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Synthesis and Cytotoxic Activities of Novel 2-(1,5-bis(aryl) penta-1,4-dien-2-yl) benzo[d]thiazol Derivatives

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Table of Contents	**Page**
S1: General Information	2
S2: Spectral data of new compounds	3
S3: Spectra of new compounds	4-8

S1: General Information

All the chemicals and solvents employed in the synthesis were supplied by Merck (Germany) and Fluka (Germany) and used without purification. The melting points were measured on an Electrothermal 9100 apparatus. The IR spectrums (KBr disc) were recorded on a Jasco FT/IR-430 spectrometer. The ^{1}H and ^{13}C NMR spectra were recorded on a Bruker Avance DPX-400 instrument. As internal standards served TMS (δ 0.00) for ^{1}H NMR and $CDCl_3$ (δ 77.0) for 13C NMR spectroscopy *J* values are given in Hz. The multiplicities of the signals in the ^{1}H NMR spectra are abbreviated by s (singlet), d (doublet), t (triplet), q (quarted), m (multiplet), br (broad) and combinations thereof. The elemental analyses were obtained from a LECO CHNS 932 Elemental Analyzer.

S2: Spectral data of new compounds

2-((1*Z*,4*E*)-1,5-di*p*-tolylpenta-1,4-dien-2-yl)benzo[d]thiazol (5a): Yellowish crystals, Yield, 55%, M.P. 171-174°C. **^{1}H-NMR** (400 MHz, $CDCl_3$): δ = 8.03 (d, *J* = 8.0 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.72 (s, 1H), 7.49 (t, *J* = 7.2 Hz, 1H), 7.45 (d, *J* = 8.0 Hz. 2H), 7.38 (t, *J* = 7.2 Hz, 1H), 7.27-7.7.23 (m, 4H), 7.09 (d, *J* = 8.0 Hz, 2H), 6.55 (d, *J* = 16.0 Hz, 1H), 6.50 (dt, *J* = 16.0, 4.8 Hz, 1H), 3.86 (d, *J* = 4.8 Hz, 2H), 2.41 (s, 3H), 2.32 (s, 3H). **^{13}C-NMR** (100MHz, $CDCl_3$): δ = 170.7, 153.8, 138.3, 136.9, 135.4, 134.8, 134.6, 133.1, 131.2, 129.9, 129.7, 126.2, 126.1, 125.1, 123.1, 121.4, 31.9, 29.7, 21.3. **IR** (KBr, cm^{-1}) 3064, 2938, 2872, 1524, 1436, 1311, 1241, 1108, 966, 759, 728. Anal. Cald. for $C_{26}H_{23}NS$: C, 81.85; H, 6.08; N, 3.67; S, 8.40; Found: C, 81.65; H, 5.98; N, 3.87; S, 8.50.

2-((1*Z*,4*E*)-1,5-bis(4-metoxyphenyl) penta-1,4-dien-2-yl) benzo[*d*]thiazol (5b): Yellowish crystals, Yield, 20%, M.P. 193-197°C. **^{1}H-NMR** (400 MHz, $CDCl_3$): δ = 8.03 (d, *J* = 7.6 Hz, 1H), 7.86 (d, *J* = 7.6 Hz, 1H), 7.70 (s, 1H), 7.53 (d, *J* = 6.8 Hz, 2H), 7.49 (dt, *J* = 7.6, 2.4 Hz, 1H), 7.38 (dt, *J* = 7.6, 1.2 Hz, 1H), 7.31 (d, *J* = 6.8 Hz, 2H), 6.96 (d, *J* = 6.8 Hz, 2H), 6.83 (d, *J* = 6.8 Hz, 2H), 6.52 (d, *J* = 16.4 Hz, 1H), 6.41 (dt, *J* = 16.4, 5.2 Hz, 1H), 3,87 (m, 5H, 3H -OCH_3, 2H –CH_2-), 3,82 (s, 3H). **^{13}C-NMR** (100MHz, $CDCl_3$): δ = 170.9, 159.6, 158.9, 153.9, 135.1, 134.8, 131.9, 130.9, 130.7, 130.3, 128.6, 127.3, 126.1, 125.0, 124.9, 122.9, 121.3, 114.1, 113.9, 55.4, 55.3, 33.3. **IR** (KBr, cm^{-1}): 3041, 2954, 2859, 1606, 1509, 1436, 1249, 1174, 1033, 964, 759, 728, 530. Anal. Cald. for $C_{26}H_{23}NO_2S$: C, 75.52; H, 5.61; N, 3.39; S, 7.75; Found: C, 75.42; H, 5.54; N, 3.57; S, 7.81.

