

Novel 1,2,3-Triazole-Based Benzothiazole Derivatives: Efficient Synthesis, DFT, Molecular Docking, and ADMET Studies

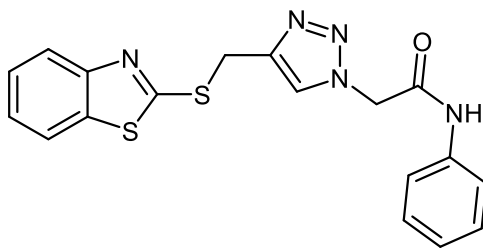
Zohreh Mirjafary ^{*a}, Mahdieh Mohammad Karbasi ^a, Parsa Hesamzadeh^a, Asghar Amiri^b,
Hamid Reza Shaker ^a, Hamid Saeidian ^b

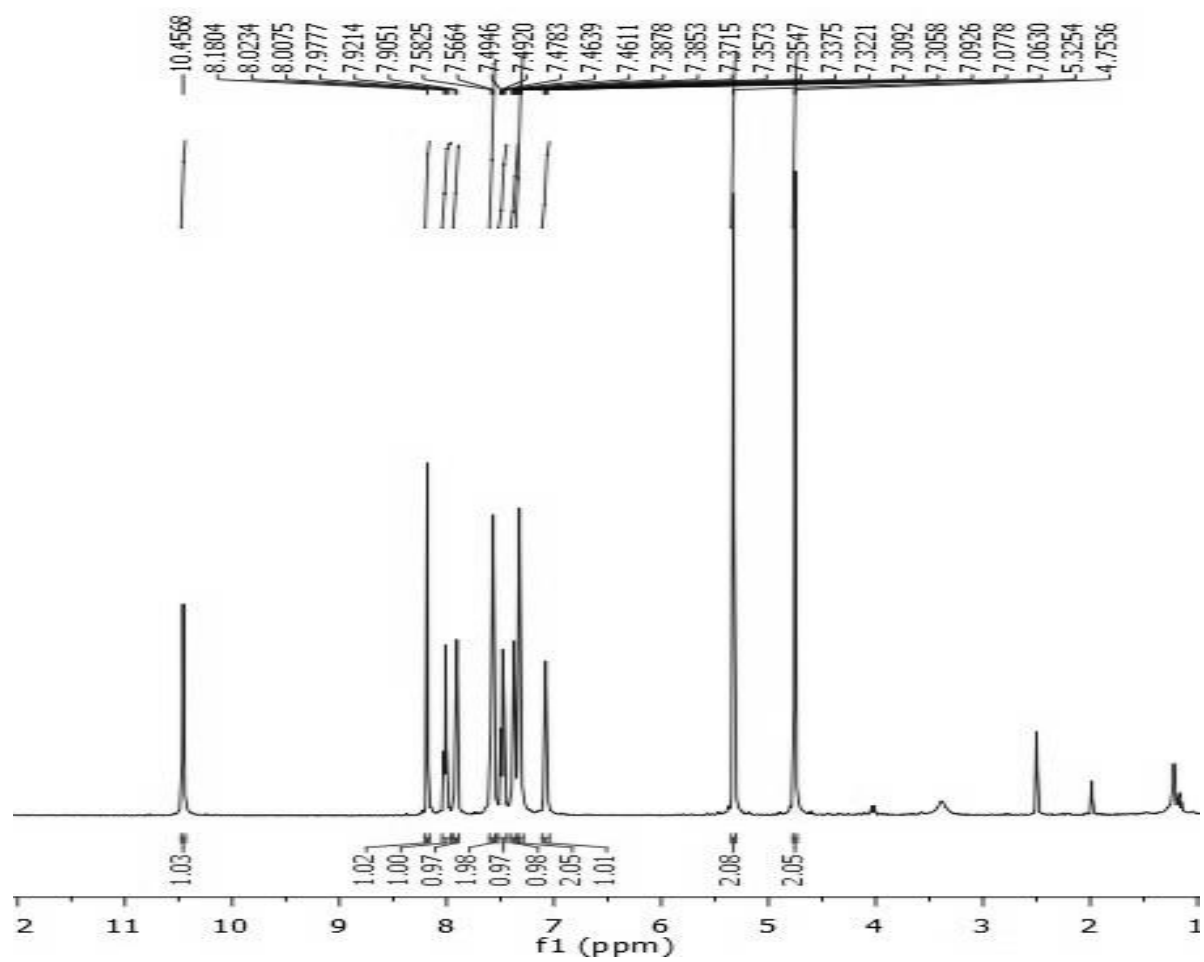
^a Department of Chemistry, Science and Research Branch, Islamic Azad University, Tehran, Iran

