Green Synthesized Al_2O_3 Nanocatalyst for Efficient Synthesis of Nicotinonitrile Derivatives: Catalytic Performance, Antimicrobial Activity and In-Silico Evaluation

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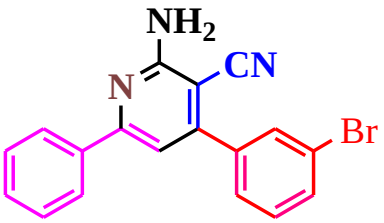
General:
Synthesis of Nicotinonitrile:

In a typical procedure, nicotinonitrile (1.0 mmol), the appropriate aromatic aldehyde (1.0 mmol), acetophenone (1.0 mmol), and ammonium acetate (1.0 mmol) were dissolved in a 1:1 (v/v) water–ethanol mixture (10 mL) in a 50 mL round-bottom flask. Aluminium oxide (Al_2O_3) nanoparticles (5 mol% relative to nicotinonitrile) were added as a heterogeneous catalyst. The reaction mixture was subjected to ultrasonication at ambient temperature to enhance mass transfer and reaction efficiency. Reaction progress was monitored by thin-layer chromatography (TLC). Upon completion, the Al_2O_3 catalyst was recovered by filtration, washed with ethanol, dried, and reused in subsequent cycles. The filtrate was concentrated under reduced pressure, and the crude product was purified by recrystallization from ethanol to yield the desired nicotinonitrile derivative. The structures of the synthesized compounds were confirmed by FT-IR spectroscopy and further characterized using ^{1}H and ^{13}C NMR spectroscopy.

[Table No.1.3,Entry-6]: 2-Amino-6-(3-bromophenyl)-4-p-tolylnicotinonitrile

FT-IR (cm^{-1}): 3400, 2900, 1600, 1450, 1000, 500.



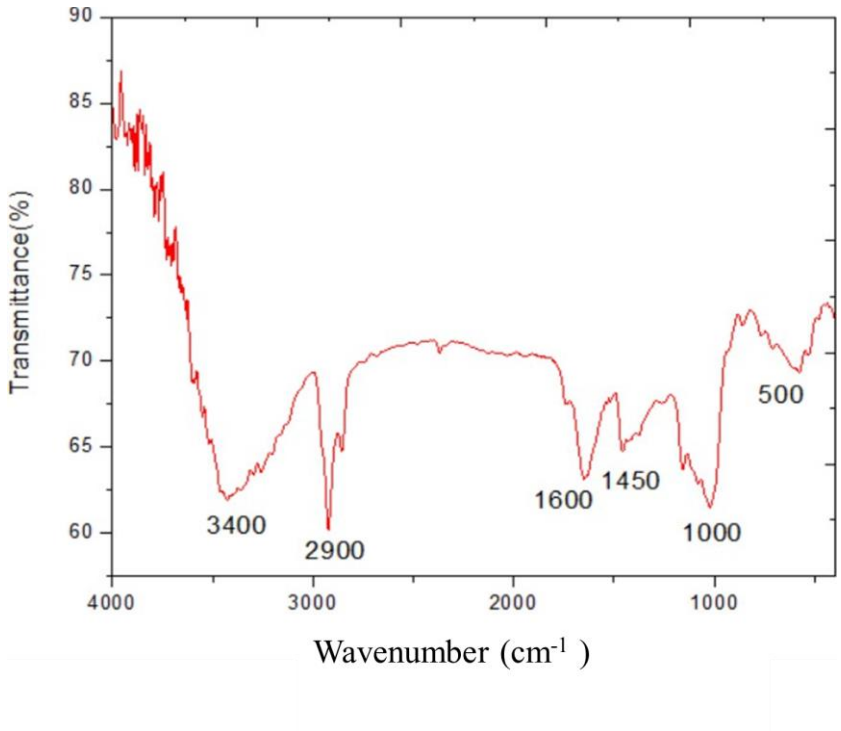


Fig.1: FT-IR Spectrum of 2-Amino-6-(3-bromophenyl)-4-p-tolylnicotinonitrile.

