

## SUPPLEMENTARY INFORMATION

# “Synthesis, Characterization and DNA Binding Kinetics of New Pd (II) and Pt (II) Thiosemicarbazone Complexes. Spectral, Structural and Anticancer Evaluation

### 1. FTIR SPECTRA DATA

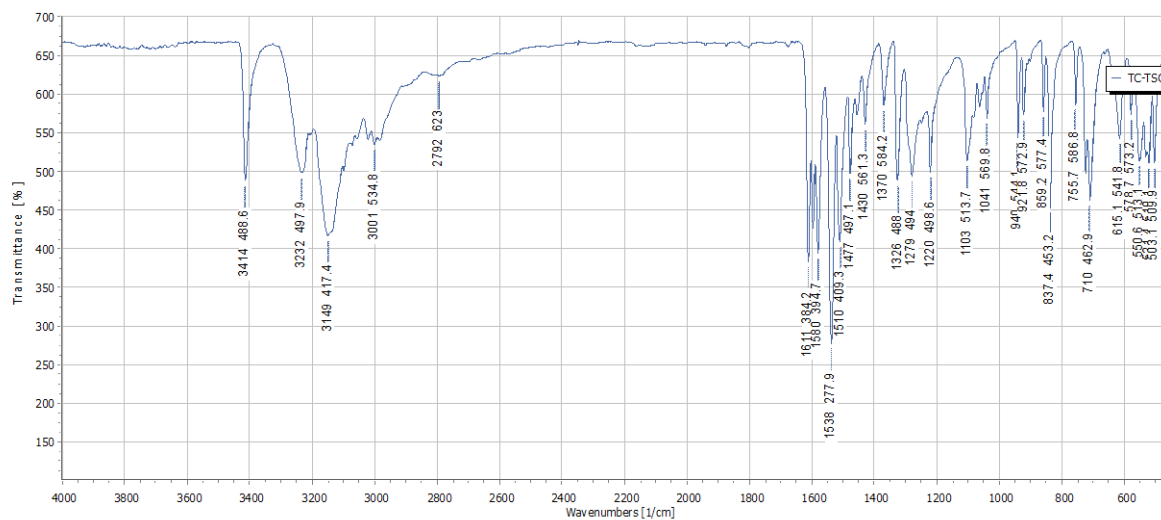


Figure ESI 1. FTIR Spectra for (E)-1-((thiophen-2-yl) methylene) thiosemicarbazide (L1)

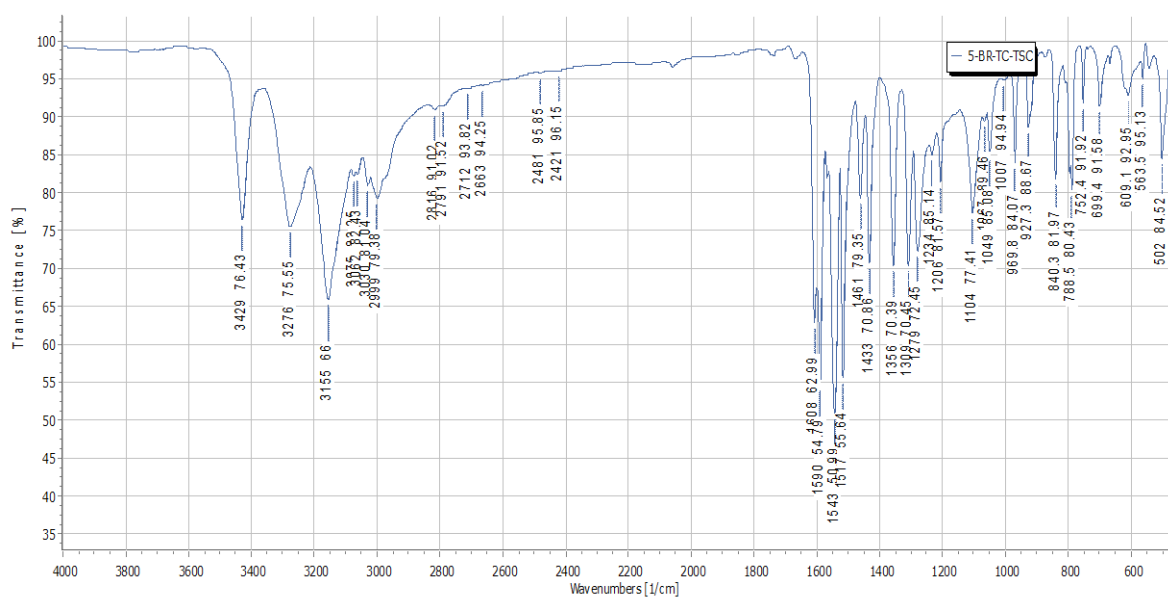
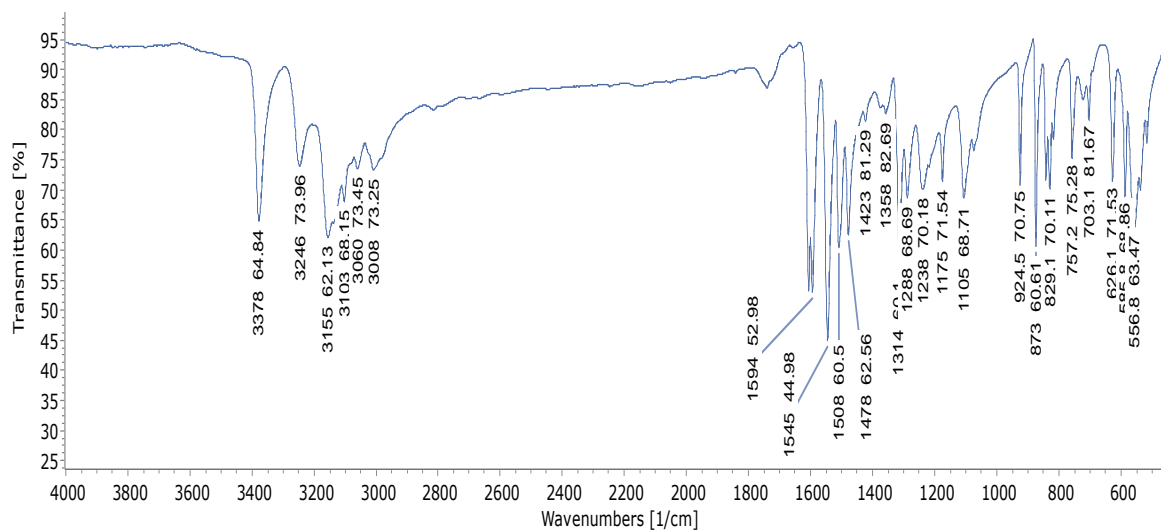
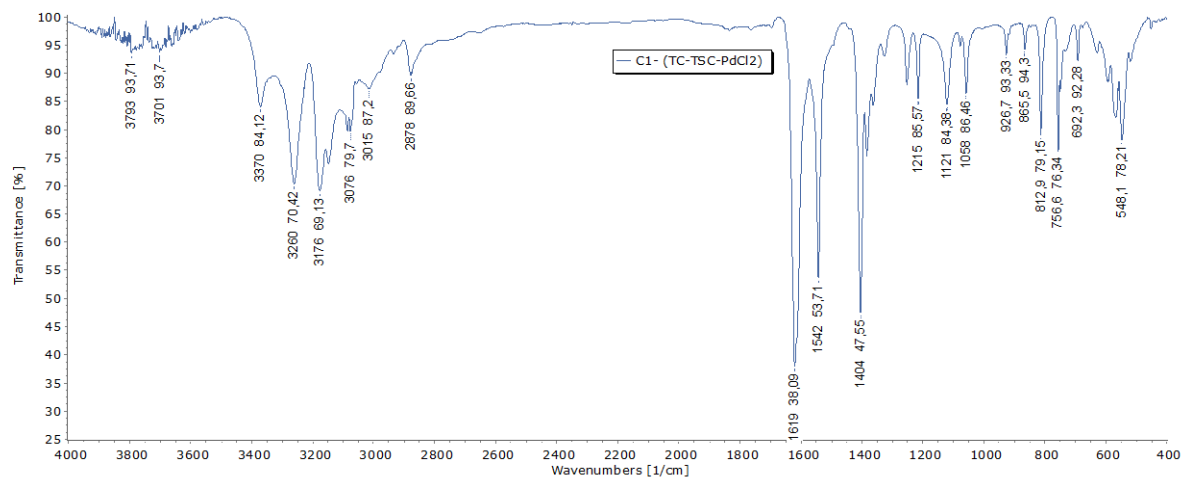


