Supporting information

Crystal structure of phenoxyl radical complex relevant to metal-site of galactose oxidase enzyme: A facile one-pot synthesis, evidence for hydrogen atom transfer and DNA cleavage via self-activation

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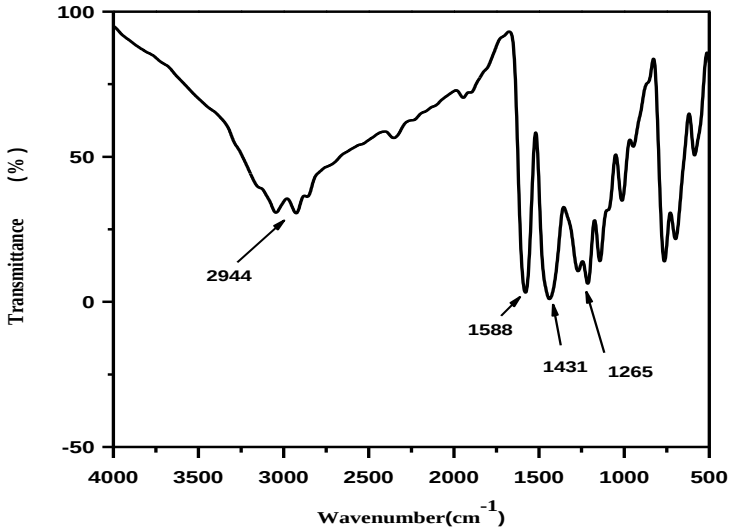


Figure S1: IR spectrum of 2,2'-((1E,1'E)-(2,2'-(pyridine-2,6-diyl)bis(2-phenylhydrazin-2-yl-1-ylidene))bis(methanylylidene))diphenol. [L^1H_2]

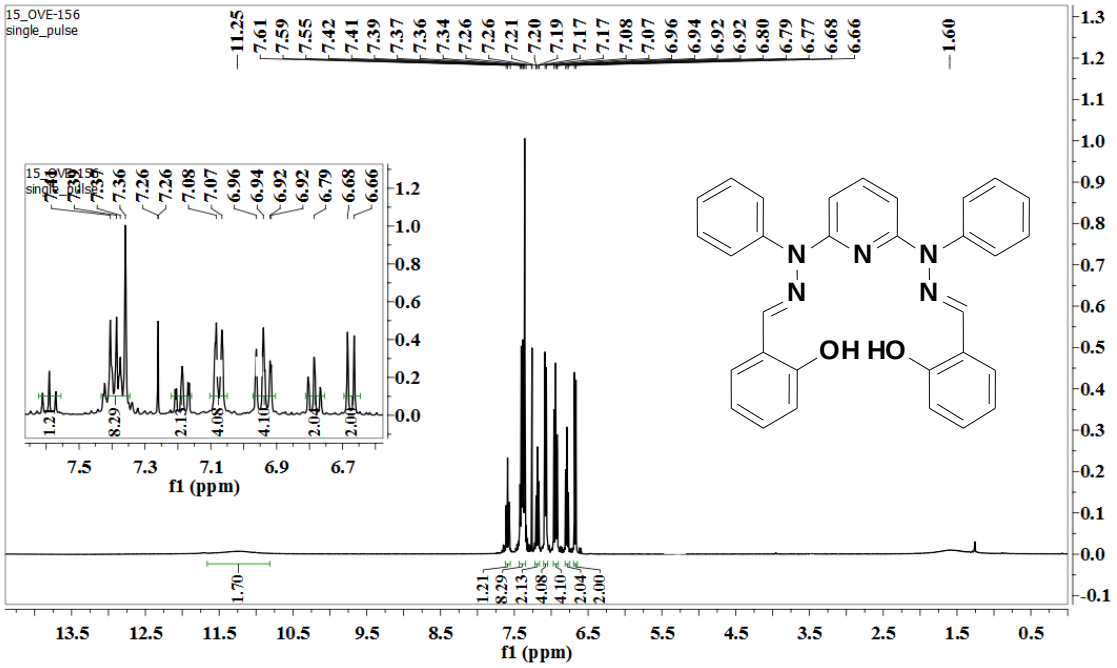


Figure S2: ^{1}H NMR spectrum of 2,2'-((1E,1'E)-(2,2'-(pyridine-2,6-diyl)bis(2-phenylhydrazin-2-yl-1-ylidene))bis(methanylylidene))diphenol. [$L^{1}H_2$]

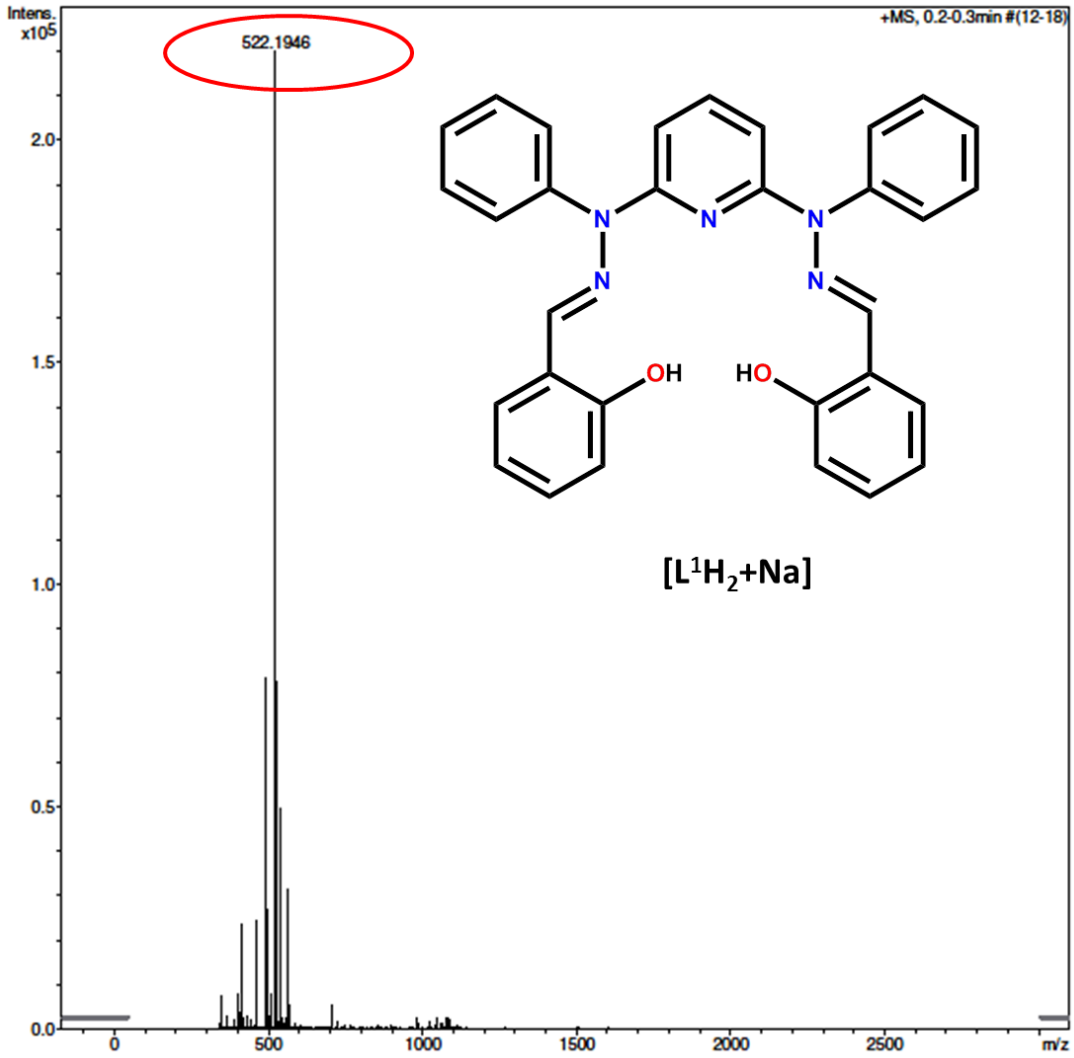


Figure S3**: ESI-MS spectra of ligand [$L^{1}H_2$+Na]**

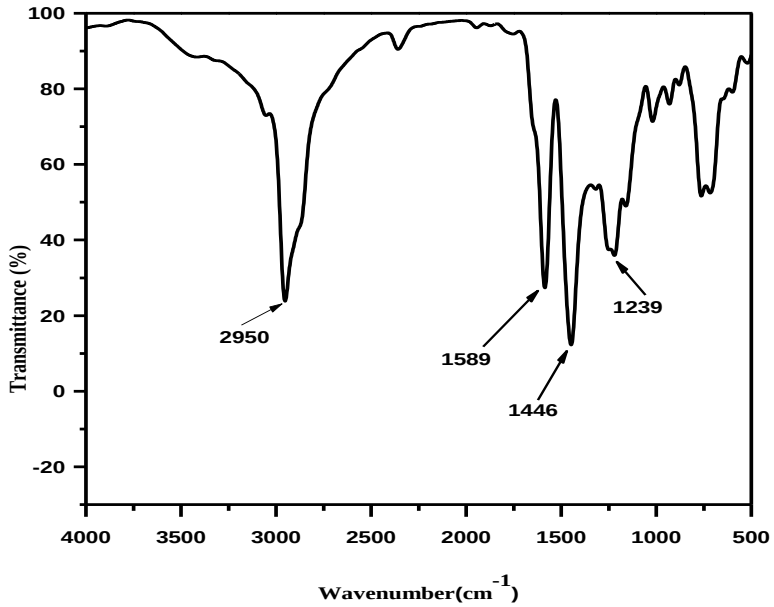


Figure S4: IR spectrum of6,6'-((1E,1'E)-(2,2'-(pyridine-2,6-diyl)bis(2-phenylhydrazin-2-yl-1-ylidene))bis(methanylylidene))bis(2,4-di-tert-butylphenol)

