



SUPPLEMENTARY MATERIAL TO
**The synthesis, characterization, antioxidant and antimicrobial
activity of some novel amides of the esters of substituted
1,4-dihydropyridines**

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CHARACTERIZATION OF SYNTHESISED COMPOUNDS

1a

Yield: 72%. M.P. 157 °C.

Elemental: C₁₉H₂₃NO₄ (M_w=329.40 gmol⁻¹): C. 69.28; H. 7.04; N. 4.25; O. 19.43 %.

Found: C. 69.30; H. 7.02; N. 4.20; O. 19.48 %.

IR(KBr. cm⁻¹) ν_{max}: 3339.60 (N-H); 3033.27 (Ar-H); 2981.98 (C-H); 1685.90 (C=O).

2a

Yield: 53%. M.P. 184 °C.

Elemental: C₁₉H₂₃NO₅ (M_w=345.16 gmol⁻¹): C. 66.07; H. 6.71; N. 4.06; O. 23.16 %.

Found: C. 66.00; H. 6.78; N. 4.09; O. 23.13 %.

IR(KBr. cm⁻¹) ν_{max}: 3348.23 (N-H); 3027.11 (Ar-H); 2978.54 (C-H); 1702.04 (C=O); 1443.47 (C–OH); 818.27 (Ar-H).

3a

Yield: 81%. M.P. 230 °C.

Elemental: C₁₉H₂₃NO₅ (M_w=345.16 gmol⁻¹): C. 66.07; H. 6.71; N. 4.06; O. 23.16 %.

Found: C. 66.10; H. 6.68; N. 4.05; O. 23.17 %.

IR(KBr. cm⁻¹) ν_{max}: 3341.89 (N-H); 3107.12 (Ar-H); 2988.47 (C-H); 1701.75 (C=O); 1485.22 (C–OH); 826.31 (Ar-H).

4a

Yield: 65% M.P. 111 °C.

Elemental: C₁₉H₂₂NO₄Cl (M_w=363.5 gmol⁻¹) C. 63; H. 5.8; N. 3.9; O. 17.6; Cl. 9.7 %.

Found: C. 63.5; H. 5.6; N. 3.6; O. 17.5; Cl. 9.8 %.

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IR(KBr. cm^{-1}) ν_{max} : 3339.60 (N-H); 3031.3 (Ar-H). 2981.98 (C-H); 1685.90 (C=O); 827.13 (Ar-H); 701.67 (C-Cl)

5a

4-(4'-bromfenil)-2.6-dimetil-3.5-dikarboetoksi-1.4-dihidropiridin

Yield: 61% M.P. 95 °C.

Elemental: $\text{C}_{19}\text{H}_{22}\text{NO}_4\text{Br}$ ($M_w=408 \text{ gmol}^{-1}$) C. 56; H. 5.1; N. 3.5; O. 15.8; Br. 19.6 %. Found: C. 56.5; H. 5.2; N. 3.2; O. 15.6; Br. 19.5 %.

IR(KBr. cm^{-1}) ν_{max} : 3342.76 (N-H); 3102.3 (Ar-H). 2990.79 (C-H); 1703.28 (C=O); 808.57 (Ar-H); 682.52 (C-Br)

6a

Yield: 52%. M.P. 163 °C.

Elemental: $\text{C}_{19}\text{H}_{22}\text{N}_2\text{O}_6$ ($M_w=374.39 \text{ gmol}^{-1}$): C. 60.95; H. 5.92; N. 7.48; O. 25.65 %. Found: C. 60.90; H. 5.97; N. 7.50; O. 25.63 %.

IR(KBr. cm^{-1}) ν_{max} : 3342.76 (N-H); 3102.27 (Ar-H); 2990.79 (C-H); 1703.28 (C=O); 1643.16 (C-NO₂); 826.35 (Ar-H).

7a

Yield: 84%. M.P. 120 °C.

Elemental: $\text{C}_{19}\text{H}_{22}\text{N}_2\text{O}_6$ ($M_w=374.39 \text{ gmol}^{-1}$): C. 60.95; H. 5.92; N. 7.48; O. 25.65 %. Found: C. 60.88; H. 5.99; N. 7.45; O. 25.68 %.

IR (KBr. cm^{-1}) ν_{max} : 3316.31 (N-H); 3100.27 (Ar-H); 2978.05 (C-H); 1699.76 (C=O); 1644.22 (C-NO₂); 823.29 (Ar-H).

8a

Yield: 70% M.P. 93 °C.

Elemental: $\text{C}_{20}\text{H}_{25}\text{NO}_5$ ($M_w=359 \text{ gmol}^{-1}$) C. 67; H. 6.8; N. 3.9; O. 22.3 %. Found: C. 67.2; H. 6.5; N. 3.9; O. 22.4 %.

IR(KBr. cm^{-1}) ν_{max} : 3341.52 (N-H); 3027.11 (Ar-H); 2991.97 (C-H); 1720.79 (C=O); 1211.44 (C-OCH₃); 809.15 (Ar-H).

9a

Yield: 68% M.P. 90 °C.

Elemental: $\text{C}_{20}\text{H}_{25}\text{NO}_4$ ($M_w=343 \text{ gmol}^{-1}$) C. 70; H. 7; N. 4; O. 19 %. Found: C. 69.9; H. 7.2; N. 3.9; O. 21 %.

IR(KBr. cm^{-1}) ν_{max} : 3348.23 (N-H); 3030.11 (Ar-H); 2978.54 (C-H); 1646.90 (C=O). 1368.29 (CH₃); 818.27 (Ar-H).

10a

Yield: 71% M.P. 98 °C.

Elemental: $\text{C}_{20}\text{H}_{25}\text{NO}_4$ ($M_w=343 \text{ gmol}^{-1}$) C. 70; H. 7; N. 4; O. 19 %. Found: C. 70.1; H. 6.9; N. 4.1; O. 18.9 %.

IR(KBr. cm^{-1}) ν_{max} : 3341.89 (N-H); 3100.40 (Ar-H); 2988.47(C-H); 1655.47 (C=O). 1485.22 (CH₃); 840.95 (Ar-H).

1b

Yield: 72%. M.P. 124 °C.

Elemental: $\text{C}_{21}\text{H}_{19}\text{N}_5\text{O}_2\text{S}_2$ ($M_w=437.54 \text{ gmol}^{-1}$): C. 57.65; H. 4.38; N. 16.01; O. 7.31; S. 14.65 %. Found: C. 55.65; H. 4.38; N. 18.01; O. 7.01; S. 14.95 %.

IR(KBr. cm^{-1}) ν_{max} : 3339.34 (N-H); 1649.04 (HNCO); 737.54 (C-S-C); 1486.63 (C=N); 3085.82 (C-H aromatic).

^1H NMR: (400 MHz, CDCl_3 , δ/ppm): 7.296 – 7.270 (2H, m, C_6H_4), 7.210 (1H, t, $J_1 = J_2 = 7.6$ Hz, C_6H_4), 7.144 – 7.091 (6H, m, C_6H_4 , $\text{C}_3\text{H}_2\text{NS}$, NH), 6.552 (2H, d, $J = 3.6$ Hz, $\text{C}_3\text{H}_2\text{NS}$), 5.625 (1H, s, $\text{C}_5\text{H}_2\text{N}$), 2.338 (6H, s, CH_3).

^{13}C NMR: (100 MHz, CDCl_3 , δ/ppm): 167.60 (2C, C=O), 147.74 (1C, C_6H_4), 143.75 (2C, $\text{C}_3\text{H}_2\text{NS}$), 138.90 (2C, $\text{C}_3\text{H}_2\text{NS}$), 128.00 (2C, C_6H_4), 127.82 (2C, C_6H_4), 126.08 (1C, C_6H_4), 108.95 (2C, $\text{C}_3\text{H}_2\text{NS}$), 104.23 (2C, $\text{C}_5\text{H}_2\text{N}$), 59.70 (2C, $\text{C}_5\text{H}_2\text{N}$), 39.63 (1C, $\text{C}_5\text{H}_2\text{N}$), 14.24 (2C, CH_3).

