Electronic Supplementary Material (ESI) for New Journal of Chemistry.

SUPPLEMENTARY MATERIAL

Metal–azole fungistatic drug complexes as anti-*Sporothrix* spp.

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Figure S1. (A) ESI-MS spectrum of complex $[Pt(KTZ)_2Cl_2]$ (**5**). (B) ESI-MS simulation of $[Pt(KTZ)_2Cl_2+H]^+$.

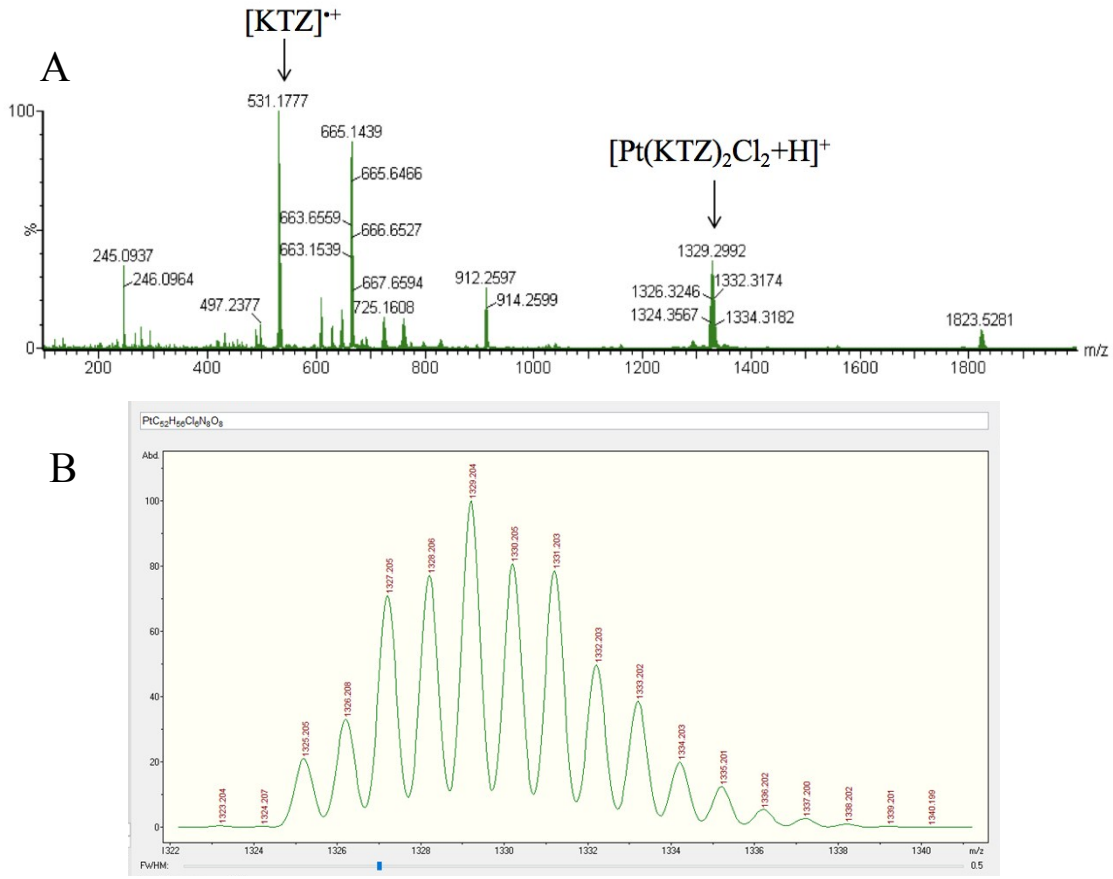
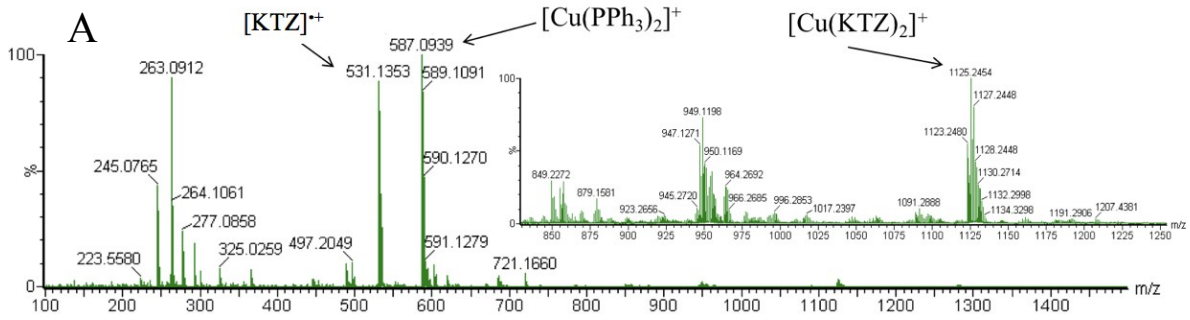
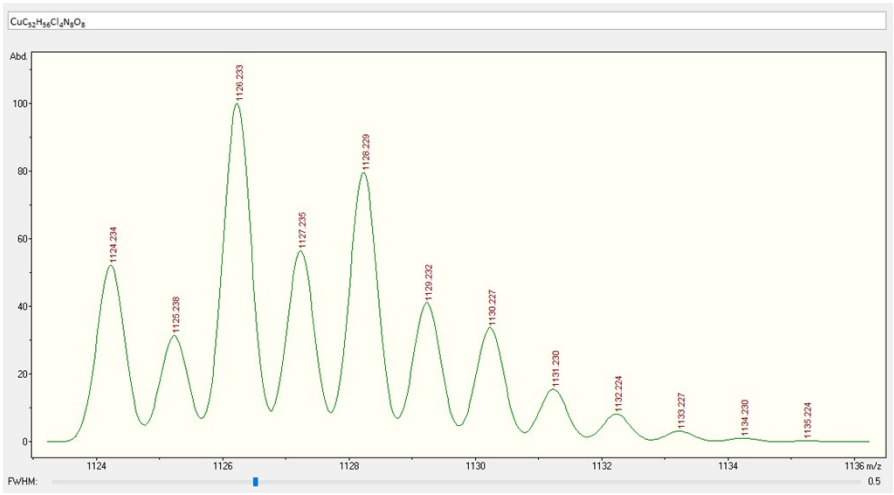


Figure S2. (A) ESI-MS spectrum of complex $[Cu(PPh_3)_2(KTZ)_2]NO_3$ (**1**). (B) ESI-MS simulation of $[Cu(KTZ)_2]^+$. (C) ESI-MS simulation of $[Cu(PPh_3)_2]^+$.





