

Exploring the untapped catalytic application of ZnO/CuI/PPy nanocomposite for the green synthesis of biologically active 2,4,5-trisubstituted imidazole scaffolds

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ELECTRONIC SUPPLEMENTARY INFORMATION (ESI)

Electronic Supplementary Information (ESI) includes FESEM, TEM and XRD of recycled ZnO/CuI/PPy nanocatalyst; Green chemistry metric calculations, ^1H NMR and ^{13}C NMR spectra of compounds.

Total No of Pages: 17, Total No of Tables: 0, Total number of Figures: 27.

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General Remarks

Chemicals and solvents were purchased from Sigma Adrich, Alfa-Aesar and Merck India Pvt. ^1H and ^{13}C spectra were recorded on a Jeol Spectrospin spectrometer at 400 MHz and 100 MHz respectively by keeping TMS as internal standard. CHNS Analyser was recorded on model Vario Micro Cube at USIC (University Science Instrument Centre), University of Delhi, Delhi, India. The X-ray diffractometer (Model No. D8 DISCOVER) at 2θ range of $2-90^\circ$ with $\text{Cu K}\alpha$ radiation. Chemical shift values were recorded in terms of δ and coupling constants (J) are in hertz (Hz). FTIR spectra were obtained on IRAffinity-1S Fourier Transform Infrared Spectrophotometer. FESEM measurement was performed on Zeiss GeminiSEM 500 at USIC, University of Delhi. Transmission electron microscopy (TEM) was obtained on a TECNAI G20 HR-TEM 200kV at SAIF (sophisticated analytical instrumentation facility), AIIMS, New Delhi, India. The elemental composition and electronic structure analysis were obtained from X-ray photoelectron spectra (XPS) of PHI 5000 Versa Probe III instrument at Institute Instrumentation Centre, Indian Institute of Technology, Roorkee – 247 667 (Uttarakhand), India. ICP-MS was measured on Agilent ICP-MS 7900 with UHMI at the ICP-MS Lab, (CRF Adopted Facility), IIT Delhi, INDIA.

Characterization of Recycled ZnO/CuI/PPy nanocatalyst

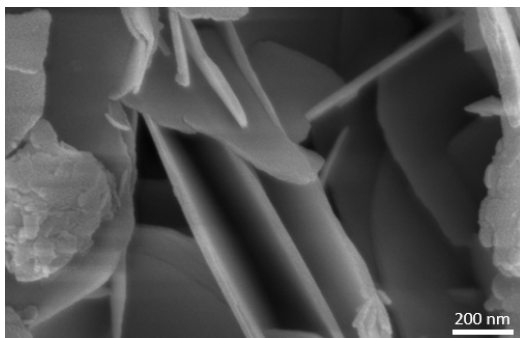


Figure S1: FESEM of recycled nanocatalyst

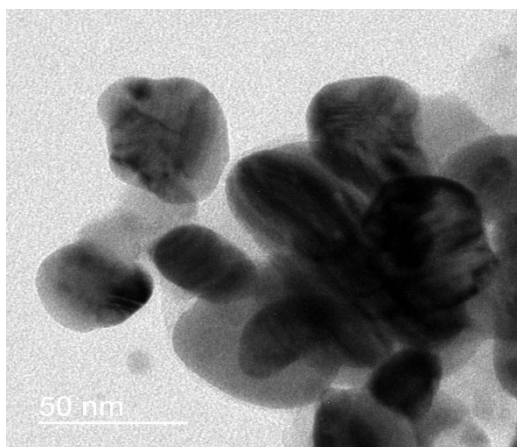


Figure S2: TEM of recycled nanocatalyst

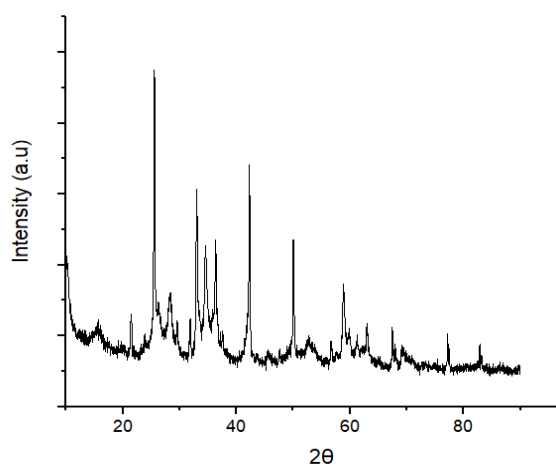
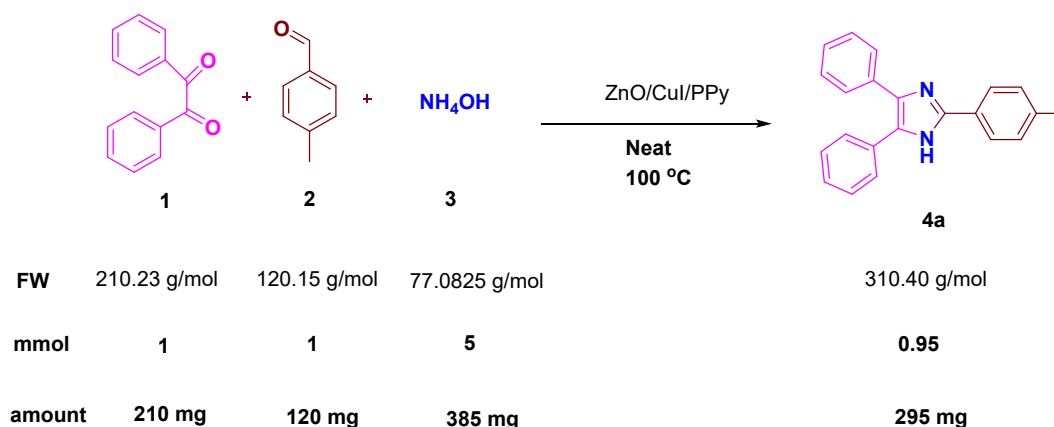


Figure S3: XRD of recycled nanocatalyst

Calculation of Green chemistry metrics



E-factor:

The ideal value of E-factor is zero.