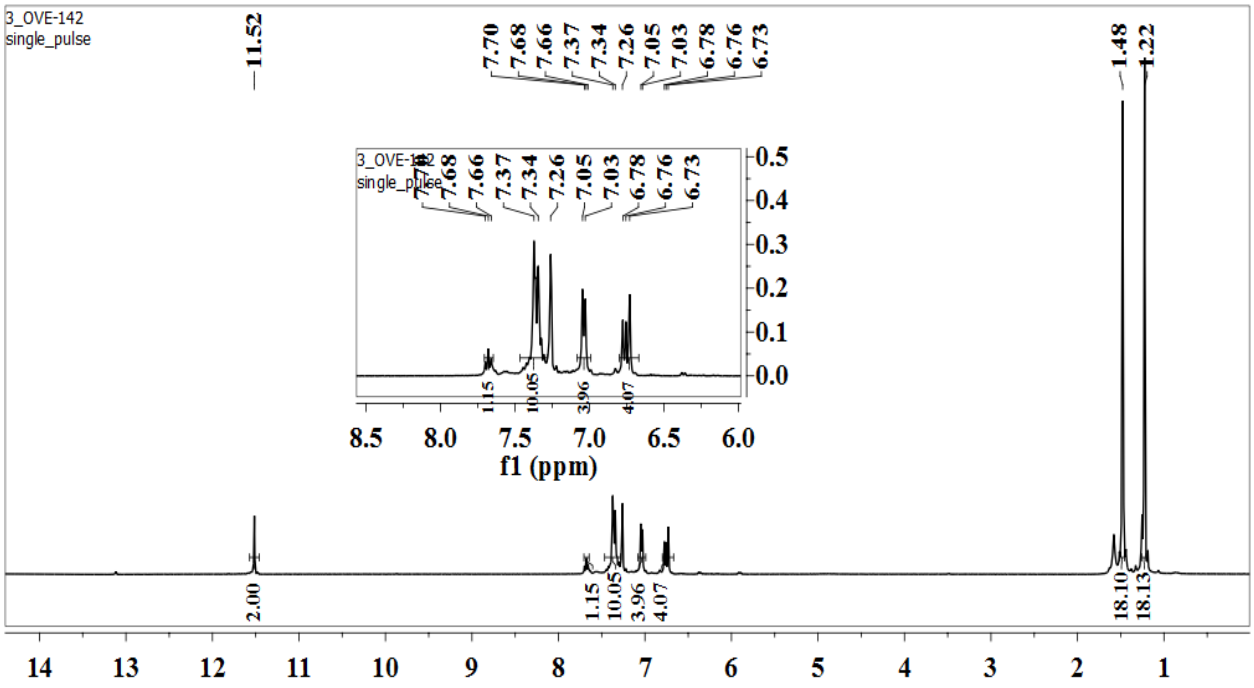


Figure S5: ^{1}H NMR spectrum of 6,6'-((1E,1'E)-(2,2'-(pyridine-2,6-diyl)bis(2-phenylhydrazin-2-yl-1-ylidene))bis(methanylylidene))bis(2,4-di-tert-butylphenol)

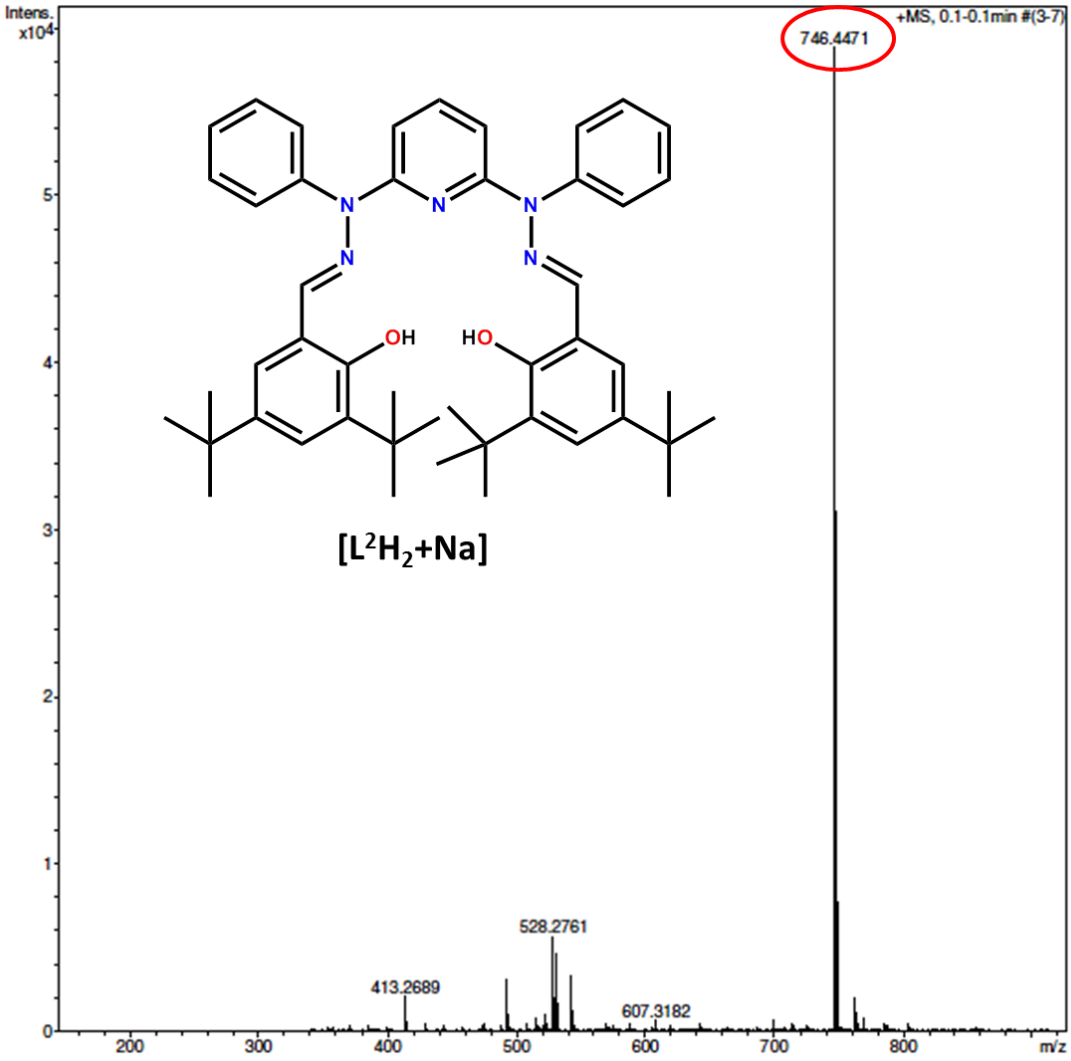


Figure S6: ESI-MS spectra of ligand [L^2H_2+Na]

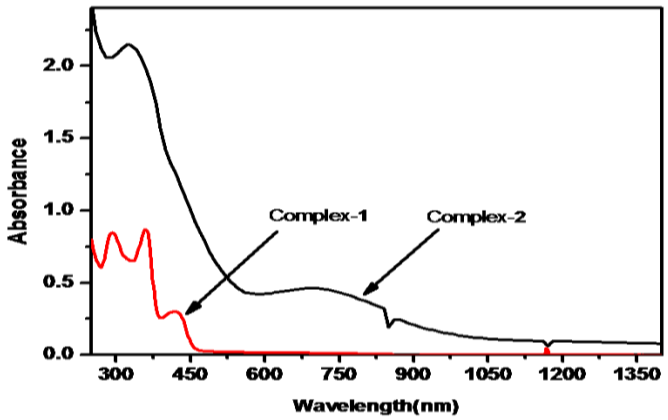


Figure S7. UV-Vis spectra of complexes [Cu(L^1H)ClO_4] (**1**) and [Cu(L^2) NO_3] (**2**) in NIR region.

