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Copper(II) complexes of functionalized 2,2′:6′,2″-terpyridines and 2,6-di(thiazol-2-yl)pyridine. Structure, spectroscopy, cytotoxicity and catalytic activity †

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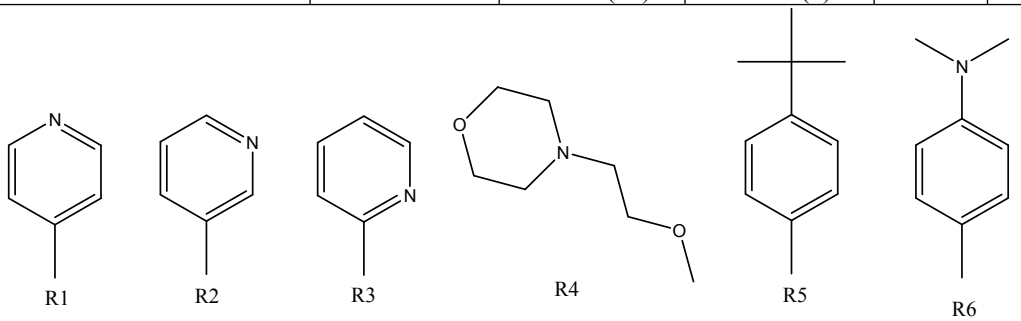
† Electronic Supplementary Information (ESI, this file) available: Bond lengths and angles, dihedral angles between aromatic rings, short intra- and intermolecular contacts, electronic absorption spectra in methanol, IR spectra, XPRD patterns, HRMS reports. CCDC 1540061–1540066.

Electronic supplementary information (ESI)

Table S1. The selected structural data for Cu(II) coordination compounds incorporating 2,2′:6′,2″-terpyridine derivatives.

terpy						
Compound	**Cu-$N_{central}$ [Å]**	**Cu-$N_{terminal}$ [Å]**	**Cu-Cl [Å]**	**τ**	**coordination geometry**	**Ref.**
$CuCl_2$(terpy) · H_2O	1.949(6)	2.049 (6) 2.048(6)	2.231(2) 2.565(2)	0.085	square pyramid	[1]
$CuCl_2$(terpy)	1.952	2.052 2.056	2.252 2.469	-	square pyramid	[2]
$CuCl_2$(terpy) · H_2O	1.944	2.039 2.044	2.221 2.554	-		
$CuCl_2$(terpy)	1.9650(8)	2.0556(8) 2.0559(8)	2.2557(3) 2.4700(3)	0.030	square pyramid	[3]
4'-R-terpy						
Compound	**Cu-$N_{central}$ [Å]**	**Cu-$N_{terminal}$ [Å]**	**Cu-Cl [Å]**	**τ**	**coordination geometry**	**Ref.**
1	1.941(2)	2.042(2) 2.045(2)	2.2176(8) 2.6007(8)	0.132	square pyramid	This publication
2	1.939(3)	2.036(4) 2.050(4)	2.2274(13) 2.5631(13)	0.072	square pyramid	
3	1.950(2)	2.043(2) 2.051(2)	2.2424(8) 2.4894(8)	0.077	square pyramid	
	1.955(2)	2.017(2) 2.023(2)	2.3034(8) 2.4008(8)	0.457	trigonal bipyramid	
4	1.976(2)	2.036(2) 2.046(2)	2.2348(8) 2.4782(8)	0.08	square pyramid	
5	1.977(2)	2.046(3) 2.047(3)	2.2392(9) 2.4643(10)	0.059	square pyramid	
6	1.979(4)	2.027(4) 2.048(4)	2.2311(15) 2.5796(14)	0.121	square pyramid	
[$CuCl_2$(4'-(H-**R1**)-terpy)]Cl · $4H_2O$	1.942(3)	2.046(3) 2.051(3)	2.218(1) 2.570(1)	0.104	square pyramid	[4]
[$CuCl^2$(4'-(**R1**)-terpy)] · H2O · MeOH	1.941(2)	2.038(1) 2.038(1)	2.225(1) 2.579(1)	0.146	square pyramid	
[$CuCl_2$(4'-(**R2**)-terpy)] · H2O	1.946(1)	2.032(1) 2.018(1)	2.2524(4) 2.5219(5)	0.064	square pyramid	
	1.948(1)	2.035(1) 2.048(1)	2.2623(5) 2.4433(5)	0.035		
[$CuCl_2$(4'-(**R3**)-terpy)] · MeOH	1.955(2)	2.038(2) 2.045(2)	2.2424(8) 2.4958(9)	0.034	square pyramid	
$CuCl_2$(4'-Cl-terpy)	1.948(3)	2.049(2) 2.049(2)	2.2379(11) 2.5001(12)	0.106	square pyramid	[5]
$CuCl_2$(4'-(**R4**)-terpy)	1.9525(18)	2.0418(18) 2.0526(17)	2.2393(5) 2.5237(6)	0.105	square pyramid	[6]
$CuCl_2$(4'-(**R5**)-terpy)	1.948(3)	2.029(3) 2.047(3)	2.228(1) 2.520(1)	0.051	square pyramid	[7]
$CuCl_2$(4'-(H-**R1**)-terpy) · H_2O · HCl	1.9536(12)	2.0425(13) 2.0525(12)	2.2320(4) 2.5518(5)	0.118	square pyramid	[3]
$CuCl_2$(4'-Ph-terpy) · H_2O	1.957(3)	2.037(4) 2.044(3)	2.251(2) 2.505(2)	0.048	square pyramid	[8]
[$CuCl_2$(4'-Ph-terpy)] · [$CuCl_2$(4'-Ph-terpy)] · CH_3OH	1.961(3)	2.036(3) 2.043(3)	2.2430(9) 2.4491(9)	0.048	square pyramid	
	1.950(2)	2.045(3)	2.247(1)	0.111	square pyramid	

		2.047(3)	2.556(1)			
$CuCl_2$(4'-Ph-terpy) · [$CuCl_2$(4'-Ph-terpy)]$_2$	1.958(2)	2.035(2) 2.043(2)	2.2469(7) 2.4410(7)	0.001	square pyramid	[9]
$CuCl_2$[4'-(**R6**)-terpy]	1.9560(19)	2.0374(18) 2.0425(19)	2.2431(6) 2.4851(6)	0.019	square pyramid	[10]
$CuCl_2$(4'-Cl-terpy)	1.963(2)	2.041(2) 2.054(2)	2.2437(7) 2.4792(8)	0.007	square pyramid	[11]
$CuCl_2$(4'-CN-terpy)	1.954(2)	2.036(2) 2.040(2)	2.2394(8) 2.4672(8)	0.033	square pyramid	
	1.967(2)	2.032(2) 2.040(2)	2.2381(8) 2.4424(8)	0.039	square pyramid	
other *terpy* compounds						
Compound	**Cu-$N_{central}$ [Å]**	**Cu-$N_{terminal}$ [Å]**	**Cu-Cl [Å]**	**τ**	**coordination geometry**	**Ref.**
[$CuCl_2$(**L1**)]	1.974(4)	2.074(4) 2.081(4)	2.3136(13) 2.3169(12)	0.576	trigonal bipyramid	[12]
[$CuCl_2$(**L2**)]	1.972(5)	2.040(6) 2.040(6)	2.311(3) 2.311(3)	0.573	trigonal bipyramid	[13]
[$CuCl_2$(**L3**)]	1.9808(13)	2.0857(12) 2.0874(12)	2.3313(5) 2.3365(5)	0.79	trigonal bipyramid	[14]



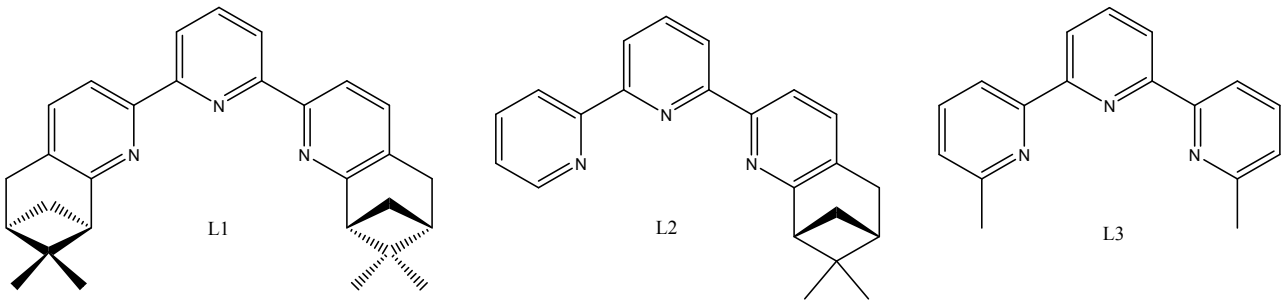


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Table S2. Bond lengths [Å] and angles [°] of prepared copper(II) complexes

Bond lengths [Å]						
	1	**2**	**3**	**4**	**5**	**6**
Cu(1)–N(1)	2.042(2)	2.036(4)	2.043(2)	2.036(2)	2.046(3)	2.027(4)
Cu(1)–N(2)	1.941(2)	1.939(3)	1.950(2)	1.976(2)	1.977(2)	1.979(4)
Cu(1)–N(3)	2.045(2)	2.050(4)	2.051(2)	2.046(2)	2.047(3)	2.048(4)
Cu(1)–Cl(1)	2.2176(8)	2.2274(13)	2.2424(8)	2.2348(8)	2.2392(9)	2.2311(15)
Cu(1)–Cl(2)	2.6007(8)	2.5631(13)	2.4894(8)	2.4782(8)	2.4643(10)	2.5796(14)
N(1)–C(1)	1.343(3)	1.334(6)	1.342(3)	1.361(3)	1.364(4)	1.368(6)
N(1)–C(3)				1.320(3)	1.321(4)	1.318(6)
N(2)–C(4)				1.343(3)	1.339(4)	1.342(6)
N(2)–C(8)				1.338(3)	1.333(4)	1.334(6)
N(3)–C(9)				1.316(3)	1.327(4)	1.309(6)
N(3)–C(11)				1.373(3)	1.377(4)	1.373(7)
S(1)–C(2)				1.707(3)	1.706(4)	1.701(6)
S(1)–C(3)				1.704(3)	1.699(3)	1.705(5)
S(2)–C(9)				1.702(3)	1.697(3)	1.700(5)
S(2)–C(10)				1.712(3)	1.710(4)	1.702(6)
N(1)–C(5)	1.358(3)	1.360(5)	1.342(3)			
N(2)–C(6)	1.332(3)	1.343(5)	1.338(3)			
N(2)–C(10)	1.341(3)	1.330(5)	1.343(3)			
N(3)–C(11)	1.352(3)	1.363(6)	1.348(4)			
N(3)–C(15)	1.336(4)	1.329(5)	1.342(4)			
Cu(2)–N(5)			2.017(2)			
Cu(2)–N(6)			1.955(2)			
Cu(2)–N(7)			2.023(2)			
Cu(2)–Cl(3)			2.3034(8)			
Cu(2)–Cl(4)			2.4008(8)			
N(5)–C(21)			1.341(4)			
N(5)–C(25)			1.352(3)			
Bond angles [°]						
	1	**2**	**3**	**4**	**5**	**6**
N(1)–Cu(1)–N(2)	79.14(9)	79.48(14)	78.83(9)	78.49(9)	78.43(10)	78.12(16)
N(1)–Cu(1)–N(3)	156.58(9)	156.74(14)	155.78(10)	153.52(8)	153.72(11)	155.32(17)
N(2)–Cu(1)–N(3)	79.52(9)	78.87(14)	78.70(9)	78.25(8)	78.13(10)	78.11(17)
N(1)–Cu(1)–Cl(1)	99.32(7)	98.44(11)	98.36(7)	97.92(7)	99.16(7)	100.94(12)
N(1)–Cu(1)–Cl(2)	94.84(7)	92.23(11)	95.03(7)	97.73(7)	96.79(8)	90.61(12)
N(2)–Cu(1)–Cl(1)	164.51(7)	161.05(11)	160.41(7)	158.32(7)	157.24(9)	162.57(12)
N(2)–Cu(1)–Cl(2)	93.68(7)	94.13(11)	95.70(7)	96.69(7)	97.06(8)	94.44(11)
N(3)–Cu(1)–Cl(1)	98.65(7)	99.25(11)	99.78(8)	99.01(7)	97.85(7)	99.73(12)
N(3)–Cu(1)–Cl(2)	96.04(6)	97.71(10)	96.05(7)	97.38(7)	97.72(8)	97.75(12)
Cl(1)–Cu(1)–Cl(2)	101.82(3)	104.79(5)	103.87(3)	104.98(3)	105.68(4)	102.99(5)
N(5)–Cu(2)–N(6)		78.96(9)				
N(5)–Cu(2)–N(7)		158.16(8)				
N(6)–Cu(2)–N(7)		79.20(9)				
N(5)–Cu(2)–Cl(3)		94.65(7)				
N(5)–Cu(2)–Cl(4)		97.61(7)				
N(6)–Cu(2)–Cl(3)		130.72(7)				
N(6)–Cu(2)–Cl(4)		119.99(7)				
N(7)–Cu(2)–Cl(3)		99.37(6)				
N(7)–Cu(2)–Cl(4)		93.49(7)				
Cl(3)–Cu(2)–Cl(4)		109.29(3)				

Table S3. Dihedral angles between aromatic rings in compounds **1-6**.