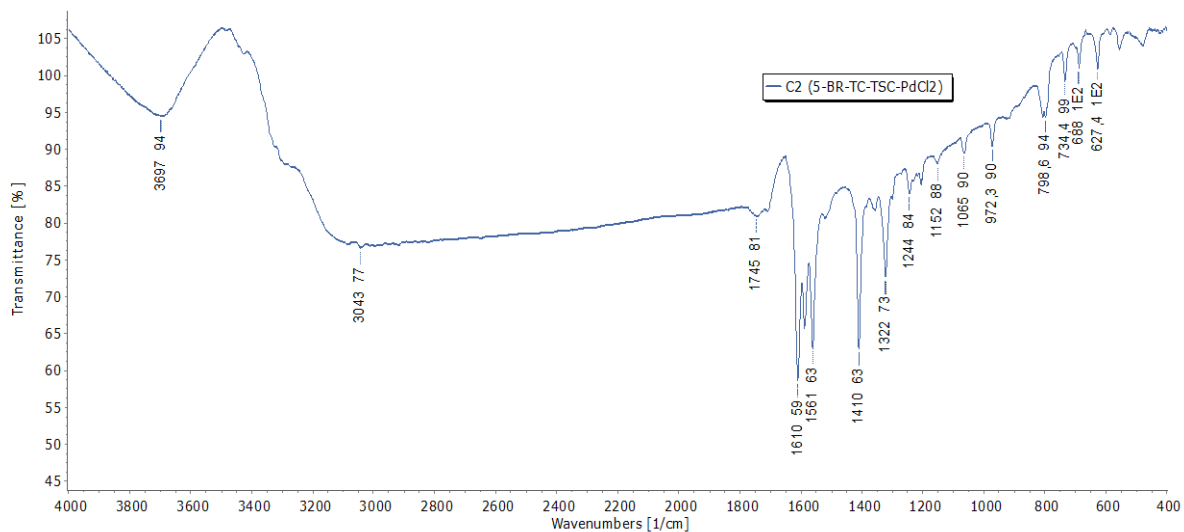
Figure ESI 2. FTIR Spectra for (E)-1-((5-bromothiophen-2-yl) methylene) thiosemicarbazide (L2)



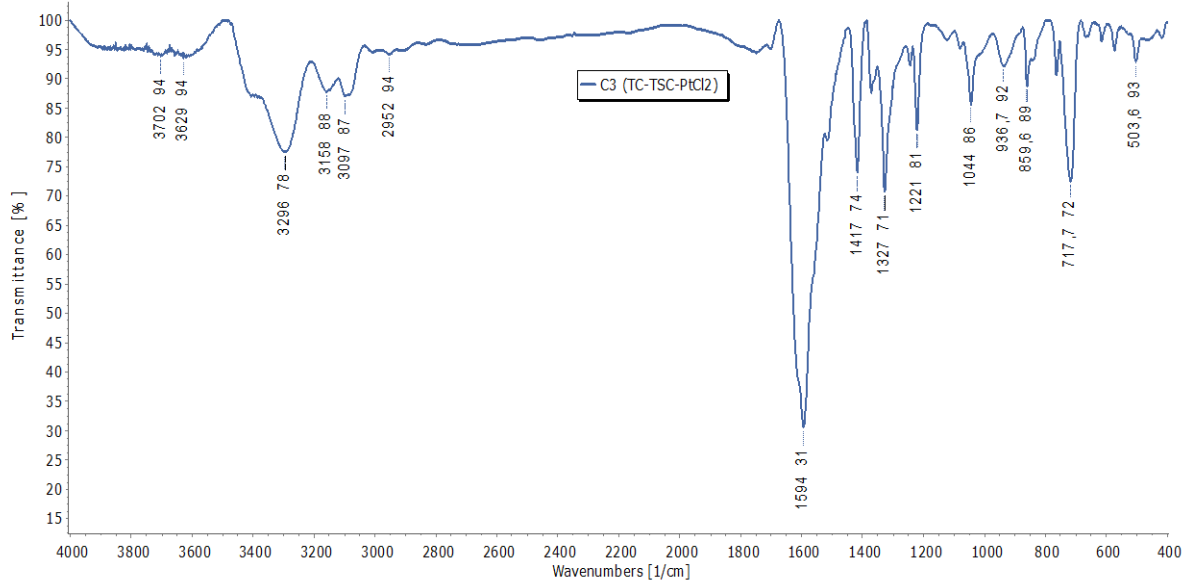
**Figure ESI 3 FTIR Spectra for (E)-1-((4-bromothiophen-2-yl) methylene) thiosemicarbazide (L3)**



