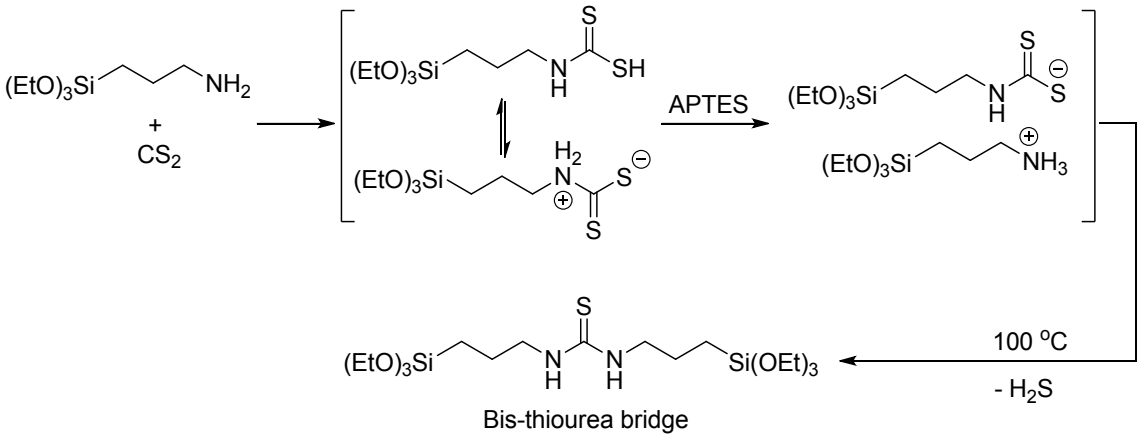


Figure S1 Procedure for synthesis of the bis-thiourea bridge.

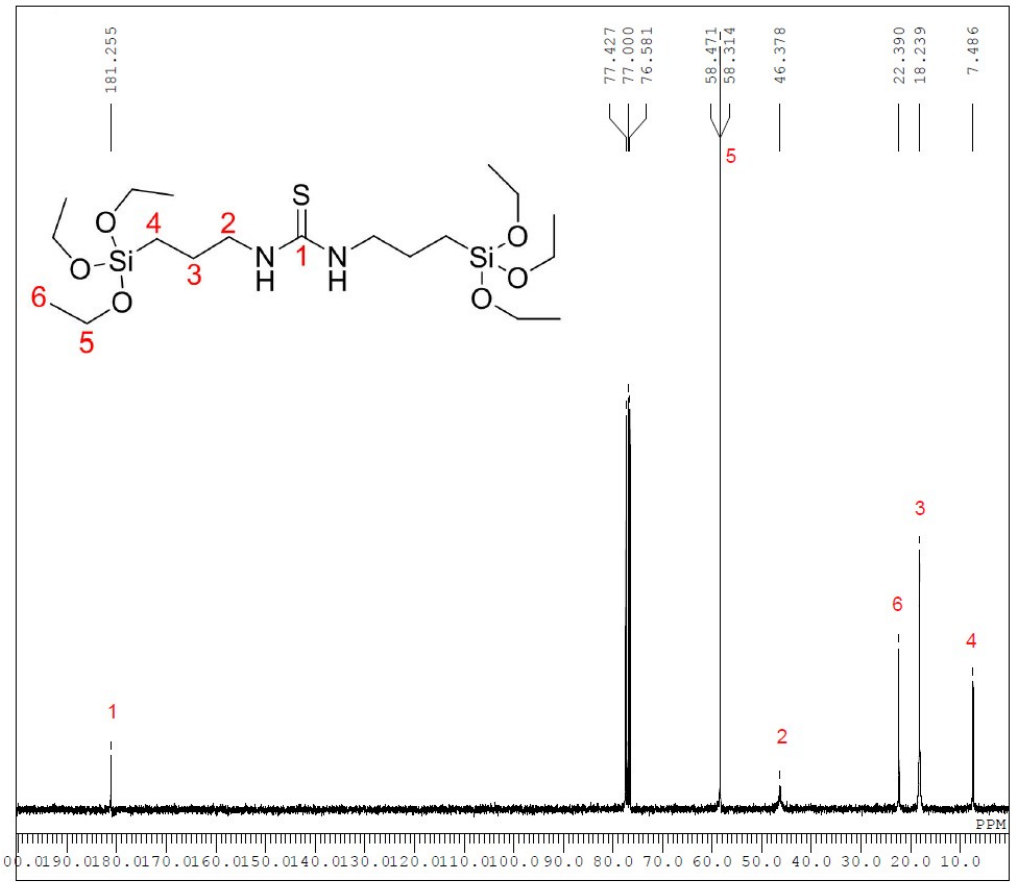


Figure S2 ^{13}C-NMR of the synthesized bis-thiourea bridge.

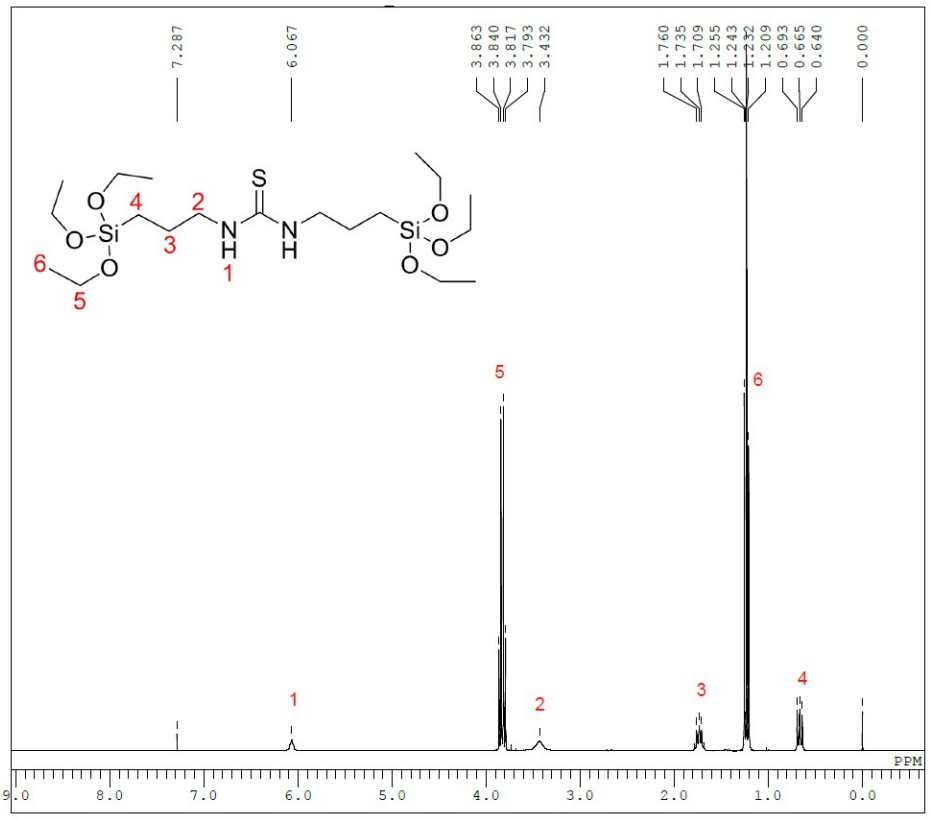


Figure S3 ^{1}H-NMR of the synthesized bis-thiourea bridge.

