Cu(II) complex of a new isoindole derivative: structure, catecholase like activity, antimicrobial properties and bio-molecular interactions

Sangita Adhikari,[a] Sisir Lohar[a], Babli Kumari,[a] Aparna Banerjee,[b] Rajib Bandopadhyay,[b] Jesús Sanmartín Matalobos[c*] and Debasis Das[a]*

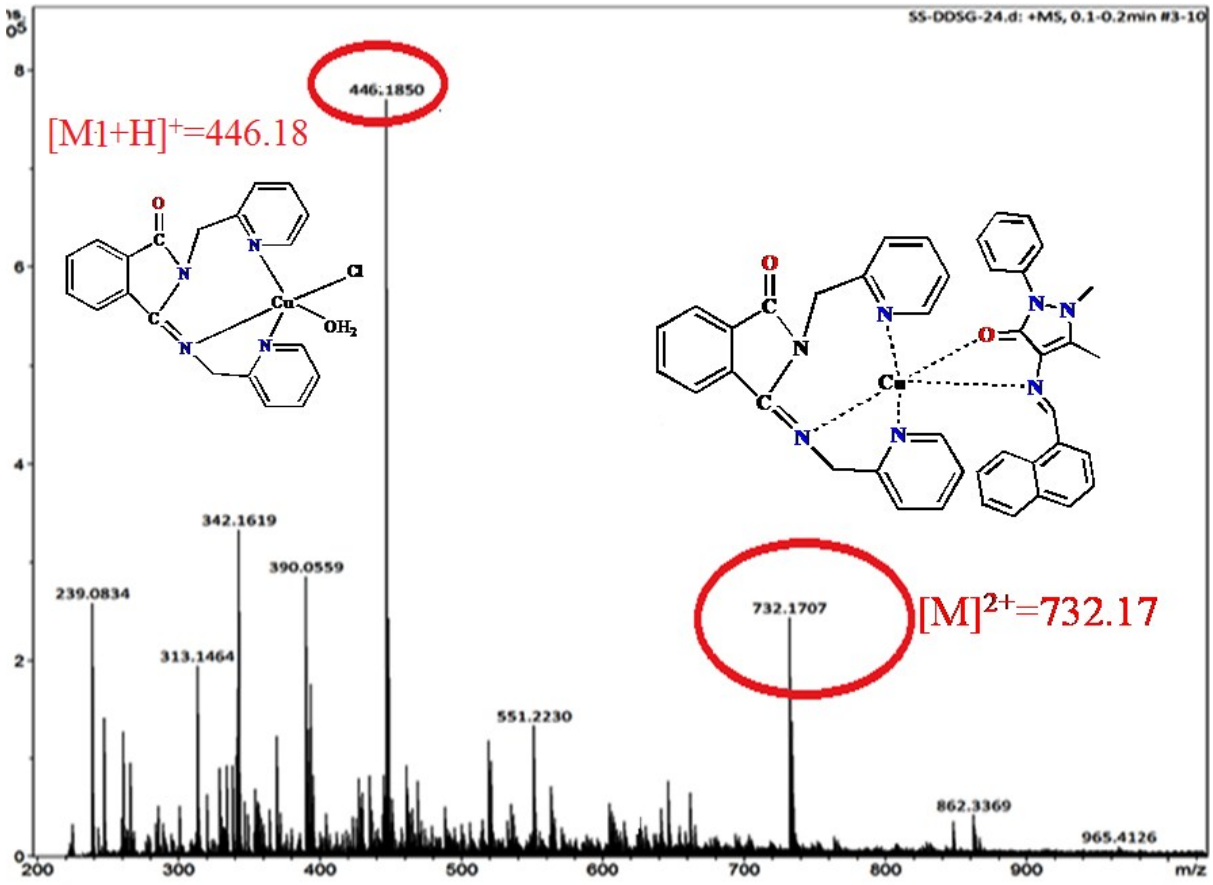

Fig. S1 ESI-MS spectrum of the adduct between ANNAP and [Cu(PICPH)Cl_2] complex.