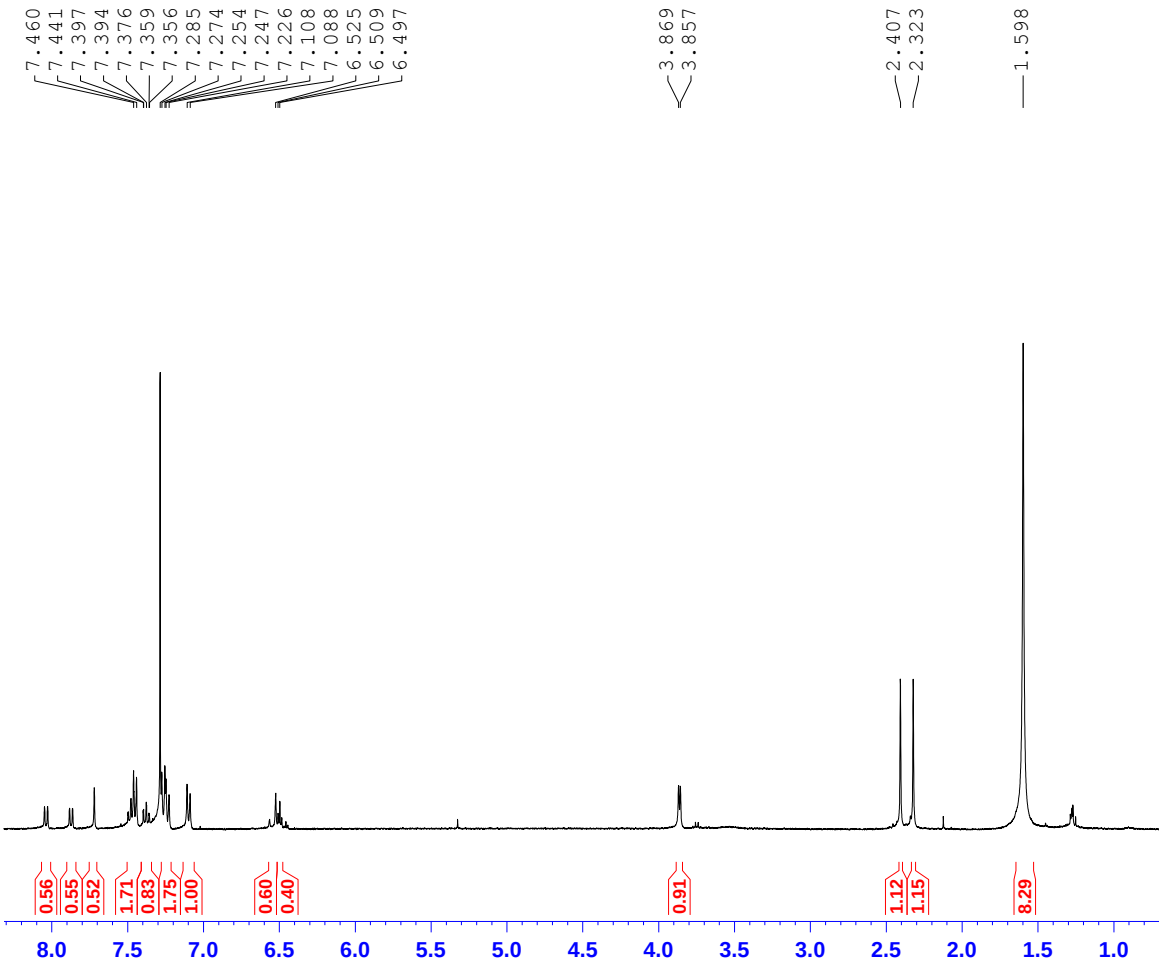
2-(((1*S*,2*S*,*E*)-2-(benzo[d]thiazol-2-yl)-1,5-di-p-tolylpent-4-en-1-yl)thio)aniline (6a): Yellowish crystals, Yield, 60%, M.P. 203-206°C. **^{1}H-NMR** (400 MHz, $CDCl_3$): δ = 8.05 (d, *J* = 7.6 Hz, 1H), 7.89 (d, *J* = 7.6 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 1H), 7.41 (t, *J* = 7.6 Hz. 1H), 7.19-7.15 (m, 4H), 7,11-7.03 (m, 4H), 6.98 (t, *J* = 7.2 Hz, 1H), 6.78 (d, *J* = 7.2 Hz, 1H), 6.58 (d, *J* = 7.2 Hz, 1H), 6.36 (t, *J* = 7.2 Hz), 6.11 (d, *J* = 15.6 Hz, 1H), 5.92 (dt, J = 15.6, 7.2 Hz, 1H), 4.49 (d, *J* = 11.2 Hz, 1H), 4.18 (brs, 2H, -NH_2), 3.87 (dt, *J* = 11.2, 6.8 Hz, 1H), 2.56 (t, *J* = 6.8 Hz, 2H), 2.36 (s, 3H), 2.29 (s, 3H). **^{13}C-NMR** (100MHz, $CDCl_3$): δ = 172.6, 152.1, 148.1, 137.4, 136.3, 135.5, 134.8, 134.2, 132.4, 129.1, 128.1, 127.4, 126.5, 125.9, 125.0, 124.4, 123.2, 122.9, 122.6, 121.7, 119.6, 117.8, 114.6, 50.2, 46.2, 36.3, 21.3, 21.1. **IR** (KBr, cm^{-1}) 3374, 3054, 3031, 2919, 2852, 1513, 1436, 1311, 1241, 1108, 966, 759, 728. Anal.

