Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Facile Synthesis of Multifunctional Magnetic Porous Organic Polymers with High Catalytic Performance and Dye Adsorption Capacity

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The adsorption kinetics for the adsorption of MB was investigated. The obtained adsorption data for MB was analyzed according to the pseudo-first-order kinetic model using Eq (1):

$$\log (q_t - q_e) = \log q_e - \frac{k}{2.303} t \qquad \text{Eq (1)}$$

where k is the rate constant of the pseudo-first-order adsorption (min^{-1}), q_t is the amount of analyte adsorbed at time t ($mg\ g^{-1}$), and q_e is the amount of analyte adsorbed per mass unit of adsorbent at equilibrium ($mg\ g^{-1}$).

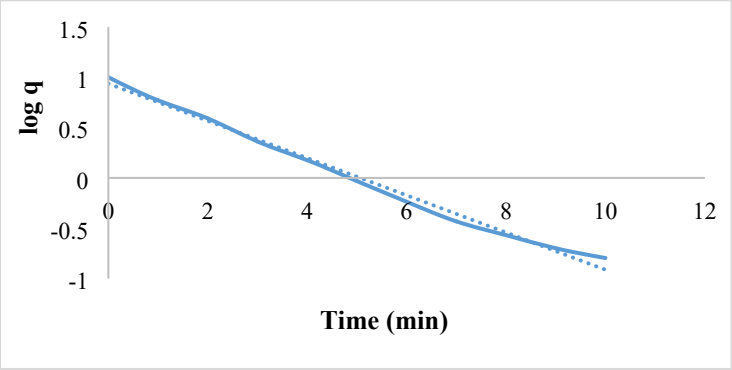


Figure S1 Pseudo-first-order kinetic of MB (10 $mg\ L^{-1}$) adsorption on MOP-F

The Langmuir equation's linear form is provided by Eq (2):

$$\frac{C}{q} = \frac{1}{q_e} C + \frac{1}{k\, q_e} \qquad \text{Eq (2)}$$

where q ($mg\ g^{-1}$) and C ($mg\ L^{-1}$) respectively are the amount of metal ion adsorbed on the sorbent surface and the metal ion concentration in solution, both at equilibrium, k ($L\ mg^{-1}$) is the Langmuir constant and q_e ($mg\ g^{-1}$) is the maximum sorption capacity for monolayer formation on the sorbent surface.

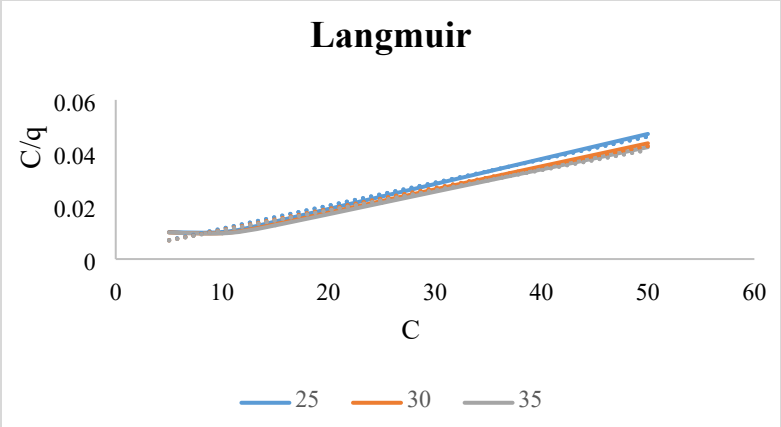


Figure S2 Linear plots of Langmuir isotherm model for MB sorption by MOP-F at different temperatures

25 ℃:

y = 0.0009x + 0.0028

$\frac{1}{q_e} = 0.0009 \rightarrow q_e = 1111.11$

$\frac{1}{k\,q_e} = 0.0028 \rightarrow k = 0.3214$

$R^2 = 0.9856$

30 ℃:

y = 0.0008x + 0.0031

$\frac{1}{q_e} = 0.0008 \rightarrow q_e = 1250$

$\frac{1}{k\,q_e} = 0.0031 \rightarrow k = 0.2580$

$R^2 = 0.9828$

35 ℃:

y = 0.0008x + 0.0032

$\frac{1}{q_e} = 0.0008 \rightarrow q_e = 1250$

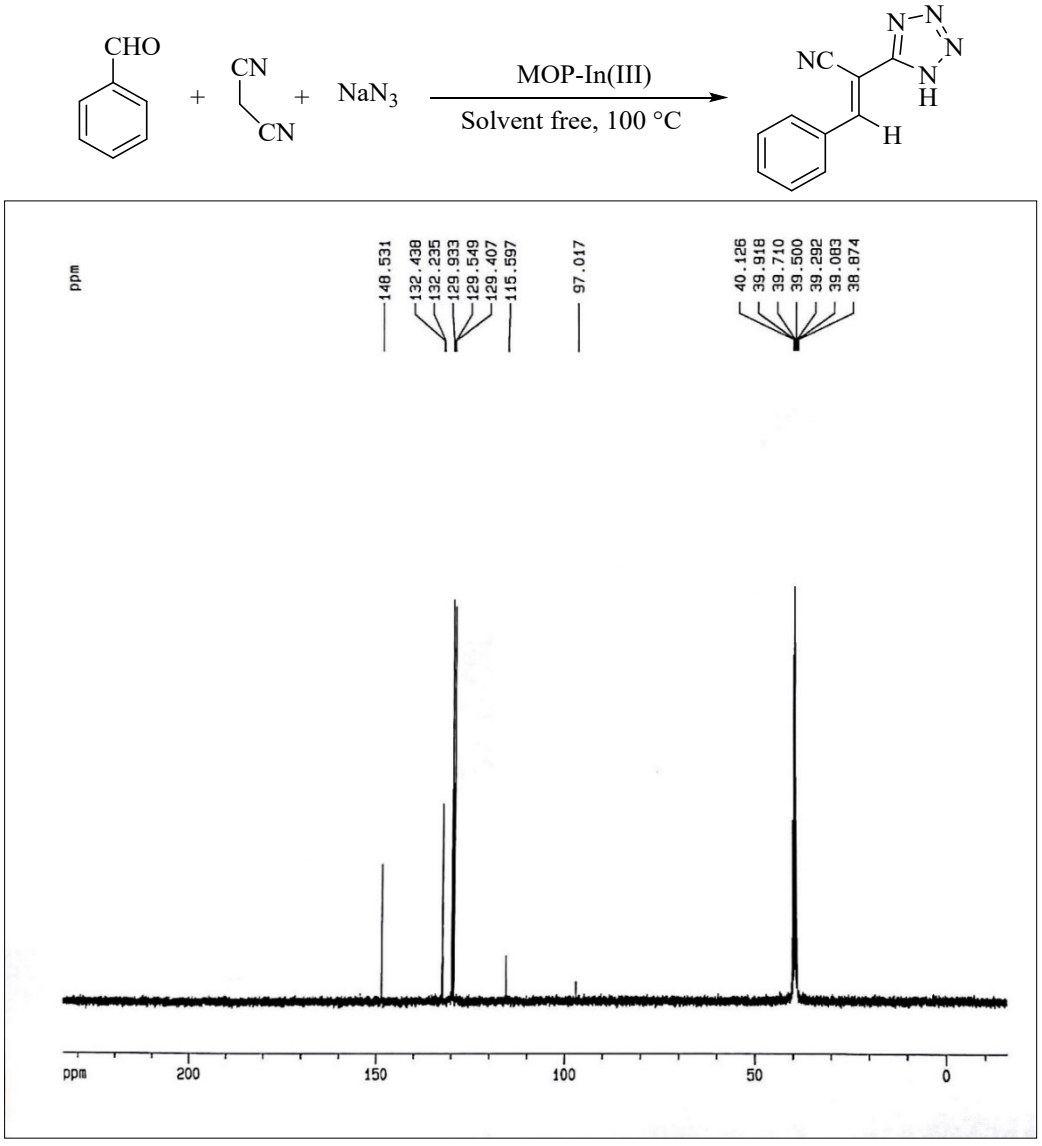
$\frac{1}{k\,q_e} = 0.0032 \rightarrow k = 0.2500$

$R^2 = 0.9811$

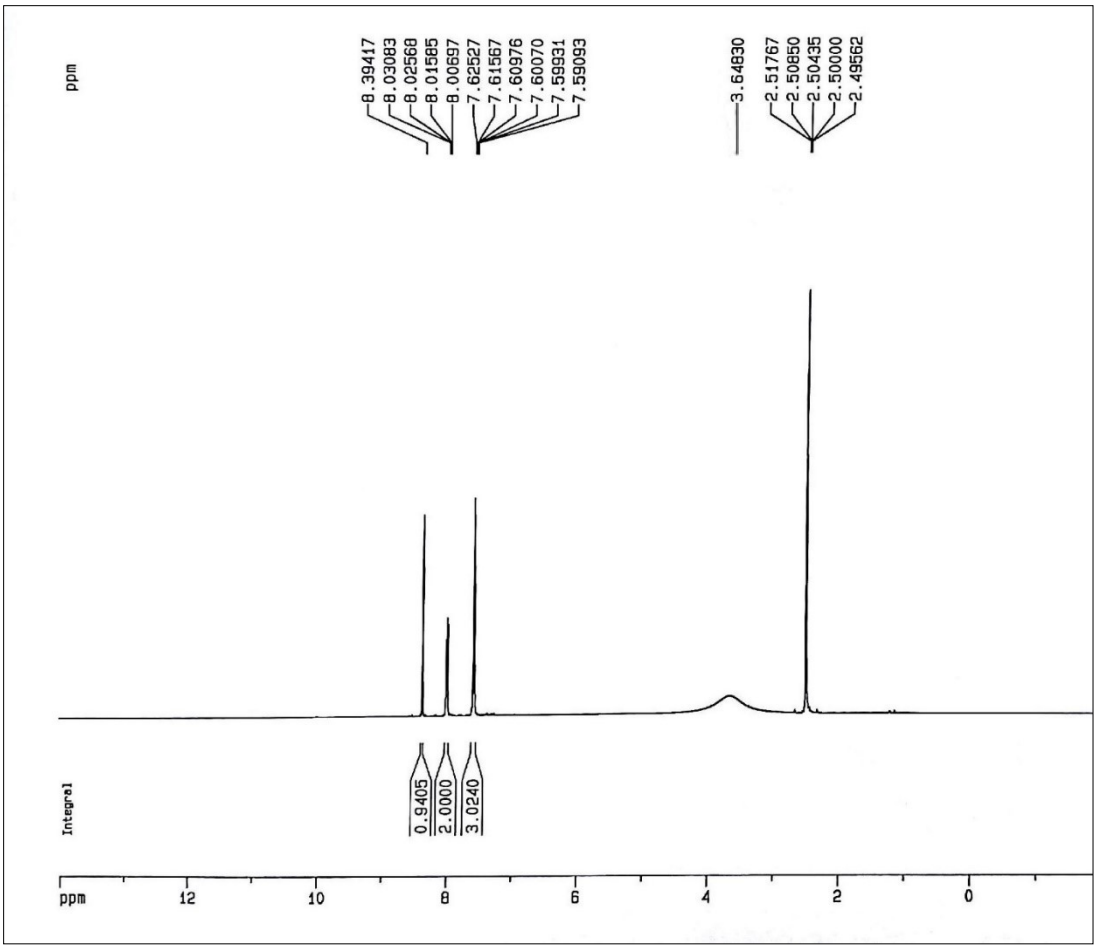
Spectral analysis of the products

Table 3, Entry 1:

