

**A novel Palladium-2-picolyamine Complex Grafted on Magnetic UiO-66-NH₂
nanocomposites: As an efficient Heterogeneous catalyst for Fast Suzuki–
Miyaura Cross-Coupling**

Parastoo Nasri ^a, Masoomeh Norouzi ^{a,*}

^a *Department of Chemistry, Faculty of Science, Ilam University, P.O. Box 69315516, Ilam, Iran.*

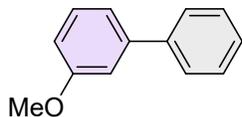
* Correspondence to: (M. Norouzi), Ilam University, Ilam, Iran, E-mail: m.norouzi@ilam.ac.ir

General

All solvents and chemical reagents were obtained from Merck Chemical Company and used without further purification. ¹H NMR and ¹³C NMR spectra were recorded on a Bruker spectrometer in CDCl₃-d₆. Chemical shifts (δ) are presented in parts per million (ppm), while coupling constants (*J*) are expressed in Hertz (Hz). The following standard abbreviations were employed to describe the multiplicity of the signals: s = singlet, d = doublet, t = triplet, q = or quartet, m = multiplet, and br = broad signals.

Spectral Data:

3-Methoxybiphenyl



Yield = 93%; $^1\text{H NMR}$ (250 MHz, $\text{CDCl}_3\text{-d}_6$), δ (ppm): 7.73 (s, 2 H), 7.57–7.46 (m, 4 H), 7.33–7.29 (d, $J = 8.4$ Hz, 2H), 7.04 (s, 1H), 3.94 (s, 3 H). $^{13}\text{C NMR}$ (63 MHz, CDCl_3) δ : 160.09, 142.87, 141.21, 129.91, 128.89, 127.56, 127.33, 119.79, 113.02, 112.78, 55.33.