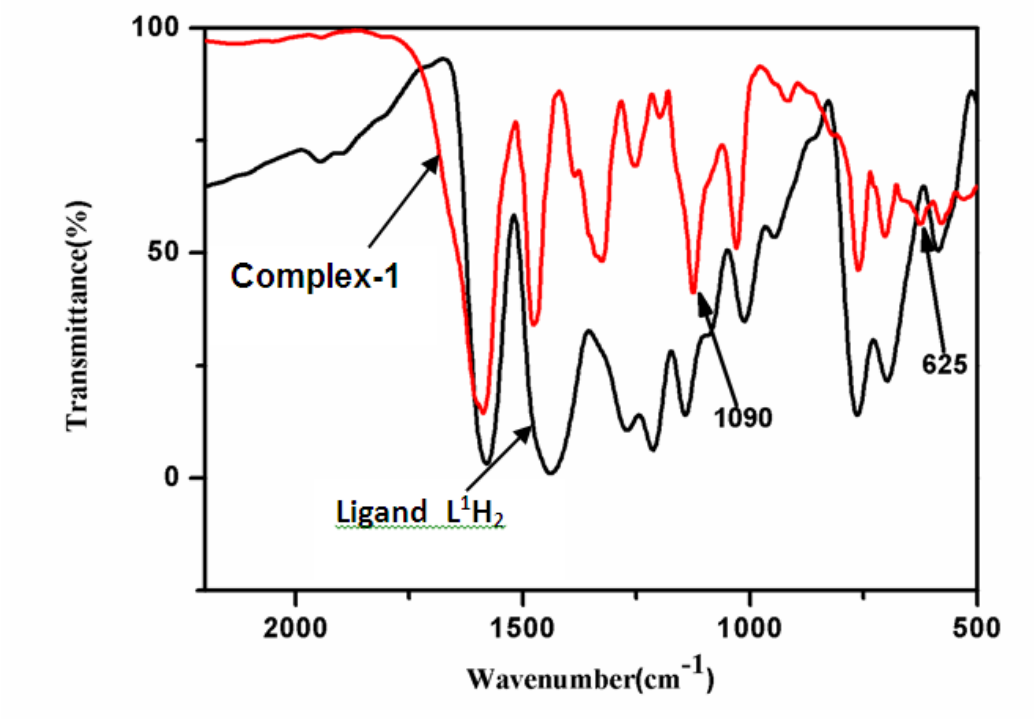


Figure S8: Infrared spectrum of complex $[Cu(L^1H)ClO_4]$**(1).** Black spectrum was for ligand and red spectrum was for corresponding metal complex

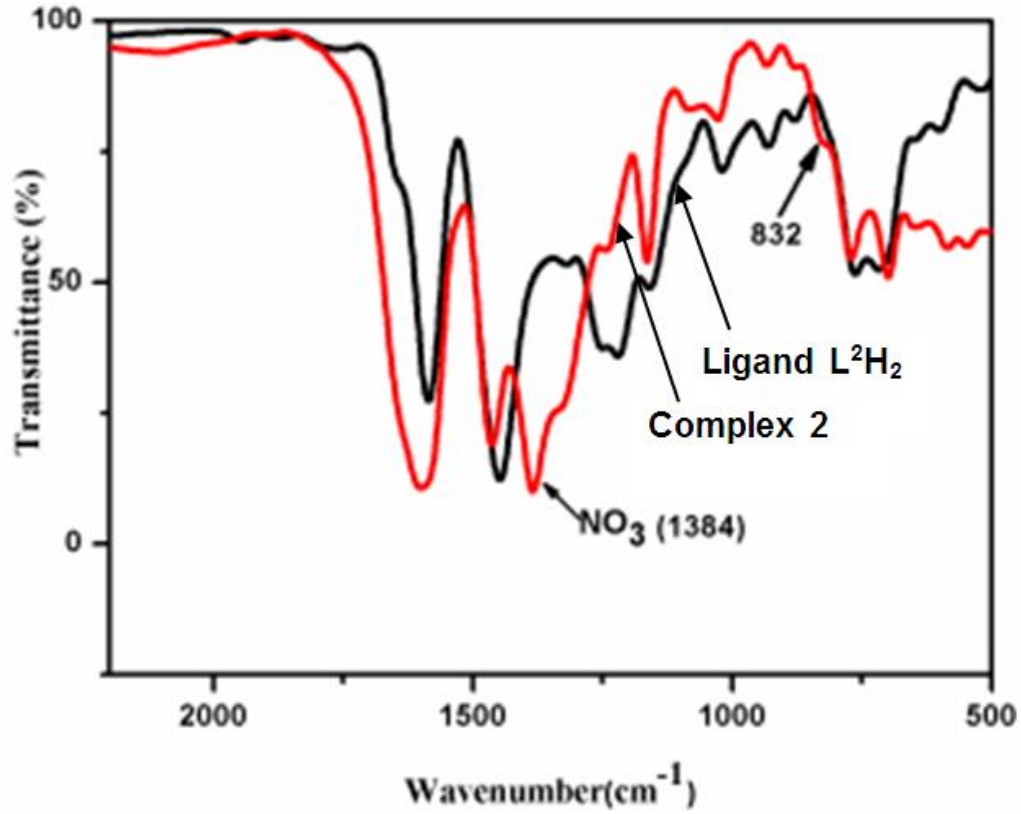


Figure S9: Infrared spectrum of complex **2.** Black spectrum was for ligands and red spectrum was for corresponding metal complex

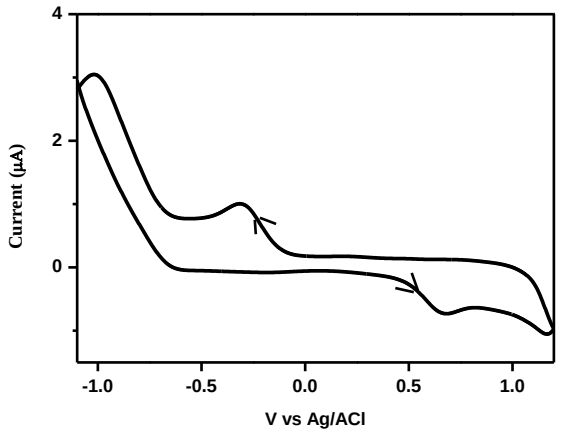


Figure S10: Cyclic voltammograms of a 10^{-3} M solution of complex **1** in dichloromethane in

presence of 0.1 M tetrabutylammonium perchlorate (TBAP), using working electrode: glassy-carbon, reference electrode: Ag/AgCl; auxiliary electrode: platinum wire, scan rate 0.1 Vs^{-1}.

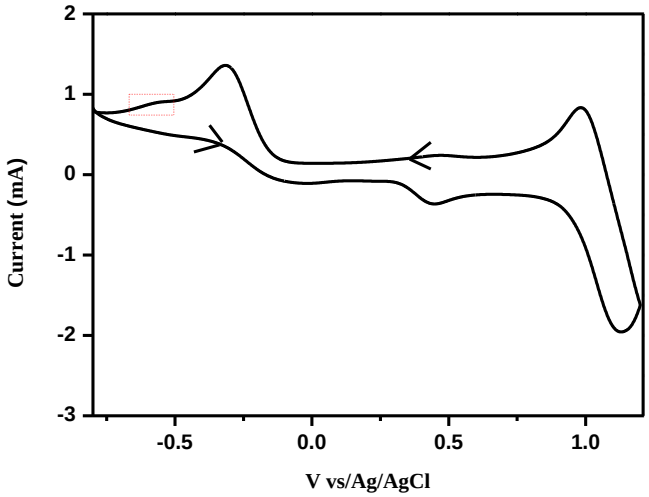


Figure S11: Cyclic voltammograms of a 10^{-3} M solution of complex **2** in dichloromethane in presence of 0.1 M tetrabutylammonium perchlorate (TBAP), using working electrode: glassy-carbon, reference electrode: Ag/AgCl; auxiliary electrode: platinum wire, scan rate 0.1 Vs^{-1}.