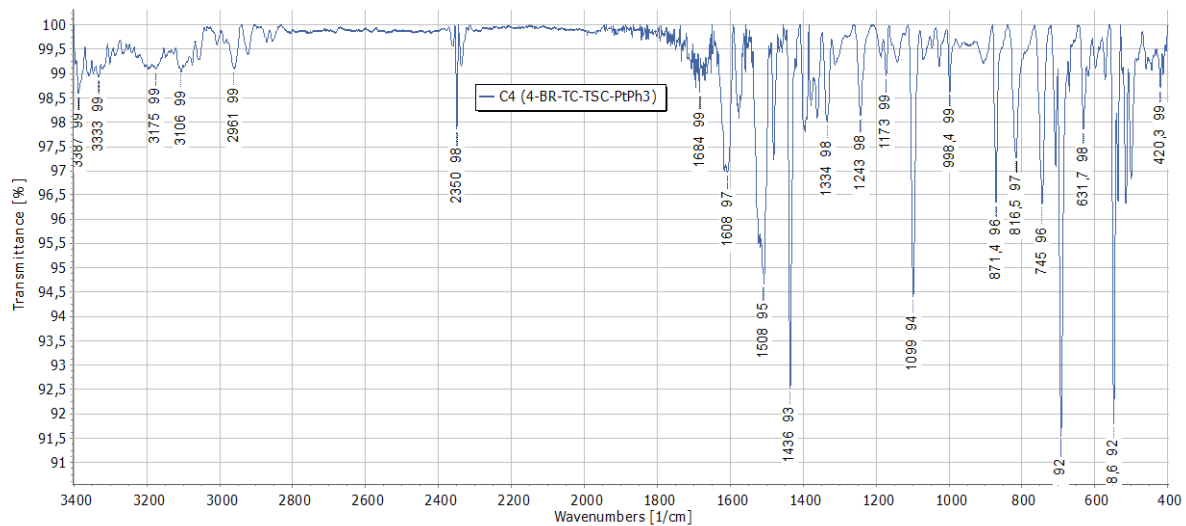
**Figure ESI 4 FTIR Spectra for Palladium Complex C1**



**Figure ESI 5 FTIR Spectra for Palladium Complex C2**



**Figure ESI 6 FTIR Spectra for Platinum Complex C3**



**Figure ESI 7 FTIR Spectra for Platinum Complex C4**

## 2. <sup>1</sup>H NMR SPECTRA

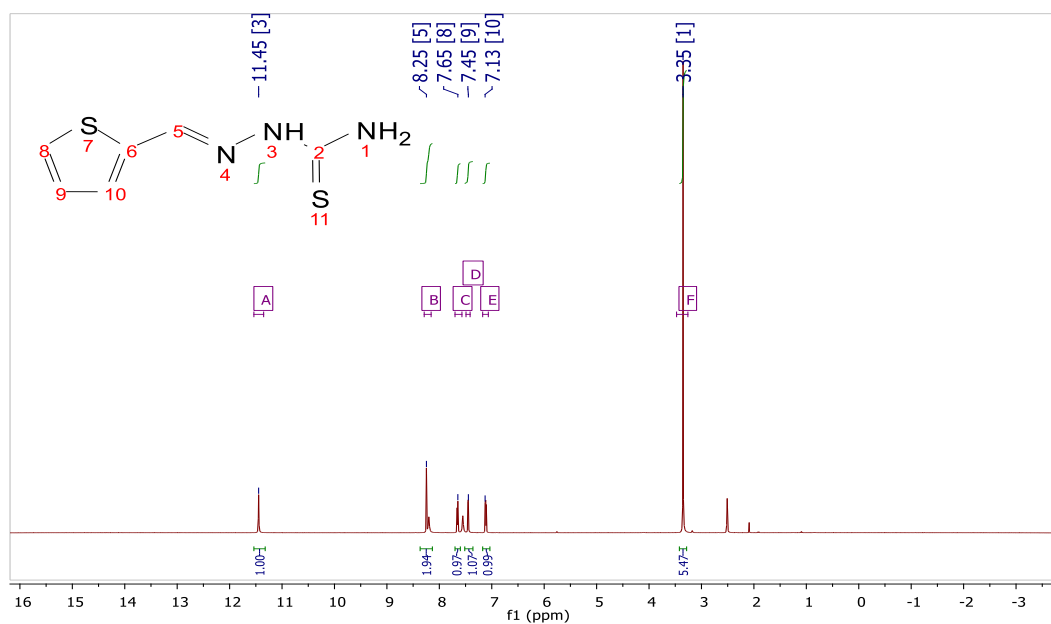


Figure ESI 8. <sup>1</sup>H NMR Spectra for (E)-1-((thiophen-2-yl)methylene)thiosemicarbazide (L1)