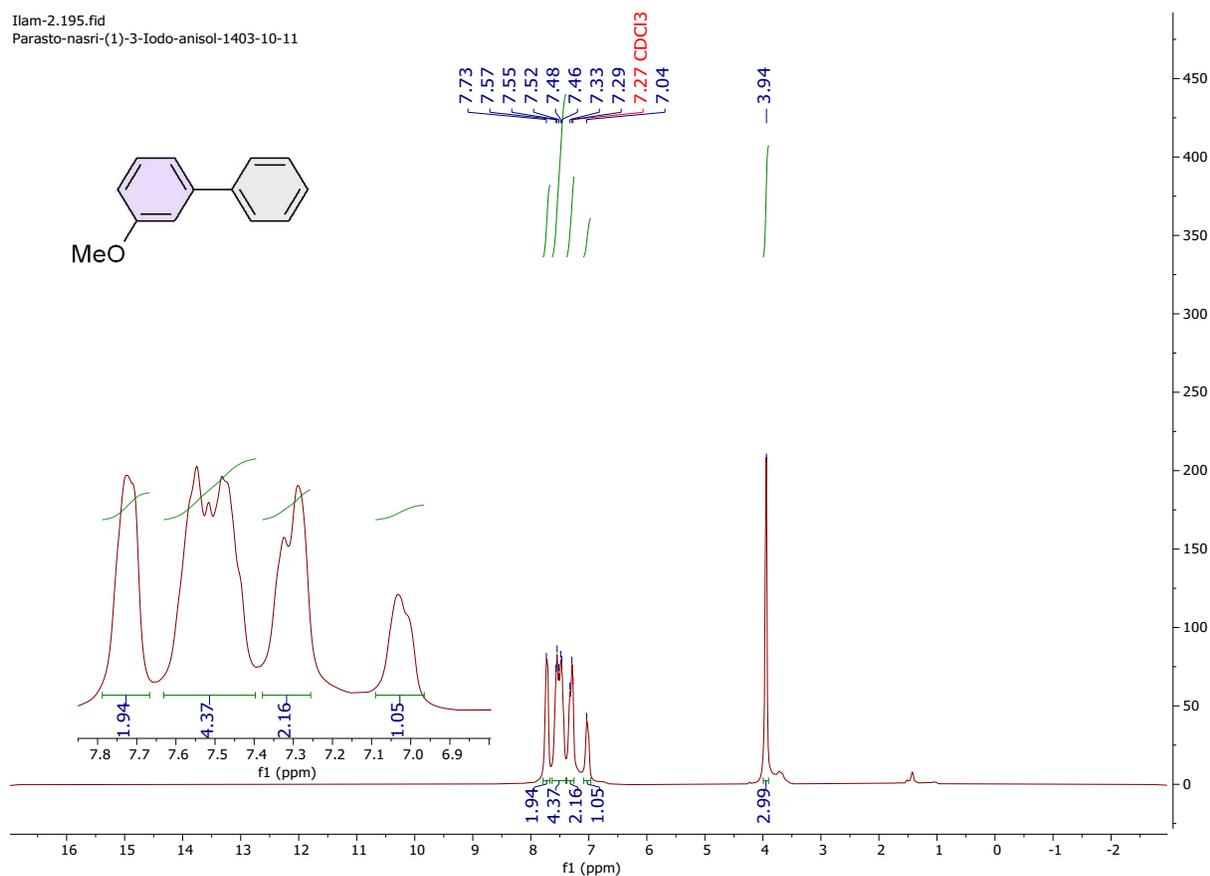


Figure S1. $^1\text{H NMR}$ spectrum of 3-Methoxybiphenyl

Ilam-2.196.fid

Parasto-nasri-(1)-3-Iodo-anisol-1403-10-11

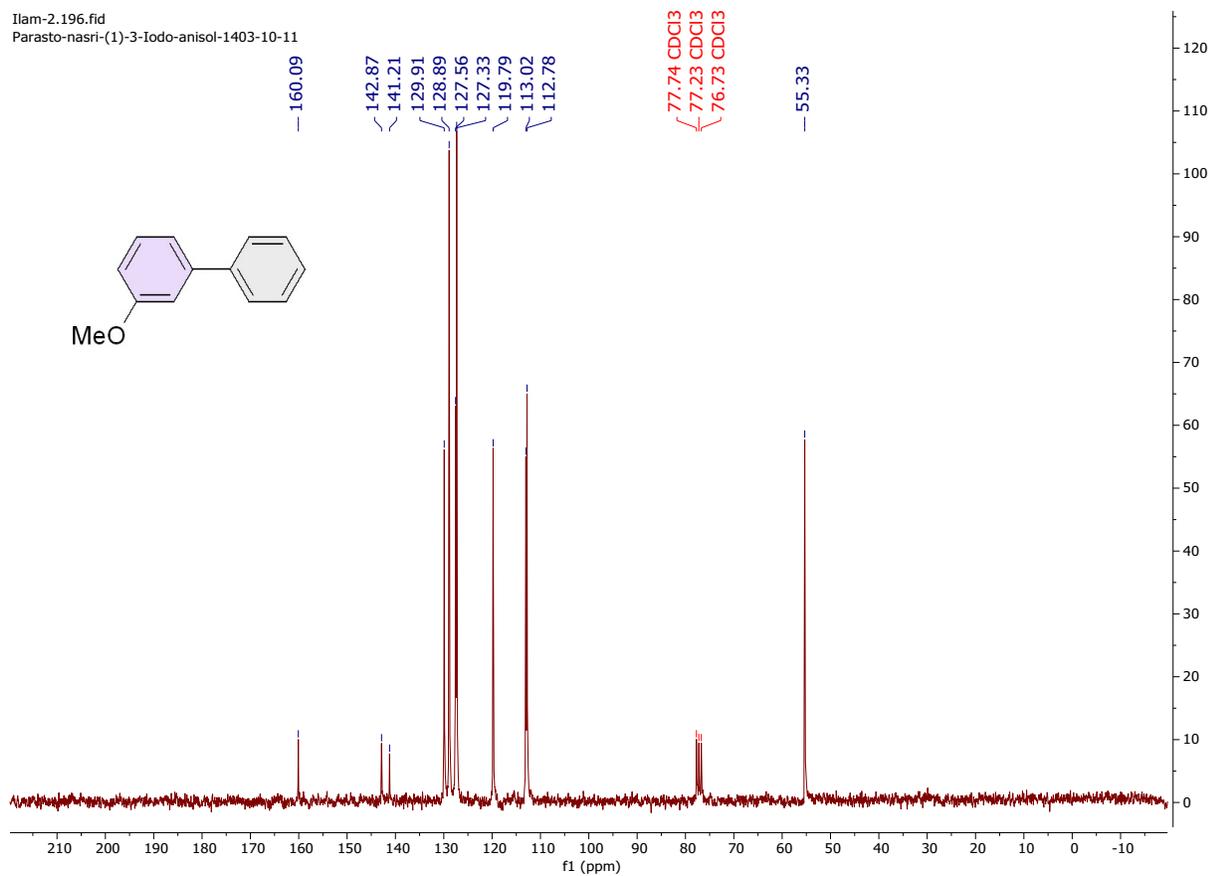
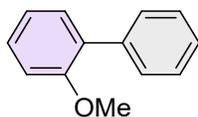


Figure S2. ^{13}C NMR spectrum of 3-Methoxybiphenyl

2-Methoxybiphenyl



Yield = 94%; $^1\text{H NMR}$ (250 MHz, $\text{CDCl}_3\text{-d}_6$), δ (ppm): 7.63-7.7.60 (d, $J = 7.8$ Hz, 2H), 7.56 – 7.52-7.39 (m, 4H), 7.13-7.03 (q, $J = 8.1$ Hz, 2H), 3.86 (s, 3H). $^{13}\text{C NMR}$ (63 MHz, CDCl_3) δ 156.50, 138.60, 130.95, 130.75, 129.61, 128.68, 128.05, 126.98, 120.88, 111.25, 55.57.

