

Supplementary Information file (S1)

Copper Borate (CuB₄O₇) catalyzed multi-component green synthesis of 2,4,5-triarylimidazole derivatives and evidence of *in-situ* conversion of Copper Borate (CuB₄O₇) into Cu(OAc)₂ in presence of NH₄OAc.

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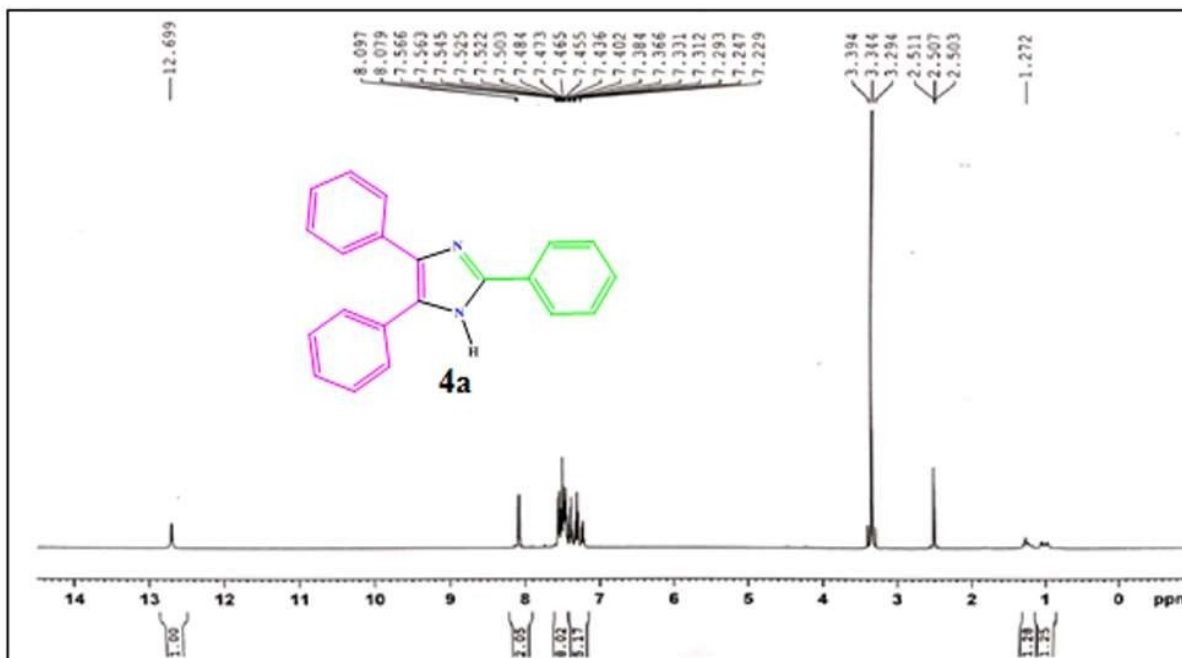
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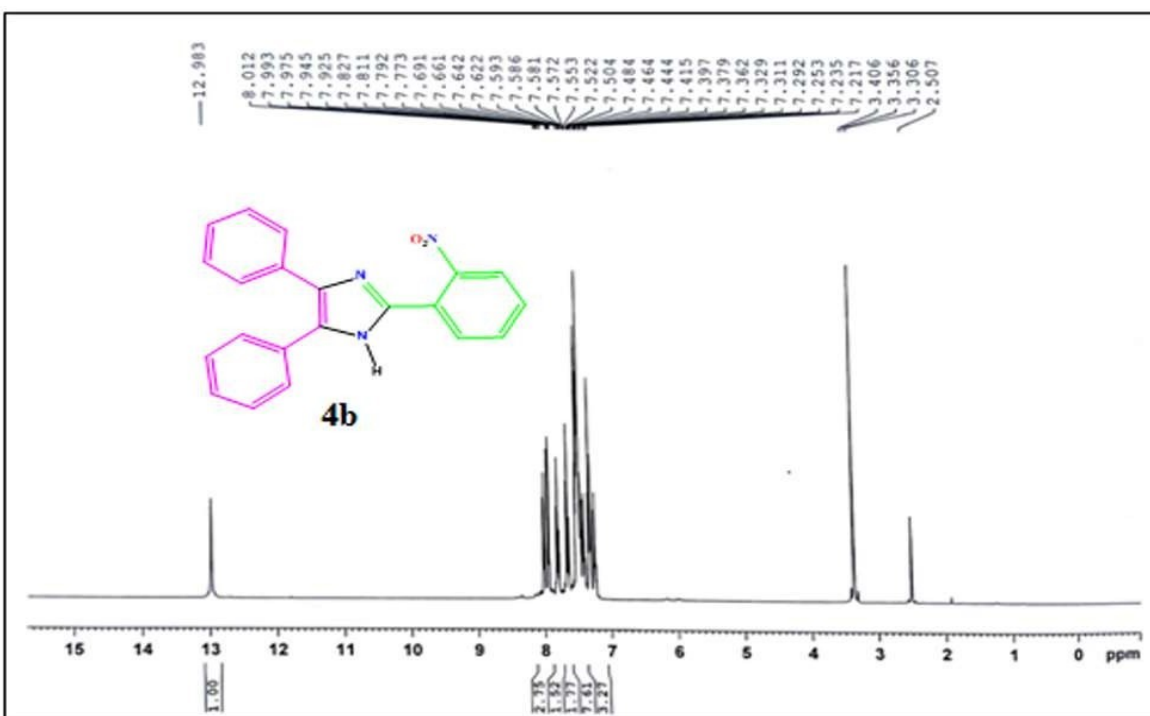
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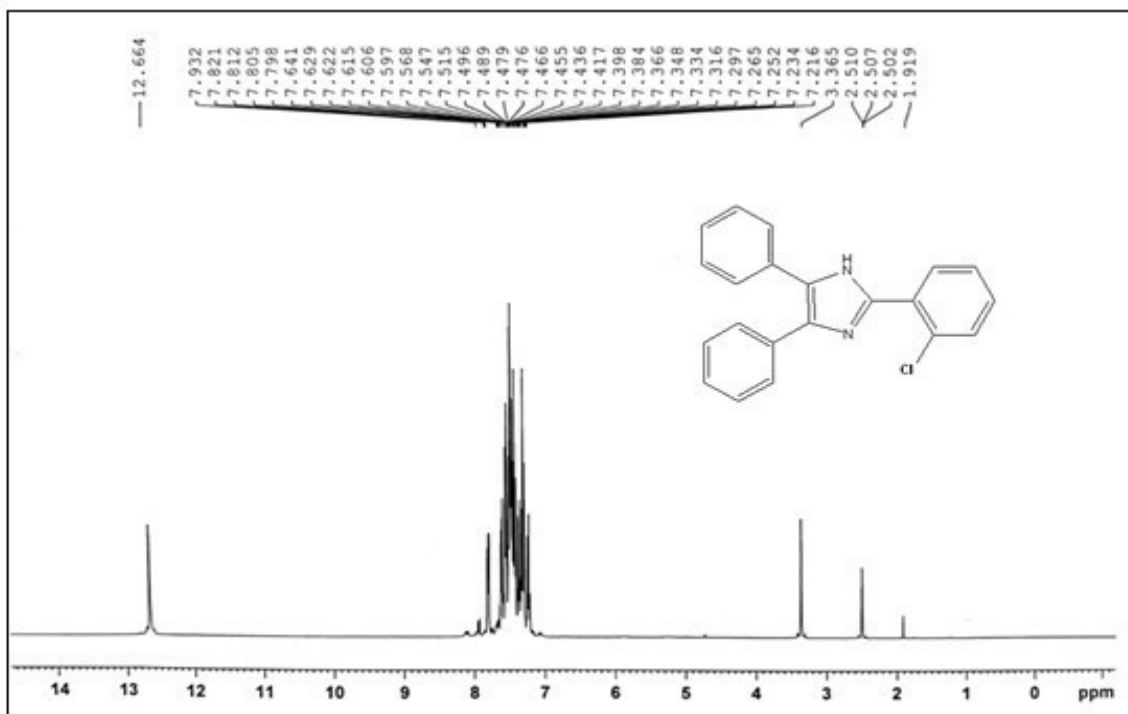
I. Copy of ^1H NMR spectra