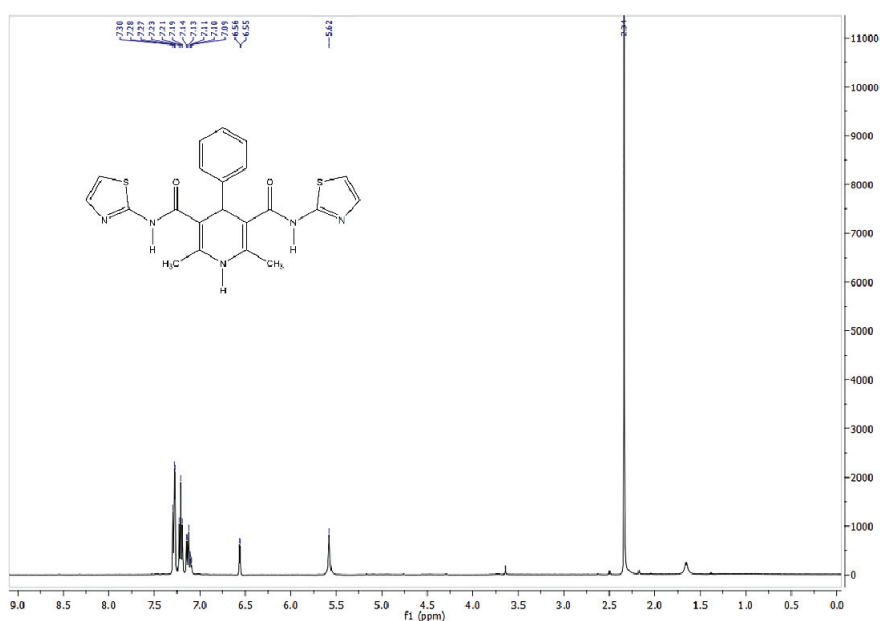
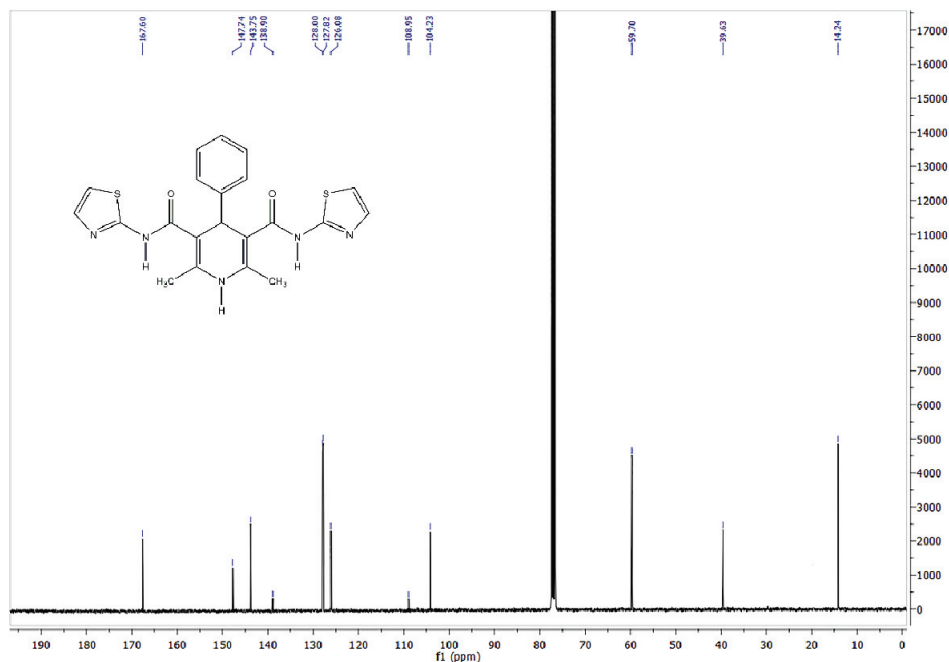


Fig S-1. The ^1H NMR spectrum of compound **1b**

Fig S-2. The ^{13}C NMR spectrum of compound **1b****2b**

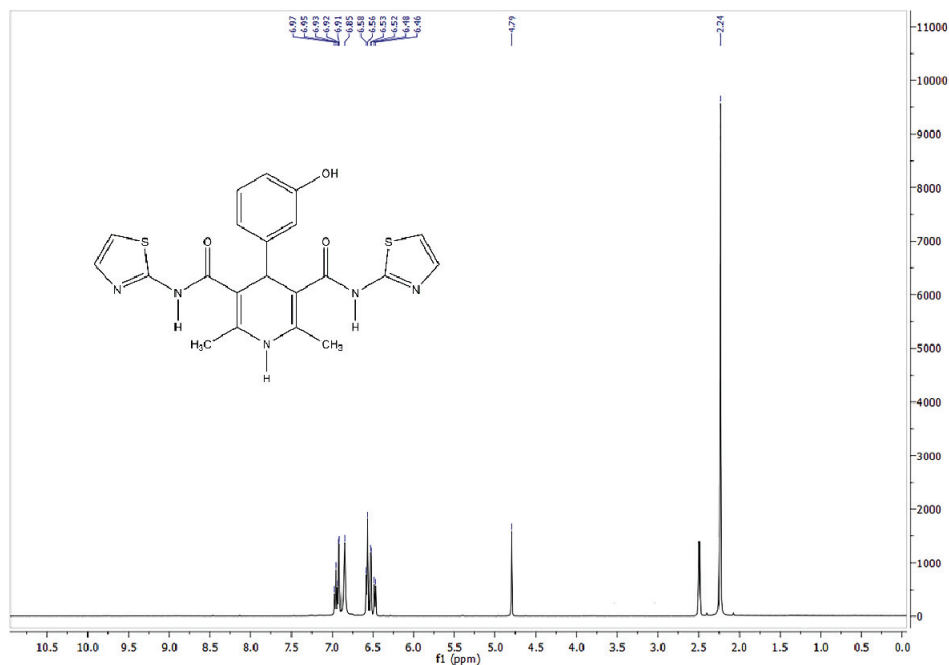
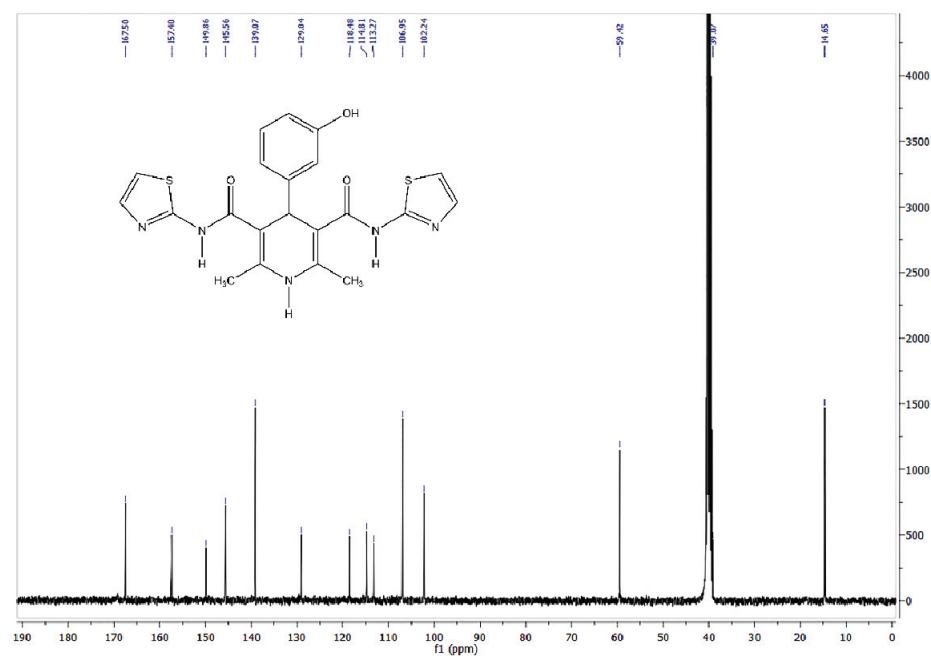
Yield: 53%. M.P. 141 °C.

Elemental: $\text{C}_{21}\text{H}_{19}\text{N}_5\text{O}_3\text{S}_2$ ($M_w=453.54 \text{ gmol}^{-1}$): C. 55.61; H. 4.22; N. 15.44; O. 10.58; S. 14.14%. Found: C. 54.25; H. 5.59; N. 15.50; O. 10.57; S. 14.09 %.

IR(KBr. cm^{-1}) ν_{max} : 3348.94 (N-H); 1647.21 (HNCO); 736.52 (C-S-C); 1479.70 (C=N); 3085.57 (C-H aromatic).