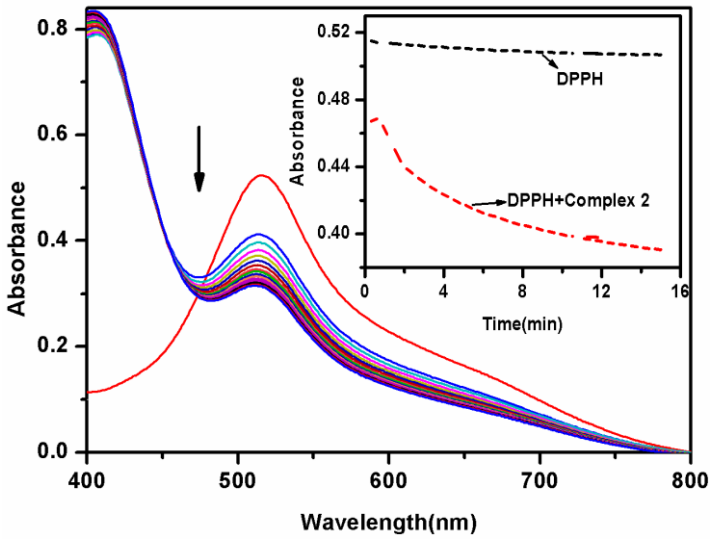
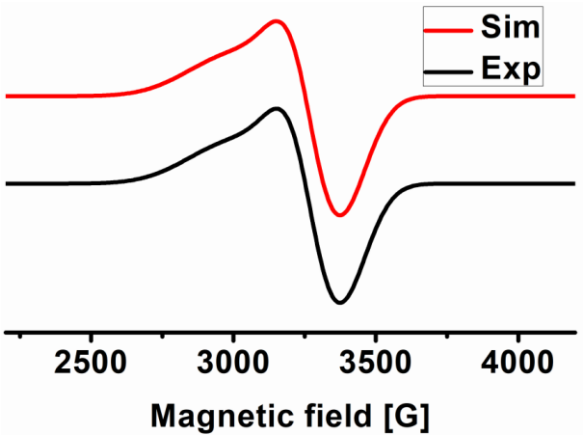
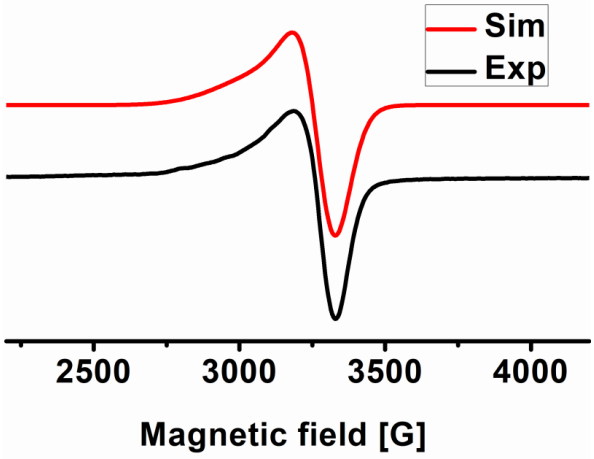


Figure S12: Reaction of pheoxyl radical from complex **2** (100µM) with DPPH radical ($3x10^{-5}$ M) MeOH solution



g_x = 1.98, g_y = 2.06, g_z = 2.28; W_x = 175 G, W_y = 155 G, W_z = 300 G.



g_x = 2.04, g_y = 2.06, g_z = 2.29; W_x = 100 G, W_y = 140 G, W_z = 300 G.

Complex-**1** Complex-**2**

Figure S13: X-Band EPR spectra of complex-**1** and complex-**2** in solid form . Microwave Frequency : 9.391028GHz, Power : 0.712 mW, Mod. Frequency : 100 kHz, Mod. Amplitude: 3G, T =100K

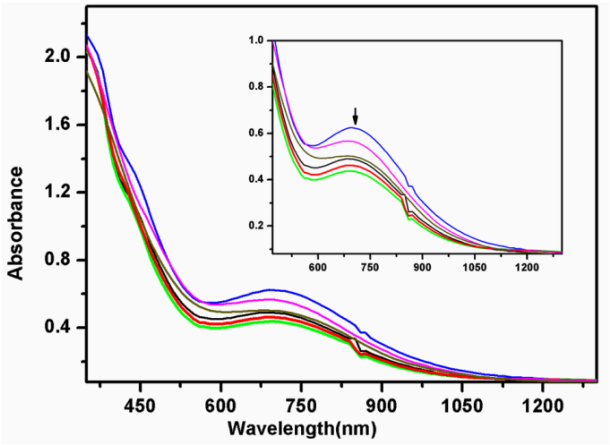


Figure S14: UV-Vis spectrum Changes of $[Cu(L^2)NO_3]$ (**2**) during the reaction with benzyl alcohol. solvent = CH_2Cl_2, [Benzyl alcohol] = 0.57 M, $[Cu(L^2)NO_3]$ (**2**) = 0.1 mM Total measuring time: 90 min.

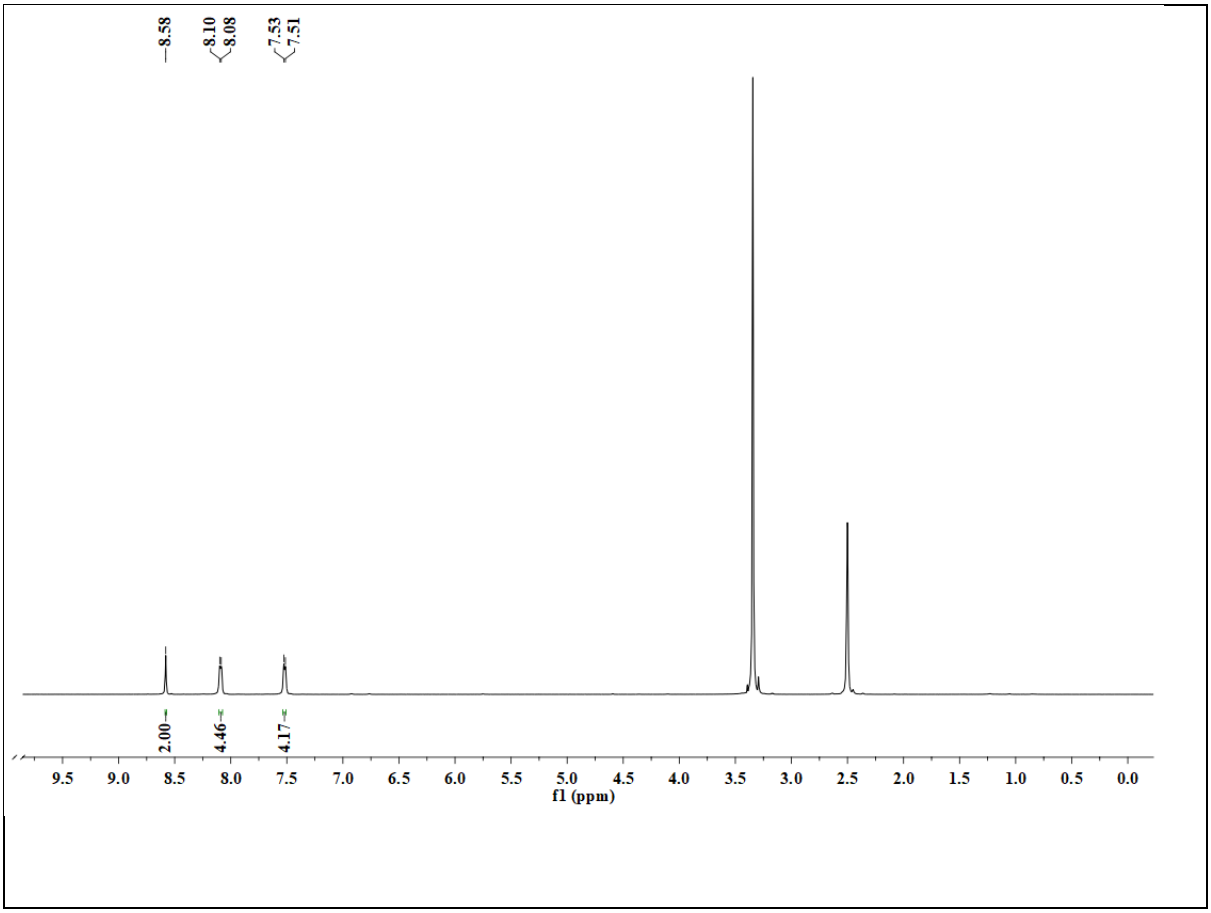


Figure S15 ^{1}H NMR data of anthracene produced from 9,10-dihydroanthracene in the presence of complex**2** in catalytic amount

