



SUPPLEMENTARY MATERIAL TO

Green chemical principles based regioselective functionalization of 2,4,6-trichloropyrimidine-5-carbaldehyde: Application in the synthesis of new pyrimidines and pyrrolopyrimidine

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SPECTRAL AND ANALYTICAL DATA FOR THE NEW COMPOUNDS

2,4-Dichloro-6-(cyclopentylamino) pyrimidine-5-carbaldehyde (7)

White powder; m.p.: 121–122 °C; ¹H-NMR (400 MHz, DMSO-*d*₆, δ / ppm): 10.20 (*s*, 1H), 9.30 (*s*, 1H), 4.4 (*m*, 1H), 2.03–1.90 (*m*, 2H), 1.80–1.55 (*m*, 6H); ¹³C-NMR (100 MHz, DMSO, δ / ppm): 190.77, 165.09, 163.41, 160.94, 112.38, 52.84, 32.17, 31.77, 23.35, 23.22; IR (cm⁻¹): 3260.00, 2951.11, 1713.14; MS (ESI): *m/z*: (M+H)⁺: 260; Anal. Calcd for C₁₀H₁₁Cl₂N₃O: C, 46.17; H, 4.26; Cl, 27.26; N, 16.15. Found: C, 46.16; H, 4.27; Cl, 27.25; N, 16.13.

Methyl (Z)-2-bromo-3-(2,4-dichloro-6-(cyclopentylamino)pyrimidin-5-yl)acrylate (9)

Brown solid; m.p.: 138–139 °C, ¹H-NMR (400 MHz, DMSO-*d*₆, δ / ppm): 7.90 (*s*, 1H), 7.45 (*m*, 1H), 4.40 (*m*, 1H), 3.82 (*s*, 3H), 1.97–1.84 (*m*, 2H), 1.79–1.65 (*m*, 2H), 1.59–1.49 (*m*, 4H); ¹³C-NMR (100 MHz, DMSO, δ / ppm): 161.61, 159.36, 157.92, 155.04, 133.87, 122.45, 109.53, 53.67, 52.85, 31.83, 341.48, 23.56, 23.31; IR (cm⁻¹): 3316.61, 2951.67, 1720.90; MS (ESI): *m/z*: (M+H)⁺: 396.0; Anal. Calcd for C₁₃H₁₄BrCl₂N₃O₂: C, 39.52; H, 3.57; Br, 20.22; Cl, 17.95; N, 10.64. Found: C, 39.53; H, 3.56; Br, 20.24; Cl, 17.92; N, 10.67.

*Methyl 2,4-dichloro-7-cyclopentyl-7H-pyrrolo[2,3-*d*]pyrimidine-6-carboxylate (10)*

Light brownish powder; m.p.: 130–131 °C; ¹H-NMR (400 MHz, DMSO-*d*₆, δ / ppm): 7.40 (*s*, 1H), 5.61–5.67 (*m*, 1H), 3.9 (*s*, 3H), 2.35–2.20 (*m*, 2H), 2.12–1.95 (*m*, 4H), 1.75–1.60 (*m*, 2H); ¹³C-NMR (100 MHz, DMSO, δ / ppm): 165.45,

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154.37, 152.36, 152.06, 130.77, 114.87, 107.06, 57.01, 52.67, 30.60 (2C), 24.68. (2C); IR (cm^{-1}): 3433.39, 2956.30, 1727.99; MS (ESI): m/z : $(\text{M}+\text{H})^+$: 314.0; Anal. Calcd for $\text{C}_{13}\text{H}_{13}\text{Cl}_2\text{N}_3\text{O}_2$: C, 49.70; H, 4.17; Cl, 22.57; N, 13.38. Found: C, 49.73; H, 4.12; Cl, 22.59; N, 13.36.

