Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Synergistic effect of the Pd-Ni bimetal/carbon nanofibers composite catalyst in Suzuki coupling reaction

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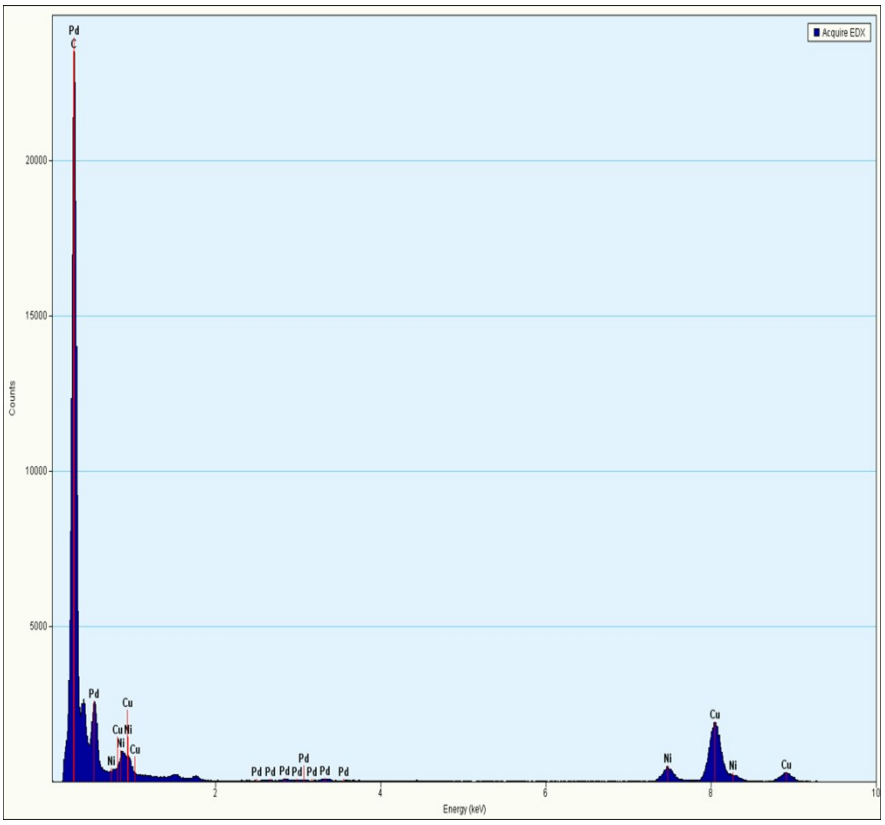

Figure S1. EDX spectrum of as-prepared Pd_1Ni_4/CNF.

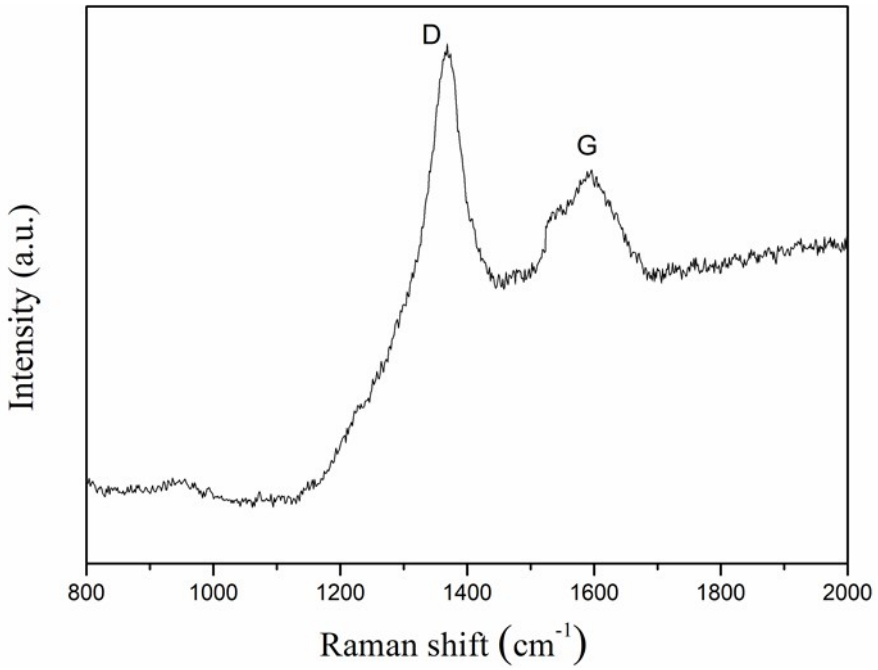

Figure S2. Raman spectrum of the catalyst Pd/CNF.

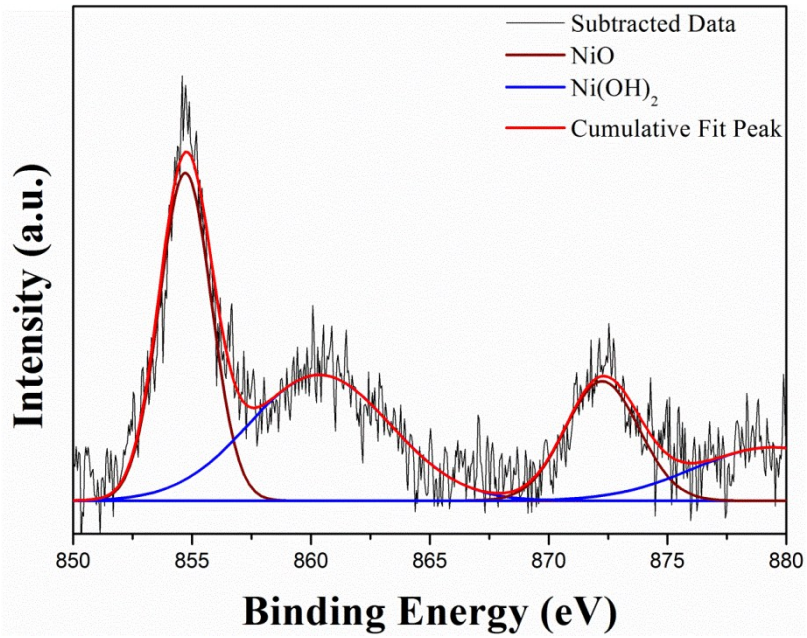

Figure S3. XPS spectrum of the catalyst Ni/CNF.