Dihedral angles [°] **in 1:**		**Dihedral angles**[°] **in 4:**	
Central ring – terminal rings	4.1(2) 2.8(2)	Central ring – terminal rings	2.3(2) 7.3(2)
Central ring – R^n-ring	4.6(2)	Central ring – R^n-ring	4.0(2)
Terminal rings	6.8(2)	Terminal rings	9.5(2)
Dihedral angles [°] **in 2:**		**Dihedral angles** [°] **in 5:**	
Central ring – terminal rings	8.2(2) 6.1(2)	Central ring – terminal rings	4.1(2) 7.9(2)
Central ring – R^n-ring	5.1(3)	Central ring – R^n-ring	4.5(2)
Terminal rings	11.7(2)	Terminal rings	11.0(2)
Dihedral angles [°] **in 3:**		**Dihedral angles** [°] **in 6:**	
A			
Central ring – terminal rings	4.5(2) 4.1(2)	Central ring – terminal rings	7.9(2) 8.0(2)
Central ring – R^n-ring	19.1(2)	Central ring – R^n-ring	14.7(2)
Terminal rings	6.0(2)	Terminal rings	3.3(2)
B			
Central ring – terminal rings	3.8(2) 1.5(2)		
Central ring – R^n-ring	11.8(2)		
Terminal rings	2.5(2)		

Table S4. Short intra- and intermolecular contacts detected in structures **1-6**.

D	**A**	**D—H** [Å]	**H•••A** [Å]	**D•••A** [Å]	**D—H•••A** [°]
1					
O(2)	Cl(2)	0.82	2.38	3.195(3)	170.10
2					
C(4)	Cl(2)[a]	0.93	2.81	3.728(5)	170.8
C(7)	Cl(2)[a]	0. 93	2.82	3.750(4)	179.1
C(9)	S(1)	0.93	2.76	3.146(4)	105.7
C(17)	Cl(2)[a]	0.93	2.68	3.588(5)	165.9
3					
C(4)	Cl(2)[b]	0.93	2.61	3.501(3)	160.9
4					
C(5)	Cl(2)[a]	0.93	2.70	3.629(3)	173.4
C(15)	Cl(1)[c]	0.93	2.81	3.713(3)	164.1
5					
C(2)	Cl(2)[d]	0.93	2.66	3.534(4)	157.1
C(5)	Cl(2)[a]	0.93	2.72	3.641(3)	173.8
C(7)	S(3)	0.93	2.70	3.095(3)	106.7
C(13)	Cl(2)[a]	0.93	2.78	3.685(4)	163.6
C(14)	Cl(2)[e]	0.93	2.83	3.743(4)	167.5
6					
C(2)	Cl(2)[f]	0.93	2.57	3.485(5)	168.8
C(5)	Cl(2)[g]	0.93	2.60	3.524(5)	173.8
C(10)	Cl(2)[h]	0.93	2.48	3.357(6)	153.3
C(13)	Cl(2)[g]	0.93	2.81	3.647(5)	151.1

Symmetry operations: (a) = 1+*x*,*y*,*z*; (b) = 2-*x*,1-*y*,1-*z*; (c) = 1+*x*,1+*y*,1+*z*; (d) = -*x*,-1-*y*,-*z*; (e) = 1-*x*,-*y*,1-*z*; (f) = 1-*x*,1-*y*,-1/2+*z*, (g) = *x*,*y*,-1+*z*, (h) = 1/2-*x*,-1/2+*y*,1/2+*z*;

Table S5. Short π•••π interactions for **1-6**.

Cg(I)•••Cg(J)	Cg(I)•••Cg(J) [Å]	α[°]	β[°]	γ [°]	Cg(I)-Perp [Å]	Cg(J)-Perp [Å]
1						
Cg(1)•••Cg(2)[a]	3.6134(19)	0.94(18)	22.16	21.88	3.3532(15)	-3.3464(13)
Cg(1)•••Cg(3)[b]	3.7030(19)	4.63(17)	23.58	20.39	3.4709(15)	3.3938(11)
Cg(2)•••Cg(4)[i]	3.8698(18)	6.79(15)	29.13	27.04	-3.4468(13)	-3.3802(12)
Cg(4)•••Cg(4)[j]	3.7929(18)	0	29.46	29.46	3.3024(12)	-3.3024(12)
2						
Cg(9)•••Cg(4)[a]	3.6762	1.067	23.23	22.48	-3.3968	3.3781
Cg(2)•••Cg(4)[i]	3.9690	1.679	20.87	30.53	3.4188	3.7087
3						
Cg(2)•••Cg(3)[b]	3.9611(18)	4.51(15)	27.63	31.20	3.3884(13)	3.5094(12)
Cg(2)•••Cg(4)[l]	3.8531(19)	5.99(16)	26.12	20.16	-3.6170(13)	-3.4597(14)
Cg(4)•••Cg(5)[l]	3.9388(18)	23.43(16)	19.84	23.73	3.6058(14)	3.7050(12)
Cg(6)•••Cg(7)[m]	3.8994(18)	11.82(17)	19.01	30.75	-3.3512(14)	3.6866(11)
Cg(7)•••Cg(8)[n]	3.4852(16)	3.82(13)	18.35	20.62	3.2620(11)	3.3079(11)
4						
Cg(10)•••Cg(11)[o]	3.7795(17)	9.55(15)	20.28	25.73	-3.4049(12)	3.5453(12)
Cg(11)•••Cg(12)[p]	3.7051(17)	3.29(17)	20.99	23.91	-3.3871(12)	3.4593(13)
5						
Cg(10)•••Cg(11)[p]	3.886(2)	11.01(18)	21.42	31.62	-3.3088(14)	-3.6171(15)
Cg(11)•••Cg(15)[r]	3.7163(18)	3.89(18)	22.05	24.23	-3.3889(14)	3.4444(15)
6						
Cg(11)•••Cg(13)[q]	3.595(3)	6.7(3)	21.71	19.25	-3.3935(19)	3.340(2)
Cg(11)•••Cg(14)[h]	3.886(2)	6.2(2)	32.57	29.19	3.3921(19)	-3.2747(17)

α = dihedral angle between *Cg*(I) and *Cg*(J); *Cg*(I)-Perp = Perpendicular distance of *Cg*(I) on ring J; *Cg*(J)-Perp = perpendicular distance of *Cg*(J) on ring I; β = angle *Cg*(I)→*Cg*(J) vector and normal to ring I; γ = angle *Cg*(I) →*Cg*(J) vector and normal to plane J.

Cg1 is the centroid of atoms = O1/C16/C17/C18/C19; Cg2 is the centroid of atoms = N1/C1/C2/C3/C4/C5; Cg3 is the centroid of atoms = N2/C6/C7/C8/C9/C10; Cg4 is the centroid of atoms = N3/C11/C12/C13/C14/C15; Cg5 is the centroid of atoms = N7/C31/C32/C33/C34/C35; Cg6 is the centroid of atoms = N8/C36/C37/C38/C39; Cg7 is the centroid of atoms = N6/C26/C27/C28/C29/C30; Cg8 is the centroid of atoms = N5/C21/C22/C23/C24/C25; Cg9 is the centroid of atoms = S1/C16/C17/C18/C19; Cg10 is the centroid of atoms = S1/C2/C1/N1/C3; Cg11 is the centroid of atoms = S2/C9/N3/C11/C10; Cg12 is the centroid of atoms = O1/C12/C13/C14/C15; Cg13 is the centroid of atoms = N4/C12/C13/C14/C15; Cg14 is the centroid of atoms = N2/C4/C5/C6/C7/C8; Cg15 is the centroid of atoms = S3/C12/C13/C14/C15.

Symmetry codes: (a) = 1+*x*,*y*,*z*; (b) = 2-*x*,1-*y*,1-*z*; (i) = 1-*x*,1-*y*,-*z*; (j) = 1-*x*,-*y*,-*z*; (l) = 1-*x*,1-*y*,1-*z*; (m) = -*x*,-*y*,2-*z*; (n) = 1-*x*,-*y*,2-*z*; (o) = -*x*,2-*y*,1-*z*; (p) = -1+*x*,*y*,*z*; (q) = *x*,*y*,1+*z*; (r) = -*x*,-*y*,-*z*; (h) = 1/2-*x*,-1/2+*y*,1/2+*z*;

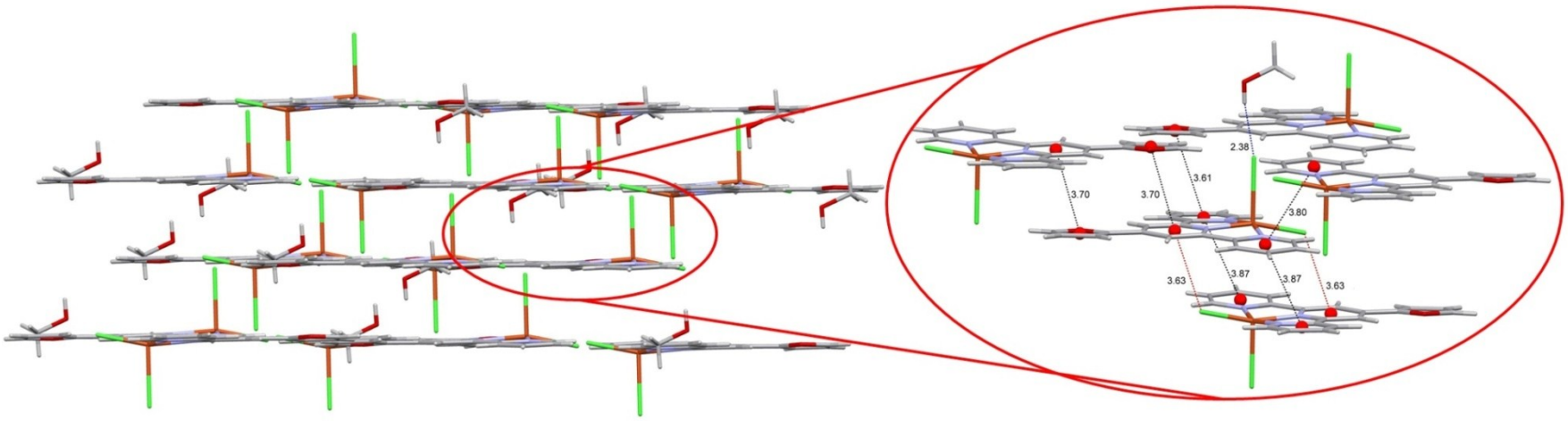
Table S6. C—X•••Cg(J)(π-ring) interactions for **1-6**.

