

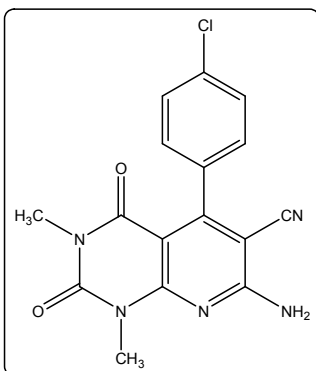
Antibacterial activity of synthetic pyrido[2,3-d]pyrimidines armed with nitrile group: POM analyses and identification of pharmacophore sites of nitriles as important *pro*-drugs

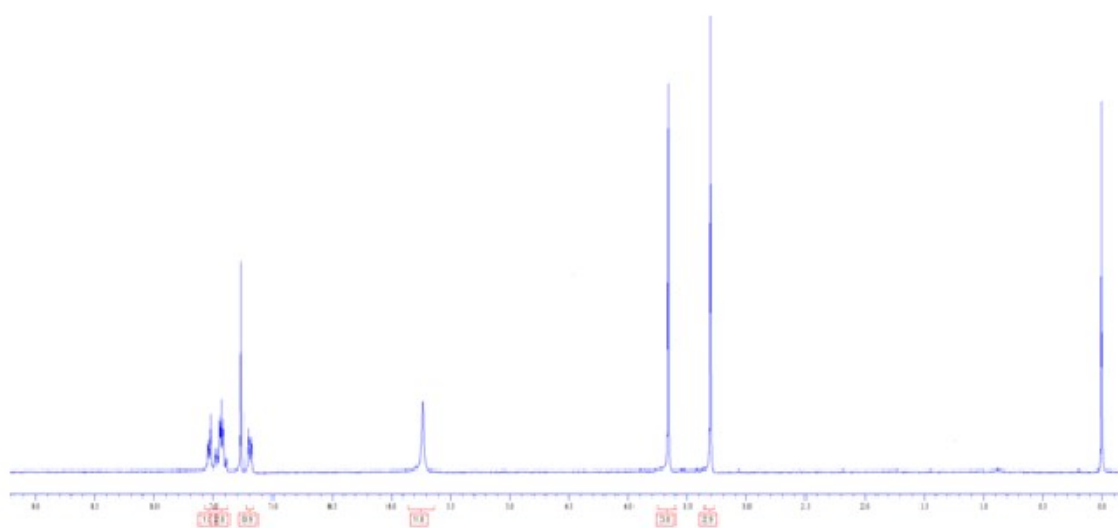
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Faisal A. Almalki,^b Taibi Ben Hadda^{*,c}

Supplementary/Spectroscopic Data of Synthesized compounds

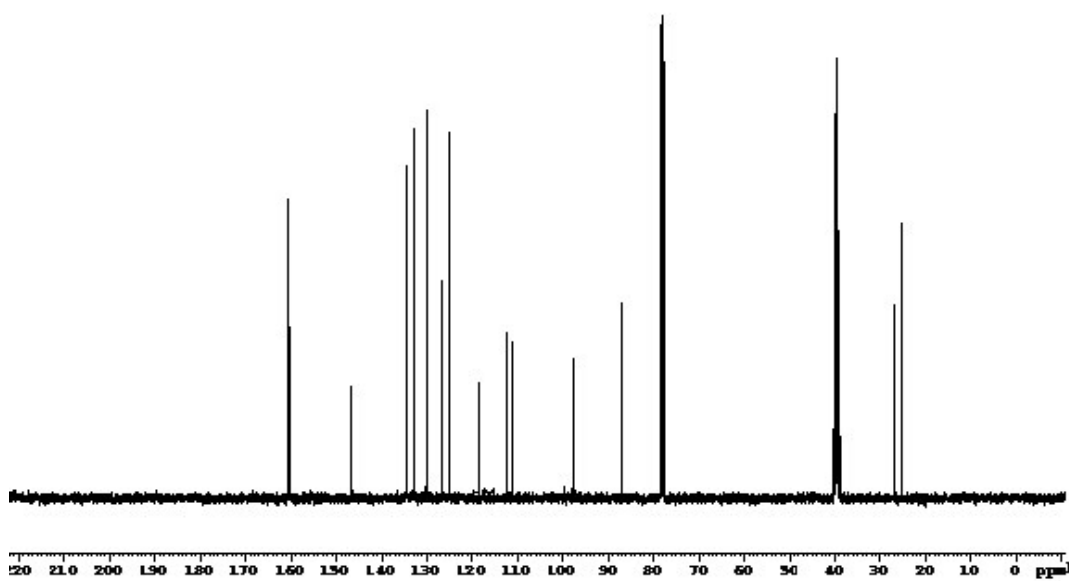
7-Amino-5-(4-chlorophenyl)-1,3-dimethyl-2,4-dioxo-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile (4e)