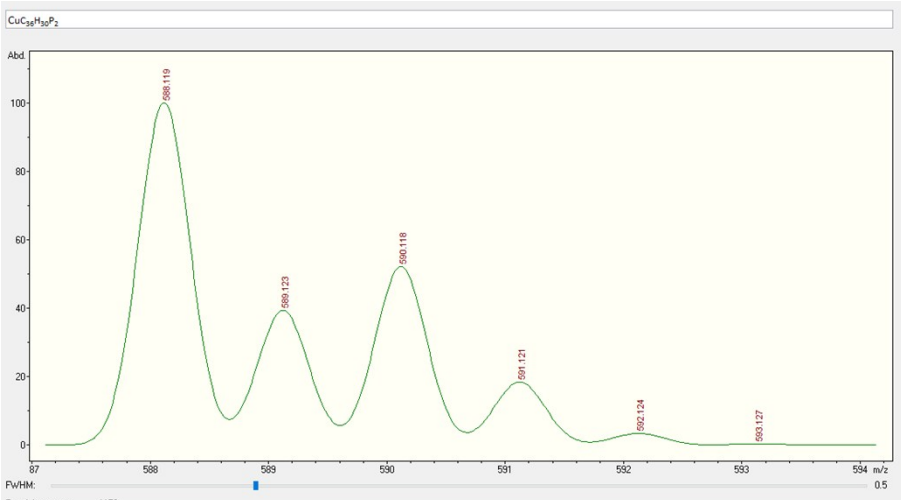
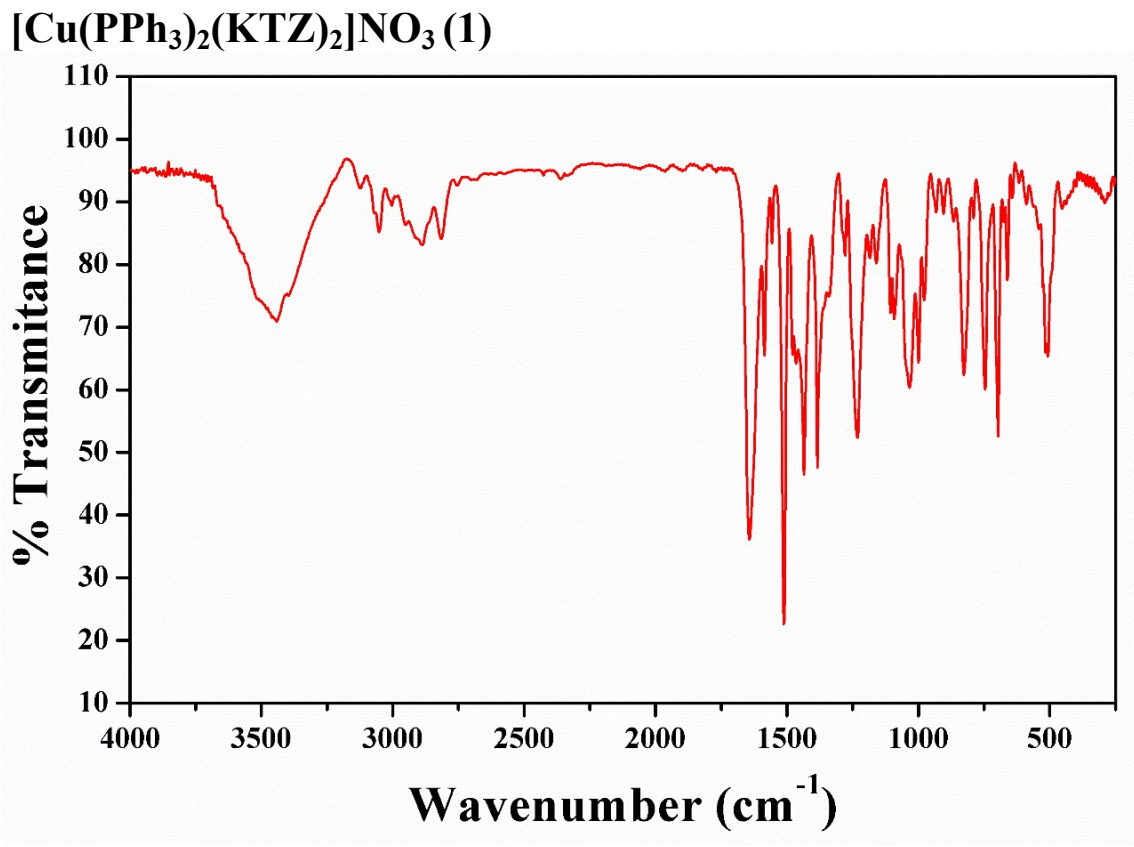
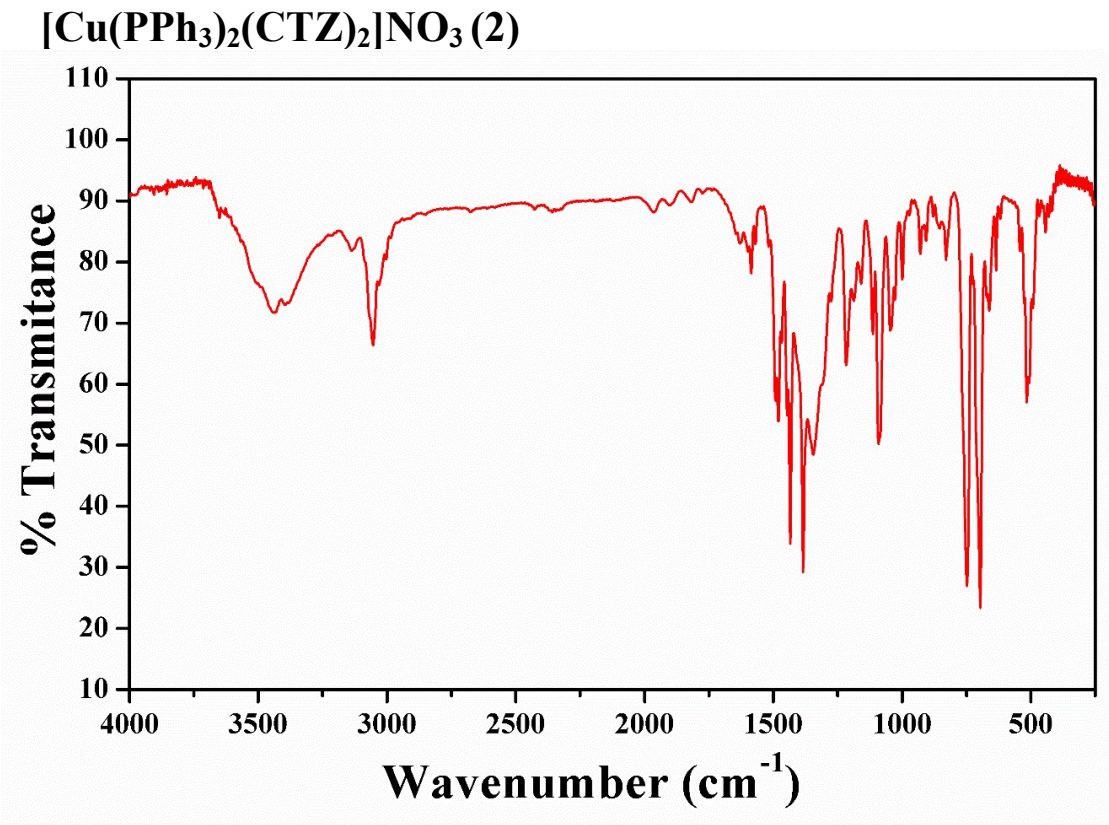
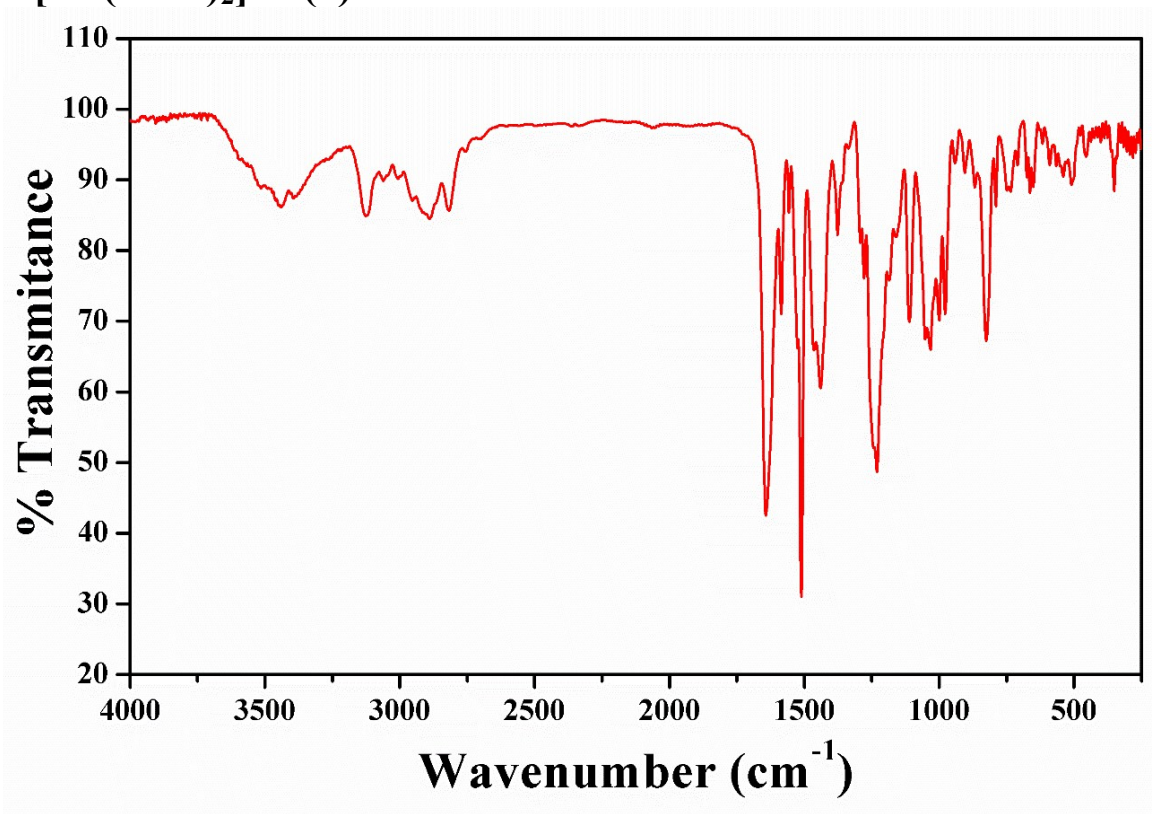


Figure S3. Infrared spectra of complexes **1-5**.

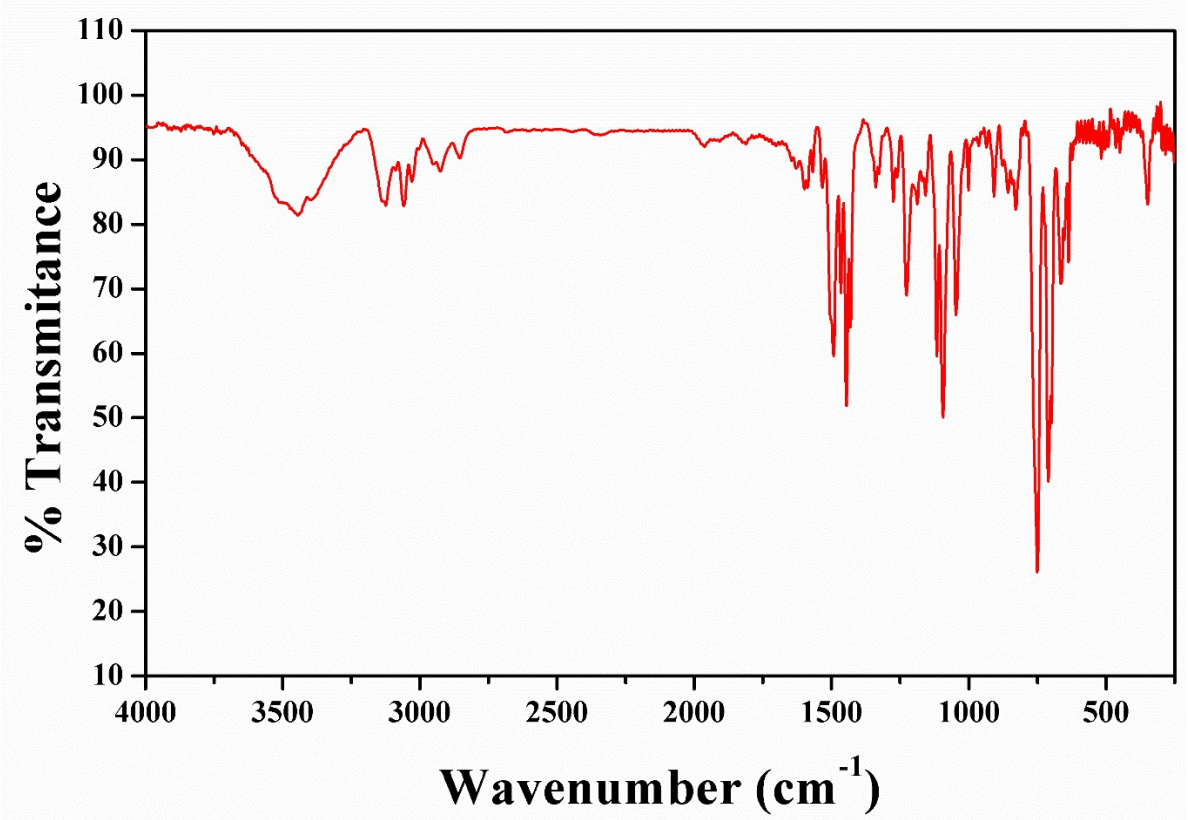




[Au(KTZ)$_2$]Cl (3)