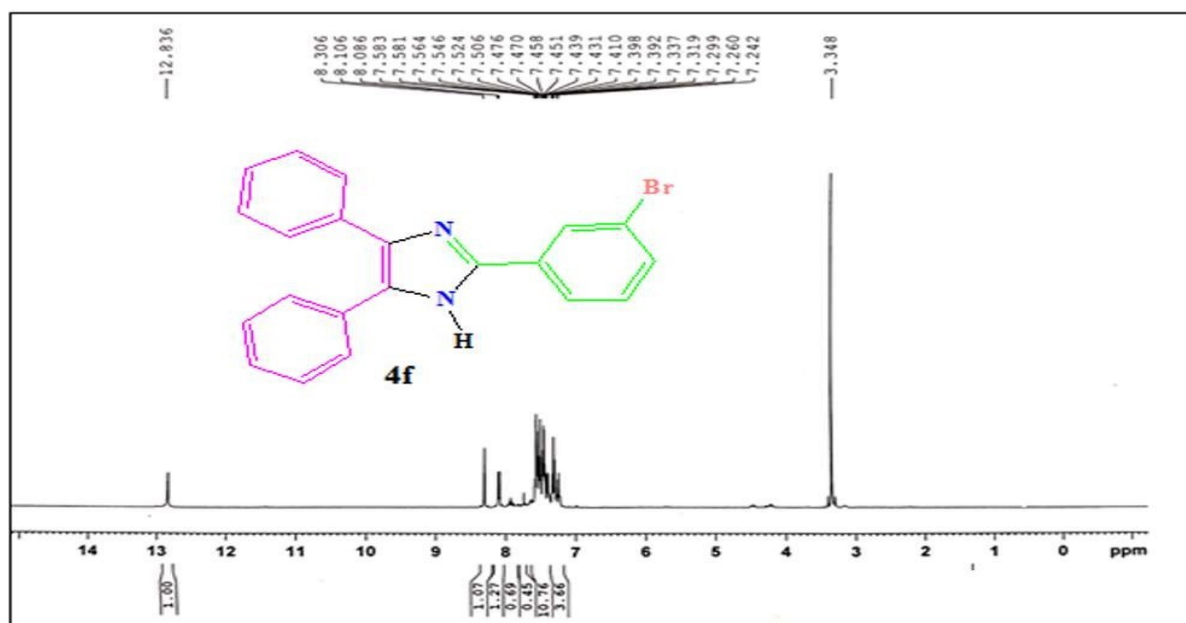
^1H NMR spectra of 2,4,5-triphenyl-1H-imidazole (4a)



