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Supporting Information

Iridium/Graphene Nanostructured Catalyst for the N-Alkylation of Amines to Synthesize Nitrogen-containing Derivatives and Heterocyclic Compounds in Green Process

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I. Characterization of the Catalyzed Products.

*N-benzylaniline (**1a**)*. It was obtained as yellow oil, yield 92 % (169 mg); ^{1}H NMR ($CDCl_3$, 600MHz) δ (ppm) = 7.37-7.32 (m, Ar, 4H), 7.27-7.24 (m, Ar, 1H), 7.18-7.15 (m, Ar, 2H), 6.72-6.69 (t, Ar, 1H), 6.64-6.62 (d, Ar, 2H, JHH = 7.8Hz), 4.32 (s, CH2, 2H), 4.01 (br. s, NH, 1H). ^{13}C NMR ($CDCl_3$, 150MHz) δ (ppm) = 148.1, 139.3, 129.2, 128.6, 127.4, 127.2, 117.5, 112.7, 48.2. HRMS (ESI/APCI): *m/z* =184.1114 g/mol, calc'd. for $C_{13}H_{14}N$: 184.1121 g/mol. FTIR IR (ATR): ν = 3410(w), 3022 (w), 1604 (m), 1507 (m), 1320 (w), 1261 (m), 731(s) cm^{-1}

*N-(4-methoxybenzyl)aniline (**1b**)*. It was obtained as yellow oil, yield 93 % (199mg); ^{1}H NMR ($CDCl_3$, 600MHz) δ (ppm) = 7.28-7.26 (d, JHH = 8.4Hz, 2H, Ar), 7.17-7.14 (m, 2H, Ar), 6.87-6.85 (m, 2H, Ar), 6.71-6.68 (t, 1H, Ar), 6.62-6.61 (m, 2H, Ar), 4.23 (br. s, NH, 1H), 3.90 (d, JHH = 13.2Hz, 1H) , 3.78 (s, 3H). .^{13}C NMR ($CDCl_3$, 150MHz) δ (ppm) = 158.8, 148.1, 131.3, 129.2, 128.7, 117.4, 113.9, 112.7, 55.2, 47.7. HRMS (ESI/APCI): *m/z* = 214.1222 g/mol, calc'd. for $C_{14}H_{16}NO$ $[M]^{+}$: 214.1226 g/mol. FTIR IR (ATR): ν = 3410 (w), 3029 (w), 2835 (w), 1604(s), 1507 (s), 1238(s),1171(m) ,1029 (m), 820 (m), 746 (s) cm^{-1}.

*N-(p-chlorobenzyl)aniline (**1c**)*. It was obtained as colorless oil, yield 85 % (185mg); ^{1}H NMR ($CDCl_3$, 600MHz) δ (ppm) = 7.28 (s, 3H, Ar), 7.16-7.13 (m, 2H, Ar), 6.72-6.69 (m, 1H, Ar), 6.59-6.58 (m, 2H, Ar), 4.29(d, 2H, JHH = 5.4Hz), 4.04 (br. s, NH, 1H). ^{13}C NMR

($CDCl_3$, 150MHz) δ (ppm) = 147.7, 137.9, 132.8, 129.2, 128.7, 128.6, 117.7, 112.8, 47.5. HRMS (ESI/APCI): *m/z* = 218.0731 g/mol, calc'd. for $C_{13}H_{13}NCl$ $[M]^+$: 218.0731 g/mol. FTIR IR (ATR): ν = 3417 (w), 3044 (w), 2843 (w), 1604(s), 1499 (s),1320(m),1253(m) ,1089 (m), 813(m), 746 (s) cm^{-1}.

*benzyl(4-methoxyphenyl)amine (**1d**)*. It was obtained as yellow oil, yield 90 % (193mg); ^1H NMR ($CDCl_3$, 600MHz) δ (ppm) = 7.36-7.31 (m, Ar, 4H), 7.26-7.24 (t, Ar, 1H), 6.76-6.75 (m, Ar, 2H), 6.58-6.59 (m, Ar, 2H), 4.26 (s, CH2, 2H), 3.72 (s, CH3, 3H).^{13}C NMR ($CDCl_3$, 150MHz) δ (ppm) = 152.1, 142.4, 139.6, 128.57, 127.52, 127.15, 114.8, 114.0, 55.7, 49.2. HRMS (ESI/APCI): *m/z* = 214.1222 g/mol, calc'd. for $C_{14}H_{16}NO$ $[M]^+$: 214.1226 g/mol. FTIR IR (ATR): ν = 3402 (w), 3029 (w), 2835 (w), 1514(s), 1231 (s), 1178 (w), 1029 (m), 820 (m), 738 (m) cm^{-1}.

*N-(4-chlorophenyl)benzylamine (**1e**)*. It was obtained as ellow oil, yield 80 % (174mg); ^1H NMR ($CDCl_3$, 600MHz) δ (ppm) = 7.33-7.19 (m, Ar, 4H), 7.10-7.06 (m, Ar, 2H), 6.54-6.51 (m, Ar, 2H), 4.61 (s, 1H), 4.29-4.28 (d, CH2 ,2H, JHH = 6.0Hz), 4.04(br. s, NH, 1H). ^{13}C NMR ($CDCl_3$, 150MHz) δ (ppm) = 146.6, 138.9, 128.9, 128.6, 127.39, 127.35, 127.0, 126.5, 122.0, 113.8 ,54.4, 48.3. HRMS (ESI/APCI): *m/z* = 218.07311 g/mol, calc'd. for $C_{13}H_{13}NCl$ $[M]^+$: 218.07310 g/mol. FTIR IR (ATR): ν = 3410 (w), 3029 (w), 2850 (w), 1596(s), 1499 (s), 1313 (m) 1178 (w), 1089 (w), 813 (m), 731 (m) cm^{-1}.

*N-Benzyl-3,5-dimethoxyaniline (**1f**)*. It was obtained as yellow oil, yield 90 % (219mg); ^1H

NMR ($CDCl_3$, 600MHz) δ (ppm) = 7.34-7.30 (m, Ar, 4H), 7.26-7.24 (t, Ar, 1H), 5.877-5.870 (m, Ar, 1H), 5.817-5.814(d, Ar, 2H, JHH = 1.8Hz), 4.28 (s, CH2, 2H), 4.03 (br. s, NH, 1H), 3.71 (s, 6H,). ^{13}C NMR ($CDCl_3$, 150MHz) δ (ppm) = 161.6, 150.0, 139.2, 128.6, 127.5, 127.2, 91.6, 89.8, 55.1, 48.3. HRMS (ESI/APCI): *m/z* =244.1333 g/mol, calc'd. for $C_{15}H_{18}O_2N$ $[M]^+$: 244.1332 g/mol. FTIR IR (ATR): ν = 3402 (w), 3007 (w), 2843 (w), 1596(s), 1455 (m),1201(s),1149(s) ,1067 (m), 805(m), 731 (m) cm^{-1}.

*N-benzyl-(2-fluorophenyl)amine (**1g**)*. It was obtained as yellow oil, yield 87 % (176mg); ^1H NMR ($CDCl_3$, 600MHz) δ (ppm) = 7.37-7.32 (m, Ar, 4H), 7.28-7.24 (m, Ar, 1H), 6.98-6.92 (m, Ar, 2H), 6.67-6.64 (m, Ar, 1H), 6.63-6.59 (m, Ar, 1H), 4.36-4.35 (d, 2H , JHH = 5.4Hz), 4.30 (br. s, NH, 1H). ^{13}C NMR ($CDCl_3$, 150MHz) δ (ppm) = 152.2, 150.6, 138.9, 136.5, 128.6, 127.3, 124.5 , 116.7, 114.4, 114.2, 112.2 , 47.8. HRMS (ESI/APCI): *m/z* = 202.1020 g/mol, calc'd. for $C_{13}H_{13}NF$ $[M]^+$: 202.1027 g/mol. FTIR IR (ATR): ν = 3432(w), 3029(w) , 2925(w), 1619(m), 1514(s), 1335(m), 1246(m), 1186(m), 746(s) cm^{-1}.

*N-ethyl-N-phenylamine (**1h**)*. It was obtained as colorless oil, yield 80 % (98mg); ^1H NMR ($CDCl_3$, 600MHz) δ (ppm) = 7.24-7.14 (m, Ar, 2H), 6.68-6.66 (t, Ar, 1H), 6.59-6.58 (d, Ar, 2H, JHH = 7.8Hz), 3.52 (br. s, NH , 1H), 3.10-3.08 (q, 2H), 0.92-0.81 (t, 3H). ^{13}C NMR ($CDCl_3$, 150MHz) δ (ppm) = 148.0, 129.8, 116.5, 112.1, 45.0, 15.6. HRMS (ESI/APCI): *m/z* = 122.0965 g/mol, calc'd. for $C_8H_{12}N$ $[M]^+$: 122.0964 g/mol. FTIR IR (ATR): ν = 3410 (w), 3051 (w),2925 (m), 2857 (m), 1604 (s), 1507 (s), 1462 (s), 1320 (m), 1261 (m),

1149 (m),1029 (s), 746 (s) cm^{-1}.

*N-propylaniline (**1i**)*. It was obtained as colorless oil, yield 68 % (93mg); ^{1}H NMR ($CDCl_3$, 600MHz) δ (ppm) = 7.16-7.14 (m, Ar, 2H), 6.68-6.65 (t, Ar, 1H), 6.60-6.58 (t, Ar, 2H,), 3.61 (br. s, NH, 1H), 3.07-3.05(t, 2H), 1.64-1.60 (m, CH2, 2H), 0.99-0.97 (t, 3H). ^{13}C NMR ($CDCl_3$, 150MHz) δ (ppm) = 148.4, 129.2, 117.0, 112.6, 45.7, 22.7, 11.6. HRMS (ESI/APCI): *m/z* = 136.1120 g/mol, calc'd. for $C_9H_{14}N$ $[M]^+$: 136.1121 g/mol. FTIR IR (ATR): ν = 3410(w), 3022 (w),2962 (w), 2932 (w), 1604 (m), 1507 (m), 1320 (m), 1253 (m) , 1149 (w), 865(w), 746 (m) cm^{-1}

*N-(n-butyl)aniline (**1j**)*. It was obtained as colorless oil, yield 75 % (113mg); ^{1}H NMR ($CDCl_3$, 600MHz) δ (ppm) = 7.16-7.13 (m, Ar, 2H), 6.67-6.65 (m, Ar, 1H), 6.59-6.57 (m, Ar, 2H), 3.56 (br. s, NH, 1H), 3.10-3.07 (t, 2H), 1.61-1.54 (m, 2H), 1.44-1.38 (m, 2H), 0.95-0.92 (t, 3H). ^{13}C NMR ($CDCl_3$, 150MHz) δ (ppm) = 148.5, 129.1, 117.0, 112.6, 43.6, 31.6, 20.2, 13.9. HRMS (ESI/APCI): *m/z* = 150.1274 g/mol, calc'd. for $C_{10}H_{16}N$ $[M]^+$: 150.1277 g/mol. FTIR IR (ATR): ν = 3417 (w), 3051 (w),2932 (m), 2865 (m), 1604 (s), 1507 (s), 1320 (m), 1261 (m), 738 (s) cm^{-1}.

*N-hexylaniline (**1k**)*. It was obtained as colorless oil, yield 72 % (128mg); ^{1}H NMR ($CDCl_3$, 600MHz) δ (ppm) = 7.16-7.13 (m, Ar, 2H), 6.67-6.65 (m, Ar, 1H), 6.59-6.57 (m, Ar, 2H), 3.56 (br. s, NH, 1H), 3.10-3.07 (t, 2H), 1.61-1.54 (m, 2H), 1.44-1.38 (m, 2H), 0.95-0.92 (t, 3H). ^{13}C NMR ($CDCl_3$, 150MHz) δ (ppm) = 148.5, 129.1, 117.0, 112.6, 43.6, 31.6, 28.7, 27.3, 23.2, 13.9. HRMS (ESI/APCI): *m/z* = 178.2920 g/mol, calc'd. for $C_{12}H_{20}N^+$ $[M]^+$: 178.2919g/mol. FTIR IR (ATR): ν = 3402 (w), 3059 (w),2925 (m), 2857 (w), 1604 (s), 1507 (s), 1320 (m), 1253 (m), 1178 (w), 865 (w), 746 (s) cm^{-1}

*4-Methoxy-N-(1-phenylethyl)aniline (**1l**)*. It was obtained as yellow oil, yield 79 % (179mg); ^{1}H NMR ($CDCl_3$, 600MHz) δ (ppm) = 7.50-7.48 (m, Ar, 2H), 7.18-7.16 (m, Ar, 2H), 6.89-6.65(m, Ar, 3H), 6.60-6.58 (m, Ar, 2H), 4.20-4.17 (q, 1H). ^{13}C NMR ($CDCl_3$, 150MHz)

δ (ppm) = 154.1, 148.5, 147.4, 142.5, 130.65, 129.1, 117.0, 112.6, 50.3, 30.8. HRMS (ESI/APCI): *m/z* = 228.3075 g/mol, calc'd. for $C_{15}H_{18}NO^+$ $[M]^+$: 228.3073 g/mol. FTIR IR (ATR): ν = 3387 (m), 3216 (w),2917 (m), 2843 (w), 1634 (m), 1507 (s), 1462 (s), 1298 (w), 1231 (s), 1126 (w),1029 (s), 820 (s) cm^{-1}.

*N-Isopropylaniline (**1m**)*. It was obtained as colorless oil, yield 90 % (123mg); ^1H NMR ($CDCl_3$, 600MHz) δ (ppm) = 7.15-7.13 (m, Ar, 2H), 6.69-6.67 (m, Ar, 1H), 6.60-6.58 (m, Ar, 2H), 3.39-3.36 (m, 1H), 1.09-1.08 (d, 6H). ^{13}C NMR ($CDCl_3$, 150MHz) δ (ppm) = 148.4, 129.2, 117.0, 112.6, 51.8, 21.8. HRMS (ESI/APCI): *m/z* = 136.1120 g/mol, calc'd. for $C_9H_{14}N$ $[M]^+$: 136.1121 g/mol. FTIR IR (ATR): ν = 3395(w), 3059(w) , 1634(m),1581(s), 1462(m), 1268(m), 738(s) cm^{-1}.

*N-Isopropyl-p-anisidine (**1n**)*. It was obtained as colorless oil, yield 92 % (153mg); ^1H NMR ($CDCl_3$, 600MHz) δ (ppm) = 7.50-7.48 (m, Ar, 2H), 6.96-6.93 (m, Ar, 2H), 4.49-4.43 (m, 1H), 1.09-1.08 (d, 6H). ^{13}C NMR ($CDCl_3$, 150MHz) δ (ppm) = 154.1, 147.4, 142.5, 130.65, 55.8, 52.8, 49.5, 22.0. HRMS (ESI/APCI): *m/z* = 166.1223 g/mol, calc'd. for $C_{10}H_{16}ON$ $[M]^+$: 166.1226 g/mol. FTIR IR (ATR): ν = 3365(w), 2962(w), 1619(w), 1507(s), 1231(s), 1171(m), 1037(m), 820(m) cm^{-1}.

*N-benzylpyridin-2-amine (**1o**)*. It was obtained as yellow solid (mp: 93-95℃), yield 95 % (176mg); ^1H NMR ($CDCl_3$, 600MHz) δ (ppm) = 8.8-8.1 (m, Ar, 1H), 7.39-7.36 (m, Ar, 1H), 7.35-7.30 (m, Ar, 4H), 7.27-7.24 (m, Ar, 1H), 6.58-6.56 (m, 1H), 6.35-6.35 (t, 1H), 4.85 (br. s, NH, 1H) , 4.49 (d, 2H , JHH = 6.0Hz,). ^{13}C NMR ($CDCl_3$, 150MHz) δ (ppm) =158.6, 148.2, 139.1, 137.4, 128.6, 127.3, 127.2, 113.1, 106.7, 46.3. HRMS (ESI/APCI): *m/z* = 185.1067g/mol, calc'd. for $C_{12}H_{13}N_2$ $[M]^+$: 185.1073 g/mol. FTIR IR (ATR): ν = 3216(m), 3022(w) , 29777(w), 1574(s), 1522(m), 1440(s), 1335(m), 1149(m), 1081(m) cm^{-1}.

*o-(benzylamino)phenol (**1p**)*. It was obtained as yellow oil, yield 75 % (150mg); ^1H NMR ($CDCl_3$, 600MHz) δ (ppm) = 11.0 (br. s, OH, 1H). 7.37-7.32 (m, Ar, 4H), 7.28-7.24 (m, Ar,

1H), 7.18-7.02 (m, Ar, 2H), 6.85-6.73 (m, Ar, 1H), 6.65-6.60 (m, Ar, 1H), 4.56-4.45 (d, 2H, JHH = 5.4Hz), 4.50 (br. s, NH, 1H). ^{13}C NMR ($CDCl_3$, 150MHz) δ (ppm) = 155.1, 155.3, 130.1, 138.5, 130.2, 129.5, 126.3, 118.6, 115.2, 114.5, 110.0, 47.8. HRMS (ESI/APCI): *m/z* =200.2542g/mol, calc'd. for $C_{13}H_{14}NO^+$ $[M]^+$: 200.2545 g/mol. FTIR IR (ATR): ν = 3100-3500(br), 3037(w), 2925 (w),2843 (w), 1581 (m), 1492 (m), 1447 (m), 1358 (m), 1238 (m), 1029 (w), 731(s) cm^{-1}

*2-(benzylamino)pyrimidine (**1q**)*. It was obtained as yellow oil, yield 56 % (104mg); ^{1}H NMR ($CDCl_3$, 600MHz) δ (ppm) = 8.25-8.24 (d, Ar, 2H, JHH = 4.8Hz) , 7.35-7.30 (m, Ar, 3H), 7.26-7.24 (m, Ar, 2H), 6.53-6.51 (t, Ar, 1H), 5.54 (br.s, NH, 1H), 4.63 (d, 2H, JHH = 4.0Hz). ^{13}C NMR ($CDCl_3$, 150MHz) δ (ppm) = 162.2, 158.0, 139.0, 128.5, 127.4, 127.2, 110.8, 45.4. HRMS (ESI/APCI): *m/z* = 186.1019 g/mol, calc'd. for $C_{11}H_{12}N_3$ $[M]^+$: 186.1026 g/mol. FTIR IR (ATR): ν = 3231(m), 3029(w) , 2857(m), 1574(s), 1529(s), 1447(s), 1261(s), 1067(m), 746(s) cm^{-1}.

*(1H-benzoimidazol-2-yl)benzylamine (**1r**)*. It was obtained as yellow oil, yield 85 % (191mg); ^{1}H NMR ($CDCl_3$, 600MHz) δ (ppm) = 7.36-7.30 (m, Ar, 4H), 7.29-7.24 (m, Ar, 4H), 7.04-7.02 (m, Ar, 2H), 4.58 (s, Ar,NH, 2H). ^{13}C NMR ($CDCl_3$, 150MHz) δ (ppm) = 154.5, 138.0, 128.9, 127.8, 127.3, 120.8, 112.4, 47.3. HRMS (ESI/APCI): *m/z* = 224.1176 g/mol, calc'd. for $C_{14}H_{14}N_3$ $[M]^+$: 224.1182 g/mol. FTIR IR (ATR): ν = 3395(w), 3059(w), 1634(m),1581(s), 1462(m), 738(s) cm^{-1}.

*N-methyl-N-phenyl-benzenemethanamine (**2a**)*. It was obtained as colorless oil, yield 82 % (163mg); ^{1}H NMR ($CDCl_3$, 600MHz) δ (ppm) = 7.35-7.30 (m, Ar, 4H), 7.25-7.22 (m, Ar, 1H), 7.15-7.13 (m, Ar, 2H), 6.70-6.67 (t, Ar, 1H), 6.68-6.64 (d, Ar, 2H, JHH = 7.8Hz), 4.35 (s, CH2, 2H), 3.10 (s, 3H). ^{13}C NMR ($CDCl_3$, 150MHz) δ (ppm) = 148.7, 139.8, 129.6, 128.8, 127.8, 127.5, 117.2, 112.5, 48.0, 45.7. HRMS (ESI/APCI): *m/z* = 198.2821 g/mol, calc'd. for $C_{14}H_{16}N^+$ $[M]^+$: 198.2819 g/mol. FTIR IR (ATR): ν = 3029 (w), 2925

(w),2857 (w), 1596 (s), 1499 (s), 1455 (m), 1350 (m), 1111(m) , 1029(m), 940(m), 746(s) , 723(s) cm^{-1}

*N-benzyl-N-(4-chloro-benzyl)-aniline (**2b**)*. It was obtained as colorless oil, yield 80 % (247mg); ^{1}H NMR ($CDCl_3$, 600MHz) δ (ppm) = 7.31-7.29 (m, Ar, 4H), 7.24-7.22 (m, Ar, 6H), 7.16-7.13 (m, Ar, 2H), 6.72-6.67 (m, Ar, 2H), 4.63-4.60 (d, Ar, 2H, JHH = 23.4Hz). ^{13}C NMR ($CDCl_3$, 150MHz) δ (ppm) = 149.1, 138.5, 132.8, 129.1, 128.6, 127.8, 127.0, 126.8, 126.6, 116.6, 117.7, 112.3, 54.5, 49.8. HRMS (ESI/APCI): *m/z* = 308.8225 g/mol, calc'd. for $C_{20}H_{19}NCl^{+}$ $[M]^{+}$: 308.8226 g/mol. FTIR IR (ATR): ν = 3051 (w), 2902 (w),2857 (w), 1596 (m), 1492 (m), 1358 (m), 1231 (m), 955 (m) , 805(m), 731 (s), cm^{-1}

*N,N-dibenzylaniline (**2c**)*. It was obtained as yellow solid (mp: 68-70°C), yield 86 % (236mg); ^{1}H NMR ($CDCl_3$, 600MHz) δ (ppm) = 7.31-7.29 (m, Ar, 4H), 7.24-7.22 (m, Ar, 6H), 7.16-7.13 (m, Ar, 2H), 6.72-6.67 (m, Ar, 2H), 4.63-4.60 (d, Ar, 2H, JHH = 23.4Hz). ^{13}C NMR ($CDCl_3$, 150MHz) δ (ppm) = 149.1, 138.5, 129.1, 128.6, 126.8, 126.6, 116.6, 112.3, 54.1. HRMS (ESI/APCI): *m/z* = 274.1588 g/mol, calc'd. for $C_{20}H_{20}N$ $[M]^{+}$: 274.1590 g/mol. FTIR IR (ATR): ν = 3037 (w), 2917 (m), 1596 (s), 1499 (s), 1455 (m), 1358 (m) 1231 (m), 1029 (w), 955 (m), 731 (s) cm^{-1}

*N-phenylpyrrolidine (**3a**)*. It was obtained as colorless oil, yield 80 % (119mg); ^{1}H NMR ($CDCl_3$, 600MHz) δ (ppm) = 7.17-7.26 (m, 3H), 6.93-6.96 (m, 2H), 6.75-6.96(m, 1H), 3.38–3.44 (m, 4H), 2.01-2.07 (m, 3H). HRMS (ESI/APCI): *m/z* =148.2231 g/mol, calc'd. for $C_{13}H_{14}N$: 148.2234 g/mol. FTIR IR (ATR): ν = 3059 (w), 3029 (w), 2962 (m),2925(s),2835(m), 1604(m), 1596(s), 1507(s), 1462 (m), 1365 (s), 1358 (w),1238(w), 1186 (m), 1156 (m), 992 (m), 746 (s), 686 (s) cm^{-1}

*N-(4-chlorophenyl) pyrrolidine (**3b**)*. It was obtained as colorless oil, yield 85 % (155mg); ^{1}H NMR ($CDCl_3$, 600MHz) δ (ppm) = 7.37-7.42 (m, 3H), 7.07-7.09 (m, 1H), 2.83-2.85 (m, 4H), 2.19-2.22 (m, 4H). HRMS (ESI/APCI): *m/z* = 182.6683 g/mol, calc'd. for $C_{11}H_{13}NCl^{+}$

$[M]^+$: 182.6686 g/mol. FTIR (ATR): *v* = 2962(w), 2925(s), 2857(m), 1738(s), 1604(m), 1470(m), 1462(m), 1373(s), 275(w), 1231(s), 1156(w), 1074(w), 1014(w), 798(m) cm^{-1}.

*N-(4-methoxyphenyl) pyrrolidine (**3c**)*. It was obtained as colorless oil, yield 89 % (159mg); ^1H NMR ($CDCl_3$, 600MHz) δ (ppm) = 6.62-6.74 (m, 4H), 3.79 (s, 3H), 3.38-3.43(t, J=6 Hz 4H), 2.01-2.06 (t, J=6 Hz 4H), 2.01–1.98 (m, 4H). ^{13}C NMR ($CDCl_3$, 150MHz) δ (ppm) = 149.2, 141.1, 116.1, 114.1, 78.1, 56.1, 51.1, 25.9. HRMS (ESI/APCI): *m/z* = 178.2485 g/mol, calc'd. for $C_{11}H_{16}NO^+$ $[M]^+$: 178.2488 g/mol. FTIR (ATR): *v* = 3044(w), 2947(m), 2925(s), 2857(m), 1619 (w), 1514(m), 1484(w), 1462(m), 1365(m), 1275(w), 1238(m), 1178(w), 1156(w), 1044(m), 970(w), 805(s),731(w)cm^{-1}.

*N-phenylpiperidine (**3d**)*. It was obtained as colorless oil, yield 75 % (122mg); ^1H NMR ($CDCl_3$, 600MHz) δ (ppm) = 7.26 (t, 2H, J=7 Hz), 6.99 (d, 2H, J=7 Hz), 6.86 (t, 1H, J=7 Hz), 3.17 (t, 4H, J=6.7 Hz), 1.75 (m, 4H), 1.61 (t, 2H, J=4.8 Hz). ^{13}C NMR ($CDCl_3$, 150MHz) δ (ppm) = 151.6, 129.0, 119.7, 116.7, 60.0, 25.7, 24.2. HRMS (ESI/APCI): *m/z* = 162.2495 g/mol, calc'd. for $C_{11}H_{16}N^+$ $[M]^+$: 162.2498 g/mol. FTIR IR (ATR): v = 2932 (m), 2853 (m), 2805 (m), 1597 (s), 1494 (s), 1450 (m), 1384 (m), 1235 (s), 1220 (s), 1131 (m), 917 (m), 753 (s) cm^{-1}.

*N-(4-methoxyphenyl) piperidine (**3e**)*. It was obtained as colorless oil, yield 78 % (150mg); ^1H NMR ($CDCl_3$, 600MHz) δ (ppm) = 6.93–6.90 (m, 2H), 6.84–6.81 (m, 2 H), 3.76 (s, 3 H), 3.03–3.01(m, 4 H), 1.74–1.70 (m, 4 H), 1.56–1.52 (m, 2 H). ^{13}C NMR ($CDCl_3$, 150MHz) δ (ppm) = 154.0, 145.2, 119.0, 114.3, 55.6, 52.7, 25.8, 23.9. HRMS (ESI/APCI): *m/z* = 192.2753g/mol, calc'd. for $C_{12}H_{18}NO^+$ $[M]^+$: 192.2752 g/mol. FTIR (ATR): *v* = 2932(m), 2850(w), 2800(w), 1507(s), 1447 (m), 1238(s), 1178(m), 1119(m), 1037(s), 917(m),858(w),820(s),798(w),701(w) cm^{-1}.

1-*(piperidine-1-yl) pyridine (**3f**)*. It was obtained as y colorless oil, yield 70 % (114mg); ^1H NMR ($CDCl_3$, 600MHz) δ (ppm) = 8.17 (s, 1H), 7.46 (t, J = 8Hz, 1H), 6.67 (d, J = 7Hz,

1H), 6.54 (dd, J = 4.9, 0.9 Hz, 1H), 3.54(s, 4H), 1.67 (s, 6H). ^{13}C NMR ($CDCl_3$, 150MHz) δ (ppm) = 159.1, 147.2, 137.7, 112.3, 107.4, 46.5, 25.4, 24.6. HRMS (ESI/APCI): *m/z* =163.2381 g/mol, calc'd. for $C_{10}H_{15}N_2^+$ $[M]^+$: 163.2380 g/mol. FTIR (ATR): *v* = 3007(w), 2925(m),2850(m), 1596(s), 1484(s), 1432(s), 1380(w), 1313(m), 1246(s),1156(w), 1126(m), 1022(w), 850(w), 768 (s),732(w) cm^{-1}.

*1-methyl-4-(pyridin-2-yl) piperazine (**3g**)*. It was obtained as colorless oil, yield 70 % (125mg); ^1H NMR ($CDCl_3$, 600MHz) δ (ppm) = 48 (dd, 1H), 7.46 (ddd, 1H), 7.18 – 7.26 (m, 2H), 3.97-3.99 (m, 4H), 2.34-2.36 (m, 4H), 1.99-2.01(m, 2H). ^{13}C NMR ($CDCl_3$, 150MHz) δ (ppm) = 138.9 , 133.2, 132.1, 130.4, 129.6, 59.9, 58.6, 52.9. HRMS (ESI/APCI): *m/z* = 178.2522g/mol, calc'd. for $C_{10}H_{16}N_3^+$ $[M]^+$: 178.2525 g/mol. IR(ATR) : *v* = 3328(s), 2932(m), 2865(m), 1626(m), 1604 (s), 1529 (w), 1514(s), 1447(m), 1156(w), 1052(m), 1029(w), 887(w),858(w),768(s),701(w) cm^{-1}.

*Benzylpiperazine (**3h**)*. It was obtained as colorless oil, yield 90 % (160mg); ^1H NMR ($CDCl_3$, 600MHz) δ (ppm) = 7.29-7.22 (m, Ar, 5H), 3.56-3.40 (m, 4H), 2.89-2.86 (m, 4H), 2.41 (br. s, NH , 1H). ^{13}C NMR ($CDCl_3$, 150MHz) δ (ppm) = 137.8, 129.2, 128.1, 127.0, 64.0, 54.1, 45.8. HRMS (ESI/APCI): *m/z* = 177.2642 g/mol, calc'd. for $C_{11}H_{17}N_2^+$ $[M]^+$: 177.2644g/mol. FTIR (ATR): *v* = 3320(s), 3029(w),2940(m),2820(m), 1641(s),1544 (m), 1492(w), 1455(s),1417(m), 1268(s), 1134(m), 999(s),910(w), 738(s) cm^{-1}.

*1-methyl-4-phenyl piperazine (**3i**)*. It was obtained as colorless oil, yield 75 % (133mg); ^1H NMR ($CDCl_3$, 600MHz) δ (ppm) = 7.26-7.31 (m, Ar, 2H), 7.05-7.09 (m, Ar, 1H), 6.92-6.99 (m, Ar, 2H), 3.63 (t, J = 4.6 Hz, 4H), 2.85-2.87 (m, 7H). ^{13}C NMR ($CDCl_3$, 150MHz) δ (ppm) = 149.3, 129.4, 121.8, 117.2, 55.4, 46.9, 43.6. HRMS (ESI/APCI): *m/z* = 177.2646 g/mol, calc'd. for $C_{11}H_{17}N_2^+$ $[M]^+$: 177.2644 g/mol.. FTIR (ATR): *v* = 3059(w), 2940(m), 2850(w), 2798(s), 1596(s), 1499 (s), 1455(m), 1373(w), 1335(w), 1417(m), 1268(s), 1134(m), 999(s), 910(w), 738(s) cm^{-1}.

Hydroxyine. It was obtained as yellow solid (mp: 190-192℃), yield 55 % (total yield of the tandem reaction, 207mg)); ^{1}H NMR ($CDCl_3$, 600MHz) δ (ppm) = 7.16-7.37 (m, Ar, 10H), 4.19 (s, 1H), 3.44-3.56 (m, 6H), 2.38-2.57 (m, 8H), 1.16 (t, 2H, JHH = 6Hz). ^{13}C NMR ($CDCl_3$, 150MHz) δ (ppm) = 142.0, 141.1, 132.4, 129.1, 128.3, 127.8, 126.9, 75.5, 67.9, 66.3, 66.1, 57.9 ,57.5, 53.9, 51.4, 15.0. HRMS (ESI/APCI): *m/z* =375.9088 g/mol, calc'd. for $C_{21}H_{28}ClN_2O_2^+$ $[M]^+$: 375.9086 g/mol. FTIR (ATR): *v* = 3300 (S), 3081 (w),3074 (w), 3014 (w),2954 (w), 2910 (w),2865 (w) ,2835 (w), 1604 (s), 1574 (s), 1529 (s), 1447 (s), 1246 (m), 1037(m), 820(s), 768(s) cm^{-1}

Cyclizine. It was obtained as yellow solid (mp: 105-107℃), yield 60 % (160mg); ^{1}H NMR ($CDCl_3$, 600MHz) δ (ppm) = 7.44-7.17 (m, 10H, Ph), 4.26 (s, 1H, N-CH), 3.31 (s, 8H, N-CH), 2.30 (s, 3H, N-CH3). ^{13}C NMR ($CDCl_3$, 150MHz) δ (ppm) = 142.6, 128.3, 127.9, 126.7, 77.4, 56.3, 46.2 HRMS (ESI/APCI): *m/z* =267.3861 g/mol, calc'd. for $C_{18}H_{23}N_2$ $[M]^+$: 267.3863 g/mol. FTIR (ATR): *v* = 3059(w), 3029(w), 2925(m), 2857(w), 1619(s), 1492(m), 1447(m), 1275(m) ,1149(w), 1074(w), 1029(w), 984(w), 925(w), 858(w), 746(s), 701(s) cm^{-1}.