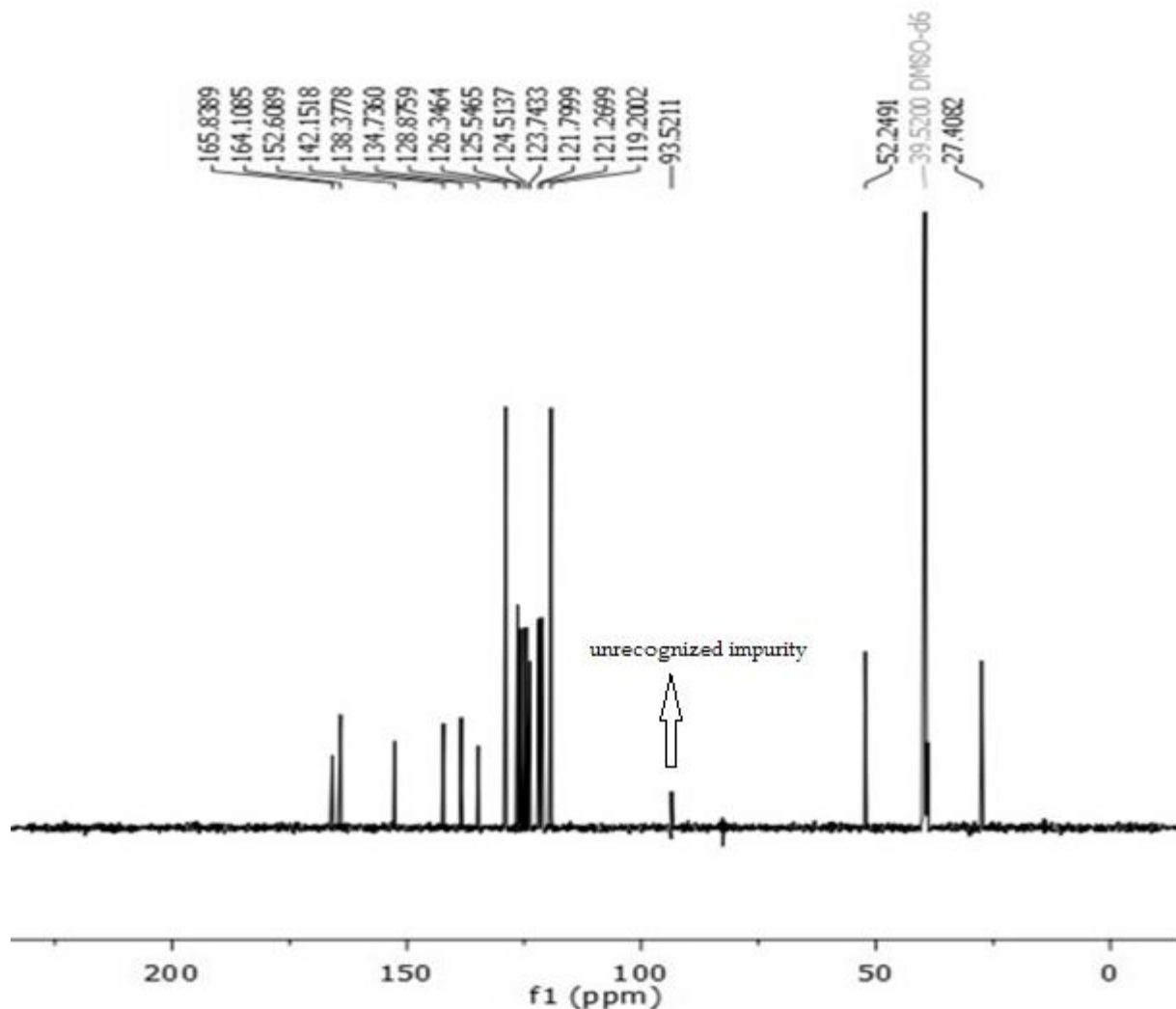
^b Department of Science, Payame Noor University (PNU), PO Box: 19395-4697, Tehran, Iran

Spectral data of the 1,2,3-triazoles 5a-f

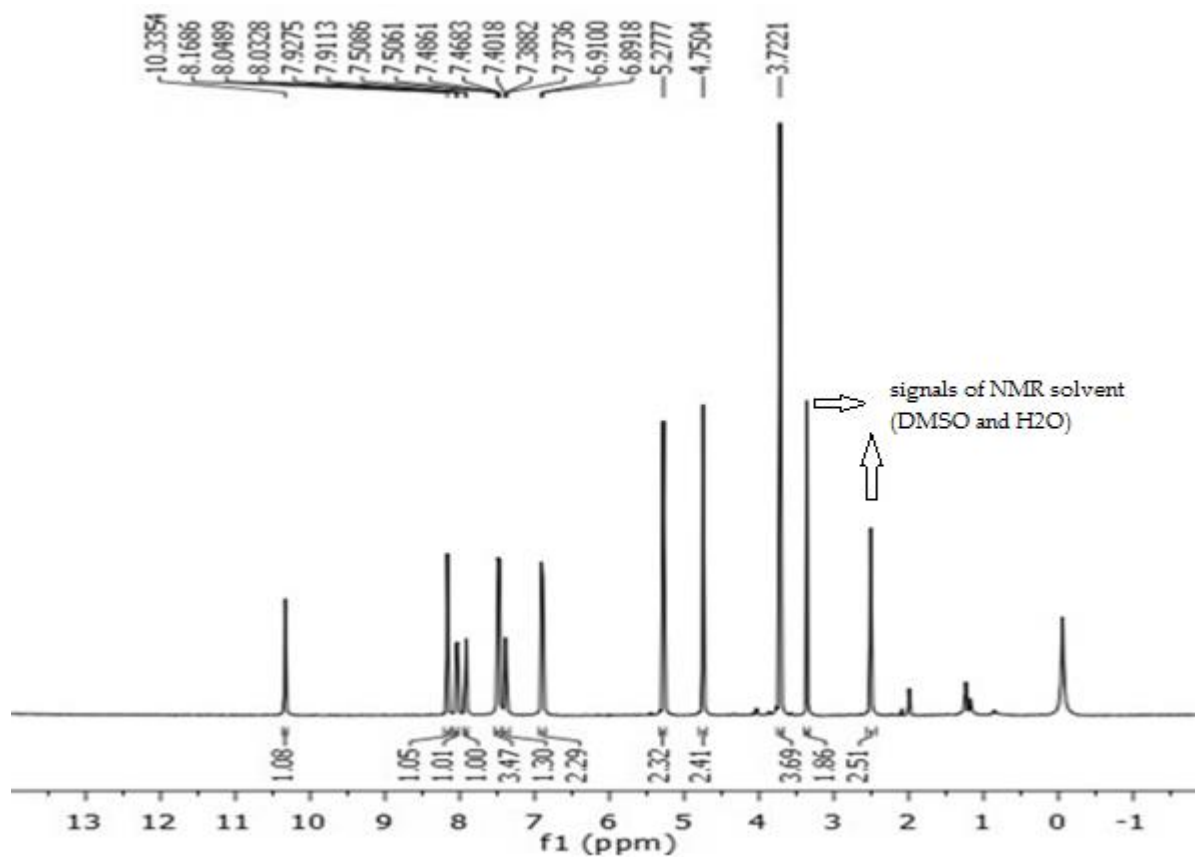
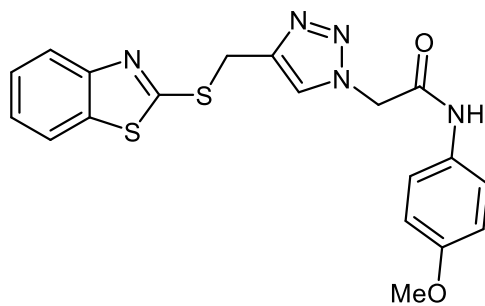
2-(4-((benzo[d]thiazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-N-phenylacetamide (**5a**): ¹H NMR (500 MHz, DMSO): δ = 4.75 (s, 2H), 5.32 (s, 2H), 7.07 (t, J = 7.4 Hz, 1H), 7.32 (t, J = 7.7 Hz, 2H), 7.37 (t, J = 7.7 Hz, 1H), 7.47 (t, J = 7.7 Hz, 1H), 7.58 (d, J = 8.5 Hz, 2H), 7.92 (d, J = 8.0 Hz, 1H), 8.02 (d, J = 8.0 Hz, 1H), 8.15 (s, 1H), 10.46 (s, 1H) ppm. ¹³C NMR (125 MHz, DMSO): δ = 27.41, 52.24, 119.20, 121.26, 121.79, 123.74, 124.51, 125.54, 126.34, 128.87, 134.74, 138.37, 142.15, 152.60, 164.10, 165.83 ppm. Anal. Calcd for C₁₈ H₁₅N₅OS₂: C, 56.67; H, 3.96; N, 18.36. found: C, 56.73; H, 4.01; N, 18.46.

