Electronic Supplementary Information

Green click synthesis of β-hydroxy-1,2,3-triazoles in water in the presence of Cu(II)-Azide catalyst: A new function for Cu(II)-Azide complexes

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Table S1. Hydrogen bonding interactions in the crystal structure of **1Ph-triazole** and **2Ph-triazole**.

D-H…A	d(D-H)	d(H…A)	d(D…A)	<(DHA)
1Ph-triazole				
O12A-H12B…N3[-x+1/2, y+1/2, -z+1/2]	0.820	2.090	2.775	141.00
O12B-H12D…O12B [-x+1/2, -y+3/2, -z]	0.820	2.165	2.926	154.47
2Ph-triazole				
O12-H12C…O12[-x+1, y+1/2, -z+1/2]	0.820	2.088	2.904	172.66
C5-H5A…N3[x,1+y,z]	0.930	2.670	3.471	144.68
O12-H12C…C12[-x+1, y+1/2, -z+1/2]	0.820	2.843	3.619	158.60

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Table S2. Selected bond lengths [Å] and angles [°] for **1Ph-triazole** and **2Ph-triazole**.

2Ph-triazole		**1Ph-triazole**	
Bond lengths [Å]			
C11-N1	1.457(8)	C11-N1	1.458(10)
N1-N2	1.333(7)	N1-N2	1.328(9)
N2-N3	1.330(8)	N2-N3	1.331(9)
N3-C4	1.342(8)	N3-C4	1.366(10)
C4-C5	1.361(8)	C4-C5	1.363(11)
C11-C12	1.506(10)	C11-C12	1.466(13)
C12-O12	1.425(8)	C12-O12A C12-O12B	1.323(14) 1.245(18)
C11-C13	1.509(9)	C12-C13	1.476(14)
Angles [°]			
C13-C11-C12	110.4(5)	C11-C12-C13	111.4(10)
C13-C11-N1	111.8(5)	C12-C11-N1	115.2(8)
C11-C12-O12	113.3(6)	C11-C12-O12A C11-C12-)12B	112.4(11) 125.7(14)
C11-N1-N2	122.3(5)	C11-N1-N2	120.2(8)
C11-N1-C5	127.2(5)	C11-N1-C5	128.7(8)
N1-N2-N3	107.2(5)	N1-N2-N3	107.1(7)
N2-N3-C4	108.2(5)	N2-N3-C4	108.4(7)
N3-C4-C5	107.4(5)	N3-C4-C5	107.5(9)
C4-C5-N1	106.9(5)	C4-C5-N1	105.8(9)
C5-N1-N2	110.2(5)	C5-N1-N2	111.2(8)

Table S3. Crystal data and structure refinement parameters for **1Ph-triazole**.

Net formula	$C_{16}H_{15}N_3O$	Density (calc.), g cm^{-3}	1.234
Formula weight, g mol^{-1}	265.31	Abs. coefficient, mm^{-1}	0.08
Wavelength, Å	0.71073	$F(000)$	1120
T, K	293(2)	Θ range, deg	2.1–28.4
Crystal size, mm	0.44 × 0.36 × 0.03	Independent reflections	3193
Crystal shape, color	Plate, colourless	Measured reflections	7072
Crystal system	Monoclinic	Reflections with $I > 2\sigma(I)$	965
Space group	*C2/c*	restraints/parameters	0/193
a, Å	30.336(6)	R_{int}	0.297
b, Å	10.076(2)	$R[F^2 > 2\sigma(F^2)]$	0.199
c, Å	9.509(2)	$wR(F^2)$	0.374
β, deg	100.65(3)	Goodness of fit on F^2	1.10
Volume, Å^3	2856.5(10)	Max electron density/eÅ^{-3}	0.33
Z	8	Min electron density/eÅ^{-3}	-0.29