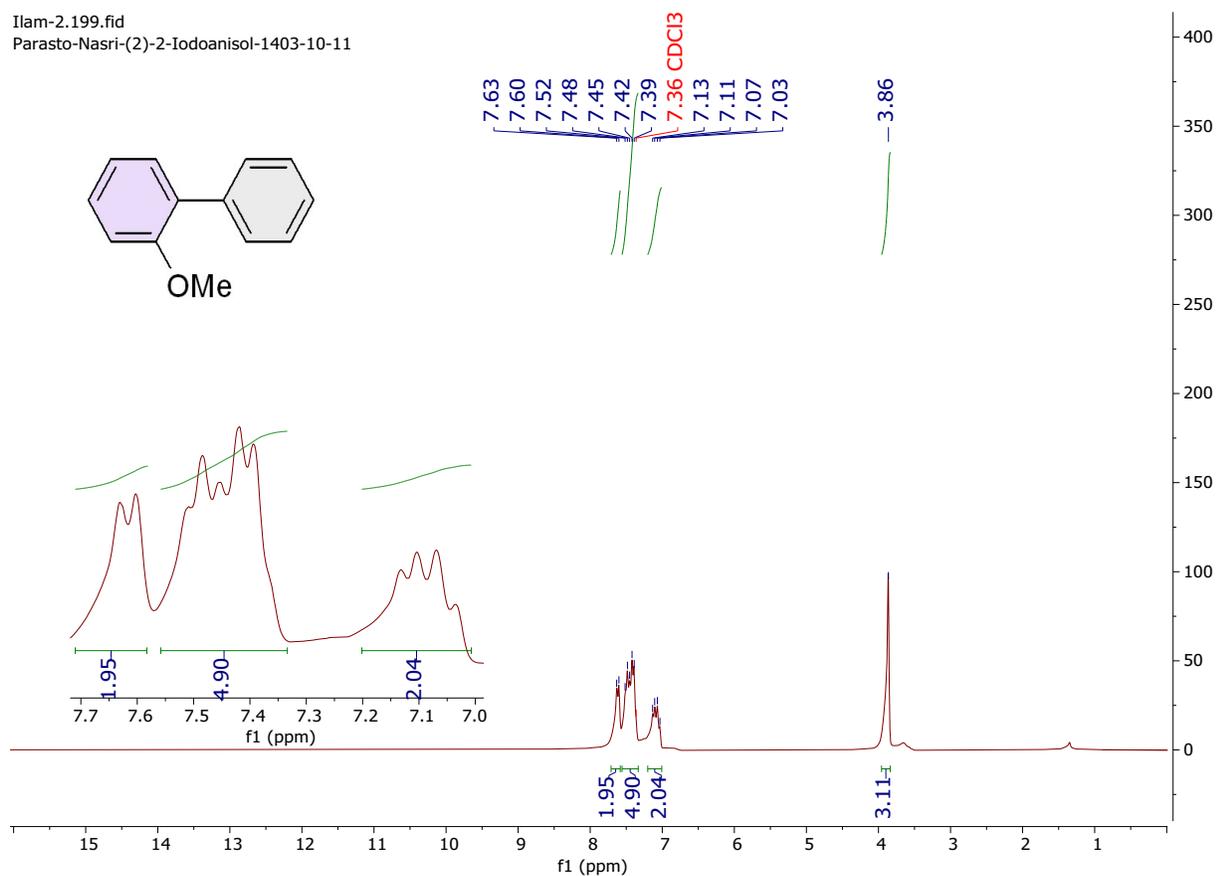


Figure S3. $^1\text{H NMR}$ spectrum of 2-Methoxybiphenyl

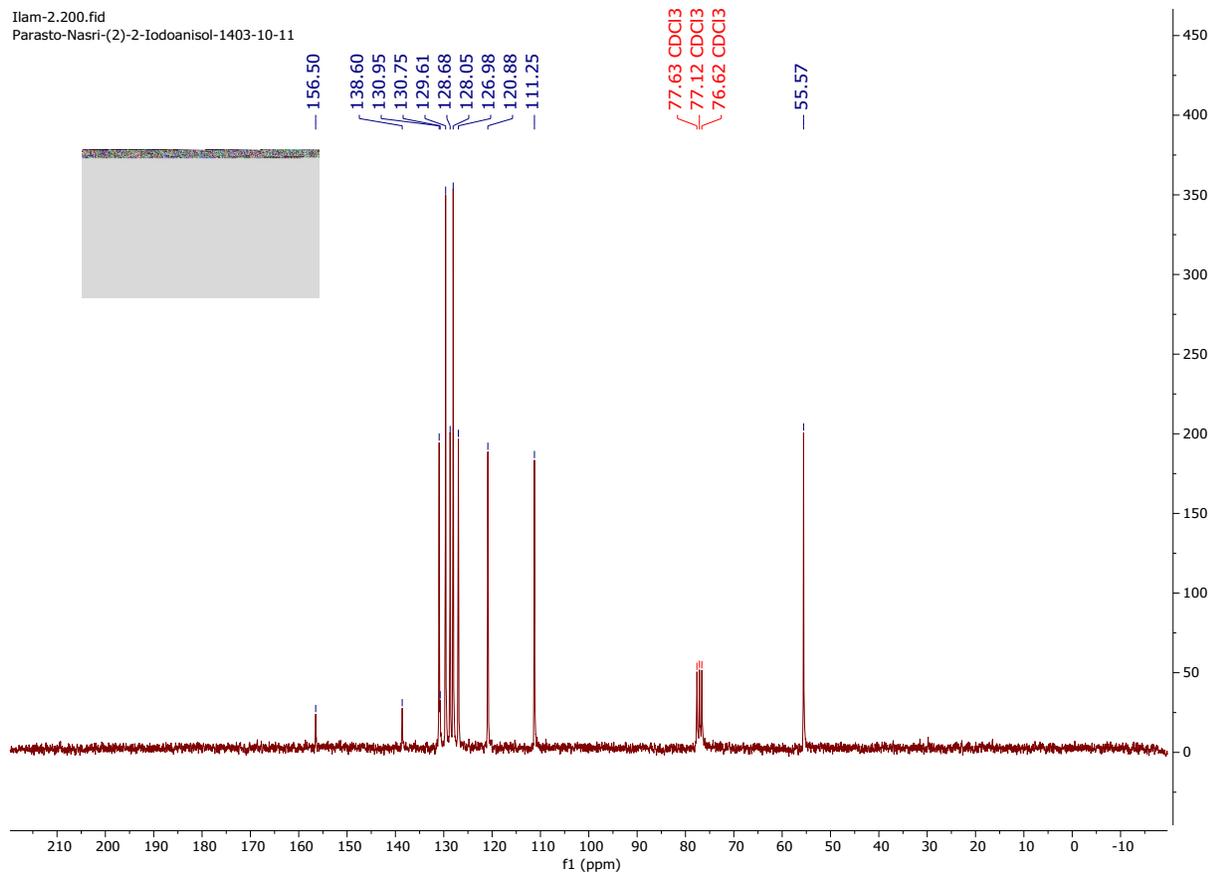
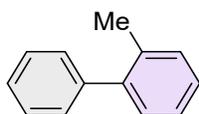


Figure S4. ^{13}C NMR spectrum of 2-Methoxybiphenyl

2-Methylbiphenyl



Yield = 94%; ^1H NMR (250 MHz, $\text{CDCl}_3\text{-d}_6$), δ (ppm): 7.43 – 7.25 (m, 9H), 2.29 (s, 3H). ^{13}C NMR (63 MHz, CDCl_3) δ 141.94, 135.35, 130.30, 129.79, 129.19, 128.06, 127.24, 126.76, 125.75, 20.48.

