Electronic Supplementary Material (ESI) for RSC Advances.

Preparation and use of combustion-derived Bi_2O_3 for the synthesis of heterocycles with anti-cancer property by Suzuki-coupling reactions

Supplementary Information

Table of contents

The EDX spectrum of SCS-Bi_2O_3 exhibits peaks for Bi and O elements confirming the presence of Bi_2O_3

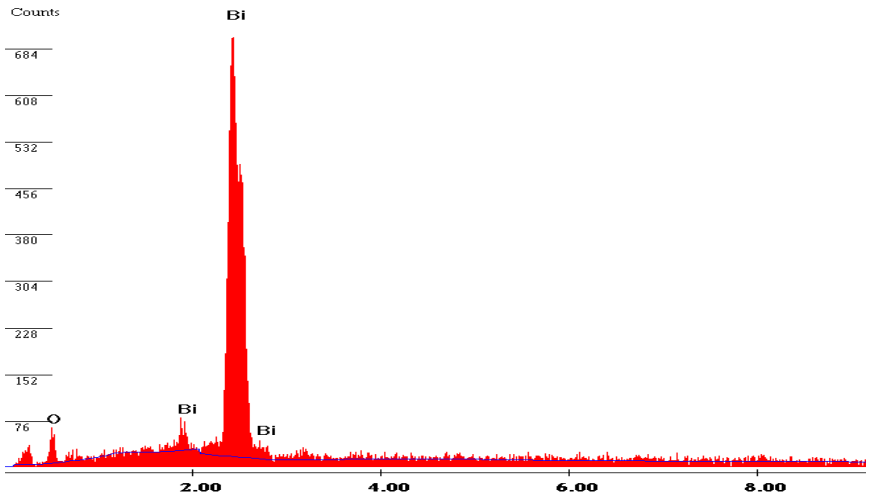


Figure SI-1. Energy dispersive X-ray analysis of SCS-Bi_2O_3

BET nitrogen adsorption-desorption of SCS- Bi_2O_3 is shown in SI Fig.2. The surface area of Bi_2O_3 was found to be of $24 m^2 g^{-1}$ and an average pore size of about 2.86 nm.

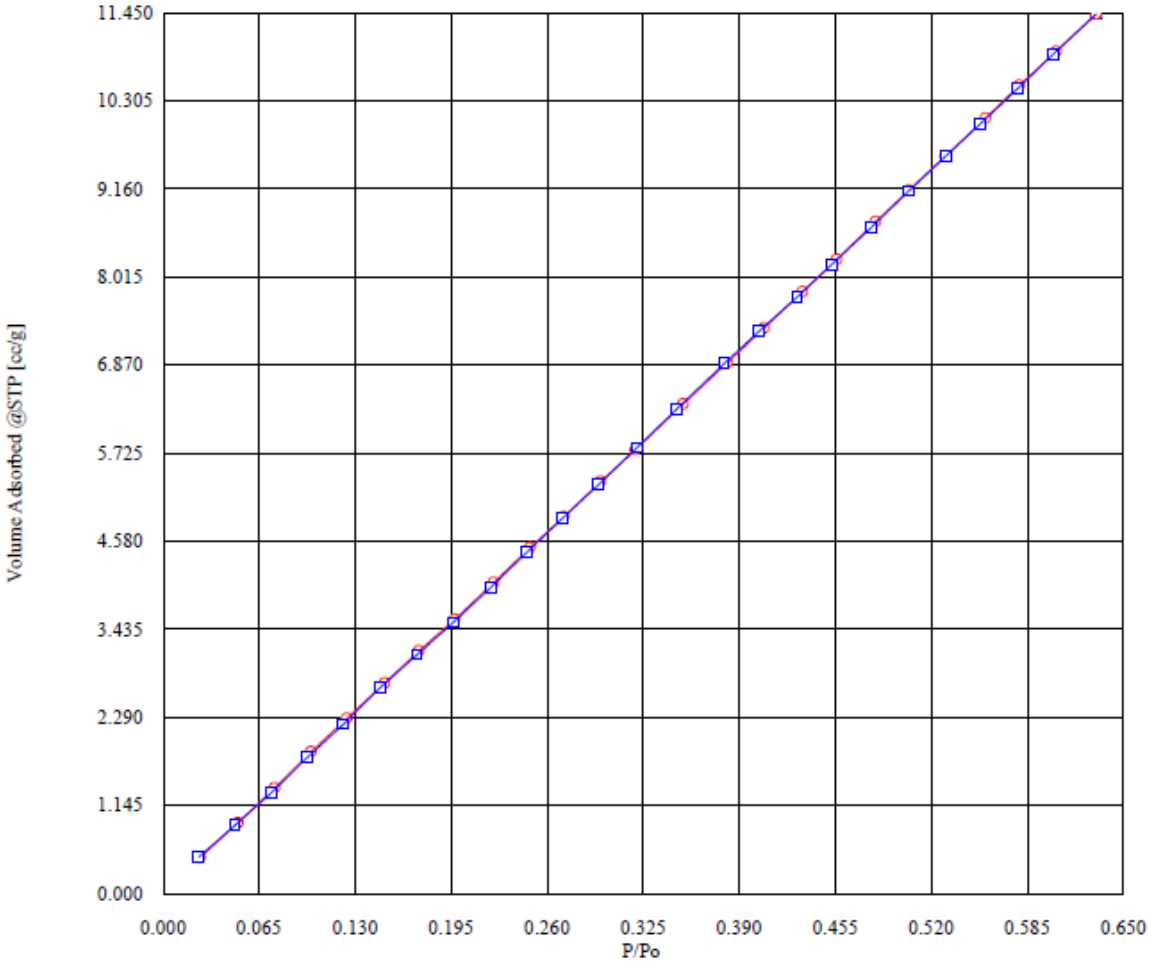


Figure SI-2. Brunauer–Emmett–Teller nitrogen adsorption-desorption Isotherm

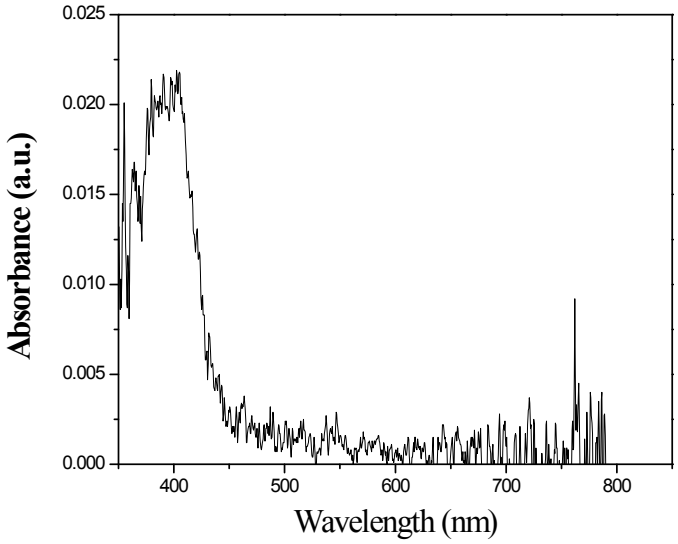
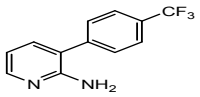


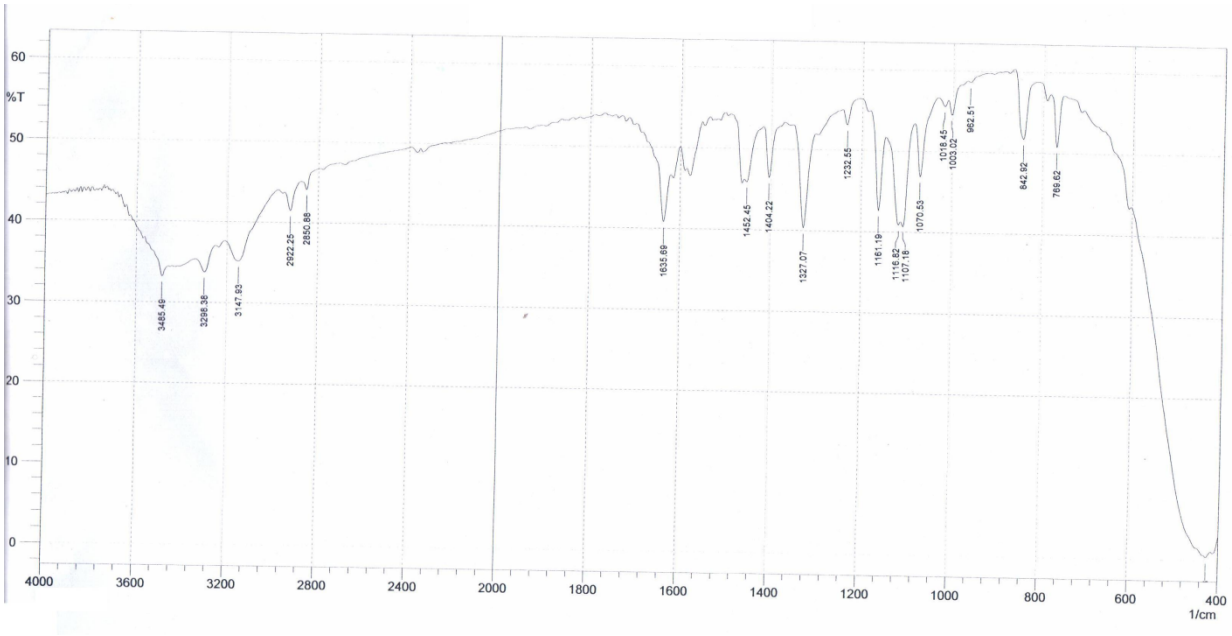
Figure SI-3. Visible spectra of Solid UV-absorbance SCS- Bi_2O_3

SI-04 Spectral characterisation of compound 3a.



(3a) 3-(4-(trifluoromethyl)phenyl)pyridin-2-amine

3a) 3-(4-(trifluoromethyl)phenyl)pyridin-2-amine: IR (cm^{-1},neat) 3485, 3147, 1635, 1116-1107; 1HNMR (300 MHz, CDCl3) 8.13(d, J=3, 1H), 7.74-7.72(d, J=6, 2H), 7.61-7.58(d, J=9, 2H), 7.39-7.37 (d, J=6, 1H), 6.81-6.77(q, J_1=6, J_2=3, 1H), 4.64(s, 2H); 13CNMR (75 MHz, CDCl3)155.61,147.90,139.98,137.67,136.18,128.75,127.18,121.45,114.61;LCMS(MM:ES+ APCI) 239.2$(M+H)^+$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1116.82
1107.18
1070.53
1018.45
1003.02
962.51
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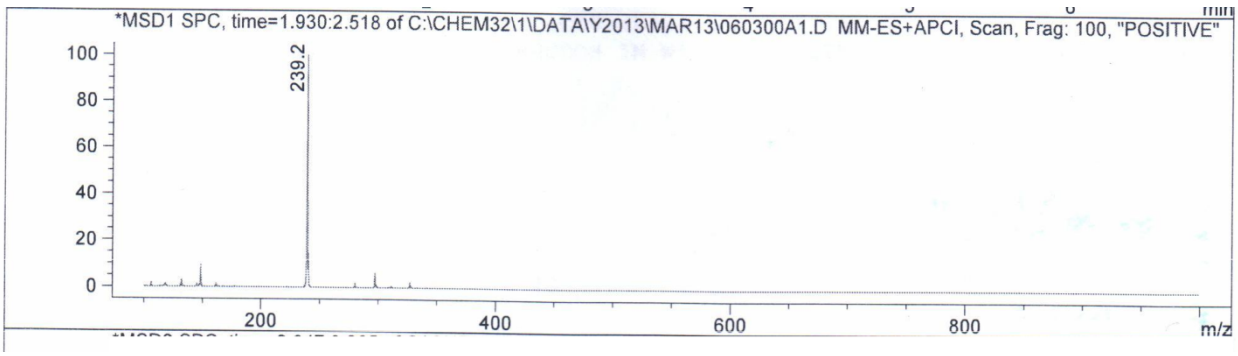
1/cm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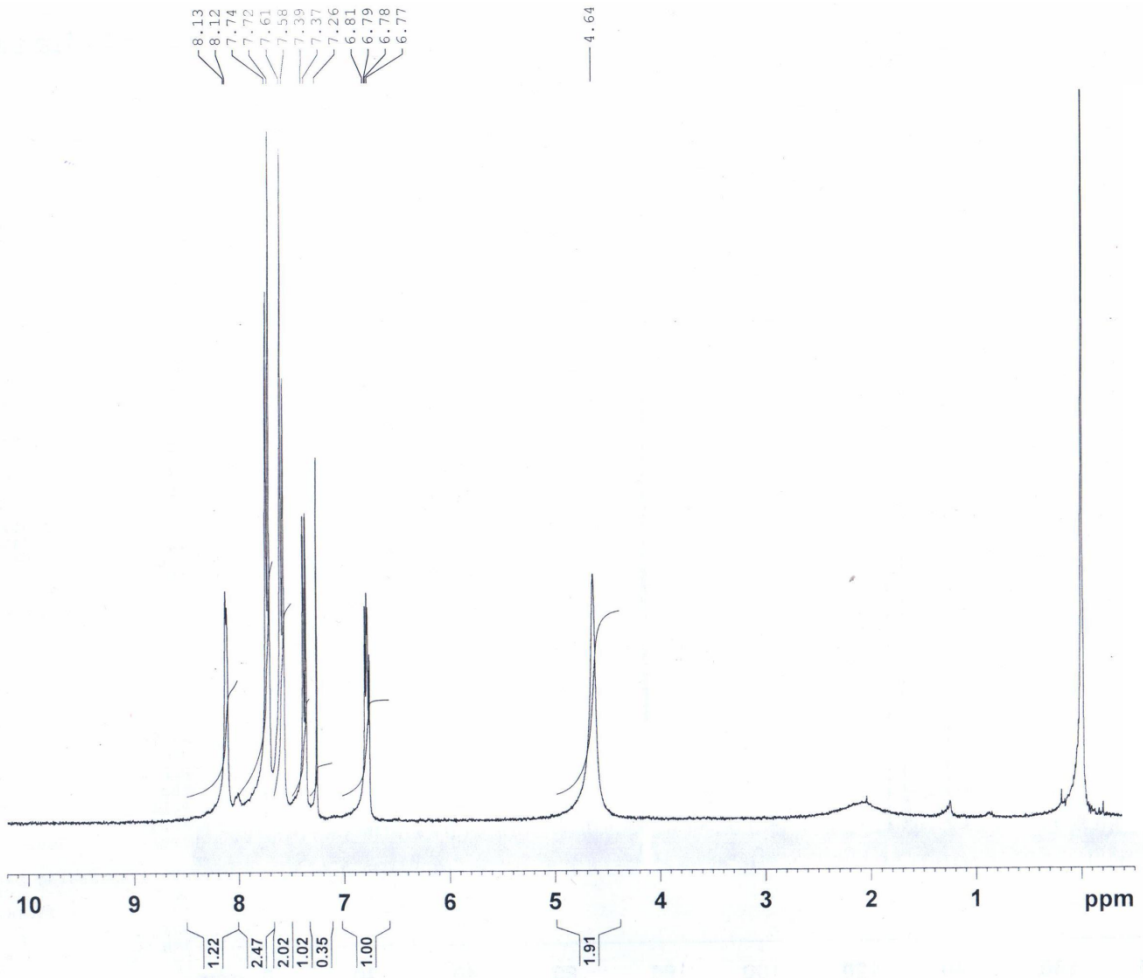
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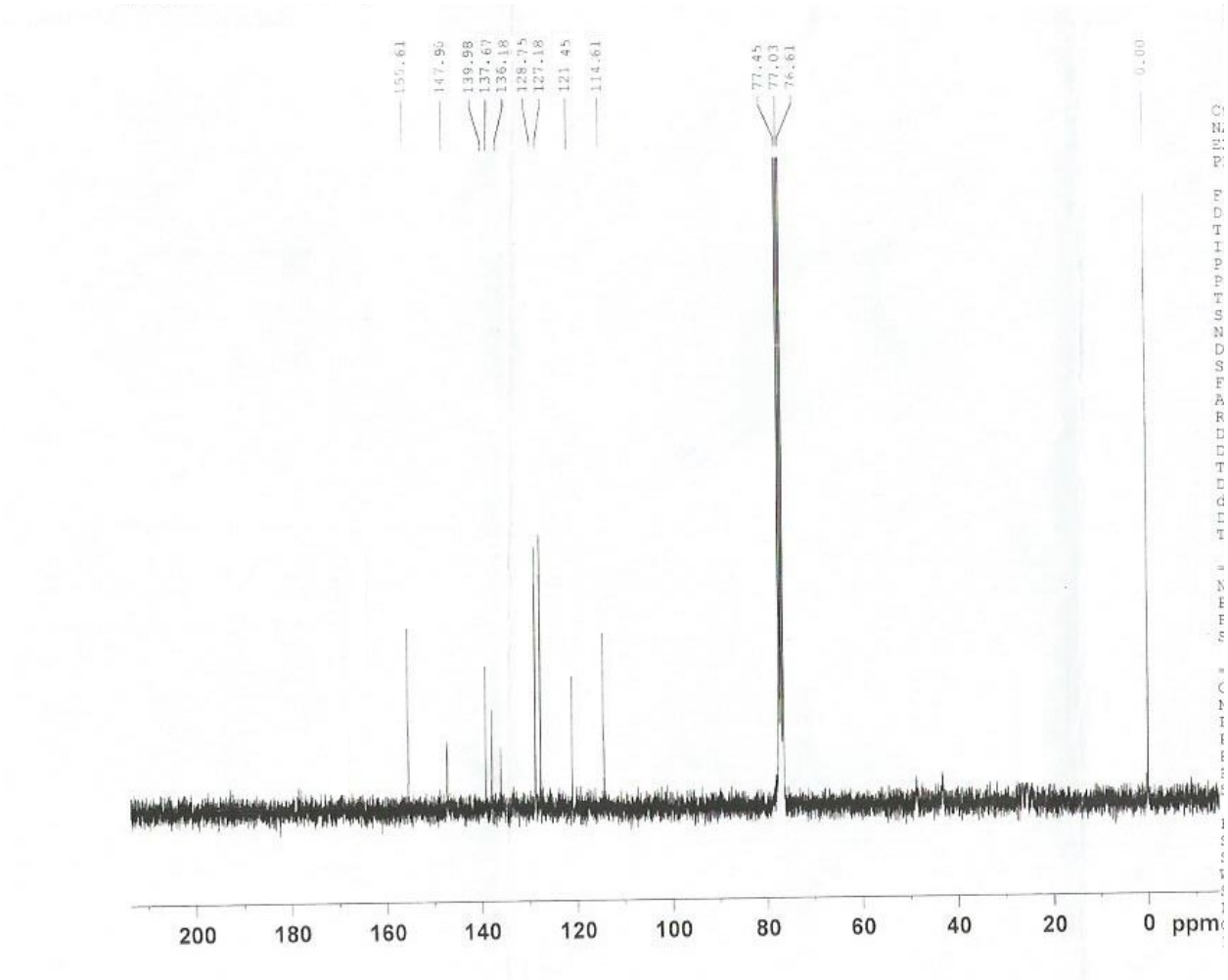
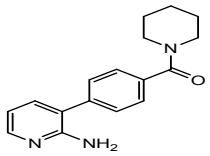
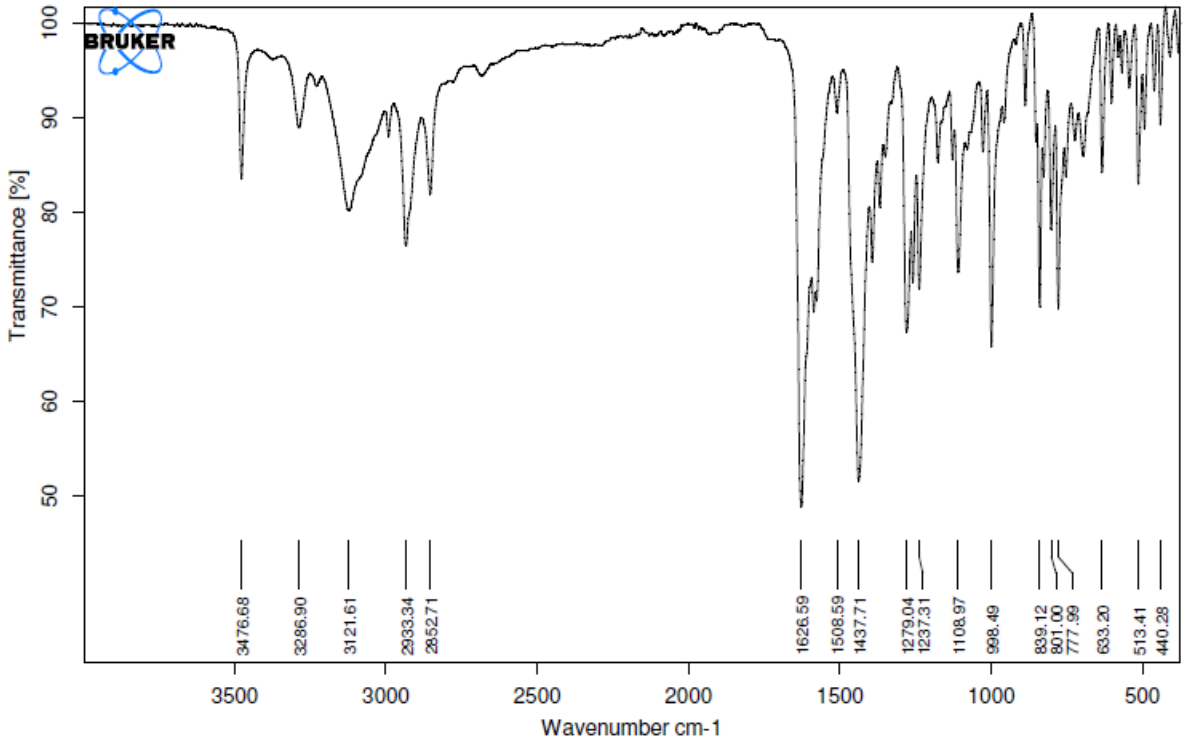


SI-05 Spectral characterisation of compound 3b.