(1)

II. Gas Chromatogram of Purified Compounds

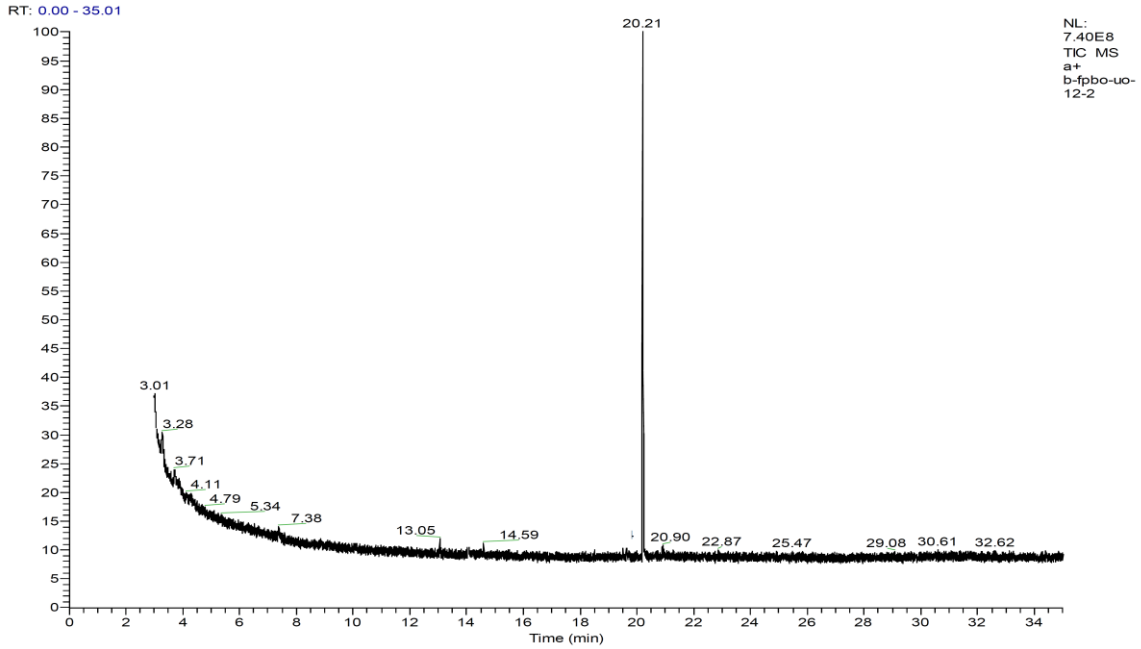


Figure S1. Gas chromatogram of purified N-benzylaniline

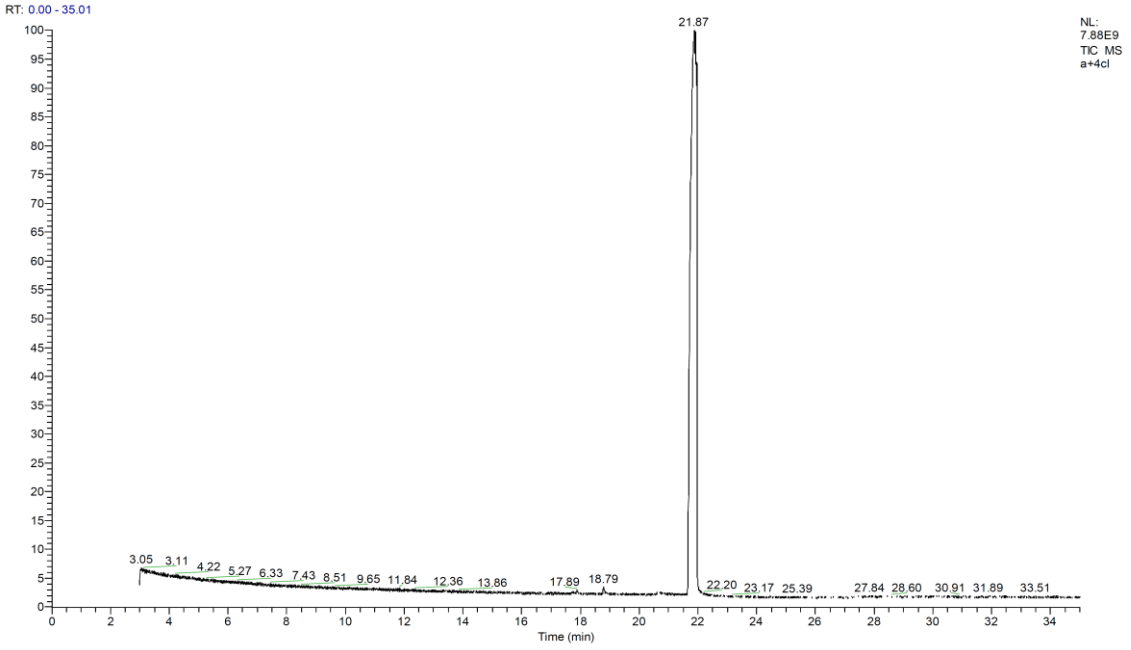


Figure S2. Gas chromatogram of purified N-(4-methoxybenzyl)aniline

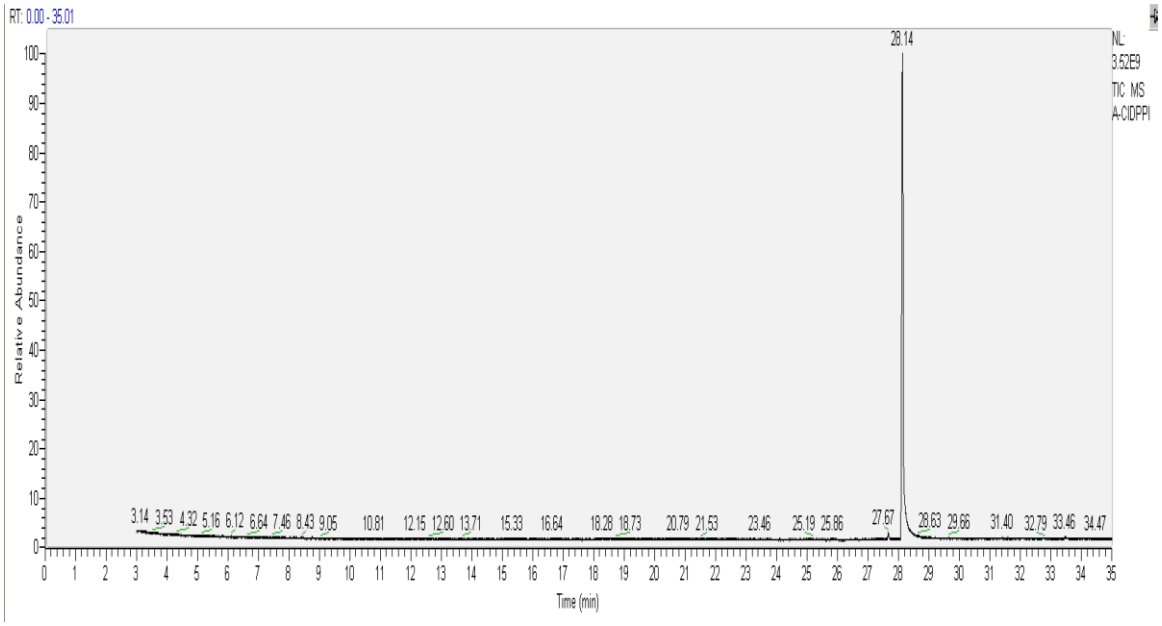


Figure S3. Gas chromatogram of purified N-(p-chlorobenzyl)aniline

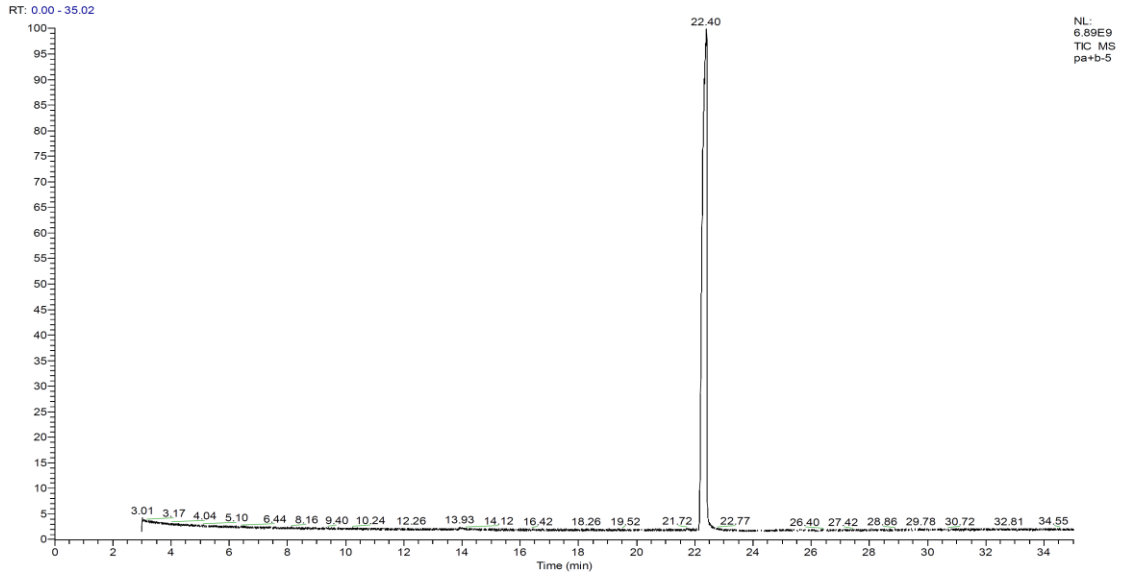


Figure S4. Gas chromatogram of purified benzyl(4-methoxyphenyl)amine

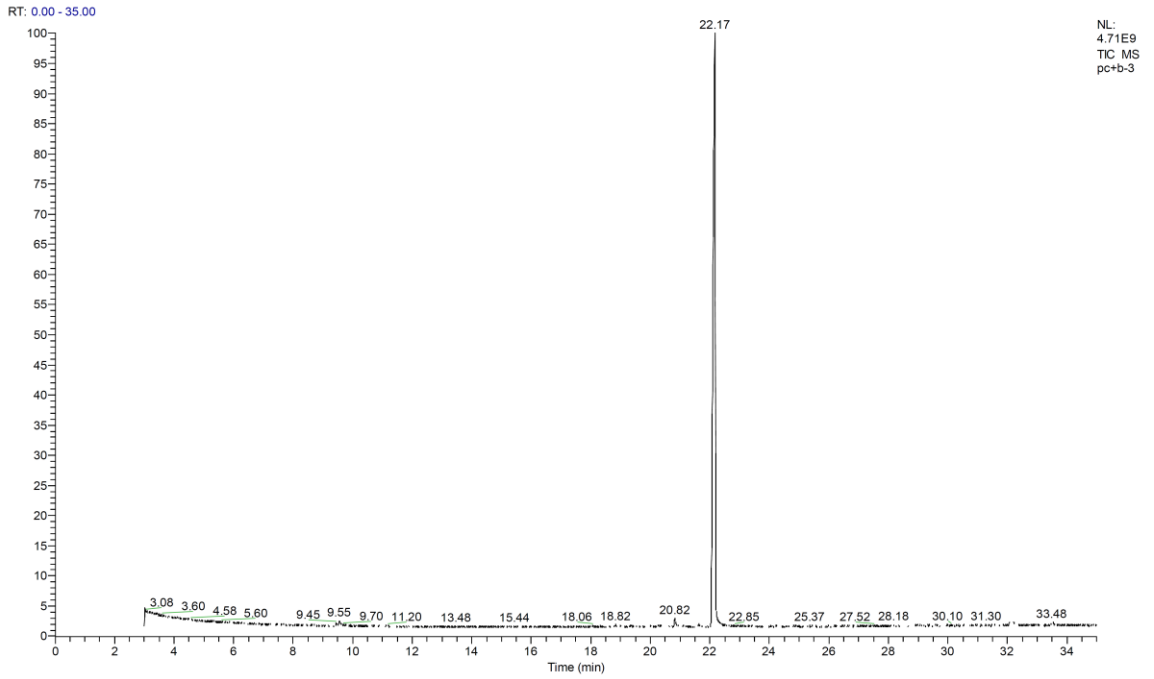


Figure S5. Gas chromatogram of purified N-(4-chlorophenyl)benzylamine

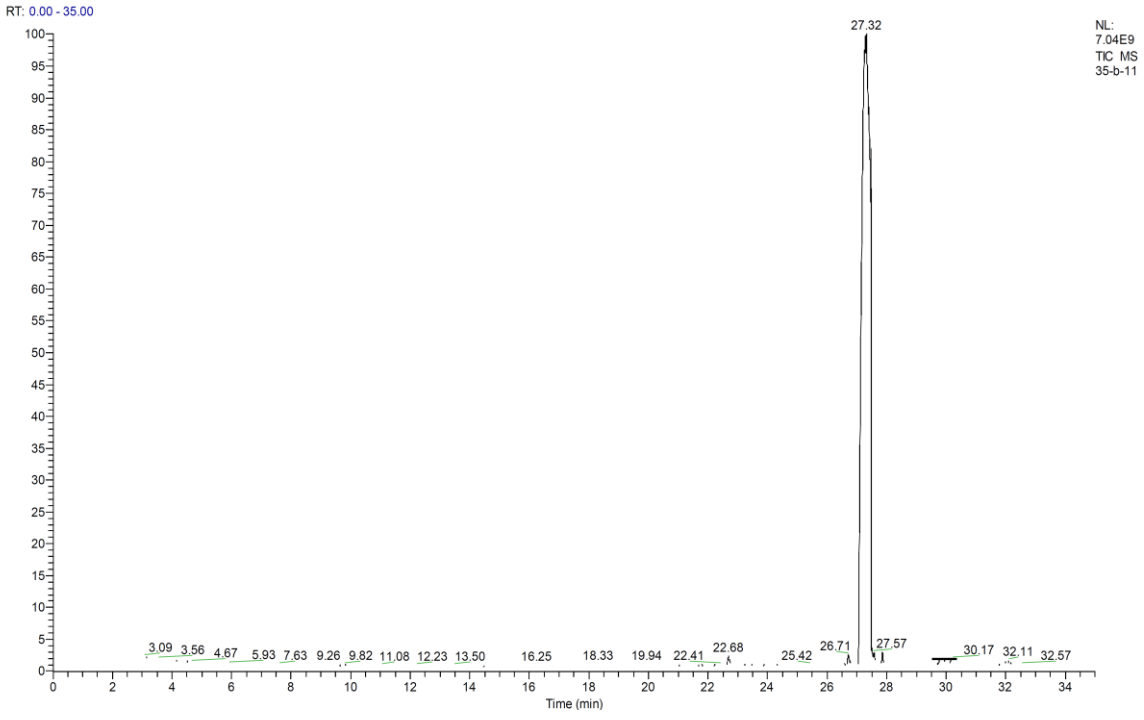


Figure S6. Gas chromatogram of purified N-Benzyl-3,5-dimethoxyaniline

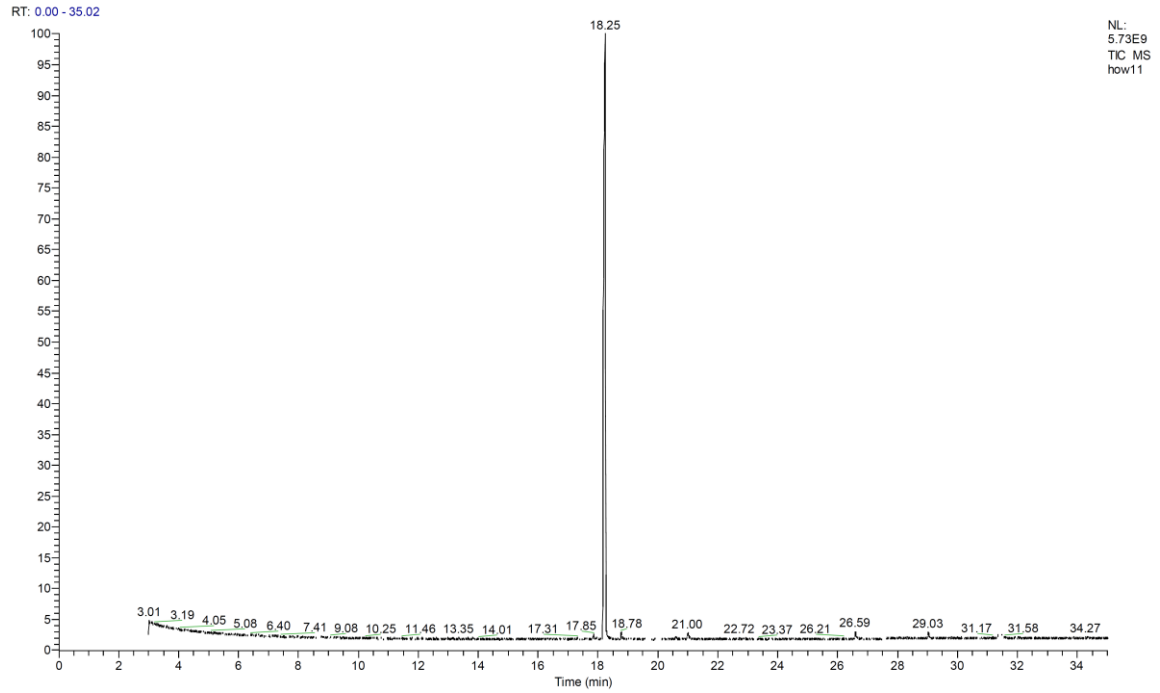


Figure S7. Gas chromatogram of purified N-benzyl-(2-fluorophenyl)amine

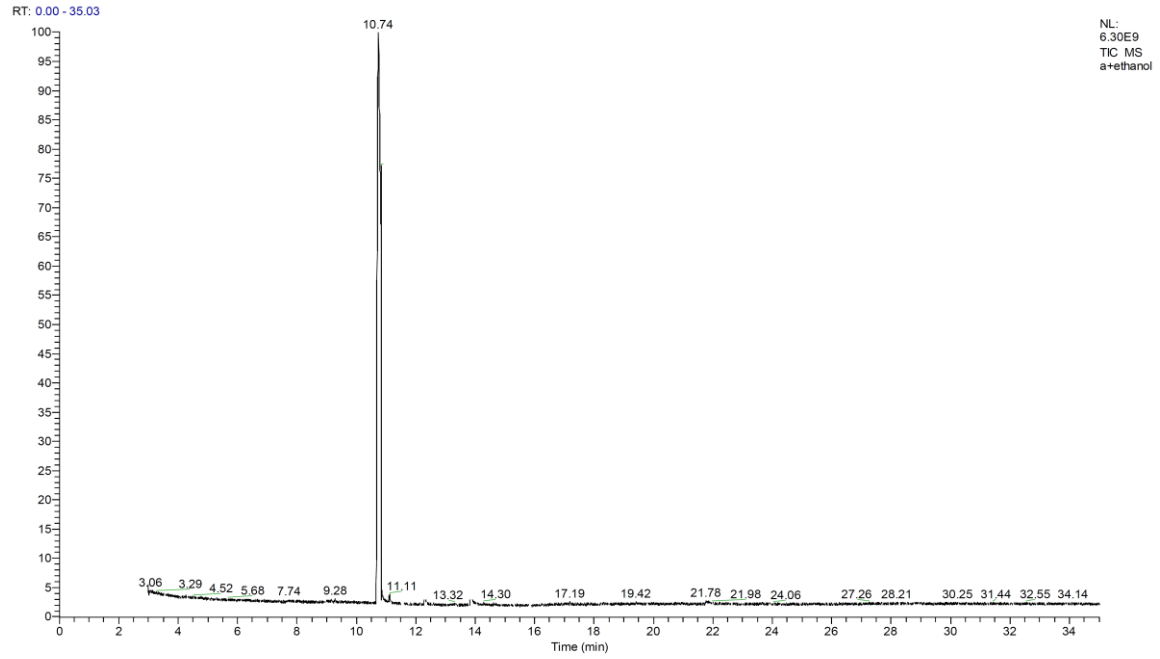


Figure S8. Gas chromatogram of purified N-ethyl-N-phenylamine

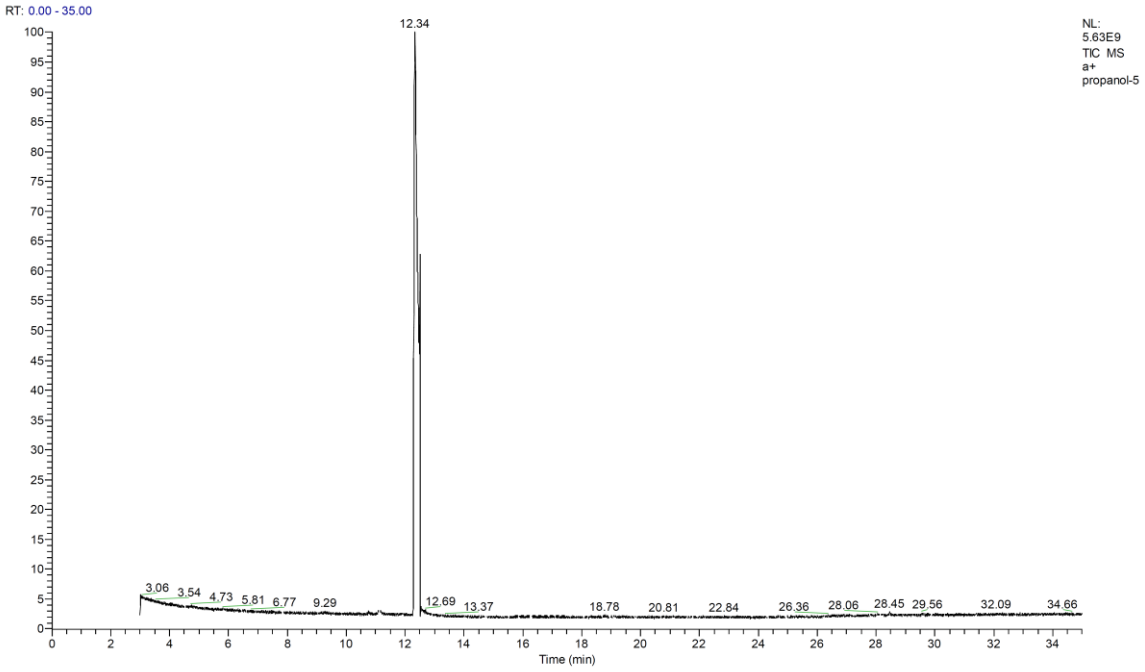


Figure S9. Gas chromatogram of purified N-propylaniline

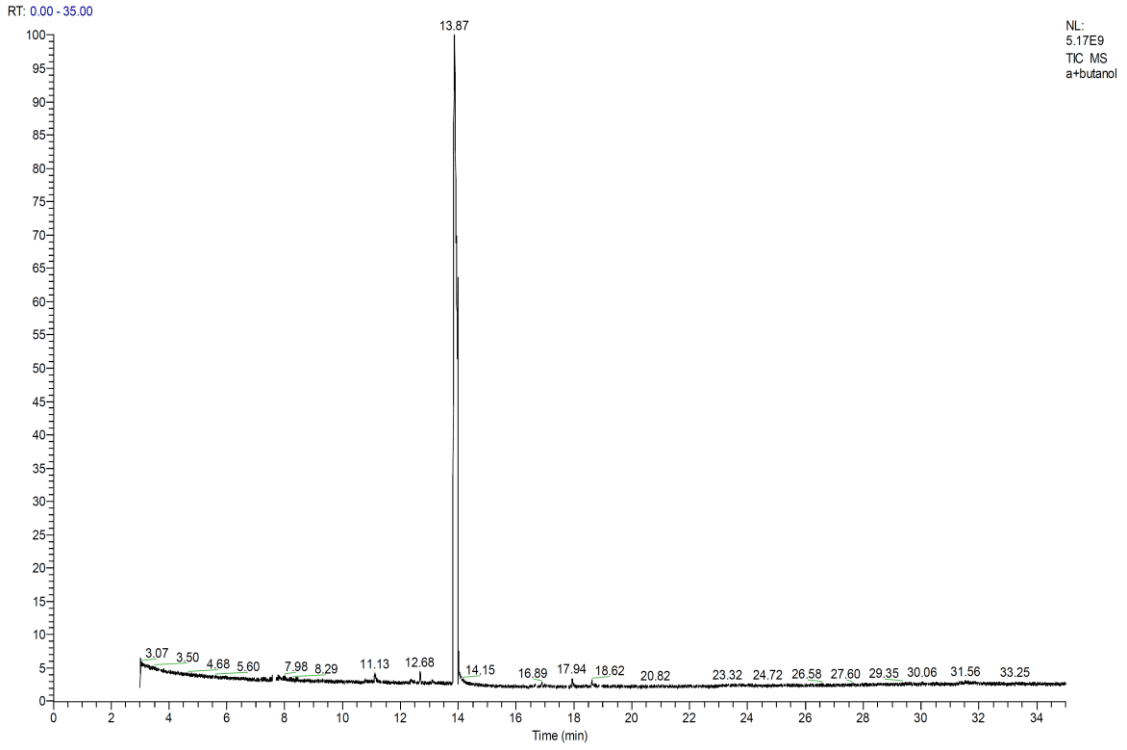


Figure S10. Gas chromatogram of purified N-(n-butyl)aniline

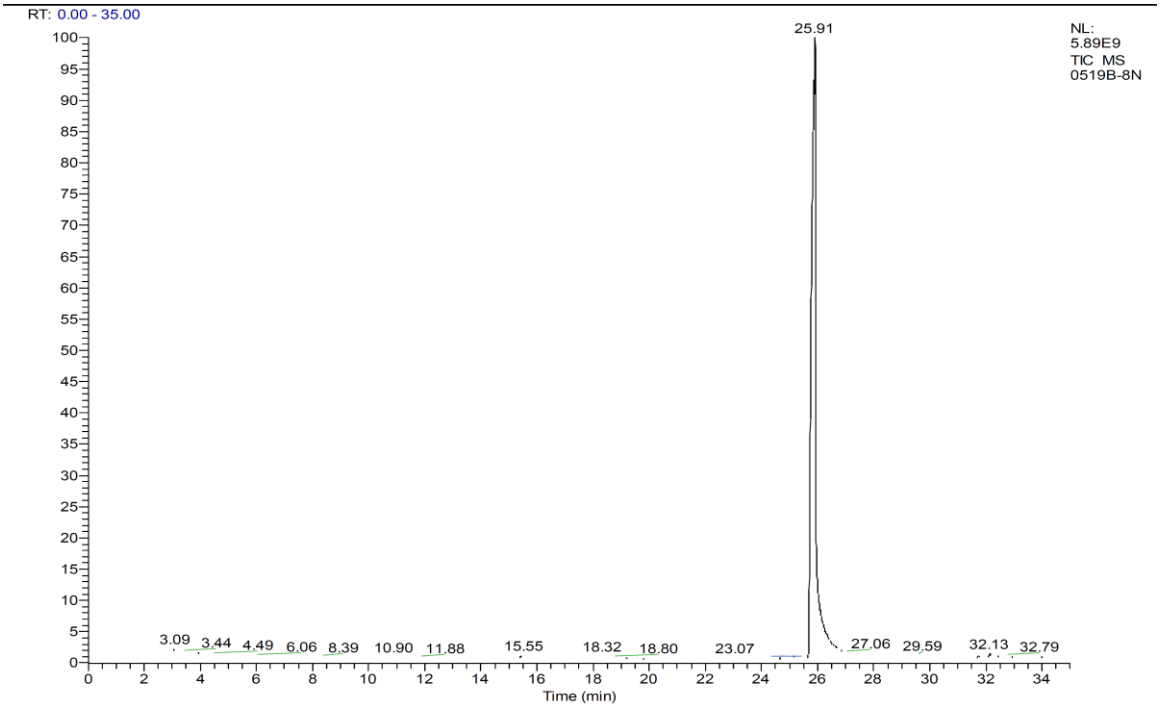


Figure S11. Gas chromatogram of purified N-hexylaniline

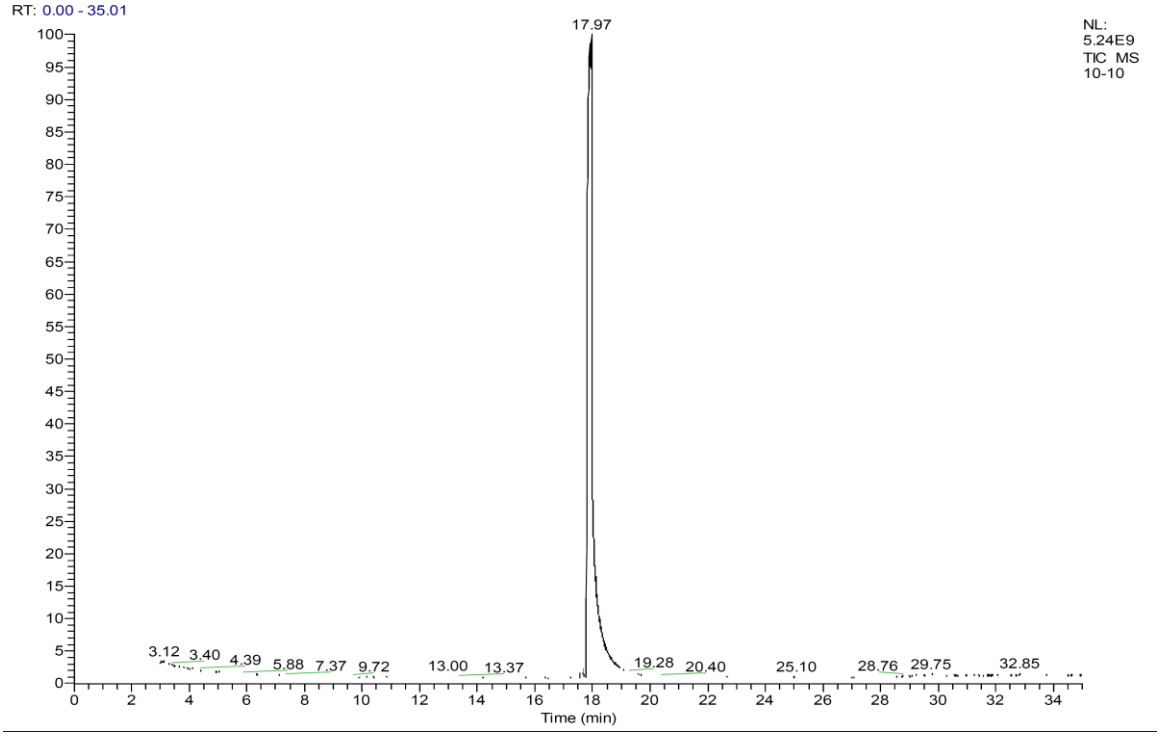


Figure S12. Gas chromatogram of purified 4-Methoxy-N-(1-phenylethyl)aniline

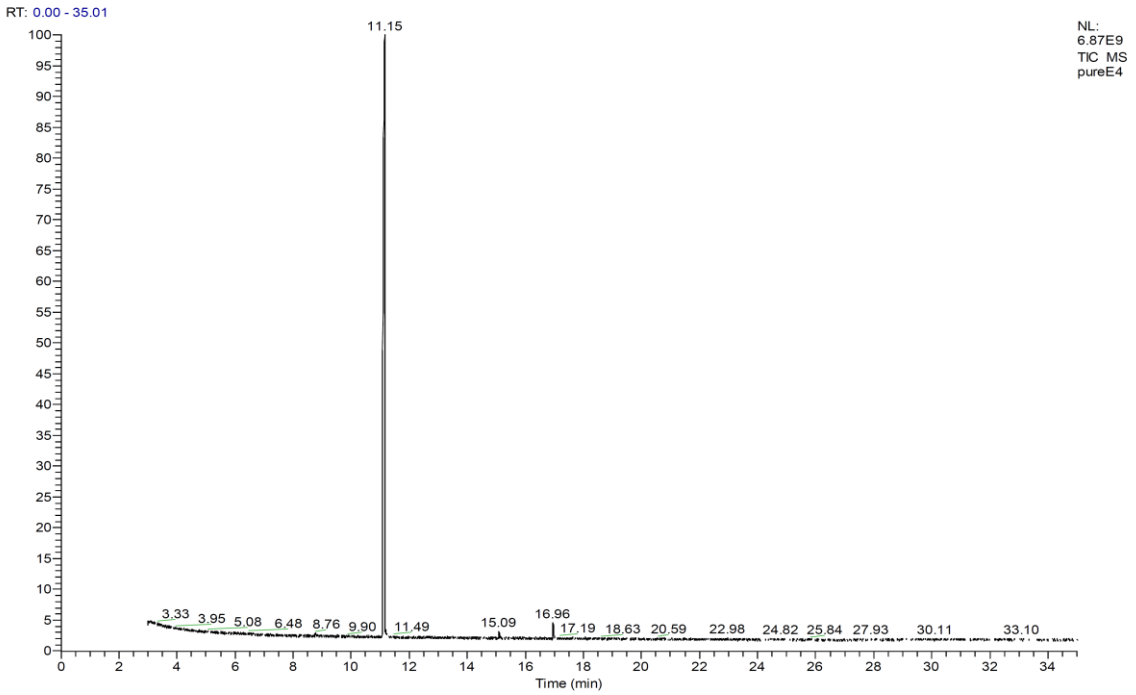


Figure S13. Gas chromatogram of purified N-Isopropylaniline

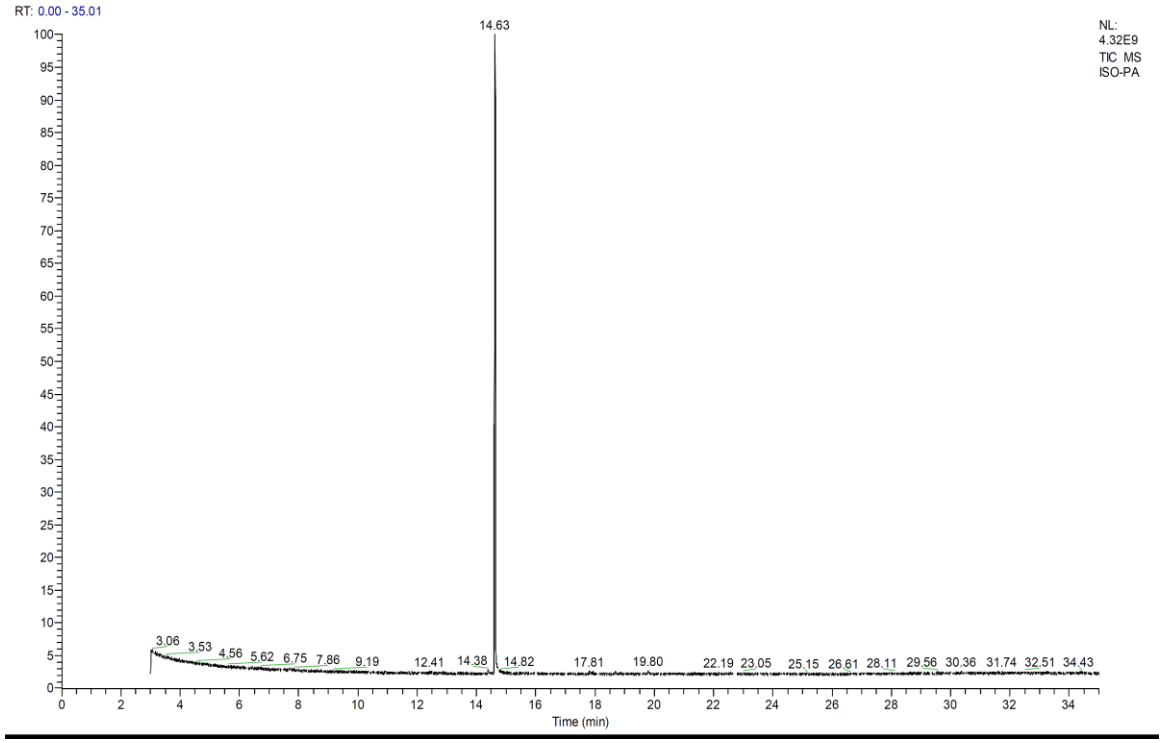


Figure S14. Gas chromatogram of purified N-Isopropyl-p-anisidine

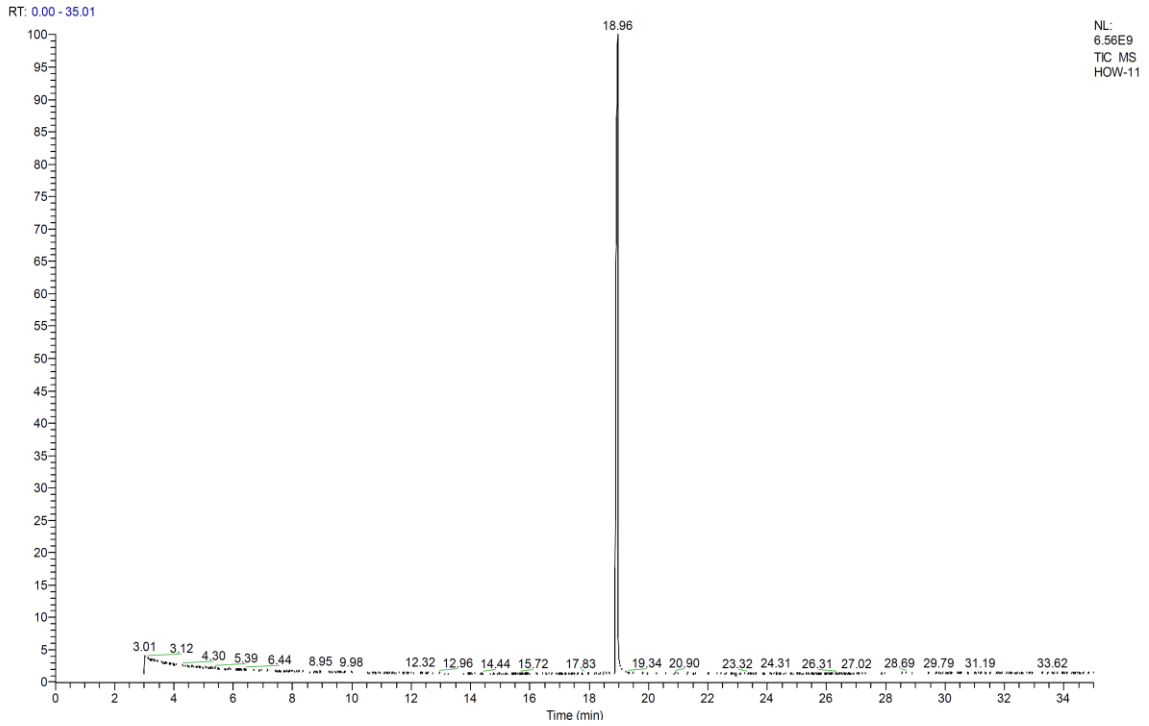


Figure S15. Gas chromatogram of purified N-benzylpyridin-2-amine

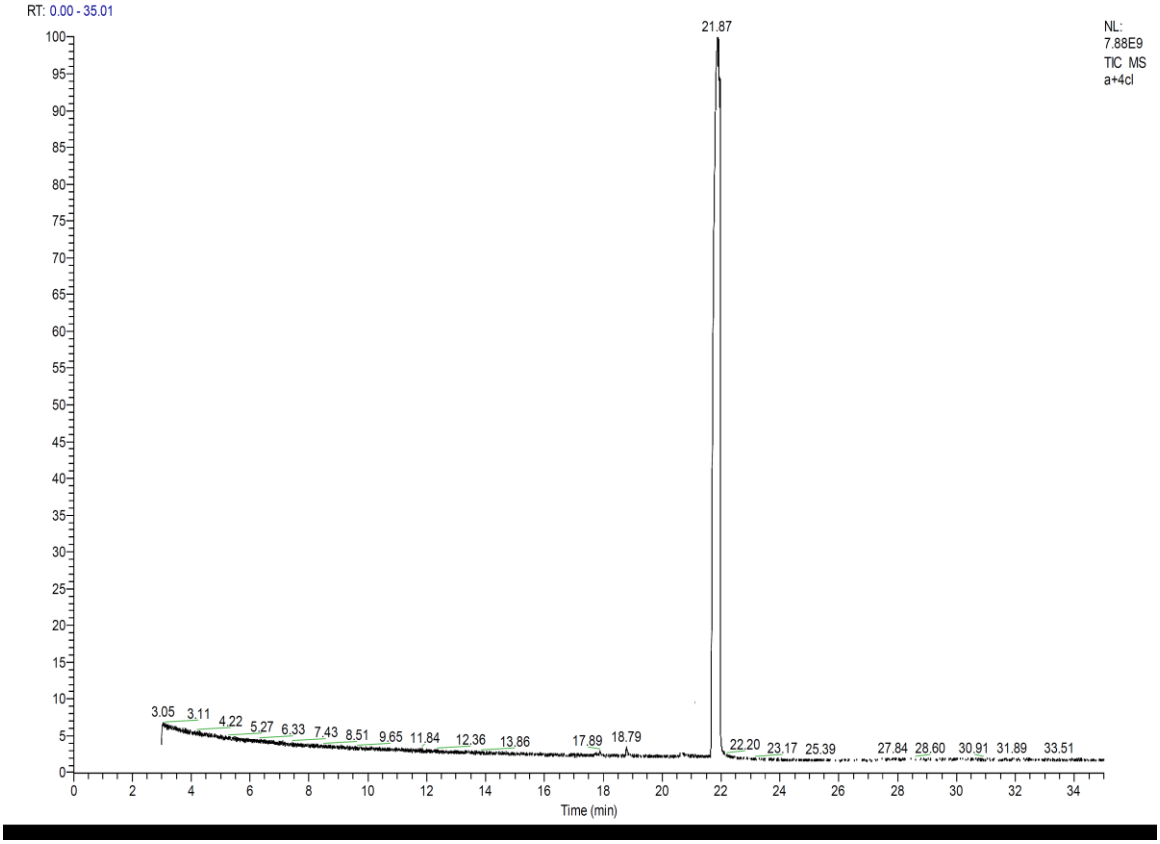


Figure S16. Gas chromatogram of purified o-(benzylamino)phenol

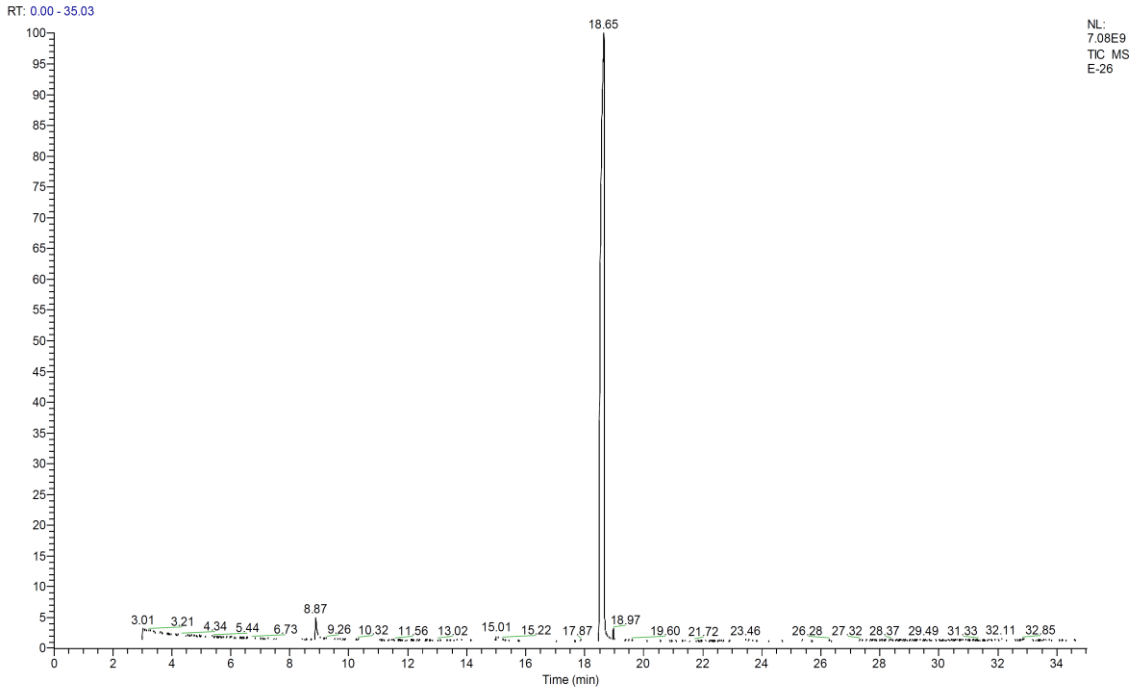


Figure S17. Gas chromatogram of purified 2-(benzylamino)pyrimidine

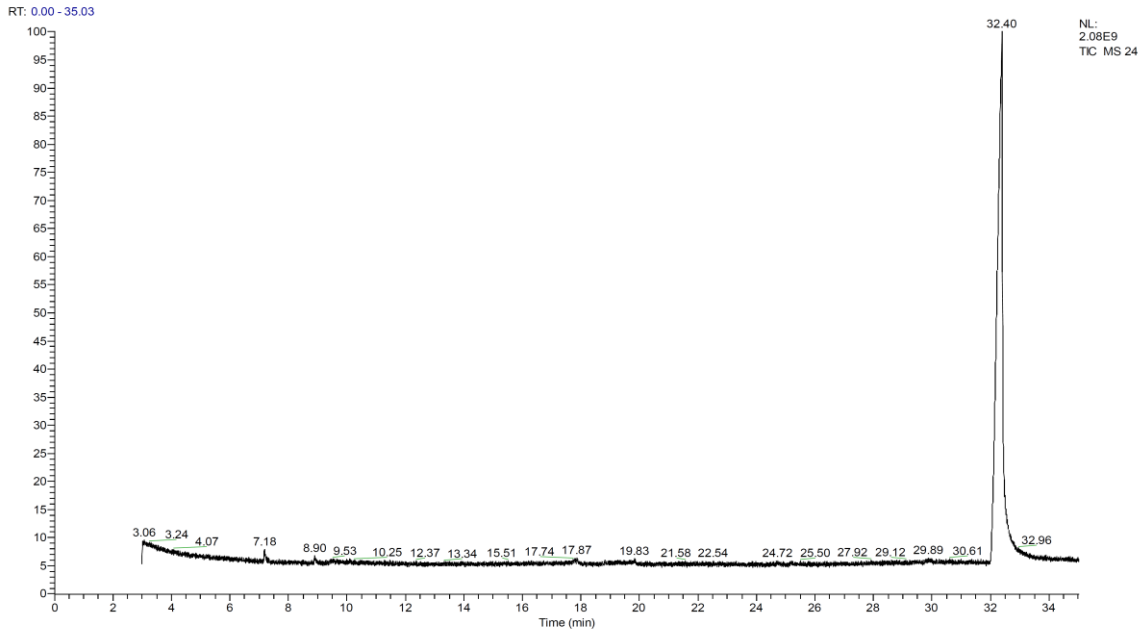