[1]H NMR (400 MHz, δ ppm): 8.26 (s,1H), 7.94 (m,1H), 7.64–7.56 (m,3H), 7.43–7.35 (m,3H), 7.19 (m,1H), 5.33 (s,2H),

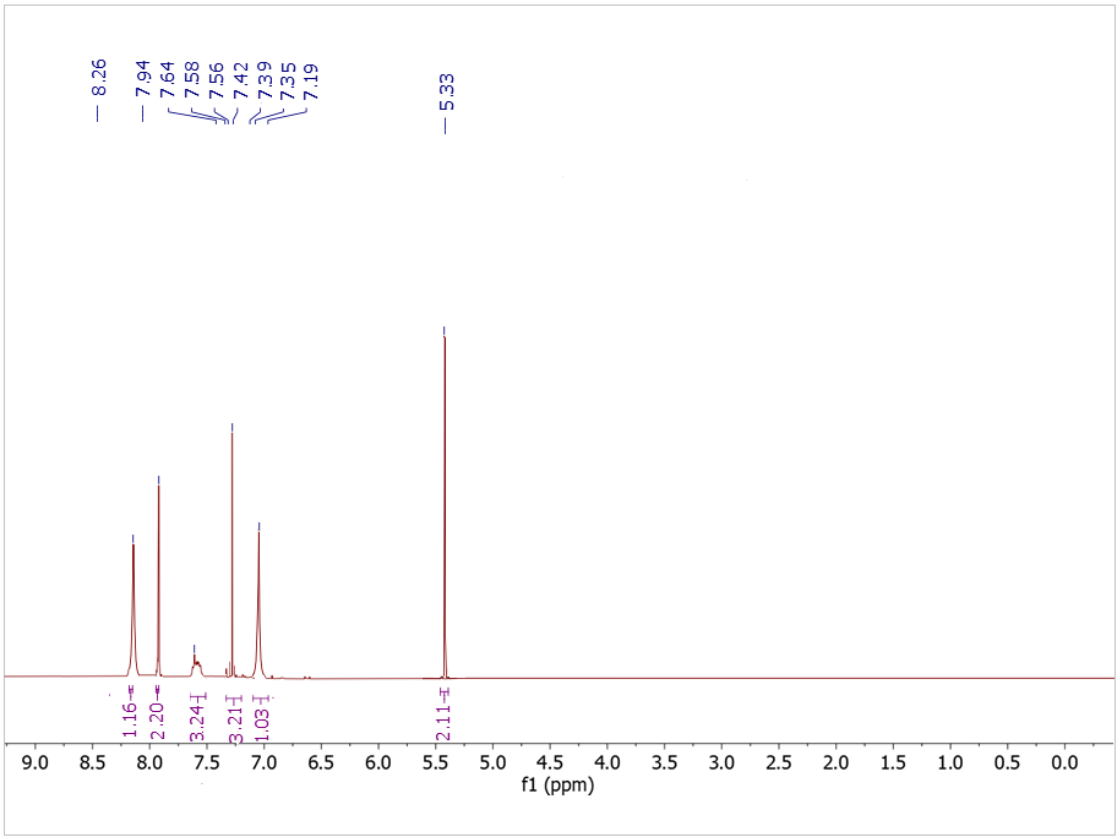


Fig.2: [1]H NMR of 2-Amino-6-(3-bromophenyl)-4-p-tolylnicotinonitrile.

^{13}C NMR (101MHz, δ ppm): 160.2, 157.2, 155.2, 140.2, 140.1, 133.1, 130.3, 130.1, 129.2, 128.8, 125.5, 122.6, 112.6, 111.6, 88.6