(3b) (4-(2-aminopyridin-3-yl)phenyl)(piperidin-1-yl)methanone

3b) (4-(2-aminopyridin-3-yl)phenyl)(piperidin-1-yl)methanone: IR (cm^{-1},neat) 3476, 3121, 2933, 1626, 1508; 1HNMR (400 MHz, CDCl3) 8.08(d, 1H), 7.50(s, 4H), 7.39-7.36(d, 1H), 6.79-6.73(t, 1H), 4.65(s, 2H), 3.85 (s, 2H), 3.45(s, 2H), 1.90-1.40(m, 6H) ; LCMS (MM:ES+APCI) 282.3$(M+H)^+$; Anal.Calcd for $C_{17}H_{19}N_3O$: C 72.57; H 6.81; N 14.94. Found: C, 71.11; H, 6.88; N, 14.56.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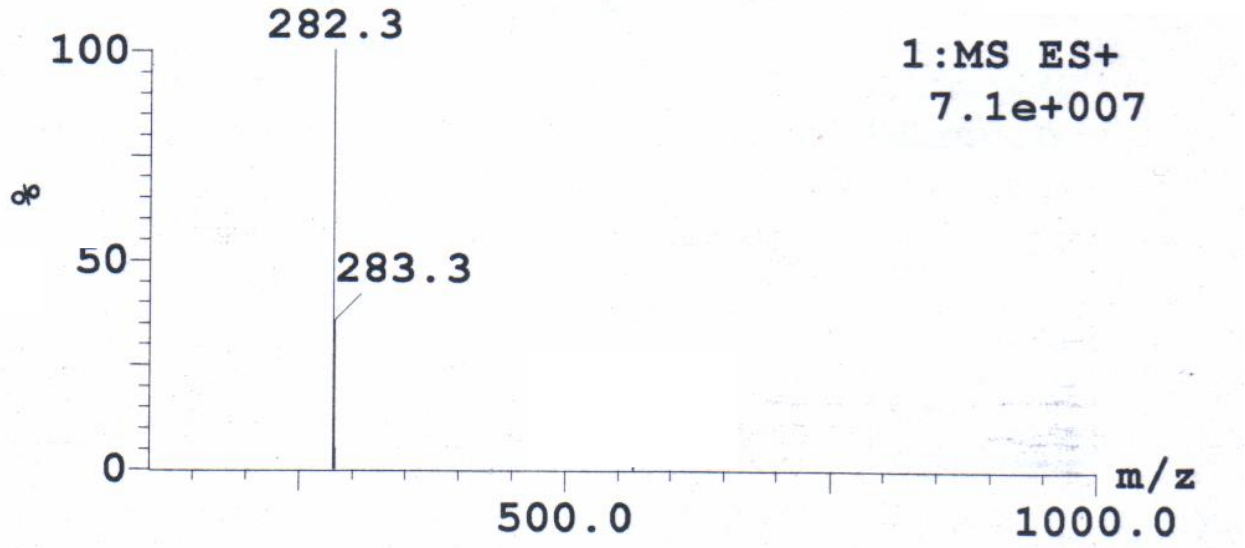
Wavenumber cm-1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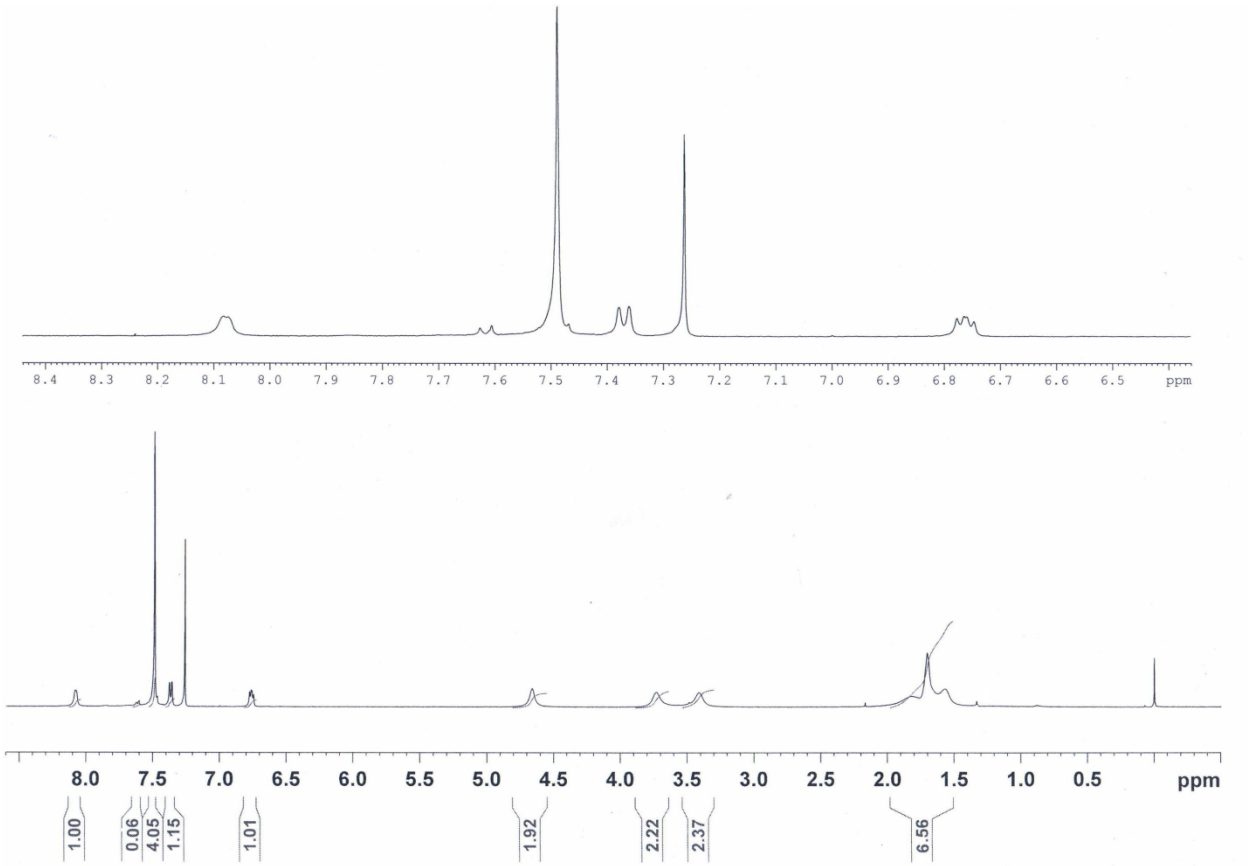
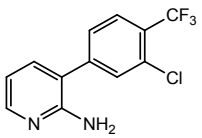
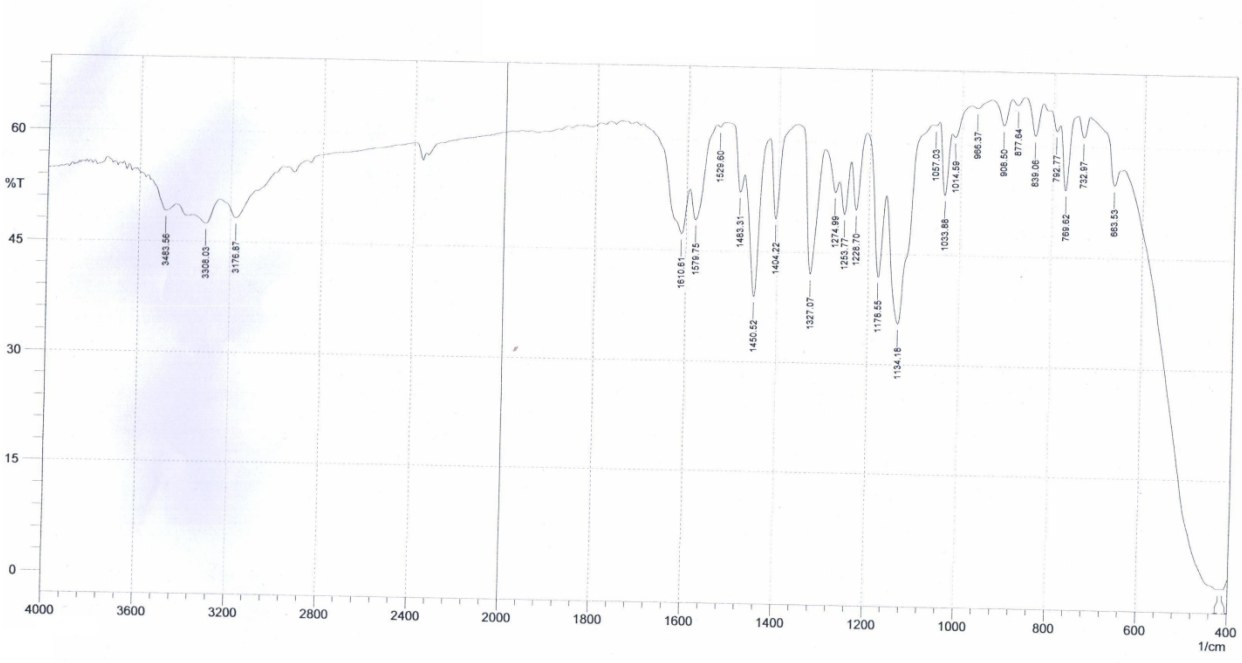


SI-06 Spectral characterisation of compound 3c.



(3c) 3-(4-chloro-3-(trifluoromethyl)phenyl)pyridin-2-amine

3c) 3-(4-chloro-3-(trifluoromethyl)phenyl)pyridin-2-amine: IR (cm^{-1},neat) 3483, 3170, 1610, 1134, 769; 1HNMR (300 MHz, CDCl3) 8.12-8.10(d, J=6, 1H), 7.79(s, 1H), 7.60(s, 2H), 7.36-7.34 (d, J=6, 1H), 6.80-6.76(q, J_1=3, J_2=6, 1H), 4.60(s, 2H); 13CNMR (75 MHz,CDCl3) 155.53, 148.36, 138.03, 135.10, 133.09, 128.44, 128.03, 127.93, 126.26, 120.82, 119.23, 114.77; LCMS (MM:ES+APCI) 273.2$(M+H)^+$; Anal.Calcd for $C_{12}H_{08}ClF_3N_2$: C 52.86; H 2.96; N 10.27. Found: C 51.34; H 3.33; N 11.09.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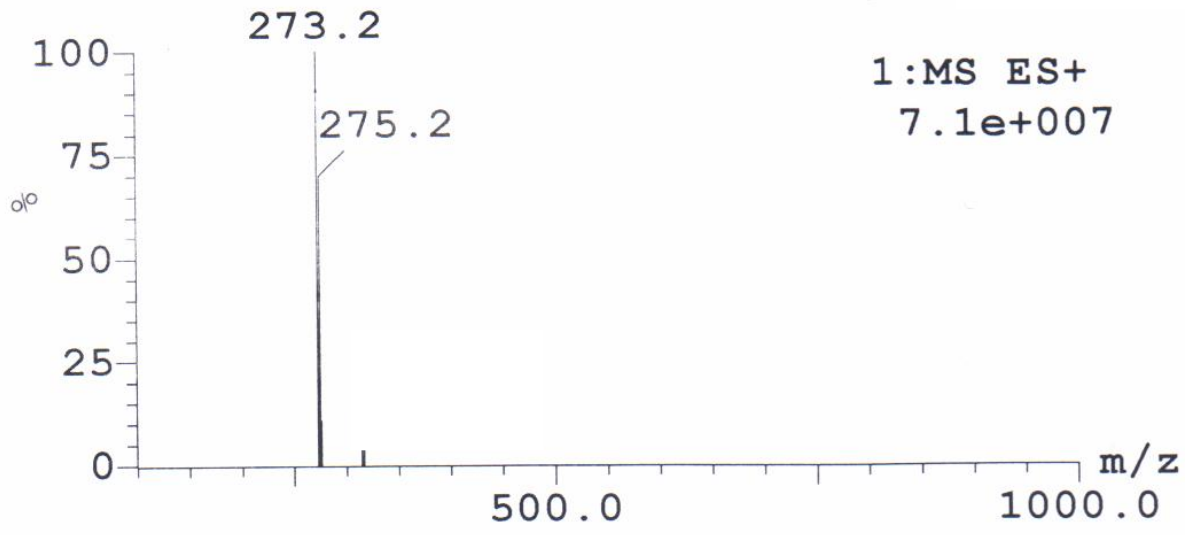
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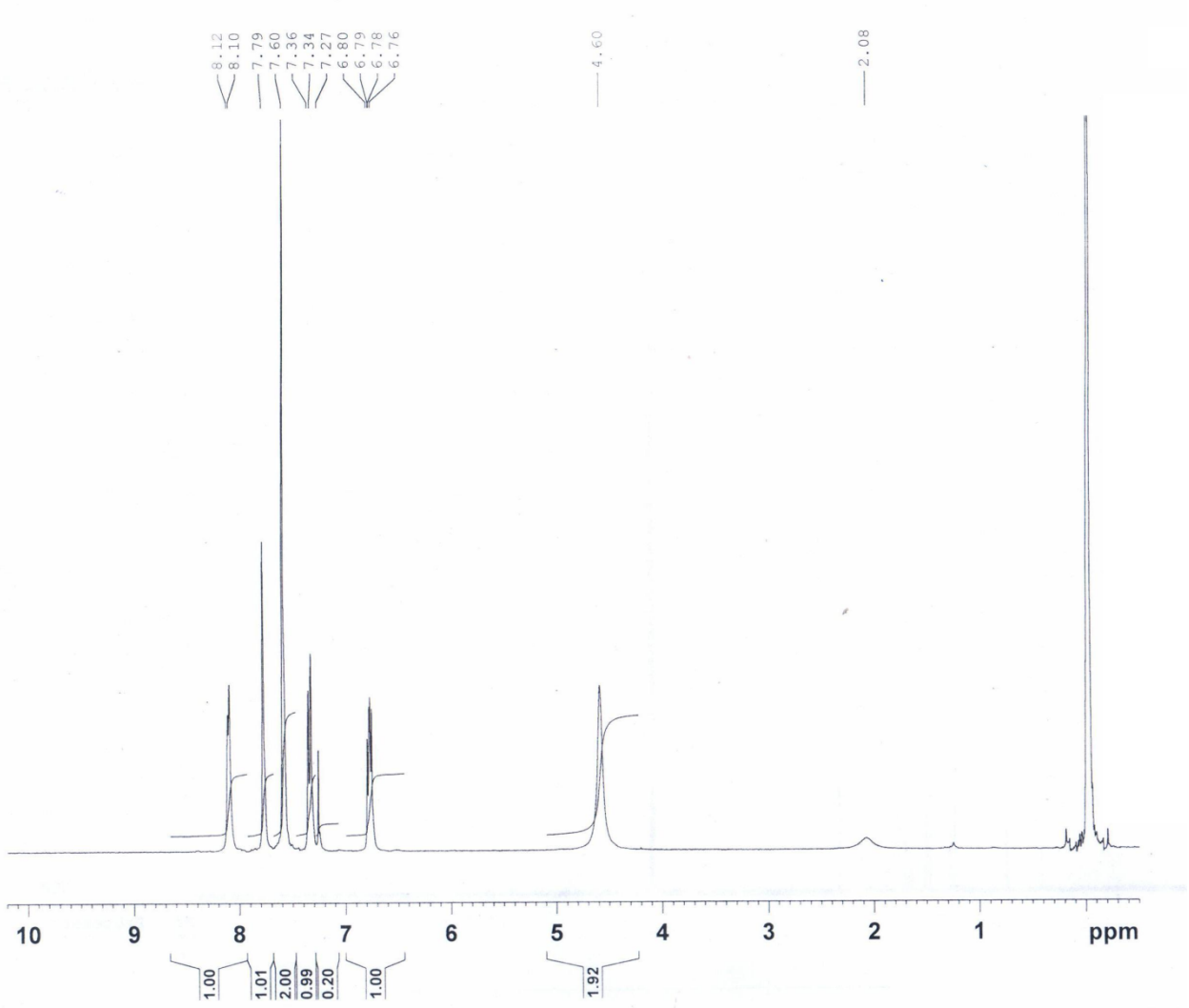
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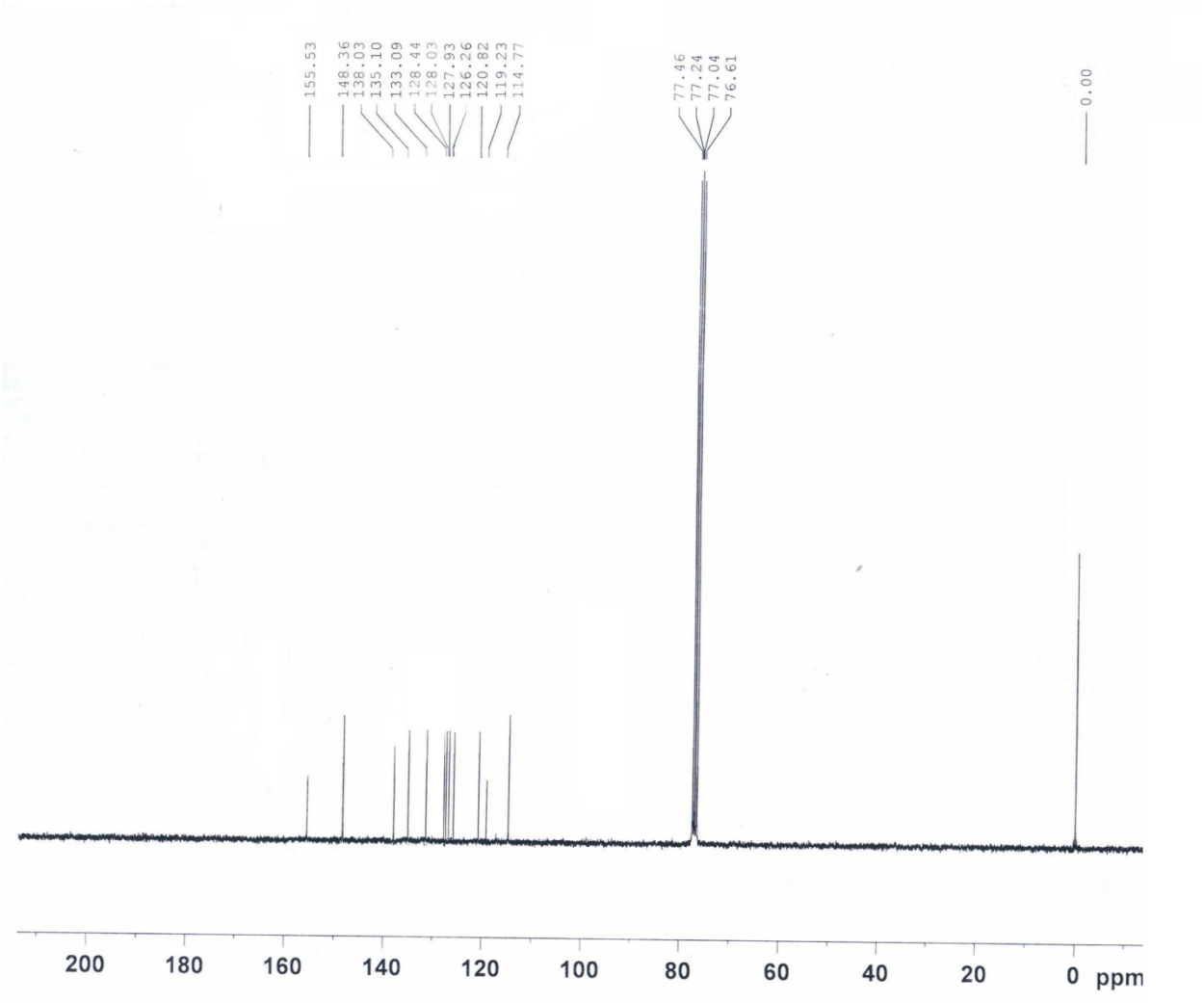
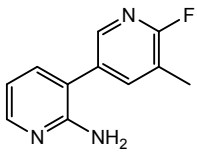
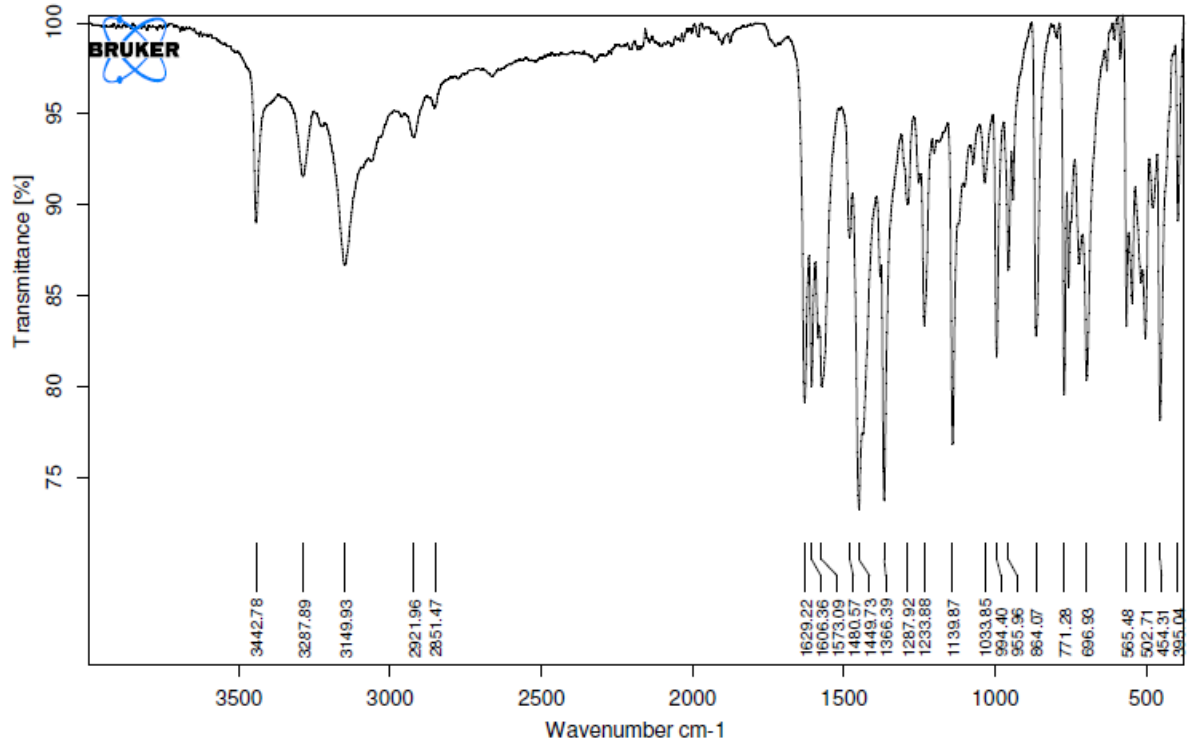