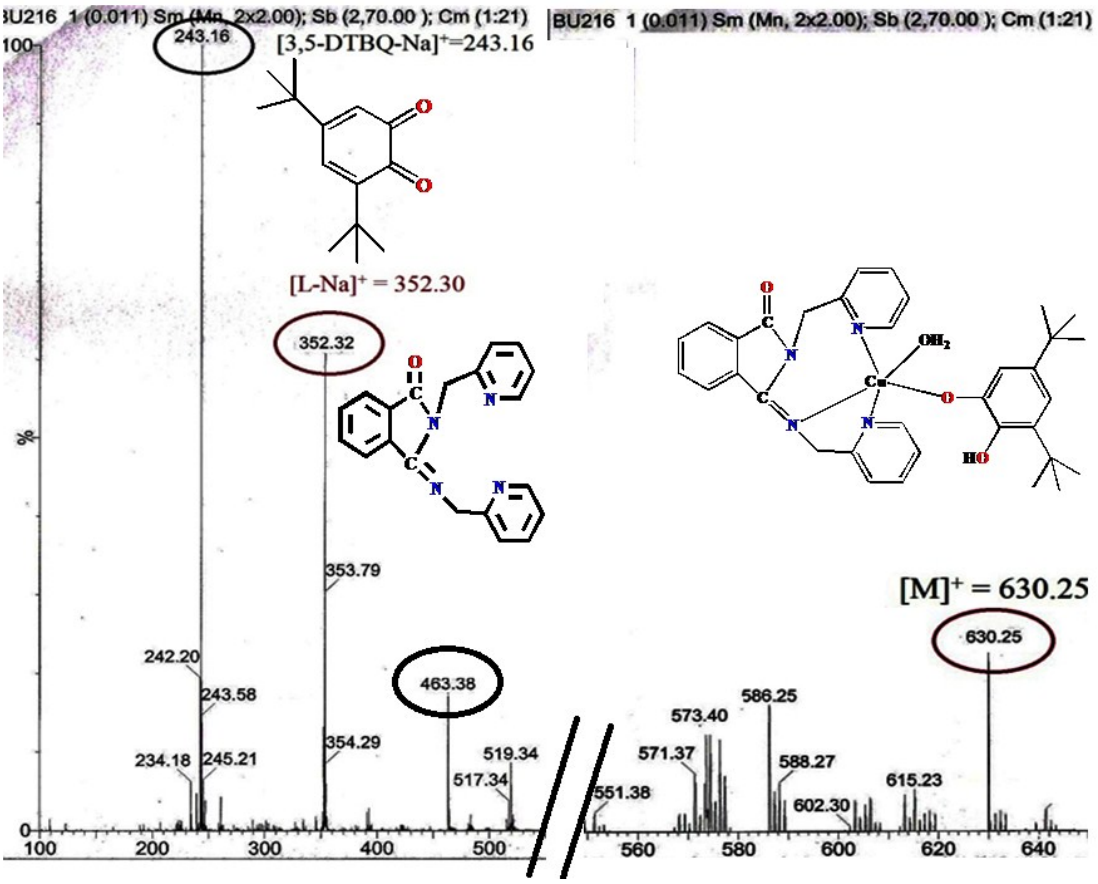

Fig. S2 ESI-MS spectrum of the mixture of [Cu(PICPH)$(Cl)_2$] and 3,5-DTBC in 1:100 mixture in MeOH

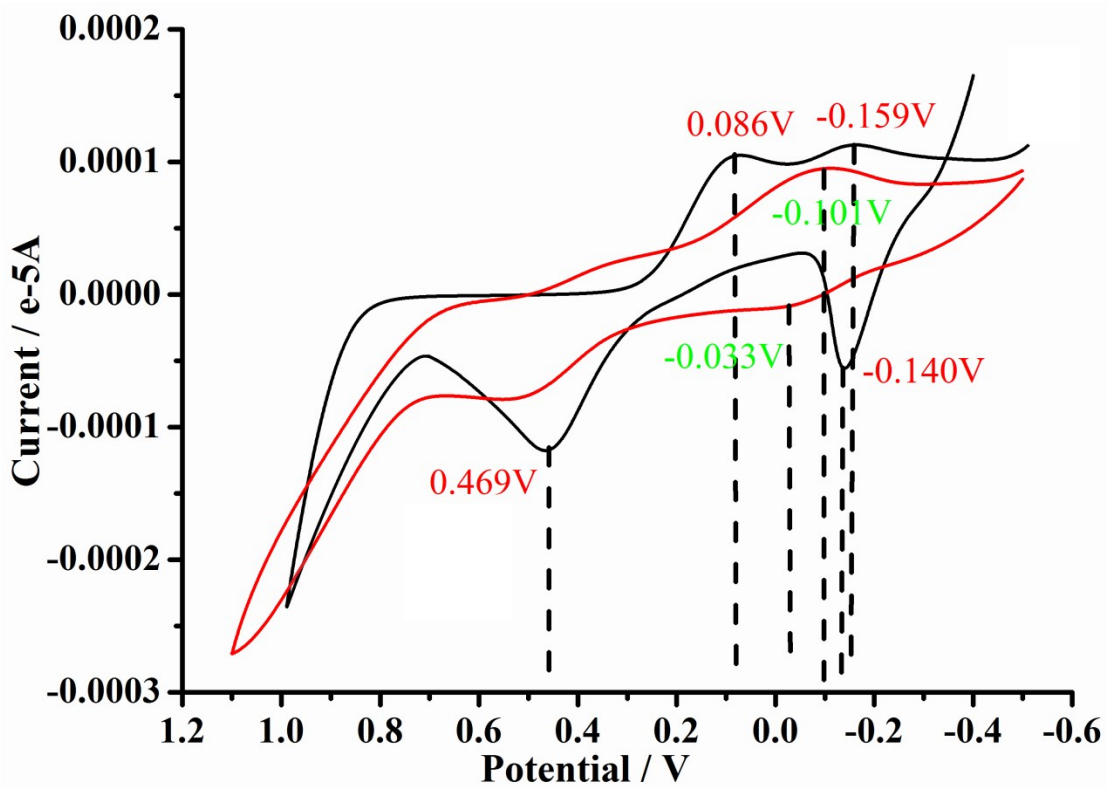

Fig. S3 Cyclic voltammograms of $[Cu(PICPH)(Cl)_2]$(black) and $[Cu(PICPH)(Cl)_2]$-catechol systems (red) in methanol using a platinum wire as auxiliary electrode and a calomel as reference electrode.