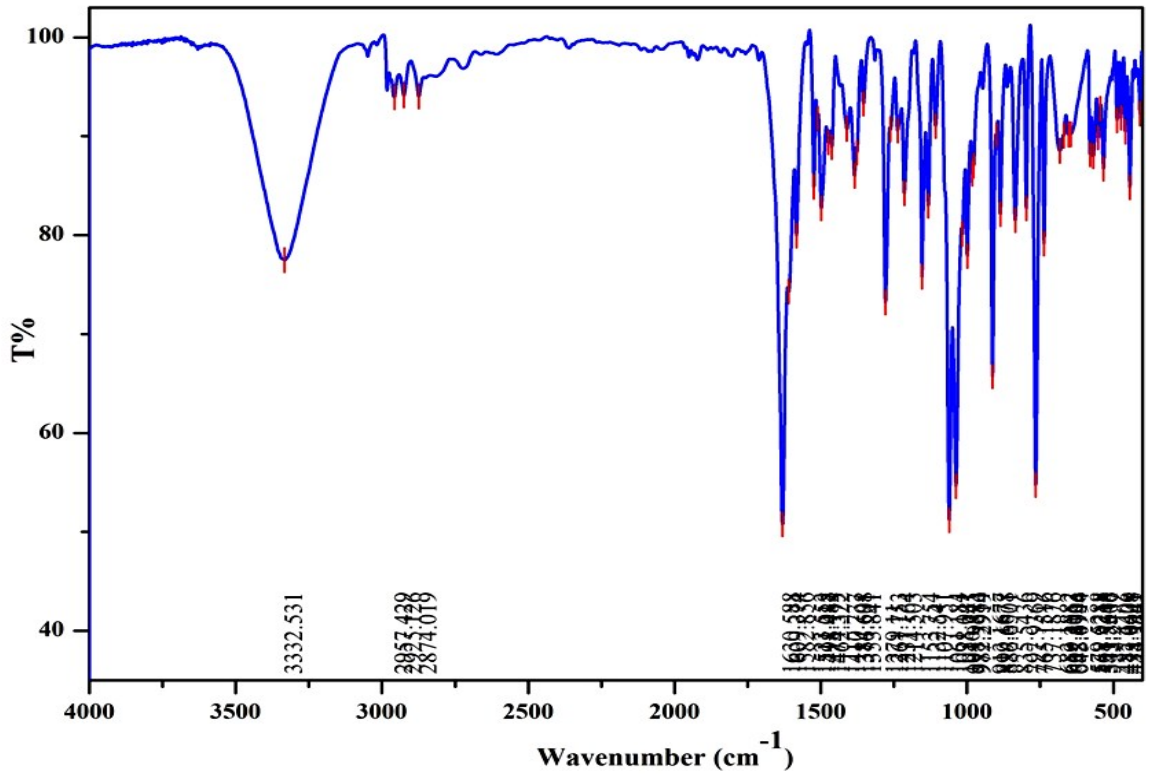


Fig. S1. FT-IR spectrum of **H_3L**

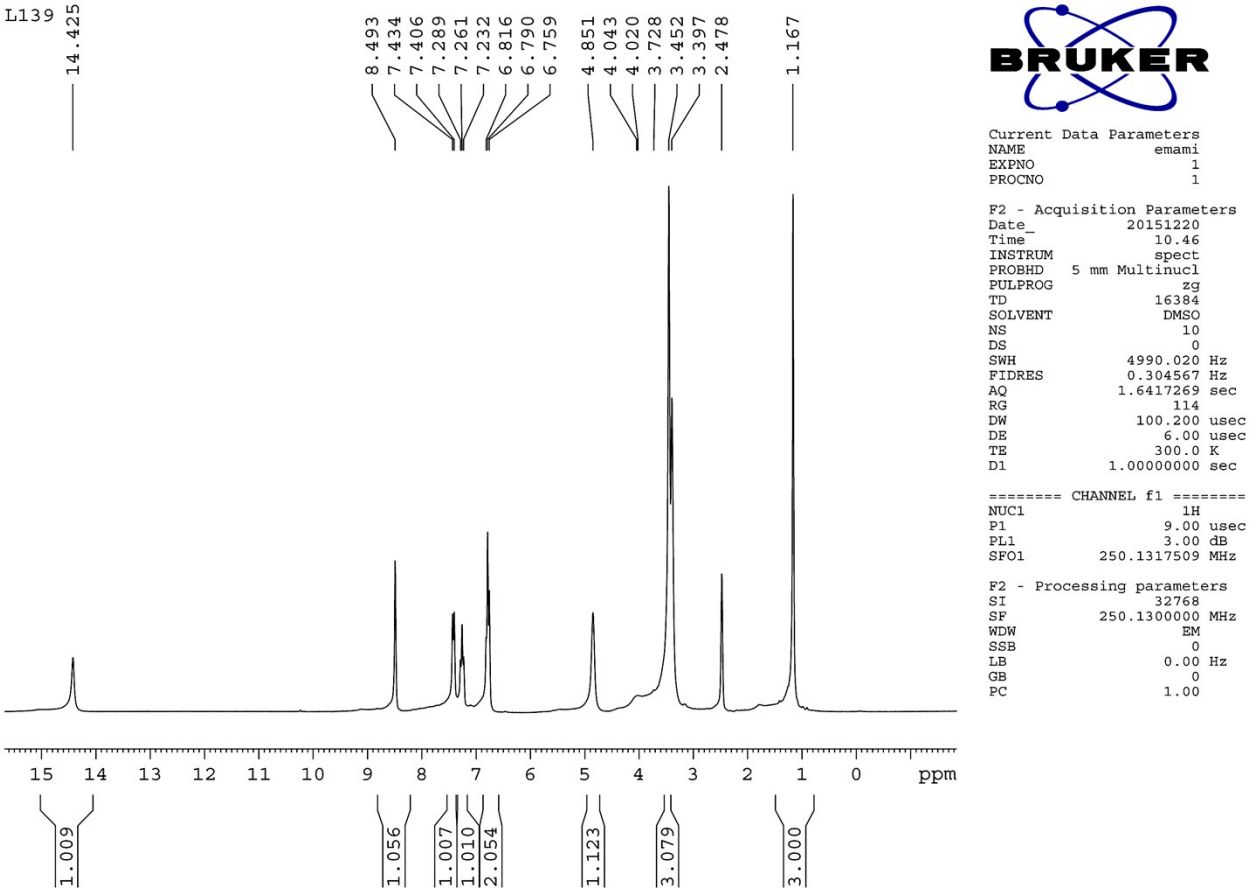


Fig. S2. ^{1}H NMR spectrum of **H_3L**

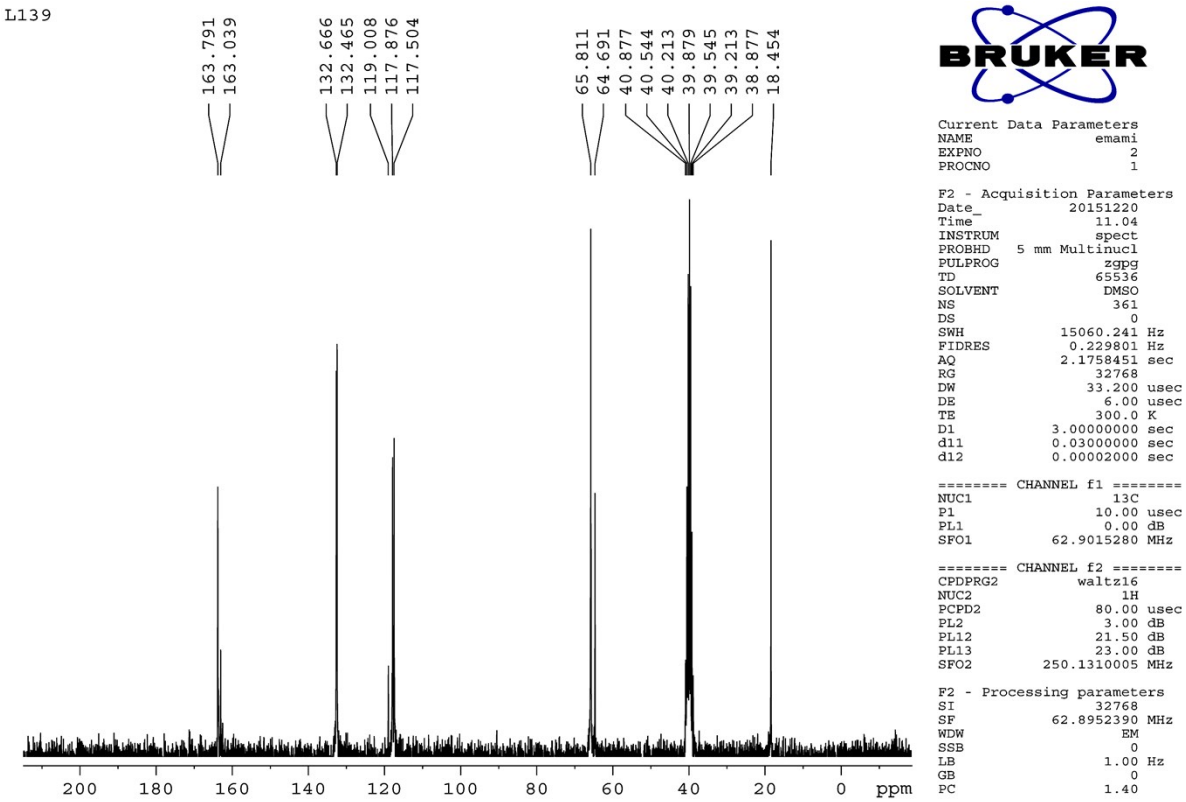