E-factor = [total mass of raw materials - the total mass of product]/ mass of product.

$$\begin{aligned} \text{E-factor of 4a} &= [(210 + 120 + 385) - 295] / 295 \\ &= 1.42. \end{aligned}$$

Process mass intensity (PMI):

$$\begin{aligned} \text{PMI} &= \sum (\text{mass of stoichiometric reactants}) / [\text{mass of product}] \\ &= (210 + 120 + 385) / 295 \\ &= 2.42 \end{aligned}$$

Reaction mass efficiency (RME):

$$\begin{aligned} \text{RME} &= [\text{mass of product} / \sum (\text{mass of stoichiometric reactants})] \times 100 \\ &= [295 / (210 + 120 + 385)] \times 100 \\ &= 41.26\% \end{aligned}$$

Carbon efficiency (CE):

$$\begin{aligned} \text{CE} &= [\text{Amount of carbon in product} / \text{Total carbon present in reactants}] \times 100 \\ &= [\text{no. of moles of product} \times \text{no. of carbons in product} / (\text{moles of 1} \times \text{carbons in 1} + \text{moles of 2} \times \text{carbons in 2})] \times 100 \\ &= [0.95 \times 22 / (1 \times 14 + 1 \times 8)] \times 100 \\ &= [20.9 / (22)] \times 100 \\ &= 95\% \end{aligned}$$