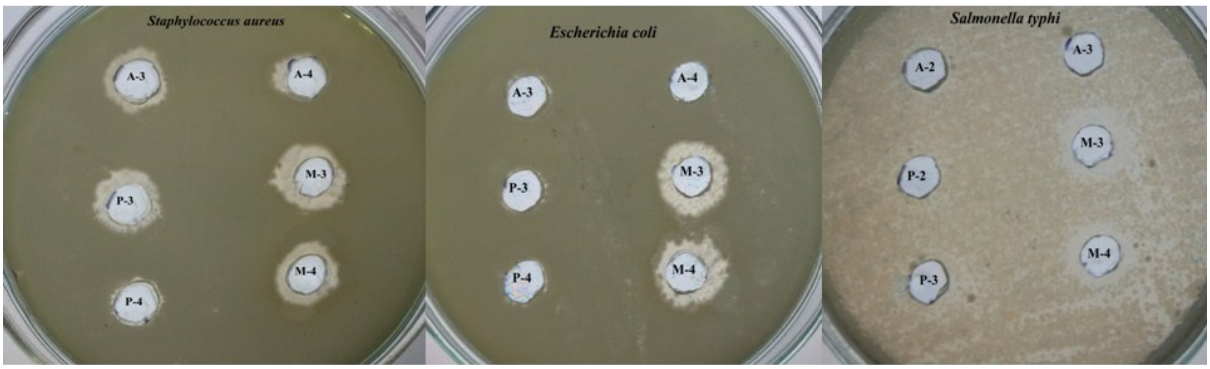

Fig. S4 Effective zone of inhibition by ANNAP (A), $[Cu(PICPH)(Cl)_2]$ (P) and their mixture (M).