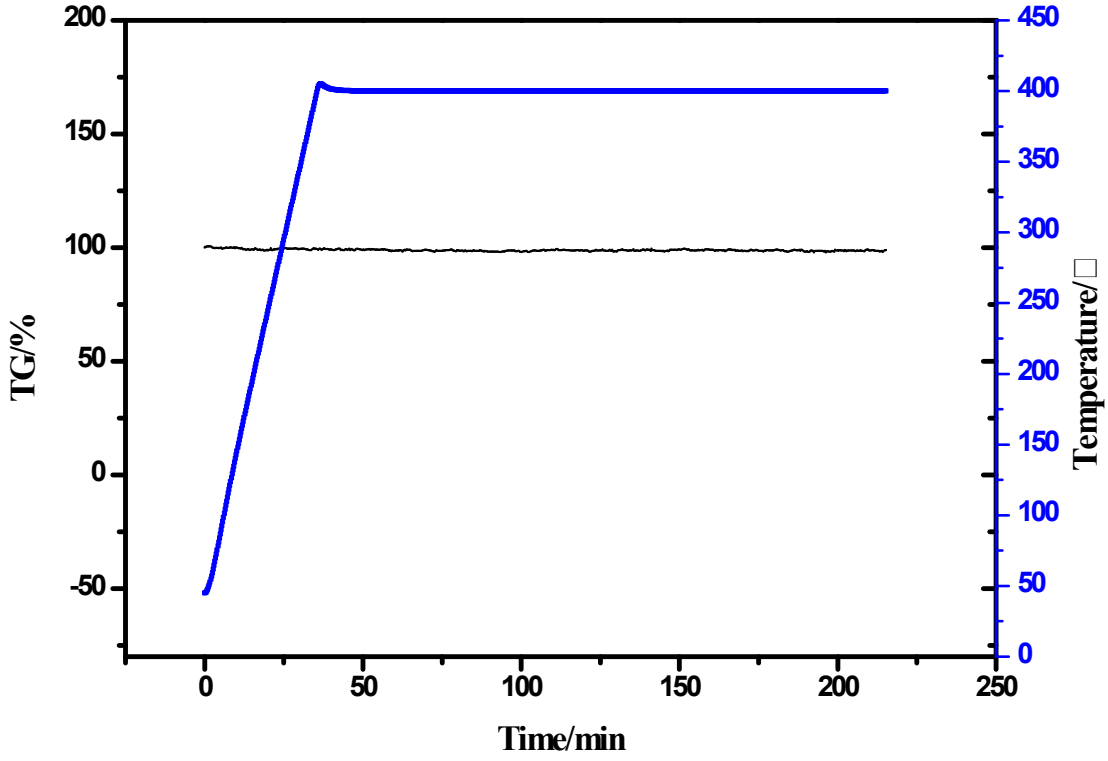

Figure S4. TG curve of the catalyst Pd_1Ni_4/CNF

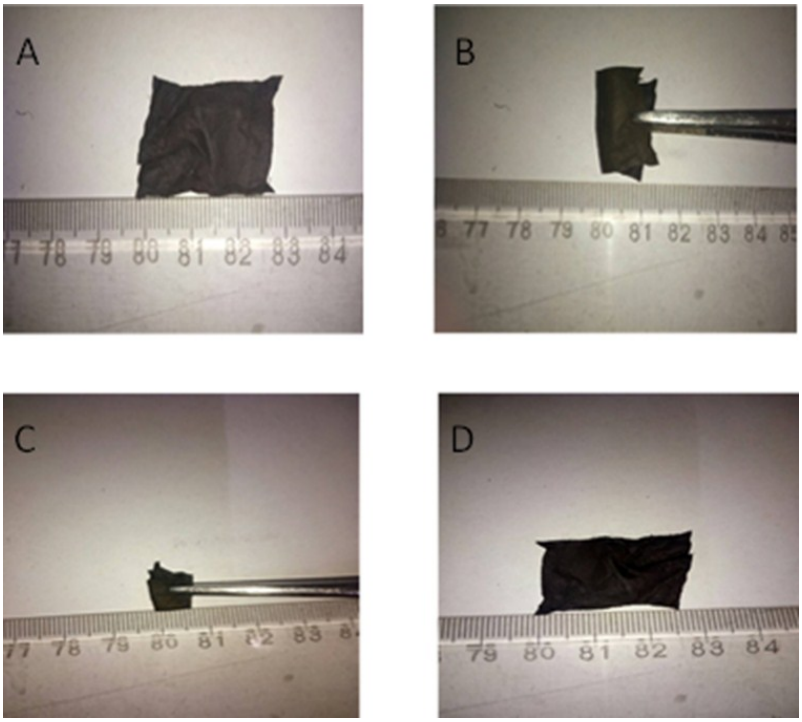

Figure S5. Representative photographs showing the flexibility of the catalyst Pd_1Ni_4/CNF sample. A is the initial sample, B and C are the photo of sample folded and D is the unfolded sample.

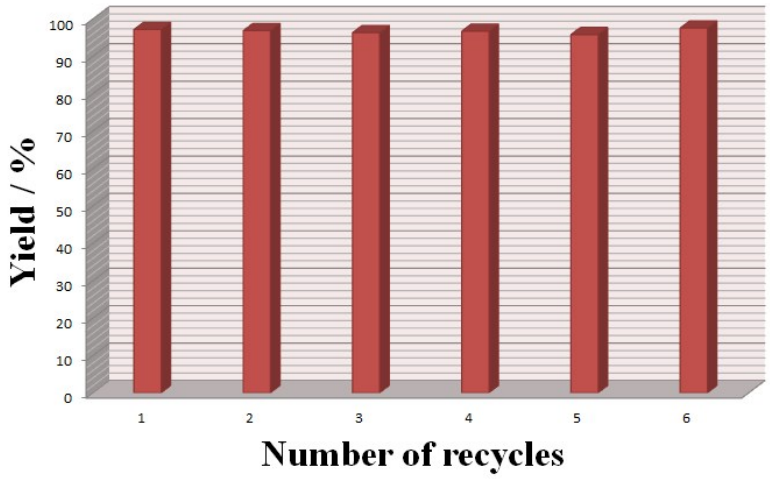

Figure S6. Recycling experiment for Suzuki coupling; Pd_1Ni_4/CNF (5 mg), bromobenzene (3 mmol 0.471g), phenylboronic acid (3.3 mmol 0.4023 g), K_2CO_3 (6 mmol, 0.8292 g), EtOH/H_20 (8 ml/8 ml), 80℃, 3 h.

1,1-Biphenyl: ^{1}H NMR (500 MHz, dmso) δ 7.65 (d, J = 7.0 Hz, 4H), 7.46 (t, J = 7.8 Hz, 4H), 7.36 (t, J = 7.4 Hz, 2H). ^{13}C NMR (125 MHz, dmso) δ 140.63, 129.38, 127.86, 127.13.

