

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)	\angle (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	1.323(14)
C11-C13	1.509(9)	C12-O12B	1.245(18)
		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	112.4(11)
		C11-C12-O12B	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 ₃ O	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 > 2σ(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 > 2σ(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

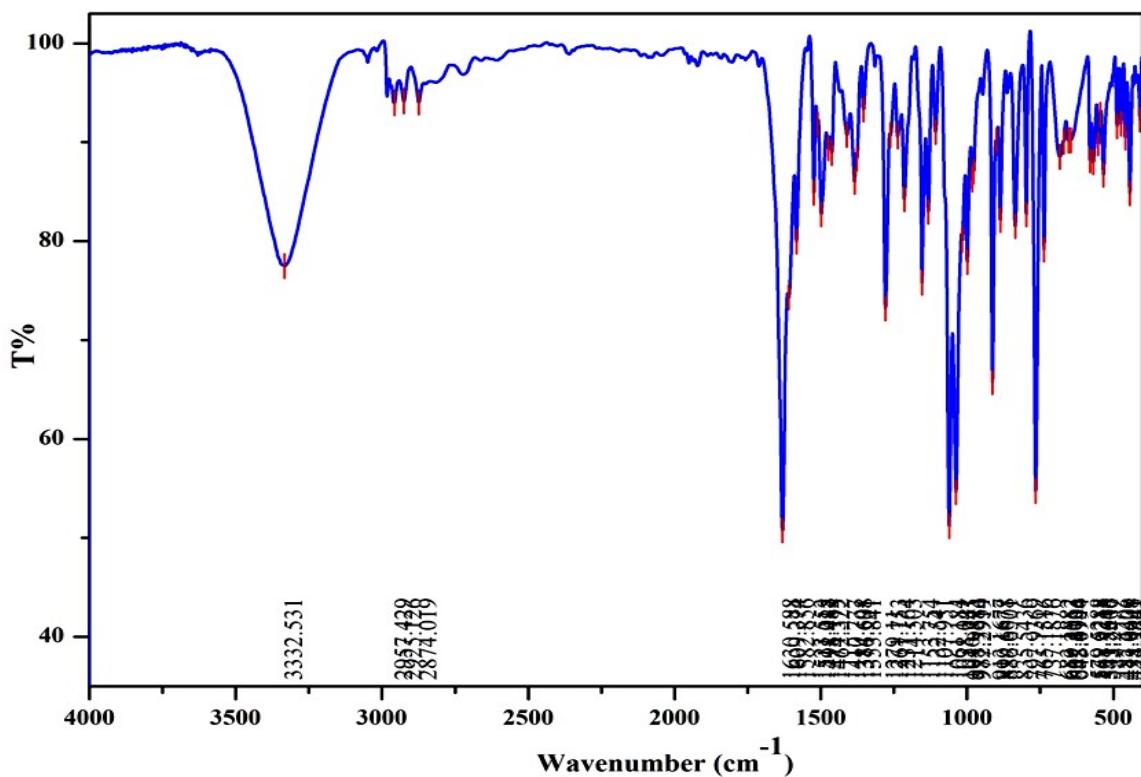


Fig. S1. FT-IR spectrum of H_3L

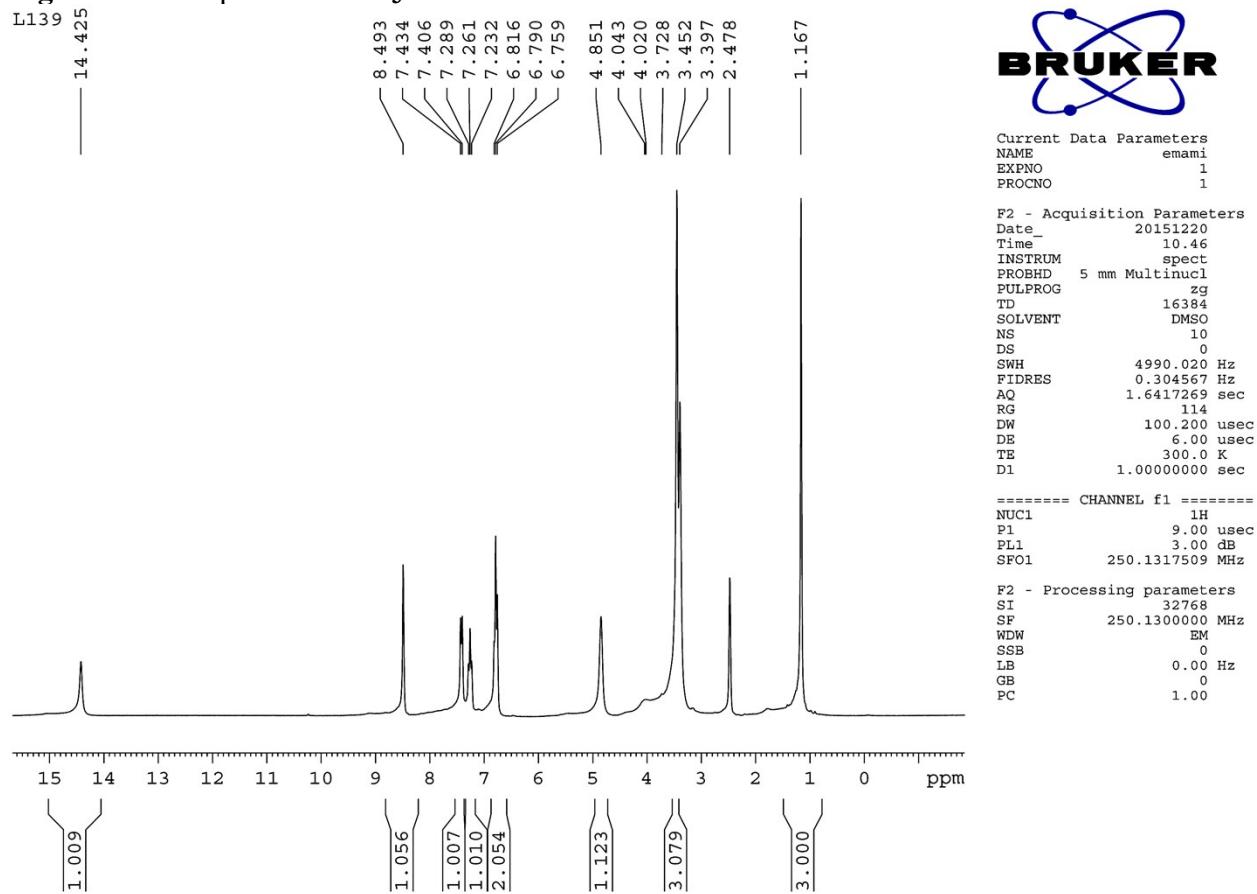


Fig. S2. ¹H NMR spectrum of H_3L

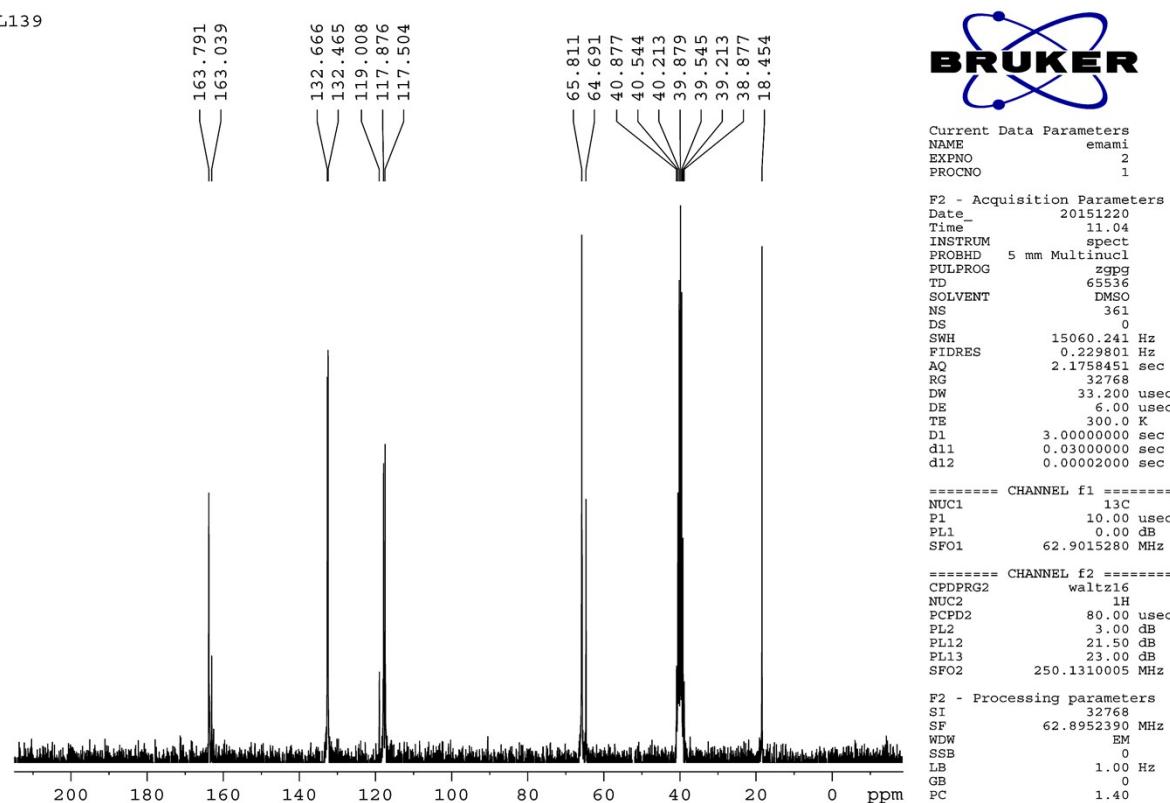
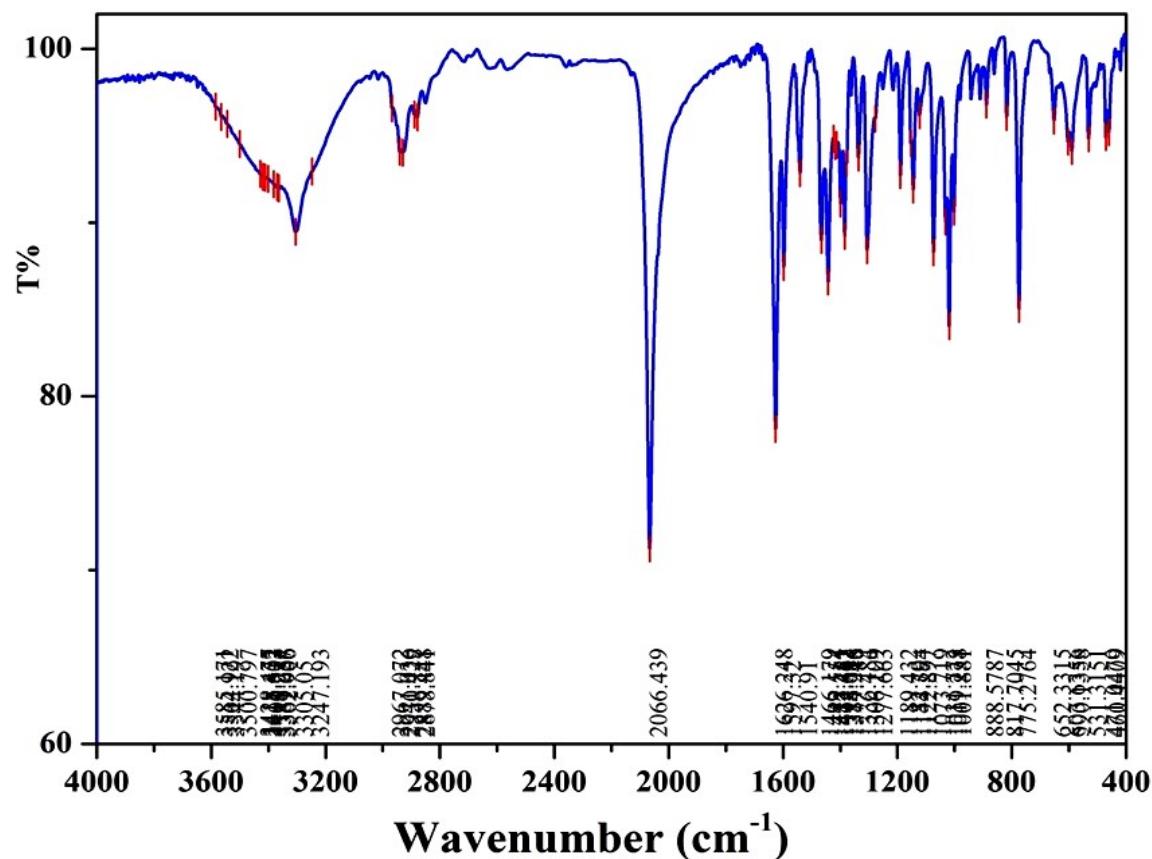
Fig. S3. ¹³C NMR spectrum of H_3L 

