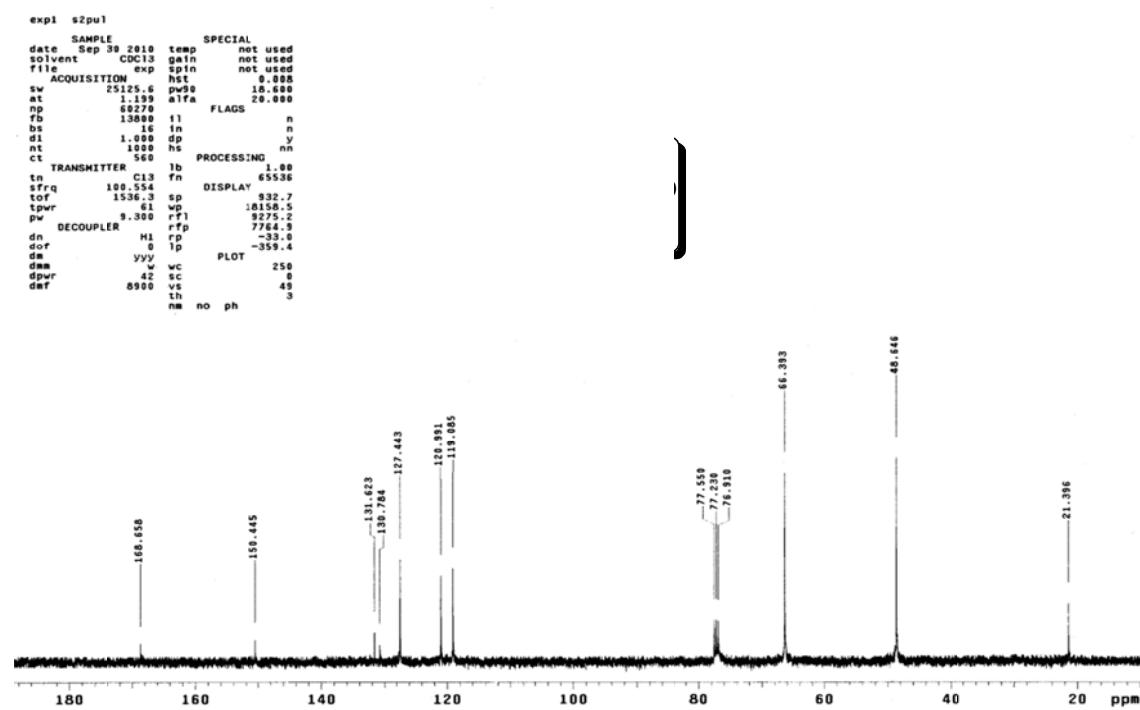
6-methyl-2-morholinobenzo[d]thiazole (18'a): ^1H NMR (400 MHz, CDCl_3):

```
expt1 s2pu1
      SAMPLE      SPECIAL
date Sep 30 2010 temp not used
solvent CDCl3 gain not used
file      exp spin not used
ACQUISITION hst    8.000
sw      6389.8 pw98 19.700
et      1.000 a1fa 20.000
np      25528 FLAGS
fb      not used 11   n
bs      1.004 in   n
dt      1.000 dp   y
nt      32   ns   nn
ct      32   PROCESSING
TRANSMITTER 1b   0.10
tn      HI fn   65536
sfrq    399.853 DISPLAY
totf    362.8 sp   -55.7
tpwr    57   w1   4257.0
pw      9.850 r1f1 300.0
DECOUPLER   rfp   2894.9
dn      C13 rp   120.0
dof     9   tp   -73.5
ds      nnc PLOT
dme     c wc   250
dpwr    50   sc   0
dmtf    15998 vs   117
      th   20
nm cdc ph
```