Y-X(I)•••Cg(J)	X(I)•••Cg(J) [Å]	X-Perp [Å]	γ [°]	Y-X•••Cg(J) [°]
1				
Cu(1)-Cl(1)•••Cg(3)^{i}	3.6348(15)	-3.364	22.26	123.68(4)
2				
C(13)-H(13)•••Cg(3)^{s}	2.96	-2.72	23.02	163
Cu(1)-Cl(1)•••Cg(3)^{i}	3.6565	3.324	24.63	127
3				
Cu(1)-Cl(1)•••Cg(3)^{l}	3.5311(14)	-3.322	19.82	115.93(4)
4				
Cu(1)-Cl(1)•••Cg(14)^{o}	3.5499(15)	-3.384	17.61	118.80(4)
5				
Cu(1)-Cl(1)•••Cg(14)^{r}	3.6710(19)	-3.384	22.80	114.35(5)
6				
Cu(1)-Cl(1)•••Cg(13)^{h}	3.795(3)	3.502	22.64	68.88(5)

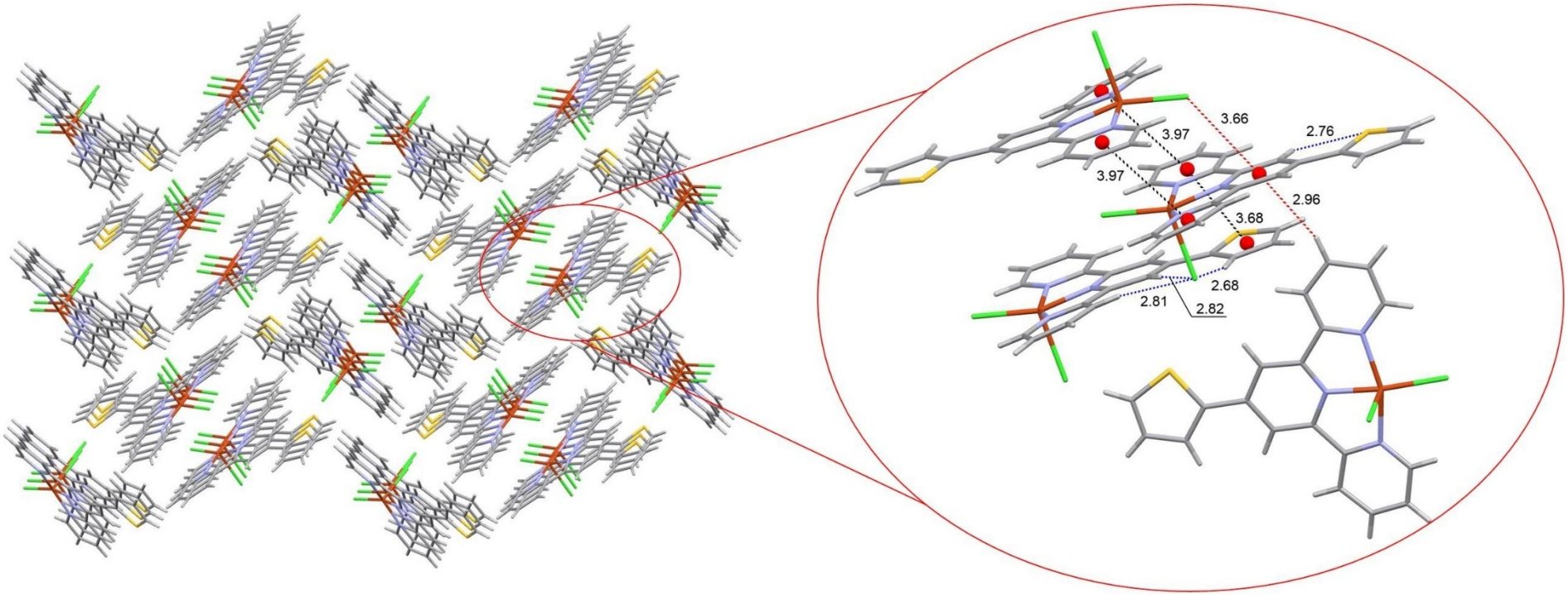
γ = angle X(I)→Cg(J) vector and normal to plane J.

Cg3 is the centroid of atoms = N2/C6/C7/C8/C9/C10; Cg14 is the centroid of atoms = N2/C4/C5/C6/C7/C8; Cg13 is the centroid of atoms = N4/C12/C13/C14/C15.

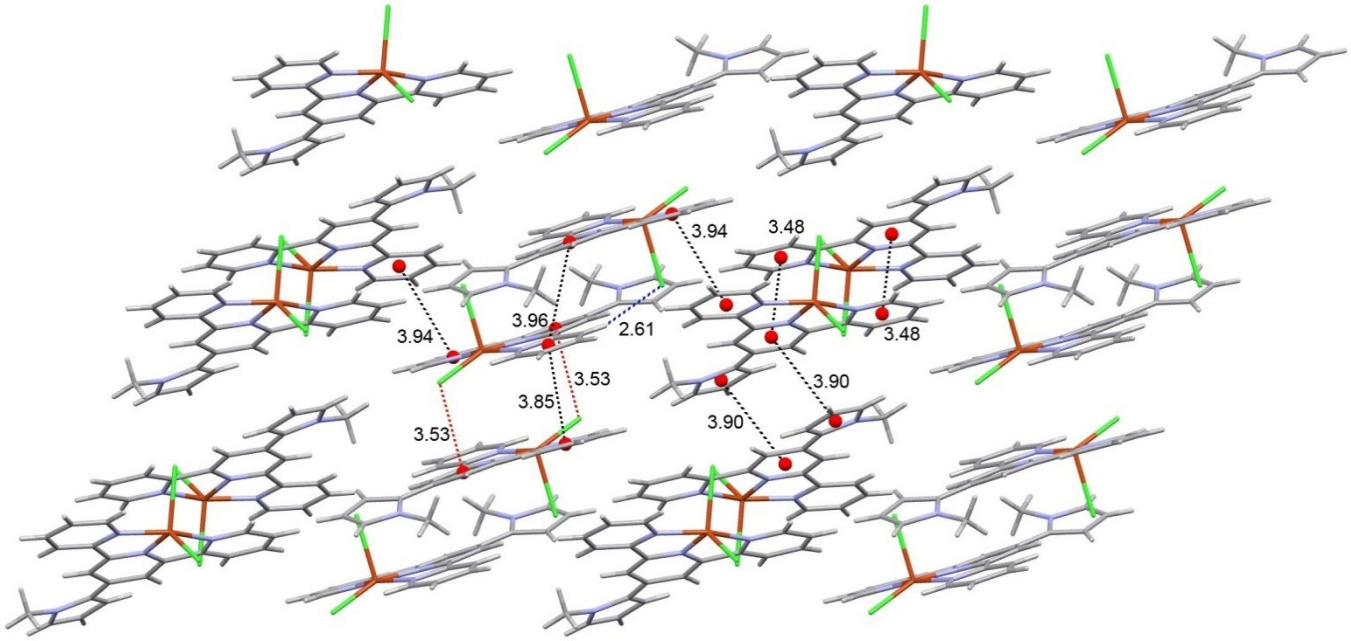
Symmetry codes: (i) = 1-*x*,1-*y*,-*z*; (s) = 1-*x*,1/2+*y*,1/2-*z*; (l) = 1-*x*,1-*y*,1-*z*; (o) = -*x*,2-*y*,1-*z*; (r) = -*x*,-*y*,-*z*; (h) = 1/2-*x*,-1/2+*y*,1/2+*z*;



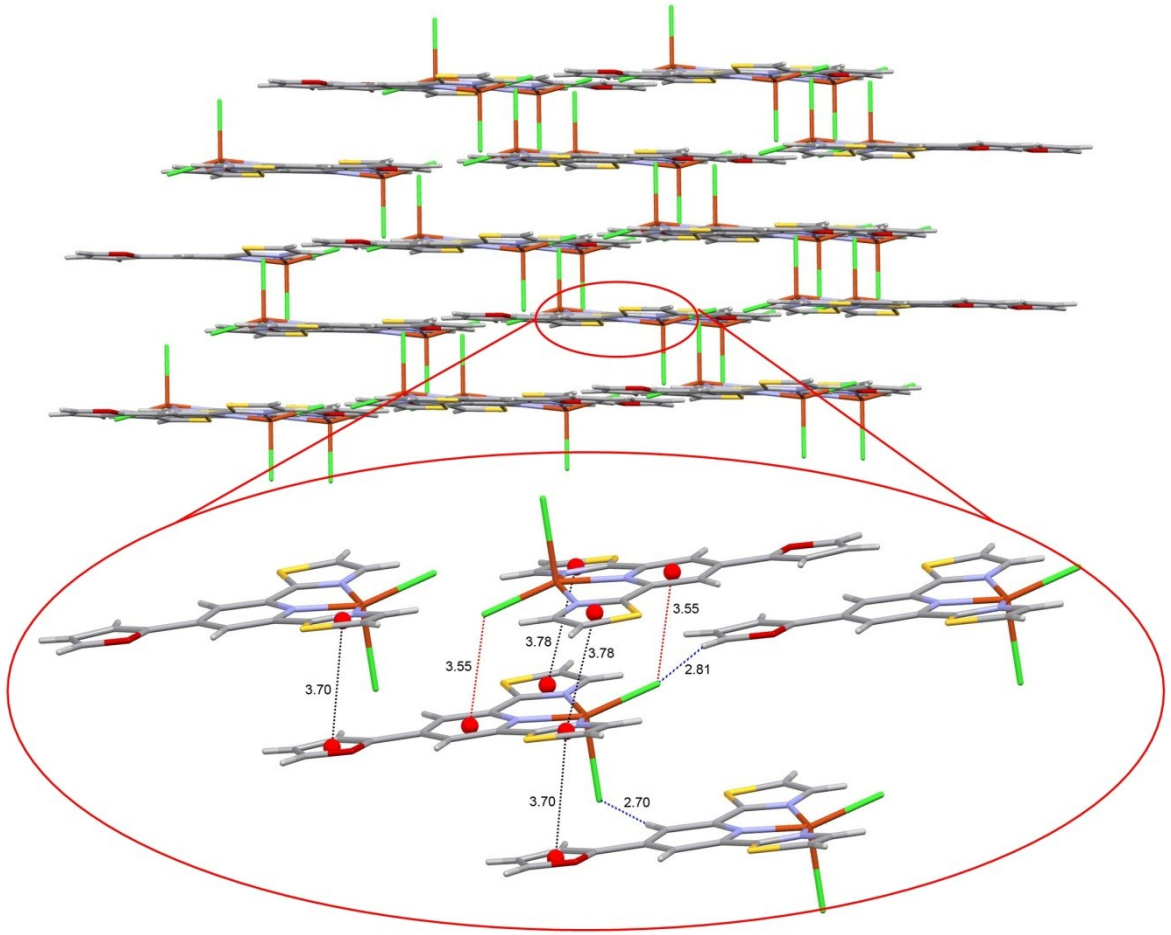
(1)



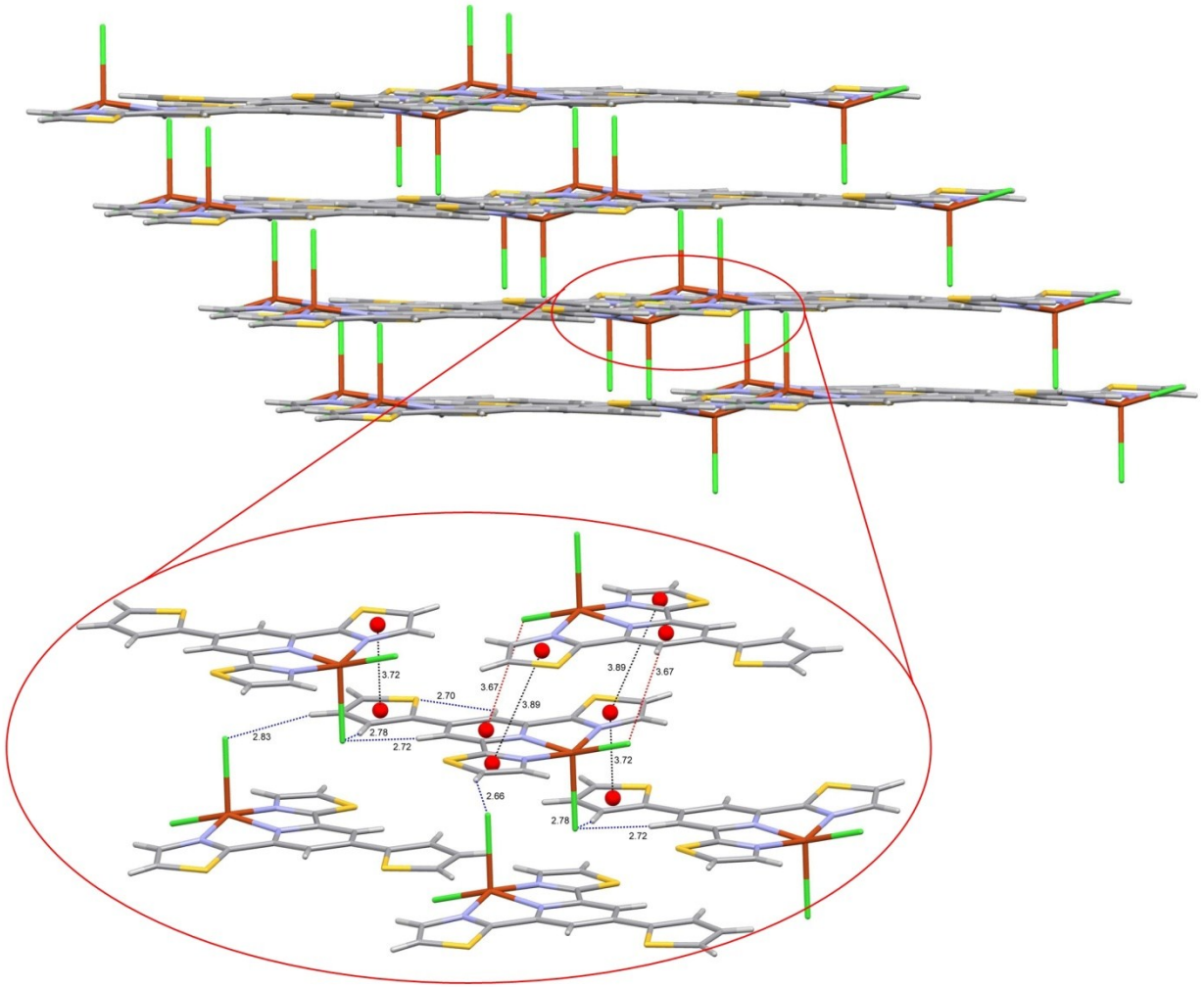
(2)