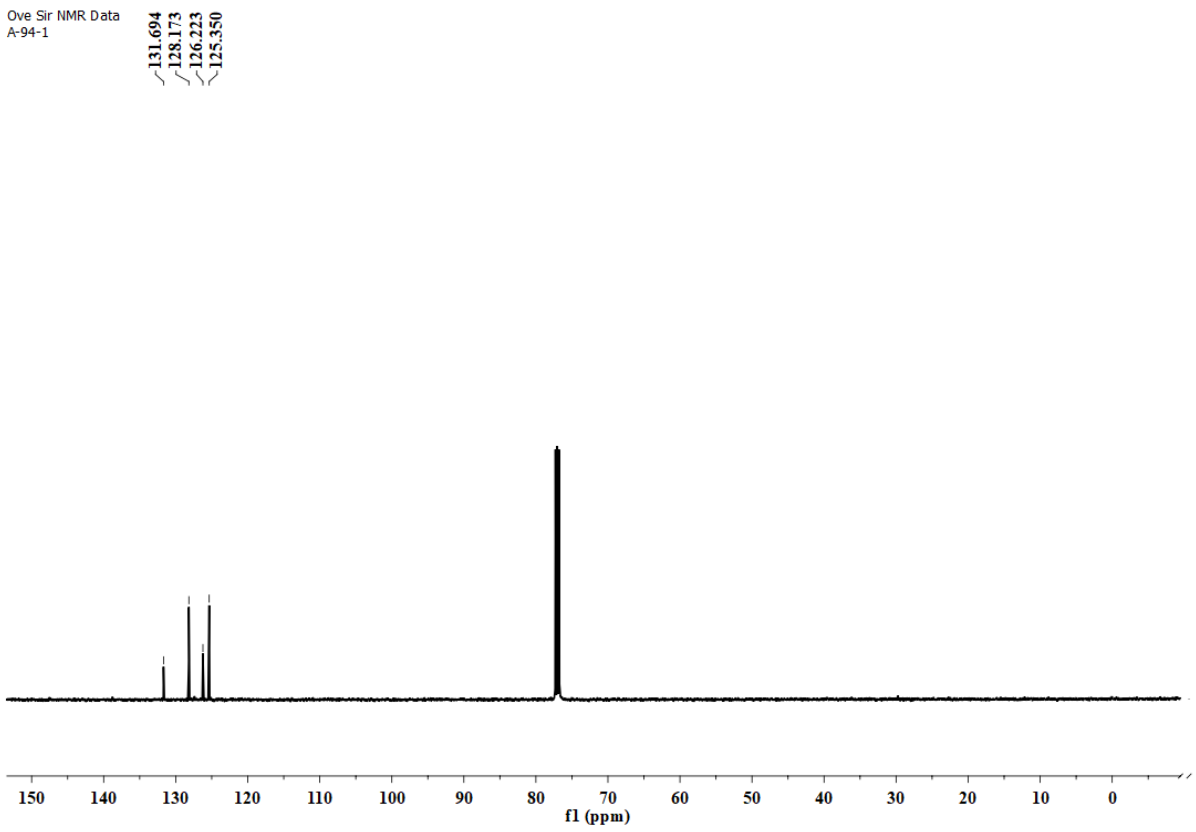


Figure S16 ^{13}C NMR data of anthracene produced from 9,10-dihydroanthracene in the presence of complex **2** in catalytic amount

Table S1: Crystallographic data for complex $[Cu(L^1H)ClO_4]$(**1**) and $[Cu(L^2)NO_3]$ (**2**)

Identification code	Complex **1**	Complex-**2**
Empirical formula	$C_{31}H_{24}ClCuN_5O_6$	$C_{47}H_{55}Cu_{0.92}N_6O_5$
Formula weight	661.54	842.587
Temperature/K	119.0	105.00
Crystal system	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/c$
a/Å	13.2622(7)	24.281(1)
b/Å	14.8135(7)	11.9133(5)
c/Å	17.2490(9)	18.1460(8)
α/°	90	90
β/°	101.332(2)	103.321(2)
γ/°	90	90
Volume/$Å^3$	3322.7(3)	5107.8(4)
Z	4	4
$\rho_{calc}g/cm^3$	1.322	1.096
μ/mm^{-1}	0.785	0.441
F(000)	1356.0	1785.3
Crystal size/mm^3	0.211 × 0.102 × 0.042	0.124 × 0.11 × 0.07
Radiation	MoKα (λ = 0.71073)	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.168 to 56.554	3.82 to 56.84
Index ranges	$-17 \le h \le 17$, $-19 \le k \le 19$, $-22 \le l \le 22$	$-32 \le h \le 32$, $-15 \le k \le 15$, $-24 \le l \le 24$
Reflections collected	69356	173918
Independent reflections	8204 [R_{int} = 0.0496, R_{sigma} = 0.0235]	12696 [R_{int} = 0.0962, R_{sigma} = 0.0539]
Data/restraints/parameters	8204/0/400	12696/0/555
Goodness-of-fit on F^2	1.051	1.097
Final R indexes [I>=2σ (I)]	R_1 = 0.0329, wR_2 = 0.0941	R_1 = 0.0597, wR_2 = 0.1646
Final R indexes [all data]	R_1 = 0.0359, wR_2 = 0.0959	R_1 = 0.0998, wR_2 = 0.1981
Largest diff. peak/hole / e $Å^{-3}$	0.46/-0.47	0.80/-0.55

GOF = $[\Sigma[w(F_o^2-F_c^2)^2]/M-N)]^{1/2}$ (M = number of reflections, N = number of parameters refined). [b] $R_1 = \Sigma \| F_o| - |F_c \| / \Sigma |F_o|$, [c] $wR_2 = [\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$

Table S2: Selected bond distances (Å) at the copper centre for complex **1**

Cu1	O1	1.8491(11)	C5	C6	1.393(2)
Cu1	N2	1.9607(12)	C7	C8	1.393(2)
Cu1	N3	1.8853(13)	C8	C9	1.389(2)
Cu1	N4	2.0900(12)	C9	C10	1.393(2)
Cl1	O3	1.4597(13)	C10	C11	1.393(2)
Cl1	O4	1.4241(15)	C12	C13	1.440(2)
Cl1	O5	1.4165(19)	C13	C14	1.415(2)
Cl1	O6	1.4257(17)	C13	C18	1.427(2)
O1	C18	1.3196(18)	C14	C15	1.375(2)
O2	C27	1.357(2)	C15	C16	1.400(2)
N1	N2	1.3947(16)	C16	C17	1.379(2)
N1	C1	1.4305(18)	C17	C18	1.411(2)
N1	C11	1.3776(18)	C19	C20	1.383(2)
N2	C12	1.2905(19)	C19	C24	1.379(2)
N3	C7	1.3358(18)	C20	C21	1.390(3)
N3	C11	1.3400(18)	C21	C22	1.389(3)
N4	N5	1.4067(17)	C22	C23	1.386(3)
N4	C25	1.2903(19)	C23	C24	1.389(2)
N5	C7	1.3802(19)	C25	C26	1.459(2)
N5	C19	1.4353(18)	C26	C27	1.408(2)
C1	C2	1.388(2)	C26	C31	1.399(2)
C1	C6	1.392(2)	C27	C28	1.395(2)
C2	C3	1.394(2)	C28	C29	1.382(3)
C3	C4	1.384(2)	C29	C30	1.391(3)
C4	C5	1.387(2)	C30	C31	1.385(2)

TableS 3: Selected bond distances (Å) at the copper centre for complex **2**

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
O1	C18	1.318(4)	C16	C17	1.372(4)
O2	N6	1.291(4)	C17	C18	1.430(4)
O3	N6	1.225(4)	C17	C27	1.547(4)
O4	N6	1.236(4)	C19	C20	1.379(5)
O5	C35	1.356(4)	C19	C24	1.375(6)
O5	Cu2	2.140(14)	C20	C21	1.392(6)
N1	N3	1.409(3)	C21	C22	1.331(7)
N1	C12	1.287(4)	C22	C23	1.381(7)
N1	Cu2	2.436(14)	C23	C24	1.397(7)
N2	N5	1.391(4)	C25	C26	1.525(5)
N2	C29	1.279(4)	C25	C36	1.543(5)
N2	Cu2	1.816(13)	C25	C37	1.534(5)

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N3	C1	1.433(5)	C27	C28	1.528(4)
N3	C7	1.382(5)	C27	C38	1.527(4)
N4	C7	1.333(5)	C27	C39	1.539(5)
N4	C11	1.351(5)	C29	C30	1.453(4)
N4	Cu2	1.972(13)	C30	C31	1.391(4)
N5	C11	1.363(5)	C30	C35	1.418(4)
N5	C19	1.432(4)	C31	C32	1.378(4)
C1	C2	1.371(5)	C32	C33	1.394(4)
C1	C6	1.342(6)	C32	C40	1.527(4)
C2	C3	1.392(7)	C33	C34	1.402(4)
C3	C4	1.348(7)	C34	C35	1.403(4)
C4	C5	1.364(8)	C34	C42	1.537(4)
C5	C6	1.380(7)	C40	C41	1.538(5)
C7	C8	1.400(4)	C40	C44	1.522(5)
C8	C9	1.374(6)	C40	C45	1.546(5)
C9	C10	1.382(6)	C42	C43	1.533(4)
C10	C11	1.390(5)	C42	C46	1.534(4)
C12	C13	1.443(4)	C42	C47	1.541(4)
O1	C18	1.318(4)	C16	C17	1.372(4)
O2	N6	1.291(4)	C17	C18	1.430(4)
O3	N6	1.225(4)	C17	C27	1.547(4)
O4	N6	1.236(4)	C19	C20	1.379(5)
O5	C35	1.356(4)	C19	C24	1.375(6)