^1H NMR: (400 MHz, $\text{DMSO}-d_6$, δ/ppm): 6.953 (1H, t, $J_1 = 8.0 \text{ Hz}$, $J_2 = 7.6 \text{ Hz}$, C_6H_4), 6.915 (2H, d, $J = 3.6 \text{ Hz}$, $\text{C}_3\text{H}_2\text{NS}$), 6.846 (2H, s, NH), 6.572 (2H, d, $J = 7.2 \text{ Hz}$, C_6H_4), 6.528 (2H, d, $J = 3.6 \text{ Hz}$, $\text{C}_3\text{H}_2\text{NS}$), 6.474 (1H, d, $J = 8.8 \text{ Hz}$, C_6H_4), 4.794 (1H, s, $\text{C}_5\text{H}_2\text{N}$), 2.237 (6H, s, CH_3).

^{13}C NMR: (100 MHz, $\text{DMSO}-d_6$, δ/ppm): 167.50 (2C, C=O), 157.40 (1C, C_6H_4), 149.86 (1C, C_6H_4), 145.56 (2C, $\text{C}_3\text{H}_2\text{NS}$), 139.07 (2C, $\text{C}_3\text{H}_2\text{NS}$), 129.04 (1C, C_6H_4), 118.48 (1C, C_6H_4), 114.81 (1C, C_6H_4), 113.27 (1C, C_6H_4), 106.95 (2C, $\text{C}_3\text{H}_2\text{NS}$), 102.24 (2C, $\text{C}_5\text{H}_2\text{N}$), 59.42 (2C, $\text{C}_5\text{H}_2\text{N}$), 39.07 (1C, $\text{C}_5\text{H}_2\text{N}$), 14.65 (2C, CH_3).

Fig S-3. The ¹H NMR spectrum of compound **2b**Fig S-4. The ¹³C NMR spectrum of compound **2b**

3b

Yield: 81%. M.P. 164 °C.

Elemental: C₂₁H₁₉N₅O₃S₂ (M_w=453.54 gmol⁻¹): C. 55.61; H. 4.22; N. 15.44; O. 10.58; S. 14.14%. Found: C. 53.21; H. 6.62; N. 15.57; O. 10.45; S. 14.15 %.

IR(KBr. cm⁻¹) ν_{max}: 3343.03 (N-H); 1655.40 (HNCO); 739.38 (C-S-C); 1485.29 (C=N); 3074.12 (C-H aromatic).

¹H NMR: (400 MHz, CDCl₃, δ/ppm): 7.137 (2H, d, *J* = 8.4 Hz, C₆H₄), 7.092 (2H, d, *J* = 3.6 Hz, C₃H₂NS), 6.659 (2H, d, *J* = 8.4 Hz, C₆H₄), 6.548 (2H, d, *J* = 4.0 Hz, C₃H₂NS), 5.513 (1H, s, C₅H₂N), 4.913 (2H, s, NH), 2.325 (6H, s, CH₃);

¹³C NMR: (100 MHz, CDCl₃, δ/ppm): 167.67 (2C, C=O), 153.83 (1C, C₆H₄), 143.40 (2C, C₃H₂NS), 140.41 (1C, C₆H₄), 138.82 (2C, C₃H₂NS), 129.20 (2C, C₆H₄), 114.63 (2C, C₆H₄), 108.94 (2C, C₃H₂NS), 104.49 (2C, C₃H₂NS), 59.70 (2C, C₅H₂N), 38.79 (1C, C₅H₂N), 14.26 (2C, CH₃).

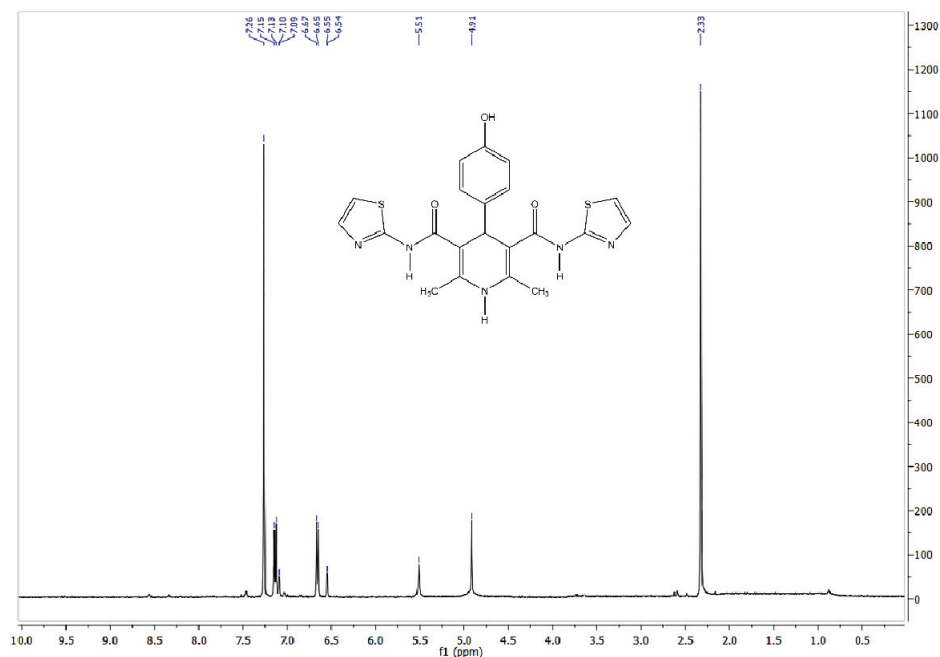
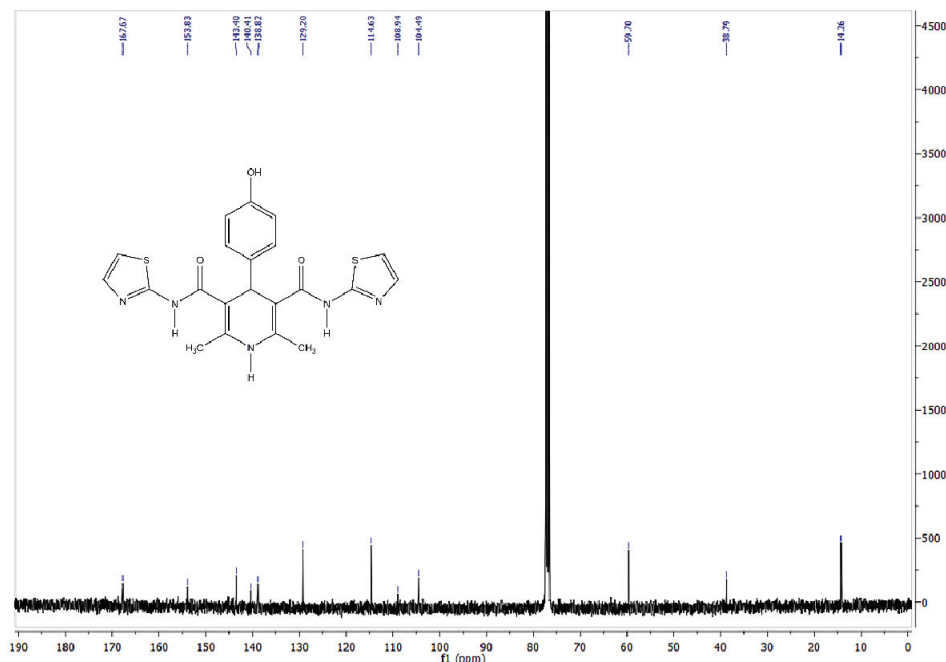