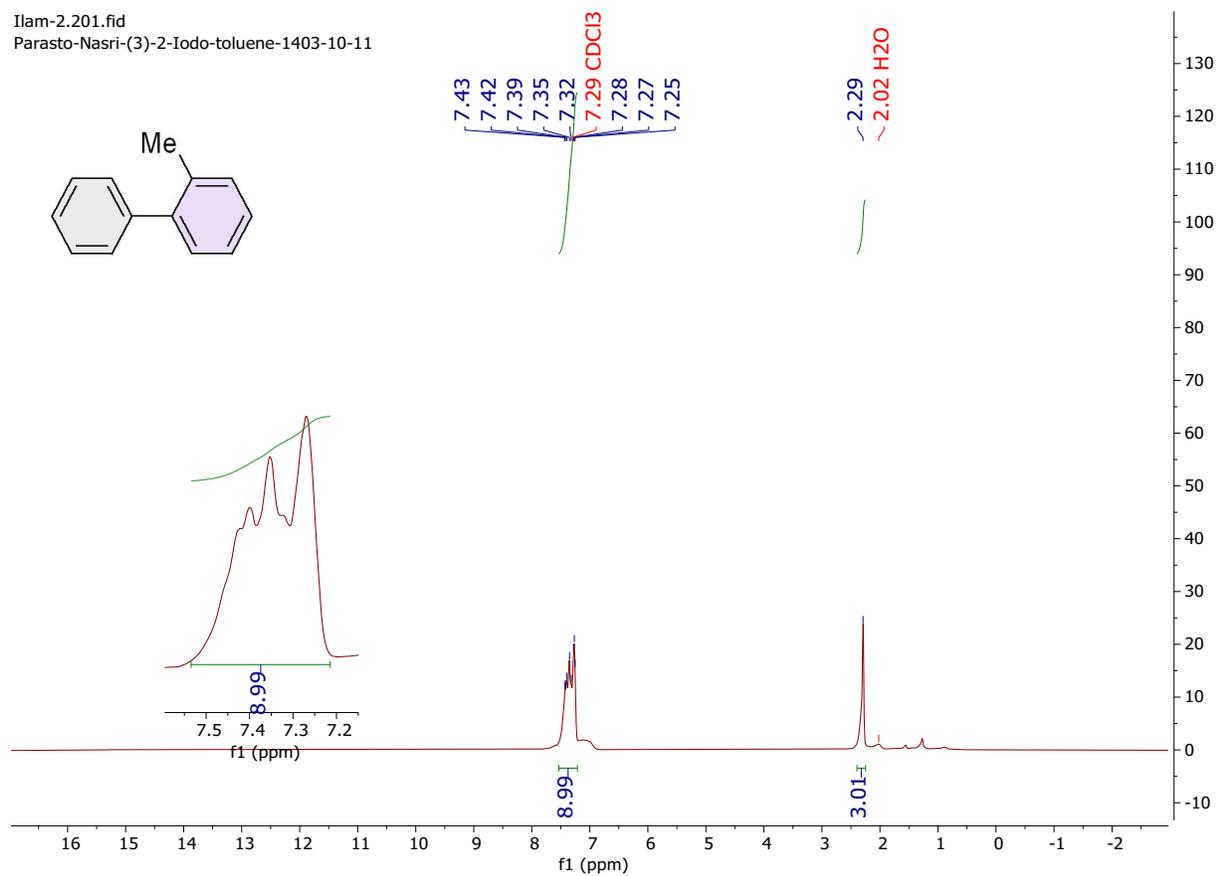


Figure S5. ^1H NMR spectrum of 2-Methylbiphenyl

Ilam-2.202.fid
Parasto-Nasri-(3)-2-Iodo-toluene-1403-10-11

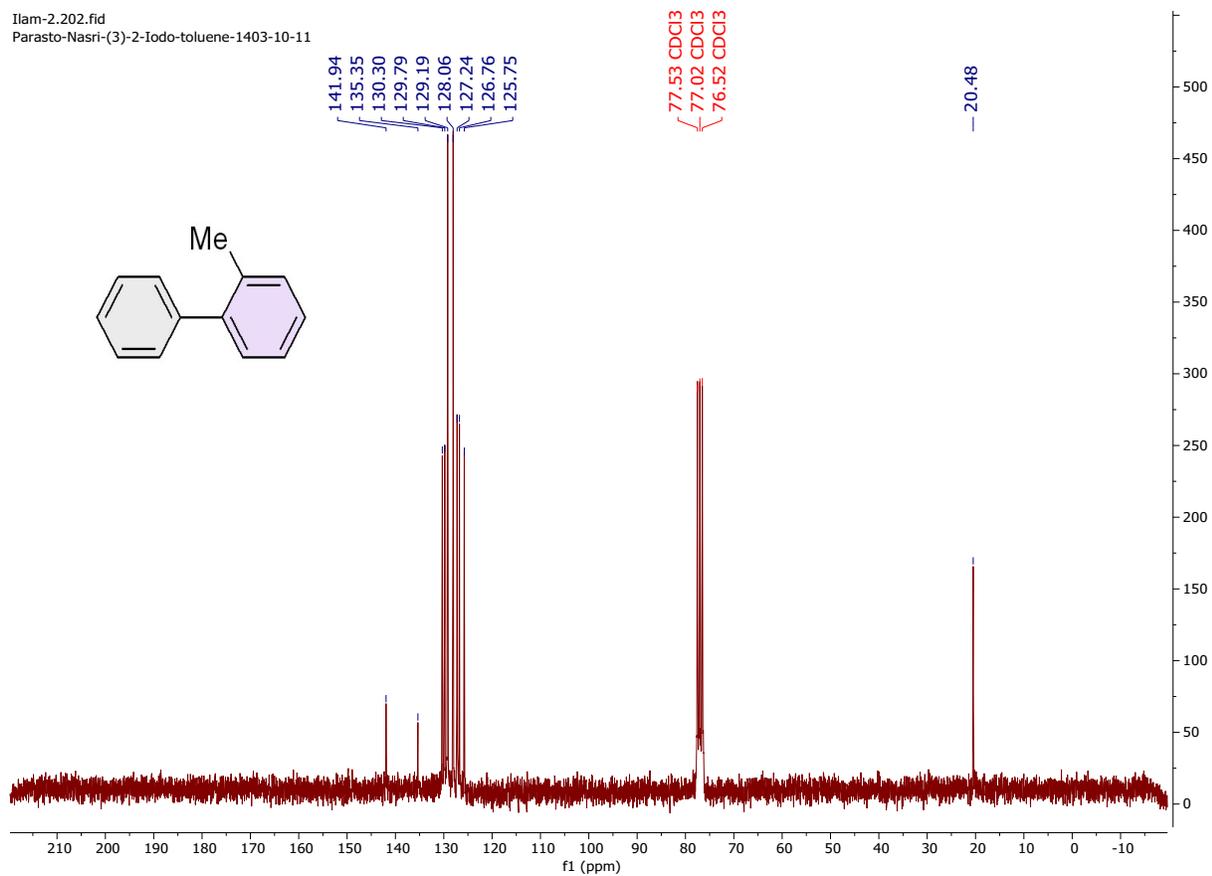
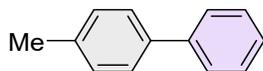