^1H and ^{13}C spectra of compounds

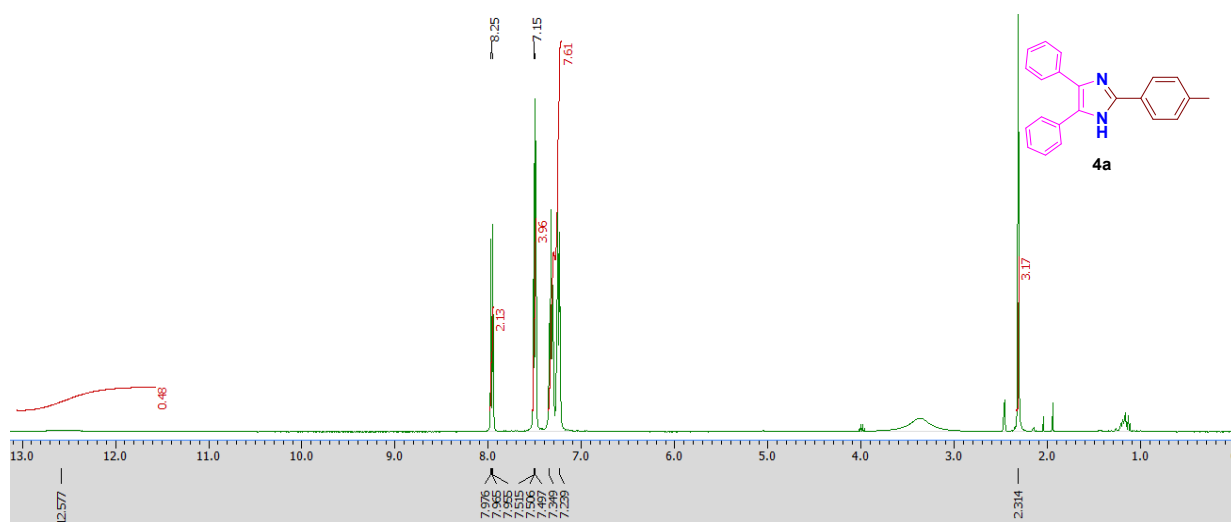


Figure S4: ^1H NMR of 2-(4-Methylphenyl)-4,5-diphenyl-1H-imidazole

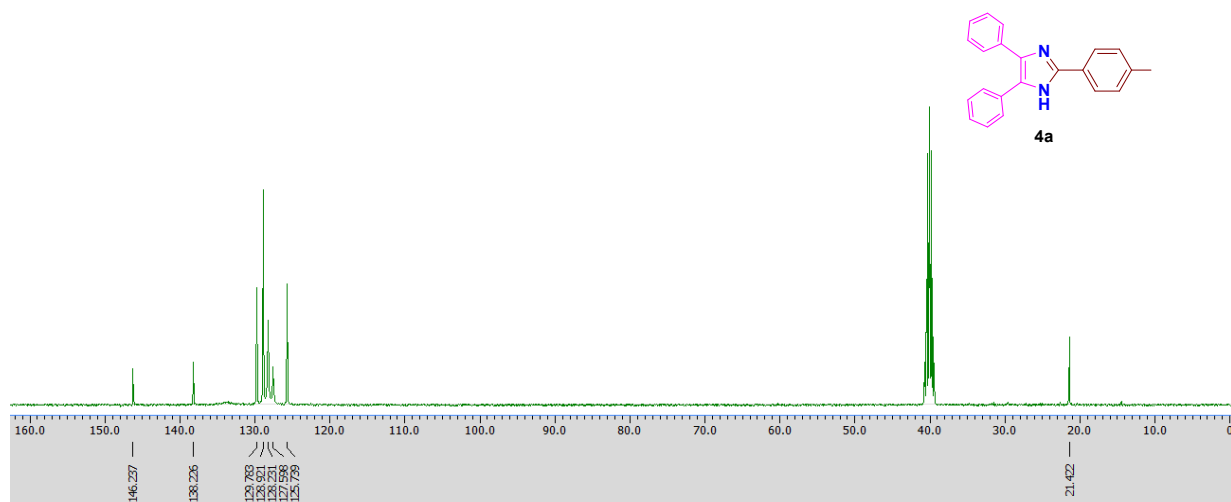


Figure S5: ^{13}C NMR of 2-(4-Methylphenyl)-4,5-diphenyl-1H-imidazole

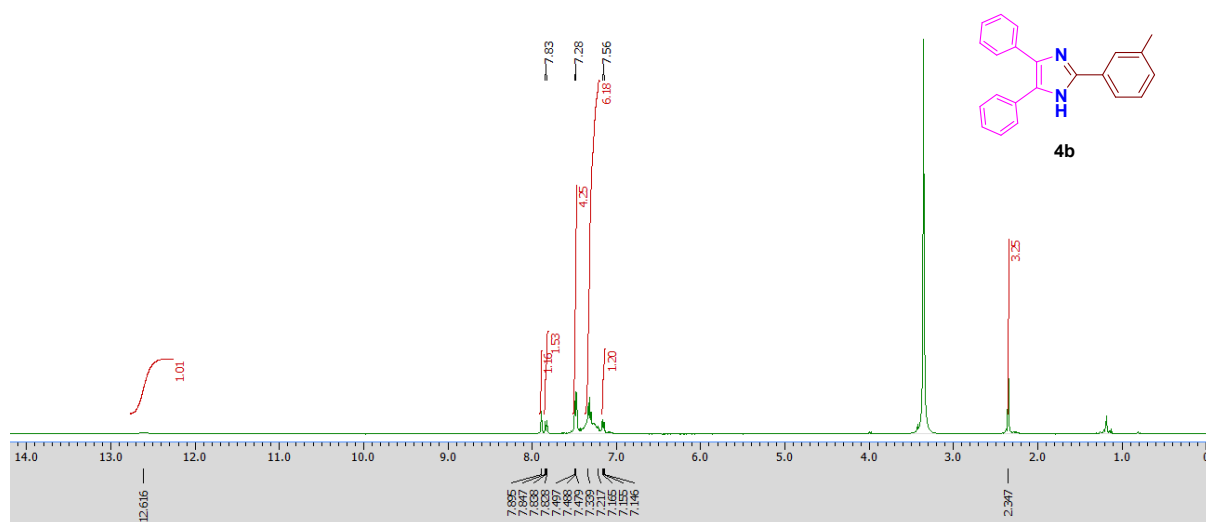


Figure S6: ¹H NMR of 2-(3-Methylphenyl)-4,5-diphenyl-1H-imidazole

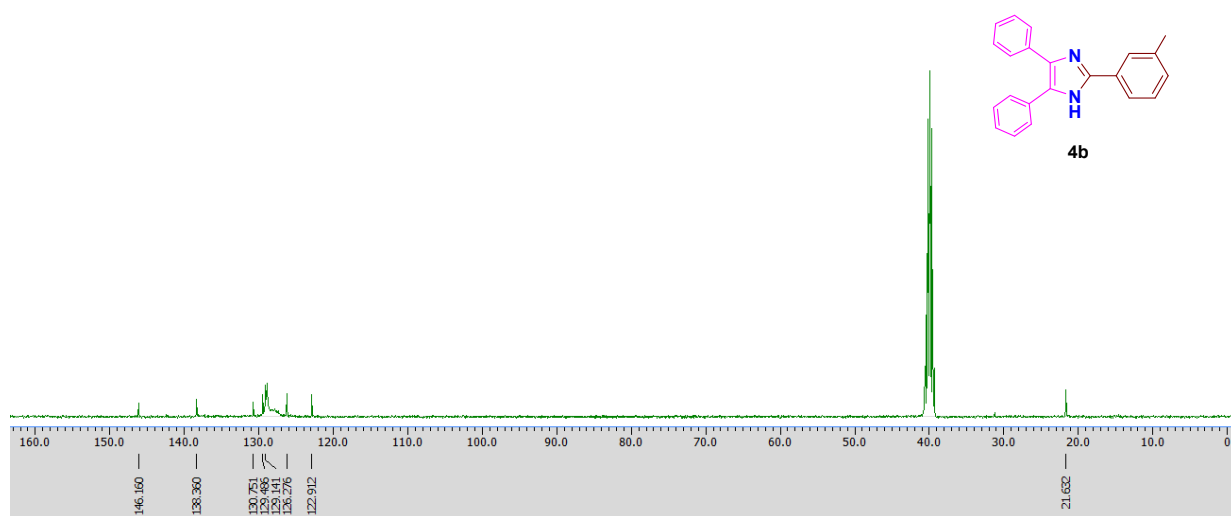