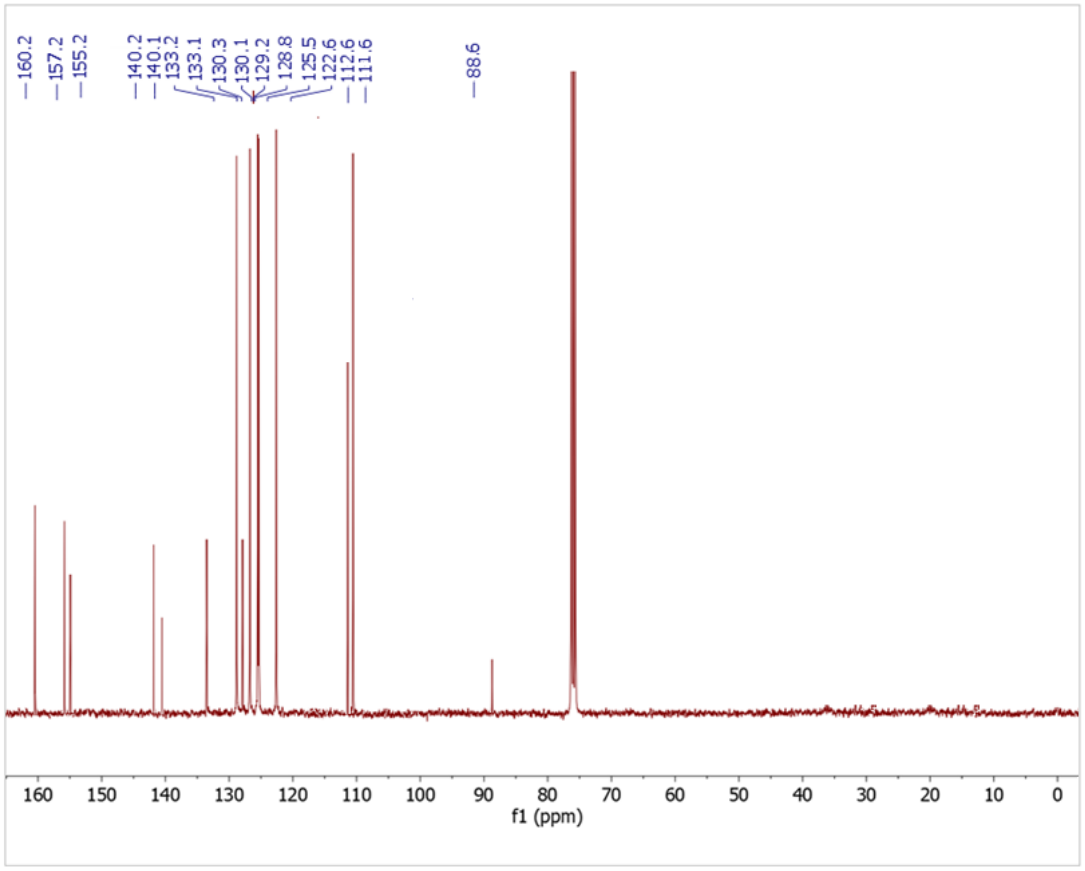
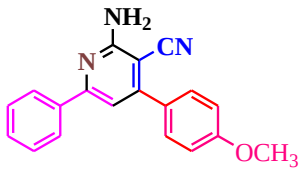


Fig.3: ^{13}C NMR of 2-Amino-6-(3-bromophenyl)-4-p-tolylnicotinonitrile.

[Table No. 1.3, Entry-7] 2-Amino-6-(4-methoxyphenyl)-4-p-tolylnicotinonitrile



FT-IR (cm^{-1}): 3400, 2900, 1600, 1450, 1000, 500.

