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SUPPLEMENTARY INFORMATION

Functionalized multi-walled carbon nanotubes as an efficient reusable heterogeneous catalyst for green synthesis of *N*-substituted pyrroles in water

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NMR data:

All ^{1}H NMR and ^{13}C NMR spectra were recorded in $CDCl_3$ or DMSO at 25 °C with a Bruker DRX-400 spectrometer Chemical shifts are given relative to the internal standard tetramethylsilane.

Spectral data:

1-Phenyl-1H-pyrrole (3a); brown solid; m.p=55-57°C, (m.p= 56-58°C) [35]; UV-Vis (CH_2Cl_2) λ_{max}: 310; IR (KBr) ν(cm^{-1}): 3033 (C-H, sp^2 stretch), 1497, 1597 (C=C Ar), 746, 692 (C-H, sp^2 OOP); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 6.35-6.36 (d, 2H, J=2.0 Hz), 7.10-7.11 (d, 2H, J=2.0 Hz), 7.25-7.44 (m, 5H).

1-p-Tolyl-1H-pyrrole (3b); black solid; m.p=79-81°C, (m.p= 80-82°C) [36]; UV-Vis (CH_2Cl_2) λ_{max}: 315; IR (KBr) *ν*(Cm^{-1}): 3050 (C-H, sp^2 stretch), 2922 (C-H, sp^3), 1509, 1616 (C=C, Ar); ^{1}H NMR($CDCl_3$, 400 MHz) *δ (ppm)*: 2.38 (s, 3H), 6.34 (s, 2H), 7.01 (s, 2H), 7.23 (d, 2H, J=8.0 Hz), 7.27-7.29 (d, 2H, J=8.0 Hz).

1-(4-Methoxy phenyl)-1H-pyrrole (3c); black solid, m.p= 87-89°C, (m.p= 88-89°C) [37]; UV-Vis (CH_2Cl_2) λ_{max}; 325; IR(KBr) *ν*(cm^{-1}): 3033(C-H, sp^2 stretch), 2926 (C-H, sp^3), 1597(C=C, Ar), 1310 (C-O), 749 (C-H sp^2 OOP); ^{1}H NMR ($CDCl_3$, 400 MHz) *δ (ppm):* 3.85 (s, 3H), 6.33 (s, 2H), 6.95-6.97 (d, 2H, J=8.4 Hz), 7.01 (s, 2H), 7.31-7.34 (d, 2H , J=8.4 Hz).

1-(3-Methoxy phenyl)-1H-pyrrole (3d); yellow solid; m.p= 46-48°C, (b.p= 98-100°C) [38]; UV-Vis (CH_2Cl_2) λ_{max}; 320; IR (KBr) *ν* (cm^{-1}): 3000 (C-H, sp^2), 2850 (C-H sp^3), 1400-1600 (C=C, Ar), 1300 (C-O), 743 (C-H sp^2 OOP); ^{1}H NMR($CDCl_3$, 400 MHz) *δ (ppm)*: 3.86 (s, 3H), 6.36 (s, 2H), 6.80-6.82 (d, 1H, J=8.0 Hz), 6.95 (s, 1H), 7.00-7.02 (d, 1H, J=8.0 Hz), 7.11 (s, 2H), 7.32-7.36 (t, 1H, J=8.4 Hz).

1-(4-Hydroxy phenyl)-1H-pyrrole (3e); brown solid, m.p= 114-116°C, (m.p=113-115°C) [39]; UV-Vis (CH_2Cl_2) λ_{max}; 325; IR (KBr) *ν* (cm^{-1}): 3448 (O-H, stretch), 3135 (C-H, sp^2), 1519 (C=C, Ar), 1024 (C-O, stretch), 732 (C-H sp^2 OOP); ^{1}H NMR (DMSO, 400 MHz) *δ (ppm)*: 6.19 (s, 2H), 6.52 (s, 1H), 6.80-6.82 (d, 2H, J= 8.8 Hz), 7.16 (s, 2H), 7.31-7.33 (d, 2H, J= 8.4 Hz).

1-(Naphthyl)-1H-pyrrole (3f); brown solid; m.p= 116-118°C, (m.p= 120°C) [40]; UV-Vis (CH_2Cl_2) λ_{max}; 356; IR (KBr) *ν*(cm^{-1}): 3054 (C-H, sp^2 stretch), 1596, 1485 (C=C, Ar), 728 (C-H sp^2 OOP); ^{1}H NMR($CDCl_3$, 400 MHz) *δ (ppm)*: 6.46 (s, 2H), 7.04 (s, 2H), 7.51-7.57 (q, 4H, J=6.8 Hz), 7.79-7.81 (d, 1H, J= 7.2 Hz), 7.90-8.00 (q, 2H, J= 7.6 Hz).