TableS 4: Selected bond angles (º) at the copper centre for complex **1** and complex **2**

Complex-**1**		Complex-**2**	
O1 Cu1 N2	94.98(5)	O1- Cu1- O2	93.82(10)
O1 Cu1 N3	168.83(5)	O1-Cu1- N1	95.44(10)
O1 Cu1 N4	105.21(5)	O1-Cu-N4	171.11(11)
N2 Cu1 N4	159.56(5)	N1- Cu1- O2	150.55(11)
N3 Cu1 N2	80.92(5)	N1- Cu1- N4	81.14(11)
N3 Cu1 N4	79.80(5)	N4 -Cu1 -O2	93.10(11)
O4 Cl1 O3	108.75(8)	Cu2 -Cu1- O1	102.8(5)
O4 Cl1 O6	109.72(13)	Cu2 -Cu1 -O2	111.6(5)
O5 Cl1 O3	109.68(12)	Cu2 -Cu1- N1	93.5(5)
O5 Cl1 O4	111.43(13)	Cu2 -Cu1- N4	69.4(5)
O5 Cl1 O6	108.69(13)	C18 -O1 -Cu1	126.4(2)
O6 Cl1 O3	108.51(10)	N6 -O2- Cu1	105.5(2)

C18 O1 Cu1	125.22(9)	C35 -O5- Cu2	114.2(4)
N2 N1 C1	122.40(11)	Cu1- N1 -Cu2	35.4(3)
C11 N1 N2	114.54(12)	N3 -N1- Cu1	112.6(2)
C11 N1 C1	123.05(12)	N3- N1 -Cu2	106.5(3)
N1 N2 Cu1	112.68(9)	C12 -N1- Cu1	126.1(2)

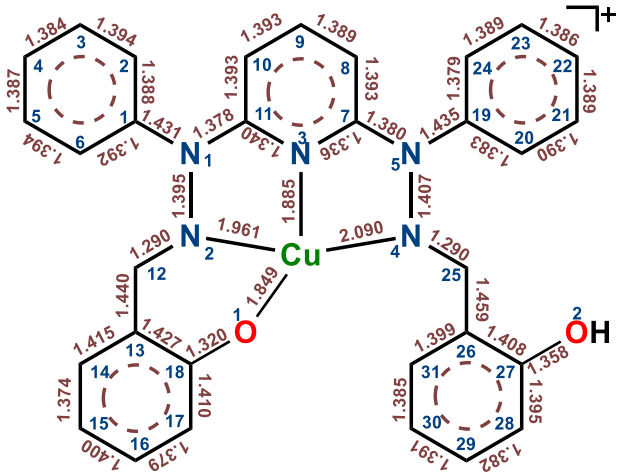


Figure S17. Bond distances [Å] in the in complex **1**

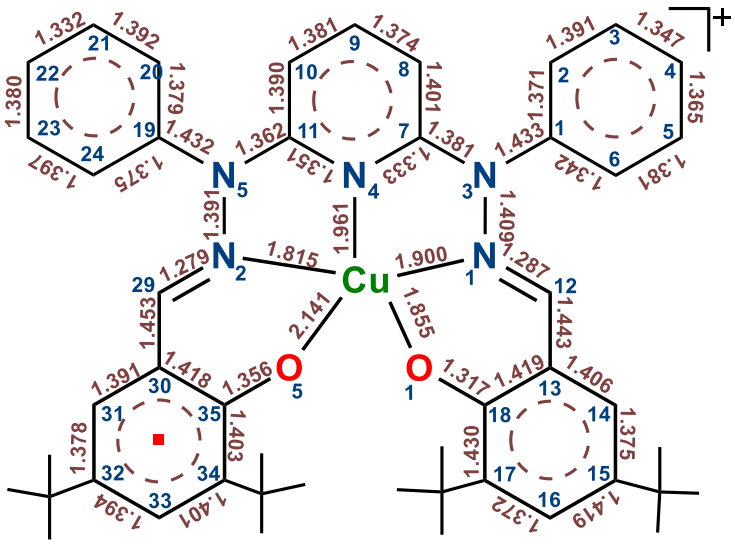


Figure S18. Bond distances [Å] in the phenoxyl and phenolate rings in complex **2**.

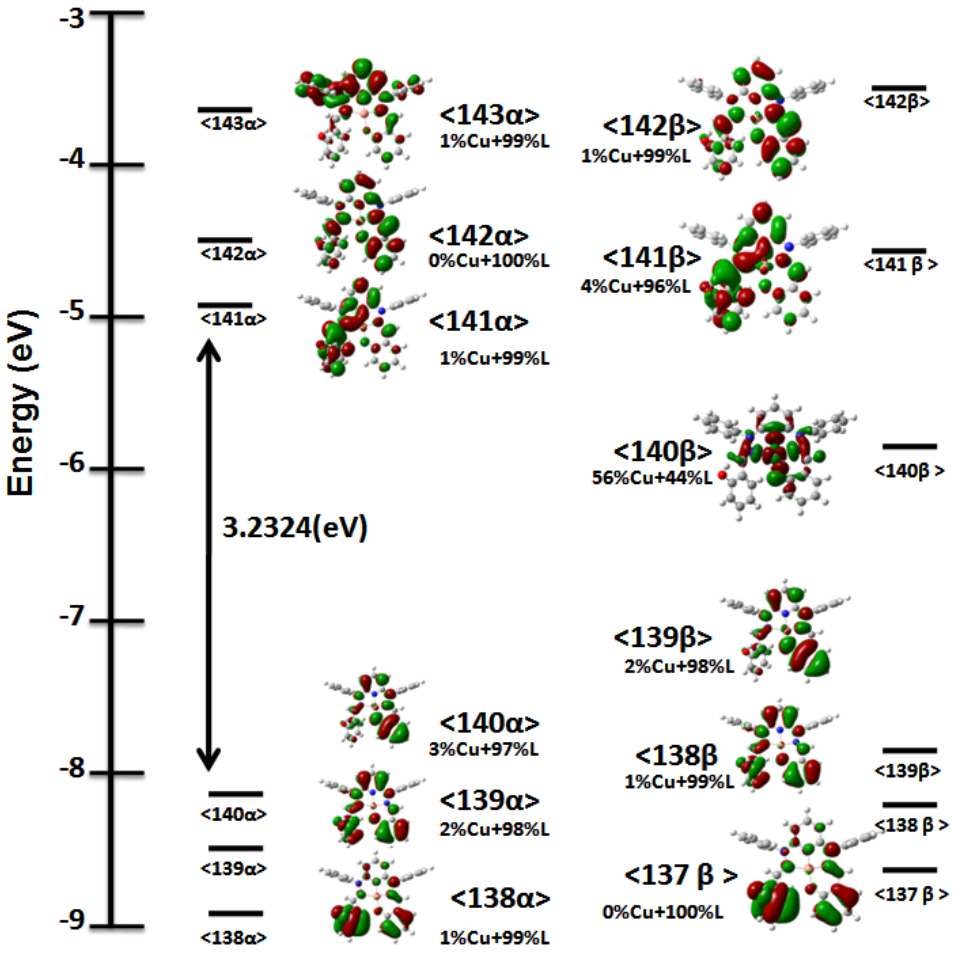


Figure S19. Single occupied frontier molecular orbitals of complex **1**. Showing significant contribution of copper and ligand L^1H_2 in SOMO.

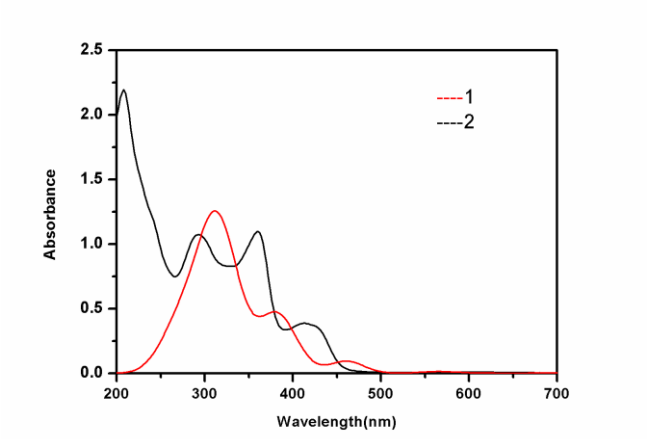


Figure S20: UV-Vis spectra of complex $[Cu(L^1H)ClO_4]$(**1**). Red coluour for theoritical calculation and black one for experimental.