SI-07 Spectral characterisation of compound 3d



(3d) 3-(6-fluoro-5-methylpyridin-3-yl)pyridin-2-amine

3d) 3-(6-fluoro-5-methylpyridin-3-yl)pyridin-2-amine: IR (cm^{-1},neat) 3442, 3149, 2921, 1606, 1033; 1HNMR (400 MHz, DMSO-d6) 7.76-7.69 (d, 2H), 7.01-6.91(d, 2H), 6.40(s, 1H), 5.39(s, 2H), 1.91(s, 3H); LCMS (MM: ES+APCI) 204.2$(M+H)^+$; Anal.Calcd for $C_{11}H_{10}FN_3$: C 65.01; H 4.96; N 20.96. Found: C 64.98; H 5.55; N 19.03.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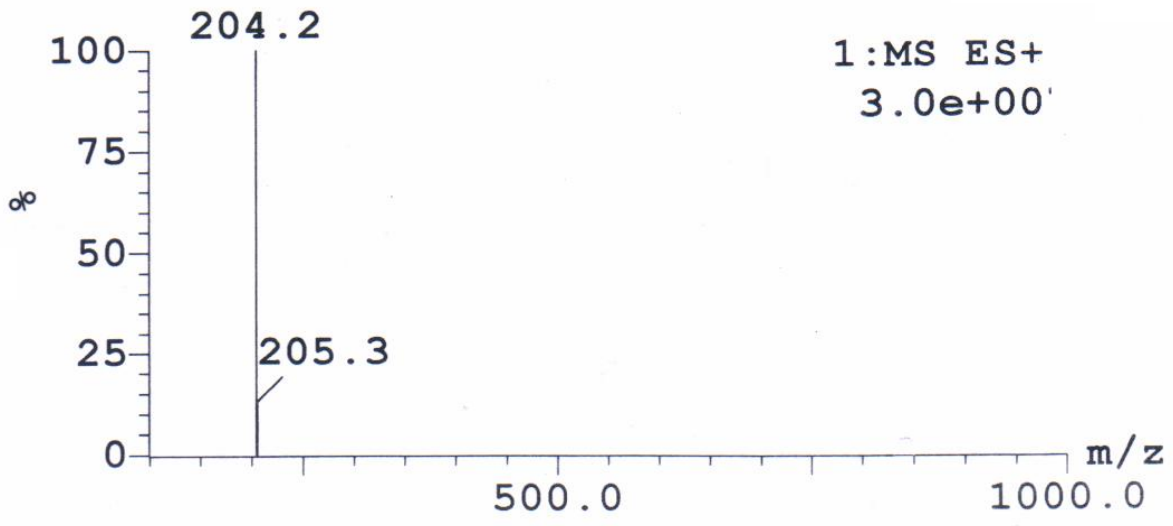
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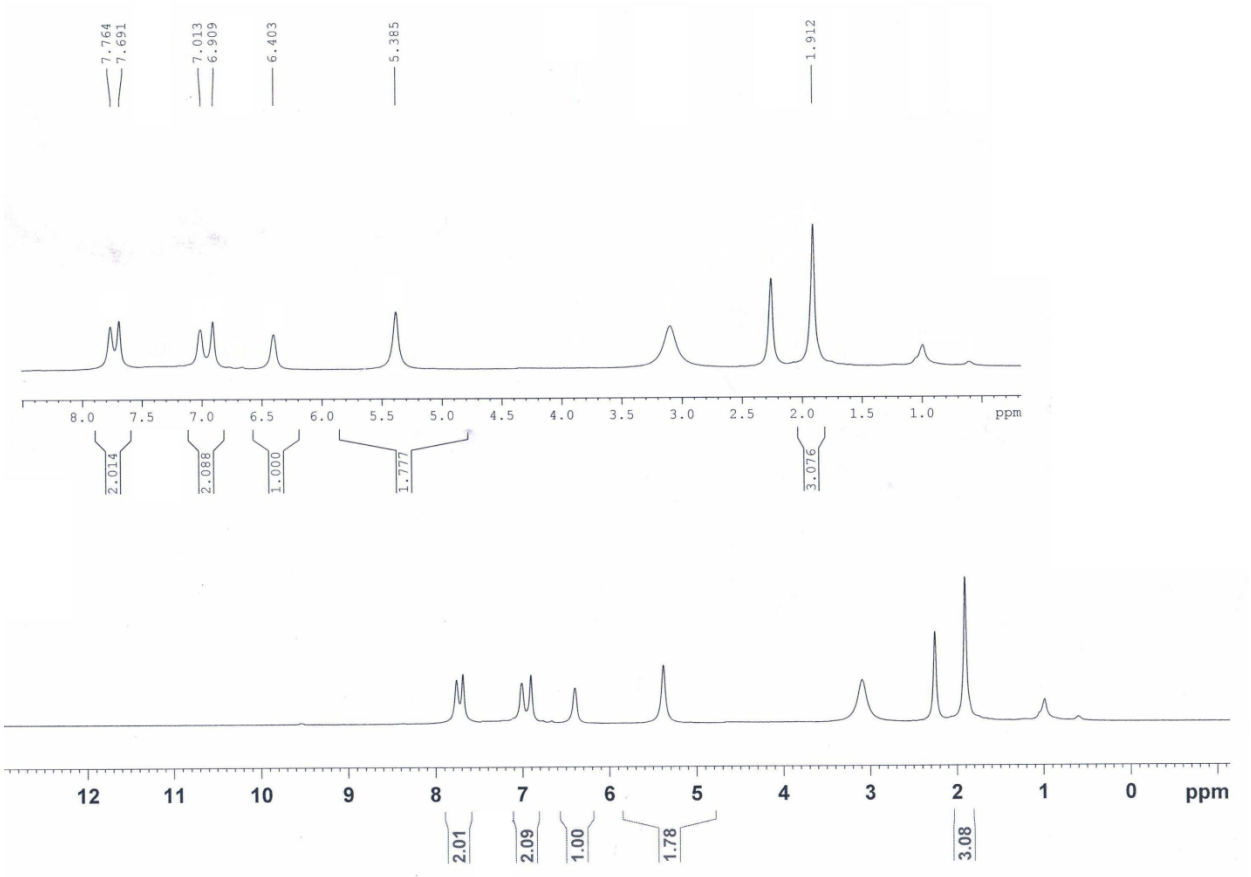
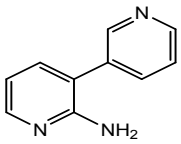
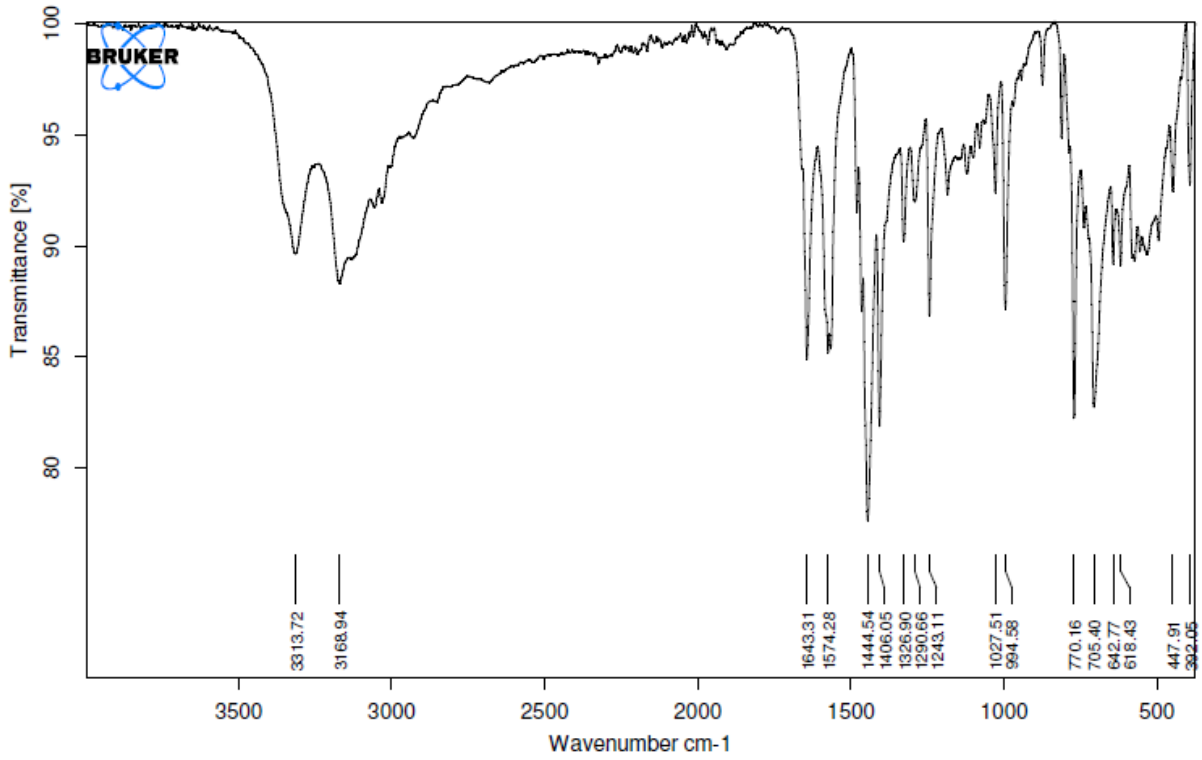


SI-08 Spectral characterisation of compound 3e.



(3e) 3-(pyridin-3-yl)pyridin-2-amine

3e) 3-(pyridin-3-yl)pyridin-2-amine : IR (cm^{-1},neat) 3313, 3168, 1643; 1HNMR (400 MHz, DMSO-d6) 8.70(s, 1H), 8.35(d, 1H), 7.90(d, 2H), 7.50(d, 1H), 7.30(m, 1H), 6.45(m, 1H), 4.10(s, 2H); LCMS (MM:ES+APCI) 172.2$(M+H)^+$; Anal.Calcd for $C_{10}H_{09}N_3$: C 70.16; H 5.30; N 24.54. Found: C 70.99; H 4.98; N 23.33.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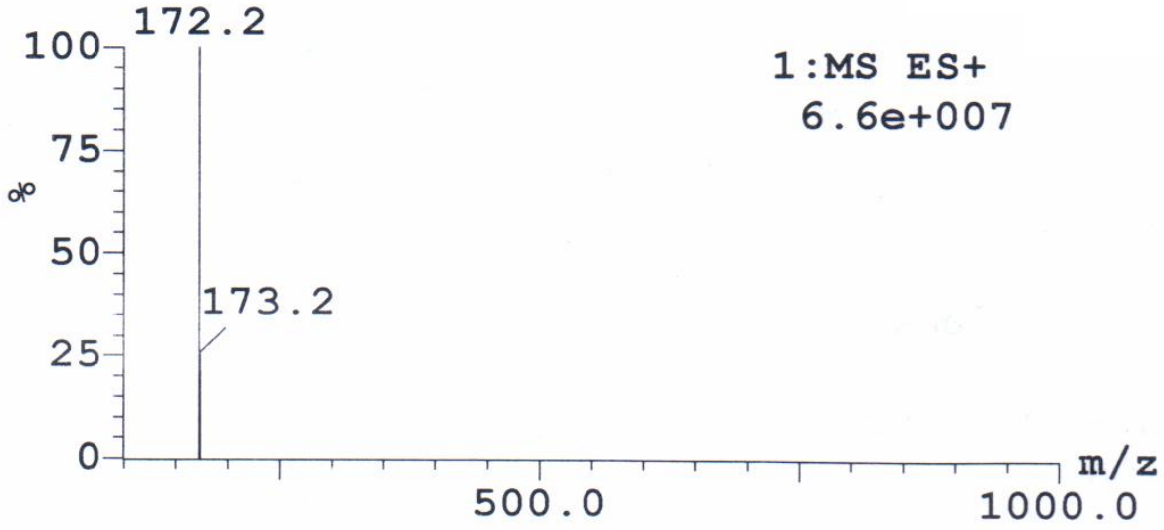
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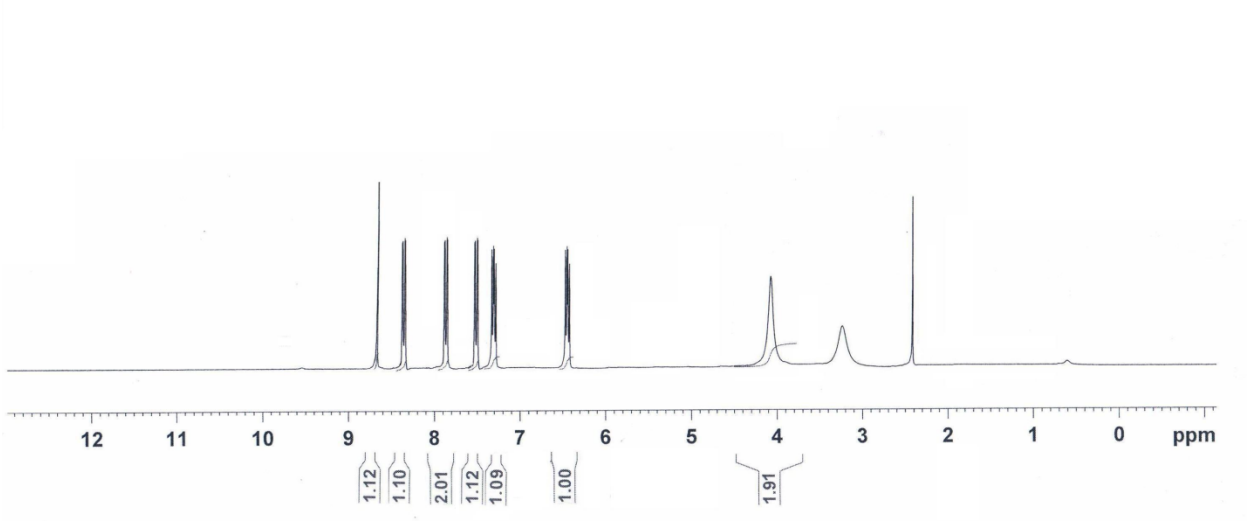
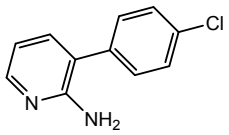
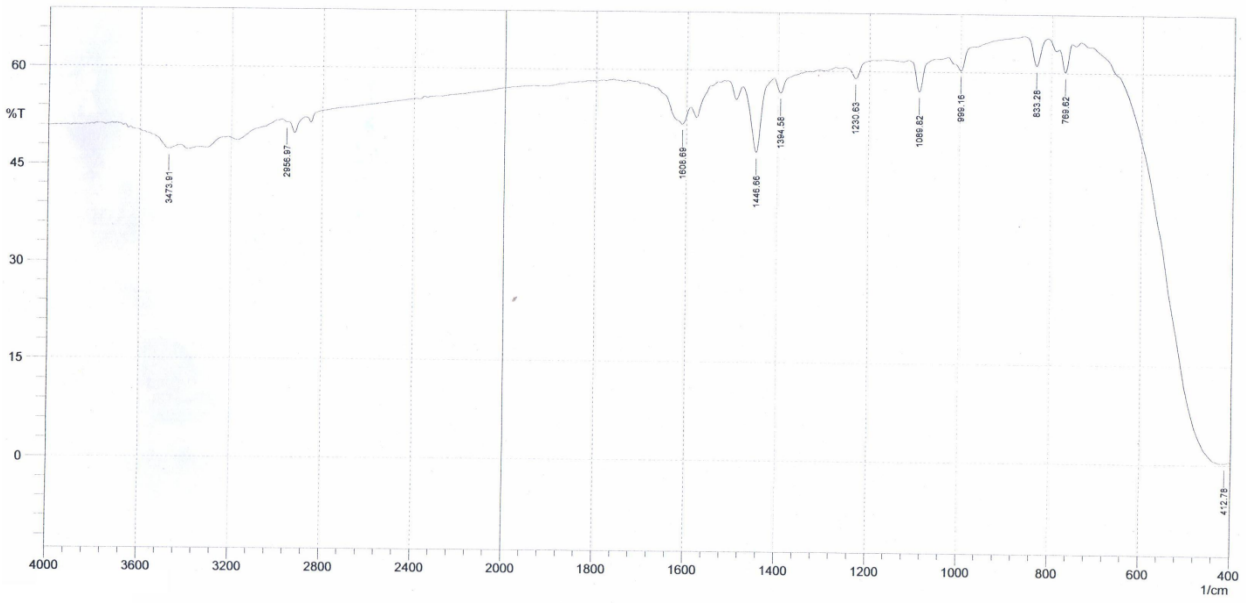


SI-09 Spectral characterisation of compound 3f.