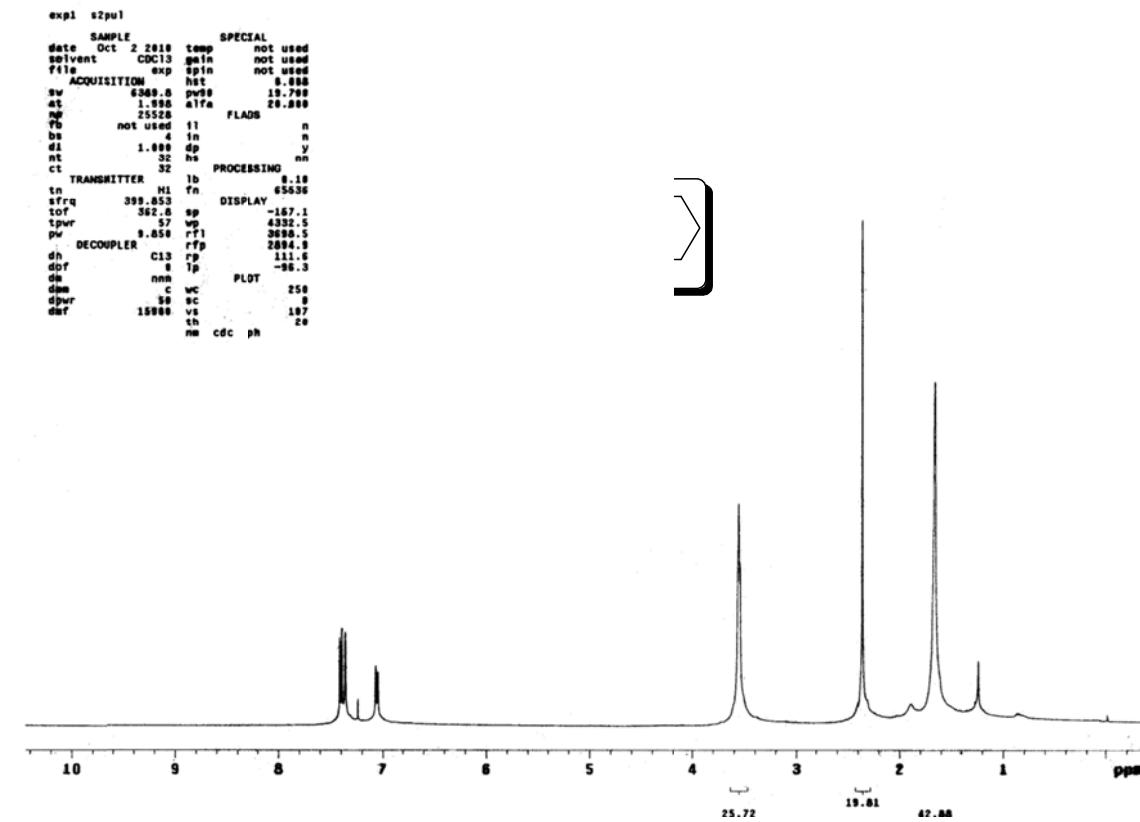


-S75 -

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

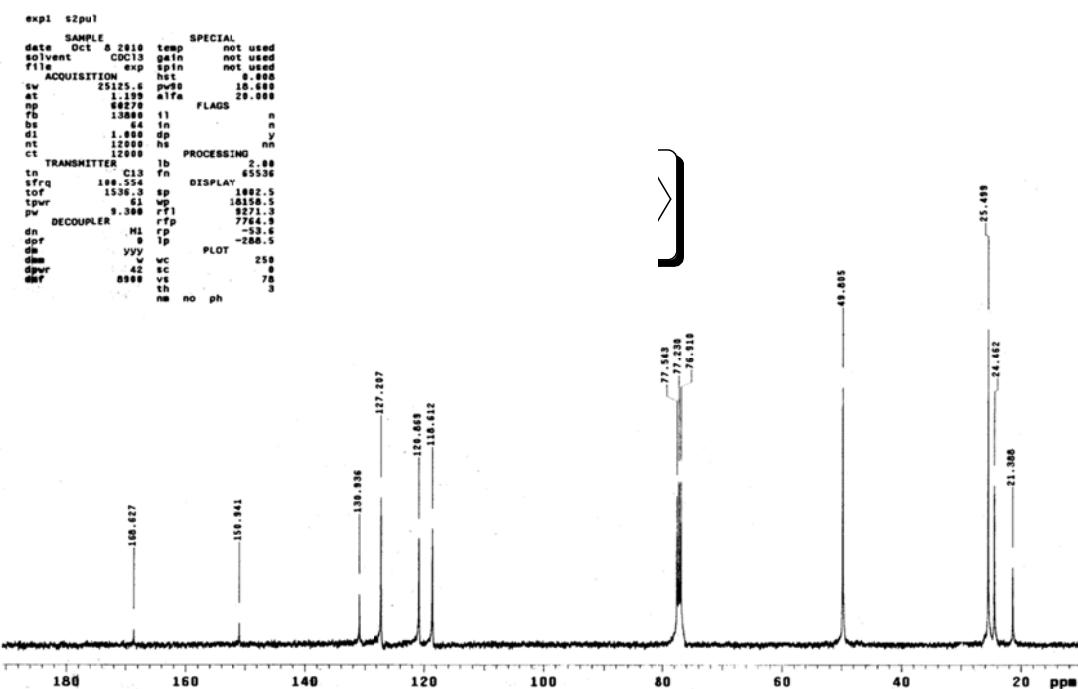


6-methyl-2-(Piperidin-1-yl)benzo[*d*]thiazole (18'd): ^1H NMR (400 MHz, CDCl_3):