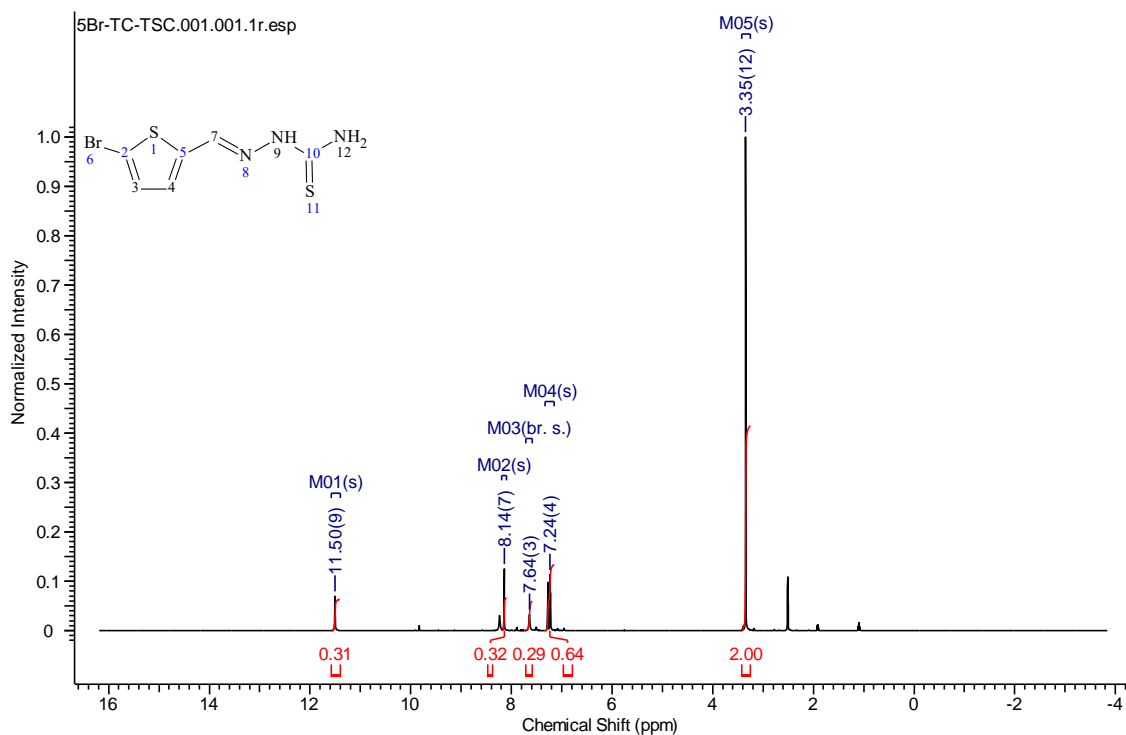
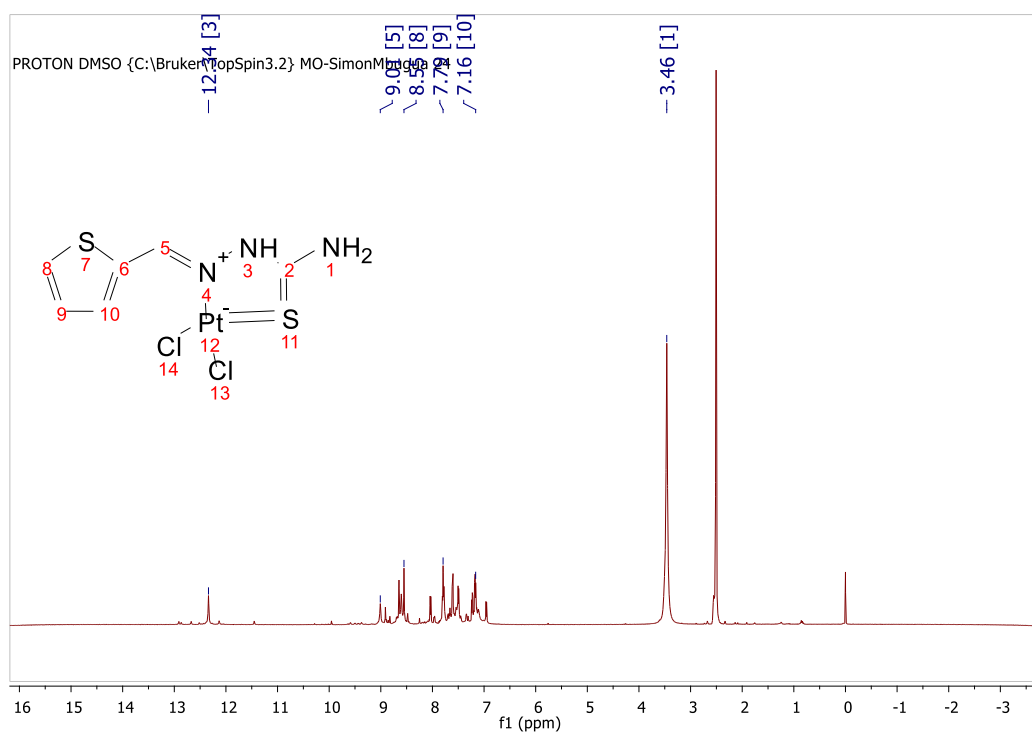
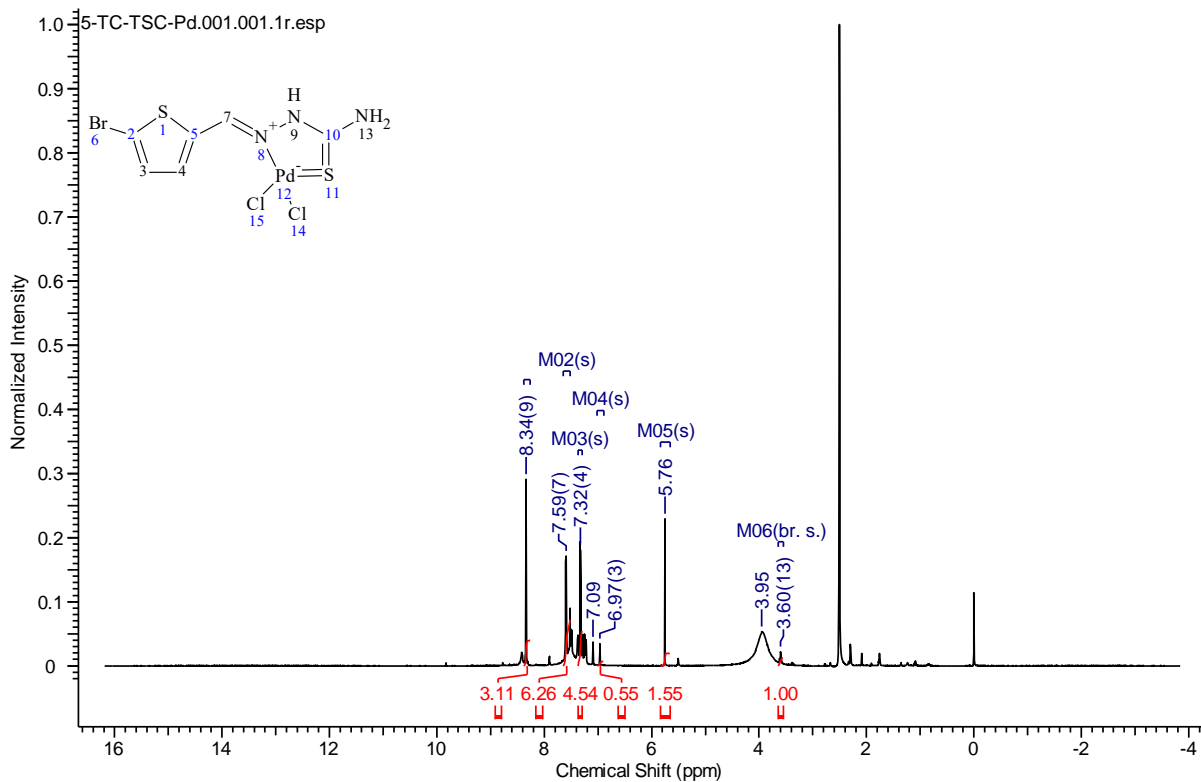


Figure ESI 9. <sup>1</sup>H NMR Spectra for (E)-1-((5-bromothiophen-2-yl)methylene)thiosemicarbazide (L2)