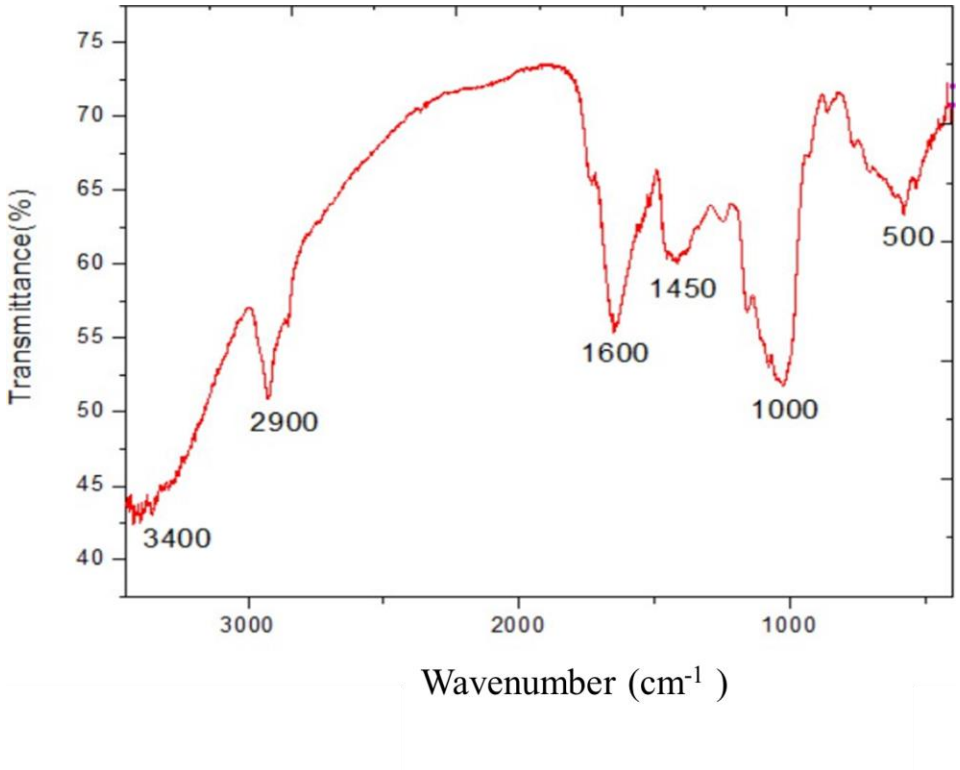


Fig. 4: FT-IR of 2-Amino-6-(4-methoxyphenyl)-4-p-tolylnicotinonitrile.

^{1}H NMR (400 MHz, δ ppm): 8.01 (s,1H), 7.97 (m,1H), 7.66–7.56 (m,2H), 7.36–7.17 (m,3H), 7.01 (m,2H), 6.76 (s,2H).

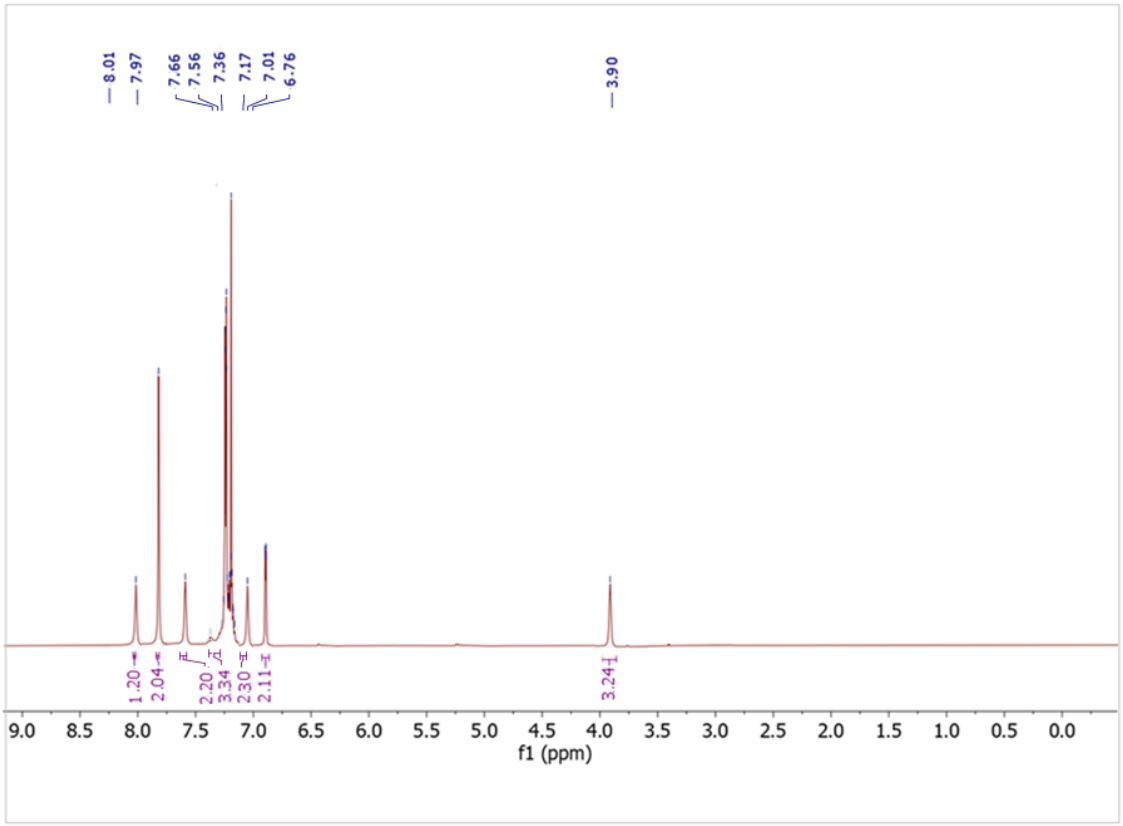


Fig. 5: ^{1}H NMR of 2-Amino-6-(4-methoxyphenyl)-4-p-tolylnicotinonitrile.