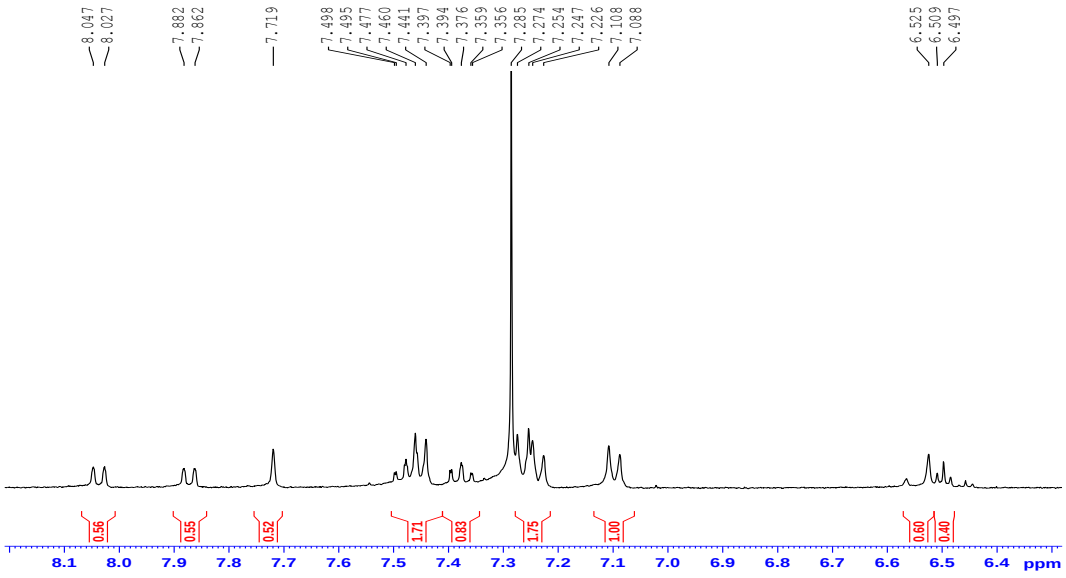
Cald. for $C_{32}H_{30}N_2S_2$: C, 75.85; H, 5.97; N, 5.53; S, 12.66. Found: C, 75.82; H, 5.99; N, 5.68; S, 12.74.