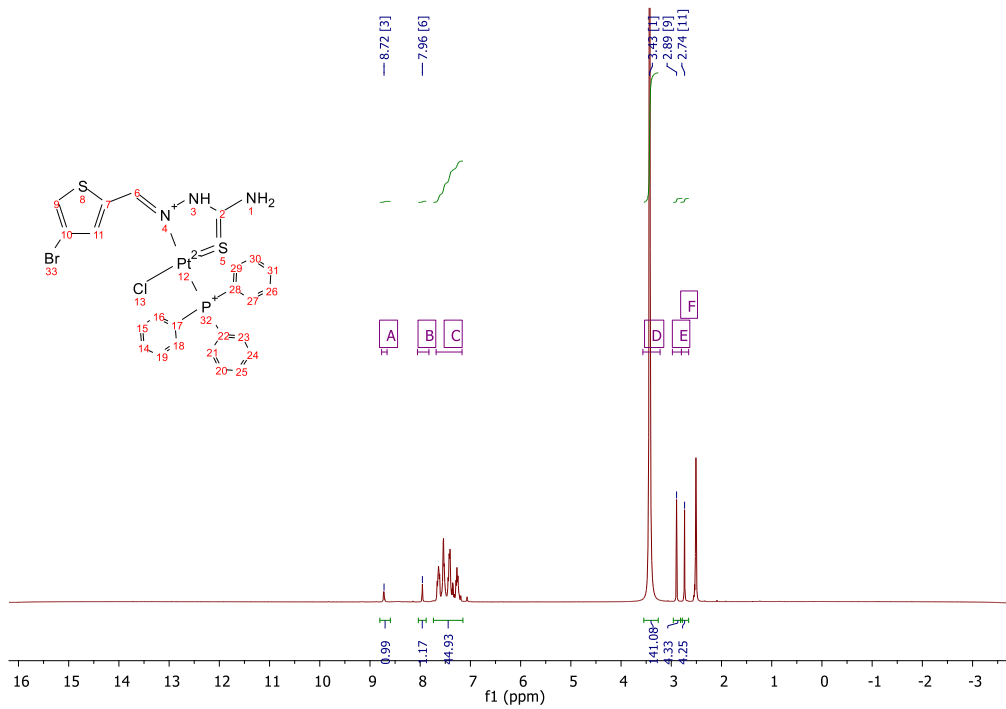


Figure ESI 12.  $^1\text{H}$  NMR Spectra for Platinum complex C4

### 3. $^{13}\text{C}$ NMR Spectra

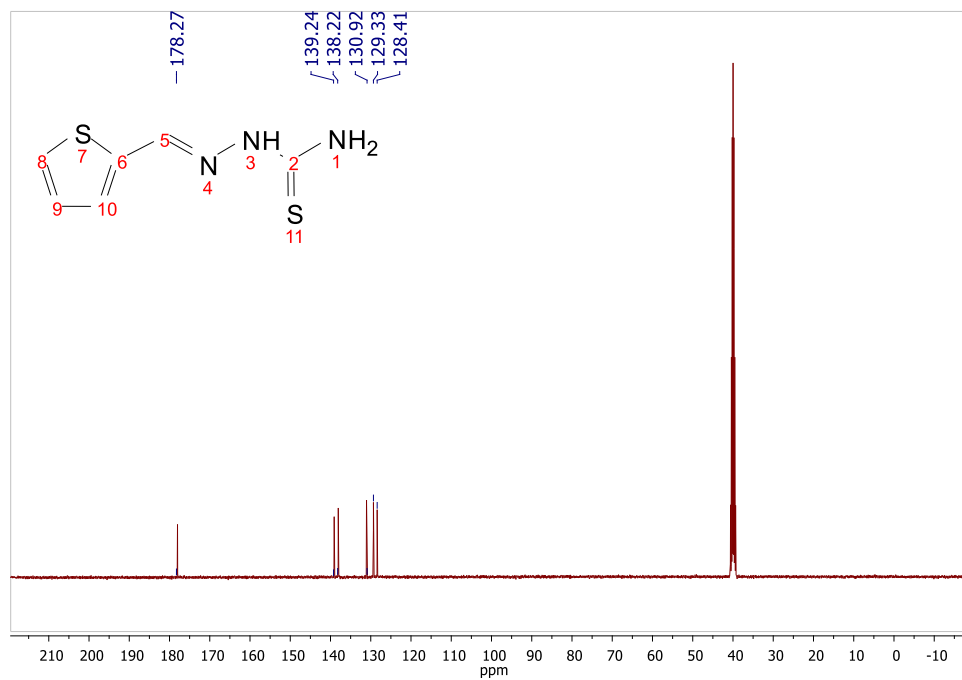


Figure ESI 13.  $^{13}\text{C}$  NMR Spectra for (E)-1-((thiophen-2-yl)methylene)thiosemicarbazide (L1)

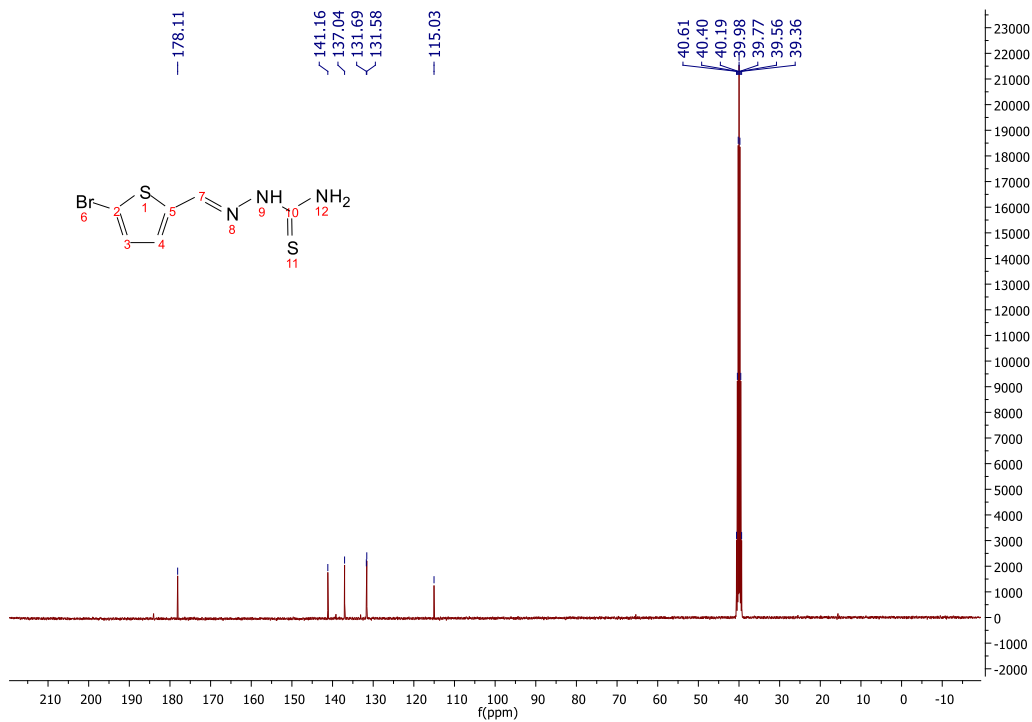


Figure ESI 14.  $^{13}\text{C}$  NMR Spectra for (E)-1-((5-bromothiophen-2-yl) methylene) thiosemicarbazide (L2)