Figure S7: ¹³C NMR of 2-(3-Methylphenyl)-4,5-diphenyl-1H-imidazole

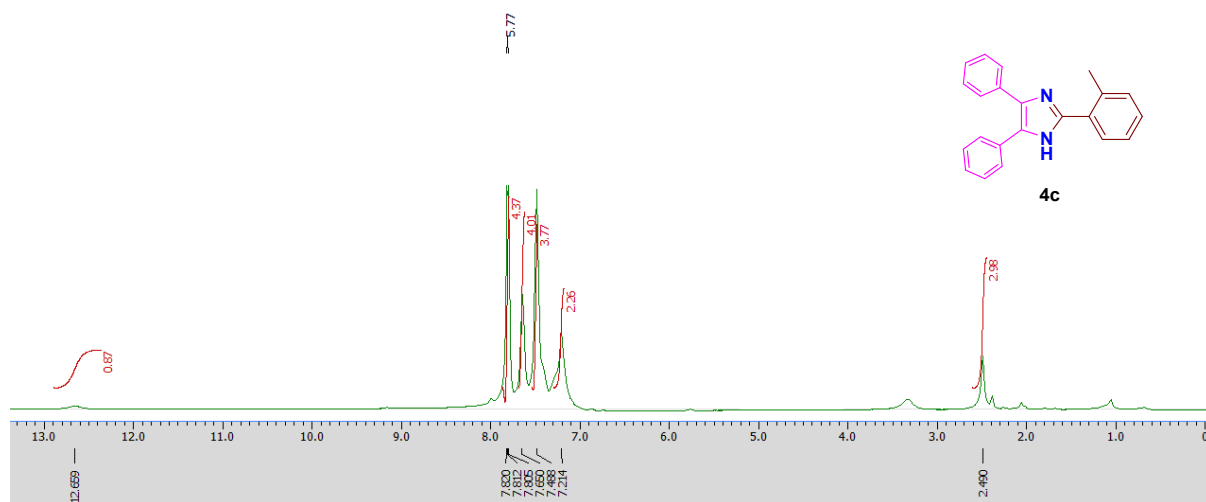


Figure S8: ¹H NMR of 2-(2-Methylphenyl)-4,5-diphenyl-1H-imidazole

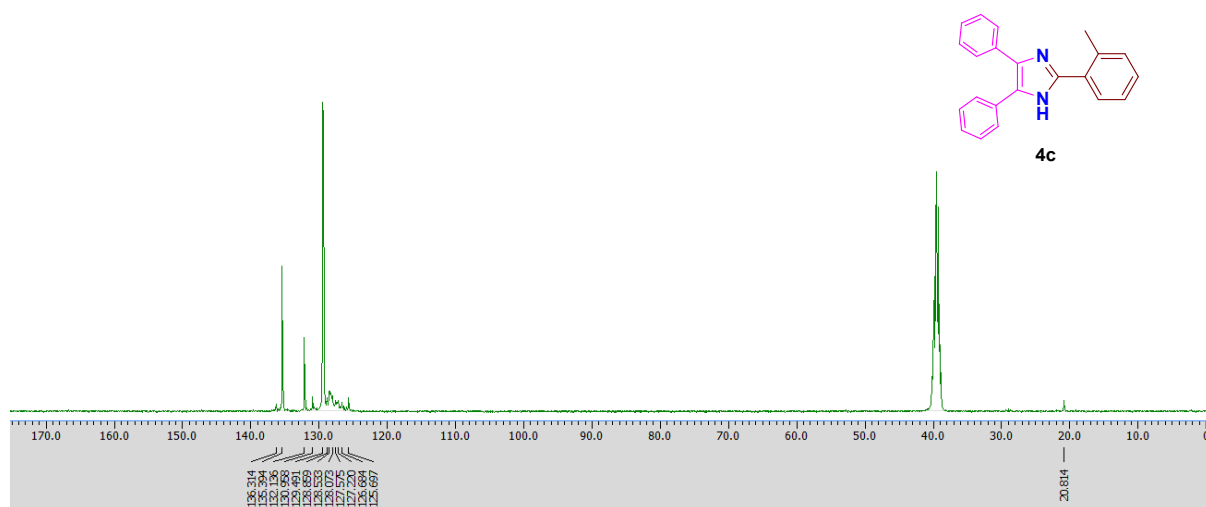


Figure S9: ¹³C NMR of 2-(2-Methylphenyl)-4,5-diphenyl-1H-imidazole

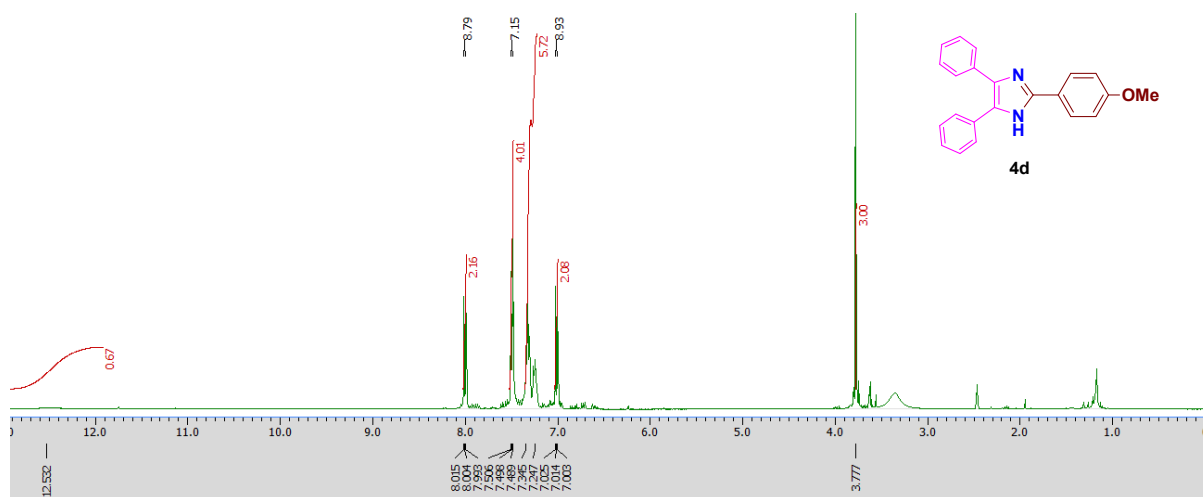


Figure S10: ¹H NMR of 2-(4-Methoxyphenyl)-4,5-diphenyl-1H-imidazole

