



SUPPLEMENTARY MATERIAL TO
**Synthesis of novel *N*-substituted benzyl *N*-(1,3-benzothiazol-2-yl)
acetamides and their *in vitro* antibacterial activities**

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N-[2-Methylphenyl)methylidene]-6-methyl-1,3-benzothiazol-2-amine (**3a**). Yield: 70%. M.p. 132-133°. FT-IR: 3042, 1610, 1597, 1530, 1505 (Fig.S1). ¹H NMR(500 MHz, DMSO-*d*₆, δ): 2.45 (s, 3H, CH₃-Benzothiazole), 2.65 (s, 3H, Ar-CH₃), 7.34 (dd, 1H, ⁴*J*_{12,14}=1.28 Hz, *J*_{11,13}=8.23 Hz, H12), 7.38 (d, 1H, *J*_{14,15}=7.81 Hz, H15), 7.39 (t, 1H, *J*_{12,14}=8.93 Hz, H13), 7.53 (dt, 1H, ⁴*J*_{H14-H12}=1.31 Hz, *J*_{13,15}=7.42 Hz, H14), 7.83 (s, 1H, H7), 7.84 (d, 1H, *J*_{5,4}=8.44 Hz, H5), 8.12 (d, 1H, *J*_{4,5}=7.81 Hz, H4), 9.34 (s, 1H, -CH=N-) (Fig.S2) (The numbering of protons of the compound is given in Scheme 1). ¹³C NMR(125 MHz, DMSO-*d*₆, δ): 19.07, 21.24, 117.88, 118.67, 121.28, 125.83, 126.45, 126.88, 127.04, 128.68, 130.90, 131.15, 136.48, 138.58, 150.54, 164.16. Anal. Calcd for C₁₆H₁₄N₂S: C 72.15, H 5.30, N 10.52, S 12.04 %; found: C 72.00, H 5.35, N 10.54, S 11.96 %.

N-[2-Methoxyphenyl)methylidene]-6-methyl-1,3-benzothiazol-2-amine (**3b**). Yield: 76%. M.p. 134-136°. FT-IR: 3045, 1615, 1595, 1551 (Fig.S3). ¹H NMR(500 MHz, DMSO-*d*₆, δ): 2.46 (s, 3H, CH₃-Benzothiazole), 3.96(s, 3H, Ar-OCH₃), 7.14 (t, 1H, *J*_{15,14}=7.51 Hz, H14), 7.24 (d, 1H, *J*_{13,12}=8.41 Hz, H12), 7.35 (dd, 1H, ⁴*J*_{5,7}=1.34 Hz, *J*_{4,5}=8.31 Hz, H5), 7.66 (dt, 1H, ⁴*J*_{13,15}=1.75 Hz, *J*_{12,14}=7.24 Hz, H13), 7.83 (d, 1H, *J*_{4,5}=8.30 Hz, H4), 7.85 (s, 1H, H7), 8.11 (dd, 1H, ⁴*J*_{15,13}=1.65 Hz, *J*_{15,14}=7.76 Hz, H15), 9.30 (s, 1H, -CH=N-)(Fig.S4 and fig. S5). ¹³C NMR (125 MHz, DMSO-*d*₆, δ): 21.21, 56.53, 112.93, 121.50, 122.35, 122.71, 122.77, 128.03, 128.56, 134.62, 135.43, 136.11, 149.86, 161.08, 161.73, 171.33. ESI-MS *m/z*= Calculated for (C₁₆H₁₄N₂SO + H⁺) 283.1, observed 283.18 (Fig.S8). Anal. Calcd for C₁₆H₁₄N₂SO: C 68.06, H 5.00, N 9.92, S 11.36 %. Found: C 68.20, H 5.20, N 9.98, S 11.35 %.

N-[2-hydroxyphenyl)methylidene]-6-methyl-1,3-benzothiazol-2-amine (**3c**). Yield: 90%. M.p. 137-138°. FT-IR: 3360, 3040, 1620, 1583, 1570, 1545 (Fig.S9).

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¹H NMR(500 MHz, DMSO-d₆, δ): 2.44 (s, 3H, CH₃-Benzothiazole); 7.01(d, 1H, $J_{15,13}$ =7.48 Hz H14), 7.04 (d, 1H, $J_{13,12}$ =8.14 Hz, H12), 7.34 (d, 1H, $J_{5,4}$ =8.43 Hz, H4), 7.52 (dt, 1H, $^4J_{13,15}$ =1.27 Hz, $J_{12,14}$ =8.40 Hz, H13), 7.83 (d, 1H, $J_{4,5}$ =8.20 Hz, H5), 7.86 (s, 1H, H7), 7.93 (dd, 1H, $^4J_{15,13}$ =1.21 Hz, $J_{15,14}$ =7.80 Hz, H15), 9.45 (s, 1H, -CH=N-), 11.5 (s, 1H, PhOH)(Fig.S10 and S11). ¹³C NMR(125 MHz, DMSO-d₆, δ): 21.58, 117.41, 120.06, 120.31, 122.40, 122.70, 128.61, 131.66, 134.47, 135.62, 135.98, 149.73, 160.98, 166.04, 169.73 (Fig.S12). Anal. Calcd. for C₁₅H₁₂N₂OS: C 67.14, H 4.51, N 10.44, S 11.95 %. Found: C 67.10, H 4.56, N 10.49, S 11.40 %.

N-[4-hydroxyphenyl)methylidene]-6-methyl-1,3-benzothiazol-2-amine (**3d**). Yield: 72%. M.p. 136-138°. FT-IR: 3350, 3044, 1618, 1585, 1572, 1543. ¹H NMR(500 MHz, DMSO-d₆, δ): 2.40 (s, 3H, CH₃-Benzothiazole), 6.96 (d, 2H, $J_{11,13}$ =8.55 Hz, H12 and H14), 7.30 (d, 1H, $J_{5,4}$ =8.11 Hz, H4), 7.77 (d, 1H, $J_{4,5}$ =8.45 Hz, H5), 7.79 (s, 1H, H7), 7.94 (d, 2H, $J_{12,14}$ =8.56 Hz, H11 and H15), 9.02 (s, 1H, -CH=N-), 10.5 (s, 1H, Ar-OH)(Fig.S13). ¹³C NMR(125 MHz, DMSO-d₆, δ): 21.54, 116.63, 122.27, 122.36, 126.37, 128.34, 133.08, 134.36, 135.07, 149.92, 163.24, 166.49, 171.41(Fig.S14). Anal. Calcd. for C₁₅H₁₂N₂OS: C 67.14, H 4.51, N 10.44, S 11.95 %. Found: C 67.02, H 4.54, N 10.40, S 11.45 %.

N-(2-methylbenzyl)-6-Methyl-1,3-benzothiazol-2-amine (**4a**). Yield: 87%. M.p. 102-103°. FT-IR: 3412, 1605, 1594, 1571. ¹H NMR(500 MHz, DMSO-d₆, δ): 2.32 (s, 3H, CH₃-Benzothiazole), 2.34 (s, 3H, Ar-CH₃), 4.55 (d, 2H, J_{CH_2-NH} =5.44 Hz, Ar-CH₂NH-), 7.03 (dd, 1H, $^4J_{5,7}$ =1.31 Hz, $J_{4,5}$ =8.15 Hz, H5), 7.18 (m, 3H, H12, H-14 and H15), 7.27 (d, 1H, $J_{5,4}$ =8.11 Hz, H4), 7.32 (d, 1H, $J_{12,14}$ =7.29 Hz, H13), 7.47 (s, 1H, H7), 8.25 (t, 1H, J_{NH-CH_2} =5.43 Hz, $NHCH_2$ -Ar)(Fig.S15). ¹³C NMR(125 MHz, DMSO-d₆, δ): 19.12, 21.22, 45.92, 118.20, 121.35, 126.27, 126.99, 127.61, 128.28, 130.51, 130.98, 136.43, 137.05, 150.81, 165.78 (Fig.S16). ESI-MS m/z = Calculated for (C₁₆H₁₆N₂S + H⁺) 269.1, observed 269.1 (Fig.S19). Anal. Calcd for C₁₆H₁₆N₂S: C 71.60, H 6.01, N 10.44, S 11.95 %. Found: C 71.52, H 6.03, N 10.50, S 11.90 %.

N-(2-methoxybenzyl)-6-Methyl-1,3-benzothiazol-2-amine (**4b**). Yield: 90%. M.p. 125-127°. FT-IR: 3430, 1608, 1567(Fig.S20). ¹H NMR(500 MHz, DMSO-d₆, δ): 2.31 (s, 3H, CH₃-Benzothiazole), 3.83 (s, 3H, Ar-OCH₃), 4.53 (d, 2H, J_{CH_2-NH} =5.67 Hz, Ar-CH₂NH-), 6.92 (t, 1H, $J_{15,13}$ =7.28 Hz, H14), 7.02 (d, 2H, $J_{12,13}$ = $J_{4,5}$ =8.09 Hz, H12 and H4), 7.25 (d, 2H, $J_{4,5}$ $J_{12,14}$ =7.03 Hz, H5 and H15), 7.29 (t, 1H, $J_{12,14}$ =7.13 Hz H13), 7.46 (s, 1H, H7); 8.22 (t, 1H, J_{NH-CH_2} =5.67 Hz, $NHCH_2$ -Ar) (Fig.S21 and S22). ¹³C NMR(125 MHz, DMSO-d₆, δ): 21.22, 42.89, 55.82, 111.06, 118.18, 120.62, 121.32, 126.79, 126.96, 128.46, 128.81, 130.44, 130.97, 150.83, 157.32, 166.00 (Fig.S23). ESI-MS m/z = Calculated for (C₁₆H₁₆N₂SO + H⁺) 285.1, observed 285.1. Anal. Calcd for C₁₆H₁₆N₂SO: C 67.58, H 5.67, N 9.85, S 11.28 %. Found: C 67.28, H 4.58, N 9.86, S 10.40 %.