Table S5: Cartesian coordinates for complex **1**

Number of atoms: 63
CuC31N5H24O2
B3LYP:

Cu	0.225046000000	0.293997000000	-0.046333000000
C	1.188925000000	3.008901000000	-0.331549000000
C	4.119856000000	-1.404844000000	0.091275000000
C	1.718042000000	-2.089194000000	0.090545000000
C	3.016966000000	1.256171000000	-0.131190000000
H	4.093584000000	1.084634000000	-0.114159000000
C	-3.124632000000	-2.472766000000	-0.063752000000
C	2.577227000000	2.619225000000	-0.261347000000
C	-0.645509000000	-2.420245000000	0.050126000000
C	1.951129000000	-3.478001000000	0.162877000000
H	2.956921000000	-3.874890000000	0.205489000000
C	4.791624000000	-1.434866000000	1.329684000000
H	4.241975000000	-1.244058000000	2.247915000000
C	0.880418000000	4.391235000000	-0.470735000000
H	-0.167806000000	4.667569000000	-0.525908000000
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H	4.038274000000	5.729940000000	-0.522423000000
C	4.810012000000	-1.648609000000	-1.113052000000
H	4.275227000000	-1.619300000000	-2.059067000000
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C	3.587591000000	3.630754000000	-0.333631000000
H	4.632519000000	3.329259000000	-0.281453000000
C	0.825133000000	-4.319558000000	0.173528000000
H	0.973575000000	-5.394288000000	0.228759000000
C	-5.048873000000	-3.430623000000	1.072005000000
H	-5.597947000000	-3.634245000000	1.986858000000
C	-3.623746000000	-2.907422000000	-1.307431000000
H	-3.062281000000	-2.704430000000	-2.216127000000
C	6.187355000000	-1.933144000000	-1.073512000000
H	6.725847000000	-2.126759000000	-1.996836000000
C	-4.841340000000	-3.611507000000	-1.356033000000
H	-5.229856000000	-3.954721000000	-2.310653000000
C	-5.554186000000	-3.870403000000	-0.168376000000
H	-6.495100000000	-4.412121000000	-0.208487000000
C	6.865928000000	-1.967986000000	0.161401000000

H	7.929428000000	-2.188866000000	0.188756000000
C	-3.830023000000	-2.731073000000	1.129007000000
H	-3.428839000000	-2.391916000000	2.080757000000
C	6.169140000000	-1.718941000000	1.361082000000
H	6.693419000000	-1.748426000000	2.311997000000
N	2.206859000000	0.218996000000	-0.037347000000
N	0.443786000000	-1.613000000000	0.038696000000
N	-1.811710000000	-0.327896000000	0.074019000000
O	0.159234000000	2.141744000000	-0.275790000000
N	2.703902000000	-1.110915000000	0.057580000000
N	-1.868540000000	-1.753468000000	-0.011101000000
C	-0.490889000000	-3.817536000000	0.115563000000
H	-1.347682000000	-4.477977000000	0.125276000000
C	-3.111417000000	1.756105000000	0.271902000000
C	-2.940836000000	0.338898000000	-0.026324000000
H	-3.852655000000	-0.209185000000	-0.273693000000
C	-2.368042000000	2.420812000000	1.282901000000
H	-1.565068000000	1.891318000000	1.784047000000
O	-4.959099000000	1.888702000000	-1.367259000000
H	-4.463482000000	1.290798000000	-1.962750000000
C	-4.173275000000	2.464083000000	-0.359617000000
C	-4.510584000000	3.767462000000	0.033323000000
H	-5.333209000000	4.266562000000	-0.468040000000
C	-2.693609000000	3.724077000000	1.670090000000
H	-2.129023000000	4.213345000000	2.457948000000
C	-3.772236000000	4.394413000000	1.049385000000
H	-4.034151000000	5.403228000000	1.356810000000

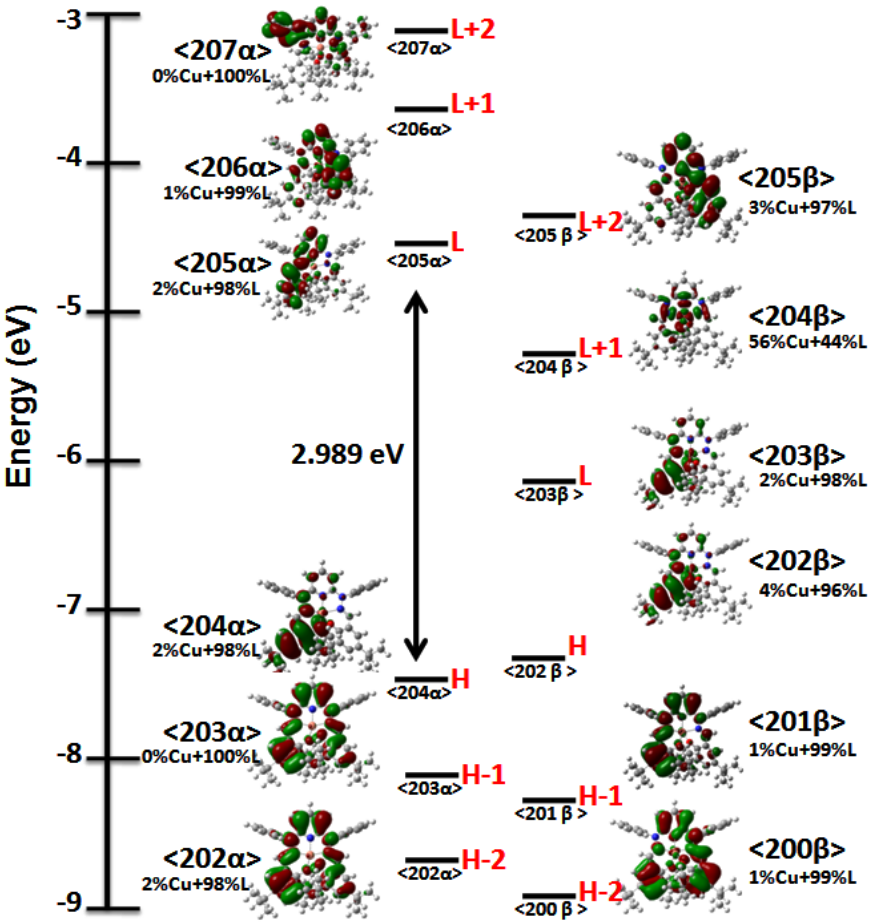

Figure S21. Single occupied frontier molecular orbitals of complex **2**. Showing significant contribution of copper and ligand L^2H_2 in SOMO.

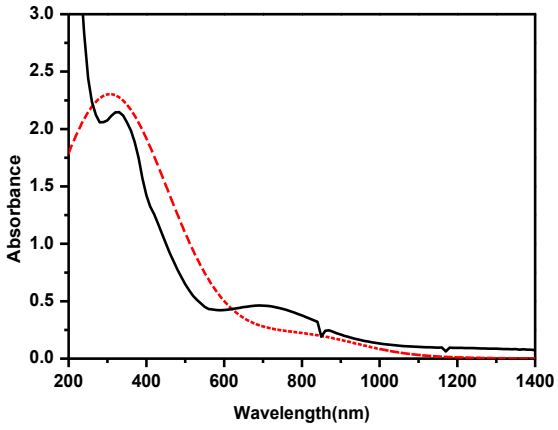

Figure S22: UV-Vis spectra of complex $[Cu(L^2))NO_3]$(**2**) in NIR region. Red coluour for theoritical calculation and black one for experimental