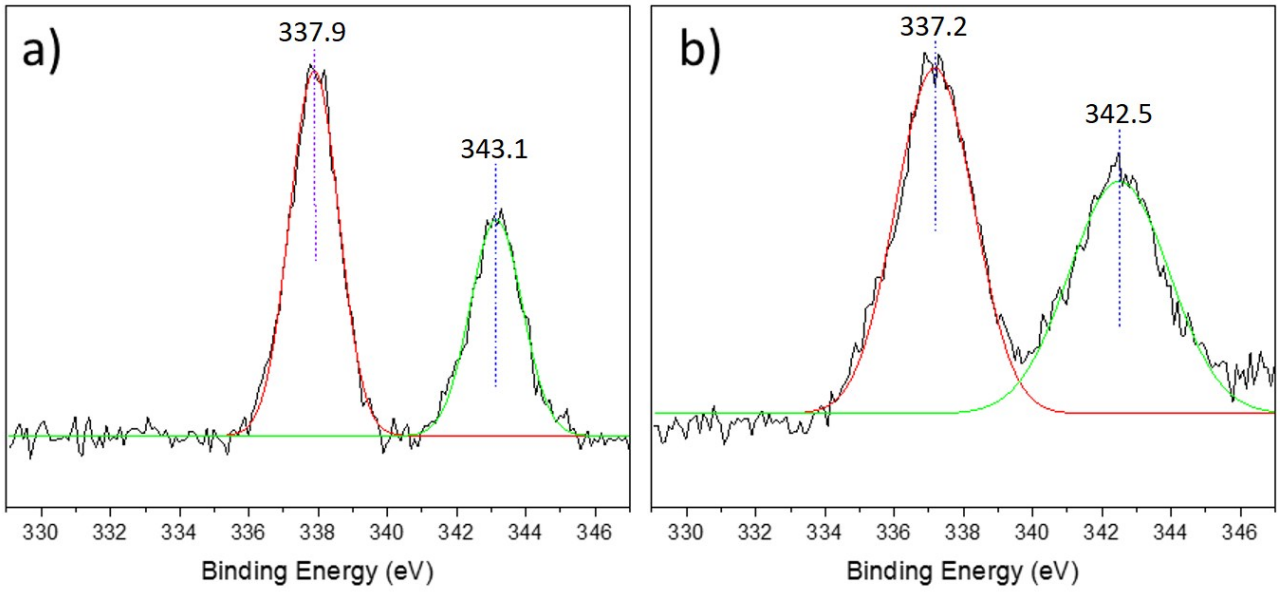


Figure S4 XPS spectra of (a) Pd^{2+}@TU-PMO and (b) Pd@TU-PMO after reduction with $NaBH_4$.

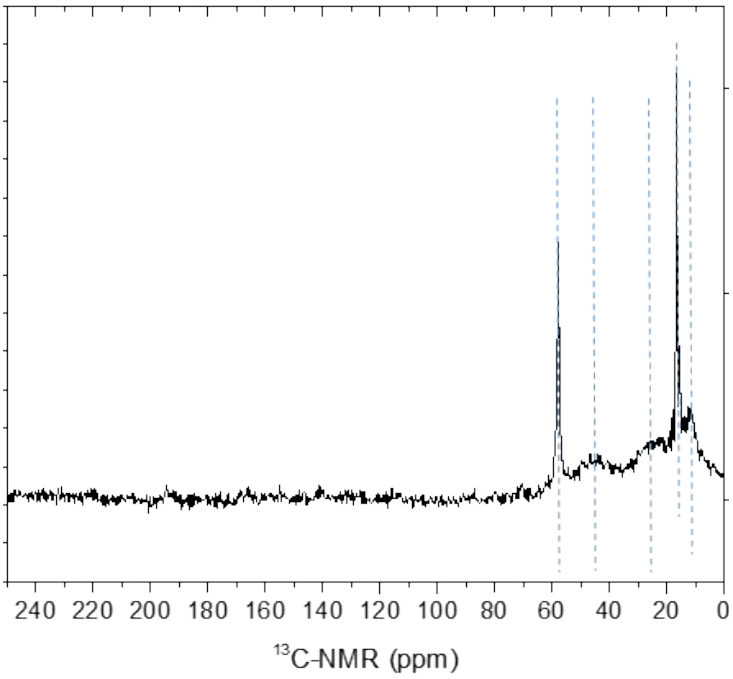


Figure S5 Solid state ^{13}C-NMR spectrum of TU-PMO. The peaks at 11.6, 16.8, 25.4, 45.0, and 57.9 ppm can be assigned to the organic structure of bis-thiourea which is preserved after embedment in TU-PMO structure.

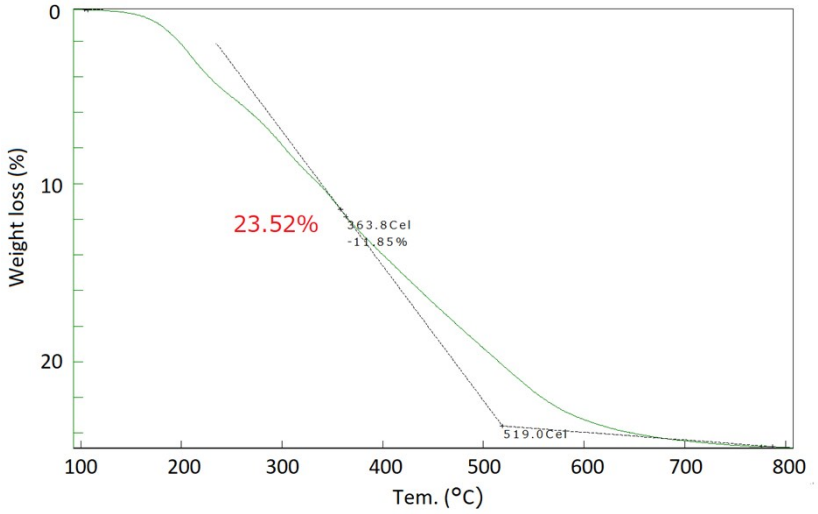


Figure S6 TGA of TU-PMO.