1-(4-Chloro phenyl)-1H-pyrrole (3g); yellow solid; m.p= 80-82°C, (m.p= 81-83) [41]; UV-Vis (CH_2Cl_2) λ_{max}; 312; IR (KBr) *ν*(cm^{-1}): 3102 (C-H, sp^2 stretch), 1501(C=C, Ar), 728 (C-Cl); ^{1}H

NMR($CDCl_3$, 400 MHz) *δ (ppm)*: 6.36-6.37 (d, 2H, J=2.0 Hz), 7.06 (d, 2H, J=1.6 Hz), 7.32-7.34 (d, 2H, J=8.8 Hz), 7.39-7.41 (d, 2H, J= 8.8 Hz).

1-(4-Bromo phenyl)-1H-pyrrole (3h); yellow solid; m.p= 91-93^oC, (m.p= 93-94.5^oC) [42]; UV-Vis (CH_2Cl_2) λ_{max}; 315; IR (KBr) *v*(cm^{-1}): 3130 (C-H, sp^2), 1497, 1590 (C=C, Ar), 727(C-H sp^2 OOP), 512 (C-Br); ^{1}H NMR($CDCl_3$, 400 MHz) *δ (ppm)*: 6.36-6.37 (d, 2H, J=2.0 Hz), 7.06 (d, 2H, J=2.0 Hz), 7.27-7.29 (d, 2H, J=9.2 Hz), 7.53-7.56 (d, 2H, J=8.8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) *δ(ppm):*110.85, 119.28, 121.62, 129.64, 131.04, 139.33.

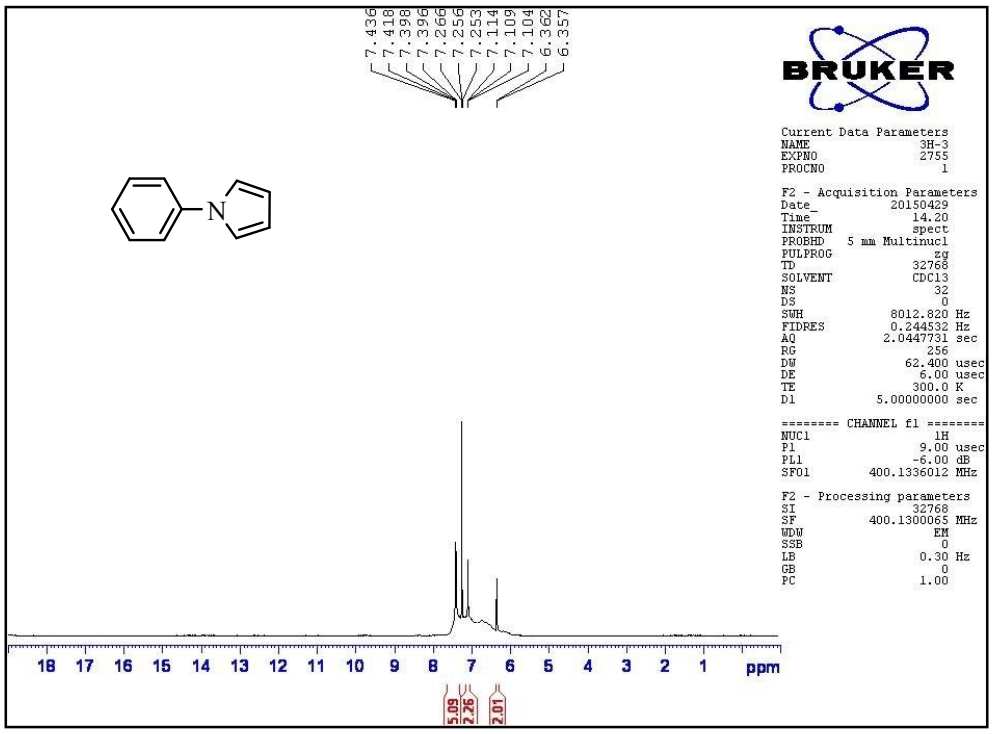
1-(3-Chloro phenyl)-1H-pyrrole (3i); brown solid; m.p= 51-53^oC, (m.p= 51-52^oC) [43]; UV-Vis (CH_2Cl_2) λ_{max}; 311; IR (KBr) *v*(cm^{-1}): 3102 (C-H, sp^2 stretch), 1500 (C=C, Ar), 720-820 (C-Cl); ^{1}H NMR ($CDCl_3$, 400 MHz) *δ (ppm)*: 6.36 (s, 2H), 7.08 (s, 2H), 7.21-7.23 (d, 1H J=7.6 Hz), 7.28-7.30 (d, 1H, J=8.4 Hz), 7.34-7.38 (t, 1H, J=8.0 Hz), 7.40 (s, 1H).

1-(2-Chloro phenyl)-1H-pyrrole (3j); black oil; UV-Vis (CH_2Cl_2) λ_{max}; 310; IR (KBr) *v*(cm^{-1}): 3050 (C-H, sp^2 stretch), 1500 (C=C, Ar), 720-820 (C-Cl); ^{1}H NMR($CDCl_3$, 400 MHz) *δ (ppm)*: 6.35-6.36 (d, 2H, J=2.7 Hz), 6.92-6.93 (d, 2H, J=2.0 Hz), 7.34-7.35 (t, 1H, J=2.0 Hz), 7.39-7.42 (m, 1H), 7.50-7.54 (m, 1H), 7.69-7.73 (m, 1H).