Figure S18. Gas chromatogram of purified (1H-benzoimidazol-2-yl)phenylamine

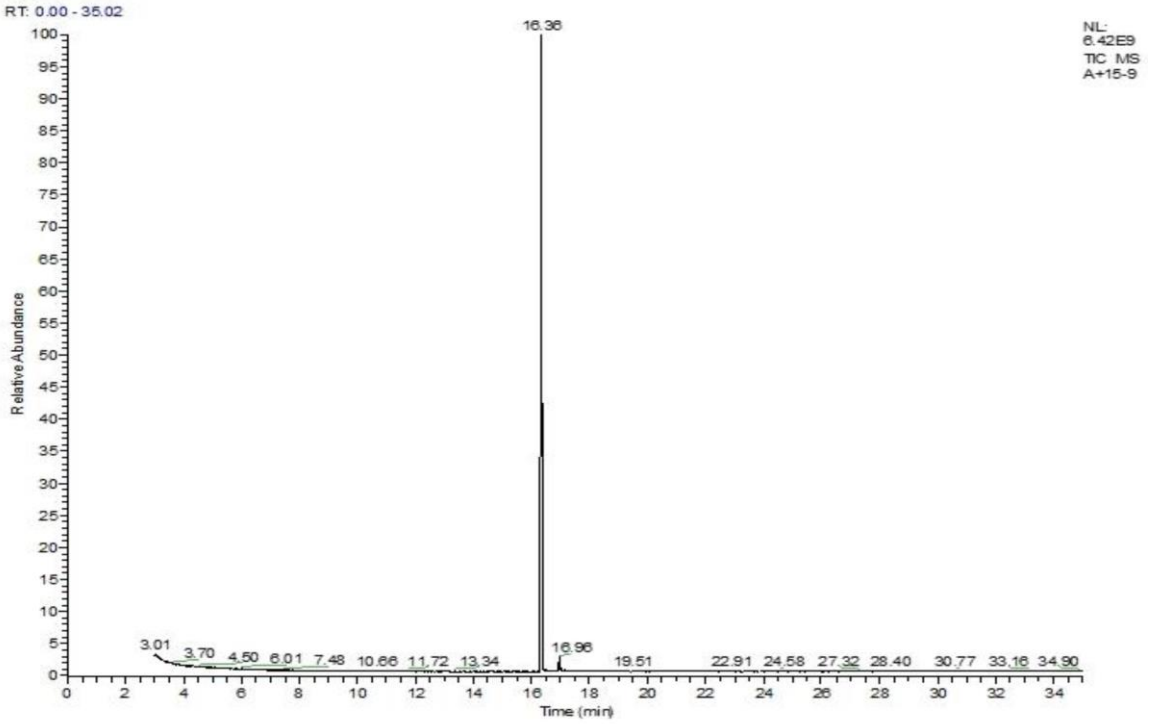


Figure S19. Gas chromatogram of purified N-methyl-N-phenyl-benzenemethanamine

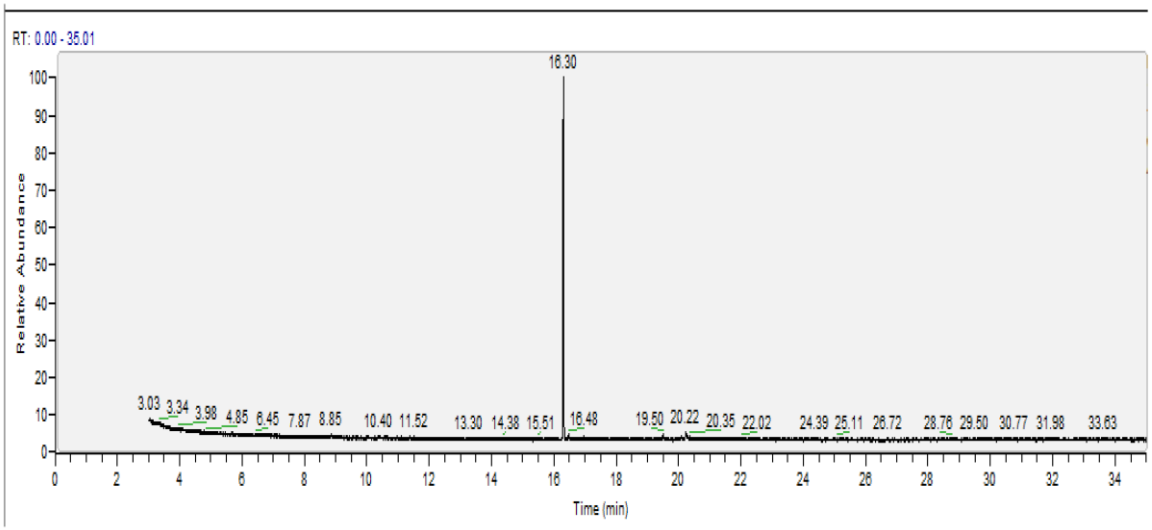


Figure S20. Gas chromatogram of purified N-benzyl-N-(4-chloro-benzyl)-aniline

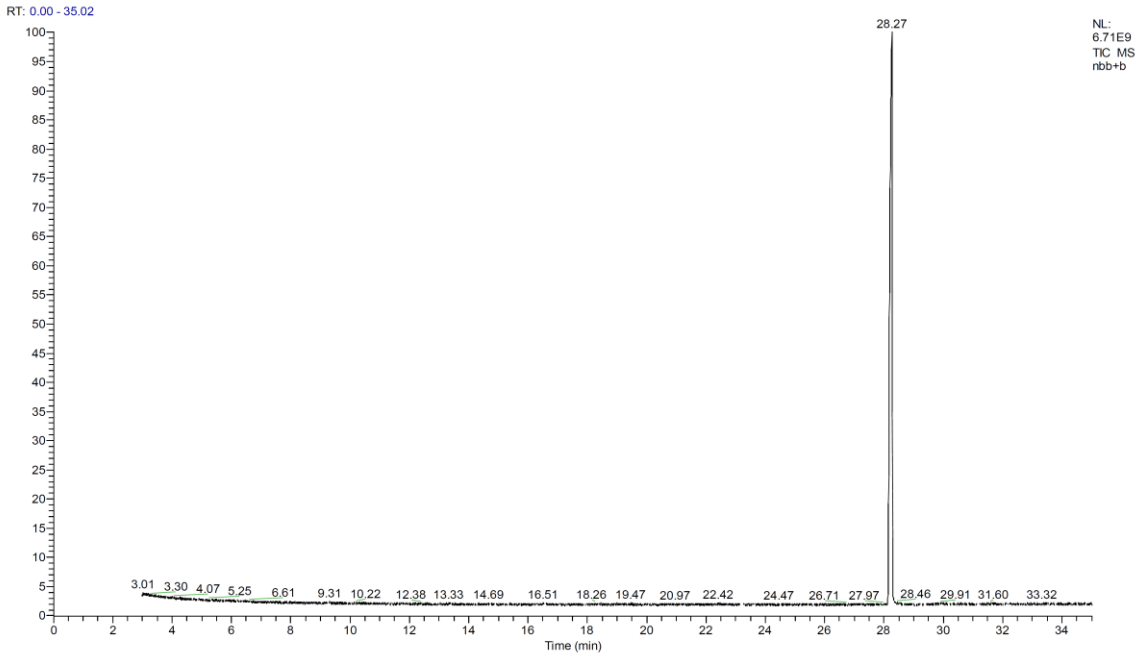


Figure S21. Gas chromatogram of purified N,N-dibenzylaniline

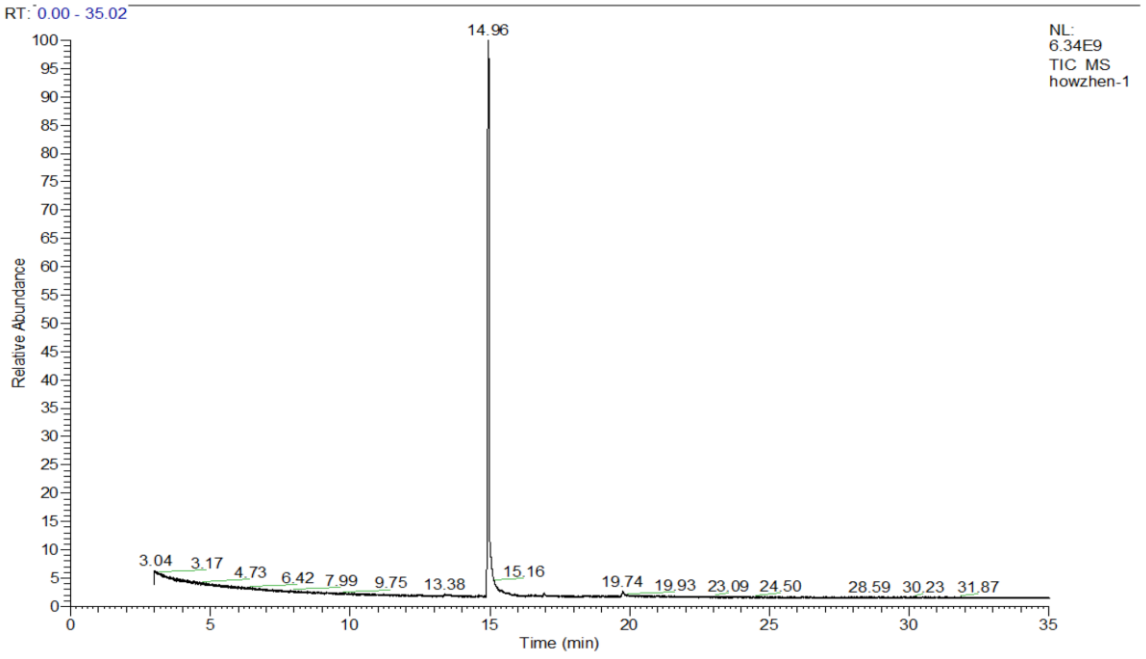


Figure S22. Gas chromatogram of purified N-phenylpyrrolidine

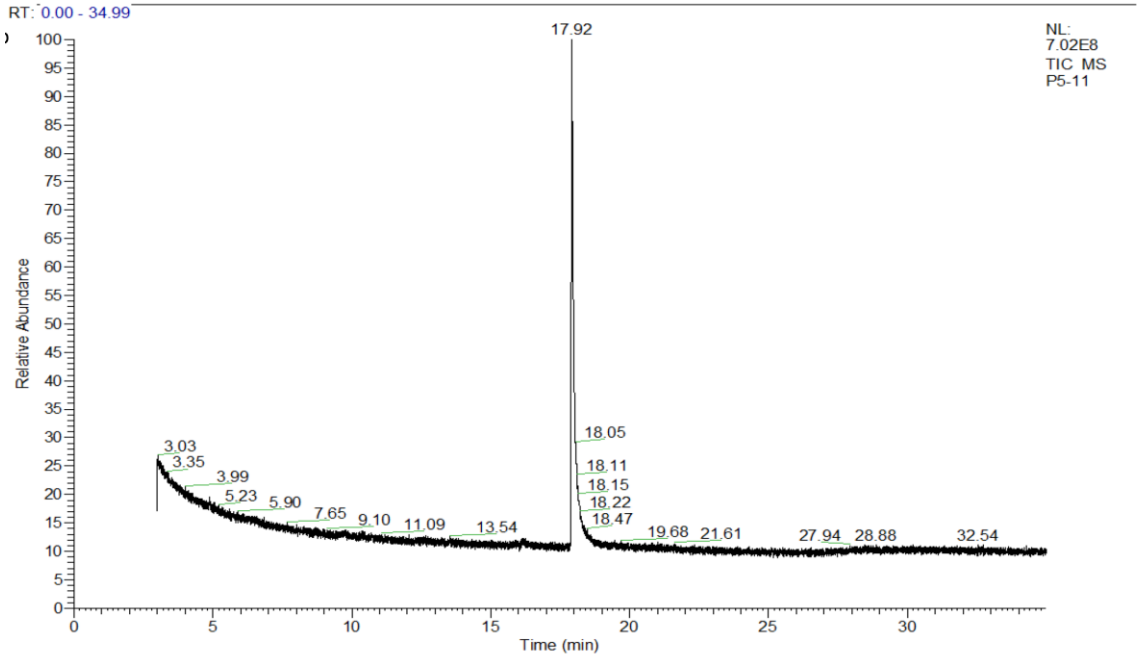


Figure S23. Gas chromatogram of purified N-(4-chlorophenyl) pyrrolidine

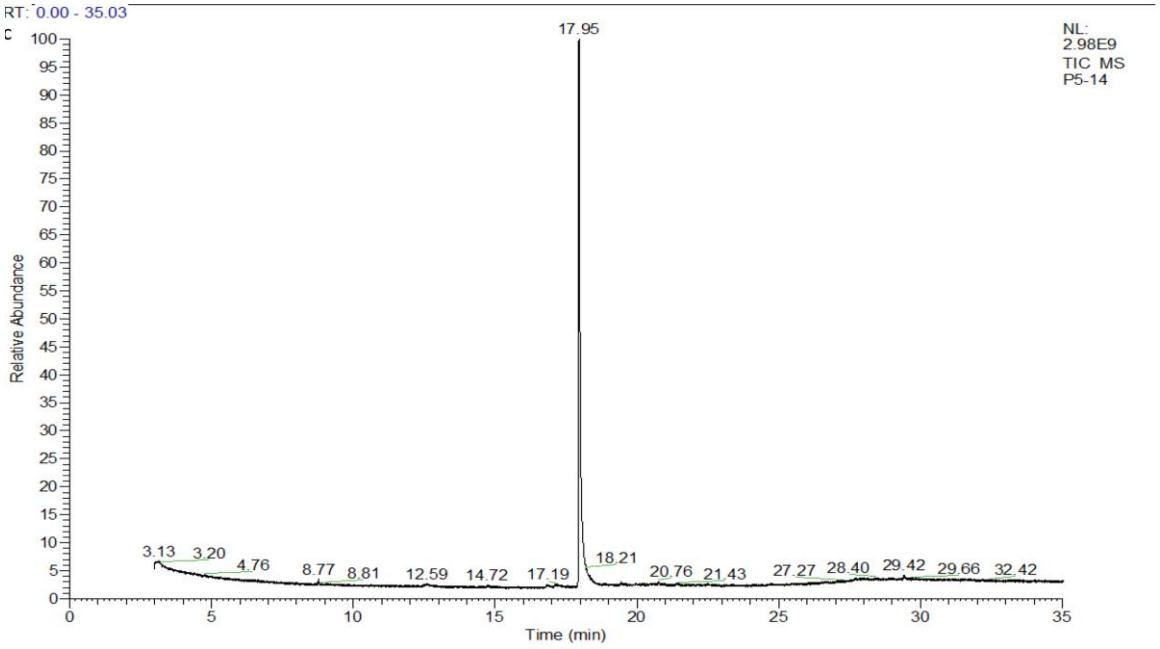


Figure S24. Gas chromatogram of purified N-(4-methoxyphenyl) pyrrolidine

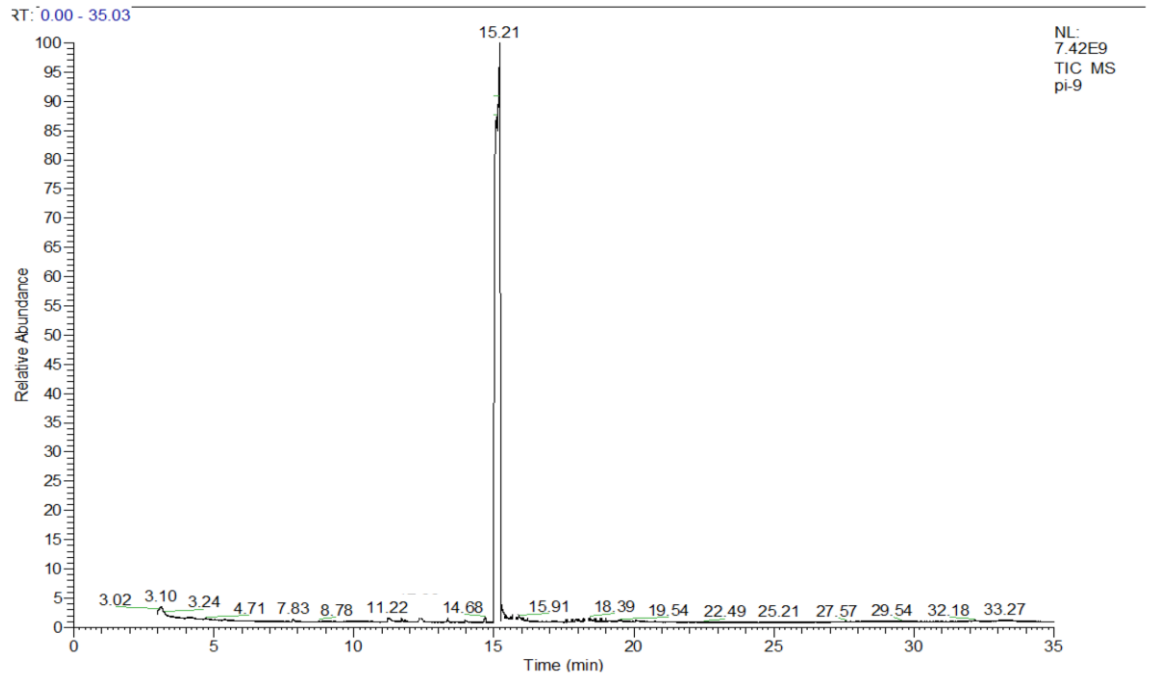


Figure S25. Gas chromatogram of purified N-phenylpiperidine

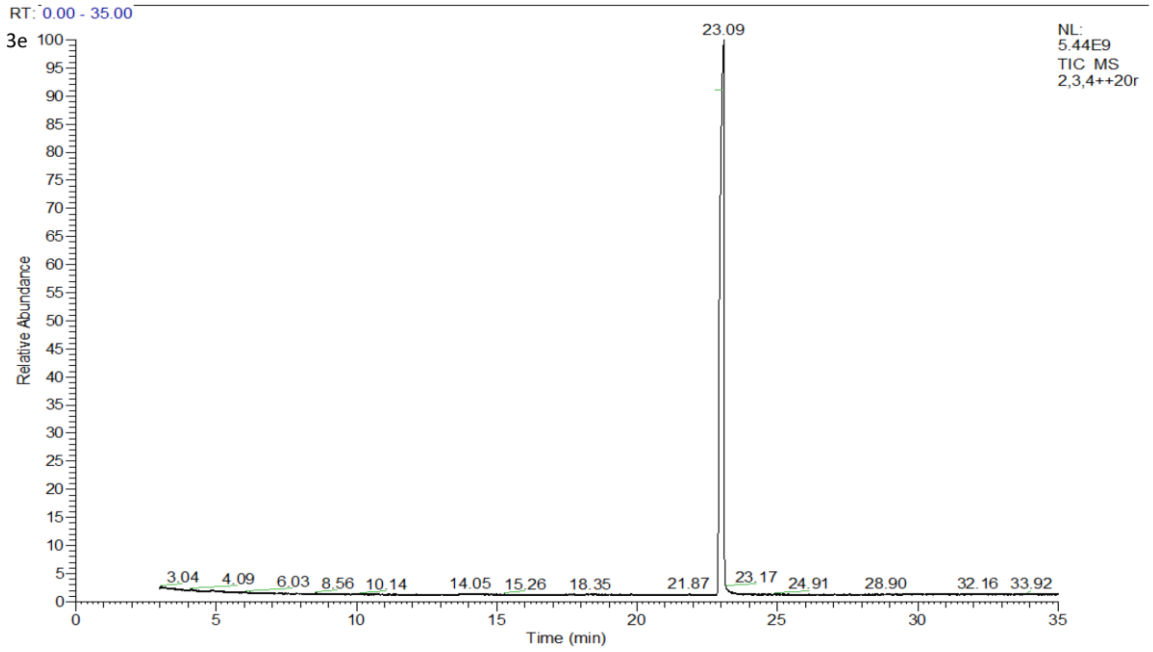


Figure S26. Gas chromatogram of purified N-(4-methoxyphenyl) piperidine

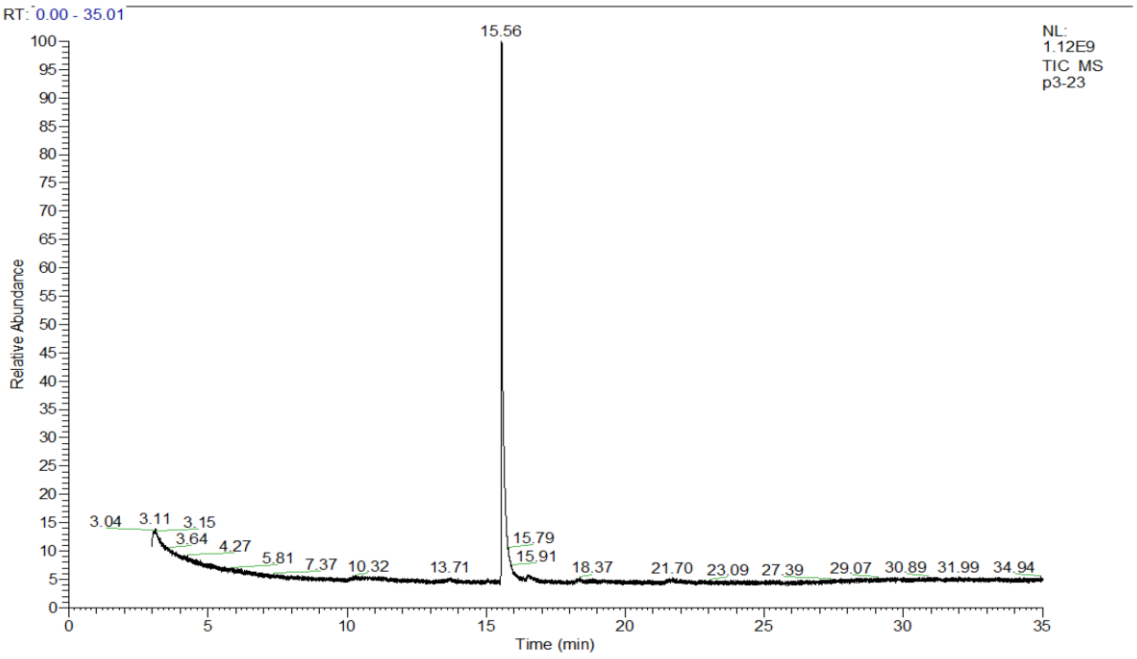


Figure S27. Gas chromatogram of purified 1-(piperidine-1-yl) pyridine

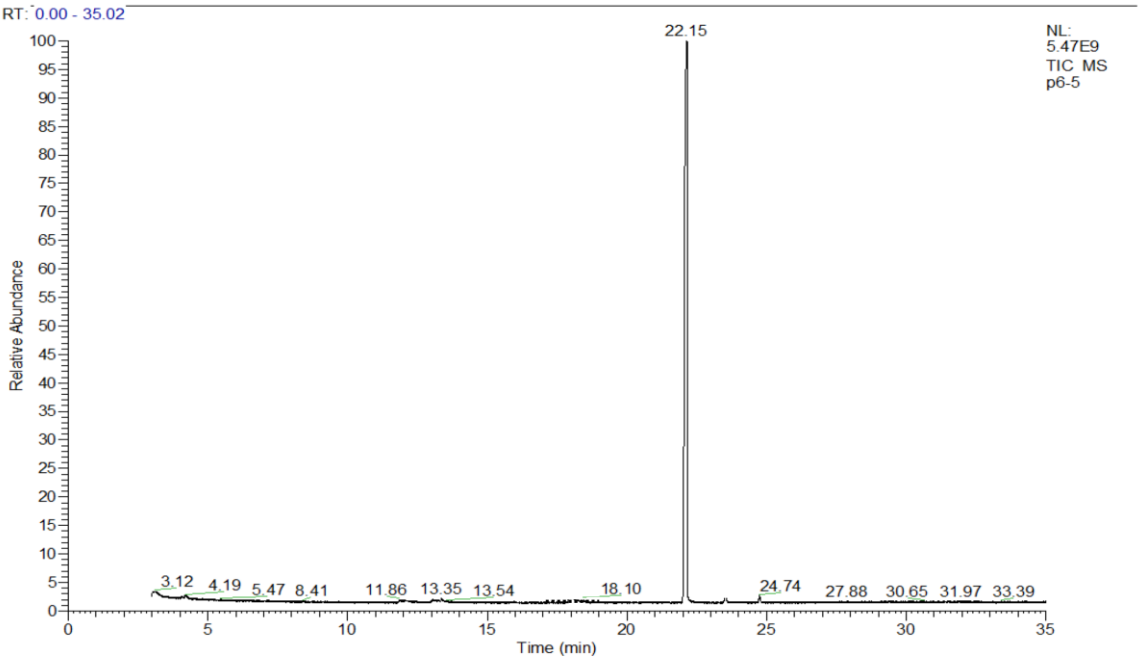


Figure S28. Gas chromatogram of purified 1-methyl-4-(pyridin-2-yl) piperazine

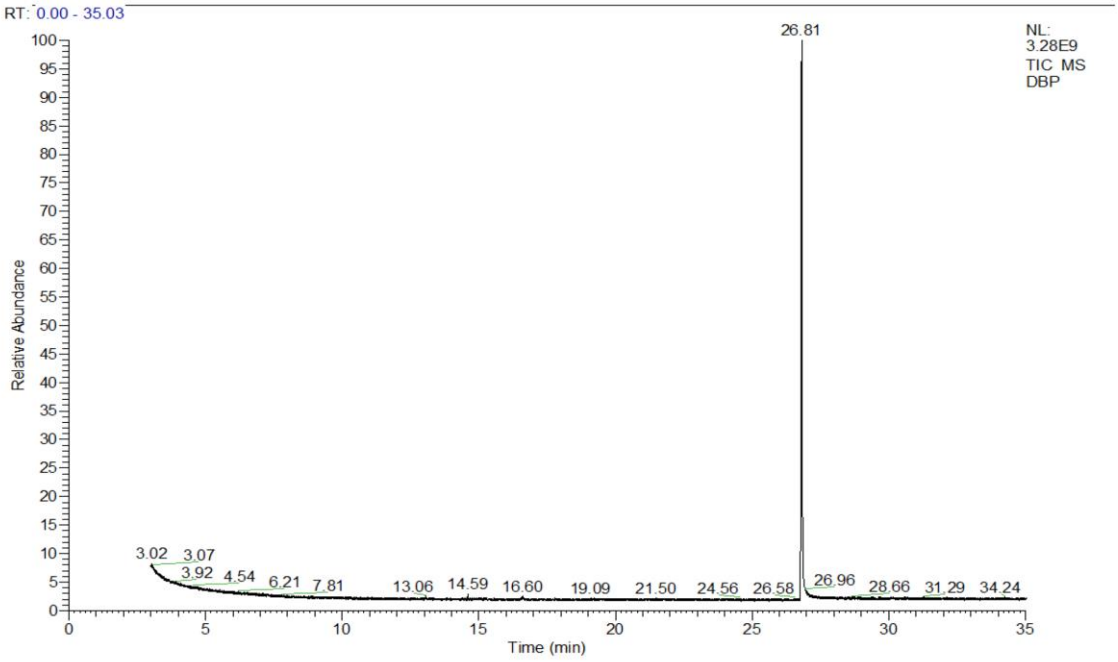


Figure S29. Gas chromatogram of purified benzylpiperazine

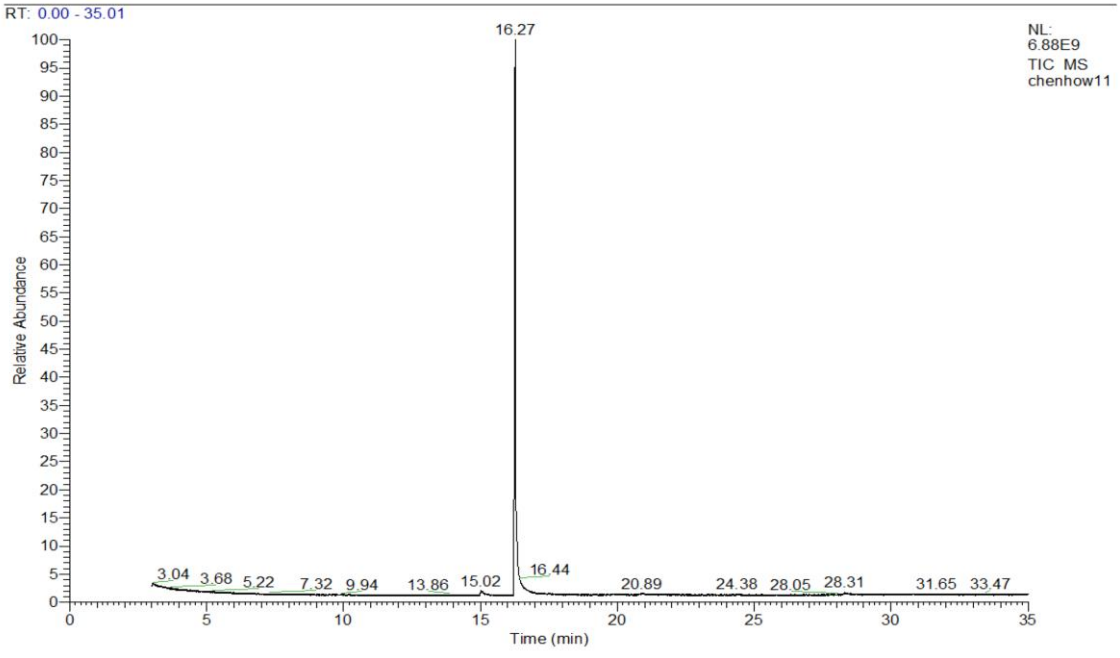


Figure S30. Gas chromatogram of purified 1-methyl-4-phenyl piperazine

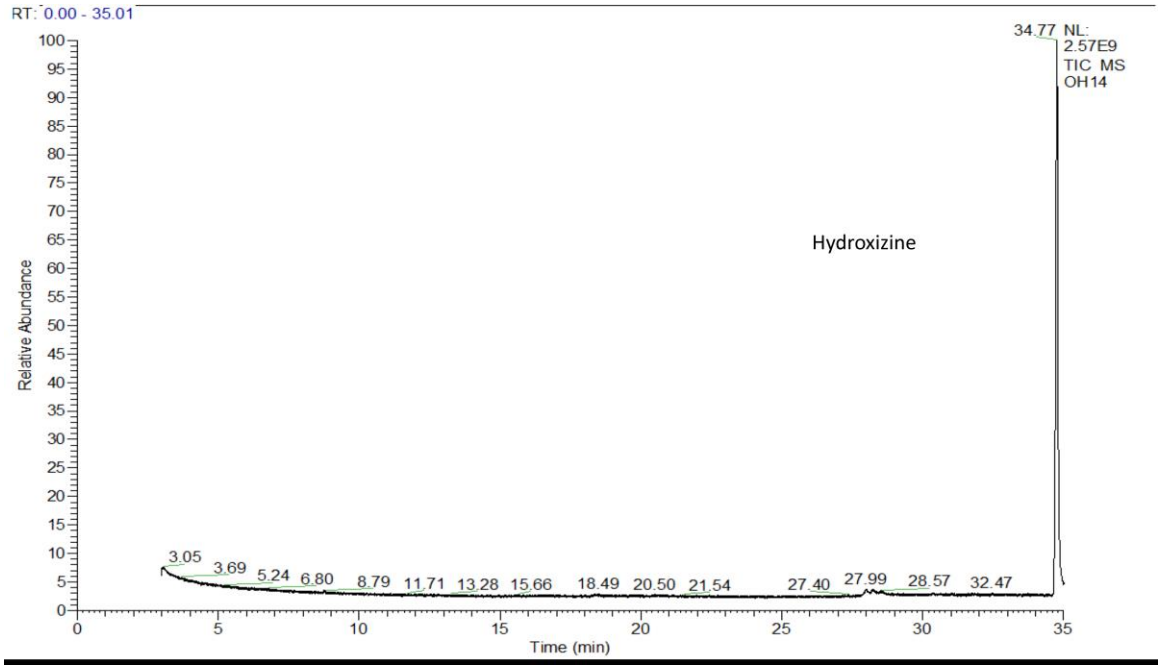


Figure S31. Gas chromatogram of purified of hydroxyzine

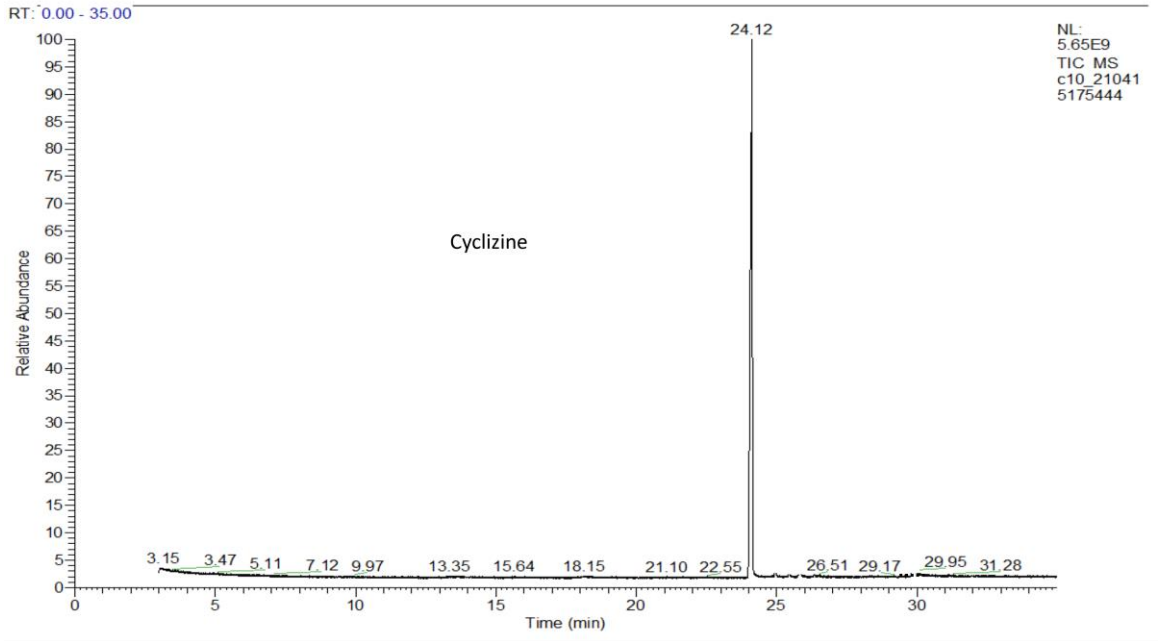


Figure S32. Gas chromatogram of purified cyclizine

III. [1]HNMR Spectra of Compounds

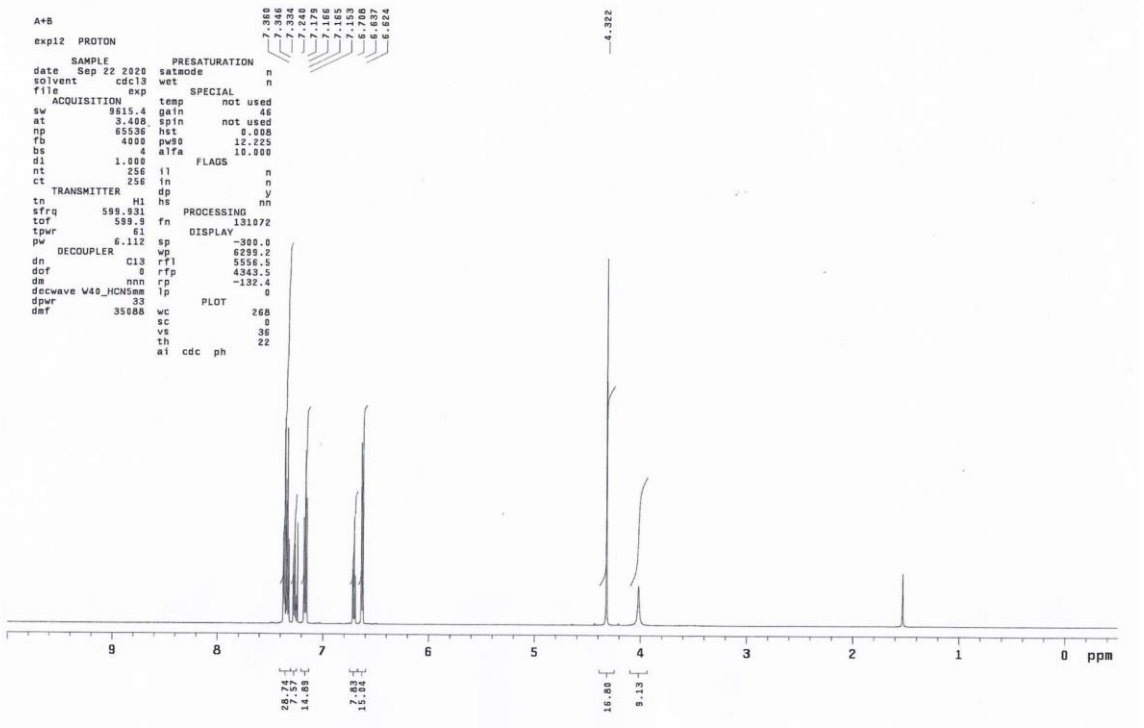


Figure S33. [1]HNMR Spectrum of N-benzylaniline

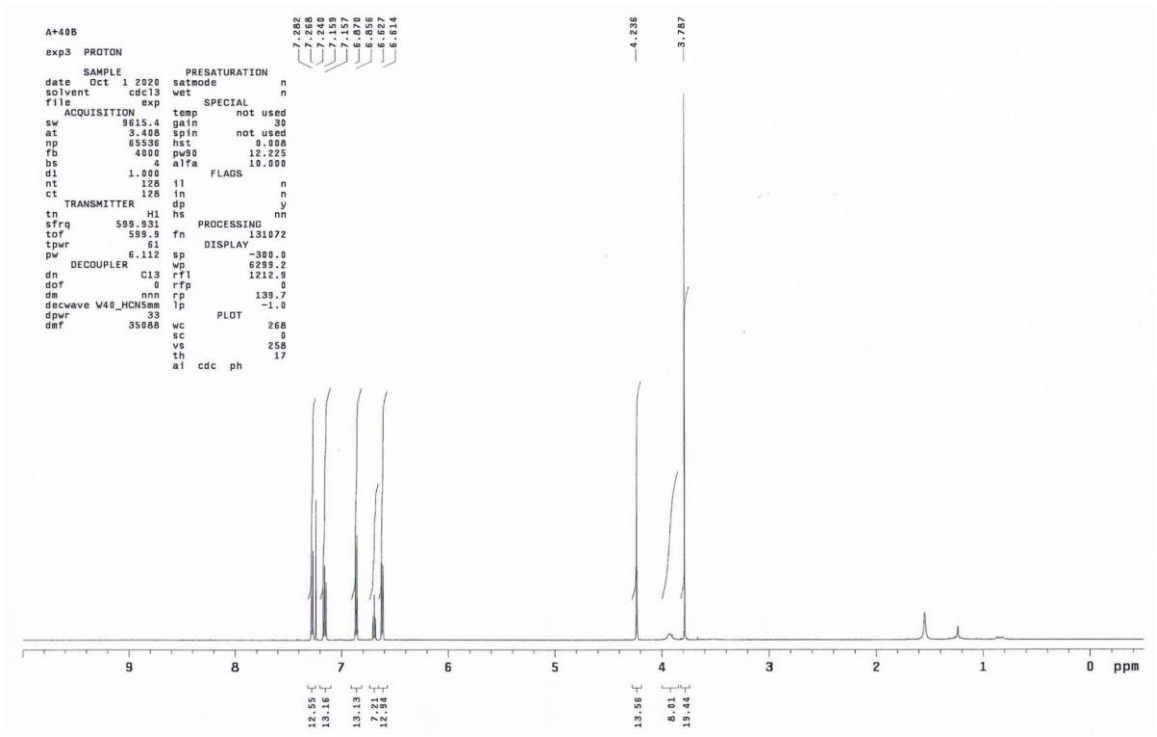


Figure S34. [1]HNMR Spectrum of N-(4-methoxybenzyl)aniline

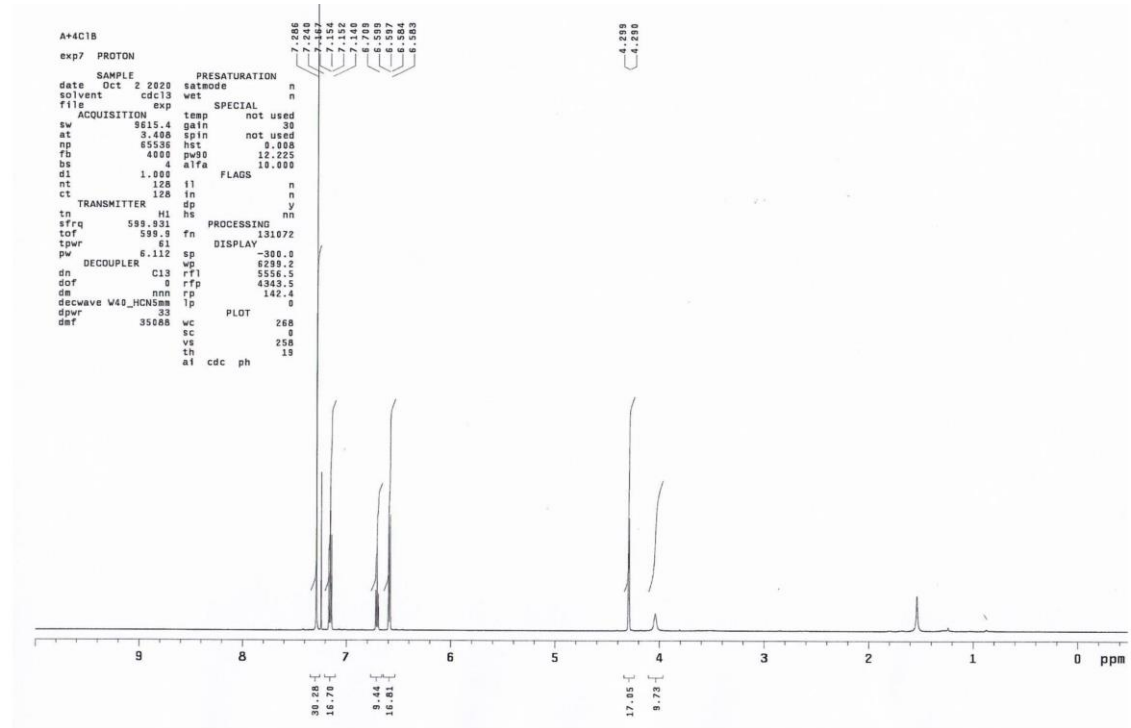


Figure S35. [1]HNMR Spectrum of N-(p-chlorobenzyl)aniline