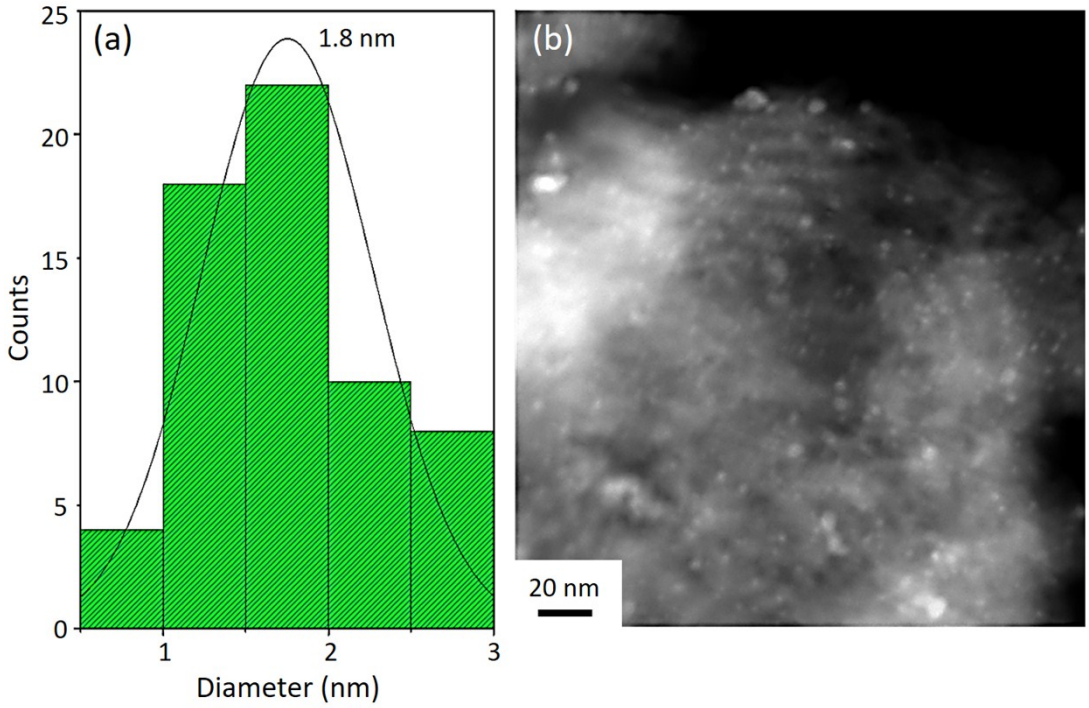


Figure S7 (a) Particle size distribution of Pd nanoparticles in TU-PMO and (b) HADDF-STEM image.

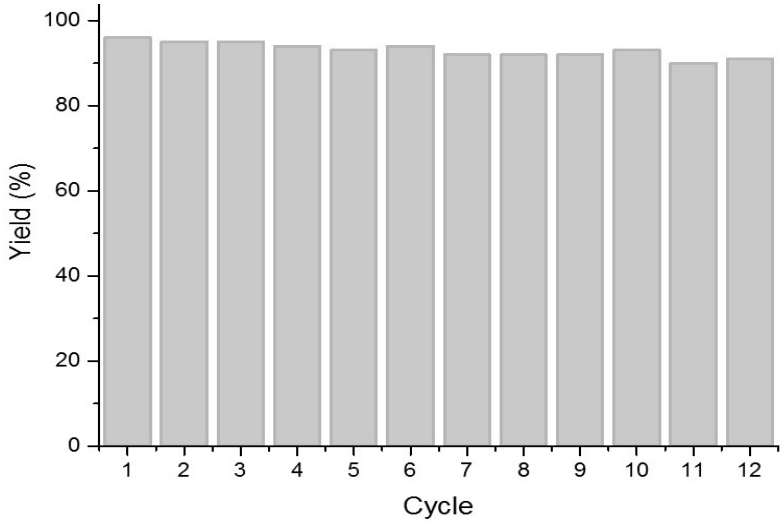


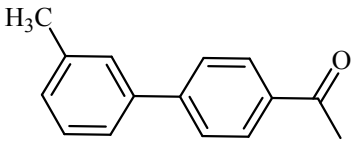
Figure S8 Recyclability of Pd@TU-PMO catalyst in Suzuki-Miyaura coupling reaction of 4-bromoacetophenone and phenylboronic acid over 12 consecutive cycles.

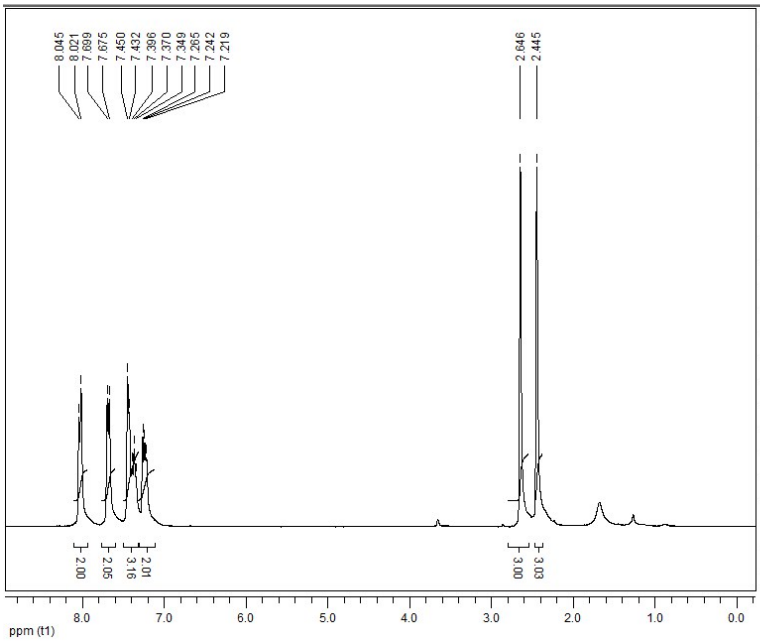
Table S1

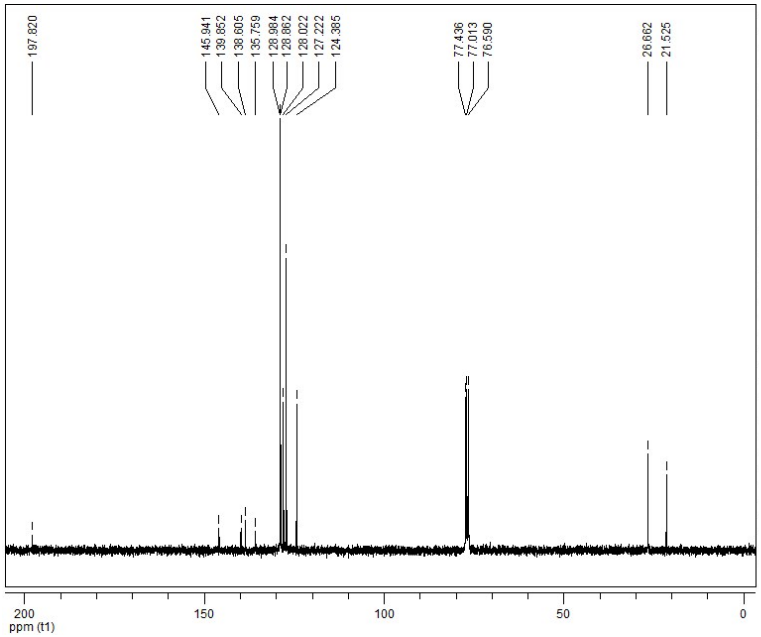
Sample	Pore diameter (nm)	Surface area ($m^2 g^{-1}$)	Vp ($cm^3 g^{-1}$)
TU-PMO	6.18	410	1.22
Pd@TU-PMO	6.18	405	1.11

Appendix:

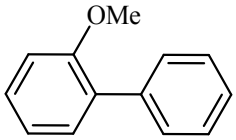
1-(3'-methyl-[1,1'-biphenyl]-4-yl)ethanone (Entry 11, 16, and 19):[R1] ^{1}H NMR (300 MHz, $CDCl_3$): δ =2.45 (s, 3 H), 2.65 (s, 3 H), 7.22-8.04 (m, 8 H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 197.8, 145.9, 139.8, 138.6, 135.9, 129.0, 128.9, 128.0, 127.2, 124.4, 26.7, 21.5.