^{13}C NMR (101MHz, δ ppm): 161.6, 160.1, 159.4, 154.6, 140.0, 134.6, 130.1, 129.8, 128.8, 128.0, 117.6, 113.1, 110.2, 88.6, 54.6

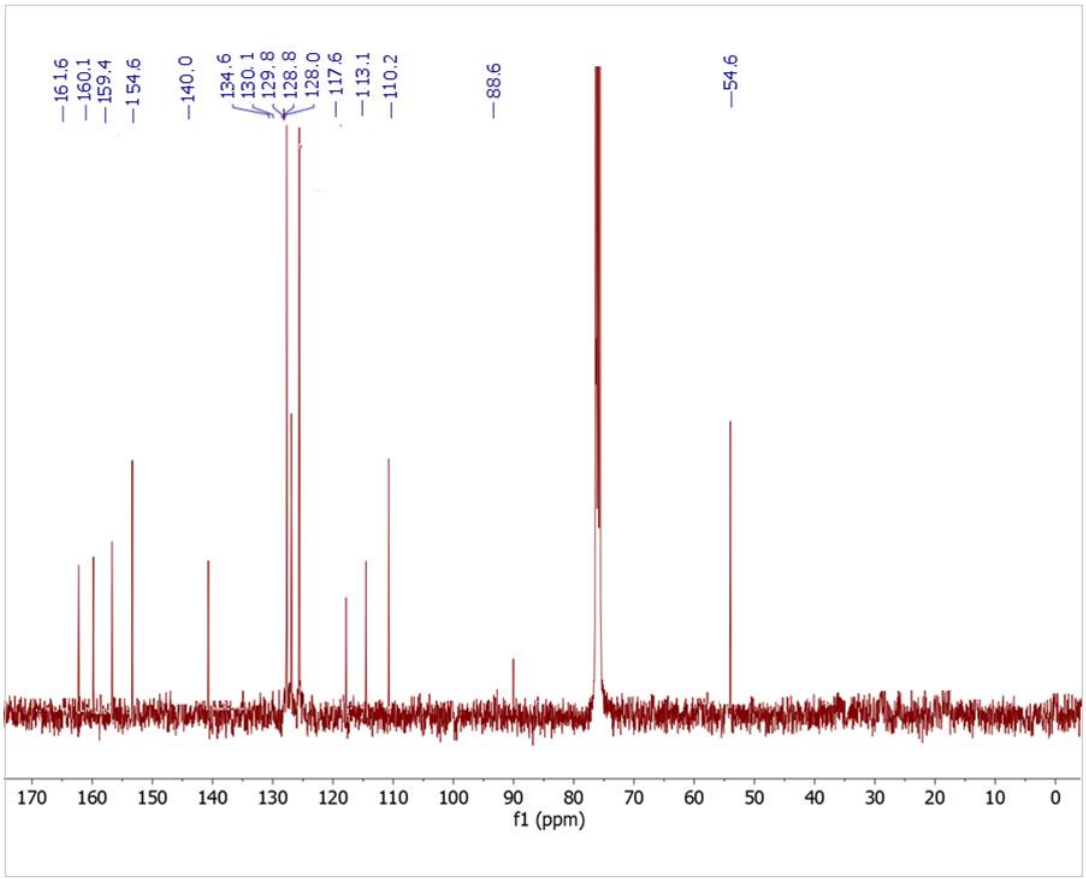
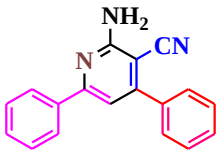


Fig. 6: ^{13}C NMR of 2-Amino-6-(4-methoxyphenyl)-4-p-tolylnicotinonitrile.

[Table No. 1.3, Entry-8] 2-Amino-6-phenyl-4-p-tolylnicotinonitrile



FT-IR (cm⁻¹): 3450, 2900, 1600, 1400, 1000, 500.