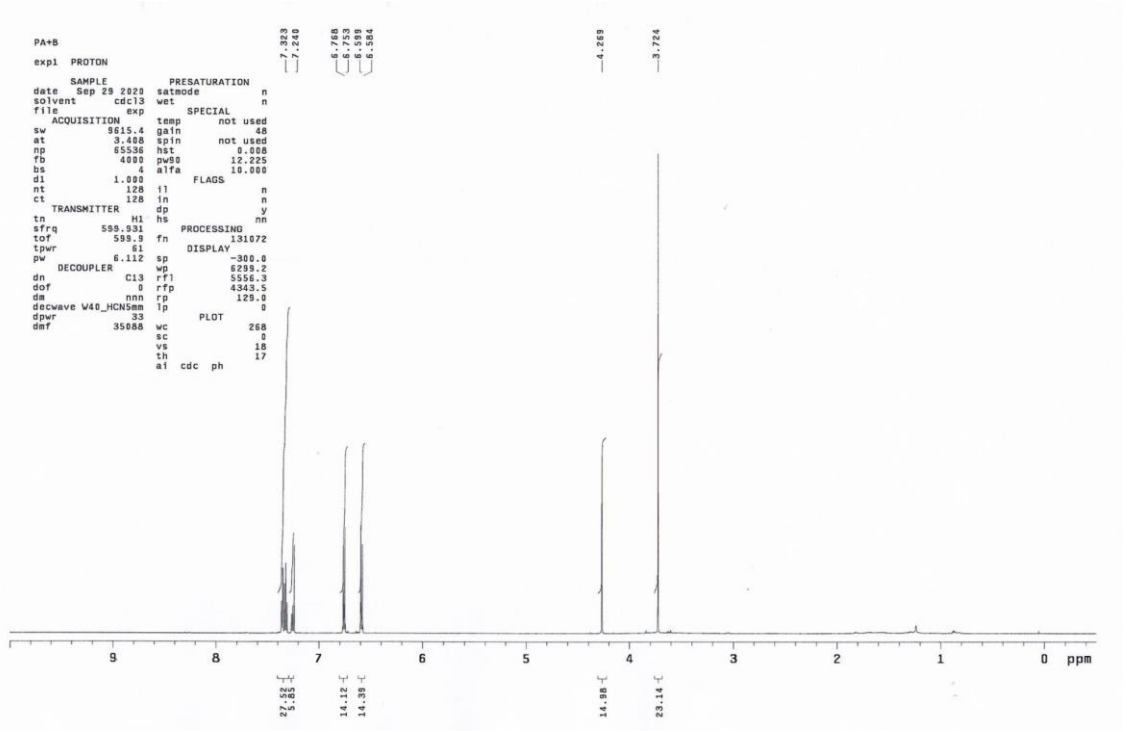


Figure S36. [1]HNMR Spectrum of benzyl(4-methoxyphenyl)amine

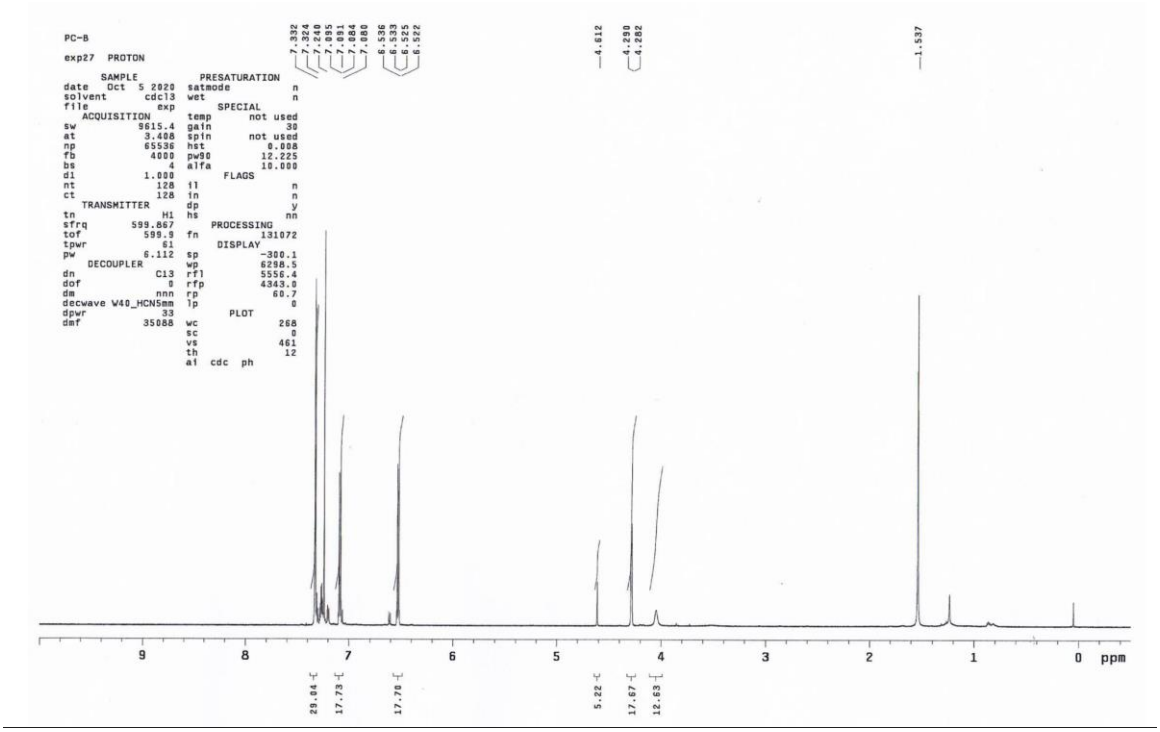


Figure S37. [1]HNMR Spectrum of N-(4-chlorophenyl)benzylamine

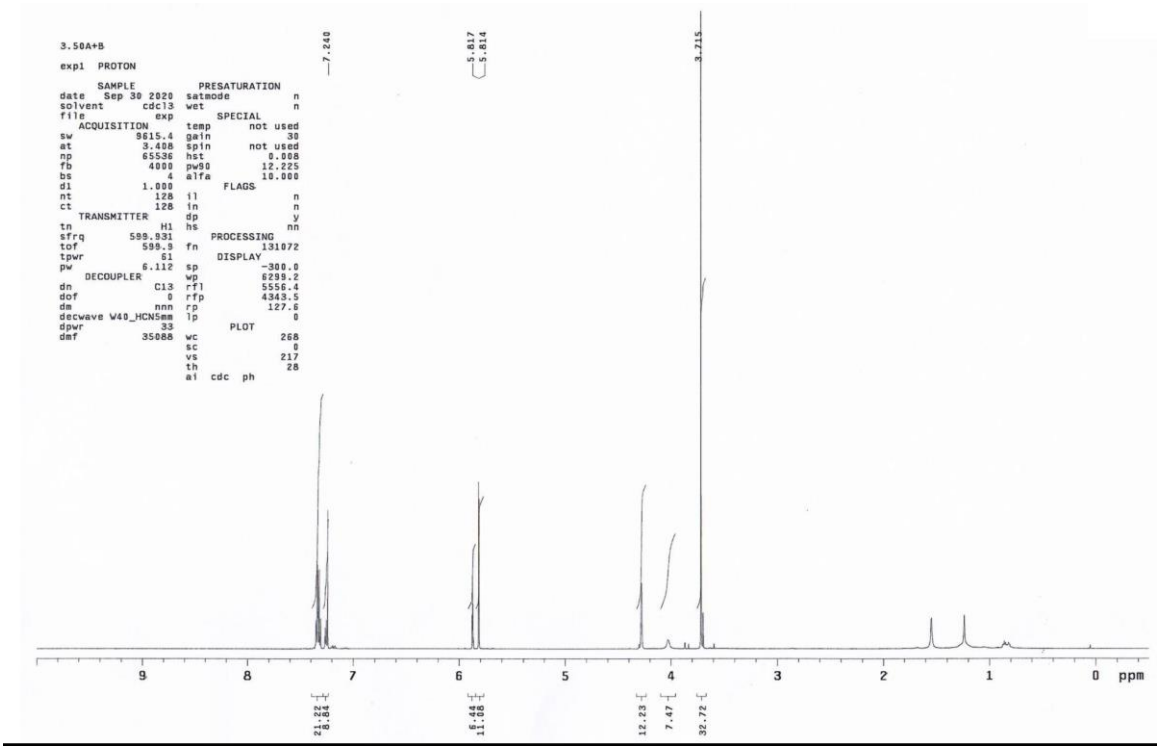


Figure S38. [1]HNMR Spectrum of N-benzyl-3,5-dimethoxyaniline

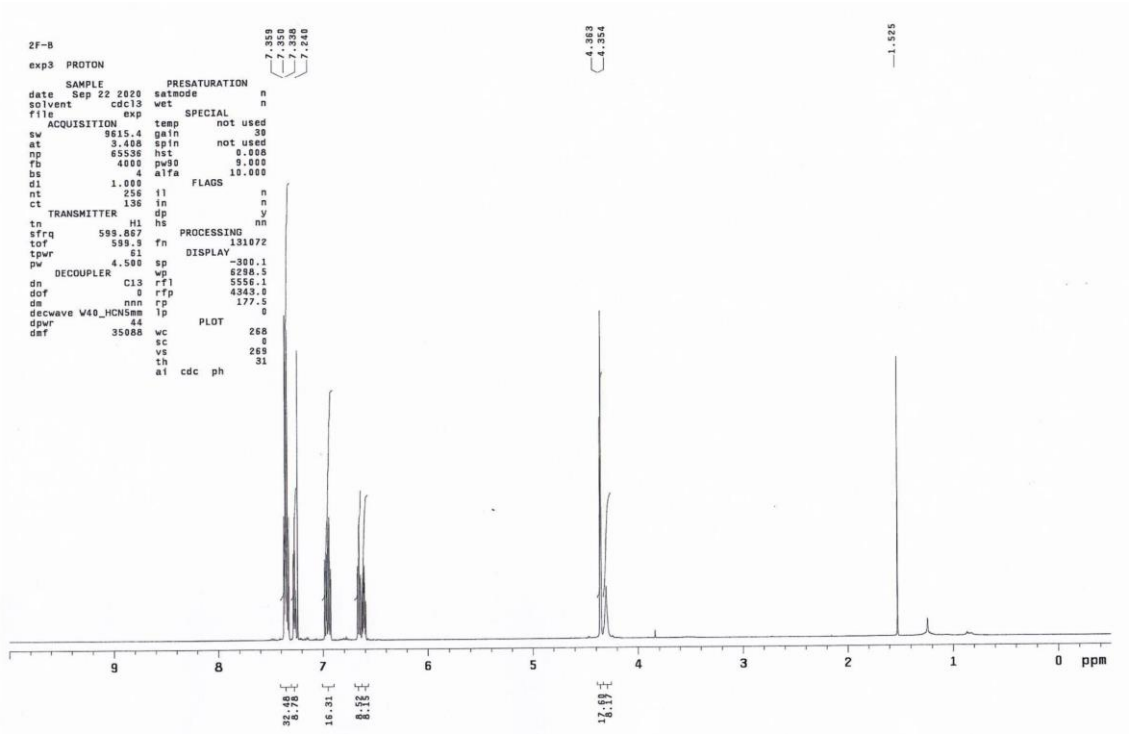


Figure S39. [1]HNMR Spectrum of N-benzyl-(2-fluorophenyl)amine

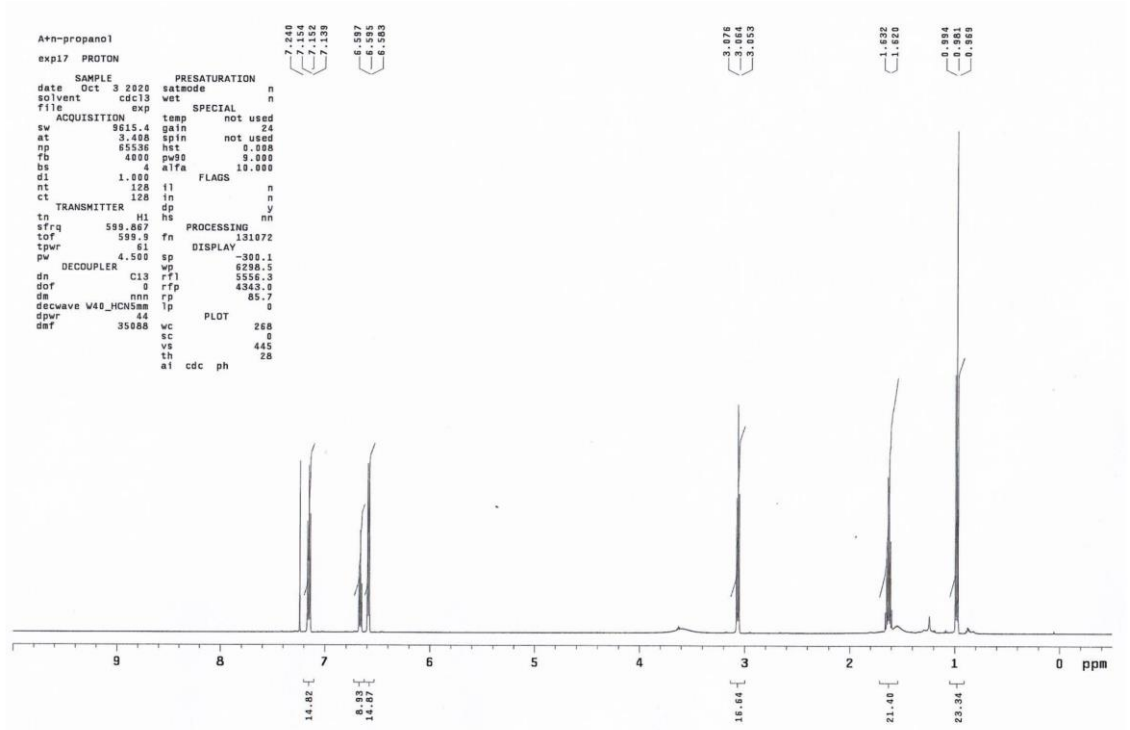


Figure S40. [1]HNMR Spectrum of N-propylaniline

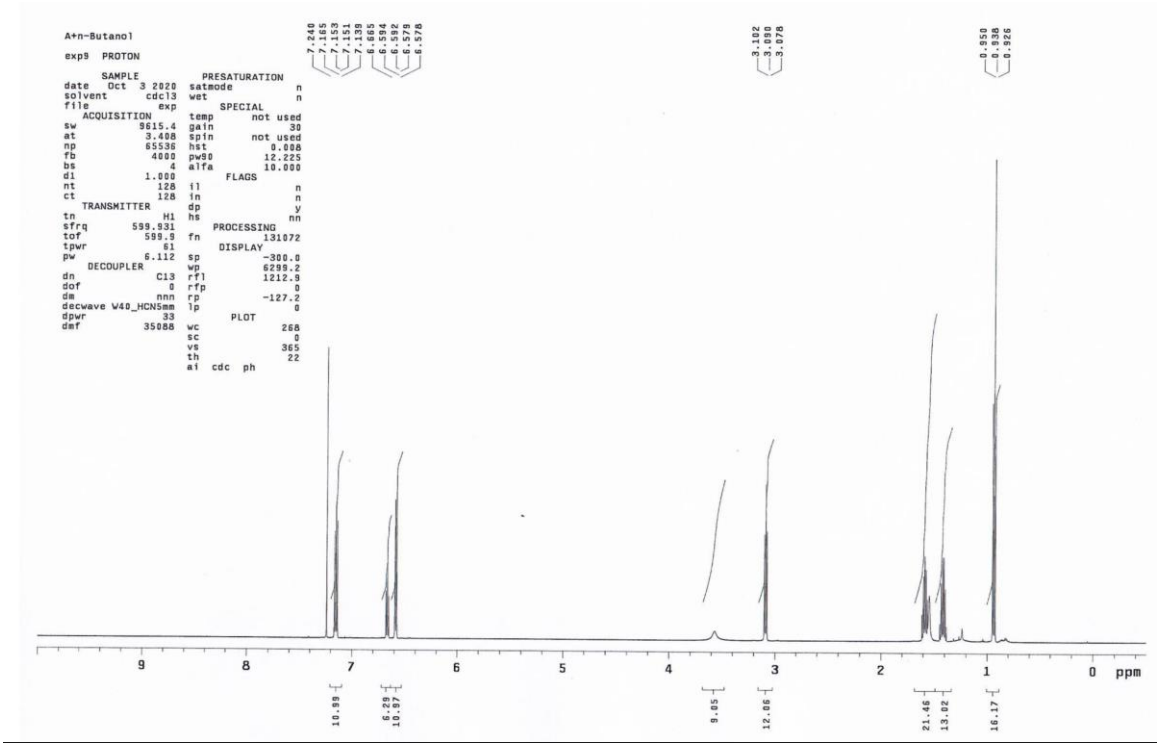


Figure S41. [1]HNMR Spectrum of N-(n-butyl)aniline

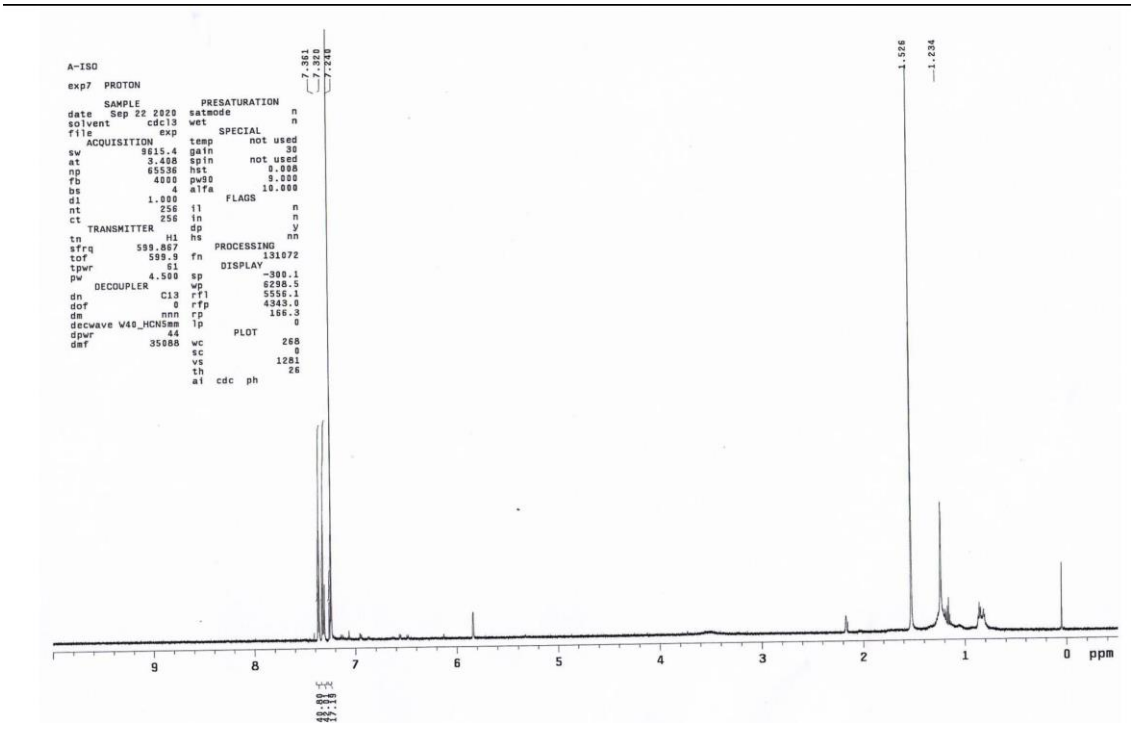


Figure S42. [1]HNMR Spectrum of N-isopropylaniline

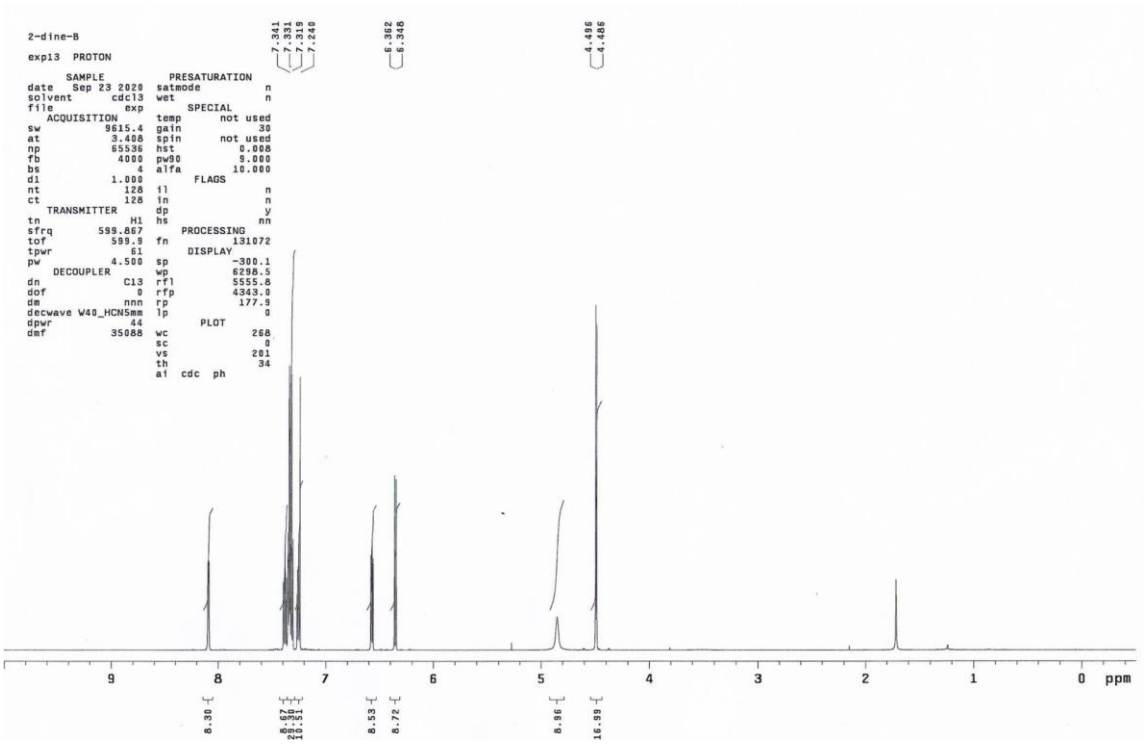


Figure S43. ^{1}HNMR Spectrum of N-benzylpyridin-2-amine

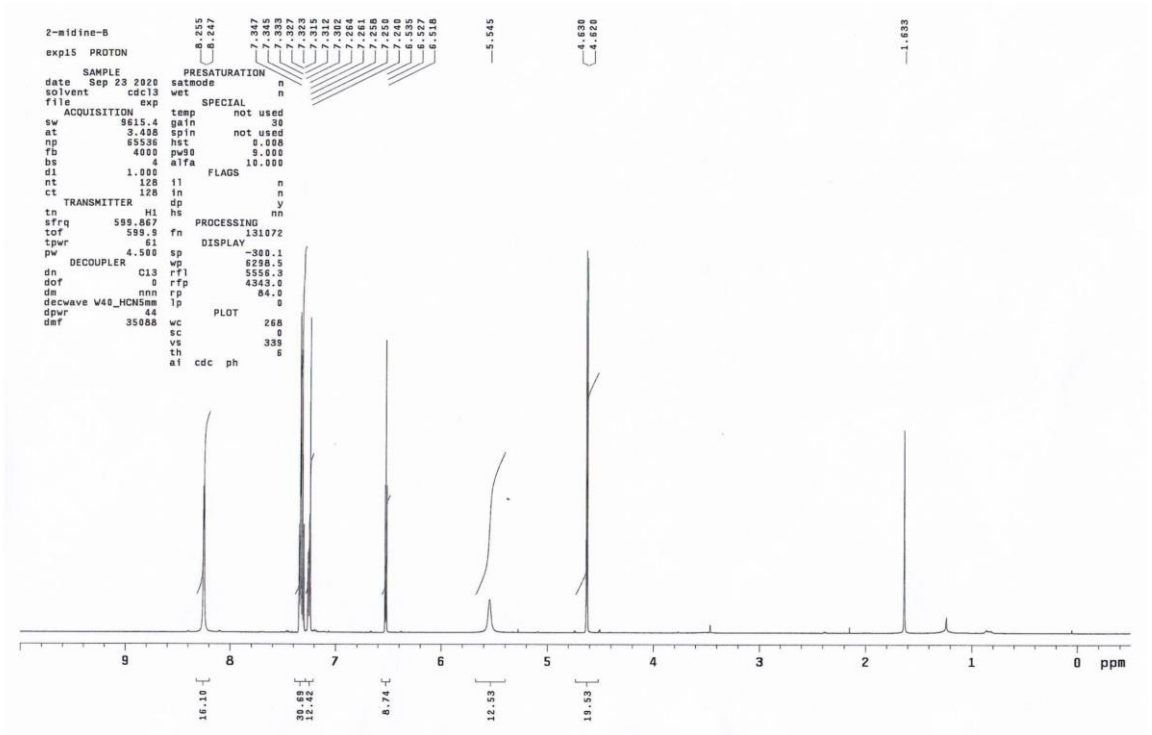


Figure S44. ^{1}HNMR Spectrum of 2-(benzylamino)pyrimidine

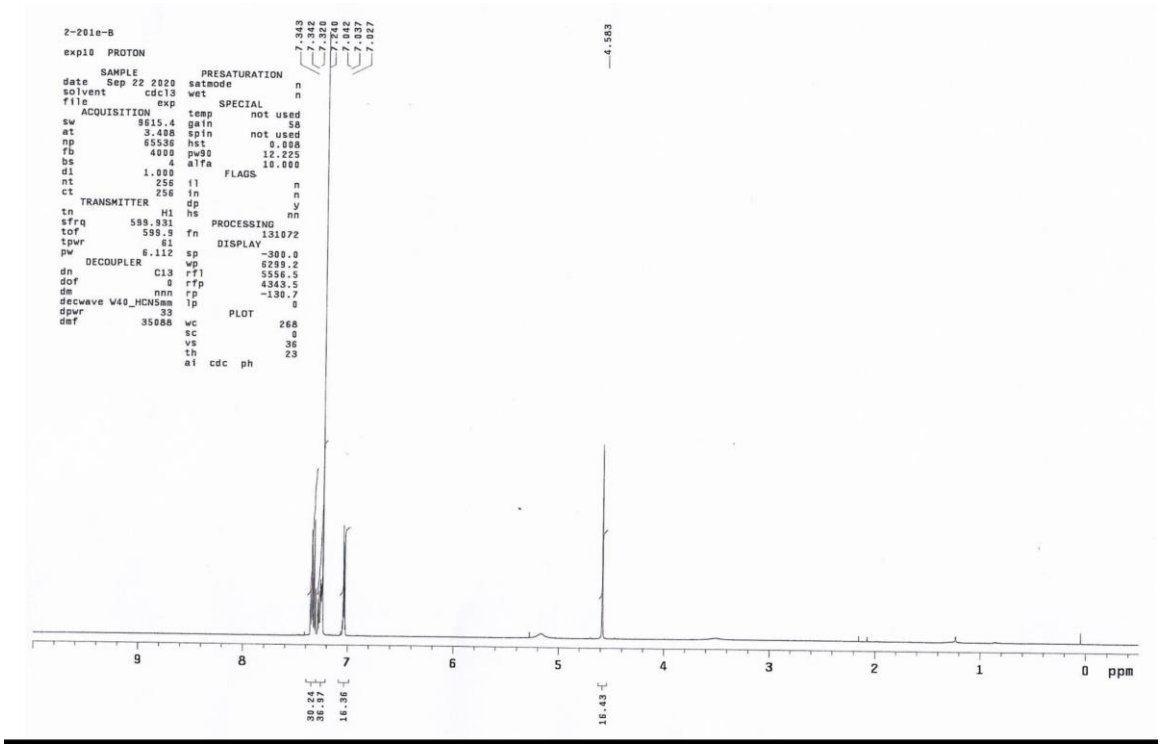


Figure S45. ^{1}HNMR Spectrum of (1H-benzoimidazol-2-yl)phenylamine

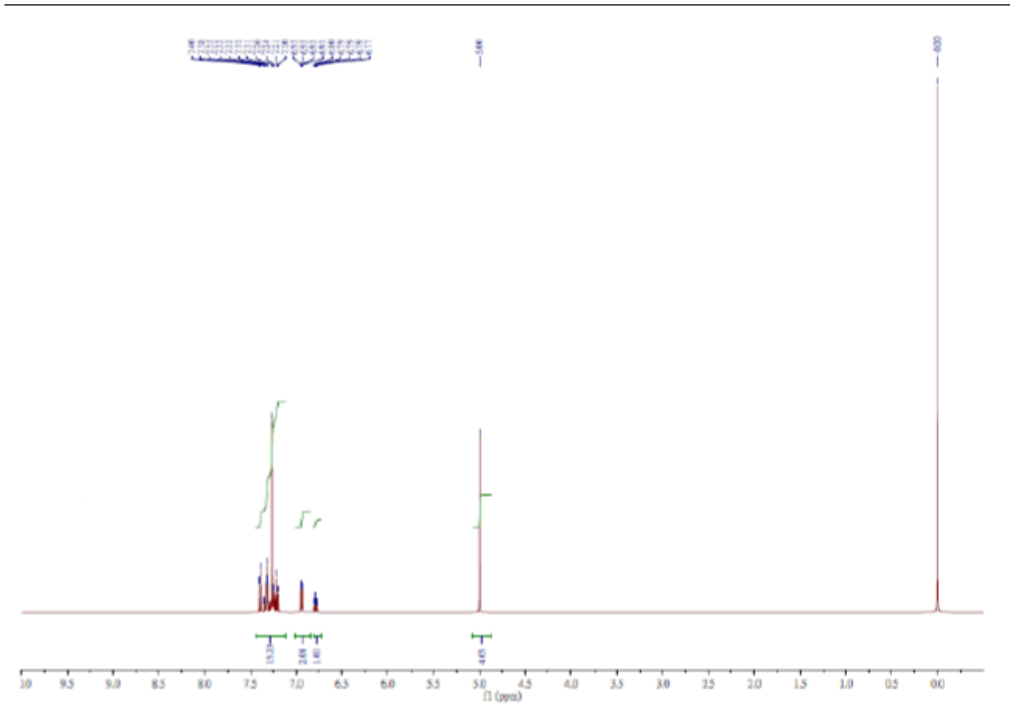


Figure S46. ^{1}HNMR Spectrum of N-benzyl-N-(4-chloro-benzyl)-aniline

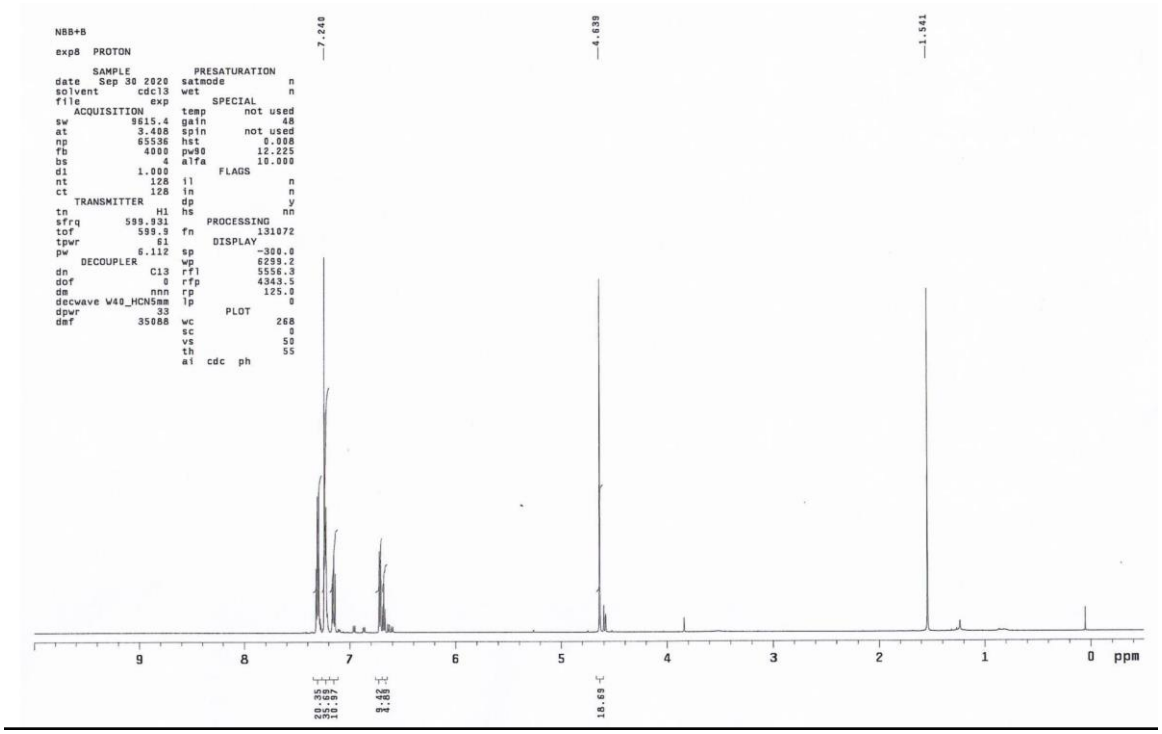


Figure S47. ^{1}HNMR Spectrum of N,N-dibenzylaniline

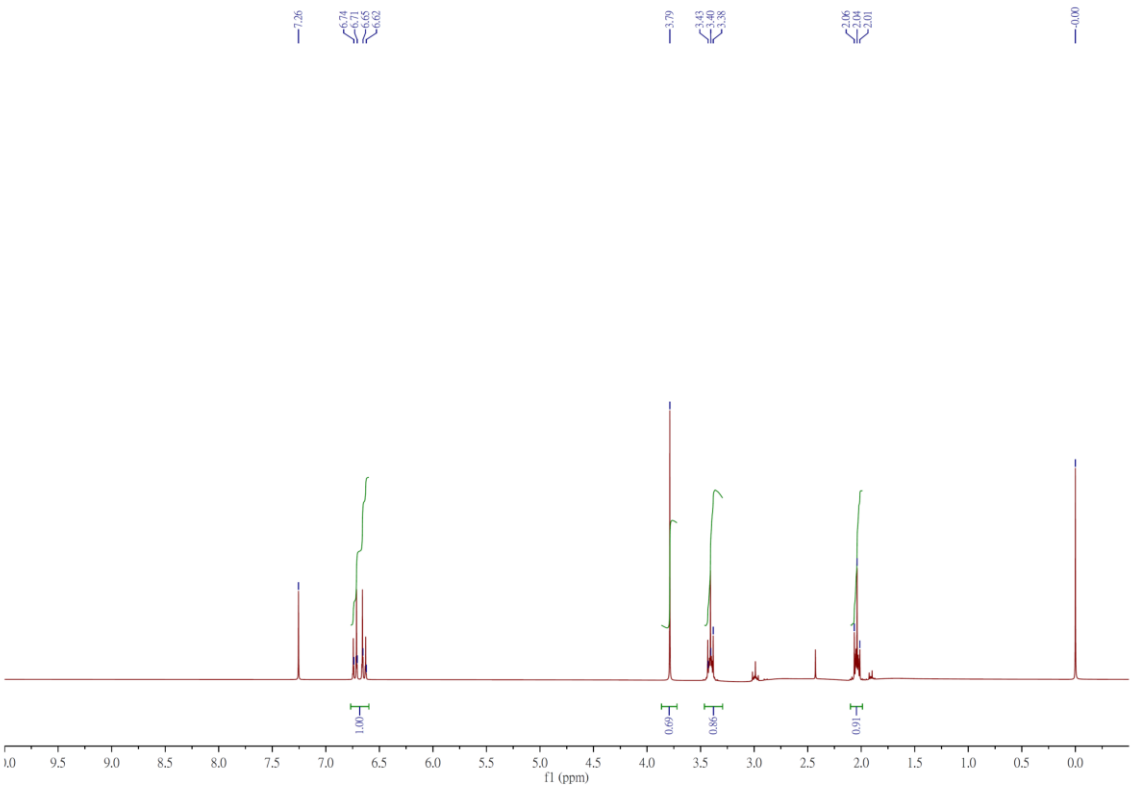


Figure S48. ^{1}HNMR Spectrum of N-(4-methoxyphenyl) pyrrolidine

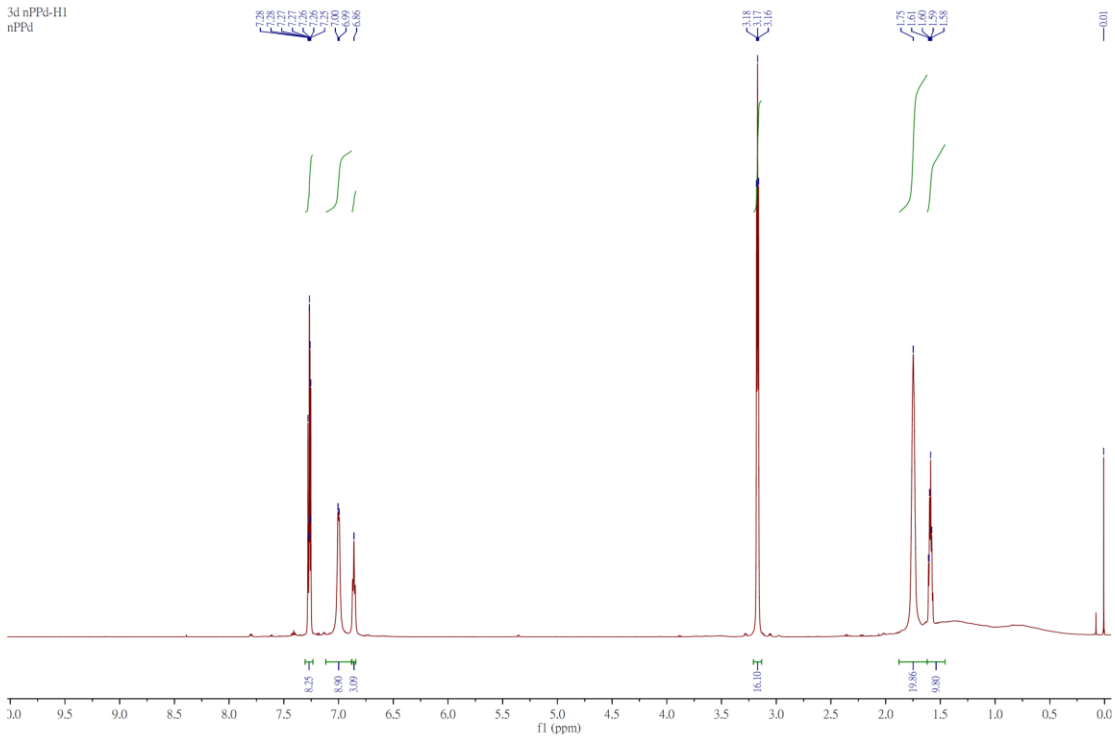


Figure S49. [1]HNMR Spectrum of N-phenylpiperidine

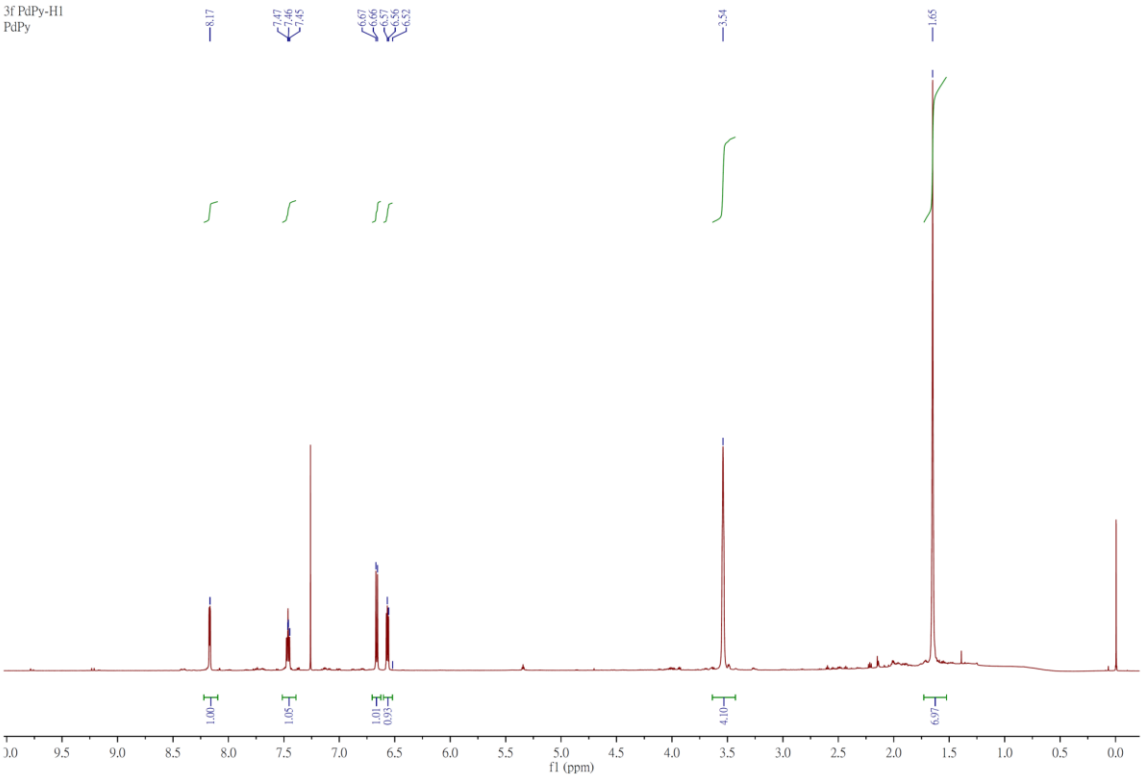


Figure S50. [1]HNMR Spectrum of 1-(piperidine-1-yl) pyridine

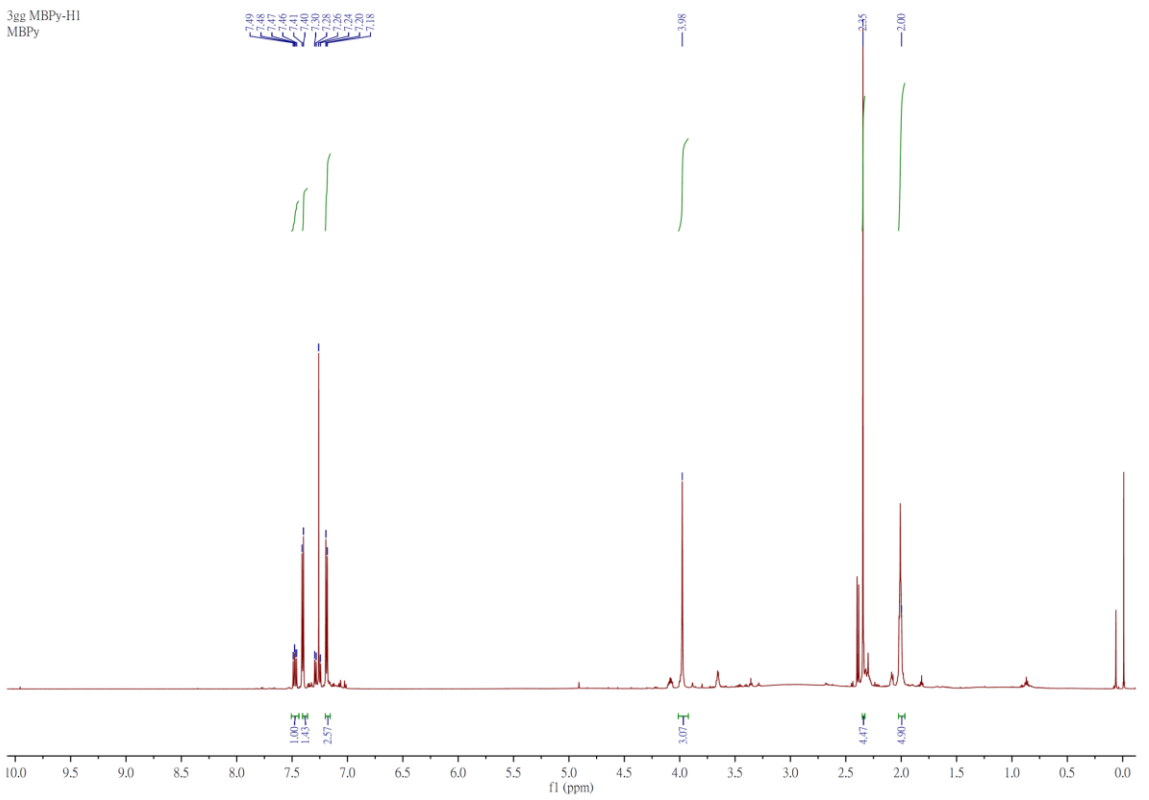


Figure S51. [1]HNMR Spectrum of 1-methyl-4-(pyridin-2-yl) piperazine

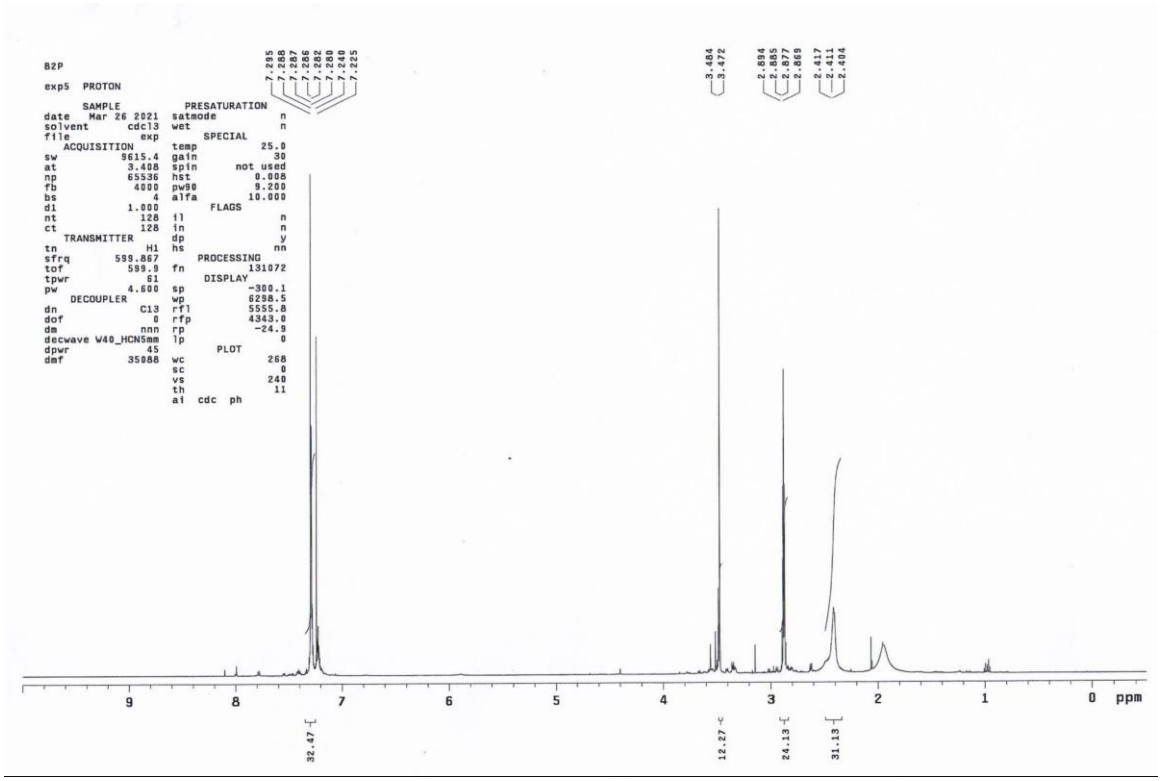


Figure S52. [1]HNMR Spectrum of Benzylpiperazine

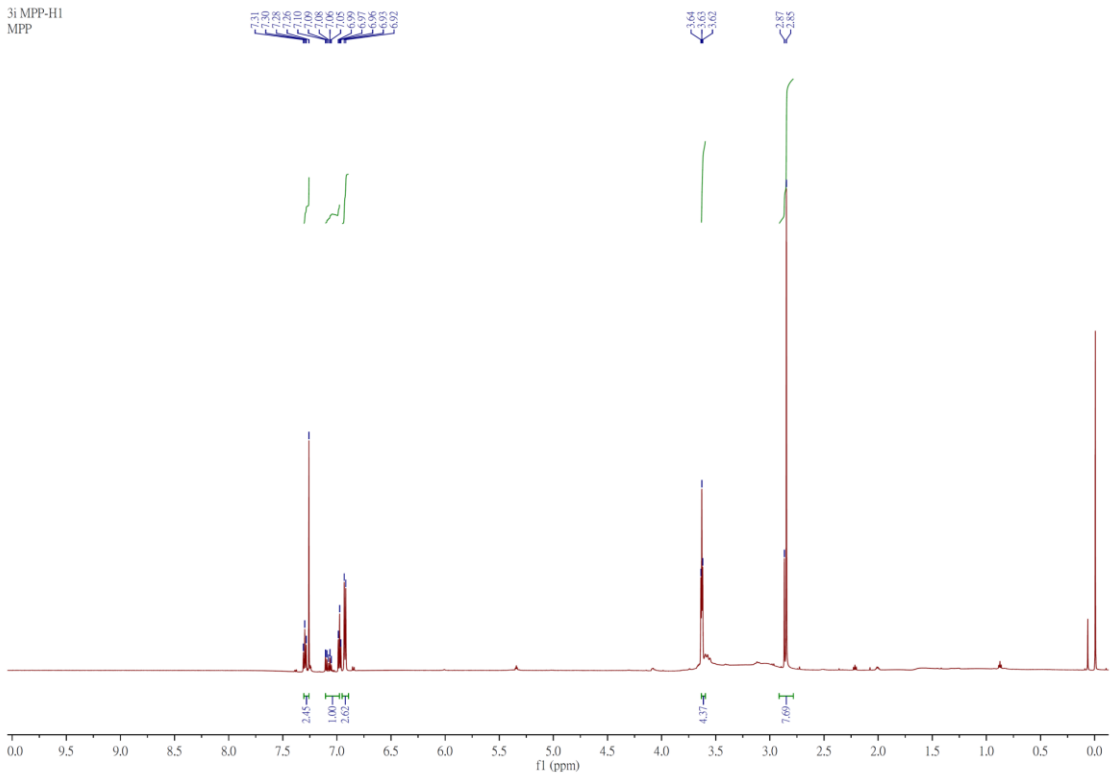


Figure S53. [1]HNMR Spectrum of 1-methyl-4-phenyl piperazine

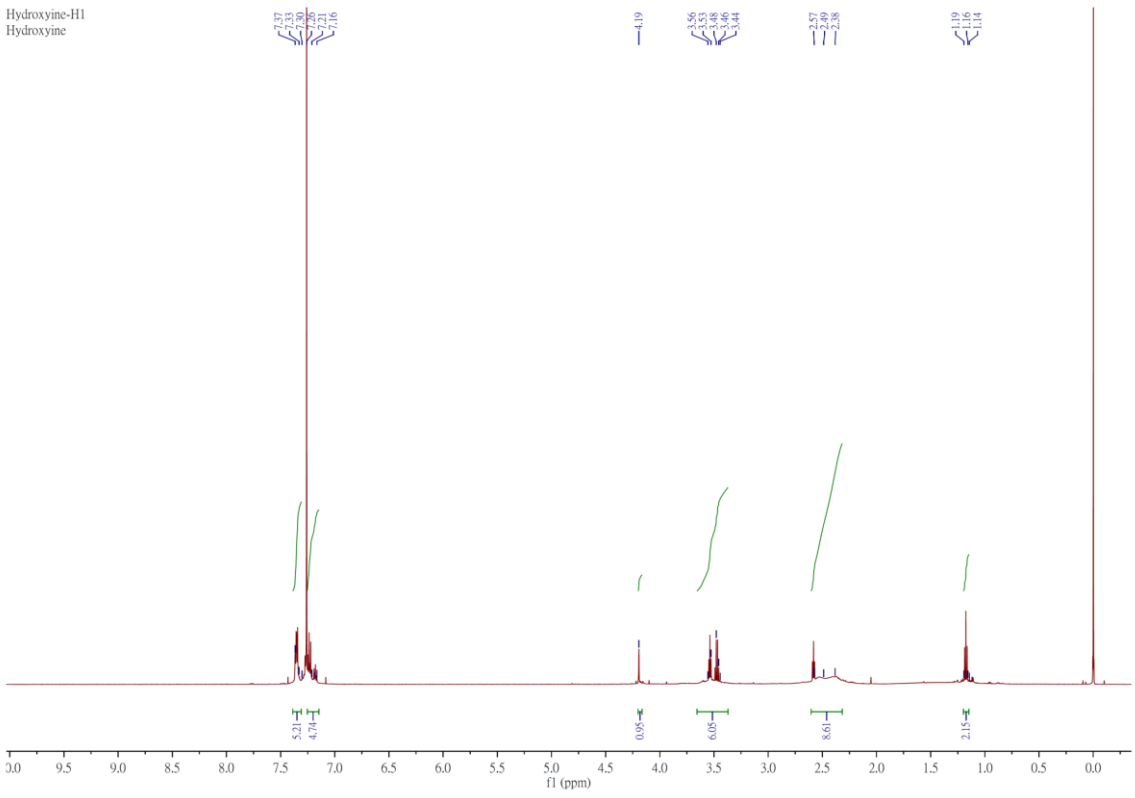


Figure S54. [1]HNMR Spectrum of hydroxyzine

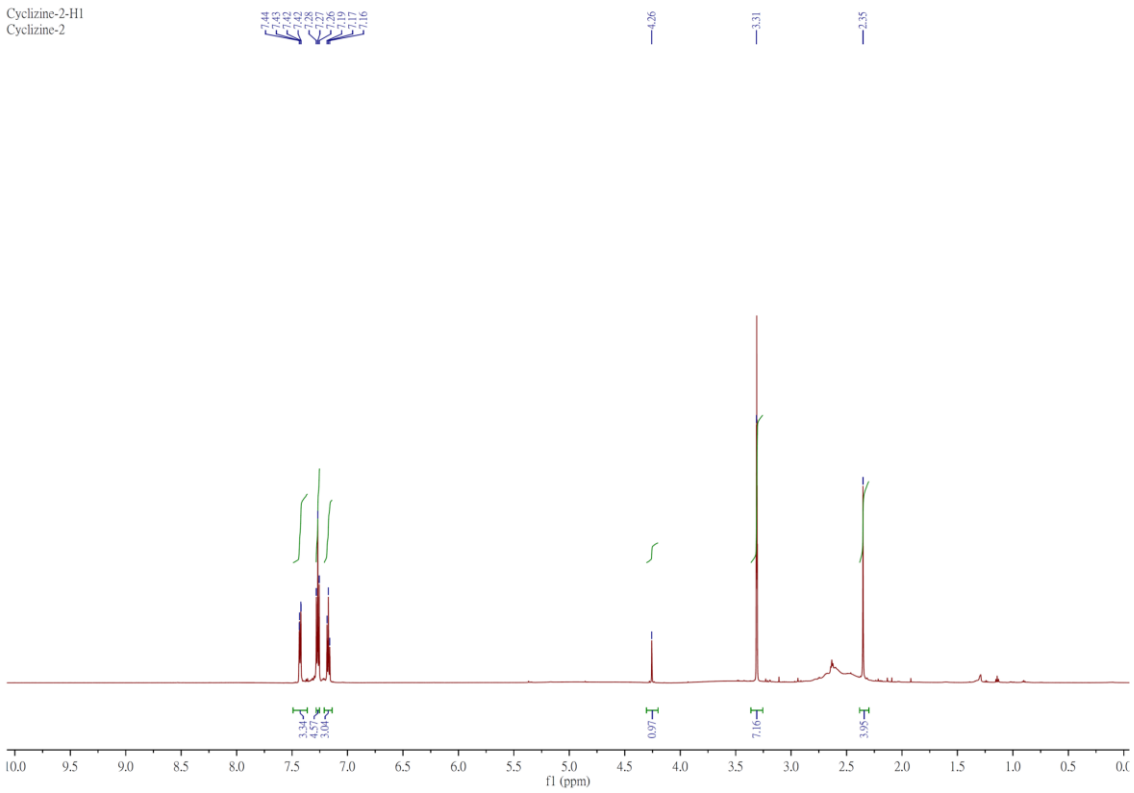