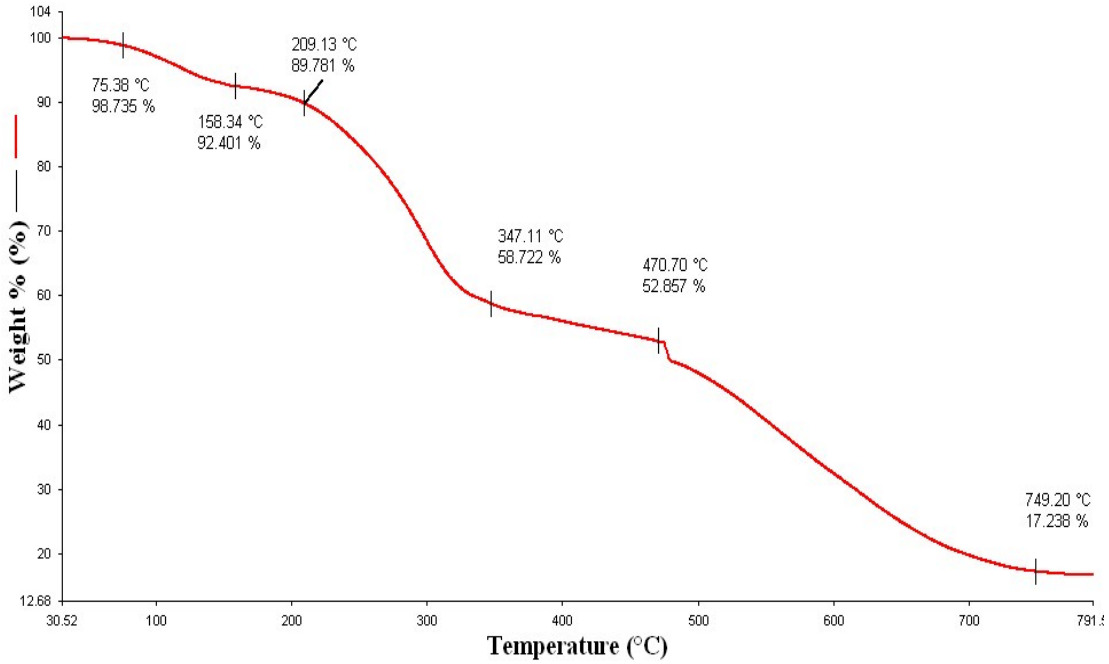

Fig. S5 TGA plot of $[Cu(PICPH)(Cl)_2]$

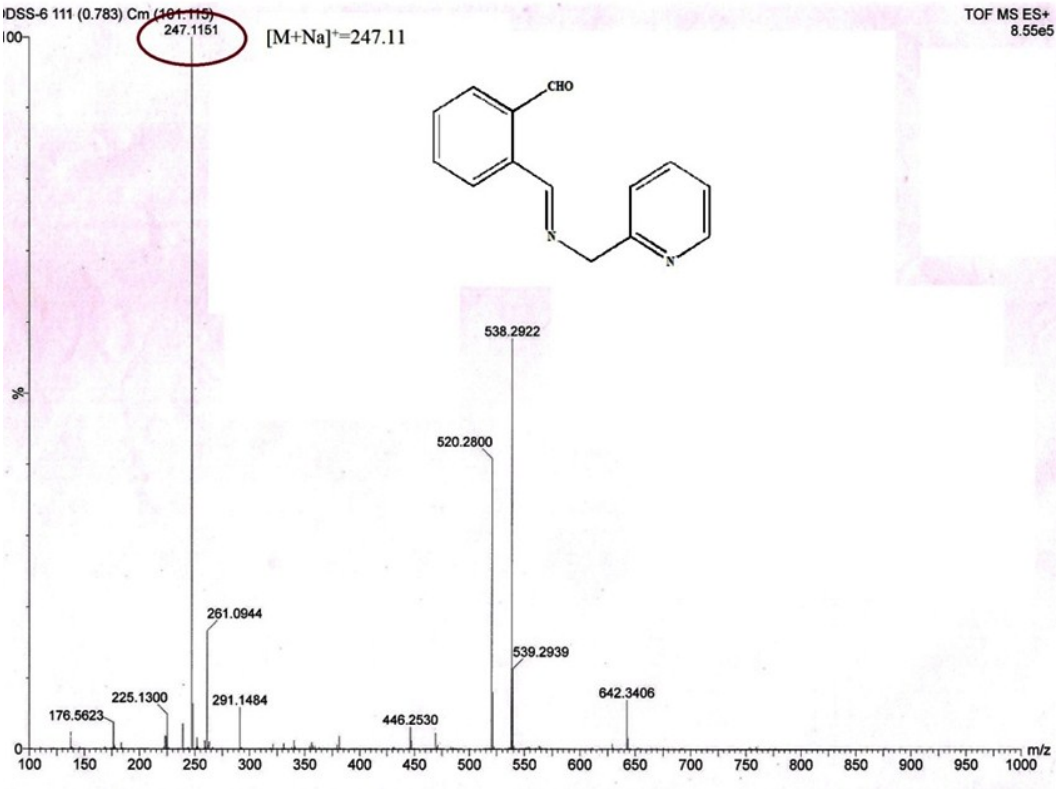

Fig.S6 ESI-MS spectrum of the mixture of 2-picolyl amine and *o*-phthaldehyde.

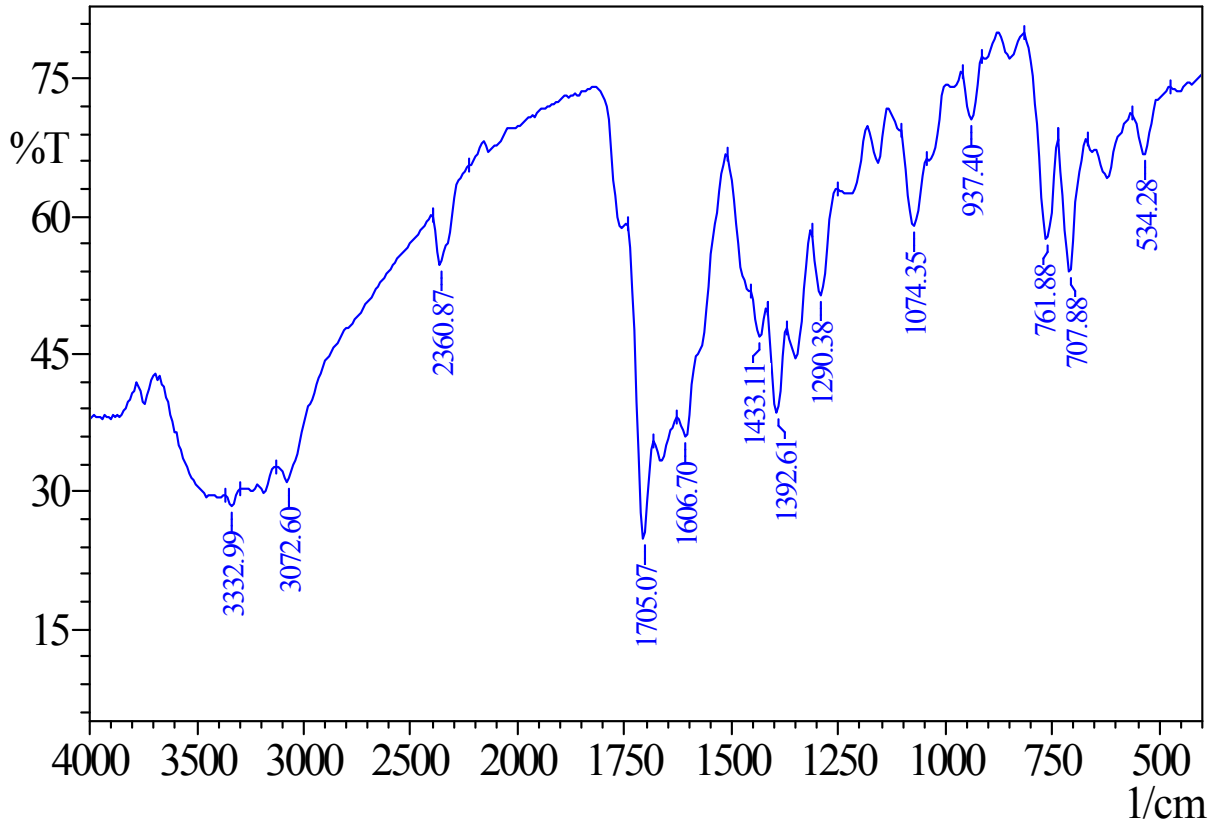

Fig. S7 FTIR spectrum of [Cu(PICPH)$(Cl)_2$]