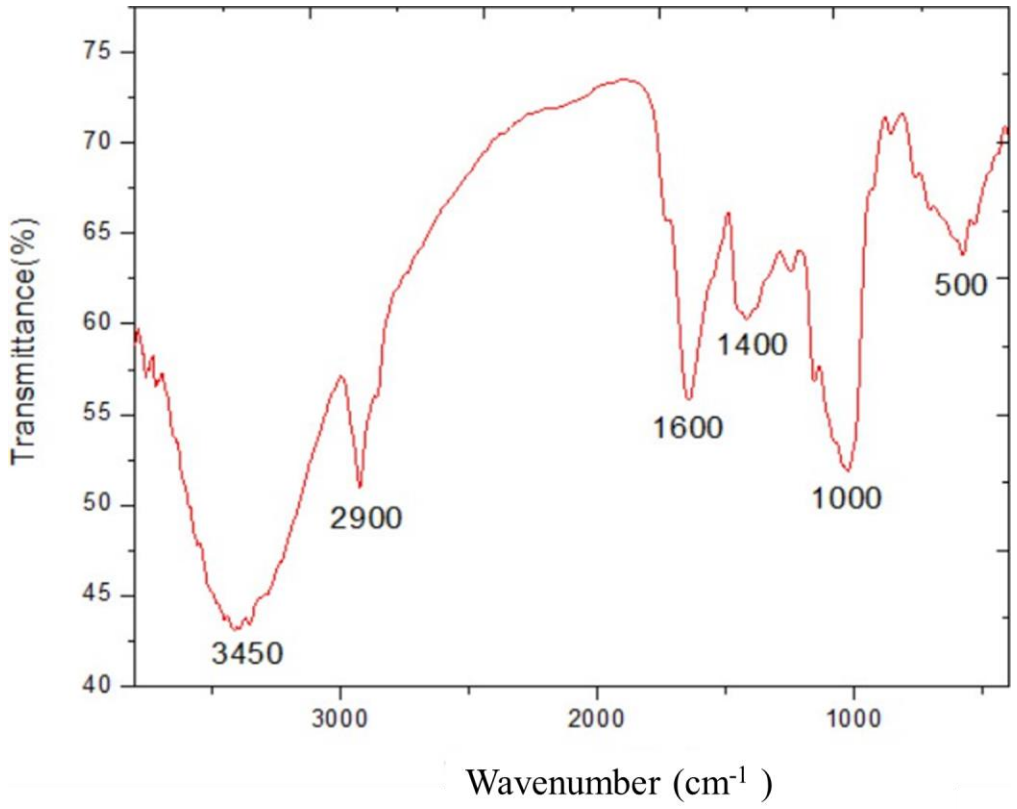


Fig. 7: FT-IR spectrum of 2-Amino-6-phenyl-4-p-tolylnicotinonitrile.

^{1}H NMR (400 MHz, δ ppm): 8.26 (s,1H), 7.87 (m,2H), 7.83–7.57 (m,4H), 7.46–7.16 (m,4H), 5.33(s,2H),