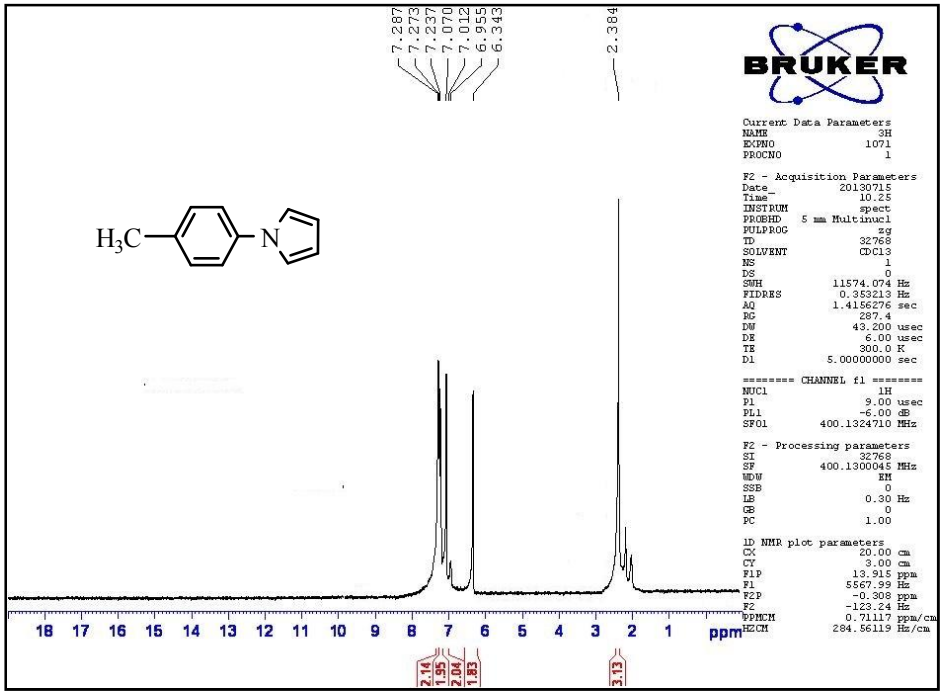
1-(4-Nitro phenyl)-1H-pyrrole (3k); yellow solid; m.p= 179-181^oC, (m.p= 180-183^oC) [44]; UV-Vis (CH_2Cl_2) λ_{max}; 335; IR (KBr) *v*(cm^{-1}): 3150 (C-H, sp^2), 1616 (C=C, Ar), 1527 (N=O), 1347 (C-N); ^{1}H NMR($CDCl_3$, 400 MHz) *δ (ppm)*: 6.44 (s, 2H), 7.20 (s, 2H), 7.52–7.55 (d, 2H, J=8.8 Hz), 8.32-8.34 (d, 2H, J=9.2 Hz).

1-(3-Nitro phenyl)-1H-pyrrole (3l); yellow solid; m.p= 67-69^oC, (m.p= 66-68^oC) [45]; UV-Vis (CH_2Cl_2) λ_{max}; 332; IR (KBr) *v*(cm^{-1}): 3150 (C-H, sp^2), 1616 (C=C, Ar), 1527 (N=O), 1347 (CN); ^{1}H NMR($CDCl_3$, 400 MHz) *δ (ppm)*: 6.42-6.43 (t, 2H, J=2.0 Hz), 7.17-7.18 (t, 2H, J=2.4 Hz), 7.60-7.64 (t, 1H, J=8.4 Hz), 7.73-7.75 (d, 1H, J=7.6 Hz), 8.10-8.12 (d, 1H, J=8.0 Hz), 8.26-8.28 (t, 1H, J=2.0 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) *δ (ppm)*: 111.84, 114.33, 119.17, 119.83, 125.65, 130.92, 141.31, 149.00.

^{1}H NMR spectra of 1-Phenyl-1H-pyrrole (3a)



^{1}H NMR spectra of 1-p-Tolyl-1H-pyrrole (3b)