White powder. Yield 92%. IR (KBr, cm^{-1}): 3377 ($-\text{NH}_2$), 2206 ($-\text{CN}$), 1759 ($-\text{C}=\text{O}$), 1618 ($-\text{C}=\text{O}$); ^1H NMR (300 MHz, $\text{DMSO}-d_6$, ppm): 3.3 (s, 3H, CH_3), 3.7 (s, 3H, CH_3), 5.8 (s, 2H, NH_2), 7.2 (s, 1H, H_{Ar}), 7.4 (br s, 1H, H_{Ar}), 7.5 (br s, 2H, H_{Ar}); ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$, ppm): 160, 146, 134, 132, 130, 126, 126, 114, 112, 111, 98, 87, 28, 27; EI-MS (m/z) = 341 (M^+).





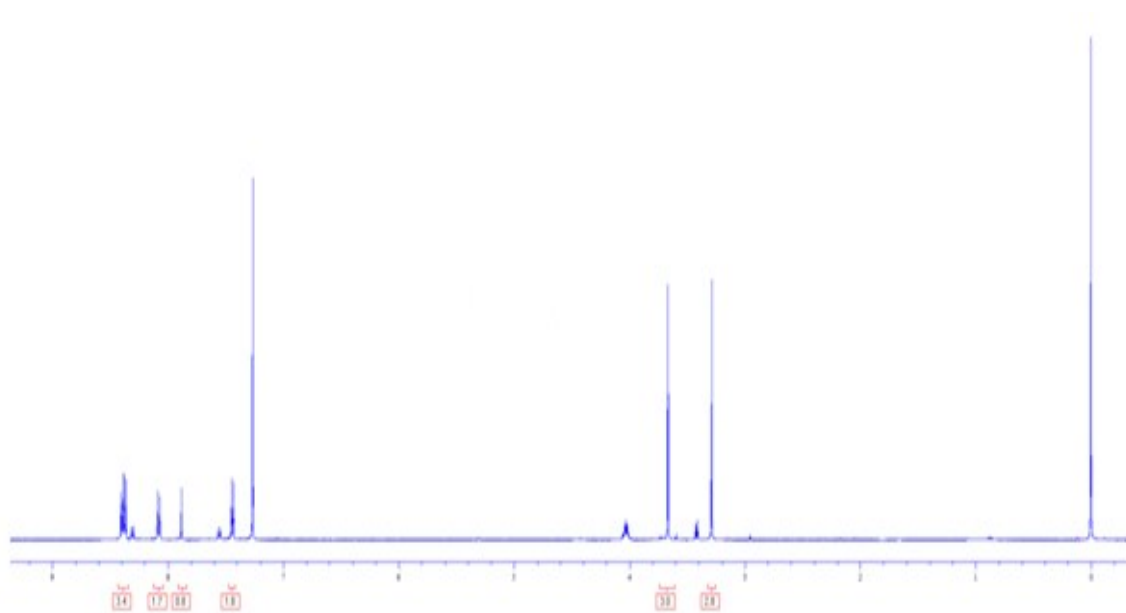
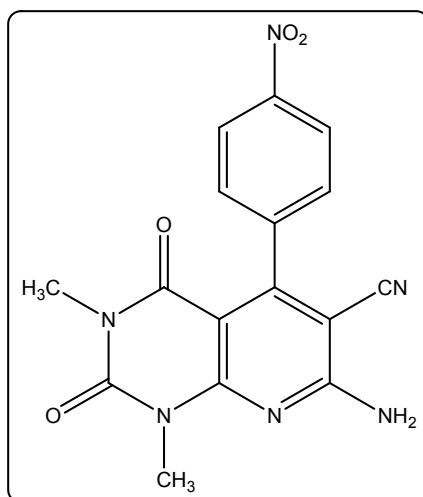
¹H Spectrum of compound 4e