Fig. S4. FT-IR spectrum of complex 1

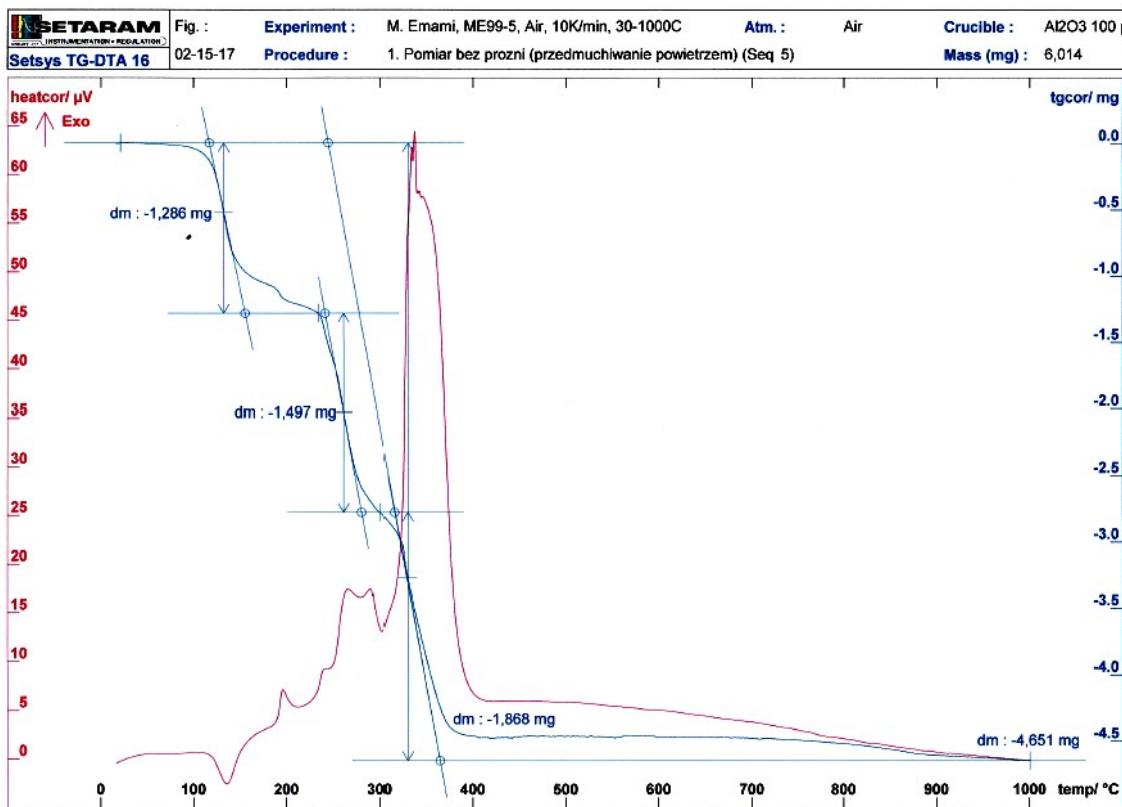


Fig. S5. TGA analysis of complex 1 under air atmosphere

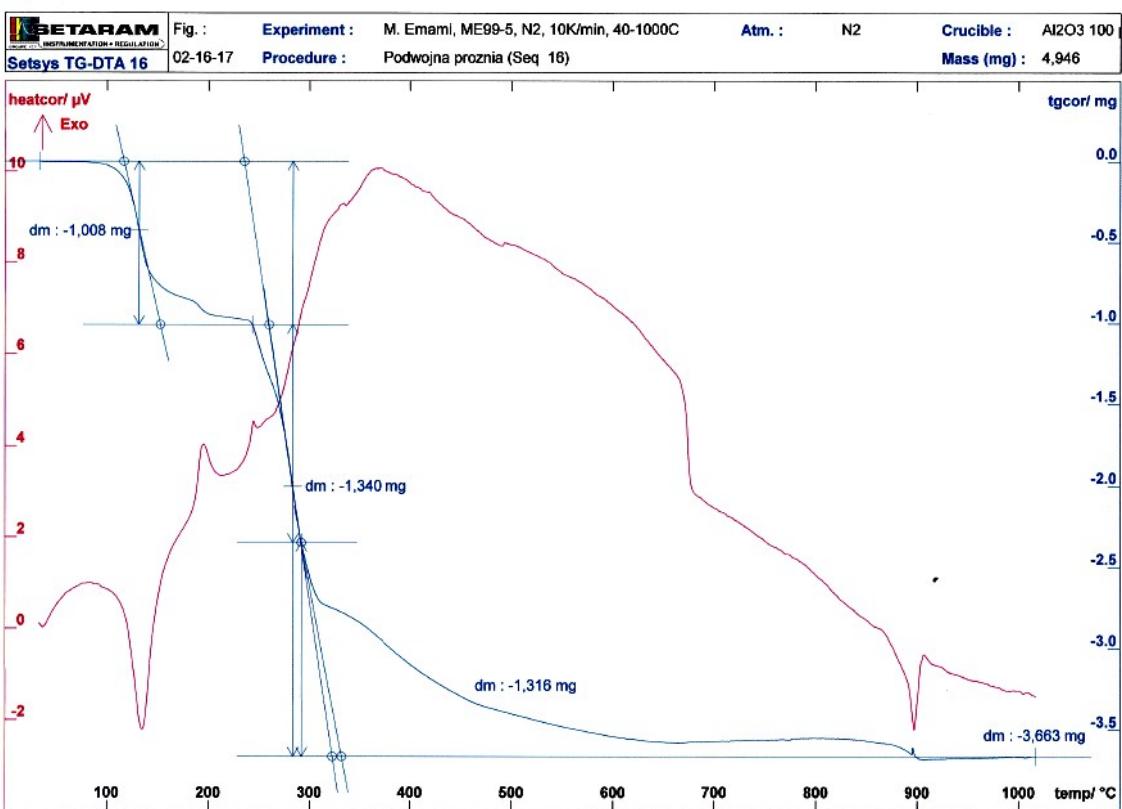


Fig. S6. TGA analysis of complex 1 under N₂ gas atmosphere

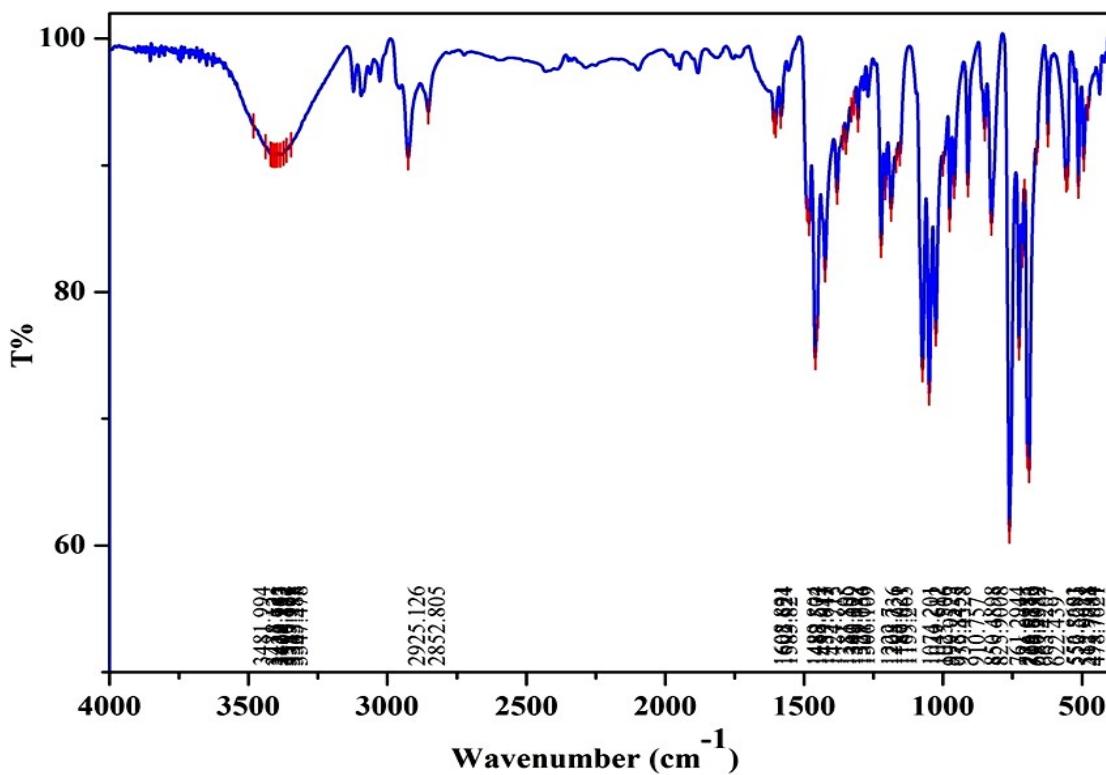


Fig. S7. FT-IR spectrum of 2Ph-triazole

emami-Triazole-1



Current Data Parameters
NAME Dr noshirzadeh
EXPNO 304
PROCNO 1

F2 - Acquisition Parameters
Date 20151109
Time 10.28
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg
TD 16384
SOLVENT CDCl₃
NS 10
DS 0
SWH 4990.020 Hz
FIDRES 0.304567 Hz
AQ 1.6417269 sec
RG 228.1
DW 100.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.00 usec
PL1 3.00 dB
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F2 - Processing parameters
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PC 1.00