N-(2-hydroxybenzyl)-6-Methyl-1,3-benzothiazol-2-amine (**4c**). Yield: 90%. M.p. 170-172°. FT-IR: 3525, 3409, 1595, 1570(Fig.S28). ¹H NMR(500 MHz, DMSO-d₆, δ): 2.32 (s, 3H, CH₃-Benzothiazole), 4.47 (d, 2H, *J*_{CH₂-NH=5.796 Hz, Ar-CH₂NH-), 6.74 (dt, 1H, ⁴*J*_{14,12}=0.79 Hz *J*_{15,13}=7.41 Hz, H14), 6.86 (dd, 1H, ⁴*J*_{12,14}=0.65 Hz, *J*_{13,12}=7.64 Hz, H12), 7.06 (dd, 1H, ⁴*J*_{15,13}=1.36 Hz, *J*_{14,15}=8.24 Hz, H15), 7.10 (dt, 1H, ⁴*J*_{13,15}=1.61 Hz, *J*_{12,14}=7.69 Hz, H13), 7.24 (dd, 1H, ⁴*J*_{5,7}=1.16 Hz, *J*_{4,5}=7.53 Hz, H5), 7.26 (d, 1H, *J*_{5,4}=8.11 Hz, H4), 7.47 (s, 1H, ⁴*J*_{7,5}=0.97 Hz, H7), 8.30 (t, 1H, *J*=5.70 Hz, NHCH₂-Ar), 9.75 (br. s, 1H, Ar-OH) (Fig.S29). ¹³C NMR(125 MHz, DMSO-d₆, δ): 21.22, 43.14, 115.85, 118.00, 119.37, 121.41, 125.34, 127.04, 128.69, 129.36, 130.55, 130.81, 150.45, 155.61, 166.29. Anal. Calcd. for C₁₅H₁₄N₂OS: C 66.64, H 5.22, N 10.36, S 11.86 %. Found: C 66.60, H 5.21, N 10.33, S 11.84 %.}

N-(4-hydroxybenzyl)-6-Methyl-1,3-benzothiazol-2-amine (**4d**). Yield: 93%. M.p. 168-170°. FT-IR: 3542, 3430, 1591, 1556. ¹H NMR(500 MHz, DMSO-d₆, δ): 2.46 (s, 3H CH₃-Benzothiazole), 4.49 (d, 2H, *J*_{CH₂-NH=5.20 Hz, Ar-CH₂NH-), 6.74 (d, 2H, *J*_{11,13}=8.43 Hz, H12 and H14), 7.02 (d, 1H, *J*_{4,5}=7.16 Hz, H5), 7.2 (d, 2H, *J*_{12,14}=8.41 Hz, H11 and H15), 7.24 (d, 1H, *J*_{5,4}=6.84 Hz, H4), 8.28 (t, 1H, *J*_{NH-CH₂}=5.44 Hz, NHCH₂-Ar), 9.30 (br. s, 1H, Ar-OH) (Fig.S30 and S31). ¹³C NMR(125 MHz, DMSO-d₆, δ): 21.22, 47.39, 115.54, 118.15, 121.32, 16.98, 129.34, 129.49, 130.42, 130.92, 150.86, 156.95, 165.91 (Fig.S32). Anal. Calcd. for C₁₅H₁₄N₂OS: C 66.64, H 5.22, N 10.36, S 11.86 %. Found: C 66.61, H 5.18, N 10.31, S 11.82 %.}

2-Chloro-*N*-[6-methyl-1,3-benzothiazol-2-yl]-*N*-[2-methylbenzyl] acetamide (**5a**). Yield: 76%. M.p. 188-190°. FT-IR: 1698, 1600, 1509(Fig.S36). ¹H NMR(500 MHz, DMSO-d₆, δ): 2.49 (s, 6H, CH₃-Benzothiazole and Ar-CH₃), 4.55 (s, 2H, Ar-CH₂N-), 5.50 (s, 2H, N(CO)CH₂Cl), 6.76 (d, 1H, *J*_{14,15}=7.59 Hz, H15), 7.11 (t, 1H, *J*_{12,14}=7.54 Hz, H13), 7.18 (t, 1H, *J*_{15,13}=7.36 Hz, H14), 7.24 (d, 1H, *J*_{13,12}=8.20 Hz, H12), 7.28 (d, 1H, *J*_{4,5}=8.63 Hz, H5), 7.62 (d, 1H, *J*_{5,4}=8.27 Hz, H4), 7.84(s, 1H, H7) (Fig.S37). ¹³C NMR(125 MHz, DMSO-d₆, δ): 19.99, 22.30, 44.62, 49.49, 122.16, 122.9, 124.72, 127.64, 128.37, 128.95, 131.69, 133.31, 134.12, 135.15, 135.54, 136.40, 152.03, 168.63 (Fig.S38). ESI-MS *m/z*= Calculated for (C₁₈H₁₇ClN₂SO + H⁺) 345.1, observed 345.1(Fig.S40). Anal. Calcd for C₁₈H₁₇ClN₂SO: C 62.69, H 4.97, N 8.12, S 9.30 %. Found: C 62.48, H 5.006, N 8.339, S 9.265 %.

2-Chloro-*N*-[6-methyl-1,3-benzothiazol-2-yl]-*N*-[2-methoxybenzyl]acetamide (**5b**). Yield: 82%. M.p. 146-149°. FT-IR: 1683, 1605, 1520 (Fig.S41). ¹H NMR(500 MHz, DMSO-d₆, δ): 2.40 (s, 3H, CH₃-Benzothiazole), 3.53 (s, 3H, Ar-OCH₃), 4.75 (s, 2H, CH₂N), 5.43 (s, 2H, N(CO)CH₂Cl), 6.87 (t, 1H, *J*_{12,14}=7.35 Hz, H13), 6.92 (d, 1H, *J*_{13,12}=6.80 Hz, H12), 7.08 (d, 1H, *J*_{14,15}=8.21 Hz, H15), 7.25 (d, 1H, *J*_{4,5}=8.94 Hz, H5); 7.29 (t, 1H, *J*_{15,13}=7.30, H14), 7.63 (d, 1H, *J*_{5,4}=8.26 Hz, H4), 7.81 (s, 1H, H7) (Fig.S42, fig.S43

and S44). ^{13}C NMR(125 MHz, DMSO- d_6 , δ): 21.48, 43.77, 46.79, 55.98, 61.29, 111.43, 121.02, 121.34, 121.61, 123.94, 126.50, 128.09, 129.16, 133.22, 134.24, 145.99, 157.00, 167.86 (Fig.S45). ESI-MS m/z = Calculated for ($\text{C}_{18}\text{H}_{17}\text{ClN}_2\text{SO}_2 + \text{H}^+$) 361.1, observed 361.1(Fig.S48). Anal. Calcd for $\text{C}_{18}\text{H}_{17}\text{ClN}_2\text{SO}_2$: C 59.91, H 4.75, N 7.76, S 8.89 %. Found: C 59.72, H 4.64, N 7.63, S 8.99 %.

2-[(Chloroacetyl)(6-methyl-1,3-benzothiazol-2-yl)aminomethyl]phenyl chloroacetate (**5c**). Yield: 78%. M.p. 159-161°. FT-IR: 1775, 1668, 1600, 1505. ^1H NMR(500 MHz, DMSO- d_6 , δ): 2.40 (s, 3H, CH_3 -Benzothiazole), 4.70 (s, 2H, Ar- CH_2N -), 4.80 (s, 2H, $\text{O}(\text{CO})\text{CH}_2\text{Cl}$), 5.50 (s, 2H, $\text{N}(\text{CO})\text{CH}_2\text{Cl}$), 7.07 (d, 1H, $J_{14,15}=7.69$ Hz, H15), 7.10 (d, 1H, $J_{4,5}=7.49$ Hz, H5), 7.20 (t, 1H, $J_{15,13}=7.49$ Hz, H14), 7.30 (d, 1H, $J_{13,12}=8.03$ Hz, H12), 7.40 (t, 1H $J_{12,14}=7.89$ Hz, H13), 7.65 (d, 1H, $J_{5,4}=8.28$ Hz, H4), 7.85 (s, 1H, H7). Anal. Calcd. for $\text{C}_{19}\text{H}_{16}\text{Cl}_2\text{N}_2\text{O}_3\text{S}$: C 53.90, H 3.81, N 6.62, S 7.58 %. Found: C 53.92, H 3.84, N 6.59, S 7.55 %.

4-[(Chloroacetyl)(6-methyl-1,3-benzothiazol-2-yl)aminomethyl]phenyl chloroacetate (**5d**). Yield: 82%. M.p. 156-158°. FT-IR: 1762, 1663, 1593, 1520. ^1H NMR(500 MHz, DMSO- d_6 , δ): 2.43 (s, 3H, CH_3 -Benzothiazole), 4.69 (s, 2H, Ar- CH_2N), 4.76 (s, 2H, $\text{O}(\text{CO})\text{CH}_2\text{Cl}$), 5.57 (s, 2H, $\text{N}(\text{CO})\text{CH}_2\text{Cl}$), 6.74 (d, 2H, $J_{11,15}=7.69$ Hz, H12 and H14), 7.10 (d, 2H, $J_{12,14}=8.5$ Hz, H11 and H15), 7.28 (d, 1H, $J_{4,5}=7.35$ Hz, H5), 7.69 (d, 1H, $J_{5,4}=8.24$ Hz, H4), 7.83 (s, 1H, H7), 8.59 (s, 1H, Ar-OH). Anal. Calcd. for $\text{C}_{19}\text{H}_{16}\text{Cl}_2\text{N}_2\text{O}_3\text{S}$: C 53.90, H 3.81, N 6.62, S 7.58 %. Found: C 53.88, H 3.83, N 6.61, S 7.55 %.

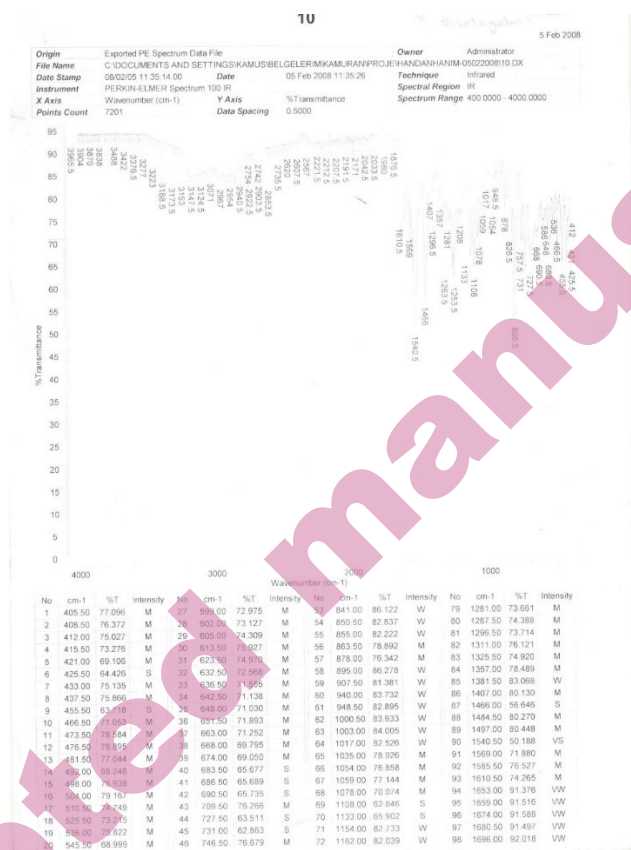
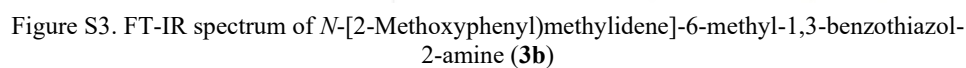
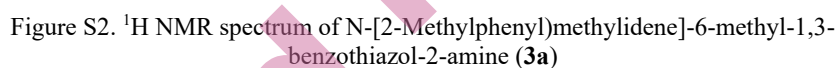


Figure S1. FT-IR spectrum of N-[2-Methylphenyl]methylidene]-6-methyl-1,3-benzothiazol-2-amine (**3a**).