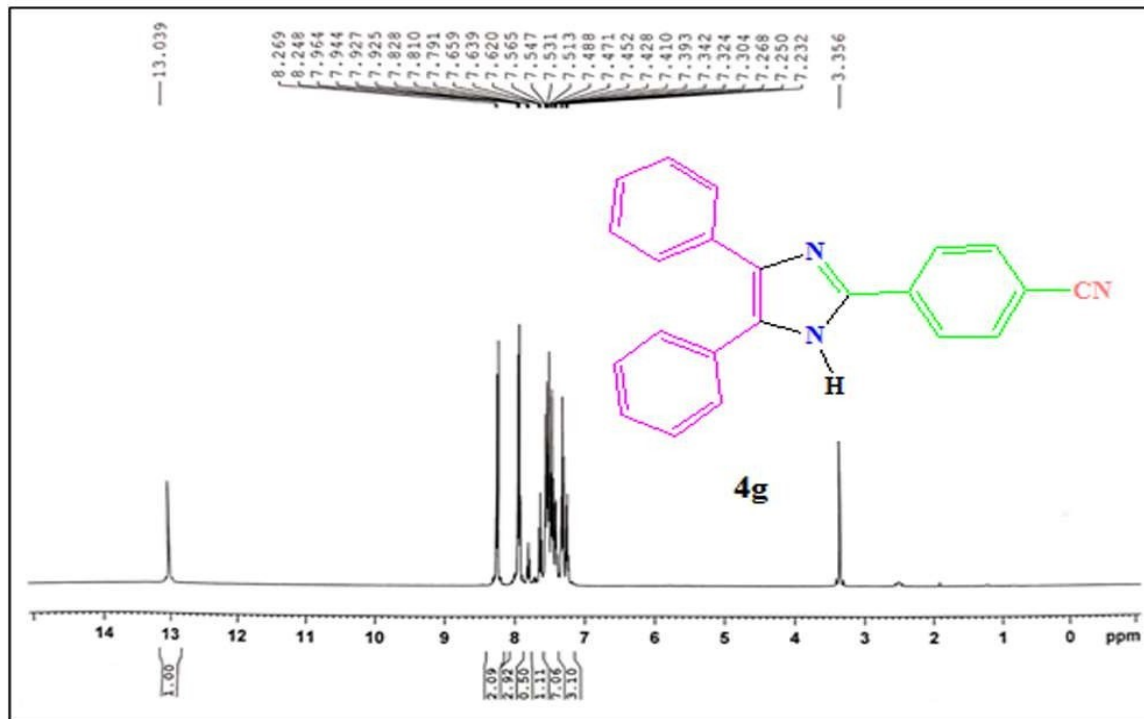
¹HNMR spectra of 2-(2-nitrophenyl)-4,5-diphenyl-1H-imidazole (4b)