2-(((1*S*,2*S*,*E*)-2-(benzo[d]thiazol-2-yl)-1,5-bis(4-methoxyphenyl)pent-4-en-1-yl)thio) aniline (6b): Yellowish crystals, Yield, 24%, M.P. 214-217°C. **^{1}H-NMR** (400 MHz, $CDCl_3$): δ = 8.06 (d, *J* = 8.0 Hz, 1H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.52 (dt, *J* = 8.0, 1.2 Hz, 1H), 7.41 (dt, *J* = 8.0, 1.2 Hz, 1H), 7.13 (d, *J* = 6.8 Hz, 2H), 7.10 (d, *J* = 6.8 Hz, 2H), 7,00 (dt, *J* = 8.0, 1.6 Hz, 1H), 6.84 (d, *J* = 6.8 Hz, 2H), 6.80 (dd, *J* = 8.0, 1.6 Hz, 1H), 6.76 (d, *J* = 6.8 Hz, 2H), 6.58 (dd, *J* = 8.0, 1.2 Hz, 1H), 6.38 (dt, *J* = 78.0, 1.2 Hz, 1H), 6.10 (d, *J* = 15.6 Hz, 1H), 5.81 (dt, *J* = 15.6, 7.6 Hz, 1H), 4.50 (d, *J* = 11.2 Hz, 1H), 4.20 (brs, 2H, -NH_2), 3.86 (dt, *J* = 11.2, 6.8 Hz, 1H), 3.82 (s, 3H), 3.77 (s, 3H), 2.57 (t, *J* = 6.8 Hz, 2H). **^{13}C-NMR** (100MHz, $CDCl_3$): δ = 173.4, 161.1, 158.8, 153.1, 149.1, 143.7, 137.4, 132.5, 131.9, 131.6, 130.2, 129.4, 127.6, 127.2, 126.8, 126.0, 124.1, 123.8, 122.8, 121.7, 117.8, 114.5, 113.8, 55.4, 55.2, 50.4, 38.1, 35.3. **IR** (KBr, cm^{-1}) 3412. 3043, 3032, 2923, 2862, 1513, 1436, 1311, 1241, 1108, 966, 759, 728. Anal. Cald. for $C_{32}H_{30}N_2O_2S_2$: C, 71.34; H, 5.61; N, 5.20; S, 11.90. Found: C, 71.45; H, 5.74; N, 5.33; S, 12.12.