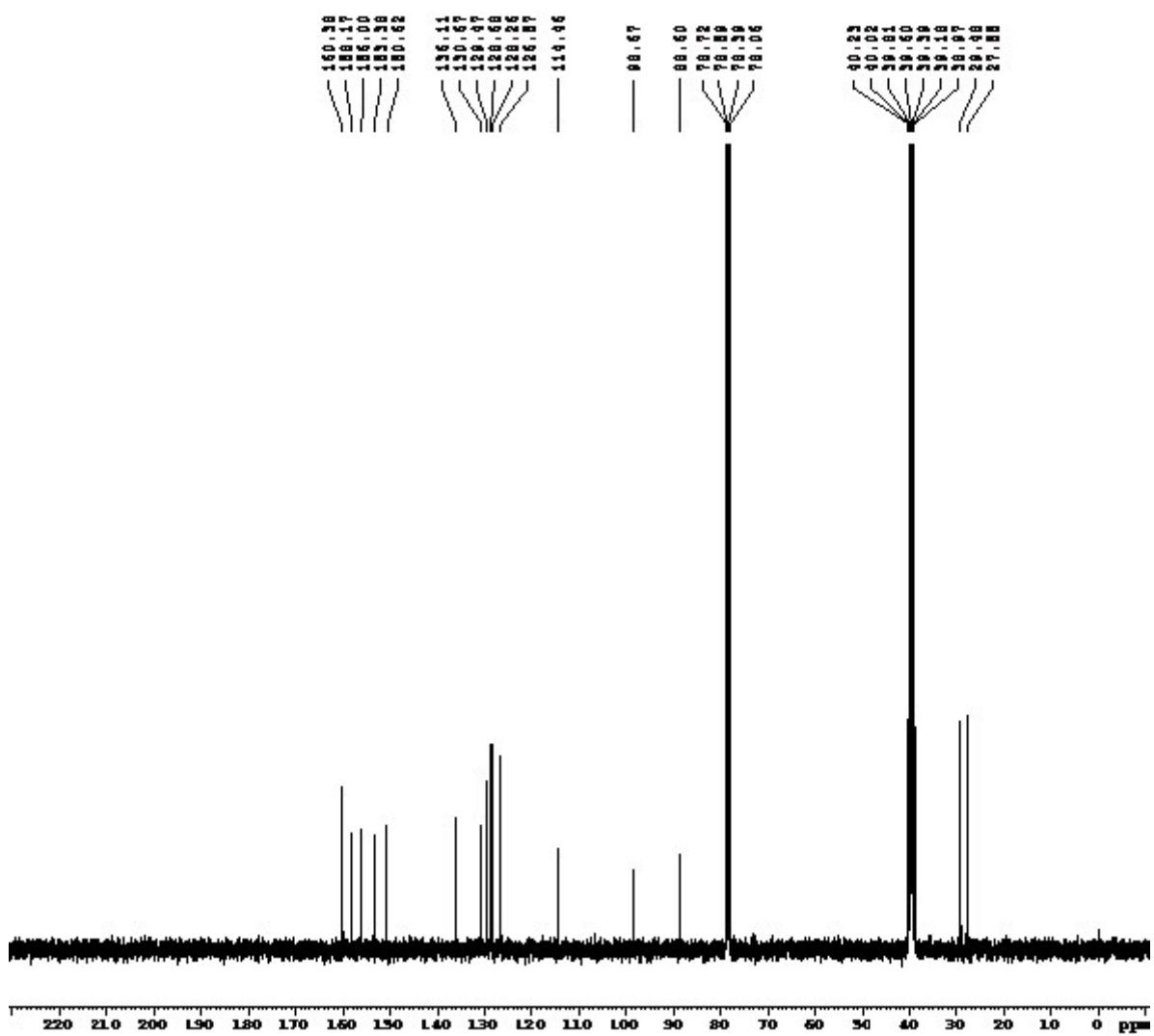
¹³C Spectrum of compound 4e

7-Amino-5-(4-nitrophenyl)-1,3-dimethyl-2,4-dioxo-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile (4f)