[Au(CTZ)$_2$]Cl (4)



trans-[Pt(KTZ)$_2$Cl$_2$] (5)

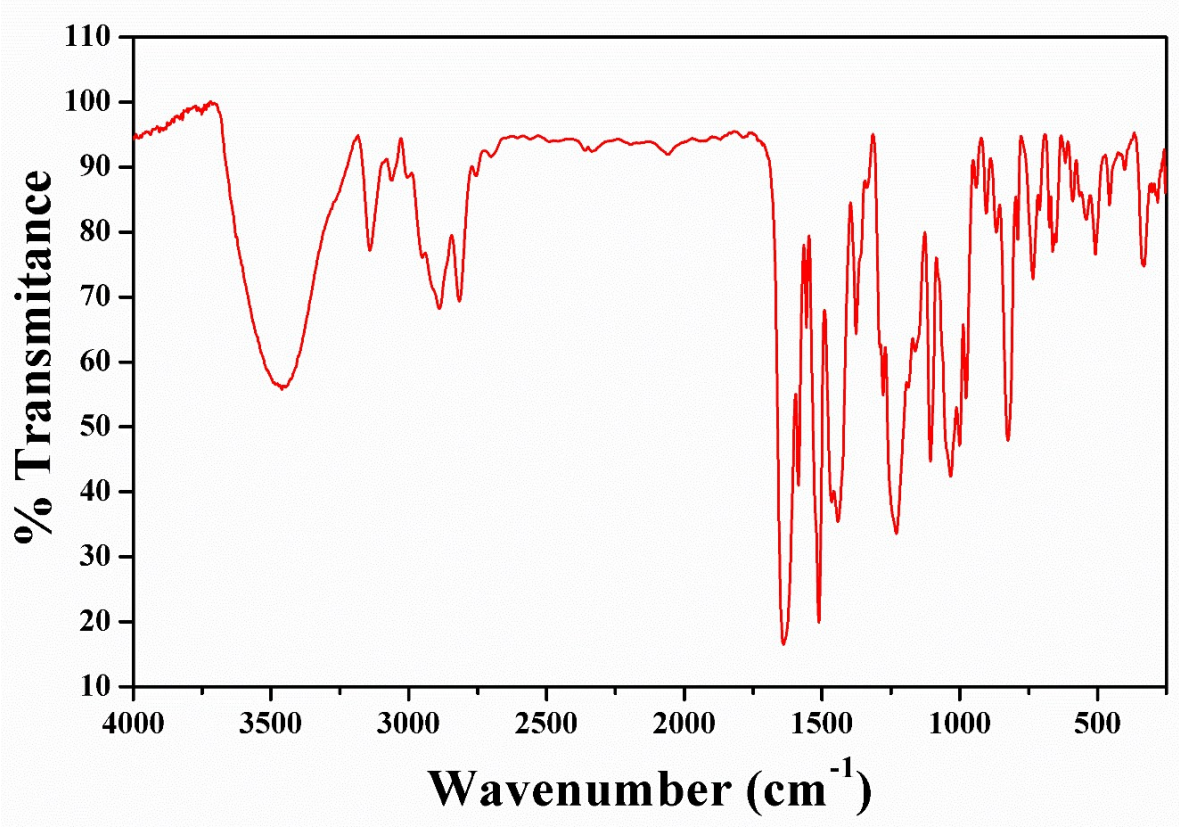
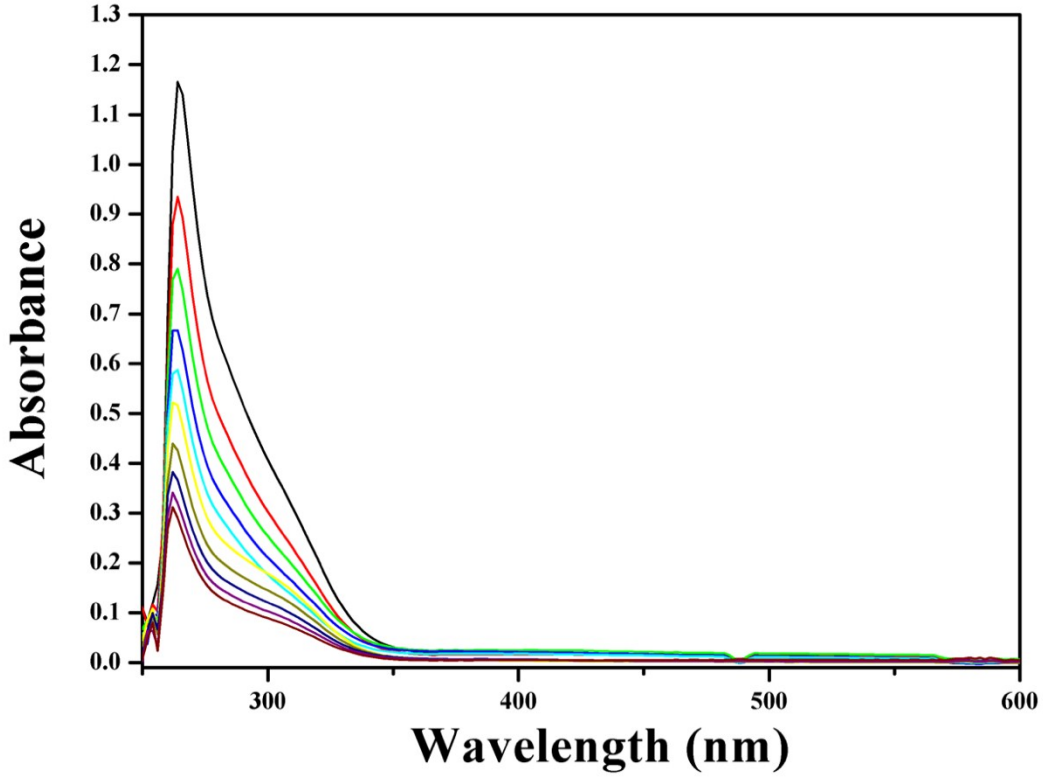
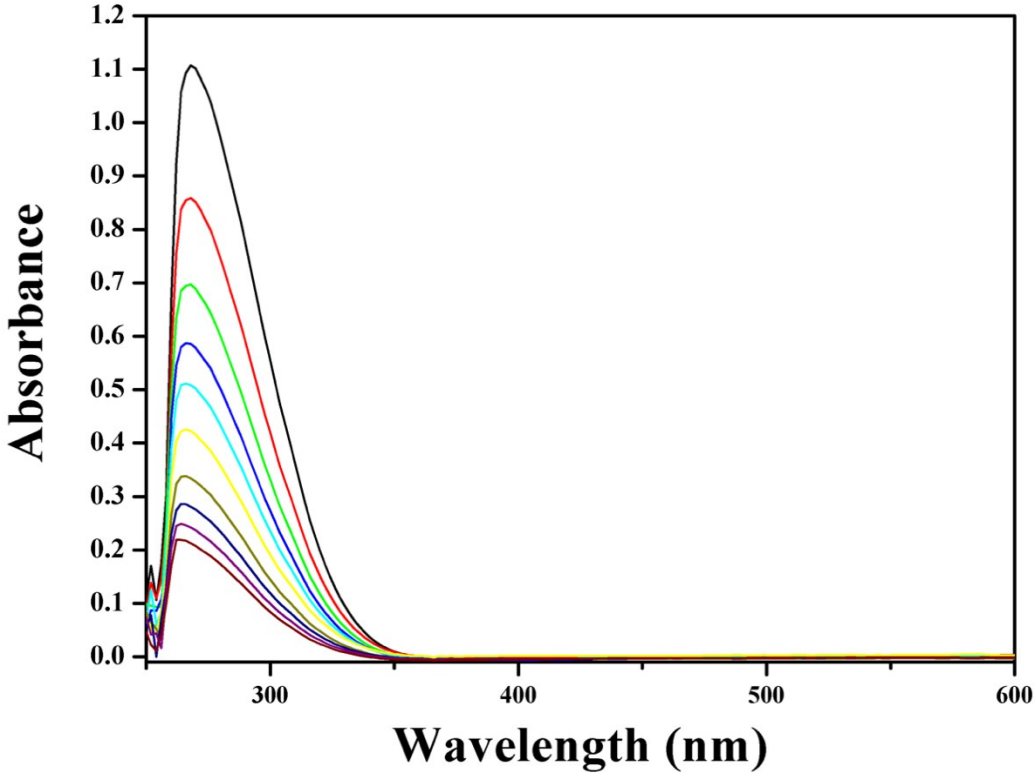


Figure S4. UV- Visible spectra of complexes 1-5 in DMSO, measured at different concentrations to calculate the molar absorptivity.