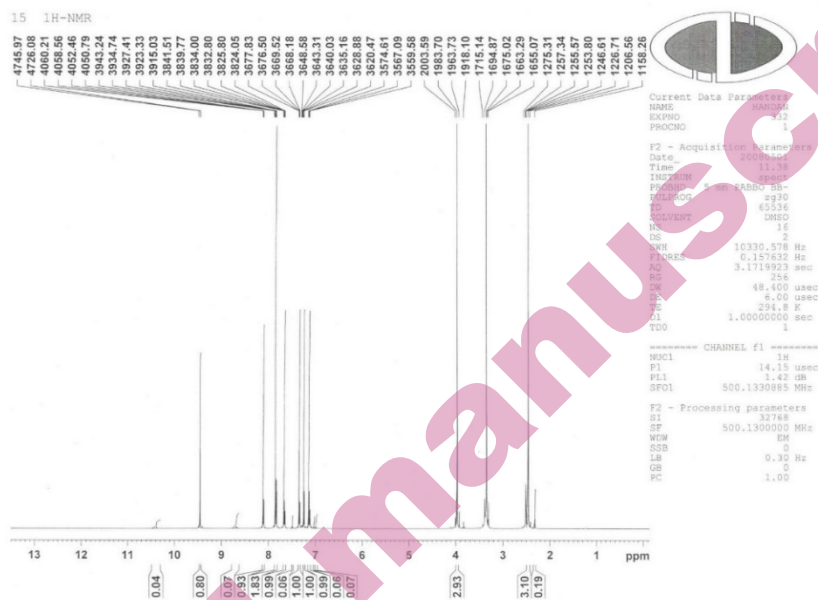


Figure S4. ¹H NMR spectrum of *N*-[2-Methoxyphenyl)methylidene]-6-methyl-1,3-benzothiazol-2-amine (**3b**)

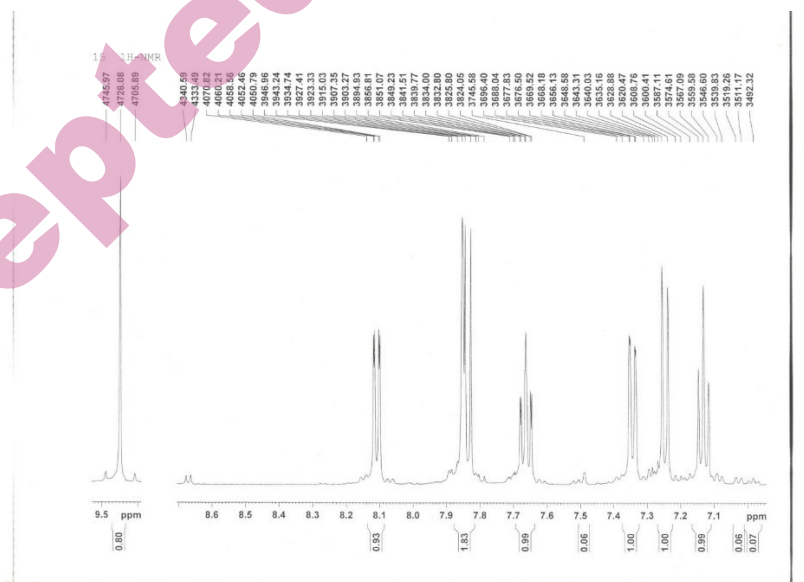


Figure S5. ¹H NMR spectrum of *N*-[2-Methoxyphenyl)methylidene]-6-methyl-1,3-benzothiazol-2-amine (**3b**)

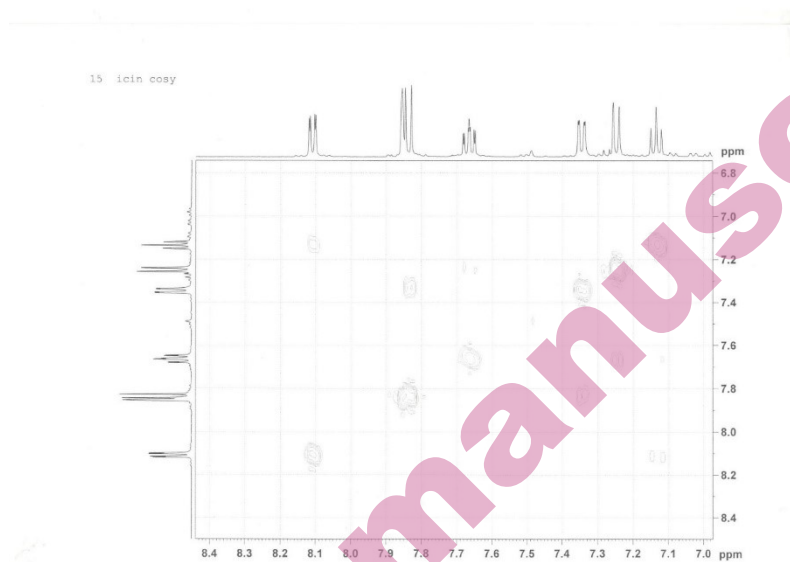


Figure S6. ¹H-¹H COSY spectrum of *N*-[2-Methoxyphenyl)methylidene]-6-methyl-1,3-benzothiazol-2-amine (**3b**).

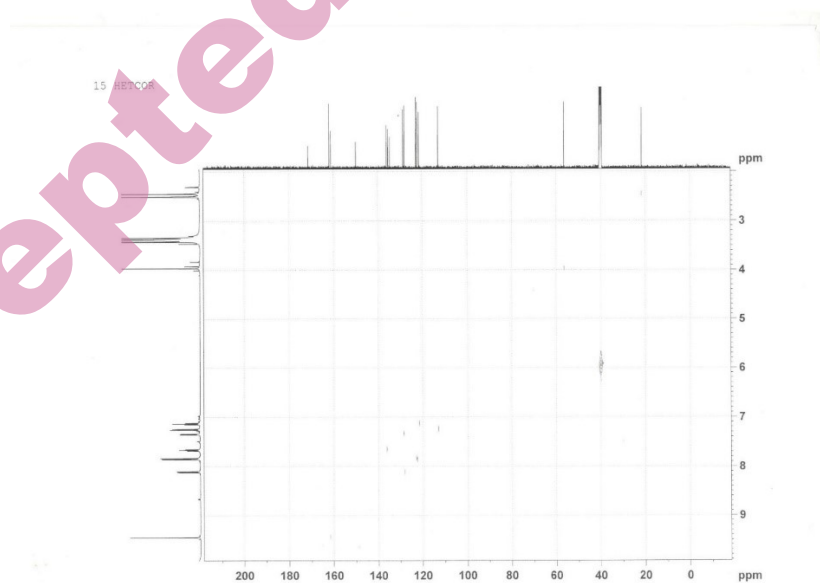
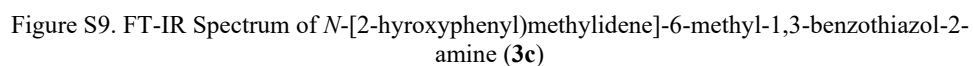
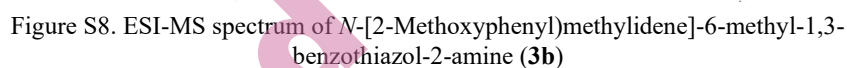


Figure S7. HETCOR spectrum of *N*-[2-Methoxyphenyl)methylidene]-6-methyl-1,3-benzothiazol-2-amine (**3b**).





27-28 ¹H-NMR

Chemical shifts (ppm): 7.82, 7.81, 7.80, 7.79, 7.78, 7.77, 7.76, 7.75, 7.74, 7.73, 7.72, 7.71, 7.70, 7.69, 7.68, 7.67, 7.66, 7.65, 7.64, 7.63, 7.62, 7.61, 7.60, 7.59, 7.58, 7.57, 7.56, 7.55, 7.54, 7.53, 7.52, 7.51, 7.50, 7.49, 7.48, 7.47, 7.46, 7.45, 7.44, 7.43, 7.42, 7.41, 7.40, 7.39, 7.38, 7.37, 7.36, 7.35, 7.34, 7.33, 7.32, 7.31, 7.30, 7.29, 7.28, 7.27, 7.26, 7.25, 7.24, 7.23, 7.22, 7.21, 7.20, 7.19, 7.18, 7.17, 7.16, 7.15, 7.14, 7.13, 7.12, 7.11, 7.10, 7.09, 7.08, 7.07, 7.06, 7.05, 7.04, 7.03, 7.02, 7.01, 7.00, 6.99, 6.98, 6.97, 6.96, 6.95, 6.94, 6.93, 6.92, 6.91, 6.90, 6.89, 6.88, 6.87, 6.86, 6.85, 6.84, 6.83, 6.82, 6.81, 6.80, 6.79, 6.78, 6.77, 6.76, 6.75, 6.74, 6.73, 6.72, 6.71, 6.70, 6.69, 6.68, 6.67, 6.66, 6.65, 6.64, 6.63, 6.62, 6.61, 6.60, 6.59, 6.58, 6.57, 6.56, 6.55, 6.54, 6.53, 6.52, 6.51, 6.50, 6.49, 6.48, 6.47, 6.46, 6.45, 6.44, 6.43, 6.42, 6.41, 6.40, 6.39, 6.38, 6.37, 6.36, 6.35, 6.34, 6.33, 6.32, 6.31, 6.30, 6.29, 6.28, 6.27, 6.26, 6.25, 6.24, 6.23, 6.22, 6.21, 6.20, 6.19, 6.18, 6.17, 6.16, 6.15, 6.14, 6.13, 6.12, 6.11, 6.10, 6.09, 6.08, 6.07, 6.06, 6.05, 6.04, 6.03, 6.02, 6.01, 6.00, 5.99, 5.98, 5.97, 5.96, 5.95, 5.94, 5.93, 5.92, 5.91, 5.90, 5.89, 5.88, 5.87, 5.86, 5.85, 5.84, 5.83, 5.82, 5.81, 5.80, 5.79, 5.78, 5.77, 5.76, 5.75, 5.74, 5.73, 5.72, 5.71, 5.70, 5.69, 5.68, 5.67, 5.66, 5.65, 5.64, 5.63, 5.62, 5.61, 5.60, 5.59, 5.58, 5.57, 5.56, 5.55, 5.54, 5.53, 5.52, 5.51, 5.50, 5.49, 5.48, 5.47, 5.46, 5.45, 5.44, 5.43, 5.42, 5.41, 5.40, 5.39, 5.38, 5.37, 5.36, 5.35, 5.34, 5.33, 5.32, 5.31, 5.30, 5.29, 5.28, 5.27, 5.26, 5.25, 5.24, 5.23, 5.22, 5.21, 5.20, 5.19, 5.18, 5.17, 5.16, 5.15, 5.14, 5.13, 5.12, 5.11, 5.10, 5.09, 5.08, 5.07, 5.06, 5.05, 5.04, 5.03, 5.02, 5.01, 5.00, 4.99, 4.98, 4.97, 4.96, 4.95, 4.94, 4.93, 4.92, 4.91, 4.90, 4.89, 4.88, 4.87, 4.86, 4.85, 4.84, 4.83, 4.82, 4.81, 4.80, 4.79, 4.78, 4.77, 4.76, 4.75, 4.74, 4.73, 4.72, 4.71, 4.70, 4.69, 4.68, 4.67, 4.66, 4.65, 4.64, 4.63, 4.62, 4.61, 4.60, 4.59, 4.58, 4.57, 4.56, 4.55, 4.54, 4.53, 4.52, 4.51, 4.50, 4.49, 4.48, 4.47, 4.46, 4.45, 4.44, 4.43, 4.42, 4.41, 4.40, 4.39, 4.38, 4.37, 4.36, 4.35, 4.34, 4.33, 4.32, 4.31, 4.30, 4.29, 4.28, 4.27, 4.26, 4.25, 4.24, 4.23, 4.22, 4.21, 4.20, 4.19, 4.18, 4.17, 4.16, 4.15, 4.14, 4.13, 4.12, 4.11, 4.10, 4.09, 4.08, 4.07, 4.06, 4.05, 4.04, 4.03, 4.02, 4.01, 4.00, 3.99, 3.98, 3.97, 3.96, 3.95, 3.94, 3.93, 3.92, 3.91, 3.90, 3.89, 3.88, 3.87, 3.86, 3.85, 3.84, 3.83, 3.82, 3.81, 3.80, 3.79, 3.78, 3.77, 3.76, 3.75, 3.74, 3.73, 3.72, 3.71, 3.70, 3.69, 3.68, 3.67, 3.66, 3.65, 3.64, 3.63, 3.62, 3.61, 3.60, 3.59, 3.58, 3.57, 3.56, 3.55, 3.54, 3.53, 3.52, 3.51, 3.50, 3.49, 3.48, 3.47, 3.46, 3.45, 3.44, 3.43, 3.42, 3.41, 3.40, 3.39, 3.38, 3.37, 3.36, 3.35, 3.34, 3.33, 3.32, 3.31, 3.30, 3.29, 3.28, 3.27, 3.26, 3.25, 3.24, 3.23, 3.22, 3.21, 3.20, 3.19, 3.18, 3.17, 3.16, 3.15, 3.14, 3.13, 3.12, 3.11, 3.10, 3.09, 3.08, 3.07, 3.06, 3.05, 3.04, 3.03, 3.02, 3.01, 3.00, 2.99, 2.98, 2.97, 2.96, 2.95, 2.94, 2.93, 2.92, 2.91, 2.90, 2.89, 2.88, 2.87, 2.86, 2.85, 2.84, 2.83, 2.82, 2.81, 2.80, 2.79, 2.78, 2.77, 2.76, 2.75, 2.74, 2.73, 2.72, 2.71, 2.70, 2.69, 2.68, 2.67, 2.66, 2.65, 2.64, 2.63, 2.62, 2.61, 2.60, 2.59, 2.58, 2.57, 2.56, 2.55, 2.54, 2.53, 2.52, 2.51, 2.50, 2.49, 2.48, 2.47, 2.46, 2.45, 2.44, 2.43, 2.42, 2.41, 2.40, 2.39, 2.38, 2.37, 2.36, 2.35, 2.34, 2.33, 2.32, 2.31, 2.30, 2.29, 2.28, 2.27, 2.26, 2.25, 2.24, 2.23, 2.22, 2.21, 2.20, 2.19, 2.18, 2.17, 2.16, 2.15, 2.14, 2.13, 2.12, 2.11, 2.10, 2.09, 2.08, 2.07, 2.06, 2.05, 2.04, 2.03, 2.02, 2.01, 2.00, 1.99, 1.98, 1.97, 1.96, 1.95, 1.94, 1.93, 1.92, 1.91, 1.90, 1.89, 1.88, 1.87, 1.86, 1.85, 1.84, 1.83, 1.82, 1.81, 1.80, 1.79, 1.78, 1.77, 1.76, 1.75, 1.74, 1.73, 1.72, 1.71, 1.70, 1.69, 1.68, 1.67, 1.66, 1.65, 1.64, 1.63, 1.62, 1.61, 1.60, 1.59, 1.58, 1.57, 1.56, 1.55, 1.54, 1.53, 1.52, 1.51, 1.50, 1.49, 1.48, 1.47, 1.46, 1.45, 1.44, 1.43, 1.42, 1.41, 1.40, 1.39, 1.38, 1.37, 1.36, 1.35, 1.34, 1.33, 1.32, 1.31, 1.30, 1.29, 1.28, 1.27, 1.26, 1.25, 1.24, 1.23,