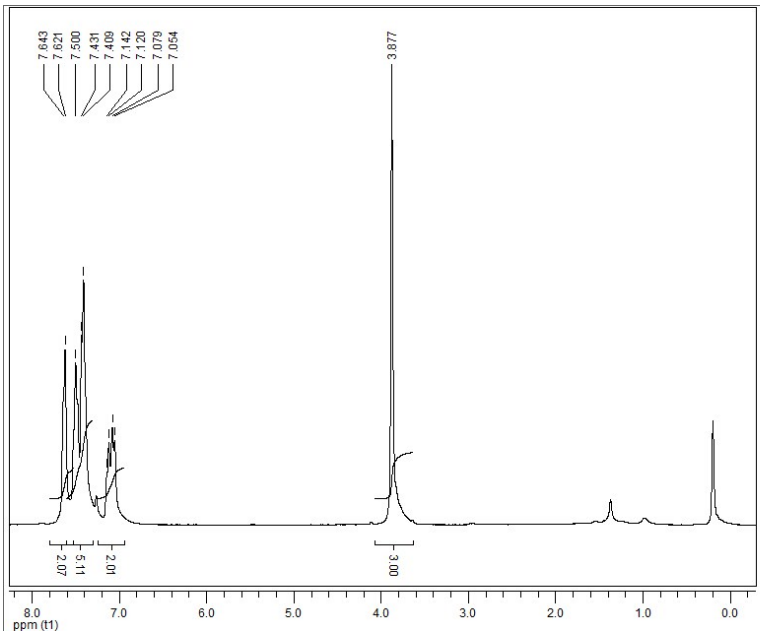


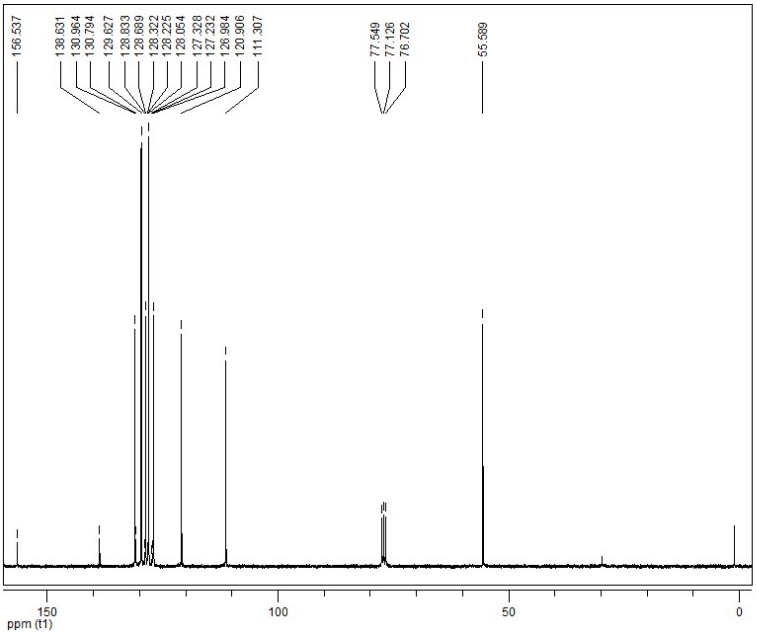




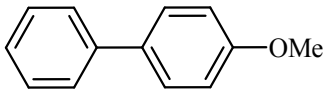
2-Methoxylbiphenyl (Entry 5):[R1] White solid, mp: 89-91 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.57-7.61 (m, 4 H), 7.44-7.48 (m, 2 H), 7.32-7.37 (m, 1 H), 7.01-7.04 (m, 2 H), 3.88 (s, 3 H); ^{13}CNMR (75 MHz, $CDCl_3$): δ = 159.2, 140.9, 133.8, 128.7, 128.2, 126.8, 126.7, 114.2, 55.3.

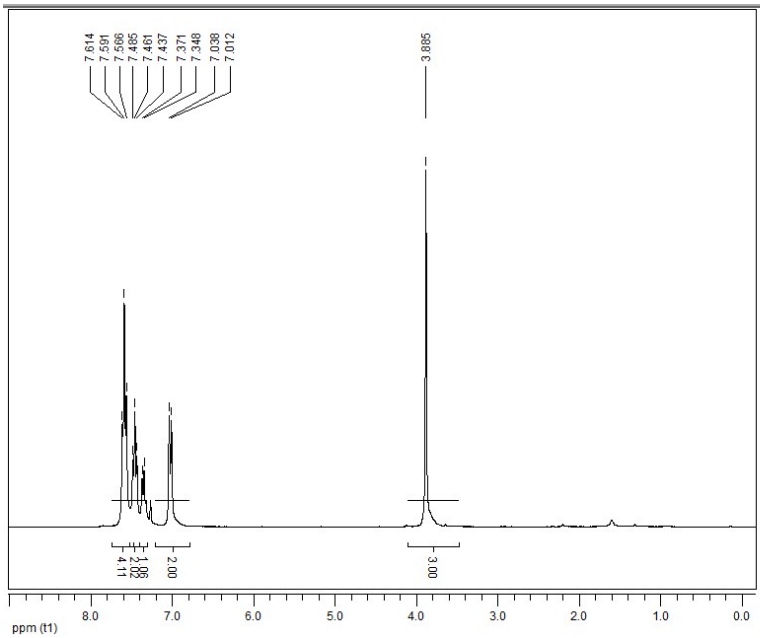


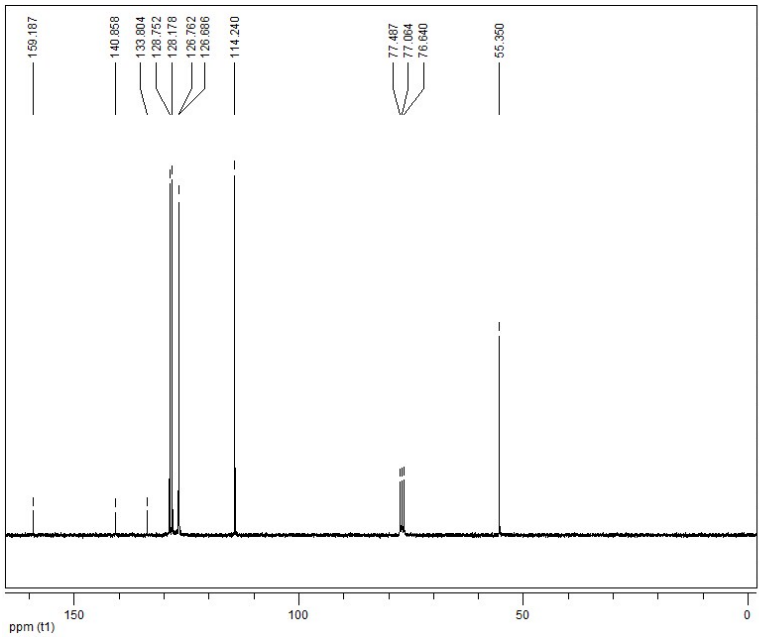




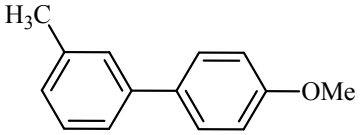
4-Methoxybiphenyl (Entry 7):[R2] White solid, mp: 89-91 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.57-7.61 (m, 4 H), 7.44-7.48 (m, 2 H), 7.32-7.37 (m, 1 H), 7.01-7.04 (m, 2 H), 3.88 (s, 3 H); ^{13}CNMR (75 MHz, $CDCl_3$): δ = 159.2, 140.9, 133.8, 128.7, 128.2, 126.8, 126.7, 114.2, 55.3.