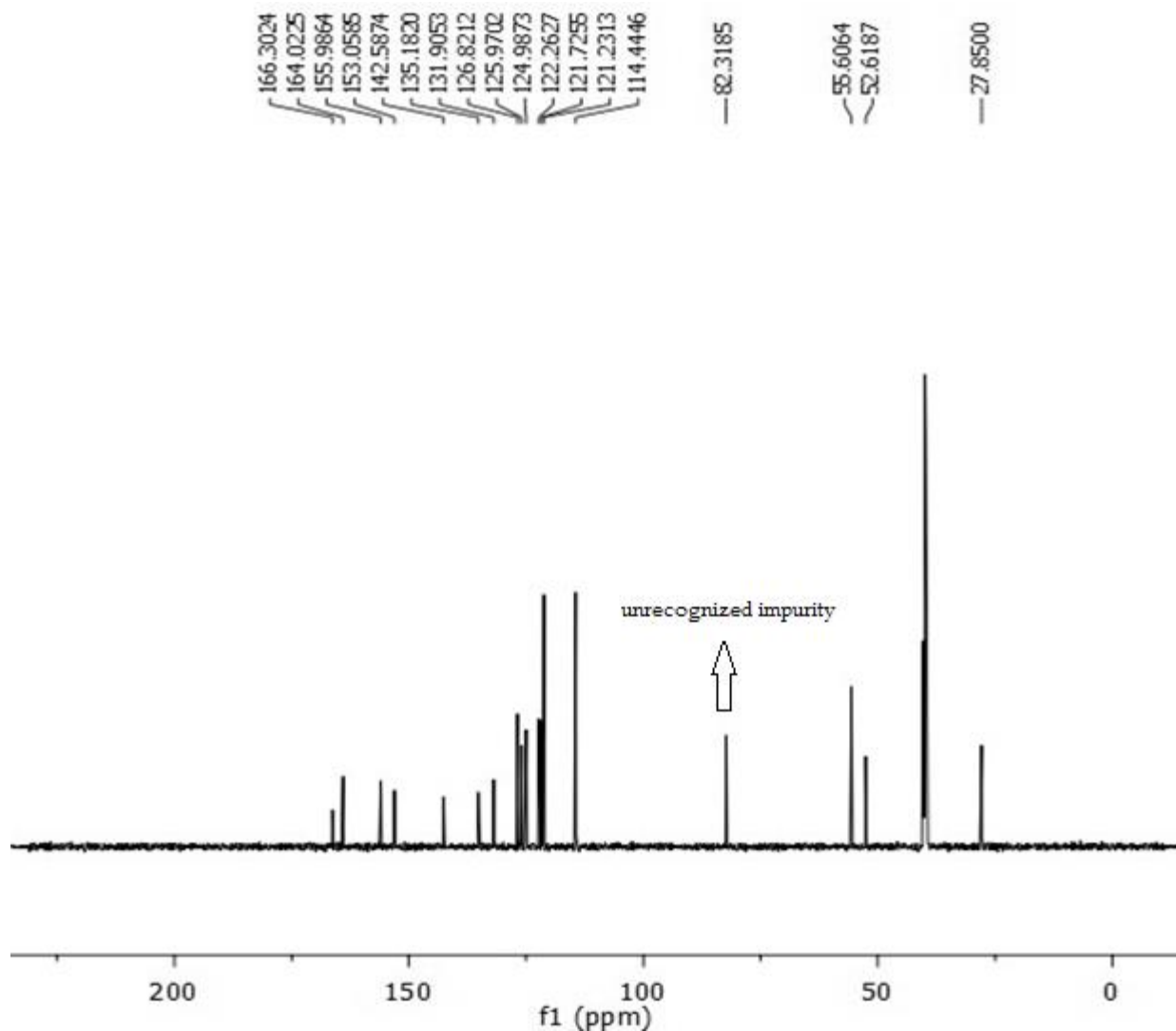




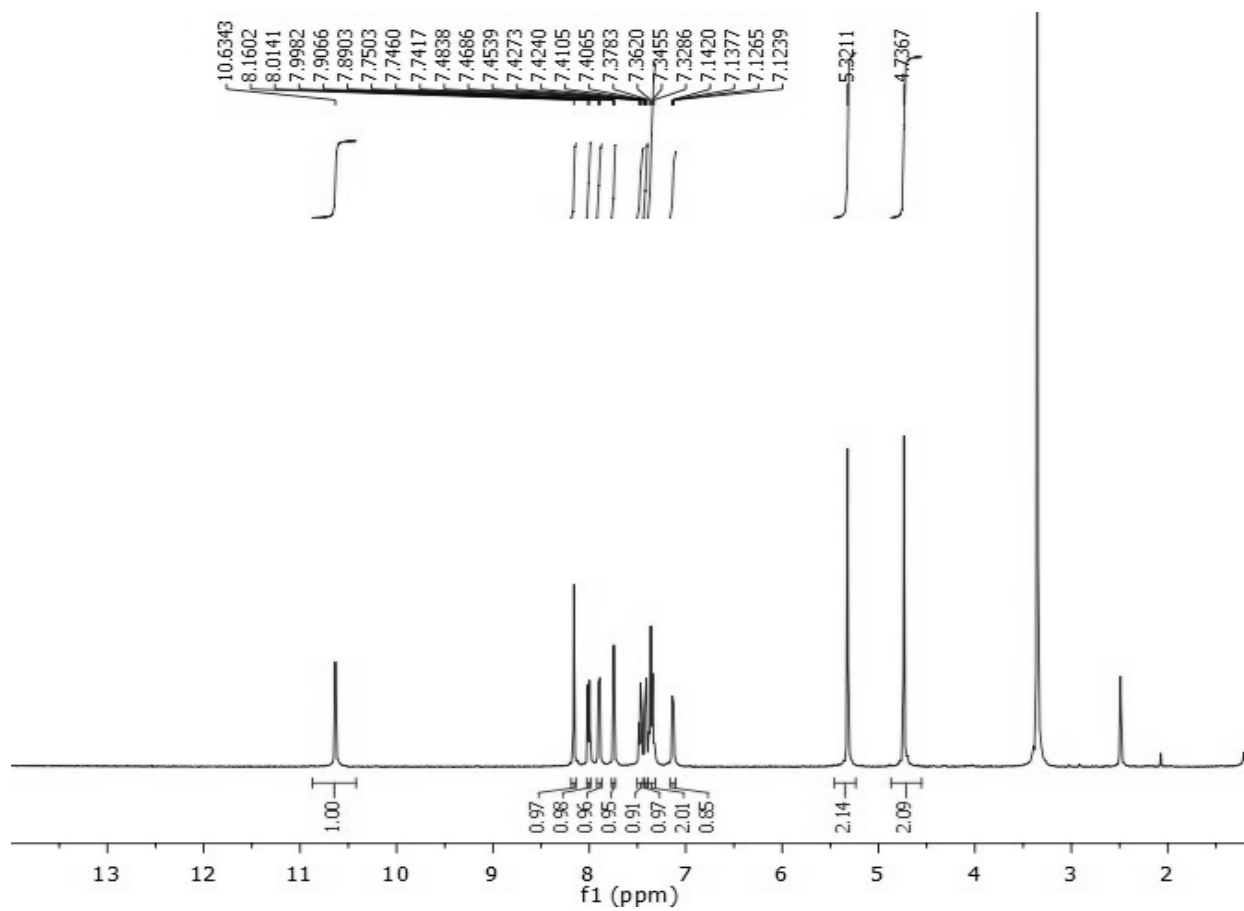
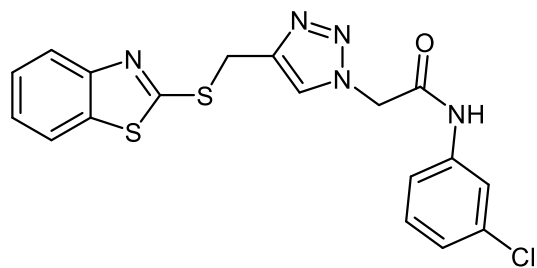