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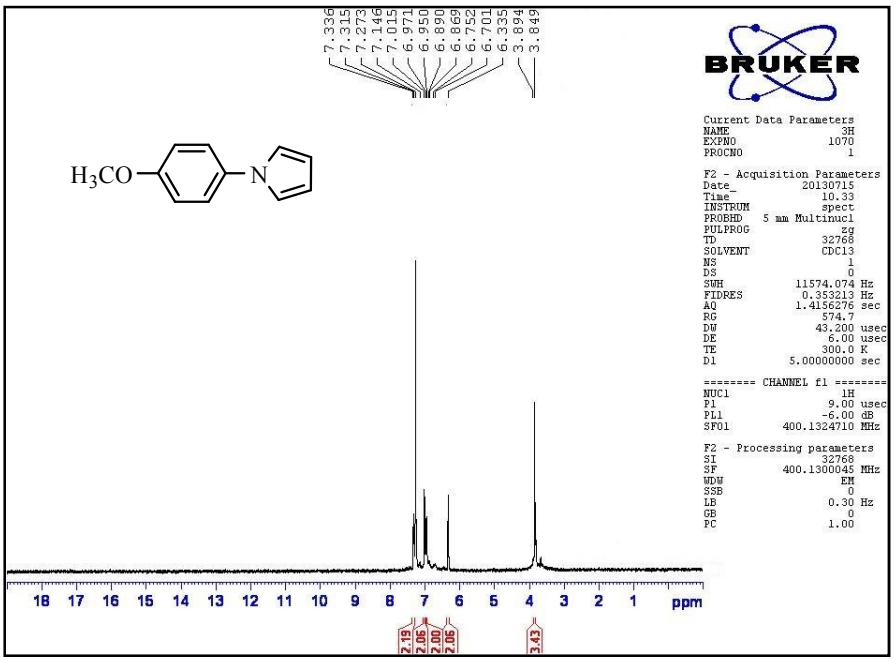
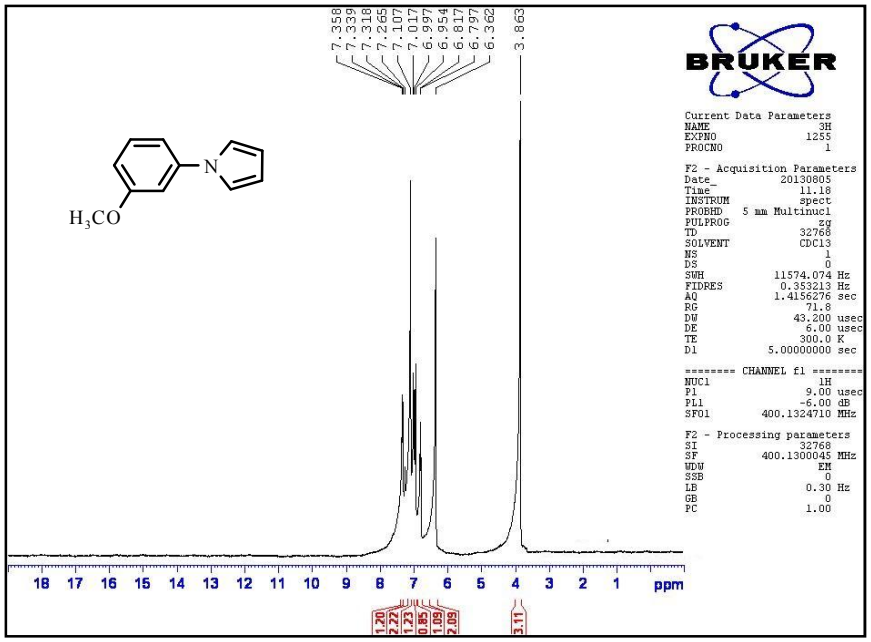
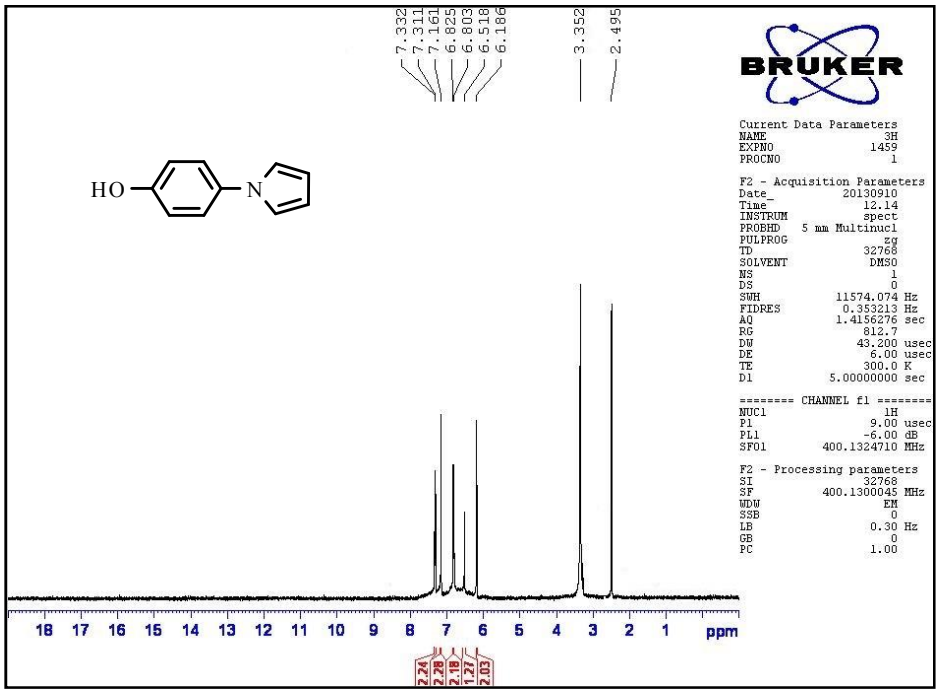