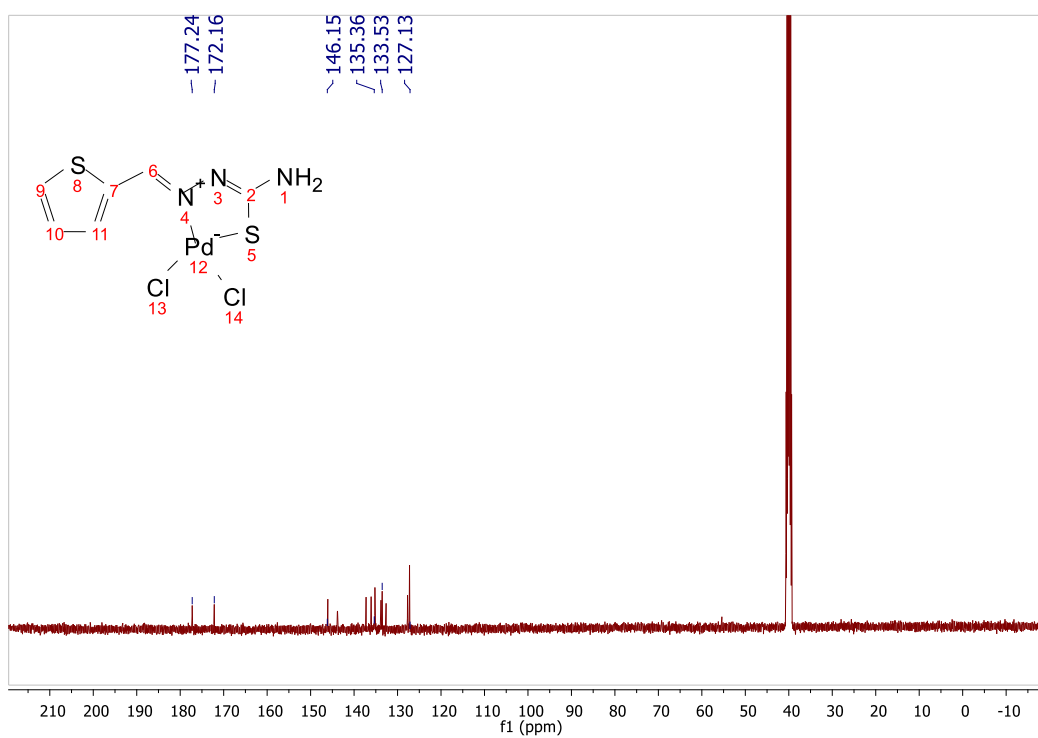


Figure ESI 15.  $^{13}\text{C}$  NMR Spectra for Palladium Complex C1

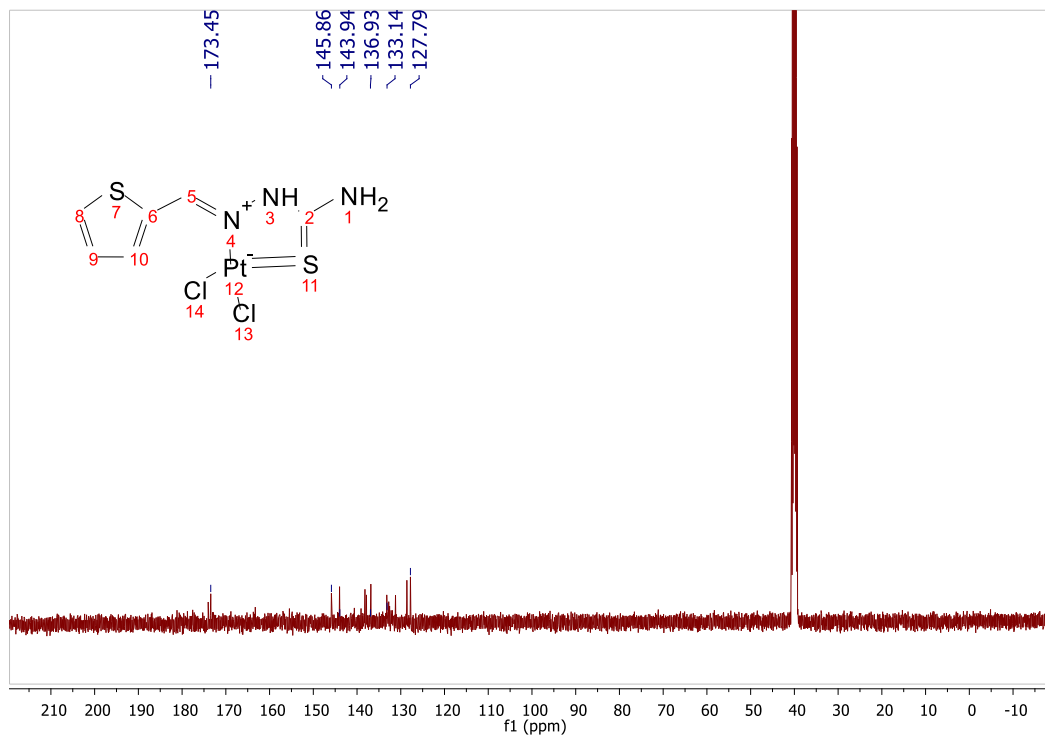


Figure ESI 16.  $^{13}\text{C}$  NMR Spectra for Platinum Complex C3

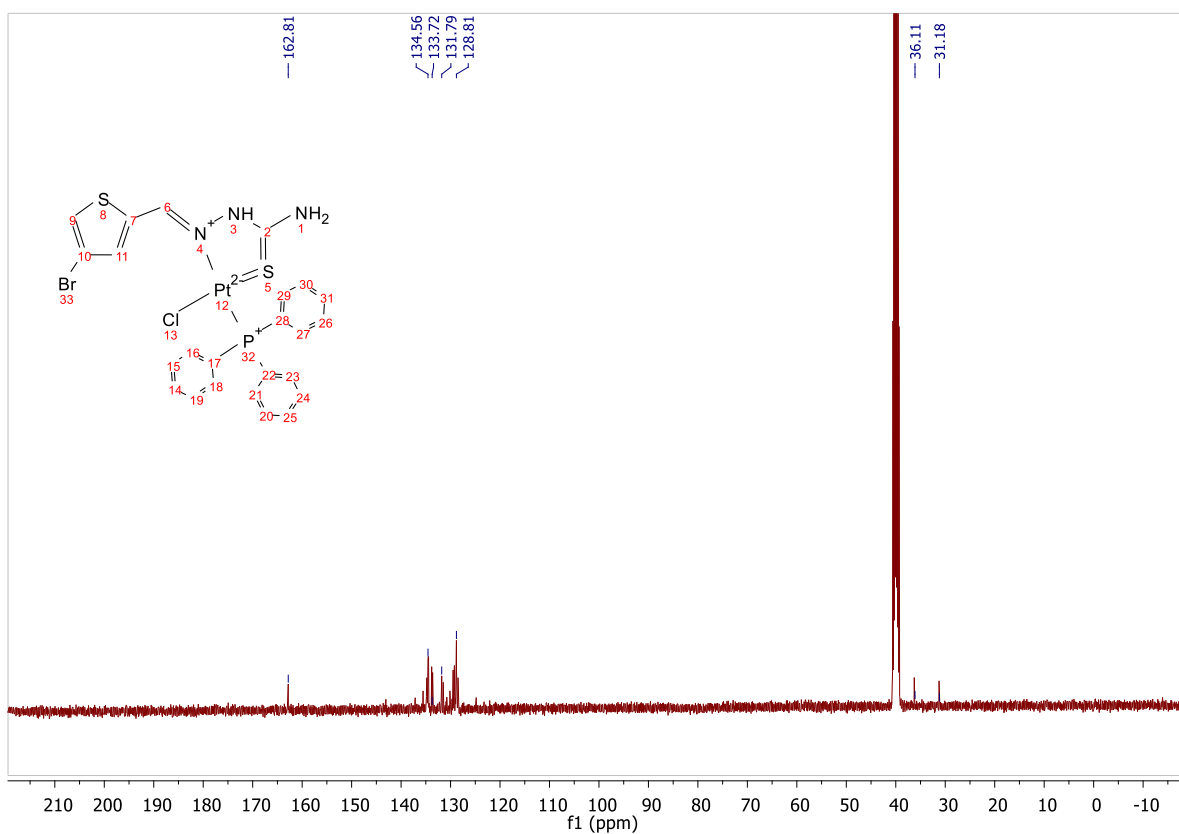