(3f) 3-(4-chlorophenyl)pyridin-2-amine

3f) 3-(4-chlorophenyl)pyridin-2-amine: IR (cm^{-1},neat) 3473, 2956, 1608, 769; 1HNMR (400 MHz, CDCl3) 8.11-8.05 (d, 1H), 7.48-7.38(m, 4H), 7.35-7.31(dd, 1H),6.75(q, 1H), 4.55(s, 2H); 13CNMR (75 MHz, CDCl3) 155.69, 147.60, 137.46, 136.87, 134.80, 131.80, 127.31, 120.84, 114.58; LCMS (MM:ES+APCI) 205.4$(M+H)^+$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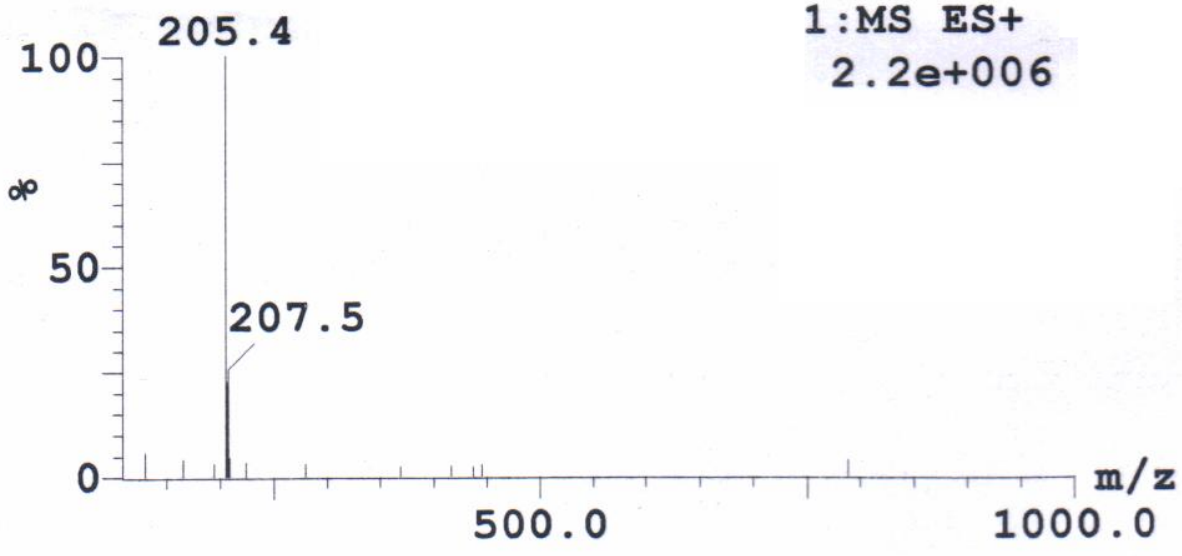
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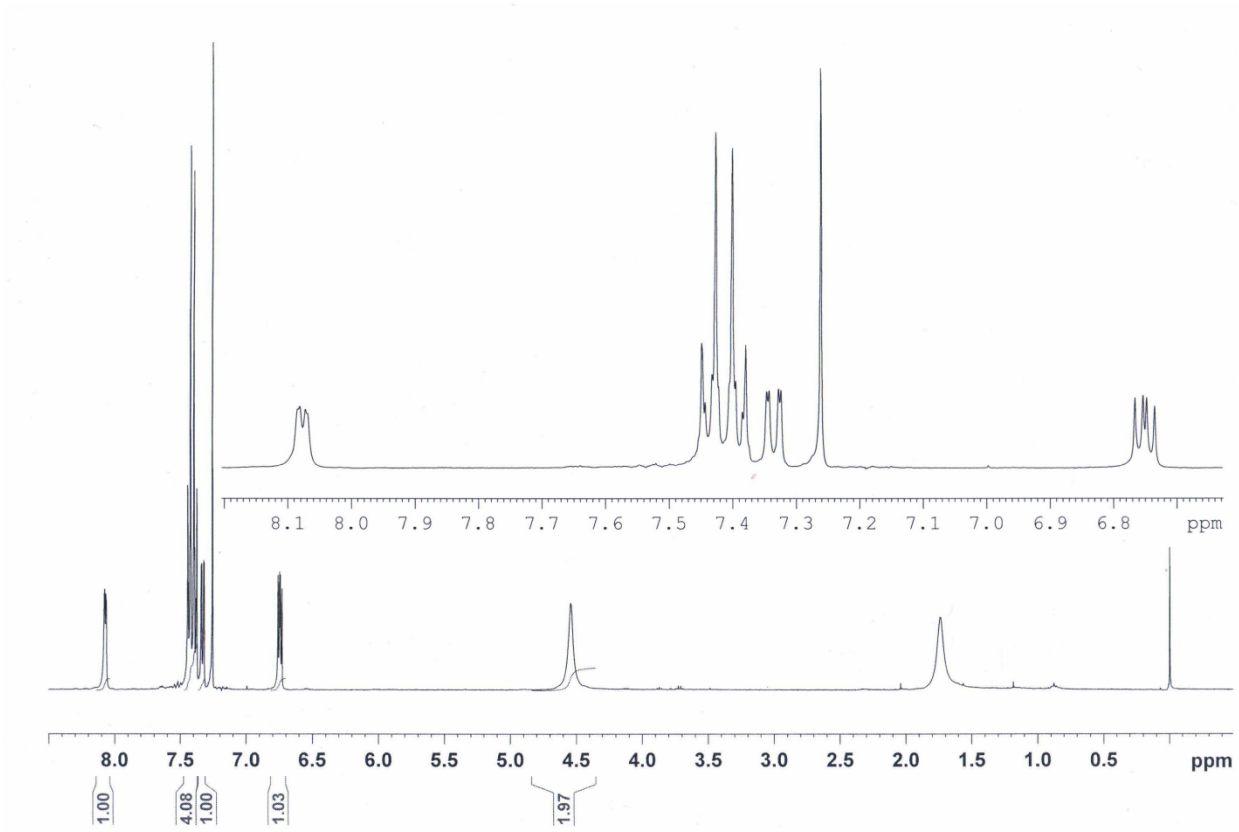
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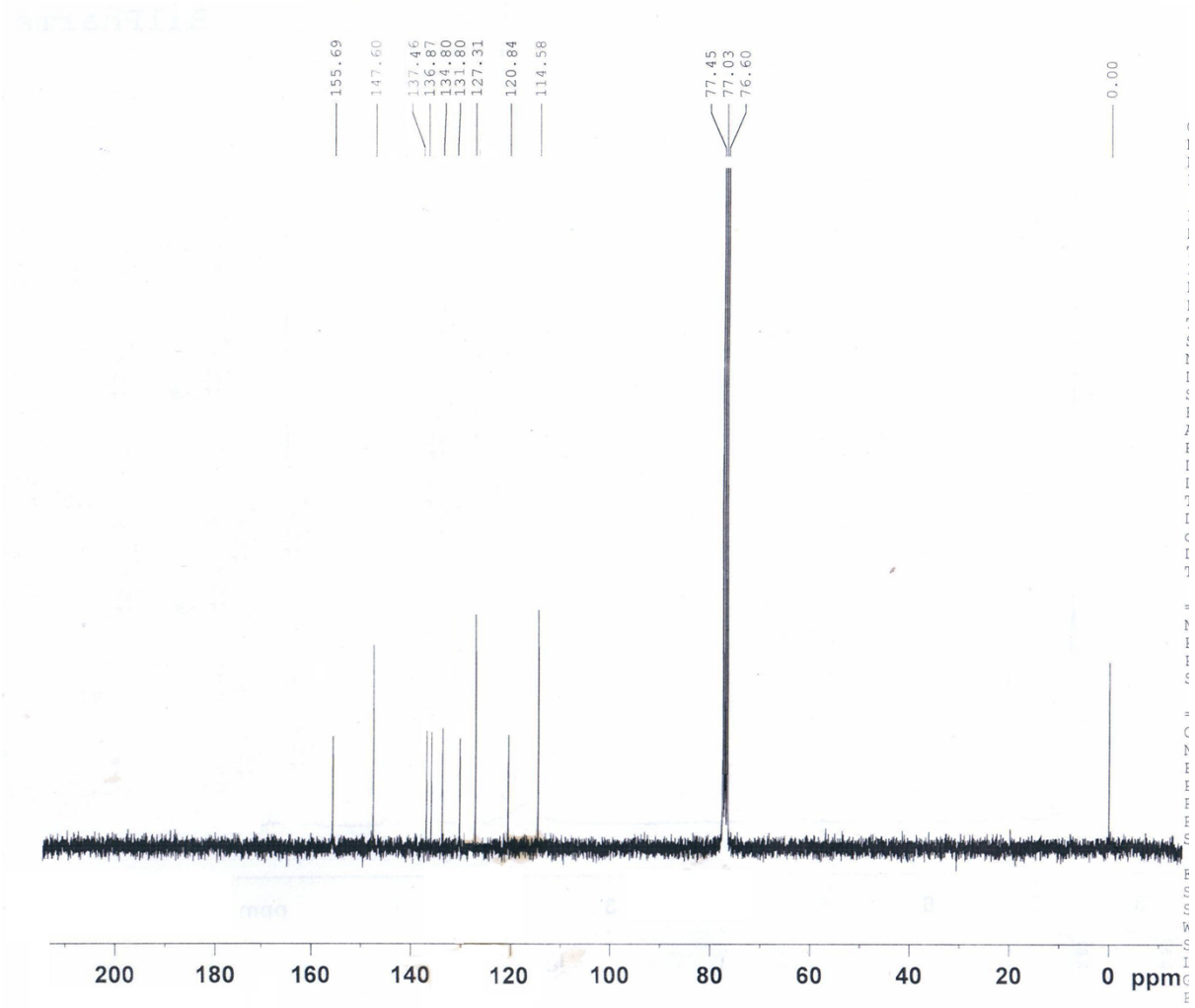
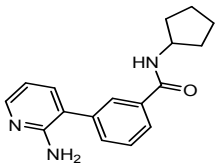
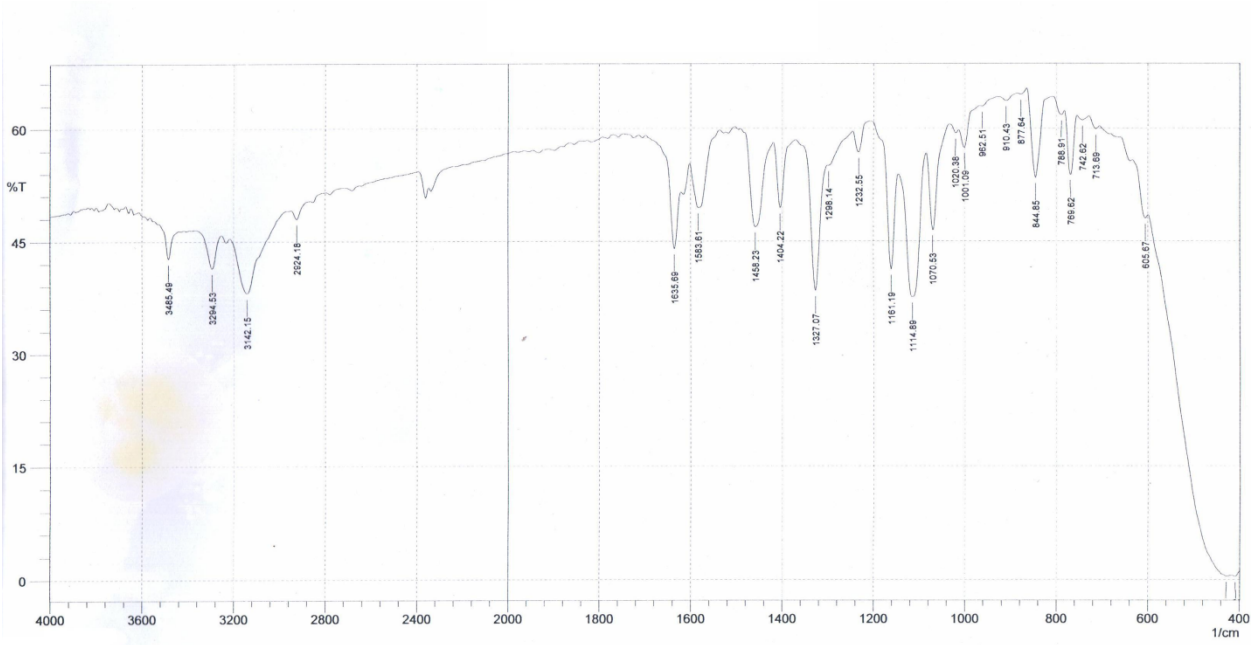


SI-10 Spectral characterisation of compound 3g.



(3g) 3-(2-aminopyridin-3-yl)-N-cyclopentylbenzamide

3g) 3-(2-aminopyridin-3-yl)-N-cyclopentylbenzamide: IR (cm^{-1},neat) 3485, 3142, 2942, 1635, 1583; 1HNMR (400 MHz, CDCl3) 8.02(s, 1H), 7.80-7.68(m, 2H), 7.52-7.43(m, 2H), 7.31-7.30(d, J=6.4, 1H), 6.93-6.69(q, 1H), 5.99(s, 1H), 4.51(s, 2H), 4.39-4.30(q, 1H), 2.06-2.02(q, 2H), 1.69-1.57(m, 2H), 1.47-1.41(m, 2H), 1.26-1.18(m, 2H) ; 13CNMR (75 MHz, CDCl3) 166.74, 155.71, 147.55, 138.43, 138.05, 135.94, 131.50, 129.38, 127.19, 126.38, 121.02, 114.53, 51.83, 35.20, 35.15, 26.66, 26.62;LCMS (MM:ES+APCI) 282.2$(M+H)^+$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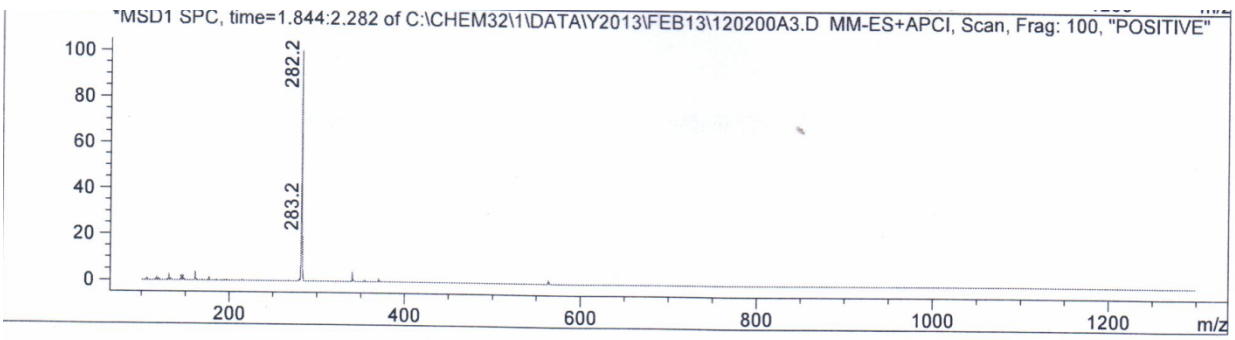
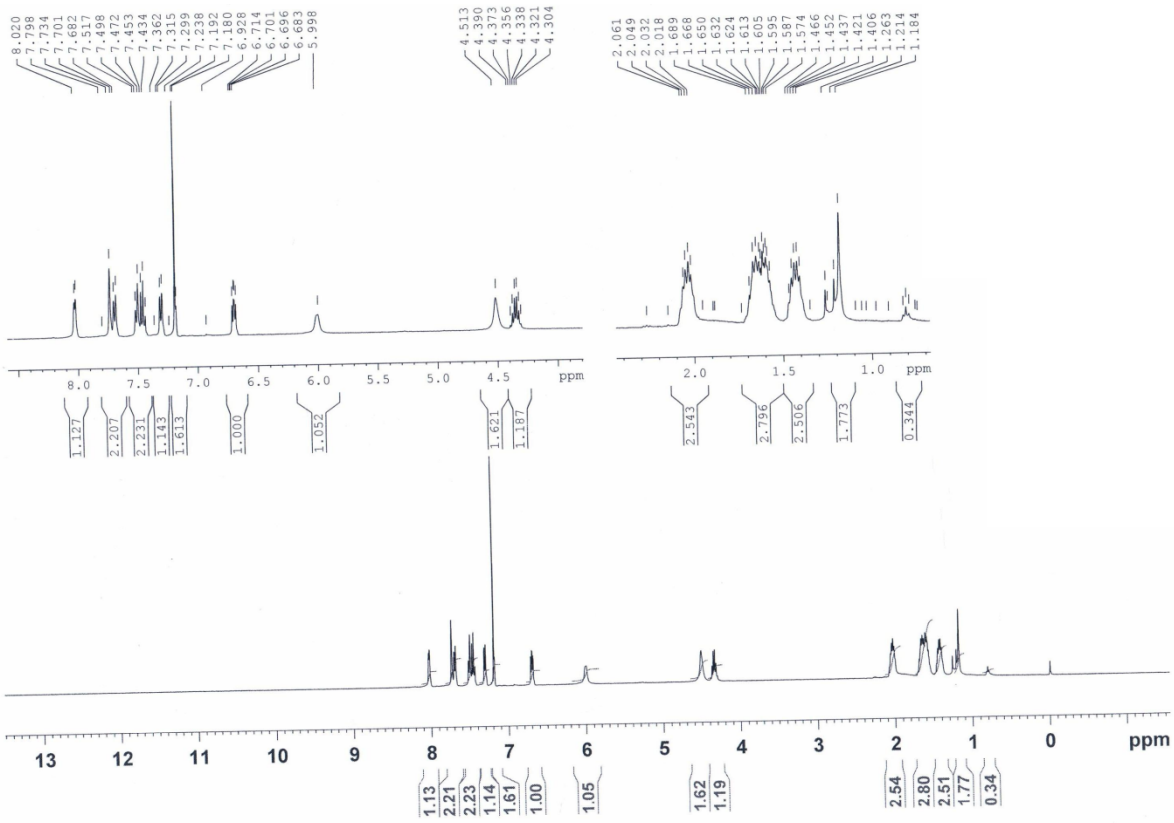
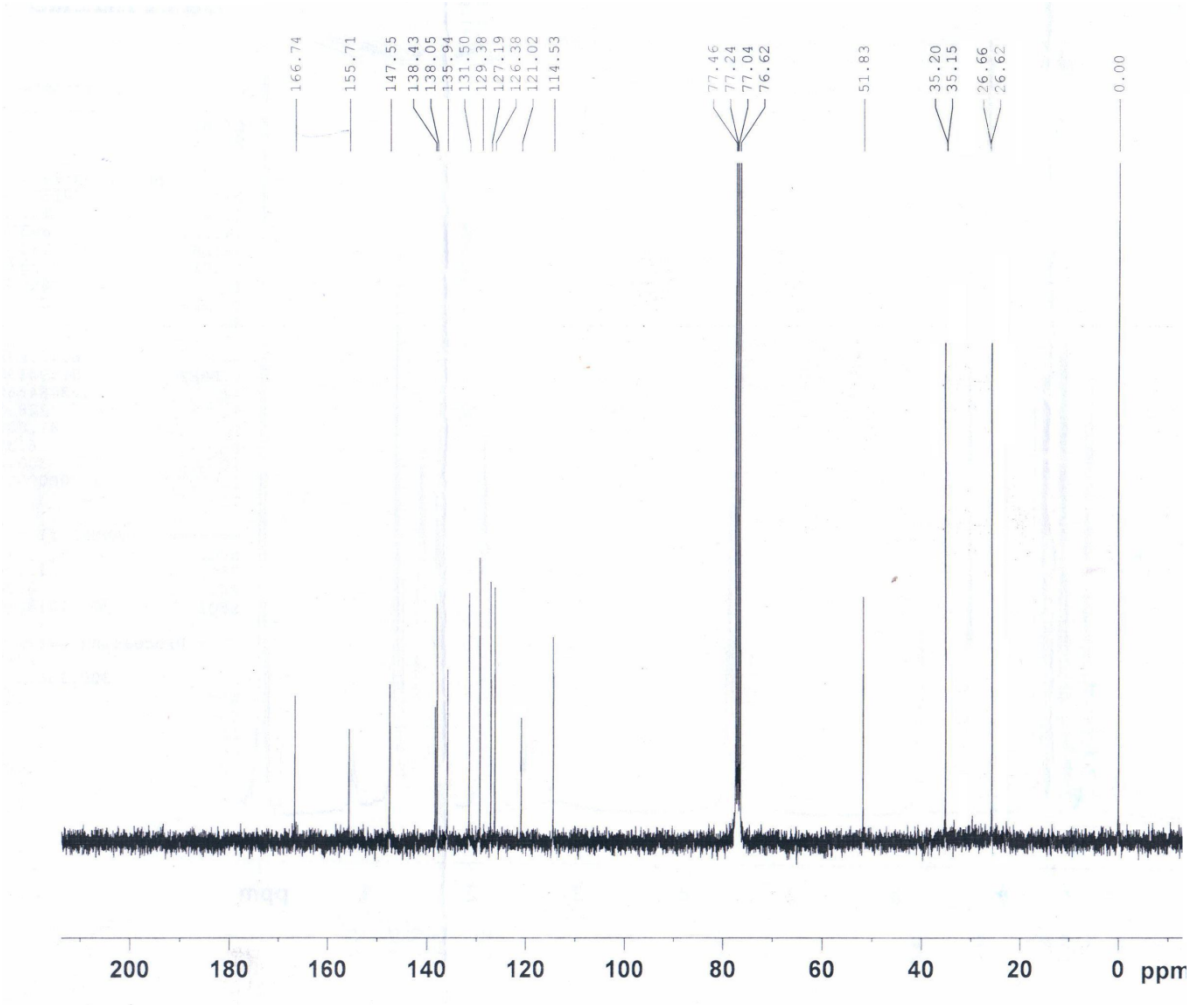
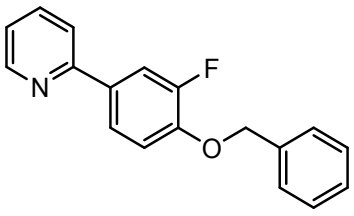
1070.53
1020.38
1001.09
962.51
910.43
877.84
844.85
788.61
766.62
742.62
713.69
605.67


*MSD1 SPC, time=1.844:2.282 of C:\CHEM32\1\DATA\Y2013\FEB13\120200A3.D MM-ES+APCI, Scan, Frag: 100, "POSITIVE"
100
80
60
40
20
0
282.2
283.2
200
400
600
800
1000
1200
m/z


8.020
7.798
7.734
7.701
7.682
7.517
7.498
7.472
7.453
7.434
7.362
7.315
7.299
7.238
7.192
7.180
6.928
6.714
6.701
6.696
6.683
5.998
4.513
4.390
4.373
4.356
4.338
4.321
4.304
2.061
2.049
2.032
2.018
1.689
1.668
1.650
1.632
1.624
1.613
1.605
1.595
1.587
1.574
1.466
1.452
1.437
1.421
1.406
1.263
1.214
1.184
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
ppm
2.0
1.5
1.0
ppm
1.127
2.207
2.231
1.143
1.613
1.000
1.052
1.621
1.187
2.543
2.796
2.506
1.773
0.344
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.13
2.21
2.23
1.14
1.61
1.00
1.05
1.62
1.19
2.54
2.80
2.51
1.77
0.34

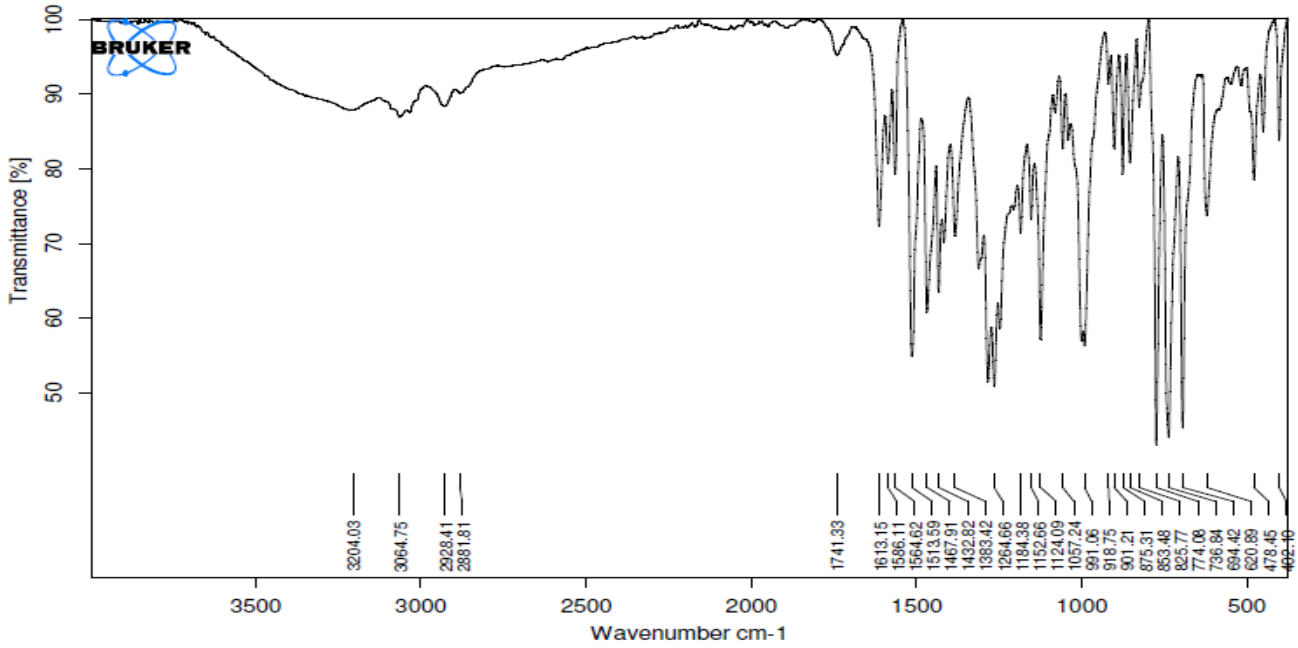


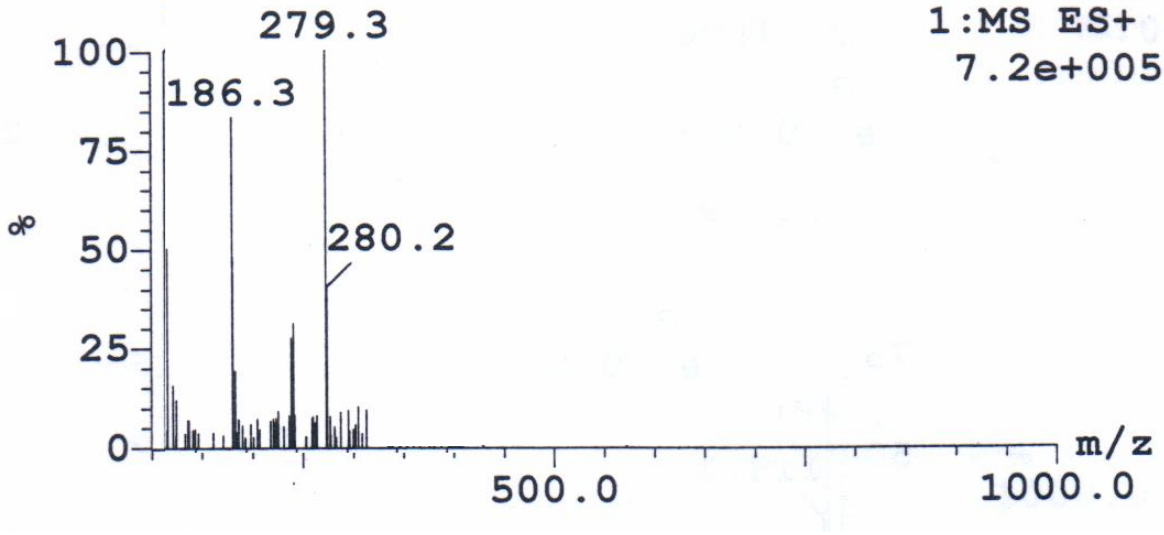
SI-11 Spectral characterisation of compound 3h.