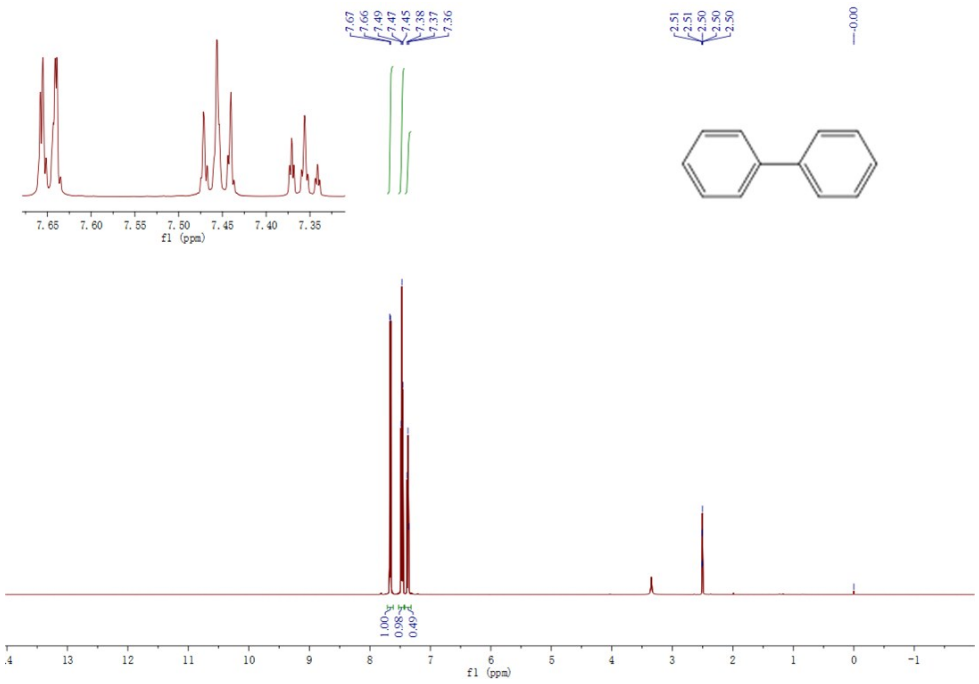

Figure S7-A: ^{1}H NMR of 1,1-Biphenyl

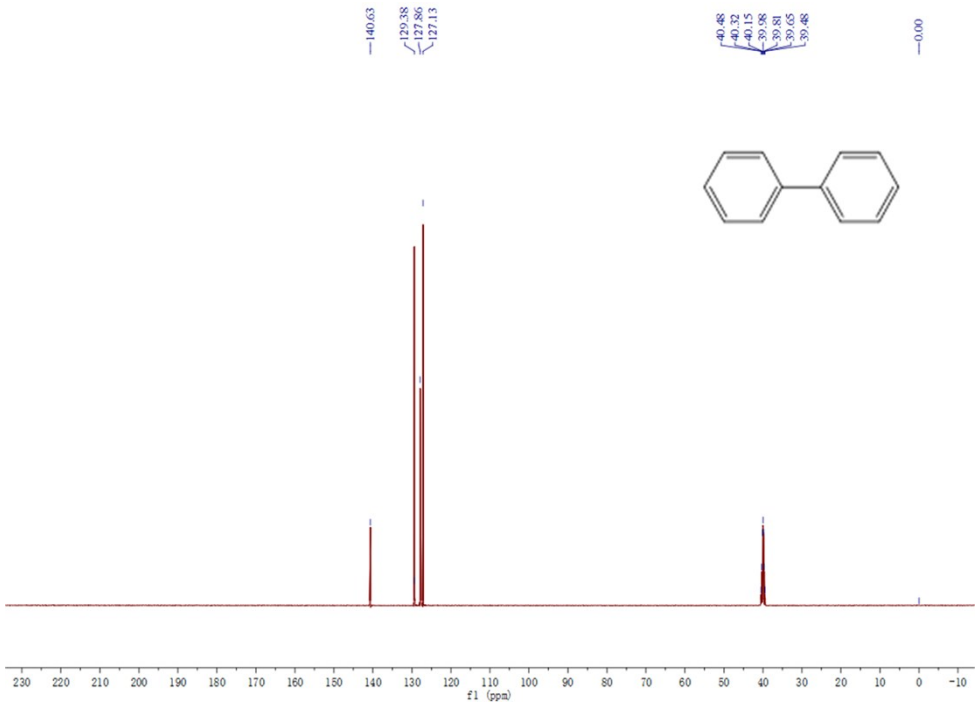

Figure S7-B: ^{13}C NMR of 1,1-Biphenyl

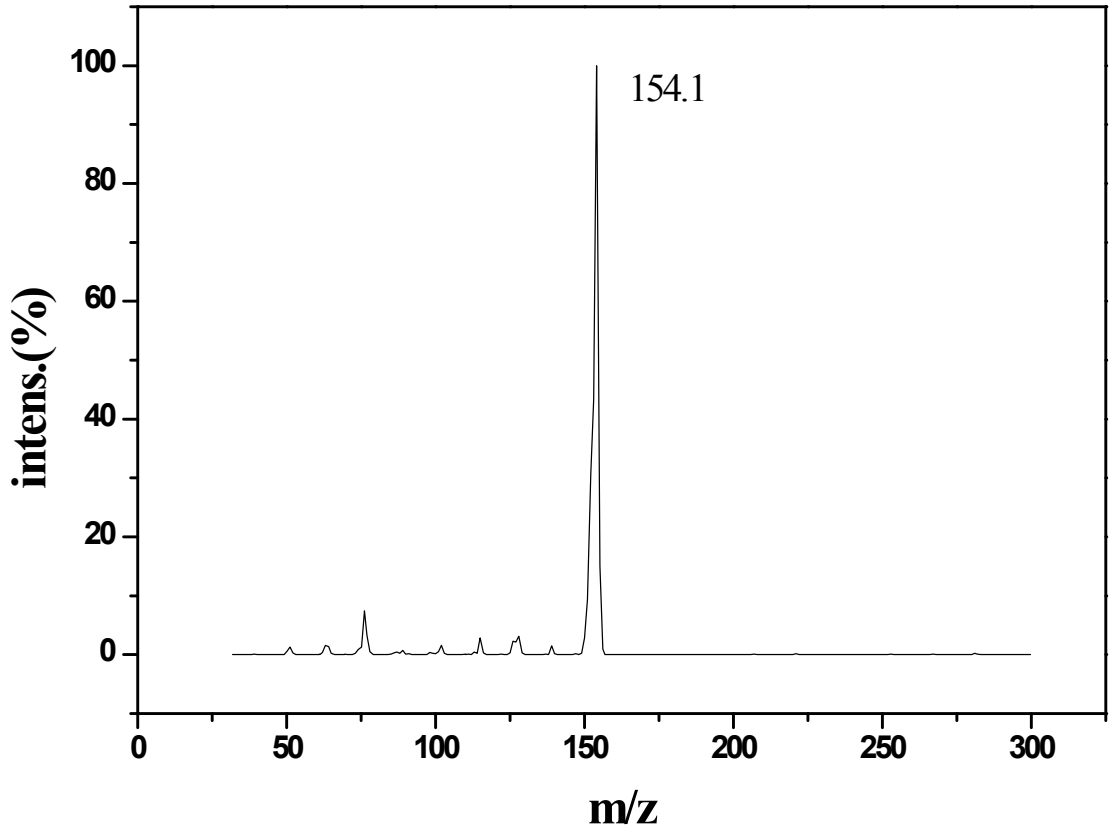

Figure S7-C: mass spectrum of 1,1-Biphenyl

2-Methyl-1,1-Biphenyl: ^{1}H NMR (500 MHz, dmso) δ 7.43 (t, J = 7.6 Hz, 2H), 7.38 –

7.30 (m, 3H), 7.30 – 7.22 (m, 3H), 7.20 – 7.17 (m, 1H), 2.22 (s, 3H). ^{13}C NMR (125 MHz, dmso) δ 141.35, 134.67, 130.32, 129.51, 128.94, 128.21, 127.29, 126.88, 125.93, 20.17.