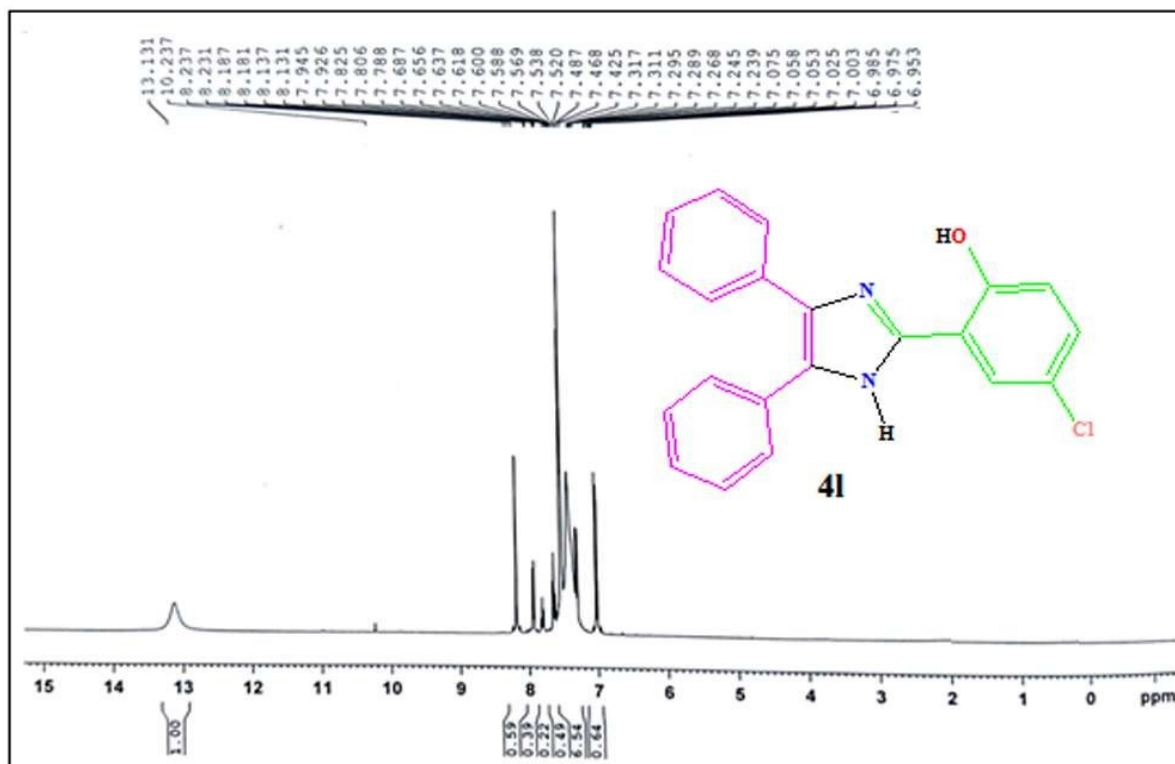
¹H NMR spectra of 2-(2-chlorophenyl)-4,5-diphenyl-1H-imidazole (4e)



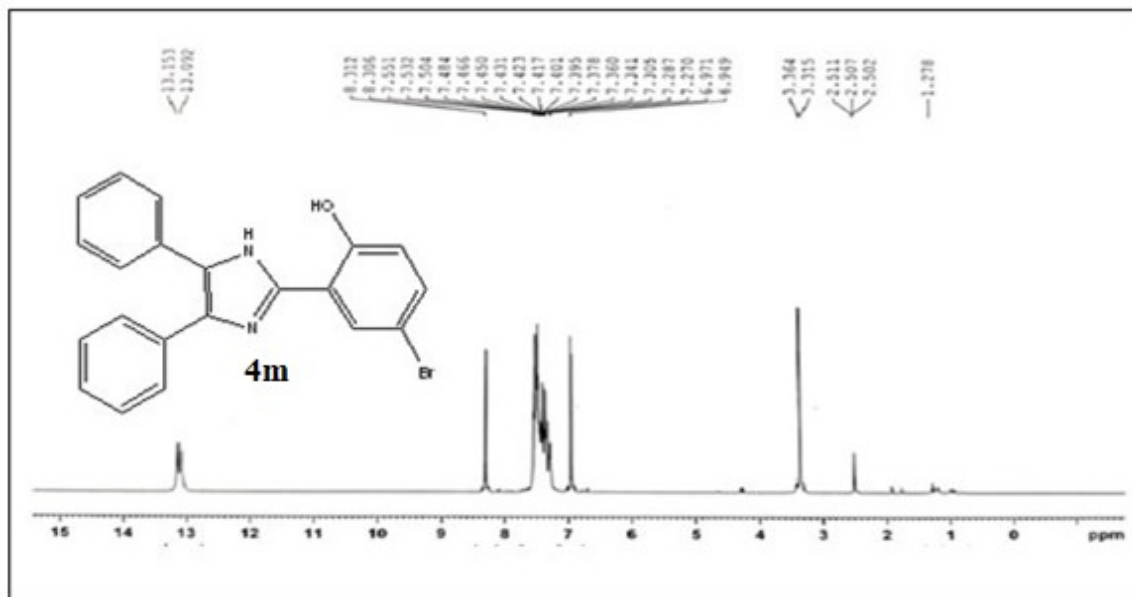
¹H NMR spectra of 2-(3-bromophenyl)-4,5-diphenyl-1H-imidazole(4f)



