## Electronic Supplementary Information

# Post Synthetically Modified Metal–Organic Framework for Copper Catalyzed Denitrative C-N Coupling of Nitroarenes under Heterogeneous Condition

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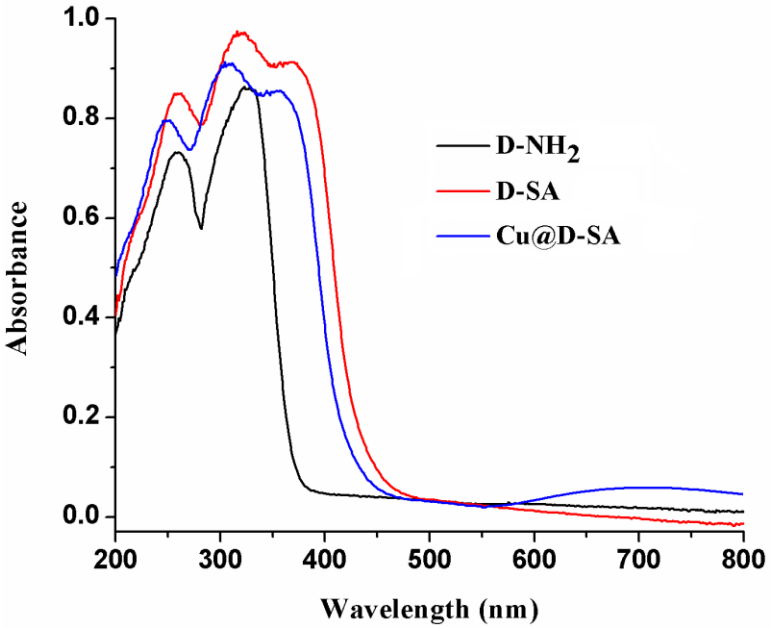



**Fig. S1** Solid state diffuse reflectance UV−Vis spectra of D–$NH_2$, D–SA and Cu@D–SA.

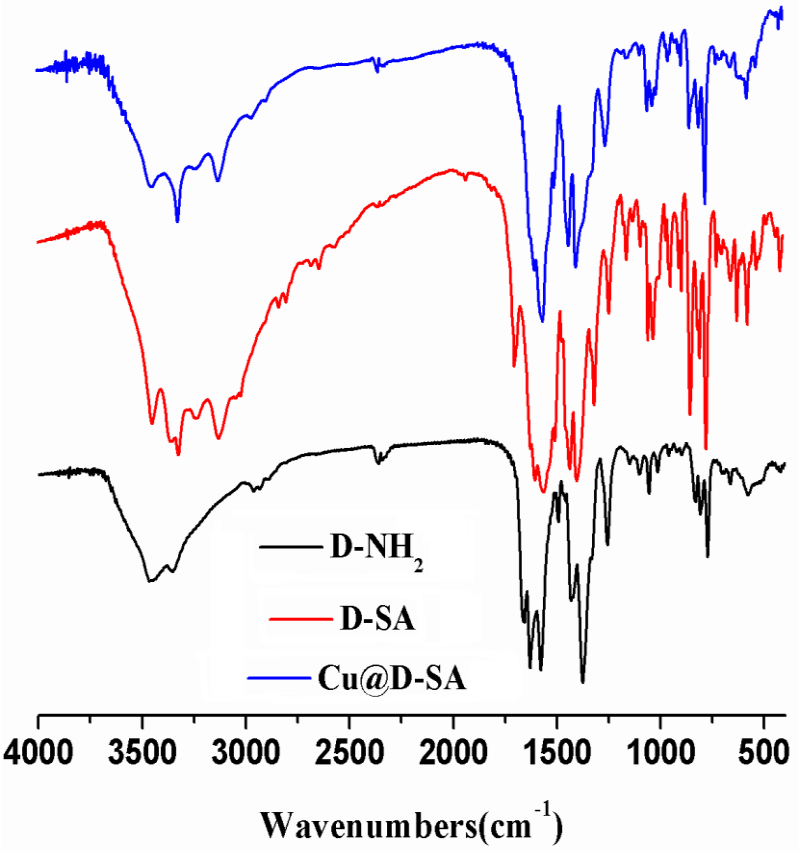



**Fig. S2** FTIR spectra of D-$NH_2$, D-SA and Cu@D-SA.

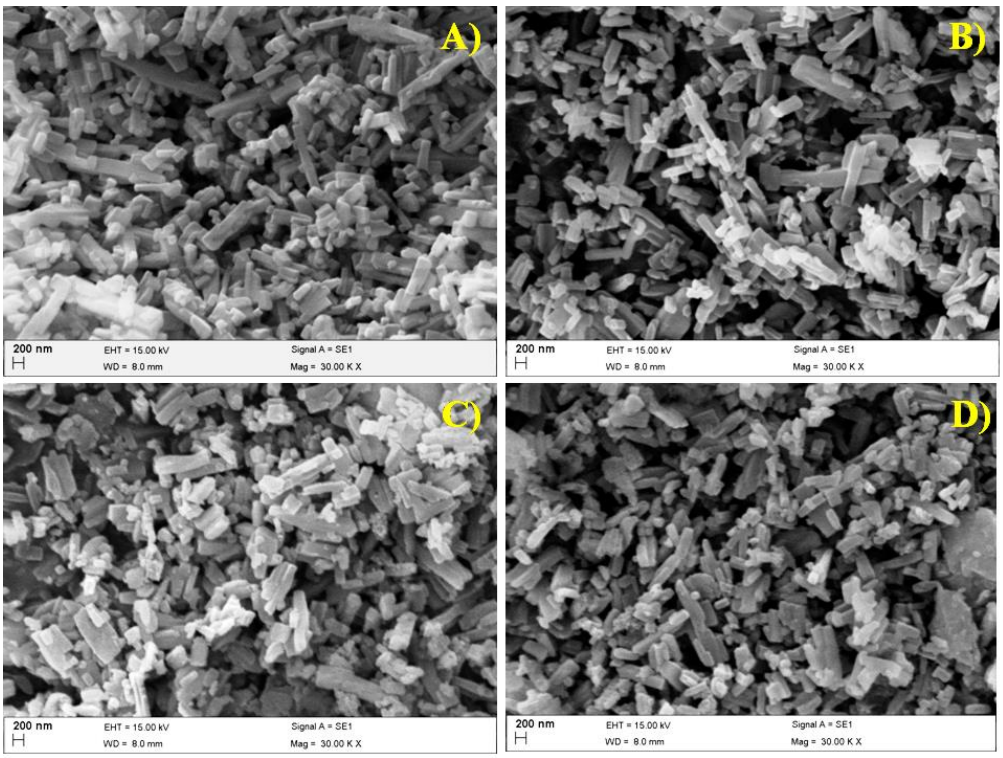



**Fig. S3** SEM image of A) D-$NH_2$, B) D-SA, C) Cu@D-SA (unreacted) and D) Cu@D-SA (recovered after 5th cycle).

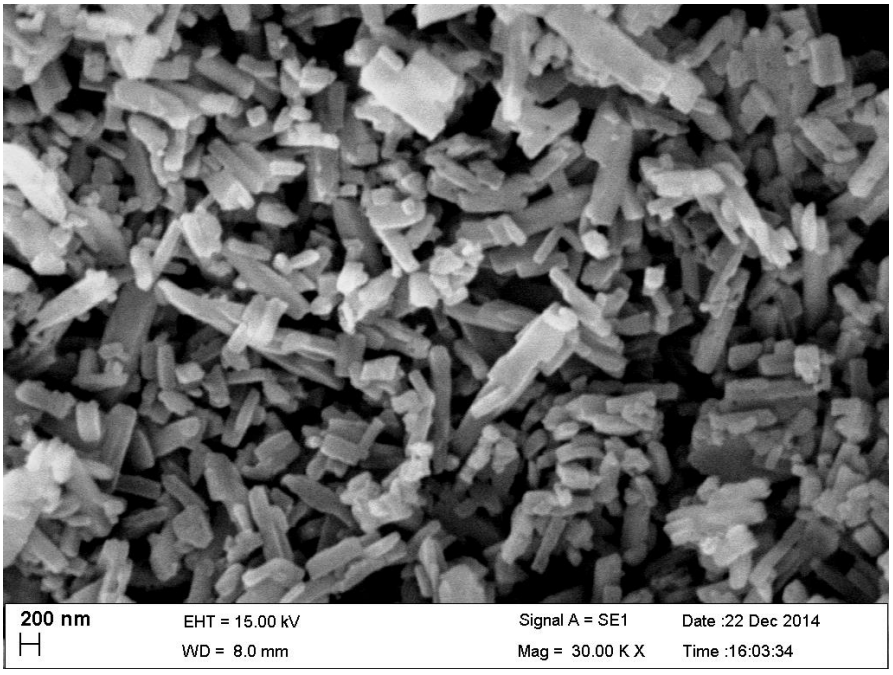
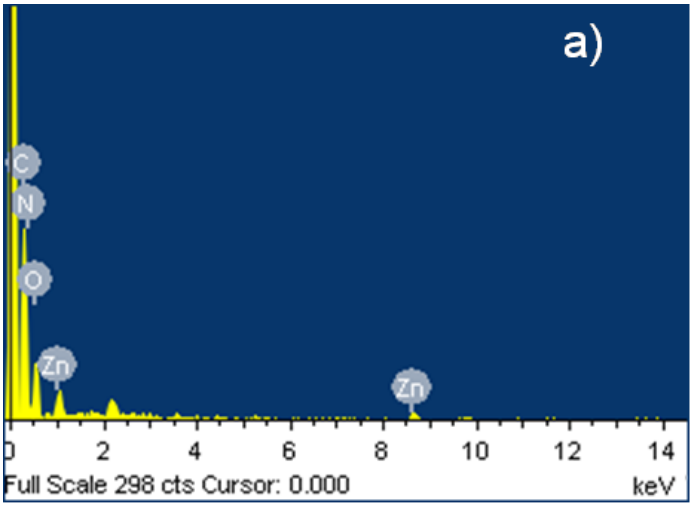
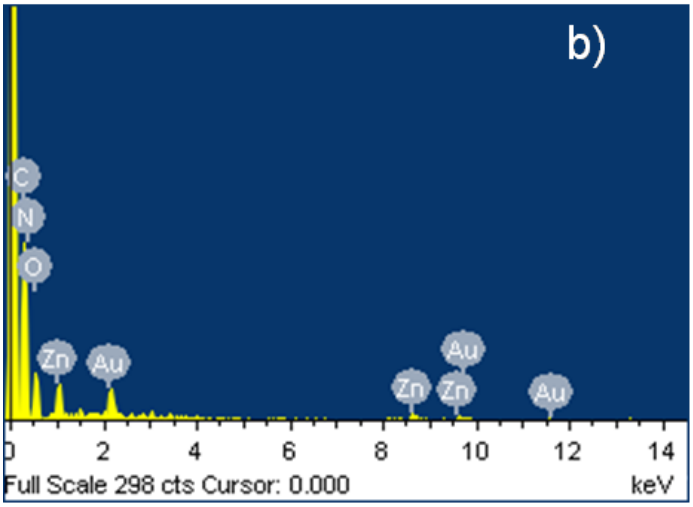



**Fig. S4** SEM image of Cu@D-SA (recovered after 10th cycle)

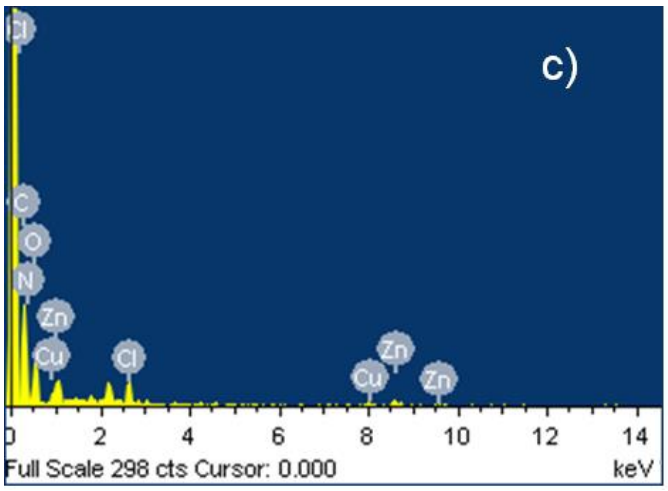



| Element | Weight% |
|---|---|
| CK | 49.59 |
| NK | 9.15 |
| OK | 20.85 |
| ZnK | 20.41 |
| Totals | 100.00 |



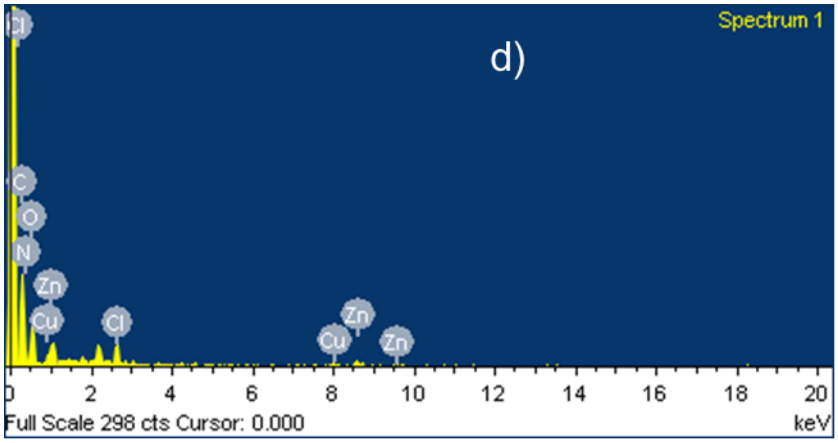

| Element | Weight% |
|---|---|
| CK | 51.57 |
| NK | 8.36 |
| OK | 20.12 |
| ZnK | 19.95 |
| Totals | 100.00 |

**Fig. S5** EDS elemental analysis of a) D-$NH_2$ and B) D-SA. Au is present in spectra due to gold coating.




| Element | Weight% |
|---|---|
| CK | 50.29 |
| NK | 7.98 |
| OK | 16.01 |
| ClK | 2.69 |
| CuK | 2.39 |
| ZnK | 20.64 |
| Totals | 100.00 |

**Fig. S6** EDS elemental analysis of c) Cu@D–SA.




| Element | Weight% |
|---|---|
| C K | 51.69 |
| N K | 7.68 |
| O K | 16.31 |
| Cl K | 2.31 |
| Cu K | 2.04 |
| Zn K | 19.97 |
| Totals | 100.00 |

**Fig. S7** EDS elemental analysis of d) Cu@D–SA recovered after 10$^{th}$ catalytic cycles.

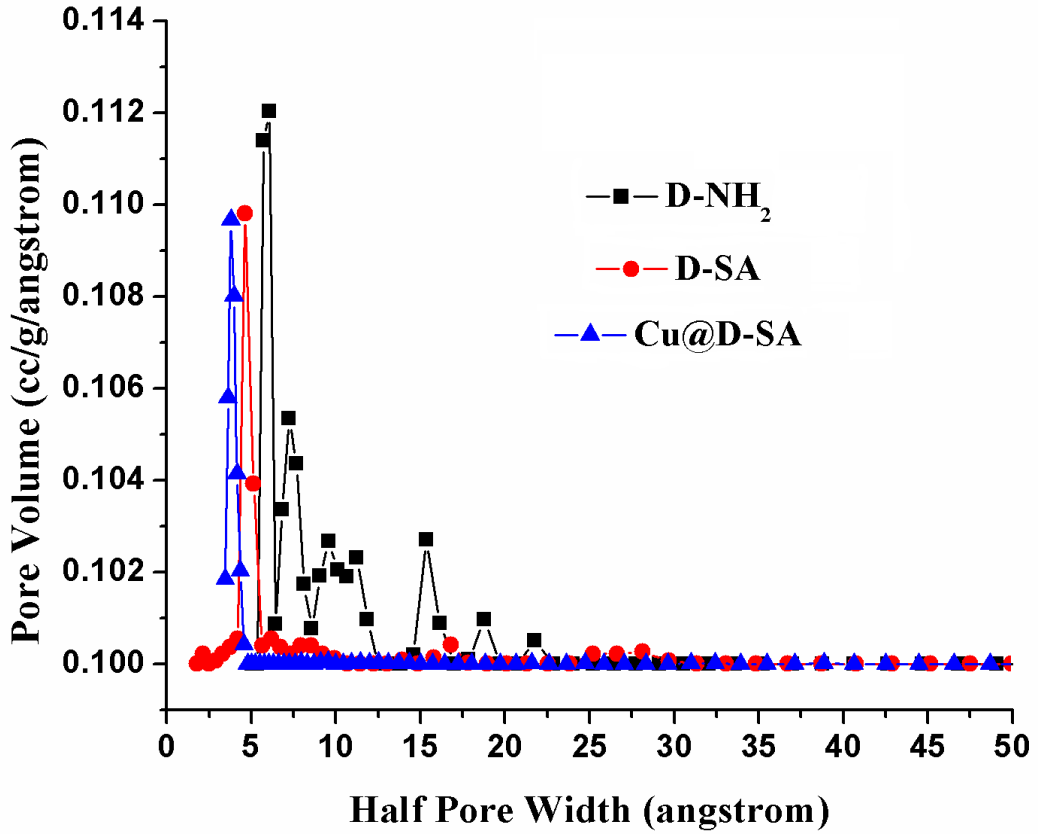



**Fig. S8** Pore size distribution of 1) D-$NH_2$ (half pore width – 6.1 Å), 2) D-SA (half pore width – 4.6 Å) and 3) Cu@D-SA (half pore width – 3.7 Å).

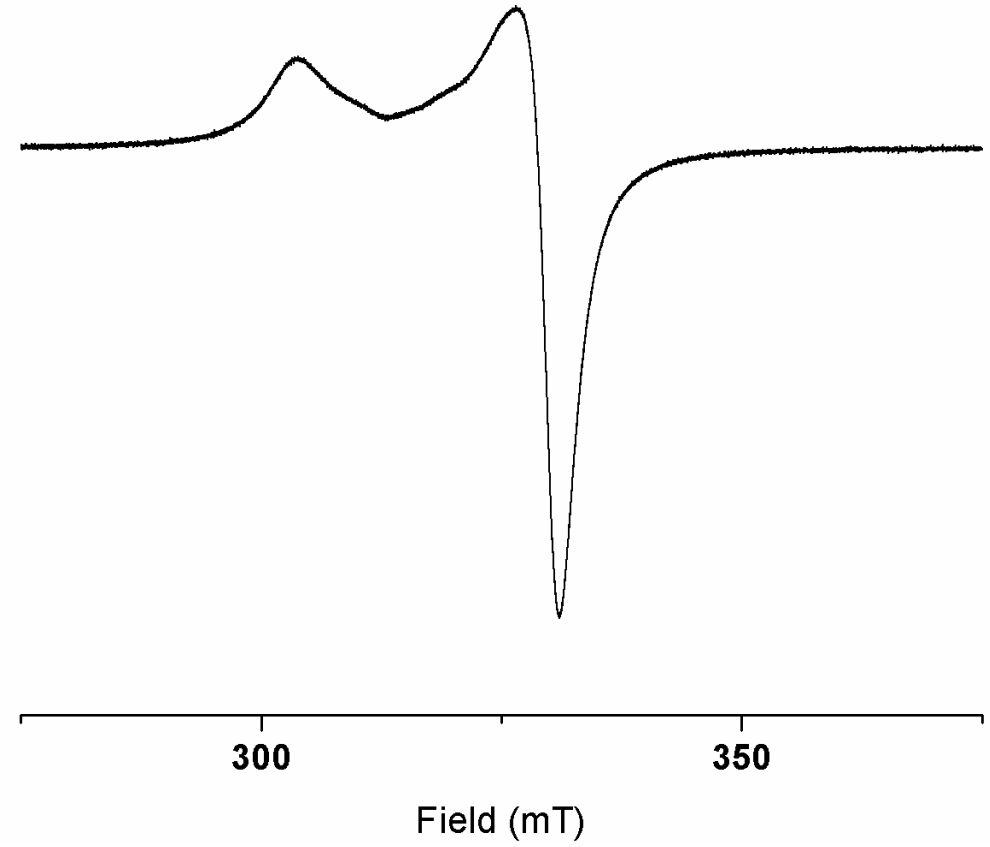



**Fig. S9** X-band EPR spectrum of the catalyst Cu@D-SA.

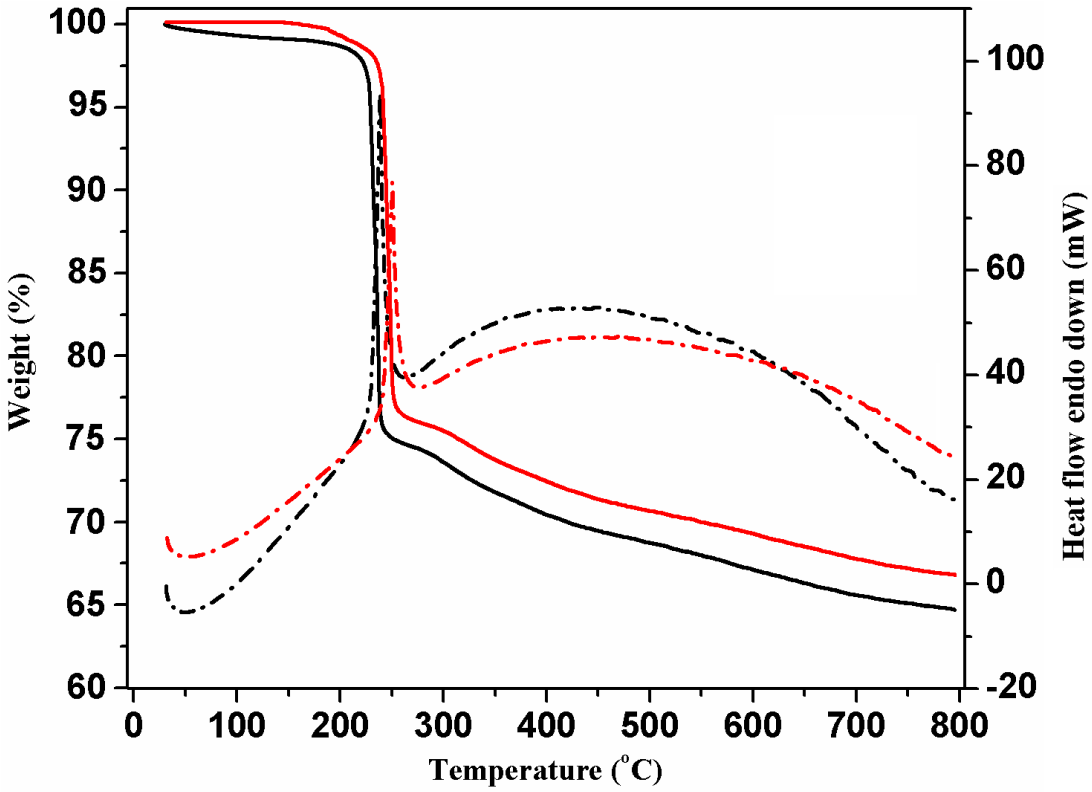



**Fig. S10** TG(—)/DTA(— - —) curve for a) Cu@D–SA (black) and b) dehydrated ($10^{-2}$ Torr, 4 hours at 90 °C) Cu@D–SA (red).

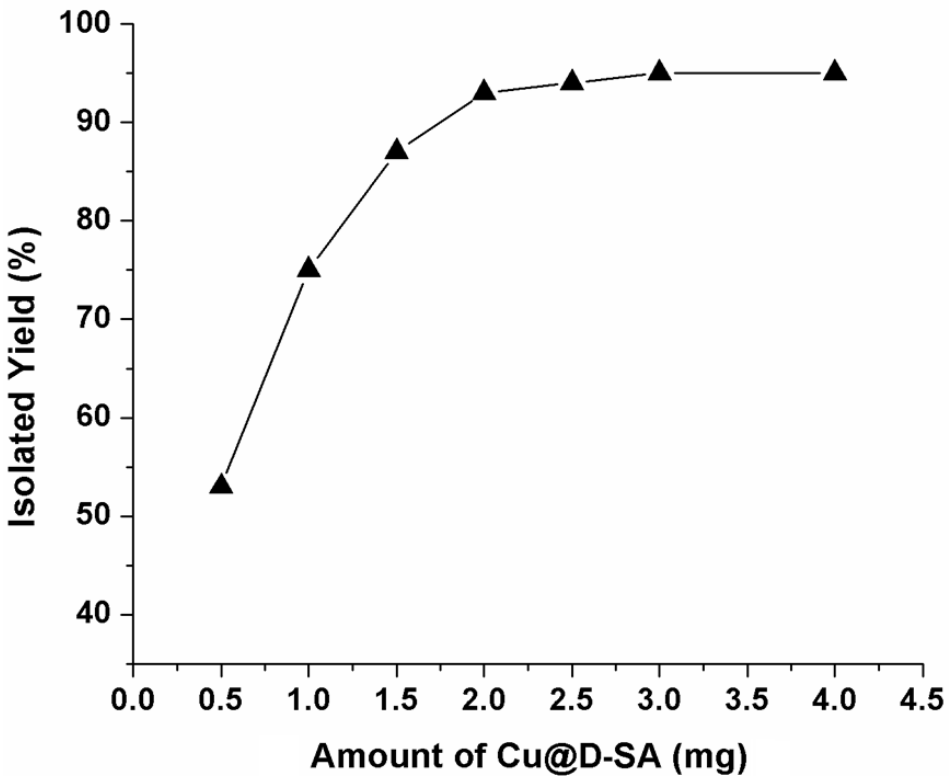



**Fig. S11** Plot showing progress of reaction for optimization of amount of catalyst Cu@D-SA in N-arylation reaction of 1,4-dinitrobenzene with pyrazole.

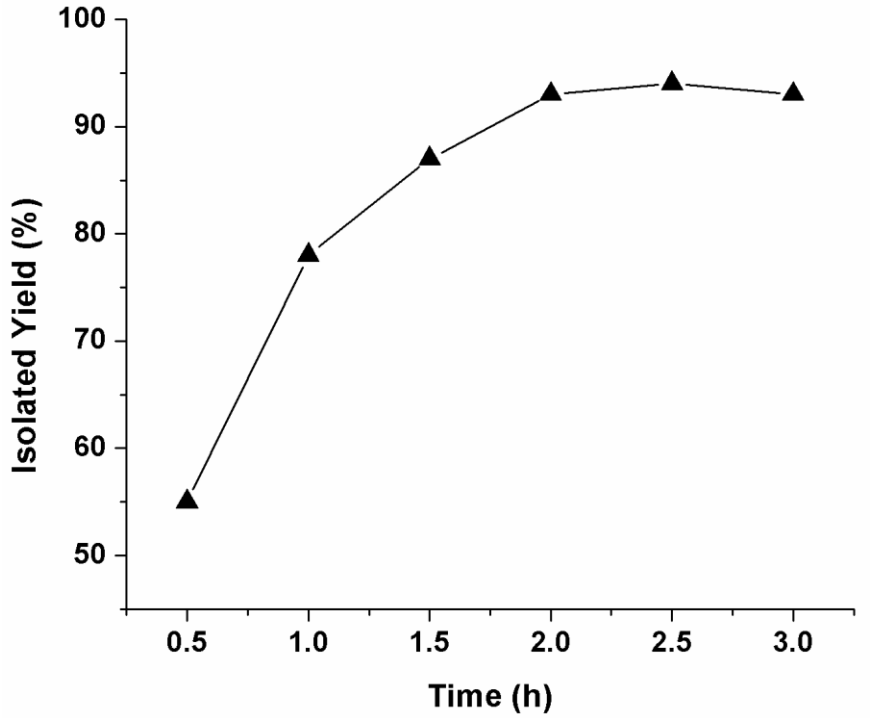



**Fig. S12** Reaction propagation plot for N-arylation reaction of 1,4-dinitrobenzene with pyrazole.

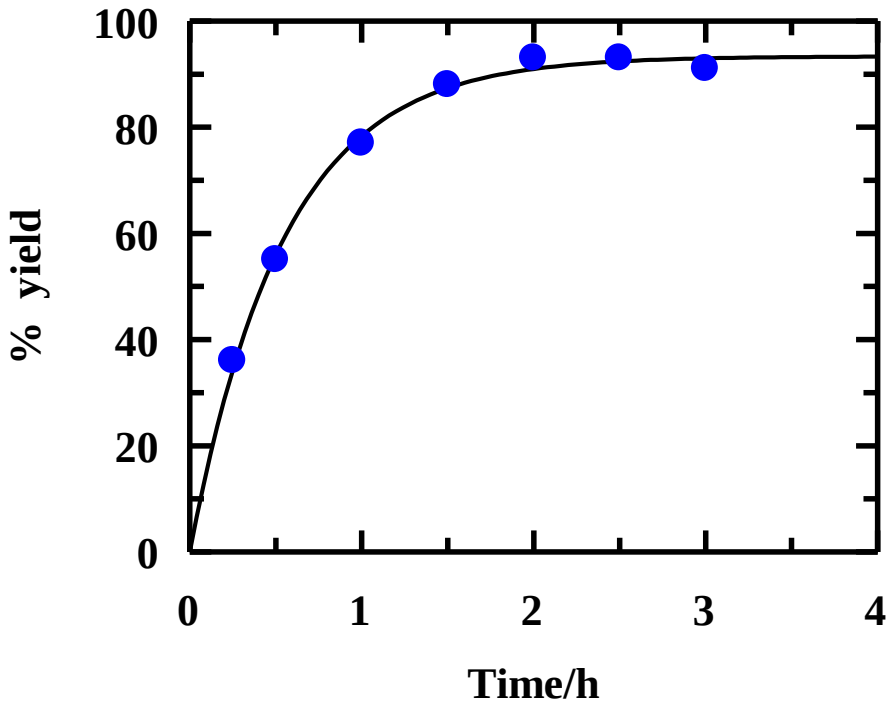



**Fig. S13** Plot showing fitting of first order rate equation of N-arylation reaction of 1,4-dinitrobenzene with pyrazole (Rate equation, $C_0$-C = $C_0[1-e^{-kt}]$ gives k = 1.83 $h^{-1}$ and $t_{½} \approx 0.4$ h).