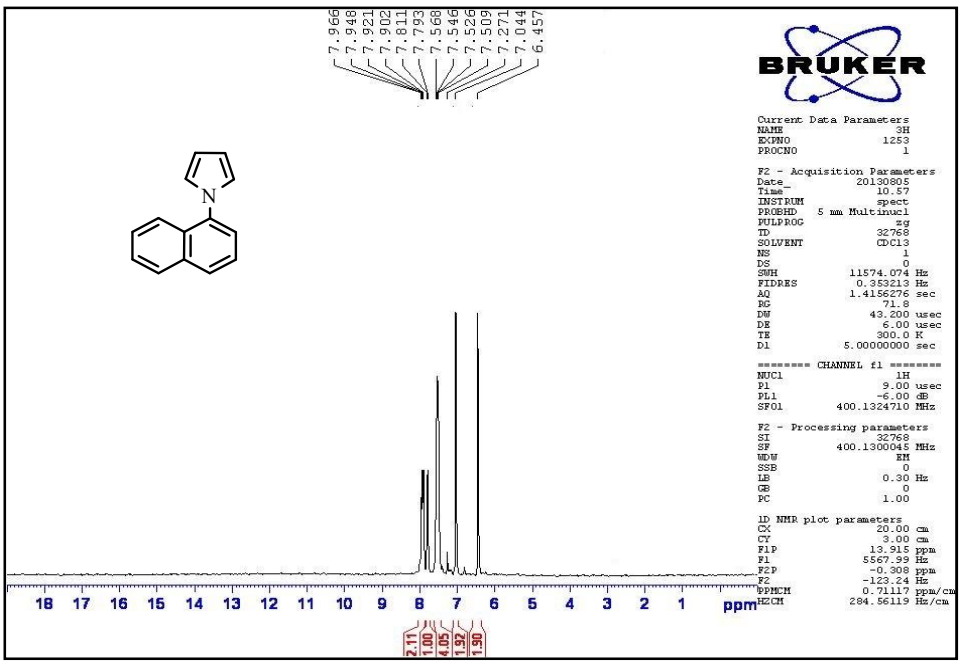
^{1}H NMR spectra of 1-(3-Methoxy phenyl)-1H-pyrrole (3d)



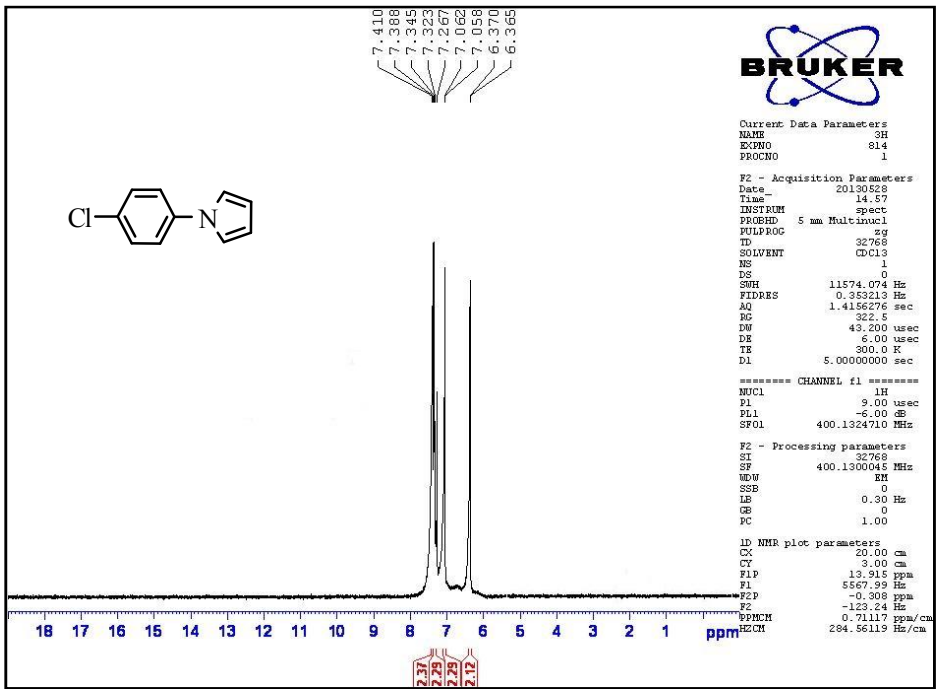
^{1}H NMR spectra of 1-(4-Hydroxy phenyl)-1H-pyrrole (3e)