Figure ESI 17.  $^{13}\text{C}$  NMR Spectra for Platinum Complex C4



#### 4. UV-Vis Spectra

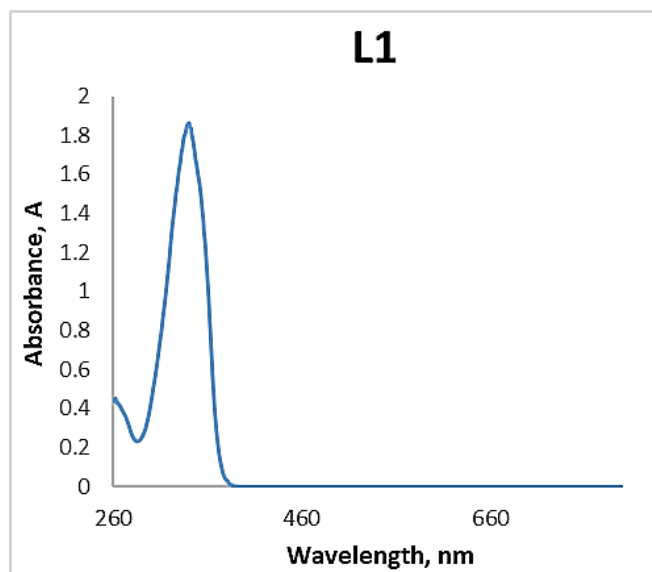


Figure ESI 18. UV-Vis Spectra for Ligand L1

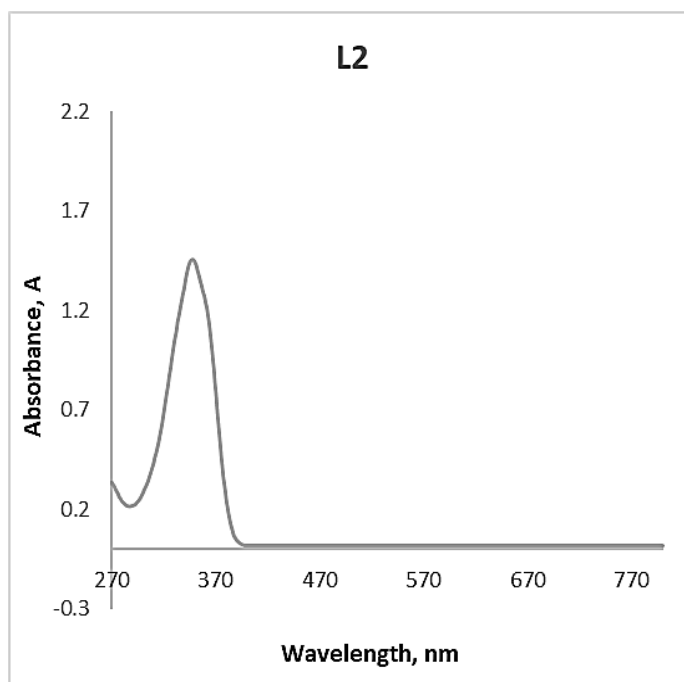
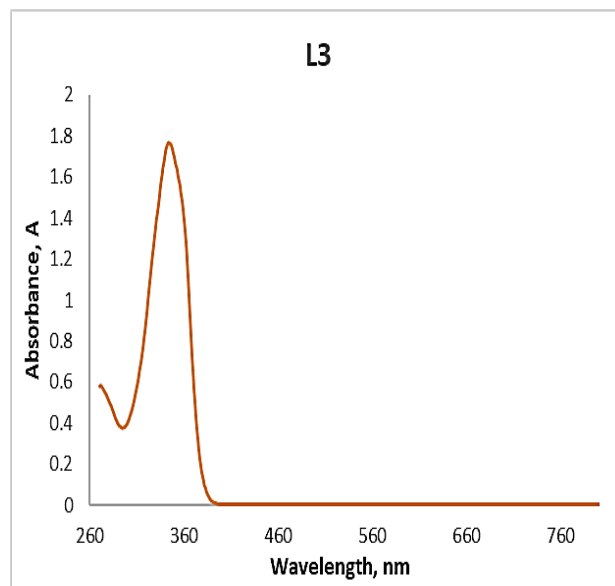
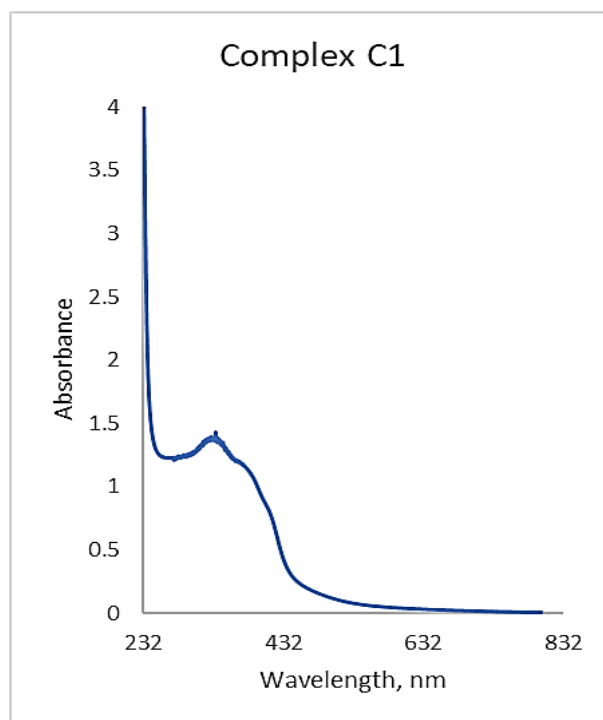