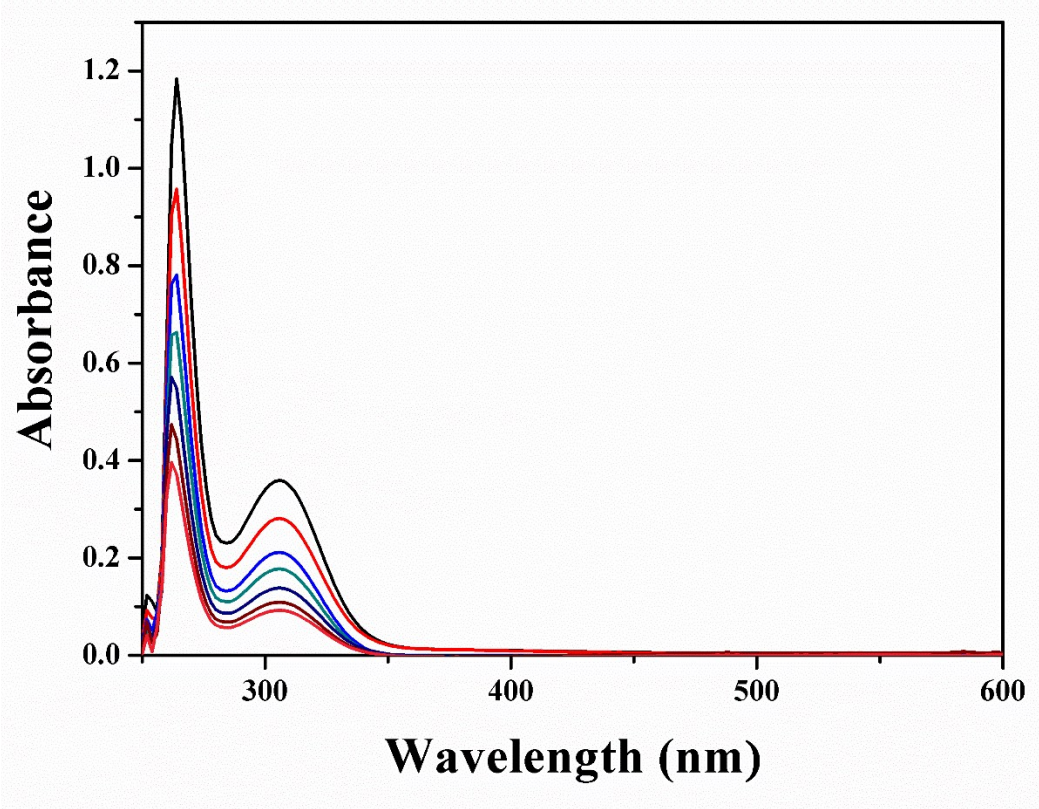
$[Cu(PPh_3)_2(KTZ)_2]NO_3$ (1)



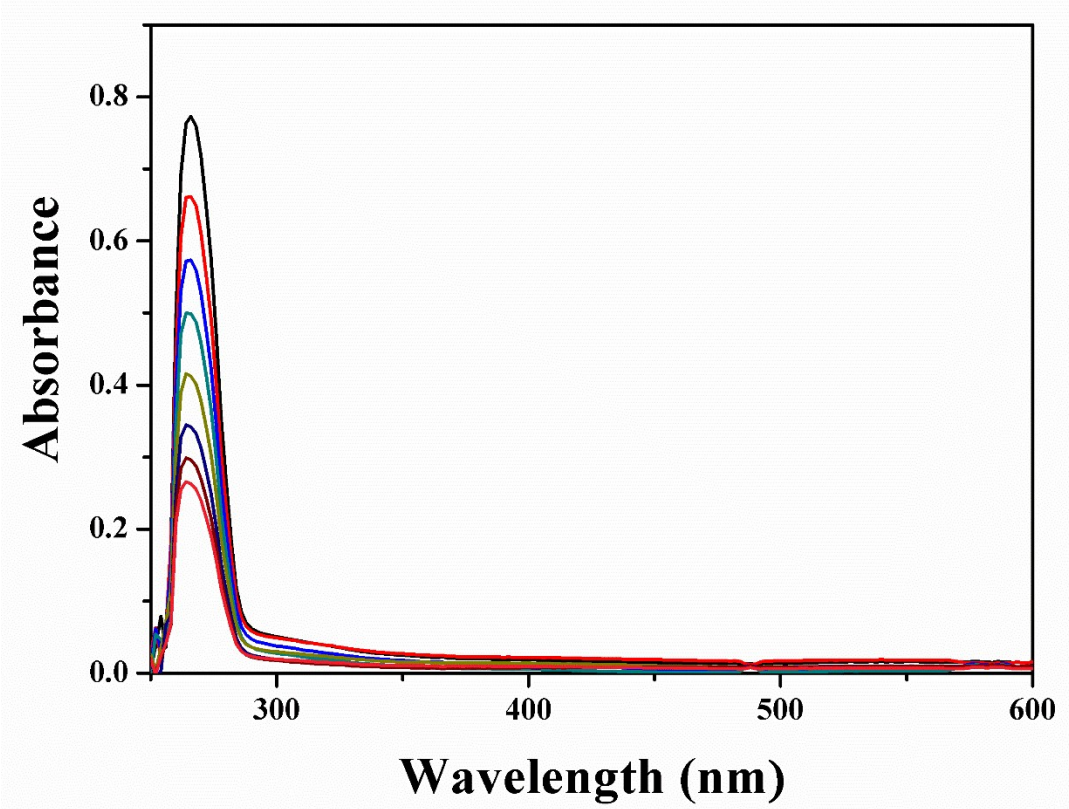
$[Cu(PPh_3)_2(CTZ)_2]NO_3$ (2)



[Au(KTZ)$_2$]Cl (3)



[Au(CTZ)$_2$]Cl (4)



trans-[$Pt(KTZ)_2Cl_2$] (5)

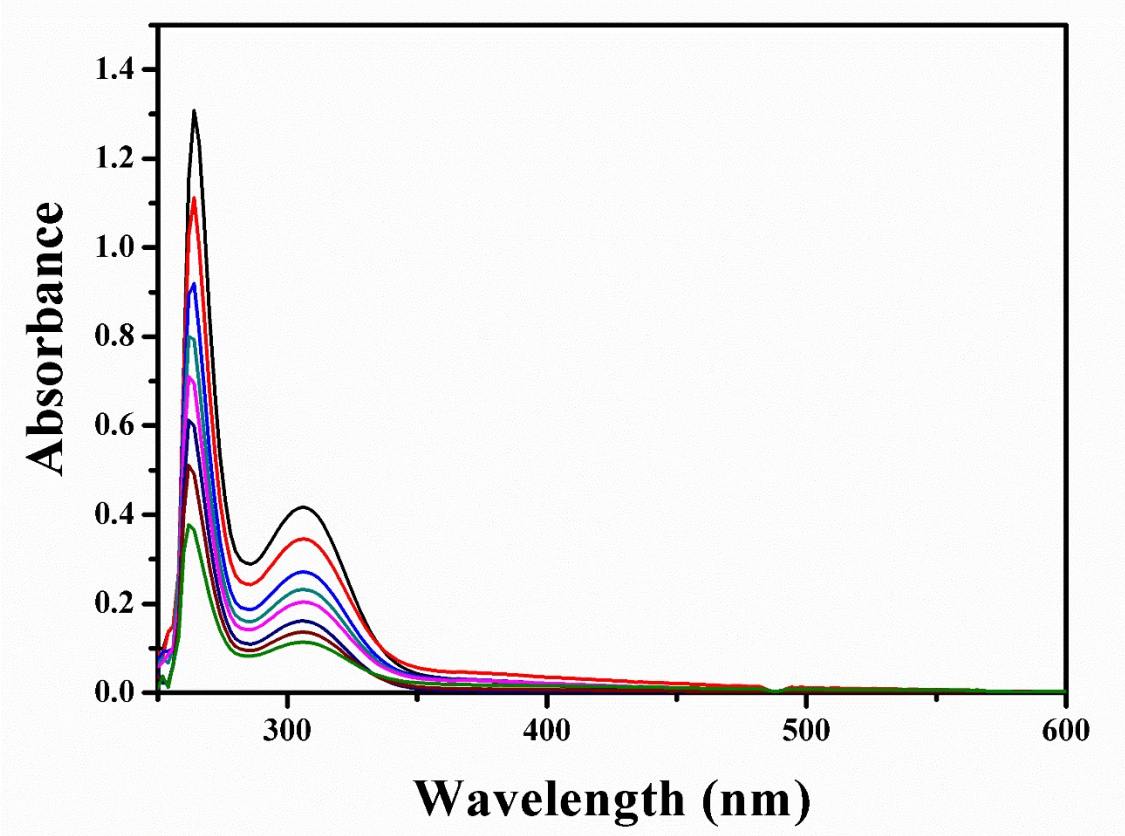


Figure S5.^{1}H-^{1}H COSY NMR spectra of complex $[Cu(PPh_3)_2(KTZ)_2]NO_3$ (**1**) in dmso-d_6.