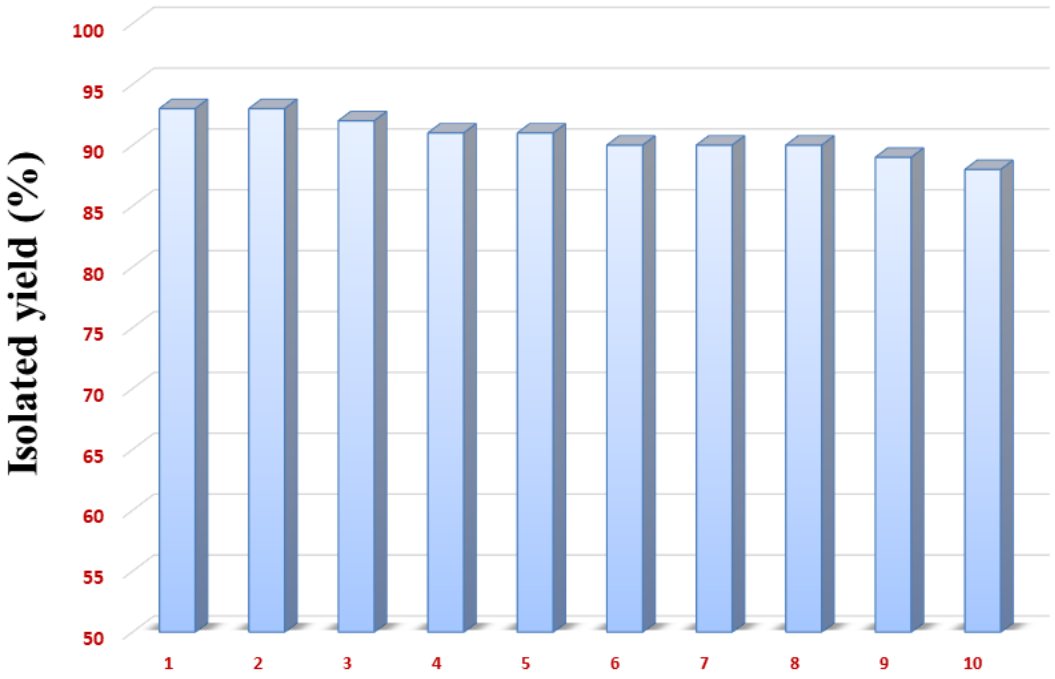



**Fig. S14** Recycling of the catalyst (up to 10 successive cycles).

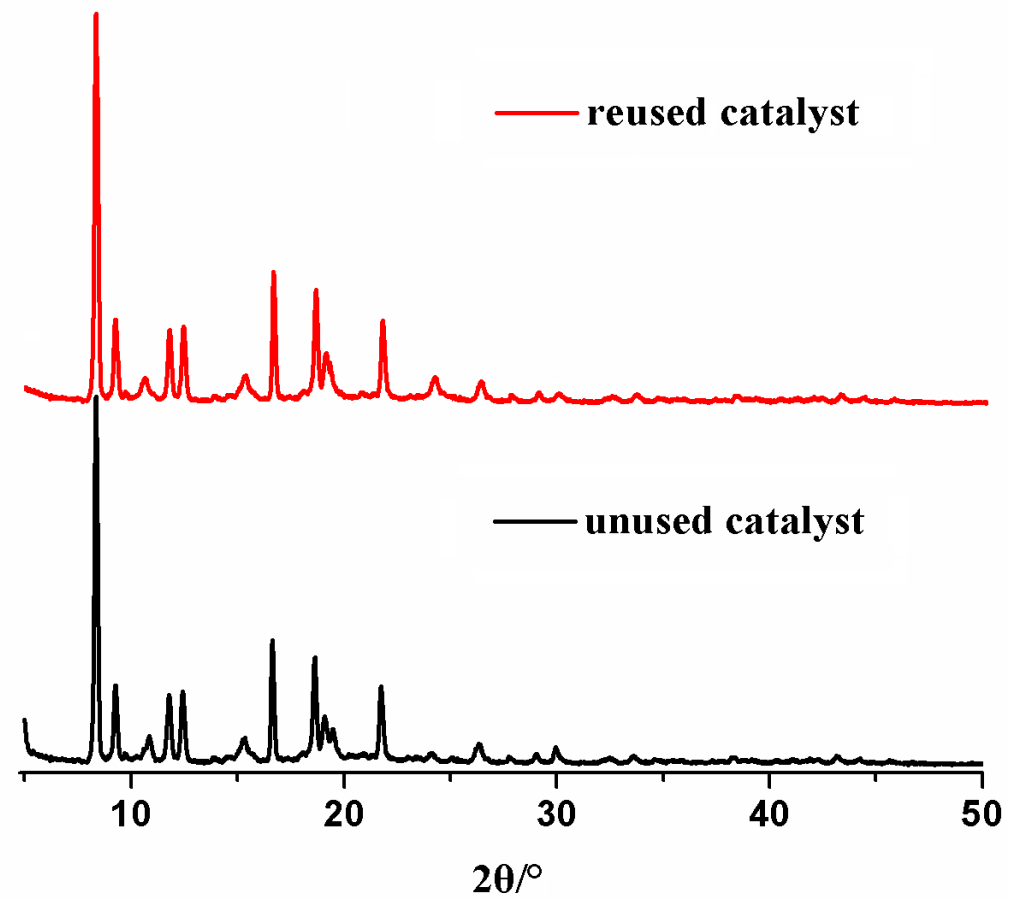



**Fig. S15** PXRD of Cu@D–SA before and after catalytic reaction.

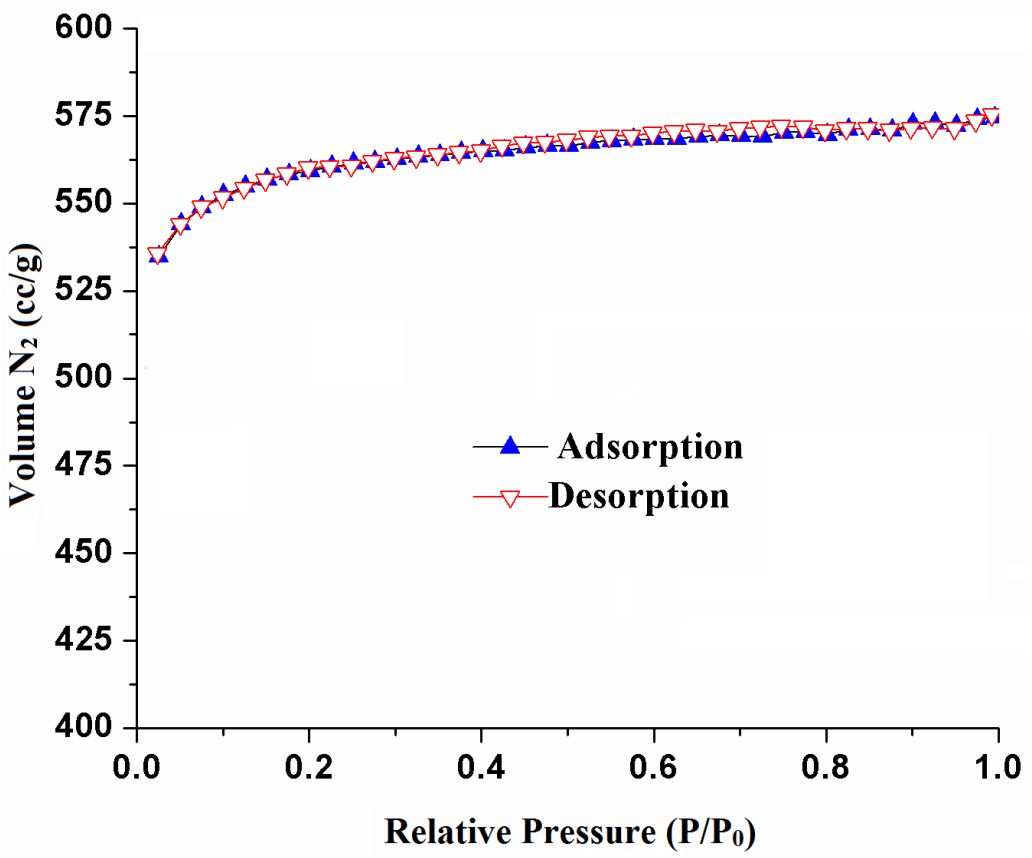



**Fig. S16** $N_2$ adsorption isotherm at 77 K of recovered Cu@D–SA catalyst after fifth cycles (BET – 1518 $cm^2/g$).

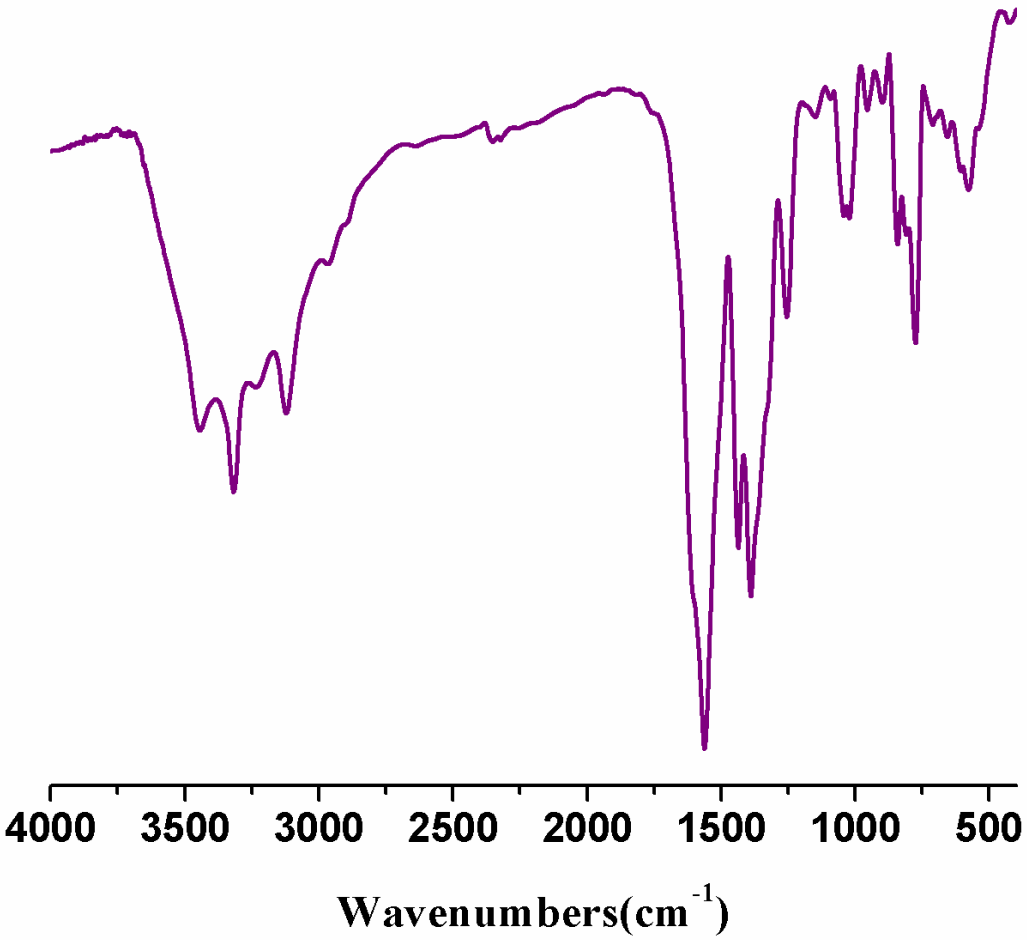



**Fig. S17** FTIR spectrum of Cu@D–SA (recovered after fifth cycle catalytic reaction).

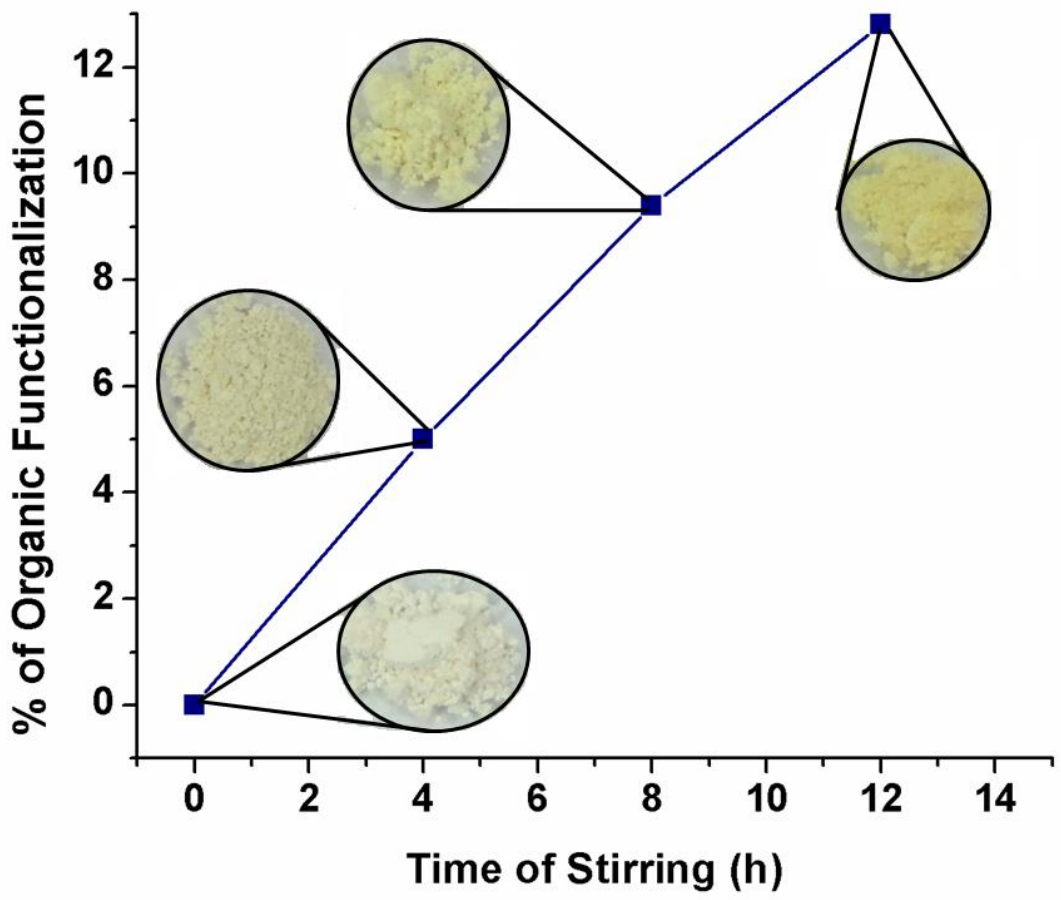



**Fig. S18** Plot showing amine functionalization in DMOF–$NH_2$ along with visual color change.

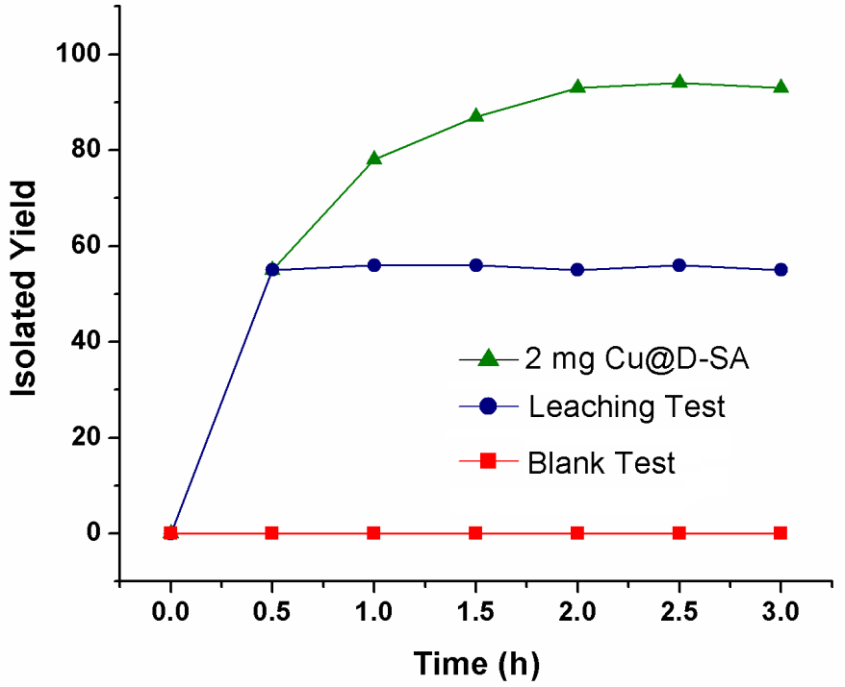
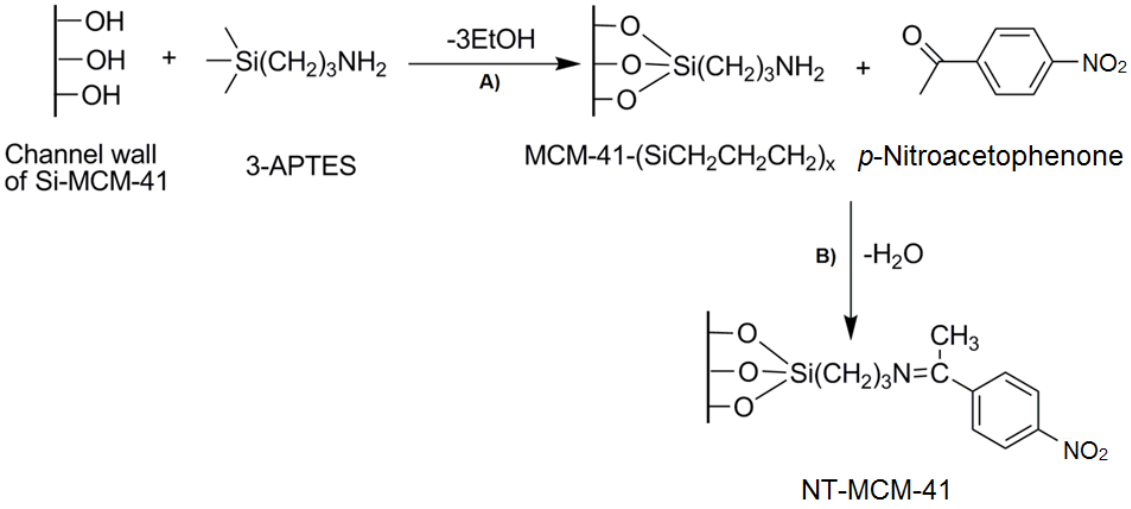
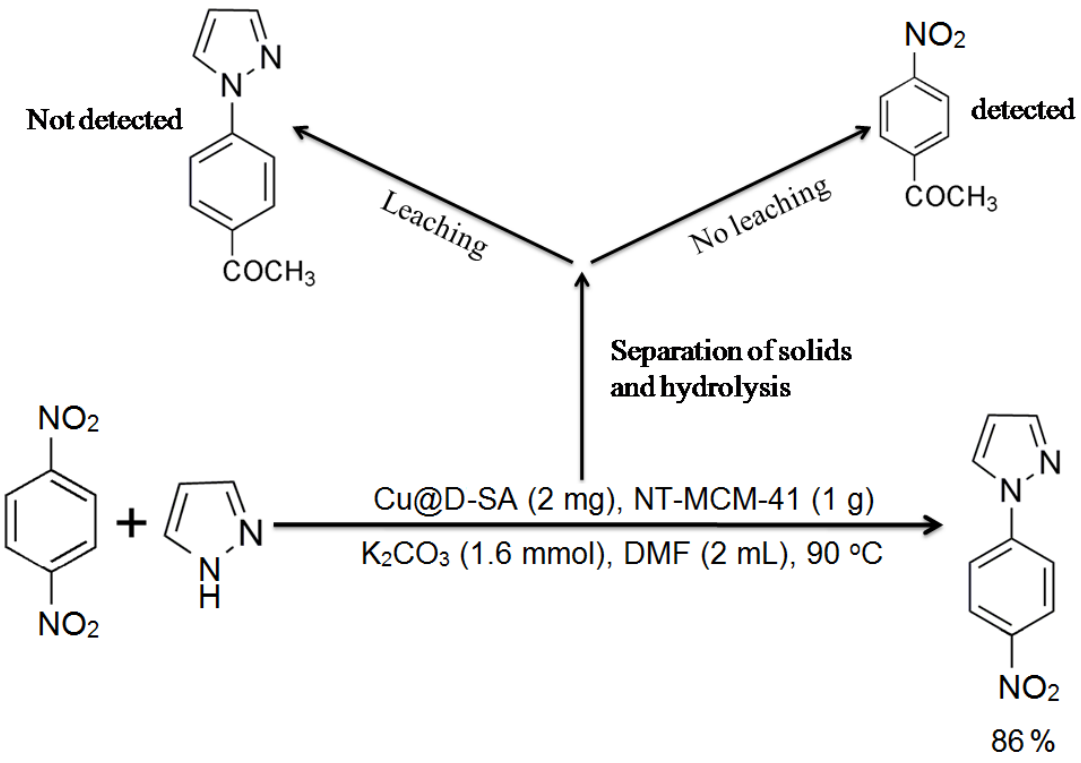



**Fig. S19** Plot supporting no leaching of copper from the catalyst.

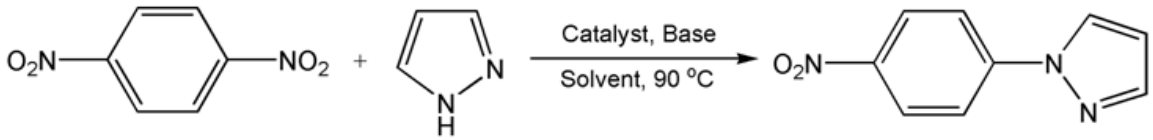



**Scheme S1** A) Organic modification of Si-MCM-41: APTES/$CHCl_3$ and B) anchoring of *p*-nitroacetophenone onto MCM-41(in ethanol).




**Scheme S2** Three-phase test for N-arylation reaction.

**Table S1** Optimization of reaction condition

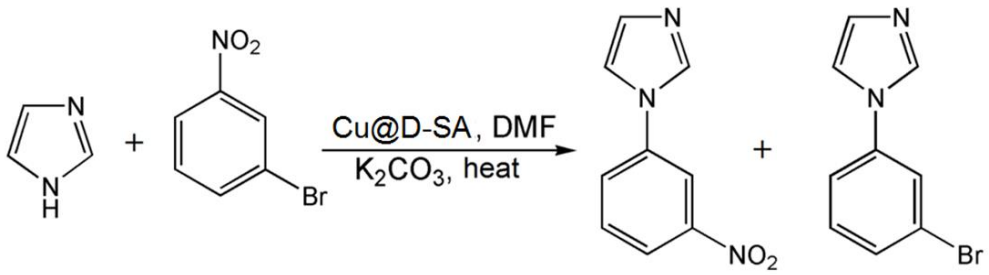



S1a = Cu@D-SA
S1b = DMOF-$NH_2$
S1c = DMOF-$NH_2$+$CuCl_2.2H_2O$
S1d = DMOF-SA+$CuCl_2.2H_2O$
S1e = $Cu(NO_3)_2.3H_2O$
S1f = $Cu(OAc)_2.H_2O$
S1g = $CuCl_2.2H_2O$

| Entry[a] | Catalyst | Base | Solvent | Yield[b] (%) | Entry[a] | Catalyst | Base | Solvent | Yield[b] (%) |
|---|---|---|---|---|---|---|---|---|---|
| 1 | S1a | $K_2CO_3$ | DMSO | 80 | 10 | S1b | $K_2CO_3$ | DMF | - |
| 2 | S1a | $K_2CO_3$ | Toluene | - | 11 | S1c | $K_2CO_3$ | DMF | 32 |
| 3 | S1a | $K_2CO_3$ | MeCN | 27 | 12 | S1d | $K_2CO_3$ | DMF | 37 |
| 4 | S1a | $K_2CO_3$ | DMF | 93 | 13 | S1e | $K_2CO_3$ | DMF | 24 |
| 5 | S1a | $Na_2CO_3$ | DMF | 47 | 14 | S1f | $K_2CO_3$ | DMF | 39 |
| 6 | S1a | $Cs_2CO_3$ | DMF | 79 | 15 | S1g | $K_2CO_3$ | DMF | 31 |
| 7 | S1a | KOH | DMF | 69 | 16[c] | S1a | $K_2CO_3$ | DMF | 59 |
| 8 | S1a | NaOH | DMF | 58 | 17[d] | S1a | $K_2CO_3$ | DMF | 94 |
| 9 | S1a | - | DMF | - | 18[e] | S1a | $K_2CO_3$ | DMF | 91 |

[a] Reaction Condition: pyrazole (1 mmol), 1,4-dinitrobenzene (1.2 mmol), imidazole (1.0 mmol), base (1.6 mmol), 0.002 g catalyst, solvent (2 mL) at 90 ºC upto 2 h. [b] Isolated yield. [c] at 60 ºC. [d] at 120 ºC. [e] fifth cycle of the recovered catalyst (entry 4). DMF = dimethyl formamide, DMSO = dimethyl sulfoxide.

**Table S2** Control experiment of m-bromonitrobenzene with imidazole to demonstrate the thermally induced chemoselectivity




**2g** **2h**

| Entry[a] | Temperature (°C) | Conversion[b] | Selectivity 2g : 2h |
|---|---|---|---|
| 1 | 70 | 67% | 94 : 6 |
| 2 | 90 | 78% | 79 : 21 |
| 3 | 110 | 85% | 56 : 44 |
| 4 | 130 | 86% | 27 : 73 |
| 5 | 150 | 89% | 9 : 91 |

[a] Reaction condition: *m*-bromonitrobenzene (1.2 mmol), imidazole (1.0 mmol), $K_2CO_3$ (1.6 mmol), Cu@D-SA (0.002 g), DMF (2 mL) at heating for 2 h. [b] Isolated yield. Reactions have been performed both in inert and open atmosphere, however, no variation of selectivity of products was observed in low and high temperatures.

**Table S3** TOF values in each recycled catalytic step using 1,4-dinitrobenzene and pyrazole as reactants under the optimized reaction conditions

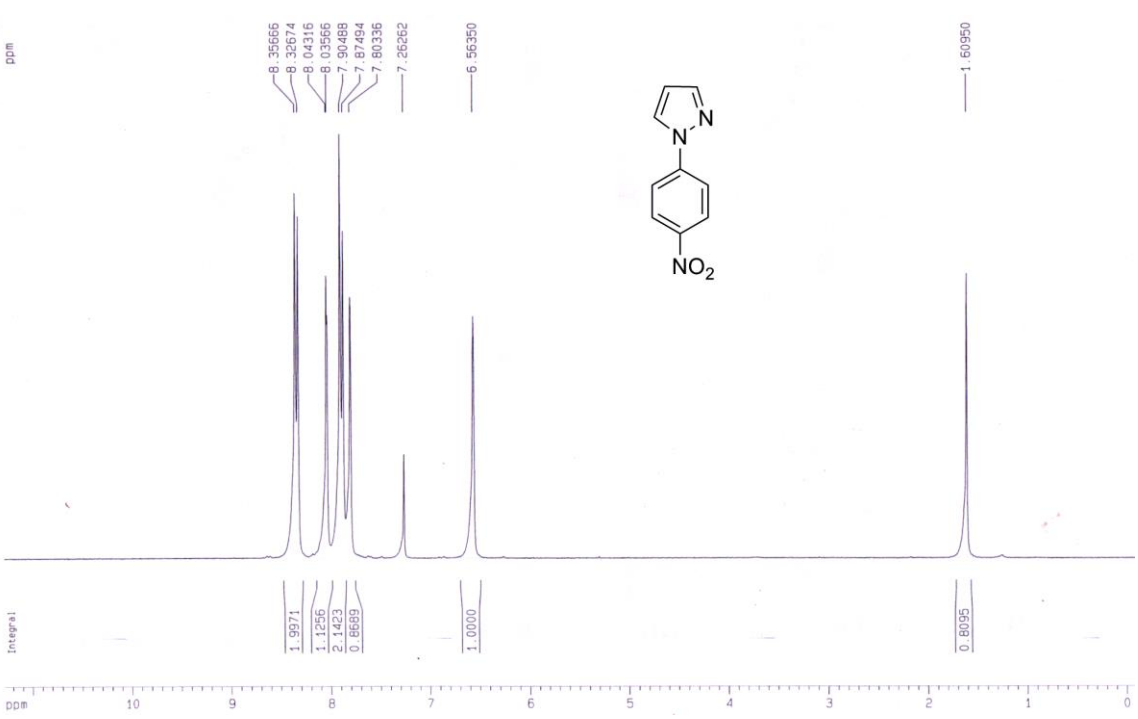
| Cycle[a] | Isolated yield[b] | TOF ($min^{-1}$)[c] |
|---|---|---|
| 1 | 93 | 315 |
| 2 | 93 | 315 |
| 3 | 92 | 312 |
| 4 | 91 | 308 |
| 5 | 91 | 308 |
| 6 | 90 | 305 |

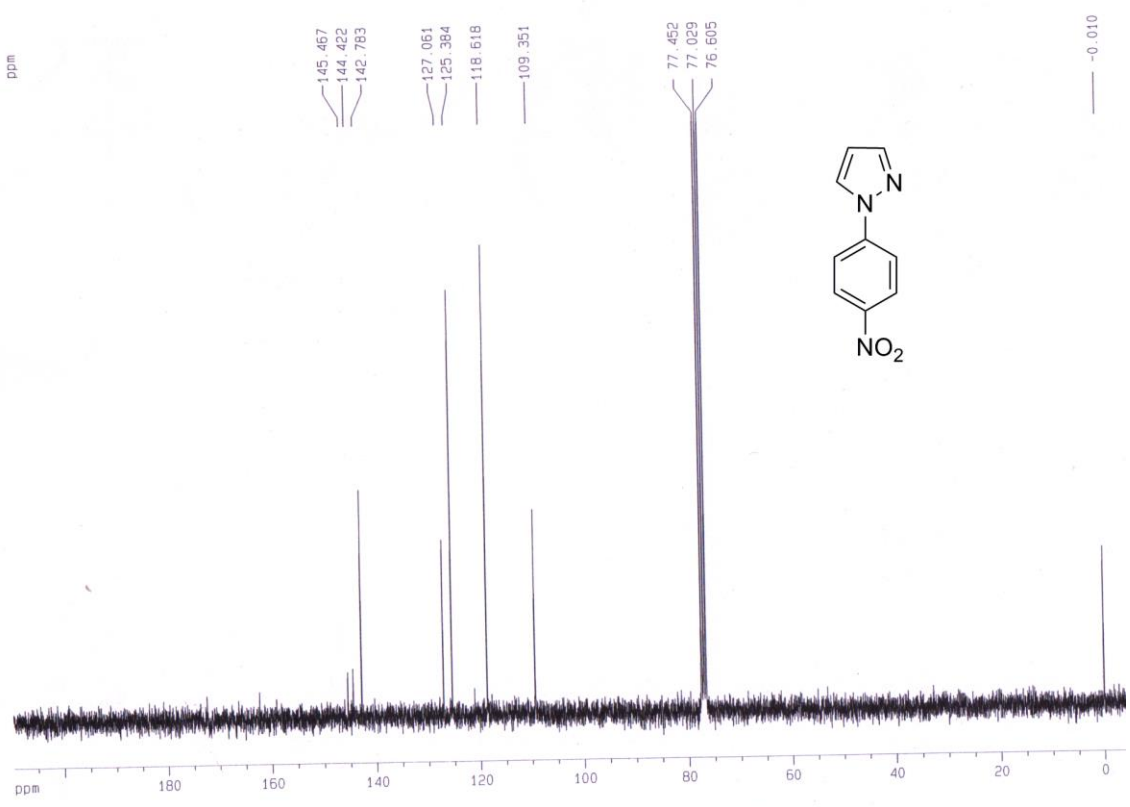
| | | |
|---|---|---|
| 7 | 90 | 305 |
| 8 | 90 | 305 |
| 9 | 89 | 298 |
| 10 | 88 | 298 |

[a] Reaction Condition: pyrazole (1 mmol), 1,4-dinitrobenzene (1.2 mmol), $K_2CO_3$ (1.6 mmol), 0.002 g catalyst, DMF (2 mL) at 90 ºC upto 2 h. [b] Isolated yield. [c] TOF = Mol.product/mol.Cu min. (unit in $min^{-1}$).

## Characterization of Products

pyrazole-*p*-nitrobenzene (Table 1, entry 1a): $^1$H–NMR (300 MHz, $CDCl_3$): δ (ppm): 8.34 (d, *J* = 8.98 Hz, 2H), 8.04 (d, *J* = 2.25 Hz, 1H), 7.89 (d, *J* = 8.98 Hz, 2H), 7.8 (s, 1H), 6.56 (s, 1H); $^{13}$C–NMR (75 MHz, $CDCl_3$): δ (ppm): 145.47, 144.42, 142.78, 127.06, 125.38, 118.62, 109.35; HRMS (ESI): calcd. for $[M+H]^+$ ($C_9H_8N_3O_2$) requires m/z 190.0617, found 190.06613; Anal. Calcd. for $C_9H_7N_3O_2$: C, 57.14%; H, 3.73%; N, 22.21%. Found: C, 57.17%; H, 3.74%; N, 22.19%.

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118.618
109.351
77.452
77.029
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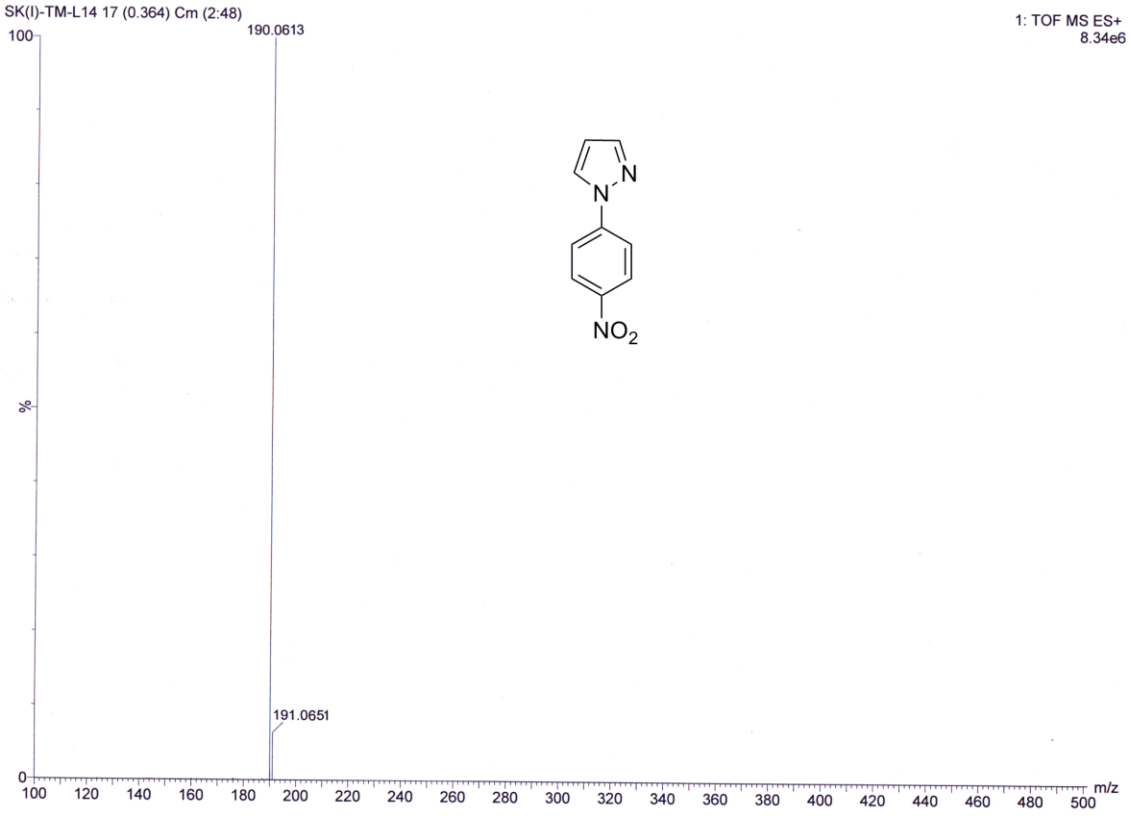
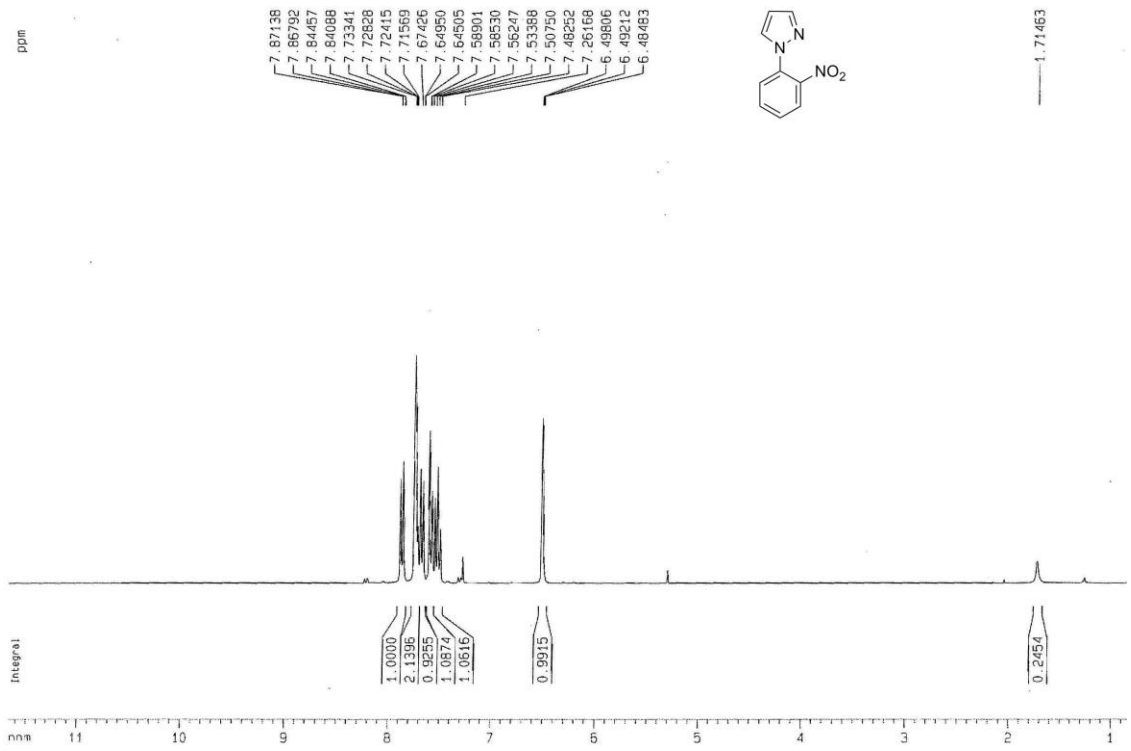
N
N
NO2
ppm
180
160
140
120
100
80
60
40
20
0




pyrazole-*o*-nitrobenzene (Table 1, entry 1b): $^{1}$H–NMR (300 MHz, $CDCl_3$): δ (ppm): 7.87-7.84 (m, 1H), 7.73-7.64 (m, 3H), 7.58-7.48 (m, 2H), 6.49-6.48 (m, 1H); $^{13}$C–NMR (75 MHz, $CDCl_3$): δ (ppm): 144.61, 142.28, 133.38, 133.09, 129.77, 128.41, 126.18, 125.01, 108.2; HRMS (ESI): calcd. for $[M+H]^+$ ($C_{13}H_{10}N_3O_2$) requires m/z 240.0773, found 240.0774; Anal. Calcd. for $C_{13}H_9N_3O_2$: C, 65.27%; H, 3.79%; N, 17.56%. Found: C, 65.26%; H, 3.80%; N, 17.55%.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7.59901
7.58530
7.56247
7.53388
7.50750
7.48252
7.26168
6.49806
6.49212
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Integral
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2.1396
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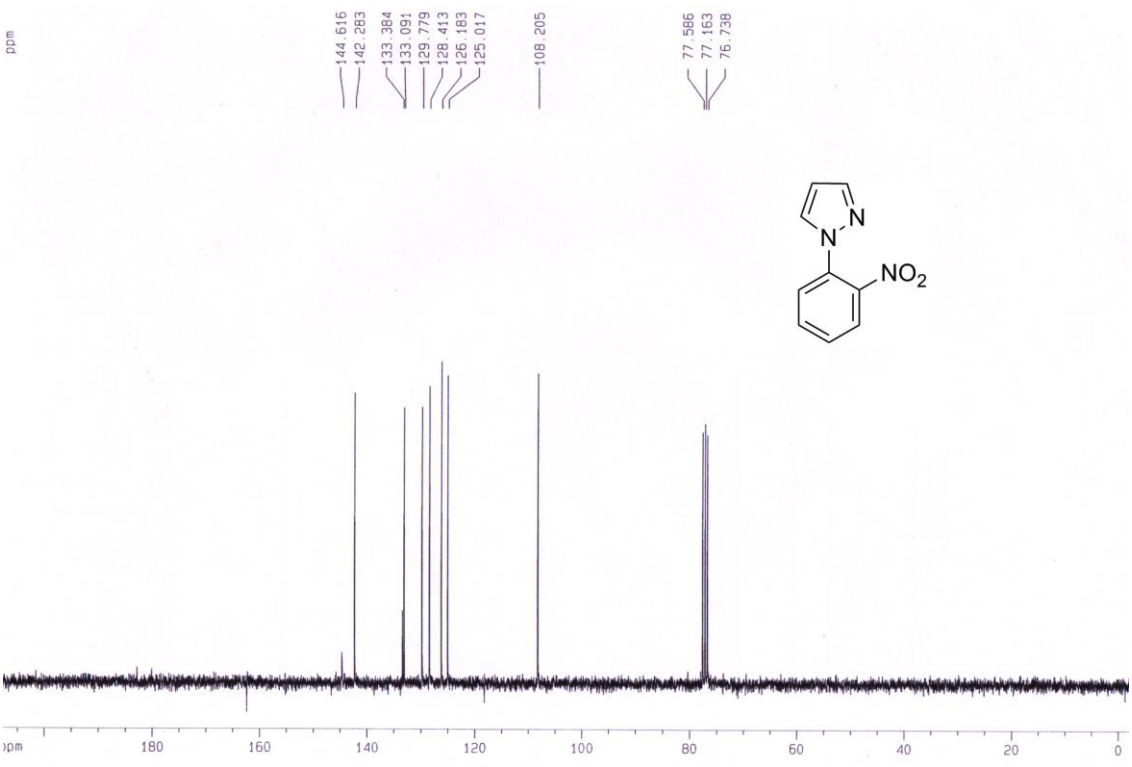
1.0616
0.9915
0.2454
ppm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129.779
128.413
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125.017
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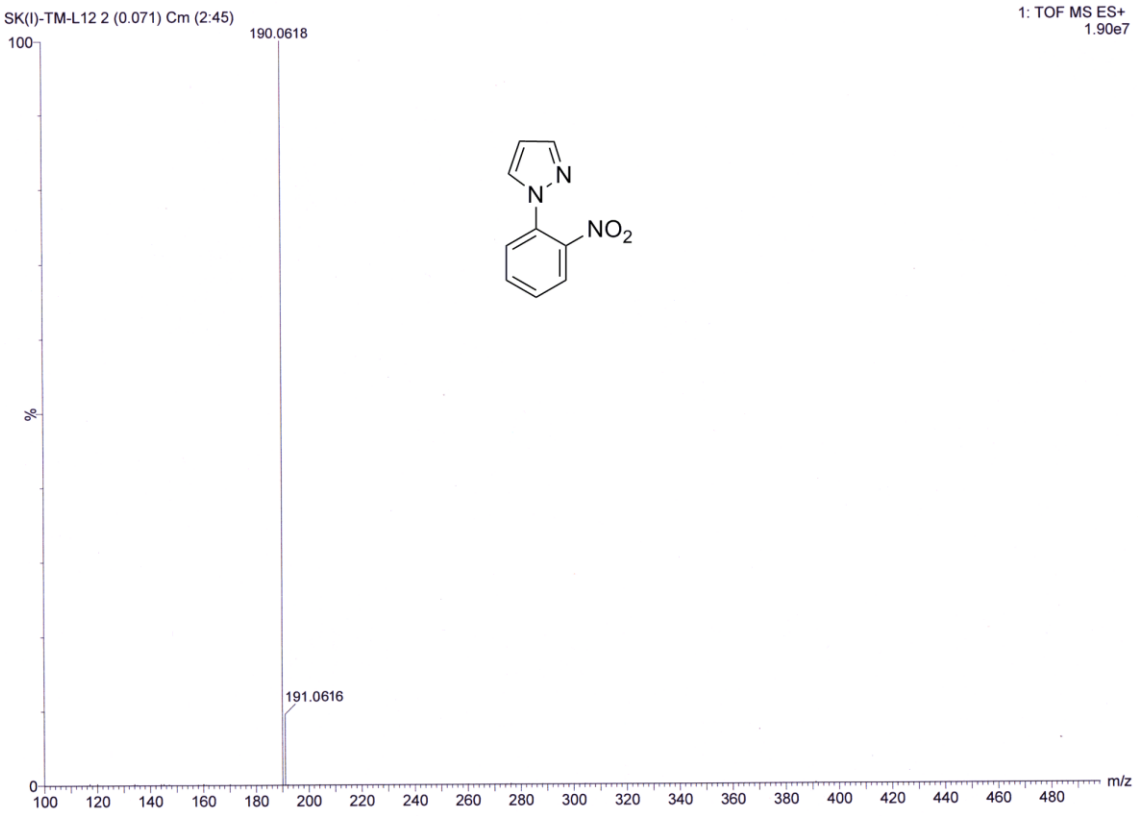
77.586
77.163
76.738
NO2
ppm




pyrazole-*p*-benzonitrile (Table 1, entry 1c): $^{1}$H–NMR (300 MHz, $CDCl_3$): δ (ppm): 7.97 (d, *J* = 2.52 Hz, 1H), 7.8 (d, *J* = 8.82 Hz, 2H), 7.74-7.67 (m, 3H), 6.49 (t, *J* = 1.8 Hz, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ (ppm): 142.94, 142.4, 133.62, 126.88, 118.9, 118.41, 109.48, 109.05; HRMS (ESI): calcd. for $[M+H]^+$ ($C_{10}H_8N_3$) requires m/z 170.0718, found 170.0717; Anal. Calcd. for $C_{10}H_7N_3$: C, 70.99%; H, 4.17%; N, 24.84%. Found: C, 70.97%; H, 4.15%; N, 24.82%.