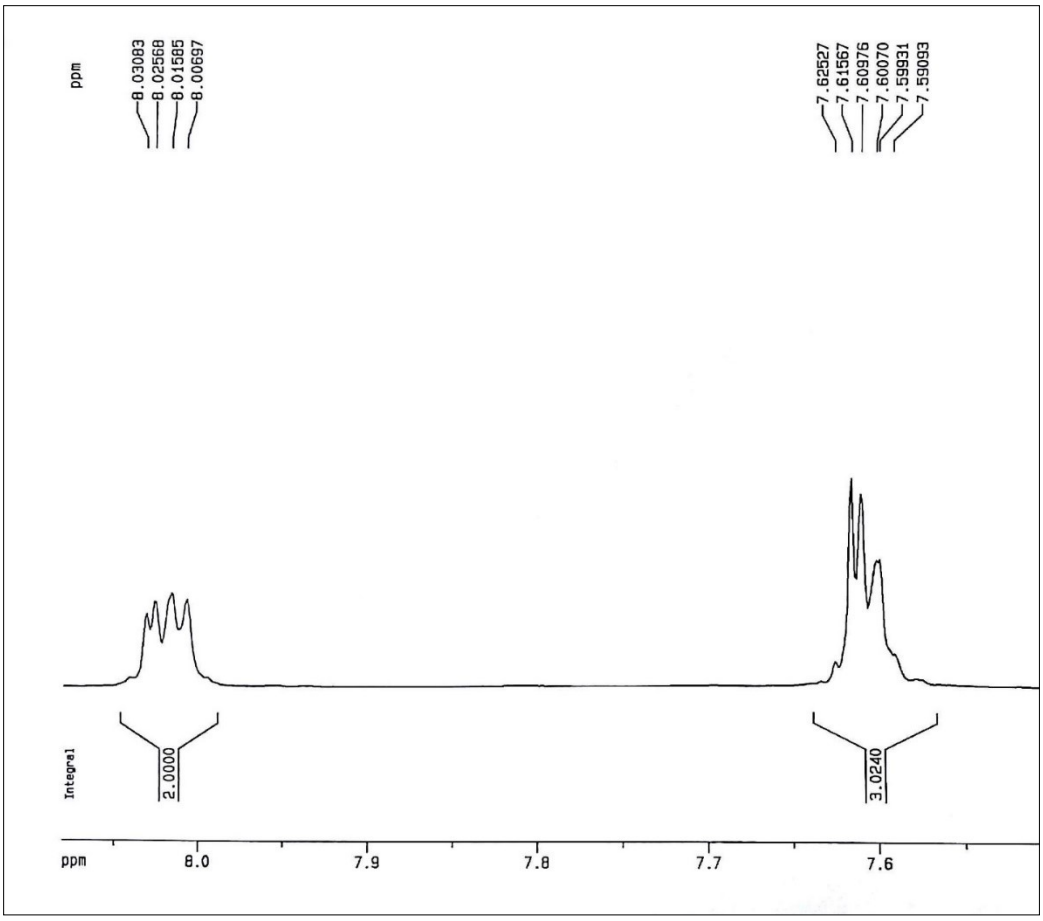
(E)-3-phenyl-2-(1H-tetrazol-5-yl)acrylonitrile. M.P: 168-170° C. ^{1}H-NMR (DMSO-d_6), δppm: 2.5(brs, NH, overlap with solvent) 7.59-7.62 (m, 3H, CH-Ar), 8.00-8.03 (m, 2H, CH-Ar), 8.39 (s, 1H, CH). ^{13}C-NMR (DMSO-d_6), δppm: 97.01, 115.59, 129.40, 129.54, 129.93, 132.23, 132.43, 148.5.



^{13}CNMR, (E)-3-phenyl-2-(1H-tetrazol-5-yl)acrylonitrile



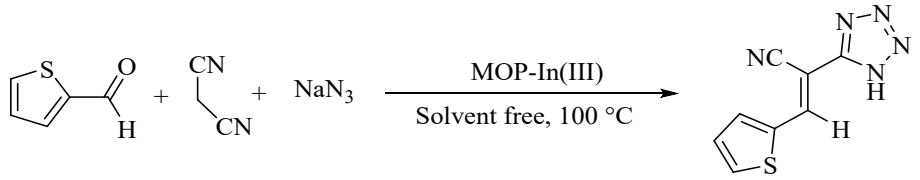
[1]HNMR, (E)-3-phenyl-2-(1H-tetrazol-5-yl)acrylonitrile

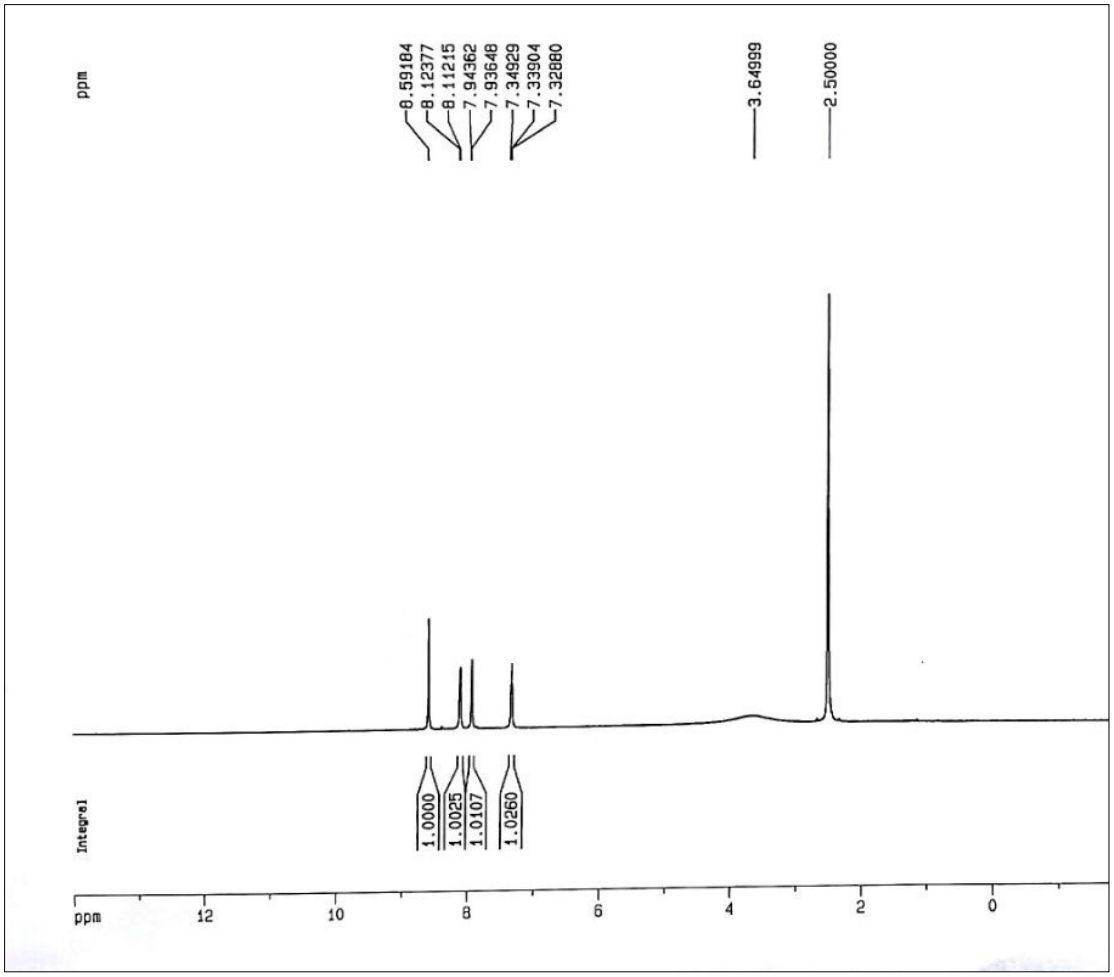


[1]HNMR, (E)-3-phenyl-2-(1H-tetrazol-5-yl)acrylonitrile

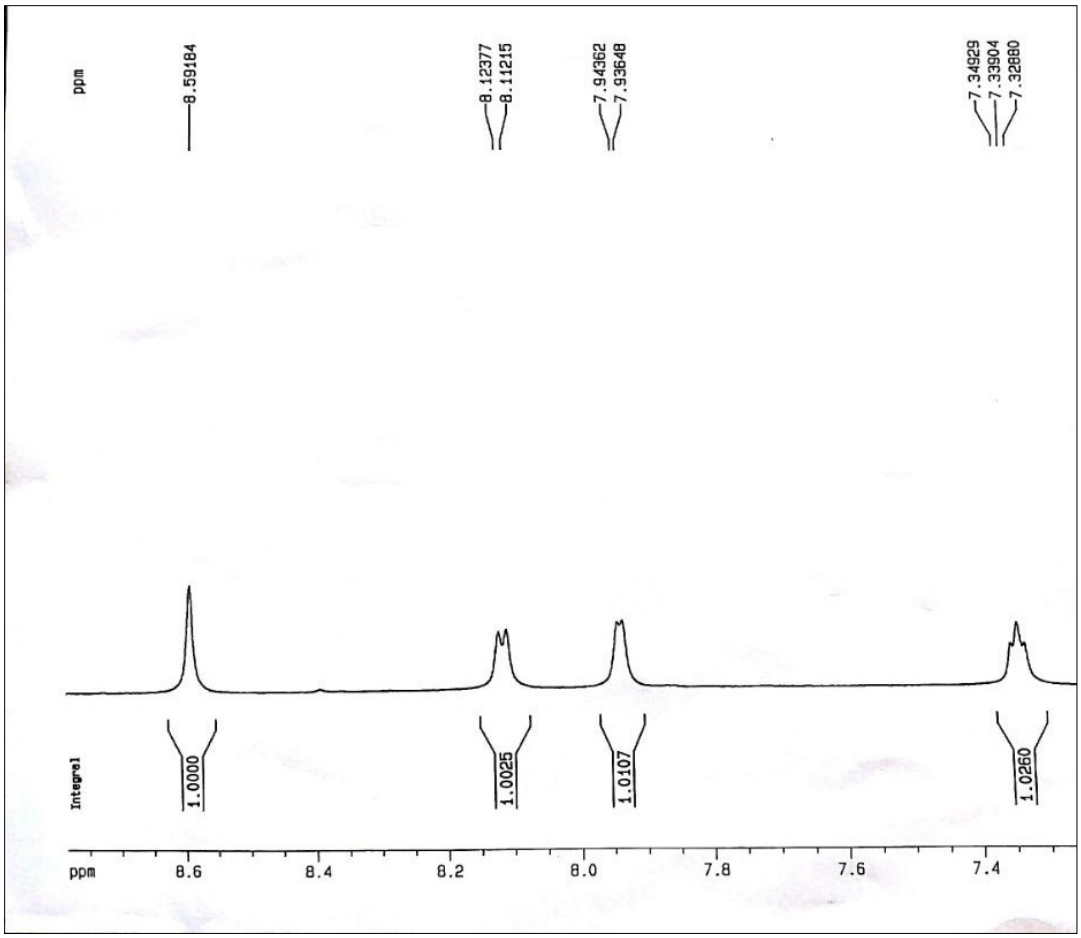
Table 3, Entry 9:

(E)-2-(1H-tetrazol-5-yl)-3-(thiophen-2-yl)acrylonitrile. M.P: 133-136° C. ^{1}H-NMR (DMSO-d_6), δppm: 2.5(brs, NH, overlap with solvent), 7.32-7.35 (t, 1 H, CH), 7.93-7.94 (d, 1 H, CH), 8.11-8.12 (d, 1 H, CH), 8.59 (s, 1 H, CH). ^{13}C-NMR (DMSO-d_6), δppm: 92.28, 115.80, 128.67, 134.95, 136.11, 137.88, ‘141.13, 155.13.