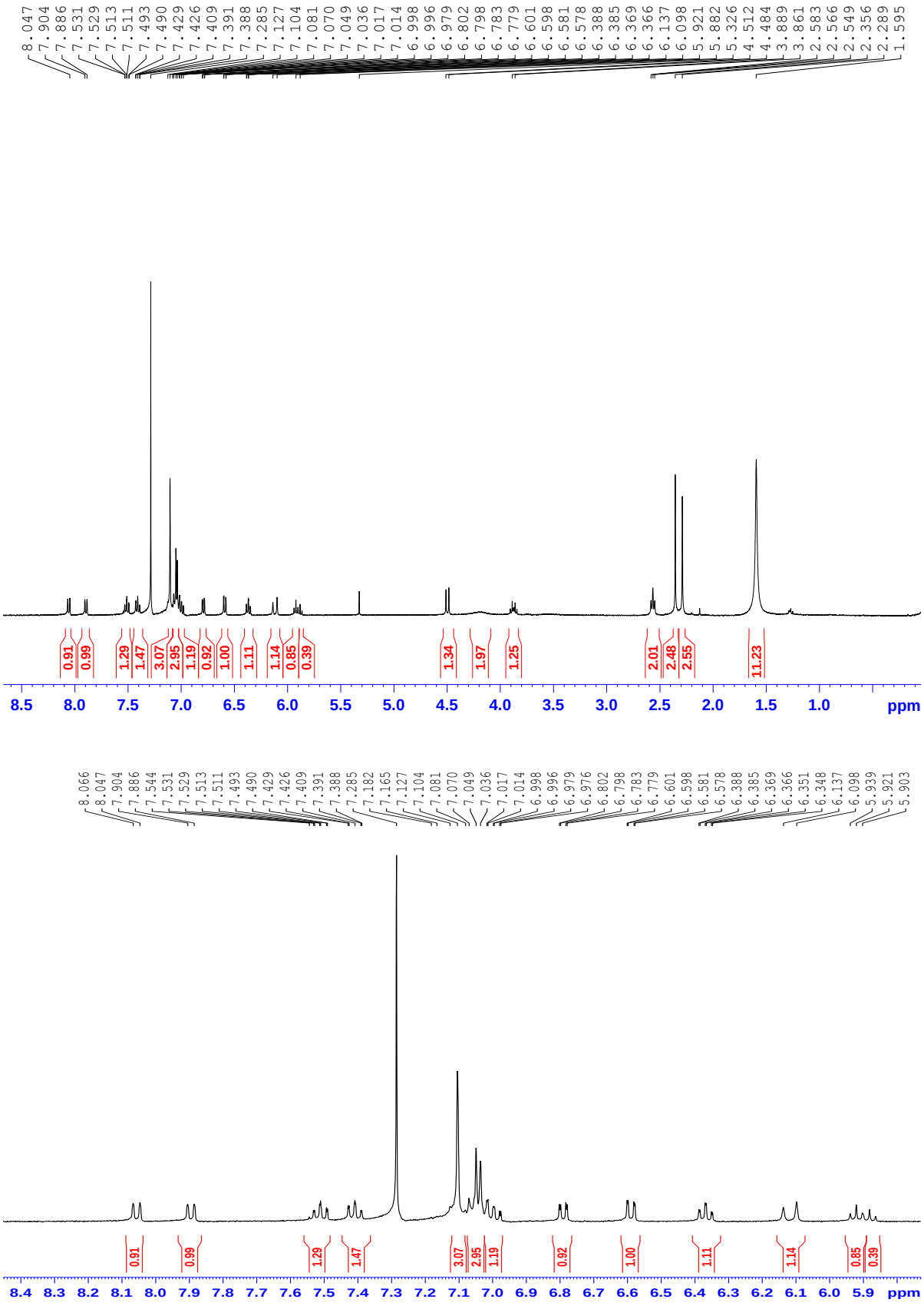
S3: Spectra of new compounds

2-((1*Z*,4*E*)-1,5-di*p*-tolylpenta-1,4-dien-2-yl)benzo[d]thiazol (5a) ^{1}H NMR($CDCl_3$):