ppm
7.9748
7.9664
7.8131
7.7837
7.7382
7.7338
7.7042
7.6978
7.6807
7.6747
6.5048
6.4987
6.4908
0.0303
N
N
CN
Integral
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3.0083
1.0000
ppm
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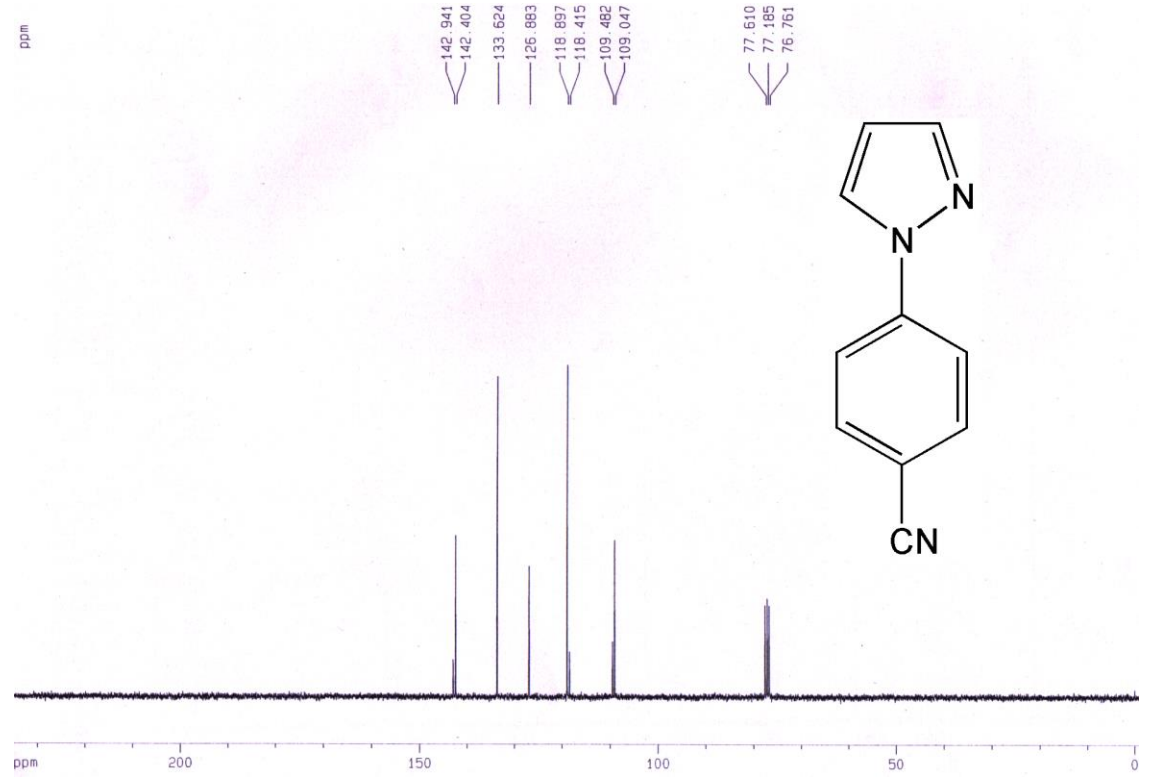
9
8
7
6
5
4
3
2
1
0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142.404
133.624
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118.897
118.415
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77.610
77.185
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N
CN
ppm
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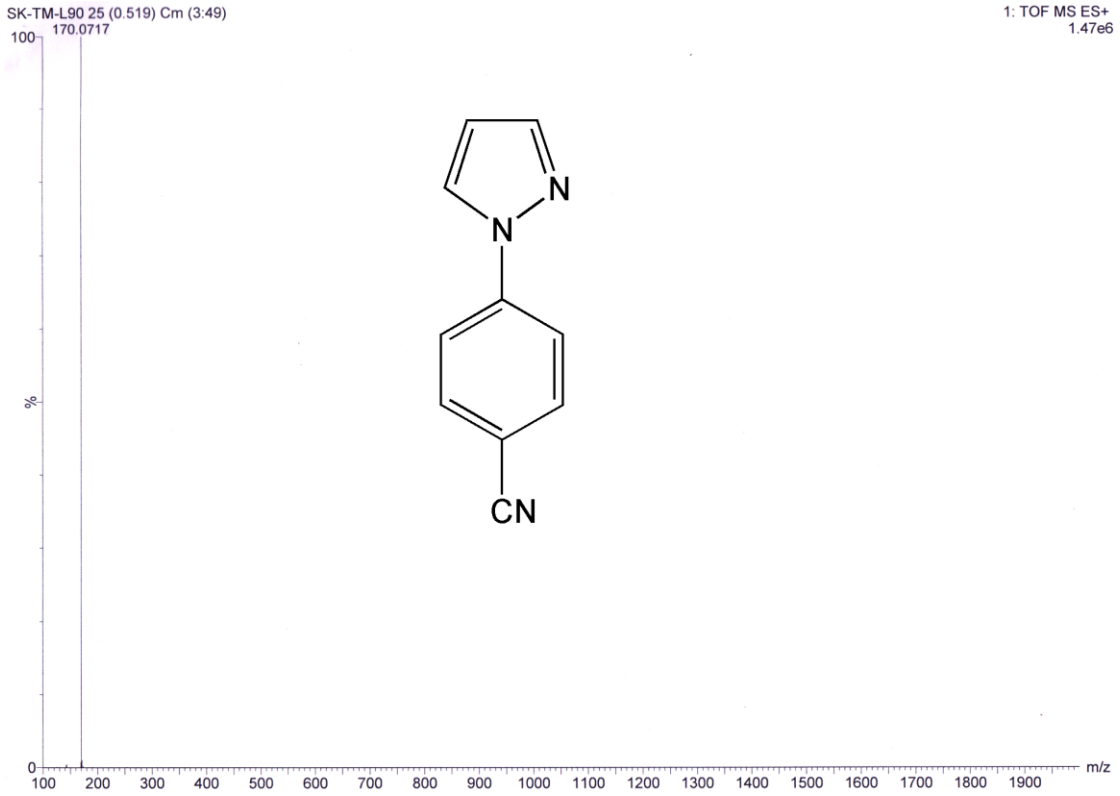
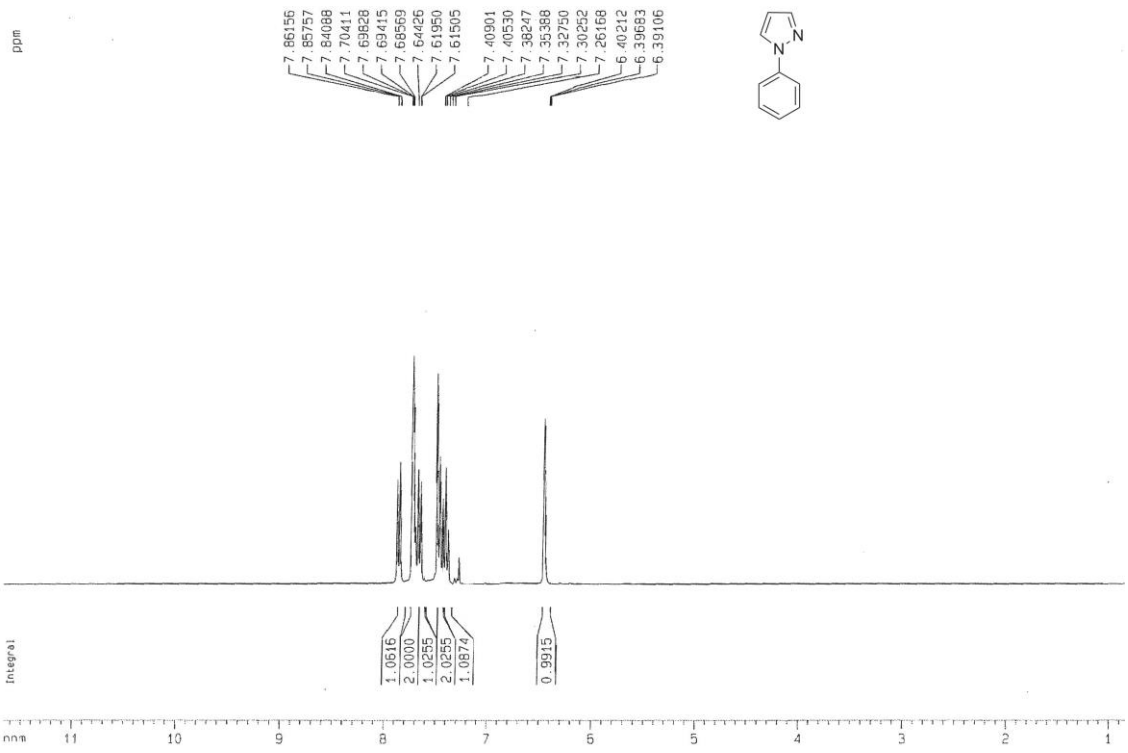
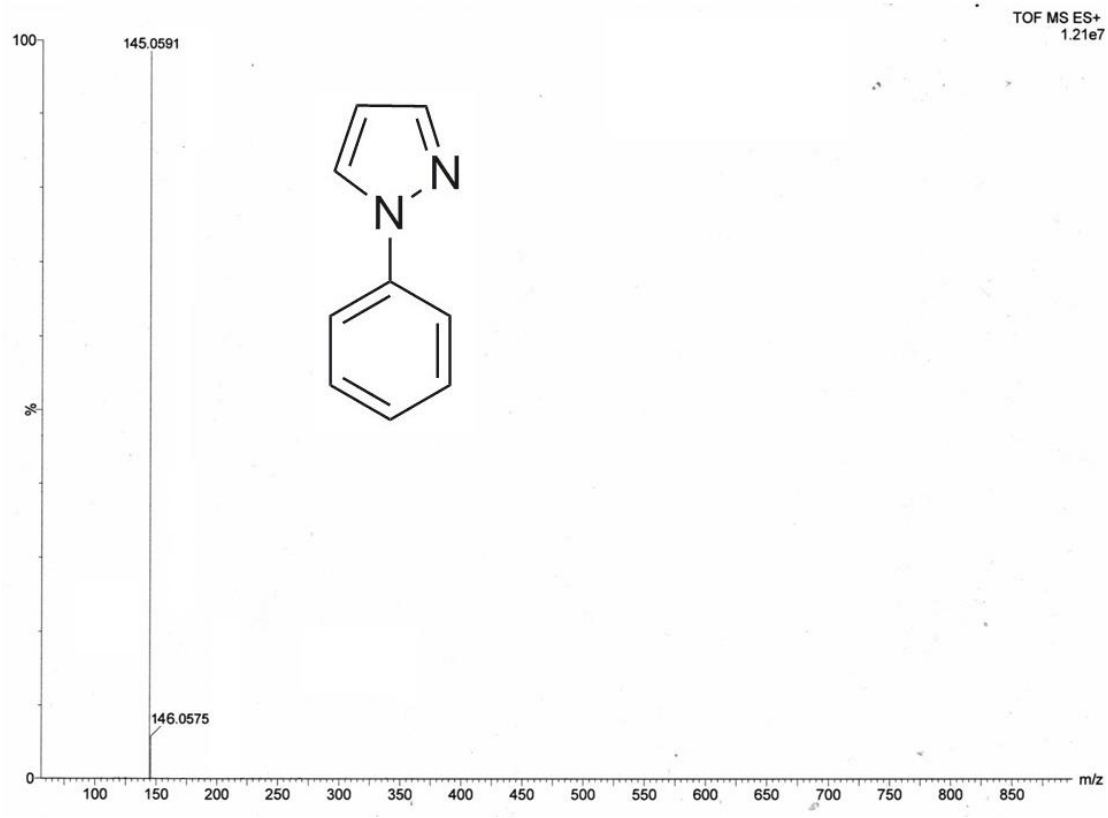
150
100
50
0

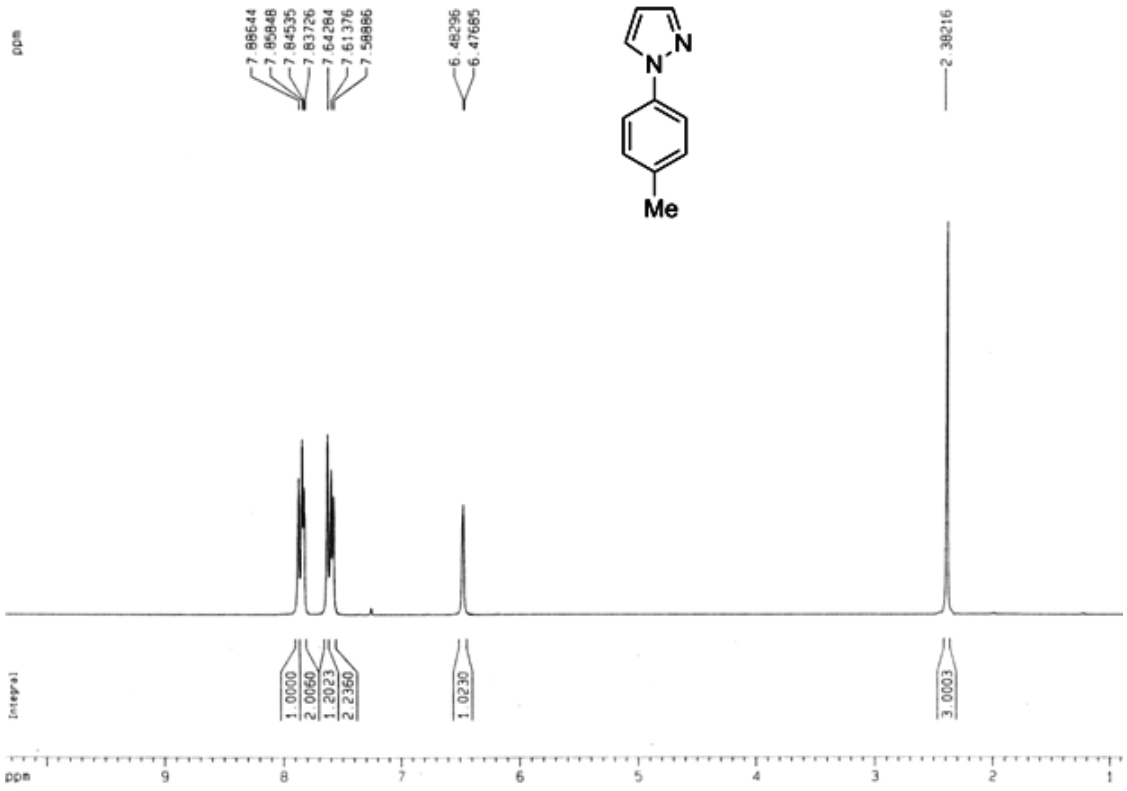


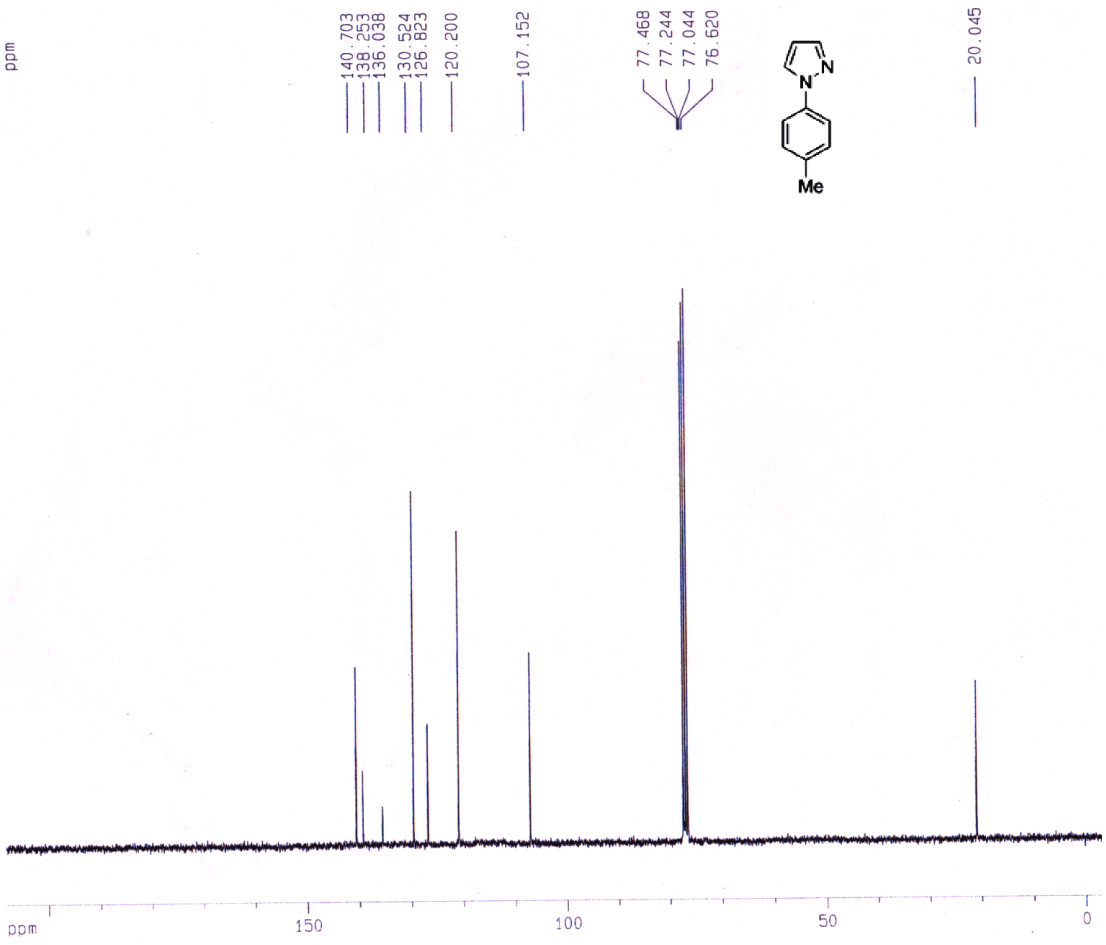

1-Phenyl-1H-pyrazole (Table 1, entry 1d): $^{1}$H–NMR (300 MHz, $CDCl_3$): δ (ppm): 7.86-7.84 (m, 1H), 7.70-7.62 (m, 3H), 7.41-7.30 (m, 3H), 6.40-6.39 (m, 1H); HRMS (ESI): calcd. for $[M+H]^+$ ($C_9H_9N_2$) requires m/z 145.0687, found 245.0591; Anal. Calcd. for $C_9H_8N_2$: C, 74.98%; H, 5.59%; N, 19.43%. Found: C, 74.91%; H, 5.63%; N, 19.50%.

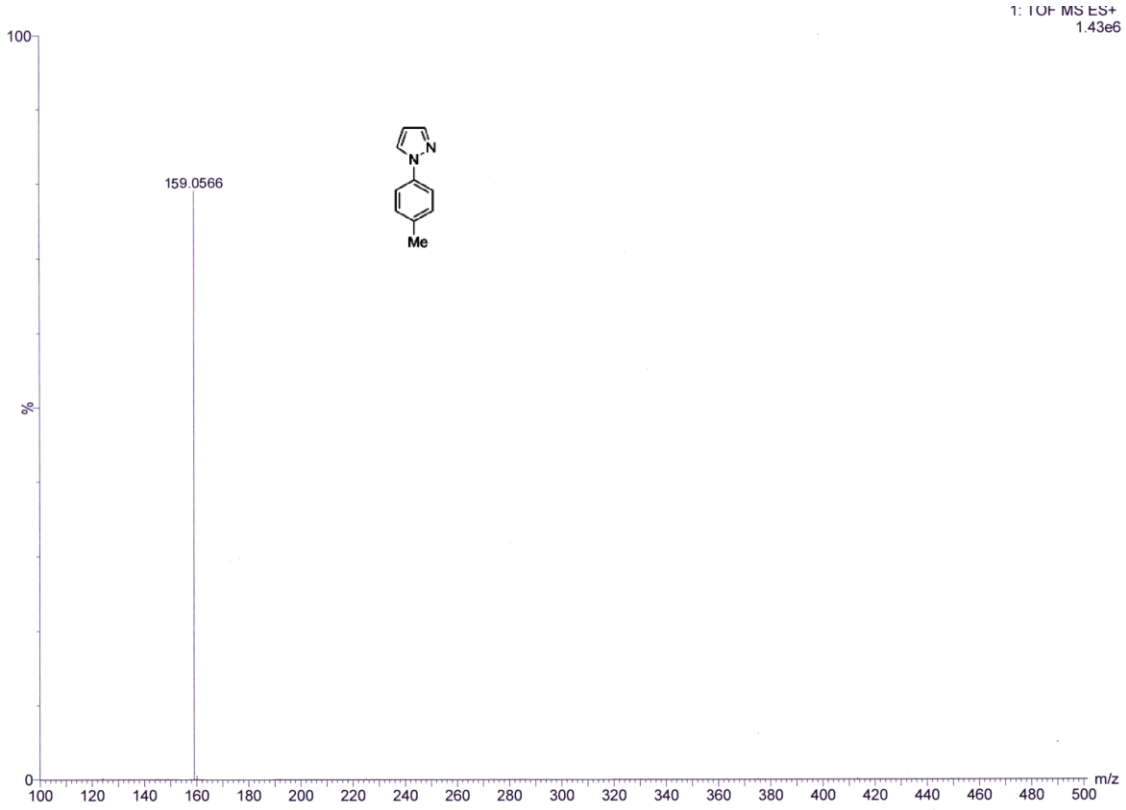

ppm
7.86156
7.85757
7.84088
7.70411
7.69828
7.69415
7.68569
7.64426
7.61950
7.61505
7.40901
7.40530
7.38247
7.35388
7.32750
7.30252
7.26168
6.40212
6.39683
6.39106
Integral
1.0616
2.0000
1.0255
2.0255
1.0874
0.9915
ppm


TOF MS ES+
1.21e7
145.0591
146.0575
%
m/z

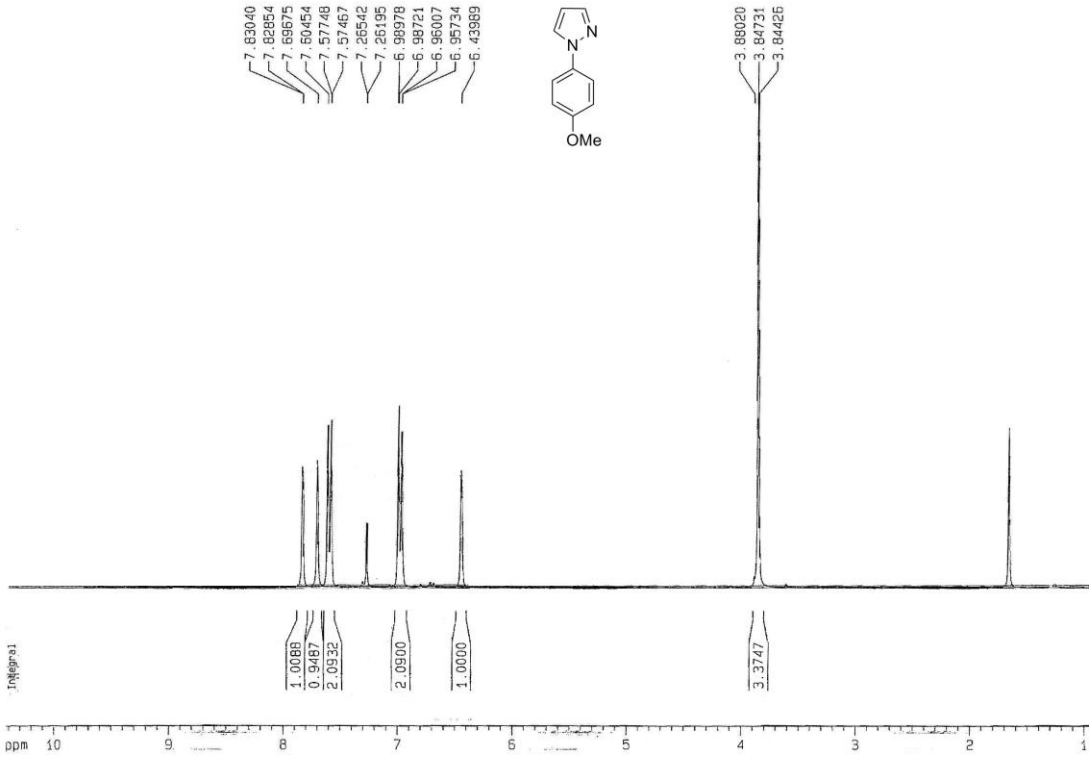
1-(4-Methylphenyl)-1H-pyrazole (Table 1, entry 1e): $^{1}$H–NMR (300 MHz, $CDCl_3$): δ (ppm): 7.89-7.59 (m, 6H), 6.48 (d, *J* = 1.83 Hz, 1H), 2.38 (s, 3H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ (ppm): 140.70, 138.25, 136.04, 130.52, 126.82, 120.20, 107.15, 20.05; HRMS (ESI): calcd. for $[M+H]^+$ ($C_{10}H_{11}N_2$) requires m/z 159.0844, found 159.0566; Anal. Calcd. for $C_{10}H_{10}N_2$: C, 75.92%; H, 6.37%; N, 17.71%. Found: C, 75.95%; H, 6.39%; N, 17.82%.

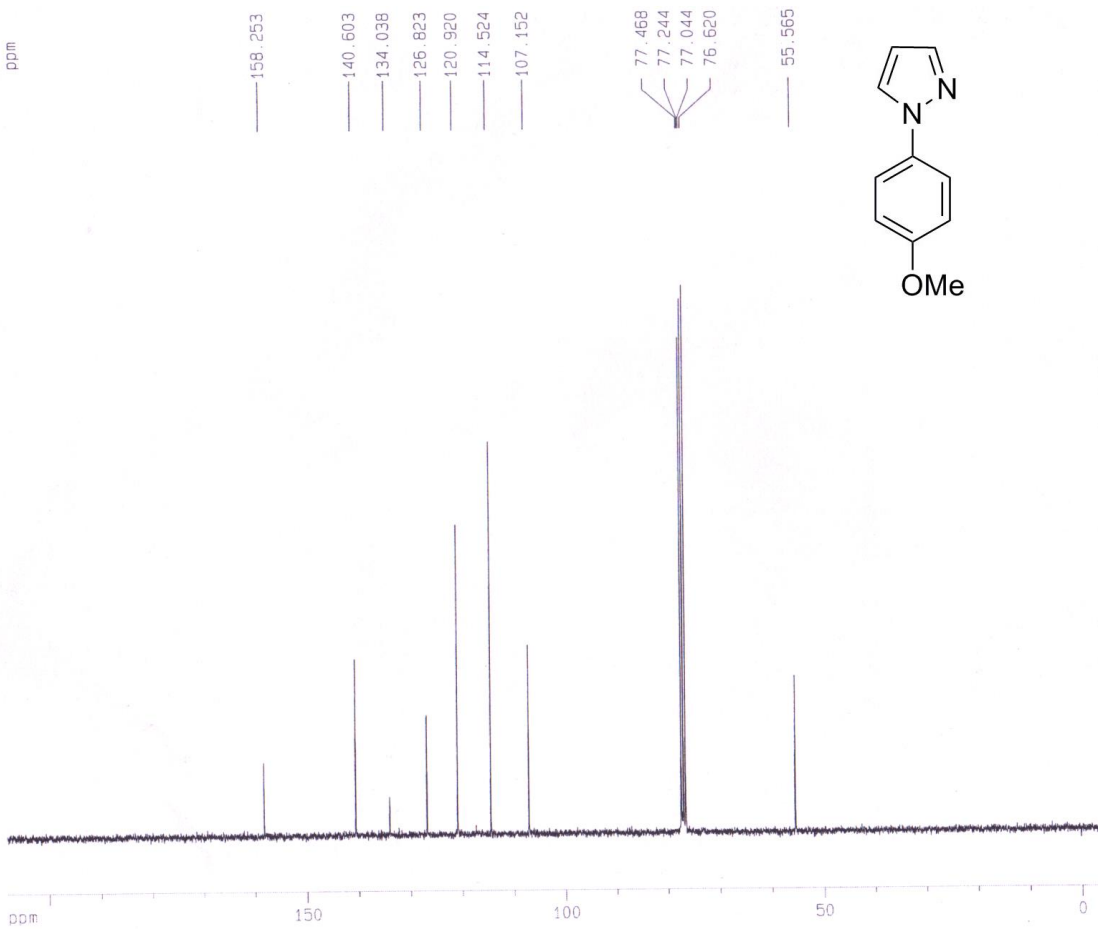


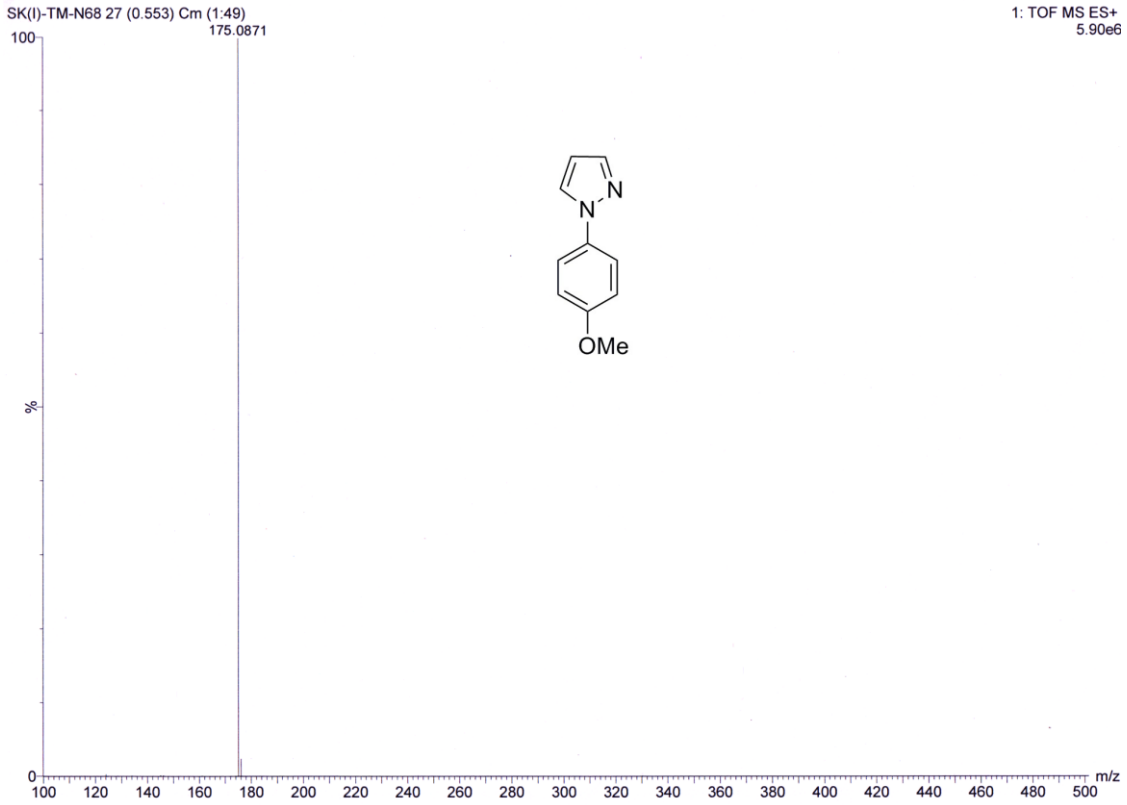

ppm
140.703
138.253
136.038
130.524
126.823
120.200
107.152
77.468
77.244
77.044
76.620
20.045
N
N
Me
ppm
150
100
50
0



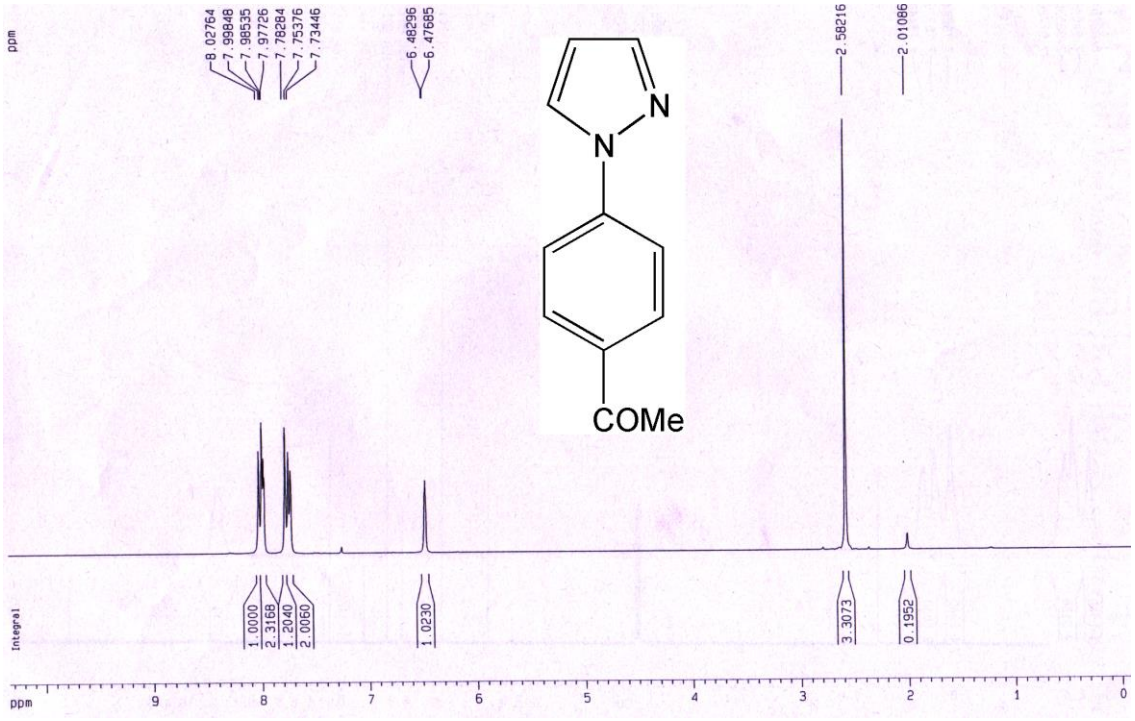

1-(4-Methoxyphenyl)-1H-pyrazole (Table 1, entry 1f): $^{1}$H–NMR (300 MHz, $CDCl_3$): δ (ppm): 7.83 (d, *J* = 0.6 Hz, 1H), 7.69 (s, 1H), 7.60-7.57 (m, 2H), 6.99-6.96 (m, 2H), 6.44 (s, 1H), 3.85 (s, 3H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ (ppm): 158.25, 140.60, 134.04, 126.82, 120.92, 114.52, 107.15, 55.57; HRMS (ESI): calcd. for $[M+H]^+$ ($C_{10}H_{11}N_2O$) requires m/z 175.0793, found 175.0871;Anal. Calcd. for $C_{10}H_{10}N_2O$: C, 68.95%; H, 5.79%; N, 16.08%. Found: C, 69.03%; H, 5.81%; N, 16.12%.