White powder. Yield 95%. IR (KBr, cm^{-1}): 3297 ($-\text{NH}_2$), 2222 ($-\text{CN}$), 1758 ($-\text{C}=\text{O}$), 1624 ($-\text{C}=\text{O}$); ^1H NMR (300 MHz, DMSO-d_6 , ppm): 3.3 (s, 3H, CH_3), 3.7 (s, 3H, CH_3), 7.4 (s, 2H, NH_2), 7.9 (d, 2H, H_{Ar}), 8.1 (d, 2H, H_{Ar}) ppm; ^{13}C NMR (100 MHz, DMSO-d_6 , ppm): 160, 158, 156, 150, 133, 124, 115, 114, 113, 98, 88, 29, 27; EI-MS (m/z) = 353 (M^+).



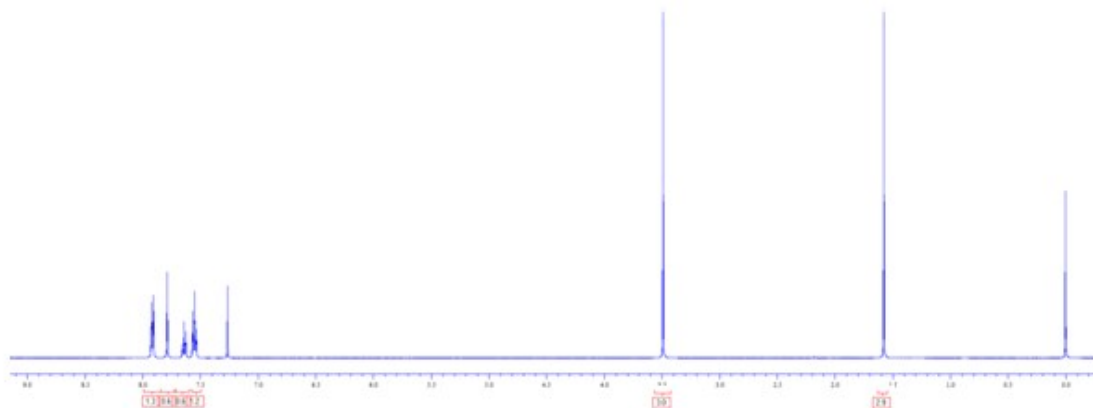
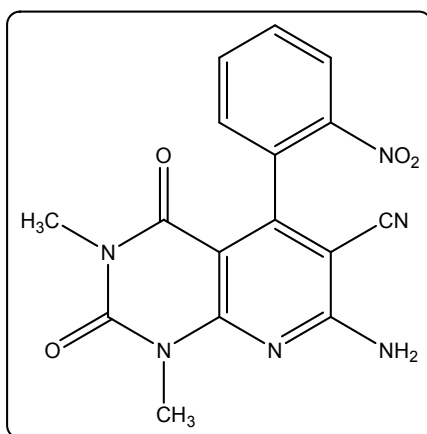
^1H Spectrum of compound 4f