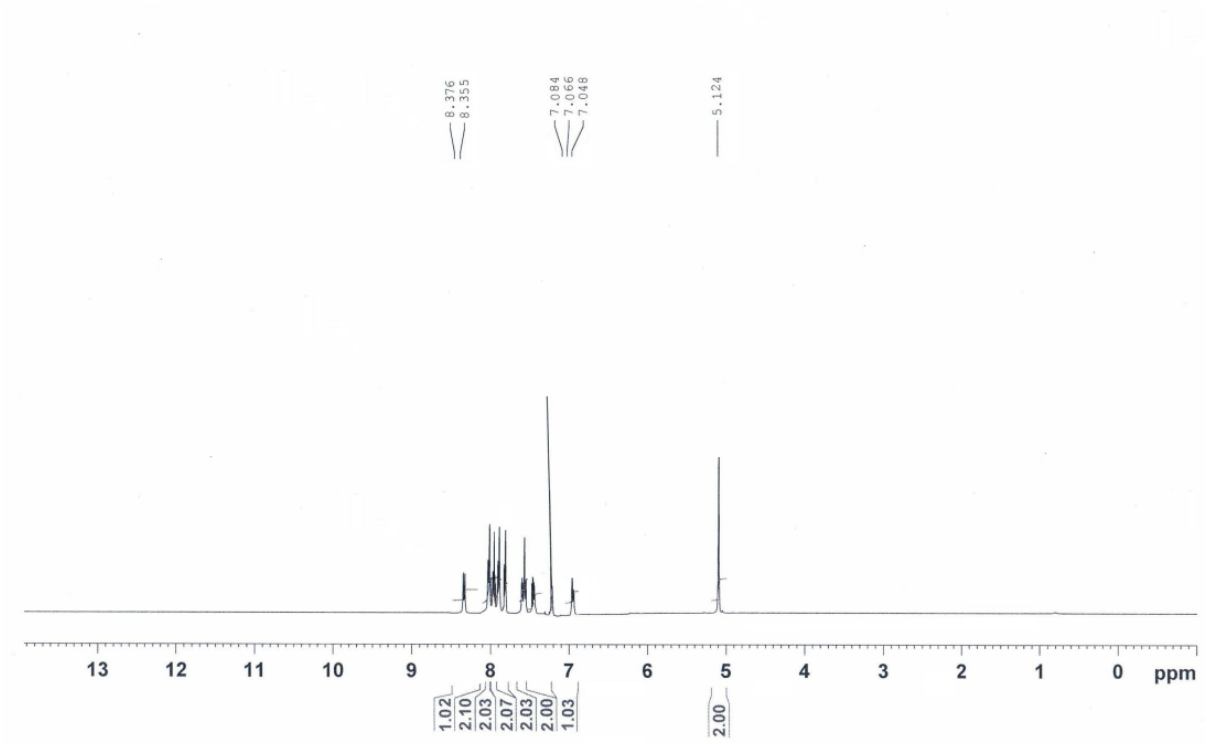


(3h) 2-(4-(benzyloxy)-3-fluorophenyl)pyridine

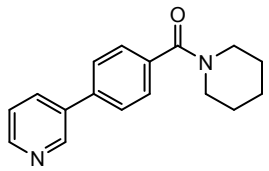
3h) 2-(4-(benzyloxy)-3-fluorophenyl)pyridine : The compound was obtained following the general procedure described above.IR (cm^{-1},neat) 3064, 2881, 1264, 1057 ; 1HNMR (400 MHz, CDCl3) 8.37-8.35 (d, J = 8.4 Hz, 1H), 8.10-8.00 (m, 2H), 7.90 (t, 2H), 7.85 (t, 2H), 7.60 (t, 2H), 7.45(m,2H), 7.08-7.04(t, J =7.2Hz, 1H), 5.12(s, 1H); LCMS (MM:ES+APCI) 280.2$(M+H)^+$; Anal.Calcd for $C_{18}H_{14}FNO$: C 77.40; H 5.05; N 5.01. Found: C, 78.45; H, 5.85; N, 5.44.


BRUKER
Transmittance [%]
100
90
80
70
60
50
3204.03
3064.75
2928.41
2881.81
1741.33
1613.15
1586.11
1564.62
1513.59
1467.91
1432.82
1383.42
1264.66
1184.38
1152.66
1124.09
1057.24
991.06
918.75
901.21
875.31
853.48
825.77
774.08
736.84
694.42
620.89
478.45
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1


279.3
1:MS ES+
7.2e+005
100
186.3
75
%
50
280.2
25
0
m/z
500.0
1000.0

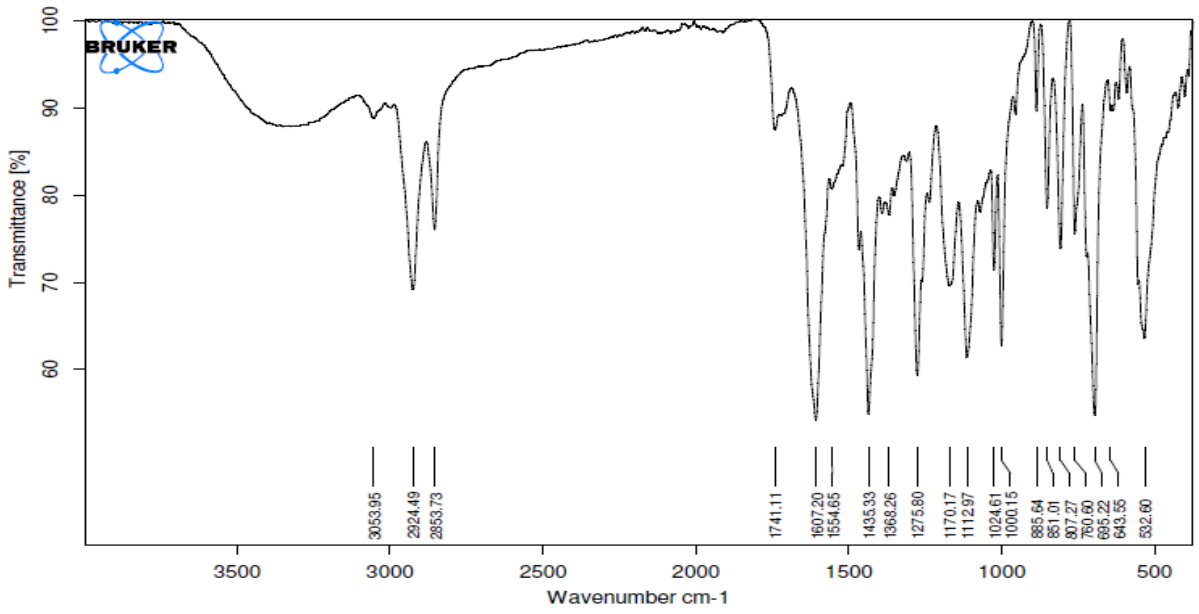


SI-12 Spectral characterisation of compound 3i.



(3i) piperidin-1-yl(4-(pyridin-3-yl)phenyl)methanone

3i) piperidin-1-yl(4-(pyridin-3-yl)phenyl)methanone: IR (cm^{-1},neat) 3054, 2924, 1607 ; 1HNMR (400 MHz, CDCl3) 8.50 (s, 1H), 8.05 (d, 1H), 7.50 (s, 4H), 7.40(d, 1H), 7.20 (t, 1H), 3.40(t,4H), 1.90-1.60(m, 6H); 13CNMR (75 MHz, CDCl3) 168.54, 147.95, 145.81, 139.04, 130.20, 129.77, 129.14, 126.12, 126.07, 125.83, 124.32, 48.79, 48.77, 24.56, 24.54, 24.52. LCMS (MM: ES+APCI) 267.3$(M+H)^+$


BRUKER
Transmittance [%]
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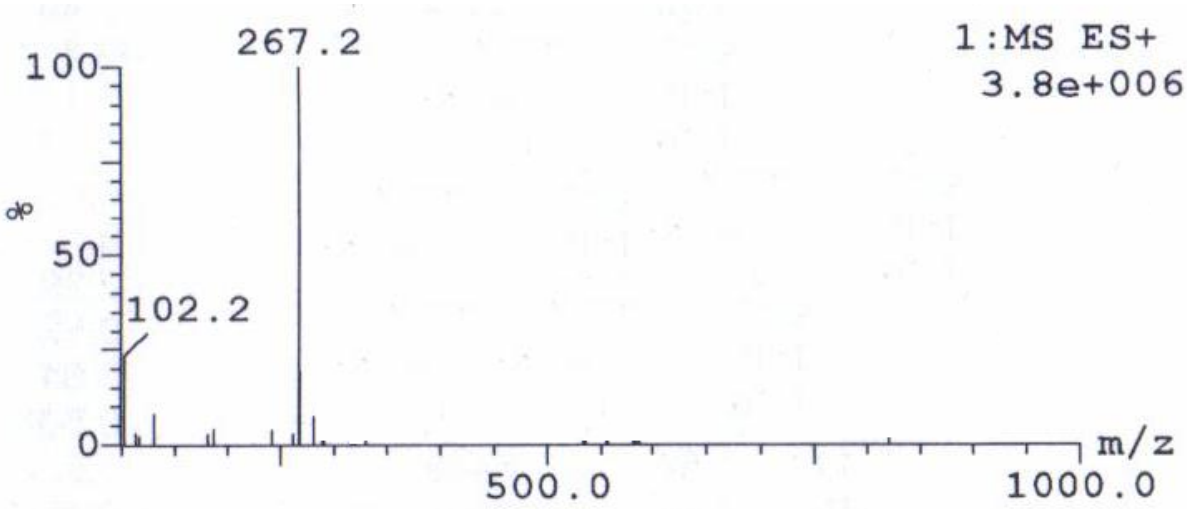
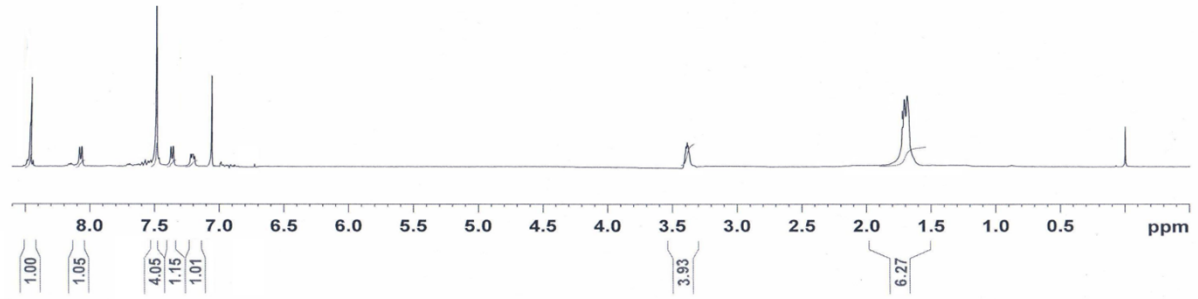
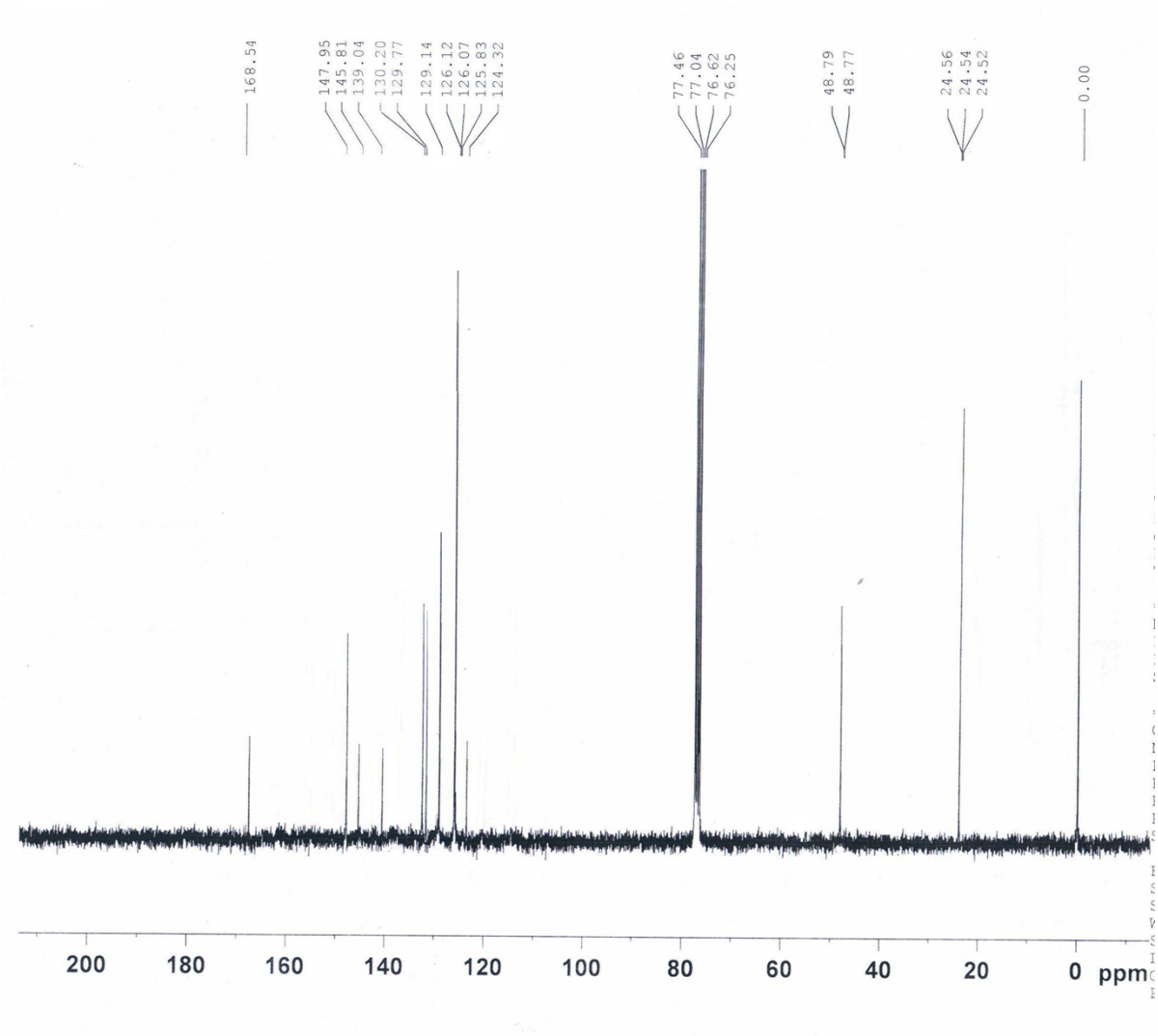
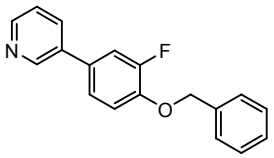
80
70
60
3053.95
2924.49
2853.73
1741.11
1607.20
1554.65
1435.33
1368.26
1275.80
1170.17
1112.97
1024.61
1000.15
885.64
851.01
807.27
760.60
695.22
643.55
532.60
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1


1:MS ES+
3.8e+006
267.2
102.2
100
50
0
%
500.0
1000.0
m/z


8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.00
1.05
4.05
1.15
1.01
3.93
6.27

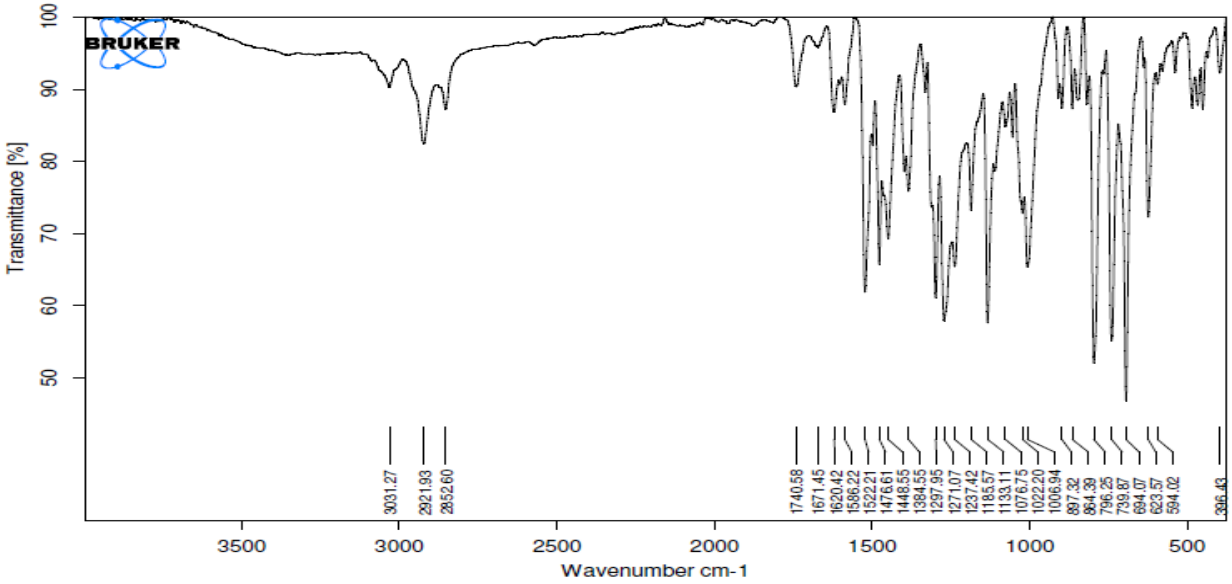


SI-13 Spectral characterisation of compound 3j.



(3j) 3-(4-(benzyloxy)-3-fluorophenyl)pyridine

3j) 3-(4-(benzyloxy)-3-fluorophenyl)pyridine : IR (cm^{-1},neat) 3031, 2852, 1297, 1022 ; 1HNMR (400 MHz, CDCl3) 8.58 (s, 1H), 8.37-8.35 (d, J= 10.8, 1H), 8.05 (m, 2H), 7.95(m, 2H), 7.85 (m, 2H), 7.65(t,1H), 7.50(t,1H), 6.95(m, 1H),6.75(d, J= 8.4Hz, 1H), 5.12(s, 2H); LCMS (MM:ES+APCI) 280.3$(M+H)^+$; Anal.Calcd for $C_{18}H_{14}FNO$: C 77.40; H 5.05; N 5.01. Found: C, 78.88; H, 5.65; N, 4.98.


BRUKER
Transmittance [%]
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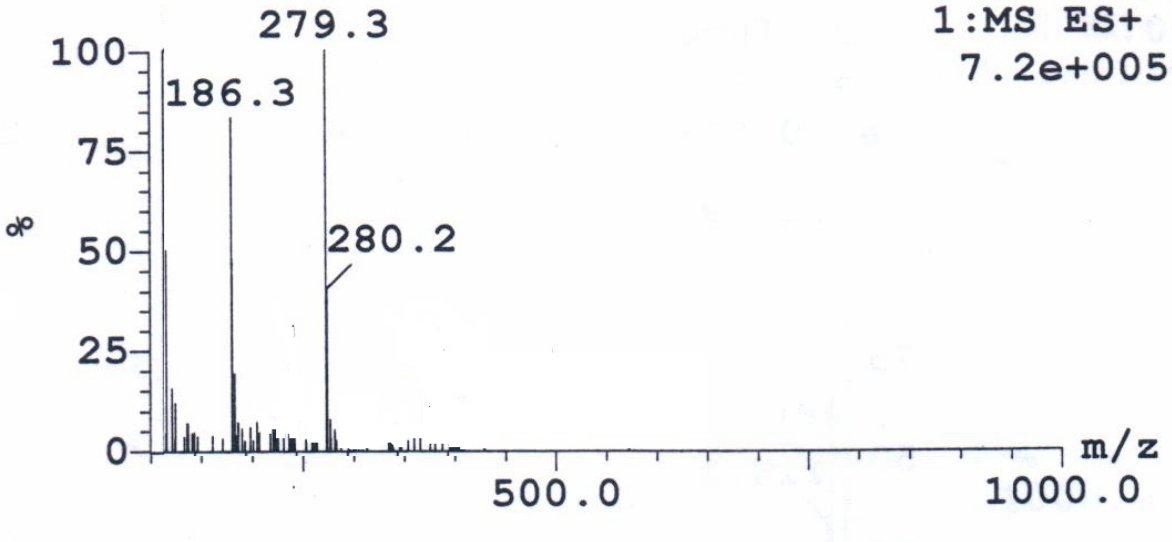
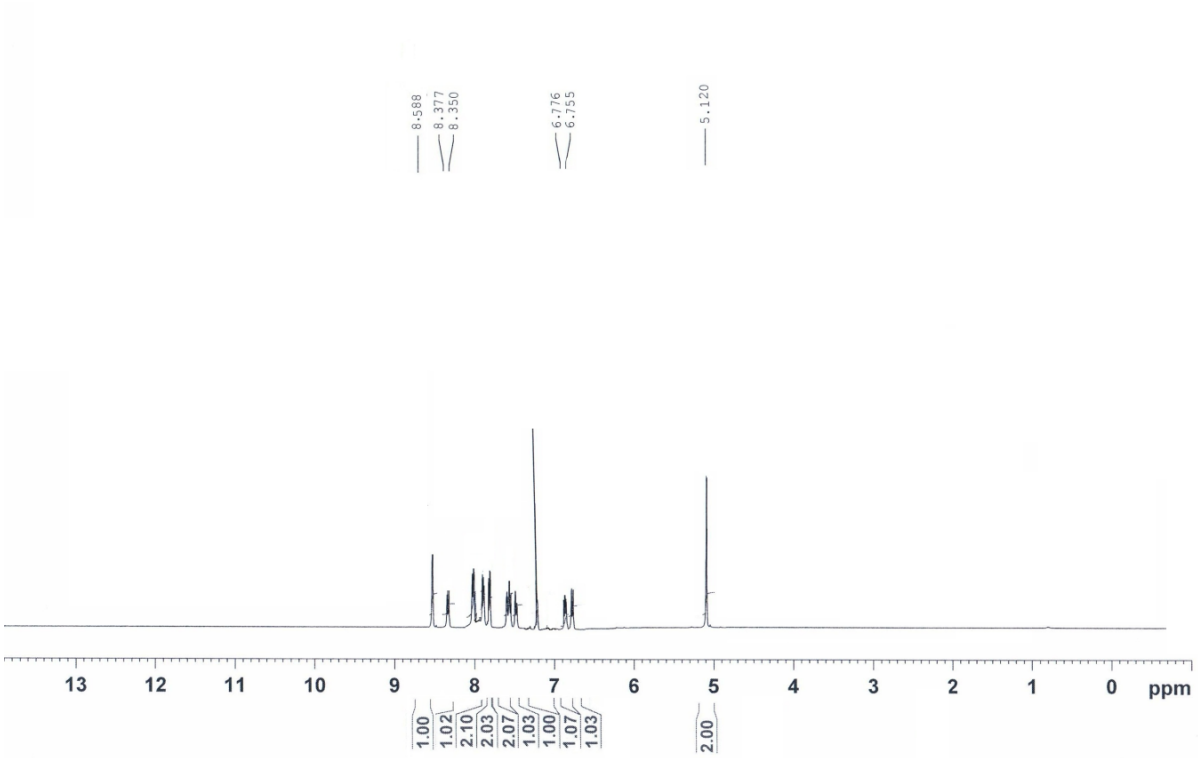
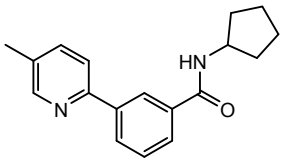
80
70
60
50
3031.27
2921.93
2852.60
1740.58
1671.45
1620.42
1586.22
1522.21
1476.61
1448.55
1384.55
1297.95
1271.07
1237.42
1185.57
1133.11
1076.75
1022.20
1006.94
897.32
864.39
796.25
739.87
694.07
623.57
594.02
396.43
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1