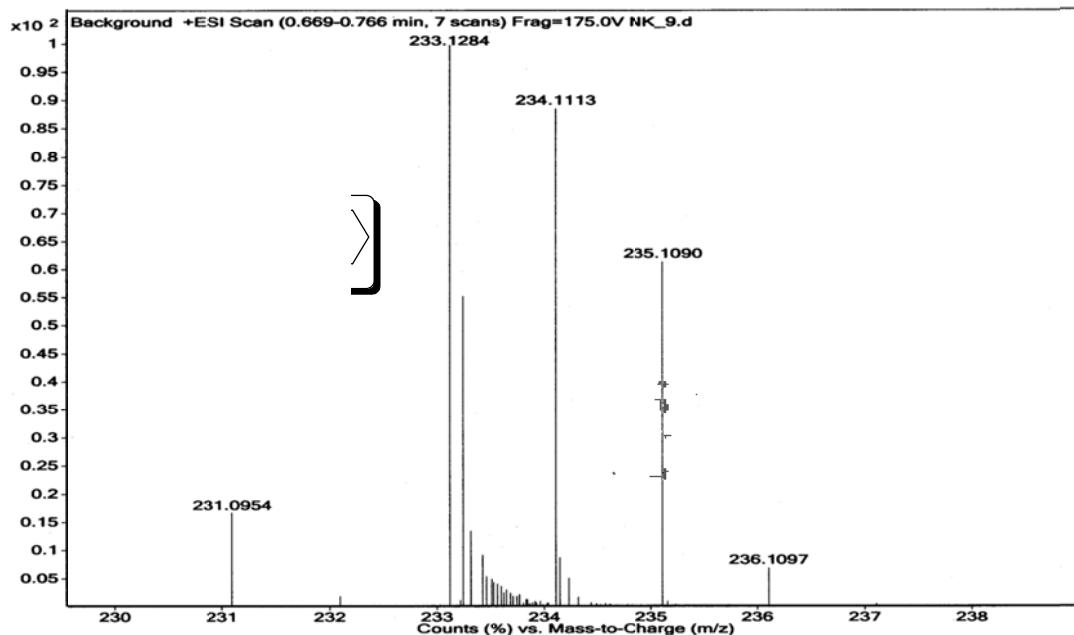
-S76 -

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



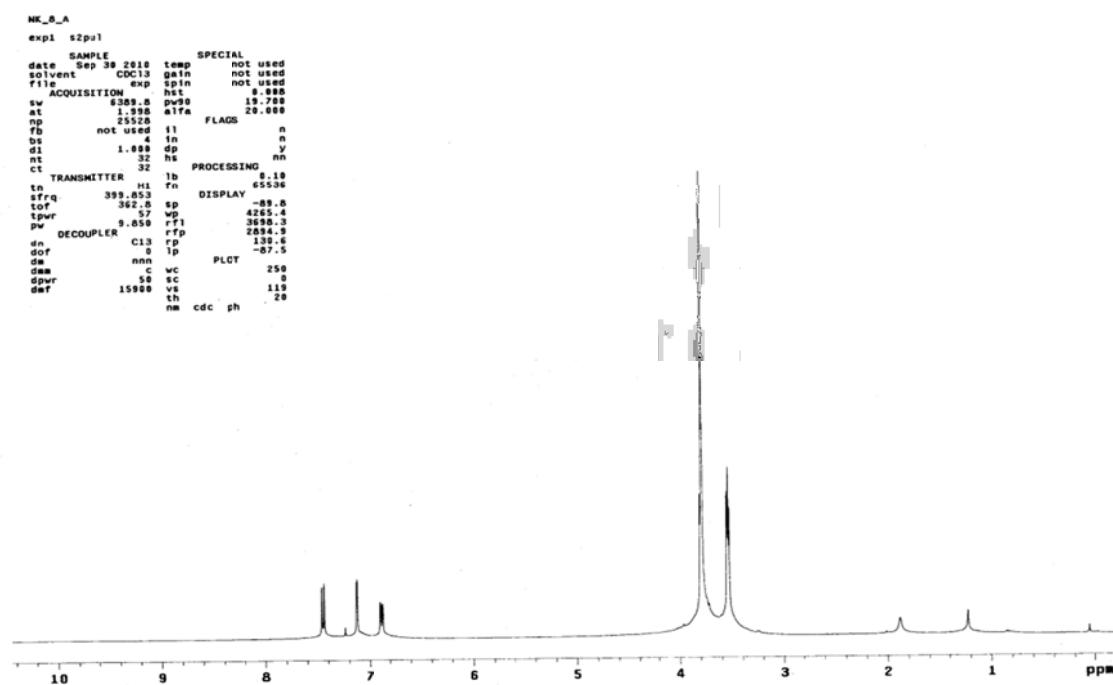
6-methyl-2-(Piperidin-1-yl)benzo[d]thiazole (18'd): MASS SPECTRA:

Sample Name	NK_9	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition		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