Spectra

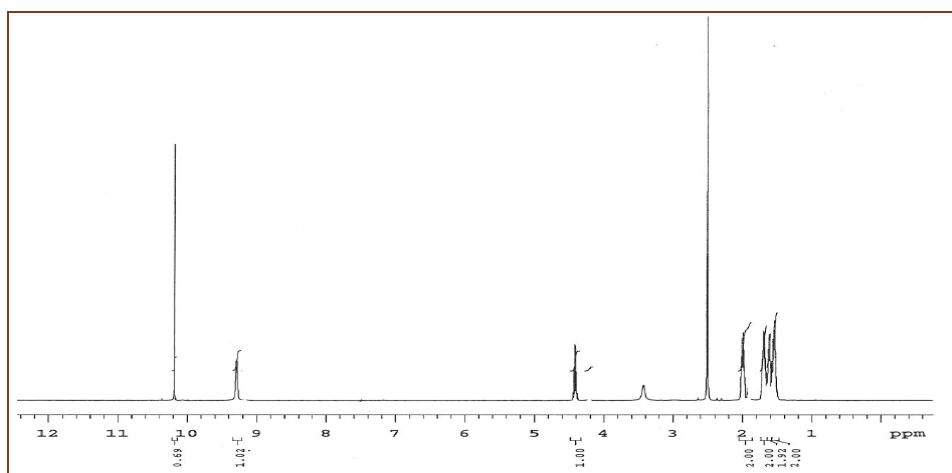


Fig. S-1. $^1\text{H-NMR}$ (400 MHz, DMSO) - 7

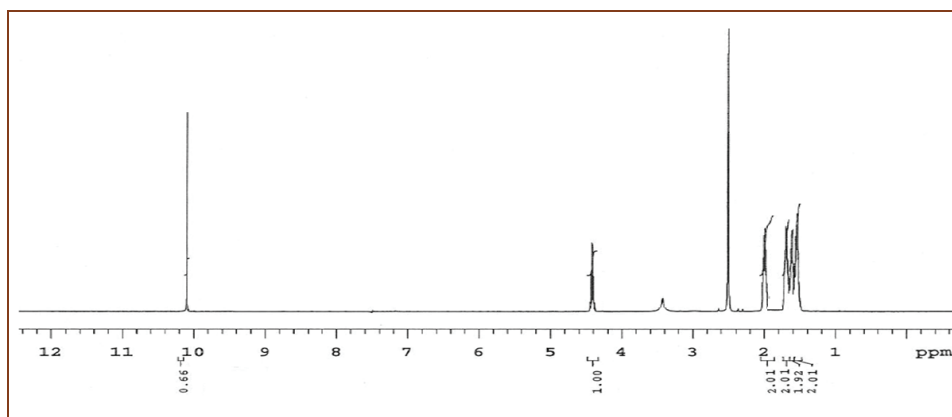


Fig. S-2. $^1\text{H-NMR}$ (400 MHz, DMSO, D_2O Exchange) - 7

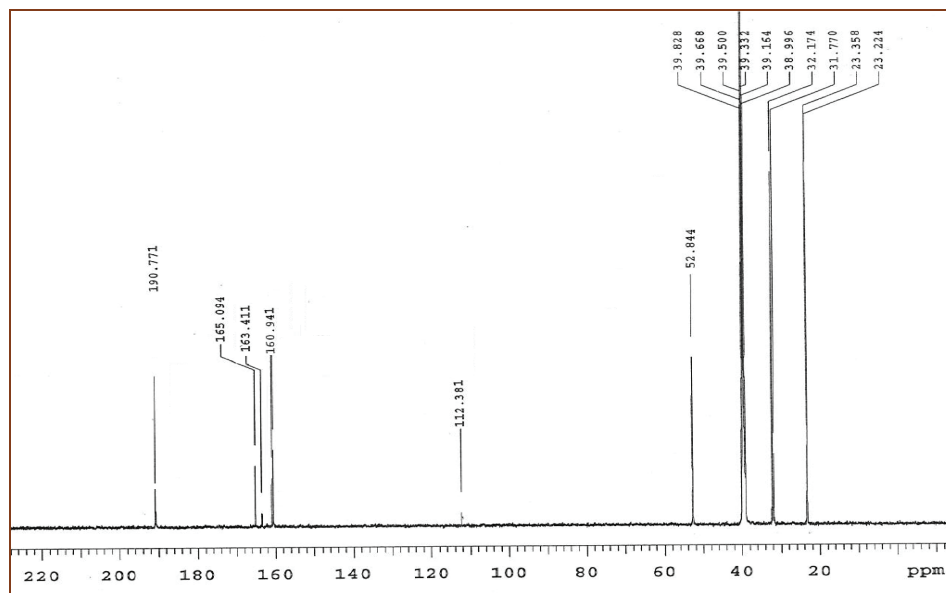


Fig. S-3. ¹³C-NMR (100 MHz, DMSO) - 7

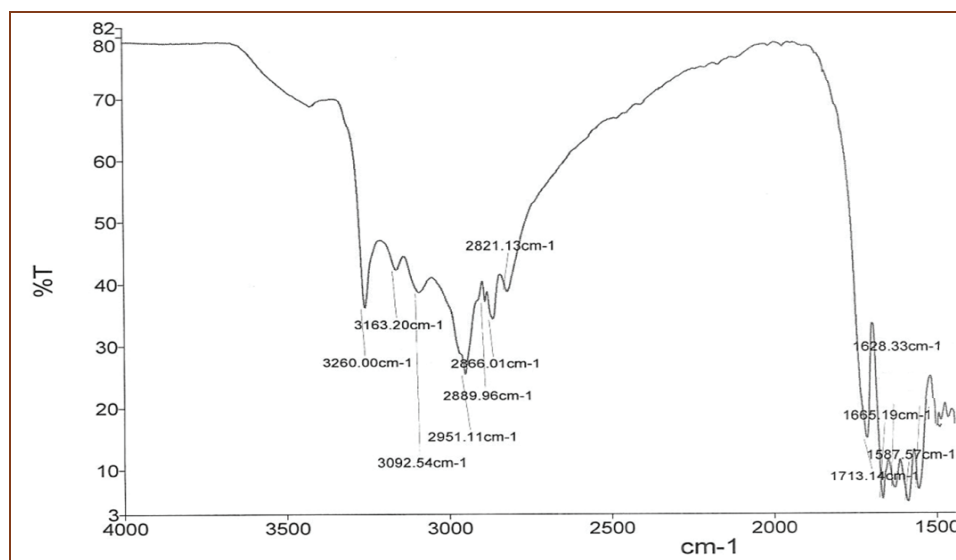


Fig. S-4. IR - 7