279.3
1:MS ES+
7.2e+005
100
186.3
75
%
50
280.2
25
0
m/z
500.0
1000.0

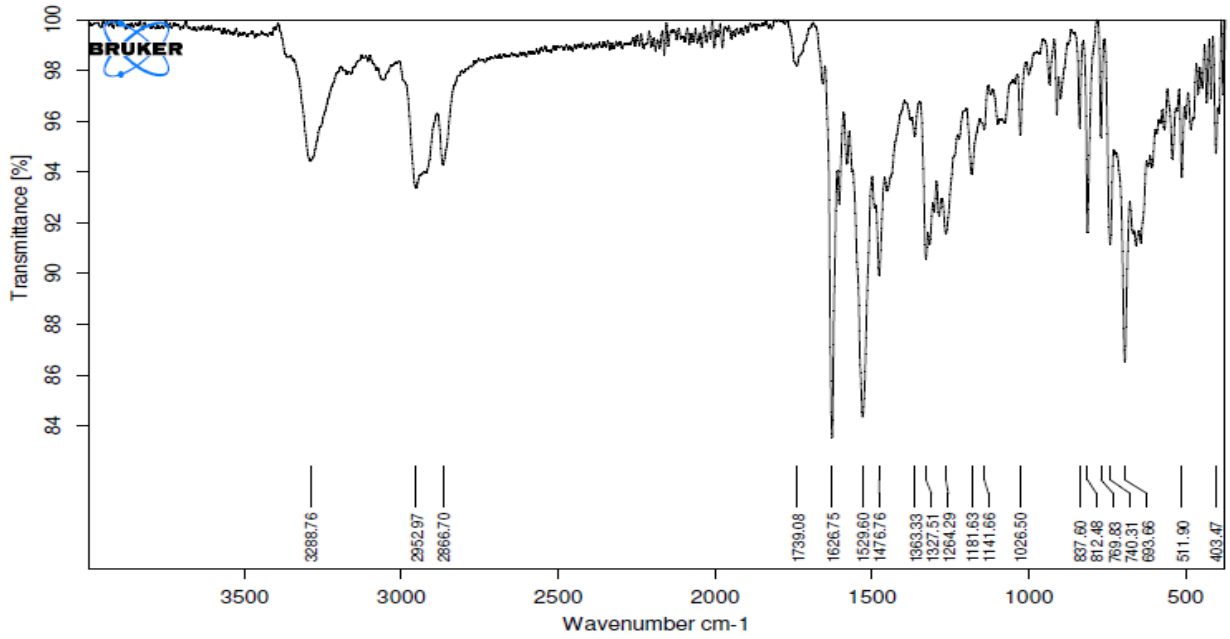


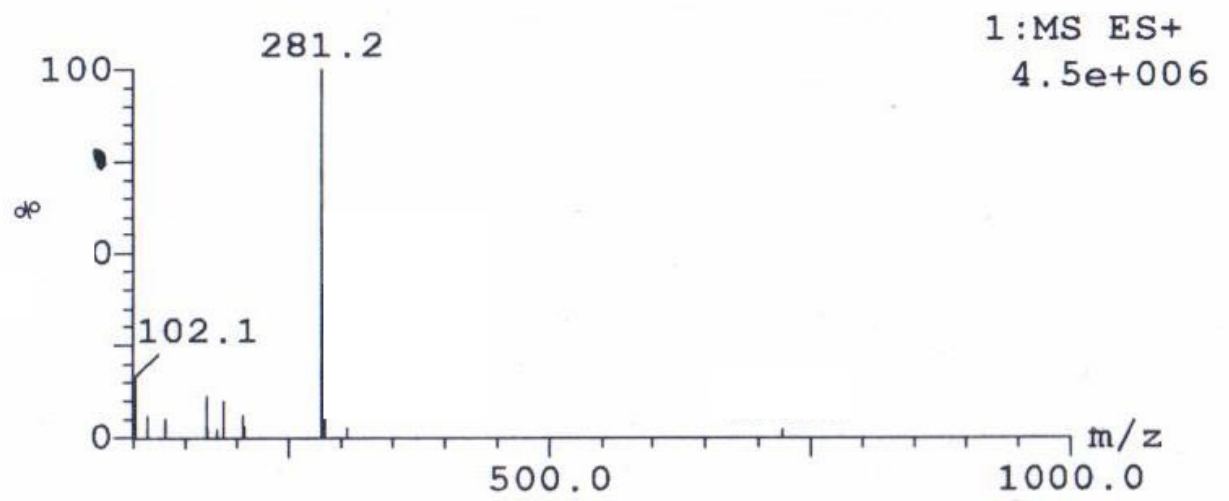
SI-14 Spectral characterisation of compound 3k.



(3k)N-cyclopentyl-3-(5-methylpyridin-2-yl)benzamide

3k) N-cyclopentyl-3-(5-methylpyridin-2-yl)benzamide : IR (cm^{-1},neat) 3288, 2952, 1739, 1626; 1HNMR (400 MHz, CDCl3) 8.30 (s, 1H), 8.00(d, 1H), 7.80(d, 1H), 7.60 -7.50(m, 2H), 7.40(m, 2H), 4.45-4.30(m,1H), 2.35(s,3H), 2.10-1.95(m, 2H),1.75-1.30(m, 4H), 1.30-1.10(m, 2H); 13CNMR (75 MHz, CDCl3) 167.20, 149.56, 138.99, 138.05, 135.54, 132.85, 130.38, 129.04, 128.50, 126.84, 124.94, 51.81, 33.22, 33.15, 23.88, 23.82, 18.20.LCMS (MM:ES+APCI) 281.2$(M+H)^+$


BRUKER
Transmittance [%]
100
98
96
94
92
90
88
86
84
3288.76
2952.97
2866.70
1739.08
1626.75
1529.60
1476.76
1363.33
1327.51
1264.29
1181.63
1141.66
1026.50
837.60
812.48
769.83
740.31
693.66
511.90
403.47
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1


1:MS ES+
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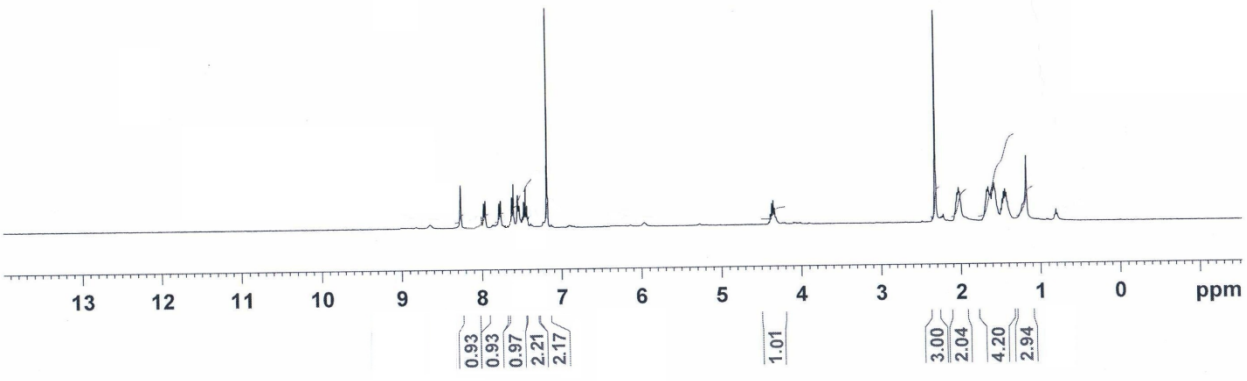
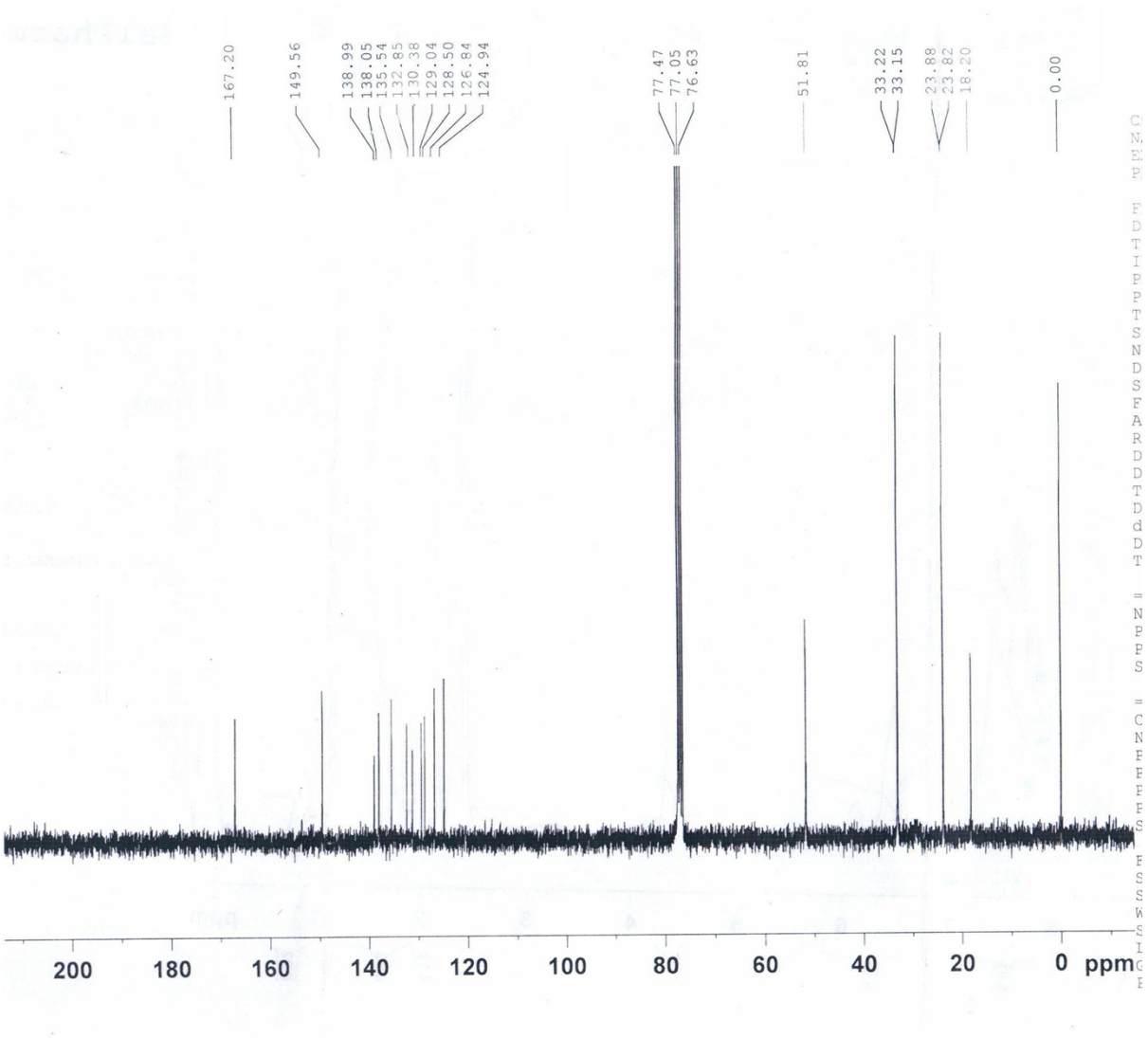
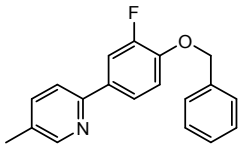
281.2
100
%
0
102.1
0
m/z
500.0
1000.0


13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.93
0.93
0.97
2.21
2.17
1.01
3.00
2.04
4.20
2.94

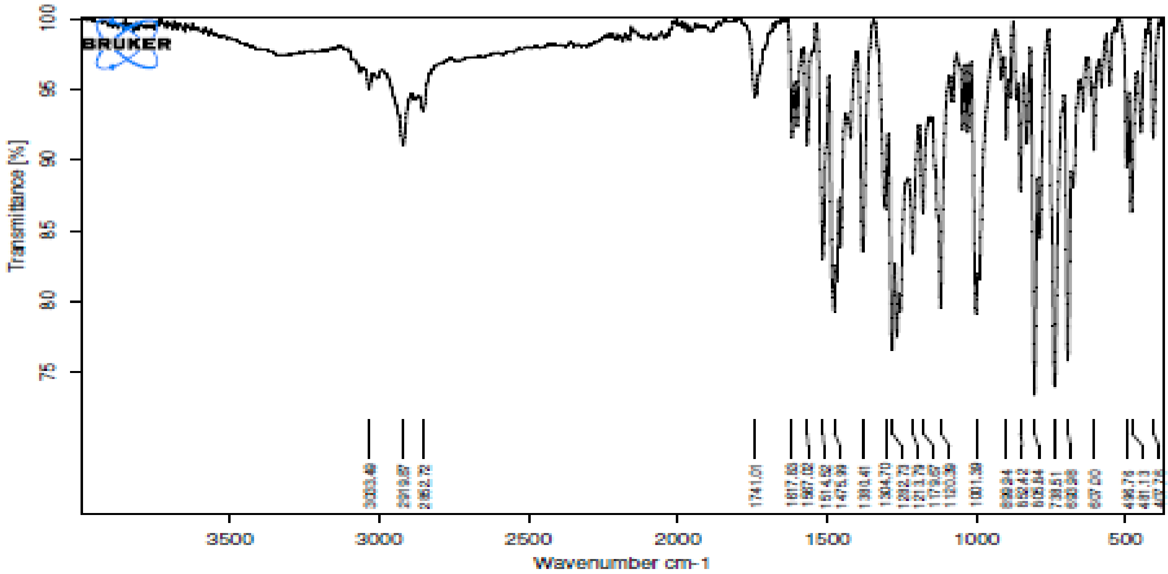


SI-15 Spectral characterisation of compound 3l.



(3l) 2-(4-(benzyloxy)-3-fluorophenyl)-5-methylpyridine

3l) 2-(4-(benzyloxy)-3-fluorophenyl)-5-methylpyridine : IR (cm^{-1},neat) 3033,2919,2852, 1179,1001; 1HNMR (400 MHz, CDCl3) 8.54-8.48 (m, 1H), 7.79-7.73(dd, 1H), 7.71-7.66(m, 1H), 7.60-7.55(m, 2H), 7.49-7.44(m, 2H), 7.43-7.38(m,2H), 7.36-7.32(m,1H), 7.11-7.05(t, 1H),5.20(s, 2H), 2.40(s, 3H); 13CNMR (75 MHz, CDCl3) 149.44,137.95, 136.35, 131.75, 128.64, 128.17, 127.46, 122.53, 122.48, 119.66, 115.60, 114.83, 114.56, 71.34, 18.13.LCMS (MM:ES+APCI) 294.5$(M+H)^+$



BRUKER
Transmittance [%]
100
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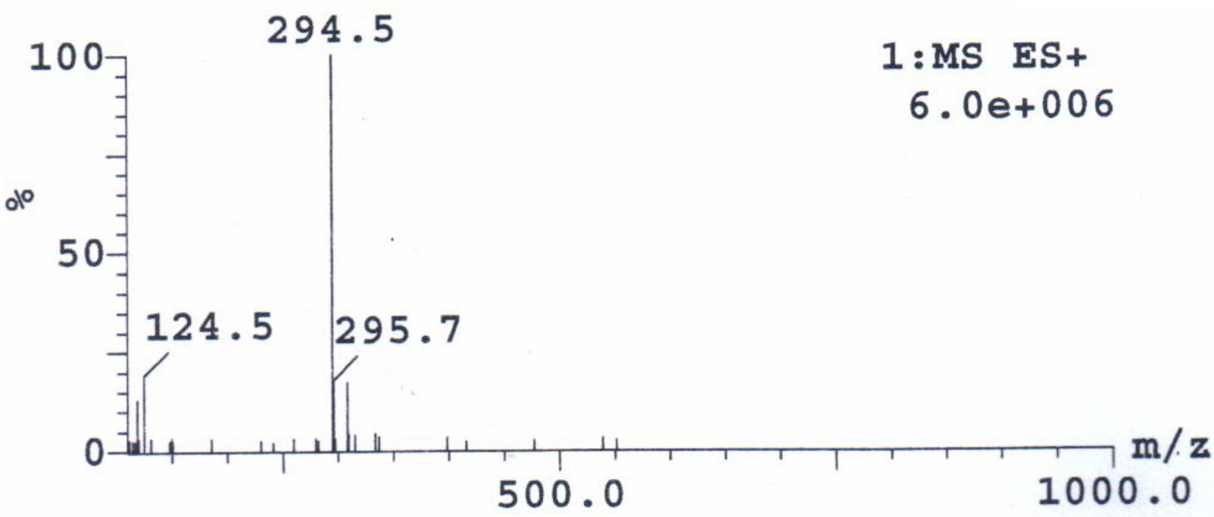
90
85
80
75
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1