Figure S11. ¹H NMR spectrum of *N*-[2-hydroxyphenyl)methylidene]-6-methyl-1,3-benzothiazol-2-amine (**3c**)

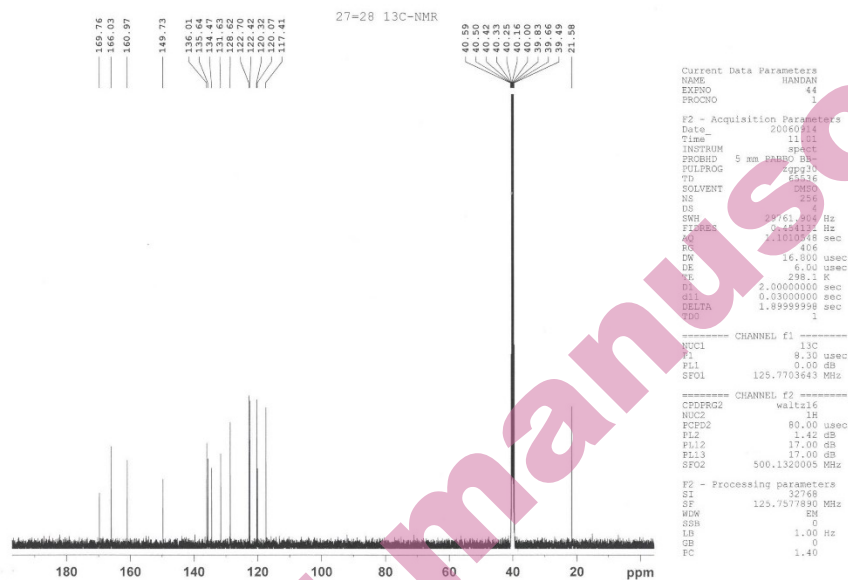


Figure S12. ^{13}C NMR spectrum of *N*-[2-hydroxyphenyl)methylidene]-6-methyl-1,3-benzothiazol-2-amine (3c).

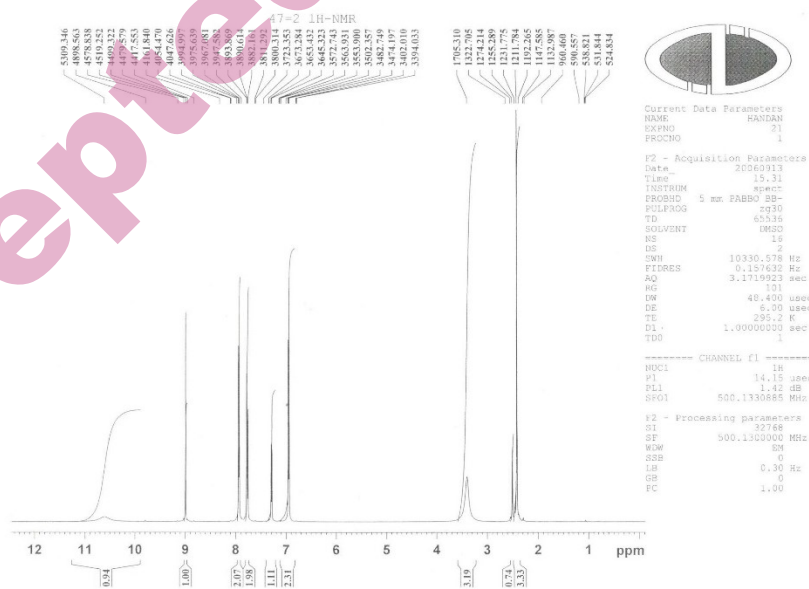


Figure S13. ^1H NMR spectrum of *N*-[4-hydroxyphenyl)methylidene]-6-methyl-1,3-benzothiazol-2-amine (3d)

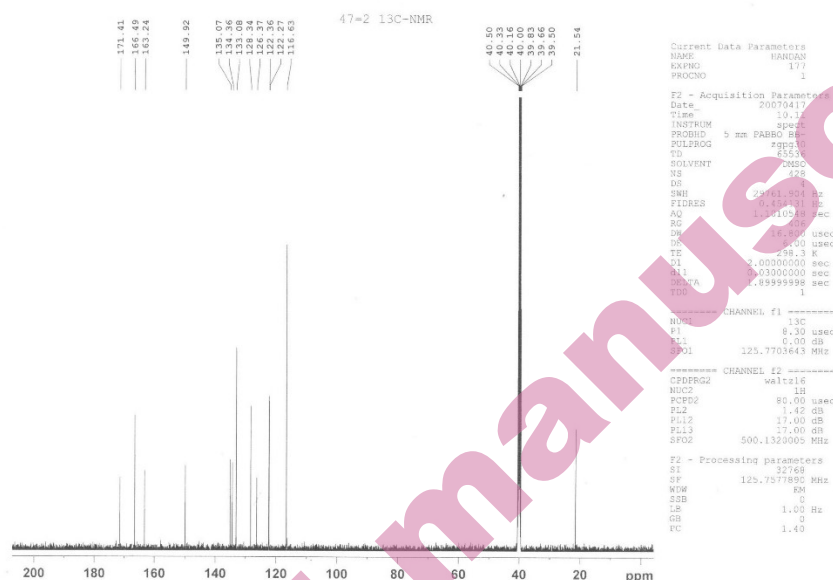


Figure S14. ^{13}C NMR spectrum of *N*-[4-hydroxyphenyl]methylidene]-6-methyl-1,3-benzothiazol-2-amine (**3d**).

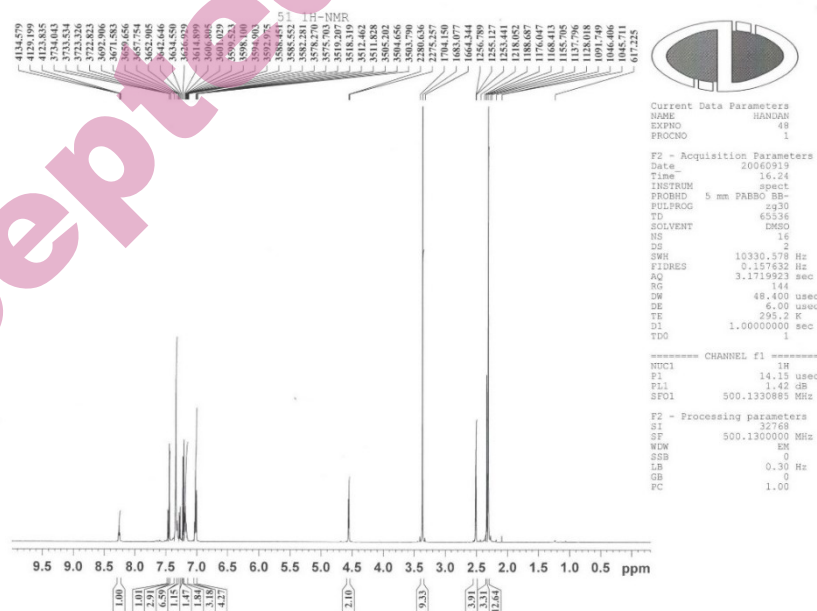


Figure S15. ^1H NMR spectrum of *N*-(2-methylbenzyl)-6-Methyl-1,3-benzothiazol-2-amine (**4a**)

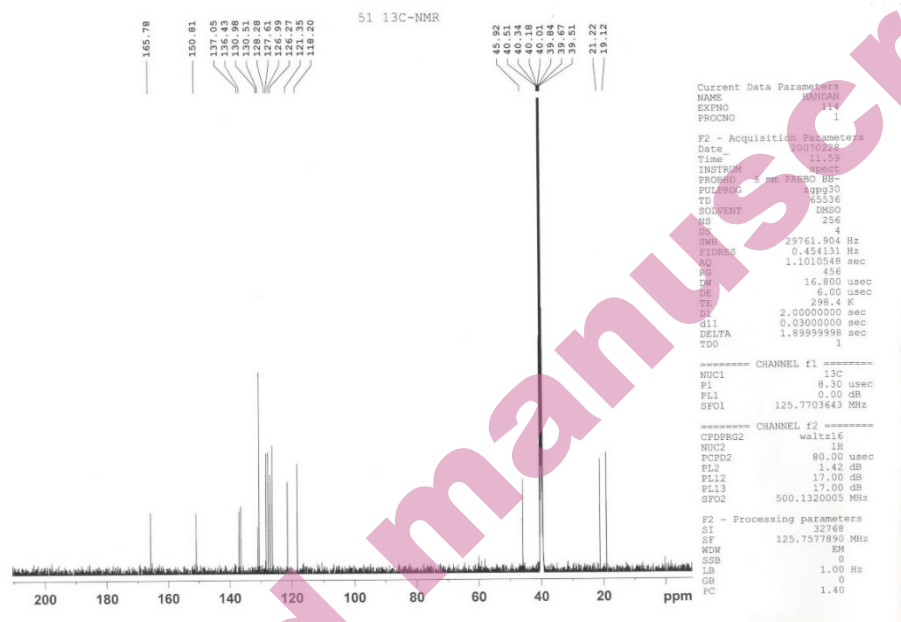


Figure S16. ^{13}C NMR spectrum of *N*-(2-methylbenzyl)-6-Methyl-1,3-benzothiazol-2-amine (**4a**)