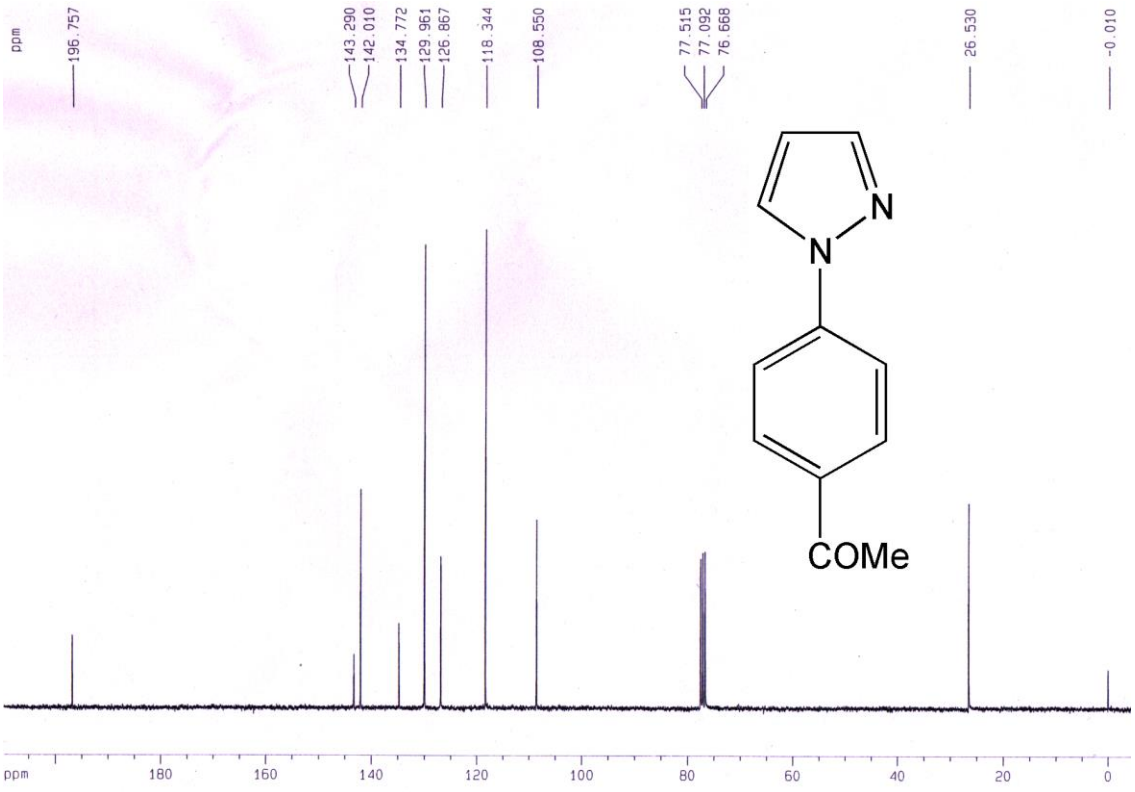

7.83040
7.82854
7.69675
7.60454
7.57748
7.57467
7.26542
7.26195
6.99978
6.98721
6.96007
6.95734
6.43989
3.88020
3.84731
3.84426
N
N
OMe
Integral
1.0088
0.9487
2.0932
2.0900
1.0000
3.3747
ppm
10
9
8
7
6
5
4
3
2
1

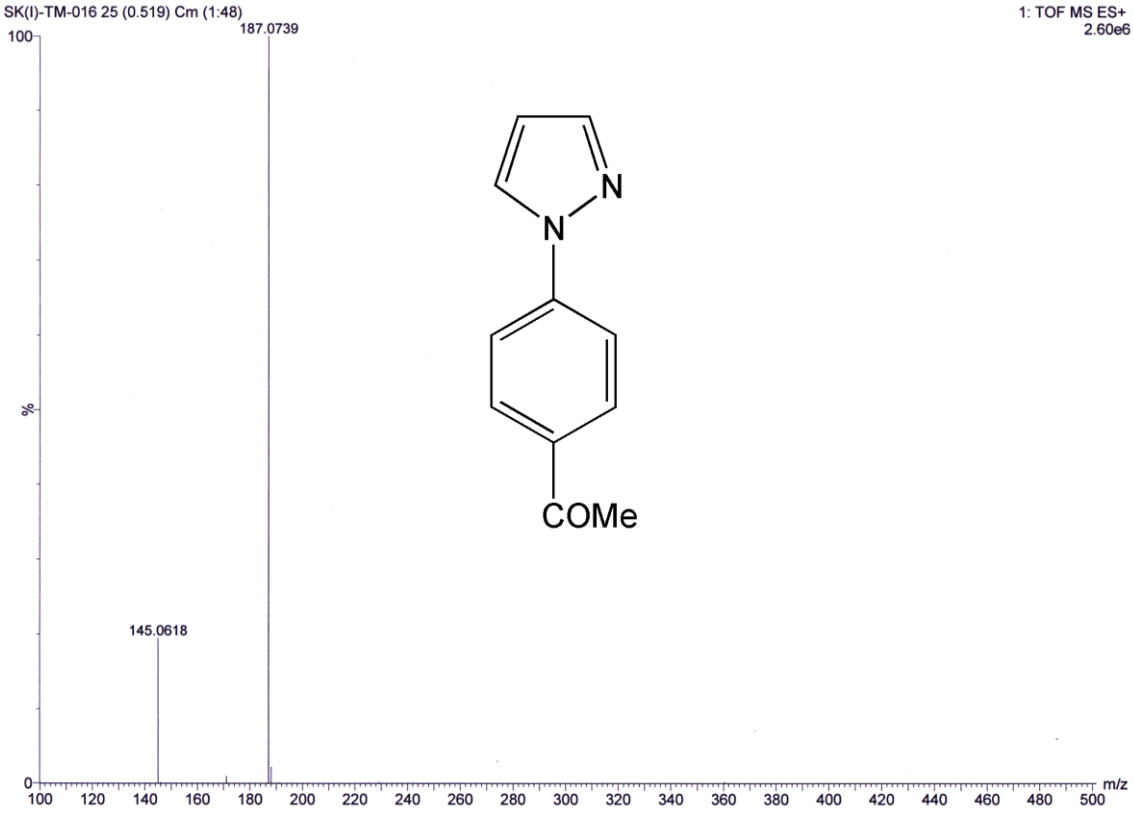

ppm
158.253
140.603
134.038
126.823
120.920
114.524
107.152
77.468
77.244
77.044
76.620
55.565
N
N
OMe
ppm
150
100
50
0



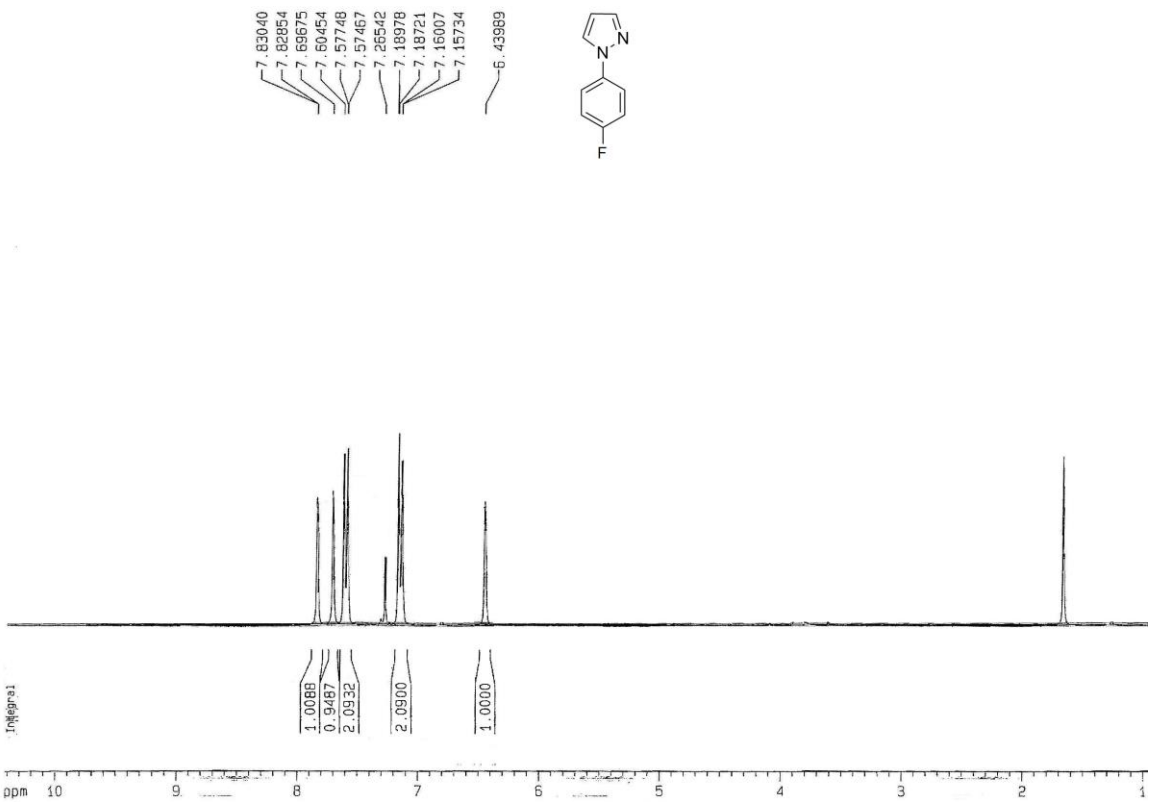

pyrazole-*p*-acetylbenzene (Table 1, 1g): δ (ppm): 8.03-7.98 (m, 3H), 7.78-7.73 (m, 3H), 6.48 (d, $J$ = 1.83 Hz, 1H); $^{13}$C–NMR (75 MHz, $CDCl_3$): δ (ppm): 196.76, 143.29, 142.01, 134.77, 129.96, 126.87, 118.34, 108.55, 26.53; HRMS (ESI): calcd. for $[M+H]^+$ ($C_{11}H_{11}N_2O$) requires m/z 187.0793, found 187.0739; Anal. Calcd. for $C_{11}H_{10}N_2O$: C, 70.95%; H, 5.41%; N, 15.04%. Found: C, 70.96%; H, 5.40%; N, 15.05%.

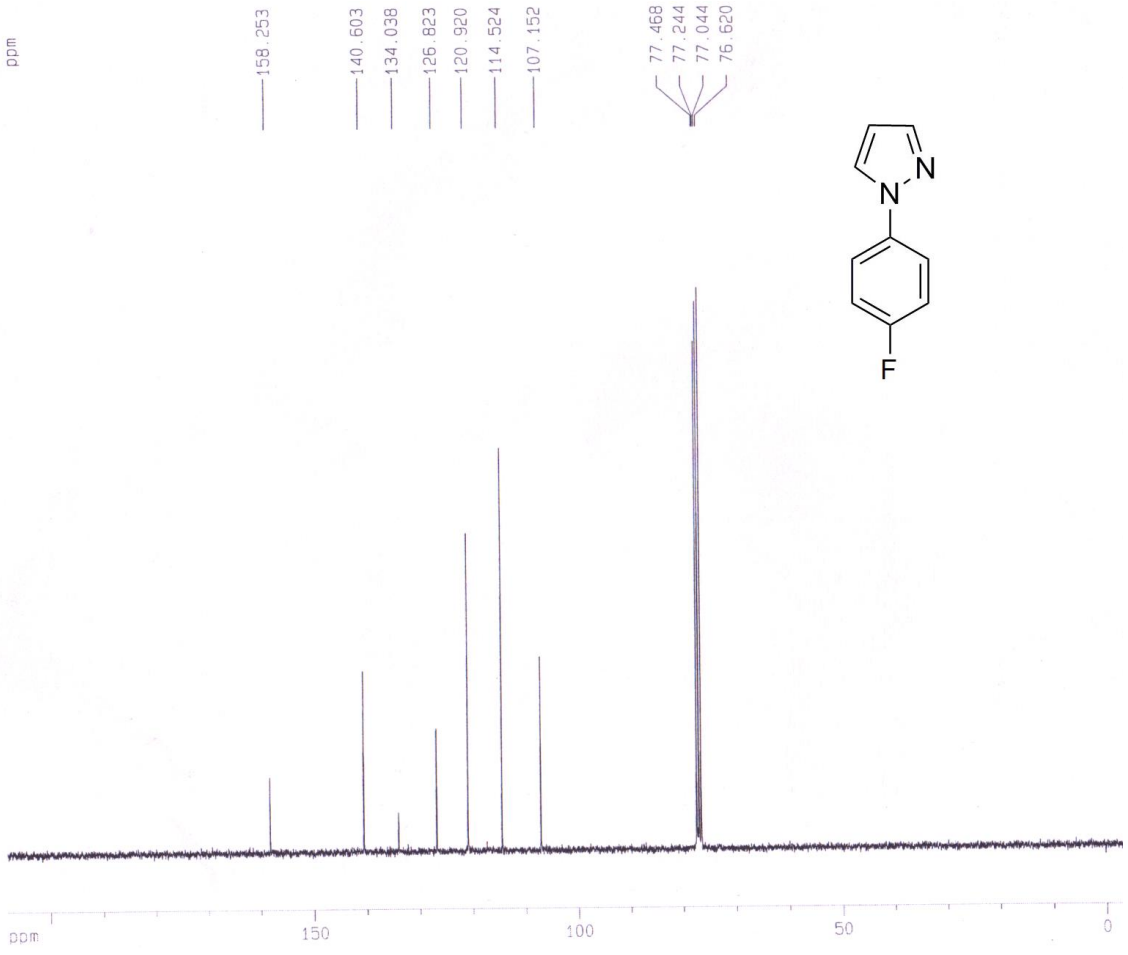

ppm
8.02764
7.99848
7.98535
7.97726
7.78284
7.75376
7.73446
6.48296
6.47685
2.58216
2.01086
N
N
COMe
Integral
1.0000
2.3168
1.2040
2.0060
1.0230
3.3073
0.1952
ppm
9
8
7
6
5
4
3
2
1
0

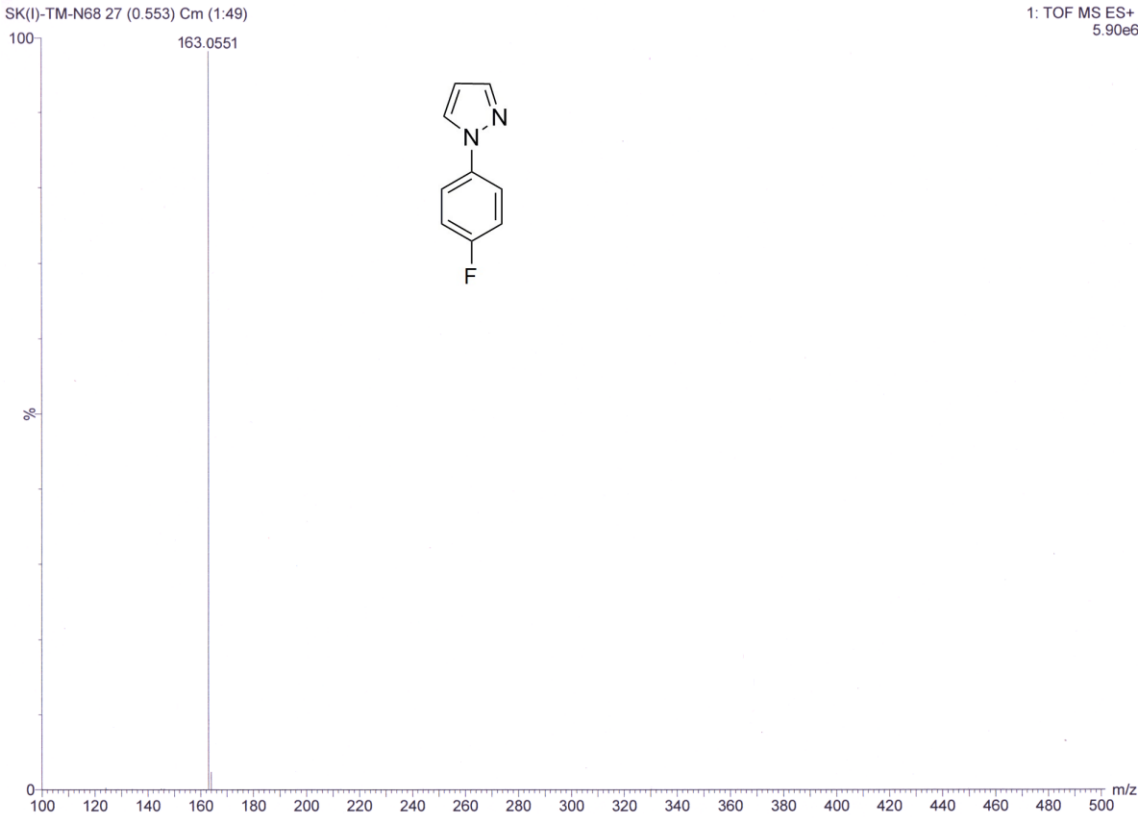

ppm
196.757
143.290
142.010
134.772
129.961
126.867
118.344
108.550
77.515
77.092
76.668
26.530
-0.010
N
N
COMe
ppm
180
160
140
120
100
80
60
40
20
0



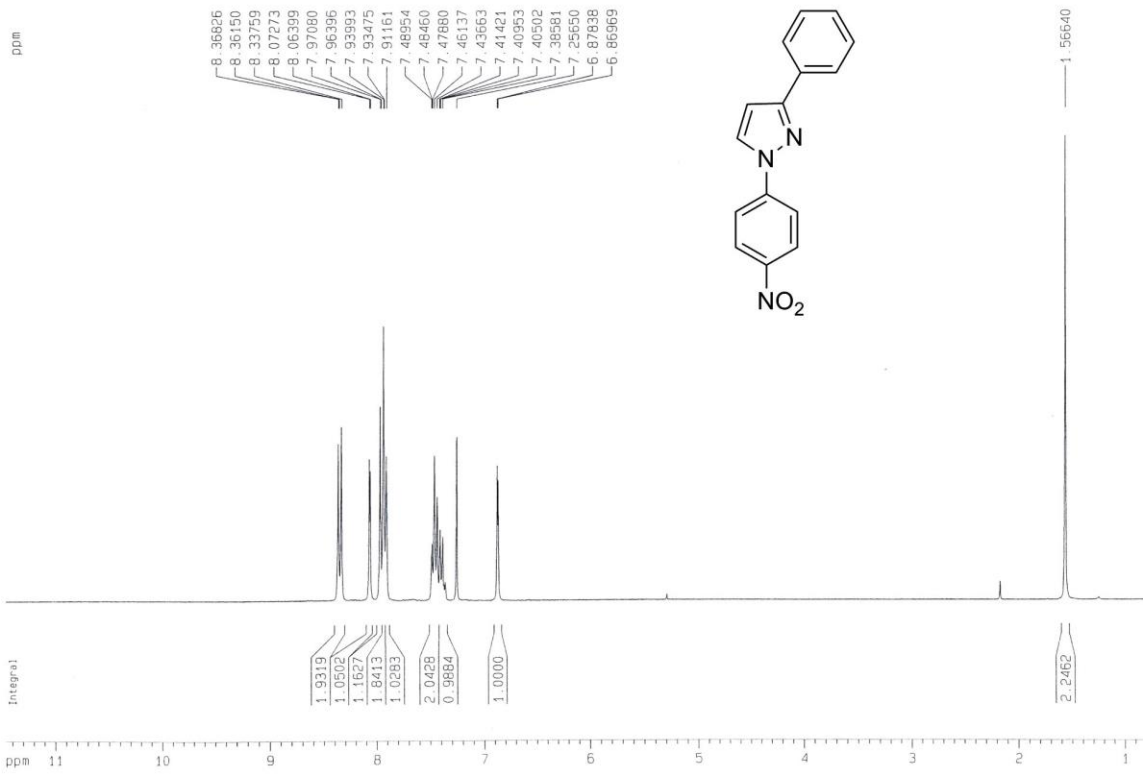

pyrazole-*p*-fluorobenzene (Table 1, 1h): $^{1}$H–NMR (300 MHz, $CDCl_3$): δ (ppm): 7.83 (d, *J* = 0.6 Hz, 1H), 7.69 (s, 1H), 7.60-7.57 (m, 2H), 7.19-7.16 (m, 2H), 6.44 (s, 1H),; $^{13}$C–NMR (75 MHz, $CDCl_3$): δ (ppm): 158.25, 140.60, 134.04, 126.82, 120.92, 114.52, 107.15; HRMS (ESI): calcd. for $[M+H]^+$ ($C_9H_8FN_2$) requires m/z 163.0759, found 187.0551; Anal. Calcd. for $C_9H_7FN_2$: C, 66.66%; H, 4.35%; N, 17.27%. Found: C, 66.76%; H, 4.40%; N, 17.29%.

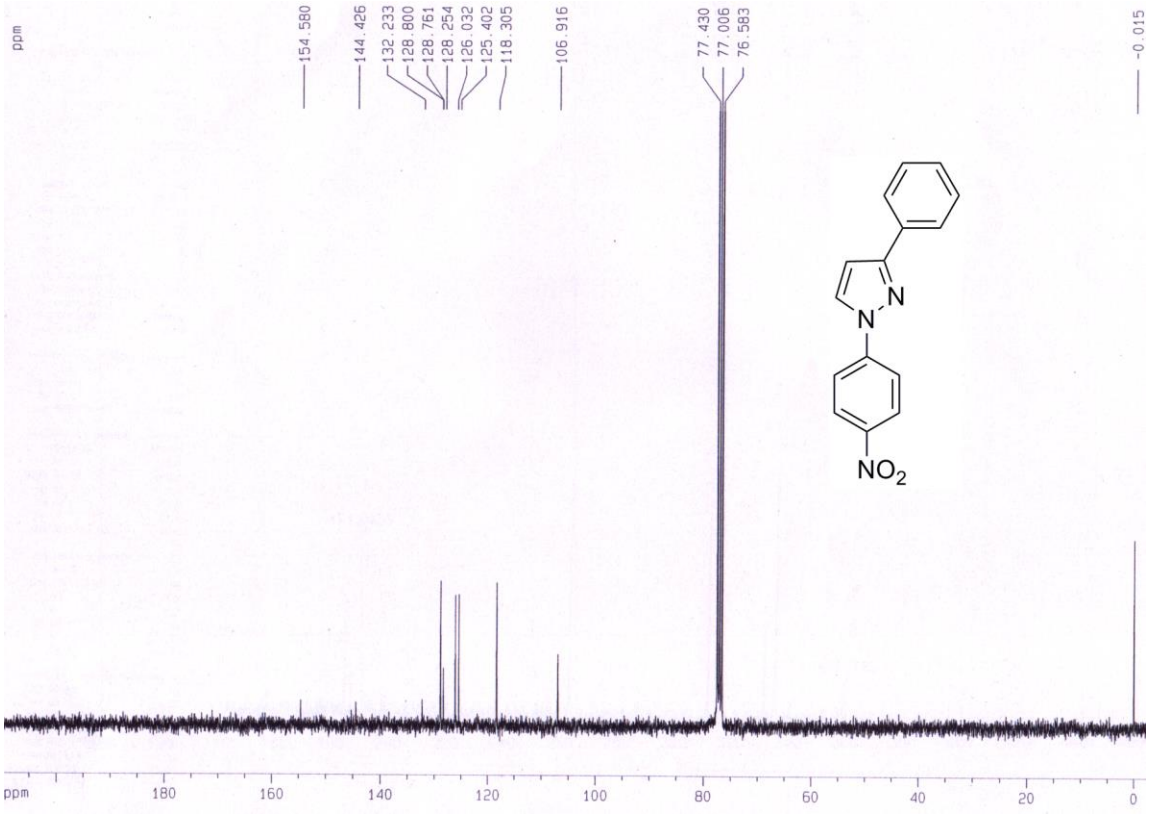

7.83040
7.82854
7.69675
7.60454
7.57748
7.57467
7.26542
7.18978
7.18721
7.16007
7.15734
6.43989
N
N
F
Integral
1.0088
0.9487
2.0932
2.0900
1.0000
ppm
10
9
8
7
6
5
4
3
2
1

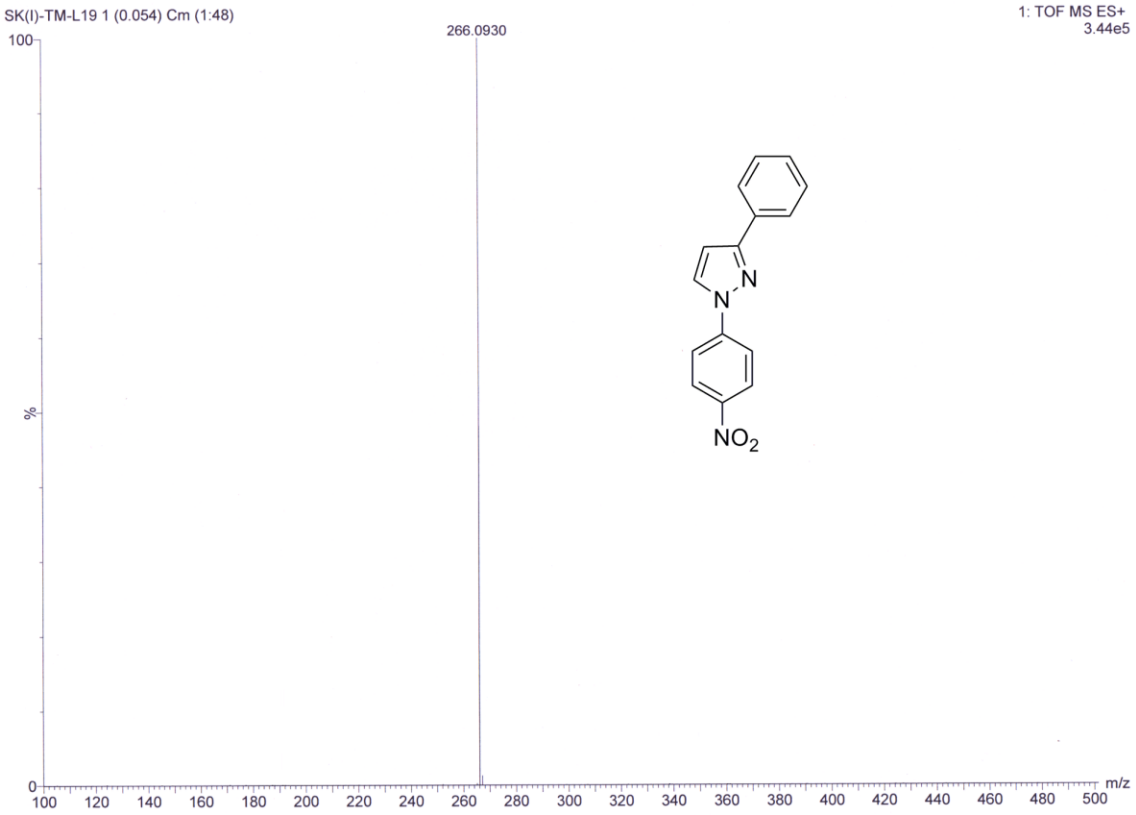

ppm
158.253
140.603
134.038
126.823
120.920
114.524
107.152
77.468
77.244
77.044
76.620
N
N
F
ppm
150
100
50
0



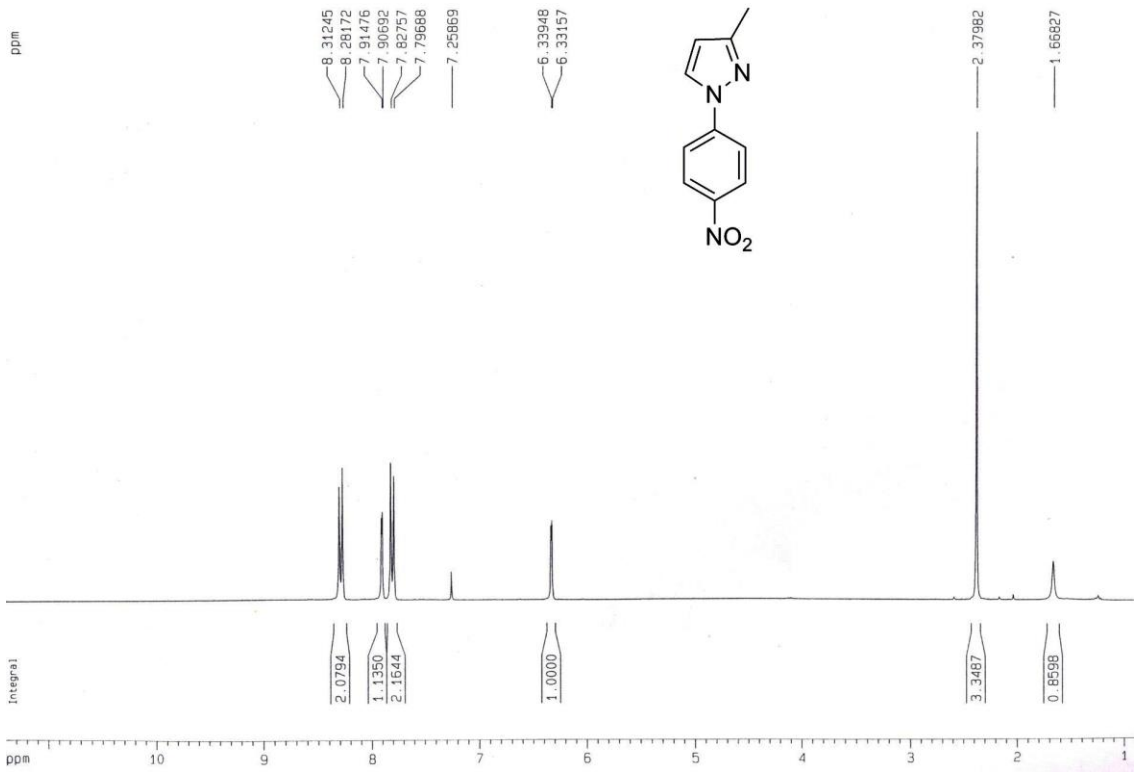

3-phenyl-pyrazole-*p*-nitrobenzene (Table 2, entry 2a): $^{1}$H–NMR (300 MHz, $CDCl_3$): δ (ppm): 8.36 (t, *J* = 2.03 Hz, 2H), 8.07 (d, *J* = 2.62 Hz, 1H), 7.91-7.97 (m, 4H), 7.26-7.49 (m, 3H), 6.87 (d, *J* = 2.60 Hz, 1H); $^{13}$C NMR (75 MHz, $CDCl_3$): δ (ppm): 154.58, 144.43, 132.23, 128.8, 128.76, 128.25, 126.03, 125.40, 118.30, 106.92; HRMS (ESI): calcd. for $[M+H]^+$ ($C_{15}H_{12}N_3O_2$) requires m/z 266.0930, found 266.0930; Anal. Calcd. for $C_{15}H_{11}N_3O_2$: C, 67.92%; H, 4.18%; N, 15.84%. Found: C, 67.95%; H, 4.19%; N, 15.82%.

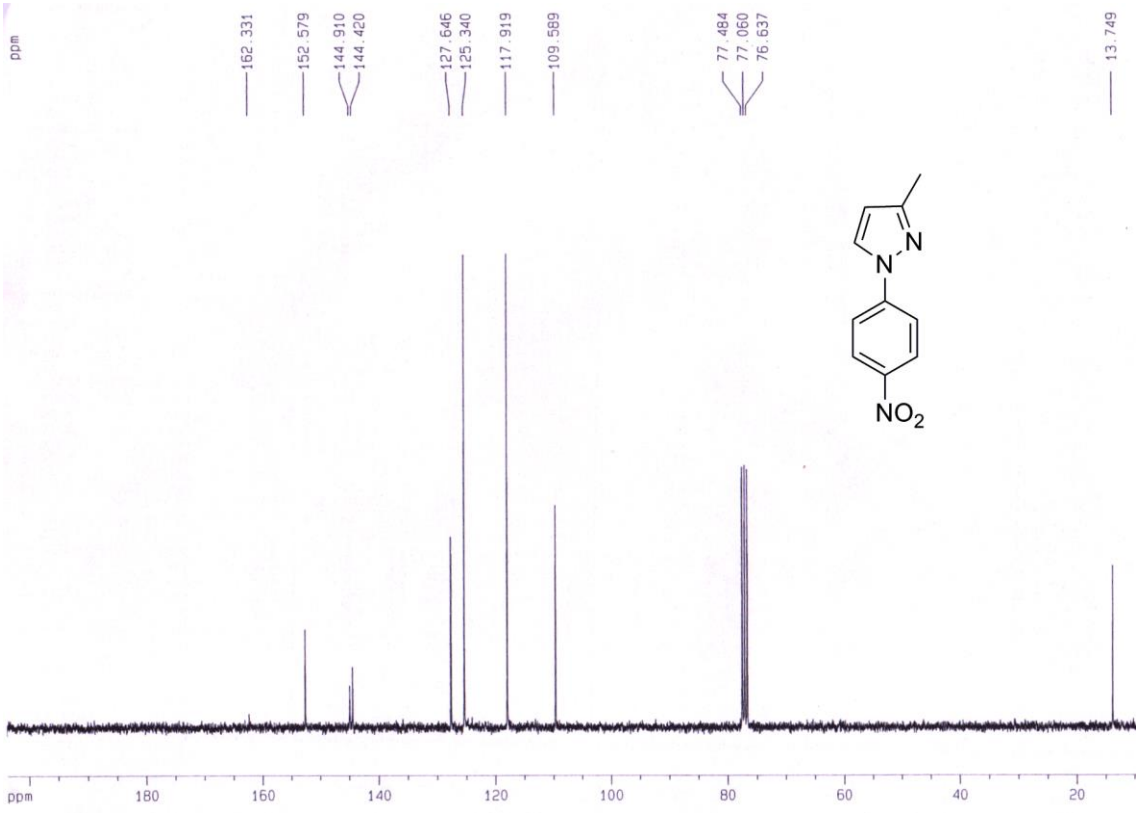

ppm
8.36826
8.36150
8.33759
8.07273
8.06399
7.97080
7.96396
7.93993
7.93475
7.91161
7.48954
7.48460
7.47880
7.46137
7.43663
7.41421
7.40953
7.40502
7.38581
7.25650
6.87838
6.86969
1.56640
N
N
NO2
Integral
1.9319
1.0502
1.1627
1.8413
1.0283
2.0428
0.9884
1.0000
2.2462
ppm 11
10
9
8
7
6
5
4
3
2
1

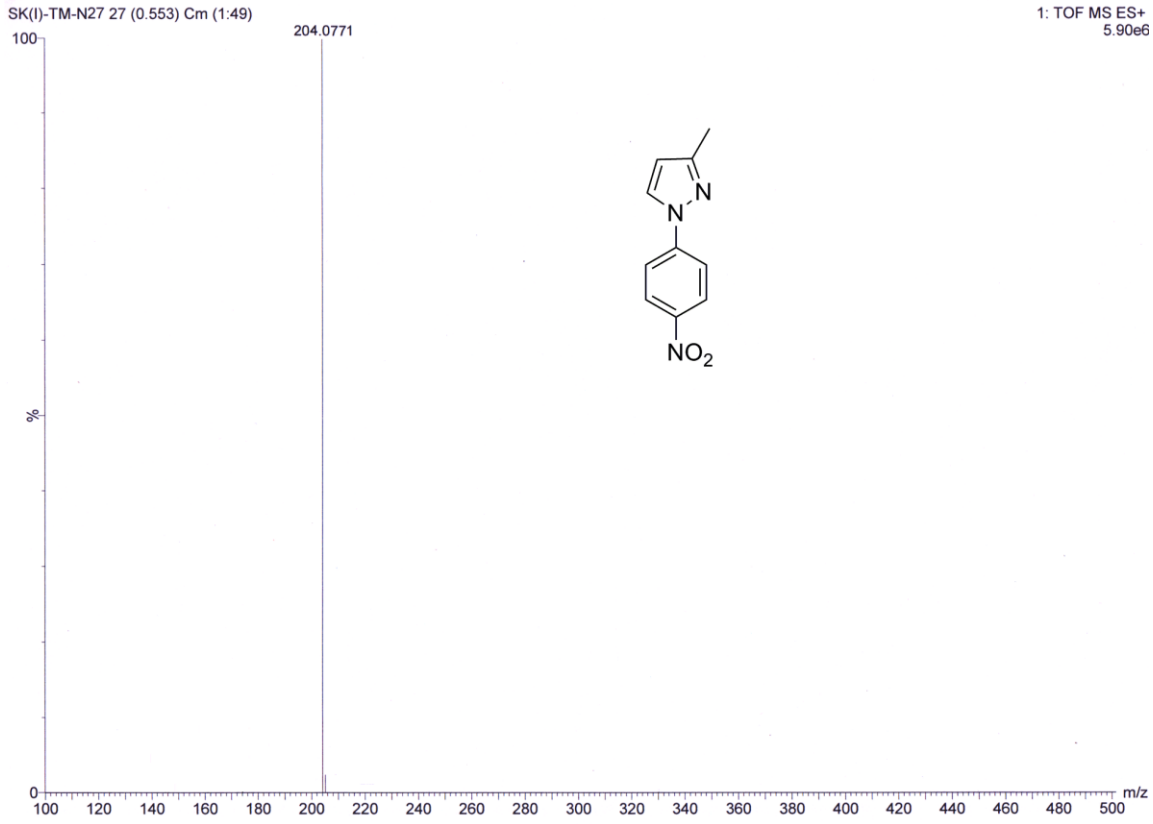

ppm
154.580
144.426
132.233
128.800
128.761
128.254
126.032
125.402
118.305
106.916
77.430
77.006
76.583
-0.015
N
N
NO2
ppm
180
160
140
120
100
80
60
40
20
0



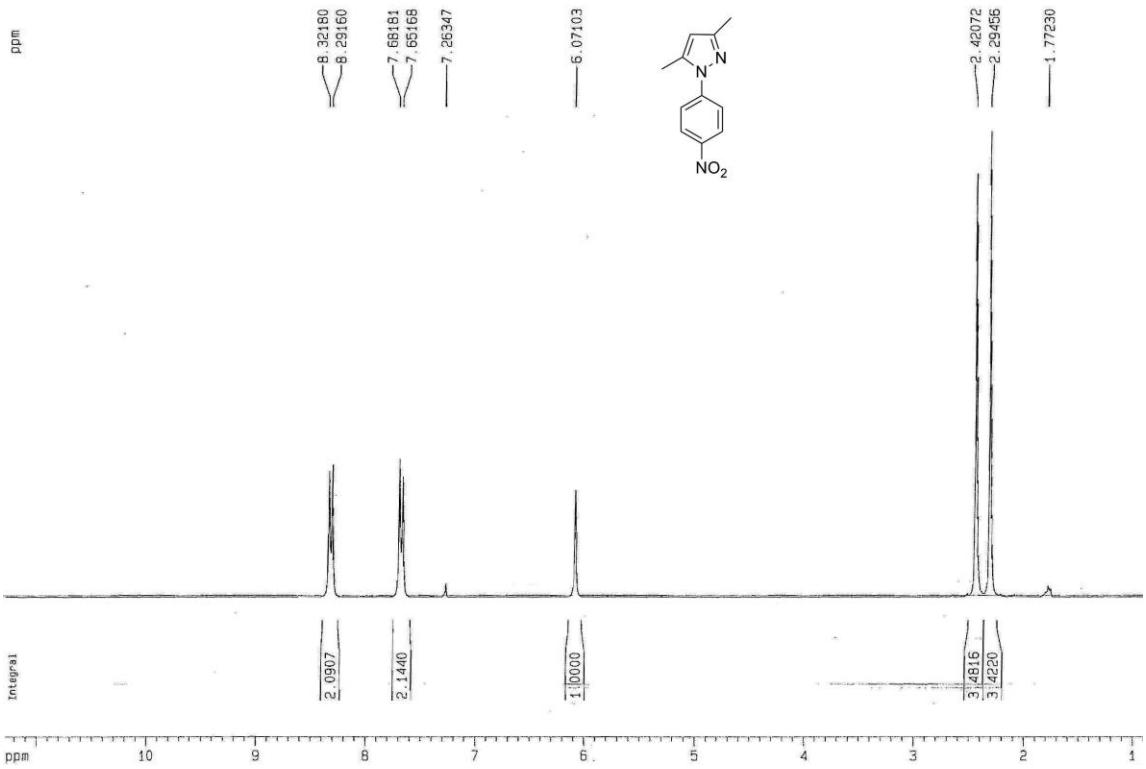

3-methyl-pyrazole-*p*-nitrobenzene (Table 2, entry 2b): $^{1}$H–NMR (300 MHz, $CDCl_3$): δ (ppm): 8.3 (d, *J* = 9.22 Hz, 2H), 7.91 (d, *J* = 2.35 Hz, 1H), 7.81 (d, *J* = 9.21 Hz, 2H), 6.33 (d, *J* = 2.34 Hz, 1H), 2.38 (s, 3H); $^{13}$C–NMR (75 MHz, $CDCl_3$): δ (ppm): 152.58, 144.91, 144.42, 127.65, 125.34, 117.92, 109.59, 13.75; HRMS (ESI): calcd. for $[M+H]^+$ ($C_{10}H_{12}N_3O_2$) requires m/z 204.0773, found 204.0771; Anal. Calcd. for $C_{10}H_{11}N_3O_2$: C, 59.11%; H, 4.46%; N, 20.68%. Found: C, 59.12%; H, 4.44%; N, 20.69%.