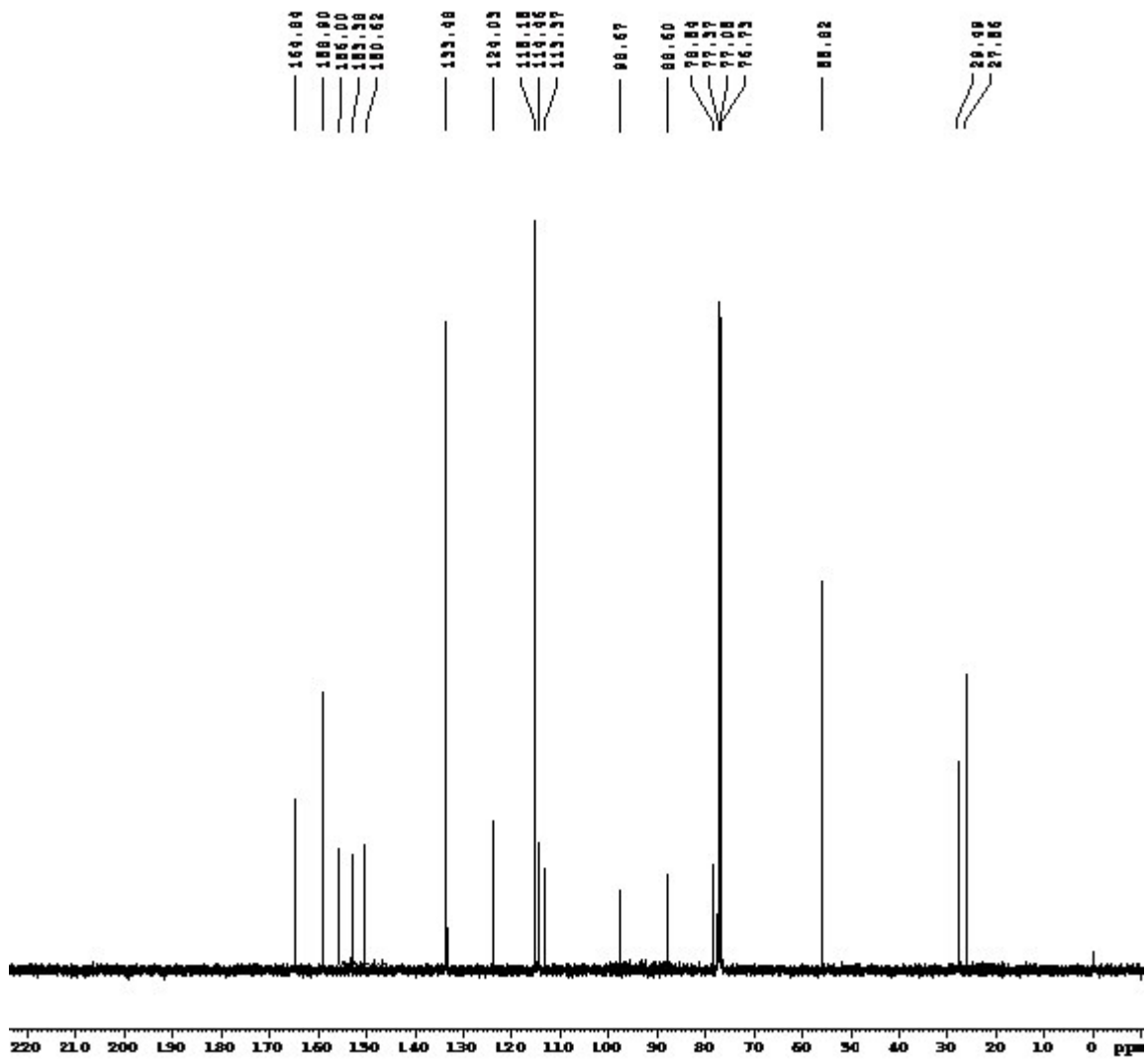
¹³C Spectrum of compound 4h

7-Amino-5-(2-nitrophenyl)-1,3-dimethyl-2,4-dioxo-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile (4h)

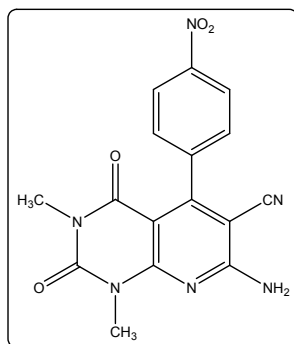
Yellow powder. Yield 89%. IR (KBr, cm^{-1}): 3403 ($-\text{NH}_2$), 2225 ($-\text{CN}$), 1707 ($-\text{C}=\text{O}$), 1613 ($-\text{C}=\text{O}$); ^1H NMR (300 MHz, DMSO-d_6 , ppm): 1.6 (s, 3H, CH_3), 3.5 (s, 3H, CH_3), 7.5 (br-s, 2H, NH_2), 7.6 (d, 1H, H_{Ar}), 7.7 (dt, 1H, H_{Ar}), 7.7-9 (t, 1H, H_{Ar}); ^{13}C NMR (100 MHz, DMSO-d_6 , ppm), 164, 158, 156, 155, 150, 133, 124, 115, 114, 113, 98, 88, 55, 29, 27; EI-MS (m/z) = 353 (M^+).