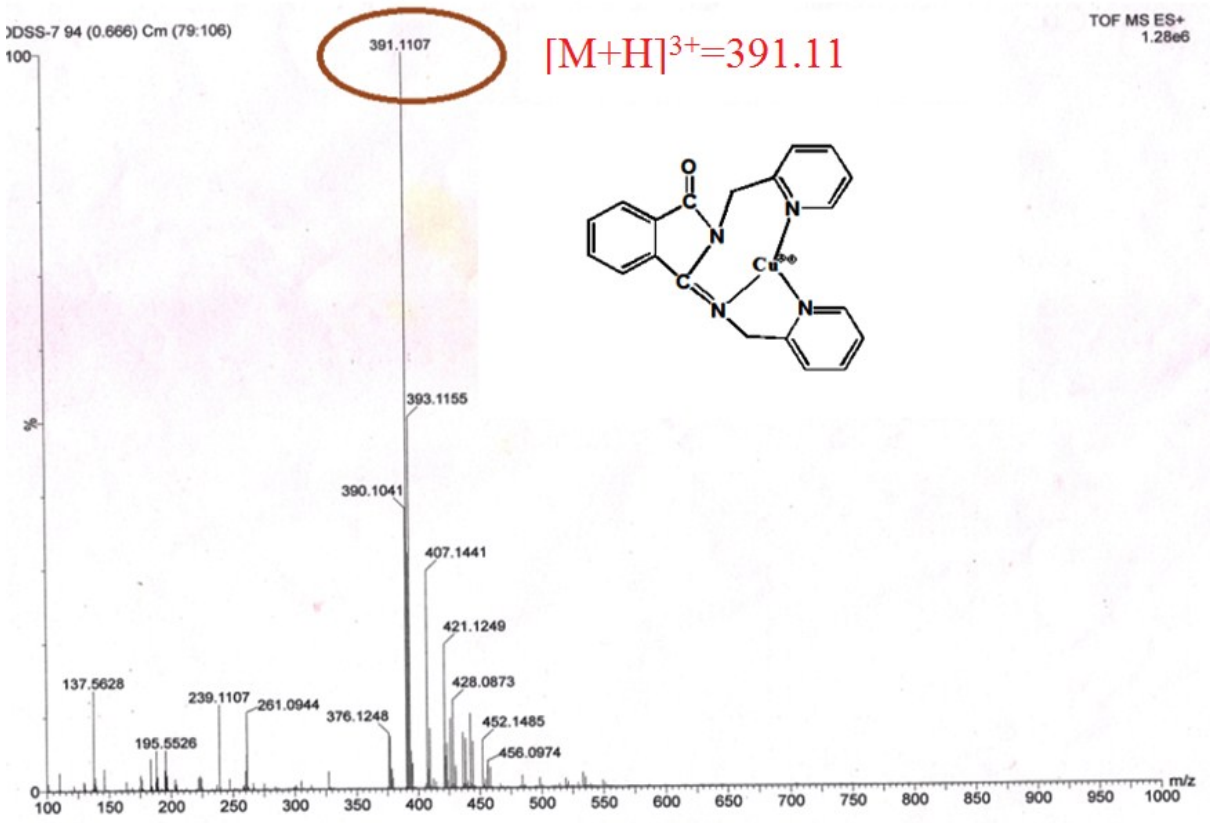

Fig. S8 ESI-MS spectrum of $[Cu(PICPH)(Cl)_2]$.