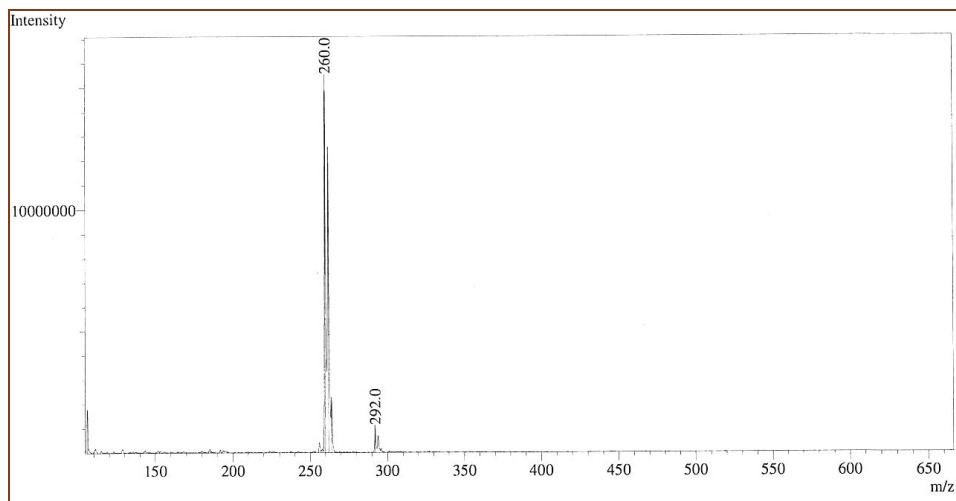
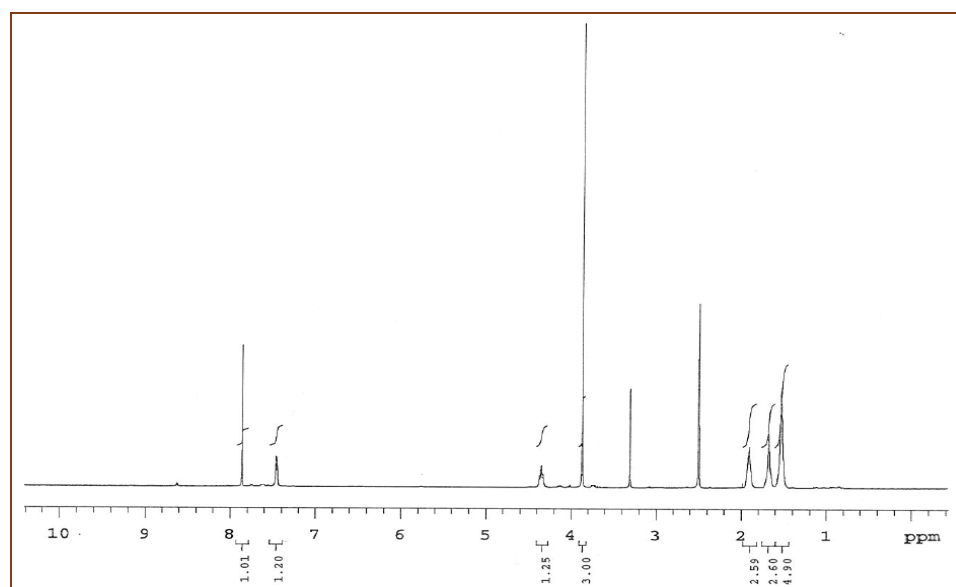
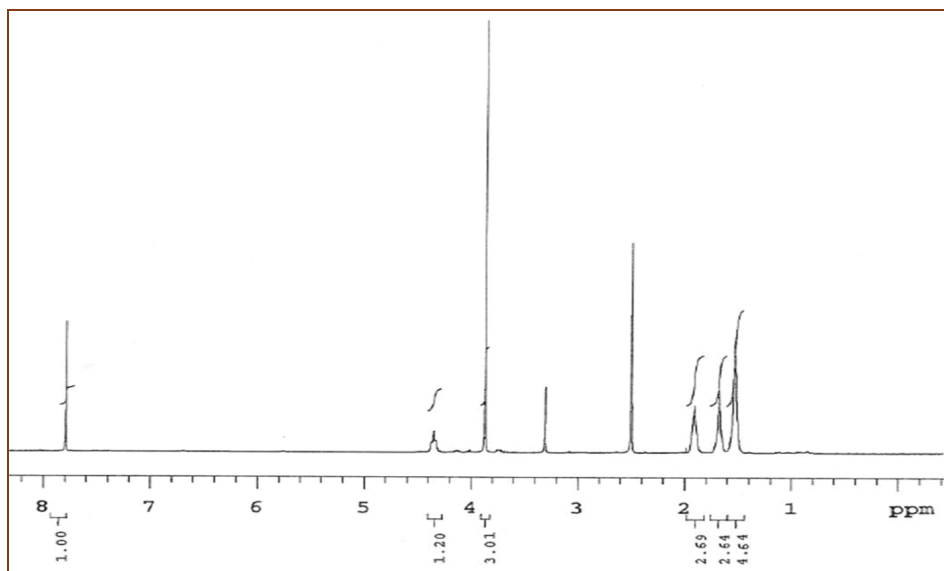
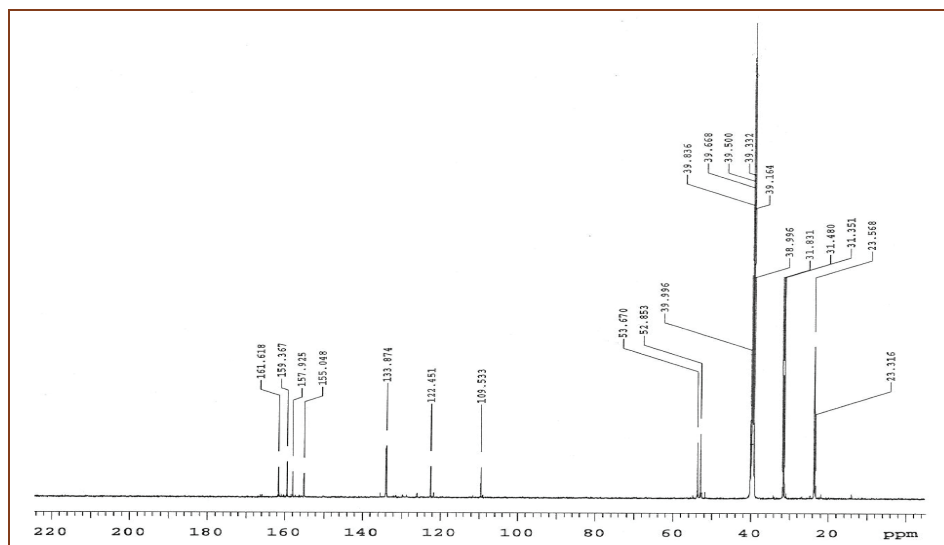