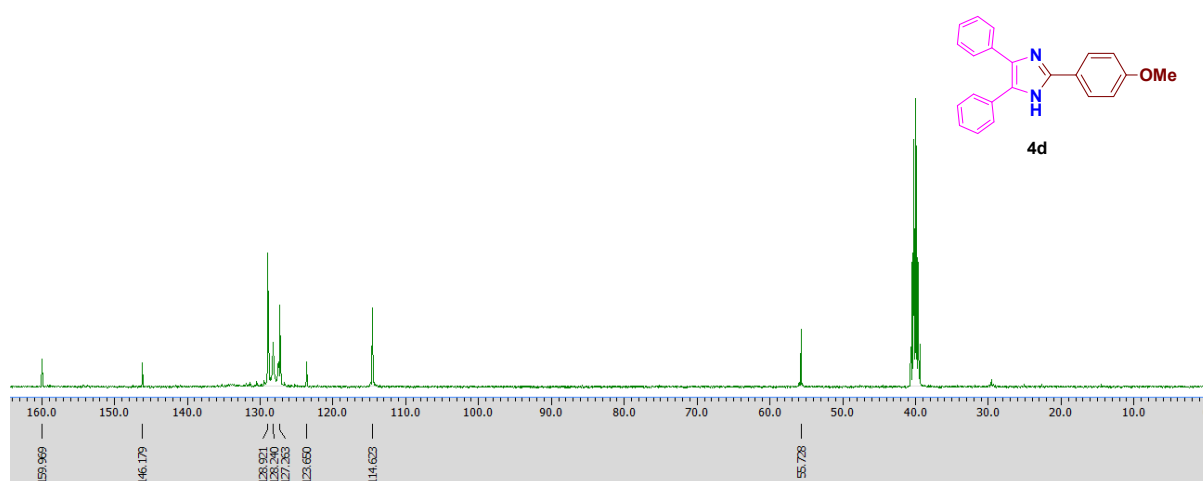


Figure S11: ¹³C NMR of 2-(4-Methoxyphenyl)-4,5-diphenyl-1H-imidazole

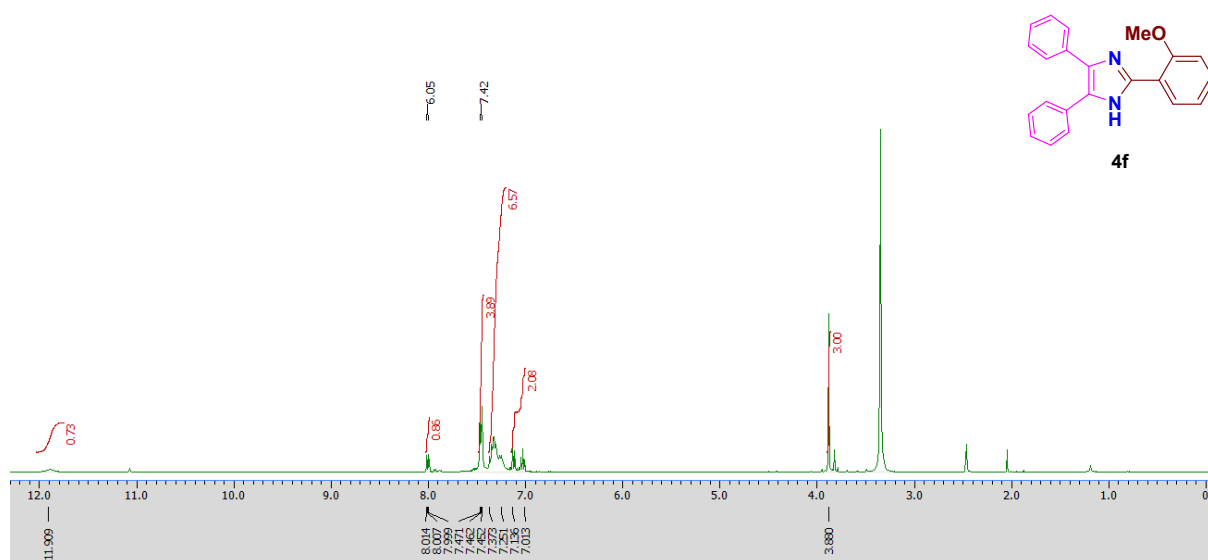


Figure S14: ¹H NMR of 2-(2-Methoxyphenyl)-4,5-diphenyl-1H-imidazole

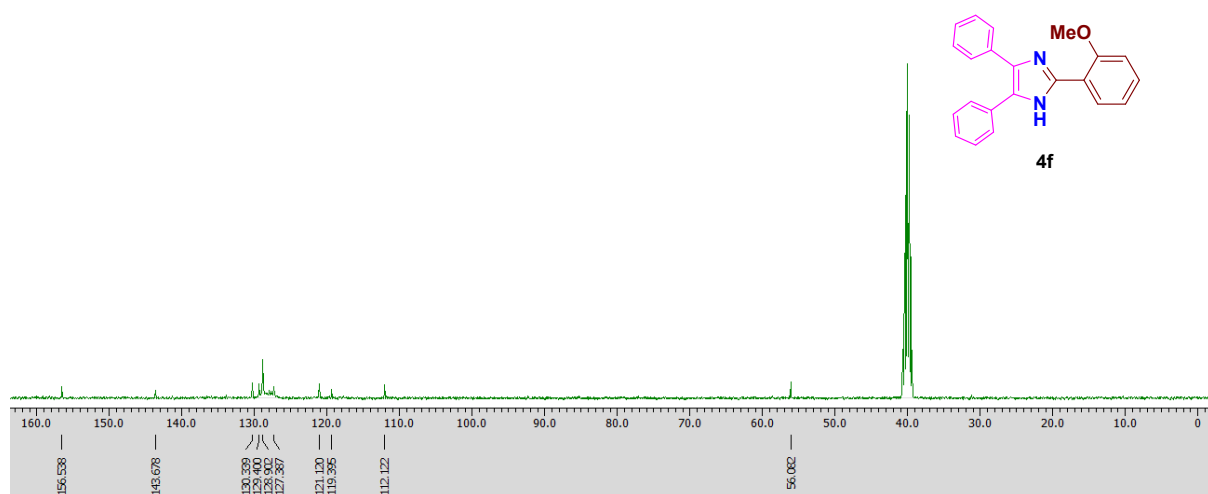


Figure S15: ¹³C NMR of 2-(2-Methoxyphenyl)-4,5-diphenyl-1H-imidazole

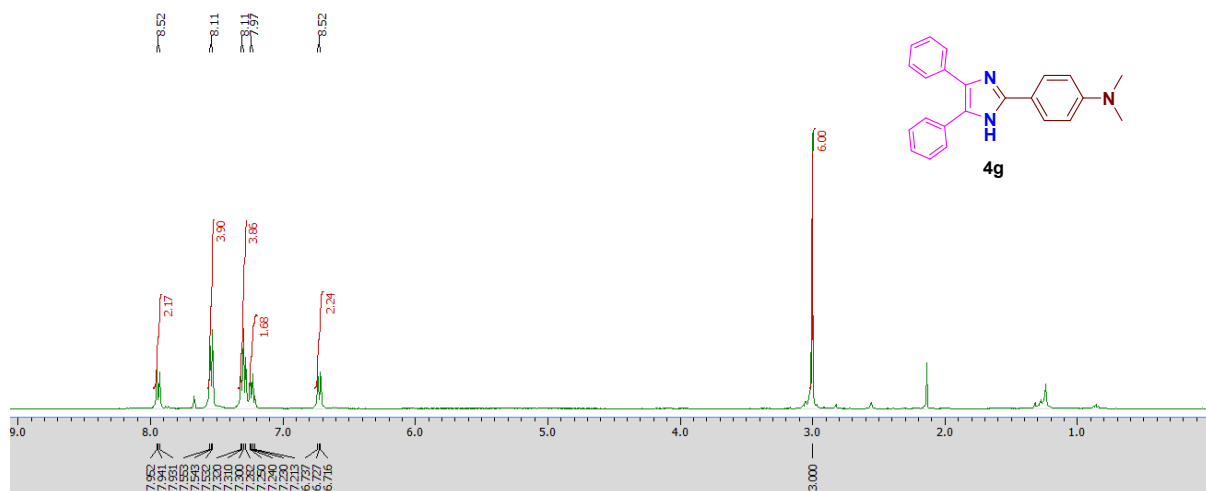


Figure S16: ¹H NMR of 2-(N,N-dimethylaminophenyl)-4,5-diphenyl-1H-imidazole