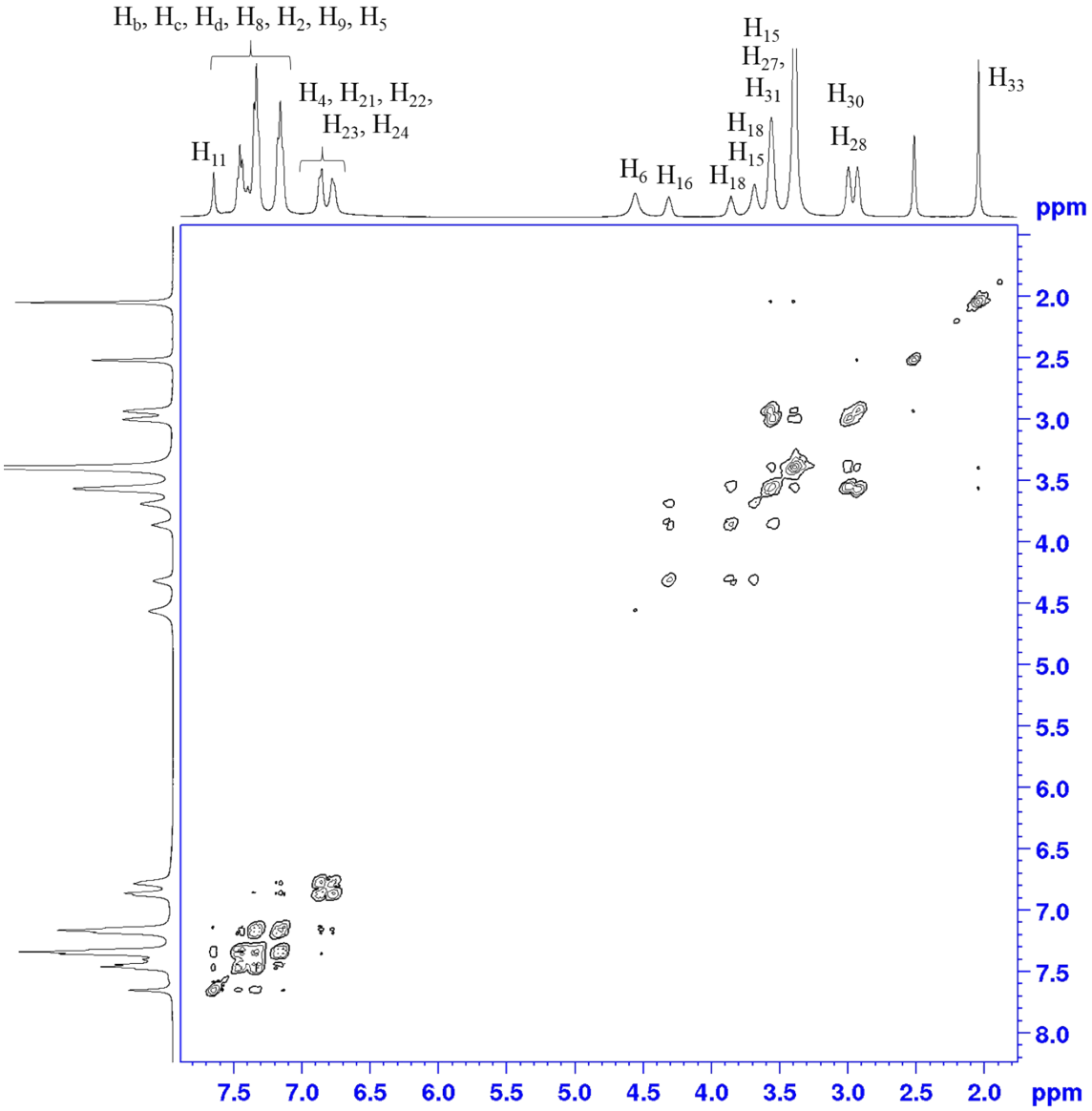


Figure S6. $^{31}P\{^{1}H\}$NMR of complex $[Cu(PPh_3)_2(KTZ)_2]NO_3$ (**1**) in dmso-d_6

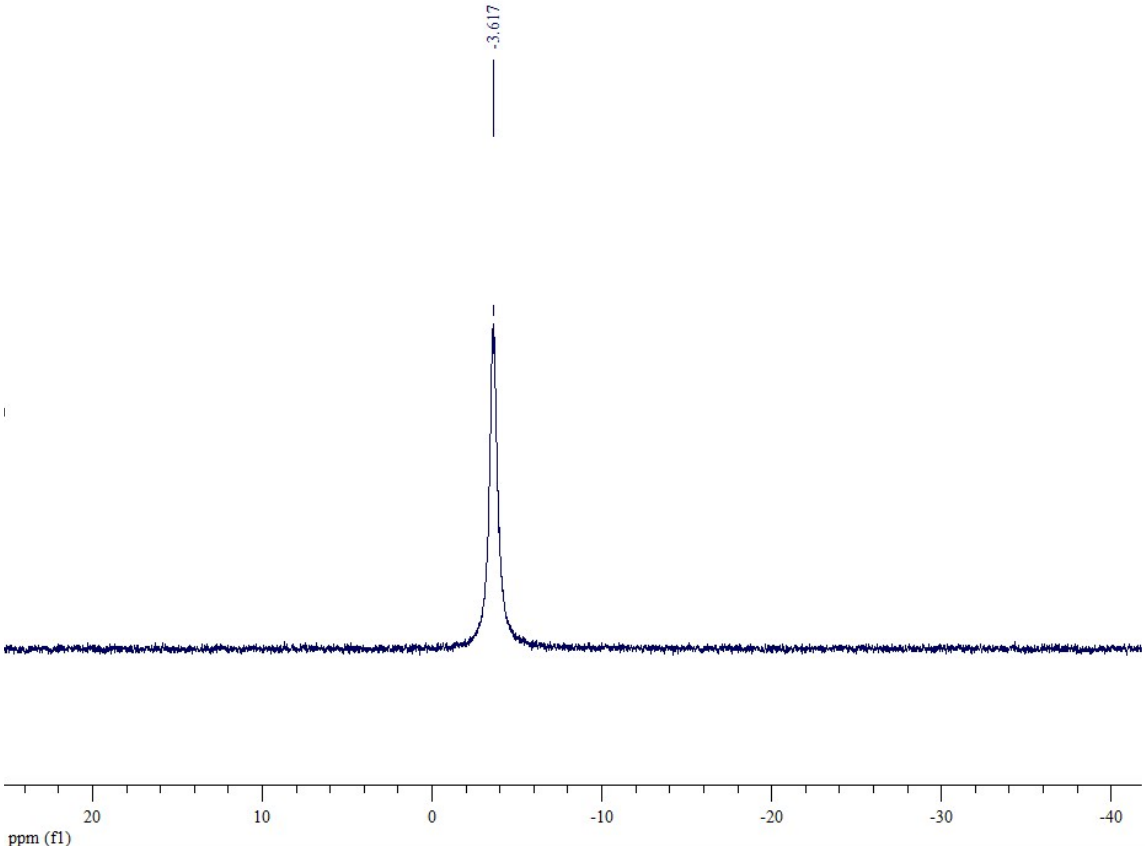


Figure S7. ^{1}H-^{1}H COSY NMR spectra of complex $[Au(KTZ)_2]Cl$ (**3**) in $CDCl_3$