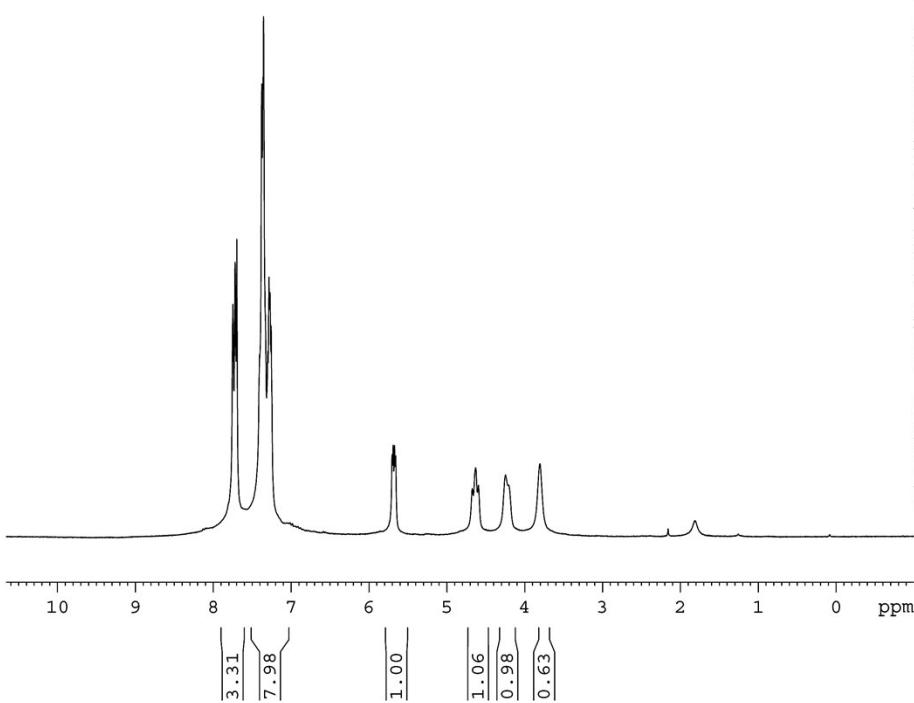


Fig. S8. ¹H NMR spectrum of 2Ph-triazole

emami-triazole-1



Current Data Parameters
NAME Dr noshiranzadeh
EXPNO 305
PROCNO 1

F2 - Acquisition Parameters
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Time 10.33
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SOLVENT CDCl3
NS 407
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SWH 15060.241 Hz
FIDRES 0.229801 Hz
AQ 2.1758451 sec
RG 32768
DW 33.200 usec
DE 6.00 usec
TE 300.0 K
D1 3.0000000 sec
d11 0.0300000 sec
d12 0.00002000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 10.00 usec
PL1 0.00 dB
SF01 62.8915280 MHz

***** CHANNEL f2 *****
CPDPGR2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 21.50 dB
PL13 23.00 dB
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F2 - Processing parameters
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SF 62.8952390 MHz
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PC 1.40