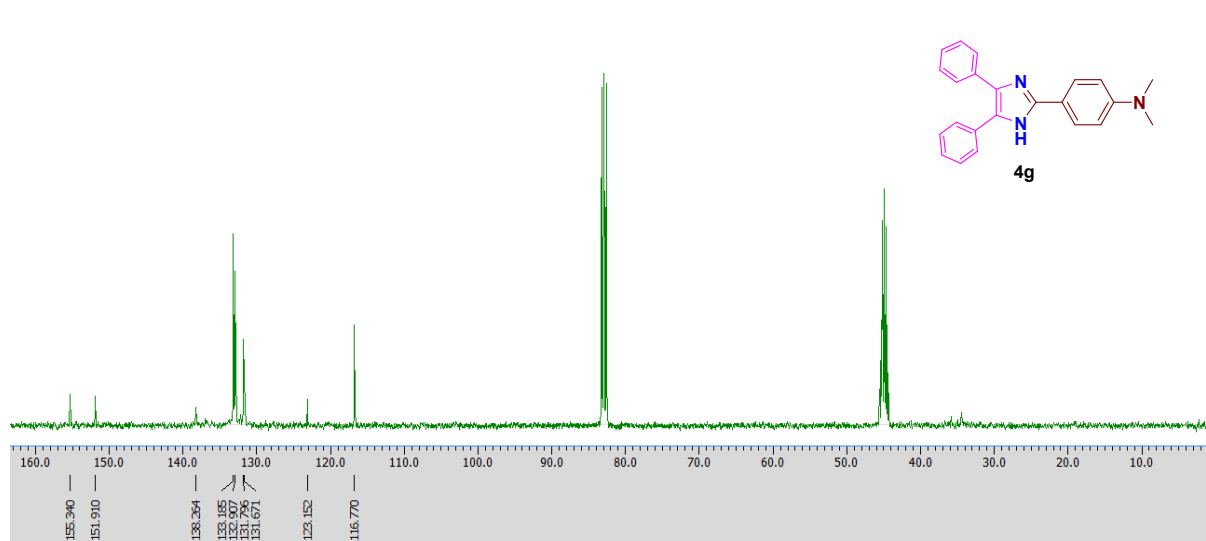


Figure S17: ¹³C NMR of 2-(N,N-dimethylaminophenyl)-4,5-diphenyl-1H-imidazole

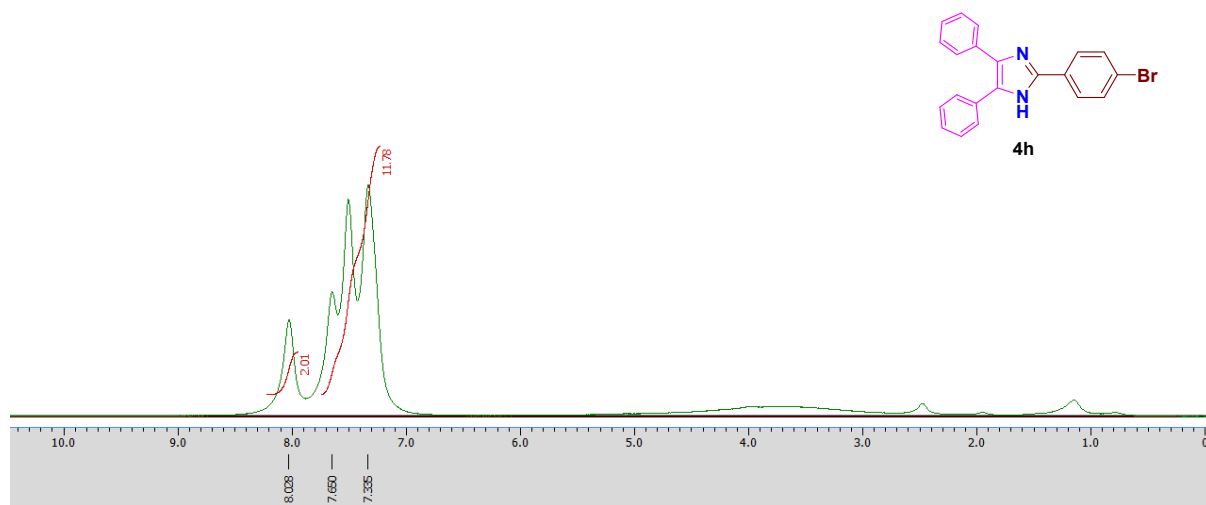


Figure S18: ^1H NMR of 2-(4-Bromophenyl)-4,5-diphenyl-1H-imidazole

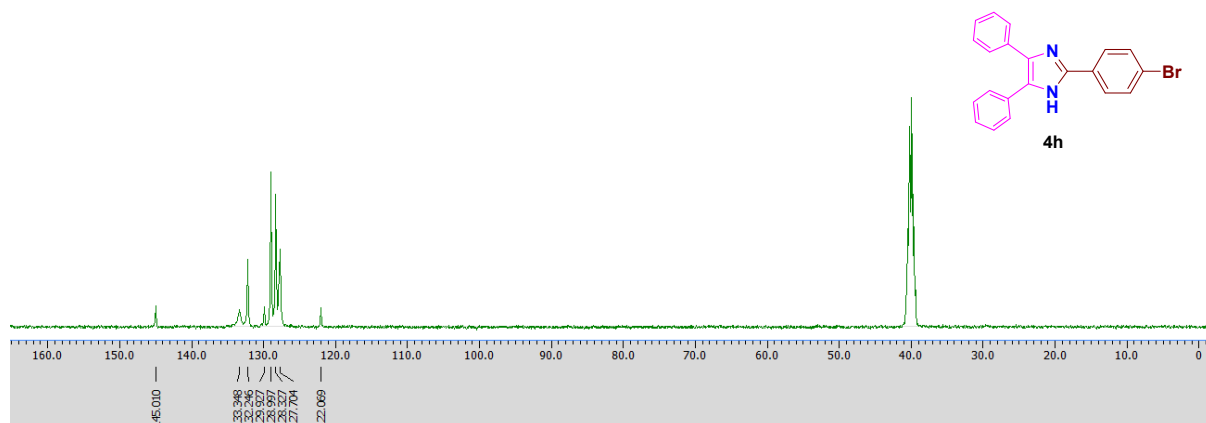


Figure S19: ^{13}C NMR of 2-(4-Bromophenyl)-4,5-diphenyl-1H-imidazole

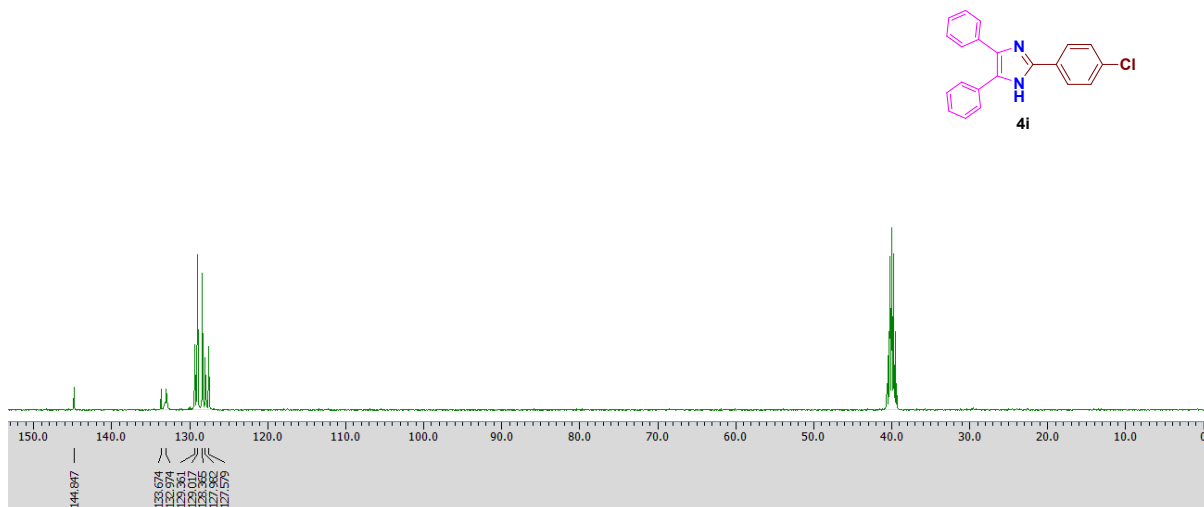