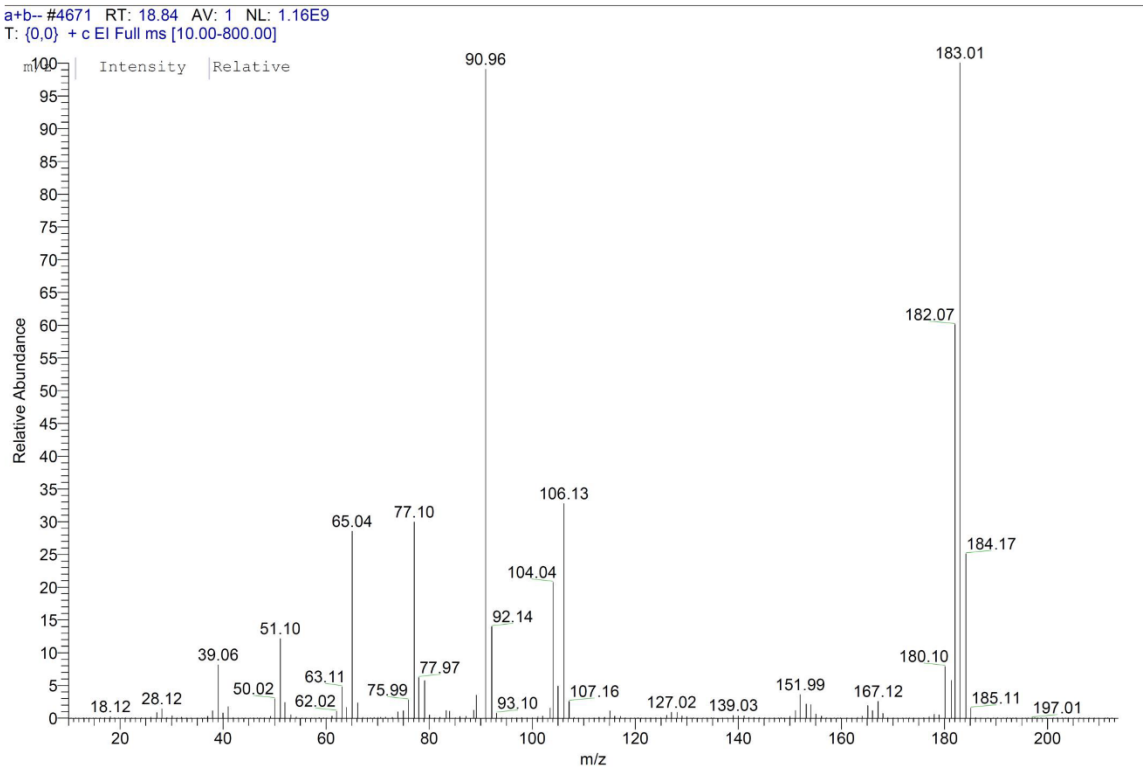


Figure S55. ^{1}HNMR Spectrum of Cyclizine

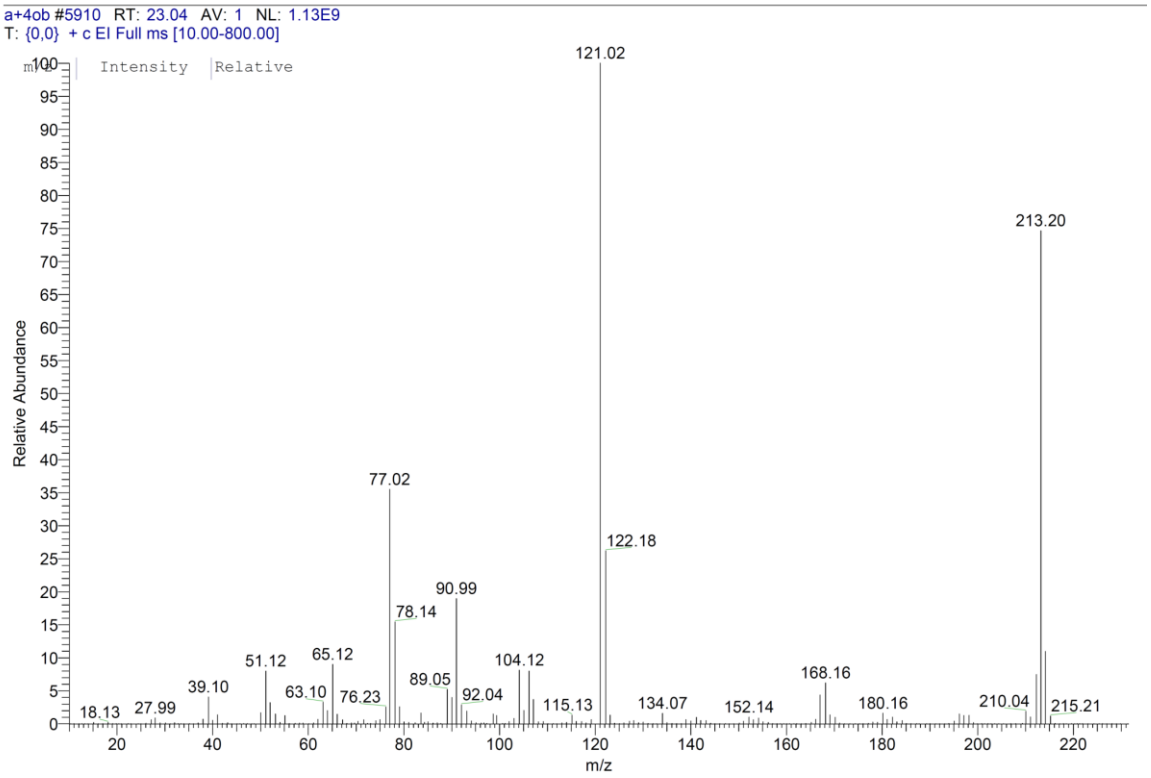
IV. Compound Mass Spectra and Data



30-A+B-APCI-H#1-20 RT: 0.01-0.54 AV: 20
T: FTMS + p APCI corona Full ms [150.00-500.00]
m/z= 183.3659-184.9091
Isotope Min Max
N-14 0 1
C-12 0 13
H-1 0 14
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
184.1114	113781720.0	100.00	184.1121	-3.72	$C_{13}H_{14}N$

Figure S56. Mass spectrum and HMS data of N-benzylaniline



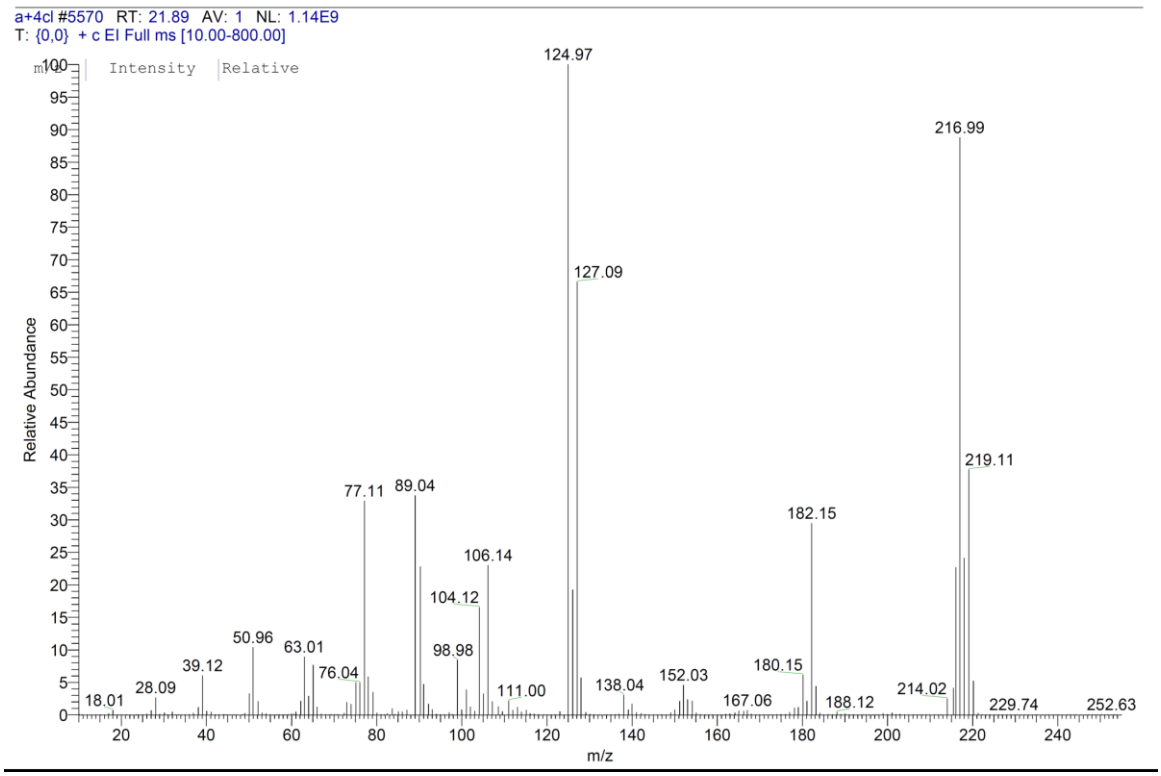
48-PA+B-H#1-20 RT: 0.00-0.27 AV: 20
T: FTMS + p ESI Full ms [50.00-1000.00]
m/z= 213.7896-214.5410

Isotope	Min	Max
C-12	0	14
H-1	0	16
N-14	0	1
O-16	0	1

Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
214.1222	53240772.0	100.00	214.1226	-1.93	$C_{14}H_{16}ON$

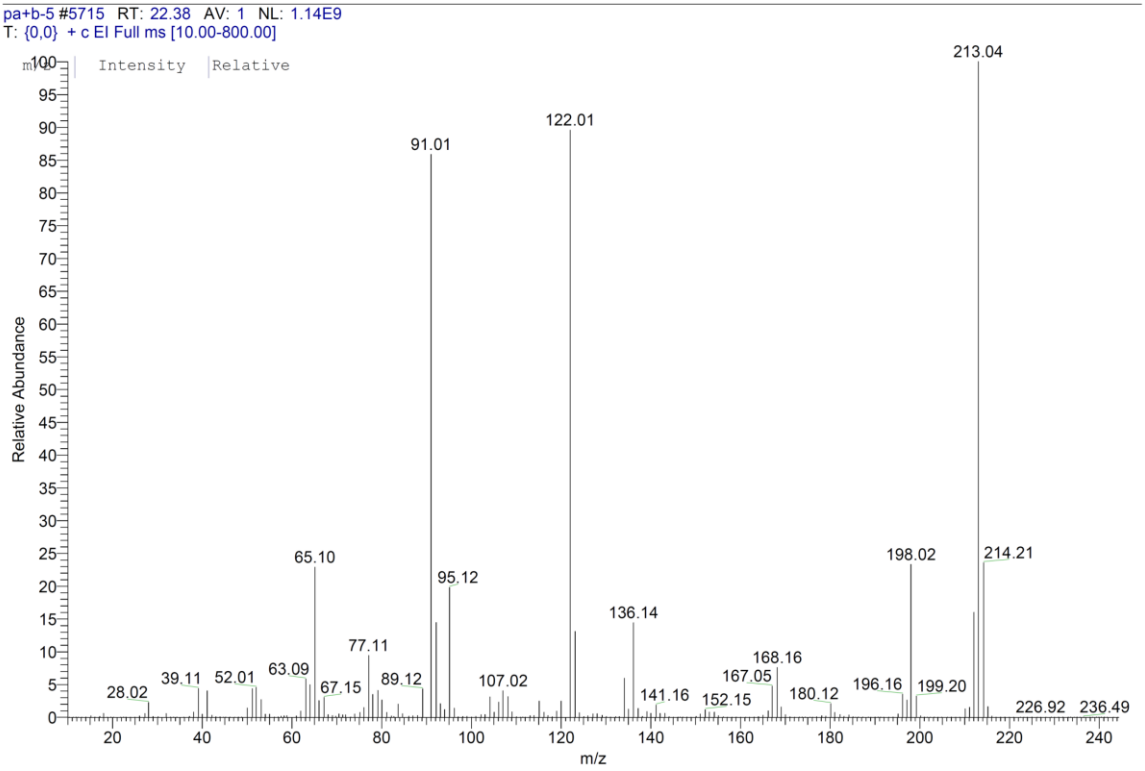
Figure S57. Mass spectrum and HMS data of N-(4-methoxybenzyl)aniline




```
64-A+4ClB-H#1-20 RT: 0.01-0.53 AV: 20
T: FTMS + p ESI Full ms [50.00-1000.00]
m/z= 217.6655-218.5323
Isotope  Min   Max
C-12       0    13
H-1        0    13
N-14       0     1
Cl-35      0     1
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1
```

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
218.0731	9187648.0	100.00	218.0731	-0.03	$C_{13}H_{13}NCl$

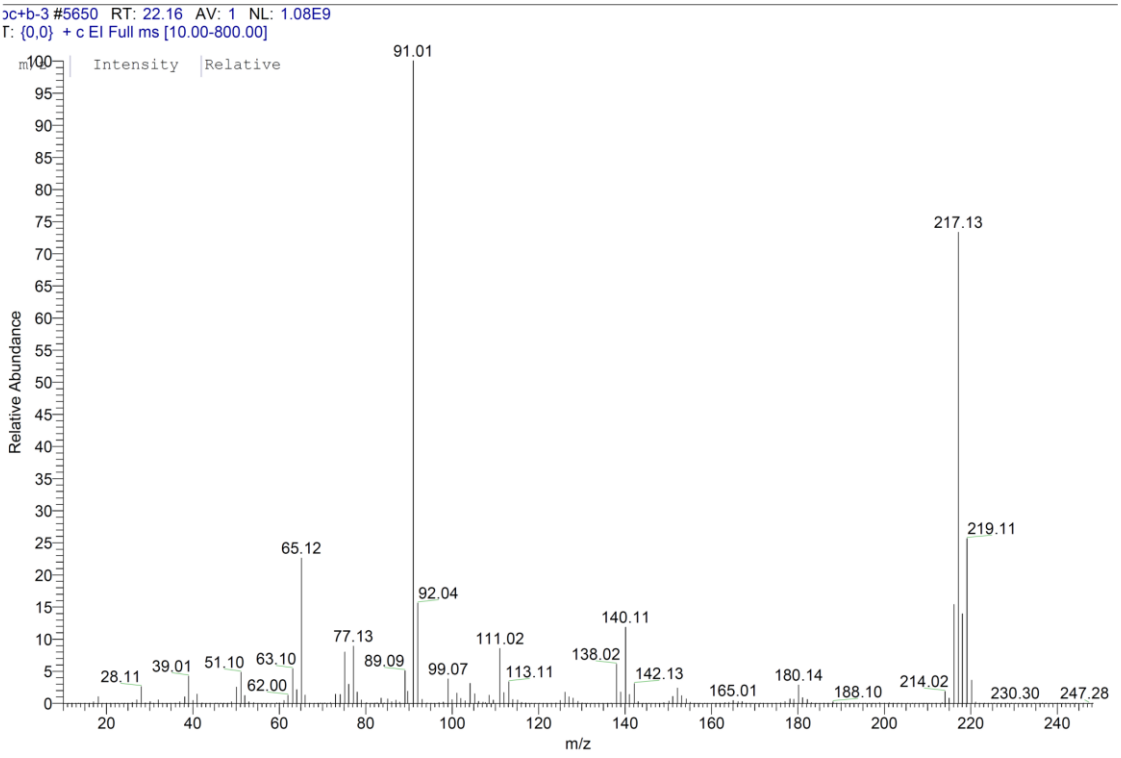
Figure S58. Mass spectrum and HMS data of N-(p-chlorobenzyl)aniline




```
48-PA+B-H#1-20 RT: 0.00-0.27 AV: 20
T: FTMS + p ESI Full ms [50.00-1000.00]
m/z= 213.7896-214.5410
Isotope  Min   Max
C-12       0    14
H-1        0    16
N-14       0     1
O-16       0     1
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1
```

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
214.1222	53240772.0	100.00	214.1226	-1.93	$C_{14}H_{16}ON$

Figure S59. Mass spectrum and HMS data of benzyl(4-methoxyphenyl)amine



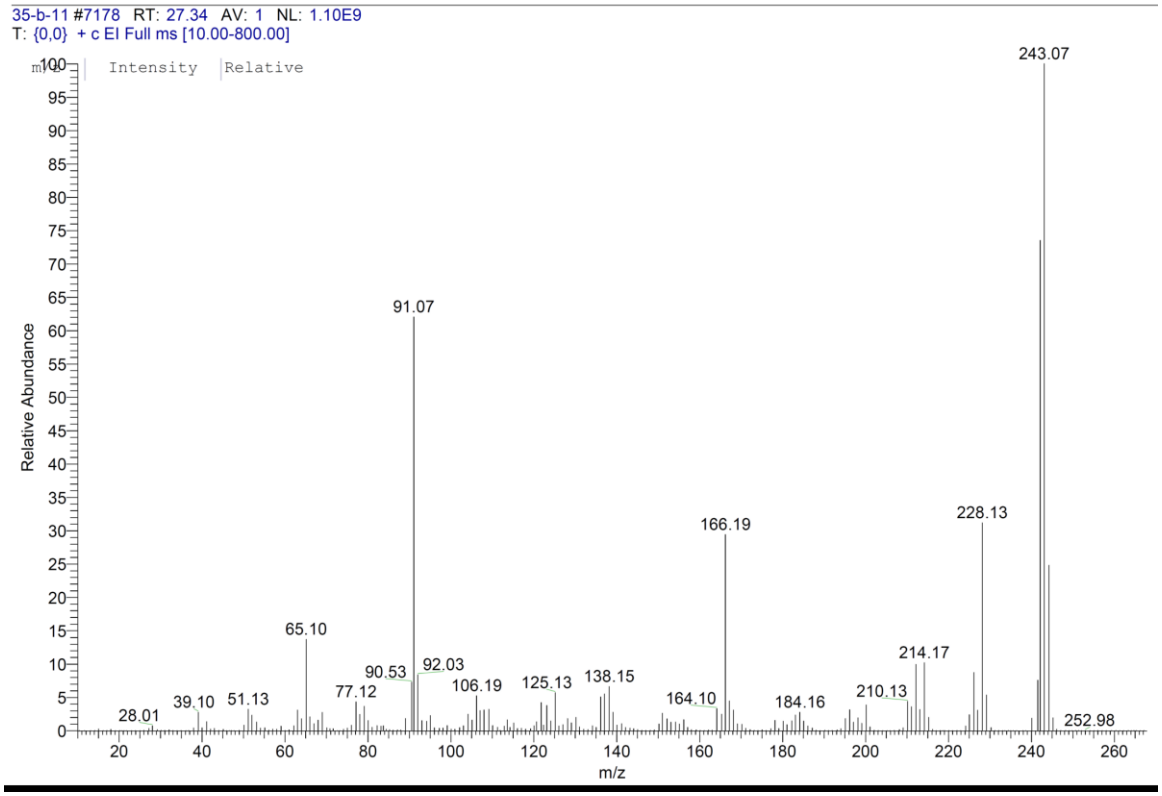
16-PC+B-H#1-20 RT: 0.01-0.52 AV: 20