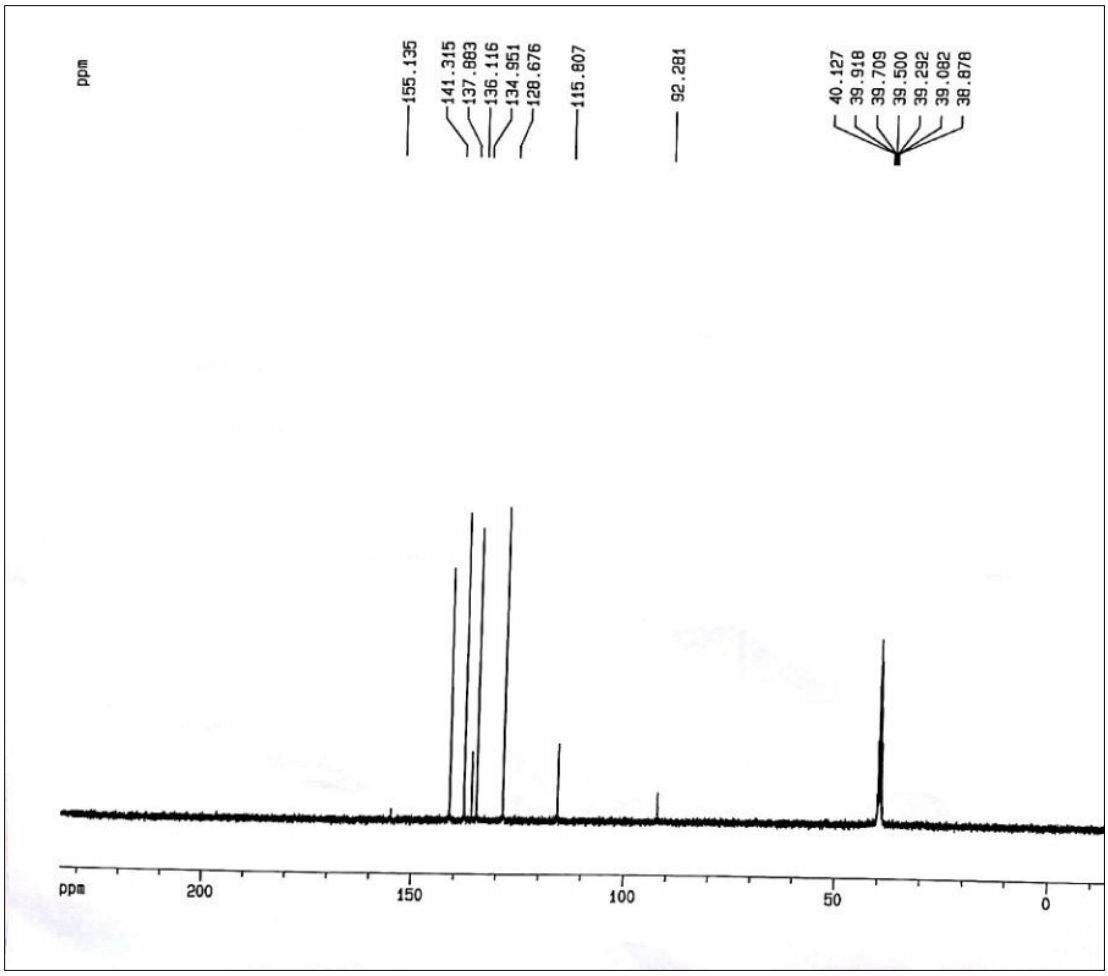




^{1}HNMR, (E)-2-(1H-tetrazol-5-yl)-3-(thiophen-2-yl)acrylonitrile.



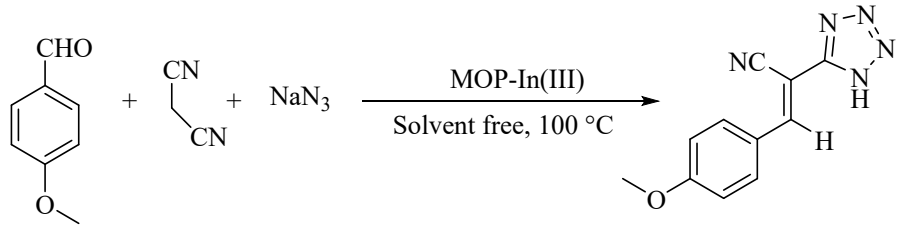
[1]HNMR, (E)-2-(1H-tetrazol-5-yl)-3-(thiophen-2-yl)acrylonitrile.

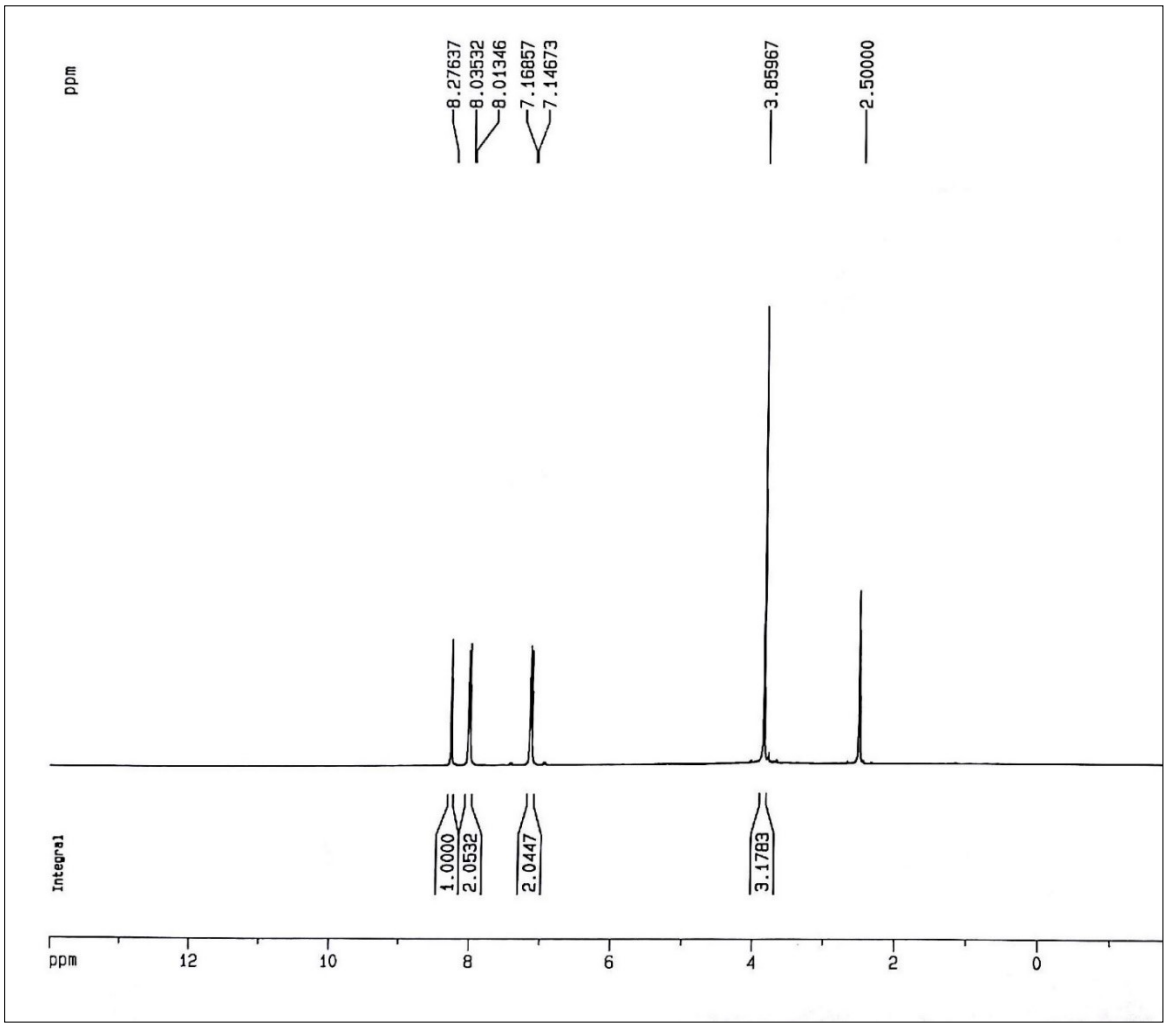


^{13}CNMR, (E)-2-(1H-tetrazol-5-yl)-3-(thiophen-2-yl)acrylonitrile.

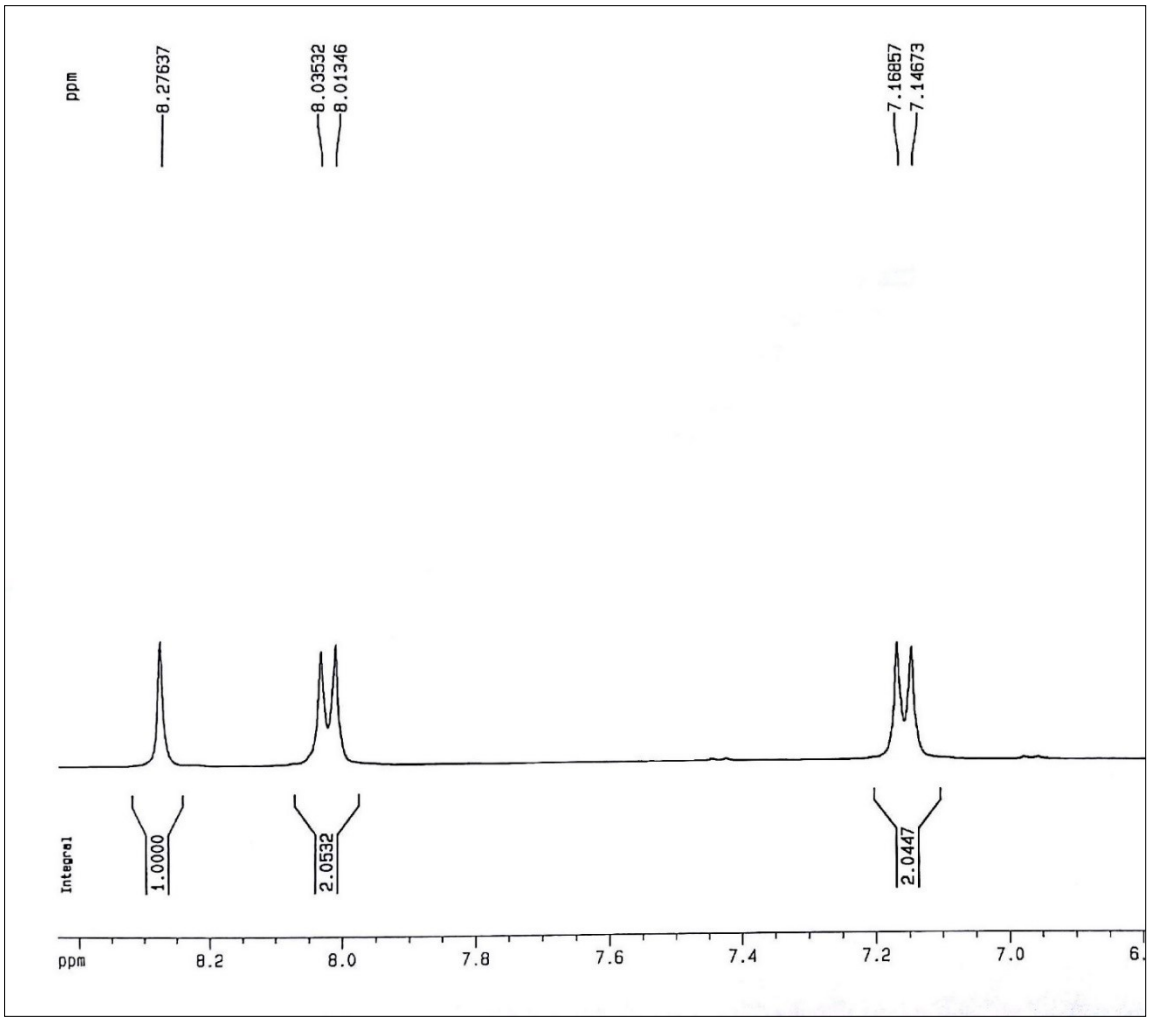
Table 3, Entry 4:

(E)-3-(4-methoxyphenyl)-2-(1H-tetrazol-5-yl)acrylonitrile. M.P: 153-155° C. ^{1}H-NMR (DMSO-d_6), δppm: 2.5(brs, NH, overlap with solvent) 3.86 (s, 3H, CH), 7.14-7.16 (d, 2H, CH-Ar), 8.01-8.03 (d, 2H, CH-Ar), 8.27 (s, 1H, CH). ^{13}C-NMR (DMSO-d_6), δppm: 55.73, 92.97, 114.99, 116.10, 124.48, 132.36, 148.16, 155.33, 162.68.