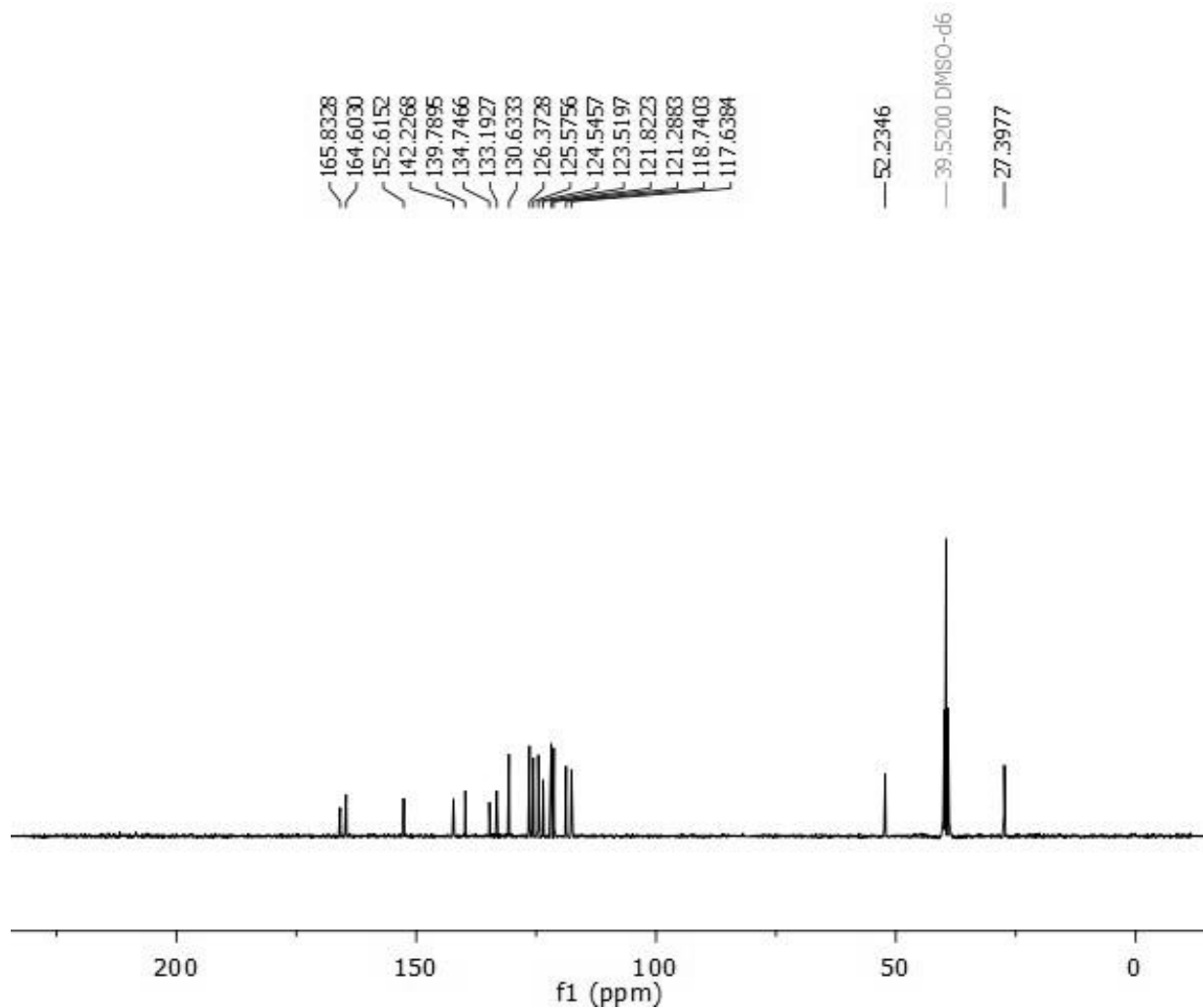
2-(4-((benzo[d]thiazol-2-ylthio)methyl)-1H-1,2,3-triazol-1-yl)-N-phenylacetamide (**5b**): ^1H NMR (500 MHz, DMSO): δ = 3.72 (s, 3H), 4.75 (s, 2H), 5.27 (s, 2H), 6.91 (d, J = 9.1 Hz, 2H), 7.38 (t, J = 7.3 Hz, 1H), 7.50-7.46 (m, 3H), 7.92 (d, J = 8.0 Hz, 1H), 8.04 (d, J = 8.0 Hz, 1H), 8.16 (s, 1H), 10.34 (s, 1H) ppm. ^{13}C NMR (125 