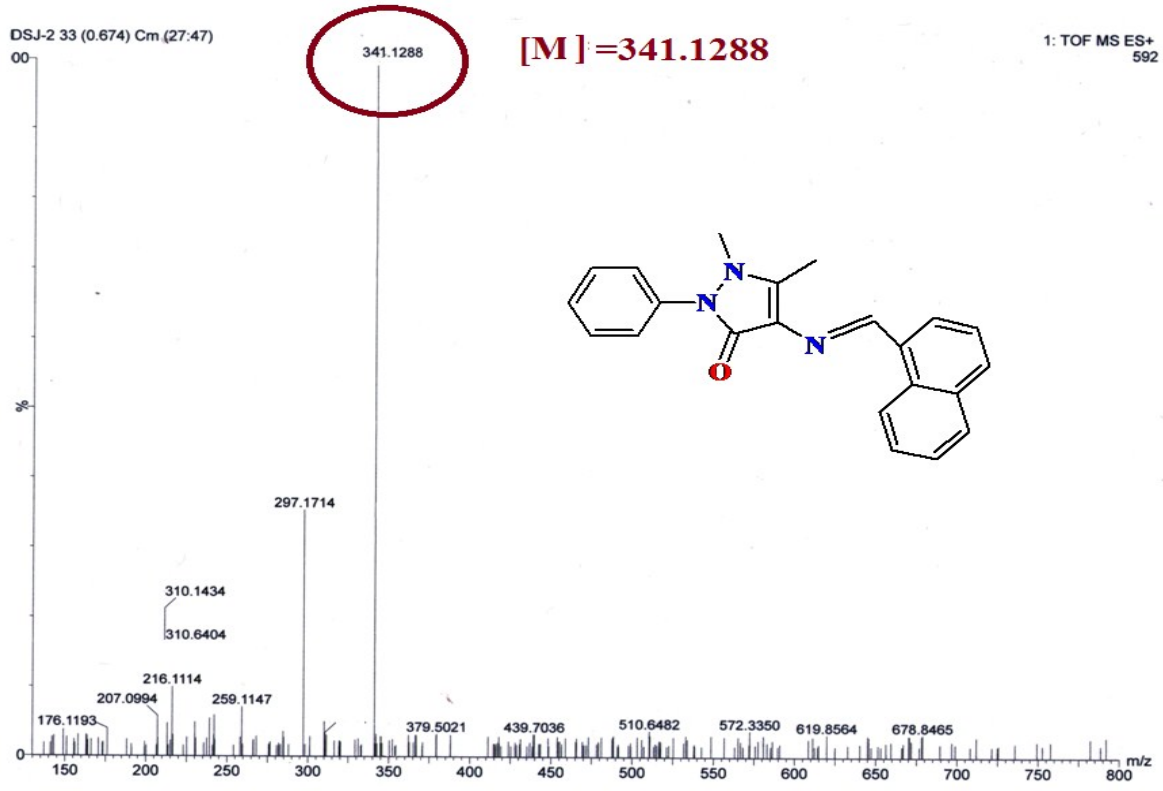

Fig.S9 ESI-MS spectrum of ANNAP in methanol.