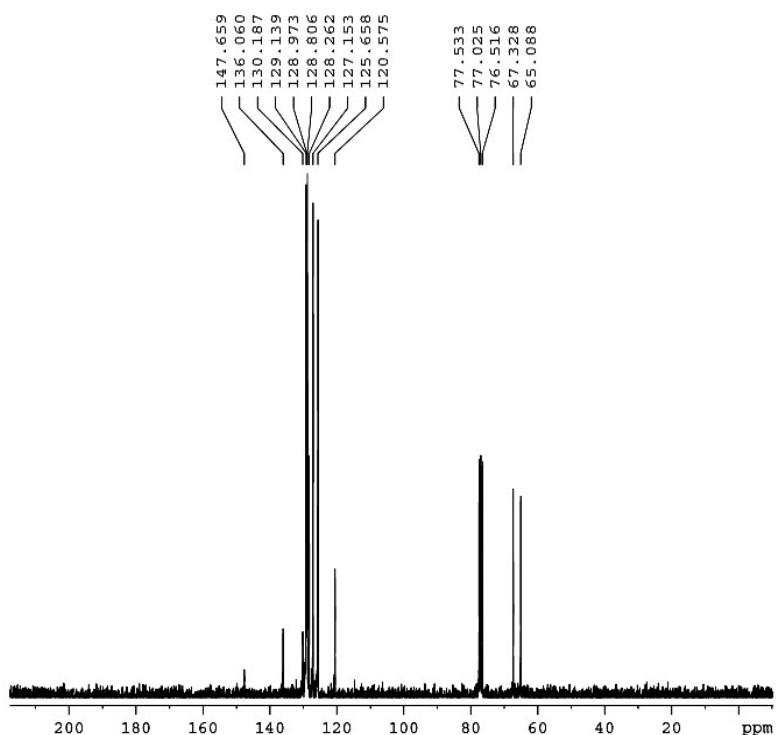


Fig. S9. ^{13}C NMR spectrum of 2Ph-triazole

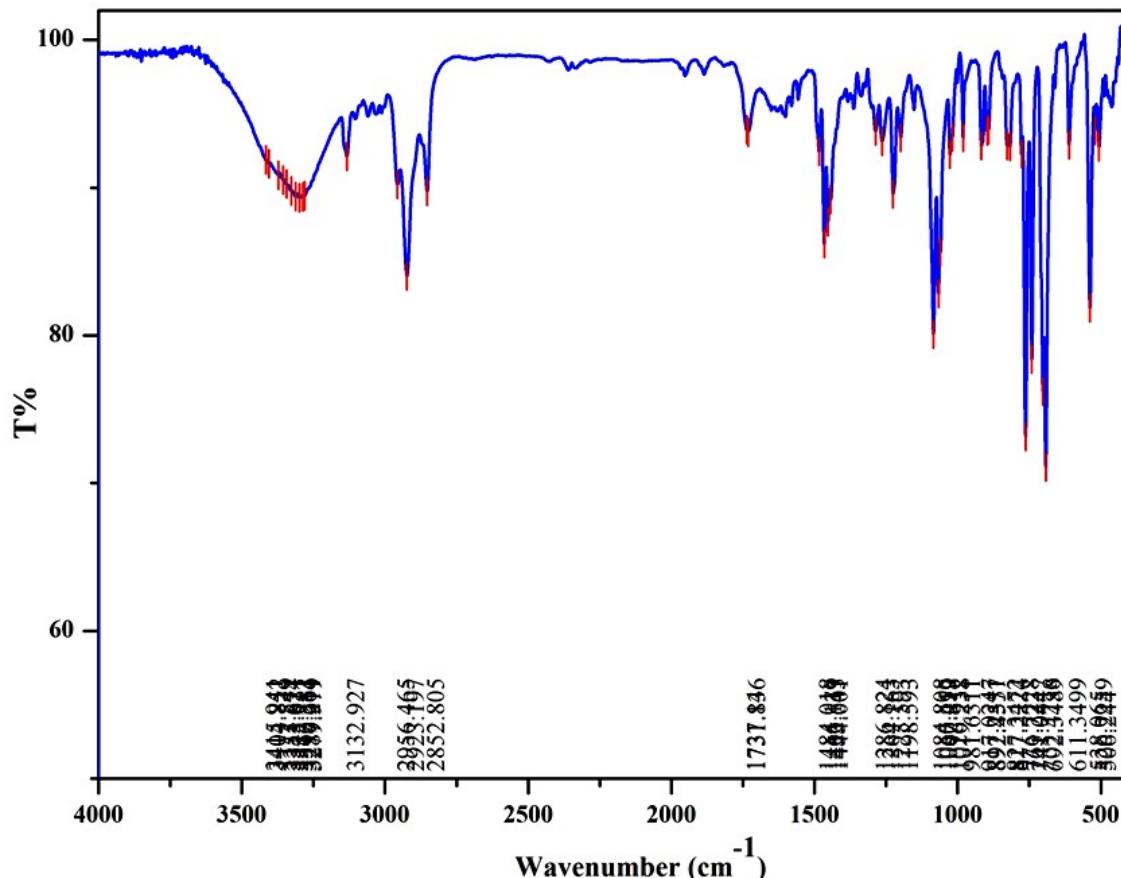


Fig. S10. FT-IR spectrum of 1Ph-triazole

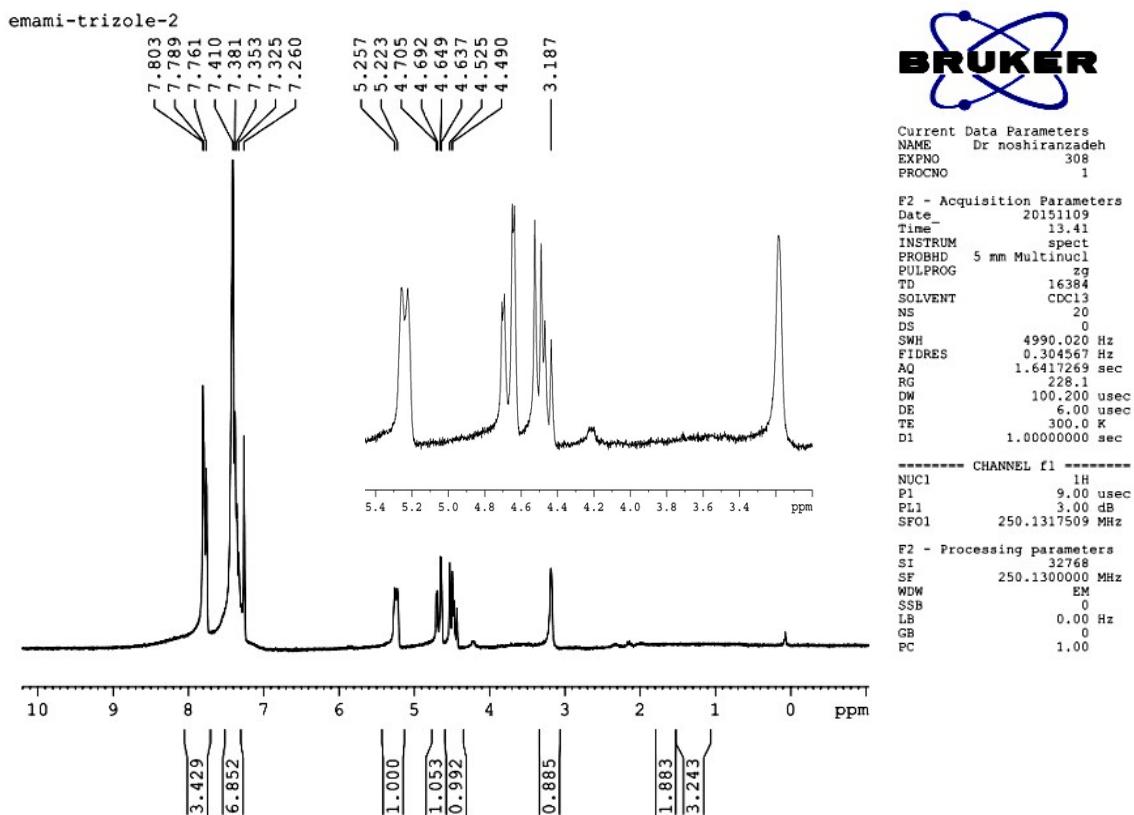