MHz, DMSO): δ = 27.85, 52.61, 55.60, 114.44, 121.23, 121.72, 122.26, 124.98, 125.97, 126.82, 131.90, 135.18, 142.58, 153.05, 155.98, 164.02, 166.30 ppm. Anal. Calcd for $\text{C}_{19}\text{H}_{17}\text{N}_5\text{O}_2\text{S}_2$: C, 55.46; H, 4.16; N, 17.02. found: C, 55.57; H, 4.09; N, 17.13.



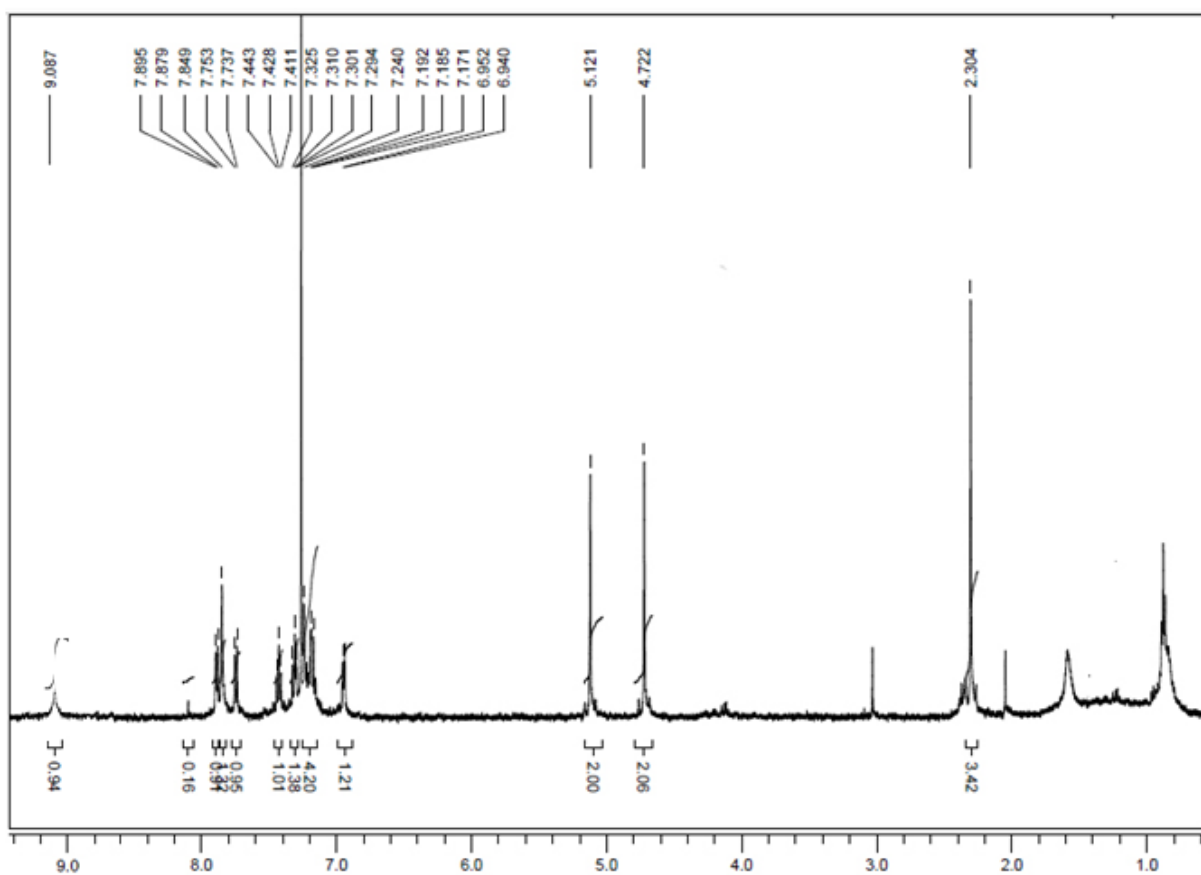
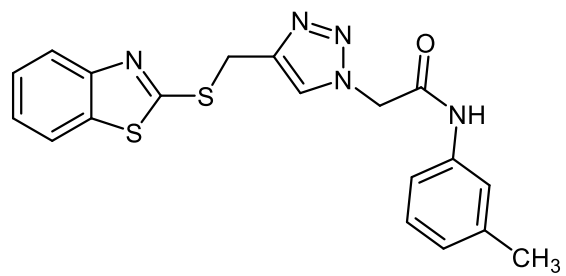