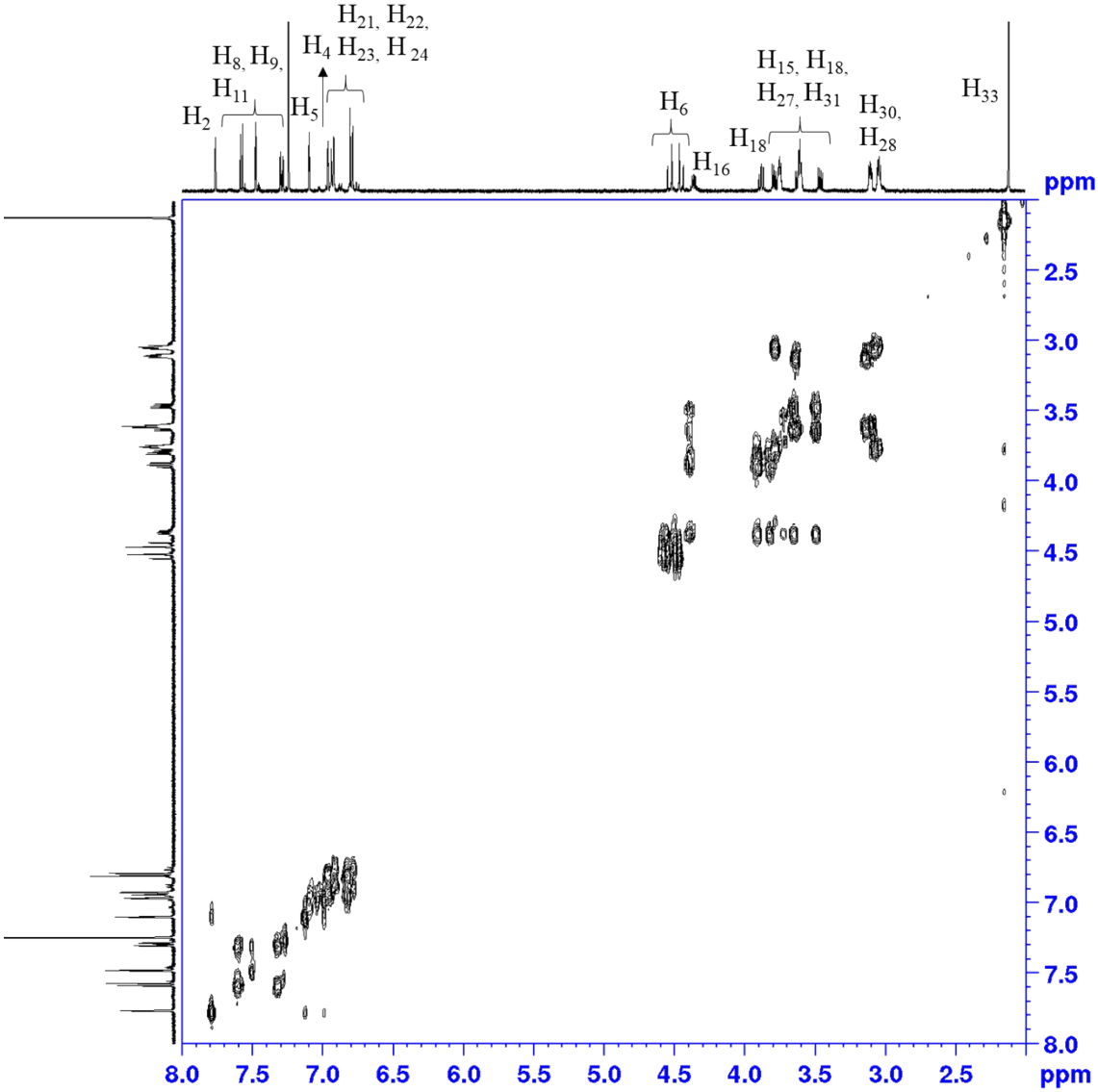


Figure S8.[1]H NMR spectra of complex *trans*-[Pt(KTZ)$_2$Cl$_2$] (**5**) and KTZ free in dmso-d$_6$

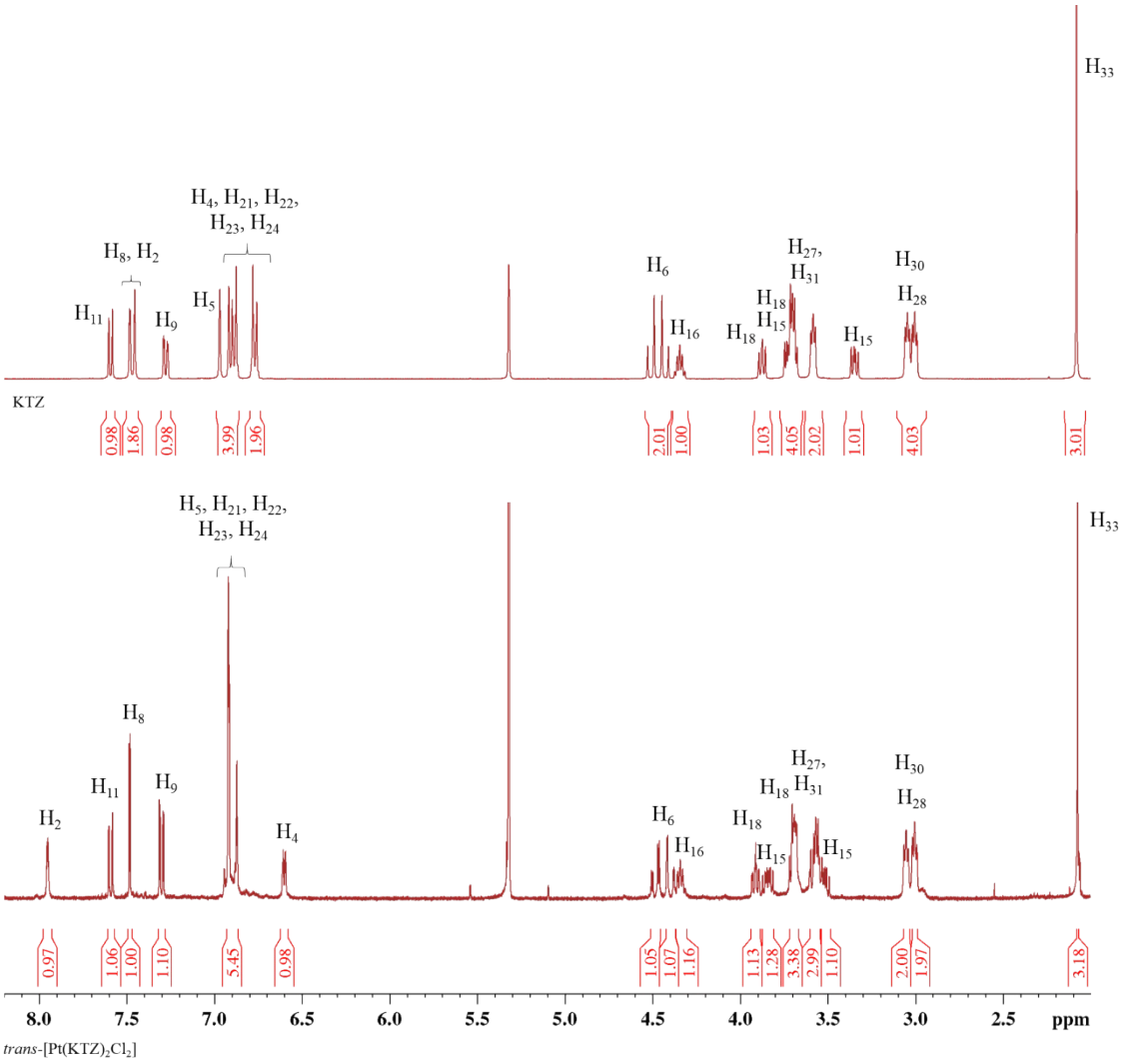


Figure S9. ^{195}Pt NMR spectra of complex *trans*-[Pt(KTZ)$_2$Cl$_2$] (**5**)

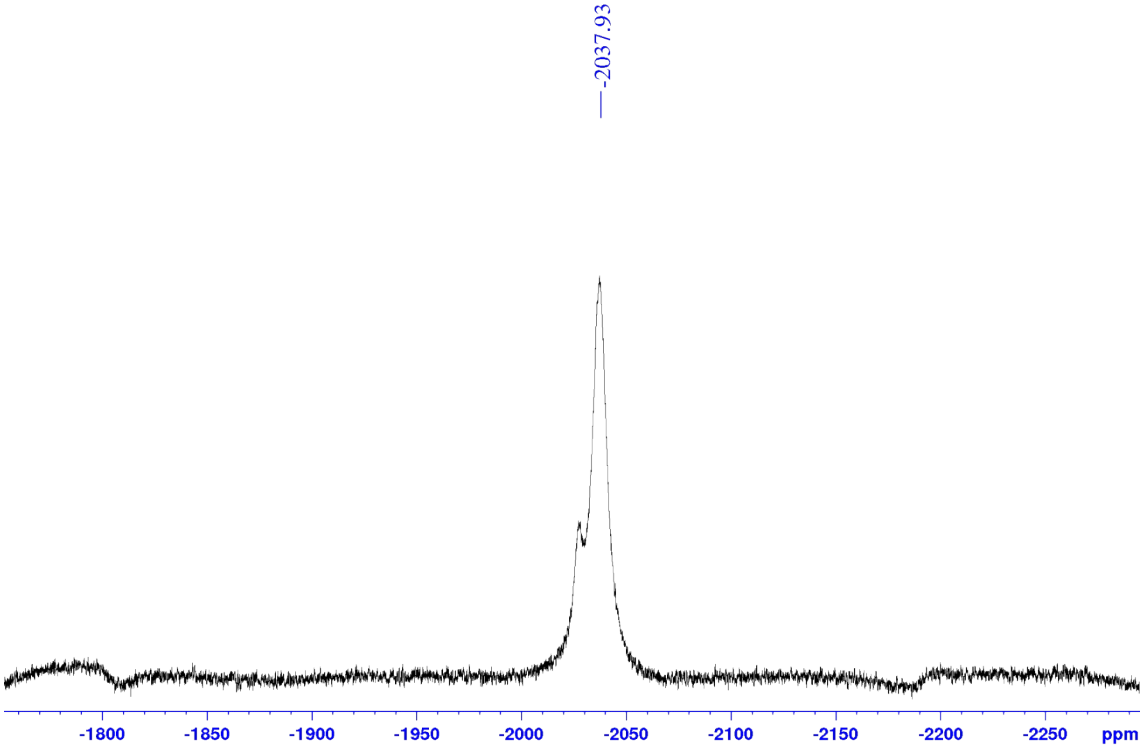
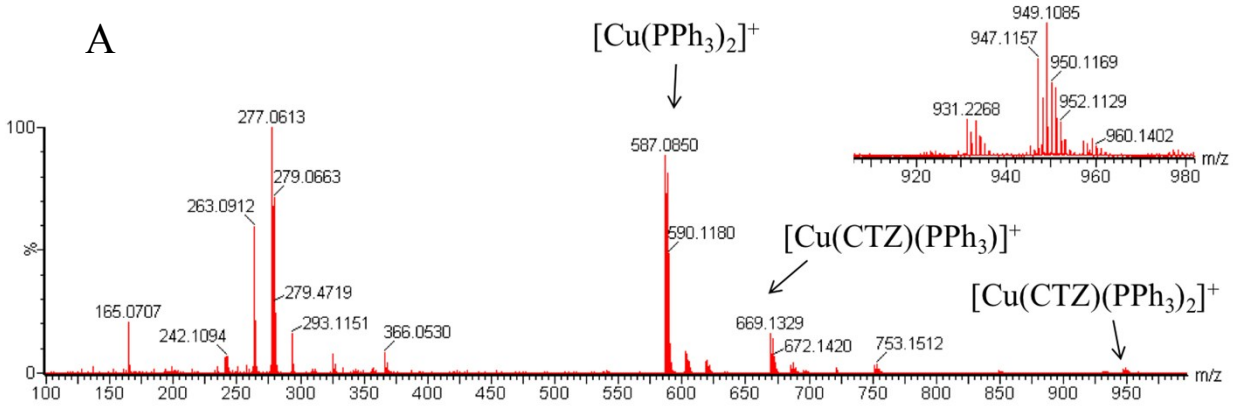


Figure S10. (A) ESI-MS spectrum of complex $[Cu(PPh_3)_2(CTZ)_2]NO_3$ (**2**). (B) ESI-MS simulation of $[Cu(CTZ)(PPh_3)_2]^+$.