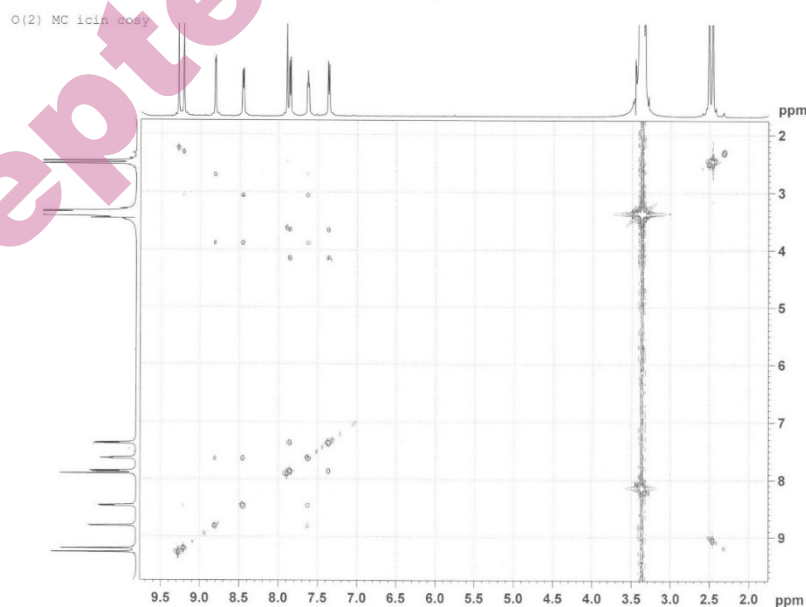


Figure S17. COSY spectrum of *N*-(2-methylbenzyl)-6-Methyl-1,3-benzothiazol-2-amine (**4a**)

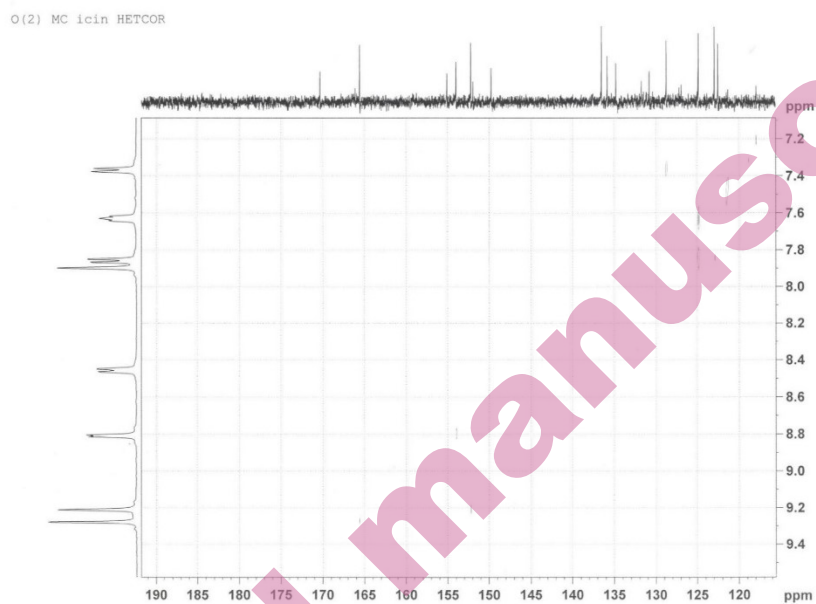


Figure S18. HETCOR spectrum of *N*-(2-methylbenzyl)-6-Methyl-1,3-benzothiazol-2-amine (4a)

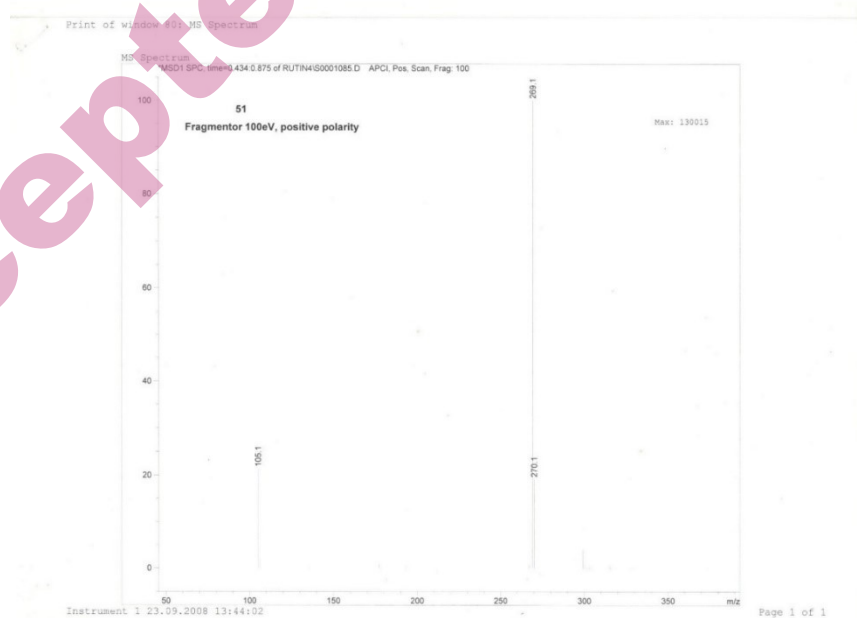


Figure S19. ESI-MS spectrum of *N*-(2-methylbenzyl)-6-Methyl-1,3-benzothiazol-2-amine (4a)

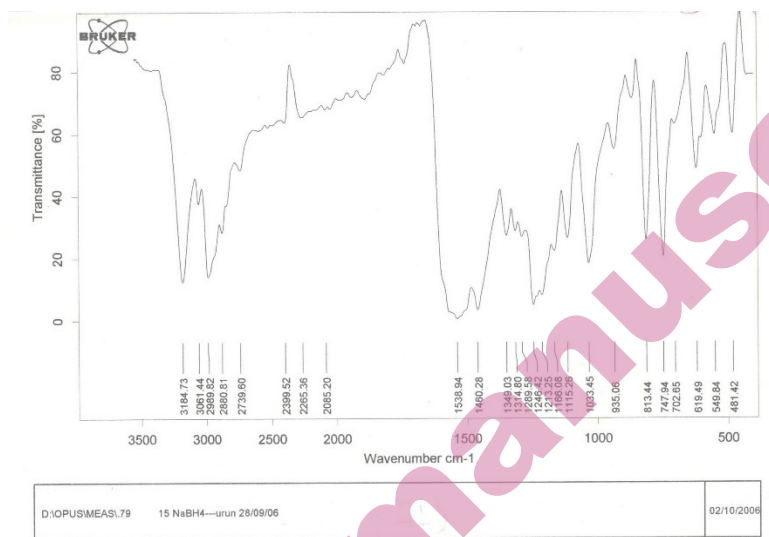


Figure S20. FT-IR spectrum of *N*-(2-methoxybenzyl)-6-Methyl-1,3-benzothiazol-2-amine (**4b**).

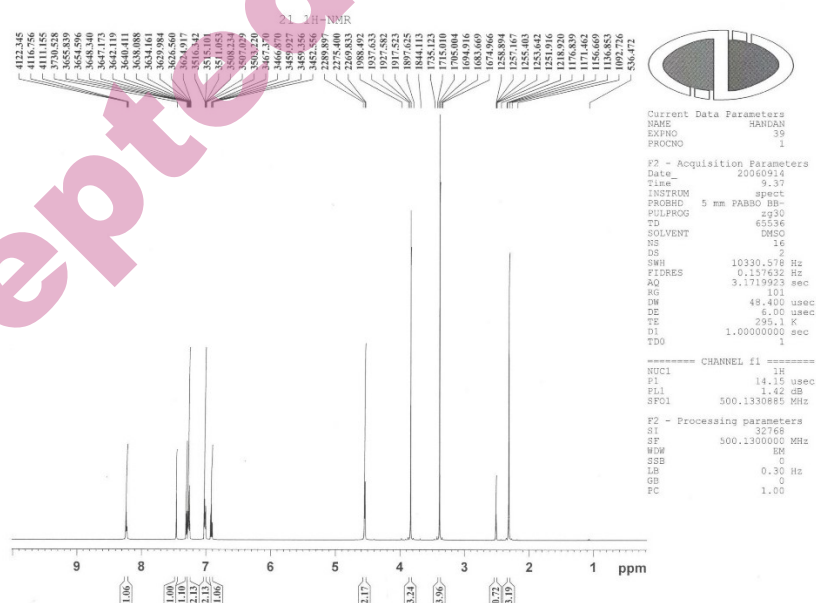


Figure S21. ^1H NMR spectrum of *N*-(2-methoxybenzyl)-6-Methyl-1,3-benzothiazol-2-amine (**4b**).

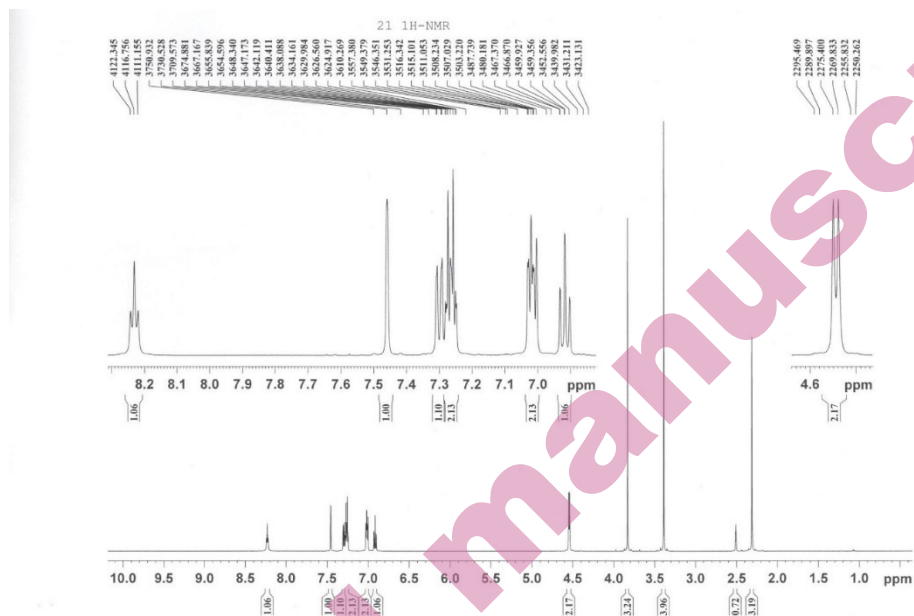


Figure S22. ¹H NMR spectrum of *N*-(2-methoxybenzyl)-6-Methyl-1,3-benzothiazol-2-amine (4b).