Fig. S-5. ESI-MS - 7

Fig. S-6. ¹H-NMR (400 MHz, DMSO) - 9

Fig. S-7. $^1\text{H-NMR}$ (400 MHz, DMSO, D_2O exchange) - **9**Fig. S-8. $^{13}\text{C-NMR}$ (100 MHz, DMSO) - **9**

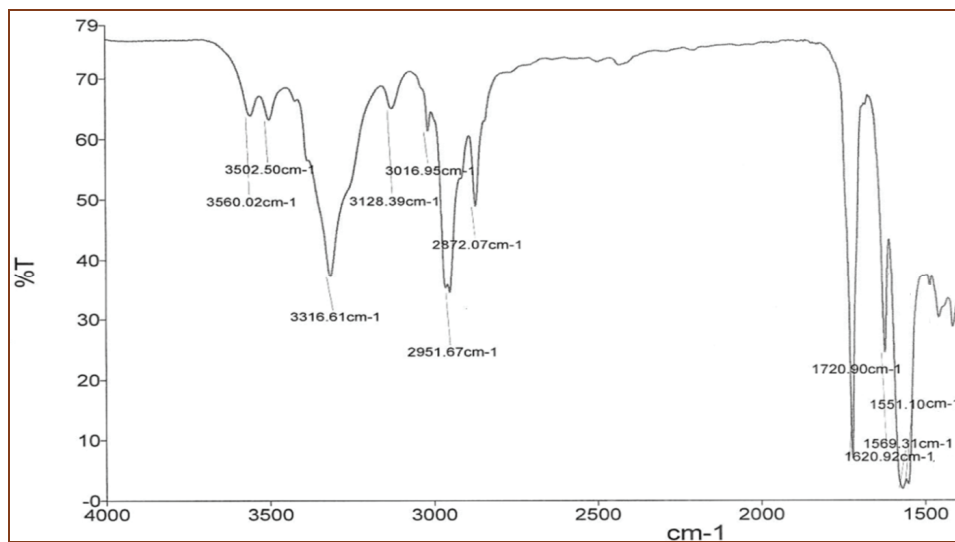


Fig. S-9. IR - 9