Fig. S3. ^{13}C NMR spectrum of $\mathbf{H_3L}$

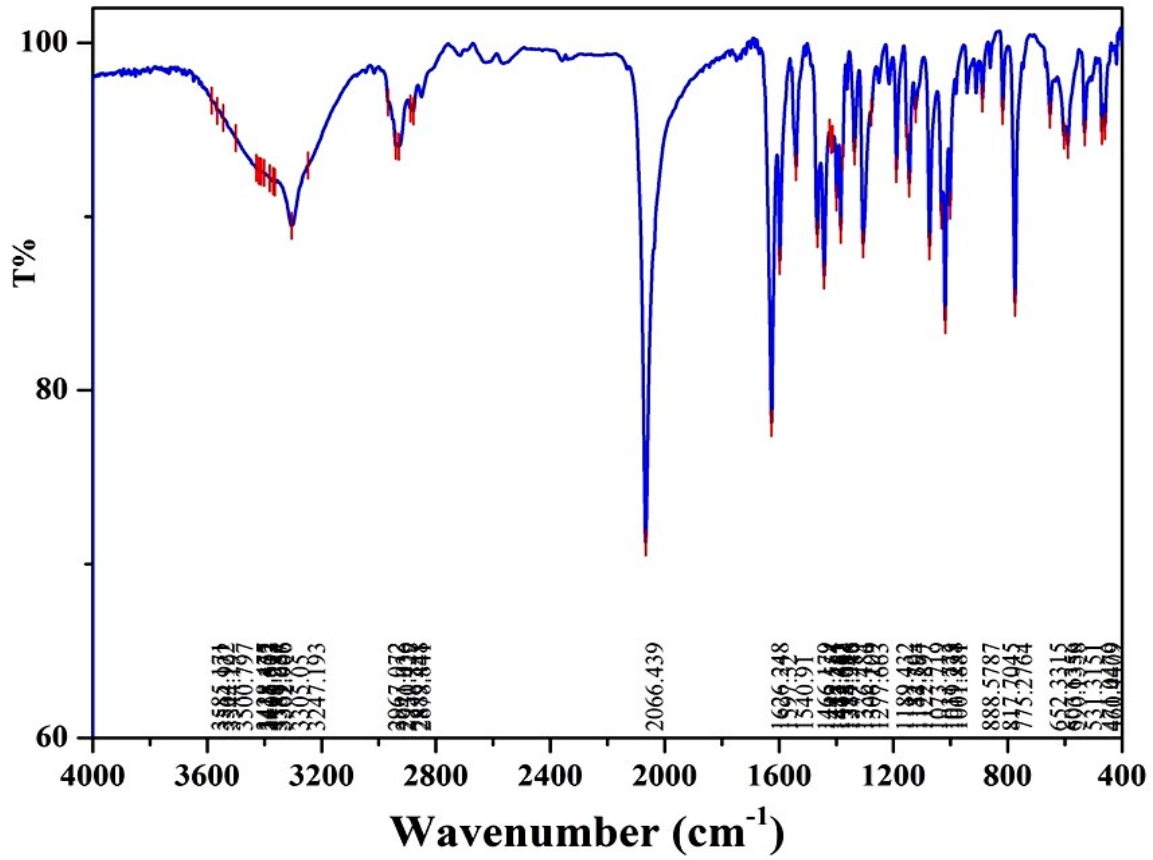


Fig. S4. FT-IR spectrum of complex **1**

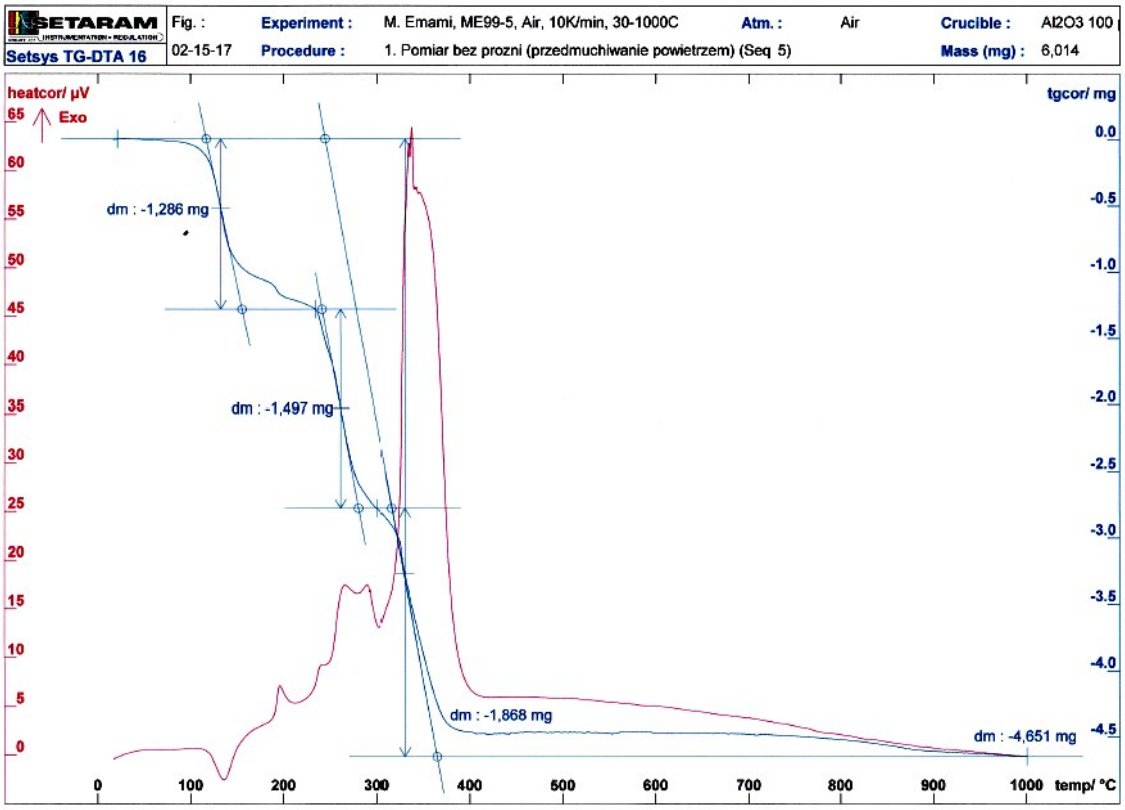


Fig. S5. TGA analysis of complex **1** under air atmosphere