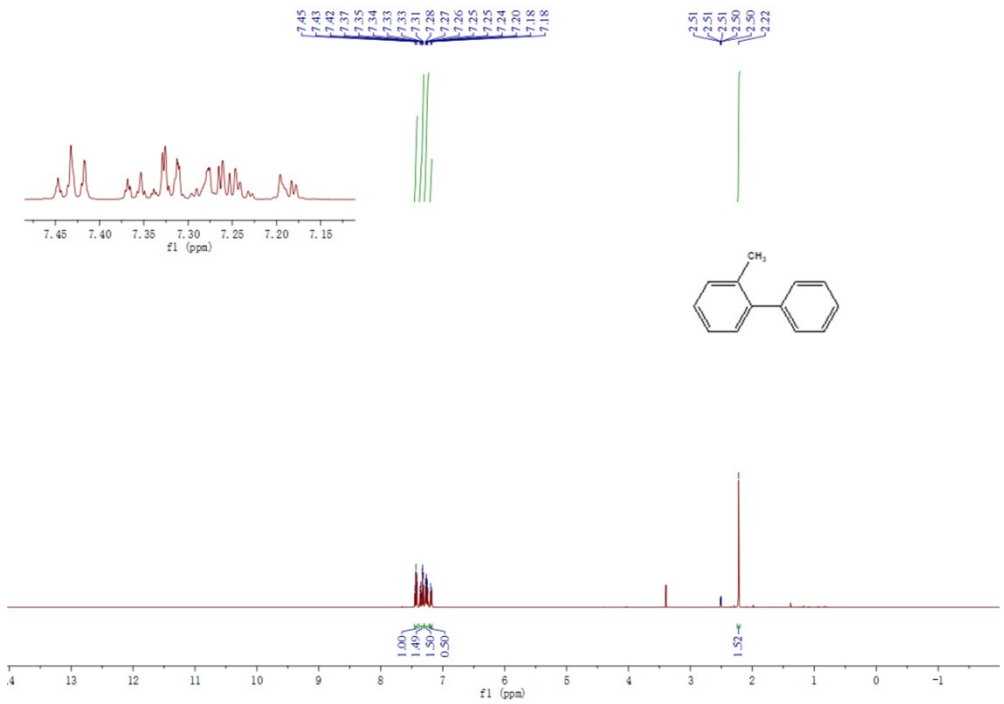

Figure S8-A: ^{1}H NMR of 2-Methyl-1,1-Biphenyl

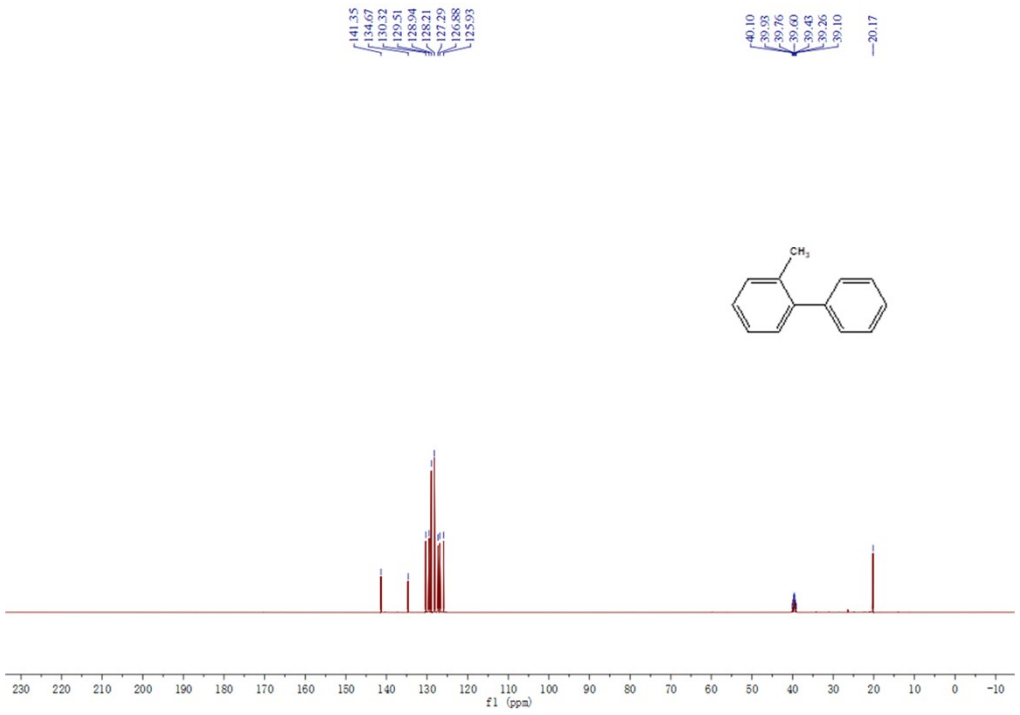

Figure S8-B: ^{13}C NMR of 2-methyl-1,1-Biphenyl

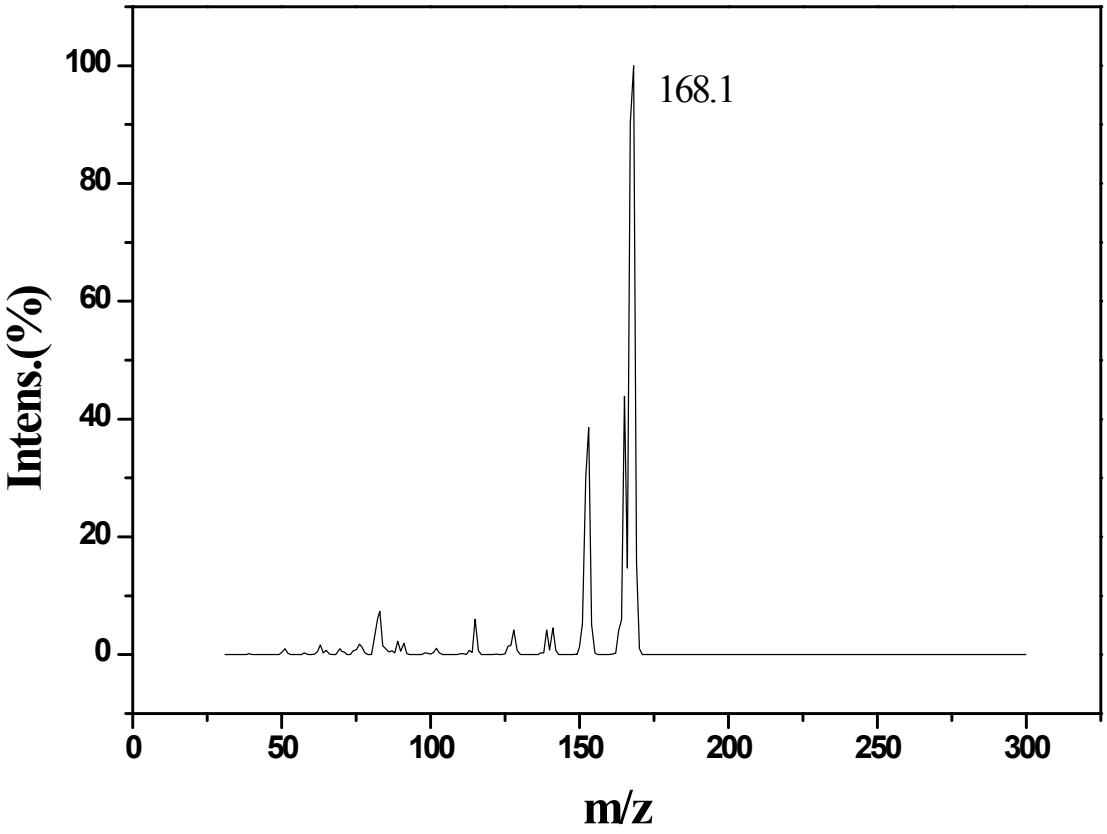

Figure S8-C: mass spectrum of 2-methyl-1,1-Biphenyl

3-Methyl-1,1-Biphenyl: ^{1}H NMR (500 MHz, dmso) δ 7.63 (d, J = 7.9 Hz, 2H), 7.44 (dd,

J = 13.7, 5.9 Hz, 4H), 7.34 (dd, J = 14.9, 7.5 Hz, 2H), 7.16 (d, J = 8.1 Hz, 1H), 2.36 (s, 3H). ^{13}C NMR (125 MHz, dmso) δ 140.65, 140.51, 138.32, 129.14, 129.08, 128.33, 127.65, 127.59, 126.97, 124.11, 21.40.