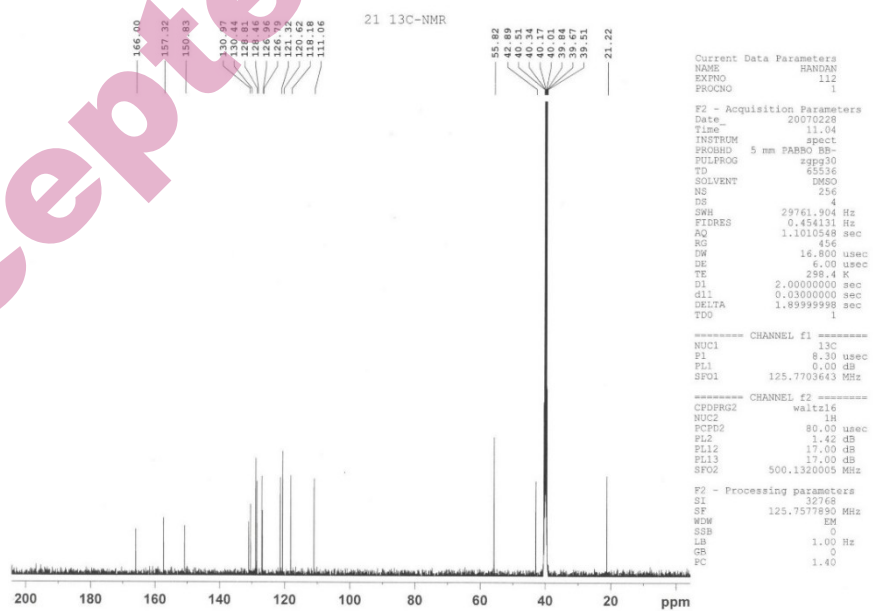


Figure S23. ¹³C NMR spectrum of *N*-(2-methoxybenzyl)-6-Methyl-1,3-benzothiazol-2-amine (4b).

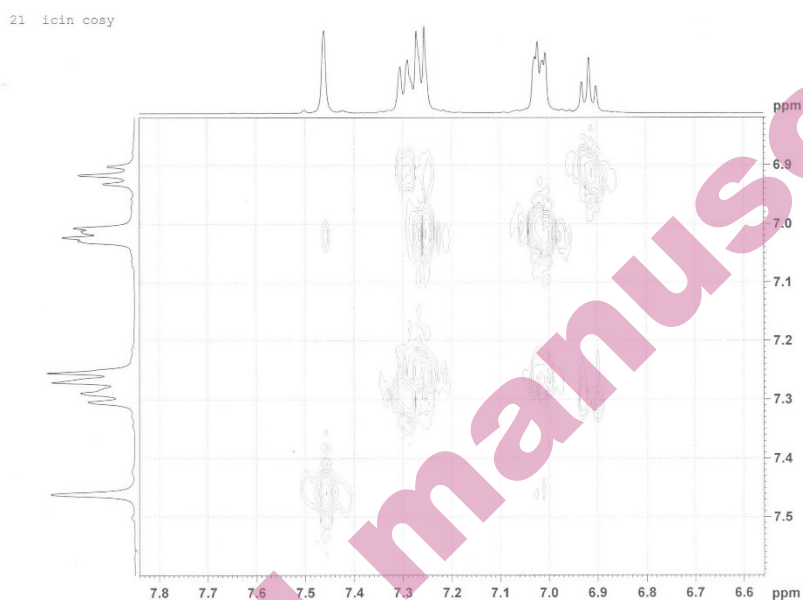


Figure S24. COSY spectrum of *N*-(2-methoxybenzyl)-6-Methyl-1,3-benzothiazol-2-amine (**4b**)

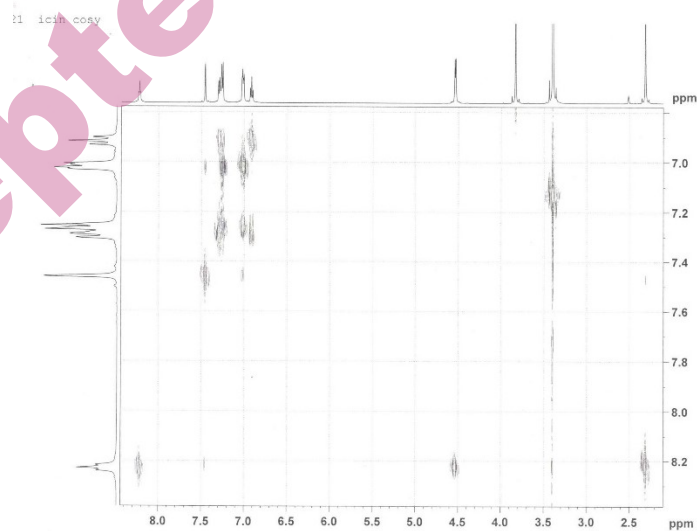


Figure S25. COSY spectrum of *N*-(2-methoxybenzyl)-6-Methyl-1,3-benzothiazol-2-amine (**4b**)

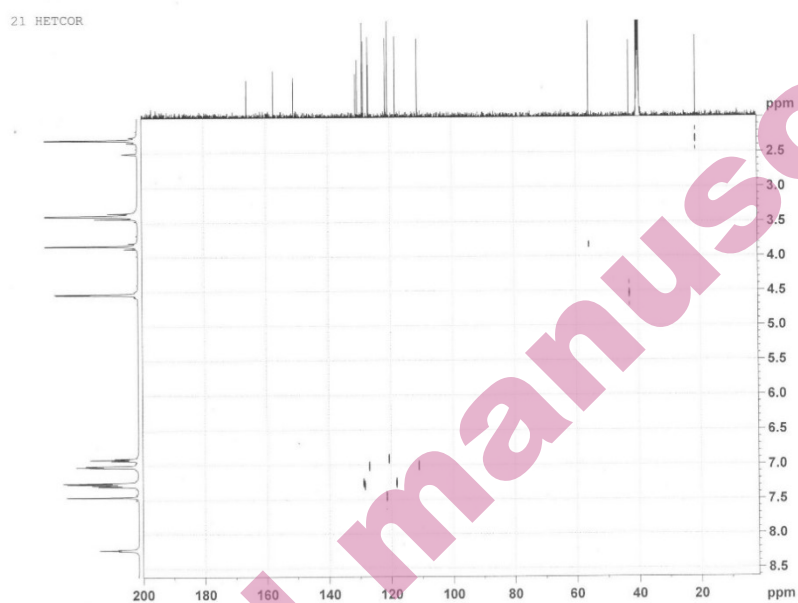


Figure S26. HETCOR spectrum of *N*-(2-methoxybenzyl)-6-Methyl-1,3-benzothiazol-2-amine (**4b**)

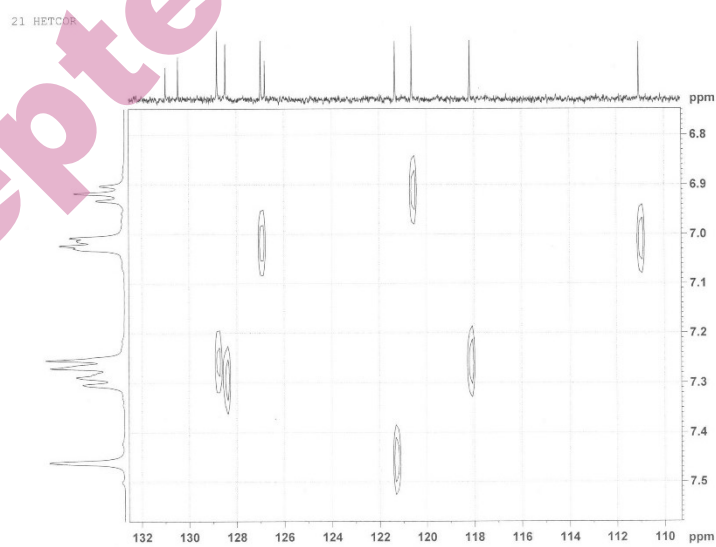
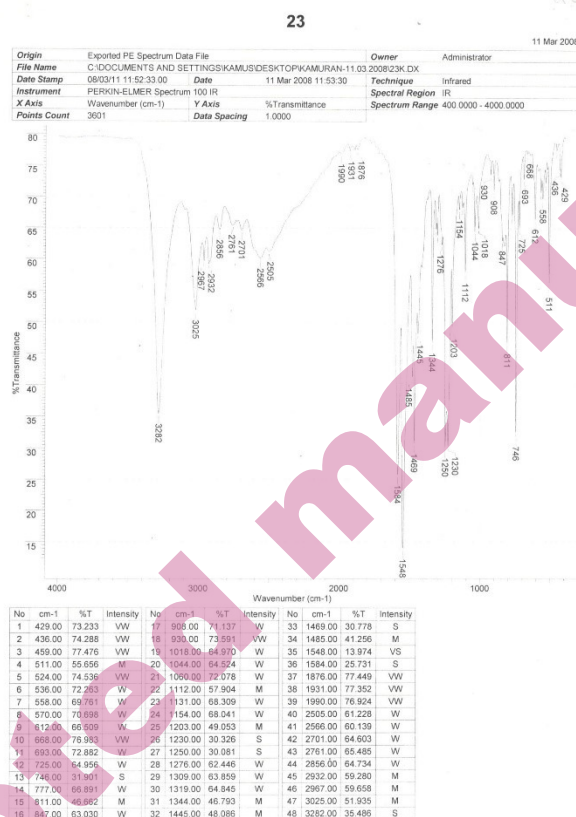


Figure S27. HETCOR spectrum of *N*-(2-methoxybenzyl)-6-Methyl-1,3-benzothiazol-2-amine (**4b**)

Figure S28. FT-IR spectrum of *N*-(2-hydroxybenzyl)-6-Methyl-1,3-benzothiazol-2-amine (**4c**).

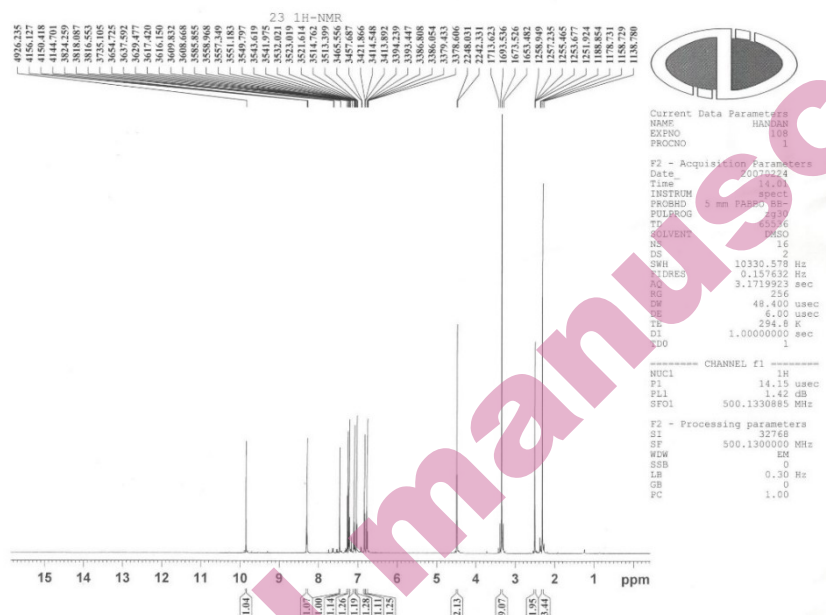


Figure S29. ¹H NMR spectrum of *N*-(2-hydroxybenzyl)-6-Methyl-1,3-benzothiazol-2-amine (4c).