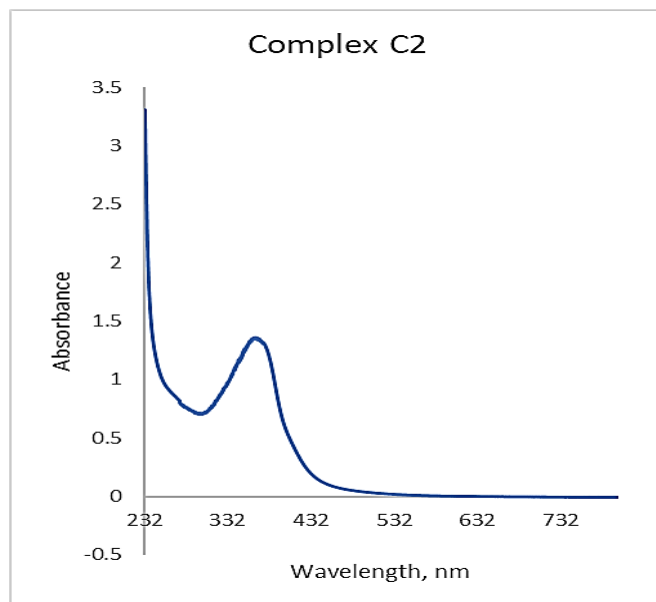
Figure ESI 19. UV-Vis Spectra for Ligand L2



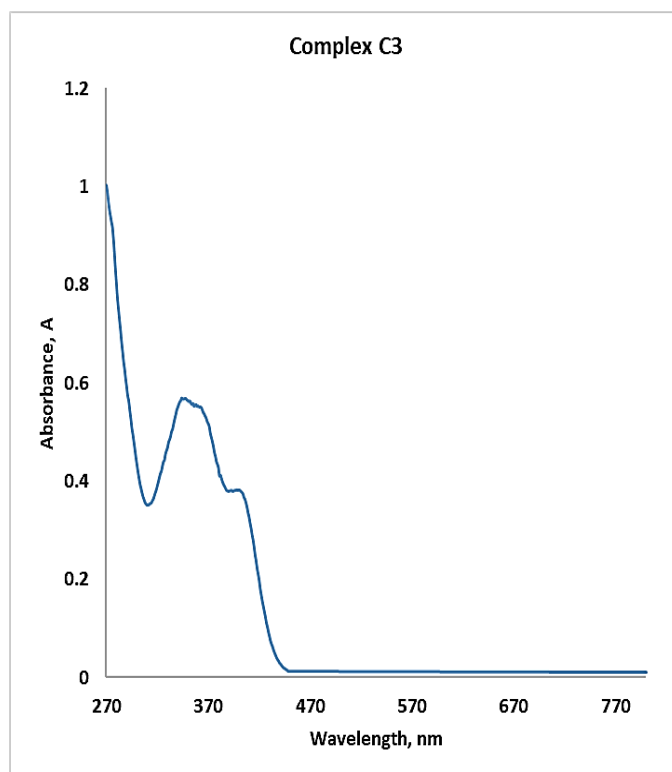
**Figure ESI 20. UV-Vis Spectra for Ligand L3**



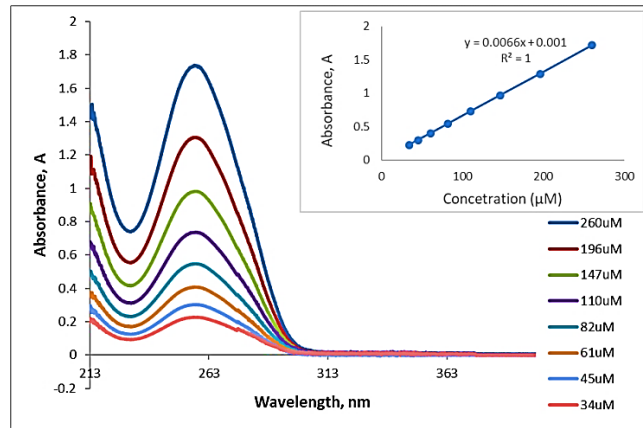
**Figure ESI 21. UV-Vis Spectra for Palladium Complex C1**



**Figure ESI 22. UV-Vis Spectra for Palladium Complex C2**



**Figure ESI 23. UV-Vis Spectra for Platinum Complex C4**



**Figure ESI 24.** Calibration curve for determination of DNA concentration used. Inset is Absorbance vs Concentration at 260nm

## 5. Crystal CIF File for Ligand L1

### checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 180924RAL\_ONANI\_TC\_TSC\_100K\_0m\_a

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found.    CIF dictionary    Interpreting this report

### Datablock: 180924RAL\_ONANI\_TC\_TSC\_100K\_0m\_a

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Bond precision:	C-C = 0.0021 A	Wavelength=1.54178	
Cell:	a=13.4381 (2)	b=5.7728 (1)	c=21.2683 (4)
	alpha=90	beta=96.302 (1)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	1639.93 (5)	1639.93 (5)	
Space group	P 21/n	P 21/n	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C6 H7 N3 S2	C6 H7 N3 S2	
Sum formula	C6 H7 N3 S2	C6 H7 N3 S2	
Mr	185.27	185.27	
Dx, g cm-3	1.501	1.501	
Z	8	8	
Mu (mm-1)	5.368	5.368	
F000	768.0	768.0	
F000'	774.83		
h,k,lmax	16,6,25	16,6,25	
Nref	2897	2897	
Tmin,Tmax	0.277,0.353	0.272,0.496	
Tmin'	0.107		

Correction method= # Reported T Limits: Tmin=0.272 Tmax=0.496  
AbsCorr = NUMERICAL

Data completeness= 1.000                      Theta(max)= 66.686

R(reflections)= 0.0264 ( 2744)              wR2(reflections)= 0.0671 ( 2897)

S = 1.036                                      Npar= 200

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The following ALERTS were generated. Each ALERT has the format  
test-name\_ALERT\_alert-type\_alert-level.  
Click on the hyperlinks for more details of the test.

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● **Alert level C**

PLAT230\_ALERT\_2\_C Hirshfeld Test Diff for S1 --C1 . 5.1 e.u.

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● **Alert level G**

PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 6 Report  
PLAT909\_ALERT\_3\_G Percentage of I>2σ(I) Data at Theta(Max) Still 93% Note  
PLAT953\_ALERT\_1\_G Reported (CIF) and Actual (FCF) Hmax Differ by . 1 Units  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 10 Info

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0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
4 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
2 ALERT type 2 Indicator that the structure model may be wrong or deficient  
1 ALERT type 3 Indicator that the structure quality may be low  
0 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check

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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special\_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

### Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

### Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

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