294.5
1:MS ES+
6.0e+006
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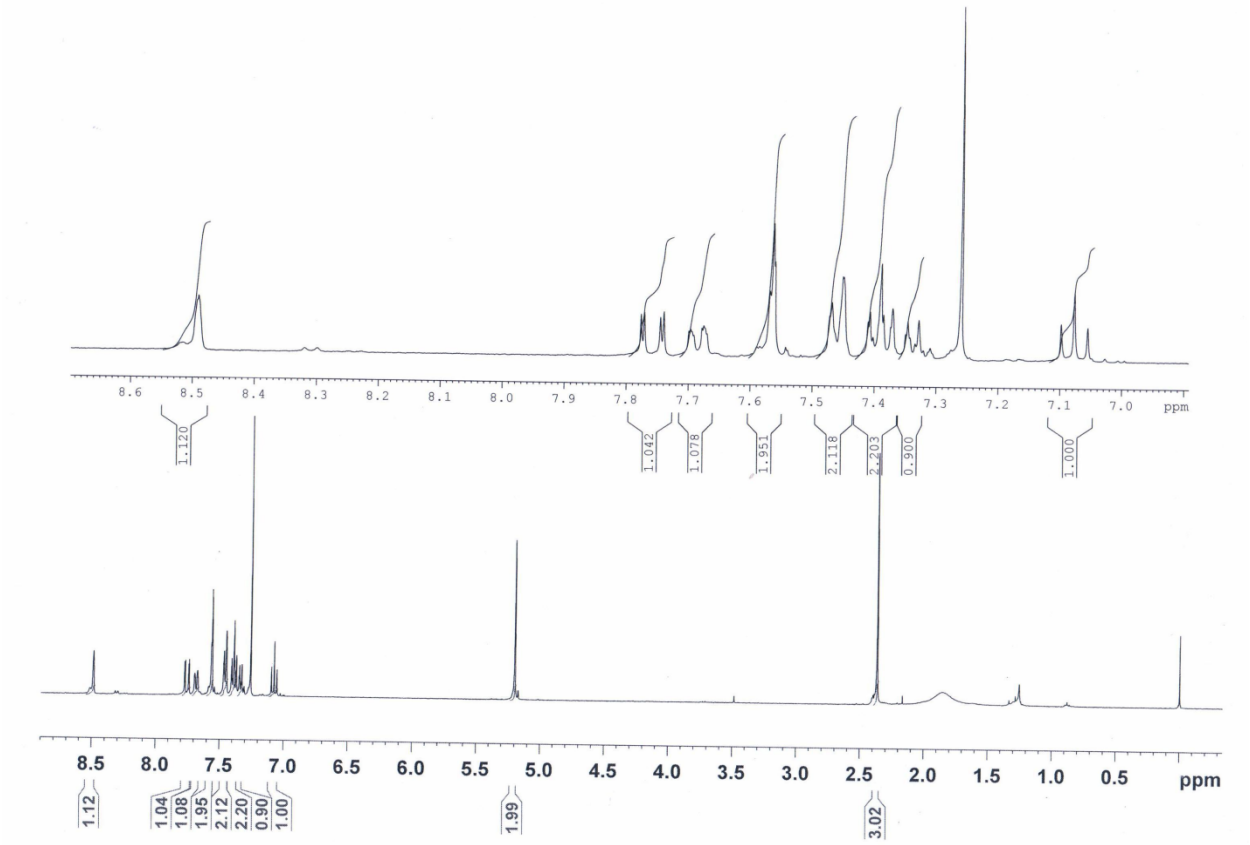
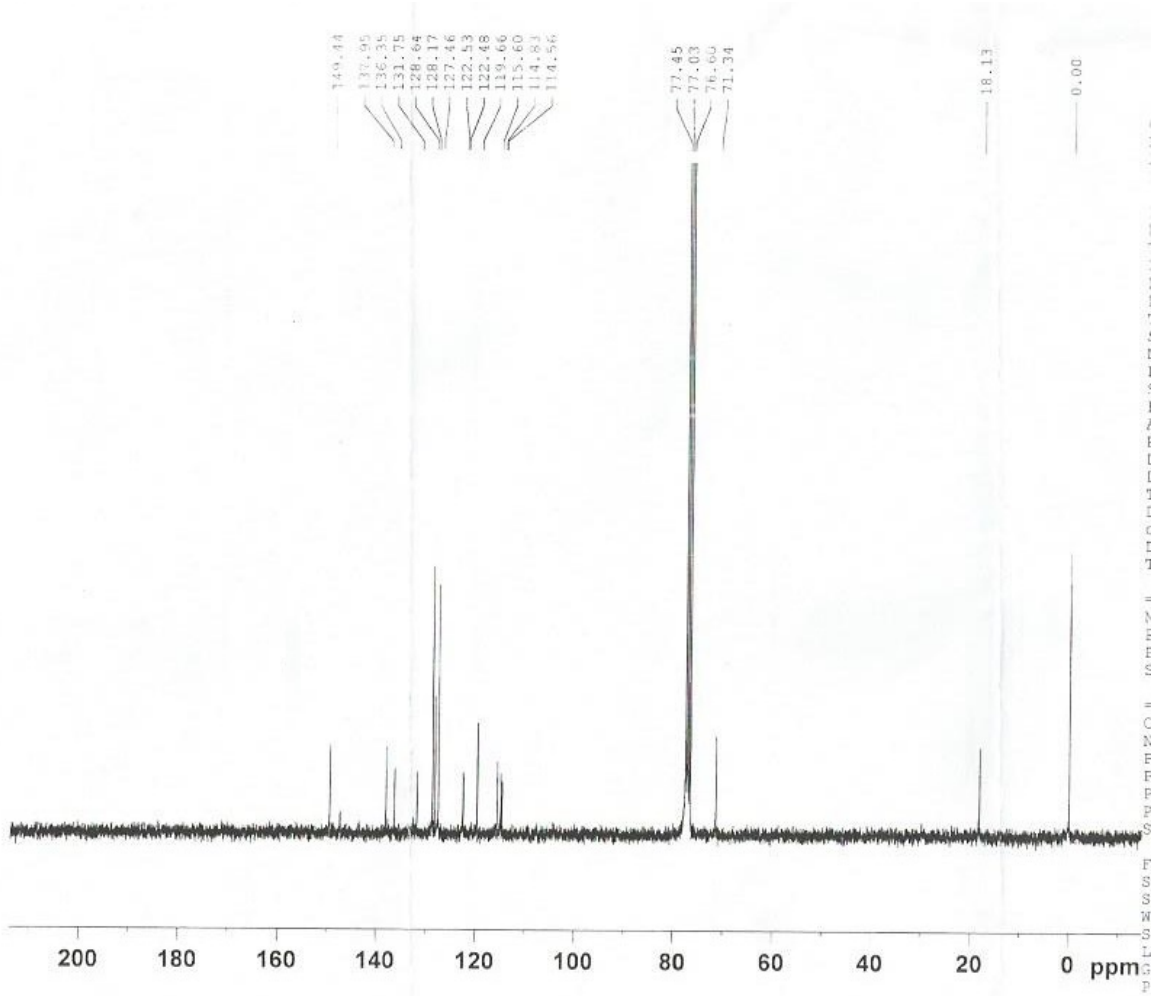
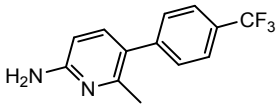
%
50
124.5
295.7
0
500.0
1000.0
m/z


8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 ppm
1.120
1.042
1.078
1.951
2.118
2.203
0.900
1.000
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.12
1.04
1.08
1.95
2.12
2.20
0.90
1.00
1.99
3.02

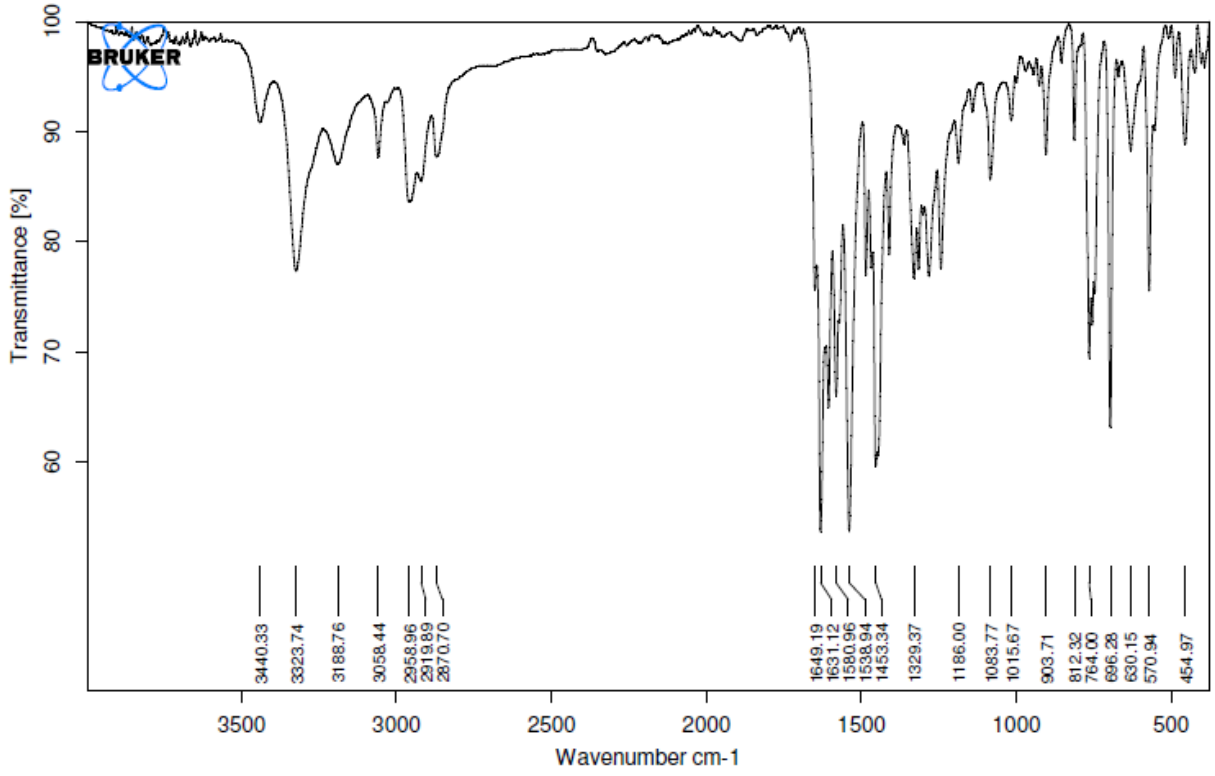


SI-16 Spectral characterisation of compound 3m.



(3m) 6-methyl-5-(4-(trifluoromethyl)phenyl)pyridin-2-amine

3m) 6-methyl-5-(4-(trifluoromethyl)phenyl)pyridin-2-amine : IR (cm^{-1},neat) 3440, 3058, 2919, 1631; 1HNMR (400 MHz, CDCl3) 7.55 (d, 1H), 7.50-7.35(q, 4H), 6.30(d, 1H), 4.70-4.40(s, 2H), 2.55(s, 3H); 13CNMR (75 MHz, CDCl3) 155.70,147.35, 139.15, 137.98, 136.03, 128.80, 127.67,121.18, 114.50, 24.59.LCMS (MM:ES+APCI) 253.2$(M+H)^+$; Anal.Calcd for $C_{13}H_{11}F_3N_2$: C 61.90; H 4.40; N 11.11. Found: C, 62.99; H, 5.18; N, 12.03.


BRUKER
Transmittance [%]
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80
70
60
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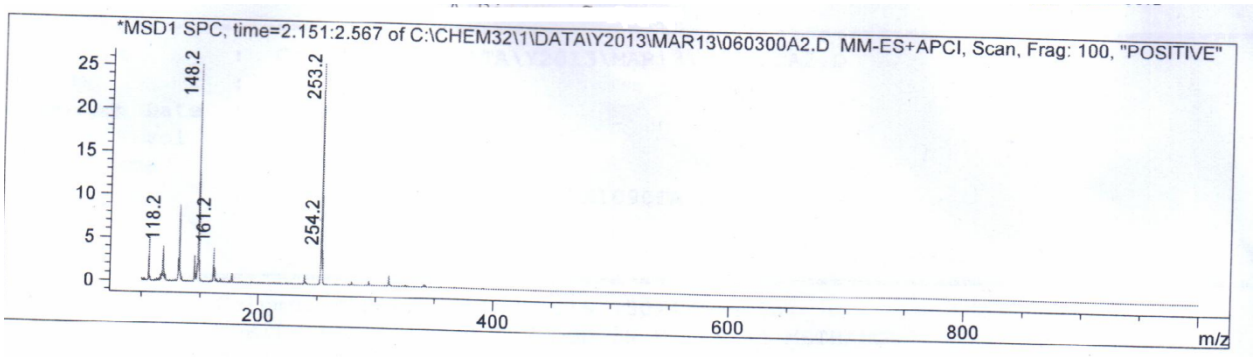
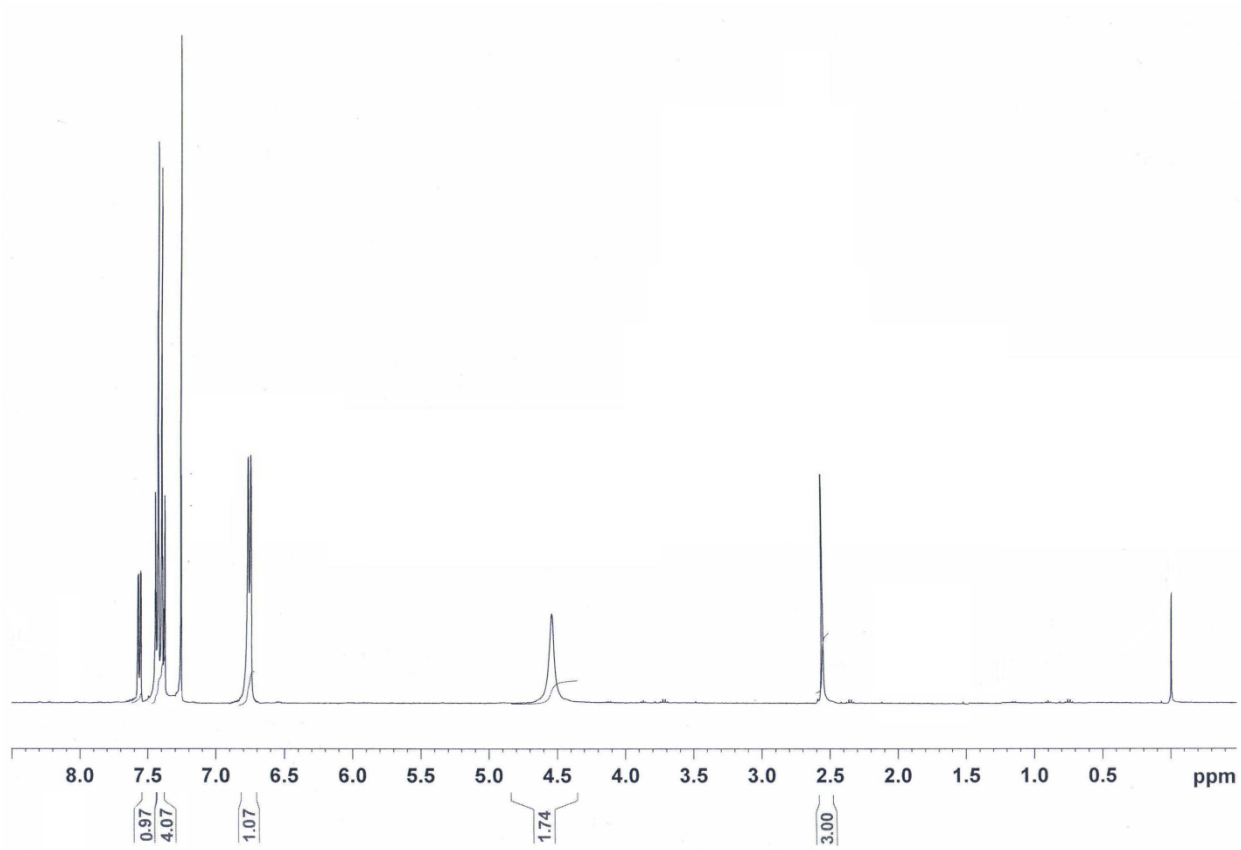
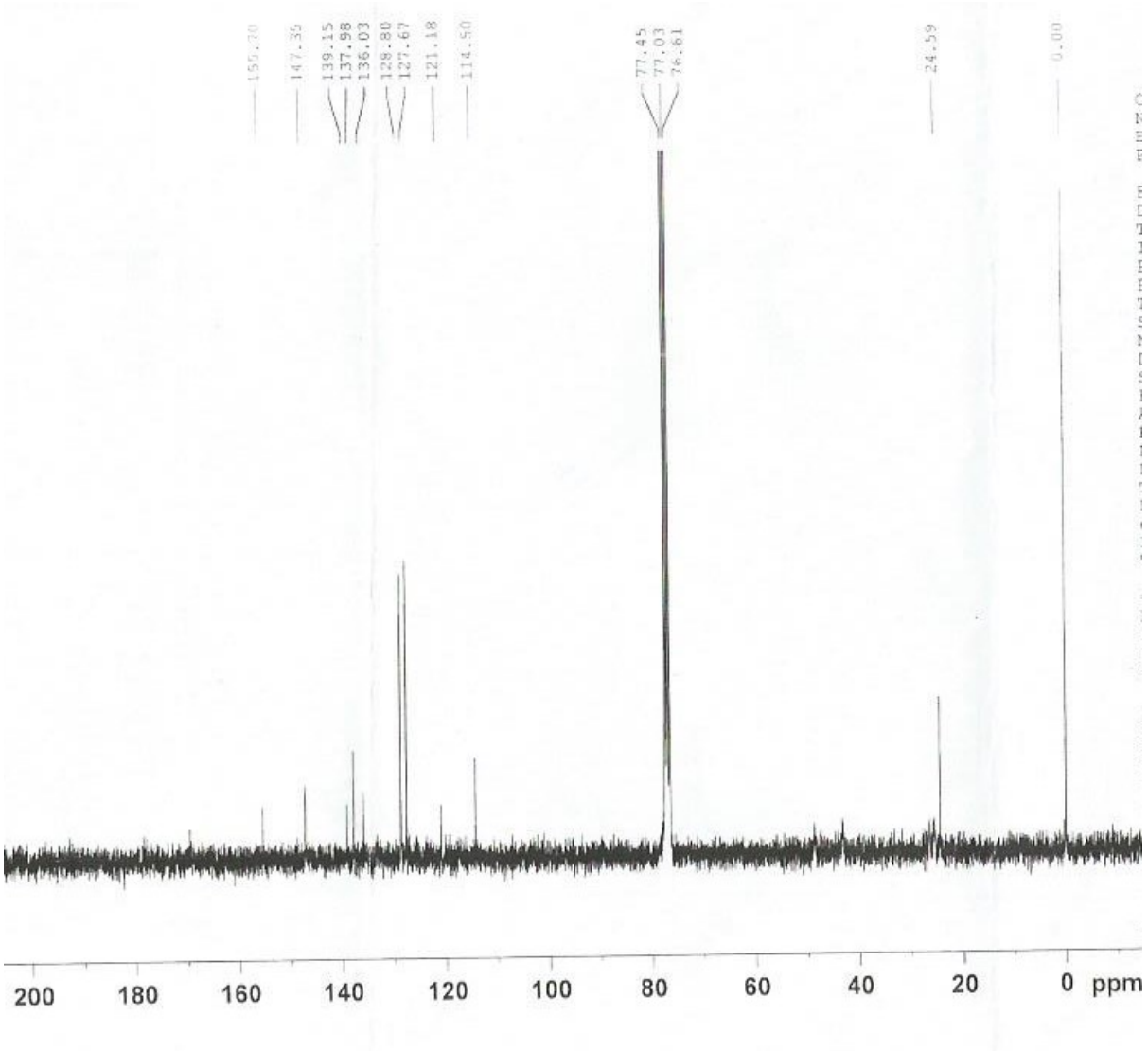
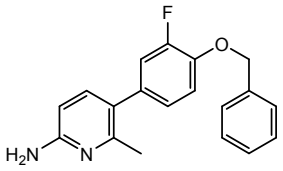
3323.74
3188.76
3058.44
2958.96
2919.89
2870.70
1649.19
1631.12
1580.96
1538.94
1453.34
1329.37
1186.00
1083.77
1015.67
903.71
812.32
764.00
696.28
630.15
570.94
454.97
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1


*MSD1 SPC, time=2.151:2.567 of C:\CHEM32\1\DATA\Y2013\MAR13\060300A2.D MM-ES+APCI, Scan, Frag: 100, "POSITIVE"
25
20
15
10
5
0
148.2
253.2
118.2
161.2
254.2
200
400
600
800
m/z


8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.97
4.07
1.07
1.74
3.00

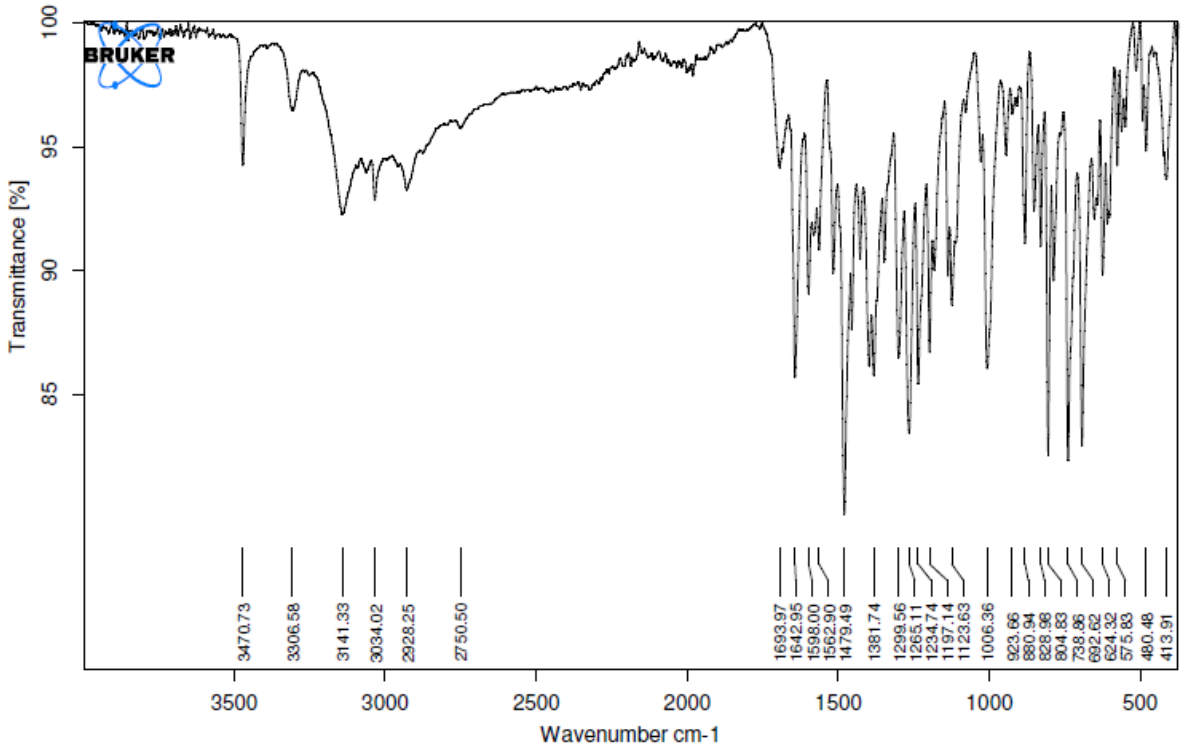


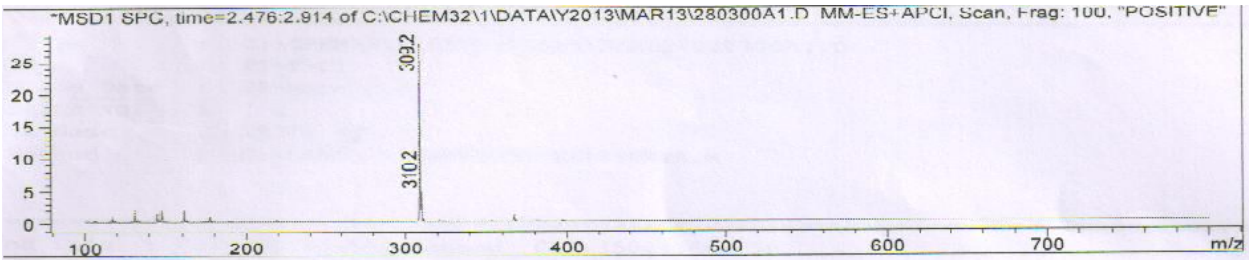
SI-17 Spectral characterisation of compound 3n.