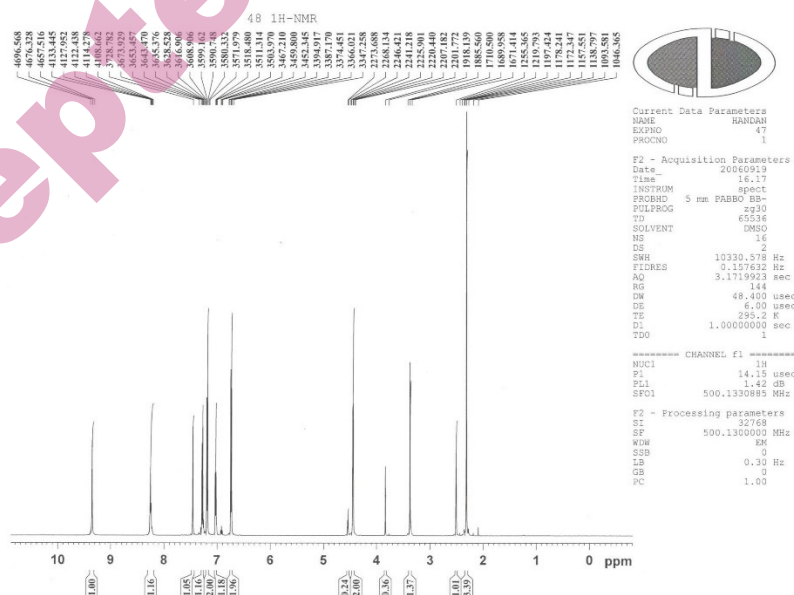


Figure S30. ¹H NMR spectrum of *N*-(4-hydroxybenzyl)-6-Methyl-1,3-benzothiazol-2-amine (4d).

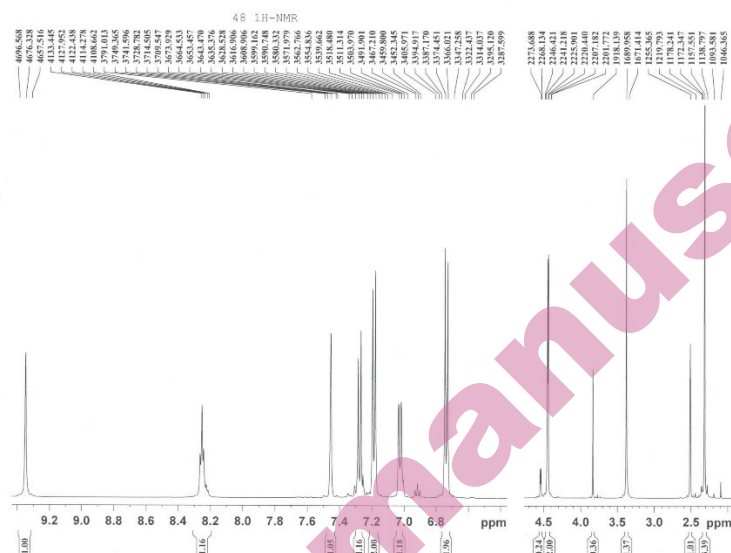


Figure S31. ¹H NMR spectrum of *N*-(4-hydroxybenzyl)-6-Methyl-1,3-benzothiazol-2-amine (**4d**).

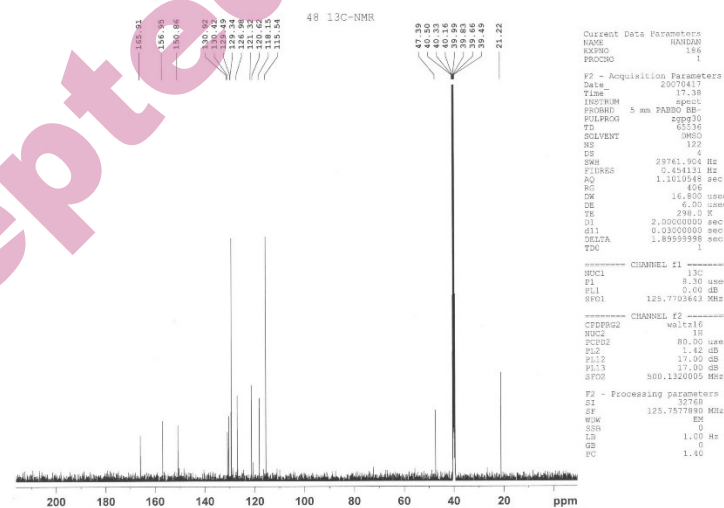


Figure S32. ¹³C NMR spectrum of *N*-(4-hydroxybenzyl)-6-Methyl-1,3-benzothiazol-2-amine (**4d**).

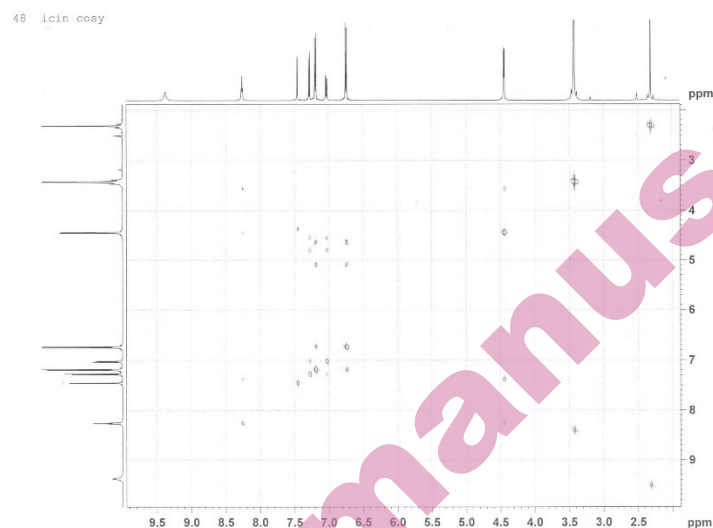


Figure S33. COSY spectrum of *N*-(4-hydroxybenzyl)-6-Methyl-1,3-benzothiazol-2-amine (**4d**).

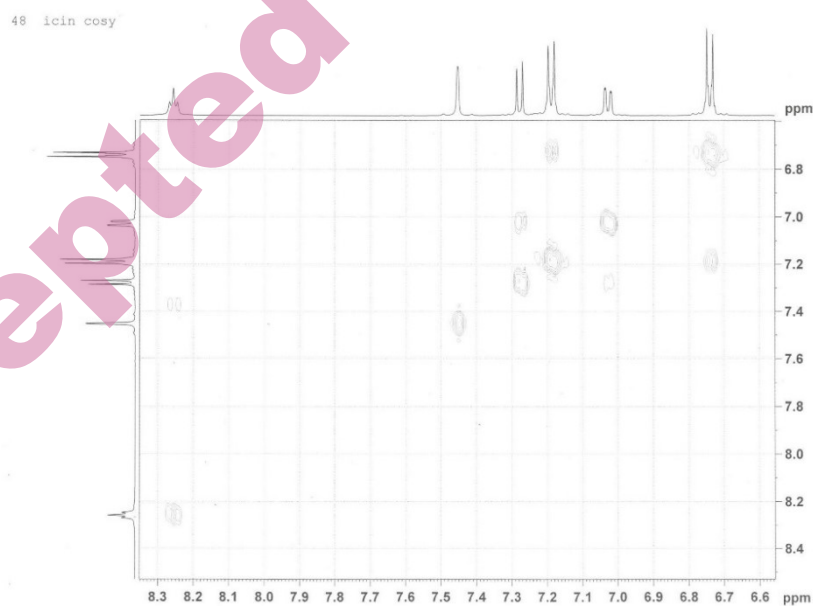


Figure S34. COSY spectrum of *N*-(4-hydroxybenzyl)-6-Methyl-1,3-benzothiazol-2-amine (**4d**).

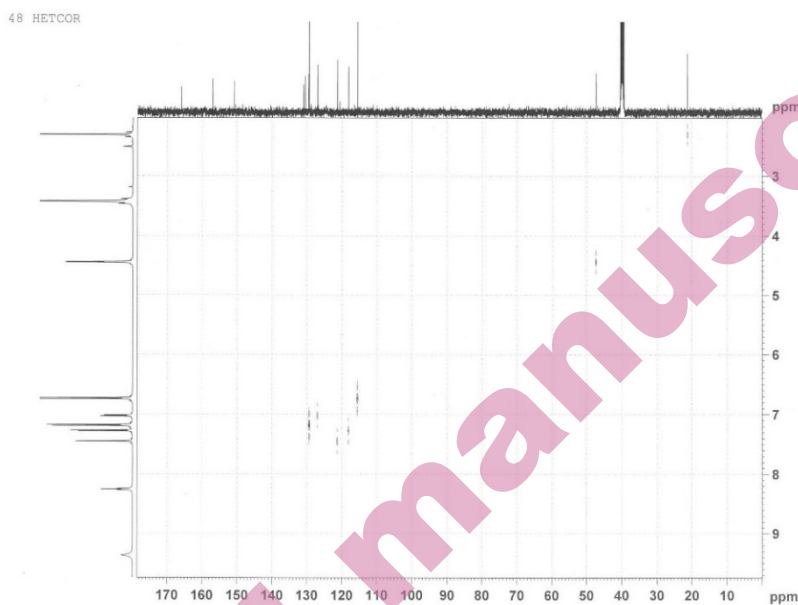


Figure S35. HETCOR spectrum of *N*-(4-hydroxybenzyl)-6-Methyl-1,3-benzothiazol-2-amine (**4d**).

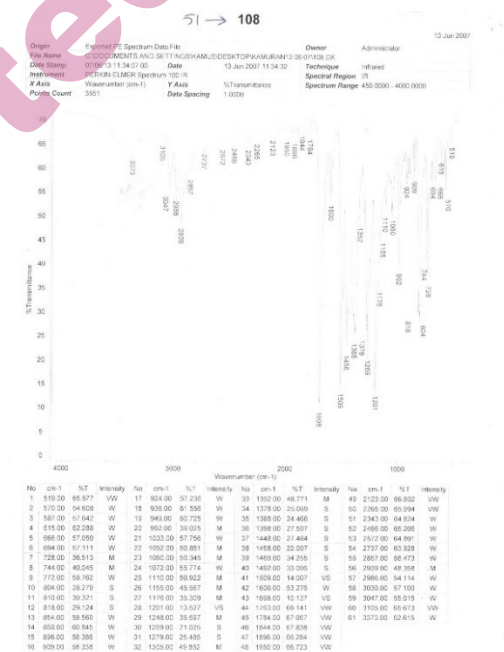


Figure S36. FT-IR spectrum of 2-Chloro-*N*-[6-methyl-1,3-benzothiazol-2-yl]-*N*-[2-methylbenzyl] acetamide (**5a**).

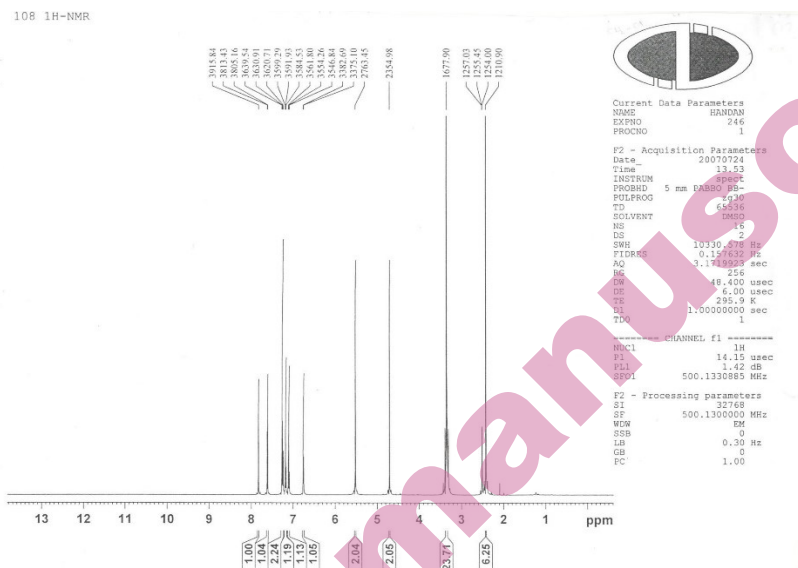


Figure S37. ^1H NMR spectrum of 2-Chloro-*N*-[6-methyl-1,3-benzothiazol-2-yl]-*N*-[2-methylbenzyl] acetamide (**5a**).