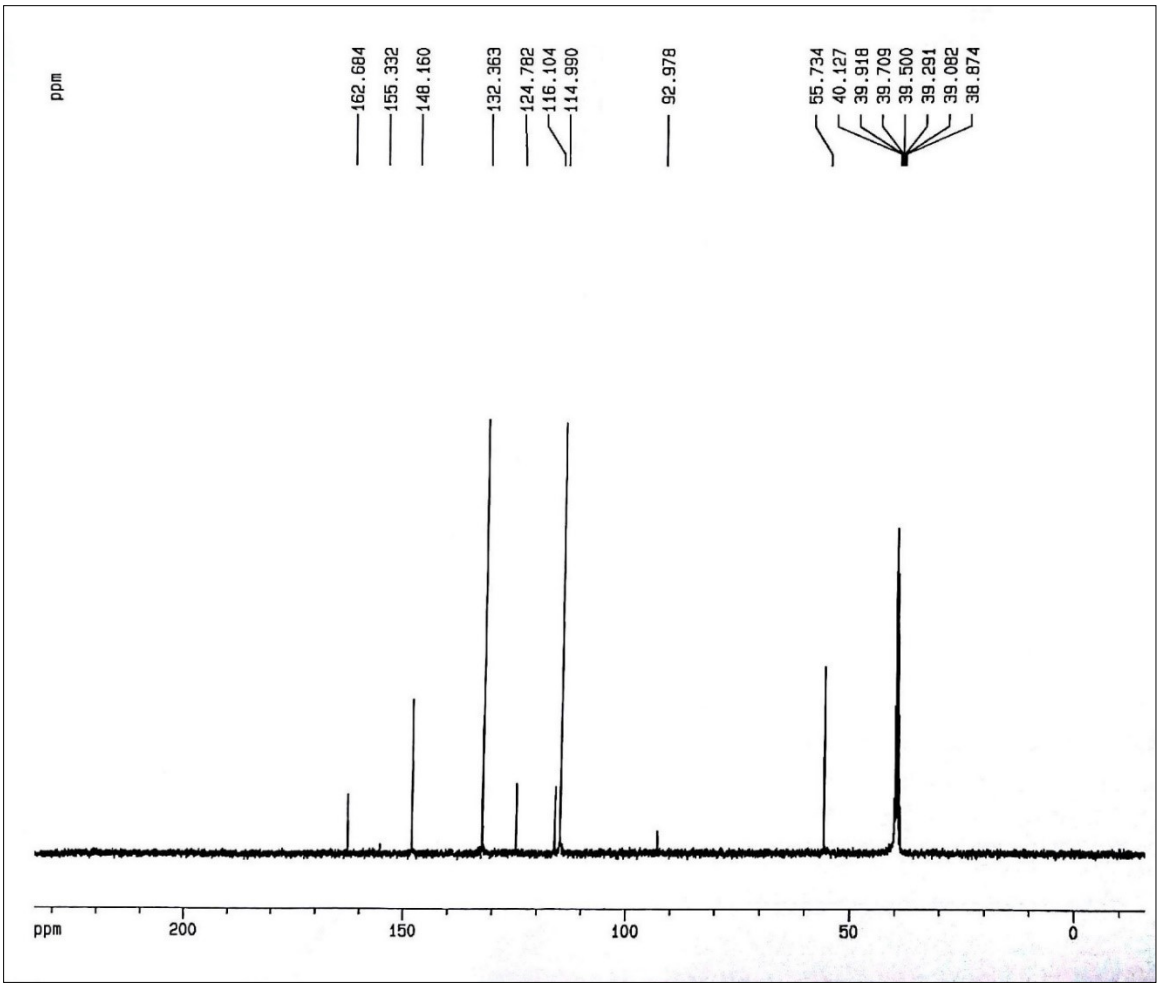




^{1}HNMR, (E)-3-(4-methoxyphenyl)-2-(1H-tetrazol-5-yl)acrylonitrile.



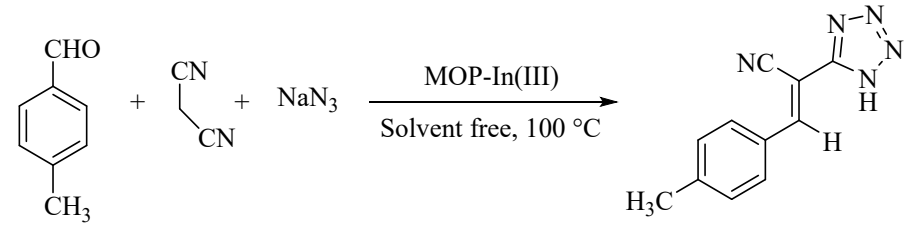
[1]HNMR, (E)-3-(4-methoxyphenyl)-2-(1H-tetrazol-5-yl)acrylonitrile.

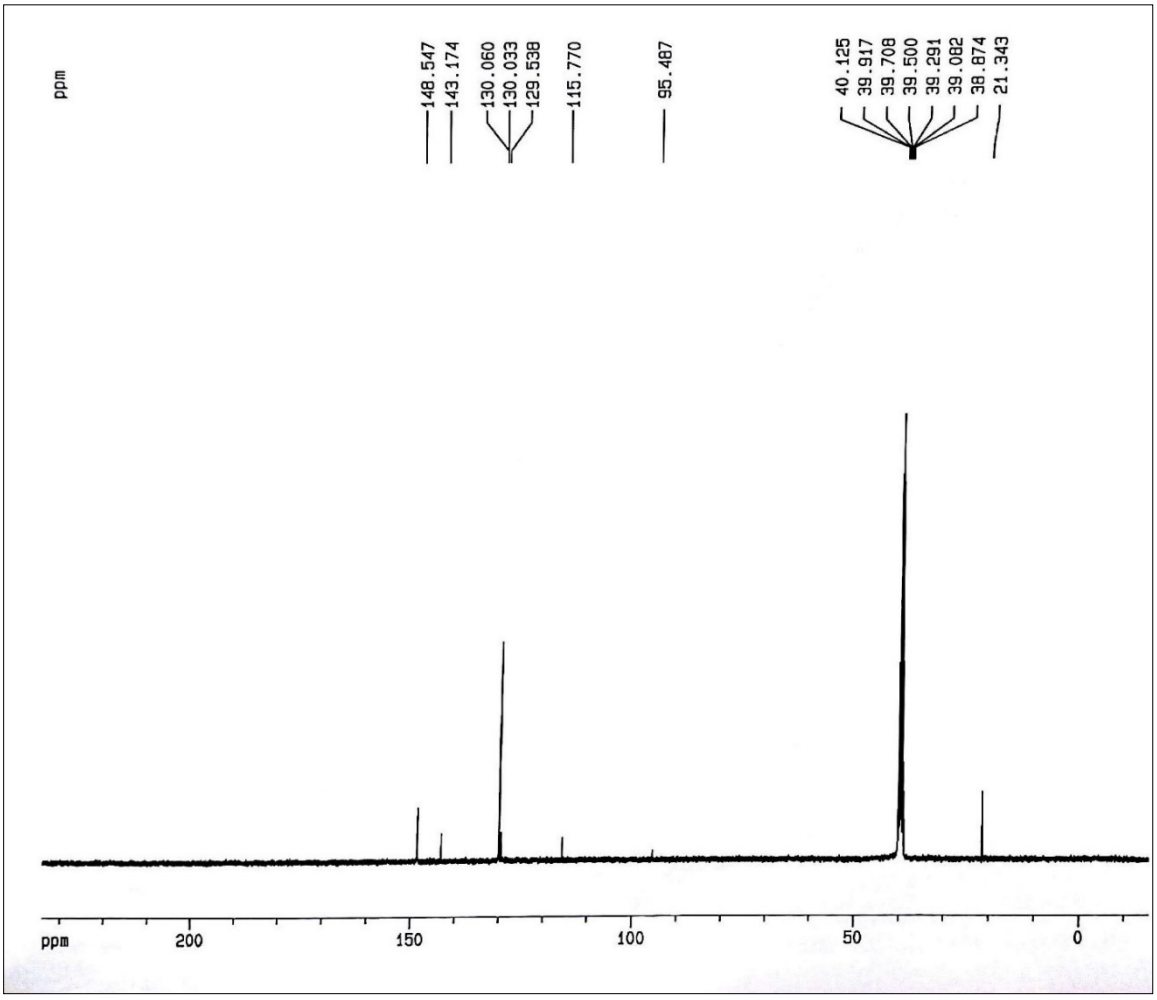


^{13}CNMR, (E)-3-(4-methoxyphenyl)-2-(1H-tetrazol-5-yl)acrylonitrile.

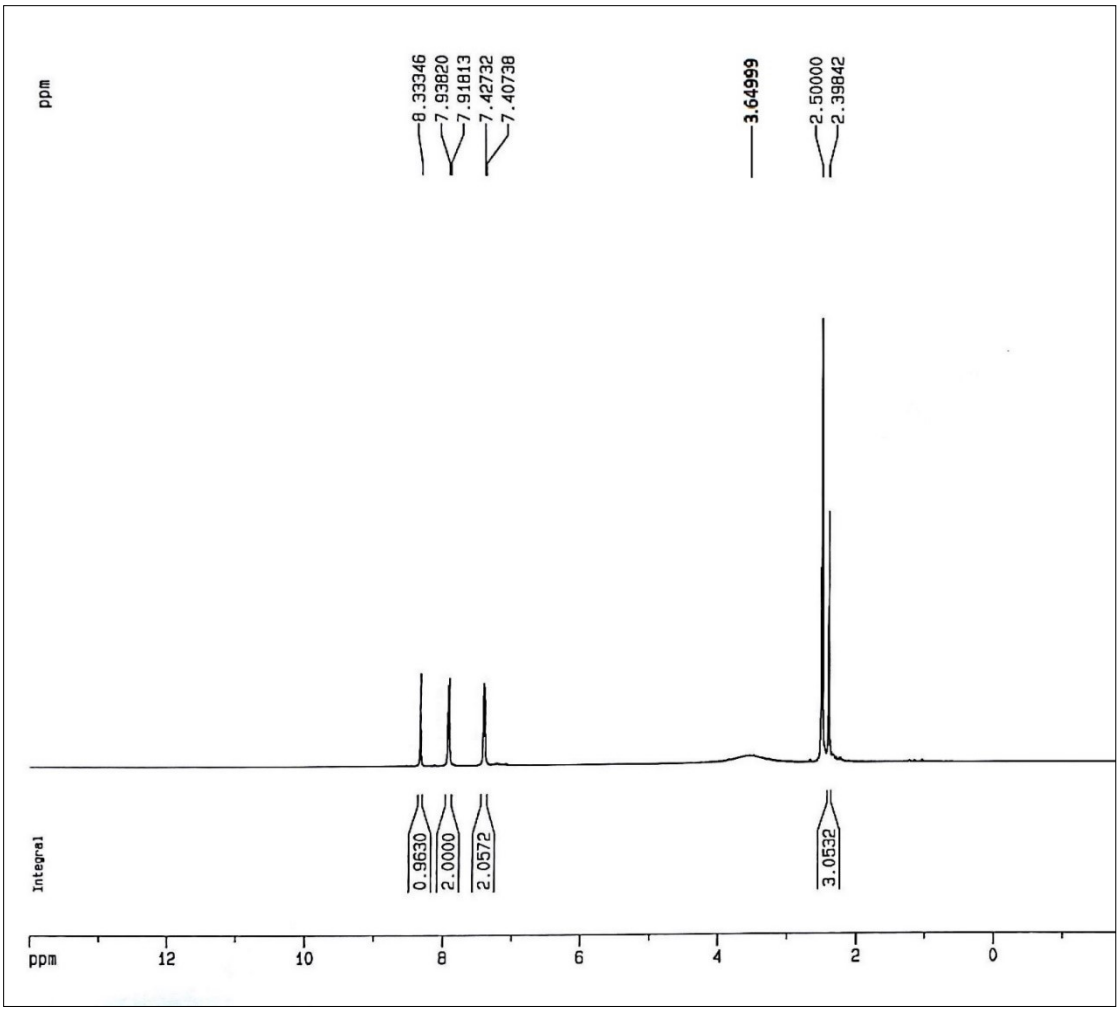
Table 3, Entry 5:

(E)-2-(1H-tetrazol-5-yl)-3-(p-tolyl)acrylonitrile. M.P: 188-191° C. ^{1}H-NMR (DMSO-d_6), δppm: 2.5 (brs, NH, overlap with solvent), 2.39 (s, 3H, CH), 7.40-7.42(d, 2H, CH-Ar), 7.91-7.93(d, 2H, CH-Ar), 8.33 (s, 1H, CH). ^{13}C-NMR (DMSO-d_6), δppm: 21.34, 95.48, 115.77, 129.53, 130.03, 130.06, 143.17, 148.54.