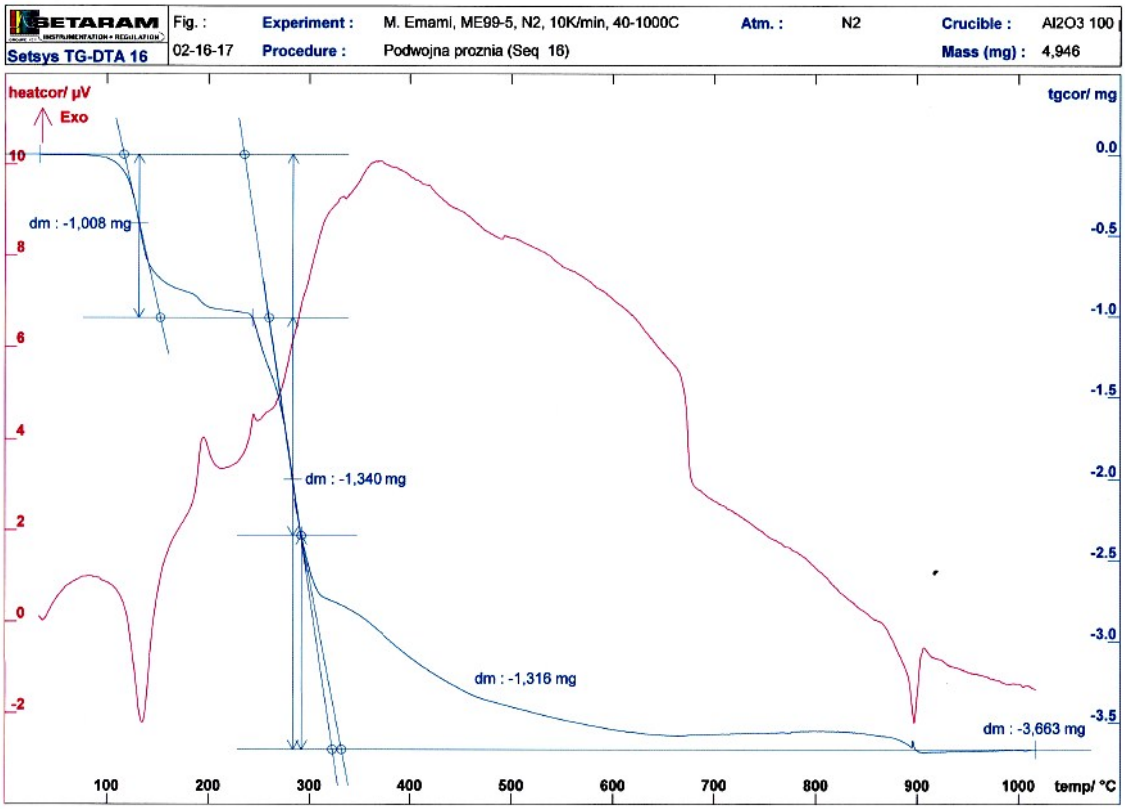


Fig. S6. TGA analysis of complex **1** under N_2 gas atmosphere

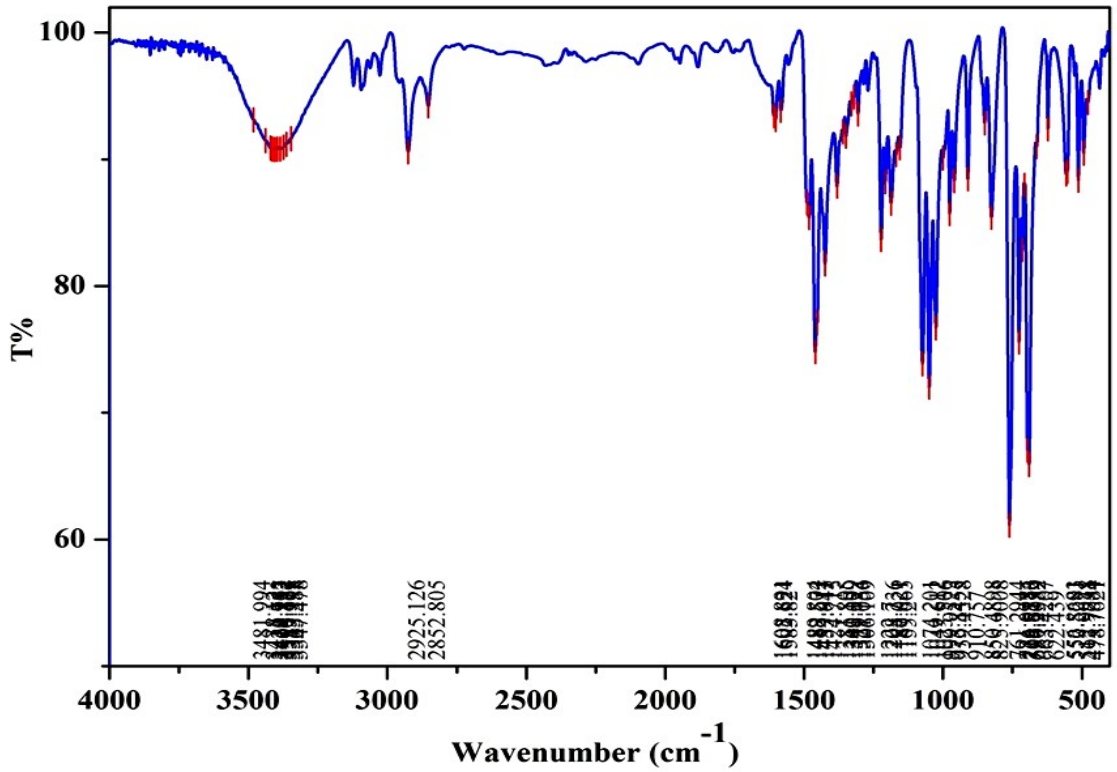


Fig. S7. FT-IR spectrum of **2Ph-triazole**

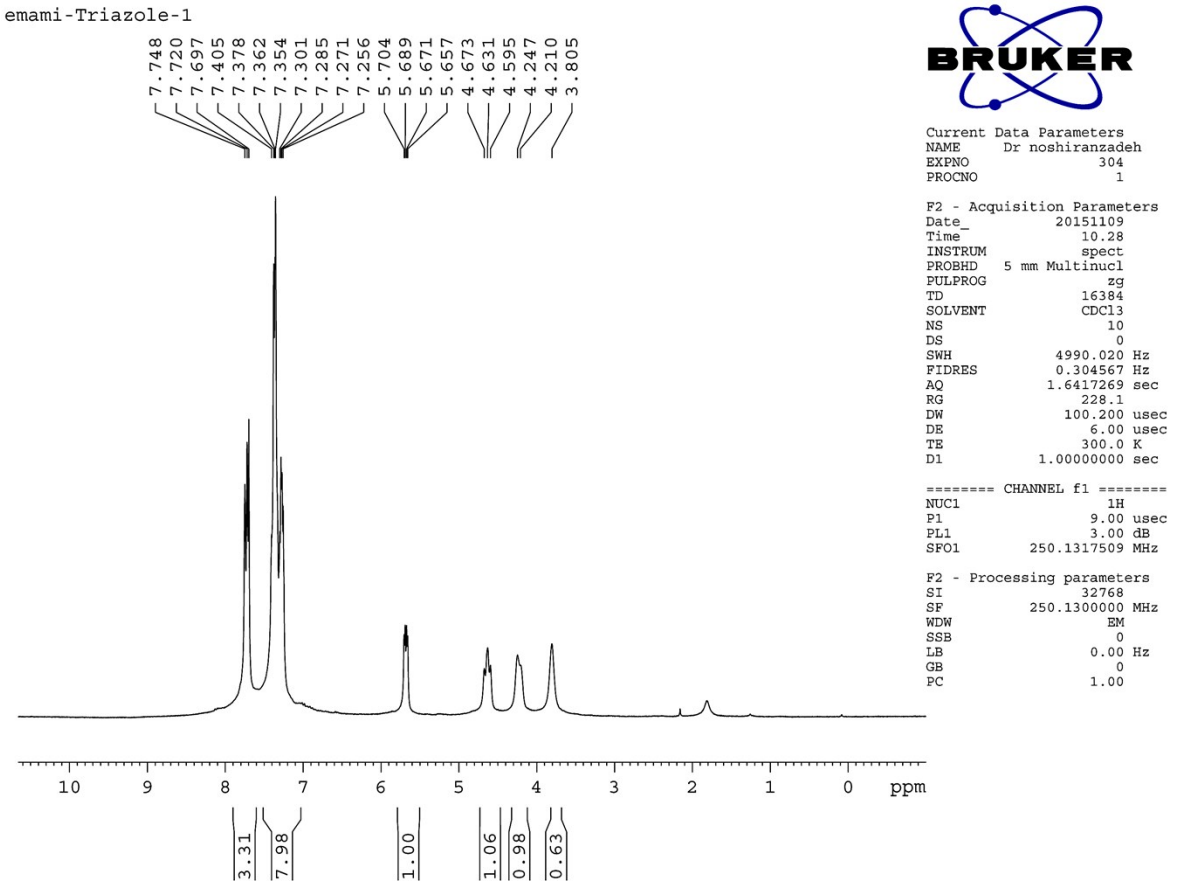