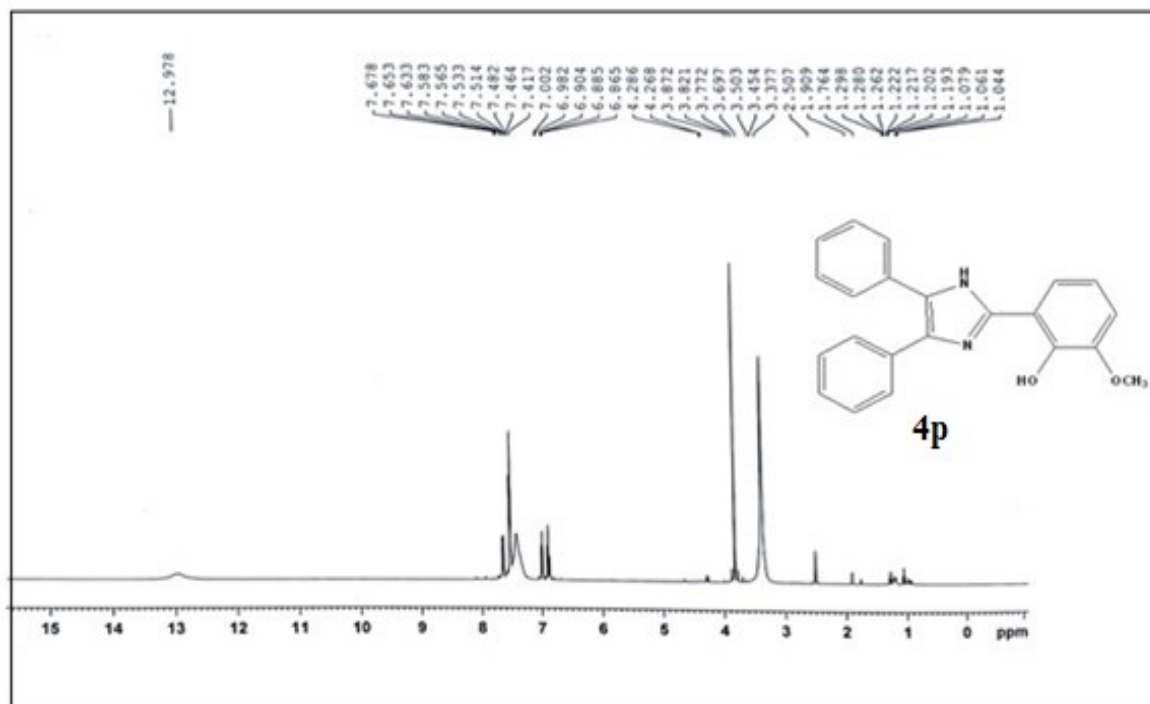
¹H NMR of 4-(4,5-diphenyl-1H-imidazol-2-yl)benzonitrile (4g)