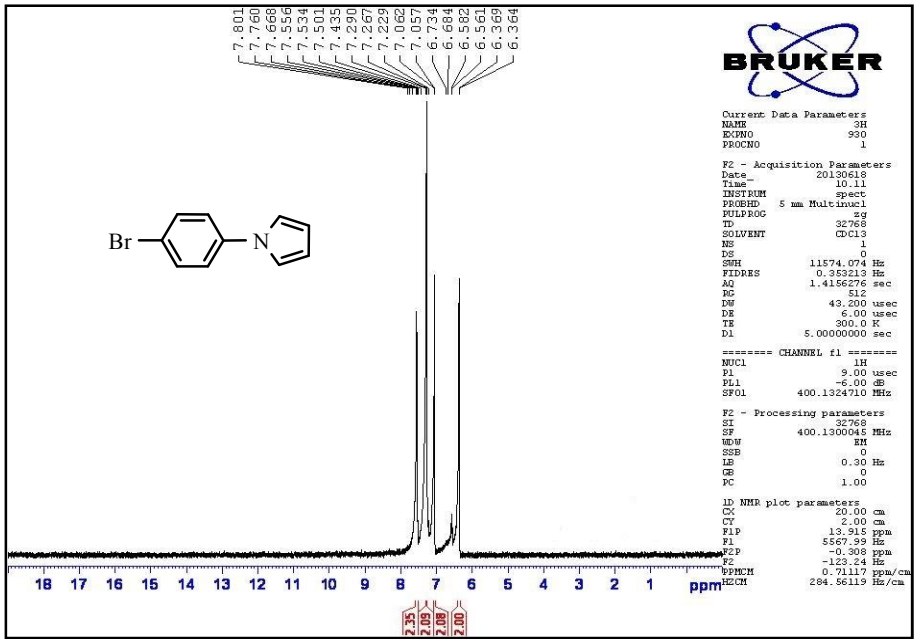
^{1}H NMR spectra of 1-(Naphthyl)-1H-pyrrole (**3f)**

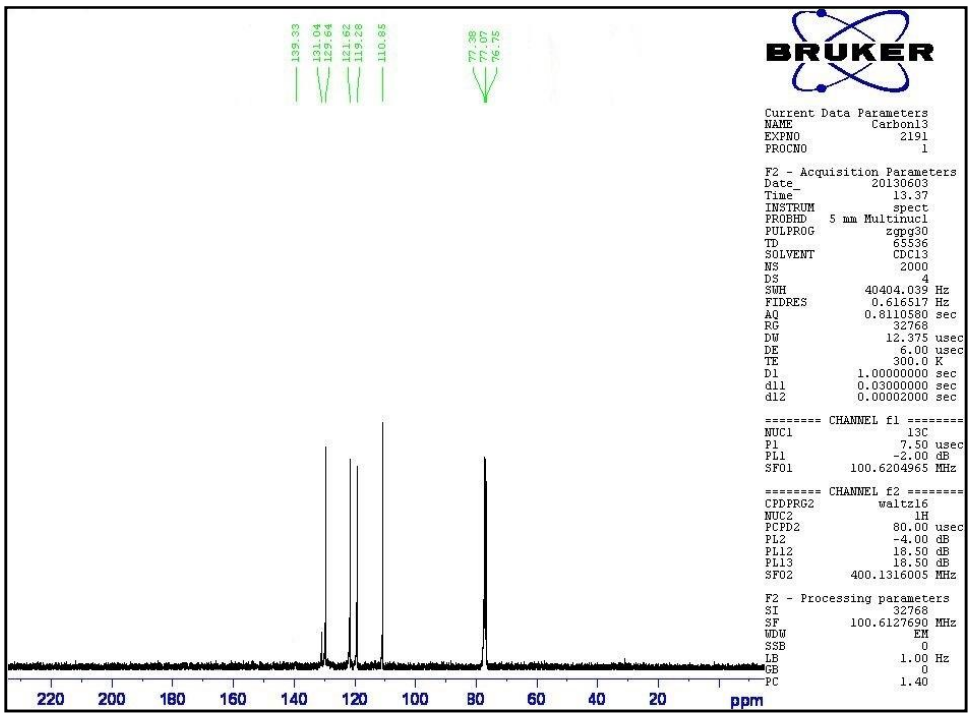


^{1}H NMR spectra of 1-(4-Chloro phenyl)-1H-pyrrole (**3g)**



^{1}H NMR and ^{13}C NMR spectra of 1-(4-Bromo phenyl)-1H-pyrrole (3h)