Fig S-5. The ¹H NMR spectrum of compound **3b**

Fig S-6. The ^{13}C NMR spectrum of compound **3b****4b**

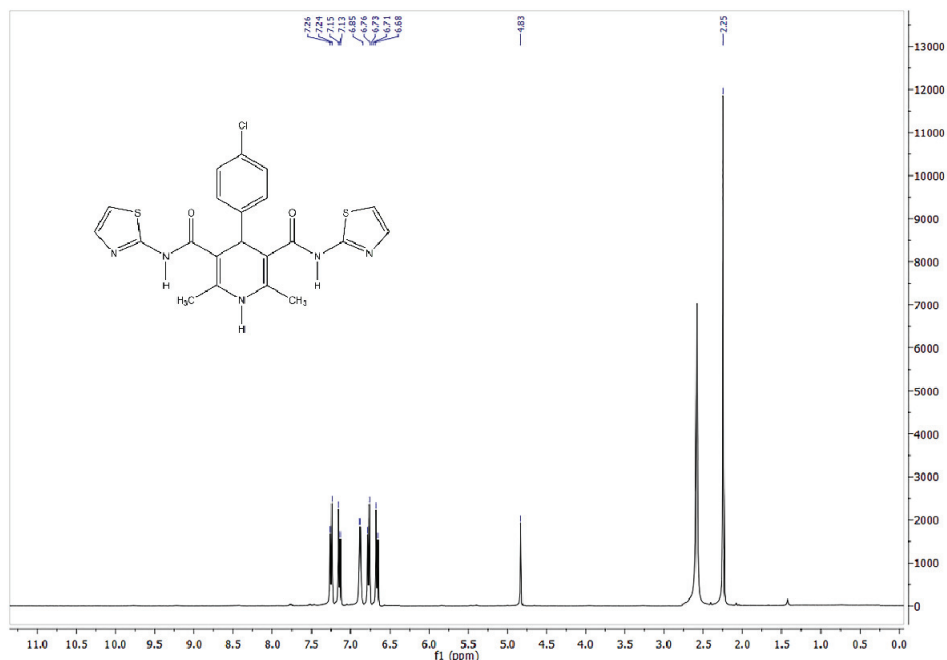
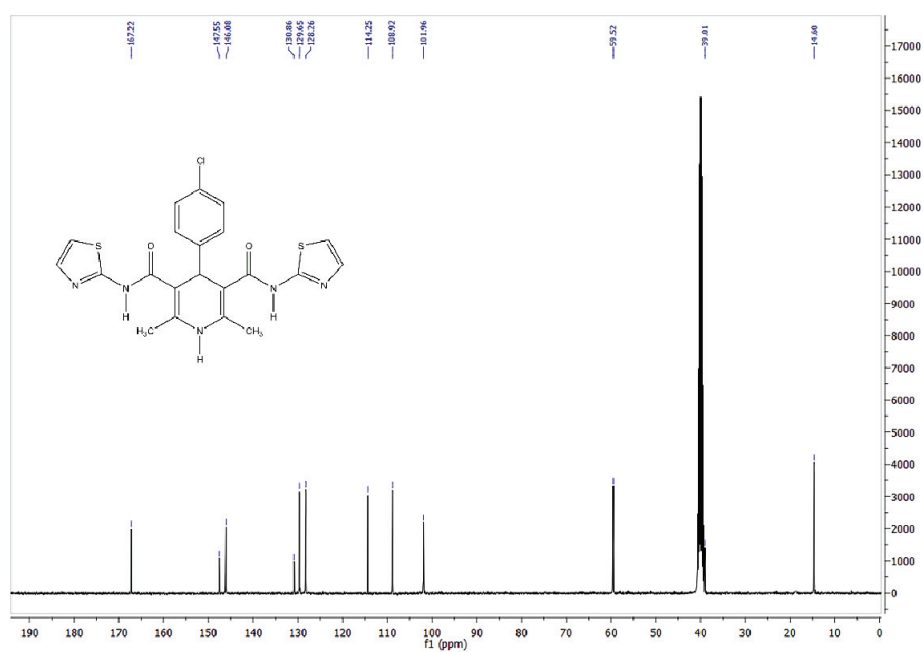
Yield: 79% M.P. 124 °C.

Elemental: $\text{C}_{21}\text{H}_{18}\text{N}_5\text{O}_2\text{S}_2\text{Cl}$ ($M_w=471.5 \text{ gmol}^{-1}$) C. 53.4; H. 3.8; N. 14.8; O. 6.8; S. 13.6; Cl. 7.5 % Found: C. 53.5; H. 3.9; N. 14.9; O. 6.7; S. 13.4; Cl. 7.5 %

IR(KBr. cm^{-1}) ν_{max} : 3339.34 (N-H); 1649.04 (HNCO); 701.52 (C-S-C); 1486.63 (C=N); 3085.82 (C-H aromatic); 737.57 (C-Cl).

^1H NMR: (400 MHz, $\text{DMSO-}d_6$, δ/ppm): 7.251 (2H, d, $J = 8.4 \text{ Hz}$, C_6H_4), 7.143 (2H, d, $J = 8.4 \text{ Hz}$, C_6H_4), 6.848 (2H, s, NH), 6.752 (2H, d, $J = 3.6 \text{ Hz}$, $\text{C}_3\text{H}_2\text{NS}$), 6.694 (2H, d, $J = 3.6 \text{ Hz}$, $\text{C}_3\text{H}_2\text{NS}$), 4.829 (1H, s, $\text{C}_5\text{H}_2\text{N}$), 2.246 (6H, s, CH_3);

^{13}C NMR: (100 MHz, $\text{DMSO-}d_6$, δ/ppm): 167.22 (2C, C=O), 147.55 (1C, C_6H_4), 146.08 (2C, $\text{C}_3\text{H}_2\text{NS}$), 130.86 (1C, C_6H_4), 129.65 (2C, C_6H_4), 128.26 (2C, C_6H_4), 114.25 (2C, $\text{C}_3\text{H}_2\text{NS}$), 108.92 (2C, $\text{C}_3\text{H}_2\text{NS}$), 101.96 (2C, $\text{C}_5\text{H}_2\text{N}$), 59.52 (2C, $\text{C}_5\text{H}_2\text{N}$), 39.01 (1C, $\text{C}_5\text{H}_2\text{N}$), 14.60 (2C, CH_3).

Fig S-7. The ¹H NMR spectrum of compound **4b**Fig S-8. The ¹³C NMR spectrum of compound **4b**

5b

Yield: 83% M.P. 105 °C.

Elemental: C₂₁H₁₈N₅O₂S₂Br (M_w=516 gmol⁻¹) C. 48.8; H. 3.5; N. 13.5; O. 6.2; S. 12.4; Br. 15.5 % Found: C. 48.9; H. 3.4; N. 13.6; O. 6.3; S. 12.4; Br. 15.4 %

IR (KBr. cm⁻¹) ν_{max}: 3315.23 (N-H); 1681.10 (HNCO). 705.45 (C-S-C); 1483.35 (C=N) i 3104.06 (C-H aromatic); 2978.34 (C-H stretch); 629.35 (C-Br)

¹H NMR: (400 MHz, DMSO-*d*₆, δ/ppm): 7.383 (2H, d, *J* = 8.0 Hz, C₆H₄), 7.089 (2H, d, *J* = 8.4 Hz, C₆H₄), 6.916 (2H, d, *J* = 3.6 Hz, C₃H₂NS), 6.862 (2H, s, NH), 6.523 (2H, d, *J* = 3.6 Hz, C₃H₂NS), 4.817 (1H, s, C₅H₂N), 2.246 (6H, s, CH₃);

¹³C NMR: (100 MHz, DMSO-*d*₆, δ/ppm): 167.24 (2C, C=O), 147.97 (1C, C₆H₄), 146.13 (2C, C₃H₂NS), 139.03 (2C, C₃H₂NS), 131.19 (2C, C₆H₄), 130.09 (2C, C₆H₄), 119.39 (1C, C₆H₄), 106.99 (2C, C₃H₂NS), 101.89 (2C, C₃H₂N), 59.55 (2C, C₅H₂N), 39.10 (1C, C₅H₂N), 14.61 (2C, CH₃).