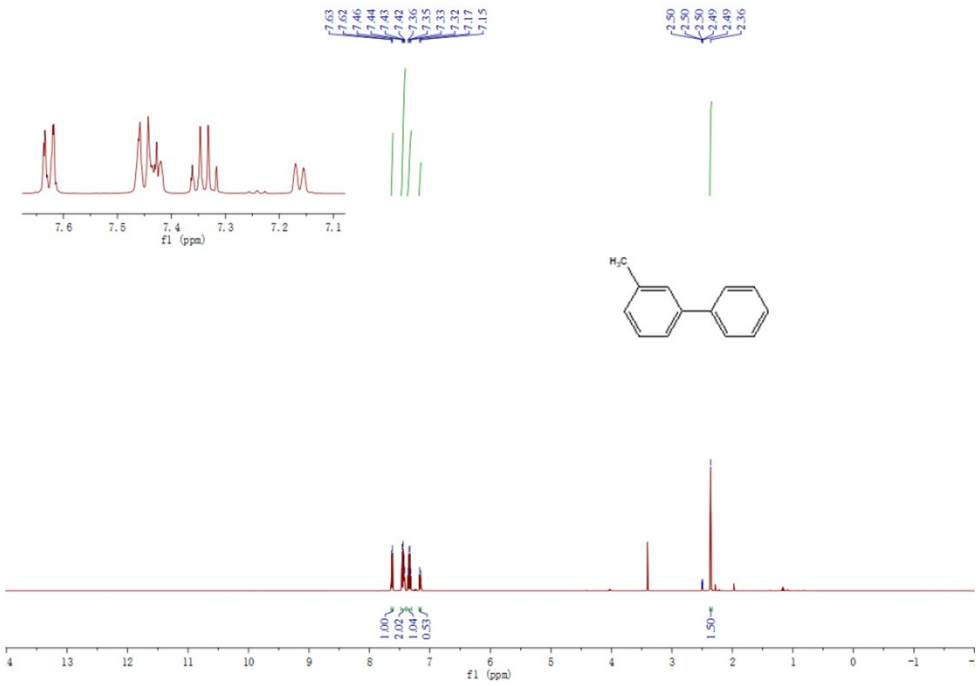

Figure S9-A: ^{1}H NMR of 3-Methyl-1,1-Biphenyl

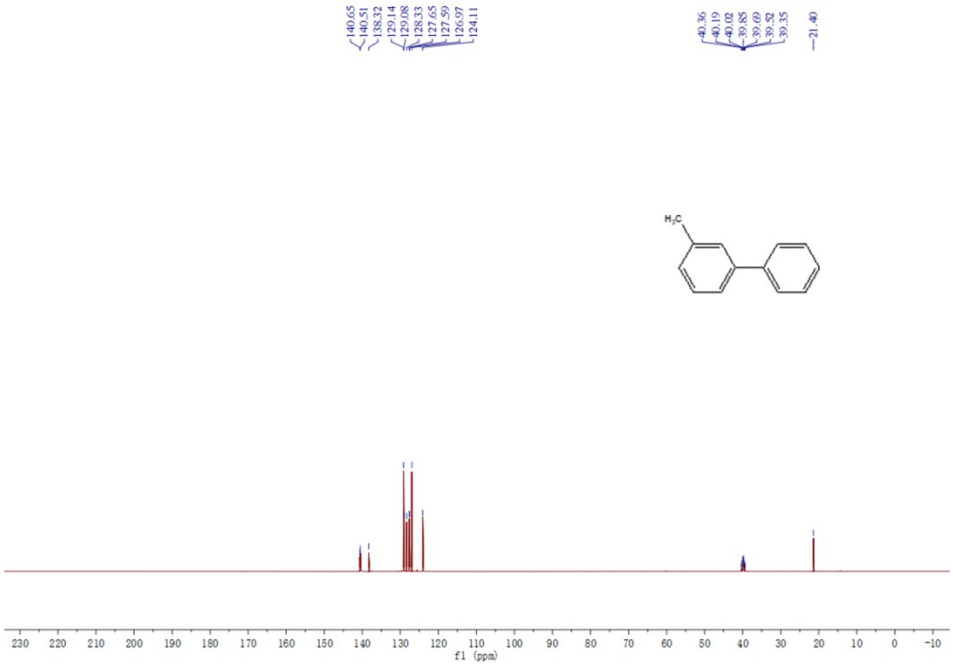

Figure S9-B: ^{13}C NMR of 3-Methyl-1,1-Biphenyl

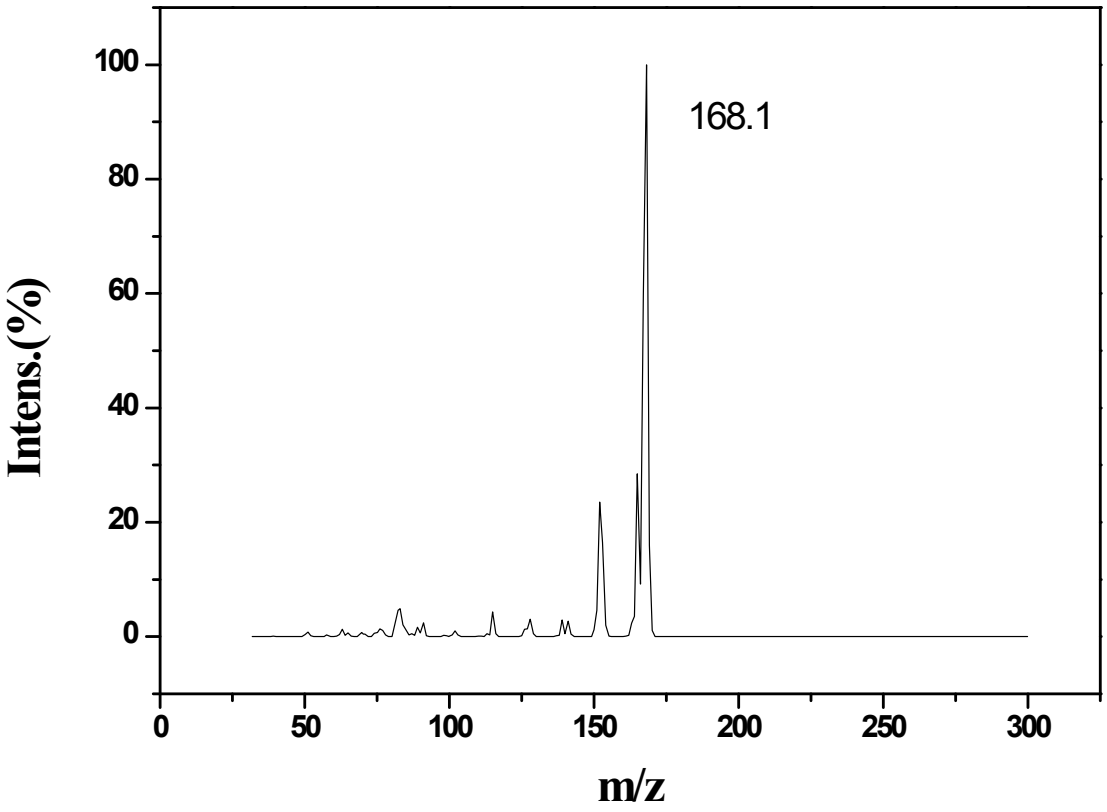

Figure S9-C: mass spectrum of 3-Methyl-1,1-Biphenyl

4-Methyl-1,1-Biphenyl: ^{1}H NMR (500 MHz, dmso) δ 7.64 (d, J = 7.0 Hz, 1H), 7.56 (d, J = 8.1 Hz, 1H), 7.45 (t, J = 7.7 Hz, 1H), 7.34 (t, J = 7.4 Hz, 1H), 7.28 (d, J = 7.9 Hz, 1H), 2.35 (s, 2H). ^{13}C NMR (125 MHz, dmso) δ 140.08, 137.27, 136.68, 129.50, 128.85, 127.08, 126.48, 126.40, 20.64.