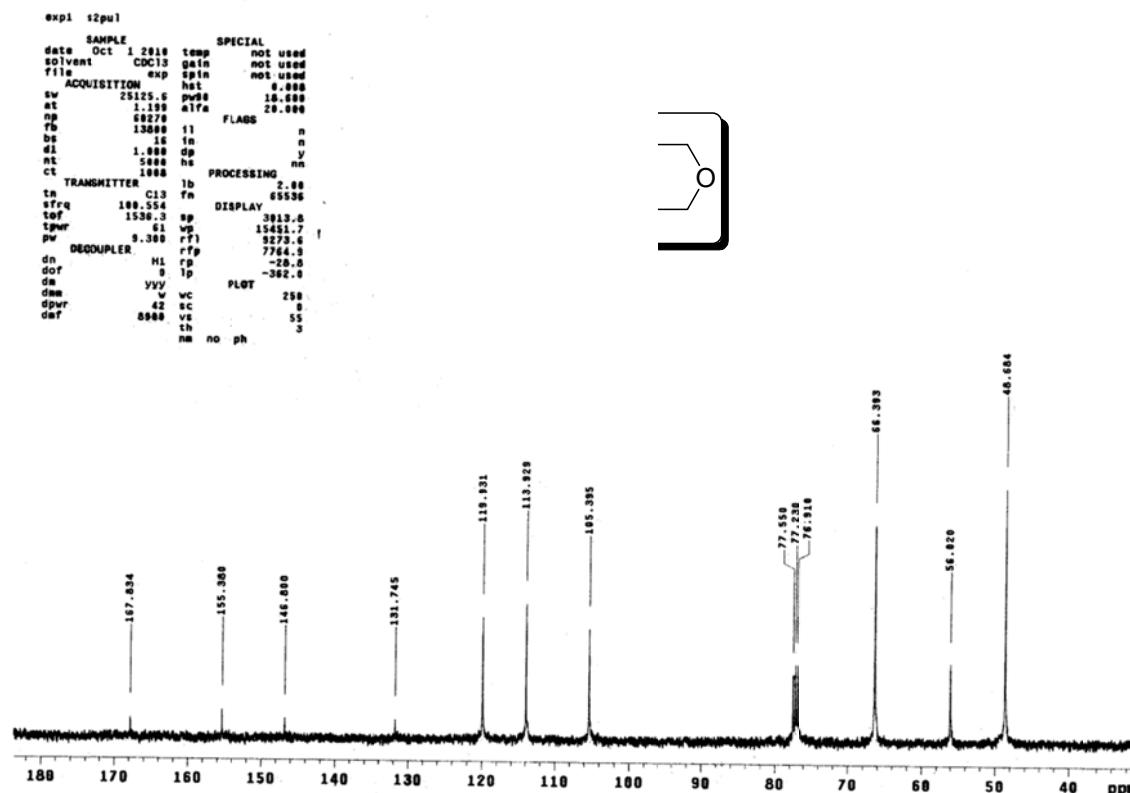


-S77 -

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



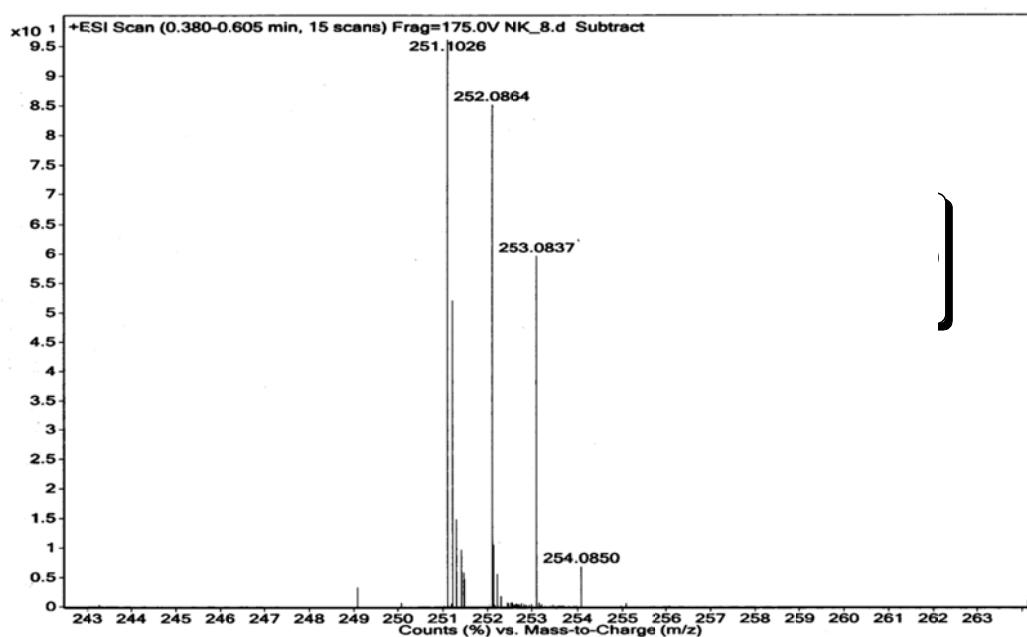
6-methoxy-2-morpholino[*d*]thiazole (19'a): ^{13}C NMR (100 MHz, CDCl_3):



-S78 -

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