Table S6: Cartesian Coordinates for complex **2**

Number of atoms: 110

CuC47N5H55O2

C	**-0.789588000000**	**-4.354072000000**	**-3.199081000000**
H	**-0.994337000000**	**-5.155120000000**	**-2.476316000000**
H	**0.087835000000**	**-4.657278000000**	**-3.783728000000**
H	**-1.637601000000**	**-4.284490000000**	**-3.892690000000**
C	**0.749345000000**	**-3.209030000000**	**-1.587285000000**
H	**0.531846000000**	**-3.948611000000**	**-0.804665000000**
H	**1.041929000000**	**-2.270693000000**	**-1.112868000000**
H	**1.595259000000**	**-3.581623000000**	**-2.182187000000**
C	**-0.144448000000**	**-1.969846000000**	**-3.623887000000**
H	**-0.995486000000**	**-1.838774000000**	**-4.305482000000**
H	**0.708547000000**	**-2.331540000000**	**-4.214487000000**
H	**0.113042000000**	**-0.996939000000**	**-3.196845000000**
C	**-5.770625000000**	**-4.051889000000**	**-2.258304000000**
H	**-4.995109000000**	**-4.533667000000**	**-2.866165000000**
H	**-6.078017000000**	**-3.131954000000**	**-2.772195000000**
H	**-6.633573000000**	**-4.729710000000**	**-2.223723000000**
C	**-4.871035000000**	**-5.075832000000**	**-0.114979000000**
H	**-4.535588000000**	**-4.891603000000**	**0.913915000000**
H	**-4.060979000000**	**-5.589660000000**	**-0.646889000000**
H	**-5.730260000000**	**-5.758389000000**	**-0.078322000000**
Cu	**-0.116204000000**	**1.156503000000**	**-0.120061000000**
N	**2.172660000000**	**2.950783000000**	**-0.619283000000**
N	**1.969909000000**	**1.593744000000**	**-0.314063000000**
N	**-2.031465000000**	**1.513836000000**	**0.218756000000**
C	**1.070285000000**	**3.775341000000**	**-0.329820000000**
N	**-2.305197000000**	**2.884533000000**	**0.509840000000**
C	**-1.226849000000**	**3.732987000000**	**0.296969000000**
C	**3.952417000000**	**-1.447682000000**	**0.143206000000**
H	**4.740246000000**	**-1.152632000000**	**-0.545730000000**
C	**-3.639044000000**	**3.358384000000**	**0.803941000000**
N	**-0.062161000000**	**3.105909000000**	**-0.009993000000**
C	**-2.843959000000**	**-0.719666000000**	**-0.365285000000**
C	**2.895012000000**	**-0.561973000000**	**0.365750000000**
C	**-1.691448000000**	**-2.482781000000**	**-1.675736000000**
C	**-2.996287000000**	**0.618248000000**	**0.141500000000**
H	**-4.005923000000**	**0.911009000000**	**0.432414000000**
C	**-1.275945000000**	**5.145611000000**	**0.346788000000**
H	**-2.187974000000**	**5.664594000000**	**0.611869000000**

C	-2.869923000000	-3.228112000000	-1.572806000000
H	-2.899729000000	-4.194529000000	-2.061792000000
C	1.915777000000	-2.216699000000	2.013536000000
C	1.816745000000	-0.930224000000	1.305213000000
C	4.021077000000	-2.713764000000	0.779878000000
C	4.321703000000	3.948972000000	0.092790000000
H	3.989330000000	3.901275000000	1.126985000000
C	3.477519000000	3.491541000000	-0.939656000000
C	-0.104351000000	5.842577000000	0.013038000000
H	-0.117176000000	6.928828000000	0.025751000000
C	2.982863000000	0.765610000000	-0.229185000000
H	3.978962000000	1.087910000000	-0.538232000000
C	1.089985000000	5.179419000000	-0.347340000000
H	1.982530000000	5.729373000000	-0.615001000000
C	5.189134000000	-3.663713000000	0.456427000000
C	-4.011309000000	-1.545233000000	-0.305610000000
H	-4.885550000000	-1.147349000000	0.201909000000
C	-1.640932000000	-1.202282000000	-1.004056000000
C	-4.044855000000	-2.808656000000	-0.877341000000
C	-5.272152000000	-3.743605000000	-0.815096000000
C	2.996641000000	-3.047561000000	1.709954000000
H	3.063480000000	-4.001914000000	2.211448000000
C	0.855710000000	-2.610650000000	3.061531000000
C	-4.077102000000	3.397666000000	2.141979000000
H	-3.407842000000	3.077444000000	2.936263000000
C	3.886565000000	3.544957000000	-2.285816000000
H	3.218451000000	3.189893000000	-3.066121000000
O	-0.500833000000	-0.491141000000	-1.013853000000
C	6.002453000000	4.531833000000	-1.577166000000
H	6.979121000000	4.938731000000	-1.824649000000
C	-4.486862000000	3.765669000000	-0.246393000000
H	-4.133694000000	3.724682000000	-1.273891000000
C	-0.488727000000	-2.998898000000	-2.505403000000
C	5.112490000000	-4.998512000000	1.238044000000
H	5.966371000000	-5.628436000000	0.962543000000
H	4.200480000000	-5.562092000000	1.002958000000
H	5.157050000000	-4.844232000000	2.323868000000
C	5.586318000000	4.472618000000	-0.231577000000
H	6.240463000000	4.832947000000	0.557415000000
C	-5.782757000000	4.225024000000	0.050459000000
H	-6.440443000000	4.544011000000	-0.753252000000

C	5.168480000000	-3.988799000000	-1.069716000000
H	5.278421000000	-3.088409000000	-1.686130000000
H	4.231322000000	-4.483216000000	-1.354745000000
H	5.998873000000	-4.663021000000	-1.313577000000
C	5.154007000000	4.068307000000	-2.602394000000
H	5.473830000000	4.118944000000	-3.639337000000
O	0.829366000000	-0.120057000000	1.521693000000
C	6.535995000000	-2.963087000000	0.816375000000
H	6.683012000000	-2.032790000000	0.254476000000
H	7.372962000000	-3.630483000000	0.576625000000
H	6.584697000000	-2.726653000000	1.886748000000
C	-6.226574000000	4.271025000000	1.387651000000
H	-7.228117000000	4.626667000000	1.613955000000
C	-5.375079000000	3.857451000000	2.431622000000
H	-5.717934000000	3.894961000000	3.461784000000
C	-6.446460000000	-3.117258000000	-0.022585000000
H	-6.167889000000	-2.900074000000	1.017257000000
H	-7.288675000000	-3.819558000000	0.001670000000
H	-6.804959000000	-2.189590000000	-0.488363000000
C	0.832375000000	-1.546257000000	4.203990000000
H	1.809683000000	-1.479075000000	4.700724000000
H	0.091793000000	-1.841374000000	4.958286000000
H	0.563271000000	-0.558502000000	3.821553000000
C	1.157407000000	-3.988807000000	3.706363000000
H	1.146147000000	-4.802929000000	2.969759000000
H	0.380249000000	-4.209923000000	4.447171000000
H	2.122114000000	-4.001510000000	4.230462000000
C	-0.551198000000	-2.696073000000	2.392995000000
H	-0.562390000000	-3.448280000000	1.593898000000
H	-0.852410000000	-1.736365000000	1.969191000000
H	-1.291024000000	-2.992604000000	3.147822000000

Table S 7 Hammett Analysis with the Para Substitution Constant (σ_P)

Substrate	k	Kx/KH	Log (Kx/kH)	σ_p	ρ
4-OMe	0.1126	1.12286	0.05032	-0.268	-0.19
4-Me	0.10941	1.09105	0.03784	-0.170	
4-H	0.10028	1	0	0	
4-NO_2	0.07112	0.70921	-0.14922	0.778	

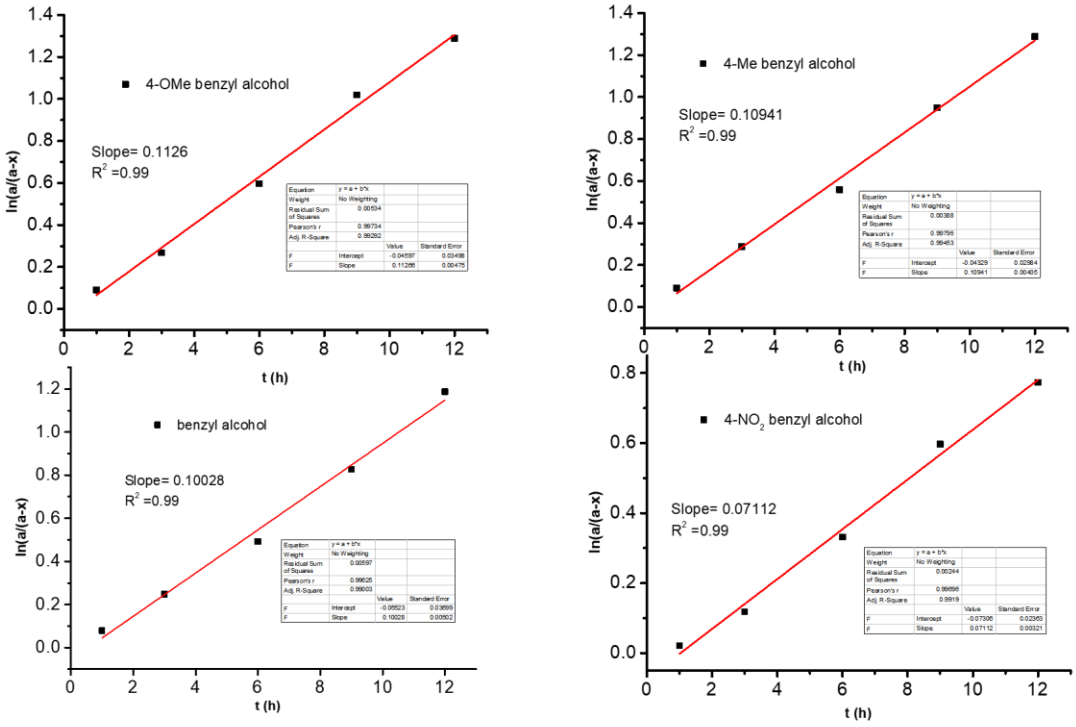

Figure S23: Determination of rate constant for the electronically disparate alcohols