Fig. S8. ^{1}H NMR spectrum of **2Ph-triazole**

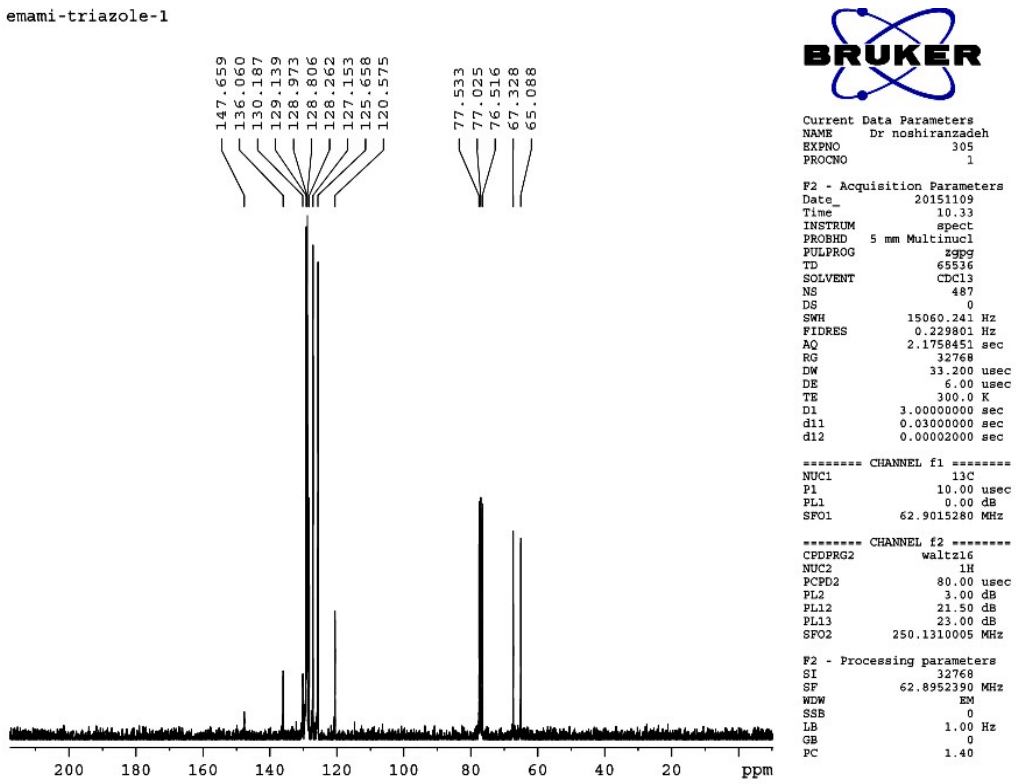


Fig. S9. ^{13}C NMR spectrum of **2Ph-triazole**

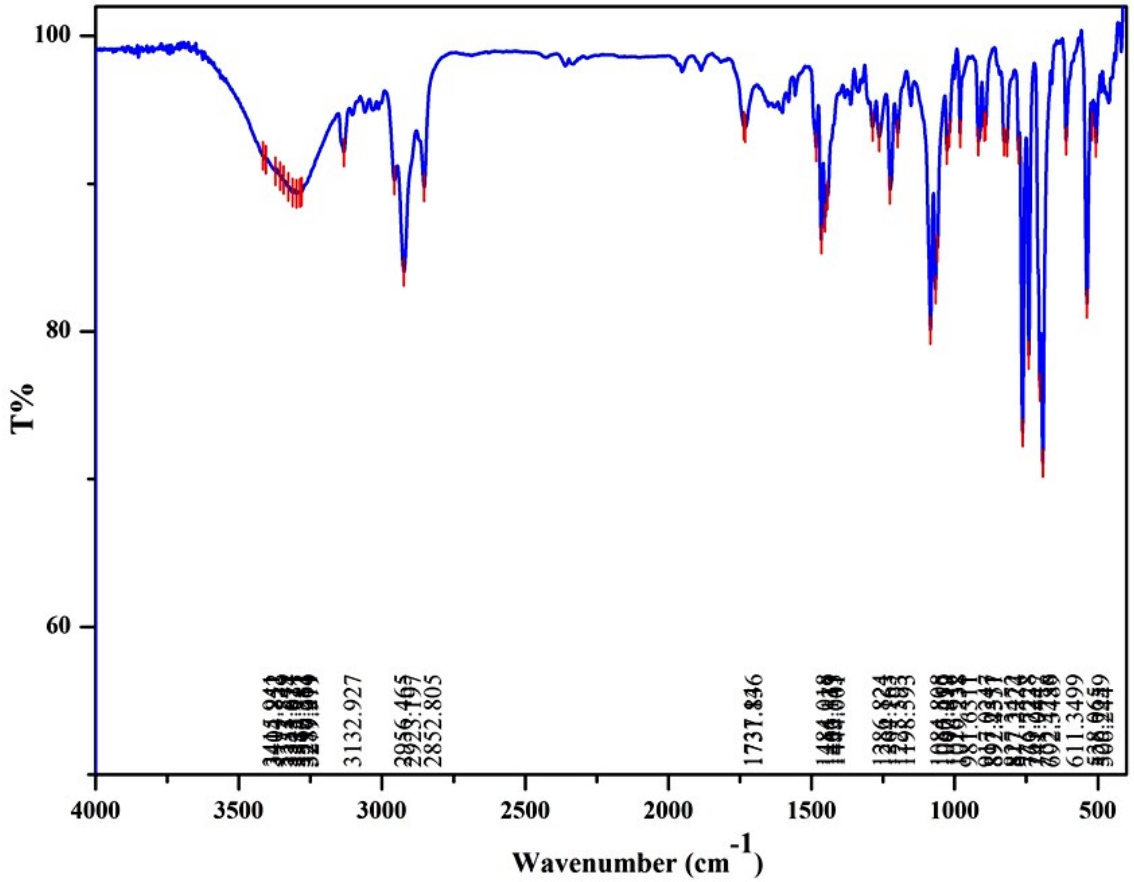


Fig. S10. FT-IR spectrum of **1Ph-triazole**