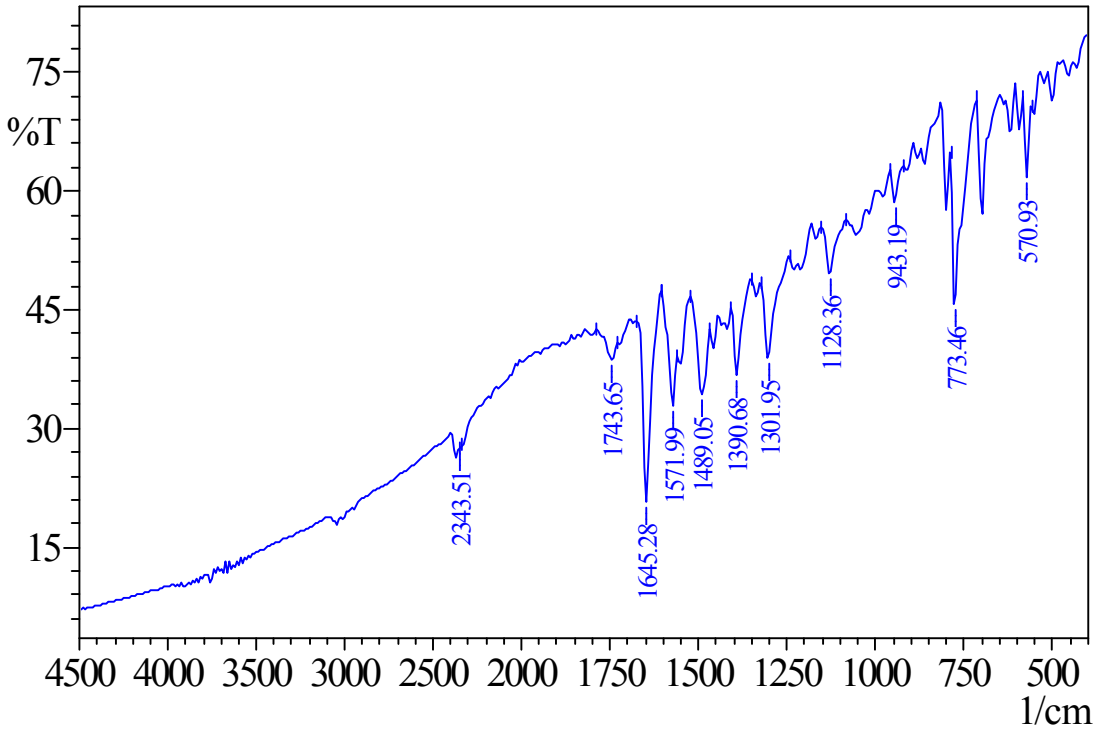

Fig. S10FTIR spectrum of ANNAP

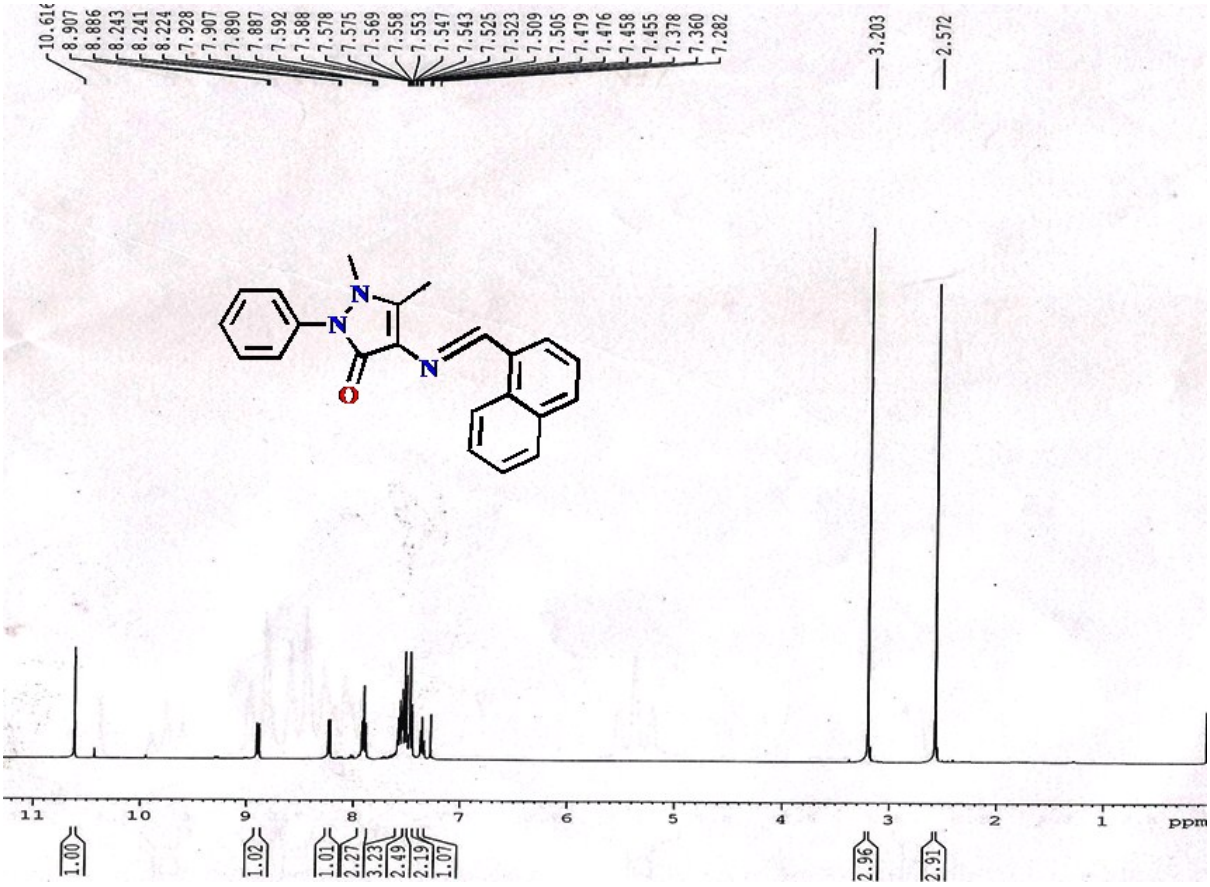

Fig.S11^{1}HNMR spectrum of ANNAP in $CDCl_3$

Table S1 Crystal data and structure refinement for [Cu(PICPH)$(Cl)_2$]

Empirical formula	$C_{20}H_{16}Cl_2CuN_4O$	
Formula weight	462.81	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 7.6364(4) Å	α= 95.949(3)°
	b = 11.0930(6) Å	β= 91.000(3)°
	c = 12.7629(6) Å	γ = 99.504(3)°
Volume	1059.91(9) $Å^3$	
Z	2	
Density (calculated)	1.450 Mg/m^3	
Absorption coefficient	1.300 mm^{-1}	
F(000)	470	
Crystal size	0.480 x 0.300 x 0.180 mm^3	
Theta range for data collection	1.605 to 27.196°	
Index ranges	-9<=h<=9, -14<=k<=14, -16<=l<=16	
Reflections collected	33783	
Independent reflections	4678 [R(int) = 0.0410]	
Completeness to theta = 25.242°	99.5 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4678 / 0 / 253	
Goodness-of-fit on F^2	1.060	
Final R indices [I>2sigma(I)]	R1 = 0.0393, wR2 = 0.0969	
R indices (all data)	R1 = 0.0465, wR2 = 0.0997	
Largest diff. peak and hole	1.109 and -0.688 e.$Å^{-3}$	

Table S2 Selected bond length (Å) and bond angle (°) of [Cu(PICPH)$(Cl)_2$]

Bond length	
CU1-N(23)	1.985(2)
CU1-N(13)	2.011(2)
CU1-N(20)	2.1435(19)
CU1-CL2	2.2969(7)
CU1-CL3	2.4120(8)
N(1)-C(9)	1.386(3)
N(1)-C(2)	1.398(3)
N(1)-C(11)	1.456(3)
C(2)-O(10)	1.199(3)
C(2)-C(3)	1.480(3)
C(3)-C(4)	1.385(3)
C(3)-C(8)	1.396(3)
C(4)-C(5)	1.384(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.386(4)
C(5)-H(5)	0.9500
C(6)-C(7)	1.394(3)
C(6)-H(6)	0.9500
C(7)-C(8)	1.382(4)
C(7)-H(7)	0.9500
C(8)-C(9)	1.487(3)
C(9)-N(20)	1.276(3)
C(11)-C(12)	1.506(3)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-N(13)	1.345(3)
C(12)-C(17)	1.378(4)
N(13)-C(14)	1.353(3)
C(14)-C(15)	1.373(4)
C(14)-H(14)	0.9500
C(15)-C(16)	1.375(4)
C(15)-H(15)	0.9500
C(16)-C(17)	1.397(4)
C(16)-H(16)	0.9500
C(17)-H(17)	0.9500
N(20)-C(21)	1.465(3)
C(21)-C(22)	1.504(3)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-N(23)	1.338(3)
C(22)-C(27)	1.387(4)
N(23)-C(24)	1.344(3)
C(24)-C(25)	1.376(4)
C(24)-H(24)	0.9500
C(25)-C(26)	1.378(4)
C(25)-H(25)	0.9500