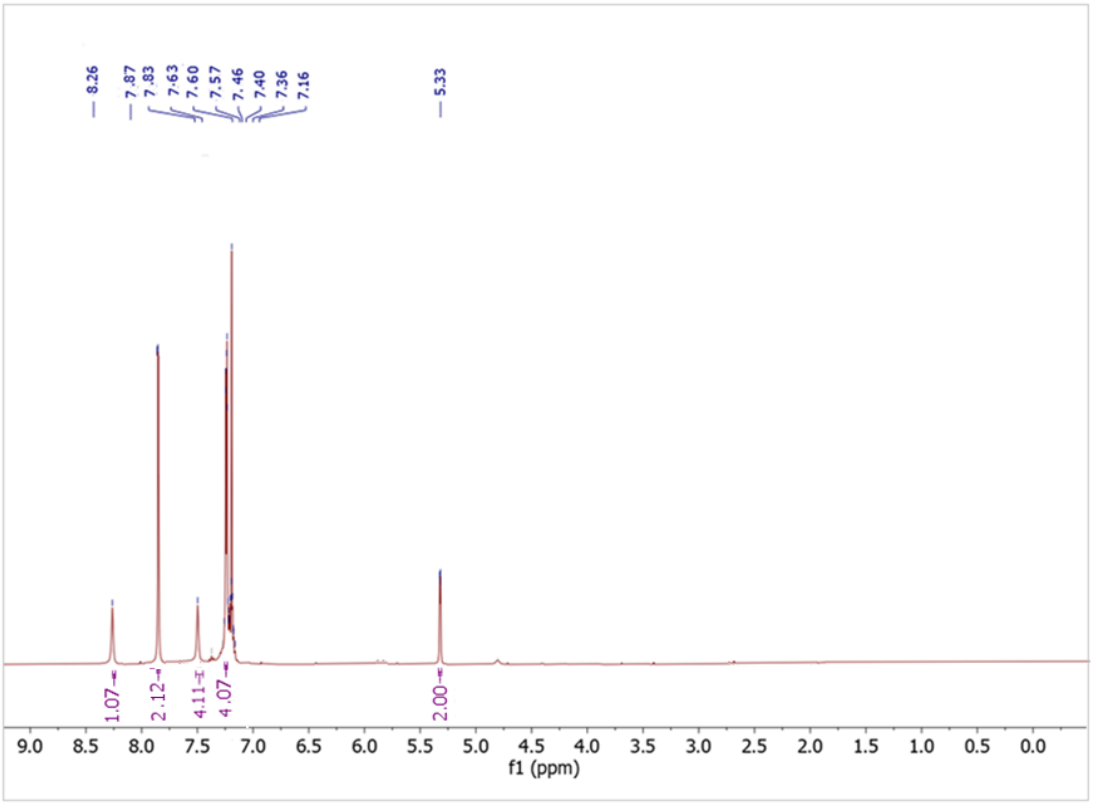


Fig. 8: ^{1}H NMR of 2-Amino-6-phenyl-4-p-tolylnicotinonitrile.

^{13}C NMR (101MHz, δ ppm): 160.2, 157.2, 155.2, 140.2, 140.1, 133.1, 130.3, 130.1, 129.2, 128.8, 125.5, 122.6, 111.6, 88.8

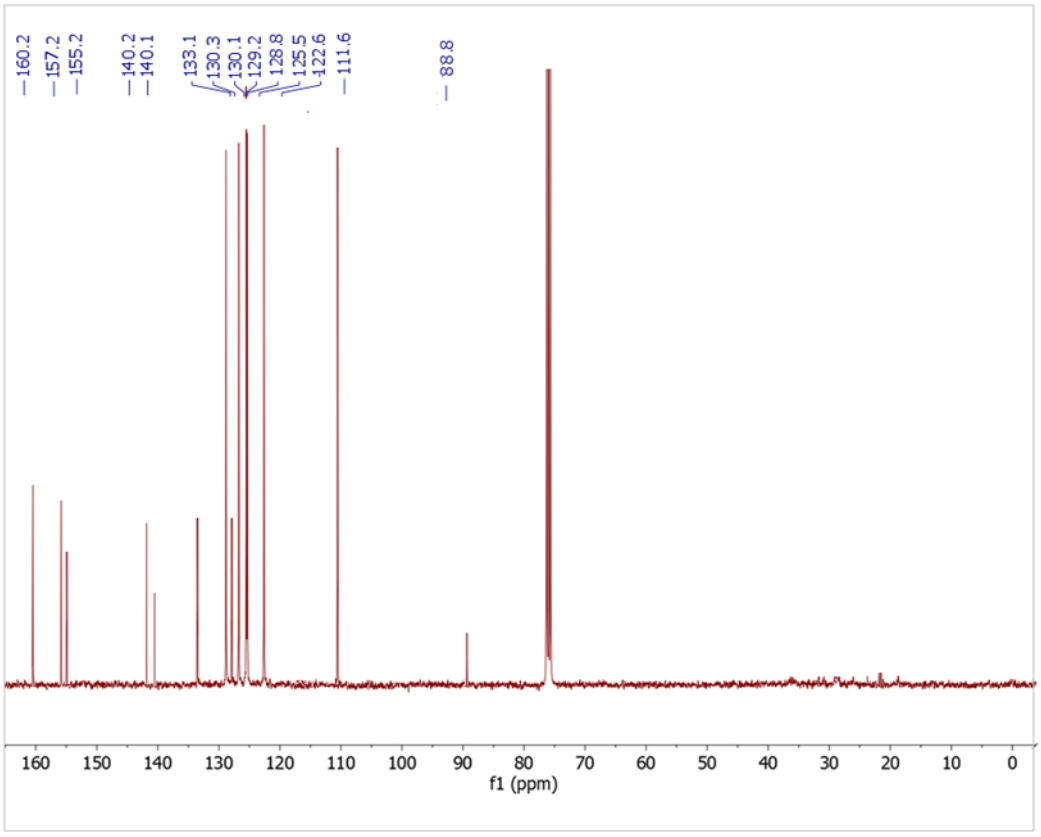


Fig. 9: ^{13}C NMR of 2-Amino-6-phenyl-4-p-tolylnicotinonitrile.