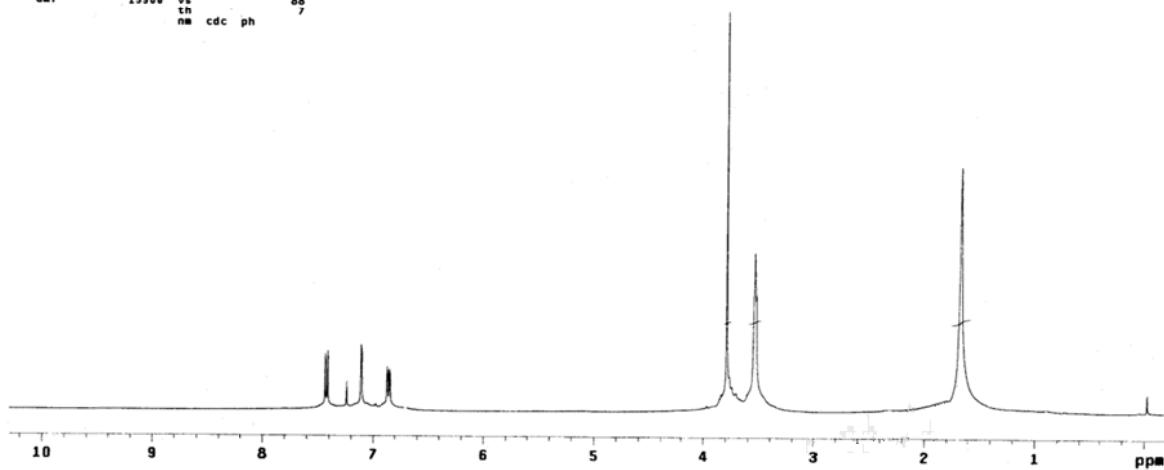
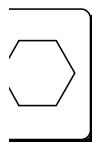
Sample Name	NK_8	Position	Vial 1	Instrument Name	Instrument 1	User Name	IRM Calibration Status	Acquired Time
Inj Vol	.1	InjPosition		SampleType	Sample			
Data Filename	NK_8.d	ACQ Method		Comment			All Ions Missed	9/28/2011 2:21:12 PM