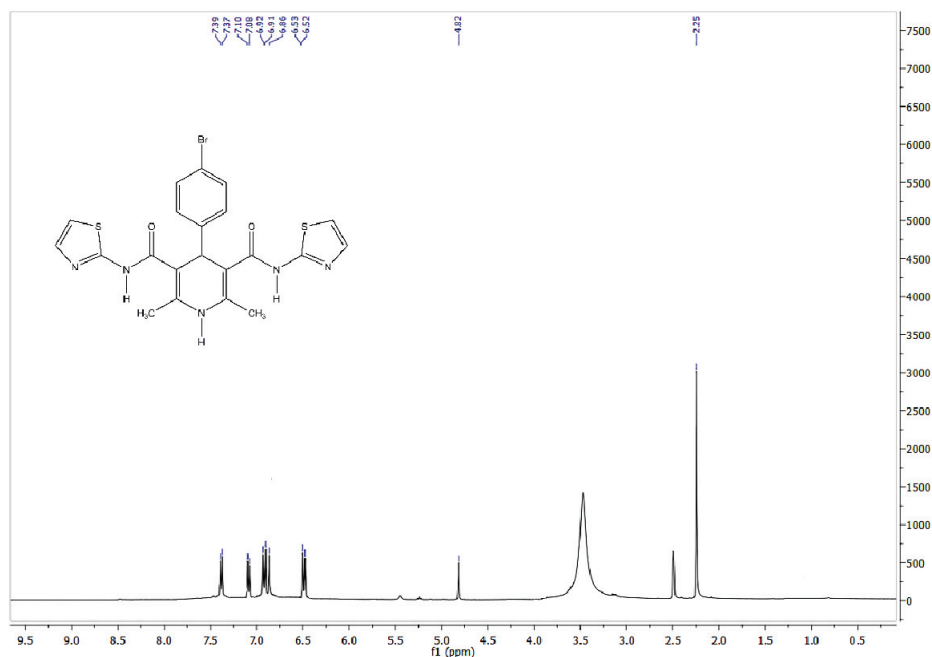
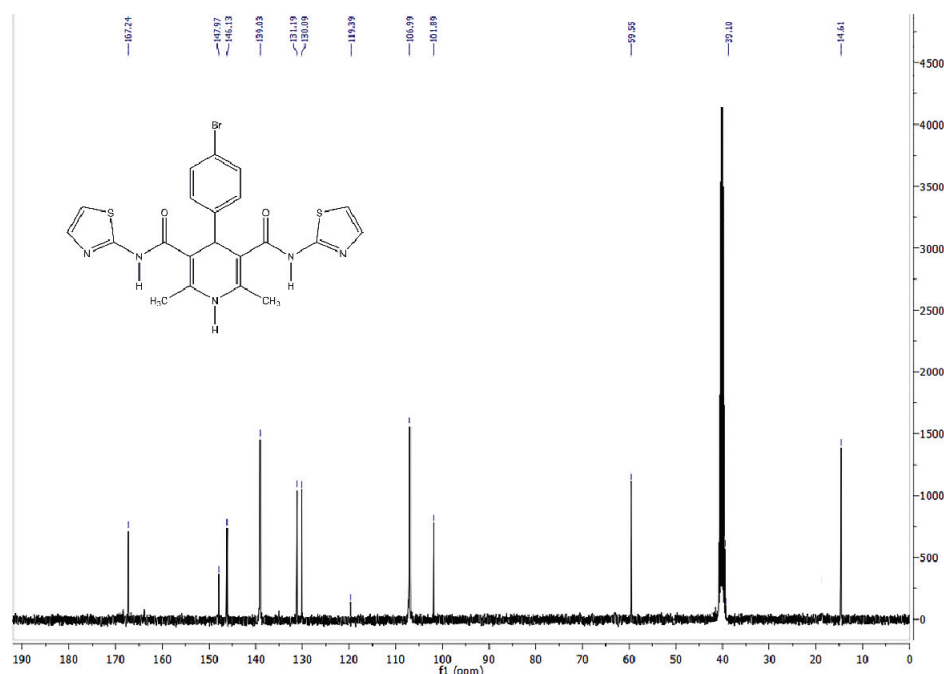


Fig S-9. The ¹H NMR spectrum of compound **5b**

Fig S-10. The ^{13}C NMR spectrum of compound **5b****6b**

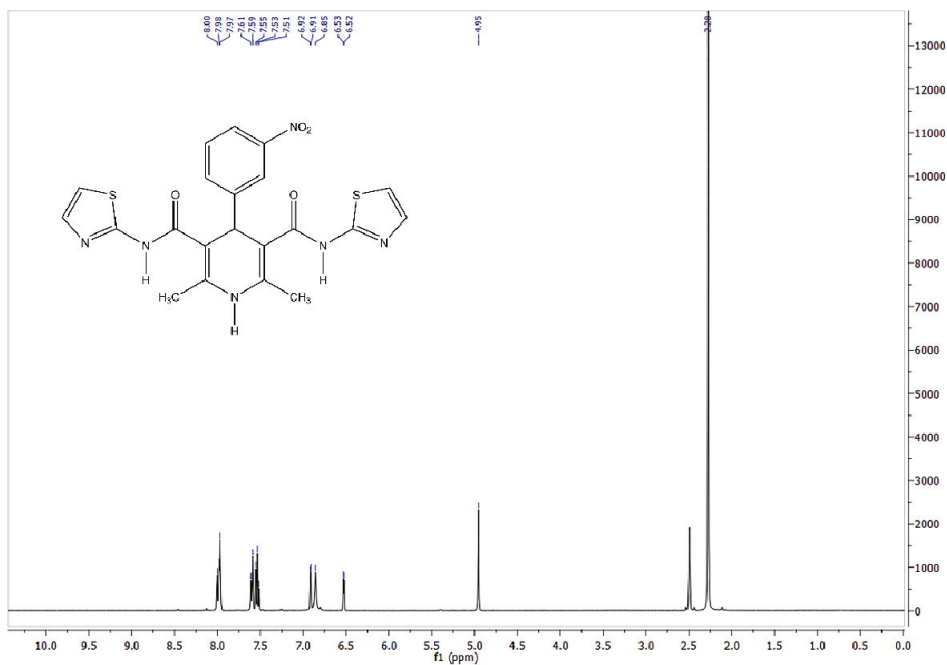
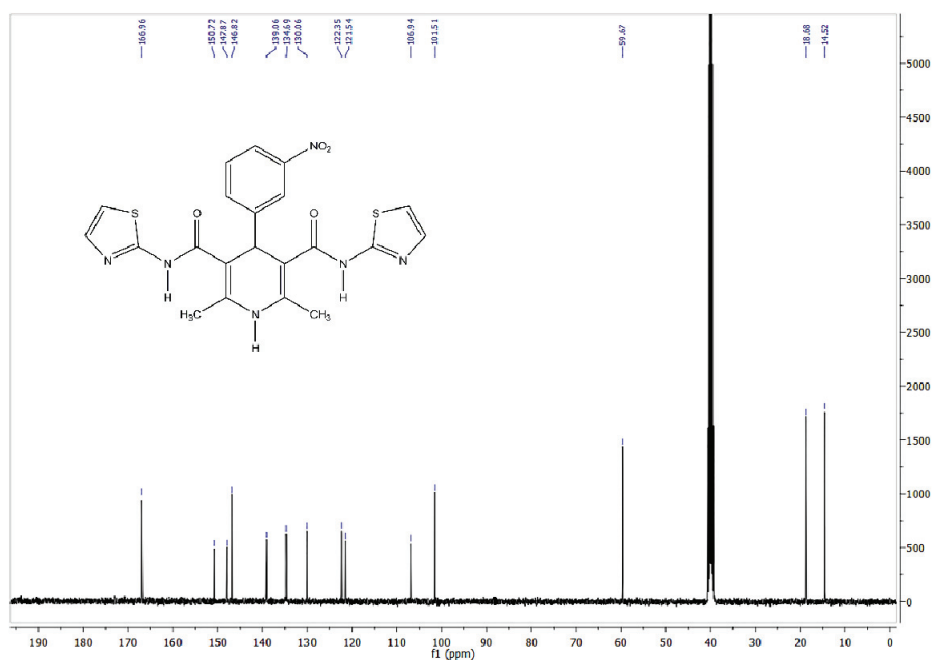
Yield: 52%. M.P. 128 °C.

Elementalna: $\text{C}_{21}\text{H}_{18}\text{N}_6\text{O}_4\text{S}_2$ ($M_w=482.53 \text{ g mol}^{-1}$): C. 52.27; H. 3.76; N. 17.42; O. 13.26; S. 13.29 %. Found: C. 52.00; H. 4.03; N. 17.01; O. 13.76; S. 13.20 %.

IR(KBr. cm^{-1}) ν_{max} : 3180.01 (N-H); 1643.61 (HNCO); 740.59 (C-S-C); 1484.01 (C=N); 3074.47 (C-H aromatic).

^1H NMR: (400 MHz, $\text{DMSO-}d_6$, δ/ppm): 8.002 – 7.969 (2H, m, C_6H_4), 7.599 (1H, d, $J=7.6$ Hz, C_6H_4), 7.533 (1H, t, $J_1=8.0$ Hz, $J_2=7.2$ Hz, C_6H_4), 6.913 (2H, d, $J=4.0$ Hz, C_6H_4), 6,855 (2H, s, NH), 6.527 (2H, d, $J=3.6$ Hz, $\text{C}_3\text{H}_2\text{NS}$), 4.954 (1H, s, $\text{C}_5\text{H}_2\text{N}$), 2.275 (6H, s, CH_3).