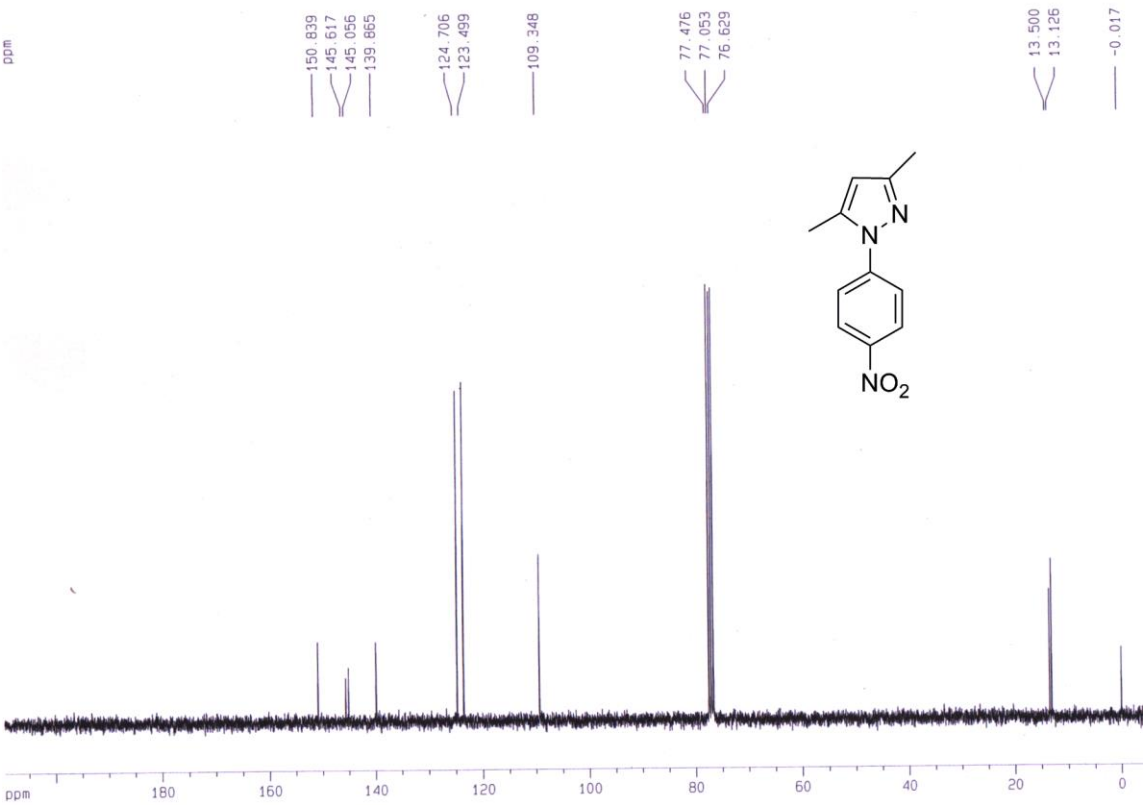

ppm
8.31245
8.28172
7.91476
7.90692
7.82757
7.79688
7.25869
6.33948
6.33157
2.37982
1.66827
Integral
2.0794
1.1350
2.1644
1.0000
3.3487
0.8598
ppm
10
9
8
7
6
5
4
3
2
1
NO2

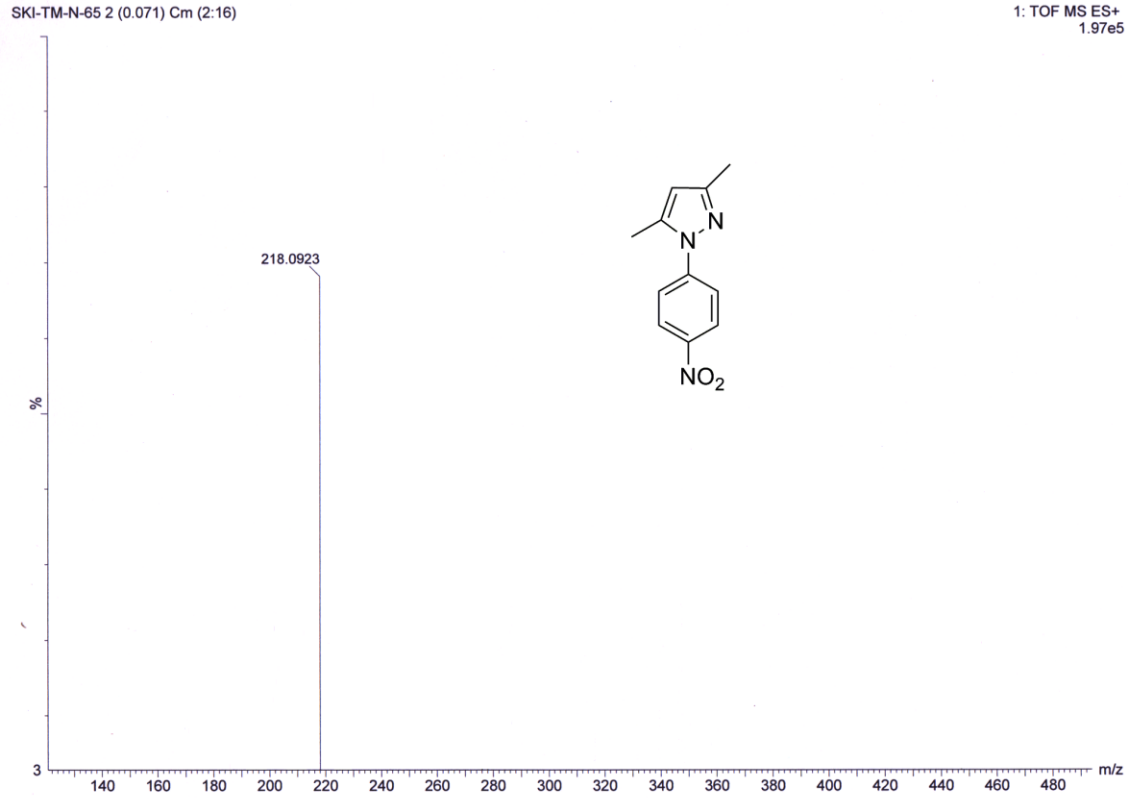

ppm
162.331
152.579
144.910
144.420
127.646
125.340
117.919
109.589
77.484
77.060
76.637
13.749
NO2
ppm
180
160
140
120
100
80
60
40
20



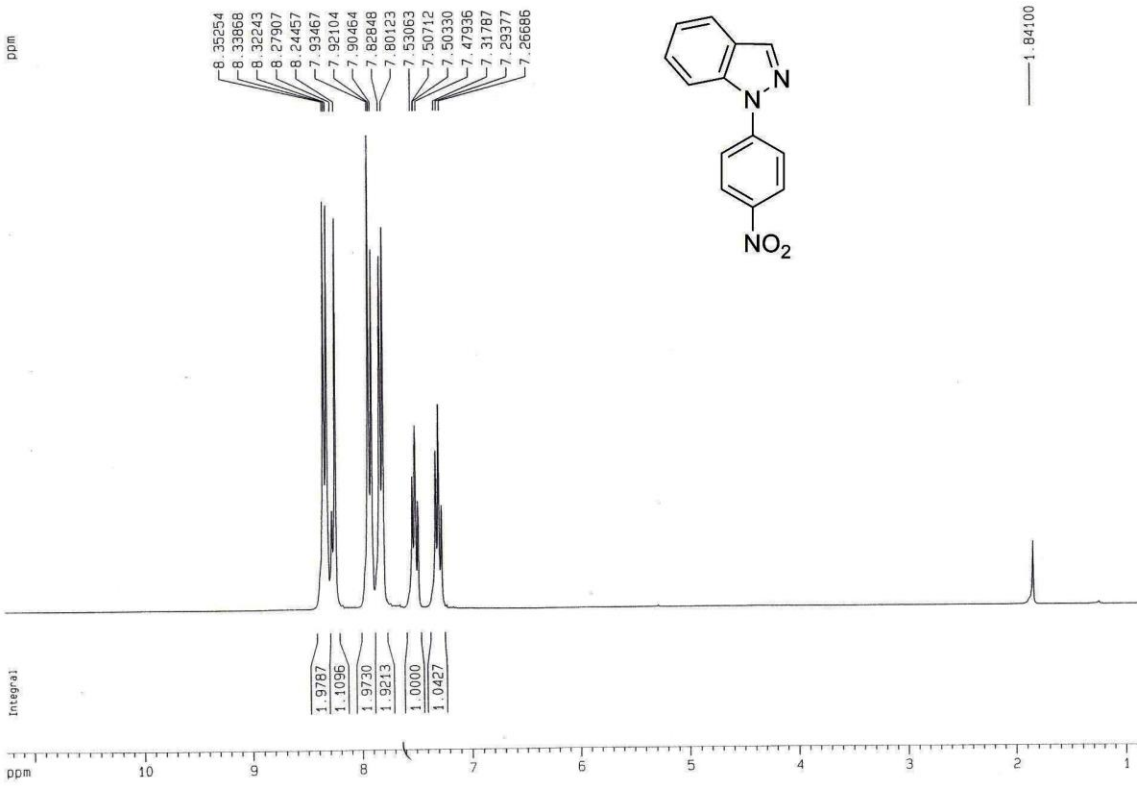

3,5-dimethyl-pyrazole-*p*-nitrobenzene (Table 2, entry 2c): $^{1}$H–NMR (300 MHz, $CDCl_3$): δ (ppm): 8.31 (d, *J* = 9.06 Hz, 2H), 7.67 (d, *J* = 9.06 Hz, 2H), 6.07 (s, 1H), 2.42 (s, 3H), 2.29 (s, 3H); $^{13}$C–NMR (75 MHz, $CDCl_3$): δ (ppm): 150.84, 145.62, 145.06, 139.86, 124.71, 123.50, 109.35, 13.50, 13.13; HRMS (ESI): calcd. for $[M+H]^+$ ($C_{11}H_{12}N_3O_2$) requires m/z 218.0930, found 218.0923; Anal. Calcd. for $C_{11}H_{11}N_3O_2$: C, 60.82%; H, 5.10%; N, 19.34%. Found: C, 60.85%; H, 5.11%; N, 19.31%.

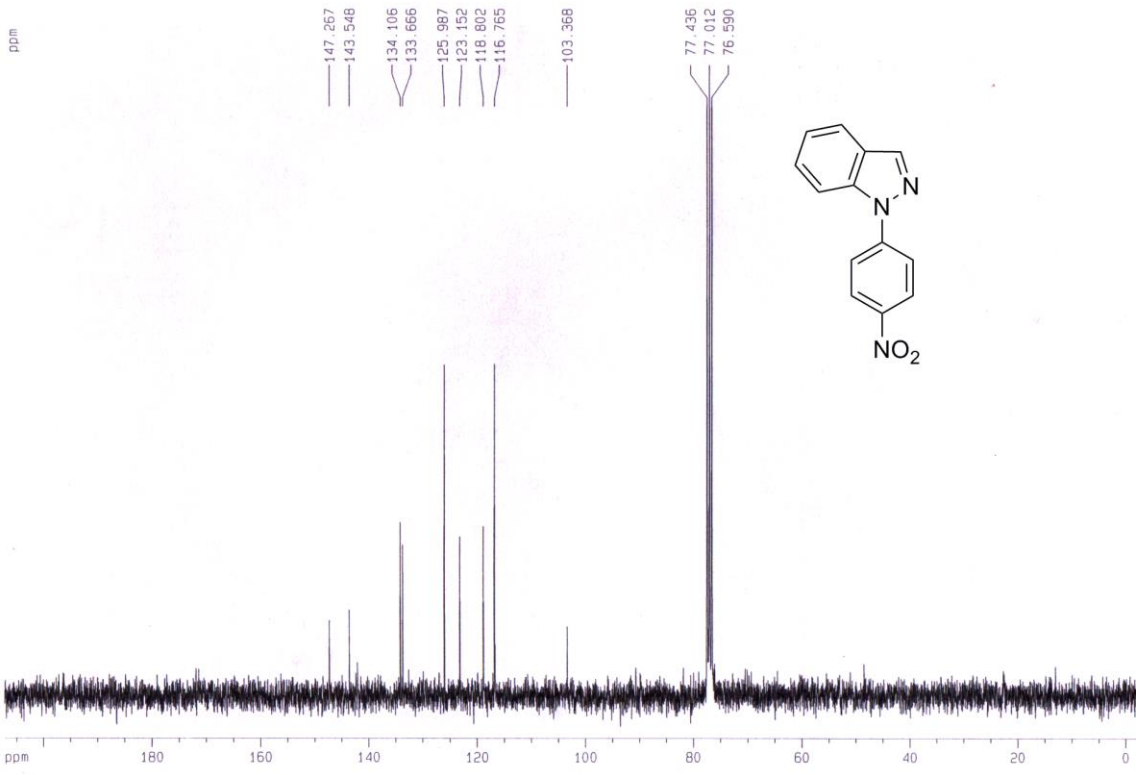

ppm
8.32180
8.29160
7.68181
7.65168
7.26347
6.07103
2.42072
2.29456
1.77230
Integral
2.0907
2.1440
1.0000
3.4816
3.4220
ppm
10
9
8
7
6
5
4
3
2
1

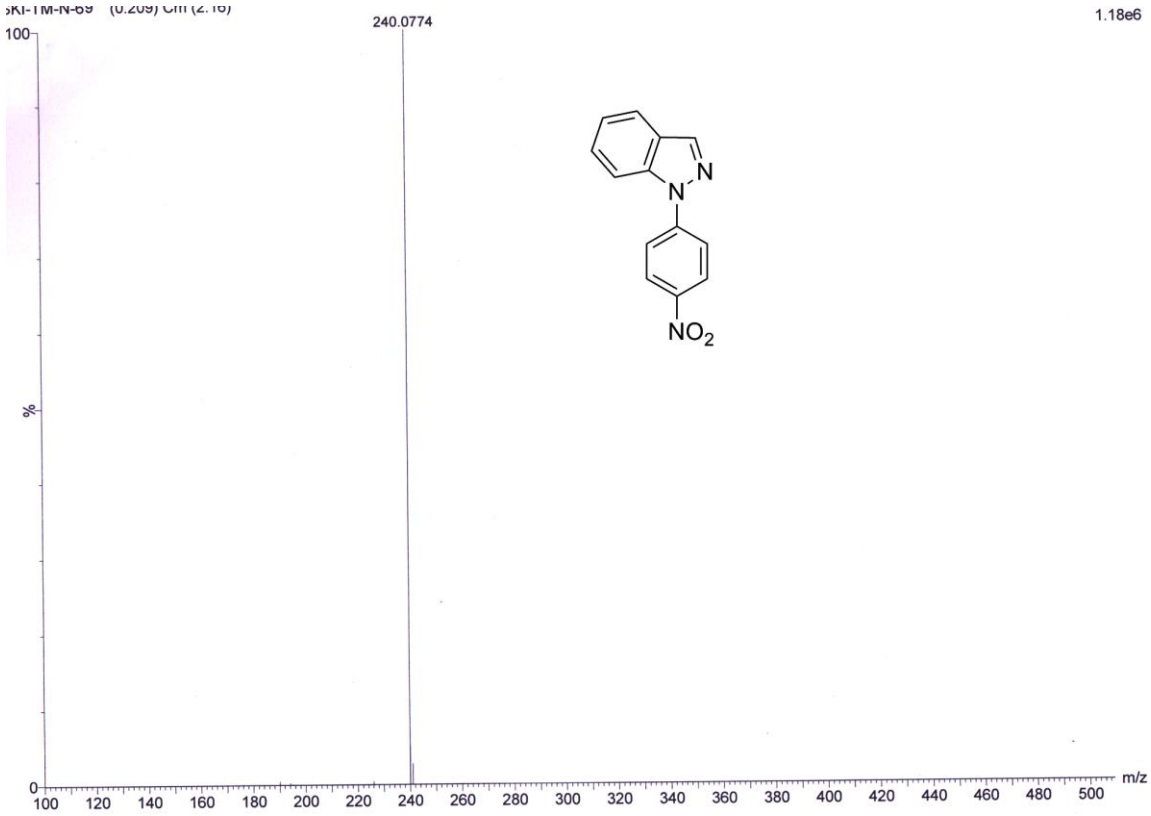

ppm
150.839
145.617
145.056
139.865
124.706
123.499
109.348
77.476
77.053
76.629
13.500
13.126
-0.017
ppm
180
160
140
120
100
80
60
40
20
0



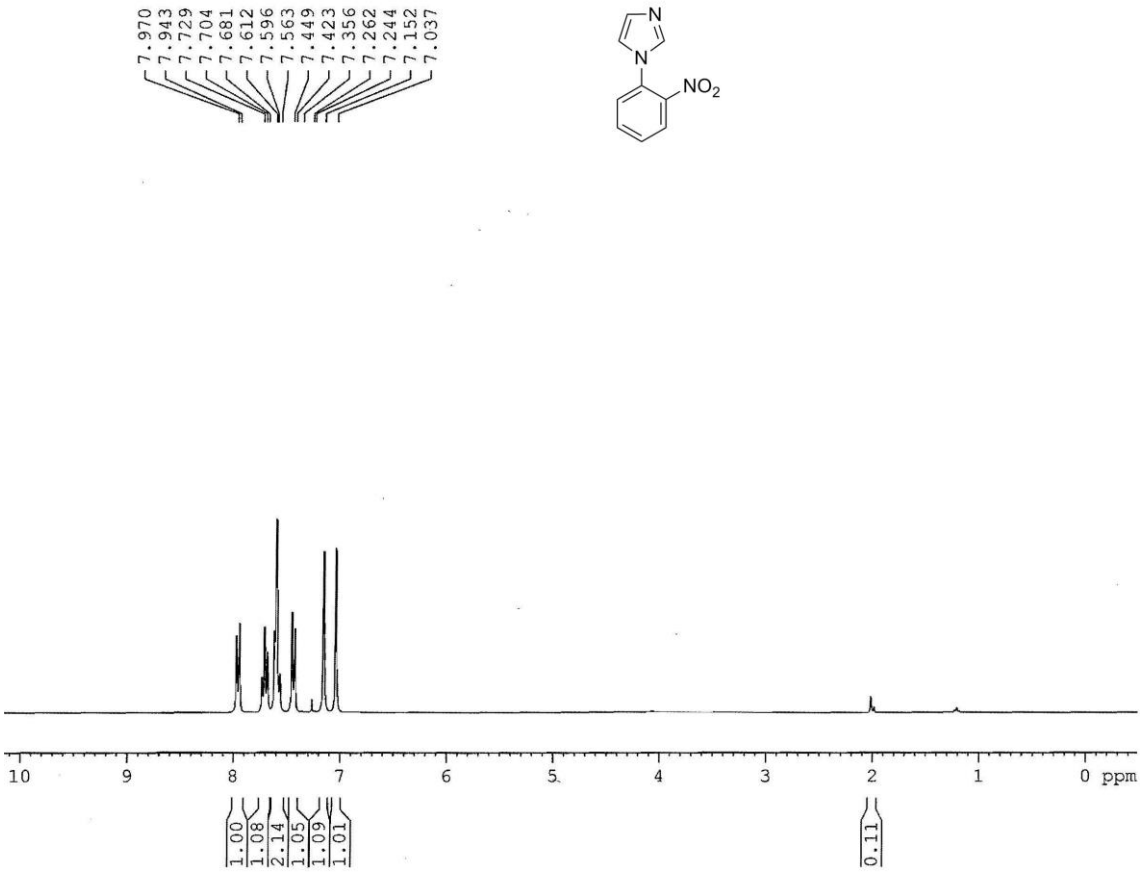

indazole-*p*-nitrobenzene (Table 2, entry 2d): $^{1}$H–NMR (300 MHz, $CDCl_3$): δ (ppm): 8.35-8.32 (m, 2H), 8.27-8.24 (m, 1H), 7.93-7.90 (m, 2H), 7.81 (d, *J* = 7.81 Hz, 2H), 7.53-7.48 (m, 1H), 7.32-7.27 (m, 1H); $^{13}$C–NMR (75 MHz, $CDCl_3$): δ (ppm): 147.27, 143.55, 134.11, 133.67, 125.99, 123.15, 118.80, 116.76, 103.37; HRMS (ESI): calcd. for $[M+H]^+$ ($C_{13}H_{10}N_3O_2$) requires m/z 240.0773, found 240.0774; Anal. Calcd. for $C_{13}H_9N_3O_2$: C, 65.27%; H, 3.79%; N, 17.56%. Found: C, 65.26%; H, 3.80%; N, 17.55%.

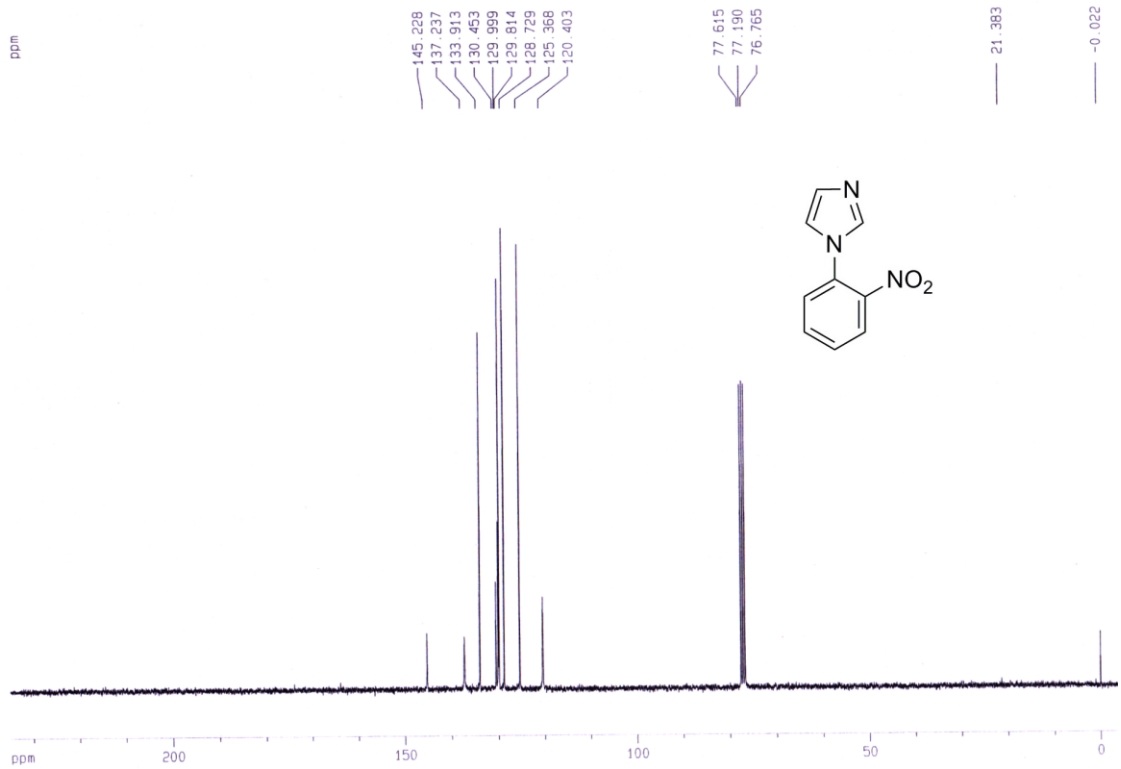

ppm
8.35254
8.33868
8.32243
8.27907
8.24457
7.93467
7.92104
7.90464
7.82848
7.80123
7.53063
7.50712
7.50330
7.47936
7.31787
7.29377
7.26686
1.84100
N
N
NO2
Integral
1.9787
1.1096
1.9730
1.9213
1.0000
1.0427
ppm
10
9
8
7
6
5
4
3
2
1

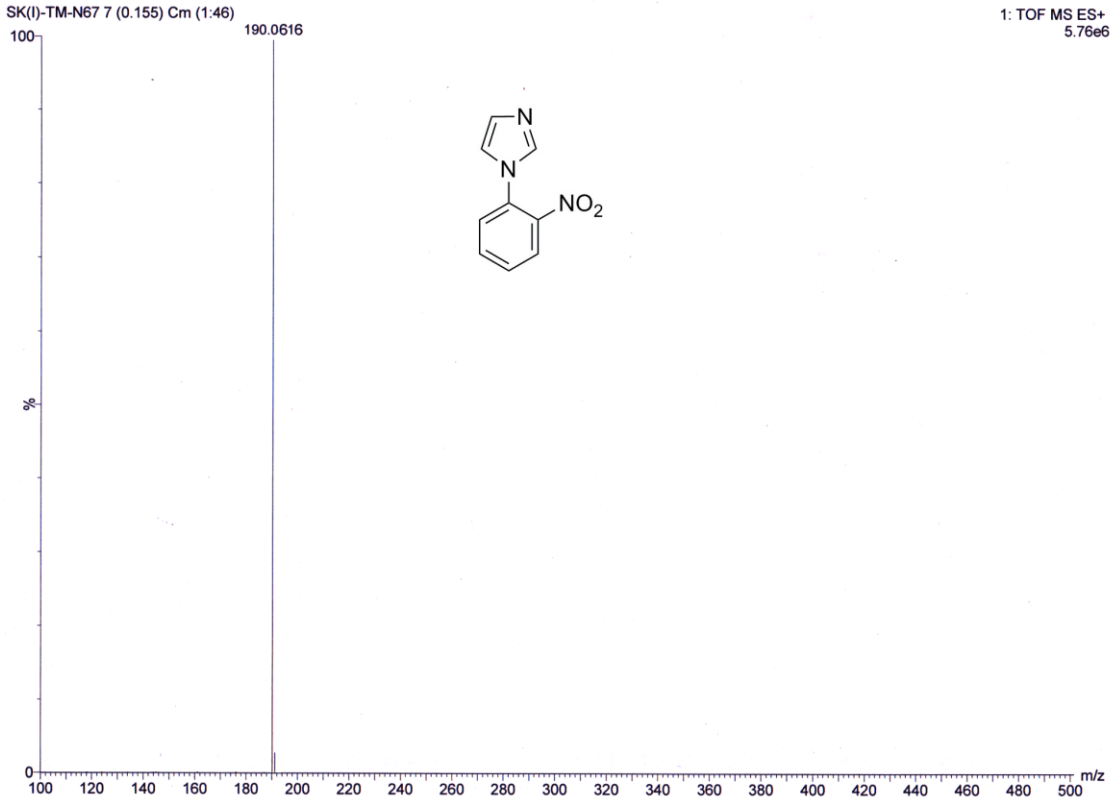

ppm
147.267
143.548
134.106
133.666
125.987
123.152
118.802
116.765
103.368
77.436
77.012
76.590
N
N
NO2
ppm
180
160
140
120
100
80
60
40
20
0



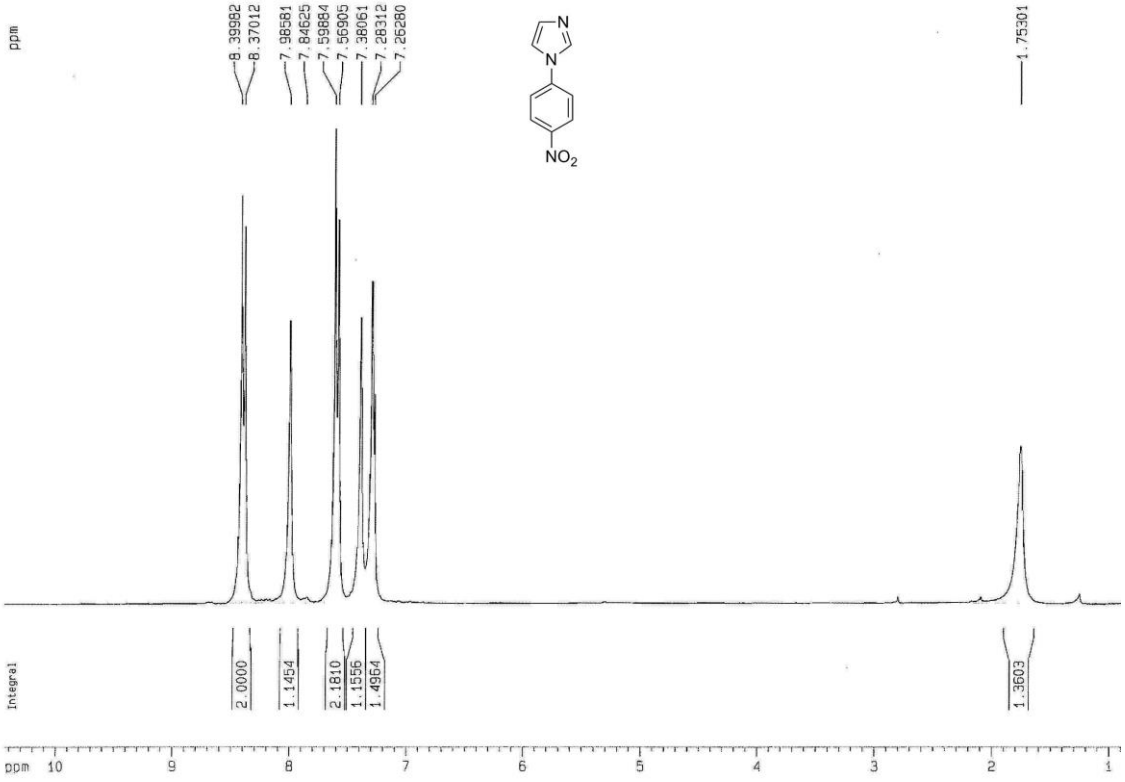

imidazole-*o*-nitrobenzene (Table 2, entry 2e): $^{1}$H–NMR (300 MHz, $CDCl_3$): δ (ppm): 7.96 (d, *J* = 8.1 Hz, 1H), 7.70 (t, *J* = 7.7 Hz, 1H), 7.61-7.56 (m, 2H), 7.45-7.35 (m, 1H), 7.15 (s, 1H), 7.03 (s, 1H); $^{13}$C–NMR (75 MHz, $CDCl_3$): δ (ppm): 145.23, 137.24, 133.91, 130.45, 130, 129.81, 128.73, 125.37, 120.40; HRMS (ESI): calcd. for $[M+H]^+$ ($C_9H_8N_3O_2$) requires m/z 190.0617, found 190.0616; Anal. Calcd. for $C_9H_7N_3O_2$: C, 57.14%; H, 3.73%; N, 22.21. Found: C, 57.15%; H, 3.72%; N, 22.23.

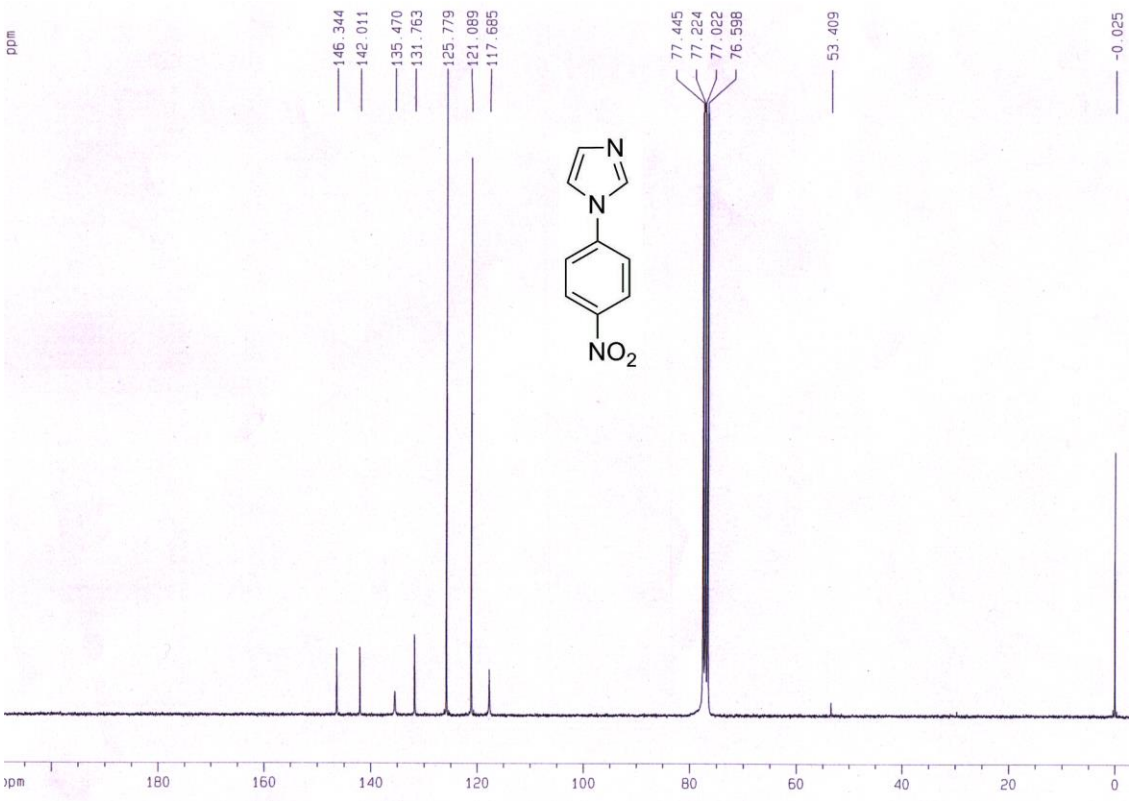

7.970
7.943
7.729
7.704
7.681
7.612
7.596
7.563
7.449
7.423
7.356
7.262
7.244
7.152
7.037
N
N
NO2
10
9
8
7
6
5
4
3
2
1
0 ppm
1.00
1.08
2.14
1.05
1.09
1.01
0.11

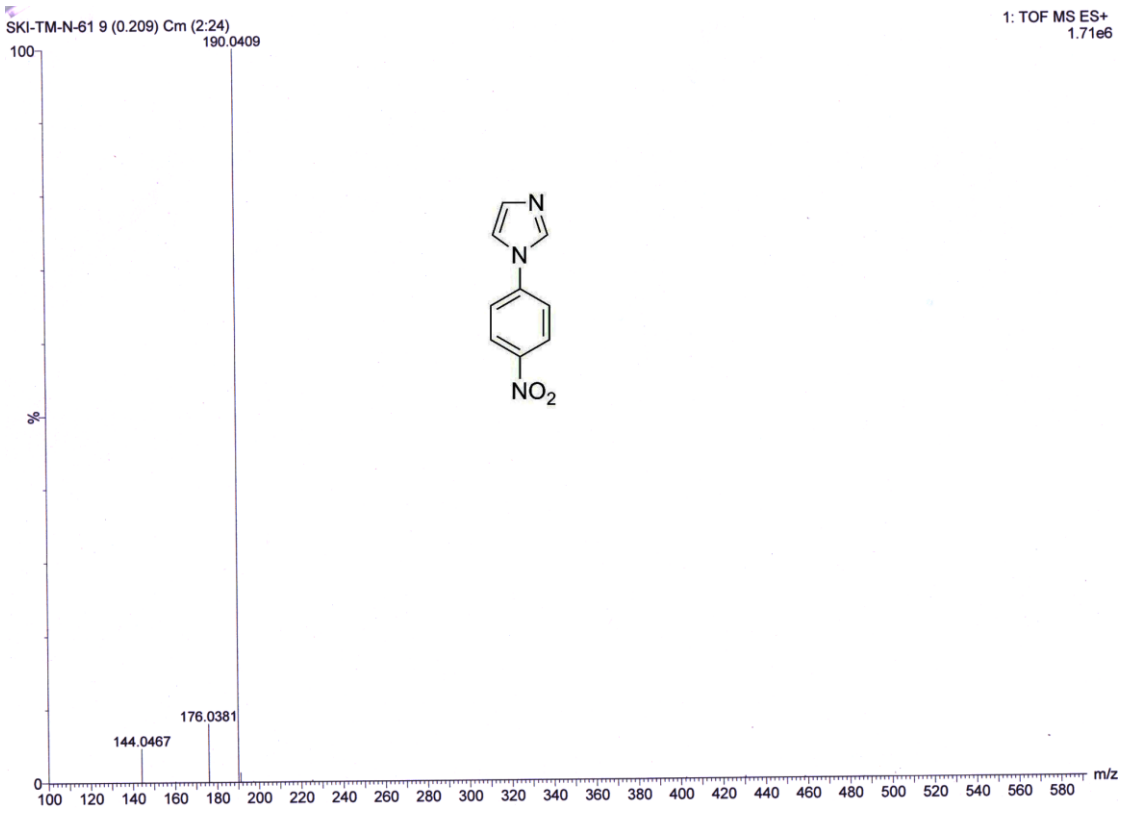

ppm
145.228
137.237
133.913
130.453
129.999
129.814
128.729
125.368
120.403
77.615
77.190
76.765
21.383
-0.022
N
N
NO2
ppm
200
150
100
50
0


SK(I)-TM-N67 7 (0.155) Cm (1:46)
1: TOF MS ES+
5.76e6
190.0616
100
%
0
N
N
NO2
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460
480
500
m/z

imidazole-*p*-nitrobenzene (Table 2, entry 2f): $^{1}$H–NMR (300 MHz, $CDCl_3$): δ (ppm): 8.38 (d, *J* = 8.91 Hz, 2H), 7.98 (s, 1H), 7.58 (d, *J* = 8.94 Hz, 2H), 7.38 (s, 1H), 7.27 (d, *J* = 6.1 Hz, 1H); $^{13}$C–NMR (75 MHz, $CDCl_3$): δ (ppm): 146.34, 142.01, 135.47, 131.76, 125.78, 121.09, 117.68; HRMS (ESI): calcd. for $[M+H]^+$ ($C_9H_8N_3O_2$) requires m/z 190.0617, found 190.0409; Anal. Calcd. for $C_9H_7N_3O_2$: C, 57.14%; H, 3.73%; N, 22.21%. Found: C, 57.17%; H, 3.73%; N, 22.19%.