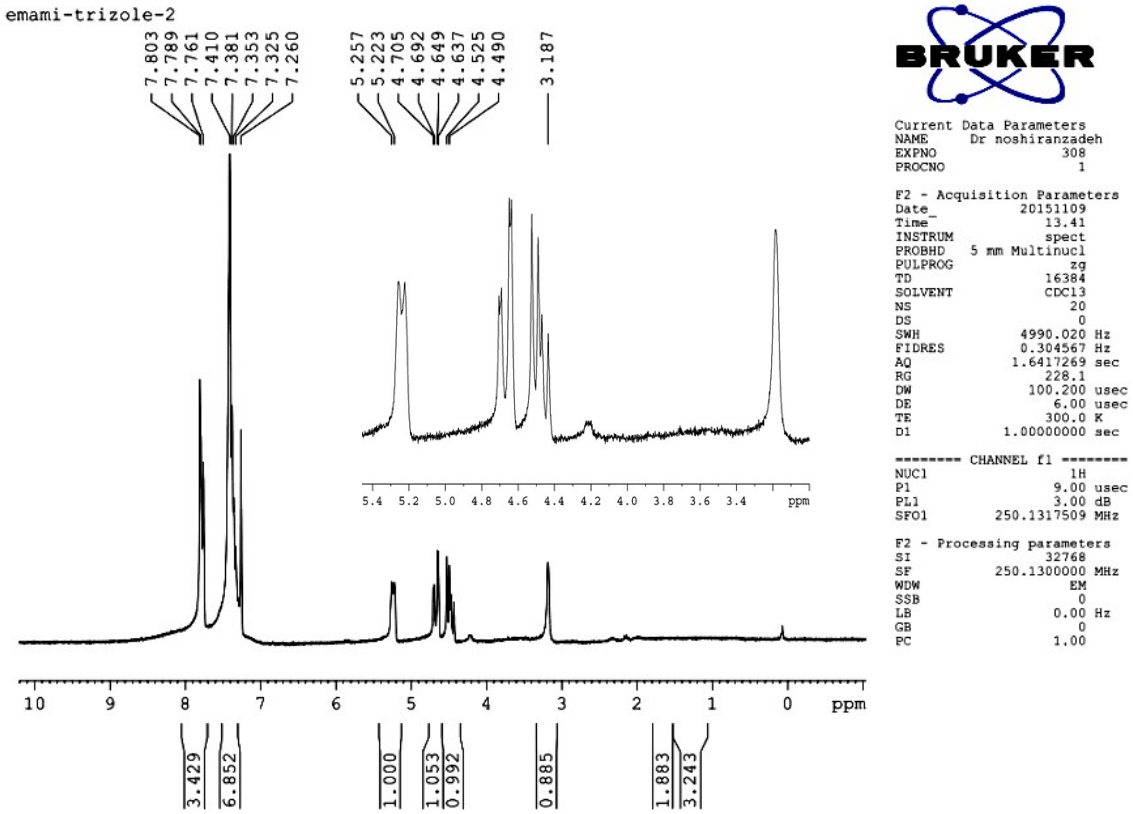


Fig. S11. ^{1}H NMR spectrum of **1Ph-triazole**

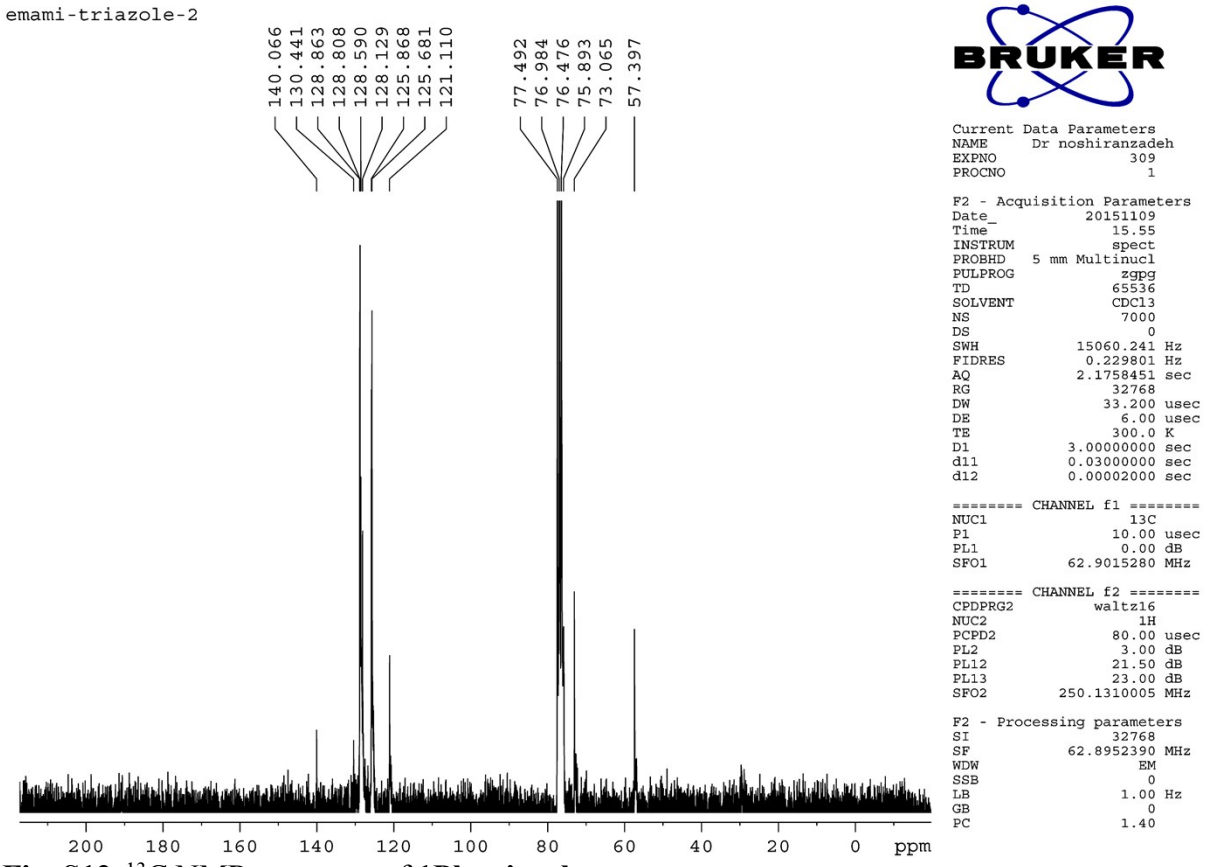


Fig. S12. ^{13}C NMR spectrum of **1Ph-triazole**