^1H Spectrum of compound 4h

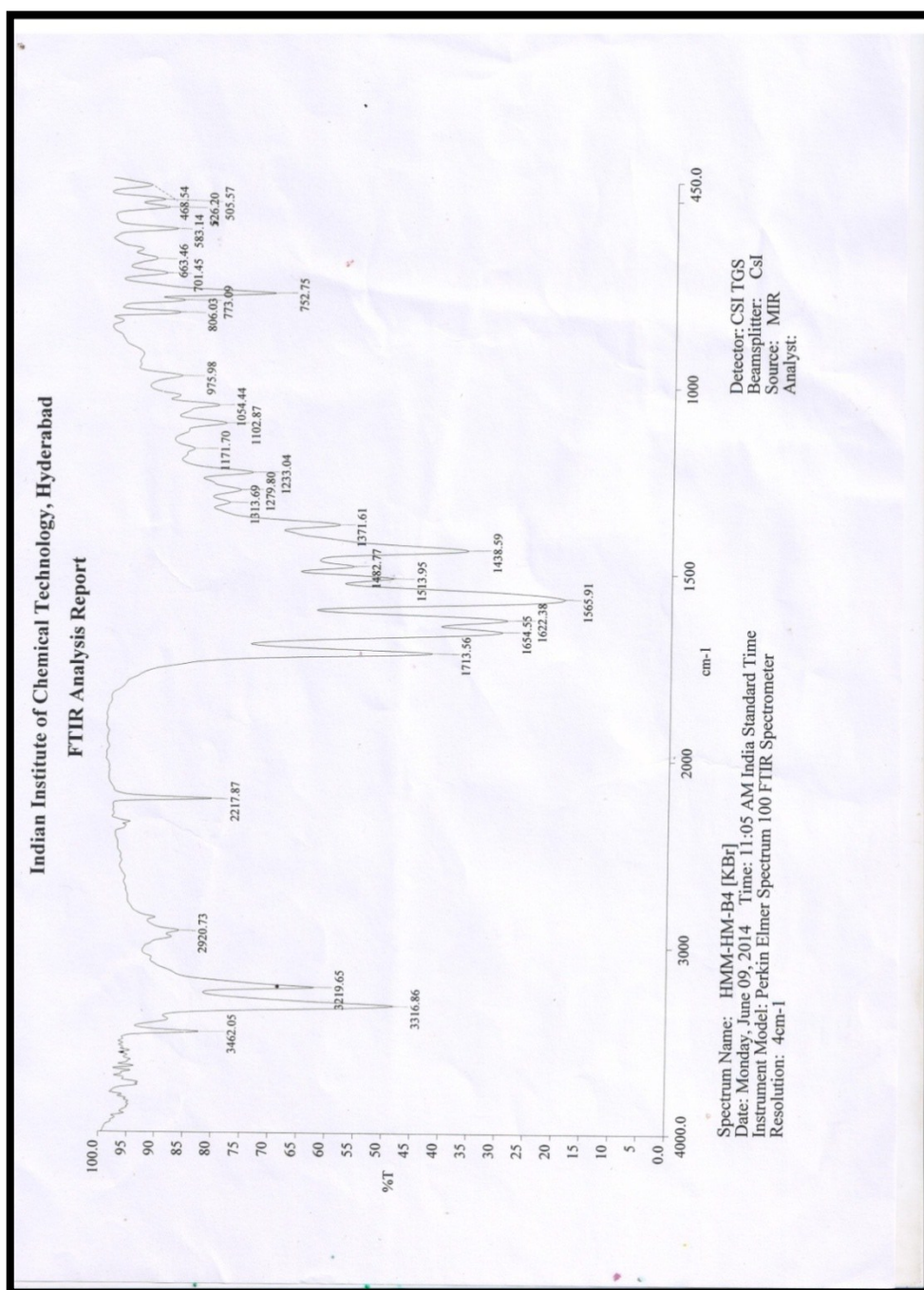


^{13}C Spectrum of compound 4h

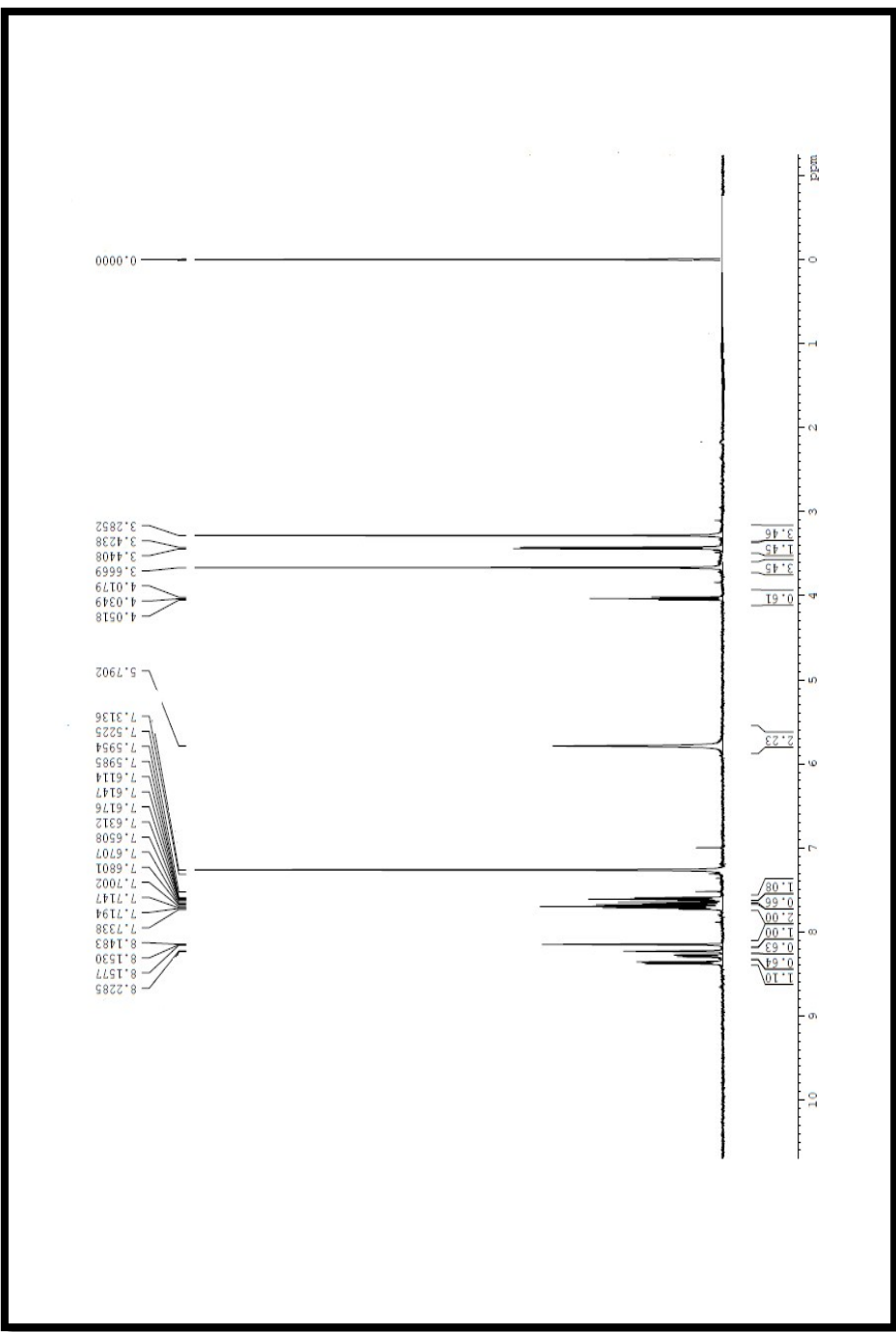


7-amino-5-(4-nitrophenyl)-1,3-dimethyl-2,4-dioxo-1,2,3,4-tetrahydropyrido [2,3-d] pyrimidine-6-carbonitrile compound 4g.