^{13}C NMR: (100 MHz, $\text{DMSO-}d_6$, δ/ppm): 166.96 (2C, C=O), 150.72 (1C, C_6H_4), 147.87 (1C, C_6H_4), 146.82 (2C, $\text{C}_3\text{H}_2\text{NS}$), 139.06 (2C, $\text{C}_3\text{H}_2\text{NS}$), 134.69 (1C, C_6H_4), 130.06 (1C, C_6H_4), 122.35 (1C, C_6H_4), 121.54 (1C, C_6H_4), 106.94 (2C, $\text{C}_3\text{H}_2\text{NS}$), 101.51 (2C, $\text{C}_5\text{H}_2\text{N}$), 59.67 (2C, $\text{C}_5\text{H}_2\text{N}$), 18.68 (1C, $\text{C}_5\text{H}_2\text{N}$), 14.52 (2C, CH_3).

Fig S-11. The ¹H NMR spectrum of compound **6b**Fig S-12. The ¹³C NMR spectrum of compound **6b**

7b

Yield 84%. M.P.105 °C.

Elemental: C₂₁H₁₈N₆O₄S₂ (M_w=482.53 gmol⁻¹): C. 52.27; H. 3.76; N. 17.42; O. 13.26; S. 13.29 %. Found: C. 53.27; H. 2.76; N. 17.72; O. 13.26; S. 12.99 %.

IR (KBr. cm⁻¹) ν_{max}: 3304.06 (N-H); 1643.97 (HNCO); 746.11 (C-S-C); 1483.35 (C=N); 2978.34 (C-H aromatic).

¹H NMR: (400 MHz, CDCl₃, δ/ppm): 8.083 (2H, d, *J* = 8.4 Hz, C₆H₄), 7.449 (2H, d, *J* = 8.8 Hz, C₆H₄), 7.084 (2H, d, *J* = 3.6 Hz, C₃H₂NS), 6.544 (2H, d, *J* = 3.6 Hz, C₃H₂NS), 5.703 (1H, s, C₅H₂N), 5.093 (2H, s, NH), 2.358 (6H, s, CH₃);

¹³C NMR: (100 MHz, CDCl₃, δ/ppm): 167.02 (2C, C=O), 155.04 (1C, C₆H₄), 146.37 (1C, C₆H₄), 144.52 (2C, C₃H₂NS), 138.76 (2C, C₃H₂NS), 128.89 (2C, C₆H₄), 123.29 (2C, C₆H₄), 108.89 (2C, C₃H₂NS), 103.27 (2C, C₃H₂N), 59.99 (2C, C₅H₂N), 40.13 (1C, C₅H₂N), 14.25 (2C, CH₃).

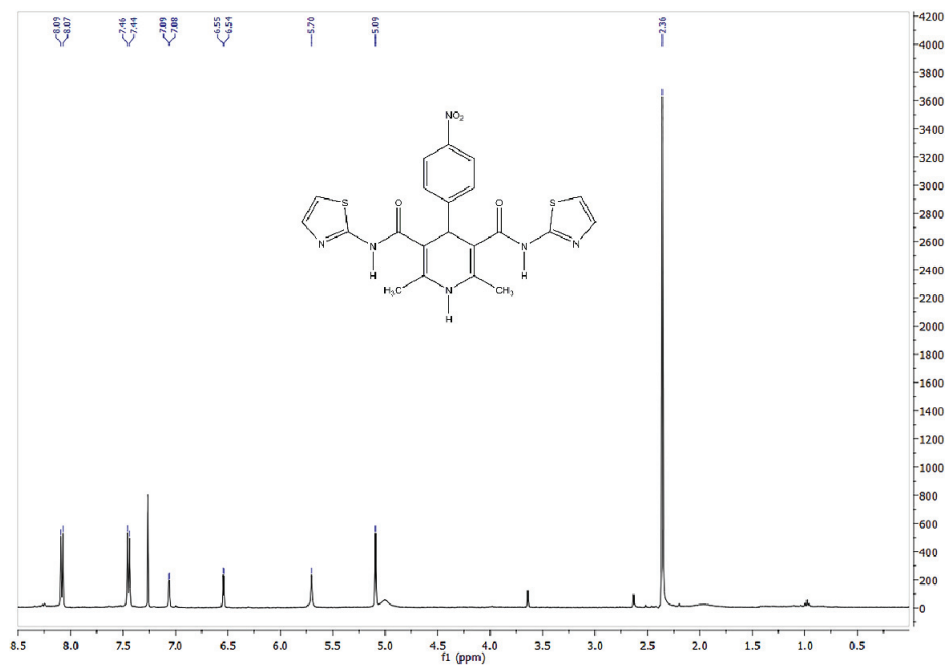
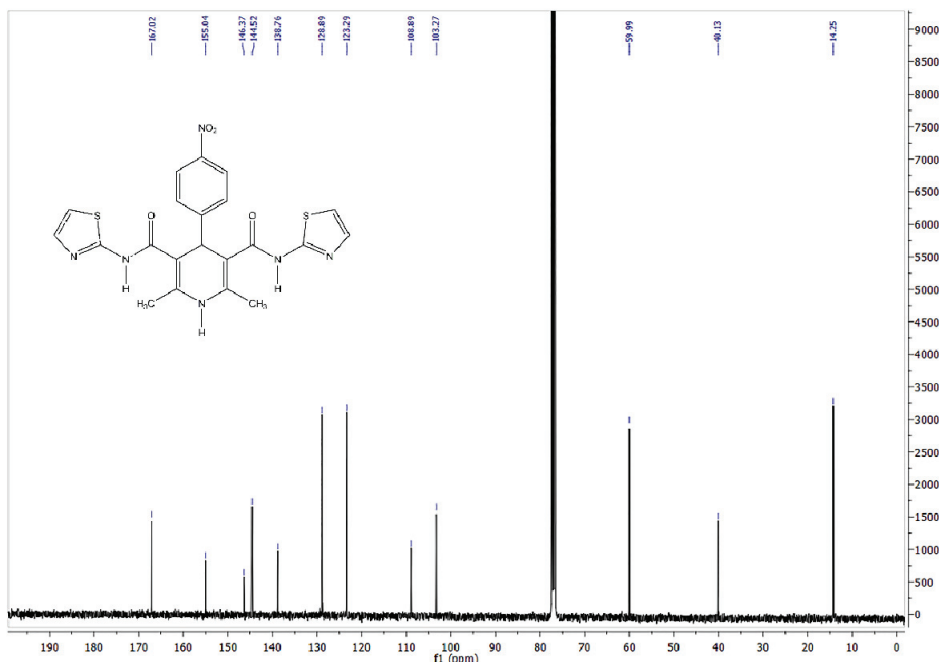


Fig S-13. The ¹H NMR spectrum of compound **7b**

Fig S-14. The ^{13}C NMR spectrum of compound **7b****8b**

Yield: 78% M.P. 141 °C.