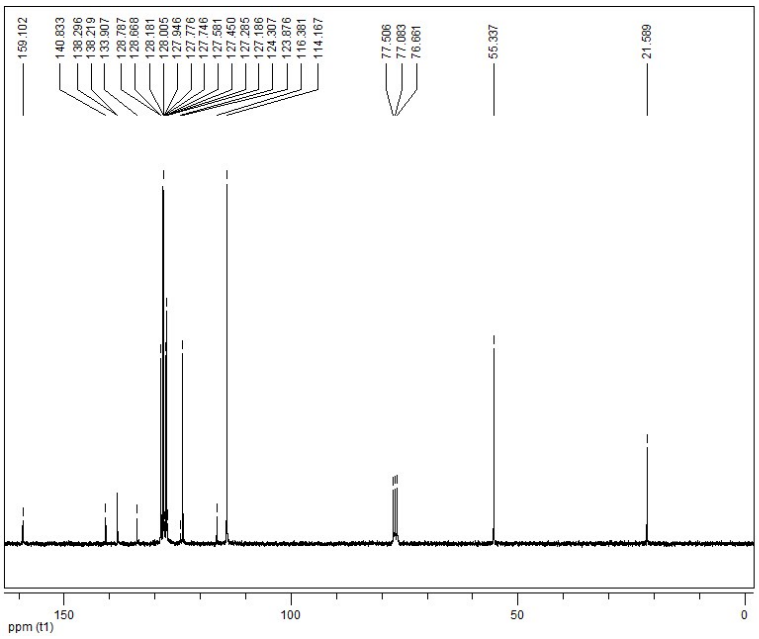


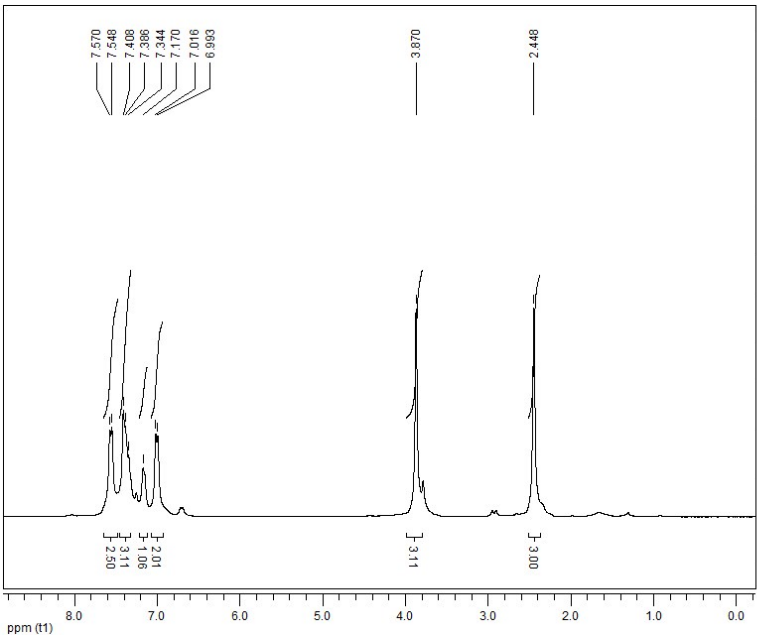




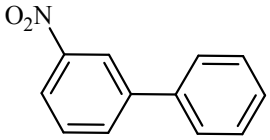
3-Methyl-4'-methoxy-biphenyl (Entry 9):[R3] Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 6.99-7.57 (m, 8 H), 3.87 (s, 3 H), 2.45 (s, 3 H). ^{13}C NMR (75MHz, $CDCl_3$): δ = 159.1, 140.8, 138.3, 133.9, 128.7, 128.2, 127.6, 127.4, 123.9, 114.2, 55.3, 21.6.

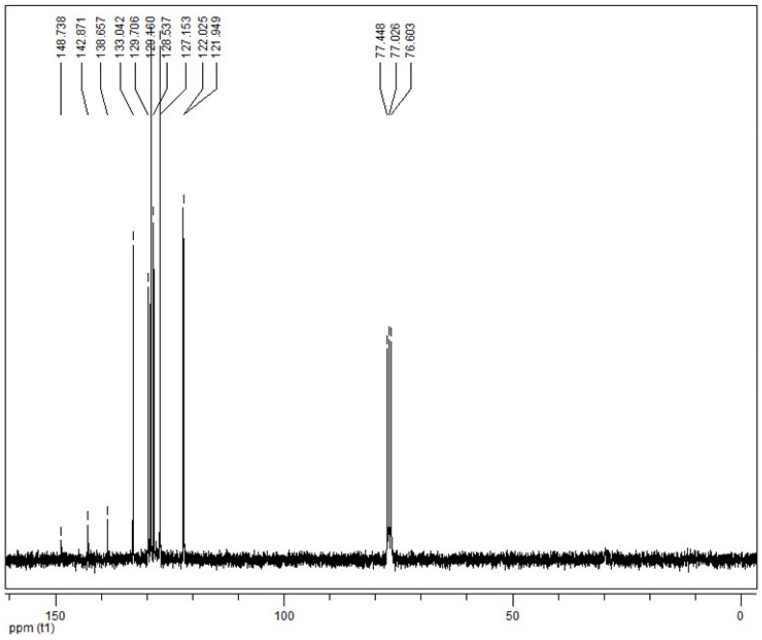




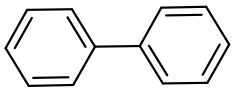


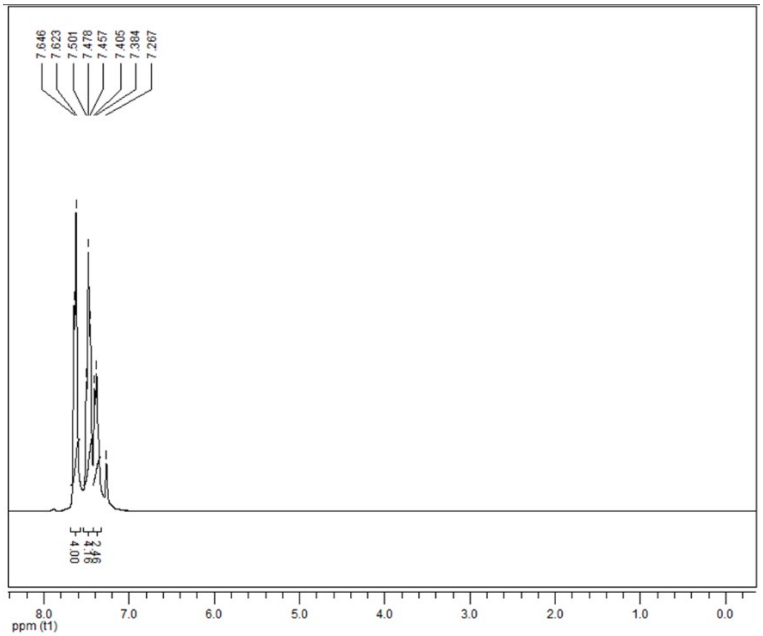
1-Nitro-3-phenylbenzene (Entry 8):[R3] ^{13}C NMR (75 MHz, $CDCl_3$): δ = 148.71, 142.85, 138.65, 133.03, 129.7, 129.2, 128.6, 127.2, 122.0, 121.9.