Figure S6. ¹³CNMR spectrum of 2-Methylbiphenyl

4-Methylbiphenyl



Yield = 96%; $^1\text{H NMR}$ (250 MHz, $\text{CDCl}_3\text{-d}_6$), δ (ppm): 7.70-7.62 (d, $J = 8.3$ Hz, 2H), 7.68-7.52 (d, $J = 8.1$ Hz, 2H), 7.49 – 7.36 (m, 5H), 2.49 (s, 3H). $^{13}\text{C NMR}$ (63 MHz, CDCl_3) δ 141.24, 138.44, 137.10, 129.59, 128.82, 127.10, 127.07, 21.21.

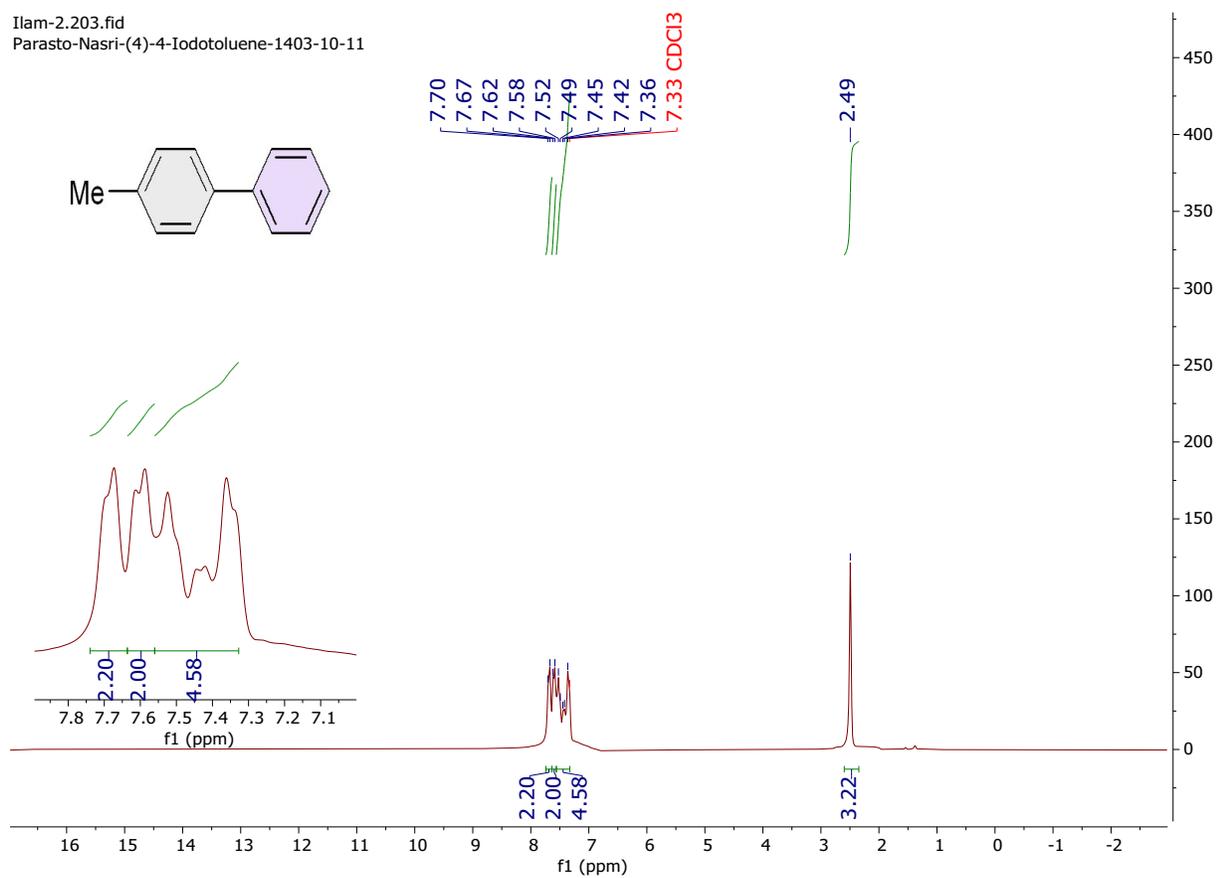


Figure S7. $^1\text{H NMR}$ spectrum of 4-Methylbiphenyl

Ilam-2.204.fid