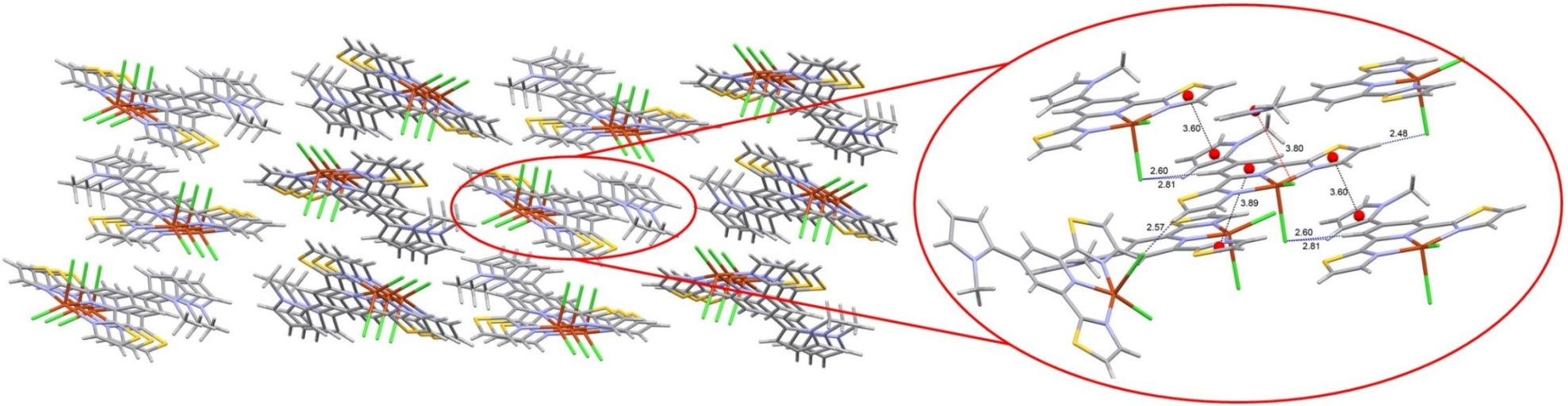
(3)



(4)

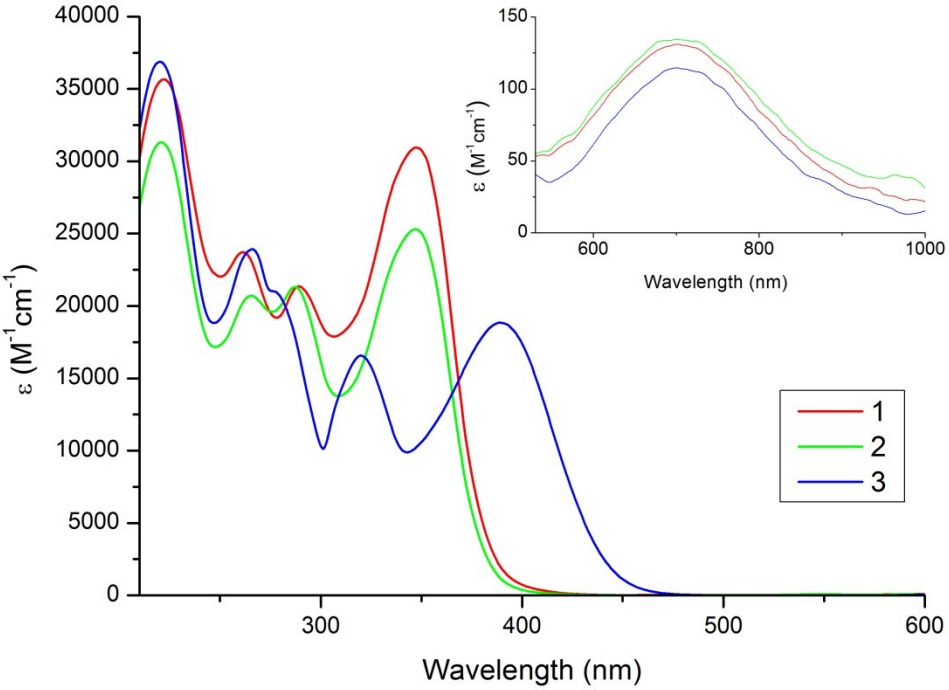


(5)

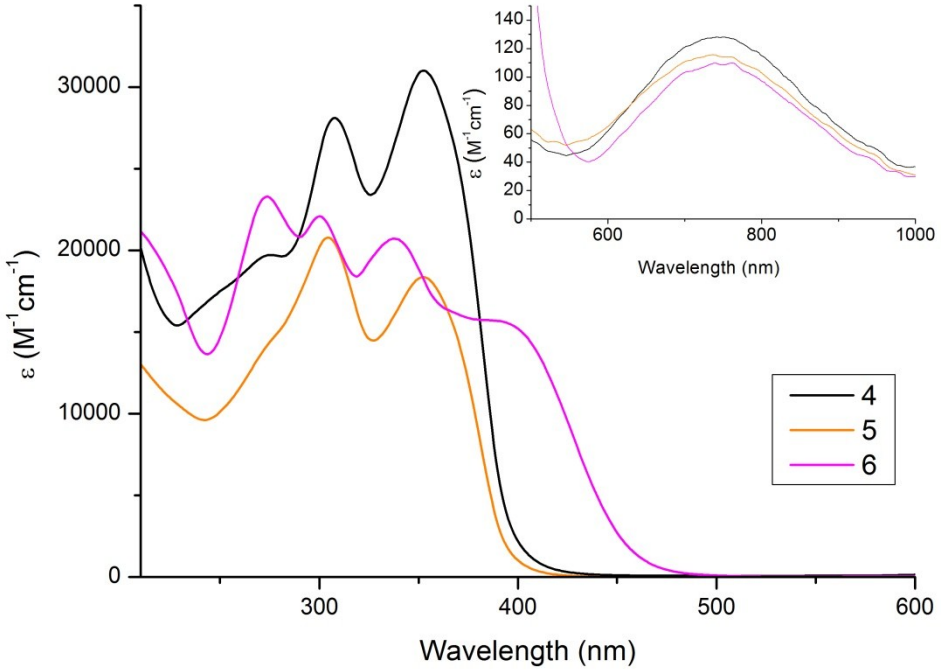


(6)

Figure S1. View of the supramolecular packing of **1-6** arising from hydrogen bonds and weak π•••π and π•••Cl type interactions.

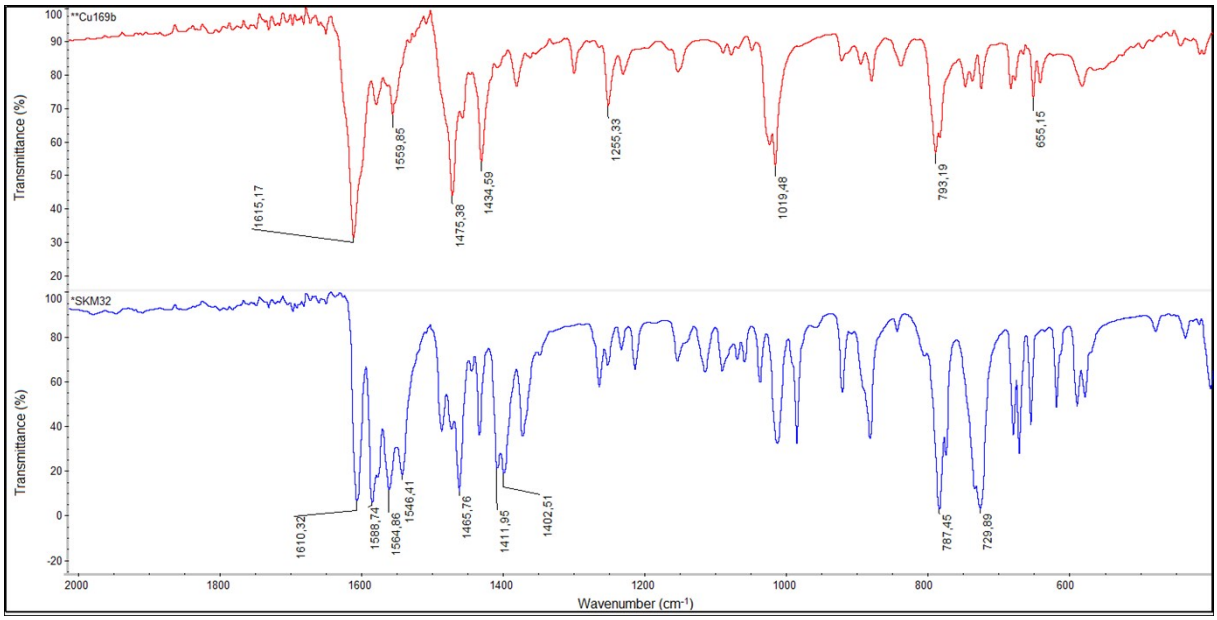


a)

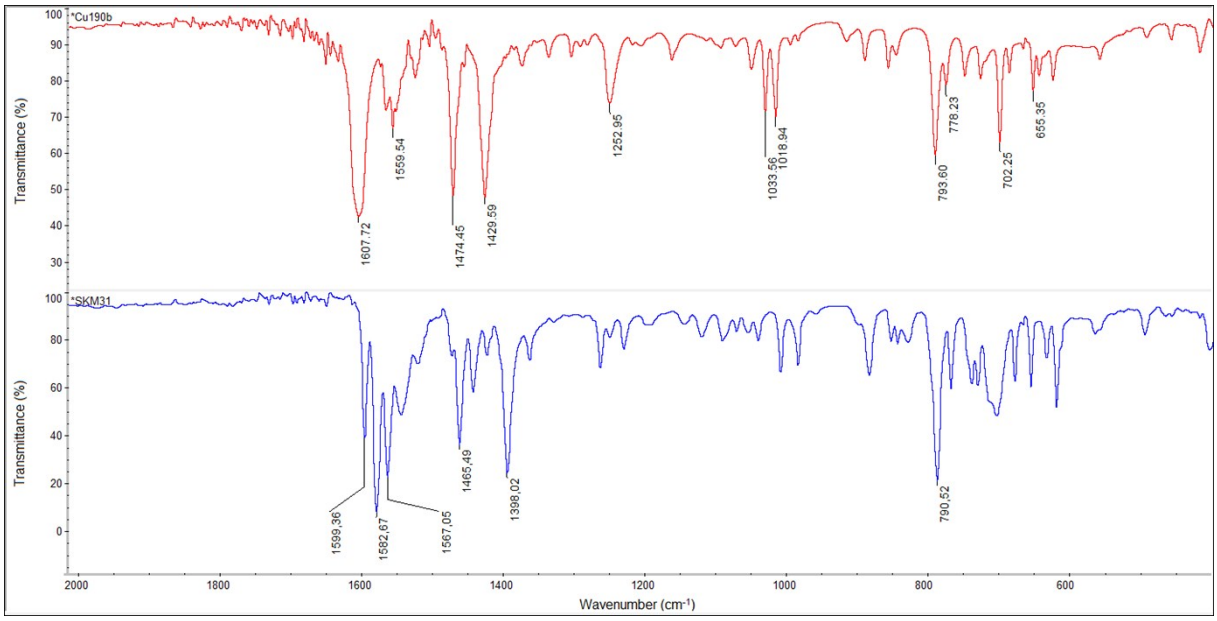


b)