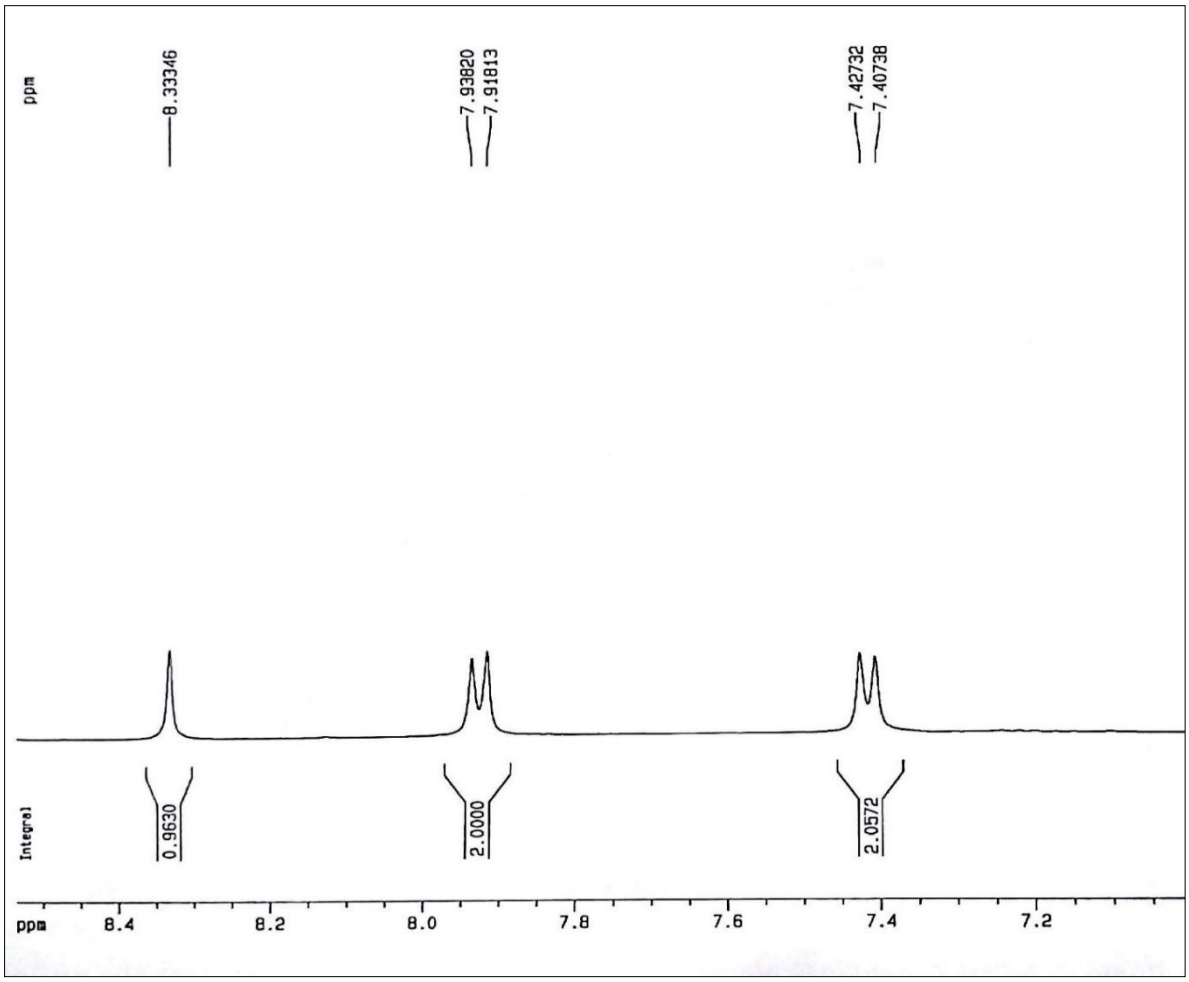




^{13}CNMR, (E)-2-(1H-tetrazol-5-yl)-3-(p-tolyl)acrylonitrile.



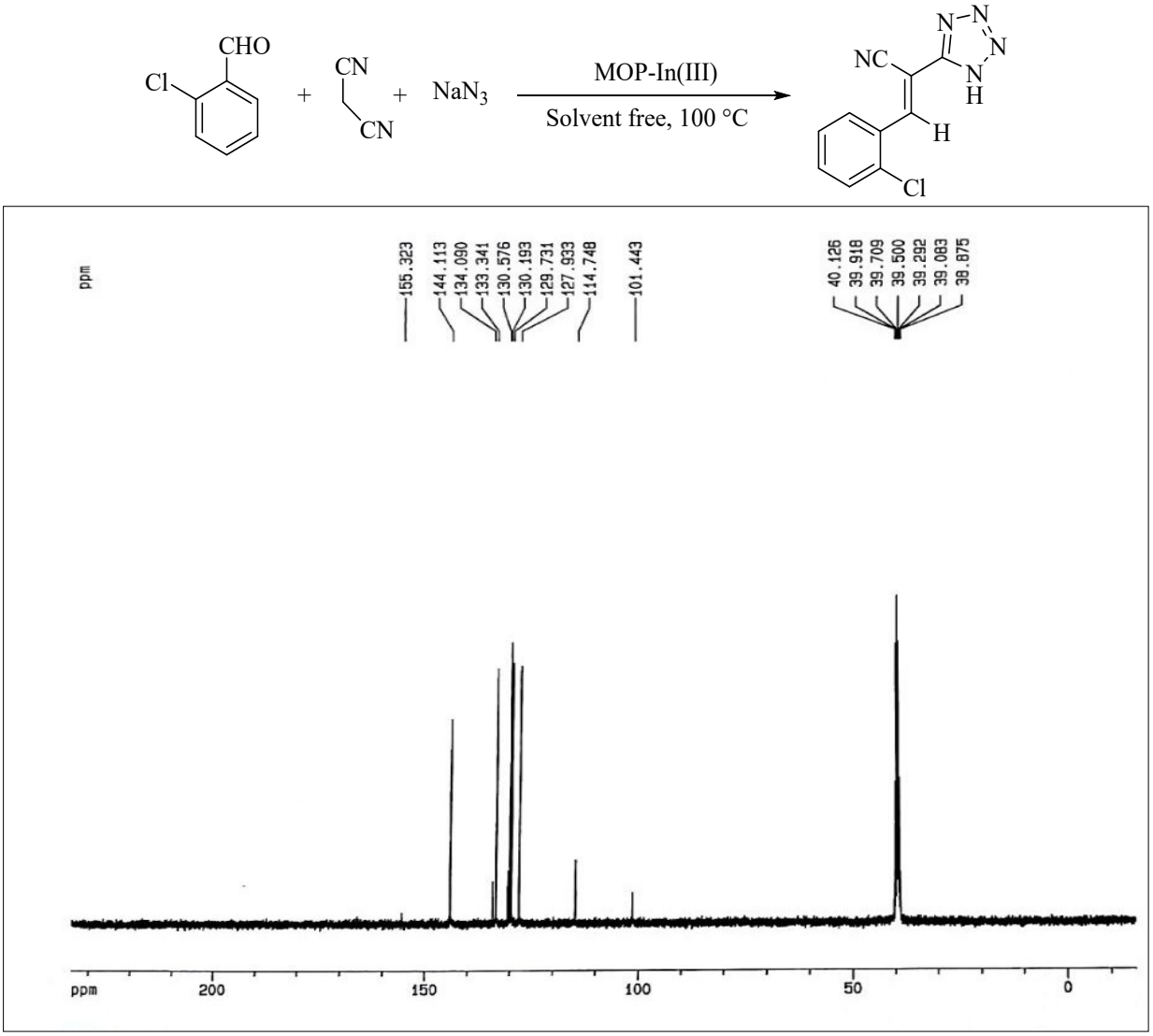
[1]HNMR, (E)-2-(1H-tetrazol-5-yl)-3-(p-tolyl)acrylonitrile.



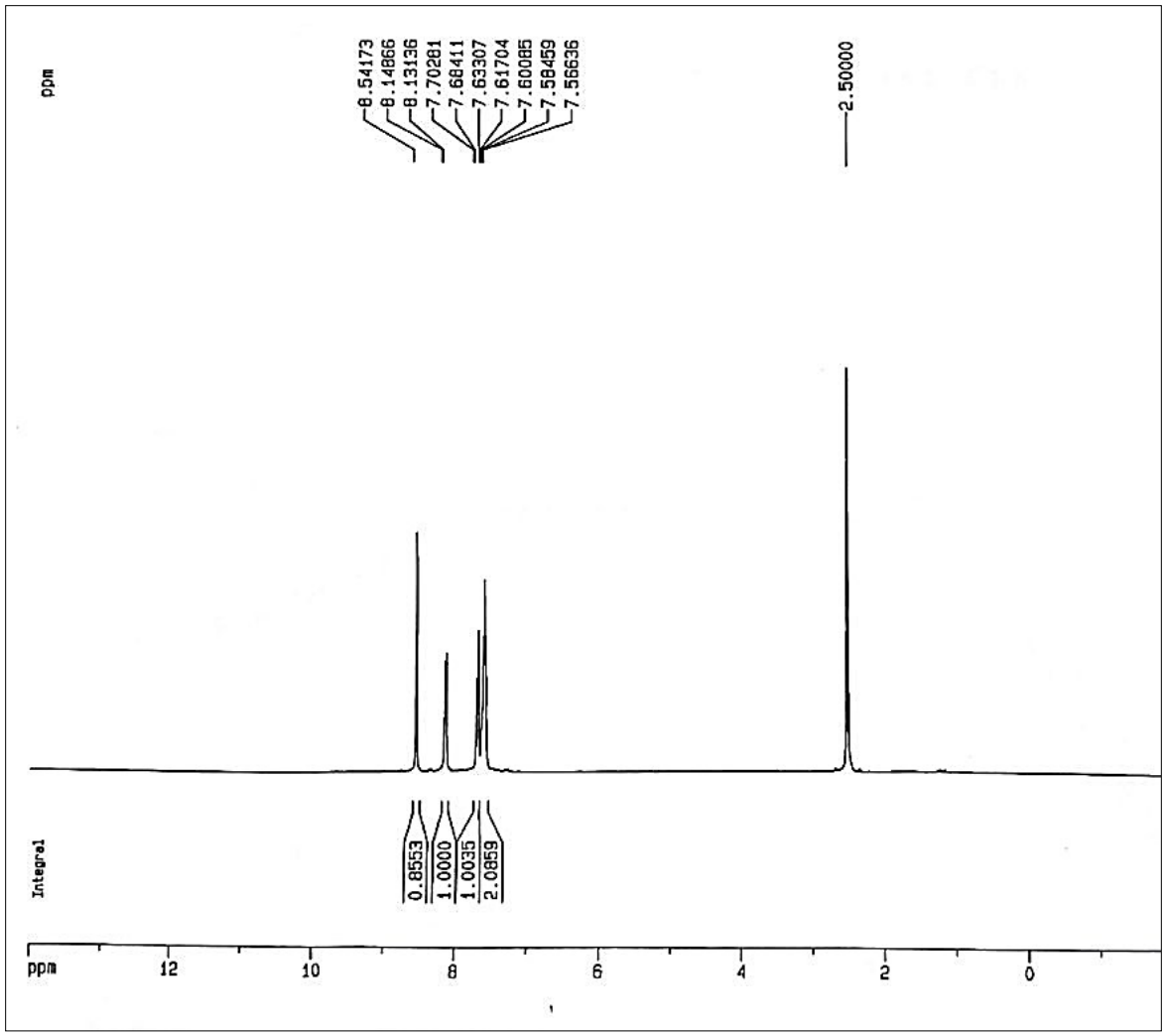
[1]HNMR, (E)-2-(1H-tetrazol-5-yl)-3-(p-tolyl)acrylonitrile.