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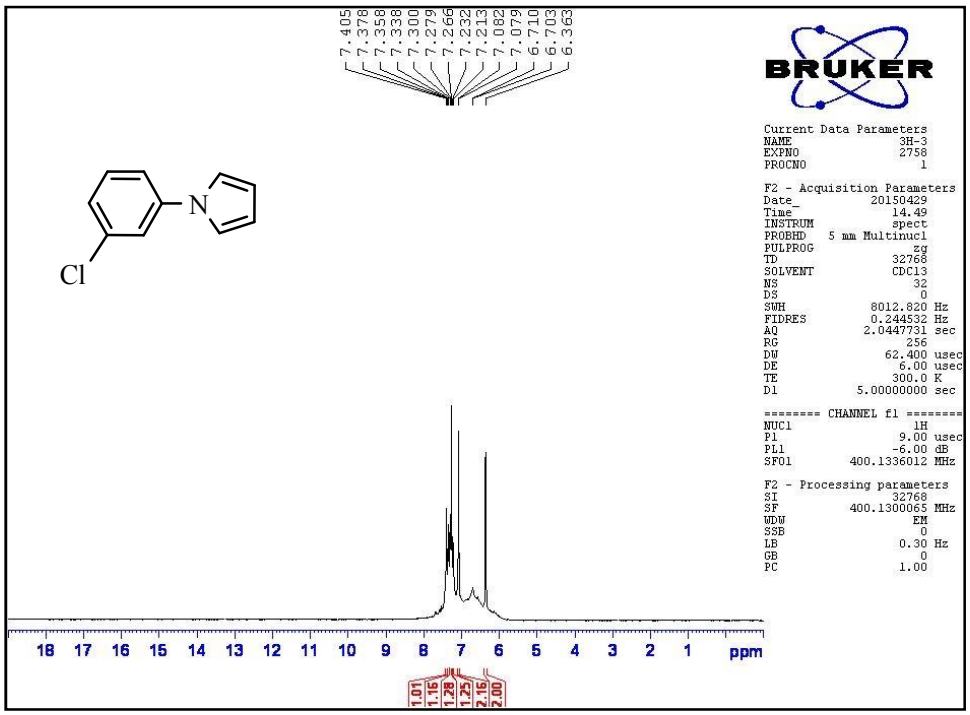
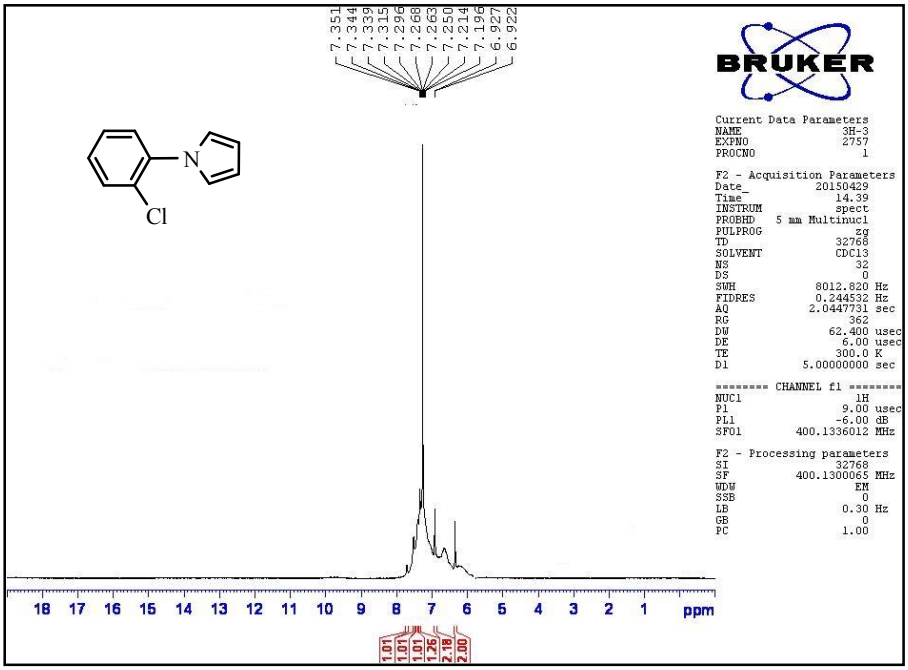
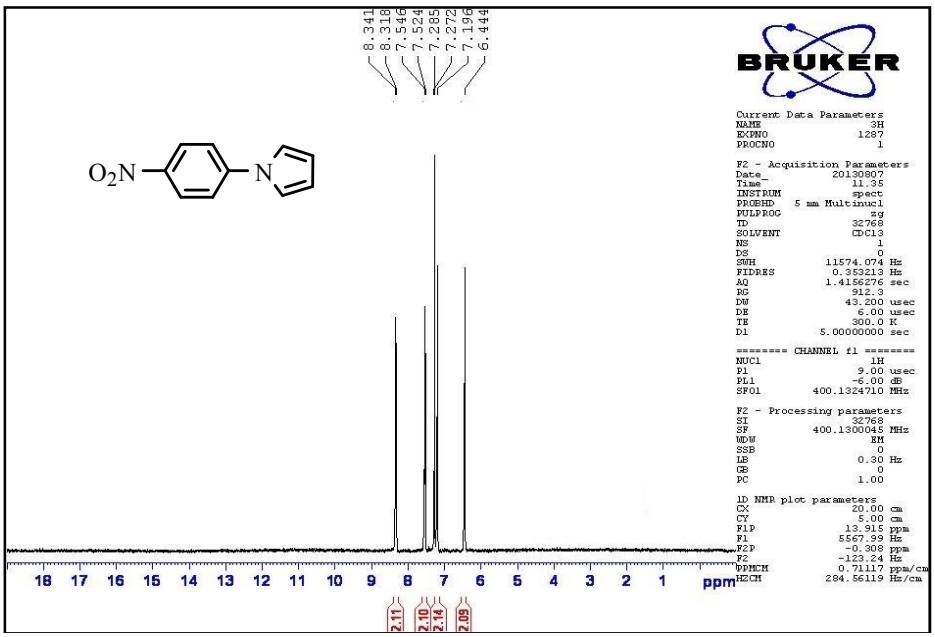
^{1}H NMR spectra of 1-(3-Chloro phenyl)-1H-pyrrole (3i)