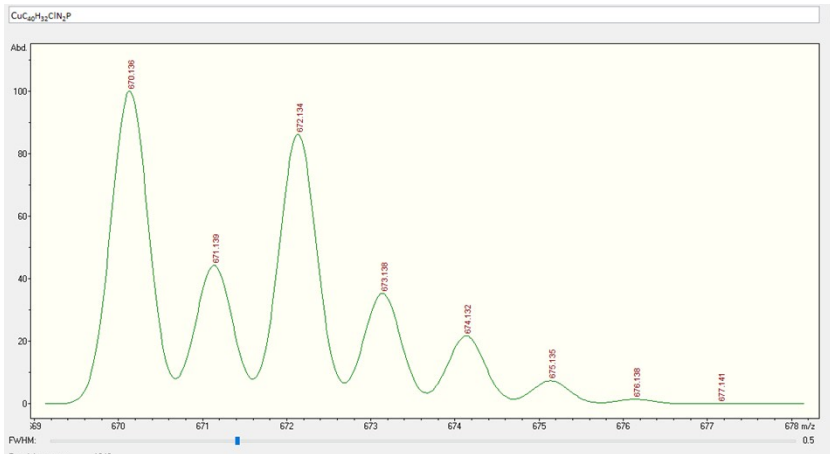
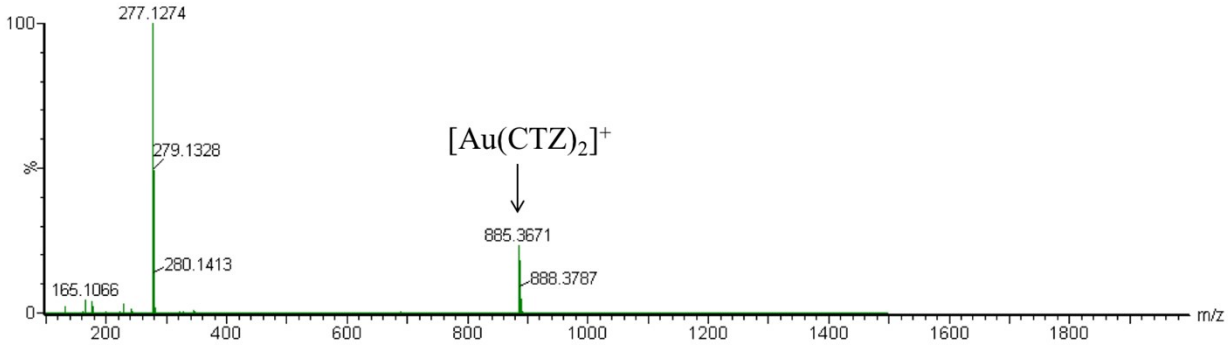
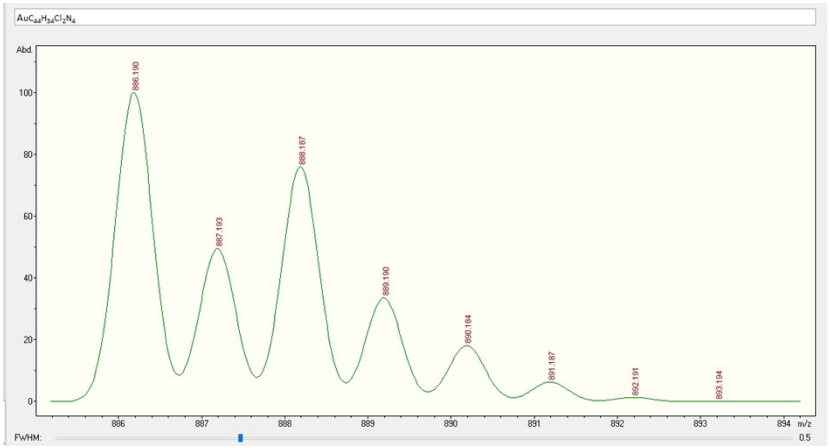


Figure S11. (A) ESI-MS spectrum of complex $[Au(CTZ)_2]Cl$ (**4**). (B) ESI-MS simulation of $[Au(CTZ)_2]^+$. (C) ESI-MS simulation of $[Au(KTZ)_2]^+$.

A



B



C

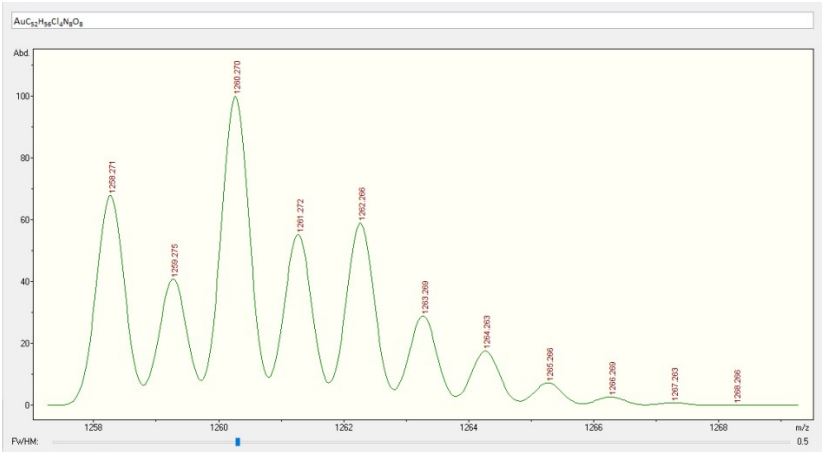


Figure S12. ^{1}H NMR spectra of complex $[Cu(PPh_3)_2(CTZ)_2]NO_3$ (**2**) and CTZ free in dmso-d_6

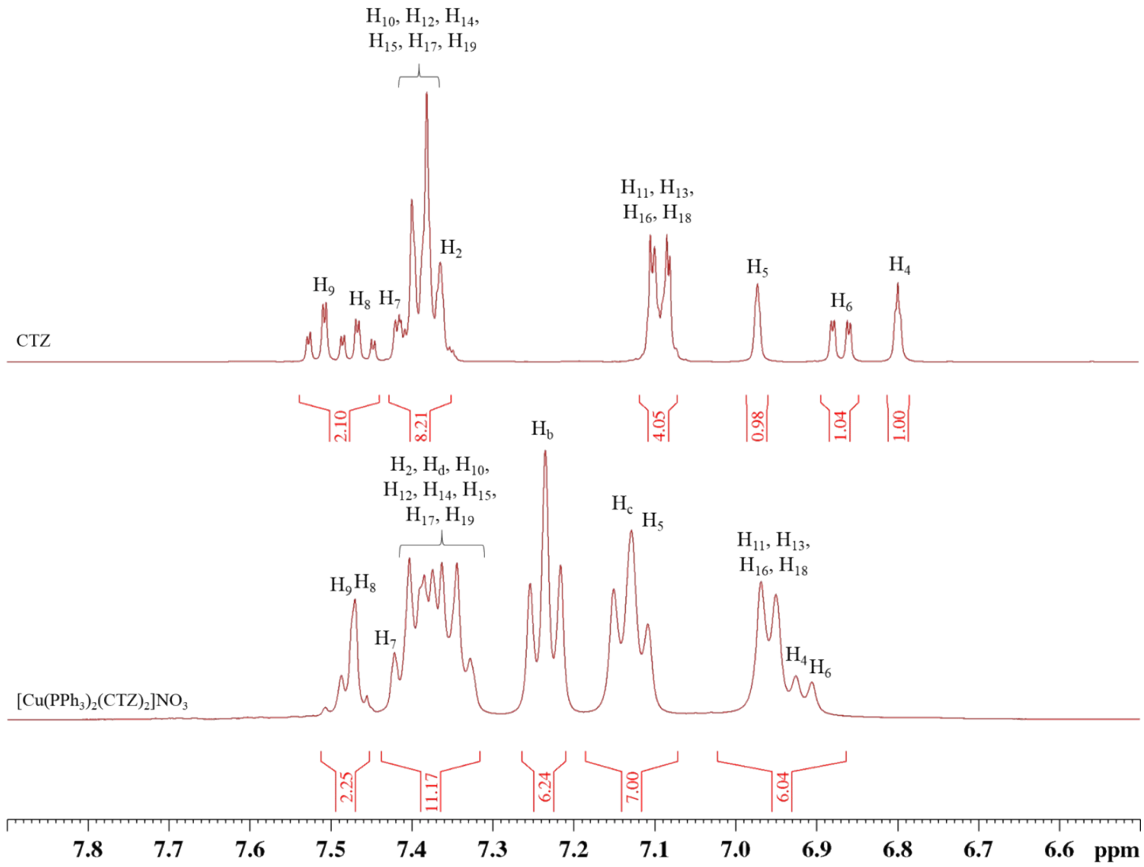


Figure S13. ^{1}H NMR spectra of complex $[Au(CTZ)_2]Cl$ (4) and CTZ free in $CDCl_3$.