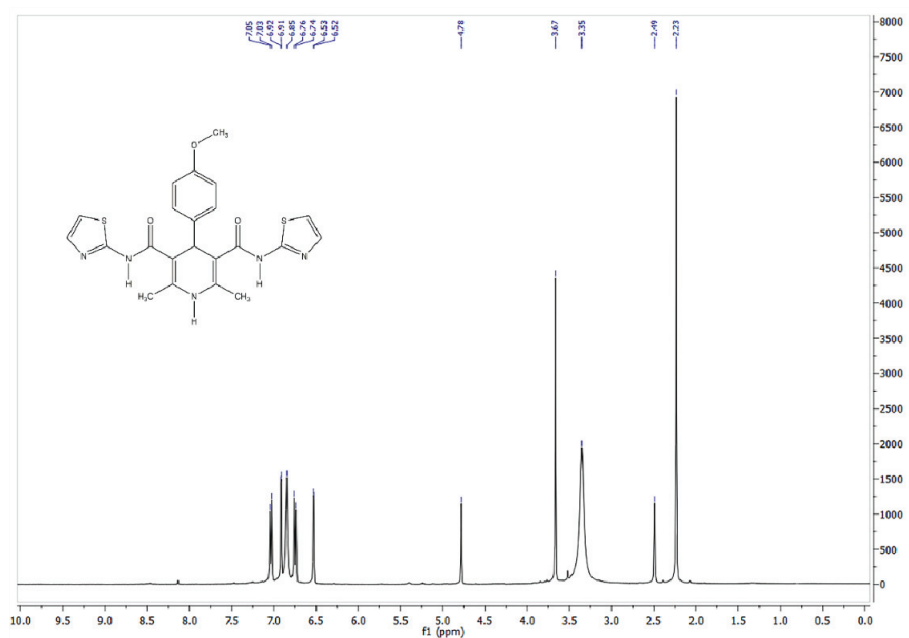
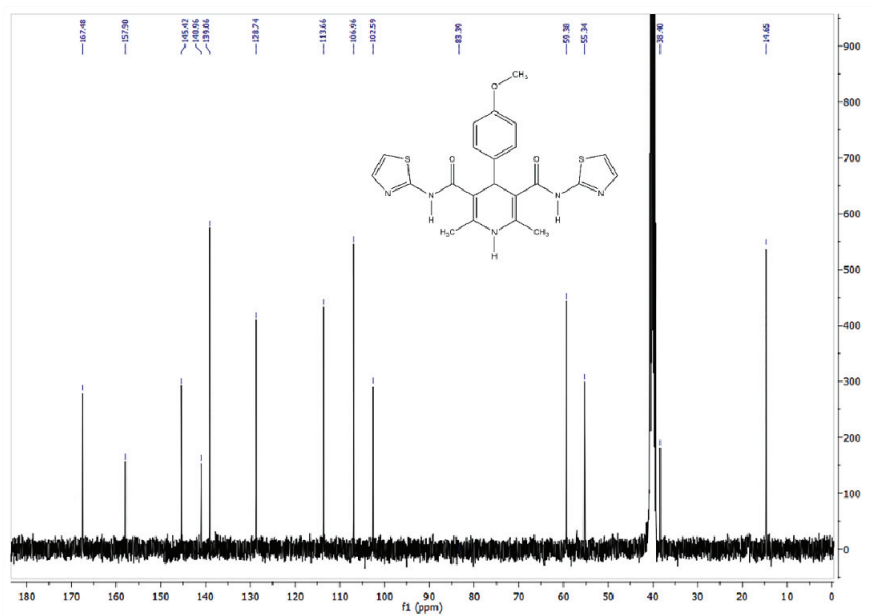
Elemental: $\text{C}_{21}\text{H}_{21}\text{N}_5\text{O}_3\text{S}_2$ ($M_w=467 \text{ gmol}^{-1}$) C. 56.5; H. 4.5; N. 15; O. 10.3; S. 13.7 %.

Found: C. 56.6; H. 4.6; N. 14.8; O. 10.4; S. 13.6 %.

IR(KBr. cm^{-1}) ν_{max} : 3348.94 (N-H); 1647.21 (HNCO); 736.52 (C-S-C); 1479.70 (C=N); 3085.57 (C-H aromatic); 1221.1 (C-OCH₃); 2978.75 (C-H stretch).

^1H NMR: (400 MHz, DMSO- d_6 , δ/ppm): 7.037 (2H, d, $J = 8.4 \text{ Hz}$, C_6H_4), 6.915 (2H, d, $J = 3.6 \text{ Hz}$, $\text{C}_3\text{H}_2\text{NS}$), 6.849 (2H, s, NH), 6.746 (2H, d, $J = 8.4 \text{ Hz}$, C_6H_4), 6.528 (2H, d, $J = 3.6 \text{ Hz}$, $\text{C}_3\text{H}_2\text{SN}$), 4.781 (1H, s, $\text{C}_5\text{H}_2\text{N}$), 3.665 (3H, s, OCH₃), 2.284 (6H, s, CH₃).

^{13}C NMR: (100 MHz, DMSO- d_6 , δ/ppm): 167.48 (2C, C=O), 157.90 (1C, C_6H_4), 145.42 (2C, $\text{C}_3\text{H}_2\text{NS}$), 140.96 (1C, C_6H_4), 139.06 (2C, C_6H_4), 128.74 (2C, $\text{C}_3\text{H}_2\text{NS}$), 113.66 (2C, $\text{C}_3\text{H}_2\text{NS}$), 106.96 (2C, C_6H_4), 102.56 (2C, $\text{C}_5\text{H}_2\text{N}$), 55.34 (1C, OCH₃), 38.40 (1C, $\text{C}_6\text{H}_4\text{N}$), 14.65 (2C, CH₃).

Fig S-15. The ¹H NMR spectrum of compound **8b**Fig S-16. The ¹³C NMR spectrum of compound **8b**

9b

Yield: 77% M.P. 251 °C.

Elemental: C₂₂H₂₁N₅O₂S₂ (M_w=451 gmol⁻¹) C. 58.5; H. 4.6; N. 15.5; O. 7.1; S. 14.2 %.
Found: C. 58.6; H. 4.4; N. 15.7; O. 6.9; S. 14.4 %.

IR(KBr. cm⁻¹) ν_{max}: 3310.35 (N-H); 1707.02 (HNCO); 781.65 (C-S-C); 1470.59 (C=N); 3022.21 (C-H aromatic).

¹H NMR: (400 MHz, DMSO-*d*₆, δ/ppm): 7.066 (1H, t, J₁ = J₂ = 7.6 Hz, C₆H₄), 6.950 – 6.854 (7H, m, C₆H₄, NH, C₃H₂NS), 6.525 (2H, d, J = 3.6 Hz, C₃H₂NS), 4.819 (1H, s, C₅H₂N), 2.245 (6H, s, CH₃), 2.210 (3H, s, CH₃).

¹³C NMR: (100 MHz, DMSO-*d*₆, δ/ppm): 167.43 (2C, C=O), 148.56 (1C, C₆H₄), 145.67 (2C, C₃H₂NS), 136.97 (2C, C₆H₄), 128.49 (1C, C₆H₄), 128.23 (1C, C₃H₂NS), 126.97 (1C, C₆H₄), 124.94 (1C, C₃H₂NS), 106.95 (2C, C₃H₂NS), 102.32 (2C, C₅H₂N), 59.39 (2C, C₅H₂N), 39.26 (1C, C₅H₂N), 21.65 (1C, CH₃), 14.62 (2C, CH₃).