Fig. S11. ¹H NMR spectrum of 1Ph-triazole
emami-trizole-2

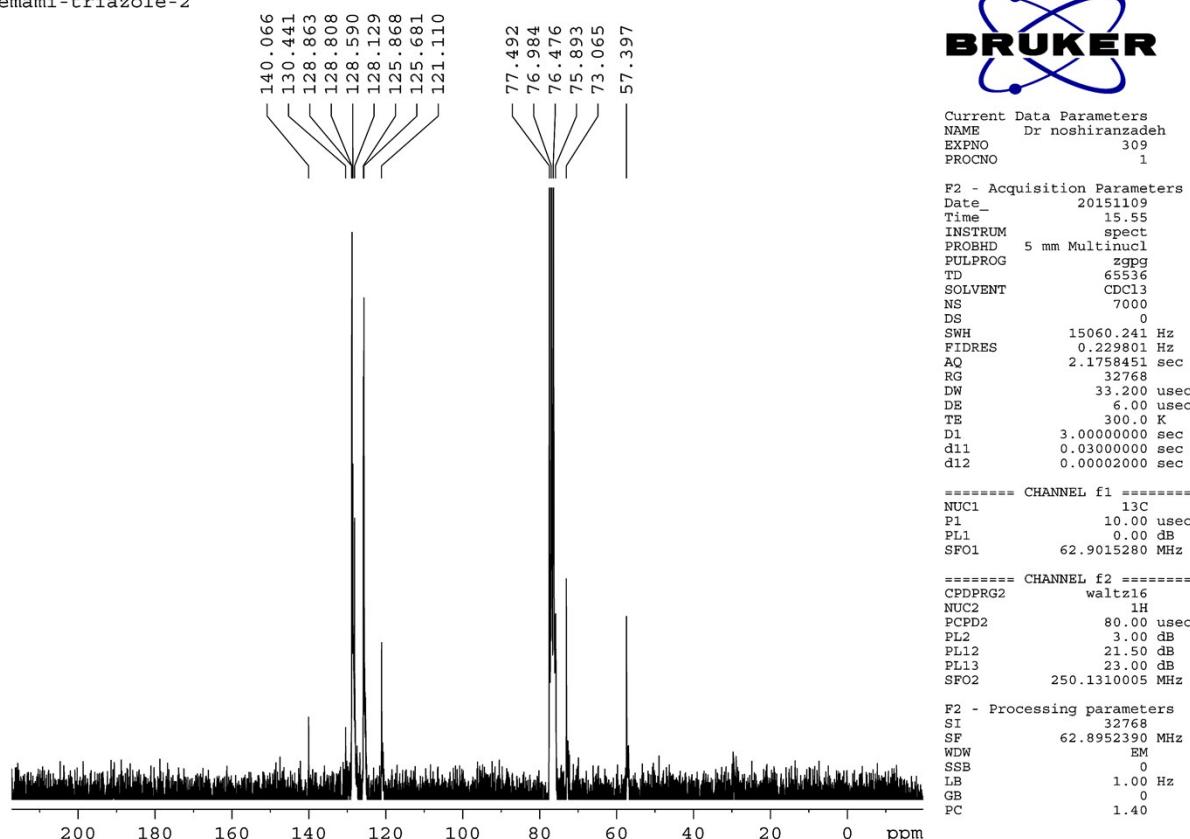


Fig. S12. ¹³C NMR spectrum of 1Ph-triazole

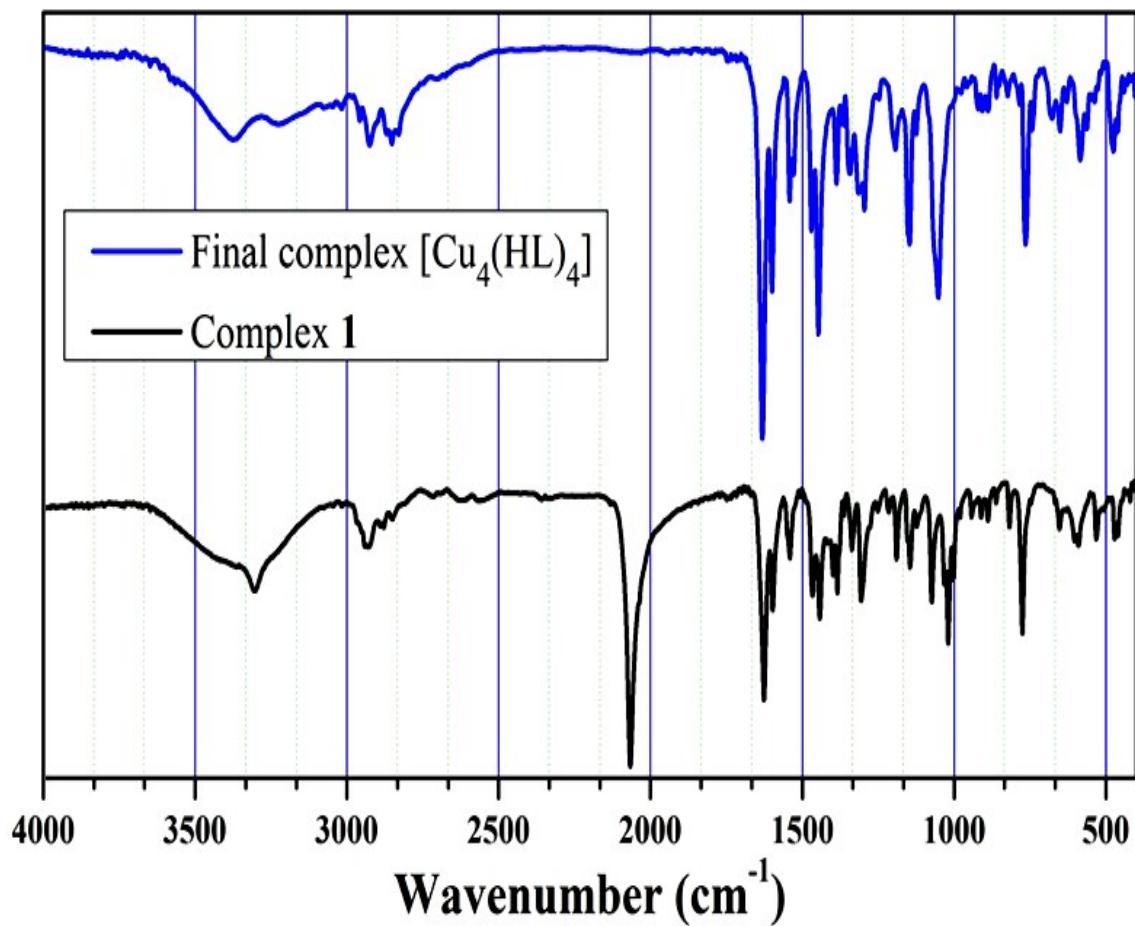


Fig. S13. Comparing the FT-IR spectrum of complex **1** (black) final green product obtained after reaction of epoxystyrene, phenylacetylene and complex **1** (blue) in the absence of sodium azide.