Table 3, Entry 8:

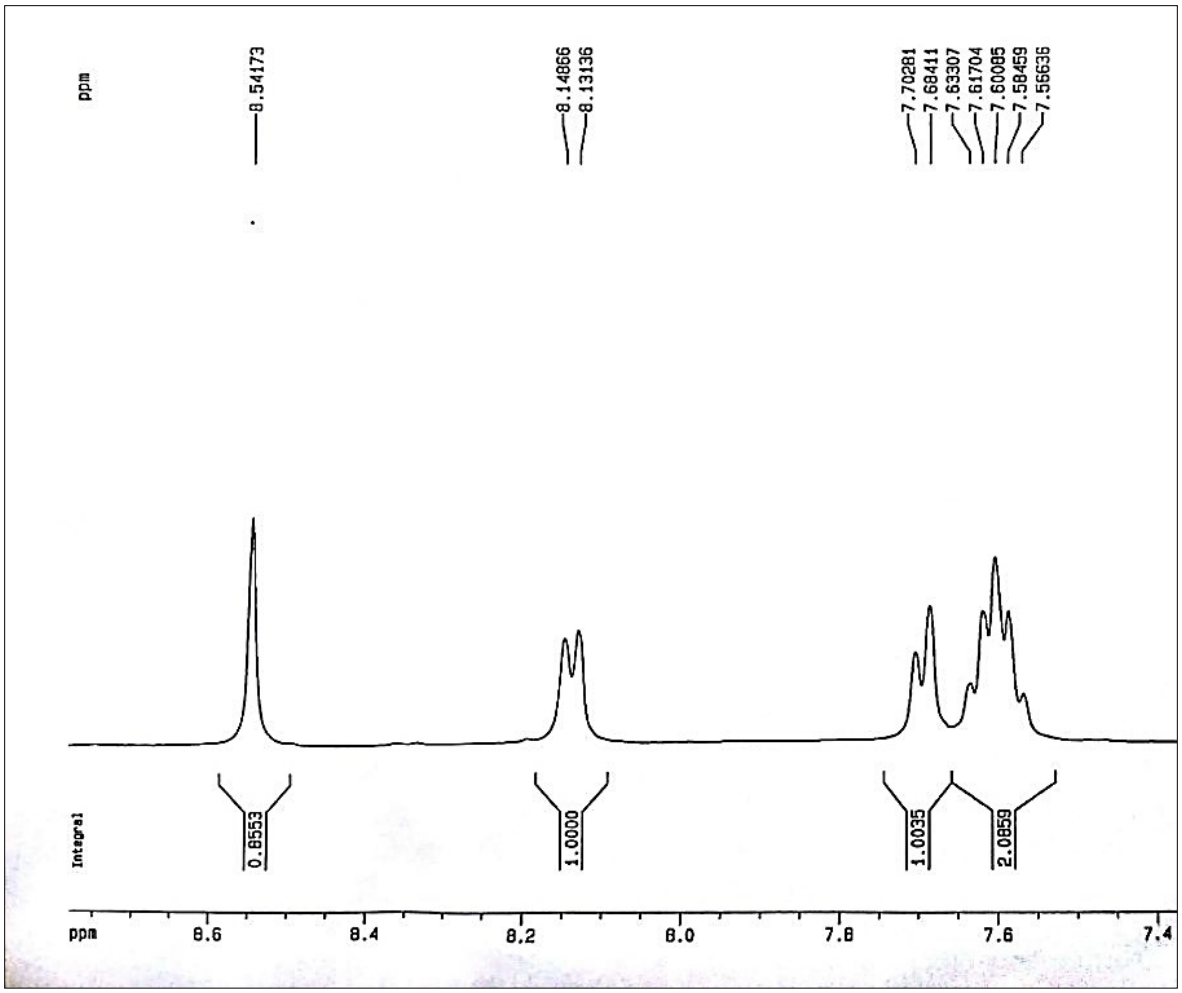
(E)-3-(2-chlorophenyl)-2-(1H-tetrazol-5-yl)acrylonitrile. M.P: 176-178° C. ^{1}H-NMR (DMSO-d_6), δppm: 2.5 (brs, NH, overlap with solvent), 7.56-7.63 (m, 2H, CH-Ar), 7.68-7.70 (d, 1H, CH-Ar), 8.13-8.14 (d, 1H, CH-Ar), 8.54(s, 1H, CH). ^{13}C -NMR (DMSO-d_6), δppm: 101.44, 114.74, 127.13, 129.73, 130,19, 130.57, 133.34, 134.09, 144.11, 155.32.



^{13}CNMR, (E)-3-(2-chlorophenyl)-2-(1H-tetrazol-5-yl)acrylonitrile.



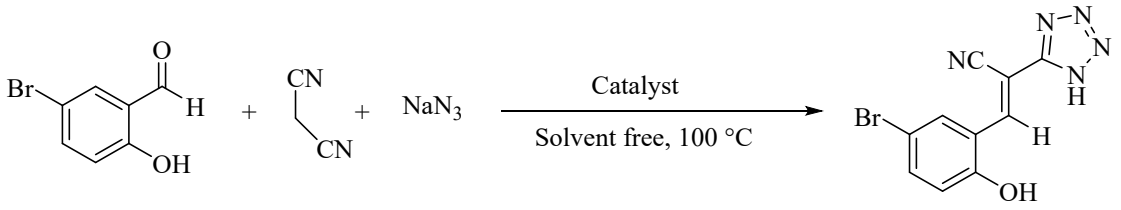
[1]HNMR, (E)-3-(2-chlorophenyl)-2-(1H-tetrazol-5-yl)acrylonitrile.

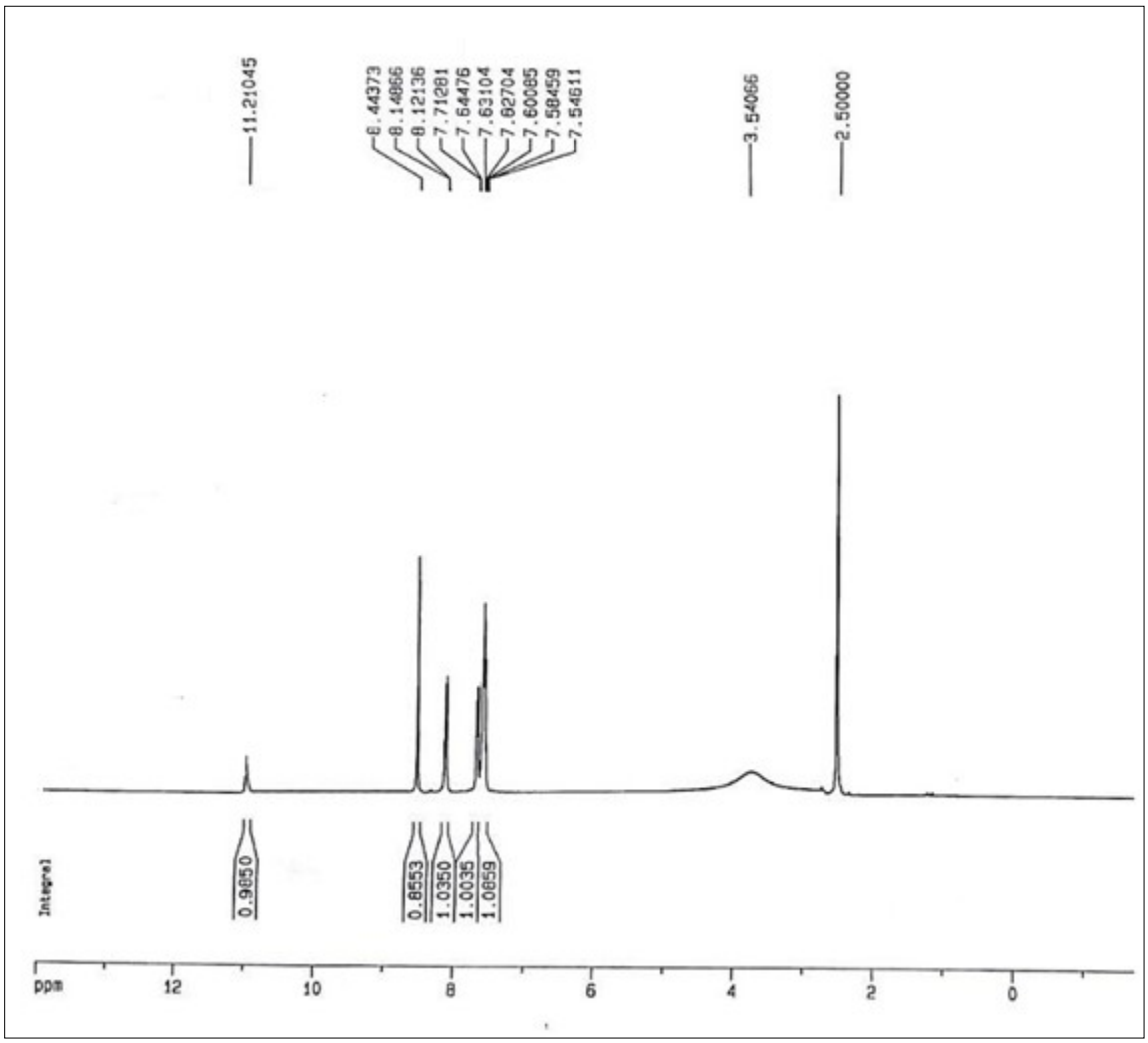


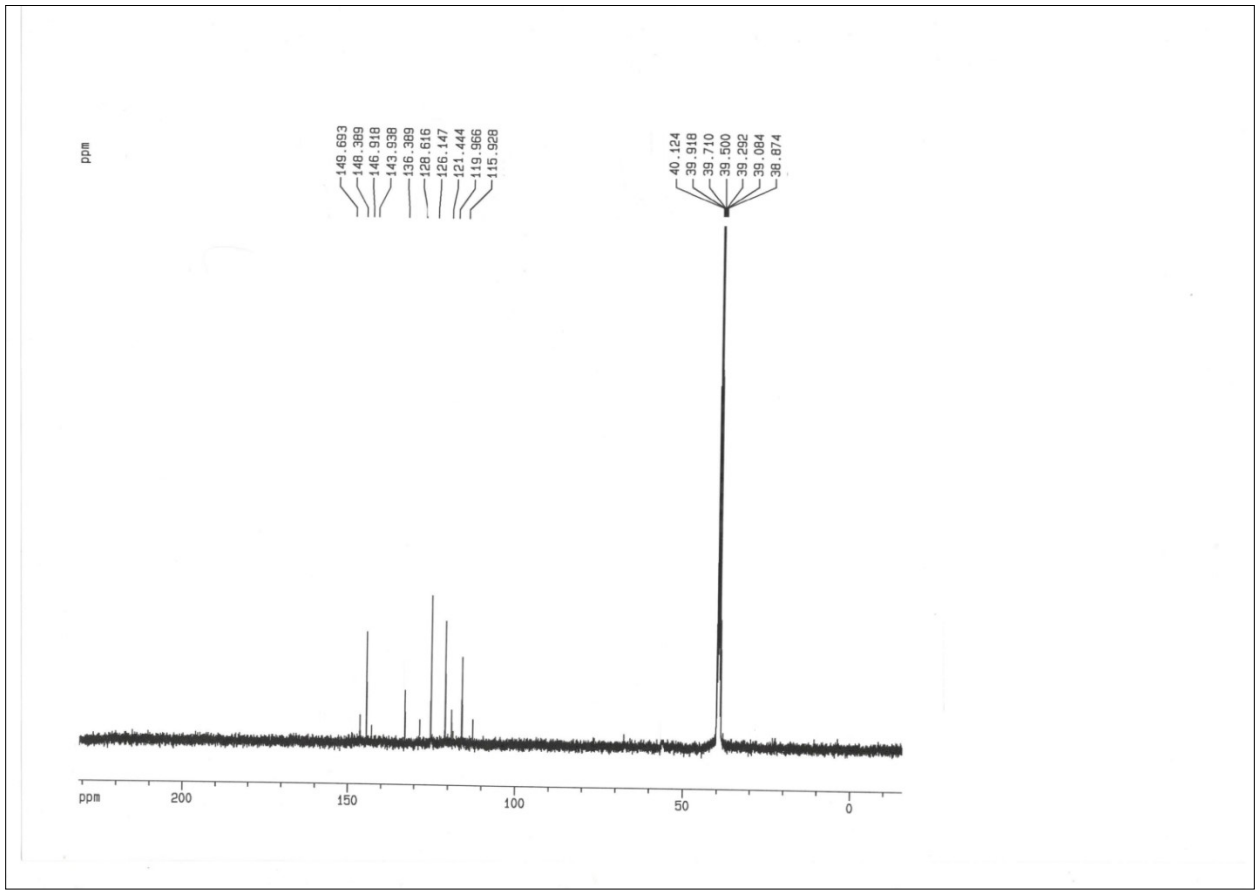
[1]HNMR, (E)-3-(2-chlorophenyl)-2-(1H-tetrazol-5-yl)acrylonitrile.