T: FTMS + p ESI Full ms [50.00-1000.00]
m/z= 218.0204-218.1504

Isotope	Min	Max
C-12	0	13
H-1	0	13
N-14	0	1
Cl-35	0	1

Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
218.07311	83306456.0	100.00	218.07310	0.03	$C_{13}H_{13}NCl$

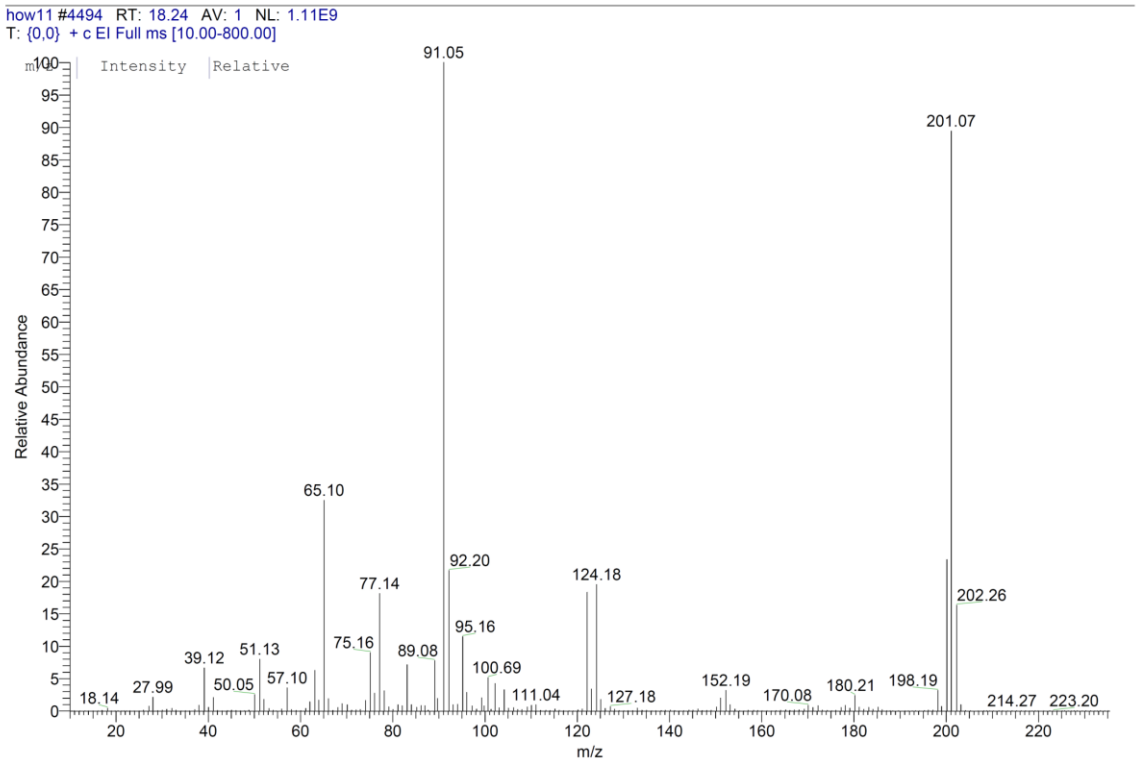
Figure S60. Mass spectrum and HMS data of N-(4-chlorophenyl)benzylamine




```
04-3,50A+B-H#1-20 RT: 0.02-0.54 AV: 20
T: FTMS + p ESI Full ms [50.00-1000.00]
m/z= 244.0767-244.2075
Isotope  Min   Max
C-12       0    15
H-1        0    18
N-14       0     1
O-16       0     2
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1
```

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
244.1333	62124160.0	100.00	244.1332	0.33	$C_{15}H_{18}O_2N$

Figure S61. Mass spectrum and HMS data of N-Benzyl-3,5-dimethoxyaniline



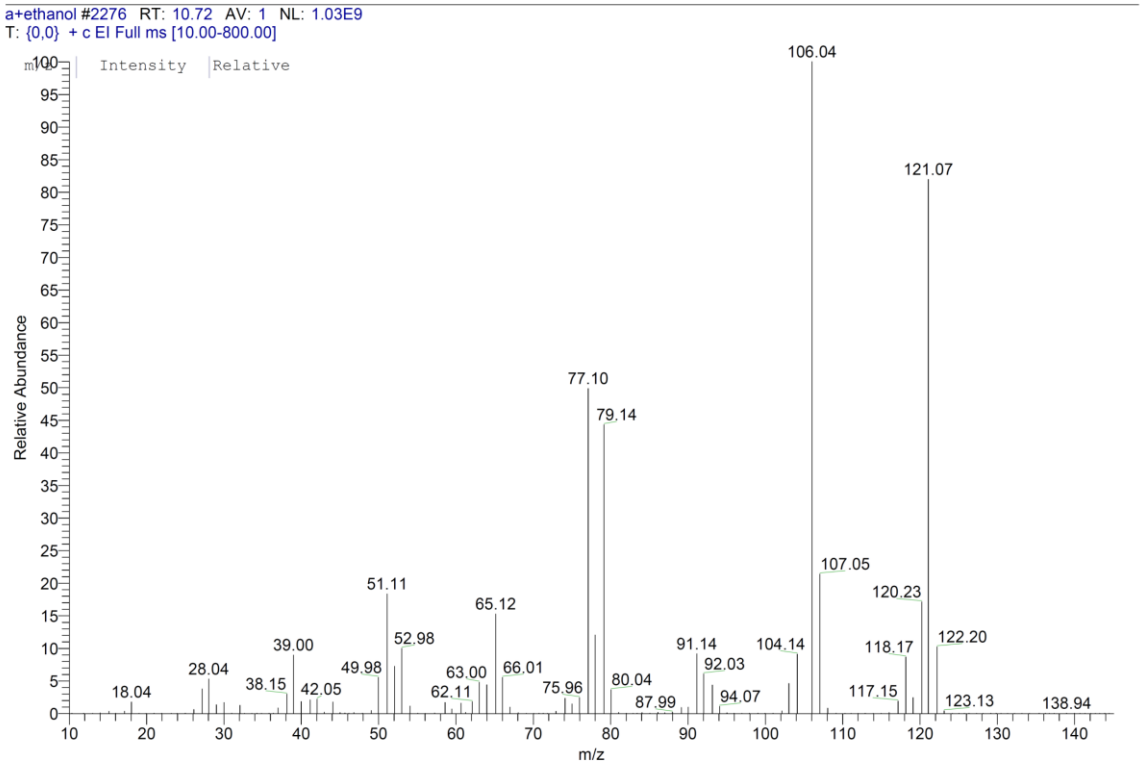
39-2F-B-APCI-H#1-20 RT: 0.02-0.54 AV: 20
T: FTMS + p APCI corona Full ms [150.00-500.00]
m/z= 201.8418-202.3504

Isotope	Min	Max
N-14	0	1
C-12	0	13
H-1	0	13
F-19	0	1

Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
202.1020	113925080.0	100.00	202.1027	-3.41	$C_{13}H_{13}NF$

Figure S62. Mass spectrum and HMS data of N-benzyl-(2-fluorophenyl)amine



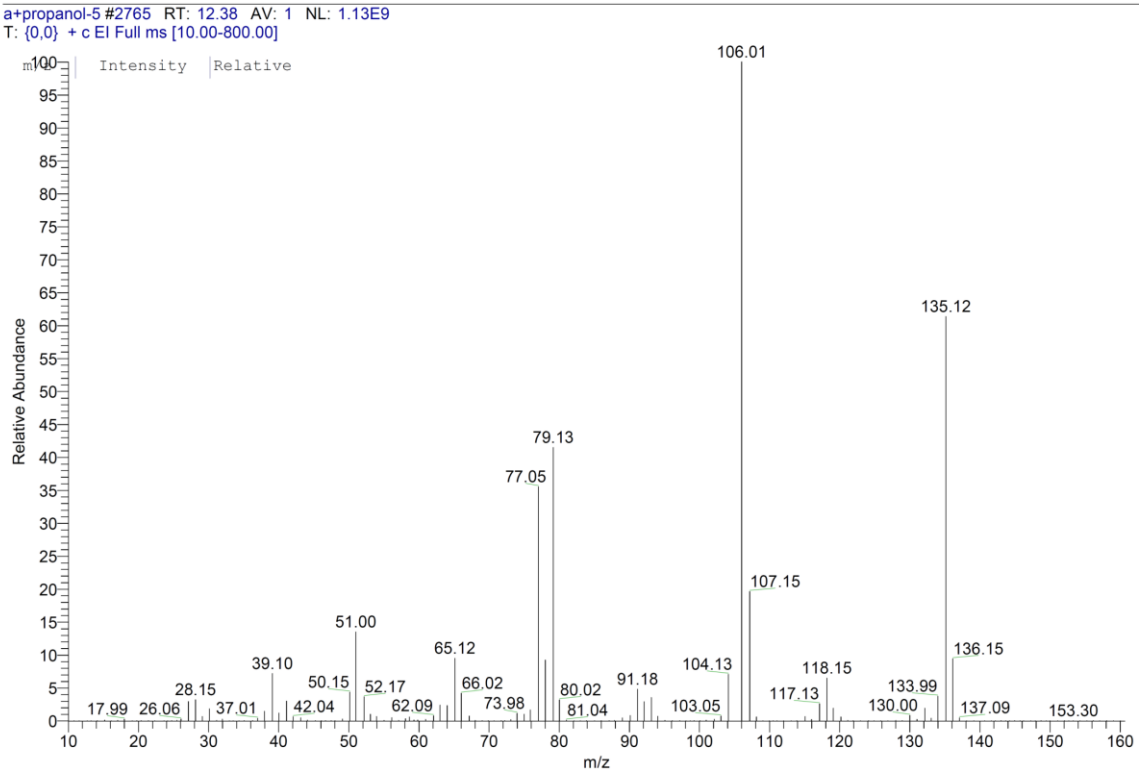
55-A+Ethanol-H#1-20 RT: 0.00-0.52 AV: 20
T: FTMS + p ESI Full ms [50.00-1000.00]
m/z= 122.0573-122.1269

Isotope	Min	Max
C-12	0	8
H-1	0	20
N-14	0	1

Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
122.0965	3147732.0	100.00	122.0964	0.54	$C_8H_{12}N$

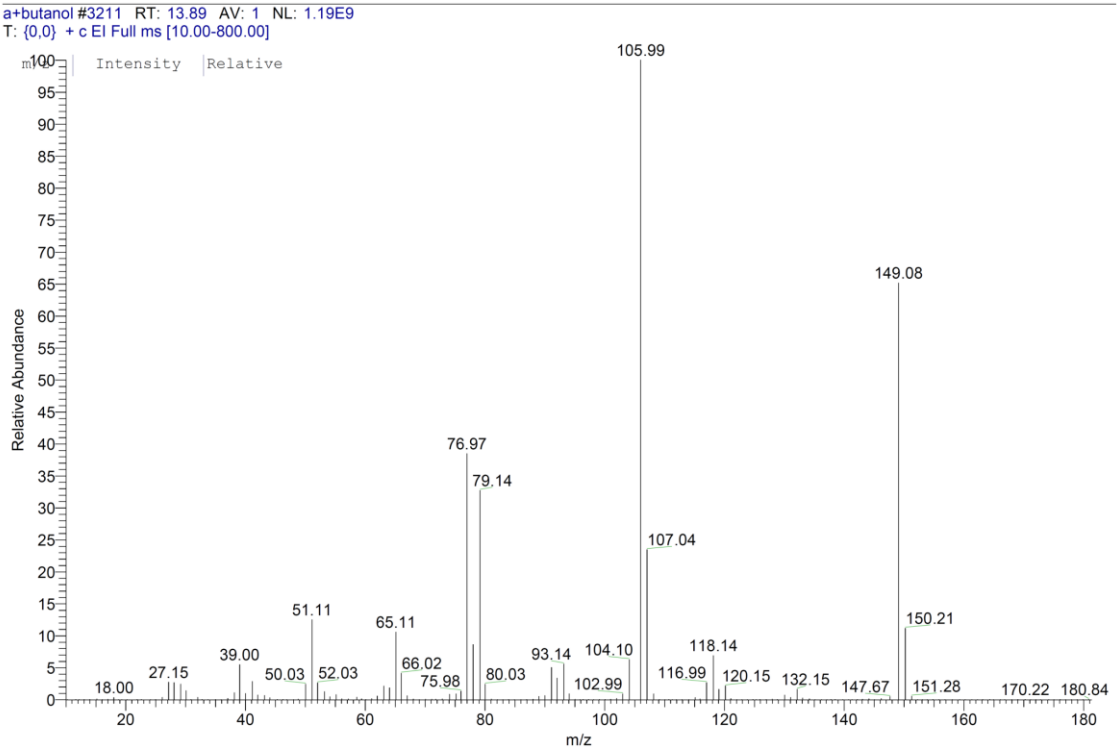
Figure S63. Mass spectrum and HMS data of N-ethyl-N-phenylamine




```
10-A+n-propanol-H#1-20 RT: 0.02-0.53 AV: 20
T: FTMS + p ESI Full ms [50.00-1000.00]
m/z= 135.9883-136.2809
Isotope  Min   Max
C-12       0     9
H-1        0    14
N-14       0     1
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1
```

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
136.1120	30461088.0	100.00	136.1121	-0.55	$C_9H_{14}N$