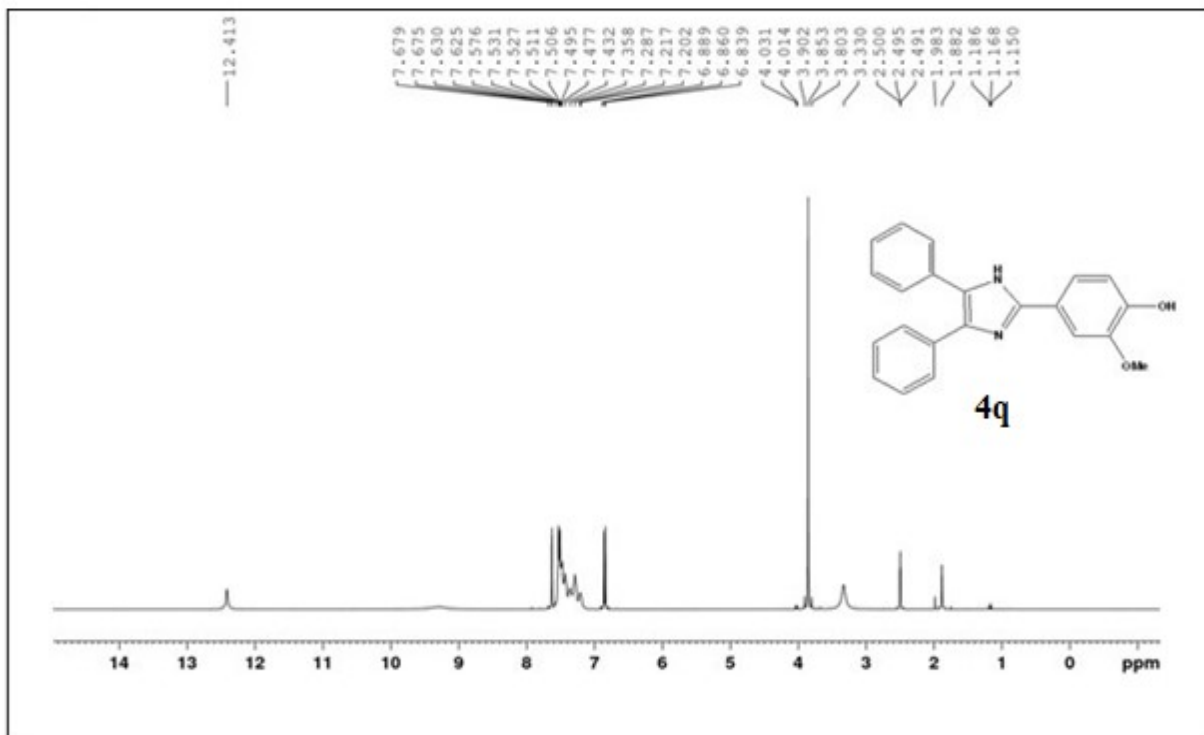
¹H NMR spectra of 4-chloro-2-(4,5-diphenyl-1H-imidazol-2-yl)phenol(4l)



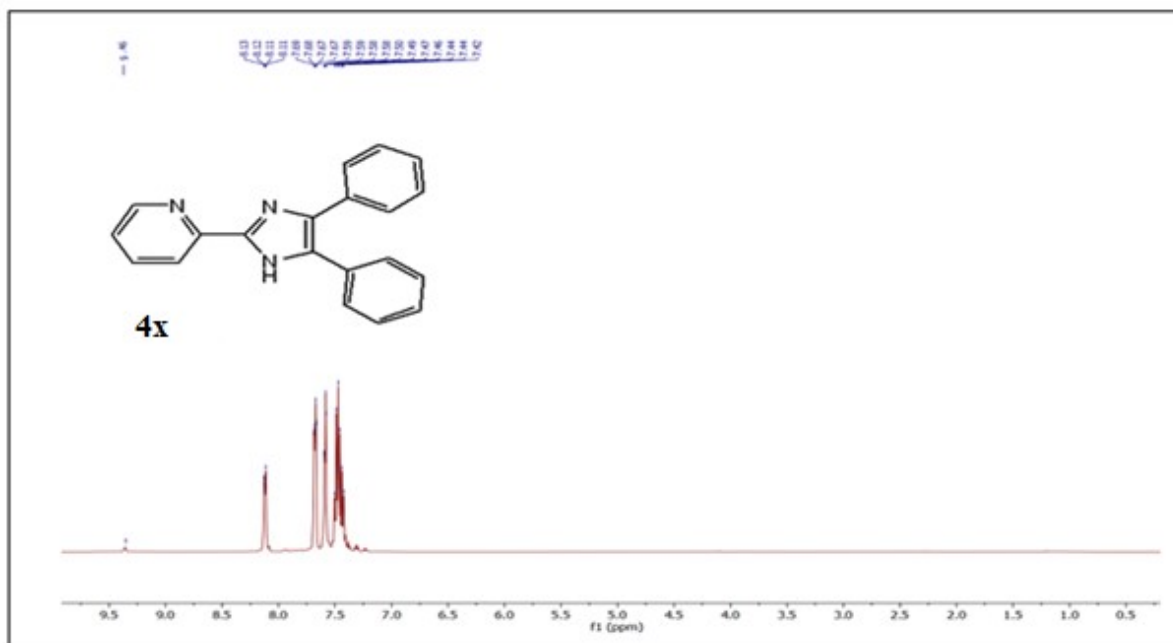
¹H NMR spectra of 4-bromo-2-(4,5-diphenyl-1H-imidazol-2-yl)phenol(4m)