Table 3, Entry 10:

3-(5-Bromo-2-hydroxyphenyl)-2-(1H-tetrazole-5-yl) acrylonitrile. MS, m/z: 292.1 (M+H)+, 314.1 (M+Na)+. 1 H NMR (400 MHz, DMSO-d6): δH (ppm) 3.54 (br s, NH, overlap with solvent), 7.54–7.63 (1H, CH-Ar), 7.64–7.71(1H, CH-Ar), 8.12–8.14 (1H, CH-Ar), 8.44(s, 1H, CH). 13C NMR (100 MHz, DMSO-d6): δC (ppm) 115.9, 119.9, 121.4, 126.1, 128.6, 136.3, 143.9, 146.9, 148.3, 149.6



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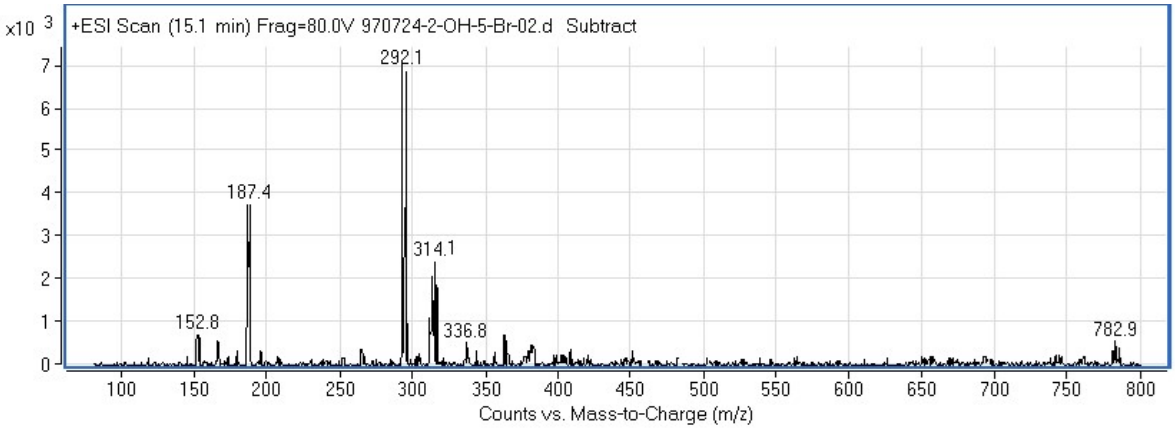
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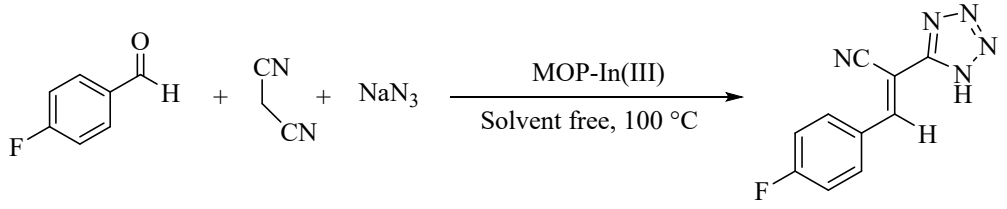
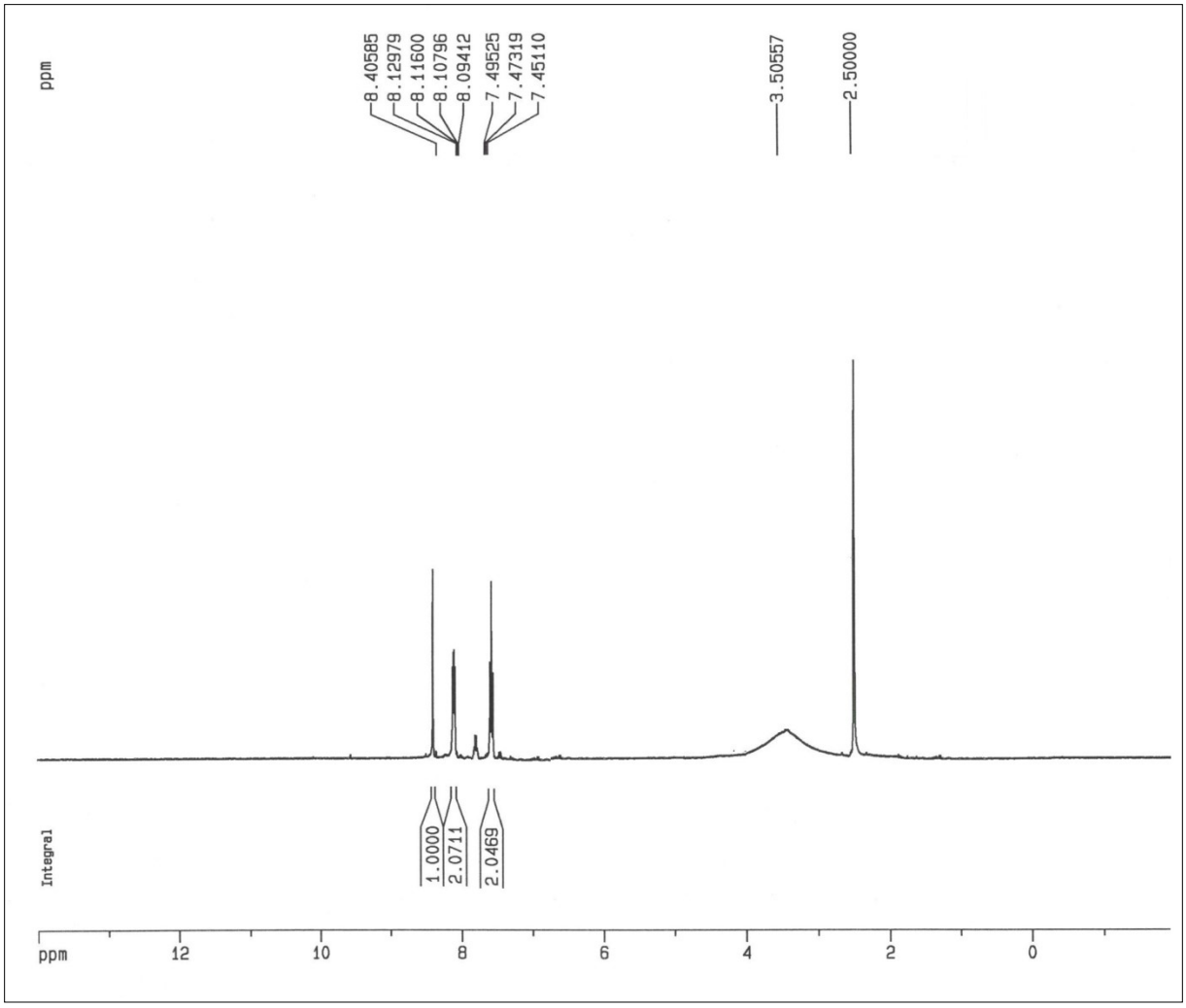
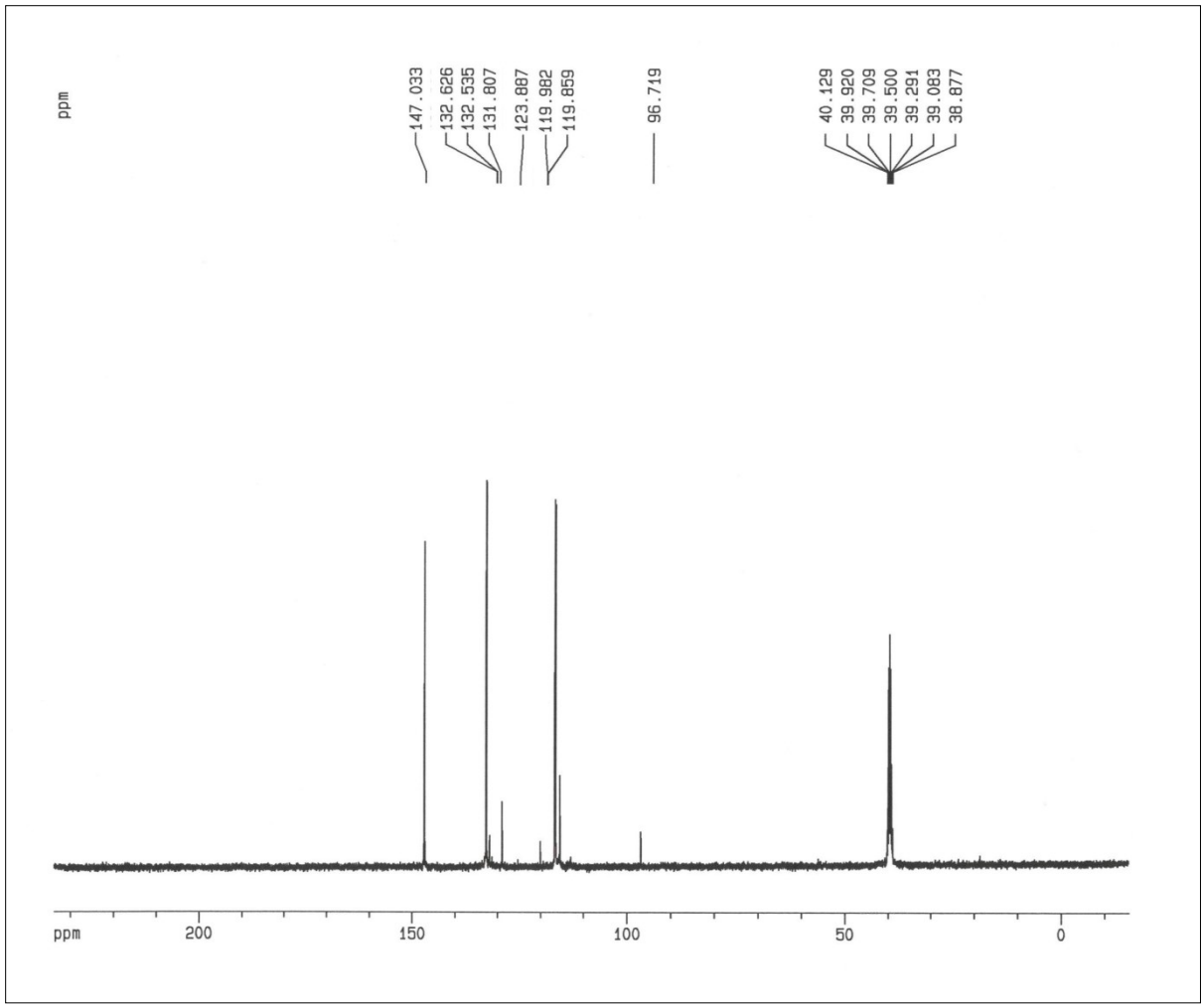
Counts vs. Mass-to-Charge (m/z)

Table 3, Entry 11:

3-(4-Fluorophenyl)-2-(1H-tetrazole-5-yl) acrylonitrile. IR (KBr) (υmax/cm−1): 3109 (NH), 2228 (CN), 1595 (C=C). MS, m/z: 216 (M+H)+, 238 (M+Na)+. 1 H NMR (400 MHz, DMSO-d6): δH (ppm) 3.50 (br s, NH, overlap with solvent), 7.45–7.49 (2H, CH-Ar), 8.098–8.120 (2H, CH-Ar), 8.40 (1H, CH). 13C NMR (100 MHz, DMSO-d6): δC (ppm) 96.7, 119.8, 119.9, 123.8, 131.8, 132.5, 132.6, 147.0