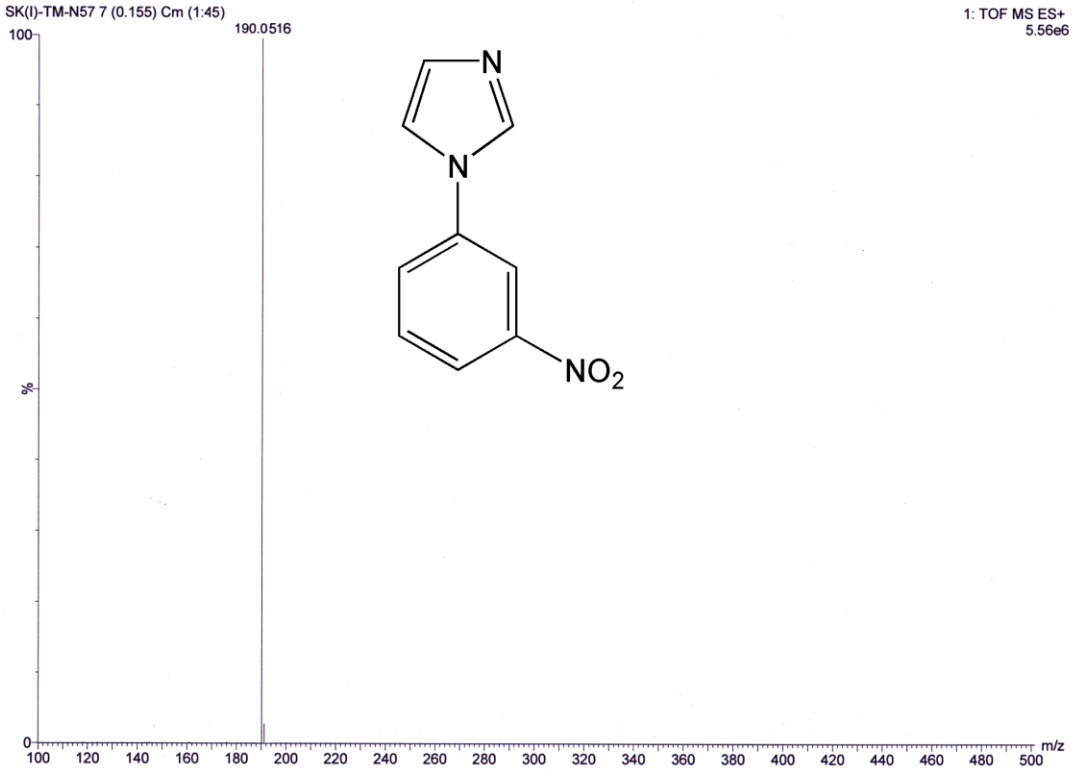



ppm
146.344
142.011
135.470
131.763
125.779
121.089
117.685
77.445
77.224
77.022
76.598
53.409
-0.025
N
N
NO2
ppm
180
160
140
120
100
80
60
40
20
0

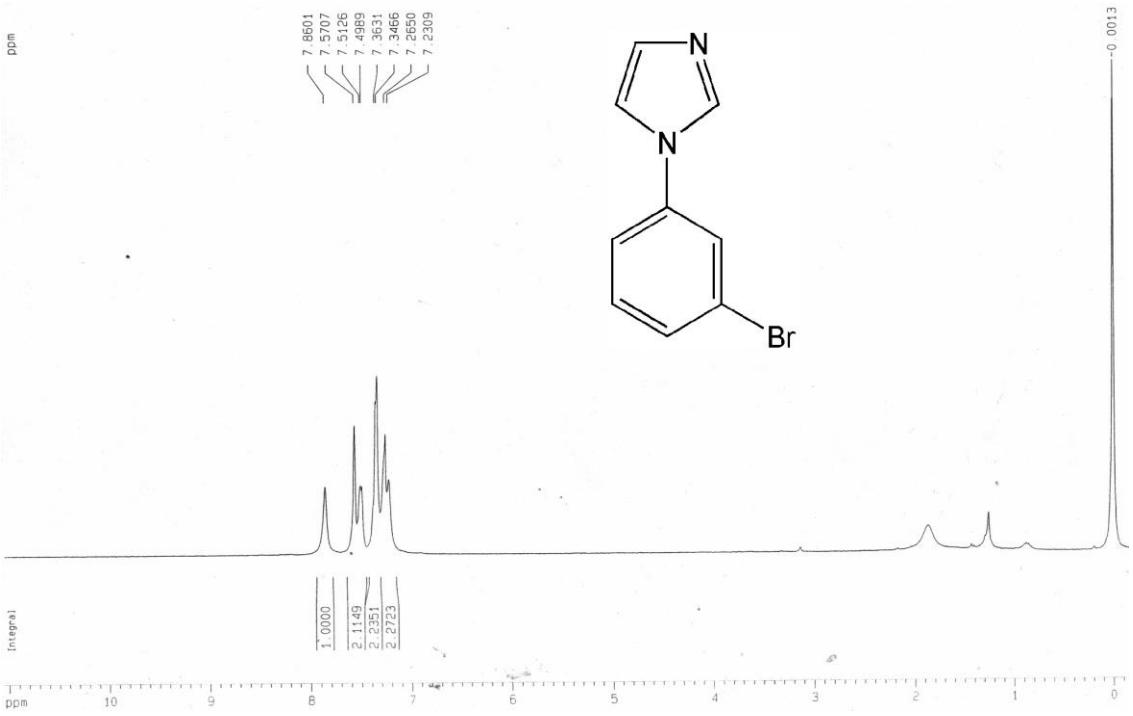


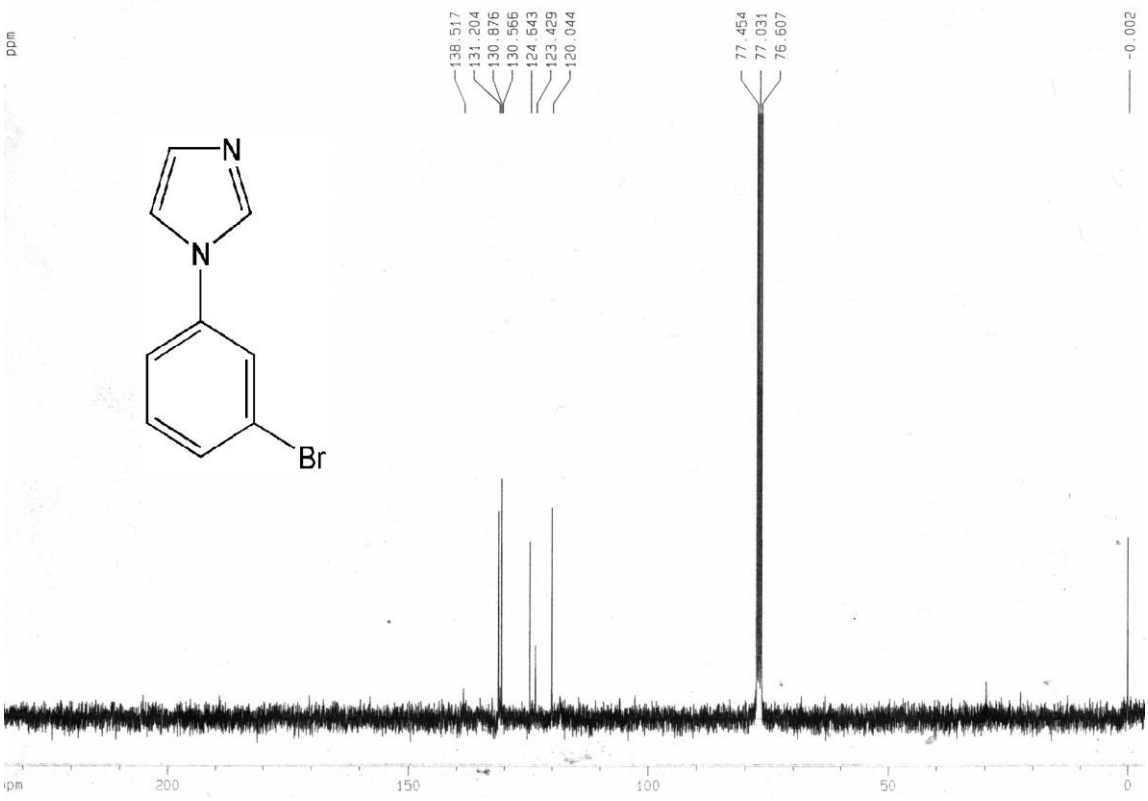

imidazole-m-nitrobenzene (Table 2, entry 2g): $^{1}$H NMR (300 MHz, $CDCl_3$): δ (ppm): 8.29-8.23 (m, 2H), 7.99 (s, 1H), 7.78-7.68 (m, 2H), 7.31 (m, 2H); HRMS (ESI): calcd. for $[M+H]^+$ ($C_9H_8N_3O_2$) requires m/z 190.0617, found 190.0516;Anal. Calcd. for $C_9H_7N_3O_2$: C, 57.14%; H, 3.73%; N, 22.21%. Found: C, 57.21%; H, 3.78%; N, 22.25%.

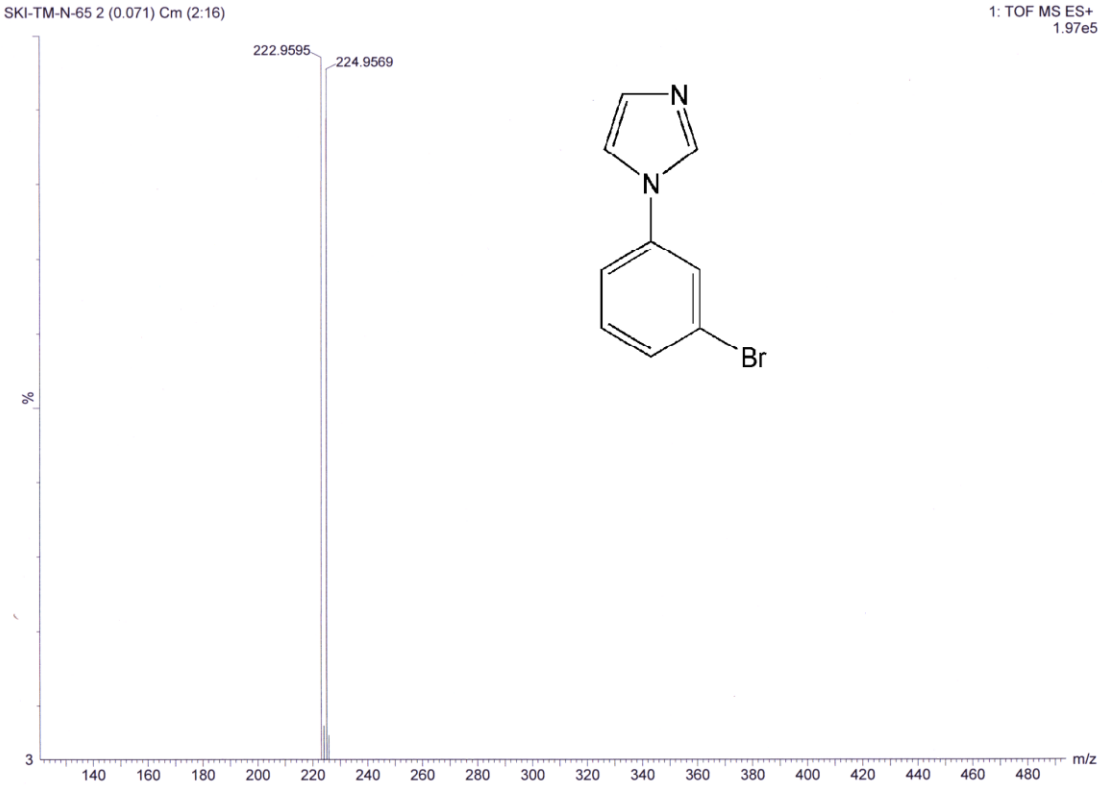

ppm
8.2895
8.2588
8.2326
7.9915
7.7783
7.7522
7.7331
7.7067
7.6804
7.3082
7.2609
0.0025
0.2007
integral
2.0530
1.0000
2.2283
2.2042
ppm
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
N
N
NO2


SK(I)-TM-N57 7 (0.155) Cm (1:45)
1: TOF MS ES+
5.56e6
190.0516
100
%
0
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460
480
500
m/z
N
N
NO2

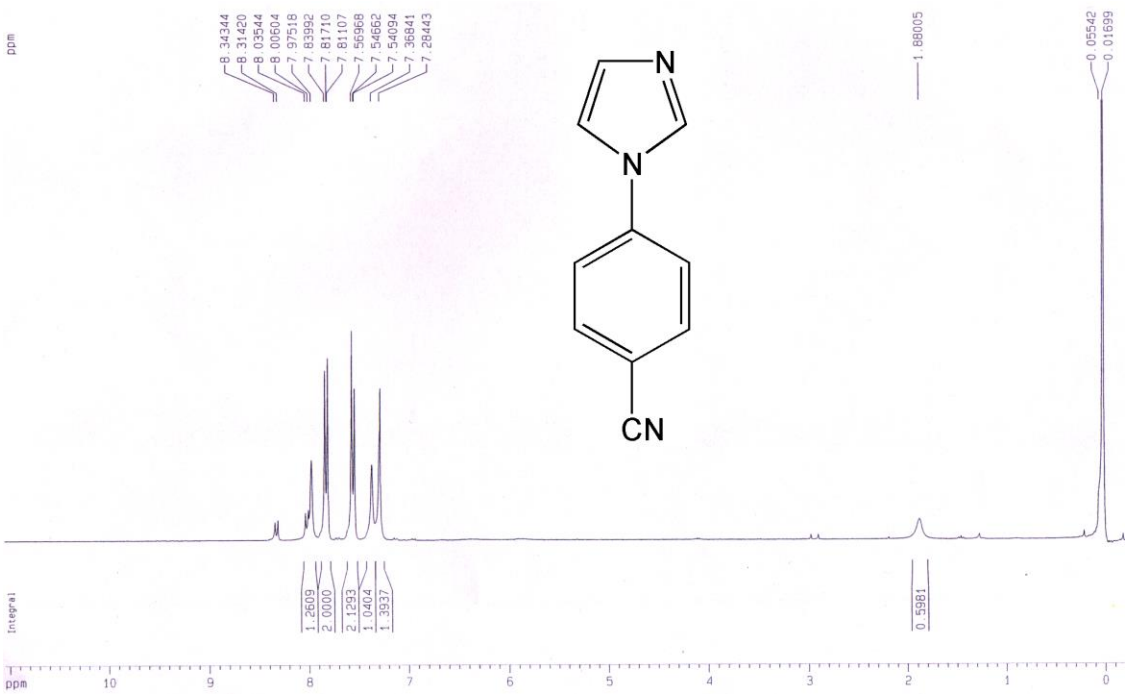
imidazole-m-bromobenzene (Table 2, entry 2h): $^{1}$H–NMR (300 MHz, $CDCl_3$): δ (ppm): 7.86 (s, 1H), 7.57-7.49 (m, 2H), 7.36-7.23 (m, 4H); $^{13}$C–NMR (75 MHz, $CDCl_3$): δ (ppm): 138.52, 131.20, 130.88, 130.57, 124.64, 123.43, 120.04; HRMS (ESI): calcd. for $[M+H]^+$ ($C_9H_8BrN_2$) requires m/z 222.9793, found 222.9593; Anal. Calcd. for $C_9H_7BrN_2$: C, 48.46%; H, 3.16%; N, 12.56%. Found: C, 48.56%; H, 3.17%; N, 12.61%.

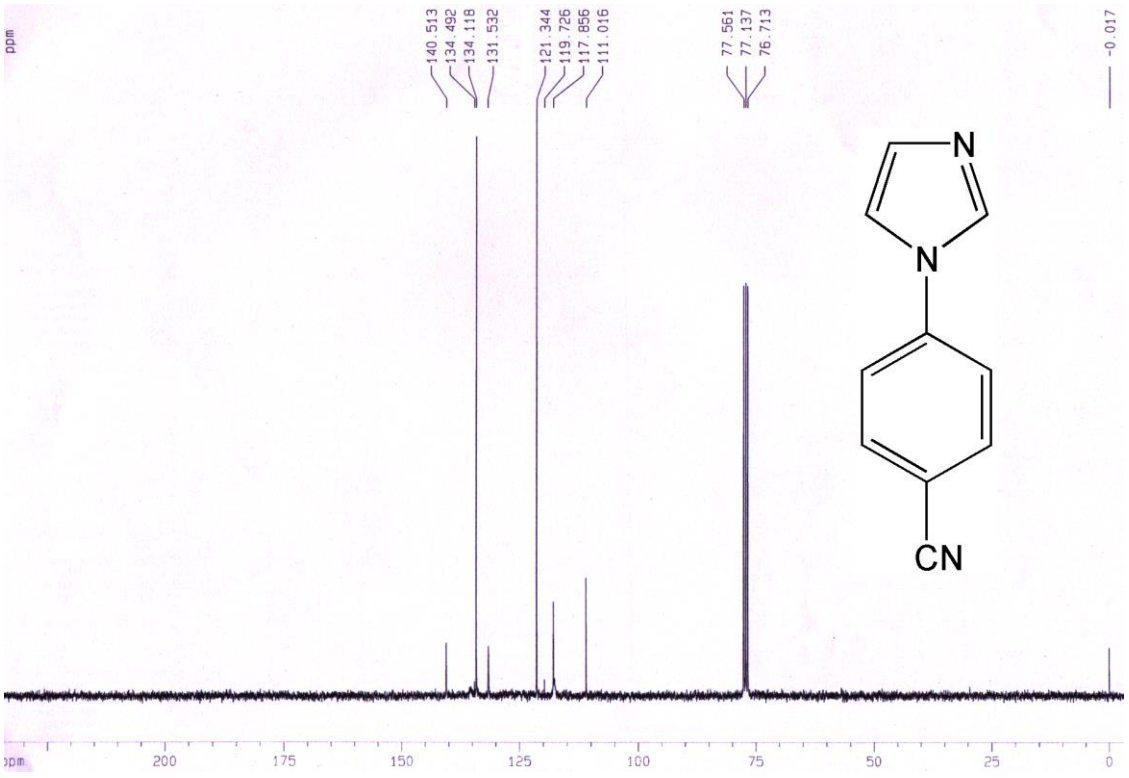


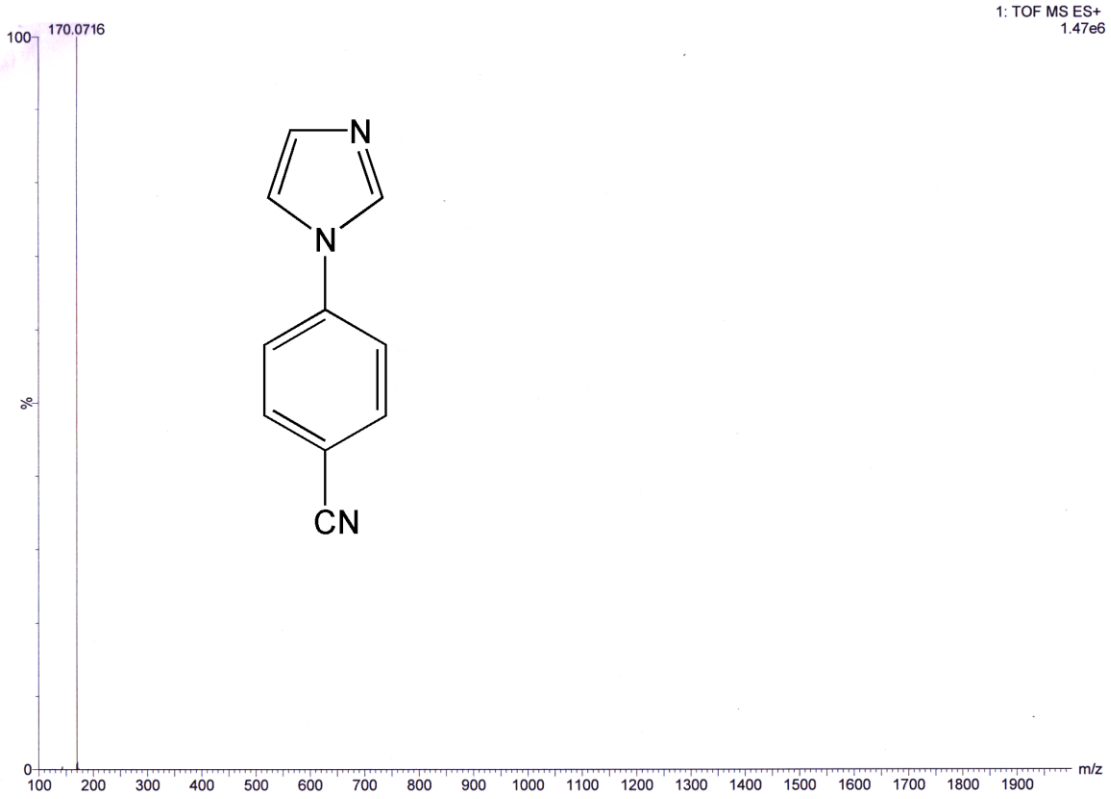

ppm
138.517
131.204
130.876
130.566
124.643
123.429
120.044
77.454
77.031
76.607
-0.002
N
N
Br
200
150
100
50
0



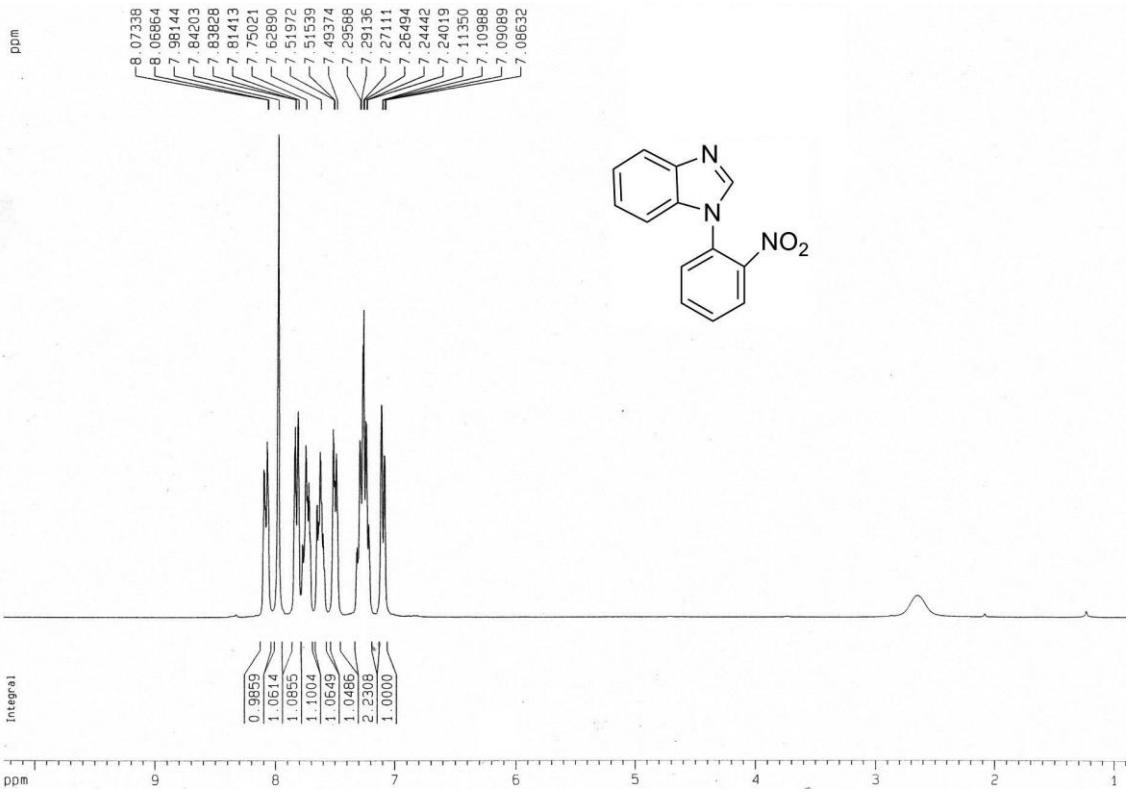

imidazole-*p*-benzonitrile (Table 2, entry 2i): $^{1}$H–NMR (300 MHz, $CDCl_3$): δ (ppm): 8.03-7.97 (m, 1H), 7.84-7.81 (m, 2H), 7.57-7.54 (m, 2H), 7.37 (s, 1H), 7.28 (s, 1H); $^{13}$C–NMR (75 MHz, $CDCl_3$): δ (ppm): 140.51, 134.49, 134.12, 131.53, 121.34, 119.73, 117.86, 111.02; HRMS (ESI): calcd. for $[M+H]^+$ ($C_{10}H_8N_3$) requires m/z 170.0718, found 170.0716; Anal. Calcd. for $C_{10}H_7N_3$: C, 70.99%; H, 4.17%; N, 24.84%. Found: C, 70.96%; H, 4.17%; N, 24.81%.

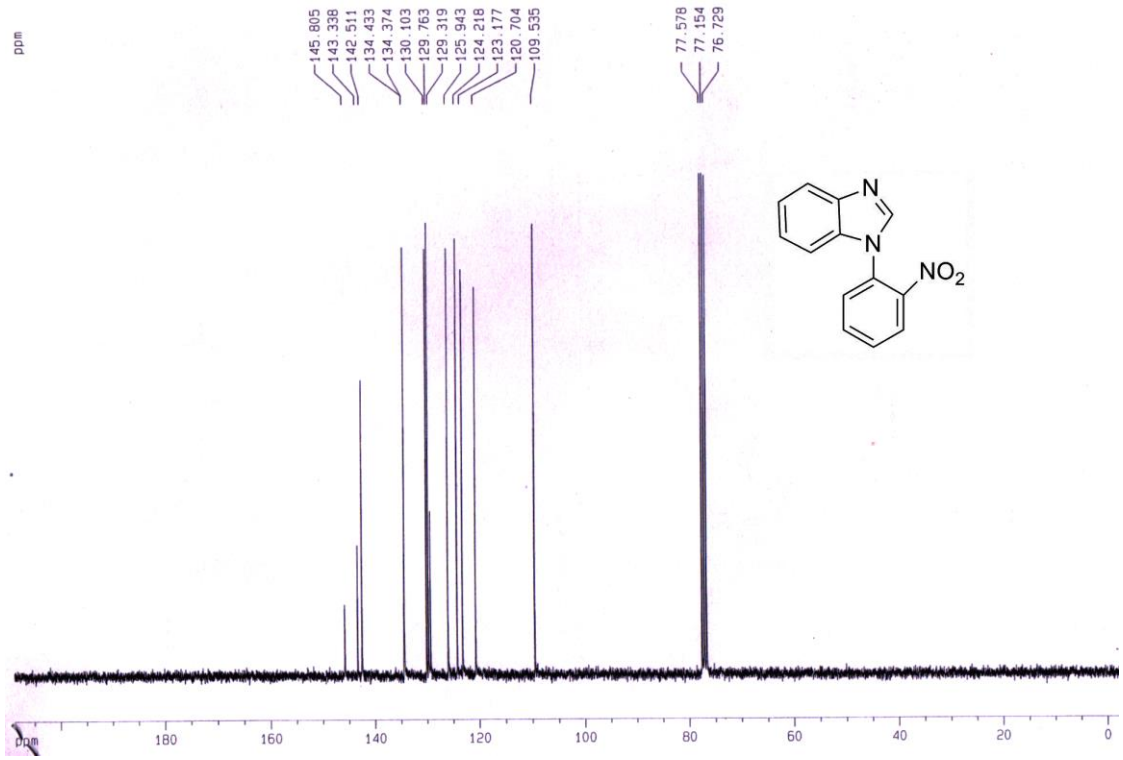

8.34344
8.31420
8.03544
8.00604
7.97518
7.83992
7.81710
7.81107
7.56968
7.54662
7.54094
7.36841
7.28443
1.88005
0.05542
0.01699
ppm
Integral
1.2609
2.0000
2.1293
1.0404
1.3937
0.5981
N
N
CN


140.513
134.492
134.118
131.532
121.344
119.726
117.856
111.016
77.561
77.137
76.713
-0.017
ppm
N
N
CN

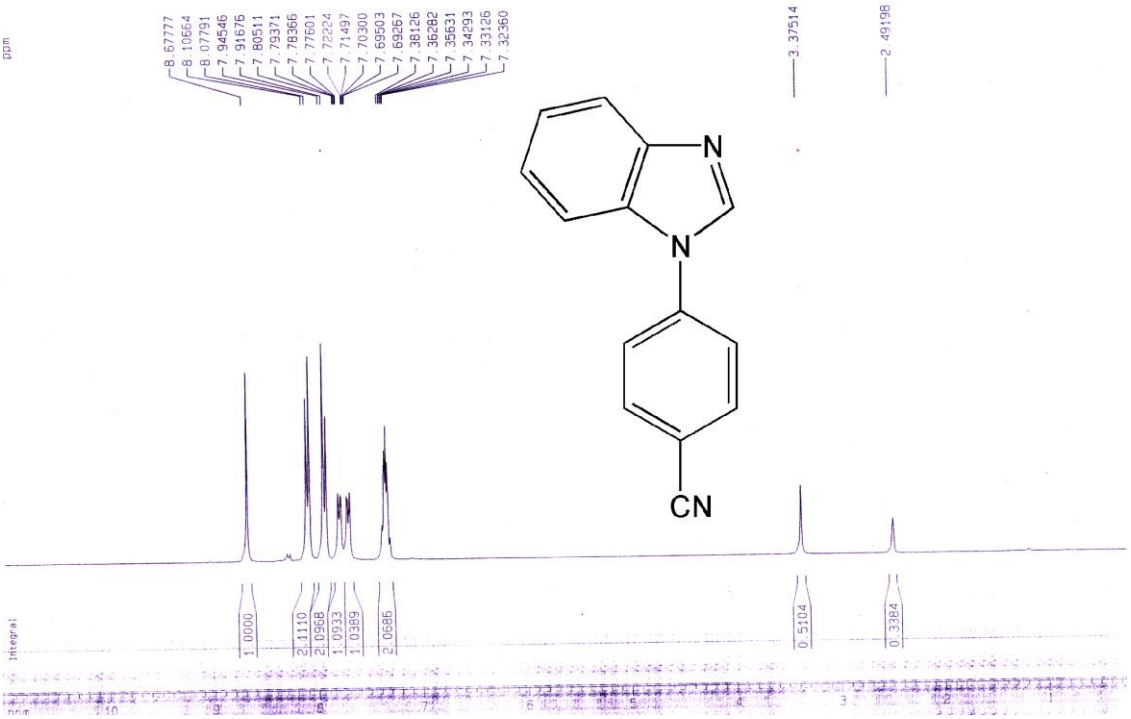


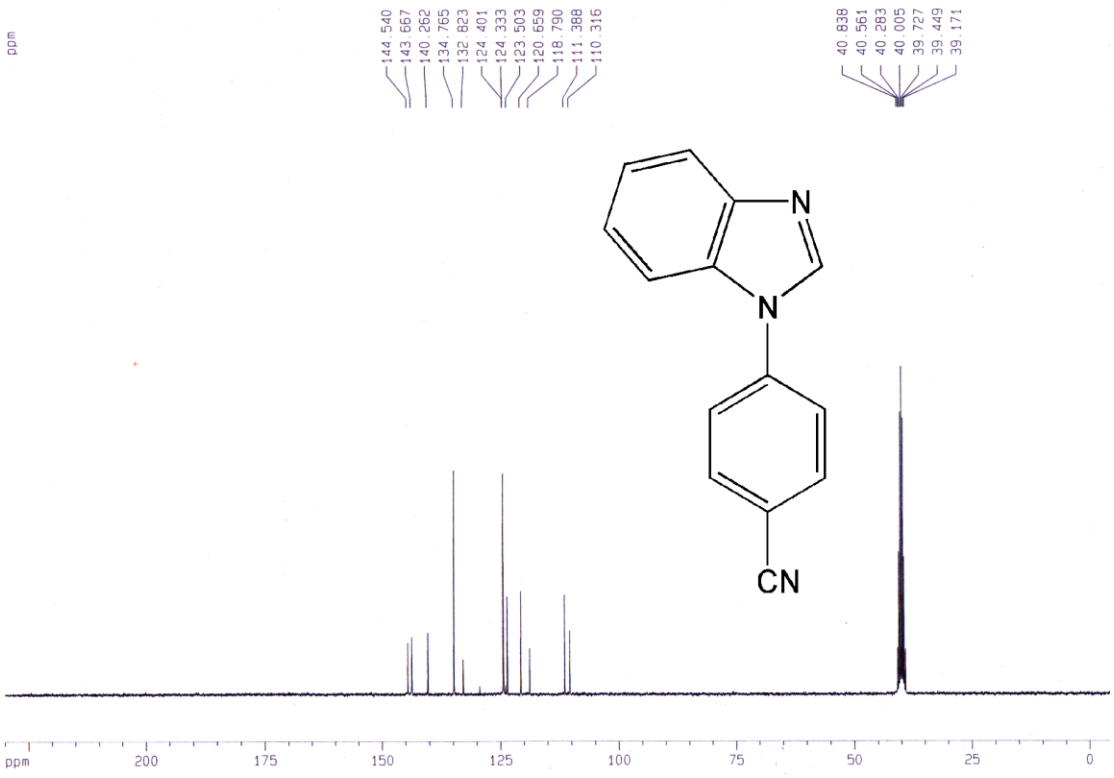

benzimidazole-*o*-nitrobenzene (Table 2, entry 2j): $^{1}$H–NMR (300 MHz, $CDCl_3$): δ (ppm): 8.07 (d, *J* = 1.42 Hz, 1H), 7.98 (s, 1H), 7.84-7.81 (m, 1H), 7.75 (m, 1H), 7.62 (m, 1H), 7.52-7.49 (m, 1H), 7.29-7.24 (m, 2H), 7.11-7.09 (m, 1H), $^{13}$C–NMR (75 MHz, $CDCl_3$): δ (ppm): 145.8, 143.34, 142.51, 134.43, 134.37, 130.1, 129.76, 129.32, 125.94, 124.23, 123.18, 120.7, 109.53; Anal. Calcd. for $C_{13}H_9N_3O_2$: C, 65.27%; H, 3.79%; N, 17.56. Found: C, 65.29%; H, 3.77%, N, 17.55.

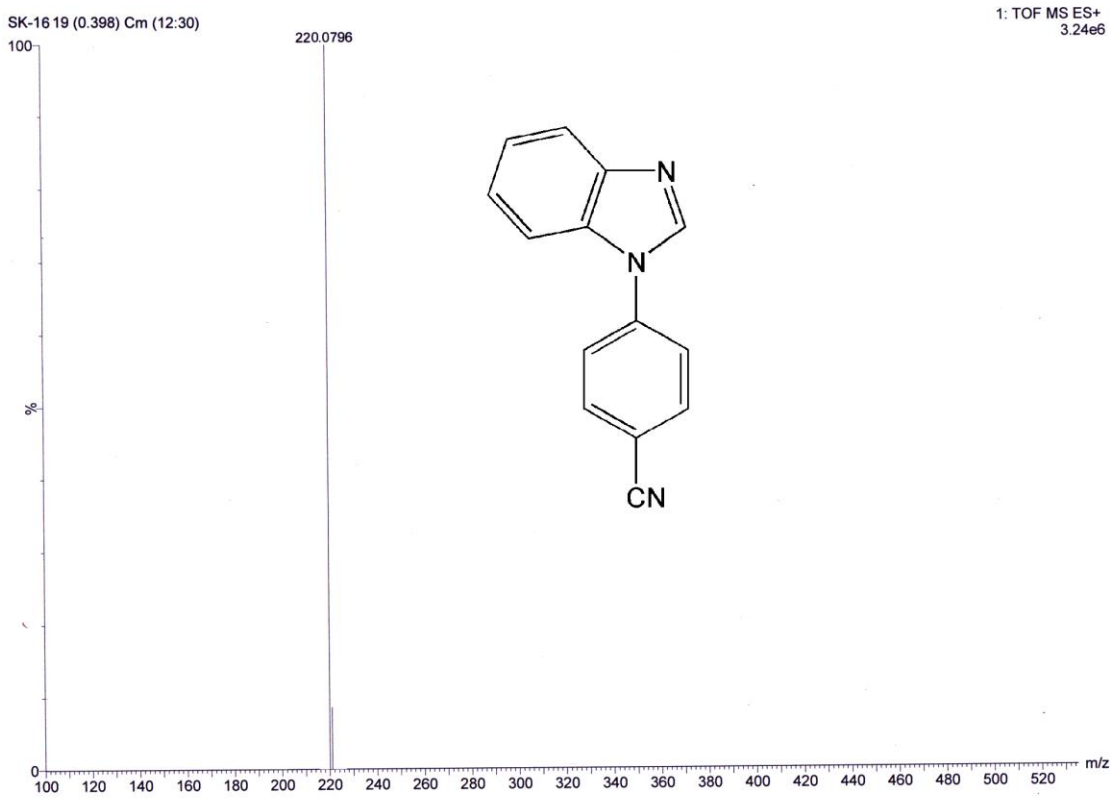

ppm
8.07338
8.06864
7.98144
7.84203
7.83828
7.81413
7.75021
7.62890
7.51972
7.51539
7.49374
7.29588
7.29136
7.27111
7.26494
7.24442
7.24019
7.11350
7.10988
7.09089
7.08632
N
N
NO2
Integral
0.9859
1.0614
1.0855
1.1004
1.0649
1.0486
2.2308
1.0000
ppm
9
8
7
6
5
4
3
2
1


ppm
145.805
143.338
142.511
134.433
134.374
130.103
129.763
129.319
125.943
124.218
123.177
120.704
109.535
77.578
77.154
76.729
N
N
NO2
ppm
180
160
140
120
100
80
60
40
20
0

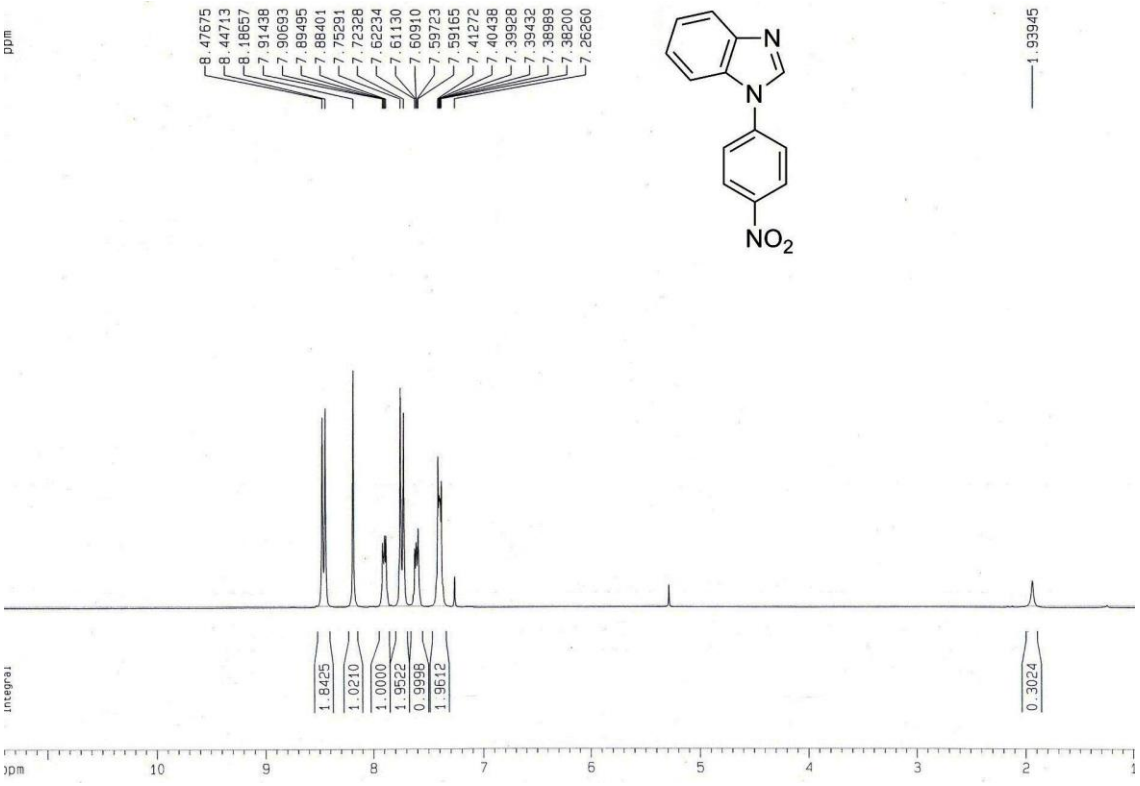
benzimidazole-*p*-benzonitrile (Table 2, entry 2k): $^{1}$H–NMR (300 MHz, DMSO-$d_6$): δ (ppm): 8.68 (s, 1H), 8.09 (d, *J* = 8.62 Hz, 2H), 7.93 (d, *J* = 8.61 Hz, 2H), 7.81-7.78 (m, 1H), 7.72-7.69 (m, 1H), 7.38-7.32 (m, 2H); $^{13}$C–NMR (75 MHz, DMSO-$d_6$): δ (ppm): 144.54, 143.67, 140.26, 134.76, 132.82, 124.40, 124.33, 123.50, 120.66, 118.79, 111.39, 110.32; HRMS (ESI): calcd. for $[M+H]^+$ ($C_{14}H_{10}N_3$) requires m/z 220.0875, found 220.0876; Anal. Calcd. for $C_{14}H_9N_3$: C, 76.70%; H, 4.14%; N, 19.17. Found: C, 76.73%; H, 4.16%, N, 19.15.