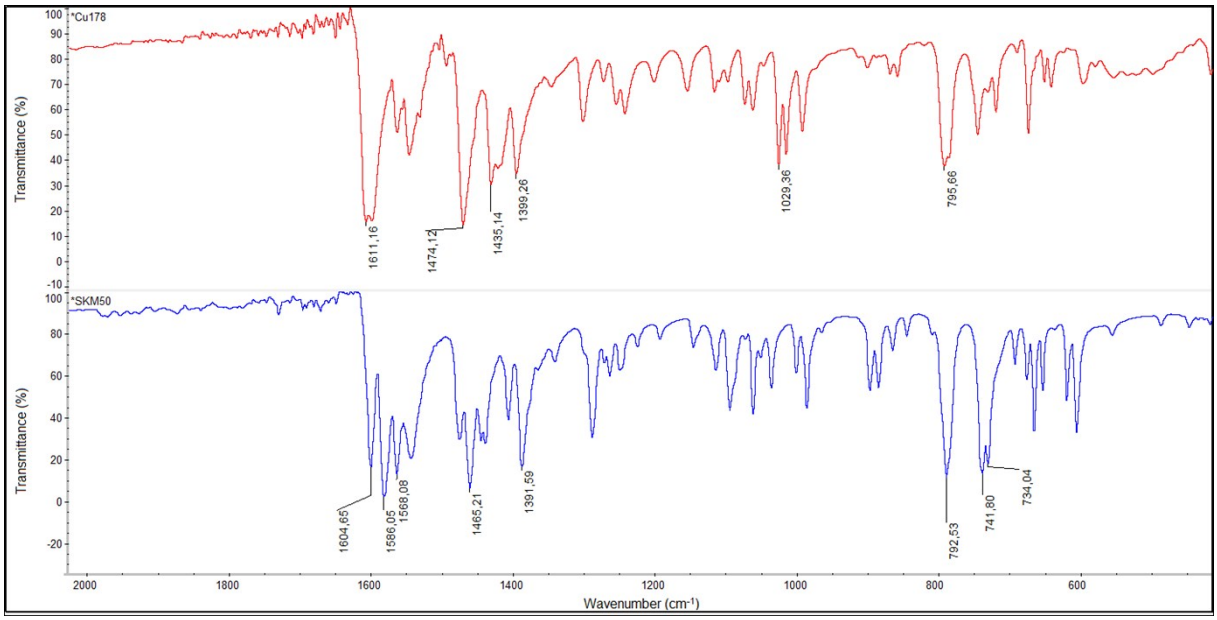
Figure S2. Electronic absorption spectra of **1-3** (a) and **4-6** (b) in methanol ($5 \cdot 10^{-5}$ M, inset: $5 \cdot 10^{-4}$ M)


**Cu169b
Transmittance (%)
1615,17
1559,85
1475,98
1434,59
1255,33
1019,48
793,19
655,15
*SKM32
Transmittance (%)
1610,32
1588,74
1564,86
1546,41
1465,76
1411,95
1402,51
787,45
729,89
Wavenumber (cm-1)

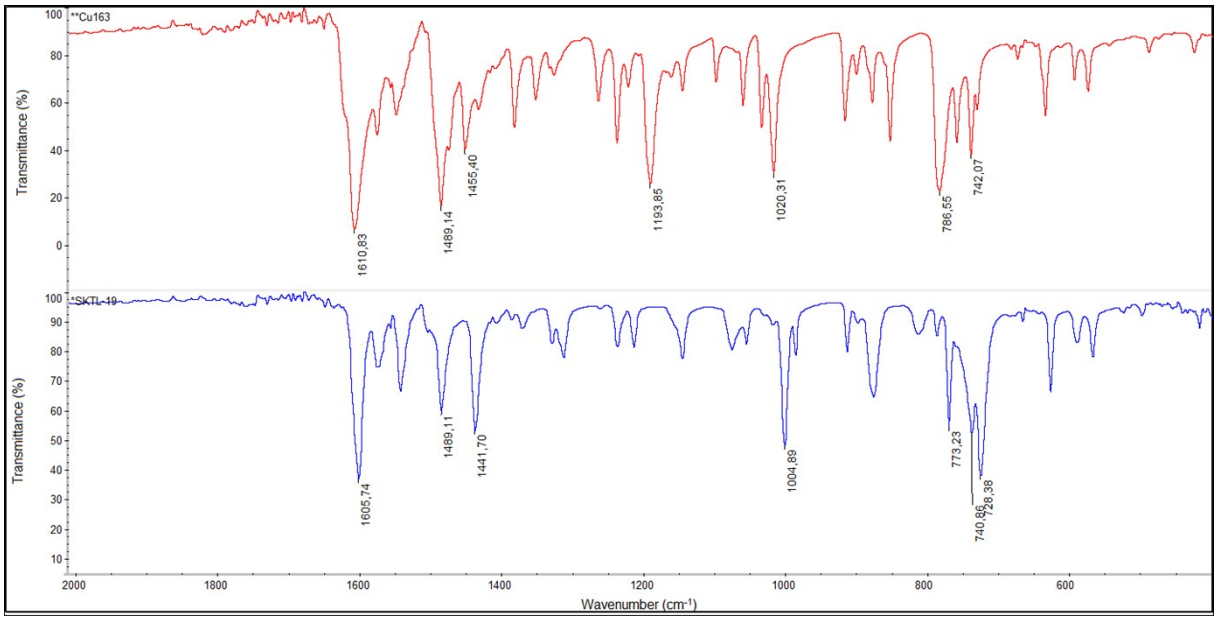
(1)


*Cu190b
Transmittance (%)
1607,72
1559,54
1474,45
1429,59
1252,95
1033,56
1018,94
793,60
778,23
702,25
655,35
*SKM31
Transmittance (%)
1599,36
1582,67
1567,05
1465,49
1398,02
790,52
Wavenumber (cm-1)

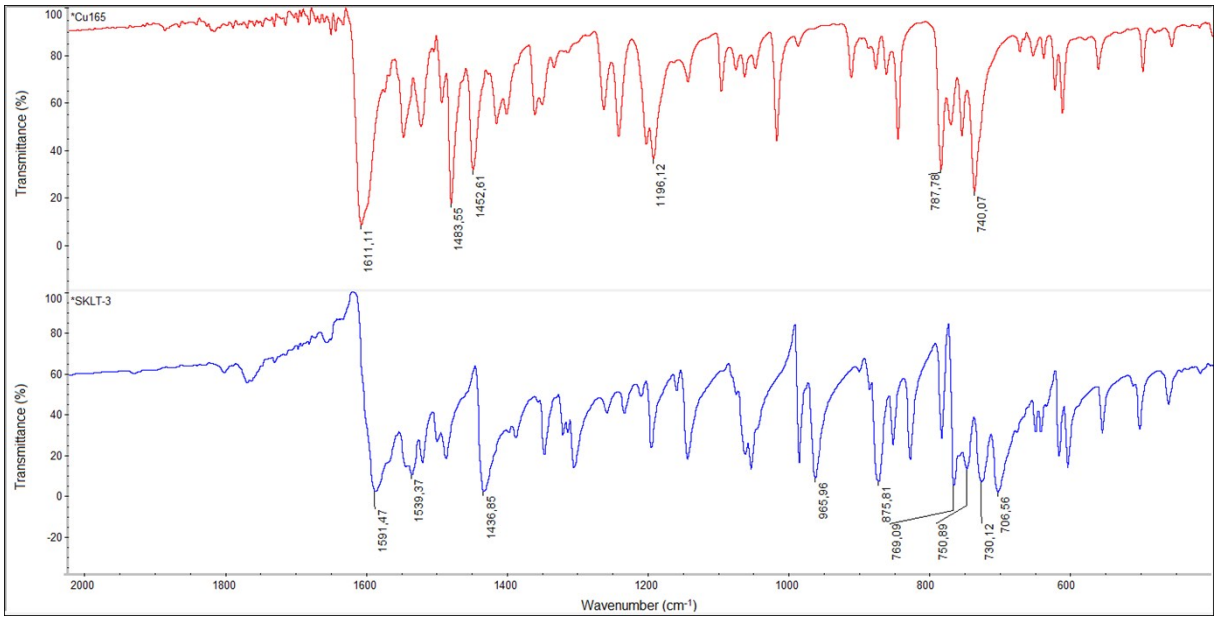
(2)


*Cu178
Transmittance (%)
1611,16
1474,12
1435,14
1399,26
1029,36
795,66
*SKM50
Transmittance (%)
1604,65
1586,05
1568,08
1465,21
1391,59
792,53
741,80
734,04
Wavenumber (cm-1)

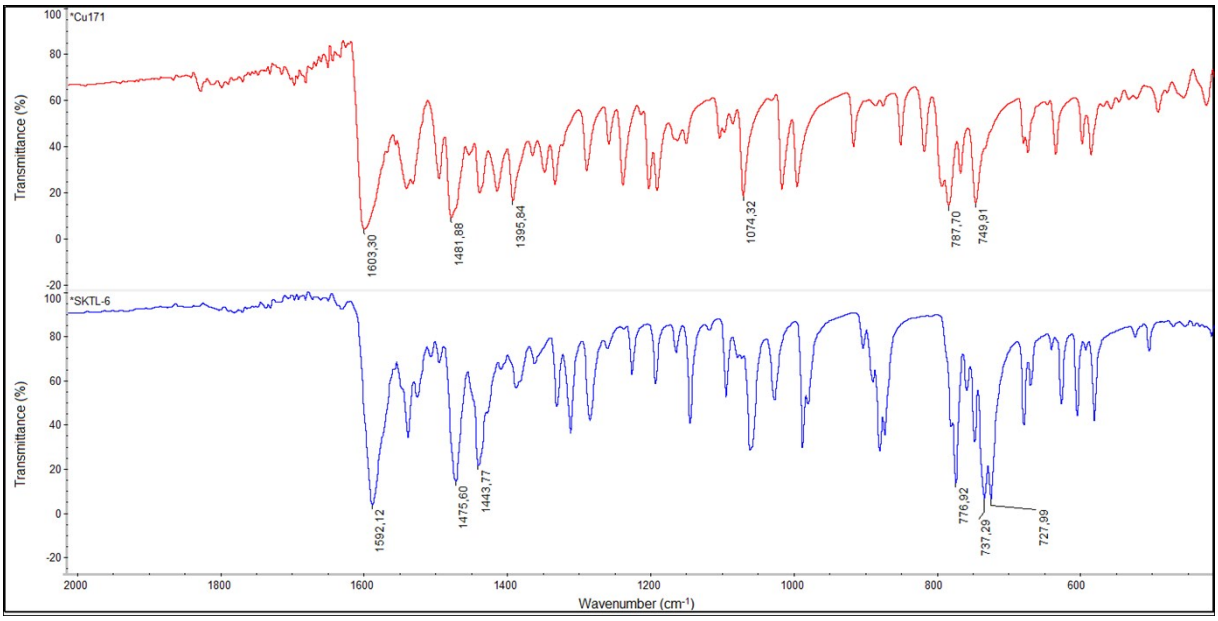
(3)


**Cu163
Transmittance (%)
1610,83
1489,14
1455,40
1193,85
1020,31
786,55
742,07
*SKTL-19
Transmittance (%)
1605,74
1489,11
1441,70
1004,89
773,23
740,86
728,38
Wavenumber (cm-1)

(4)