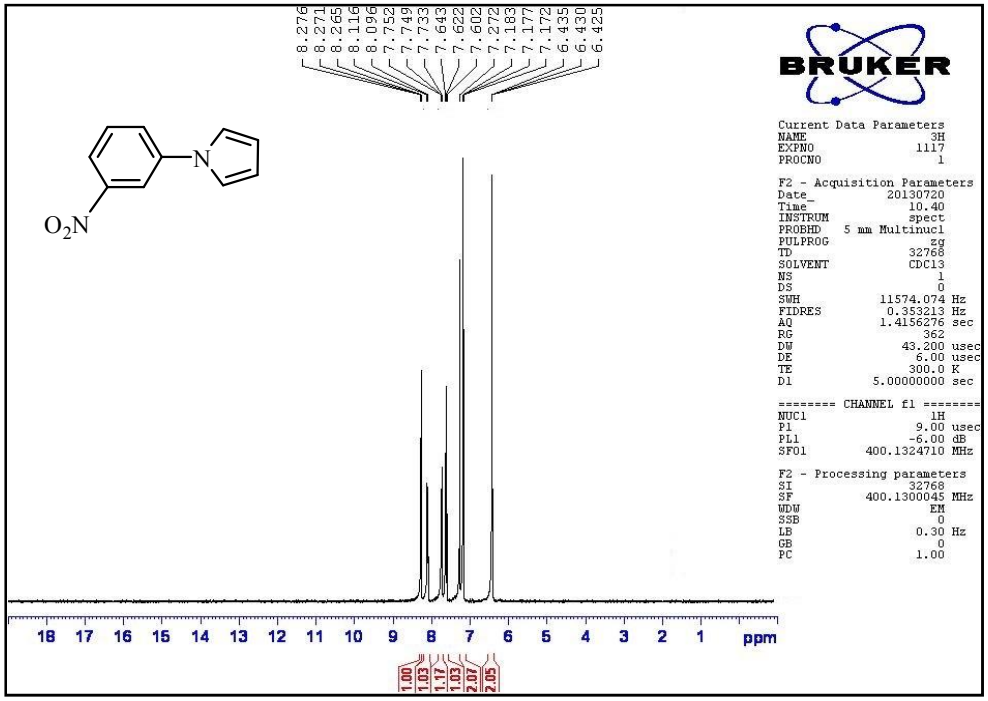
^{1}H NMR spectra of 1-(2-Chloro phenyl)-1H-pyrrole (3j)

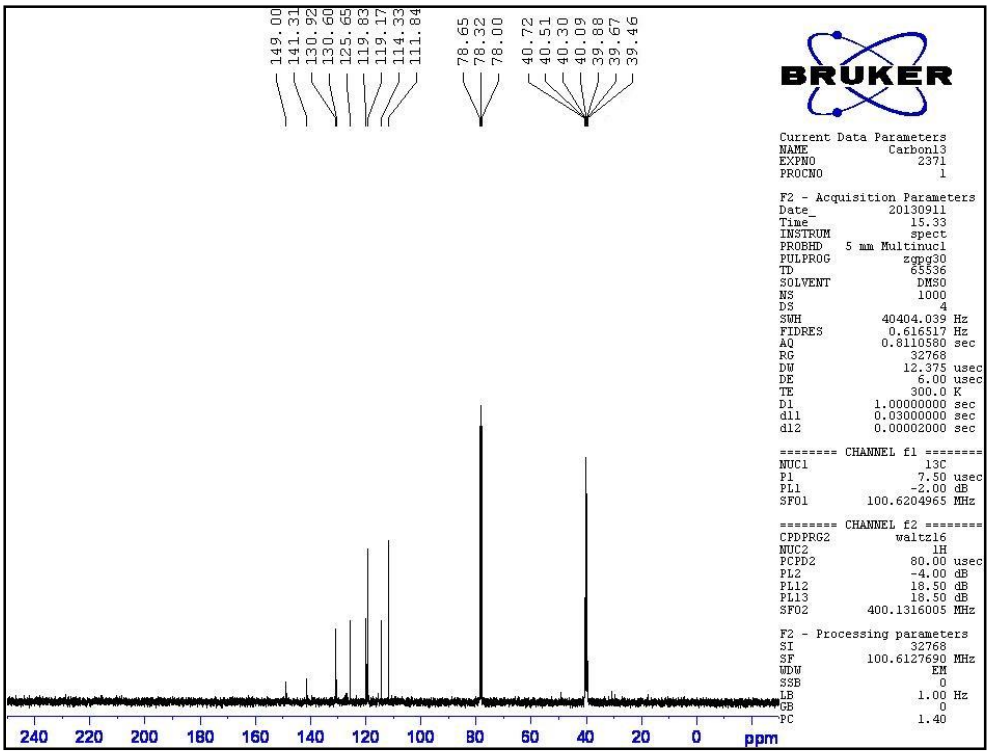


^{1}H NMR spectra of 1-(4-Nitro phenyl)-1H-pyrrole (3k)



^{1}H NMR and ^{13}C NMR spectra of 1-(3-Nitro phenyl)-1H-pyrrole (3l)

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