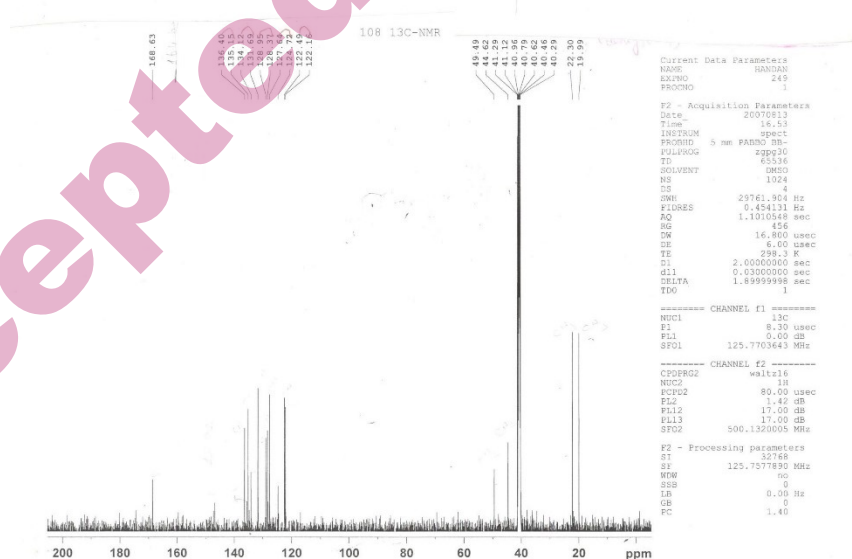


Figure S38. ^{13}C NMR spectrum of 2-Chloro-*N*-[6-methyl-1,3-benzothiazol-2-yl]-*N*-[2-methylbenzyl] acetamide (**5a**).

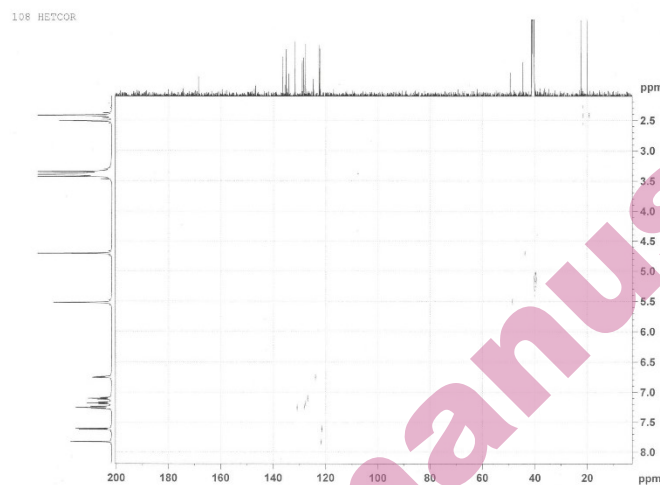


Figure S39. HETCOR spectrum of 2-Chloro-*N*-[6-methyl-1,3-benzothiazol-2-yl]-*N*-[2-methylbenzyl] acetamide (**5a**).



Figure S40. ESI-MS spectrum of 2-Chloro-*N*-[6-methyl-1,3-benzothiazol-2-yl]-*N*-[2-methylbenzyl] acetamide (**5a**)



Figure S41. FT-IR spectrum of 2-Chloro-N-[6-methyl-1,3-benzothiazol-2-yl]-N-[2-methoxybenzyl]acetamide (**5b**).

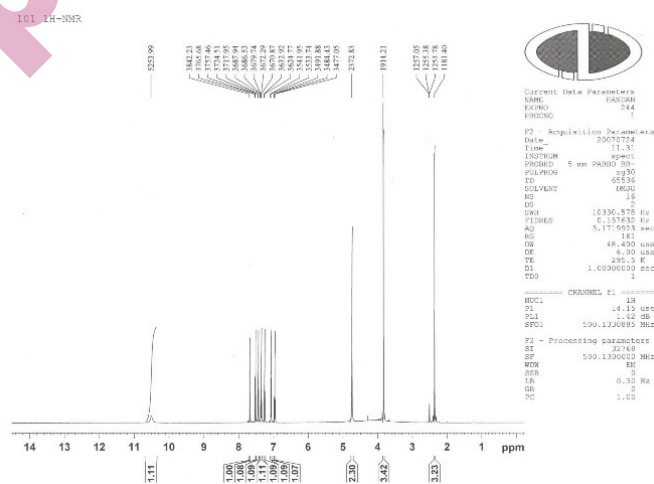


Figure S42. ¹H NMR spectrum of 2-Chloro-N-[6-methyl-1,3-benzothiazol-2-yl]-N-[2-methoxybenzyl]acetamide (**5b**).

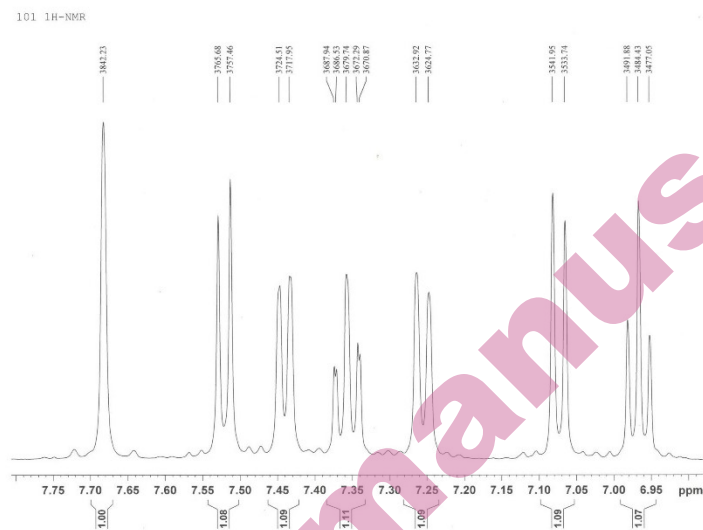


Figure S43. ¹H NMR spectrum of 2-Chloro-N-[6-methyl-1,3-benzothiazol-2-yl]-N-[2-methoxybenzyl]acetamide(**5b**).

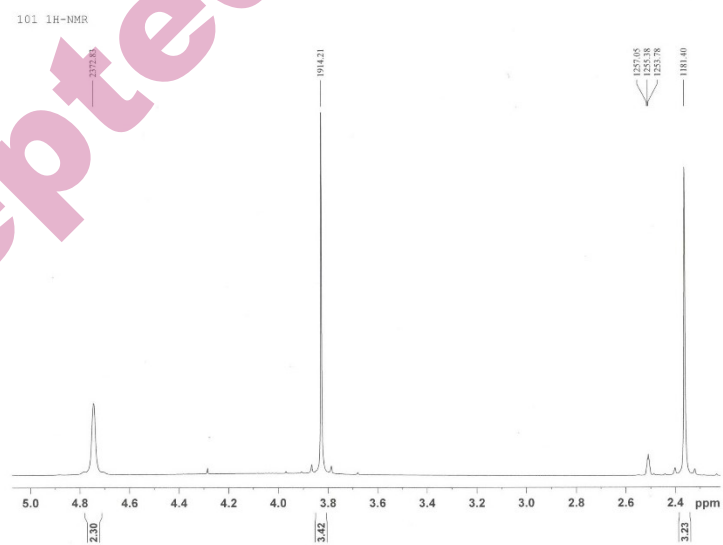
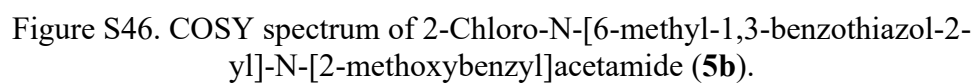
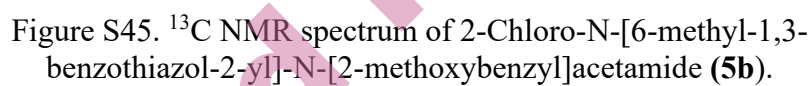


Figure S44. ¹H NMR spectrum of 2-Chloro-N-[6-methyl-1,3-benzothiazol-2-yl]-N-[2-methoxybenzyl]acetamide(**5b**).



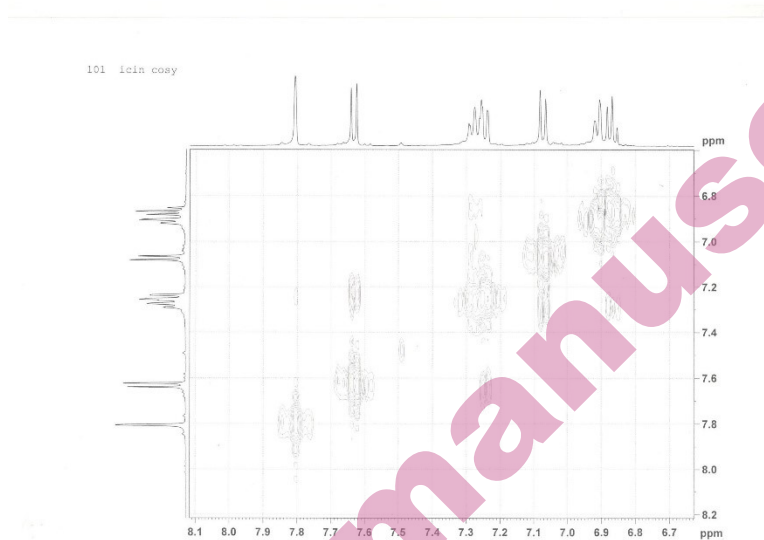


Figure S47. COSY spectrum of 2-Chloro-*N*-[6-methyl-1,3-benzothiazol-2-yl]-*N*-[2-methoxybenzyl]acetamide (**5b**).

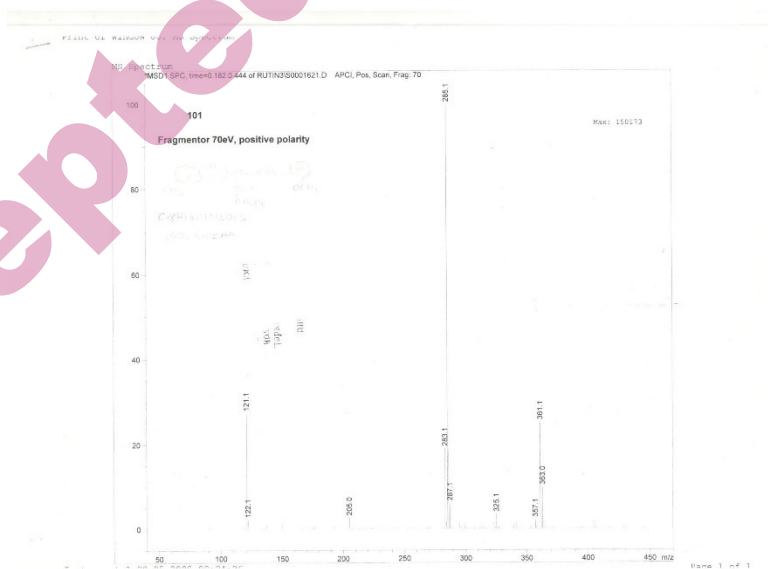


Figure S48. ESI-MS spectrum of 2-Chloro-*N*-[6-methyl-1,3-benzothiazol-2-yl]-*N*-[2-methoxybenzyl]acetamide (**5b**).