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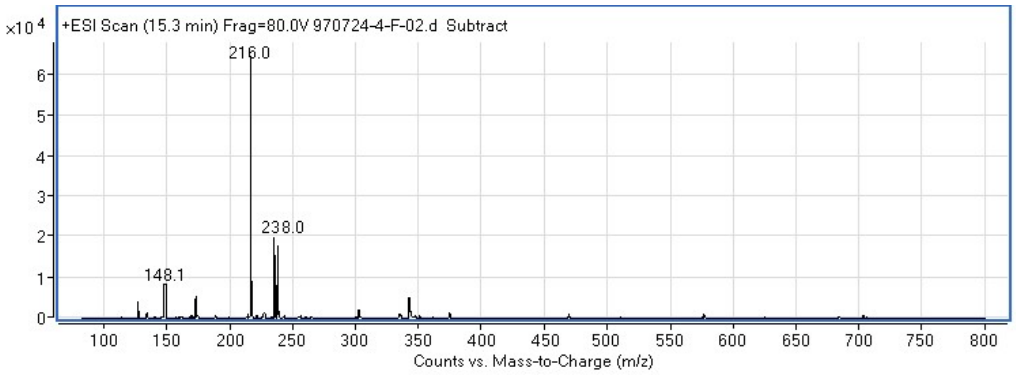
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4
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1
0
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300
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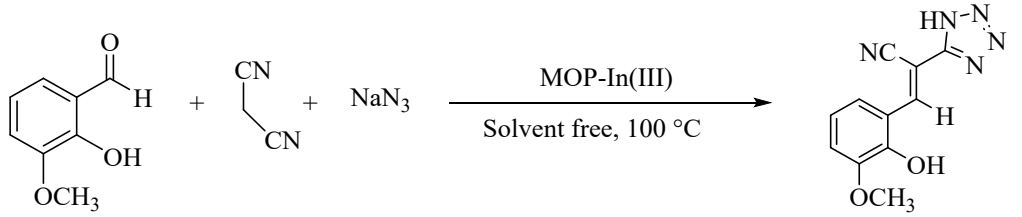
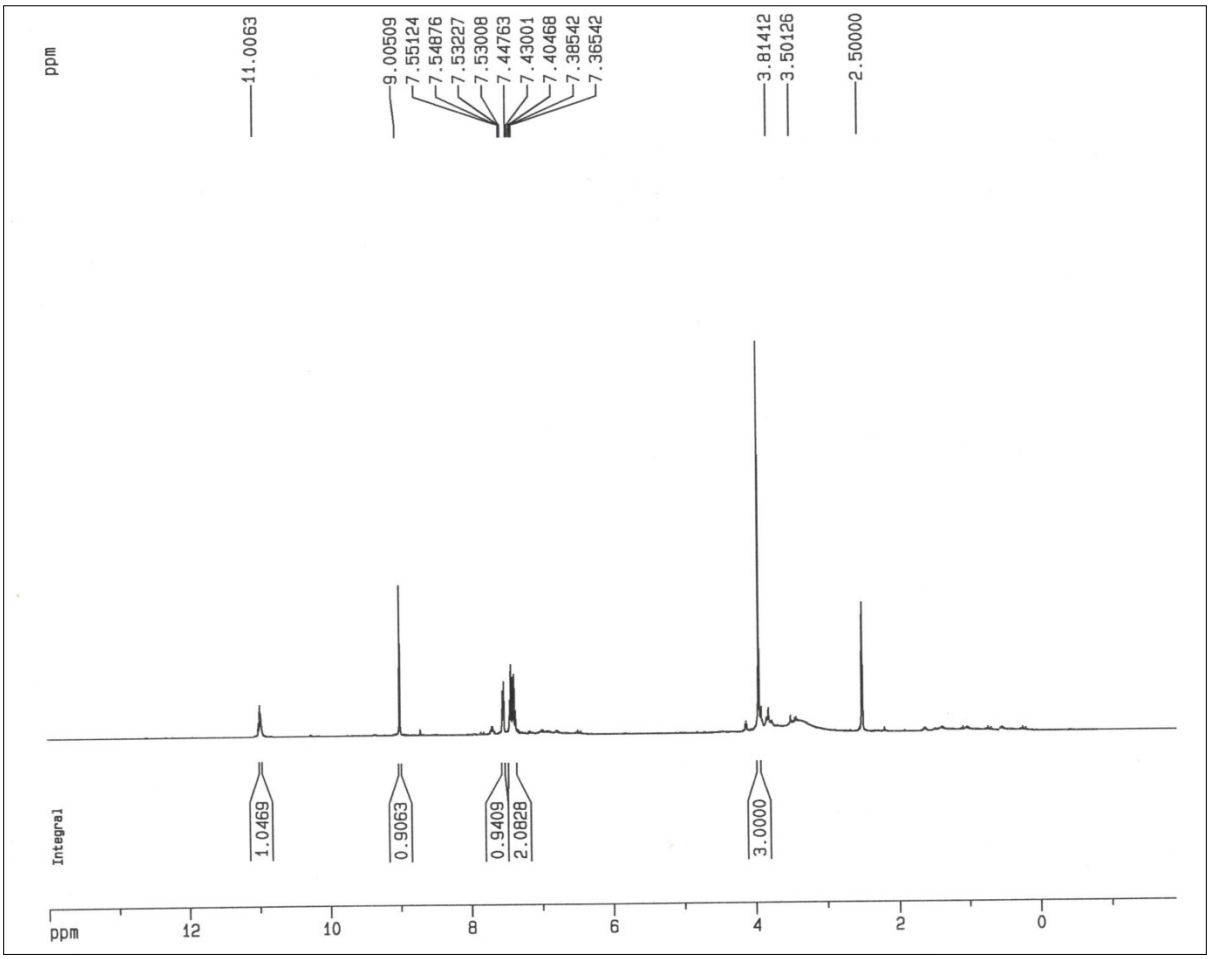
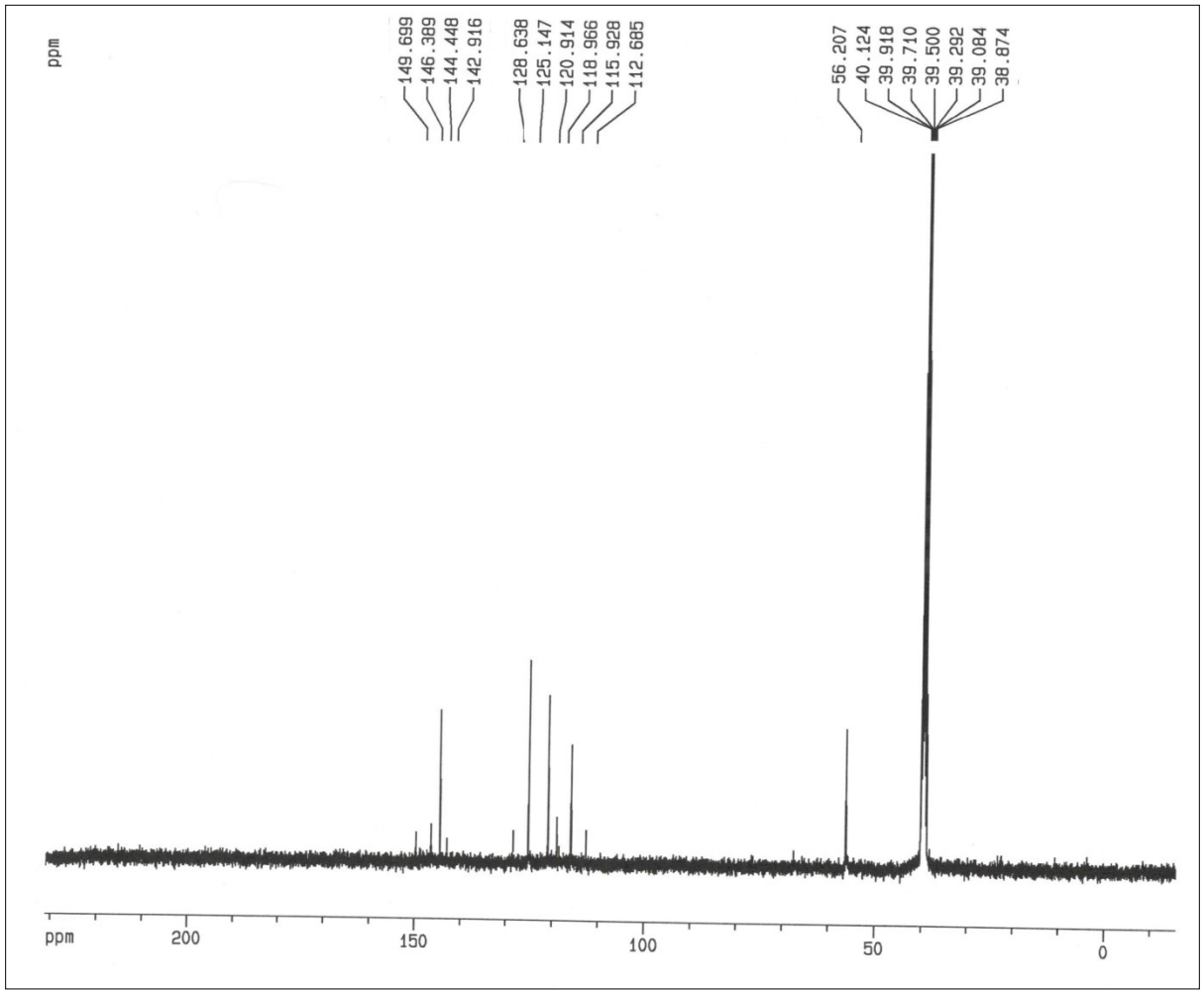
400
450
500
550
600
650
700
750
800
Counts vs. Mass-to-Charge (m/z)

Table 3, Entry 12:

3-(2-Hydroxy-3-methoxyphenyl)-2-(1H-tetrazole-5-yl) acrylonitrile. IR (KBr) (υmax/cm−1): 3174 (NH), 2201 (CN), 1580 (C=C). MS, m/z: 243 (M+H)+, 266 (M+Na)+. 1 H NMR (400 MHz, DMSOd6): δH (ppm) 3.50 (br s, NH, overlap with solvent), 3.81 (3H, OCH3), 7.36–7.44 (2H, CH-Ar), 7.53–7.55 (2H, CH-Ar), 9.00 (1H, CH), 11.00 (1H, OH). 13C NMR (100 MHz, DMSO-d6): δC (ppm) 56.2, 112.6, 115.9, 118.9, 120.9, 125.1, 128.6, 142.9, 144.4, 146.3, 149.6.



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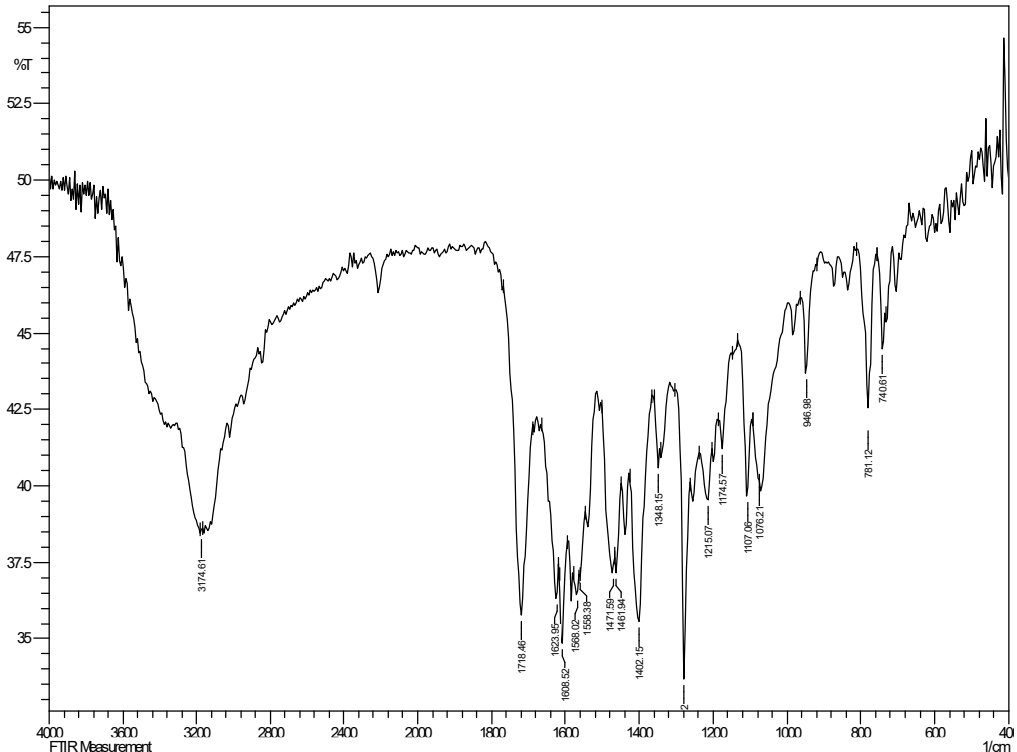
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FTIR Measurement
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