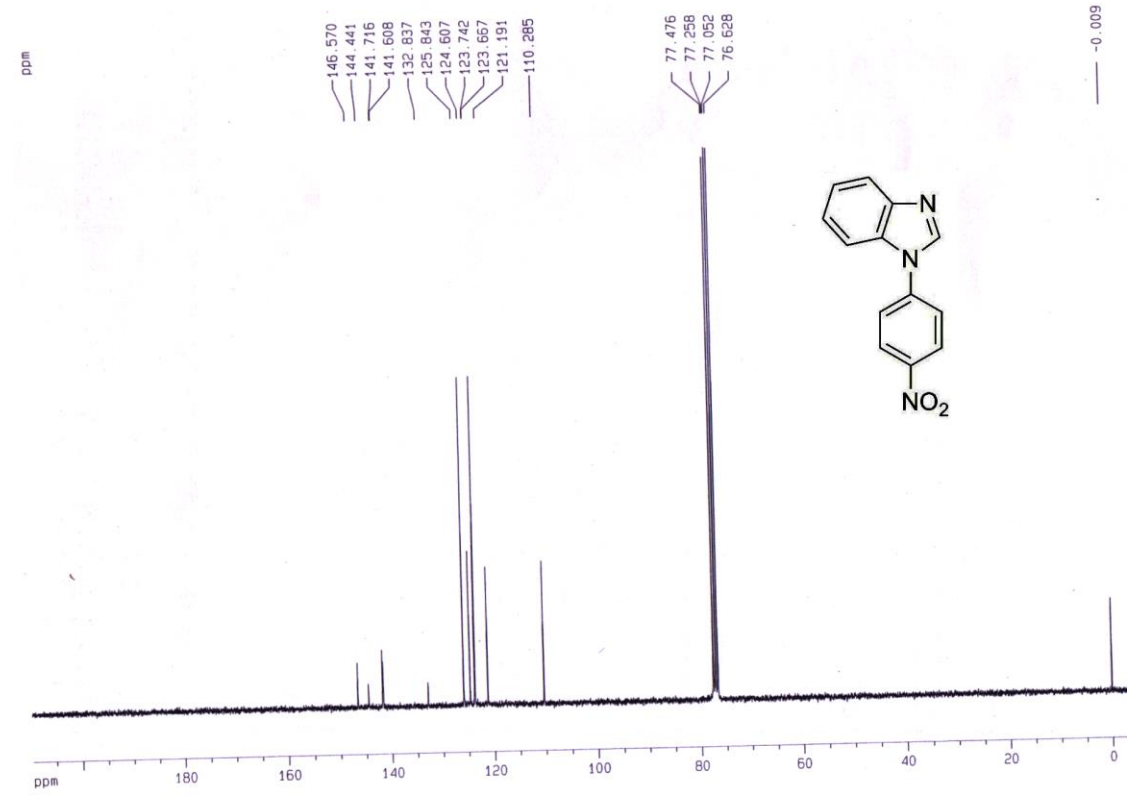


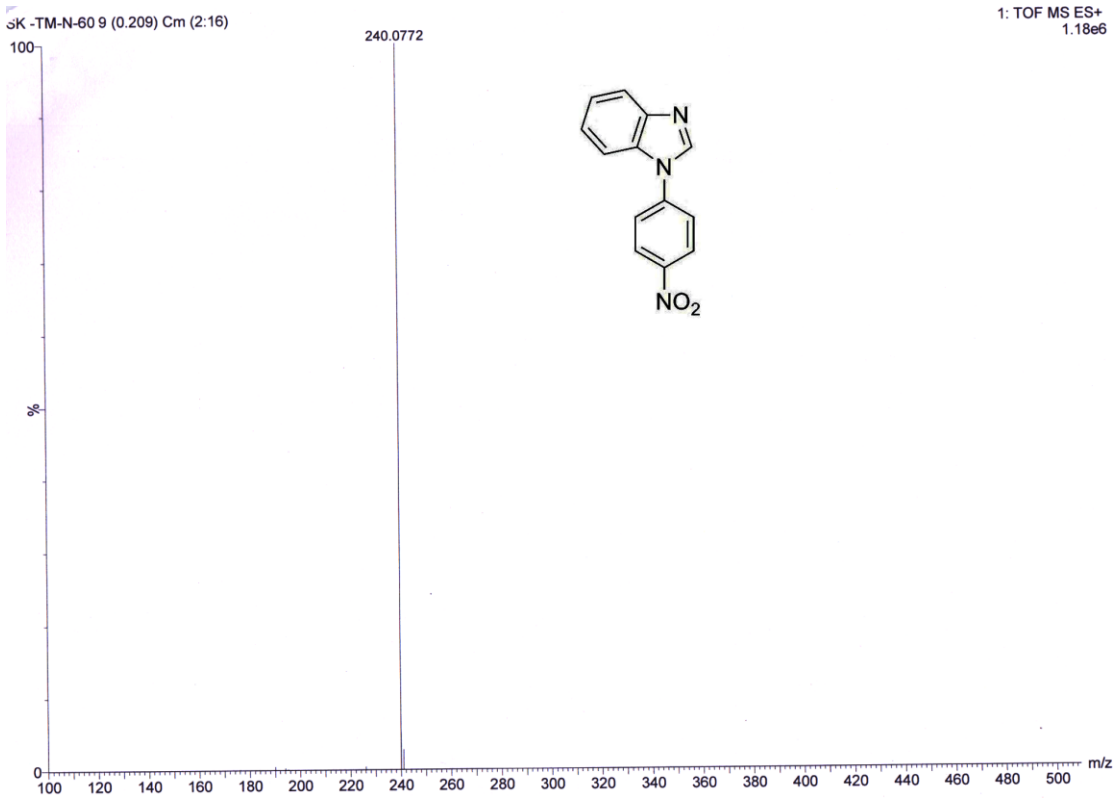

ppm
144.540
143.667
140.262
134.765
132.823
124.401
124.333
123.503
120.659
118.790
111.388
110.316
40.838
40.561
40.283
40.005
39.727
39.449
39.171
N
N
CN
ppm
200
175
150
125
100
75
50
25
0



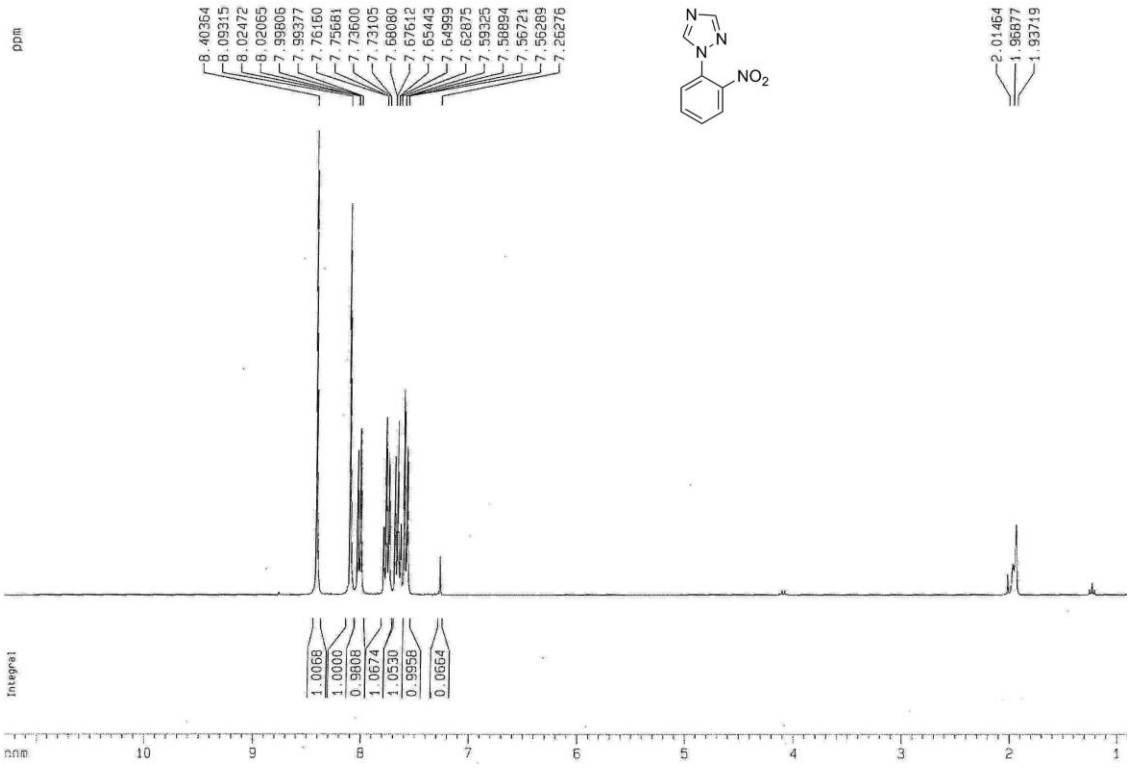

benzimidazole-*p*-nitrobenzene (Table 2, entry 2l): $^{1}$H–NMR (300 MHz, $CDCl_3$): δ (ppm): 8.46 (d, *J* = 8.89 Hz, 2H), 8.19 (s, 1H), 7.91-7.88 (m, 1H), 7.74 (d, *J* = 8.89 Hz, 2H), 7.62-7.59 (s, 1H), 7.41-7.38 (m, 2H); $^{13}$C–NMR (75 MHz, $CDCl_3$): δ (ppm): 146.57, 144.44, 141.72, 141.61, 132.84, 125.84, 124.61, 123.74, 123.67, 121.19, 110.28; HRMS (ESI): calcd. for $[M+H]^+$ ($C_{13}H_{10}N_3O_2$) requires m/z 240.0773, found 240.0772; Anal. Calcd. for $C_{13}H_9N_3O_2$: C, 65.27%; H, 3.79%; N, 17.56. Found: C, 65.25%; H, 3.78%, N, 17.56.

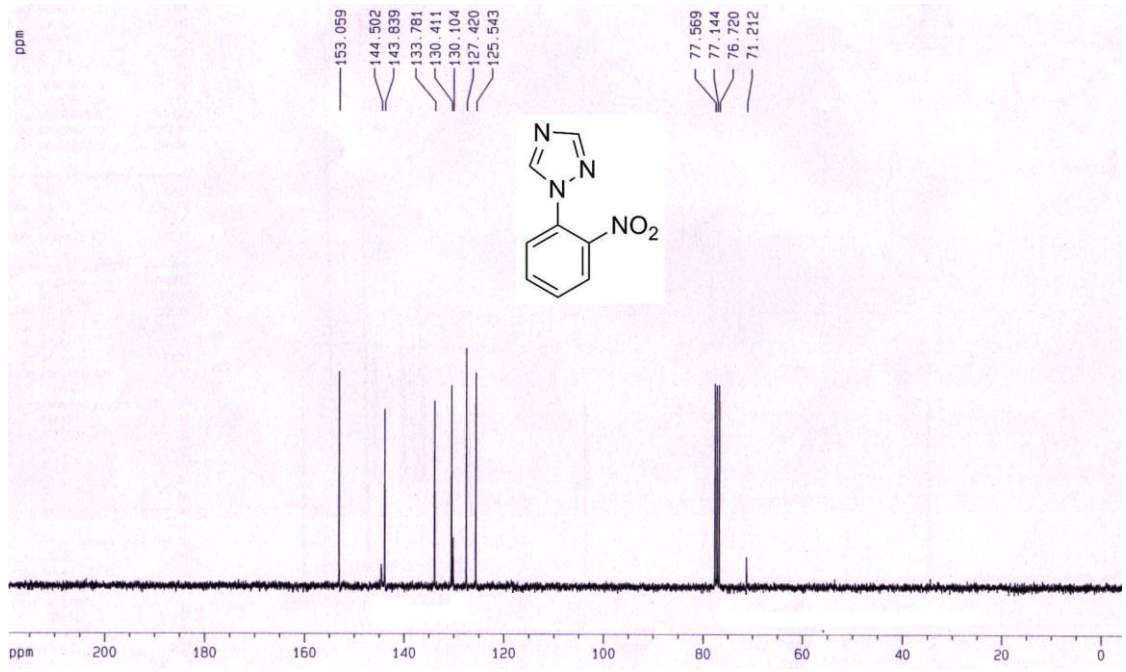

ppm
8.47675
8.44713
8.18657
7.91438
7.90693
7.89495
7.88401
7.75291
7.72328
7.62234
7.61130
7.60910
7.59723
7.59165
7.41272
7.40438
7.39928
7.39432
7.38989
7.38200
7.26260
1.93945
N
N
NO2
Integral
1.8425
1.0210
1.0000
1.9522
0.9998
1.9612
0.3024
ppm
10
9
8
7
6
5
4
3
2

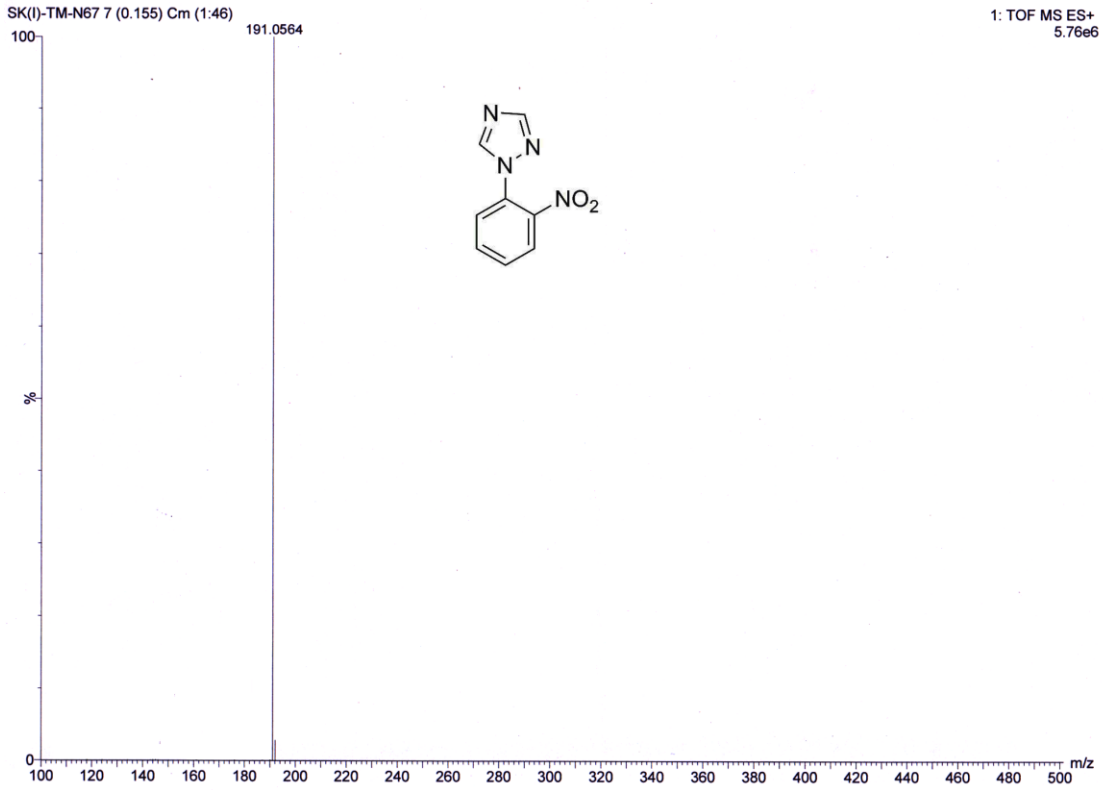

ppm
146.570
144.441
141.716
141.608
132.837
125.843
124.607
123.742
123.667
121.191
110.285
77.476
77.258
77.052
76.628
-0.009
N
N
NO2
ppm
180
160
140
120
100
80
60
40
20
0



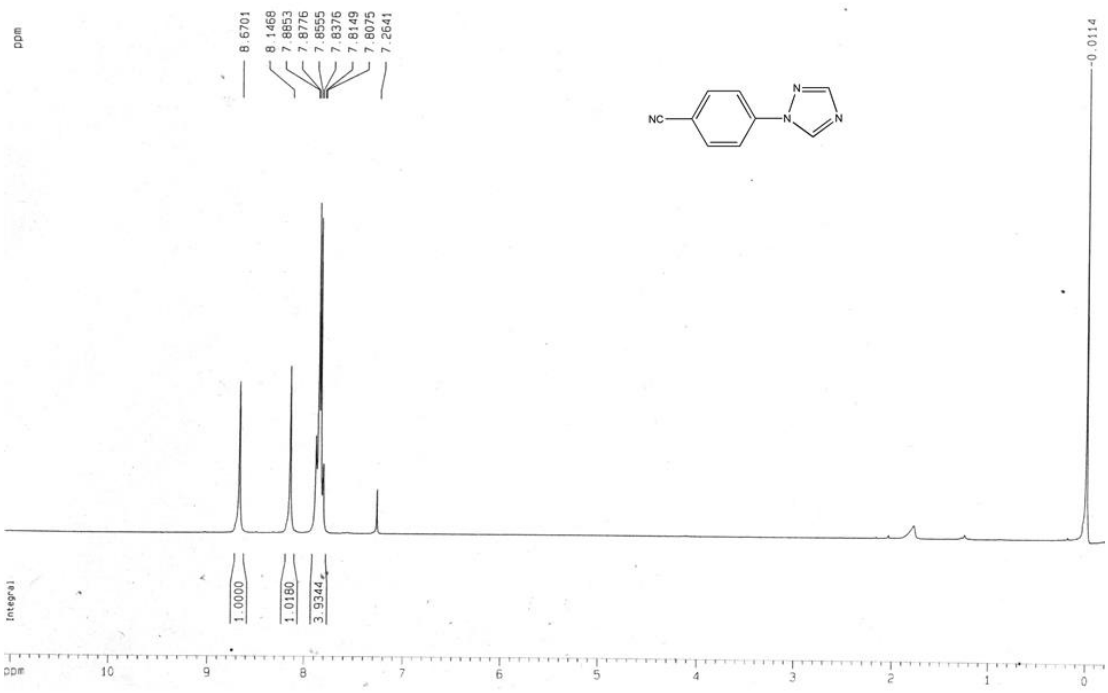

1,2,4-triazole-*o*-nitrobenzene (Table 2, entry 2m): $^{1}$H–NMR (300 MHz, $CDCl_3$): δ (ppm): 8.4 (s, 1H), 8.09 (s, 1H), 8.02-7.99 (m, 1H), 7.76-7.73 (m, 1H), 7.68-7.64 (m, 1H), 7.62-7.56 (m, 1H); $^{13}$C–NMR (75 MHz, $CDCl_3$): δ (ppm): 153.05, 144.5, 143.83, 133.78, 130.41, 130.1, 127.4, 125.5; HRMS (ESI): calcd. for $[M+H]^+$ ($C_8H_7N_4O_2$) requires m/z 191.0569, found 191.0564; Anal. Calcd. for $C_8H_6N_4O_2$: C, 50.53%; H, 3.18%; N, 29.46%. Found: C, 50.55%; H, 3.19%; N, 29.44%.

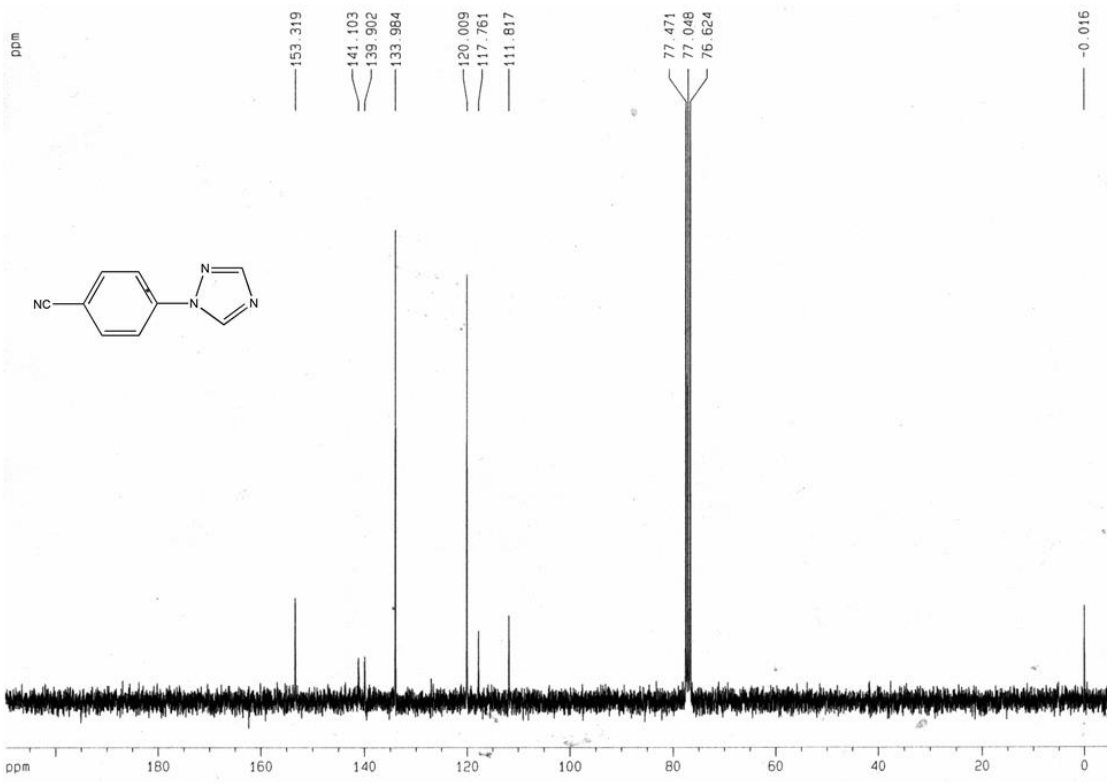

ppm
8.40364
8.09315
8.02472
8.02065
7.99805
7.99377
7.76160
7.75681
7.73600
7.73105
7.68080
7.67612
7.65443
7.64999
7.62875
7.59325
7.58894
7.56721
7.56289
7.26276
2.01464
1.96877
1.93719
Integral
1.0068
1.0000
0.9808
1.0674
1.0530
0.9956
0.0664
ppm
10
9
8
7
6
5
4
3
2
1

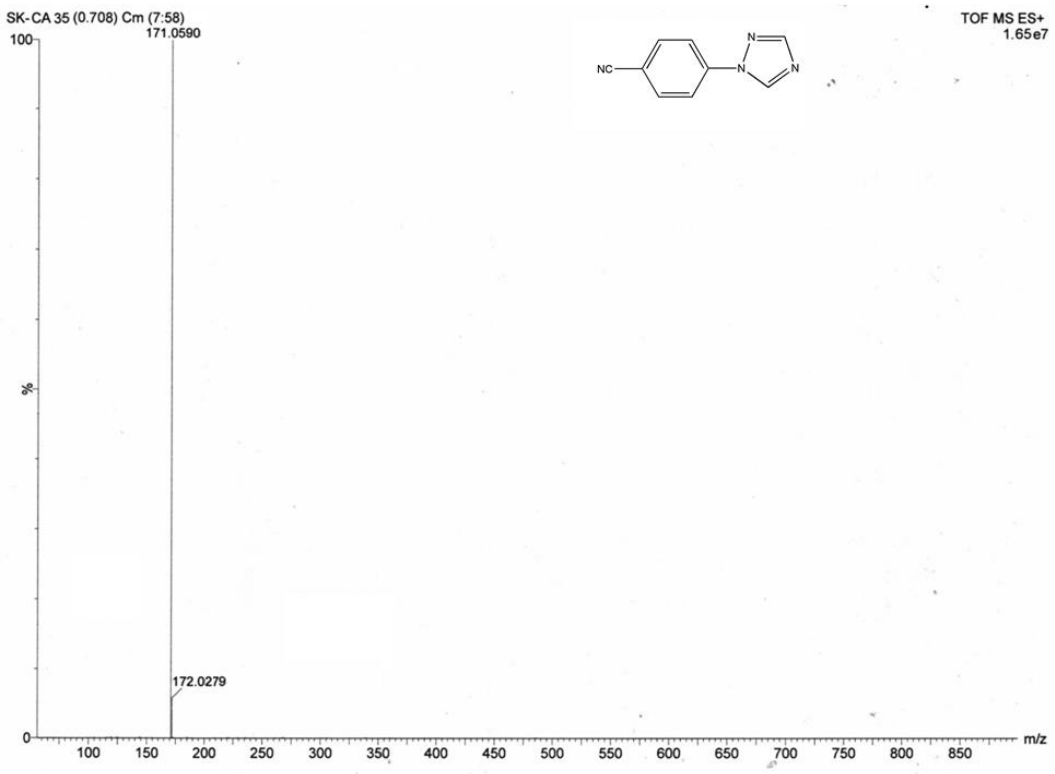

ppm
153.059
144.502
143.839
133.781
130.411
130.104
127.420
125.543
77.569
77.144
76.720
71.212
ppm
200
180
160
140
120
100
80
60
40
20
0



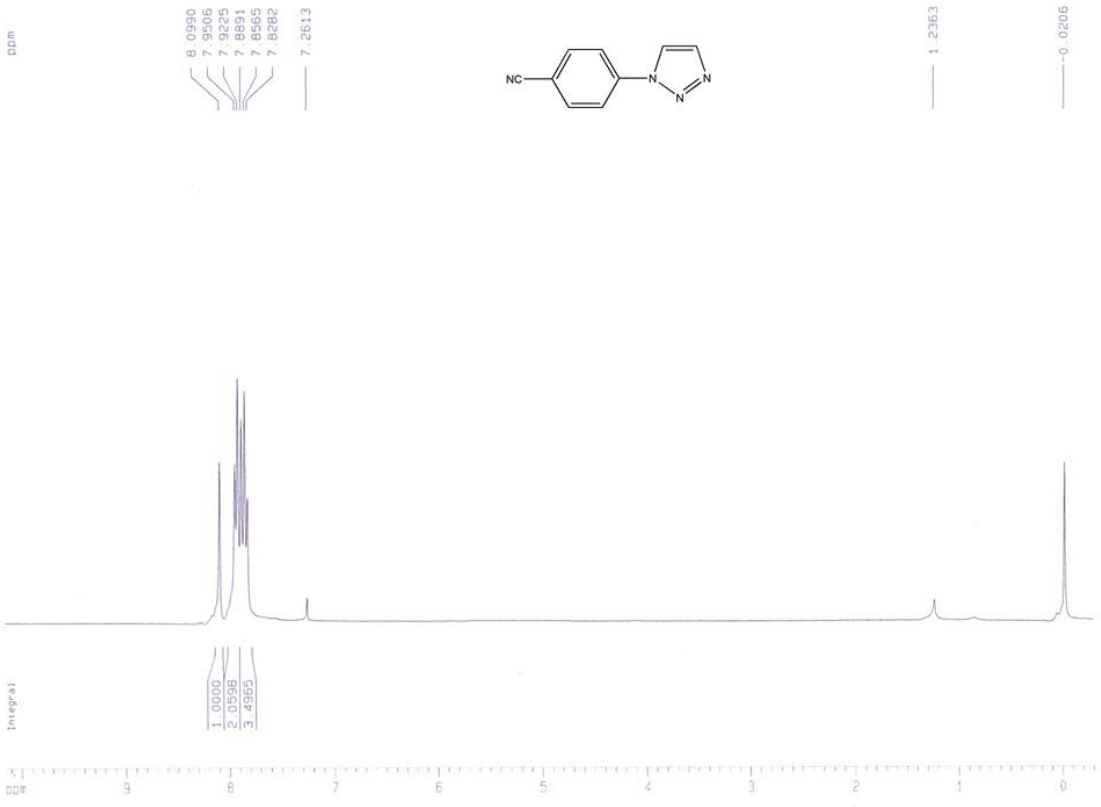

1,2,4-triazole-*p*-benzonitrile (Table 2, entry 2n): $^{1}$H–NMR (300 MHz, $CDCl_3$): δ (ppm): 8.67 (s, 1H), 8.15 (s, 1H), 7.88-7.81 (m, 4H); $^{13}$C–NMR (75 MHz, $CDCl_3$): δ (ppm): 153.32, 141.10, 139.90, 133.98, 120.01, 117.76, 111.82; HRMS (ESI): calcd. for $[M+H]^+$ ($C_{14}H_{10}N_3$) requires m/z 171.0626, found 171.0590; Anal. Calcd. for $C_9H_6N_4$: C, 63.52%; H, 3.55%; N, 32.92. Found: C, 63.63%; H, 3.61%, N, 32.95.

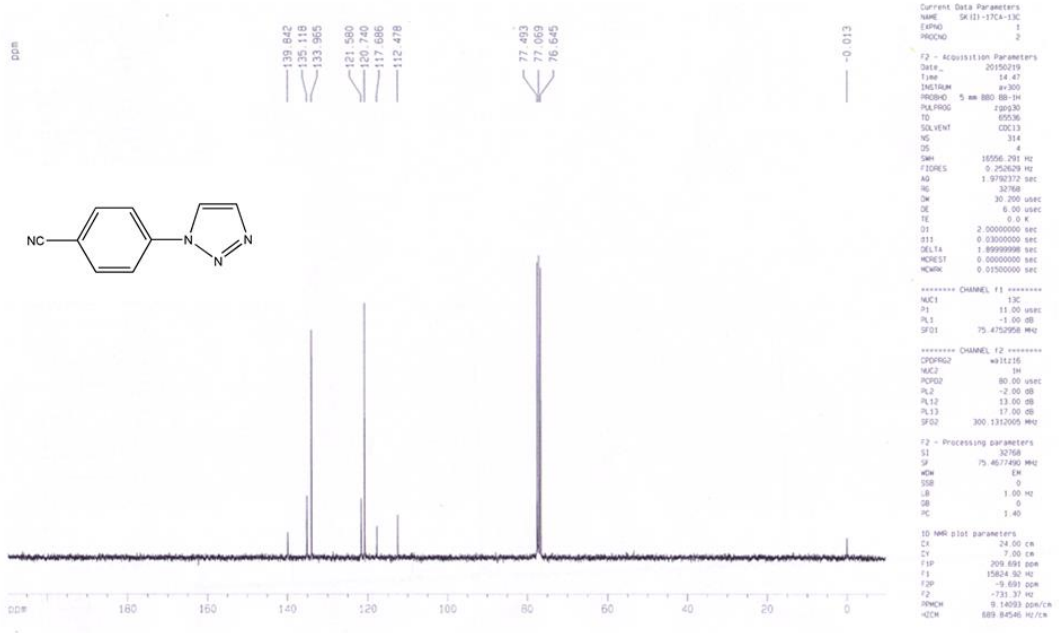

ppm
8.6701
8.1468
7.8853
7.8776
7.8555
7.8376
7.8149
7.8075
7.2641
-0.0114
NC
N
N
N
Integral
1.0000
1.0180
3.9344
ppm
10
9
8
7
6
5
4
3
2
1
0


ppm
153.319
141.103
139.902
133.984
120.009
117.761
111.817
77.471
77.048
76.624
-0.016
NC
N
N
N
ppm
180
160
140
120
100
80
60
40
20
0




1,2,3-triazole-*p*-benzonitrile (Table 2, entry 2o): $^{1}$H–NMR (300 MHz, $CDCl_3$): δ (ppm): 8.09 (s, 1H), 7.95-7.83 (m, 5H); $^{13}$C–NMR (75 MHz, $CDCl_3$): δ (ppm): 139.84, 135.12, 133.97, 121.58, 120.74, 117.69, 112.48; HRMS (ESI): calcd. for $[M+H]^+$ ($C_{14}H_{10}N_3$) requires m/z 171.0626, found 171.0591; Anal. Calcd. for $C_9H_6N_4$: C, 63.52%; H, 3.55%; N, 32.92. Found: C, 63.49%; H, 3.50%, N, 32.85.