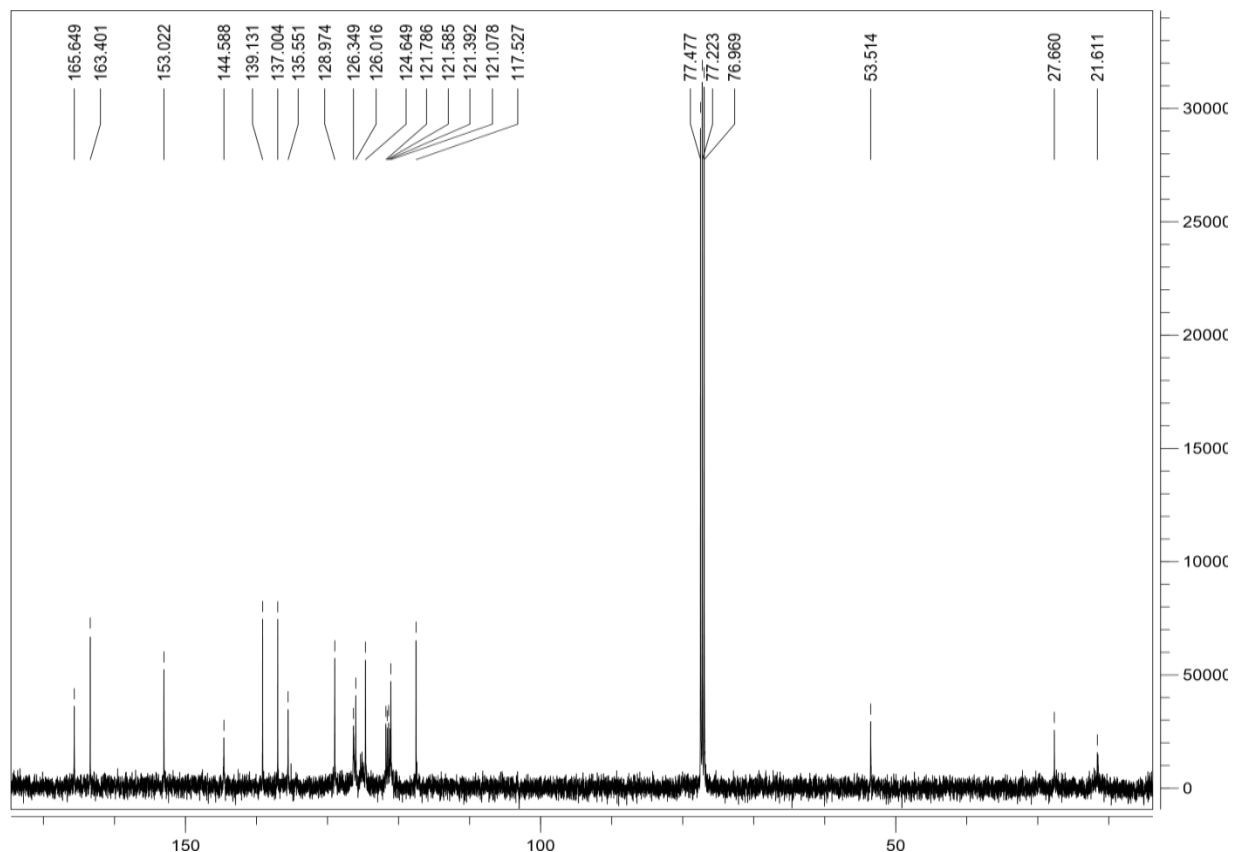
2-(4-((benzo[d]thiazol-2-ylthio) methyl)-1H-1,2,3-triazol-yl)-N-(3-chlorophenyl)acetamide (5c): ¹H NMR (500 MHz, DMSO): δ = 4.73 (s, 2H), 5.33 (s, 2H), 7.14 (d, *J* = 8.7 Hz, 1H), 7.36 (dd, *J*₁ = 16.5 Hz, *J*₂ = 8.4 Hz, 2H), 7.42 (d, *J* = 7.7 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.74 (s, 1H), 7.90 (d, *J* = 8.2 Hz, 1H), 8.01 (d, *J* = 8.0 Hz, 1H), 8.16 (s, 1H), 10.63 (s, 1H) ppm. ¹³C NMR (125 MHz, DMSO): δ = 27.39, 52.33, 117.63, 118.74, 121.28, 121.82, 123.51, 124.54, 125.57, 126.37, 130.63, 133.19, 134.74, 139.78, 142.22, 152.81, 164.60, 165.83 ppm. Anal. Calcd for C₁₈H₁₄ClN₅OS₂: C, 51.98; H, 3.39; N, 16.84. found: C, 52.05; H, 3.44; N, 16.96.