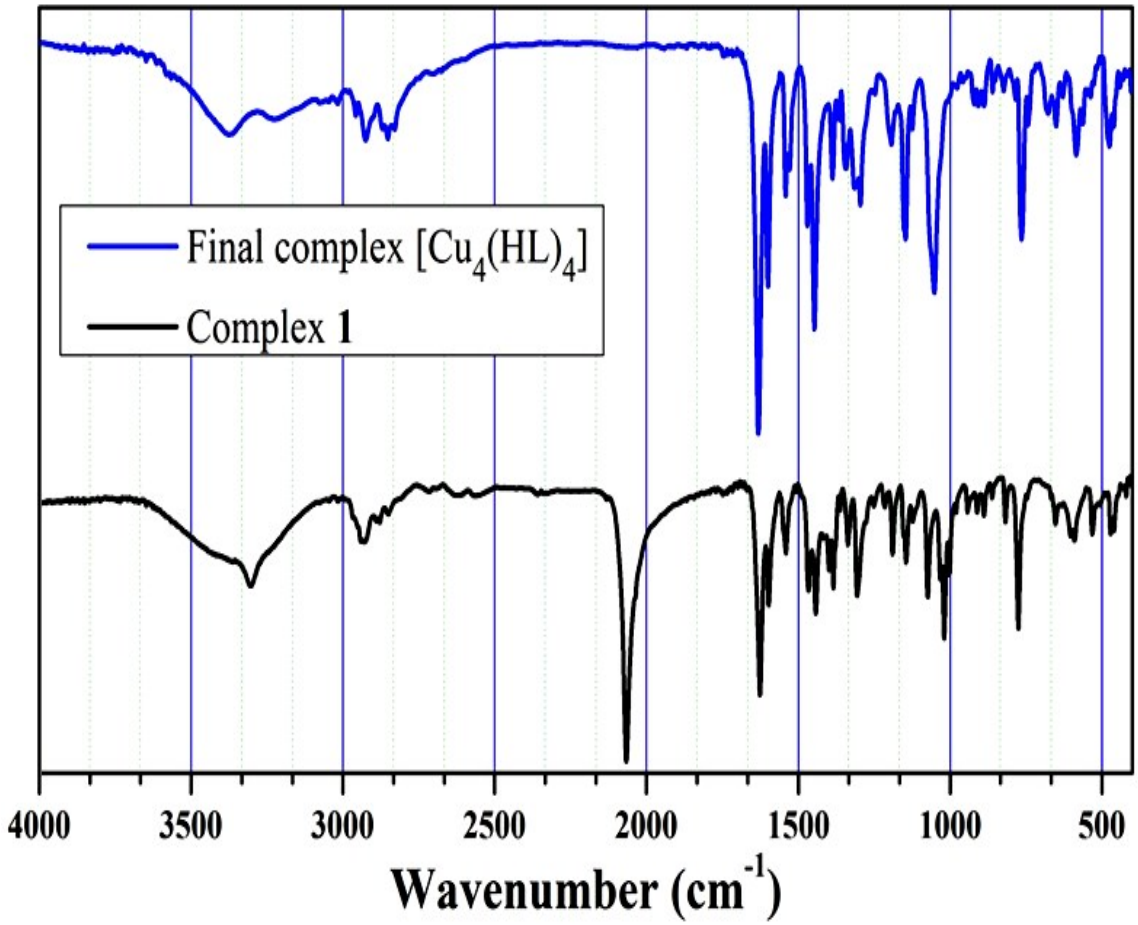


Fig. S13. Comparing the FT-IR spectrum of complex **1** (black) final green product obtained after reaction of epoxystyrene, phenylacethylene and complex **1** (blue) in the absence of sodium azide.