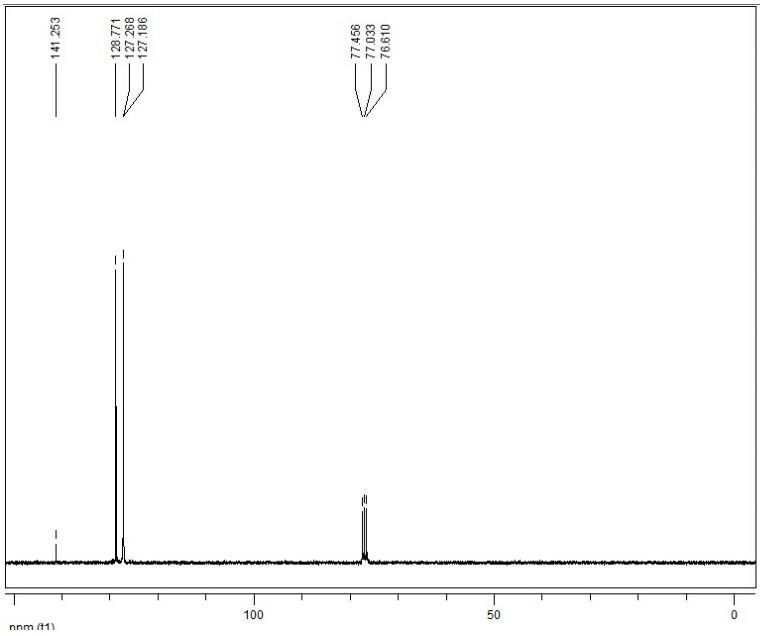




Biphenyl (Entry 1 and 12):[R2] White solid, mp: 45-47 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.28-7.63 (m, Ar-H, 9 H), 2.44 (s, CH_3, 3 H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 141.2, 138.4, 137.0, 129.5, 128.7, 127.2, 127.2, 127.0, 21.1.

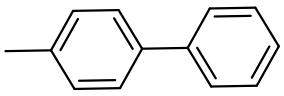


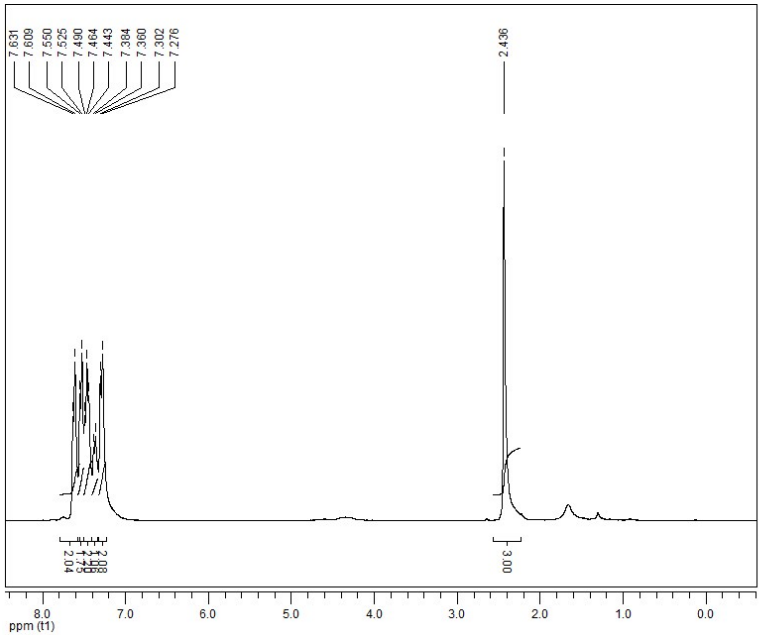


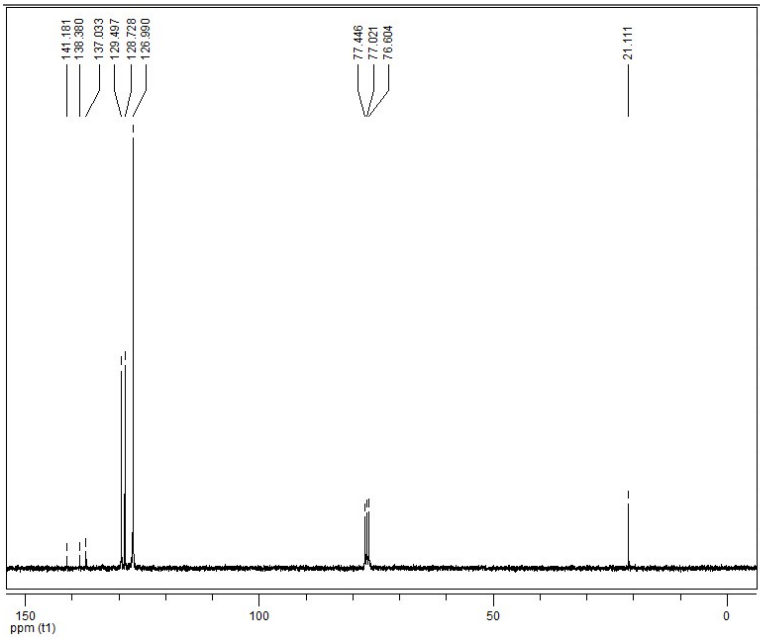


4-Methylbiphenyl (Entry 2 and 4):[R3]

White solid, mp: 45-47 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.28-7.63 (m, Ar-H, 9 H), 2.44 (s, CH_3, 3 H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 141.2, 138.4, 137.0, 129.5, 128.7, 127.23, 127.2, 127.0, 21.1.