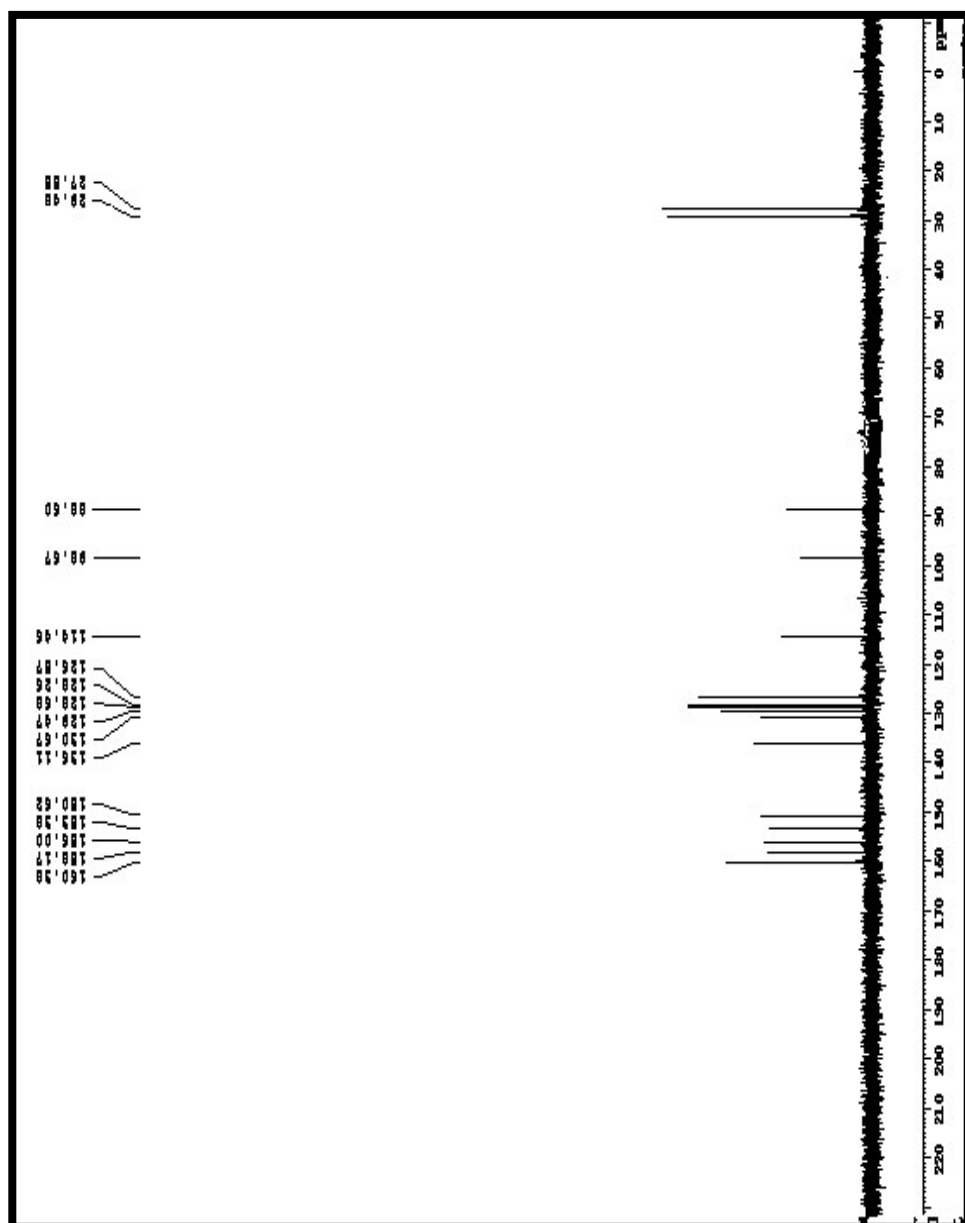
IR spectrum of compound 4g.



H^1 -NMR spectrum of compound 4g.



¹³C-NMR spectrum of compound 4g.



LC-MS spectrum of compound 4g.