Parasto-Nasri-(4)-4-Iodotoluene-1403-10-11

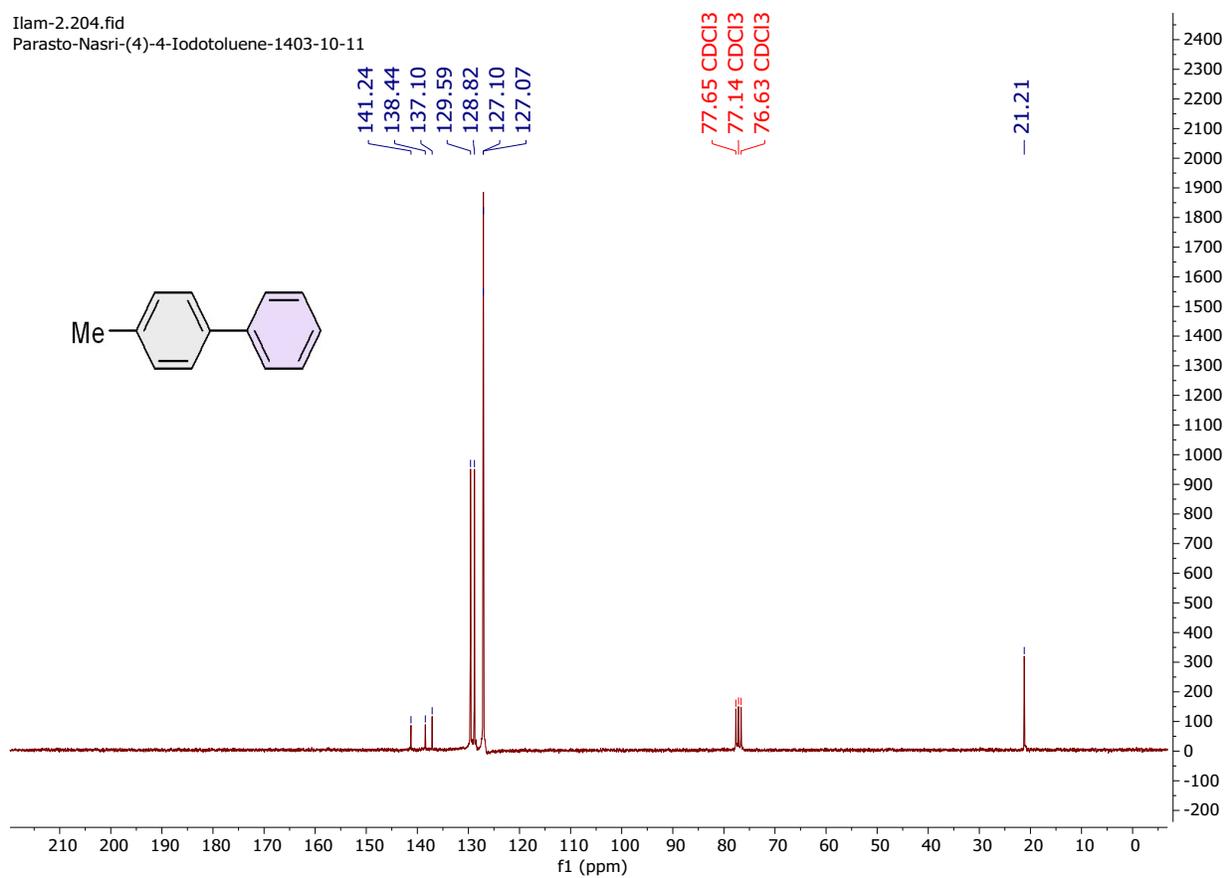
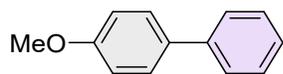


Figure S8. ¹³CNMR spectrum of 4-Methylbiphenyl

4-Methoxybiphenyl



Yield = 95%; $^1\text{H NMR}$ (250 MHz, CDCl_3) δ 7.61 (t, $J = 7.4$ Hz, 4H), 7.48 (t, $J = 7.6$ Hz, 2H), 7.38 (d, $J = 7.5$ Hz, 1H), 7.04 (d, $J = 8.6$ Hz, 2H), 3.89 (s, 3H).. $^{13}\text{C NMR}$ (63 MHz, CDCl_3) δ 159.18, 140.86, 133.78, 128.79, 128.20, 126.79, 126.72, 114.24, 55.36.