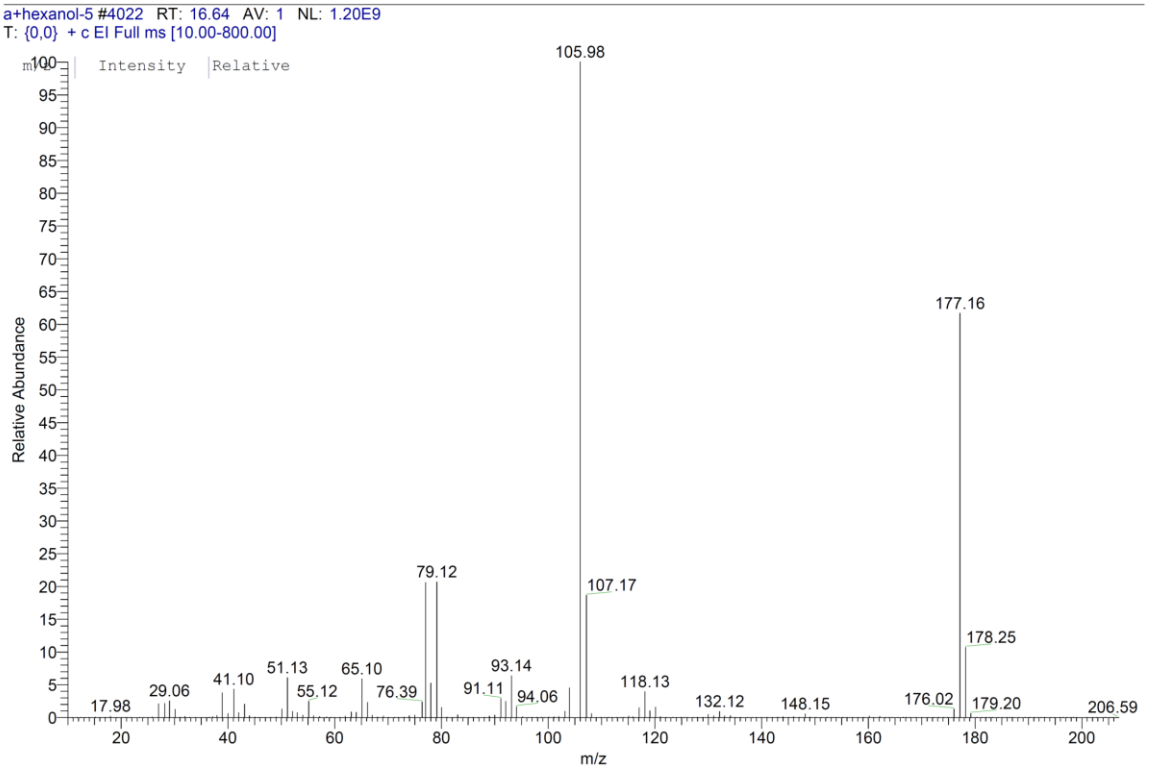
Figure S64. Mass spectrum and HMS data of N-propylaniline



45-A+n-Butanol-H#1-20 RT: 0.00-0.28 AV: 20
T: FTMS + p ESI Full ms [50.00-1000.00]
m/z= 149.9308-150.3671
Isotope Min Max
C-12 0 10
H-1 0 16
N-14 0 1
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1

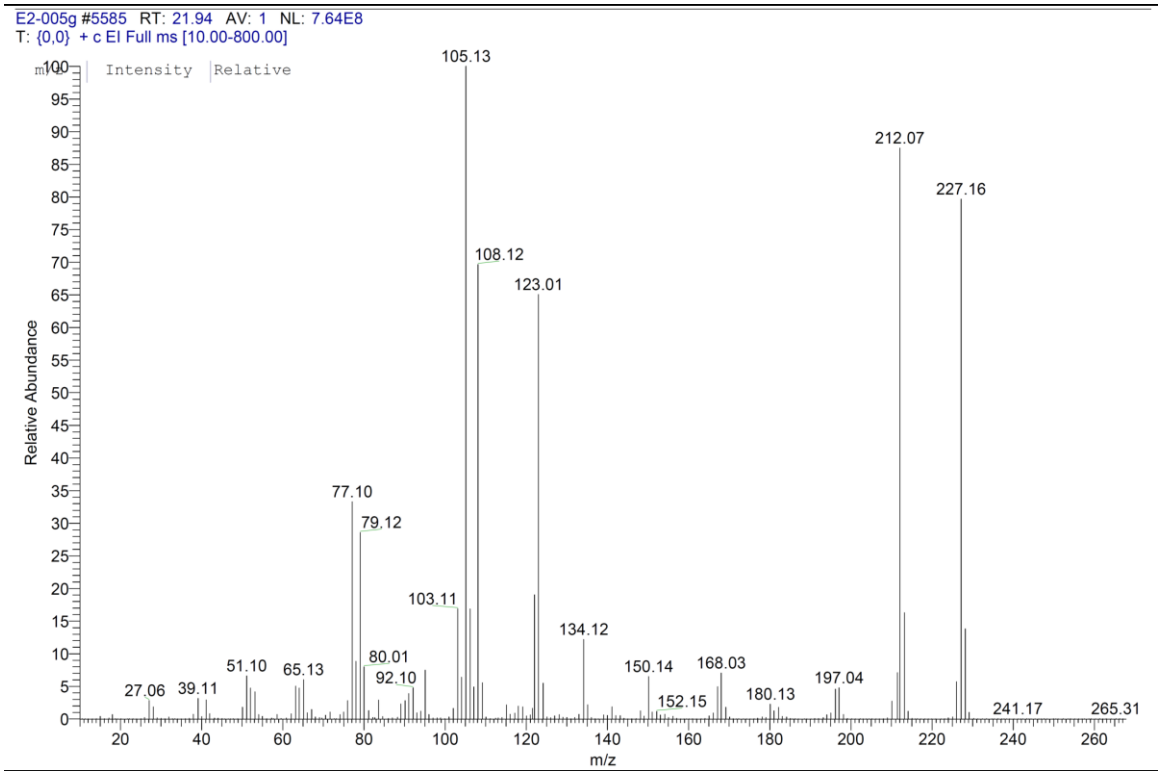
m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
150.1274	38473784.0	100.00	150.1277	-1.97	$C_{10}H_{16}N$

Figure S65. Mass spectrum and HMS data of N-(n-butyl)aniline



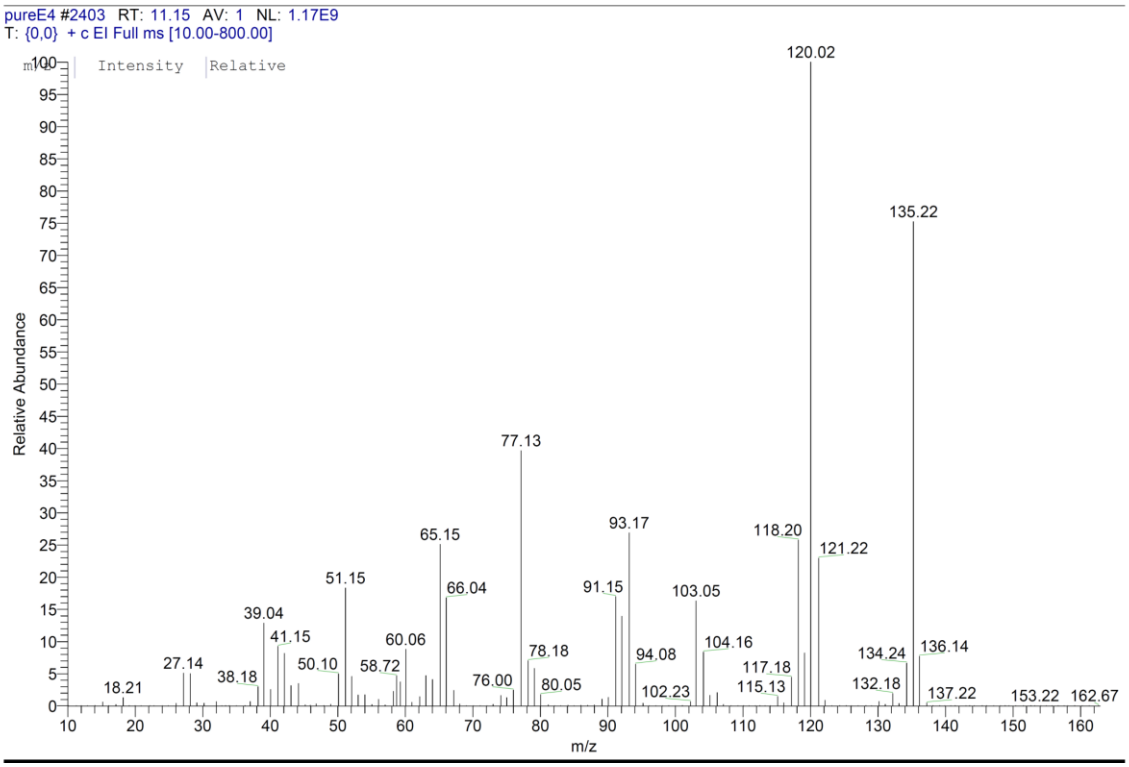

```
01-12, K-H#1-20 RT: 0.02-0.40 AV:20
T: FTMS + p ESI Full ms [50.00-1000.00]
m/z = 178.2353-178.3661
Isotope     Min    Max
C-12          0     12
H-1           0     20
N-14          0      1
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
Max results 1
    m/z      Intensity   Relative   Theo. Mass     Delta     Composition
                                                   (ppm)
 178.2920  45346102.0    100.00     178.2919       0.56     C12H20N
```

Figure S66. Mass spectrum and HMS data of N-hexylaniline




```
04-13, L-H#1-20 RT: 0.01-0.38 AV:20
T: FTMS + p ESI Full ms [50.00-1000.00]
m/z = 228.2507-228.3815
Isotope     Min    Max
C-12          0     15
H-1           0     18
N-14          0      1
O-16          0      1
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
Max results 1
    m/z      Intensity   Relative   Theo. Mass     Delta     Composition
                                                   (ppm)
 228.3075  48916661.0    100.00     228.3073       0.78     C15H18ON
```

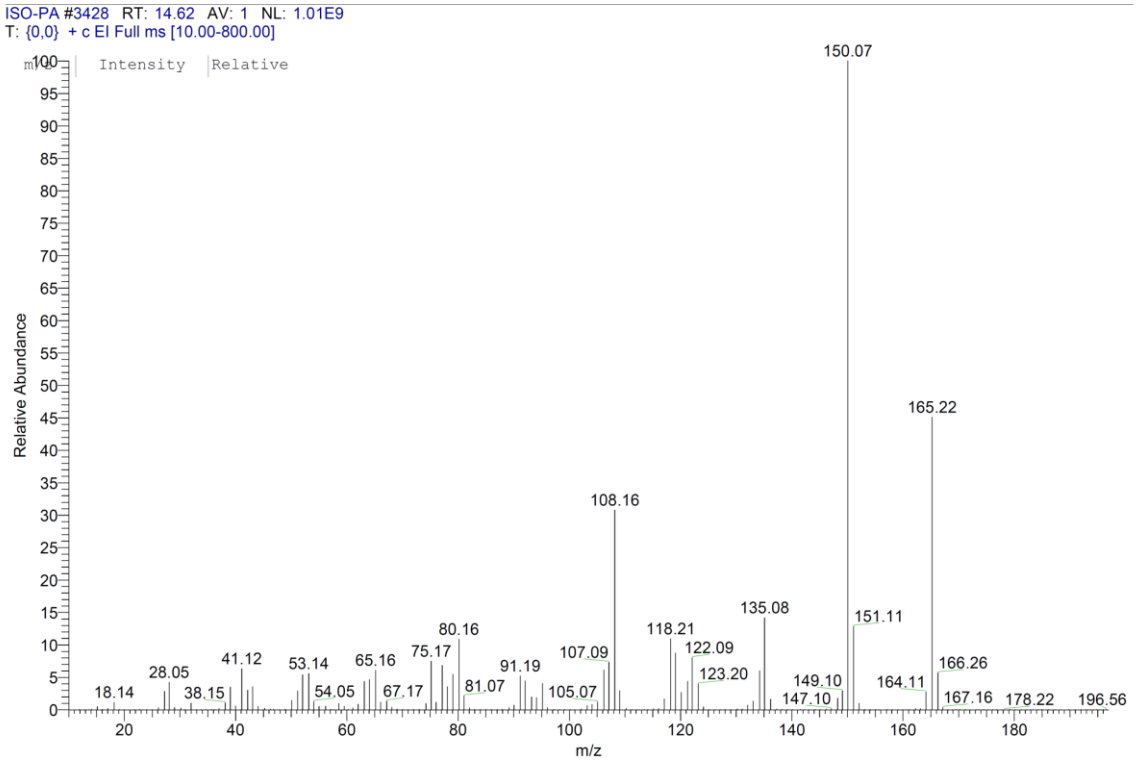
Figure S67. Mass spectrum and HMS data of 4-Methoxy-N-(1-phenylethyl)aniline



T: FTMS + p ESI Full ms [50.00-1000.00]
m/z= 135.9883-136.2809
Isotope Min Max
C-12 0 9
H-1 0 14
N-14 0 1
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
136.1120	30461088.0	100.00	136.1121	-0.55	$C_9H_{14}N$

Figure S68. Mass spectrum and HMS data of N-Isopropylaniline



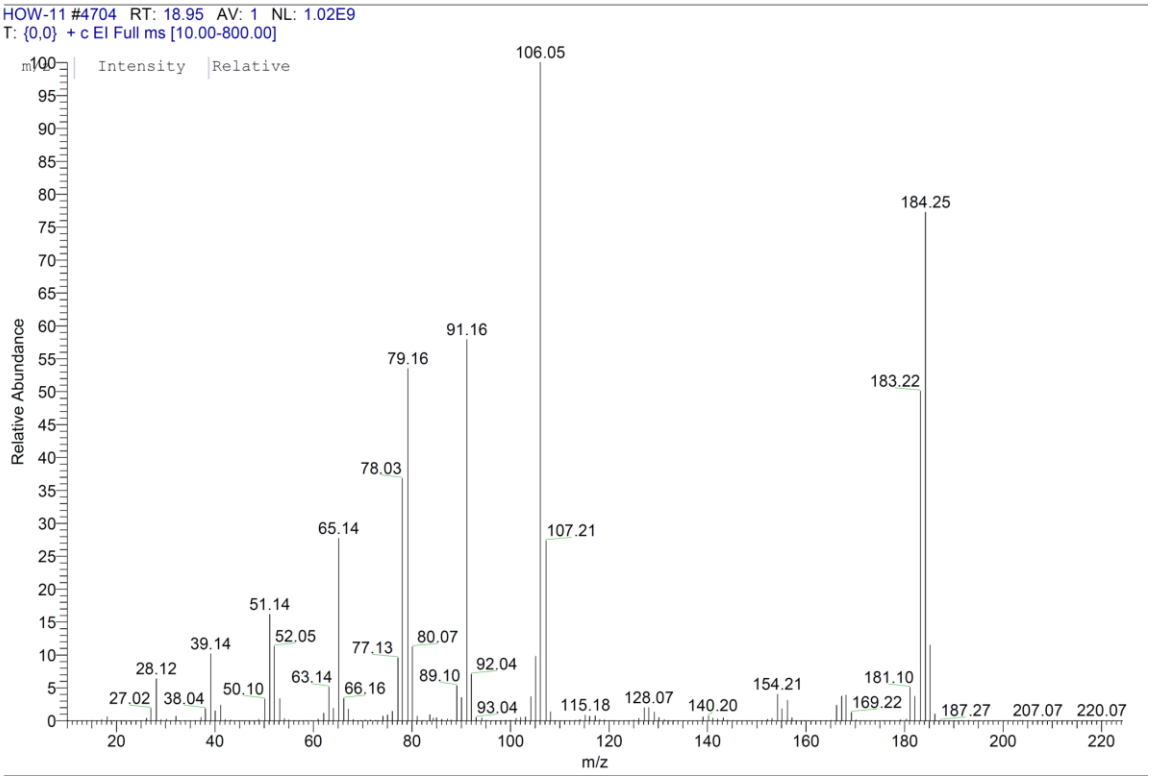
56-PA-ISO-APCI-H#1-20 RT: 0.02-0.58 AV: 20
T: FTMS + p APCI corona Full ms [100.00-500.00]
m/z= 166.0162-166.2431

Isotope	Min	Max
N-14	0	1
C-12	0	10
H-1	0	16
O-16	0	1

Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
166.1223	9010727.0	100.00	166.1226	-2.12	$C_{10}H_{16}ON$

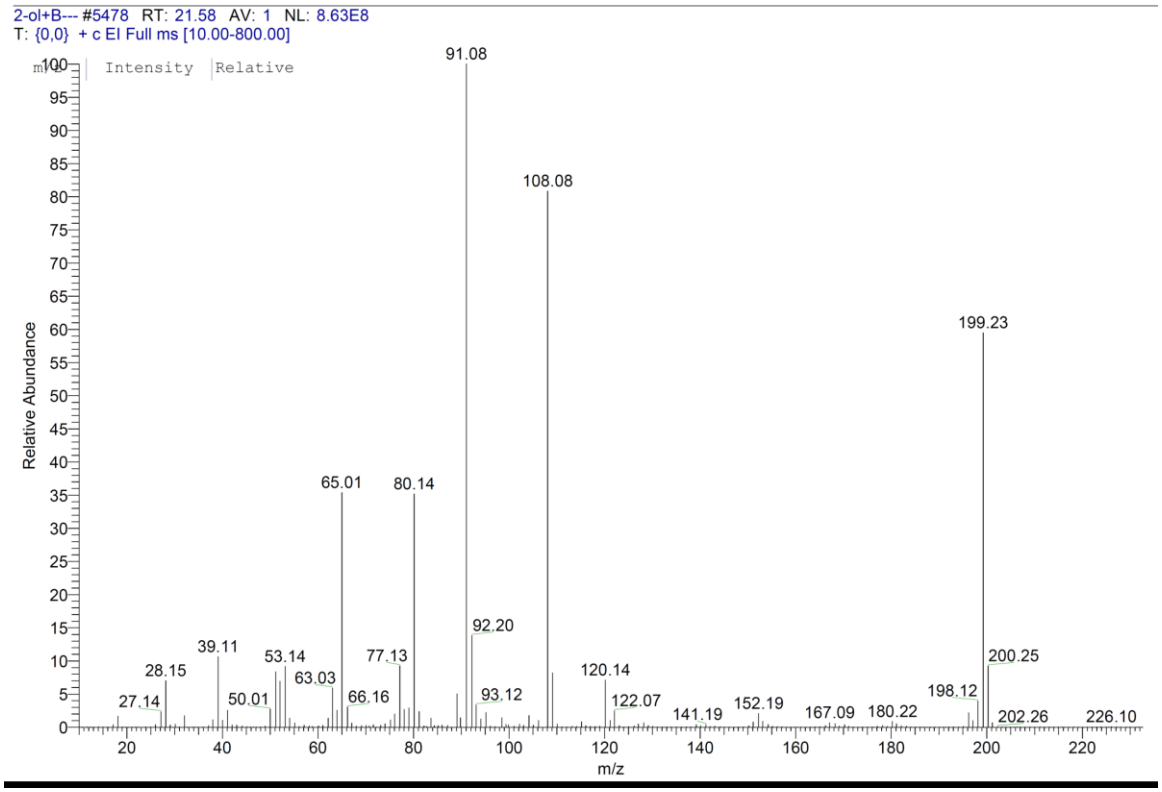
Figure S69. Mass spectrum and HMS data of N-Isopropyl-p-anisidine




```
65-2-dine-B-APCI-H#1-20 RT: 0.01-0.53 AV: 20
T: FTMS + p APCI corona Full ms [100.00-500.00]
m/z= 184.7356-185.6442
Isotope  Min   Max
N-14       0     2
C-12       0    12
H-1        0    13
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1
```

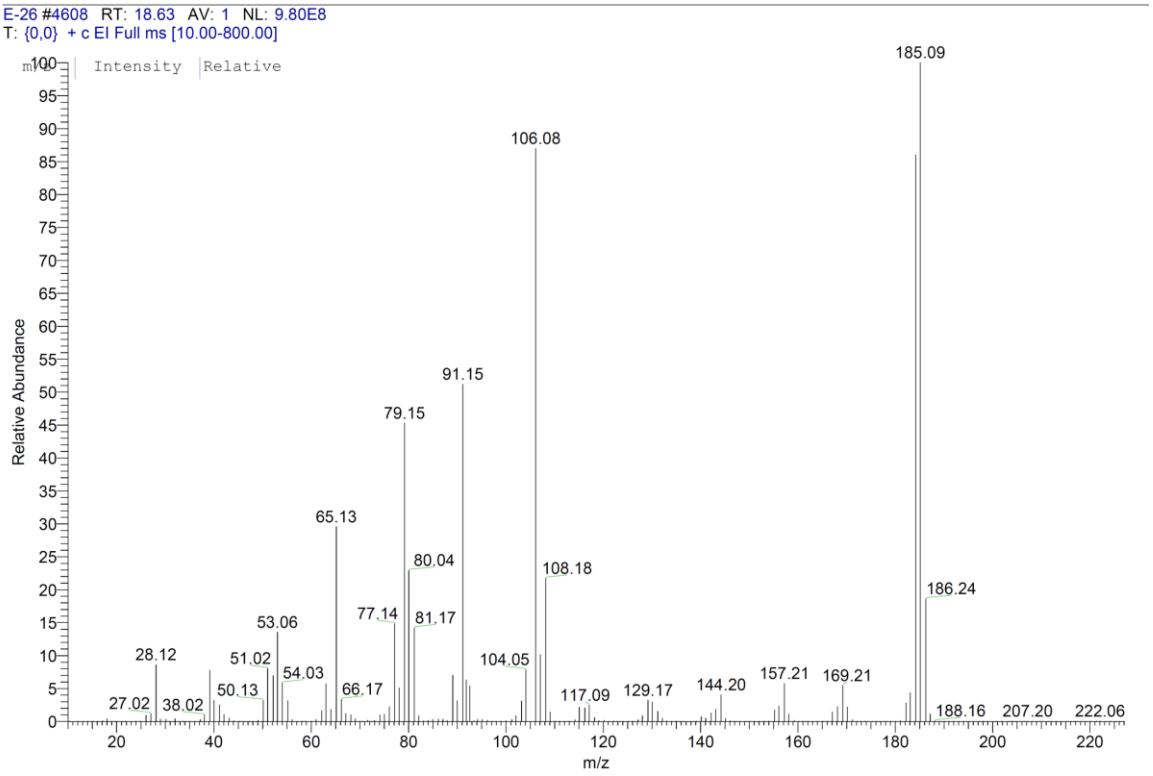
m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
185.1067	122861736.0	100.00	185.1073	-3.45	$C_{12}H_{13}N_2$

Figure S70. Mass spectrum and HMS data of N-benzylpyridin-2-amine




```
04-15, P-H#1-20 RT: 0.00-0.25 AV:20
T: FTMS + p ESI Full ms [50.00-1000.00]
m/z = 200.1979-200.3288
Isotope     Min    Max
C-12          0     13
H-1           0     14
N-14          0      1
O-16          0      1
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
Max results 1
    m/z      Intensity   Relative   Theo. Mass     Delta     Composition
                                                   (ppm)
 200.2542  56476509.0    100.00     200.2546       -1.79     C13H14ON
```

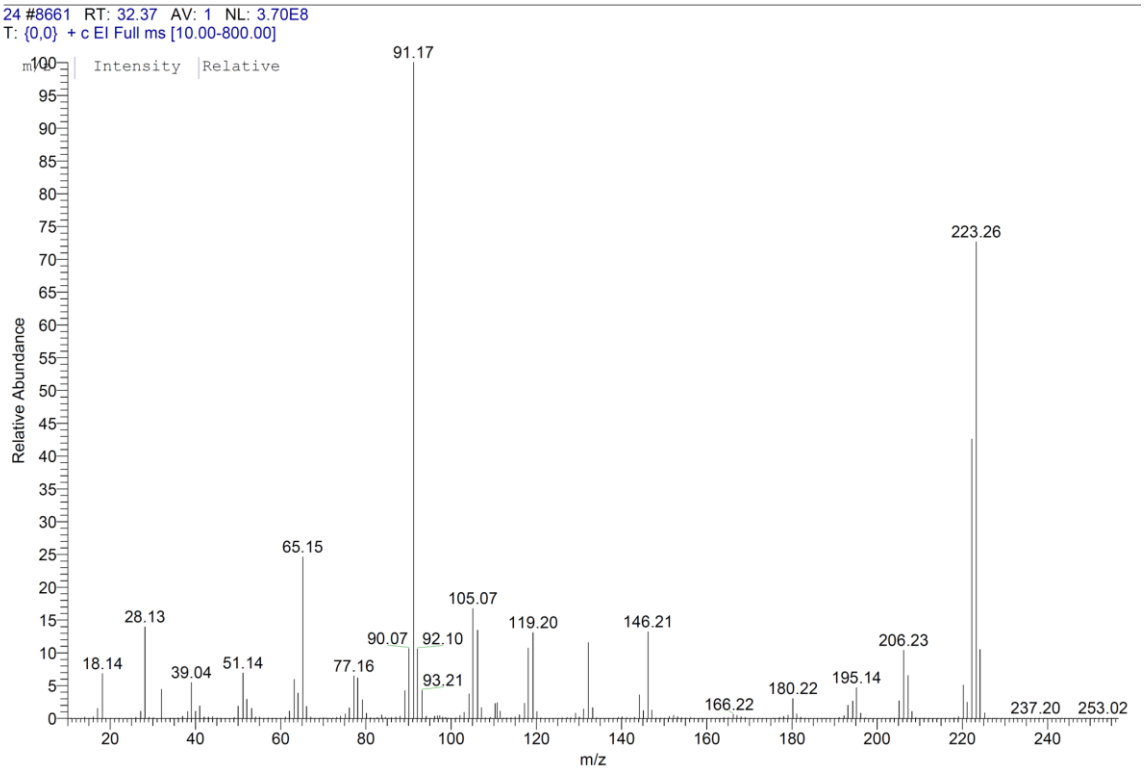
Figure S71. Mass spectrum and HMS data of o-(benzylamino)phenol




```
44-midine-B-APCI-H#1-20 RT: 0.01-0.54 AV: 20
T: FTMS + p APCI corona Full ms [150.00-500.00]
m/z= 185.8620-186.3691
Isotope  Min   Max
N-14       0     3
C-12       0    11
H-1        0    12
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1
```

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
186.1019	108207144.0	100.00	186.1026	-3.47	$C_{11}H_{12}N_3$

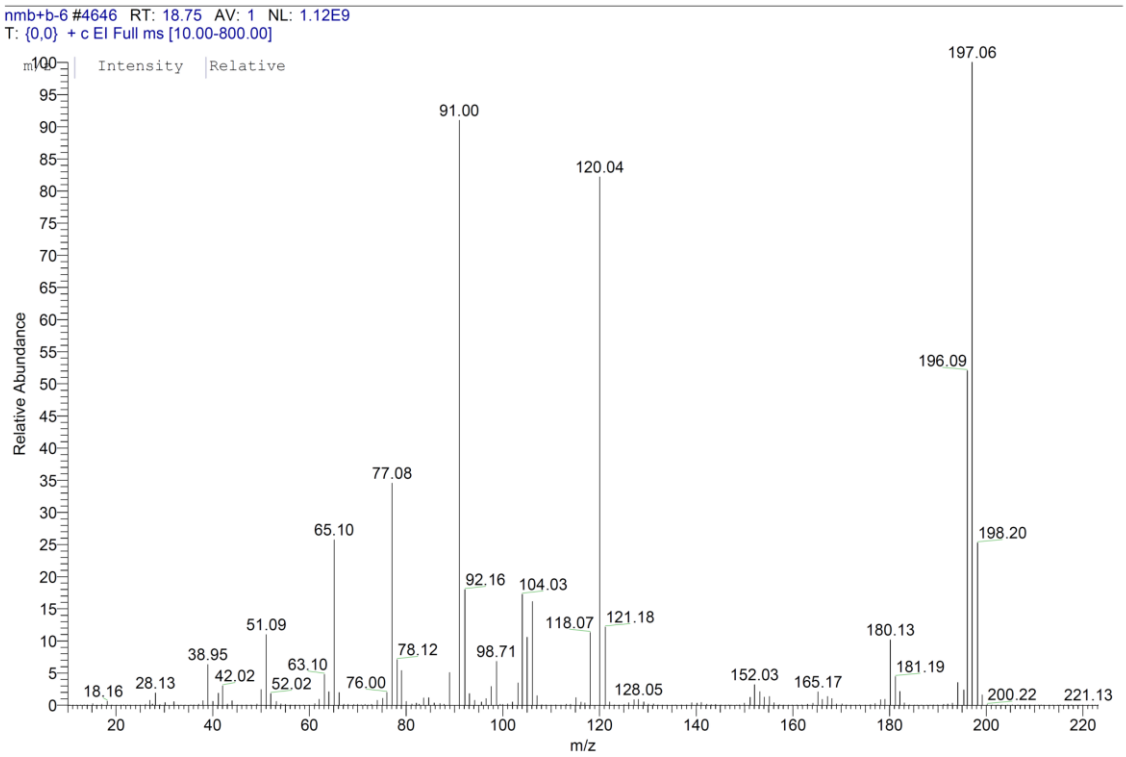
Figure S72. Mass spectrum and HMS data of 2-(benzylamino)pyrimidine




```
71-2-zole-B-APCI-H#1-20 RT: 0.02-0.54 AV: 20
T: FTMS + p APCI corona Full ms [100.00-500.00]
m/z= 223.8487-224.4695
Isotope  Min   Max
N-14       0     3
C-12       0    14
H-1        0    14
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1
```

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
224.1176	113778352.0	100.00	224.1182	-2.97	$C_{14}H_{14}N_3$

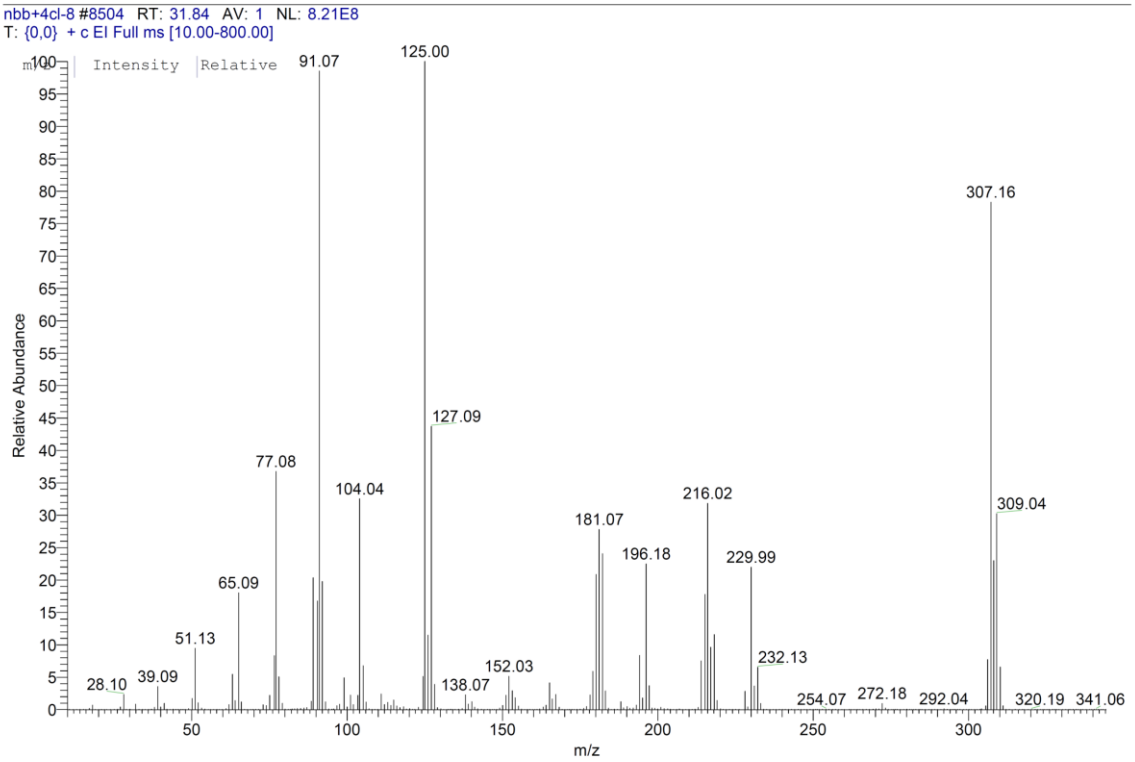
Figure S73. Mass spectrum and HMS data of (1H-benzoimidazol-2-yl)phenylamine




```
04-2, A-H#1-20 RT: 0.03-0.36 AV:20
T: FTMS + p ESI Full ms [50.00-1000.00]
m/z = 198.2253-198.3561
Isotope     Min    Max
C-12          0     14
H-1           0     16
N-14          0      1
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
Max results 1
```

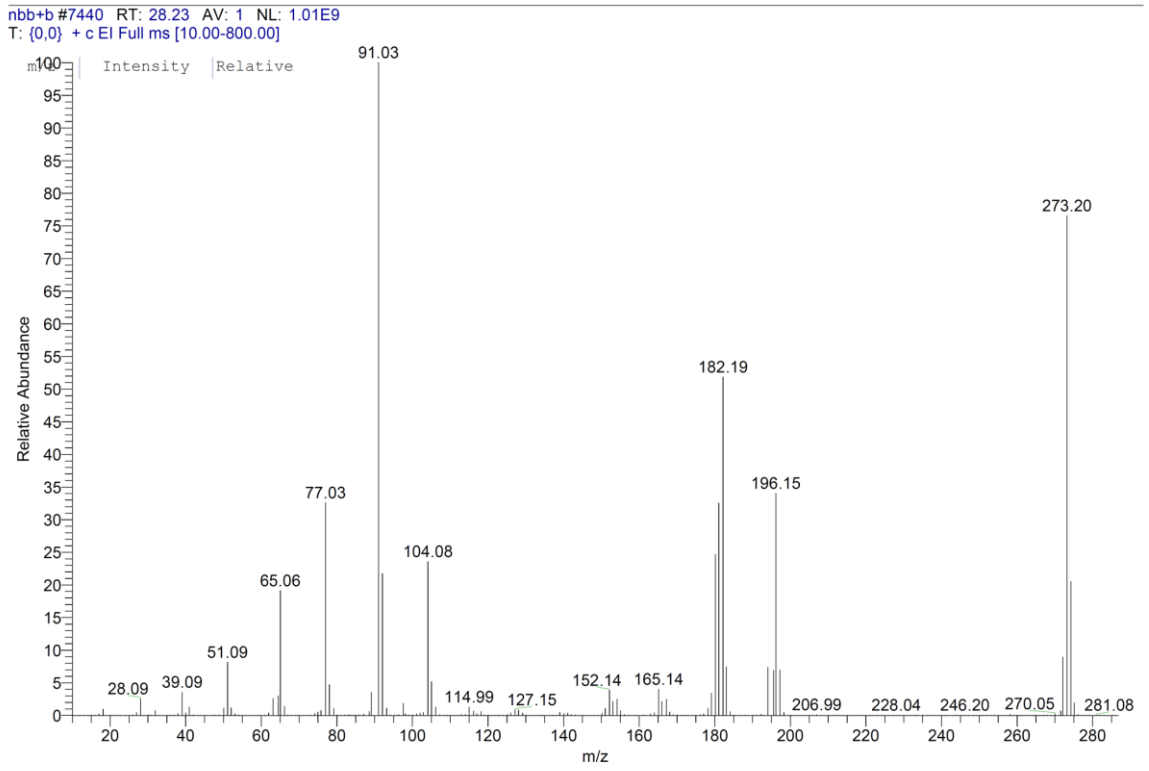
m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
198.2821	46709894.0	100.00	198.2819	0.81	$C_{14}H_{16}N$