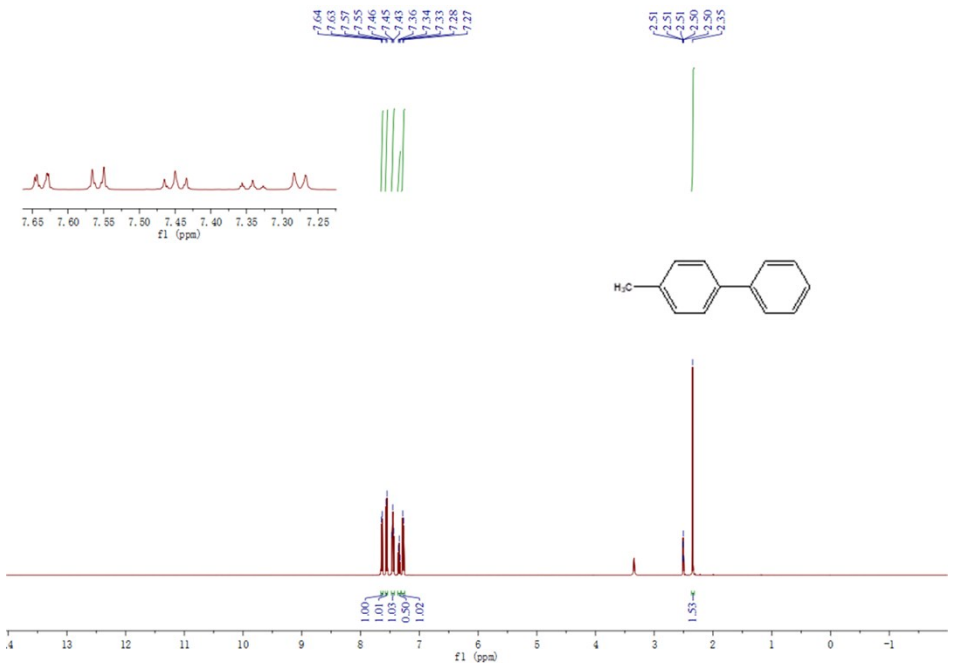

Figure S10-A: ^{1}H NMR of 4-Methyl-1,1-Biphenyl

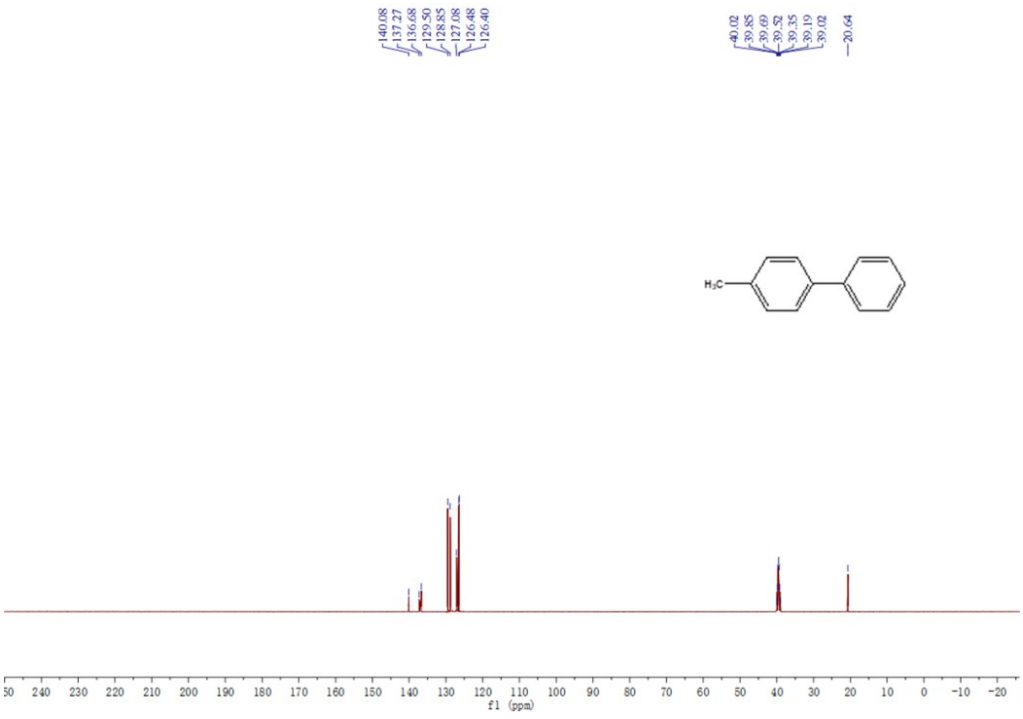

Figure S10-B: ^{13}C NMR of 4-Methyl-1,1-Biphenyl

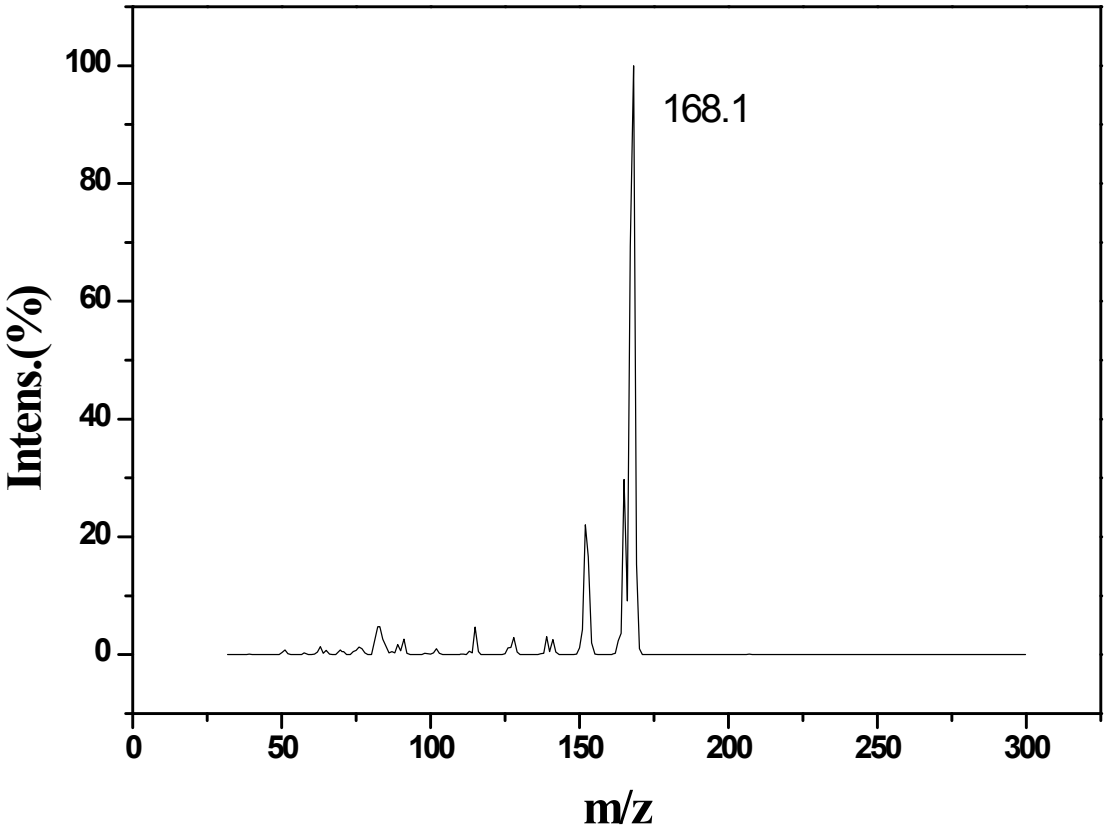

Figure S10-C: mass spectrum of 4-Methyl-1,1-Biphenyl

2-Methoxy-1,1-Biphenyl: ^{1}H NMR (500 MHz, dmso) δ 7.52 (d, J = 7.6 Hz, 2H), 7.45

(t, J = 7.7 Hz, 2H), 7.41 – 7.31 (m, 3H), 7.16 (d, J = 8.3 Hz, 1H), 7.08 (t, J = 7.4 Hz, 1H), 3.80 (s, 3H). ^{13}C NMR (125 MHz, dmso) δ 156.07, 138.18, 130.36, 129.79, 129.22, 128.82, 127.93, 126.75, 120.74, 111.70, 55.41.

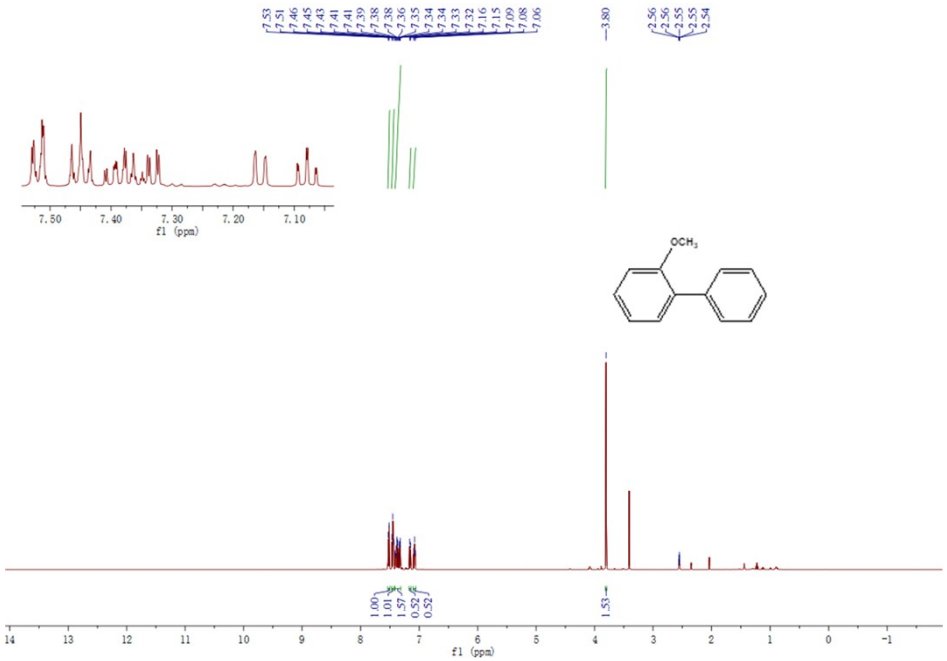

Figure S11-A: ^{1}H NMR of 2-Methoxy-1,1-Biphenyl

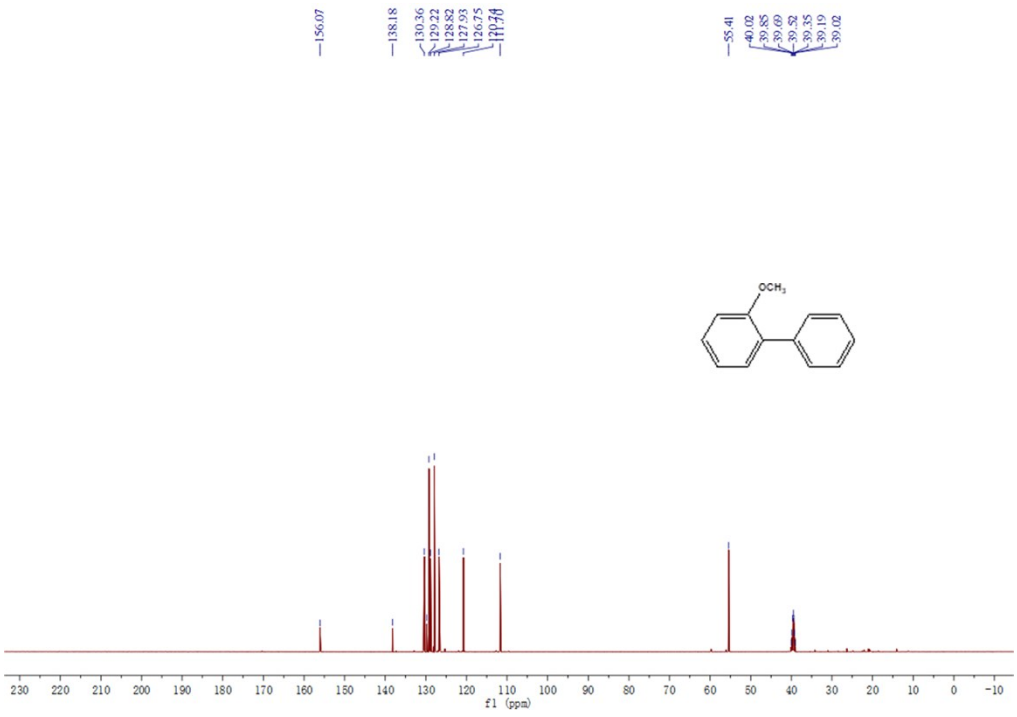

Figure S11-B: ^{13}CNMR of 2-Methoxy-1,1-Biphenyl

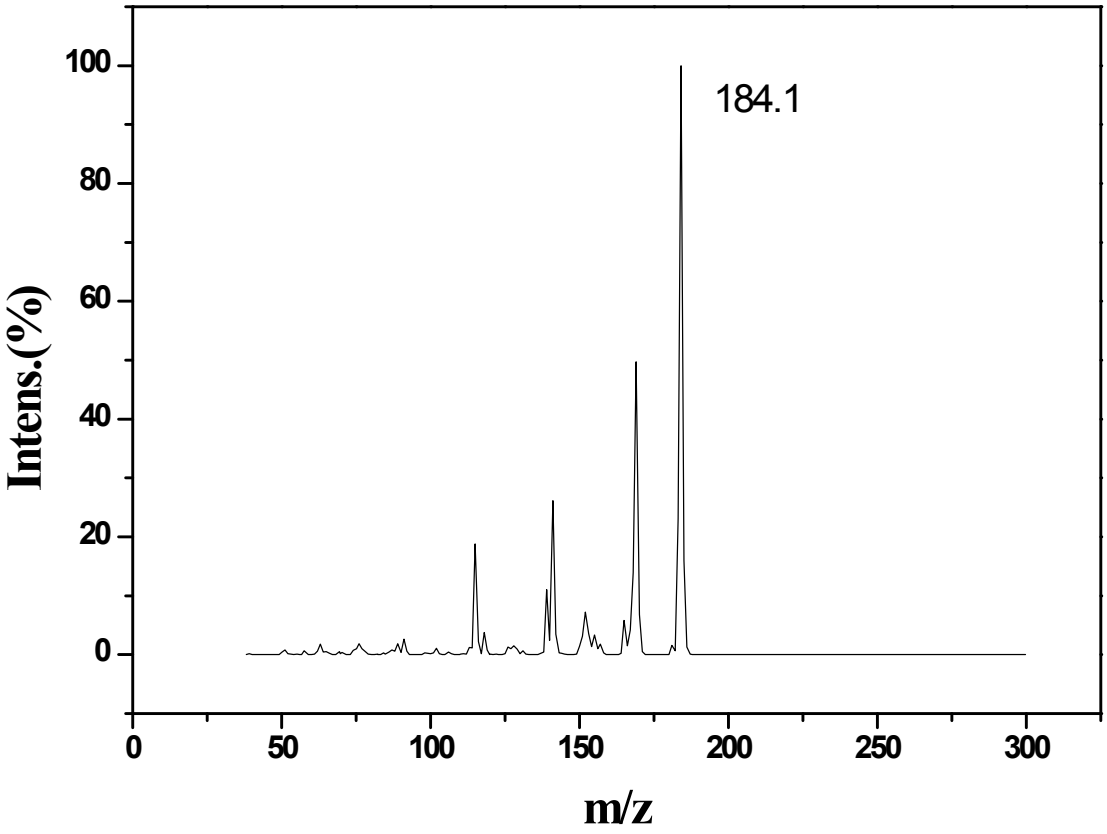

Figure S11-C: mass spectrum of 2-Methoxy-1,1-Biphenyl

3-Methoxy-1,1-Biphenyl: ^{1}H NMR (500 MHz, dmso) δ 7.67 (d, J = 8.2 Hz, 2H), 7.46 (t,