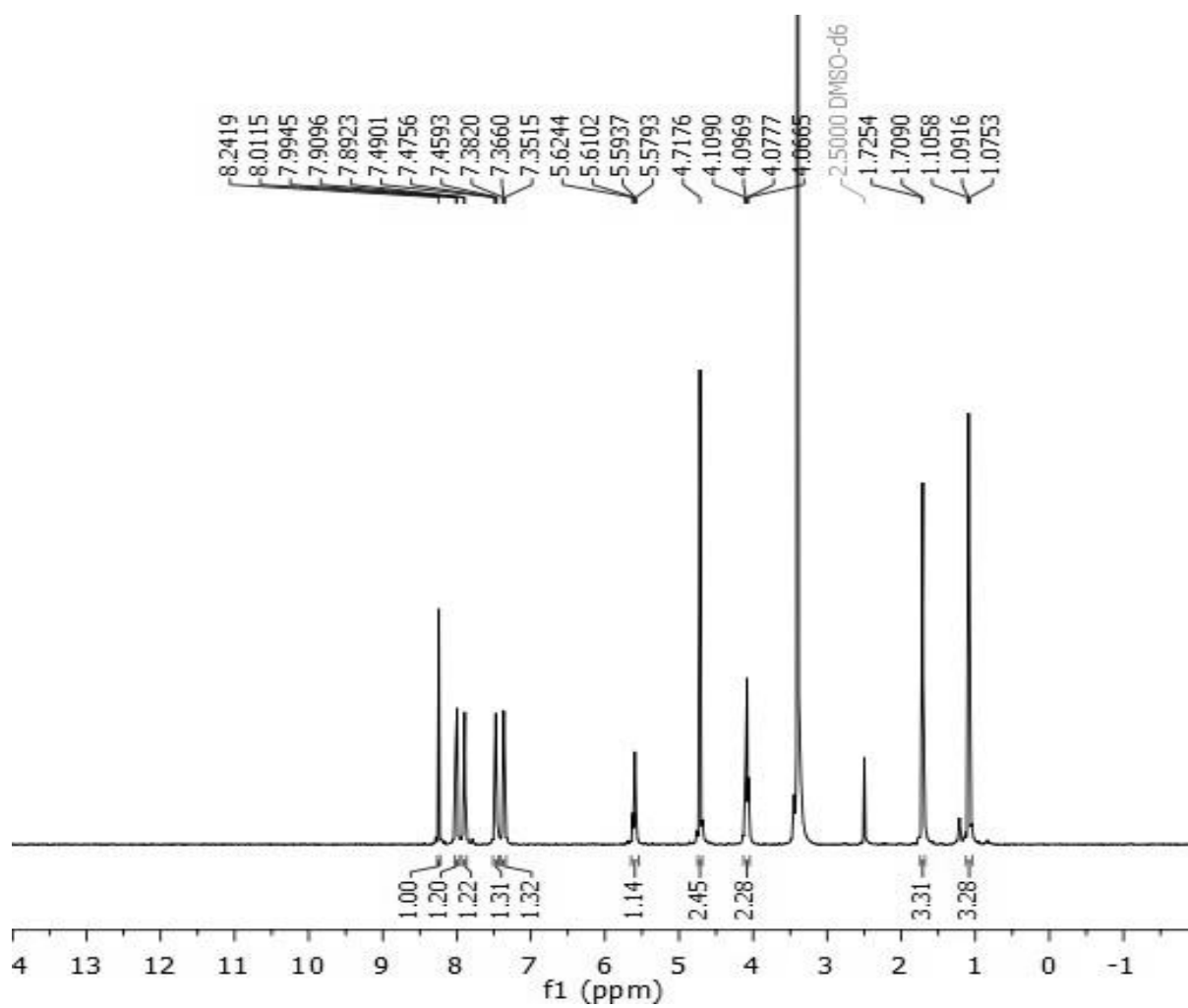
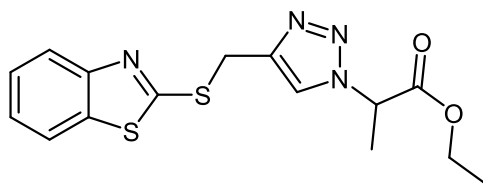