C(26)-C(27)	1.381(4)
C(26)-H(26)	0.9500
C(27)-H(27)	0.9500

Bond angles

N(23)-CU1-N(13)	178.13(8)
N(23)-CU1-N(20)	79.79(8)
N(13)-CU1-N(20)	98.57(8)
N(23)-CU1-CL2	93.61(6)
N(13)-CU1-CL2	88.16(6)
N(20)-CU1-CL2	132.91(6)
N(23)-CU1-CL3	87.82(7)
N(13)-CU1-CL3	91.42(6)
N(20)-CU1-CL3	93.78(6)
CL2-CU1-CL3	132.82(3)
C(9)-N(1)-C(2)	112.78(19)
C(9)-N(1)-C(11)	124.70(19)
C(2)-N(1)-C(11)	122.1(2)
O(10)-C(2)-N(1)	124.5(2)
O(10)-C(2)-C(3)	130.8(2)
N(1)-C(2)-C(3)	104.7(2)
C(4)-C(3)-C(8)	121.7(2)
C(4)-C(3)-C(2)	128.9(2)
C(8)-C(3)-C(2)	109.4(2)
C(5)-C(4)-C(3)	117.6(2)
C(5)-C(4)-H(4)	121.2
C(3)-C(4)-H(4)	121.2
C(4)-C(5)-C(6)	121.1(2)
C(4)-C(5)-H(5)	119.5
C(6)-C(5)-H(5)	119.5
C(5)-C(6)-C(7)	121.2(3)
C(5)-C(6)-H(6)	119.4
C(7)-C(6)-H(6)	119.4
C(8)-C(7)-C(6)	118.0(2)
C(8)-C(7)-H(7)	121.0
C(6)-C(7)-H(7)	121.0
C(7)-C(8)-C(3)	120.3(2)
C(7)-C(8)-C(9)	132.8(2)
C(3)-C(8)-C(9)	106.8(2)

N(20)-C(9)-N(1)	121.0(2)
N(20)-C(9)-C(8)	132.7(2)
N(1)-C(9)-C(8)	106.28(19)
N(1)-C(11)-C(12)	110.45(19)
N(1)-C(11)-H(11A)	109.6
C(12)-C(11)-H(11A)	109.6
N(1)-C(11)-H(11B)	109.6
C(12)-C(11)-H(11B)	109.6
H(11A)-C(11)-H(11B)	108.1
N(13)-C(12)-C(17)	122.4(2)
N(13)-C(12)-C(11)	116.8(2)
C(17)-C(12)-C(11)	120.7(2)
C(12)-N(13)-C(14)	117.9(2)
C(12)-N(13)-CU1	123.17(17)
C(14)-N(13)-CU1	118.78(17)
N(13)-C(14)-C(15)	122.8(2)
N(13)-C(14)-H(14)	118.6
C(15)-C(14)-H(14)	118.6
C(14)-C(15)-C(16)	119.2(3)
C(14)-C(15)-H(15)	120.4
C(16)-C(15)-H(15)	120.4
C(15)-C(16)-C(17)	118.8(2)
C(15)-C(16)-H(16)	120.6
C(17)-C(16)-H(16)	120.6
C(12)-C(17)-C(16)	118.9(2)
C(12)-C(17)-H(17)	120.6
C(16)-C(17)-H(17)	120.6
C(9)-N(20)-C(21)	118.5(2)
C(9)-N(20)-CU1	131.16(17)
C(21)-N(20)-CU1	107.59(14)
N(20)-C(21)-C(22)	109.8(2)
N(20)-C(21)-H(21A)	109.7
C(22)-C(21)-H(21A)	109.7
N(20)-C(21)-H(21B)	109.7
C(22)-C(21)-H(21B)	109.7
H(21A)-C(21)-H(21B)	108.2
N(23)-C(22)-C(27)	121.7(2)
N(23)-C(22)-C(21)	117.5(2)

C(27)-C(22)-C(21)	120.8(2)
C(22)-N(23)-C(24)	119.3(2)
C(22)-N(23)-CU1	115.74(16)
C(24)-N(23)-CU1	124.49(18)
N(23)-C(24)-C(25)	122.1(2)
N(23)-C(24)-H(24)	119.0
C(25)-C(24)-H(24)	119.0
C(24)-C(25)-C(26)	118.6(2)
C(24)-C(25)-H(25)	120.7
C(26)-C(25)-H(25)	120.7
C(25)-C(26)-C(27)	119.7(3)
C(25)-C(26)-H(26)	120.2
C(27)-C(26)-H(26)	120.2
C(26)-C(27)-C(22)	118.6(2)
C(26)-C(27)-H(27)	120.7
C(22)-C(27)-H(27)	120.7

Table S3. Dependence of initial rates on the concentration of DTBC (conc. of [Cu(PICPH)$(Cl)_2$] = 1x10^{-4} mol dm^{-3}).

[3,5-DTBC] (mol dm^{-3})	V (mol dm-3 s-1) [Cu(PICPH)Cl_2]
1E-3	2.5826E-4
3E-3	2.7805E-4
5E-3	2.8228E-4
7E-3	2.8497E-4
1E-2	2.8706E-4