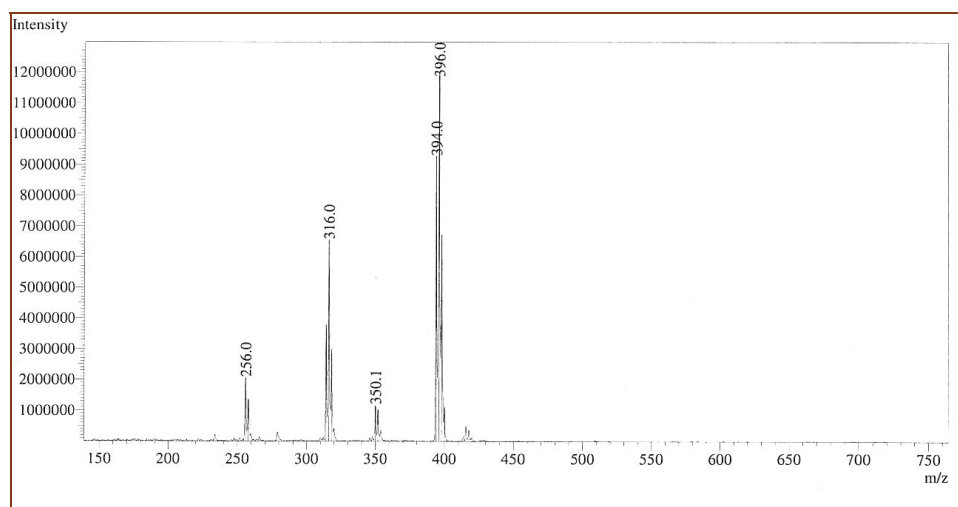
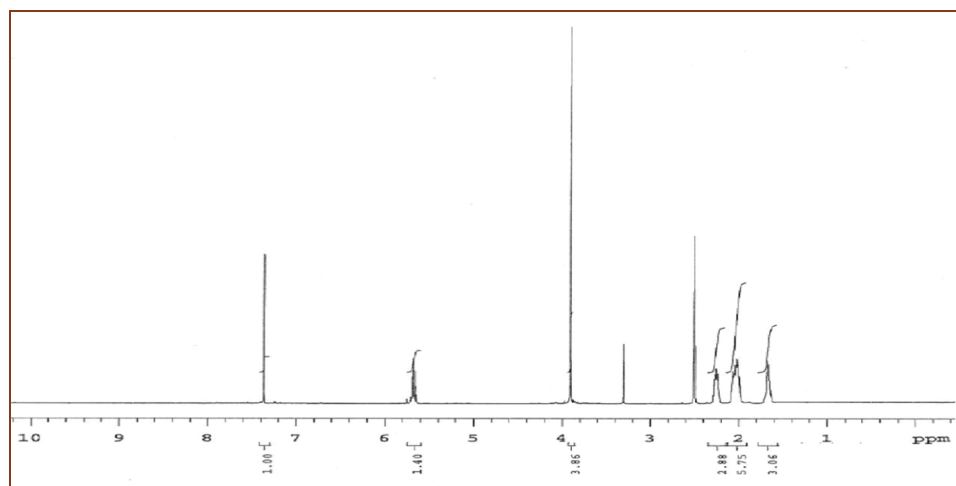
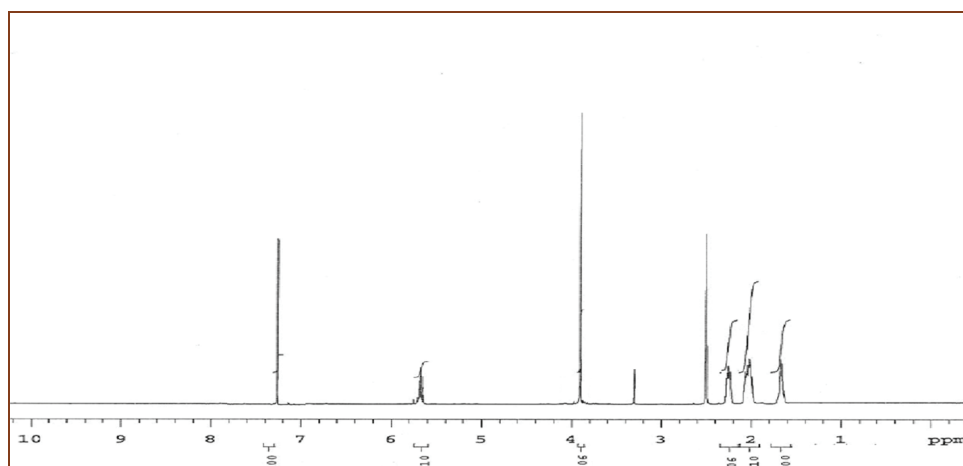


Fig. S-10. ESI-MS - 9

Fig. S-11. ¹H-NMR (400 MHz, DMSO) - **10**Fig. S-12. ¹H-NMR (400 MHz, DMSO, D₂OExchange) - **10**