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

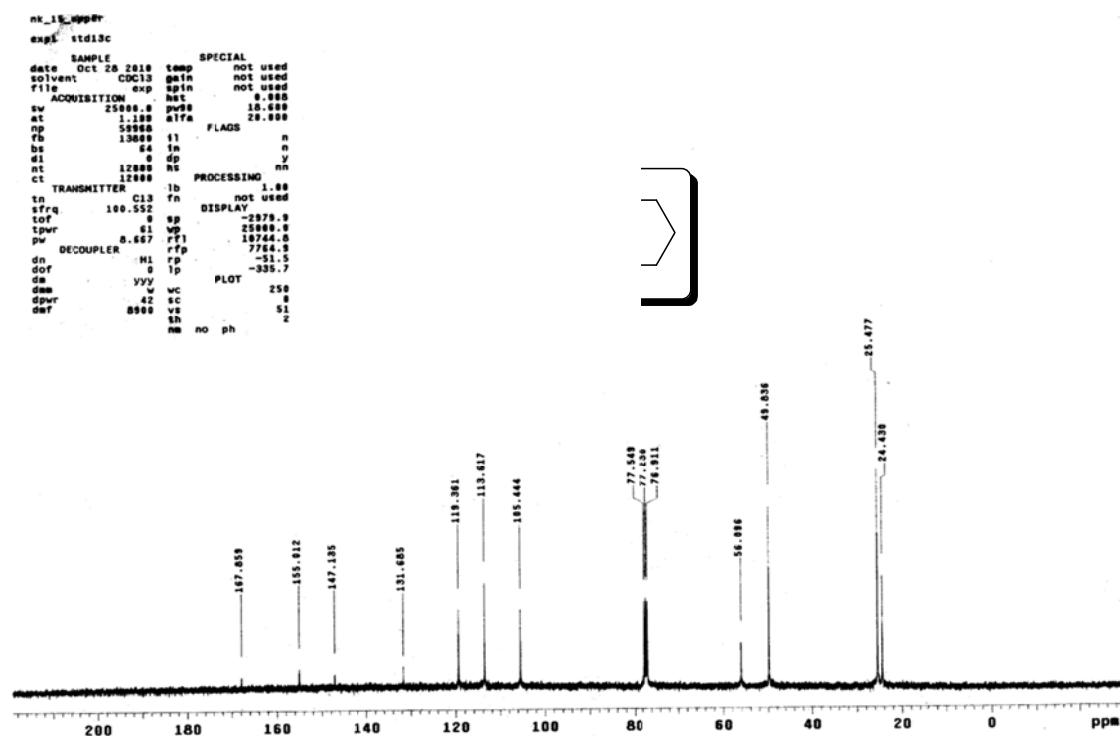
```
exp1 s2pul
SAMPLE          SPECIAL
date  Oct 25 2010 temp    not used
solvent   CDCl3 gain    not used
file      exp      fin    not used
ACQUISITION hst      0.005
sw       6389.8 pw90   19.700
at        1.990 a1fa   20.000
np       256      16
dpb     255      16
rb       not used  il      n
bs        4      in      n
d1      1.000 dp      y
nt       32      hs      nn
ct       32      PROCESSING
tn      TRANSMITTER 1b      0.10
th      H1      fm      65536
trig     399.853  DISPLAY
t0f      362.8 sp      -90.2
tpw     1.57      wp      4288.5
pw      9.850 rfp     3688.7
DECOUPLER C13      rfp     2684.9
dn      C13      rp      123.6
dof      8      lp      -76.3
dm      nnn      PLOT
dme      c      wc      250
dprw    58      sc      0
dav     15900   vt      88
nm      cdc      ph

```



-S79 -

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:

Sample Name	NK_15	Position	Vial 1	Instrument Name	Instrument 1	User Name
Inj Vol	-1	Inj/Position		SampleType	Sample	IRN Calibration Status
Data Filename	NK_15.d	ACQ Method		Comment		Acquired Time

All Ions Missed
9/28/2011 12:24:31 PM