Figure S74. Mass spectrum and HMS data of N-methyl-N-phenyl-benzenemethanamine




```
04-2, B-H#1-20 RT: 0.01-0.35 AV:20
T: FTMS + p ESI Full ms [50.00-1000.00]
m/z = 308.7660-308.8969
Isotope     Min    Max
C-12          0     20
H-1           0     19
N-14          0      1
Cl-35         0      1
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
Max results 1
    m/z      Intensity   Relative   Theo. Mass     Delta      Composition
                                                   (ppm)
 308.8225  40080103.0    100.00     308.8226       -0.51     C15H18NCl
```

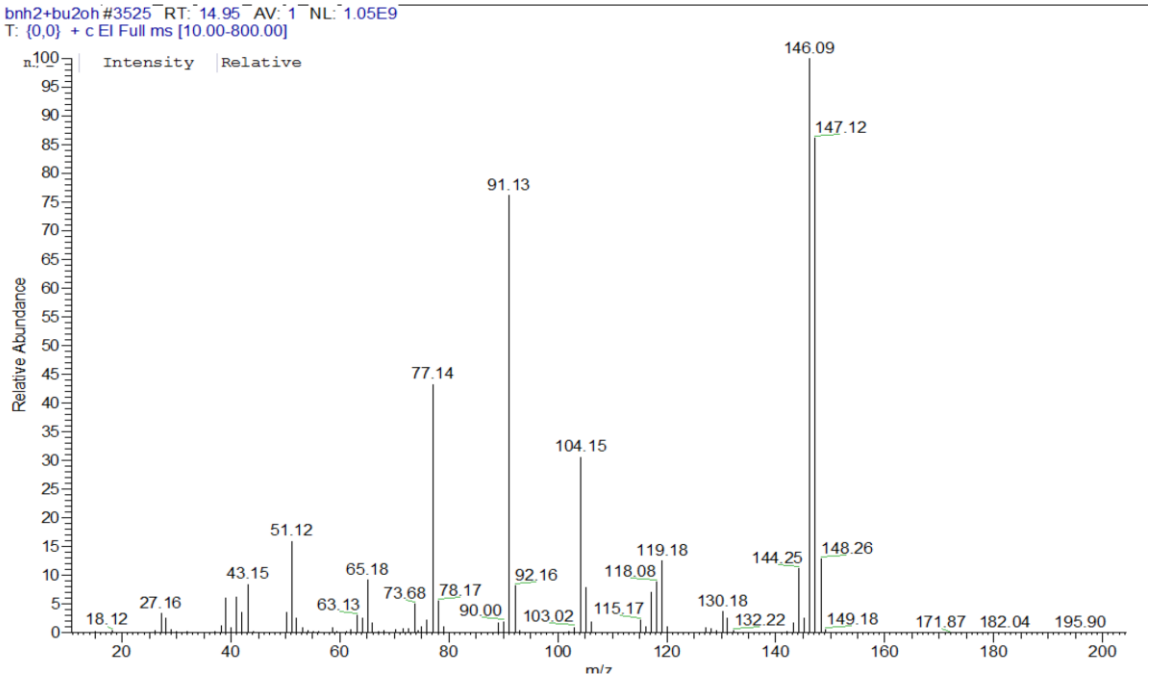
Figure S75. Mass spectrum and HMS data of N-benzyl-N-(4-chloro-benzyl)-aniline




```
47-N-BB+B-H#1-20 RT: 0.02-0.54 AV: 20
T: FTMS + p ESI Full ms [50.00-1000.00]
m/z= 274.0350-274.2826
Isotope  Min   Max
C-12       0    20
H-1        0    20
N-14       0     1
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
max results 1
```

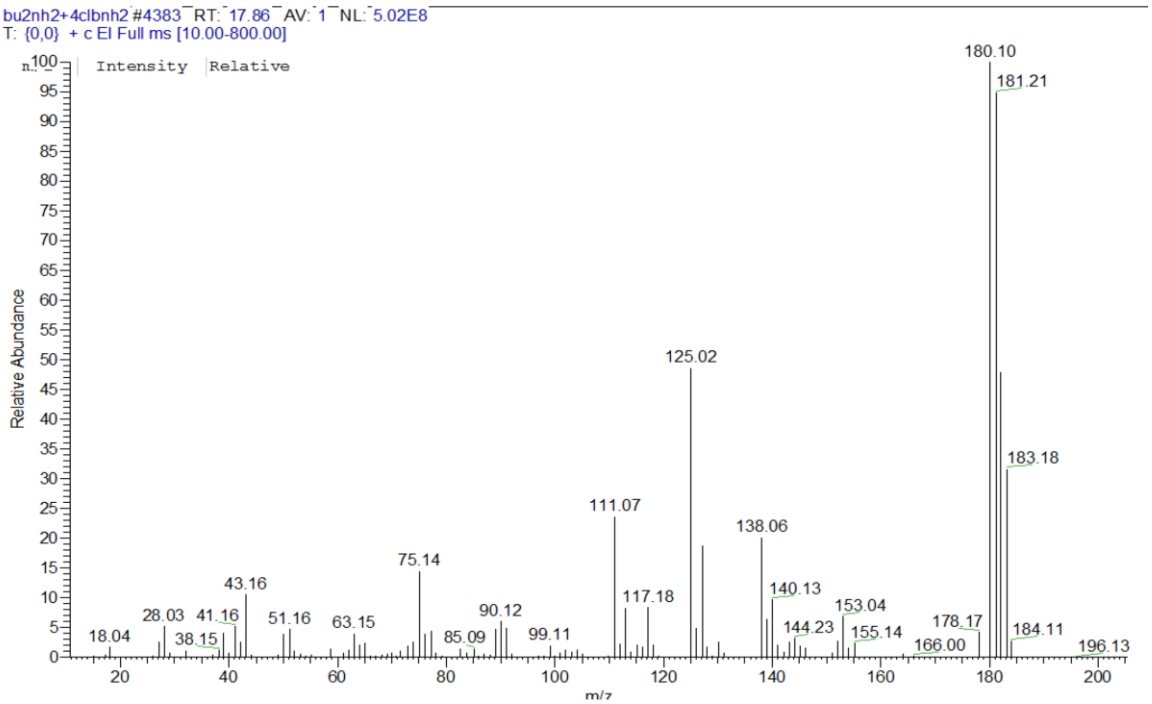
m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
274.1588	17067946.0	100.00	274.1590	-0.89	$C_{20}H_{20}N$

Figure S76. Mass spectrum and HMS data of N,N-dibenzylaniline



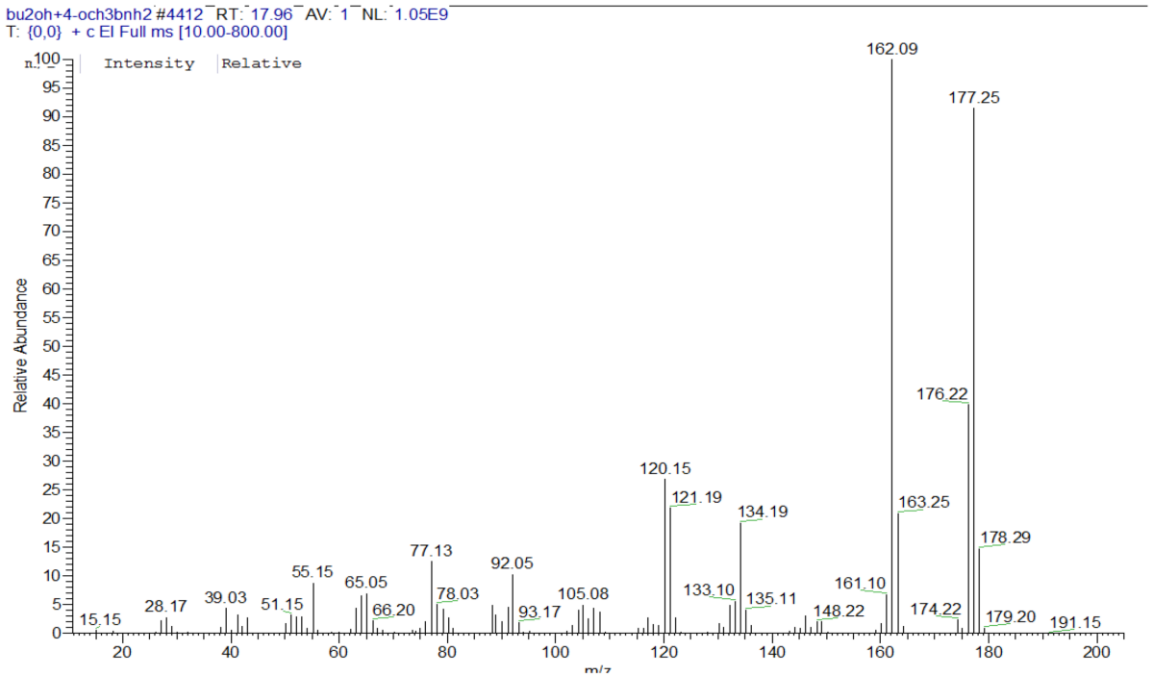

```
04-3, A-H#1-20 RT: 0.01-0.38 AV:20
T: FTMS + p ESI Full ms [50.00-1000.00]
m/z = 148.1669-148.2977
Isotope     Min    Max
C-12          0     13
H-1           0     14
N-14          0      1
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
Max results 1
    m/z      Intensity   Relative   Theo. Mass     Delta      Composition
                                                   (ppm)
 148.2231  51770133.0    100.00     148.2234       -2.42     C13H14N
```

Figure S77. Mass spectrum and HMS data of N-phenylpyrrolidine



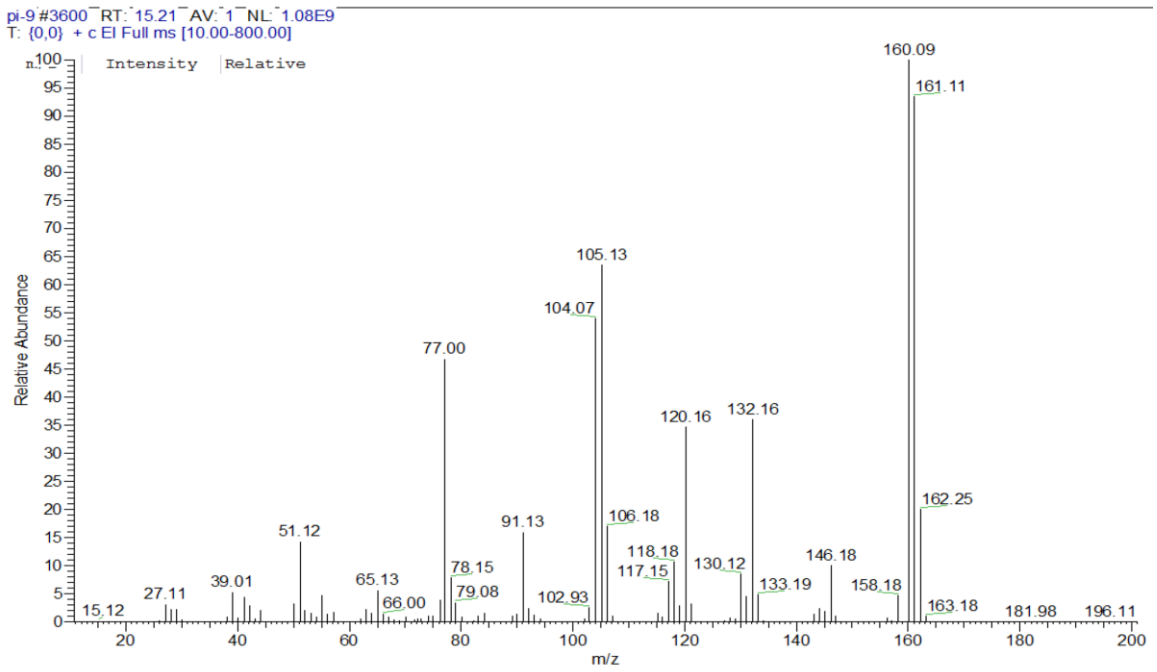

```
04-3, B-H#1-20 RT: 0.00-0.52 AV:20
T: FTMS + p ESI Full ms [50.00-1000.00]
m/z = 182.6120-182.7428
Isotope     Min    Max
C-12          0     11
H-1           0     13
N-14          0      1
Cl-35         0      1
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
Max results 1
    m/z      Intensity   Relative   Theo. Mass     Delta     Composition
                                                   (ppm)
 182.6683  47787815.0    100.00     182.6686      -1.75     C11H13NCl
```

Figure S78. Mass spectrum and HMS data of N-(4-chlorophenyl) pyrrolidine



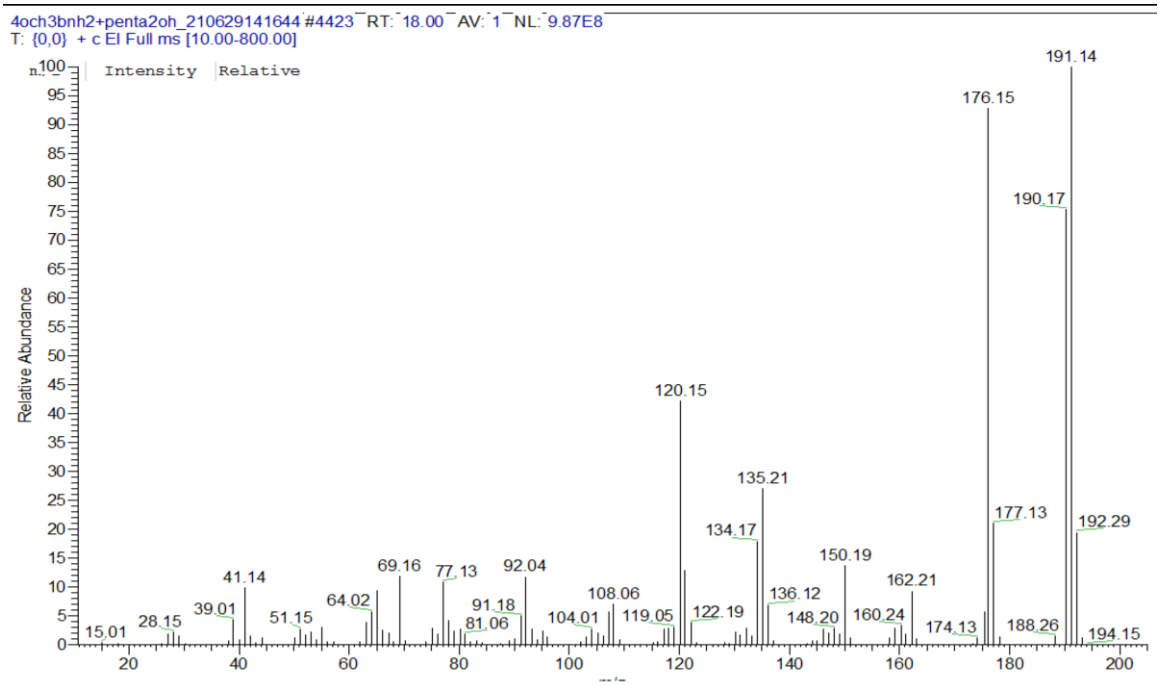

```
04-3, C-H#1-20 RT: 0.00-0.38 AV:20
T: FTMS + p ESI Full ms [50.00-1000.00]
m/z = 178.1922-178.3230
Isotope     Min    Max
C-12          0     11
H-1           0     16
N-14          0      1
O-16          0      1
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
Max results 1
    m/z      Intensity   Relative   Theo. Mass     Delta      Composition
                                                   (ppm)
 178.2485  44374400.0    100.00     178.2488      -1.90     C17H16ON
```

Figure S79. Mass spectrum and HMS data of N-(4-methoxyphenyl) pyrrolidine




```
04-3, D-H#1-20 RT: 0.00-0.45 AV:20
T: FTMS + p ESI Full ms [50.00-1000.00]
m/z = 162.1932-162.3240
Isotope     Min    Max
C-12          0     11
H-1           0     16
N-14          0      1
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
Max results 1
    m/z      Intensity   Relative   Theo. Mass     Delta      Composition
                                                   (ppm)
 162.2495  40080103.0    100.00     162.2498       -2.09     C11H16N
```

Figure S80. Mass spectrum and HMS data of N-phenylpiperidine



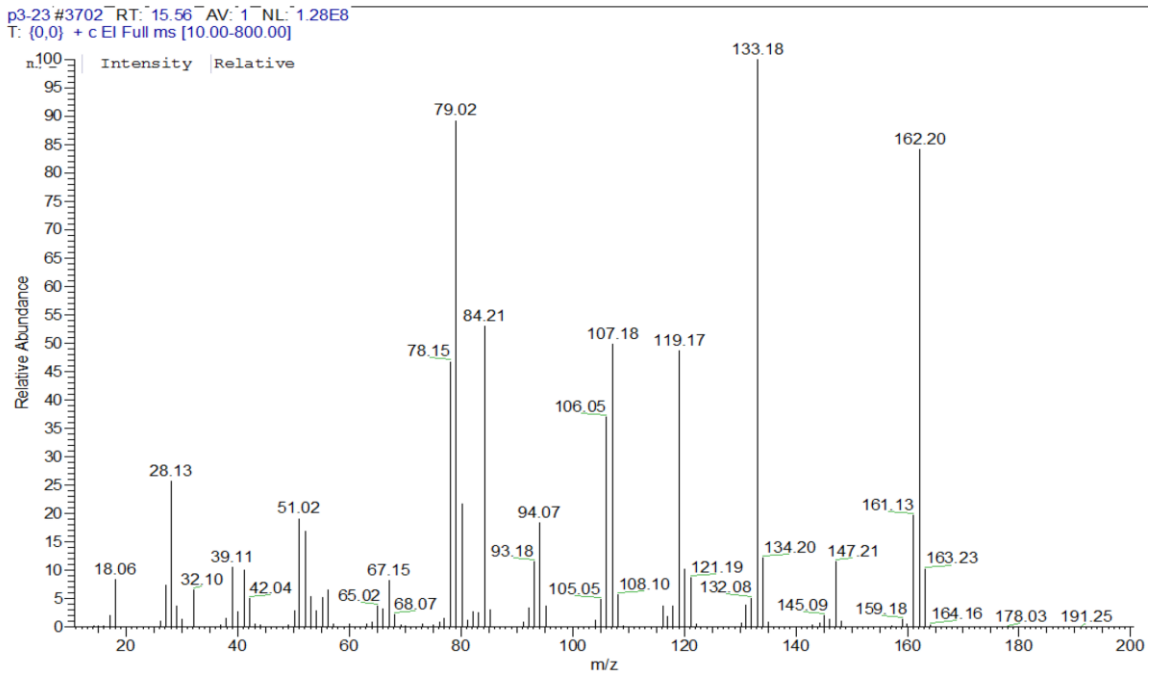
04-3, E-H#1-20 RT: 0.00-0.39 AV:20
T: FTMS + p ESI Full ms [50.00-1000.00]
m/z = 192.2186-192.3494

Isotope	Min	Max
C-12	0	12
H-1	0	18
N-14	0	1
O-16	0	1

Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
Max results 1

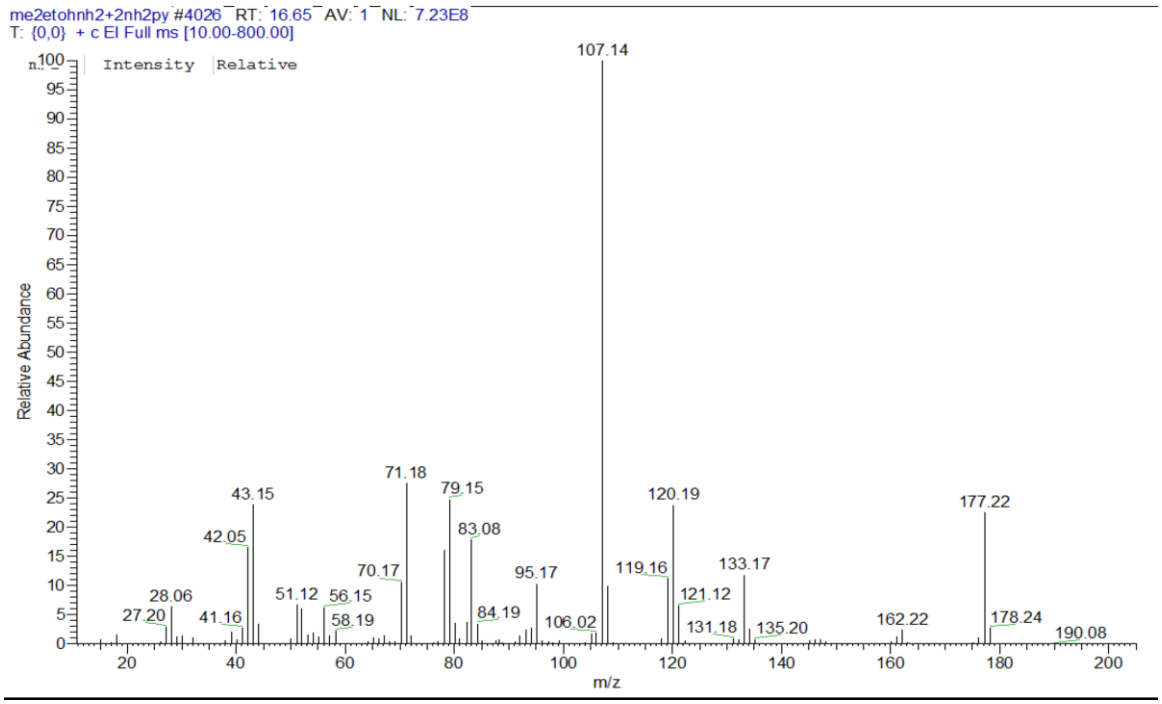
m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
192.2753	38827600.0	100.00	192.2752	0.41	$C_{12}H_{18}ON$

Figure S81. Mass spectrum and HMS data of N-(4-methoxyphenyl) piperidine




```
04-3, F-H#1-20 RT: 0.00-0.51 AV:20
T: FTMS + p ESI Full ms [50.00-1000.00]
m/z = 163.1814-163.3122
Isotope     Min    Max
C-12          0     10
H-1           0     15
N-14          0      2
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
Max results 1
    m/z      Intensity   Relative   Theo. Mass     Delta      Composition
                                                   (ppm)
 163.2381  37651006.0    100.00     163.2380       0.61      C10H15N2
```

Figure S82. Mass spectrum and HMS data of 1-(piperidine-1-yl) pyridine



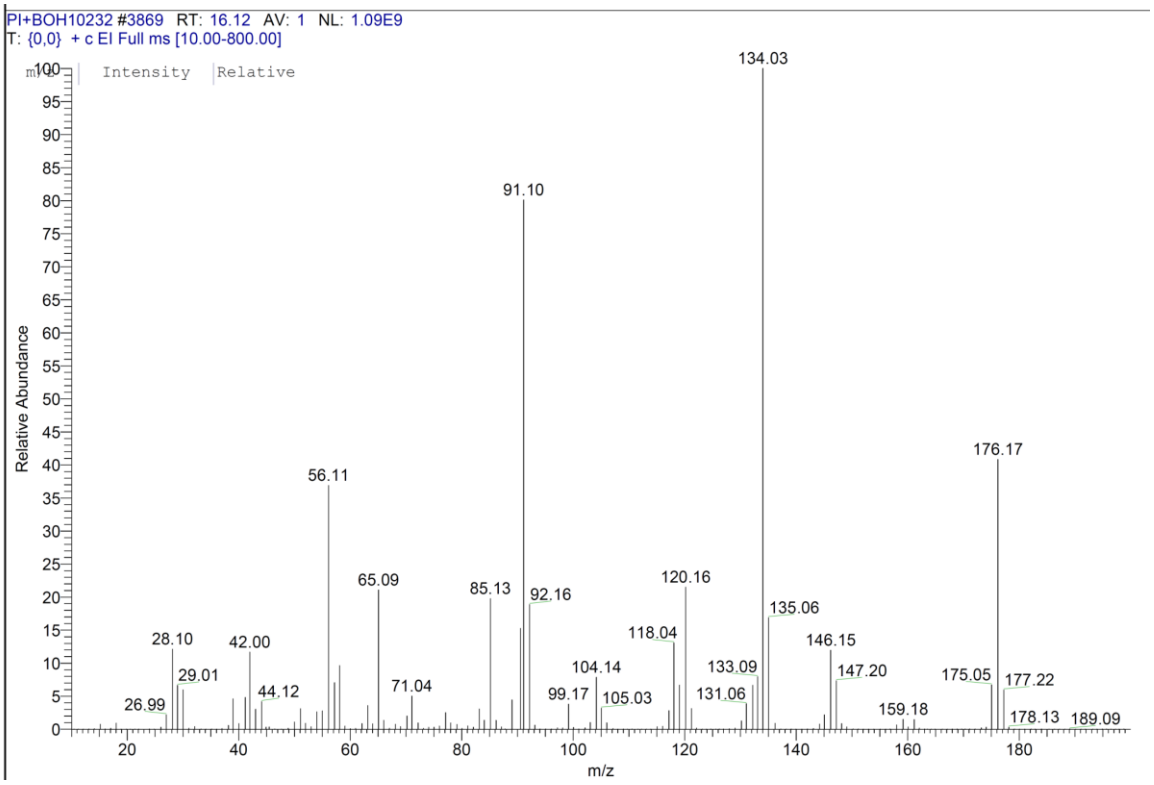
04-3, G-H#1-20 RT: 0.00-0.45 AV:20
T: FTMS + p ESI Full ms [50.00-1000.00]
m/z = 178.1959-178.3267

Isotope	Min	Max
C-12	0	10
H-1	0	16
N-14	0	3

Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
Max results 1

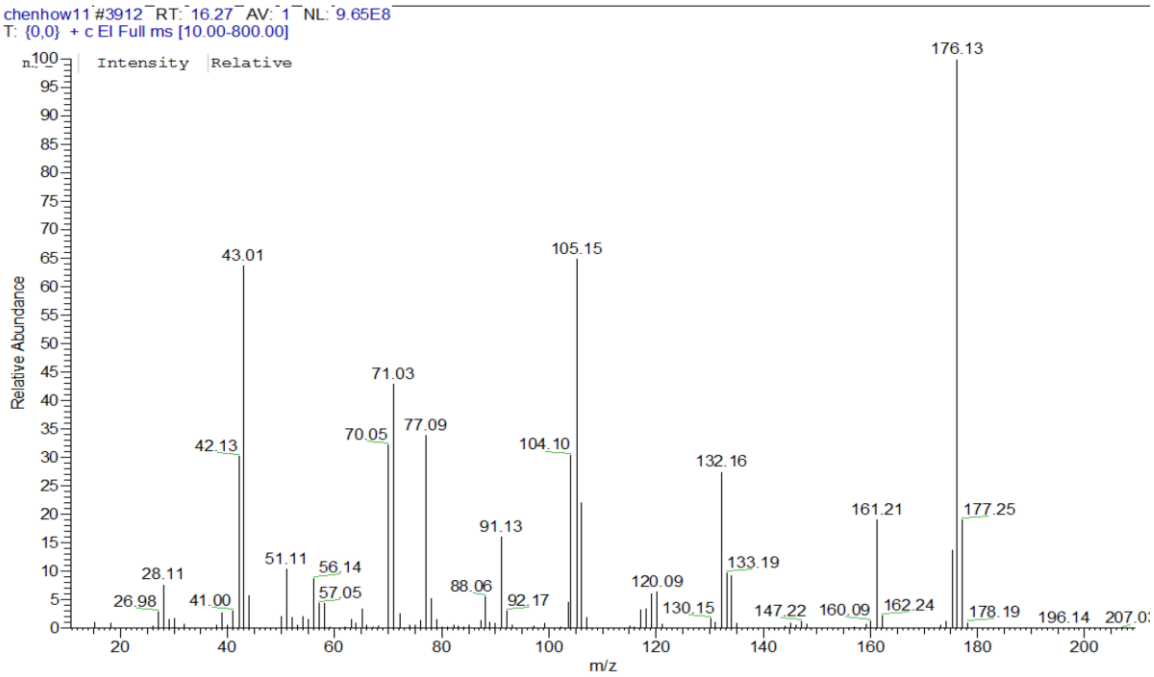
m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
178.2522	47063757.0	100.00	178.2525	-1.90	$C_{10}H_{16}N_3$

Figure S83. Mass spectrum and HMS data of 1-methyl-4-(pyridin-2-yl) piperazine



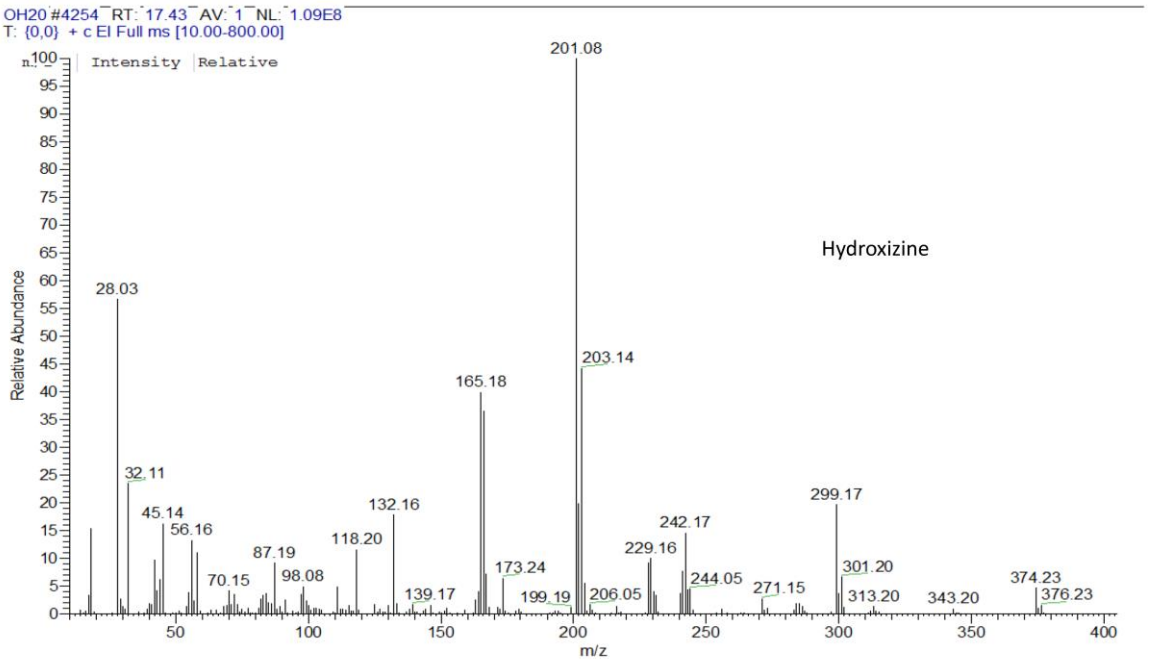

```
04-3, H+B-H#1-20 RT: 0.01-0.38 AV:20
T: FTMS + p ESI Full ms [50.00-1000.00]
m/z = 177.2078-177.3386
Isotope     Min    Max
C-12          0     11
H-1           0     17
N-14          0      2
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
Max results 1
    m/z      Intensity   Relative   Theo. Mass     Delta      Composition
                                                   (ppm)
 177.2642  43749408.0    100.00     177.2644       -1.01     C11H17N2
```

Figure S84. Mass spectrum and HMS data of benzylpiperazine



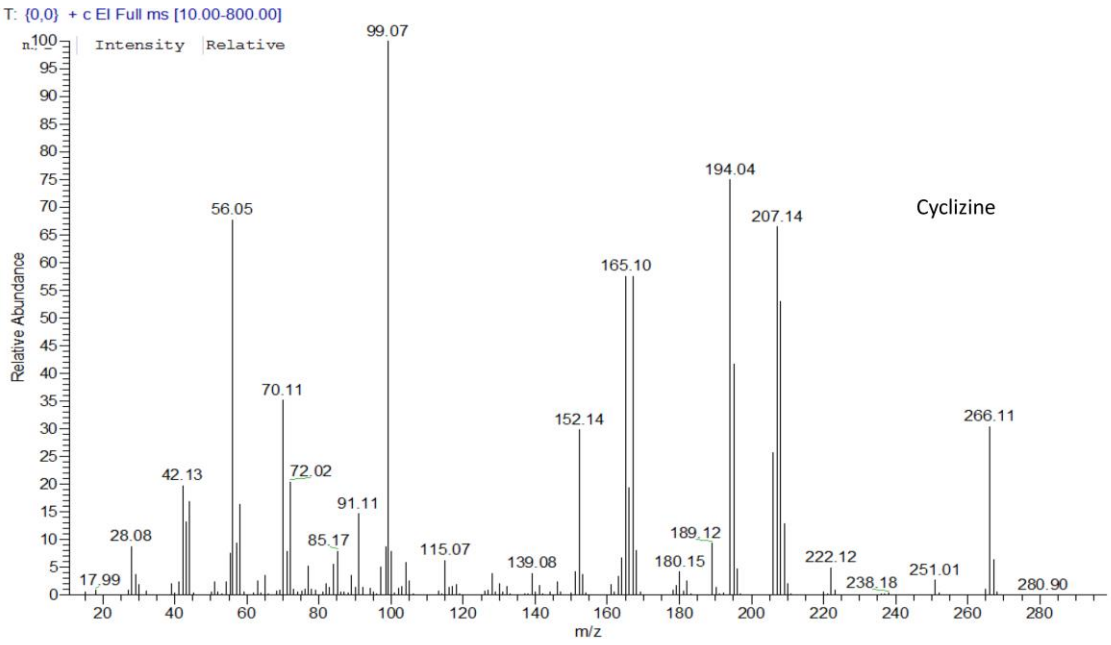

```
04-3, I-H#1-20 RT: 0.02-0.39 AV:20
T: FTMS + p ESI Full ms [50.00-1000.00]
m/z = 177.2138-177.3346
Isotope     Min    Max
C-12          0     11
H-1           0     17
N-14          0      2
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
Max results 1
    m/z      Intensity   Relative   Theo. Mass     Delta      Composition
                                                    (ppm)
 177.2646  45017507.0    100.00     177.2644       1.24      C11H17N2
```

Figure S85. Mass spectrum and HMS data of 1-methyl-4-phenyl piperazine




```
04-3, HY-H#1-20 RT: 0.02-0.55 AV:20
T: FTMS + p ESI Full ms [50.00-1000.00]
m/z = 375.8520-375.9828
Isotope     Min    Max
C-12          0     21
H-1           0     28
N-14          0      2
O-16          0      2
Cl-35         0      1
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
Max results 1
    m/z      Intensity   Relative   Theo. Mass     Delta      Composition
                                                    (ppm)
 375.9088   42785234.0    100.00     375.9086       0.48     C21H28N2O2Cl
```

Figure S86. Mass spectrum and HMS data of of hydroxyzine




```
04-3, CY-H#1-20 RT: 0.02-0.50 AV:20
T: FTMS + p ESI Full ms [50.00-1000.00]
m/z = 267.3297-267.4605
Isotope     Min    Max
C-12          0     18
H-1           0     23
N-14          0      2
Charge 1
Mass tolerance 1000.00 ppm
Nitrogen rule not used
RDB equiv -1.00-100.00
Max results 1
    m/z      Intensity   Relative   Theo. Mass     Delta      Composition
                                                   (ppm)
 267.3861   42261333.0    100.00     267.3863      -0.82     C18H23N2
```

Figure S87. Mass spectrum and HMS data of cyclizine