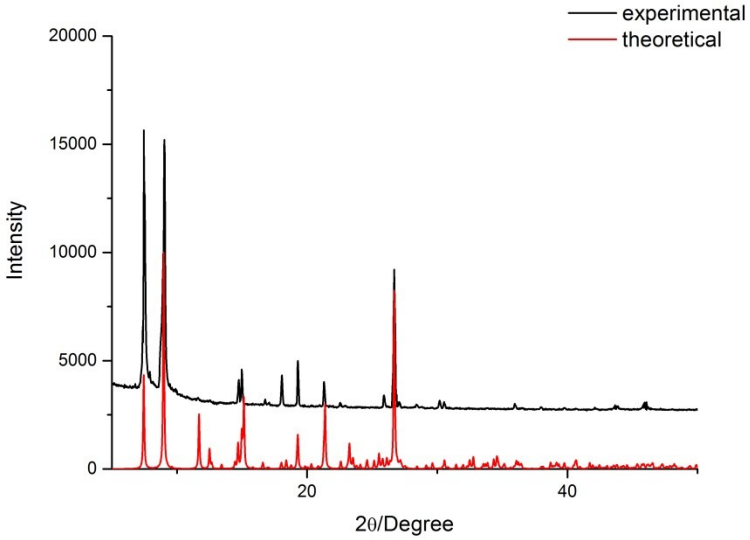


(5)

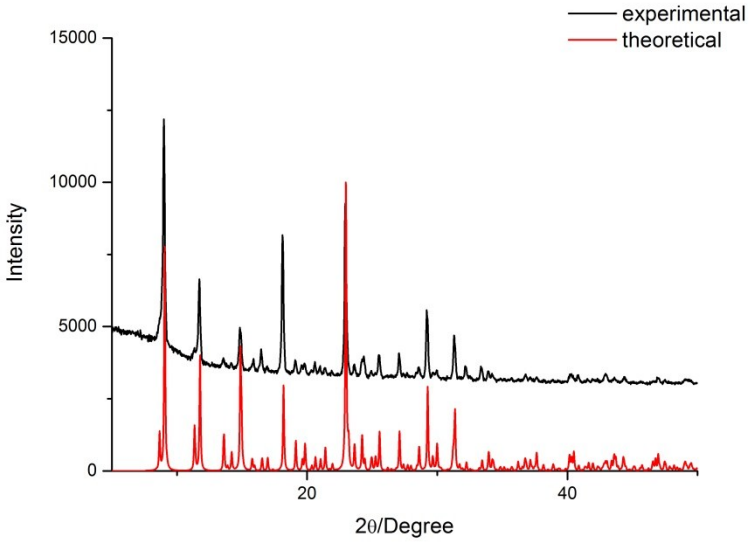


(6)

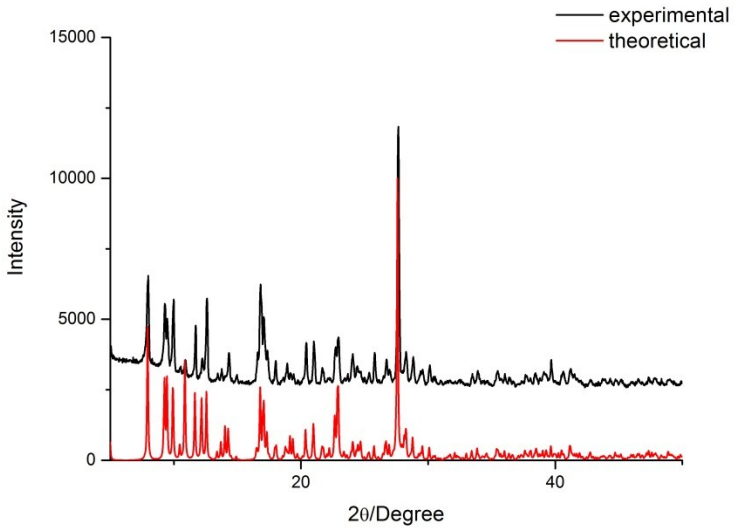
Figure S3. IR spectra of complexes **1**-**6** (red) and free ligands (blue).


experimental
theoretical
Intensity
2θ/Degree

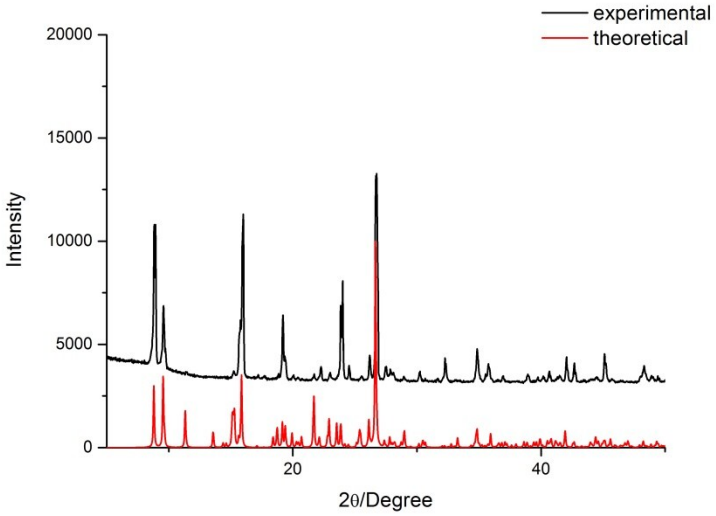
(1)


experimental
theoretical
Intensity
2θ/Degree

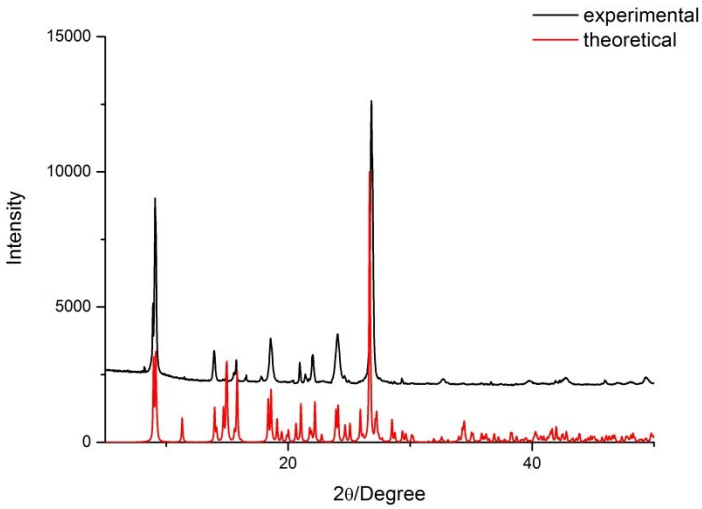
(2)


experimental
theoretical
Intensity
2θ/Degree

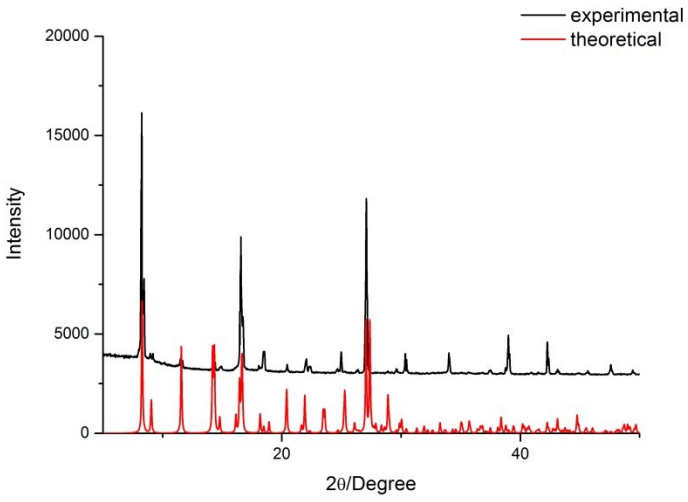
(3)



(4)

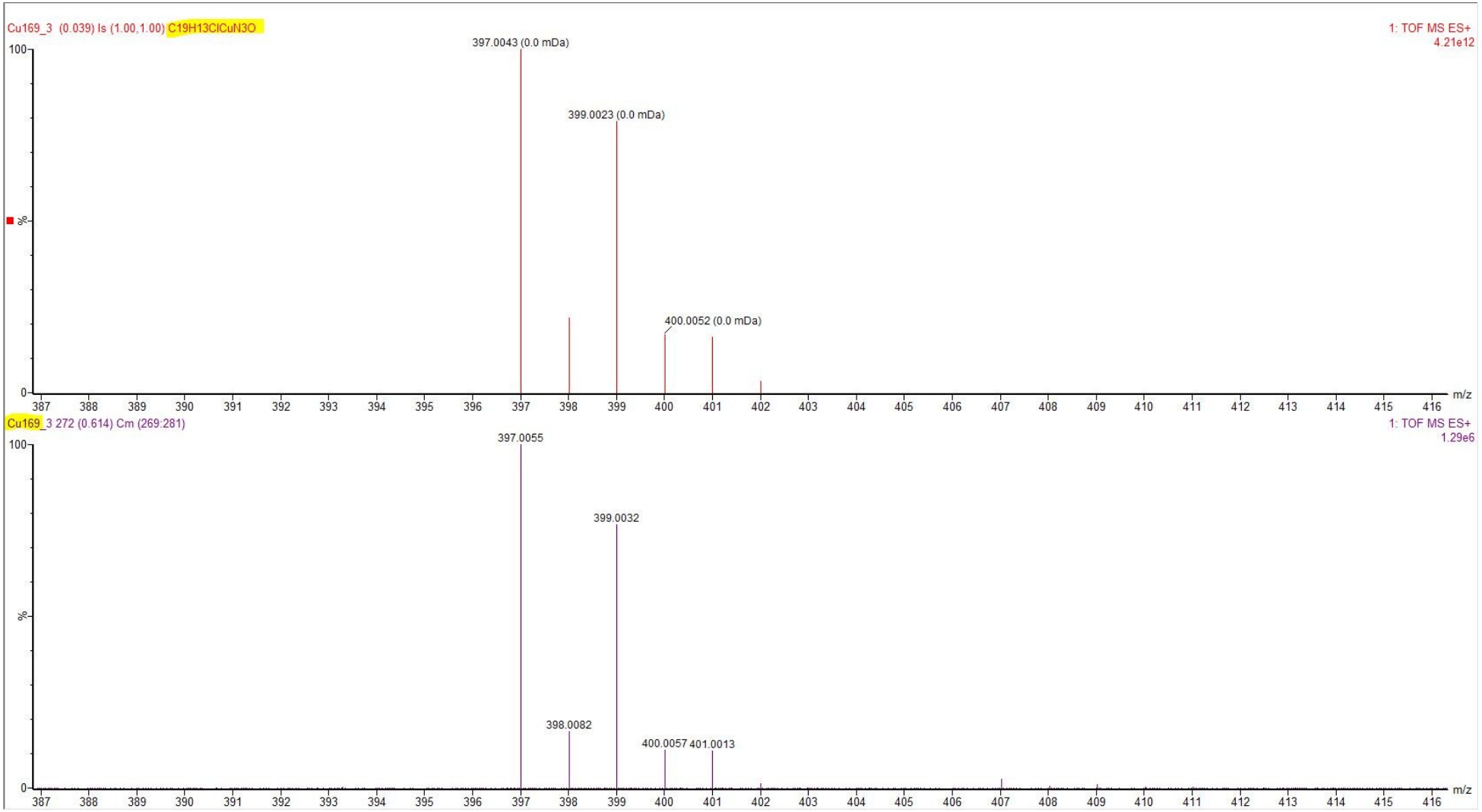


(5)