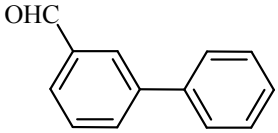


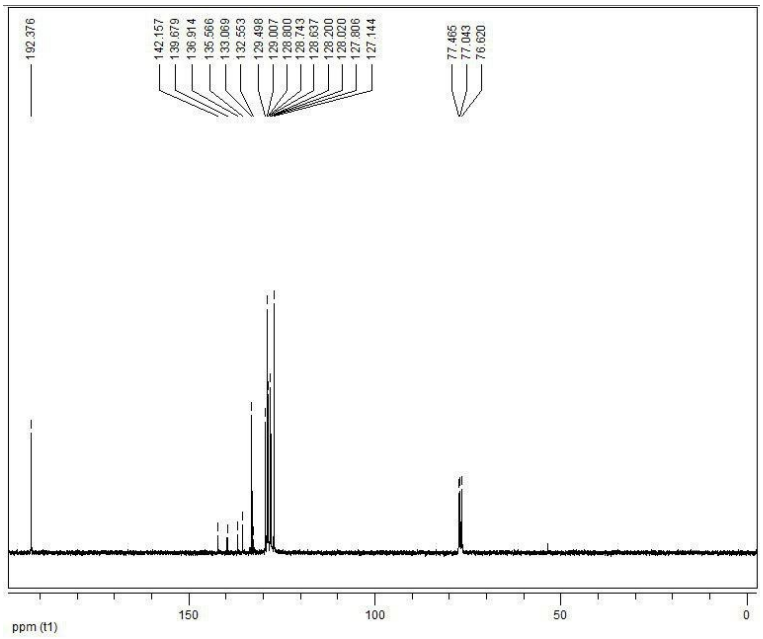


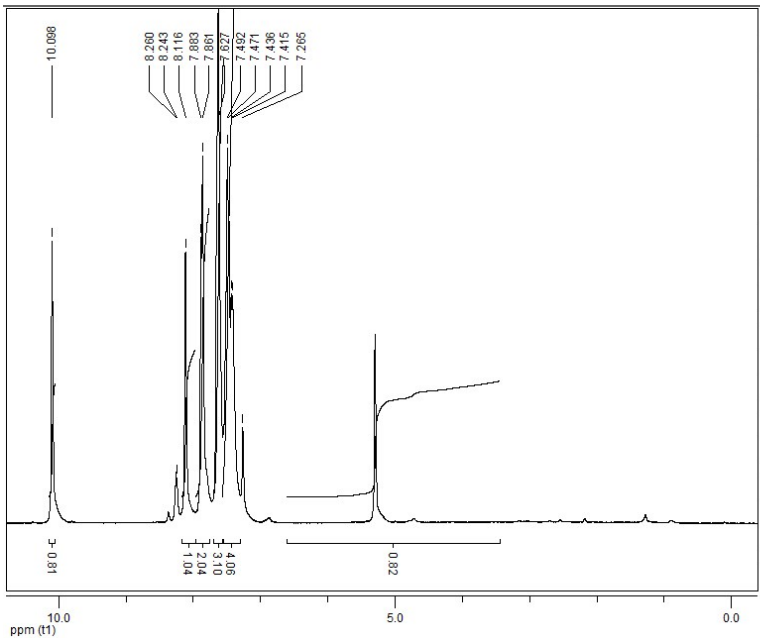


3-Phenylbenzaldehyde (Entry 13 and 18):[R3]

^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.26-8.12 (m, 9 H), 10.10 (s, 1 H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 192.4, 142.2, 136.9, 135.6, 133.1, 129.5, 129.0, 128.7, 128.2, 128.0, 127.1.

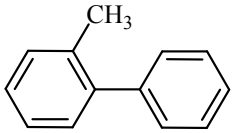


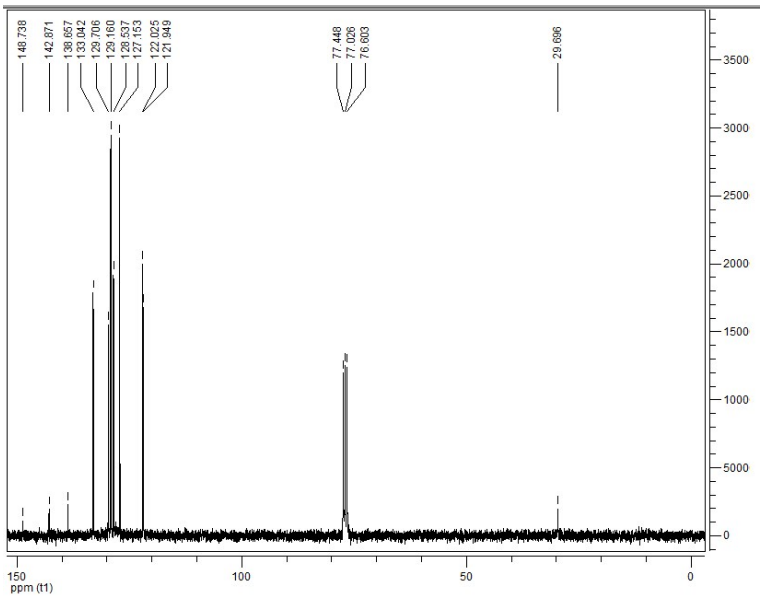




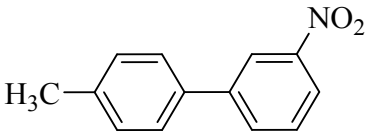
2-Methoxylbiphenyl (Entry 3):[R3]

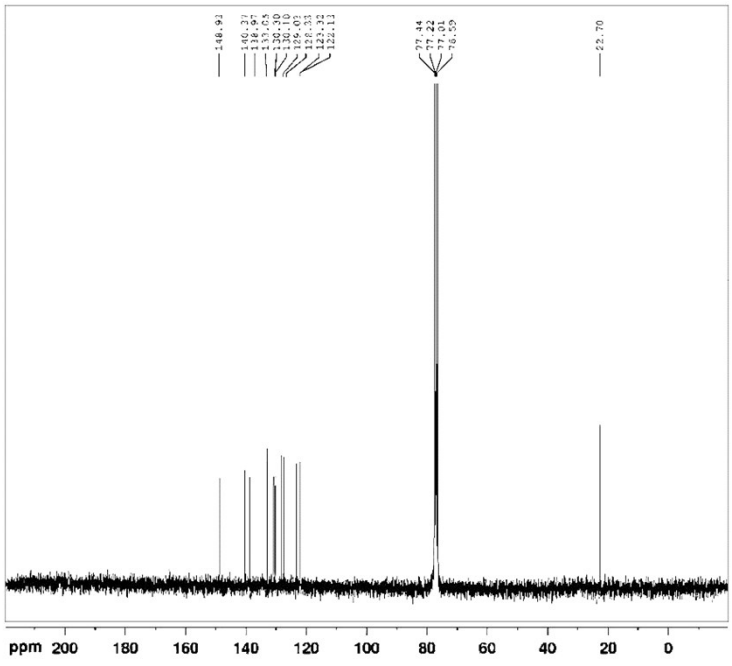
Colorless viscous liquid. ^{13}C NMR (75 MHz, $CDCl_3$): δ = 156.6, 138.7, 131.0, 130.8, 129.6, 128.8, 128.0, 127.0, 120.9, 111.3, 55.6.



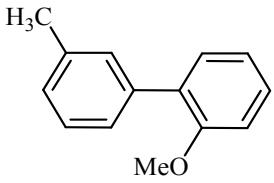


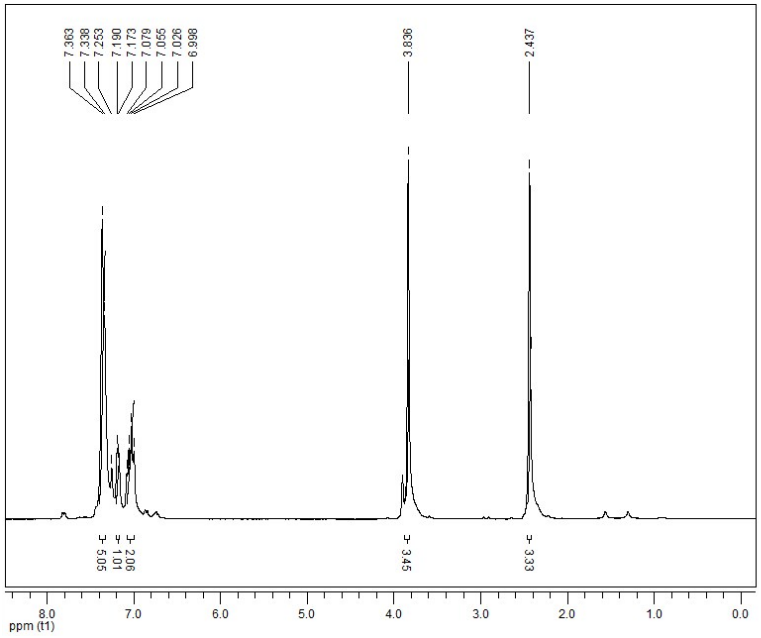
4'-methyl-3-nitro-1,1'-biphenyl (Entry 15):[R3] ^{13}C-NMR ($CDCl_3$, 75 MHz): δ = 22.7, 122.1, 123.3, 128.3, 129.0, 130.1, 130.3, 133.0, 139.0, 140.4, 148.9.