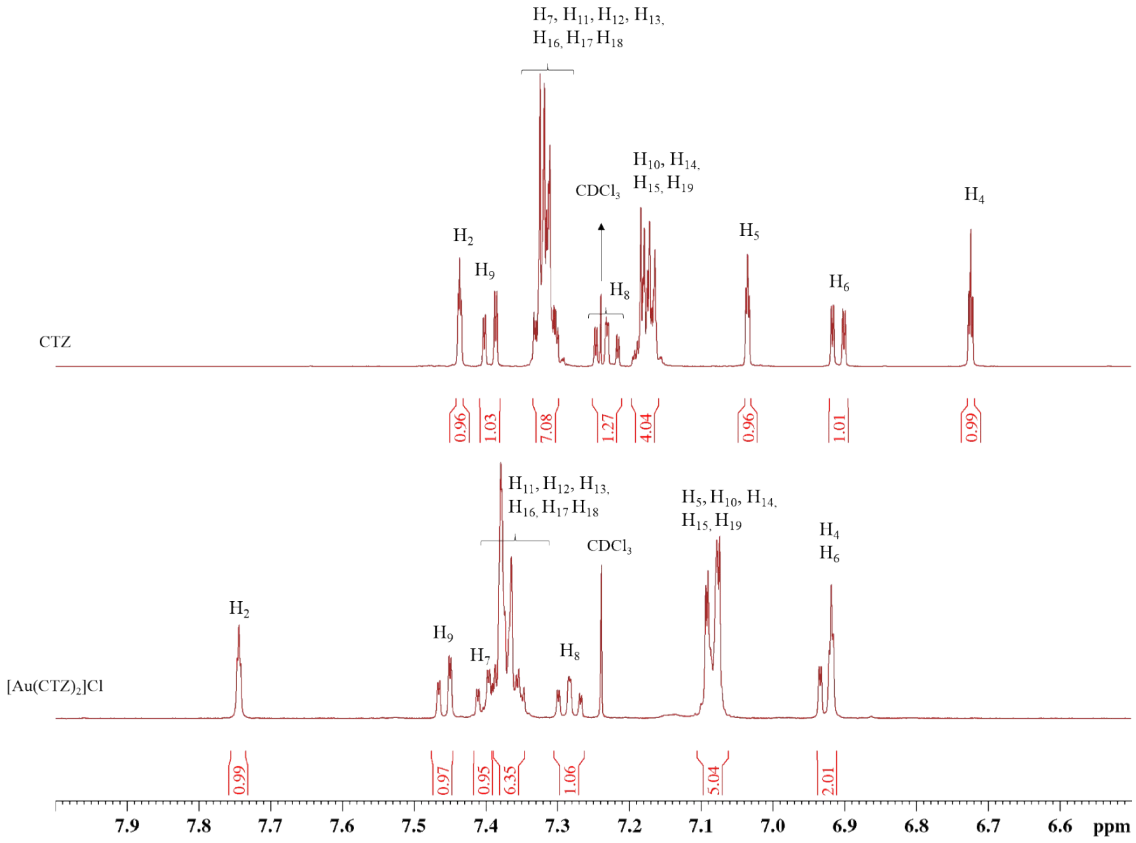


Figure S14. $^{31}P\{^{1}H\}$NMR of complex $[Cu(PPh_3)_2(CTZ)_2]NO_3$ (**2**) in dmso-d_6

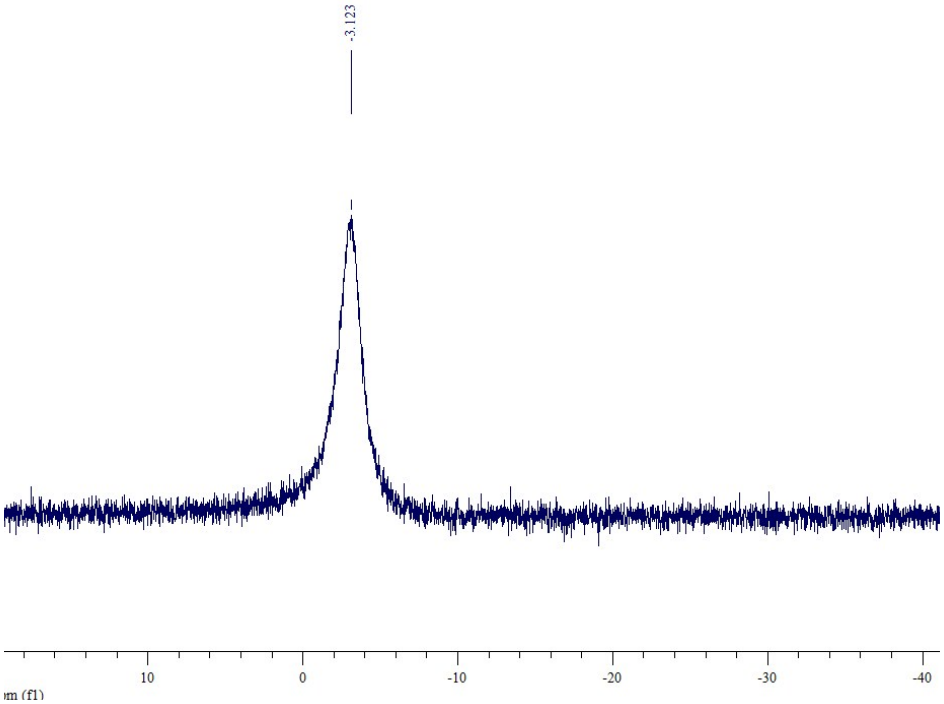


Figure S15. Optimized structure of complex **5** in a *cis* geometry.

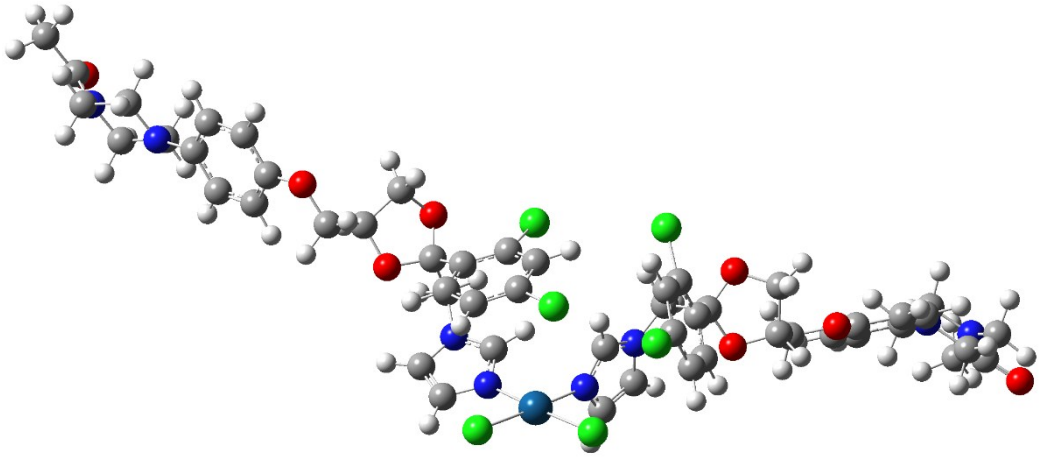


Table S1. Minimum Inhibitory Concentration (MIC) and Minimum Fungicidal Concentration (MFC) of azoles (clotrimazole and ketoconazole), metal-azole complexes and metal salts, against yeasts of *Sporothrix* spp. Results are expressed in nM.

Compounds	***Sporothrix schenckii***				***Sporothrix brasiliensis***				***Sporothrix globosa***			
	Isolate 1		Isolate 2		Isolate 3		Isolate 4		Isolate 5		Isolate 6	
	MIC	MFC	MIC	MFC	MIC	MFC	MIC	MFC	MIC	MFC	MIC	MFC
CTZ	1	40	5	20	5	>40	10	>40	1	2	1	4
$[Cu(PPh_3)_2(CTZ)_2]NO_3$ (**2**)	0.3	5	2	10	1	>10	1	>10	0.1	>10	0.7	1
$[Au(CTZ)_2]Cl$ (**4**)	0.2	2	3	10	3	>20	3	>20	0,2	6	1	20
$[AuPPh_3(CTZ)]PF_6$ (**8**)	1	2	1	1	2	4	1	2	1	1	2	8
KTZ	0.1	0.5	0.9	>40	1	10	7	>40	0.2	1	0.1	0.5
$[Cu(PPh_3)_2(KTZ)_2]NO_3$(**1**)	0.05	2	2	4	0.5	4	0.5	4	0.5	>9	0.1	1
$[Au(KTZ)_2]Cl$ (**3**)	0.06	1	5	>20	2	20	1	10	2	>20	0.06	0.5
$[Pt(KTZ)_2Cl_2]$ (**5**)	0.6	5	3	>10	1	>10	2	>10	1	>10	0.6	5
$[AuPPh_3(KTZ)]PF_6$ (**7**)	0.8	6	0.2	1	0.8	6	0.8	6	0.2	0.4	0.4	0.8
Itraconazole	1	20	1	5	1	20	1	10	0.3	0.7	0.3	20
$AuClPPh_3$	4	4	2	8	4	4	4	4	2	2	2	2
$Cu(PPh_3)_2NO_3$	>20	>20	>20	>20	>20	>20	>20	>20	>20	>20	>20	>20
$K[AuCl_4]$	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40	>40
$K_2[PtCl_4]$	>30	>30	>30	>30	>30	>30	>30	>30	>30	>30	>30	>30
KPF_6	>8	>8	>8	>8	>8	>8	>8	>8	>8	>8	>8	>8

Itraconazole values are shown for comparison