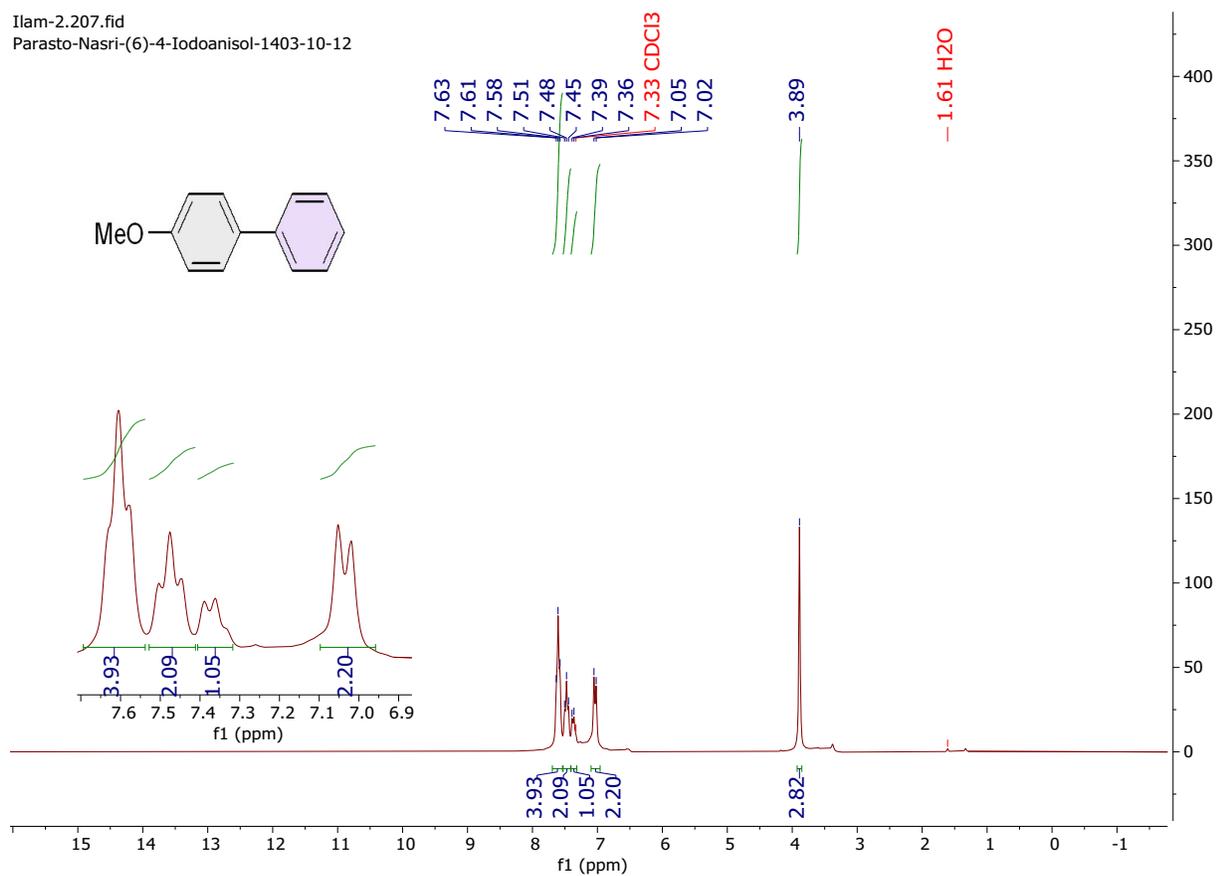


Figure S9. $^1\text{H NMR}$ spectrum of 4-Methoxybiphenyl

Ilam-2.208.fid
Parasto-Nasri-(6)-4-Iodoanisol-1403-10-12

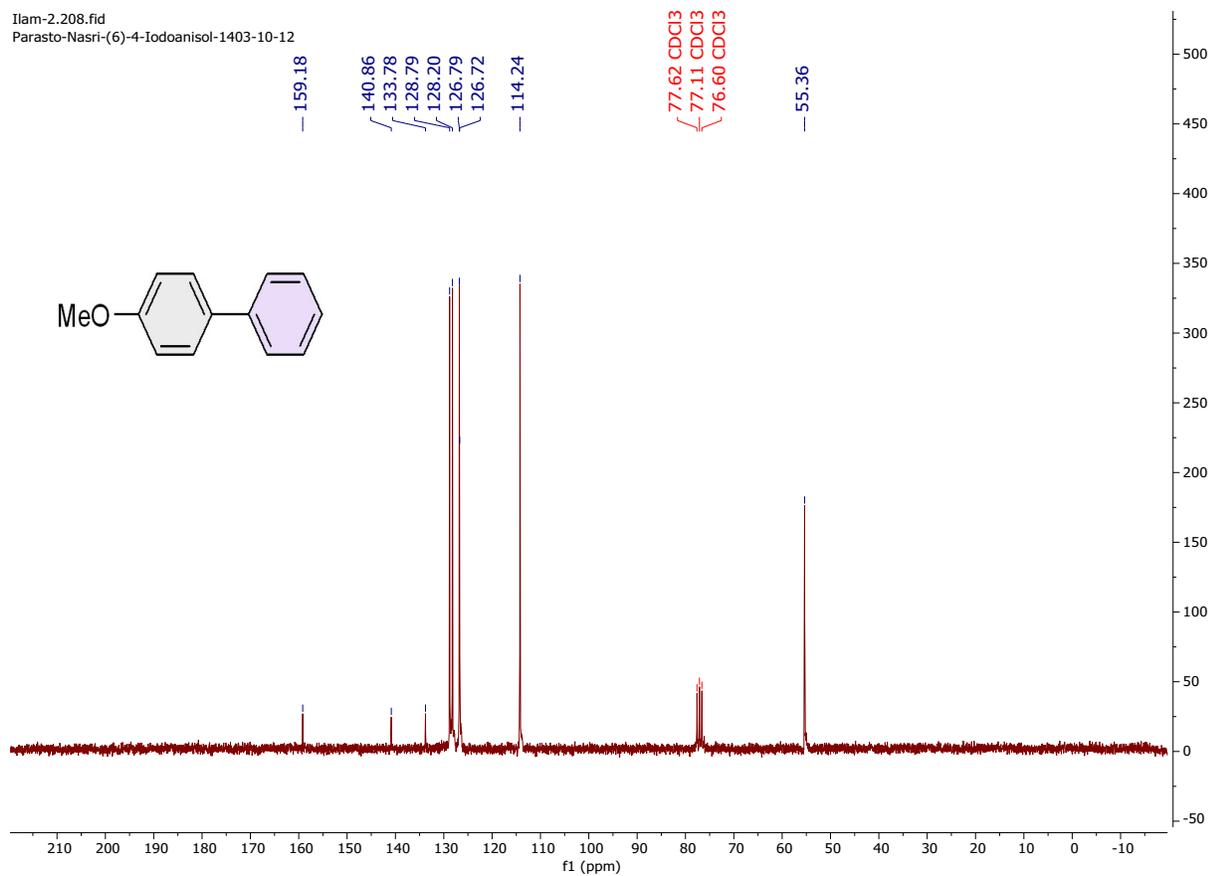
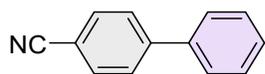


Figure S10. ¹³CNMR spectrum of 4-Methoxybiphenyl

Biphenyl-4-carbonitrile:



Yield = 98%, ^1H NMR (250 MHz, DMSO) δ 7.86 (d, $J = 6.0$ Hz, 4H), 7.71 (d, $J = 7.8$ Hz, 2H), 7.47 (d, $J = 7.6$ Hz, 3H). ^{13}C NMR (63 MHz, DMSO) δ 145.07, 138.69, 133.28, 129.61, 129.20, 128.00, 127.52, 119.32, 110.49.