J = 7.7 Hz, 2H), 7.41 – 7.34 (m, 2H), 7.23 (d, J = 7.2 Hz, 2H), 6.98 – 6.93 (m, 1H), 3.83 (s, 3H). ^{13}C NMR (125 MHz, dmso) δ 160.30, 142.29, 140.67, 130.45, 129.35, 128.03, 127.31, 119.55, 113.46, 112.78, 55.56.

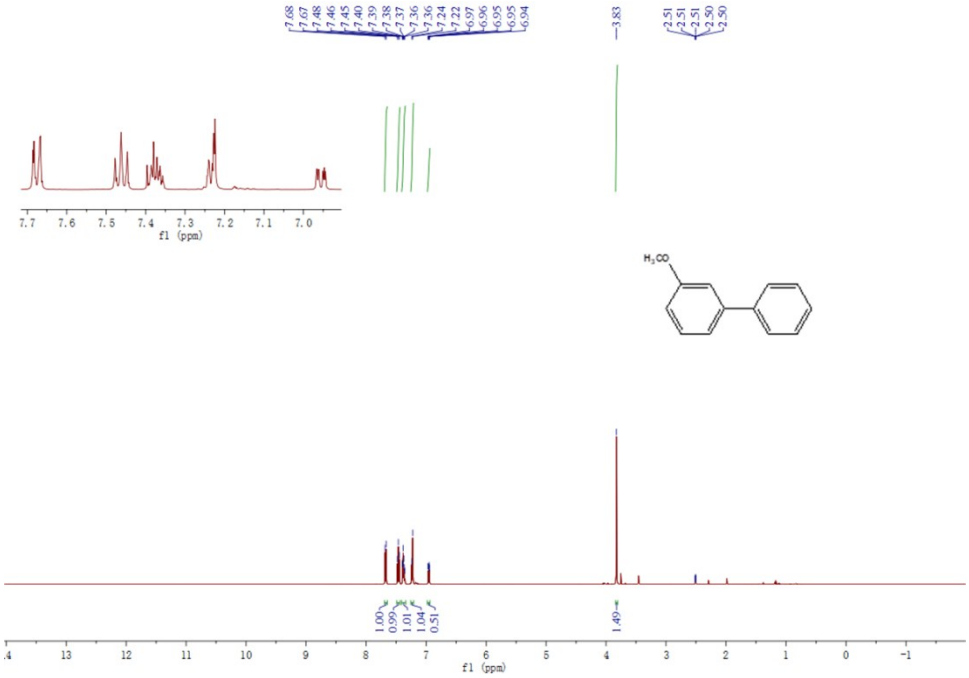

Figure S12-A: ^{1}H NMR of 3-Methoxy-1,1-Biphenyl

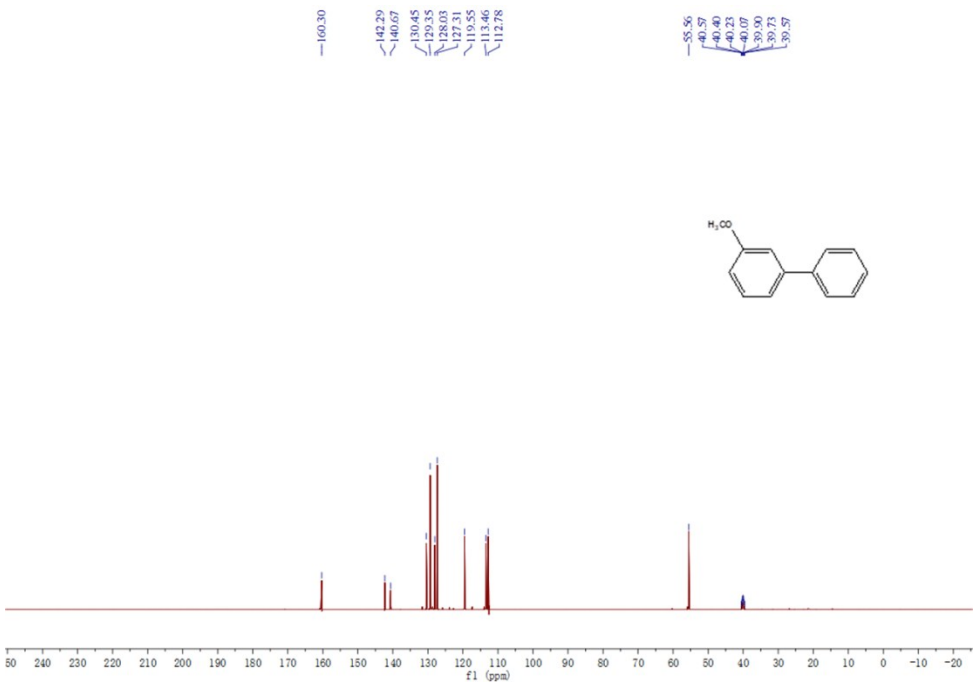

Figure S12-B: ^{13}CNMR of 3-Methoxy-1,1-Biphenyl

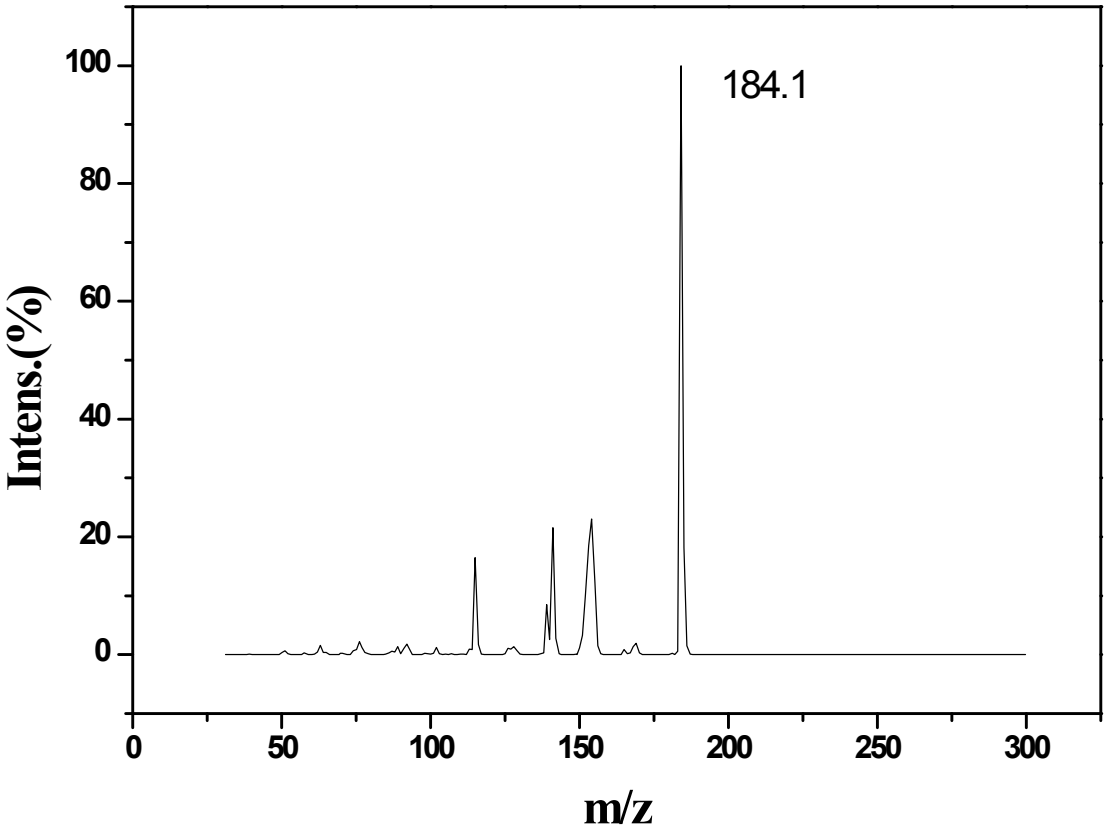

Figure S12-C: mass spectrum of 3-Methoxy-1,1-Biphenyl

4-Methoxy-1,1-Biphenyl: ^{1}H NMR (500 MHz, dmso) δ 7.63 – 7.59 (m, 4H), 7.43 (t, J

= 7.8 Hz, 2H), 7.31 (t, J = 7.4 Hz, 1H), 7.03 (d, J = 8.8 Hz, 2H), 3.80 (s, 3H). ^{13}C NMR (125 MHz, dmso) δ 159.20, 140.15, 132.85, 129.17, 128.06, 127.01, 126.49, 114.68, 55.49.