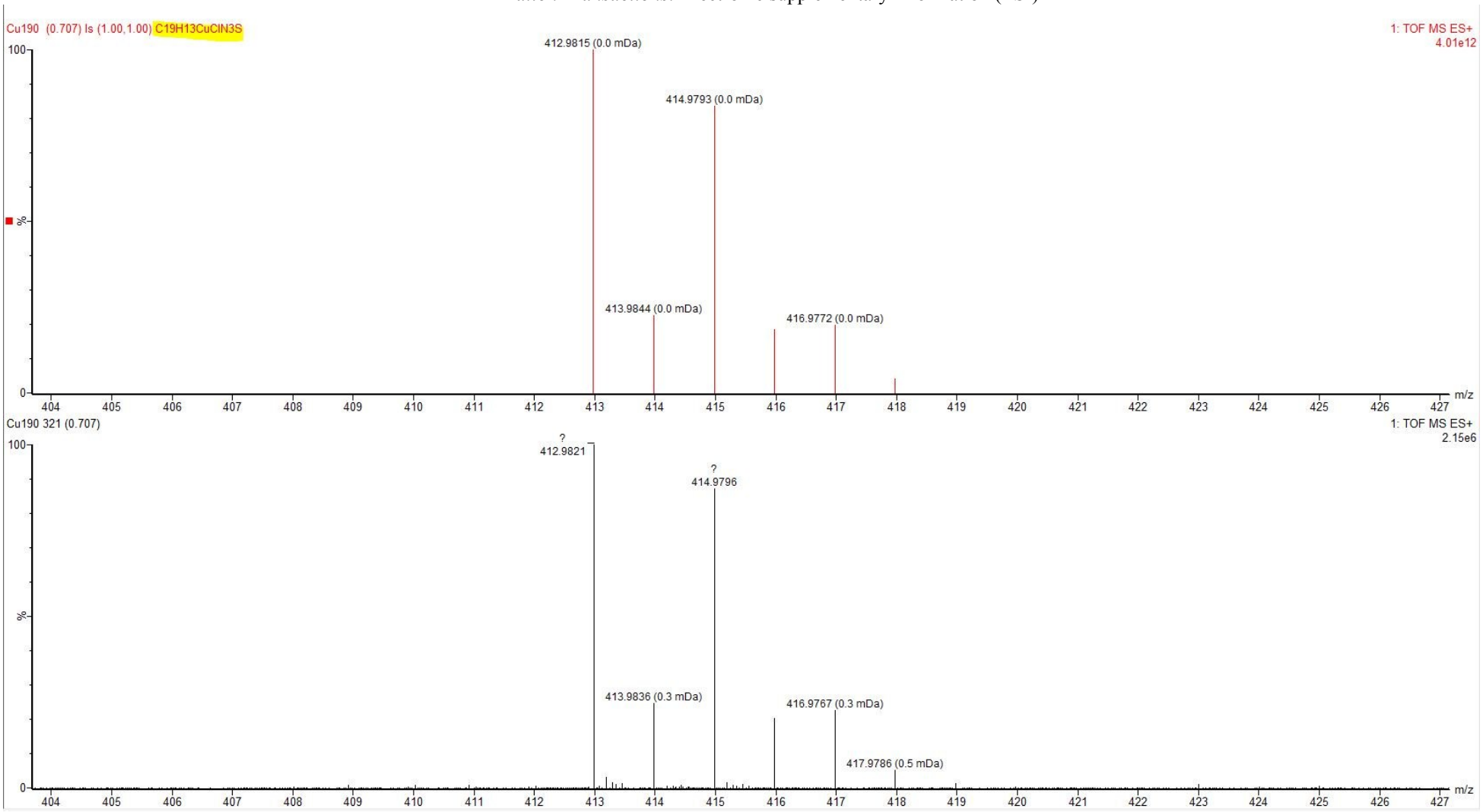


(6)

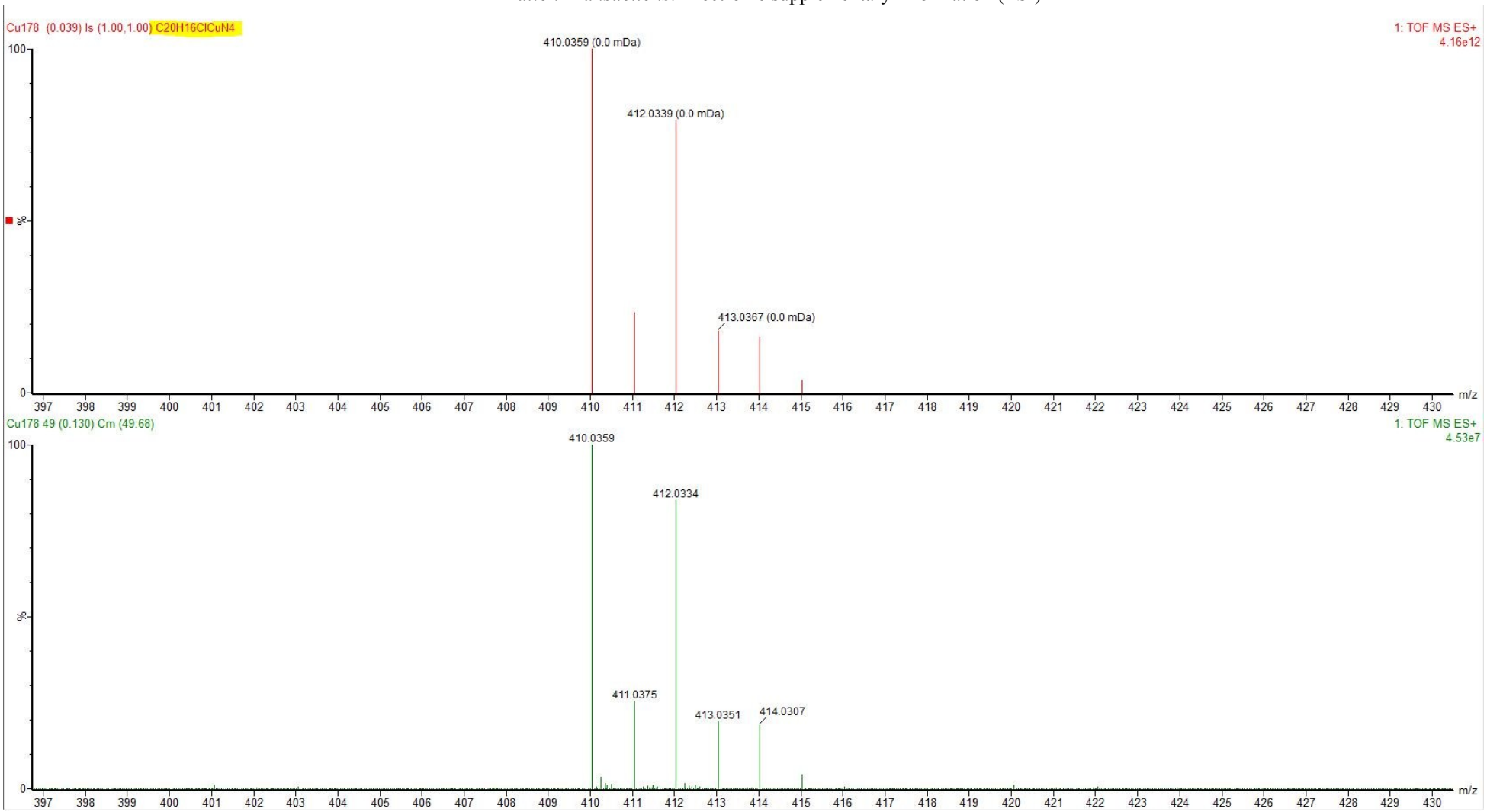
Figure S4. XRPD pattern of complexes **1-6** (experimental - black) and the simulation of its powder pattern from the crystal structure (theoretical - red).


Cu169_3 (0.039) Is (1.00,1.00) C19H13ClCuN3O
1: TOF MS ES+
4.21e12
397.0043 (0.0 mDa)
399.0023 (0.0 mDa)
400.0052 (0.0 mDa)
100
%
0
m/z
387 388 389 390 391 392 393 394 395 396 397 398 399 400 401 402 403 404 405 406 407 408 409 410 411 412 413 414 415 416
Cu169_3 272 (0.614) Cm (269:281)
1: TOF MS ES+
1.29e6
397.0055
399.0032
398.0082
400.0057
401.0013
100
%
0
m/z
387 388 389 390 391 392 393 394 395 396 397 398 399 400 401 402 403 404 405 406 407 408 409 410 411 412 413 414 415 416

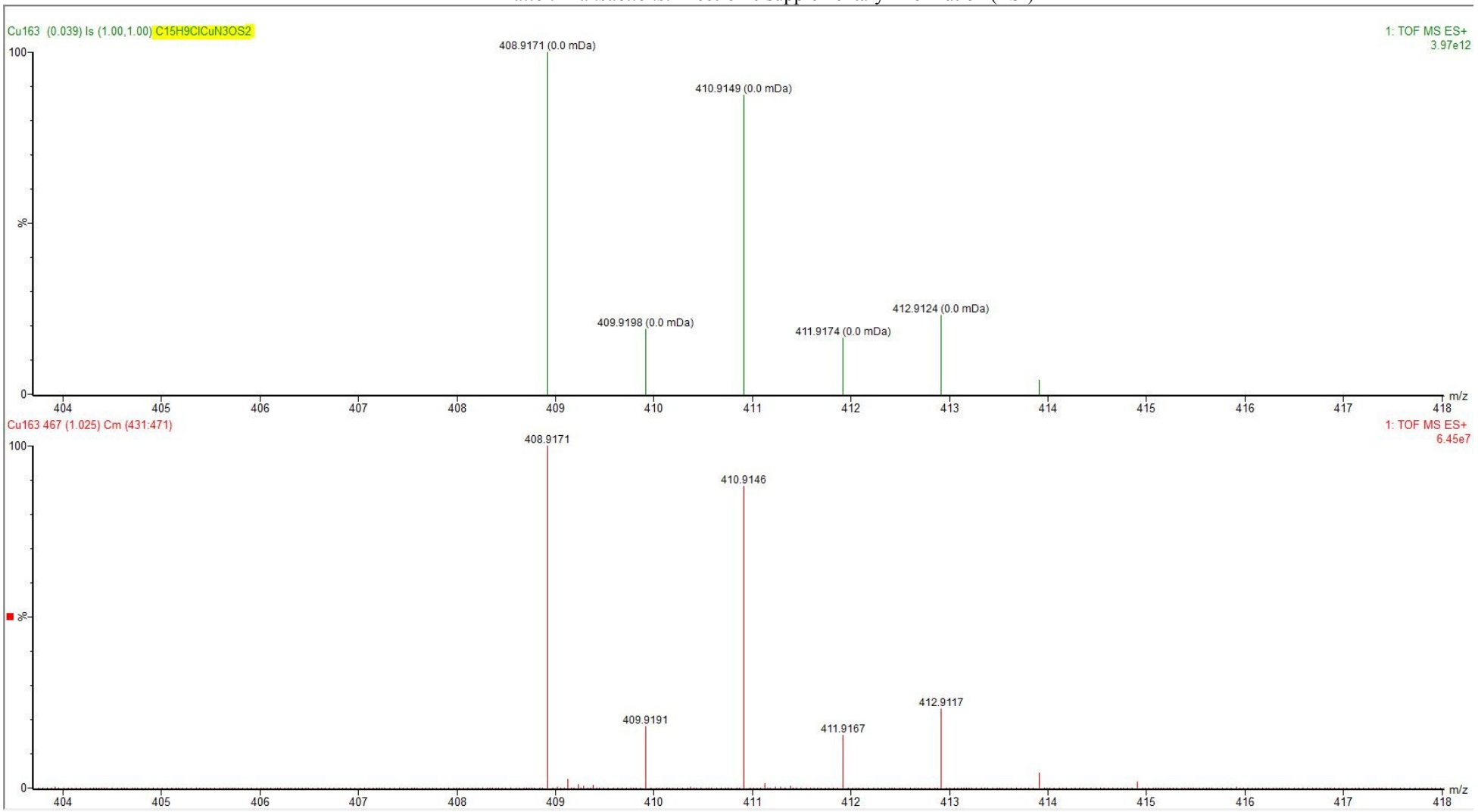
(1)


Cu190 (0.707) Is (1.00,1.00) C19H13CuClN3S
1: TOF MS ES+
4.01e12
412.9815 (0.0 mDa)
414.9793 (0.0 mDa)
413.9844 (0.0 mDa)
416.9772 (0.0 mDa)
100
%
0
m/z
404 405 406 407 408 409 410 411 412 413 414 415 416 417 418 419 420 421 422 423 424 425 426 427
Cu190 321 (0.707)
1: TOF MS ES+
2.15e6
? 412.9821
? 414.9796
413.9836 (0.3 mDa)
416.9767 (0.3 mDa)
417.9786 (0.5 mDa)