Figure S20: ¹³C NMR of 2-(4-Chlorophenyl)-4,5-diphenyl-1H-imidazole

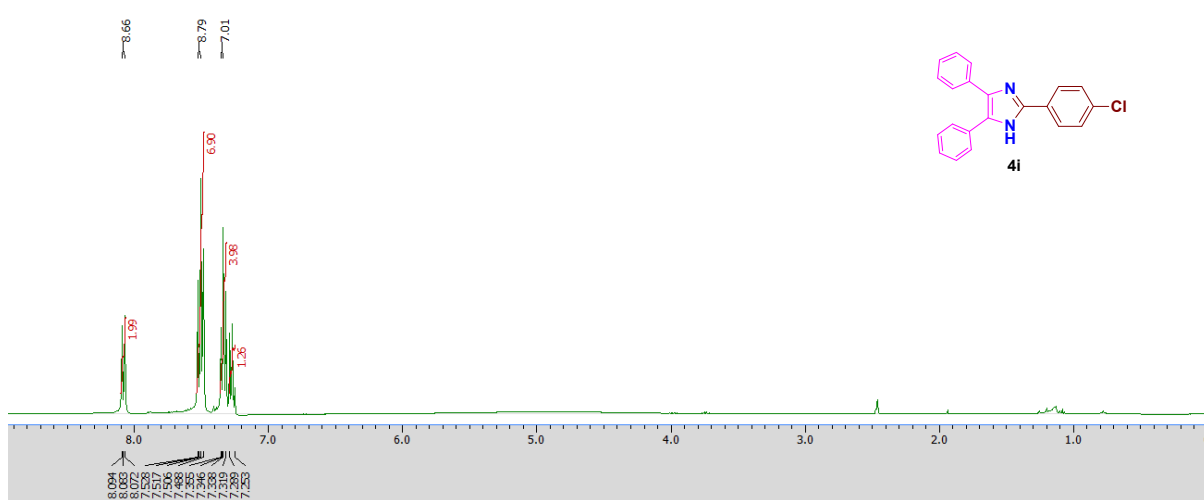


Figure S21: ¹H NMR of 2-(4-Chlorophenyl)-4,5-diphenyl-1H-imidazole

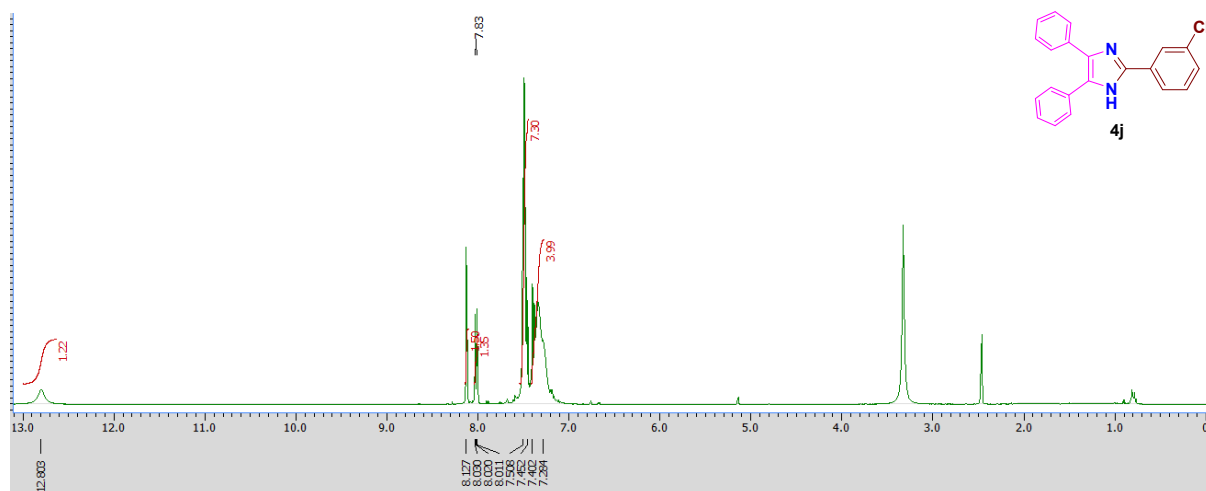


Figure S22: ^1H NMR of 2-(3-Chlorophenyl)-4,5-diphenyl-1H-imidazole

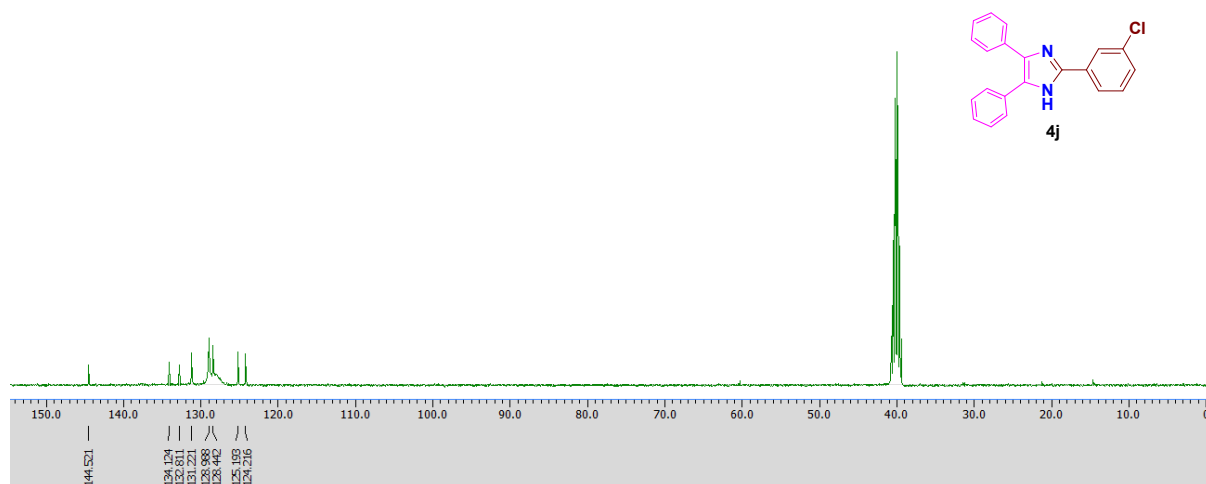


Figure S23: ^{13}C NMR of 2-(3-Chlorophenyl)-4,5-diphenyl-1H-imidazole

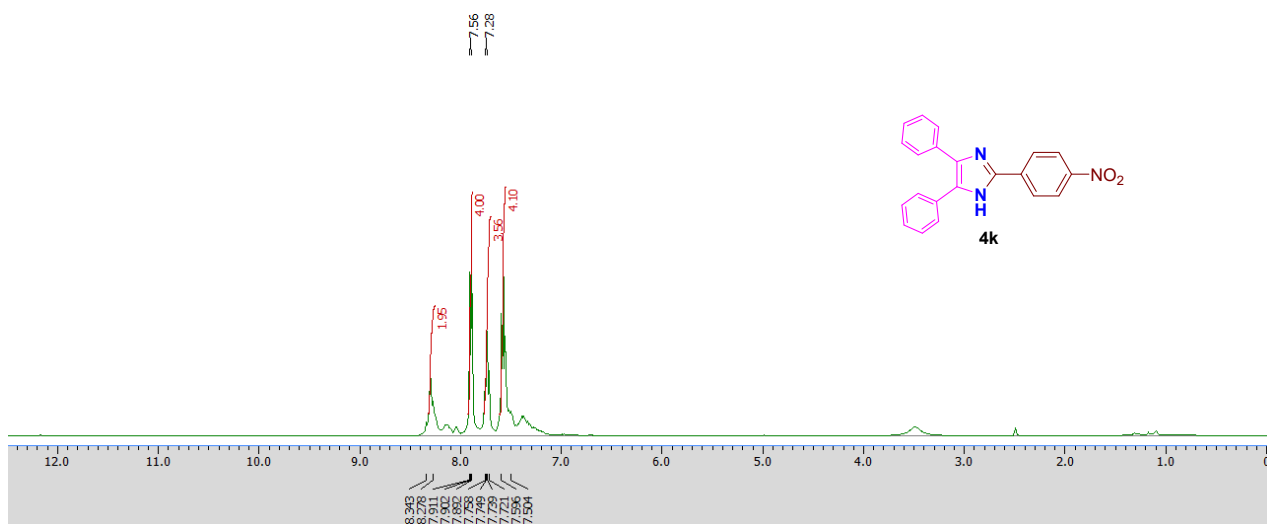