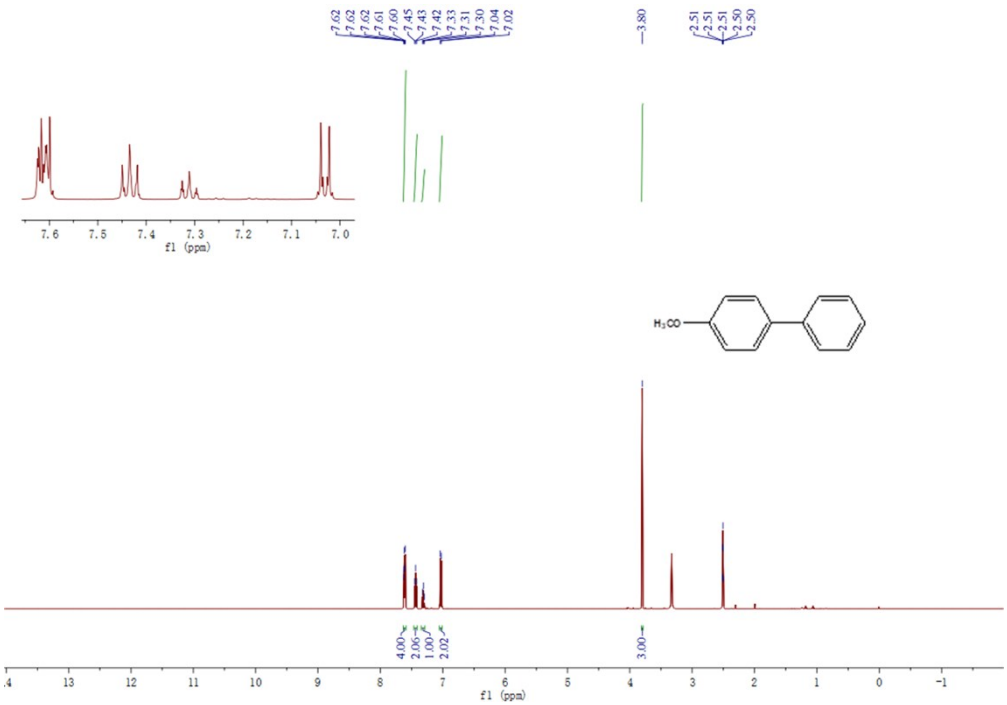

Figure S13-A: ^{1}H NMR of 4-Methoxy-1,1-Biphenyl

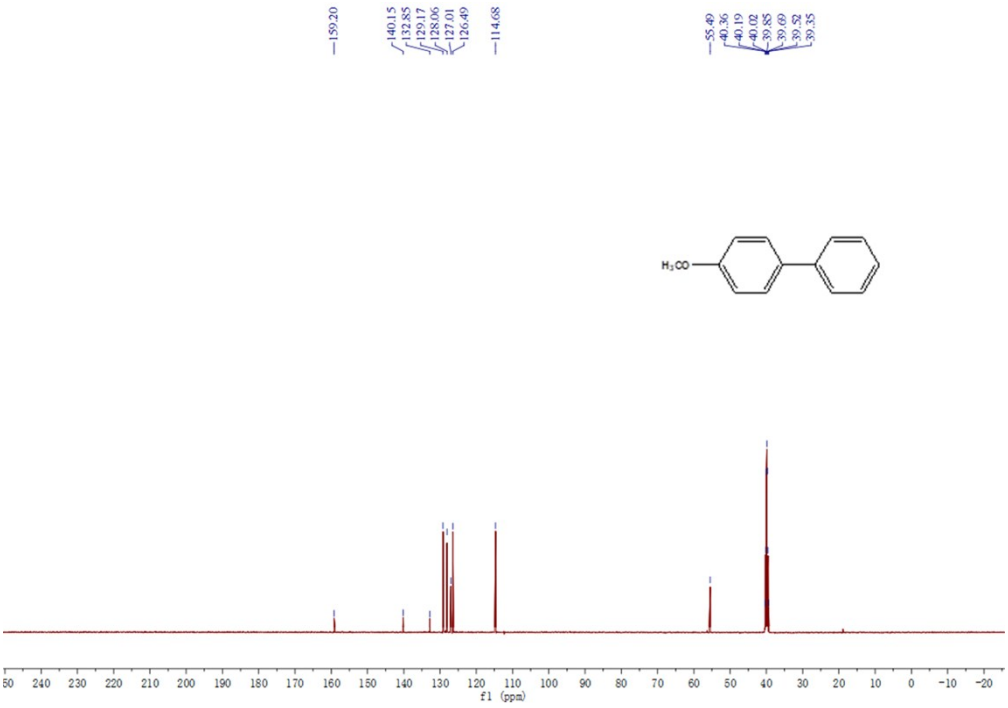

Figure S13-B: ^{13}CNMR of 4-Methoxy-1,1-Biphenyl

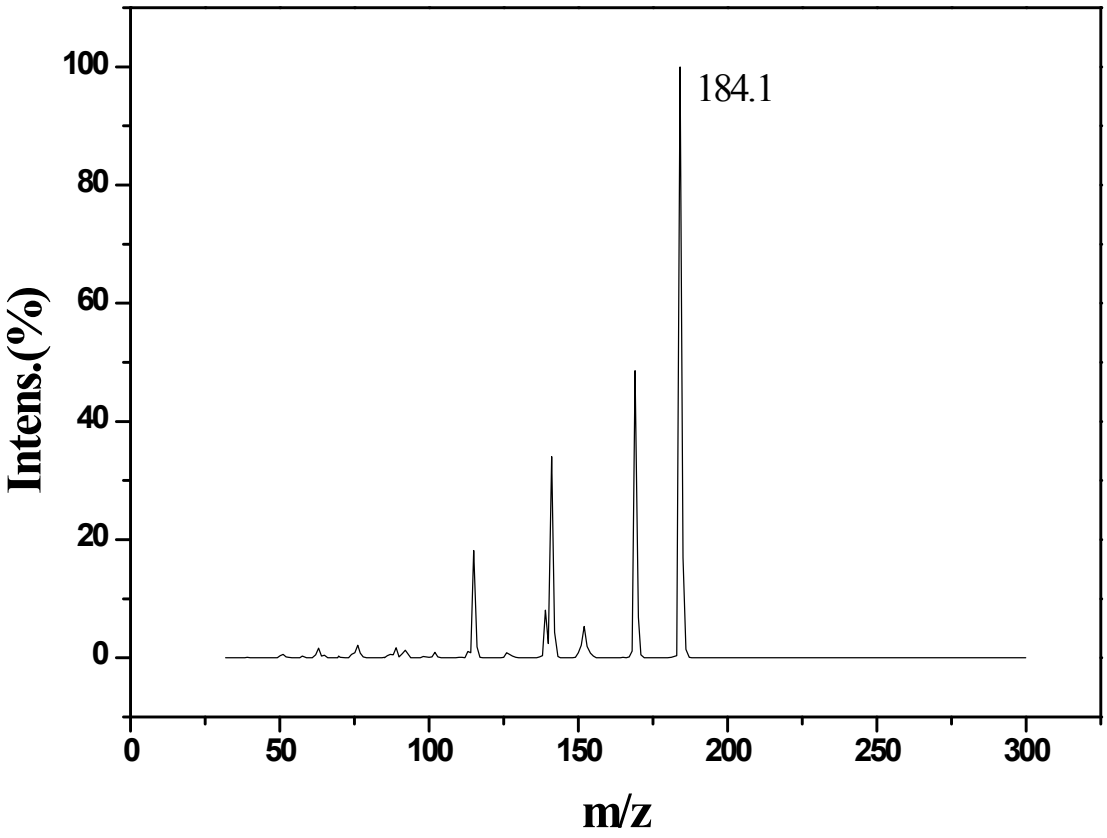

Figure S13-C: mass spectrum of 4-Methoxy-1,1-Biphenyl