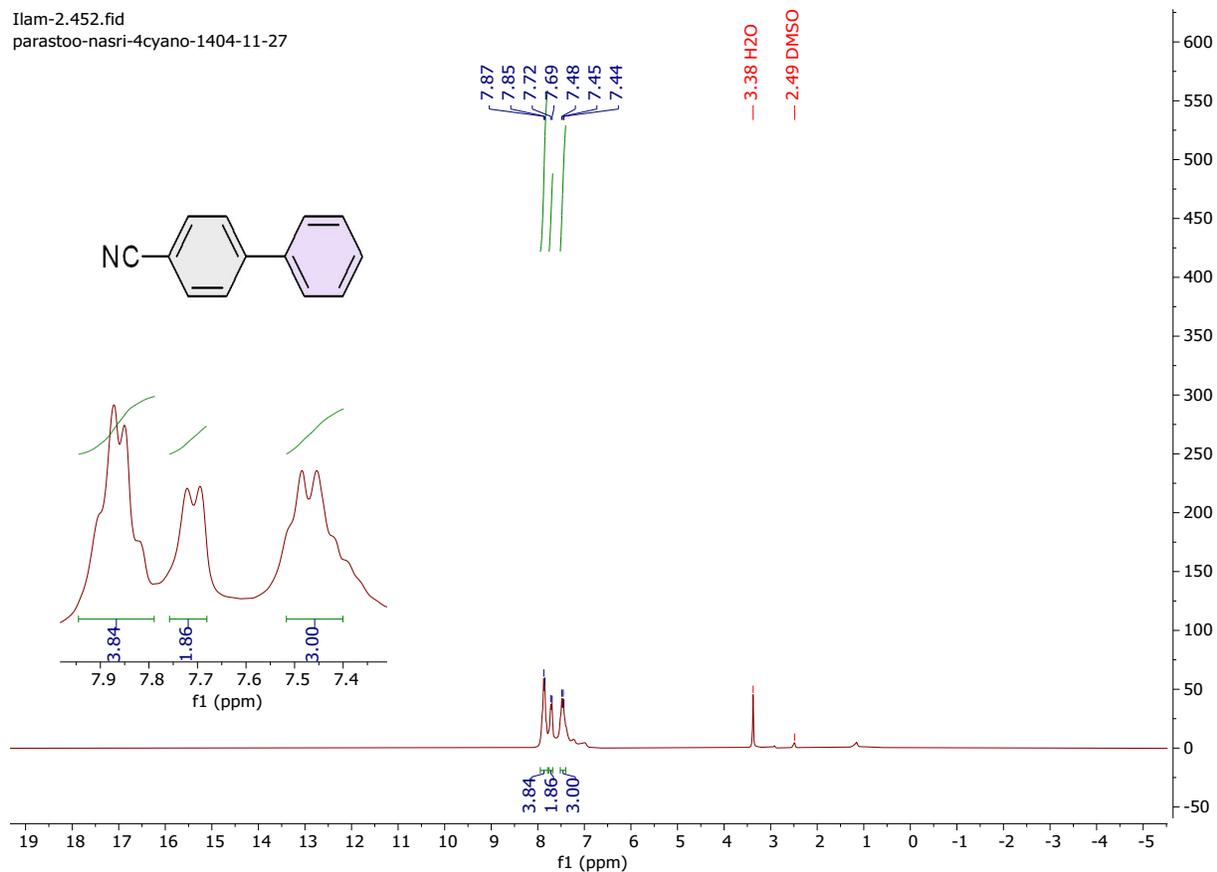


Figure S11. ^1H NMR spectrum of Biphenyl-4-carbonitrile

Ilam-2.453.fid
parasto-nasri-4-cyano-1404-11-27

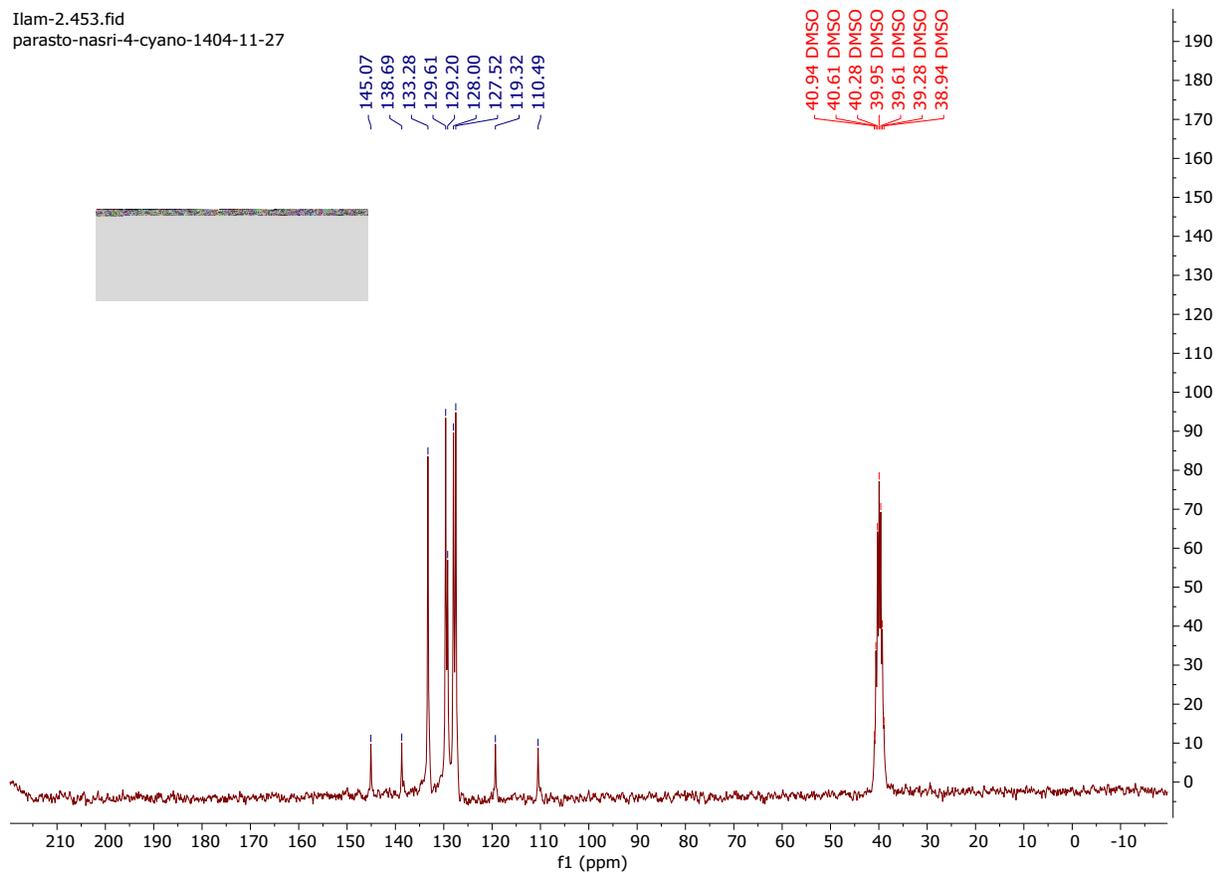


Figure S12. ^{13}C NMR spectrum of Biphenyl-4-carbonitrile

Biphenyl:



Yield = 98%, $^1\text{H NMR}$ (250 MHz, DMSO) δ 7.69 – 7.59 (m, 4H), 7.45 (t, $J = 7.5$ Hz, 4H), 7.36 (d, $J = 7.4$ Hz, 2H).