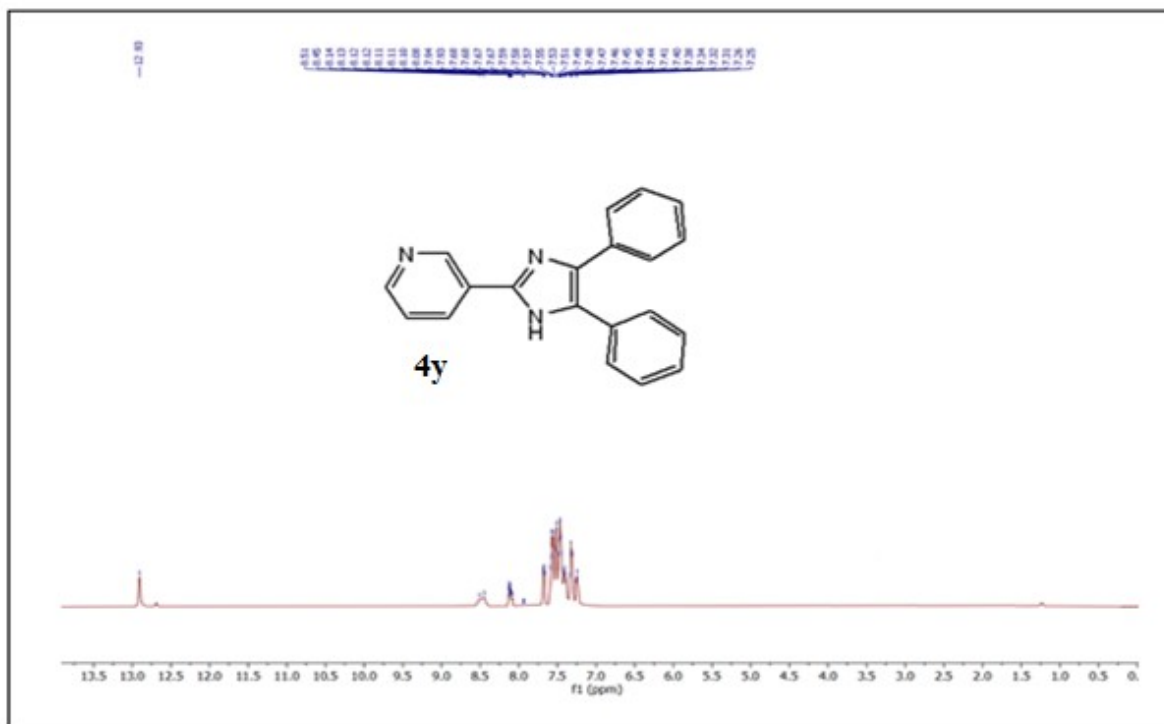
¹H NMR spectra of 2-methoxy-6-(4,5-diphenyl-1H-imidazol-2-yl)phenol(4p)



¹H NMR spectra of 4-(4,5-diphenyl-1H-imidazol-2-yl)-2-methoxyphenol(4q)



¹H NMR spectra of 2-(4,5-diphenyl-1H-imidazol-2-yl)pyridine(4x)



¹H NMR spectra of 3-(4,5-diphenyl-1H-imidazol-2-yl)pyridine(4y)