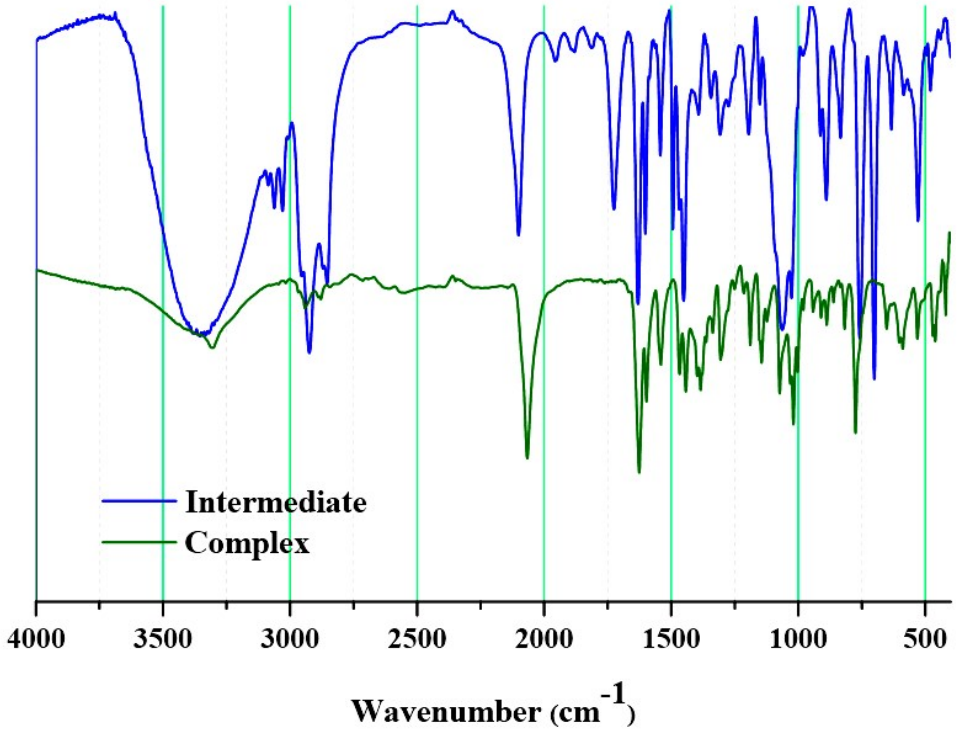
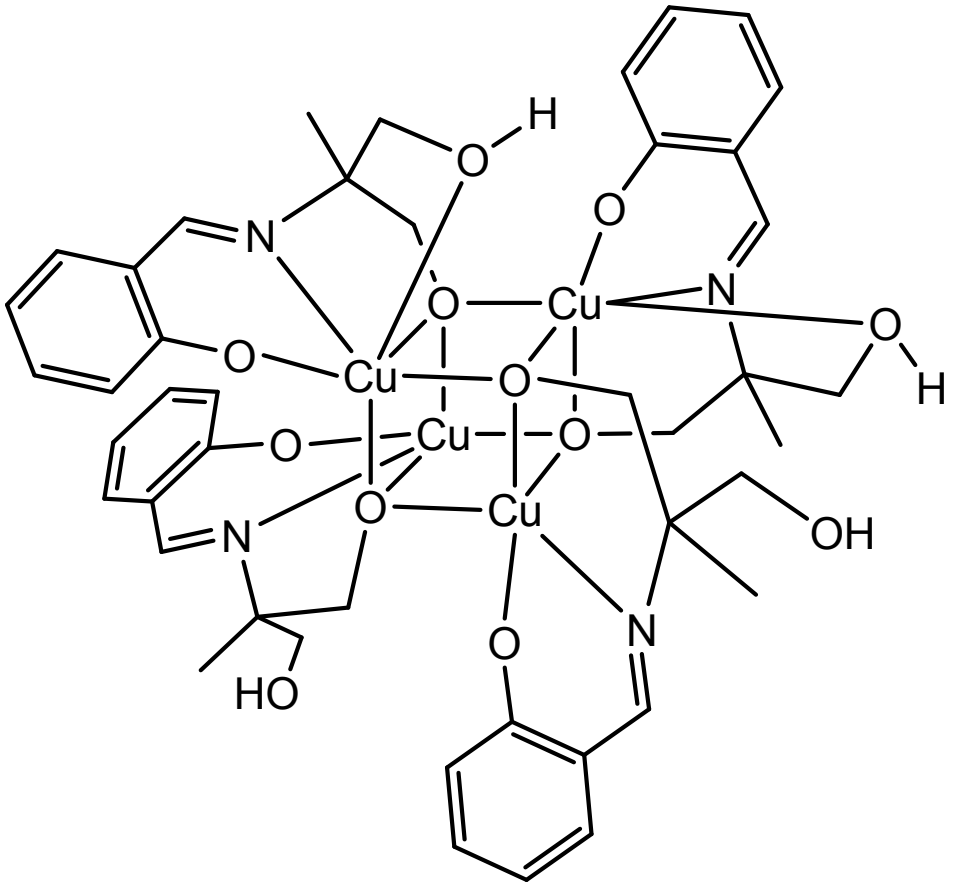


Fig. S14. Comparing the FT-IR spectrum of complex **1** with the Cu-complex obtained by the reaction of epoxystyrene with complex **1** in the absence of sodium azide and phenylacetylene.



Scheme S1. The molecular structure of the complex obtained after catalytic cycloaddition reaction in the absence of sodium azide.