Current Data Parameters
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EXPNO 1
PROCNO 2

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TD 65536
SOLVENT CDCl3
NS 314
DS 4
SWH 16556.291 Hz
FIDRES 0.252629 Hz
AQ 1.9782372 sec
RG 32768
DW 30.200 usec
DE 6.00 usec
TE 0.0 K
D1 2.00000000 sec
D11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 11.00 usec
PL1 -1.00 dB
SFO1 75.4752958 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 13.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
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SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
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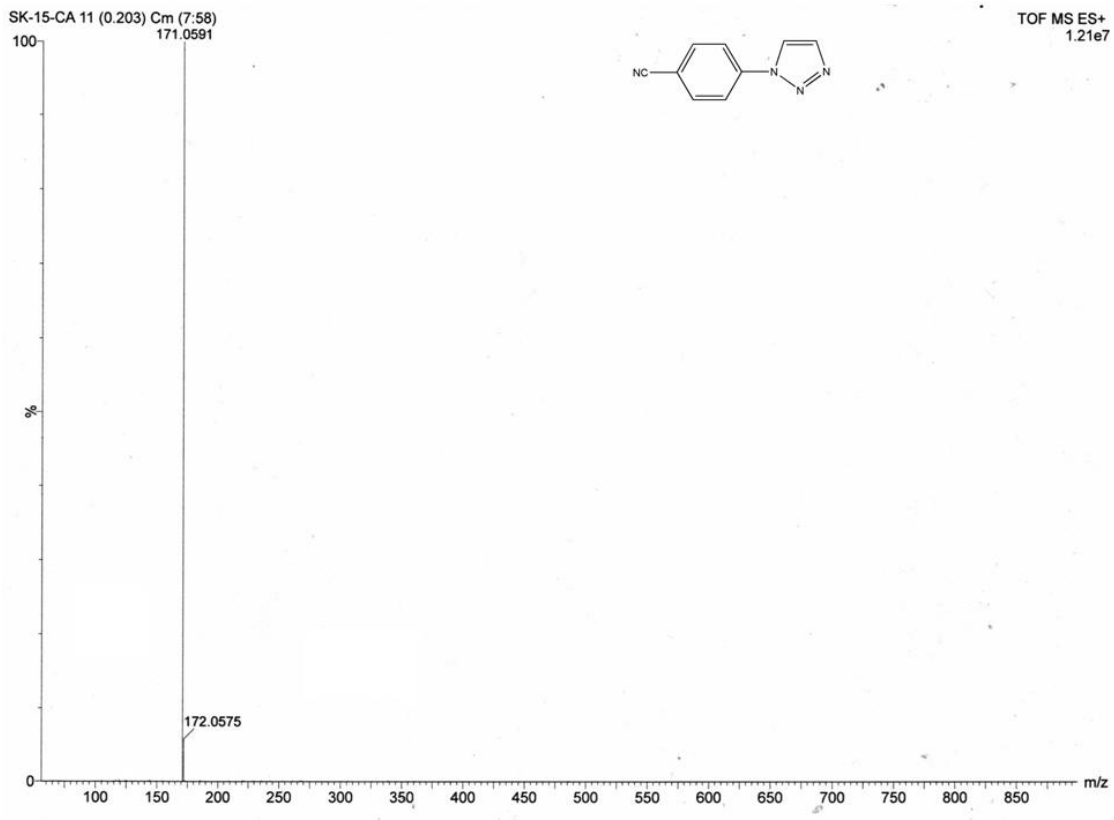
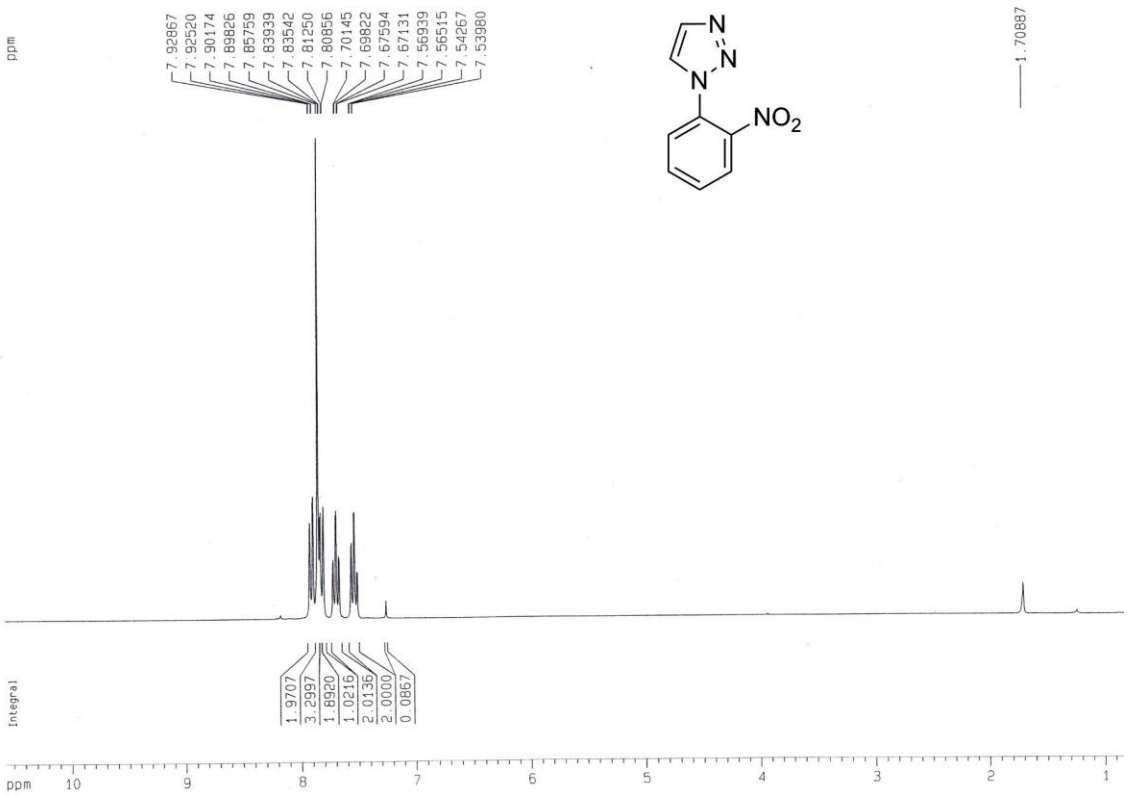
CY 7.00 cm
F1P 209.691 ppm
F1 15824.92 Hz
F2P -9.691 ppm
F2 -731.37 Hz
PPMCM 9.14093 ppm/cm
HZCM 689.84546 Hz/cm




1,2,3-triazole-*o*-nitrobenzene (Table 2, entry 2p): $^{1}$H–NMR (300 MHz, $CDCl_3$): δ (ppm): 7.93-7.90 (m, 1H), 7.89-7.81 (m, 3H), 7.70-7.67 (m, 1H), 7.57-7.54 (m, 1H); $^{13}$C–NMR (75 MHz, $CDCl_3$): δ (ppm): 153.06, 144.5, 143.84, 133.78, 130.41, 130.10, 127.42, 125.54; HRMS (ESI): calcd. for $[M+H]^+$ ($C_8H_7N_4O_2$) requires m/z 191.0569, found 191.0569; Anal. Calcd. for $C_8H_6N_4O_2$: C, 50.53%; H, 3.18%; N, 29.46%. Found: C, 50.51%; H, 3.19%; N, 29.43%.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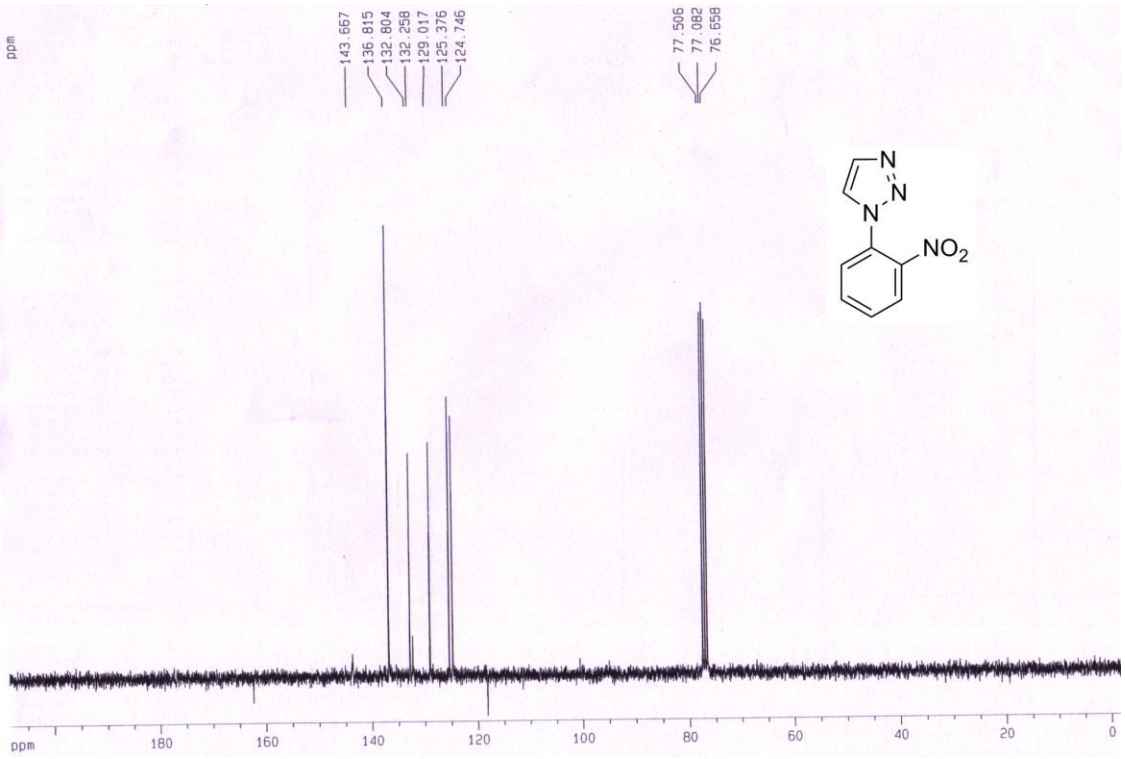
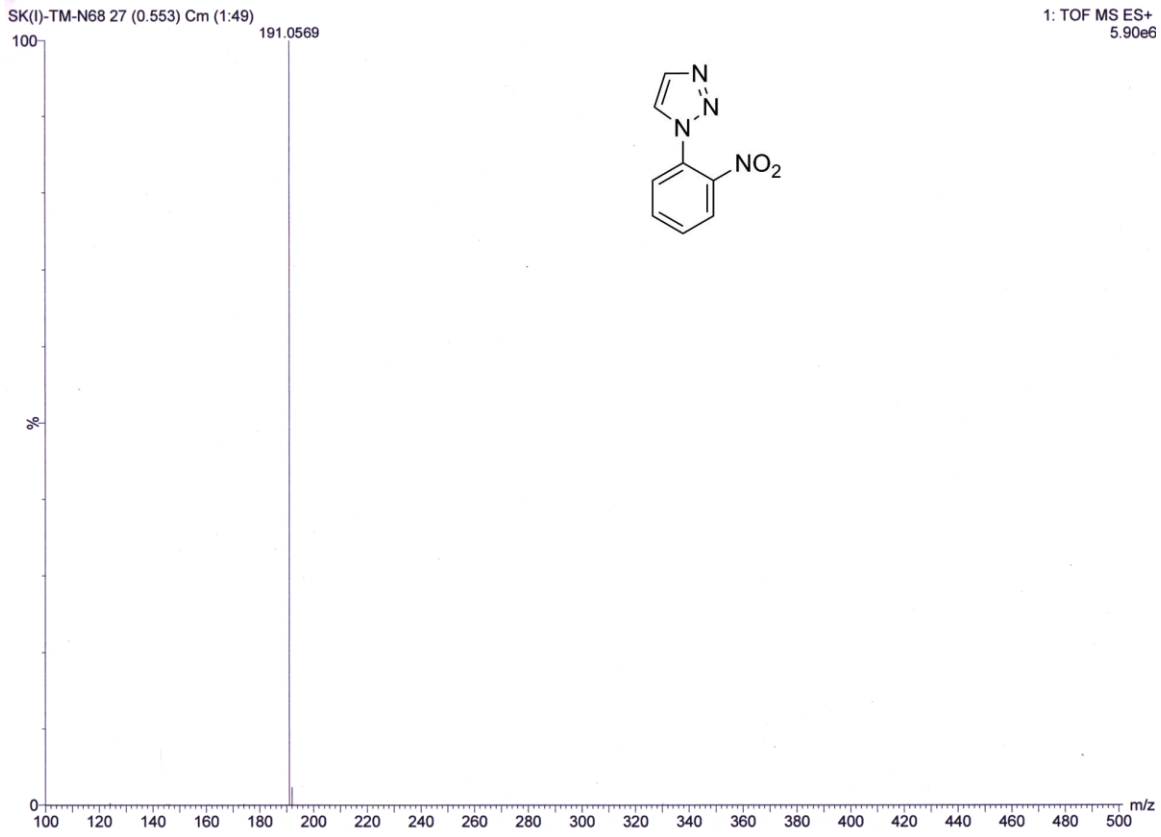
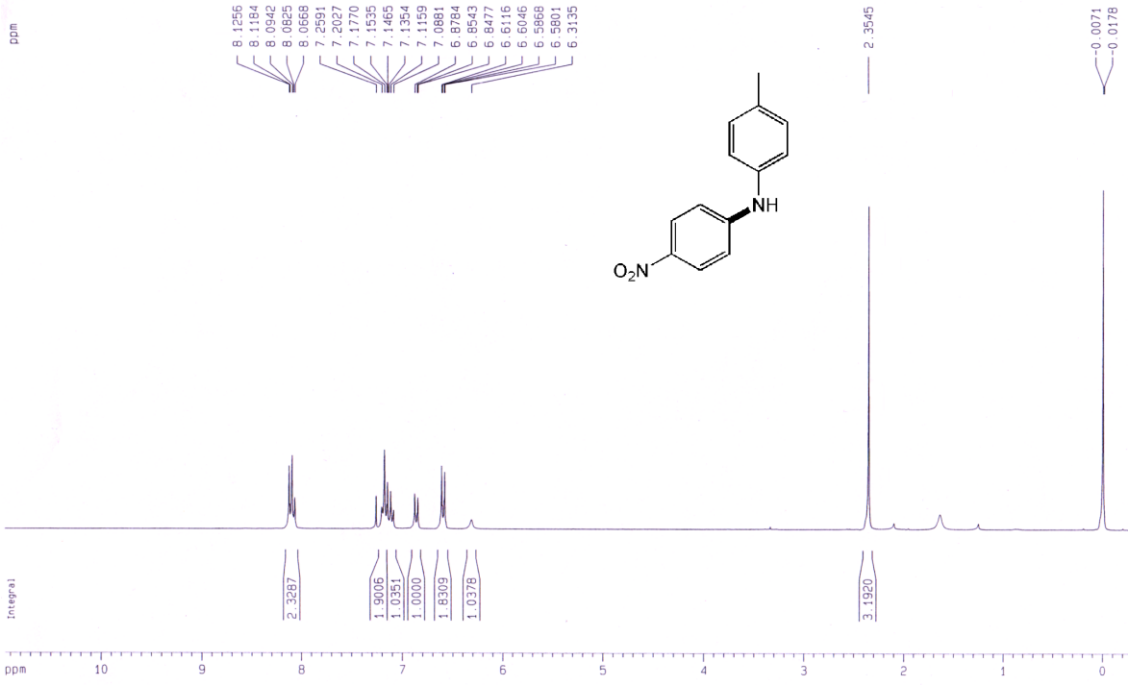
7.92520
7.90174
7.89826
7.85759
7.83939
7.83542
7.81250
7.80856
7.70145
7.69822
7.67594
7.67131
7.56939
7.56515
7.54267
7.53980
1.70887
N
N
N
NO2
Integral
1.9707
3.2997
1.8920
1.0216
2.0136
2.0000
0.0867
ppm 10 9 8 7 6 5 4 3 2 1


ppm
143.667
136.815
132.804
132.258
129.017
125.376
124.746
77.506
77.082
76.658
N
N
N
NO2
ppm 180 160 140 120 100 80 60 40 20 0




N-(4-nitrobenzene)-4-methylaniline (Table 2, entry 2q): $^{1}$H–NMR (300 MHz, $CDCl_3$): δ (ppm): 8.13-8.07 (m, 2H), 7.20-7.09 (m, 3H), 6.88-6.85 (m, 1H), 6.61-6.58 (m, 2H), 6.31 (s, 1H), 2.35 (s, 3H); $^{13}$C–NMR (75 MHz, $CDCl_3$): δ (ppm): 150.88, 139.39, 134.78, 130.28, 126.25, 126.11, 122.66, 113.20, 20.92; HRMS (ESI): calcd. for $[M+H]^+$ ($C_{13}H_{13}N_2O_2$) requires m/z 229.0898, found 229.0977; Anal. Calcd. for $C_{13}H_{12}N_2O_2$: C, 68.41%; H, 5.30%; N, 12.27%. Found: C, 68.51%; H, 5.39%; N, 12.29%.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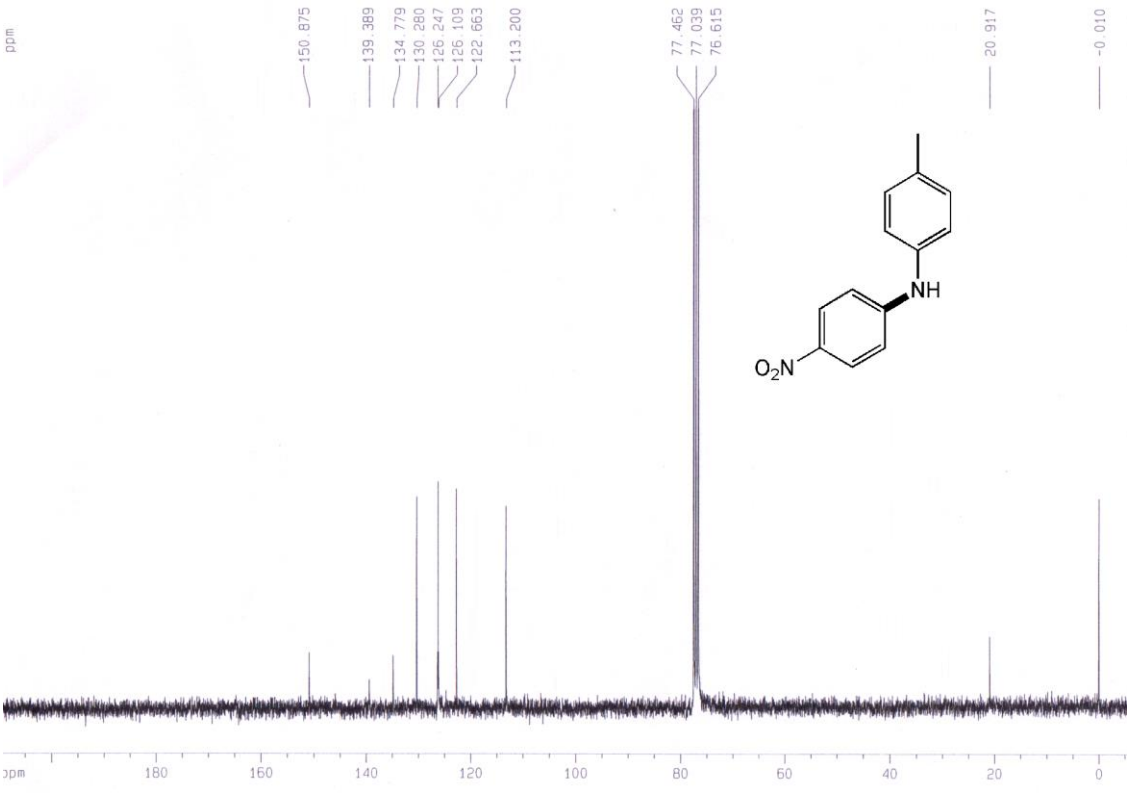
8.1256
8.1184
8.0942
8.0825
8.0668
7.2591
7.2027
7.1770
7.1535
7.1465
7.1354
7.1159
7.0881
6.8784
6.8543
6.8477
6.6116
6.6046
6.5968
6.5801
6.3135
2.3545
-0.0071
-0.0178
NH
O2N
Integral
2.3287
1.9006
1.0351
1.0000
1.8309
1.0378
3.1920
ppm
10
9
8
7
6
5
4
3
2
1
0


ppm
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139.389
134.779
130.280
126.247
126.109
122.663
113.200
77.462
77.039
76.615
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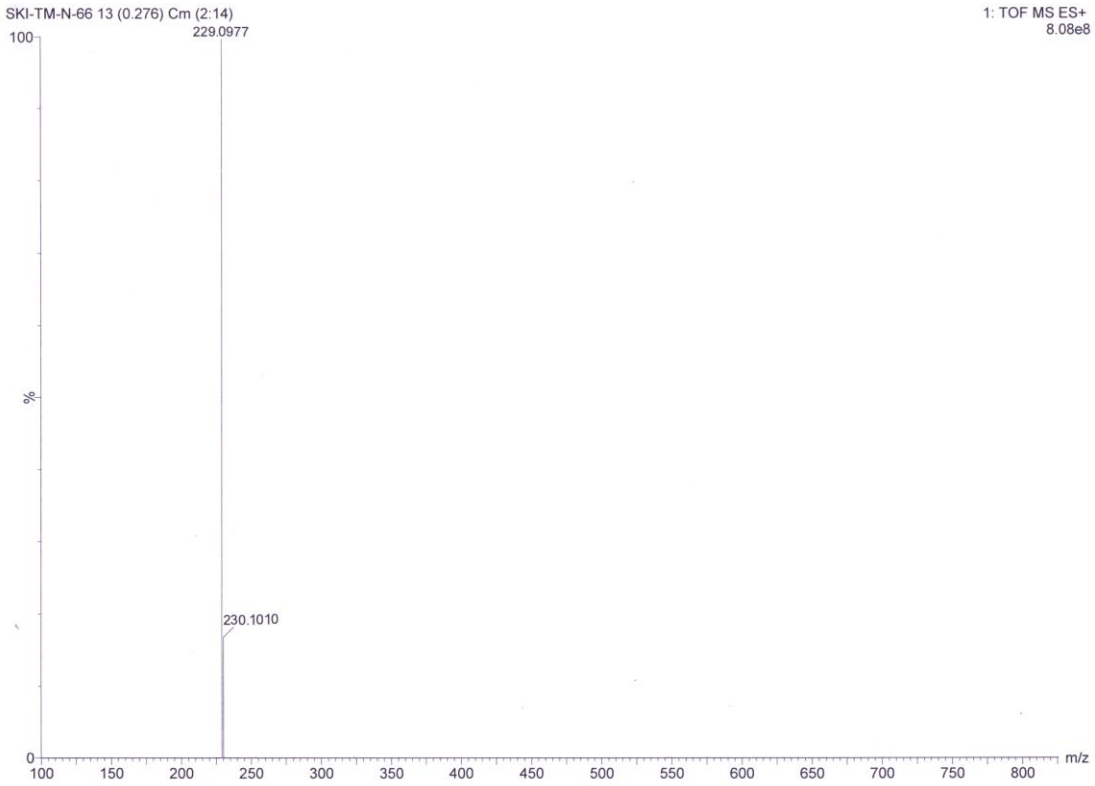
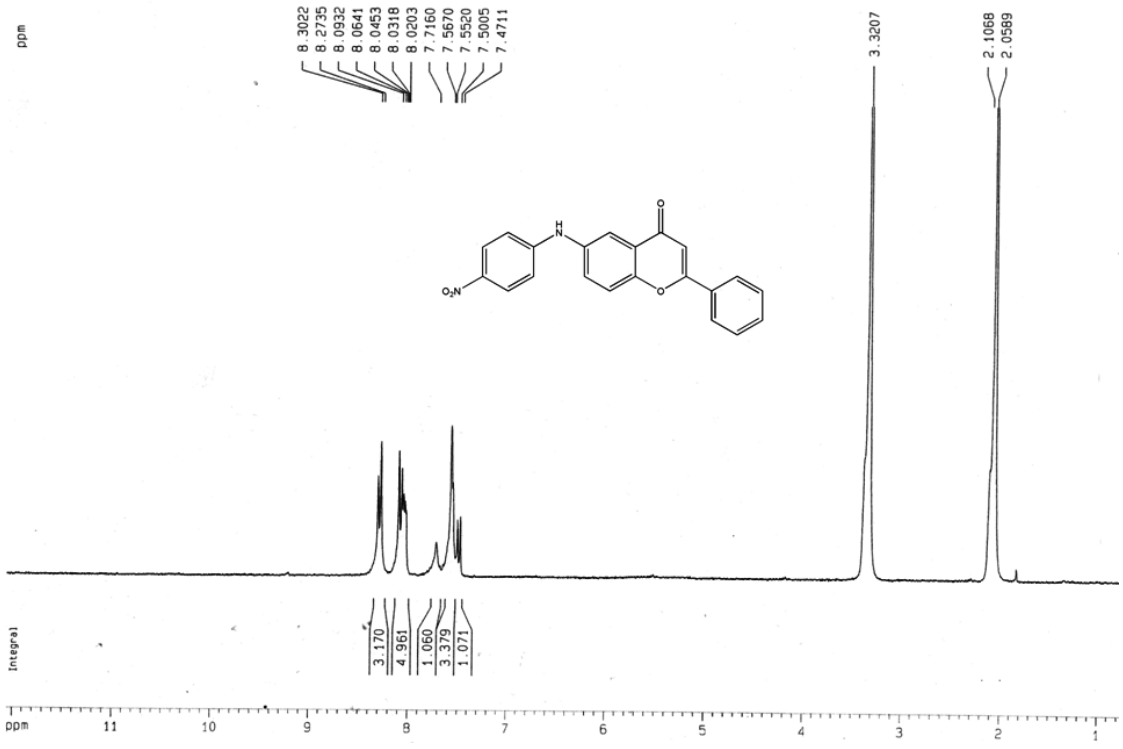
-0.010
NH
O2N
ppm
180
160
140
120
100
80
60
40
20
0




N-(4-nitrobenzene)-6-aminoflavone (Table 2, entry 2r): $^{1}$H–NMR (300 MHz, DMSO-$d_6$): δ (ppm): 8.28 (d, *J* = 8.6Hz, 3H), 8.09-8.02 (m, 5H), 7.72 (s, 1H), 7.56 (d, *J* = 4.5Hz, 3H), 7.48 (d, *J* = 8.8Hz, 1H); $^{13}$C–NMR (75 MHz, $CDCl_3$): δ (ppm): 179.33, 159.59, 148.60, 146.51, 138.68, 132.52,130.94, 128.59, 128.08, 126.81, 125.10, 124.70, 121.66, 120.38, 118.15, 117.64, 110.39; HRMS (ESI): calcd. for $[M+H]^+$ ($C_{21}H_{15}N_2O_4$) requires m/z 359.0953, found 359.0951; Anal. Calcd. for $C_{21}H_{14}N_2O_4$: C, 70.39%; H, 3.94%; N, 7.82%. Found: C, 70.41%; H, 3.89%; N, 7.89%.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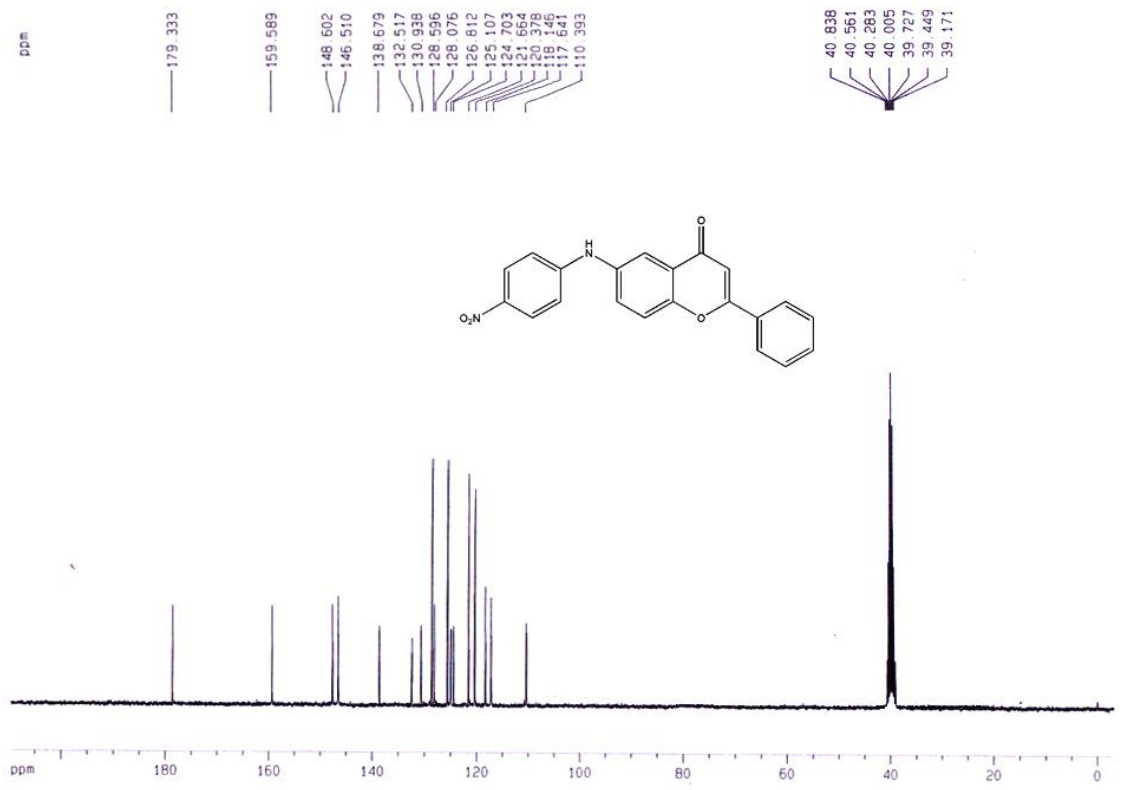
8.2735
8.0932
8.0641
8.0453
8.0318
8.0203
7.7160
7.5670
7.5520
7.5005
7.4711
3.3207
2.1068
2.0589
Integral
3.170
4.961
1.060
3.379
1.071
ppm
11
10
9
8
7
6
5
4
3
2
1


ppm
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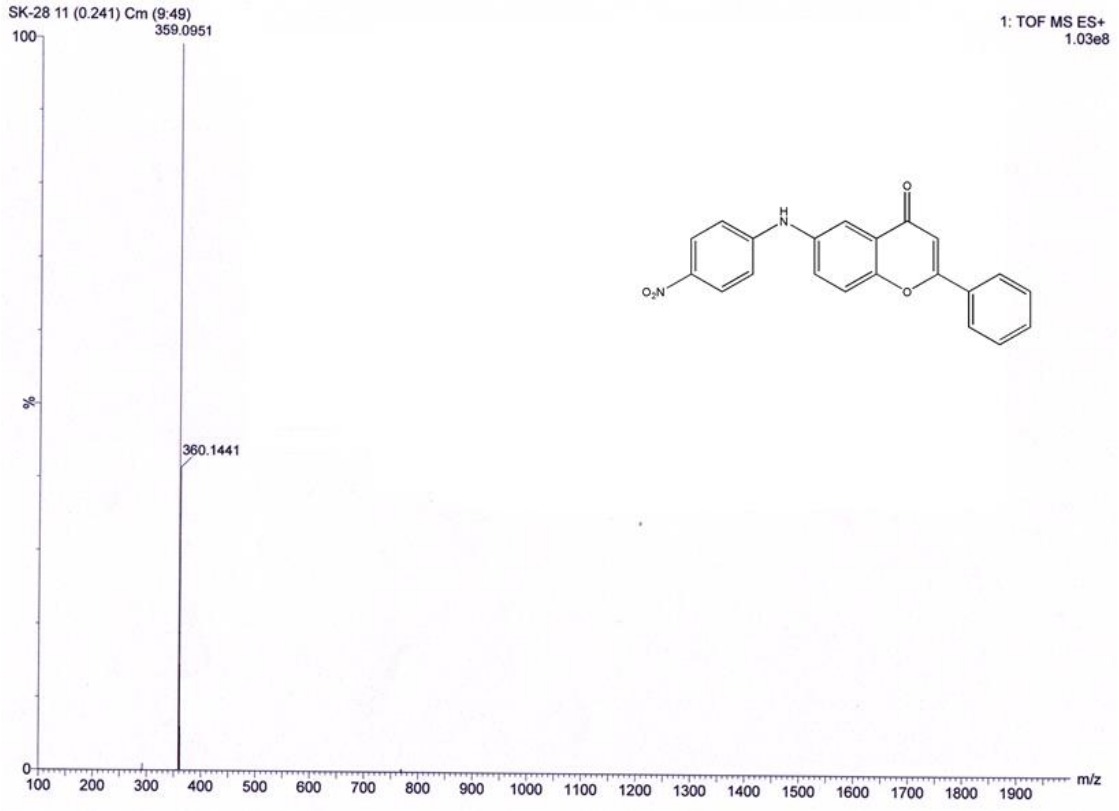
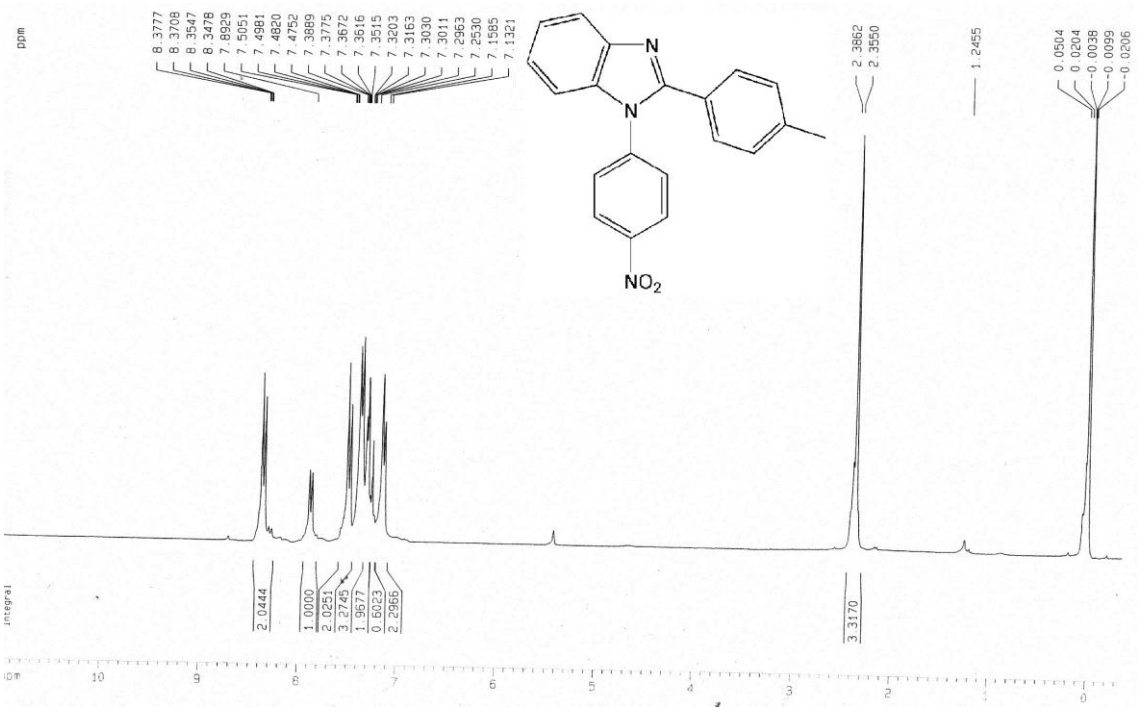
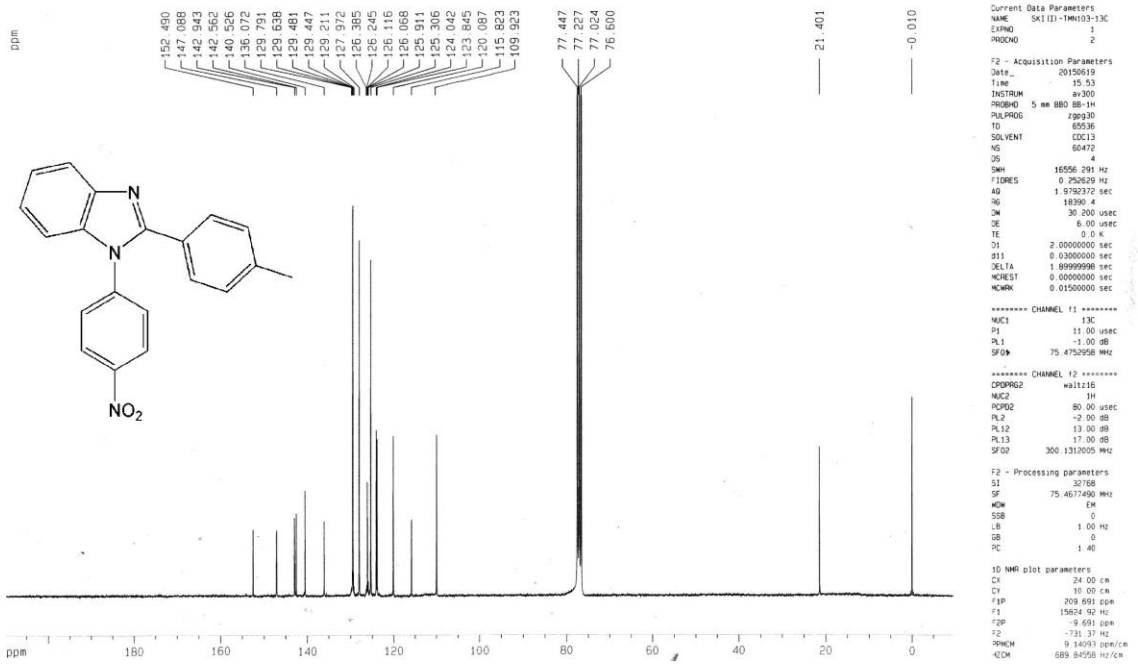
148.602
146.510
138.679
132.517
130.938
128.596
128.076
126.812
125.107
124.703
121.664
120.378
118.146
117.641
110.393
40.838
40.561
40.283
40.005
39.727
39.449
39.171
ppm
180
160
140
120
100
80
60
40
20
0




2-(4-methylphenyl)-benzimidazole-*p*-nitrobenzene (Table 2, entry 2s): $^{1}$H–NMR (300 MHz, $CDCl_3$): δ (ppm): 8.38-8.35 (m, 2H), 7.89 (m, 1H), 7.51-7.48 (m, 2H), 7.39-7.29 (m, 5H), 7.14 (d, *J* = 7.9 Hz, 2H), 2.38 (s, 3H); $^{13}$C–NMR (75 MHz, $CDCl_3$): δ (ppm): 152.49, 147.08, 142.94, 142.56, 140.53, 136.07, 129.79, 129.48, 129.21, 127.97, 126.39, 126.07, 125.91, 125.30, 124.04, 123.85, 120.09, 115.83, 109.92, 21.40; HRMS (ESI): calcd. for $[M+H]^+$ ($C_{20}H_{16}N_3O_4$) requires m/z 330.1164, found 330.1151; Anal. Calcd. for $C_{20}H_{15}N_3O_4$: C, 72.94%; H, 4.59%; N, 12.79%. Found: C, 72.91%; H, 4.64%; N, 12.86%.

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PROCNO                      2

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PULPROG             zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                       60472
DS                           4
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FIDRES              0.252629 Hz
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RG                     18390.4
DW                    30.200 usec
DE                     6.00 usec
TE                        0.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
DELTA              1.89999998 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

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P1                      11.00 usec
PL1                     -1.00 dB
SFO1               75.4752958 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                   80.00 usec
PL2                     -2.00 dB
PL12                    13.00 dB
PL13                    17.00 dB
SFO2              300.1312005 MHz

F2 - Processing parameters
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LB                      1.00 Hz
GB                             0
PC                      1.40

1D NMR plot parameters
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CY                     10.00 cm
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F1                  15824.92 Hz
F2P                   -9.691 ppm
F2                   -731.37 Hz
PPMCM               9.14093 ppm/cm
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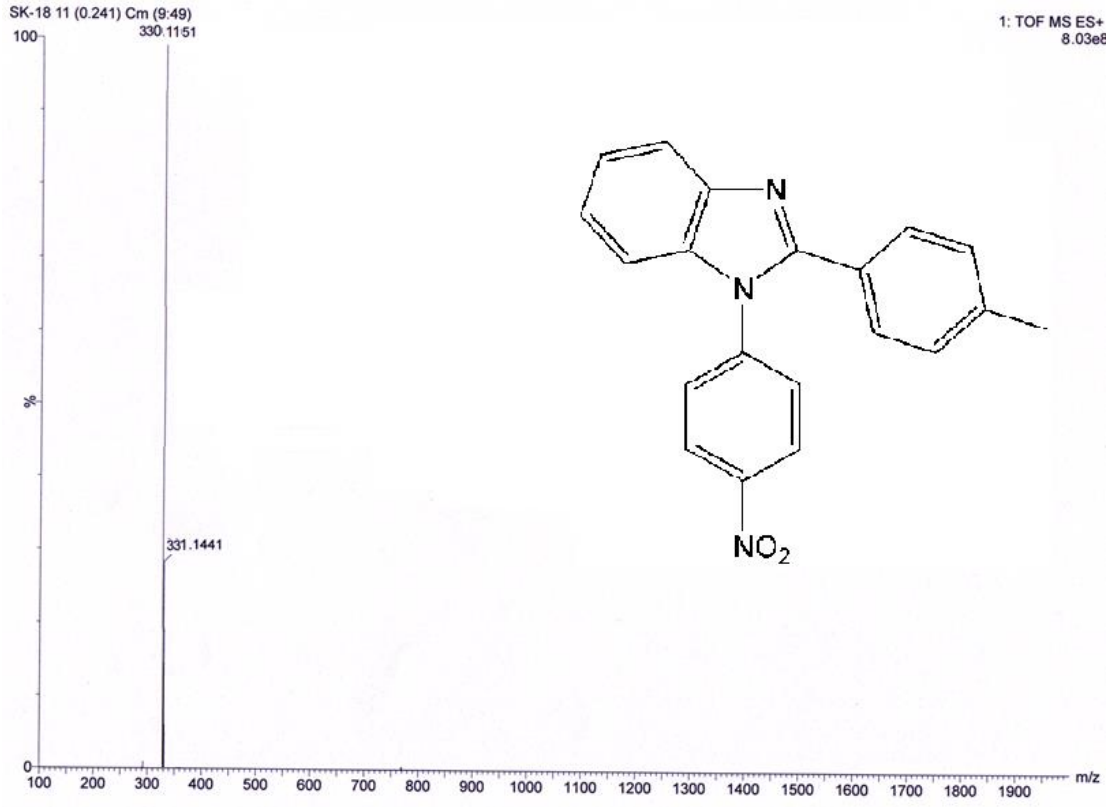
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330.1151
331.1441
%
0
100 200 300 400 500 600 700 800 900 1000 1100 1200 1300 1400 1500 1600 1700 1800 1900
m/z
N
N
NO2