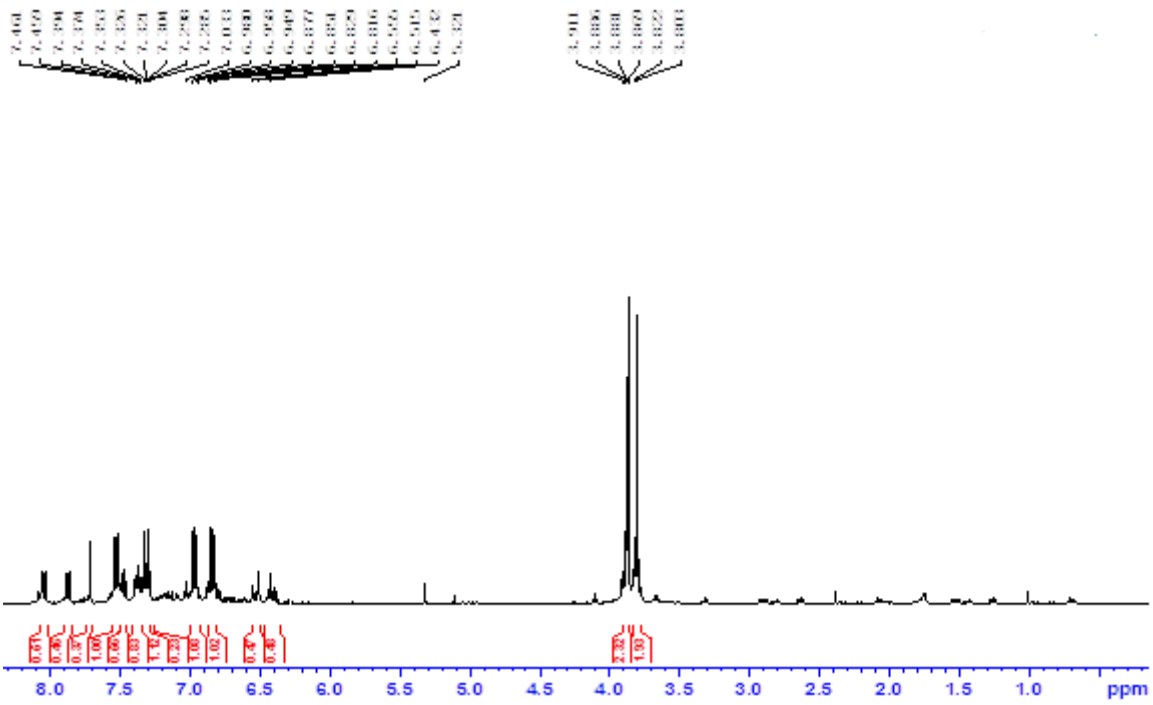


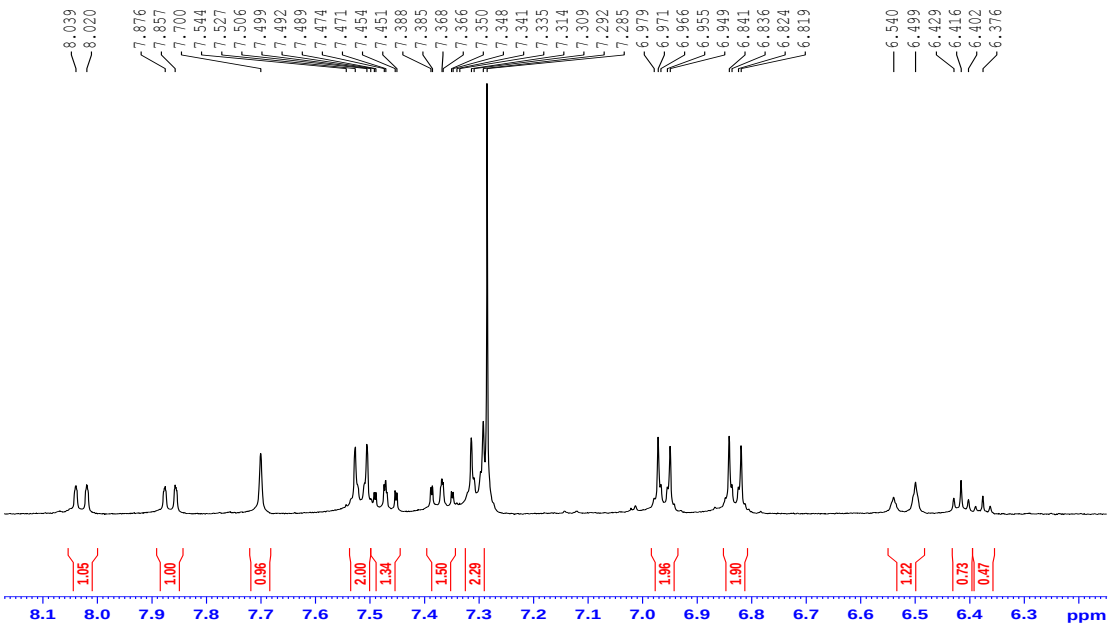


2-((1*Z*,4*E*)-1,5-bis(4-metoxyphenyl) penta-1,4-dien-2-yl) benzo[*d*]thiazol (5b) ^{1}H NMR ($CDCl_3$):



2-(((1*S*,2*S*,*E*)-2-(benzo[d]thiazol-2-yl)-1,5-di-p-tolylpent-4-en-1-yl)thio)aniline (6a) ^{1}H NMR ($CDCl_3$):





2-(((1*S*,2*S*,*E*)-2-(benzo[d]thiazol-2-yl)-1,5-bis(4-methoxyphenyl)pent-4-en-1-yl)thio) aniline (6b) ^{1}H NMR ($CDCl_3$):