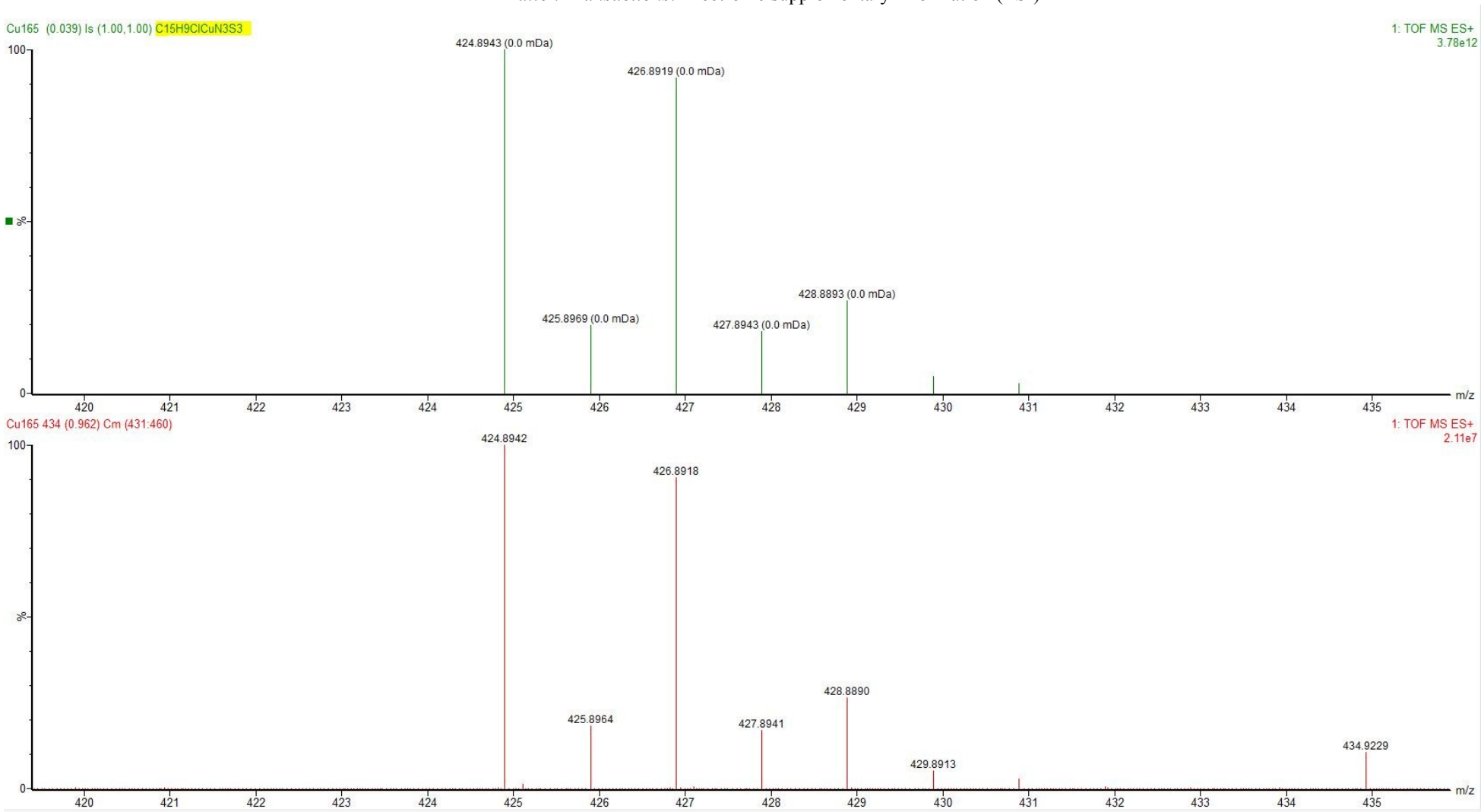
(2)


Cu178 (0.039) Is (1.00,1.00) C20H16ClCuN4
1: TOF MS ES+
4.16e12
410.0359 (0.0 mDa)
412.0339 (0.0 mDa)
413.0367 (0.0 mDa)
100
%
0
m/z
397 398 399 400 401 402 403 404 405 406 407 408 409 410 411 412 413 414 415 416 417 418 419 420 421 422 423 424 425 426 427 428 429 430
Cu178 49 (0.130) Cm (49:68)
1: TOF MS ES+
4.53e7
410.0359
412.0334
411.0375
413.0351
414.0307
100
%
0
m/z
397 398 399 400 401 402 403 404 405 406 407 408 409 410 411 412 413 414 415 416 417 418 419 420 421 422 423 424 425 426 427 428 429 430

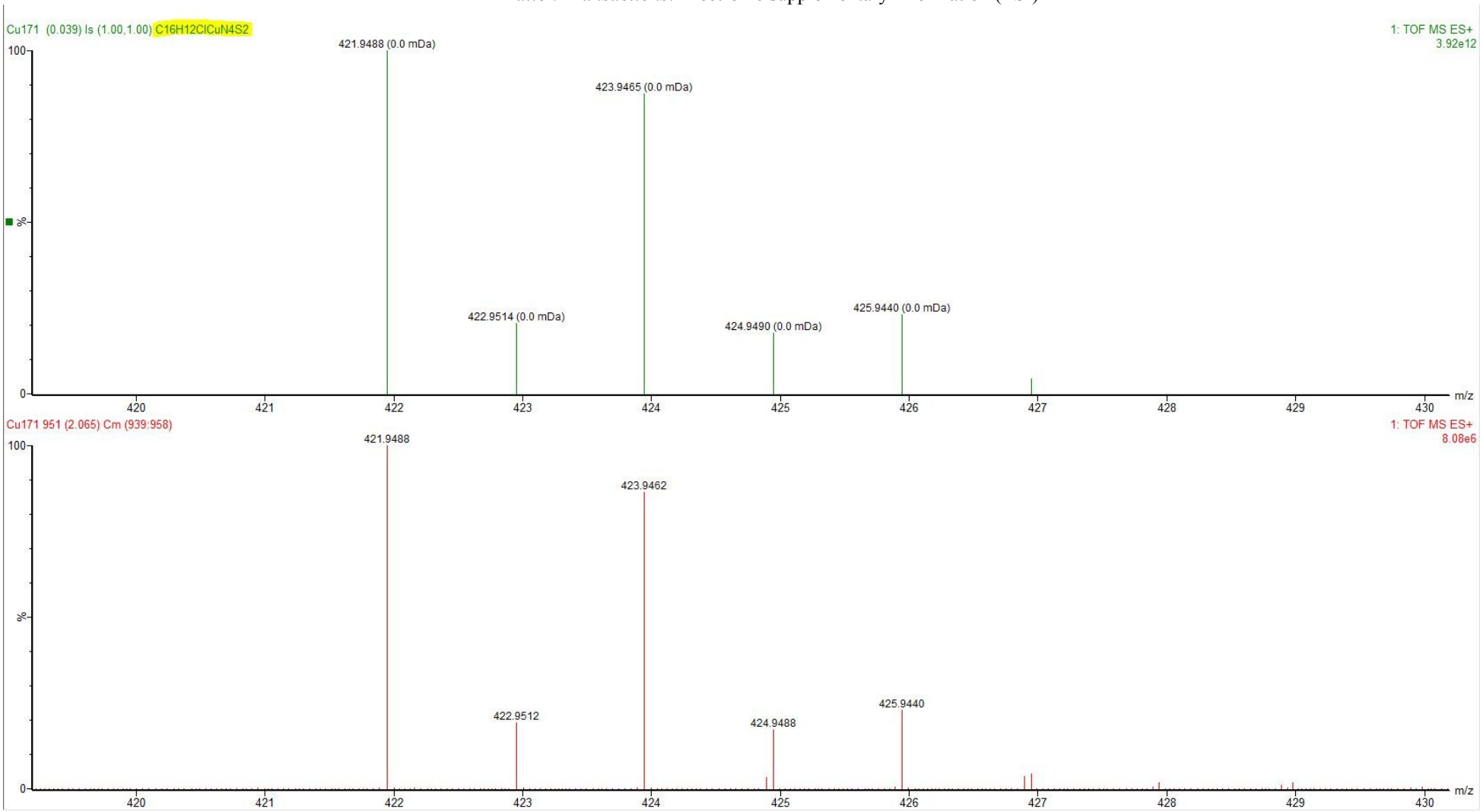
(3)


Cu163 (0.039) Is (1.00,1.00) C15H9ClCuN3OS2
1: TOF MS ES+
3.97e12
408.9171 (0.0 mDa)
410.9149 (0.0 mDa)
409.9198 (0.0 mDa)
411.9174 (0.0 mDa)
412.9124 (0.0 mDa)
100
%
0
404 405 406 407 408 409 410 411 412 413 414 415 416 417 418
m/z
Cu163 467 (1.025) Cm (431:471)
1: TOF MS ES+
6.45e7
408.9171
410.9146
409.9191
411.9167
412.9117
100
%
0
404 405 406 407 408 409 410 411 412 413 414 415 416 417 418
m/z

(4)


Cu165 (0.039) Is (1.00,1.00) C15H9ClCuN3S3
1: TOF MS ES+
3.78e12
424.8943 (0.0 mDa)
426.8919 (0.0 mDa)
425.8969 (0.0 mDa)
427.8943 (0.0 mDa)
428.8893 (0.0 mDa)
100
%
0
m/z
420 421 422 423 424 425 426 427 428 429 430 431 432 433 434 435
Cu165 434 (0.962) Cm (431:460)
1: TOF MS ES+
2.11e7
424.8942
426.8918
425.8964
427.8941
428.8890
429.8913
434.9229
100
%
0
m/z
420 421 422 423 424 425 426 427 428 429 430 431 432 433 434 435

(5)



(6)

Figure S5. HRMS of complexes **1-6**.

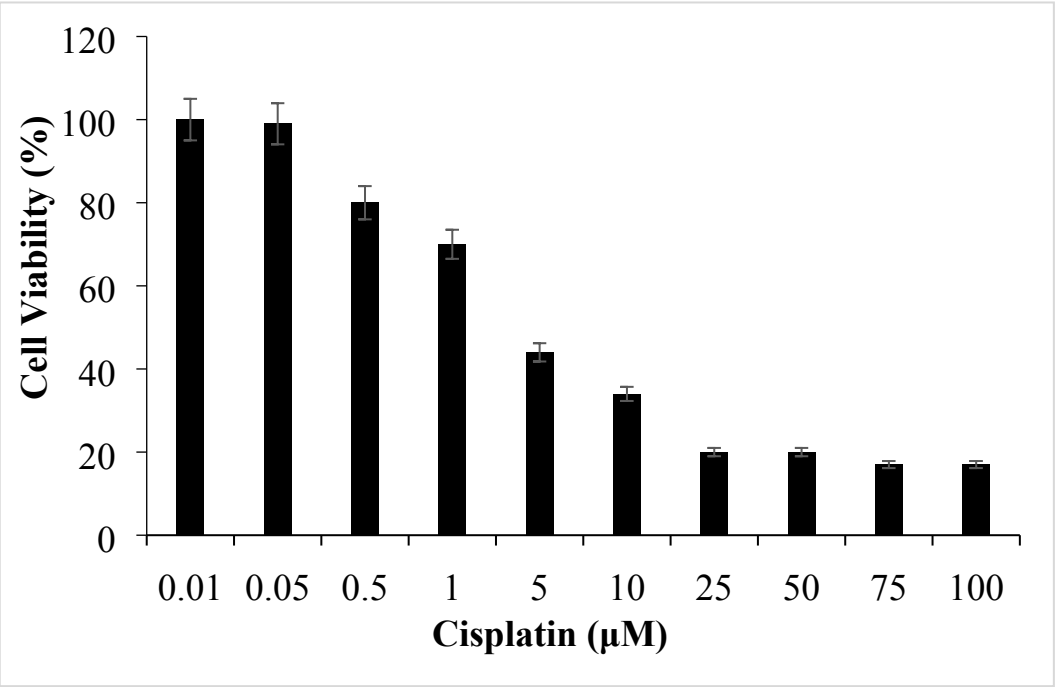


Figure S6 Cytotoxicity of cisplatin in A2780 cell line. A2780 cells were treated with increasing concentrations of the cisplatin for 48 h and cell viability was determined by MTS assay. The data were normalized against the control treated with 0.1 % (v/v) DMSO. The results showed are expressed as mean ± SEM of three independent assays. The symbol * in the figure means that the results are statistically significant with a $p < 0.05$ (as compared to control).