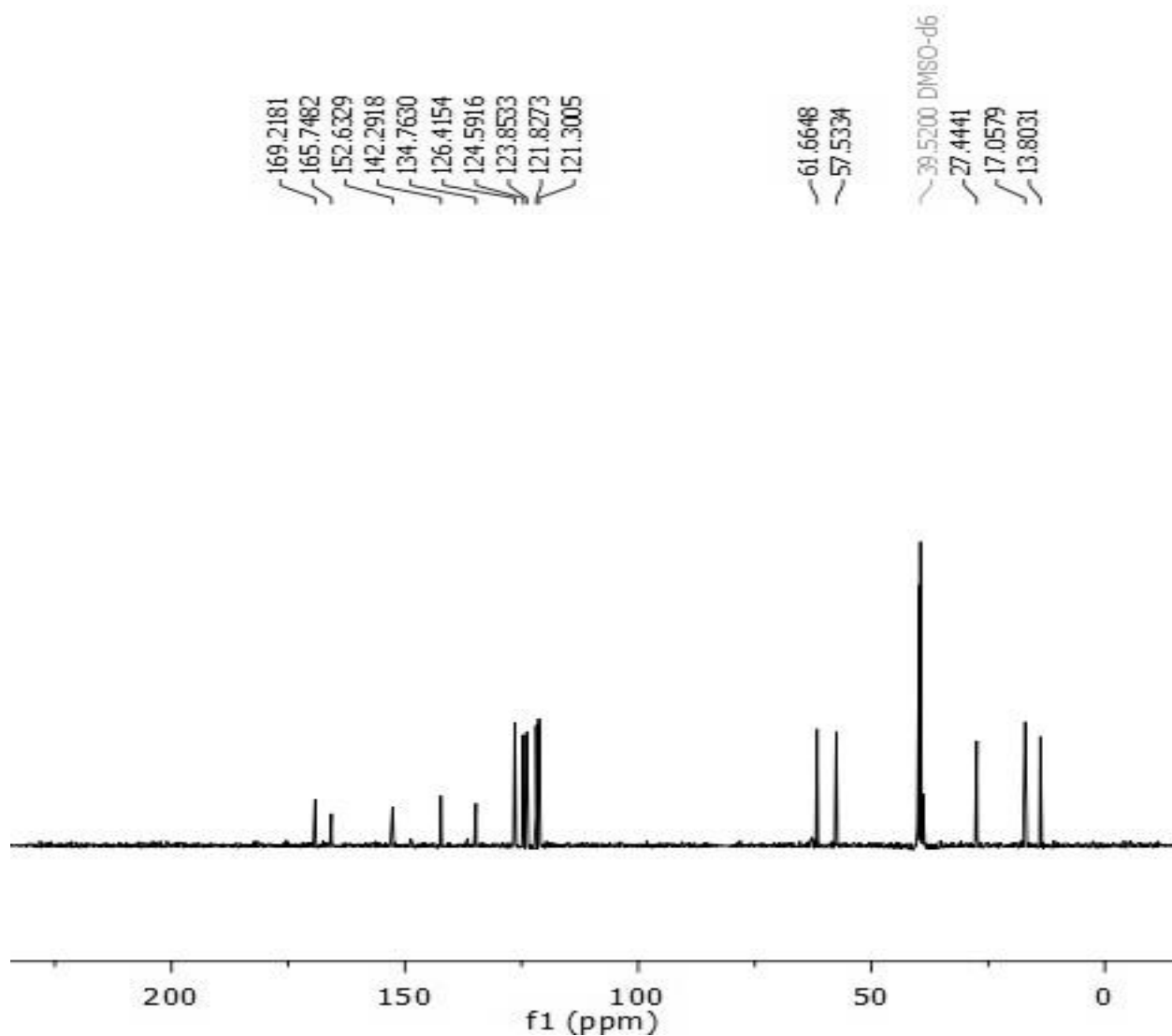
2-(4-((benzo[d]thiazol-2-ylthio) methyl)-1H-1,2,3-triazol-yl)-N-(m-tolyl)acetamide (5d): ¹H NMR (500 MHz, CDCl₃): δ = 2.30 (s, 3H), 4.72 (s, 2H), 5.12 (s, 2H), 6.95 (d, *J* = 7.4 Hz, 1H), 7.17-7.28 (m, 4H), 7.31-7.33 (m, 1H), 7.43 (t, *J* = 7.8 Hz, 1H), 7.74 (d, *J* = 8.1 Hz, 1H), 7.85 (s, 1H), 7.88 (d, *J* = 8.2 Hz, 1H), 9.09 (s, 1H) ppm. ¹³C NMR (125 MHz, CDCl₃): δ = 21.61, 27.66, 53.51, 117.53, 121.08, 121.39, 121.58, 121.77, 124.65, 126.02, 126.35, 128.97, 135.55, 137.00, 139.13, 144.59, 153.02, 163.40, 165.65 ppm. Anal. Calcd for C₁₉H₁₇N₅OS₂: C, 57.70; H, 4.33; N, 17.71. found: C, 57.77; H, 4.29; N, 17.68.





Ethyl 2-(4-((benzo[d]thiazol-2-ylthio)methyl)- 1H-1,2,3-triazol-1-yl)propanoate (5e): ^1H NMR (500 MHz, DMSO): δ = 1.09 (t, J = 7.1 Hz, 3H), 1.72 (d, J = 7.3 Hz, 3H), 4.10 (dd, J_1 = 8.6 Hz, J_2 = 5.6 Hz, 2H), 4.71 (s, 2H), 5.61 (dd, J_1 = 8.2 Hz, J_2 = 7.1 Hz, 1H), 7.38 (t, J = 7.2 Hz, 1H), 7.47 (t, J = 7.2 Hz, 1H), 7.90 (d, J = 8.6 Hz, 1H), 8.01 (d, J = 8.5 Hz, 1H), 8.24 (s, 1H) ppm. ^{13}C NMR (125 MHz, DMSO): δ = 13.80, 17.05, 27.44, 57.53, 61.66, 121.30, 121.82, 123.85, 124.59, 126.41, 134.76, 142.29, 152.63, 165.74, 169.21 ppm. Anal. Calcd for $\text{C}_{15}\text{H}_{16}\text{N}_4\text{O}_2\text{S}_2$: C, 51.71; H, 4.63; N, 16.08. found: C, 51.79; H, 4.78; N, 16.14.





Methyl 2-(4-((benzo[d]thiazol-2-ylthio) methyl)-1H-1,2,3-triazol-1-yl)acetate (5f) ^1H NMR (500 MHz, DMSO): δ = 3.64 (s, 3H), 4.74 (s, 2H), 5.39 (s, 2H), 7.37 (dt, J_1 = 7.7 Hz, J_2 = 2.9 Hz, 1H), 7.48 (dt, J_1 = 7.8 Hz, J_2 = 1.3 Hz, 1H), 7.89 (dd, J_1 = 8.2 Hz, J_2 = 1.3 Hz, 1H), 8.01 (dd, J_1 = 8.0 Hz, J_2 = 1.3 Hz, 1H), 8.14 (s, 1H) ppm. ^{13}C NMR (125 MHz, DMSO): δ = 27.79, 50.78, 52.95, 121.75, 122.78, 125.00, 125.77, 126.82, 135.21, 142.99, 153.06, 166.21, 168.10 ppm. Anal. Calcd for $\text{C}_{13}\text{H}_{12}\text{N}_4\text{O}_2\text{S}_2$: C, 48.74; H, 3.78; N, 17.49. found: C, 48.68; H, 3.86; N, 17.56.