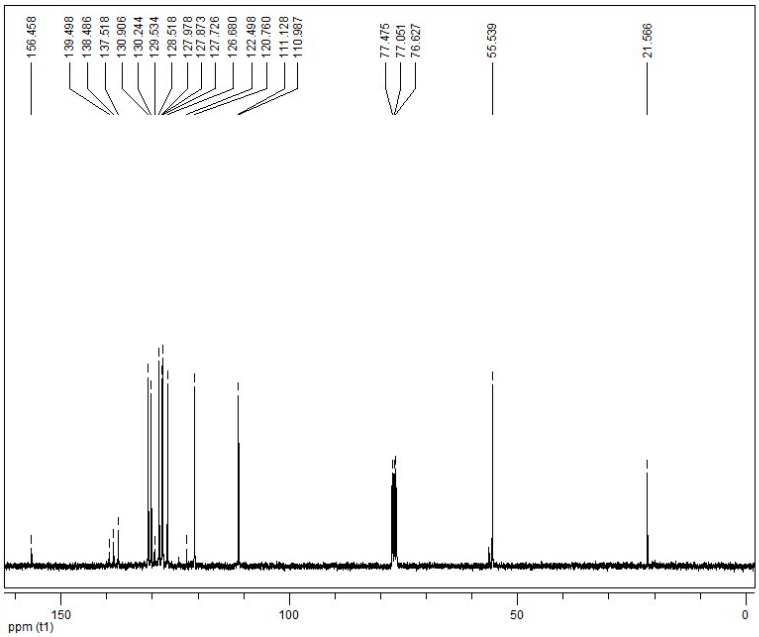




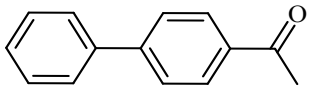
3-Methyl-2'-methoxy-biphenyl (Entry 6 and 14):[R3] Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$) : δ = 7.00-7.36 (m, 8 H), 3.84 (s, 3 H), 2.44 (s, 3 H). ^{13}C NMR (75MHz, $CDCl_3$): δ = 156.5, 139.5, 138.5, 137.52, 130.9, 130.2, 128.5, 127.9, 127.7, 126.7, 120.7, 111.1, 55.5, 21.6.

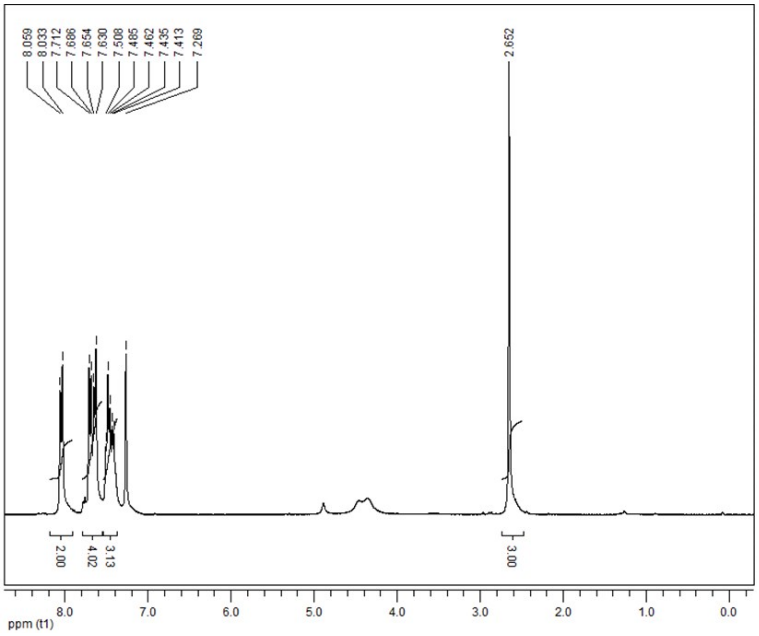


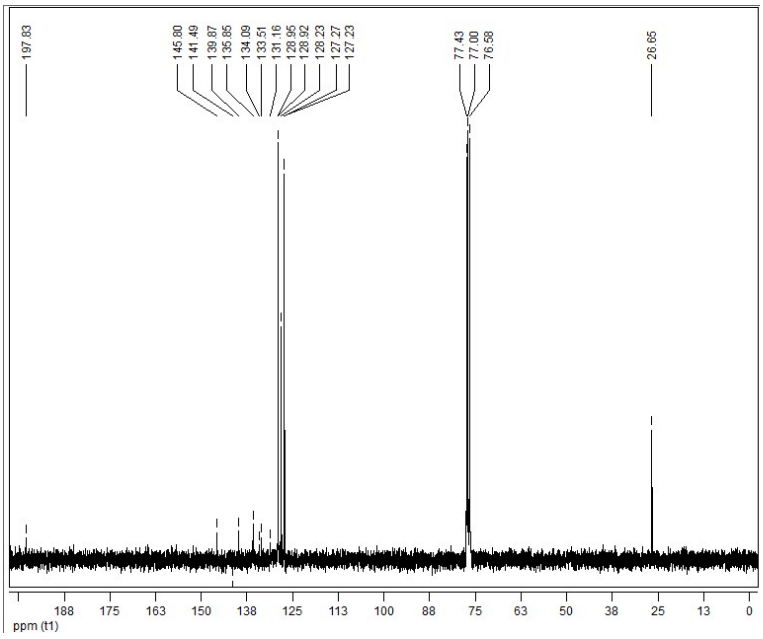




1-Biphenyl-4-yl-ethanone (Entry 17 and 10):[R3] White solid, mp: 121-123 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.03-8.06 (m, 2 H), 7.63-7.78 (m, 4 H), 7.41-7.50 (m, 3 H), 2.65 (s, 3 H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 197.8, 145.8, 139.9, 135.8, 128.9, 128.9, 128.2, 127.3, 127.2, 26.6.







Reference

R1 E. Doustkhah, S. Rostamnia, H. G. Hossieni and R. Luque, *ChemistrySelect*, **2017**, 2, 329.

R2 S. Rostamnia, E. Doustkhah and B. Zeynizadeh, *Microporous Mesoporous Mater.*, **2016**, 222, 87.

R3 S. Rostamnia and H. Xin, *Appl. Organomet. Chem.*, **2013**, 27, 348.