Figure S24: ¹H NMR of 2-(4-nitrophenyl)-4,5-diphenyl-1H-imidazole

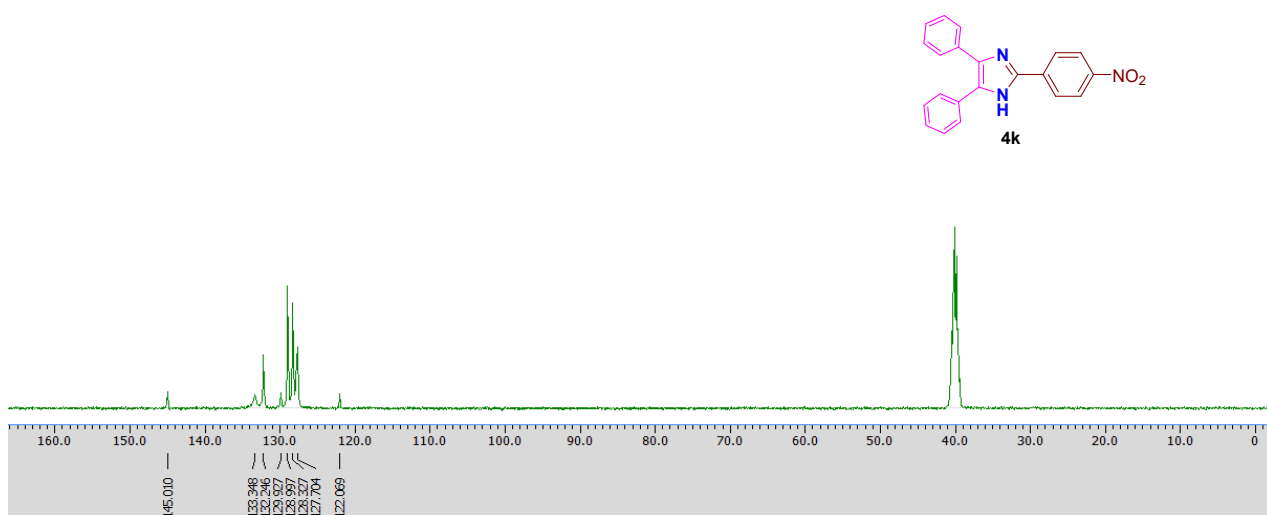


Figure S25: ¹³C NMR of 2-(4-nitrophenyl)-4,5-diphenyl-1H-imidazole

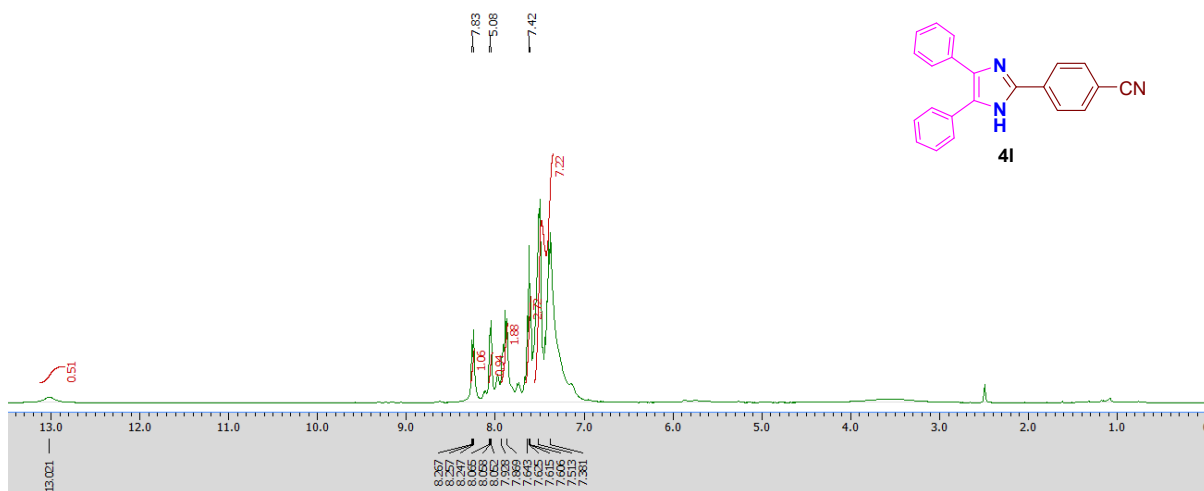


Figure S26: ¹H NMR of 2-(4-cyanophenyl)-4,5-diphenyl-1H-imidazole

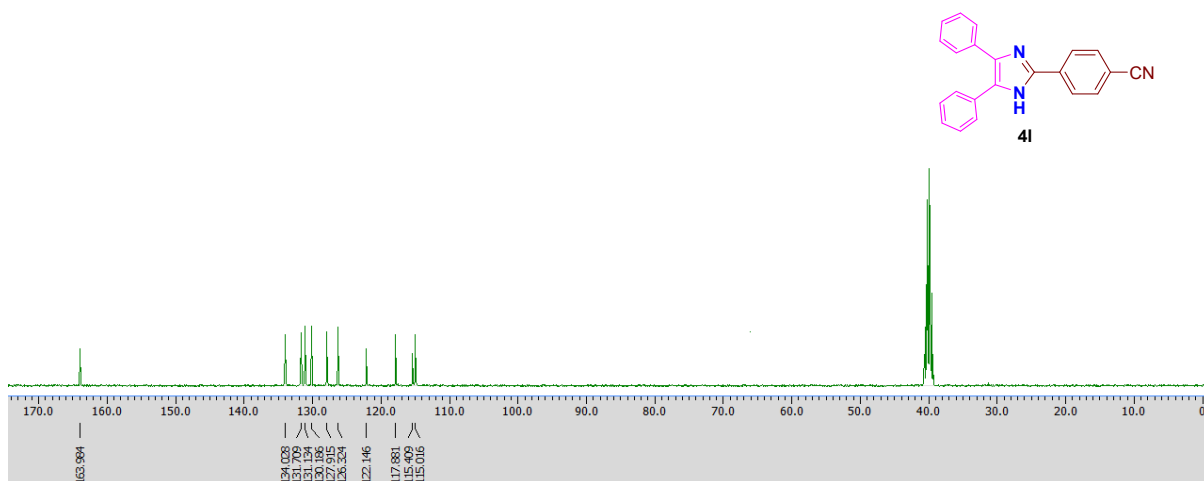


Figure S27: ¹³C NMR of 2-(4-cyanophenyl)-4,5-diphenyl-1H-imidazole