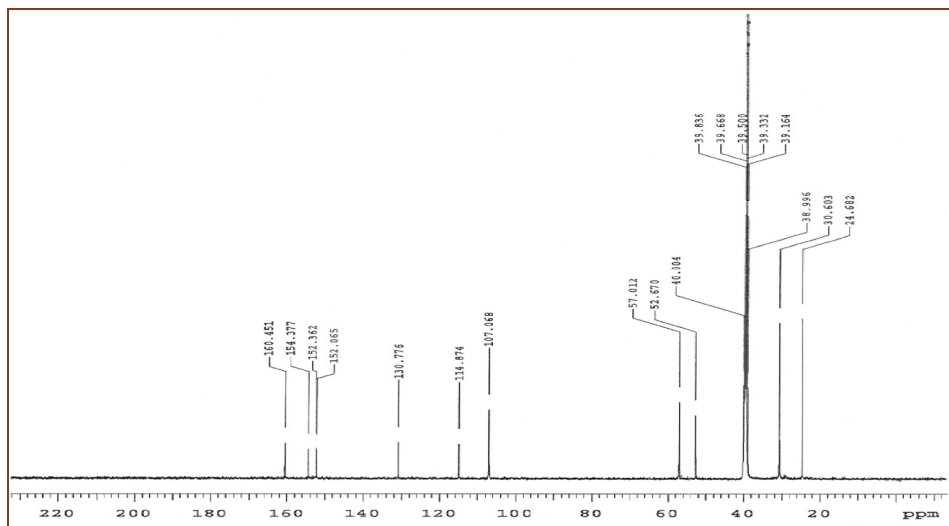
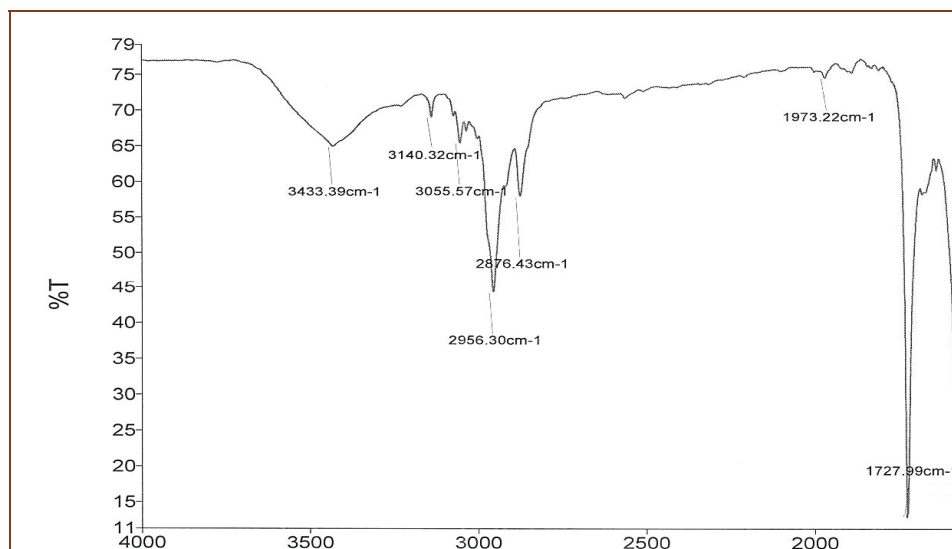
Fig. S-13. ^{13}C -NMR (100 MHz, DMSO) - 10

Fig. S-14. IR - 10

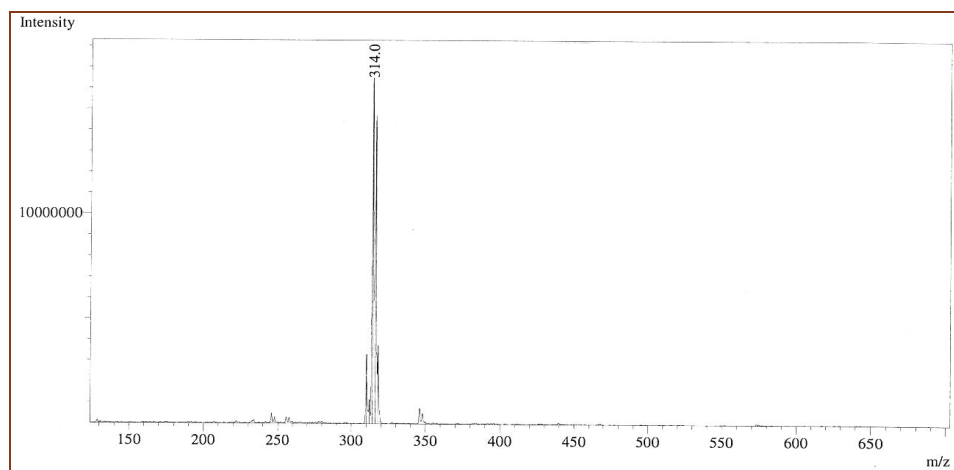


Fig. S-15. ESI-MS - 10