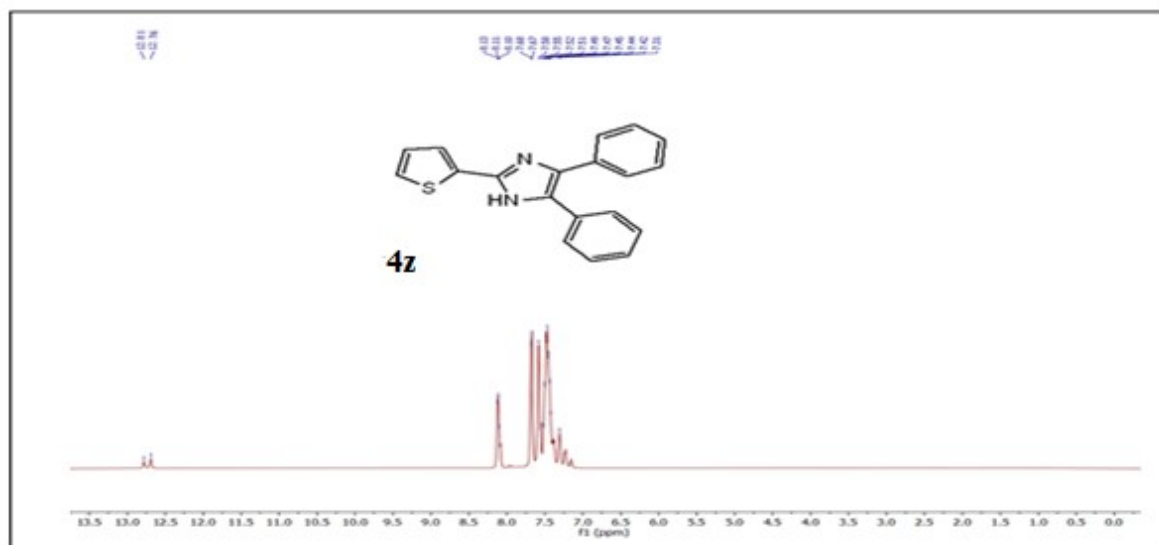


Table S1. Crystal data collection and structure refinement for compound (6)

Crystal data	
Moiety formula, Chemical formula	$\text{Cu}_2\text{C}_8\text{H}_{16}\text{O}_{10}$, $\text{Cu}_2(\text{O}_2\text{CCH}_3)_4 \cdot 2\text{H}_2\text{O}$
Formula weight	399.31
Crystal system, Space group	Monoclinic, $C 2/c$
Colour, Size, mm	Blue, $0.24 \times 0.22 \times 0.20$
Unit cell dimensions	
a, b, c	13.0799 (8) Å, 8.5056(4) Å, 13.7429(7) Å
α , β , γ	90° , $116.887(7)^\circ$, 90°
Volume Å ³ , Z	1363.65(13), 4
Density (calculated), Mg/m ³	1.945
Absorption coefficient, mm ⁻¹	3.164
F(000)	808
Data collection	
Temperature, K	119.98(10)
Theta range for data collection	2.96° to 29.01°
Index ranges	$-17 \leq h \leq 17$, $-11 \leq k \leq 10$, $-18 \leq l \leq 17$
Reflections collected	8716
Unique reflections	1660
Observed reflections ($>2\sigma(I)$)	1438
R_{int}	0.0387
Completeness to θ , %	29.01° , 91.1
Absorption correction	Multi-scan (Rigaku Oxford Diffraction, 2017) $T_{\text{min}} = 0.473$, $T_{\text{max}} = 0.531$
Refinement	
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1660 / 0 / 101
Goodness-of-fit on F^2	1.052
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0266$, $wR_2 = 0.0582$
R indices (all data)	$R_1 = 0.0328$, $wR_2 = 0.0603$
Largest diff. peak and hole	0.532 and -0.566 e.Å^{-3}

III. Table S2 selected bond lengths (Å) and bond angles (°) for compound (6)

Bond lengths (Å)			
Cu(1)-Cu(1) ⁱ	2.6118(5)	Cu(1)-O(3)	1.9847(15)
Cu(1)-O(1)	2.1411(17)	Cu(1)-O(4)	1.9415(15)
Cu(1)-O(2)	1.9907(15)	Cu(1)-O(5)	1.9559(15)

Symmetry Code: (i) -x+1, -y+1, -z+1

Bond angles (°)			
O(2)-Cu(1)-O(1)	92.58(7)	O(4)-Cu(1)-O(2)	90.29(6)
O(3)-Cu(1)-O(1)	98.35(7)	O(5)-Cu(1)-O(2)	89.42(6)
O(4)-Cu(1)-O(1)	97.28(7)	O(4)-Cu(1)-O(3)	87.20(6)
O(5)-Cu(1)-O(1)	93.52(7)	O(5)-Cu(1)-O(3)	91.06(6)

Table S3. Hydrogen bonded geometries in compound (6)

Bond	D - H	H···A	D···A	D - H···A
O(1)-H(1A)···O(3) ⁱⁱⁱ	0.73(3)	2.16(3)	2.892(3)	171(3)
O(1)-H(1B)···O(2) ^{iv}	0.77(3)	2.02(3)	2.786(2)	175(4)
C(4)-H(4A)···O(5) ^v	0.96	2.58	3.522(3)	168

Symmetry Code: (iii) -1/2-x, 1/2-y, -z; (iv) -x, y, 1/2-z; (v) 1/2+x, 1/2+y, z