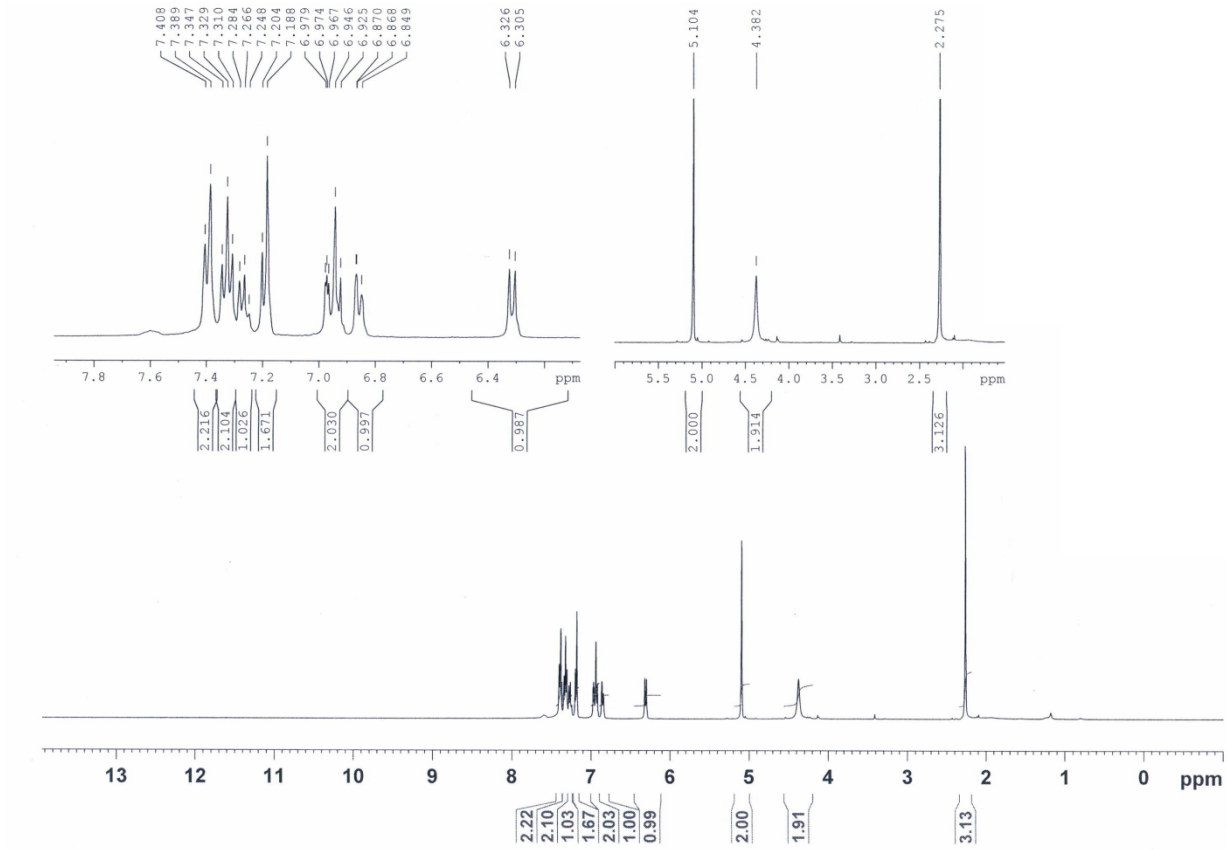


(3n) 5-(4-(benzyloxy)-3-fluorophenyl)-6-methylpyridin-2-amine

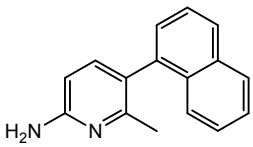
3n) 5-(4-(benzyloxy)-3-fluorophenyl)-6-methylpyridin-2-amine : IR (cm^{-1},neat) 3470, 3141, 2928, 1643, 1299, 1006 ; 1HNMR (400 MHz, CDCl3) 7.41-7.39 (m, 2H), 7.35-7.31(t, J=7.2, 2H), 7.28-7.25(m, 1H),7.20-7.19(m, 1H), 6.98-6.92(m, 2H), 6.87-6.85(m,1H), 6.33-6.31(d, J=8.4,1H), 5.10(s, 2H), 4.38(s, 2H), 2.28(s, 3H); LCMS (MM:ES+APCI) 309.2$(M+H)^+$; Anal.Calcd for $C_{19}H_{17}FN_2O$: C 74.01; H 5.56; N 9.08. Found: C, 75.02; H, 5.77; N, 8.86.


BRUKER
Transmittance [%]
100
95
90
85
3470.73
3306.58
3141.33
3034.02
2928.25
2750.50
1693.97
1642.95
1598.00
1562.90
1479.49
1381.74
1299.56
1265.11
1234.74
1197.14
1123.63
1006.36
923.66
880.94
828.98
804.83
738.86
692.62
624.32
575.83
480.48
413.91
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1


"MSD1 SPC, time=2.476:2.914 of C:\CHEM32\1\DATA\Y2013\MAR13\280300A1.D MM-ES+APCI, Scan, Frag: 100, "POSITIVE"
309.2
310.2
25
20
15
10
5
0
100
200
300
400
500
600
700
m/z

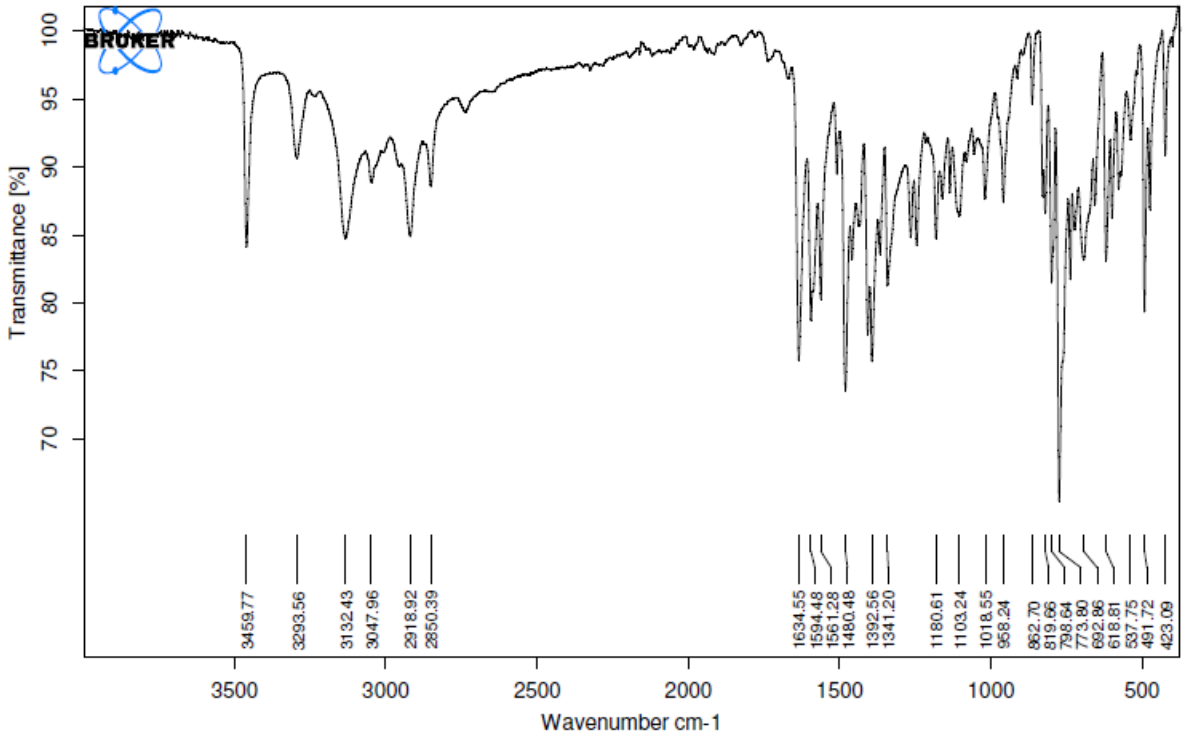


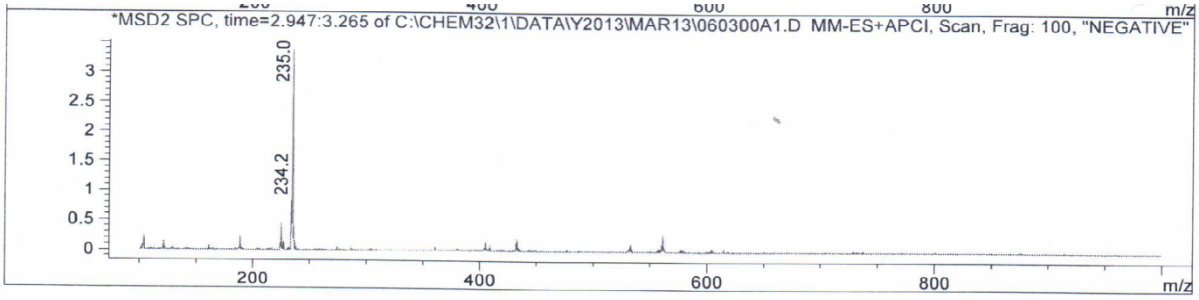
SI-18 Spectral characterisation of compound 3o.

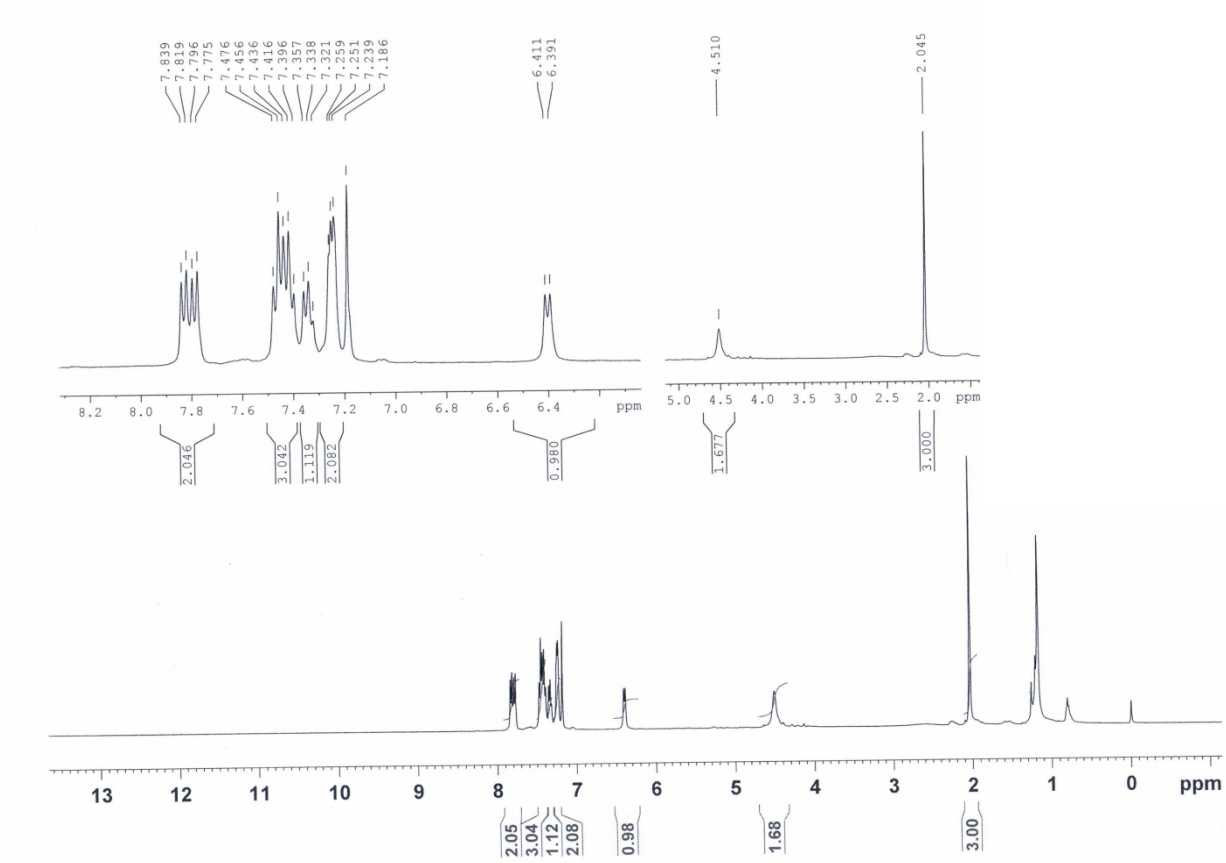


(3o) 6-methyl-5-(naphthalen-1-yl)pyridin-2-amine

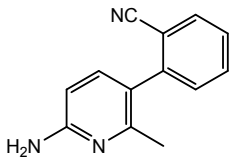
3o) 6-methyl-5-(naphthalen-1-yl)pyridin-2-amine: IR (cm^{-1},neat) 3459, 3132, 2918, 1634; 1HNMR (400 MHz, CDCl3) 7.84-7.78 (dd, J_1=8, J_2=8.4, 2H), 7.48-7.40(m, 3H), 7.36-7.32(t, J=6.8, 1H),7.26-7.24(m, 1H), 7.19(s, 1H), 6.41-6.39(d, J=8, 1H), 4.51(s,2H), 2.05(s, 3H); LCMS (MM:ES+APCI) 235.3$(M+H)^+$; Anal.Calcd for $C_{17}H_{15}N$: C 87.52; H 6.48; N 6.00. Found: C 87.88; H 6.99; N 5.94.


BRUKER
Transmittance [%]
100
95
90
85
80
75
70
3459.77
3293.56
3132.43
3047.96
2918.92
2850.39
1634.55
1594.48
1561.28
1480.48
1392.56
1341.20
1180.61
1103.24
1018.55
958.24
862.70
819.66
798.64
773.80
692.86
618.81
537.75
491.72
423.09
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1


*MSD2 SPC, time=2.947:3.265 of C:\CHEM32\1\DATA\Y2013\MAR13\060300A1.D MM-ES+APCI, Scan, Frag: 100, "NEGATIVE"
m/z
235.0
234.2
3
2.5
2
1.5
1
0.5
0
200
400
600
800
m/z

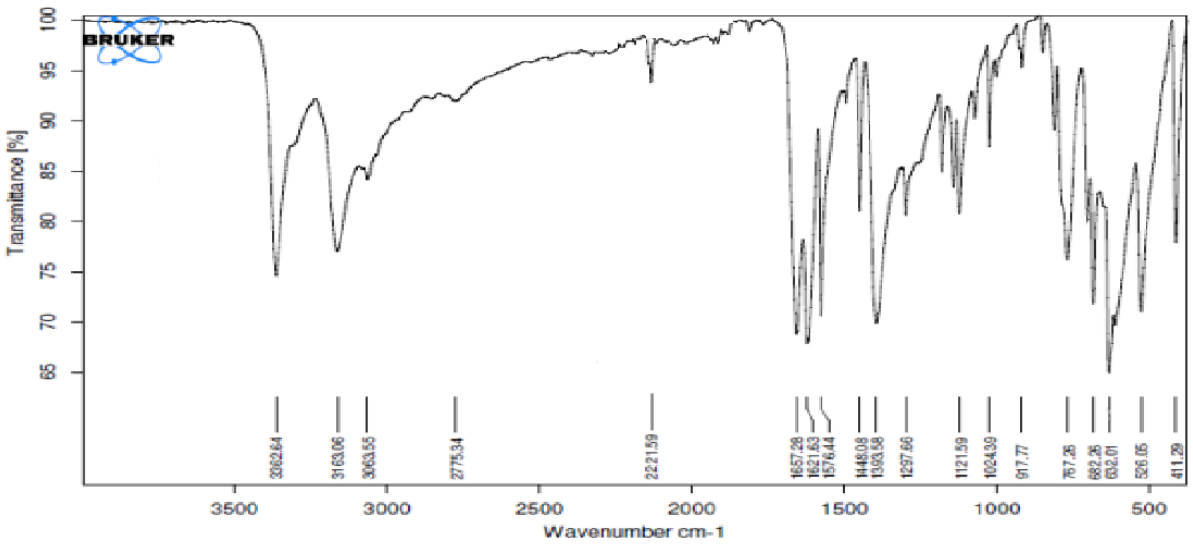


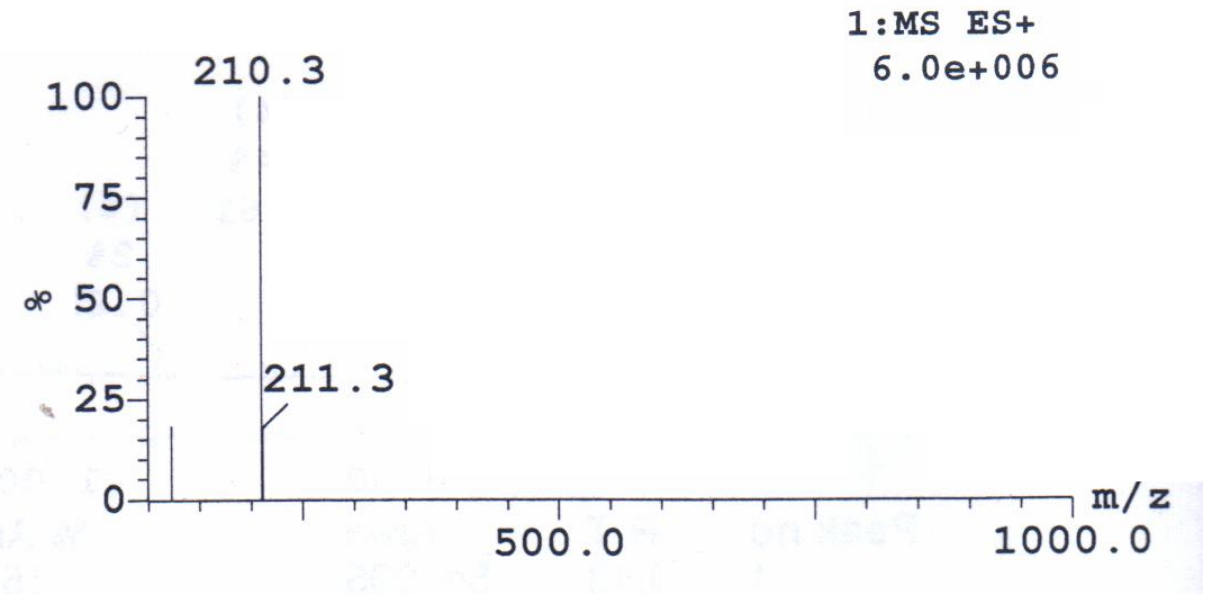
SI-19 Spectral characterisation of compound 3p.

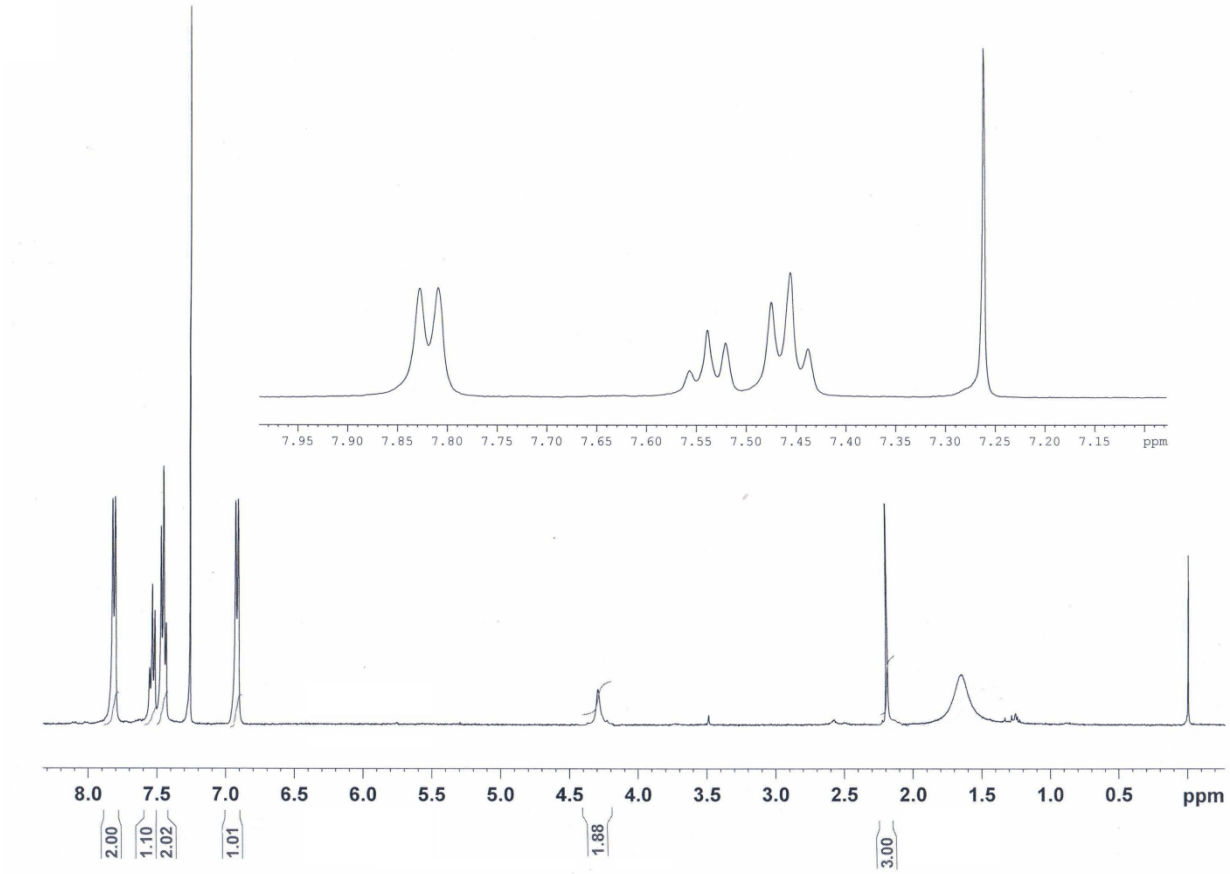


3p) 2-(6-amino-2-methylpyridin-3-yl)benzonitrile

3p) 2-(6-amino-2-methylpyridin-3-yl)benzonitrile : IR (cm^{-1},neat) 3362, 3163, 2200, 1621; 1HNMR (400 MHz, CDCl3) 7.85-7.80 (d, 2H), 7.58-7.52(t, 1H), 7.50-7.42(t, 2H),6.95 (d, 1H), 4.30(s, 2H), 2.10(s, 3H); LCMS (MM:ES+APCI) 210.3$(M+H)^+$; Anal.Calcd for $C_{13}H_{11}N_3$: C 74.62; H 5.30; N 20.08. Found: C 75.66; H 5.17; N 20.54.


BRUKER
Transmittance [%]
100
95
90
85
80
75
70
65
3062.64
3163.06
3063.55
2775.34
2221.59
1657.28
1621.53
1576.44
1448.08
1393.58
1297.66
1121.59
1024.39
917.77
767.25
682.25
632.01
526.05
411.29
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1


1:MS ES+
6.0e+006
210.3
211.3
100
75
%
50
25
0
500.0
1000.0
m/z


7.95 7.90 7.85 7.80 7.75 7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30 7.25 7.20 7.15 ppm
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.00
1.10
2.02
1.01
1.88
3.00