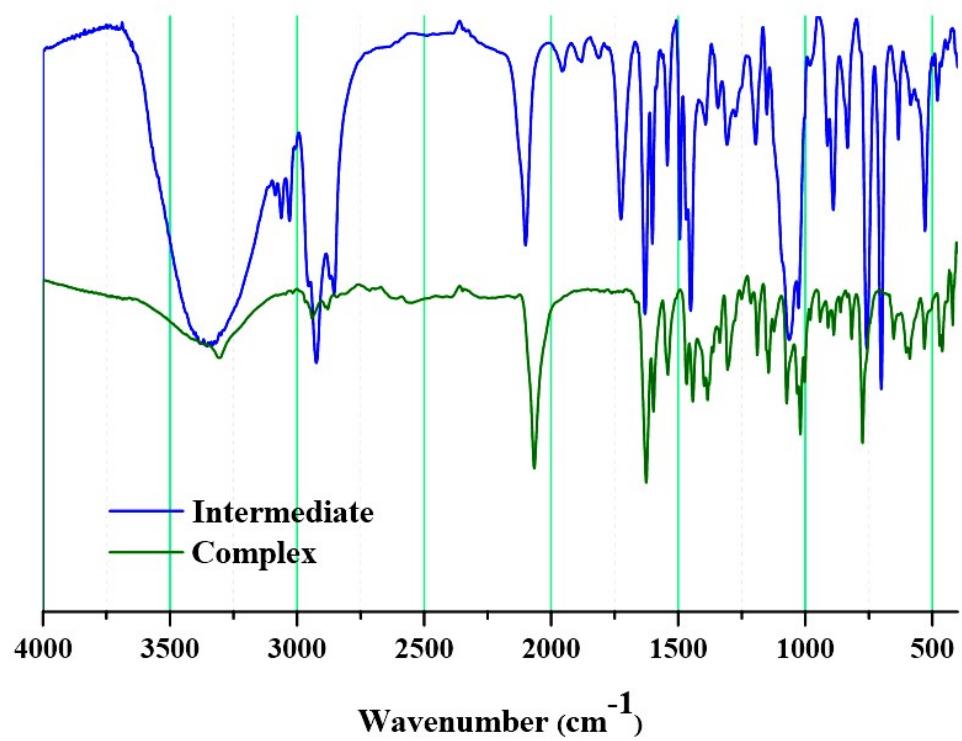
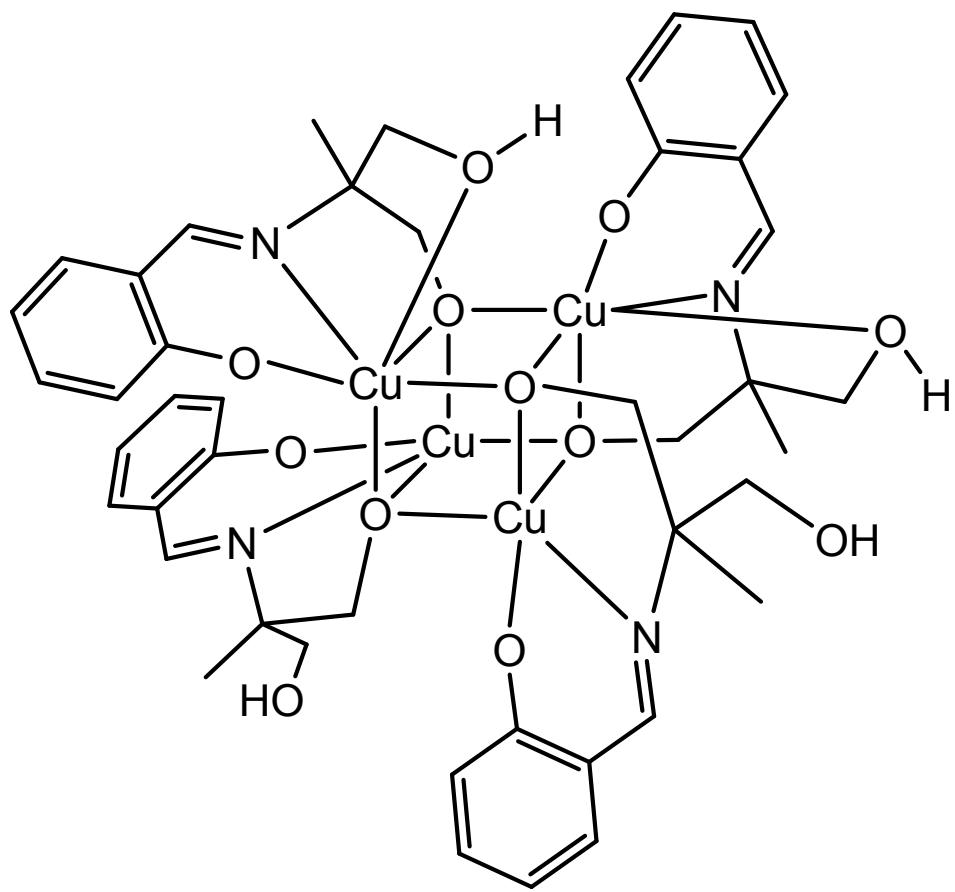


Fig. S14. Comparing the FT-IR spectrum of complex **1** with the Cu-complex obtained by the reaction of epoxystyrene with complex **1** in the absence of sodium azide and phenylacetylene.



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