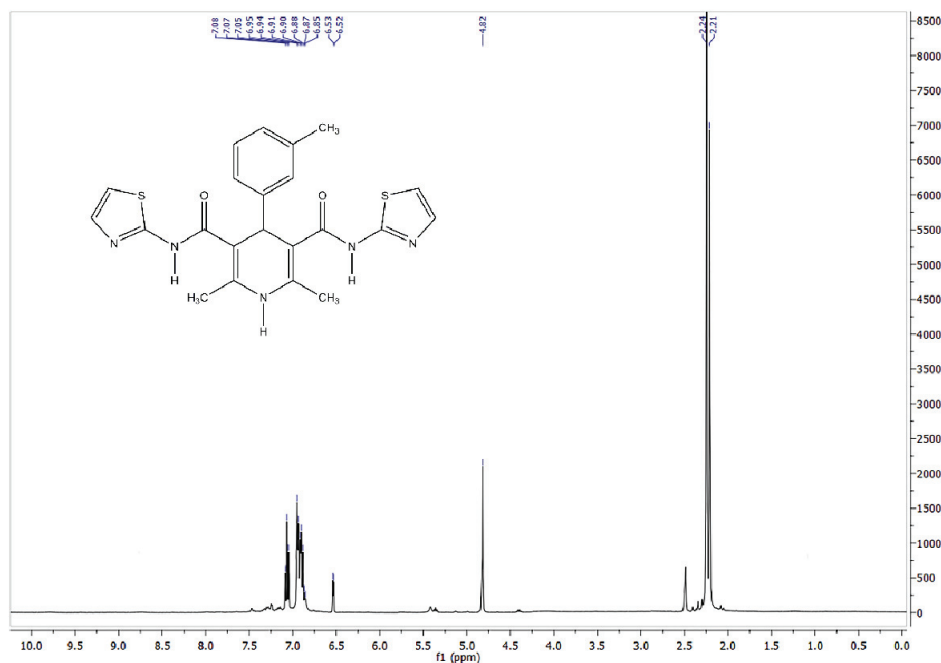
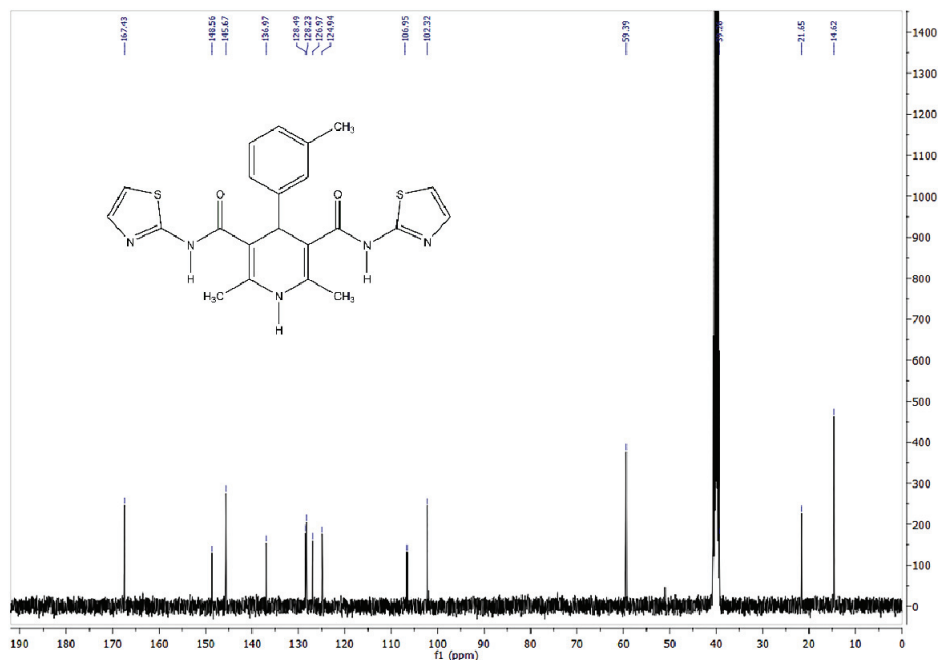


Fig S-17. The ¹H NMR spectrum of compound **9b**

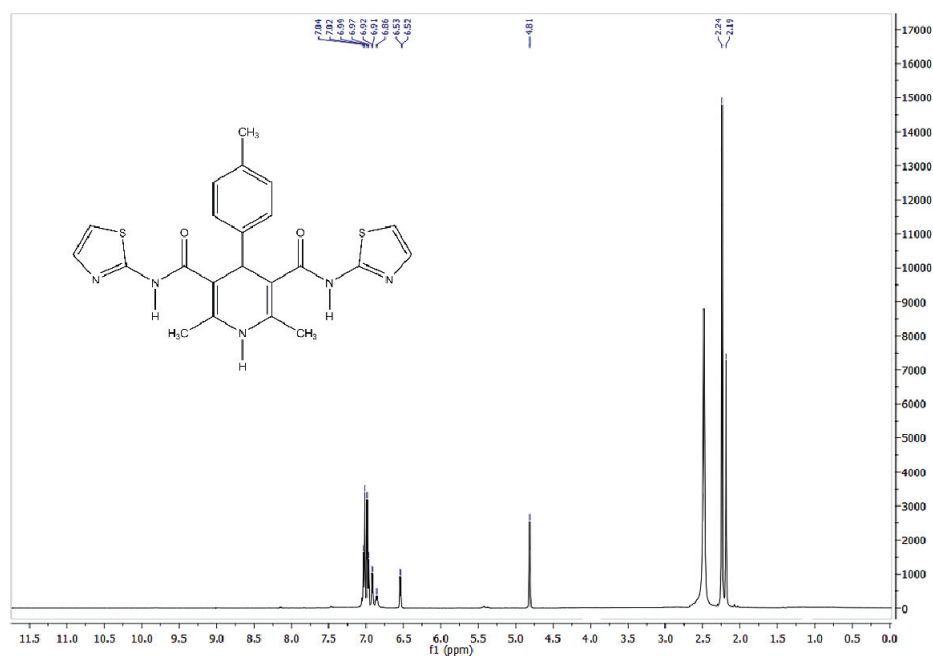
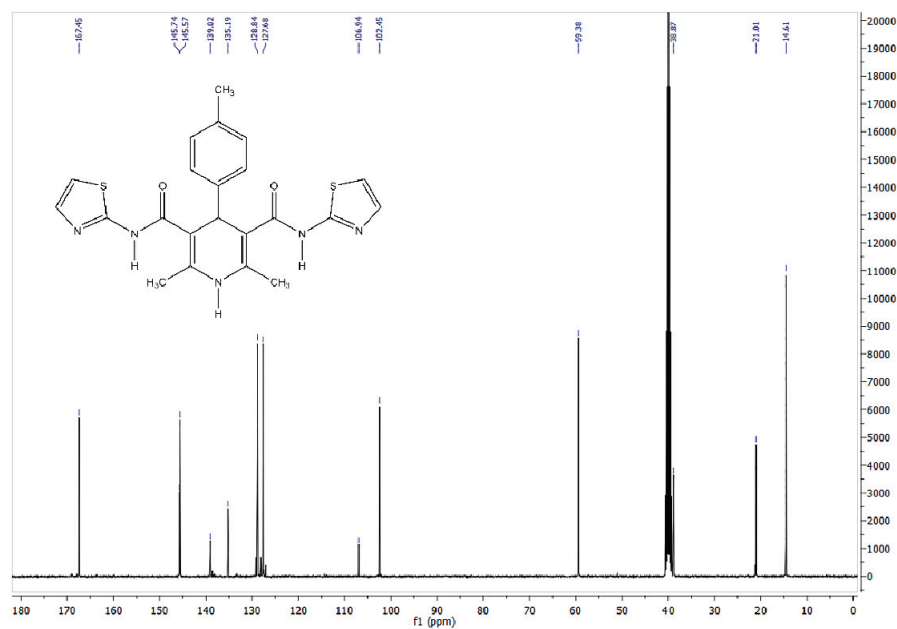
Fig S-18. The ^{13}C NMR spectrum of compound **9b****10b**

Yield: 80% M.P. 164 °C.

Elemental: $\text{C}_{22}\text{H}_{21}\text{N}_5\text{O}_2\text{S}_2$ ($M_w=451 \text{ gmol}^{-1}$) C. 58.5; H. 4.6; N. 15.5; O. 7.1; S. 14.2 %.

Found: C. 58.7; H. 4.5; N. 15.6; O. 7.2; S. 14 %.

IR(KBr. cm^{-1}) ν_{max} : 3343.03 (N-H); 1695.40 (HNCO); 779.38 (C-S-C); 1477.29 (C=N); 3027.12 (C-H aromatic). ^1H NMR: (400 MHz, $\text{DMSO}-d_6$, δ/ppm): 7.026 (2H, d, $J = 8.0$ Hz, C_6H_4), 6.978 (2H, d, $J = 8.0$ Hz, C_6H_4), 6.920 (2H, d, $J = 3.6$ Hz, $\text{C}_3\text{H}_2\text{NS}$), 6.858 (2H, s, NH), 6.522 (2H, d, $J = 3.6$ Hz, $\text{C}_3\text{H}_2\text{NS}$), 4.814 (1H, s, $\text{C}_5\text{H}_2\text{N}$), 2.243 (6H, s, CH_3), 2.190 (3H, s, CH_3); ^{13}C NMR: (100 MHz, $\text{DMSO}-d_6$, δ/ppm): 167.45 (2C, C=O), 145.74 (1C, C_6H_4), 145.57 (2C, $\text{C}_3\text{H}_2\text{NS}$), 139.02 (2C, $\text{C}_3\text{H}_2\text{NS}$), 135.19 (1C, C_6H_4), 128.84 (2C, C_6H_4), 127.68 (2C, C_6H_4), 106.94 (2C, $\text{C}_3\text{H}_2\text{NS}$), 102.45 (2C, $\text{C}_5\text{H}_2\text{N}$), 59.38 (2C, $\text{C}_5\text{H}_2\text{N}$), 38.87 (1C, $\text{C}_5\text{H}_2\text{N}$), 21.01 (1C, CH_3), 14.61 (2C, CH_3).

Fig S-19. The ¹H NMR spectrum of compound **10b**Fig S-20. The ¹³C NMR spectrum of compound **10b**.