IR spectroscopy

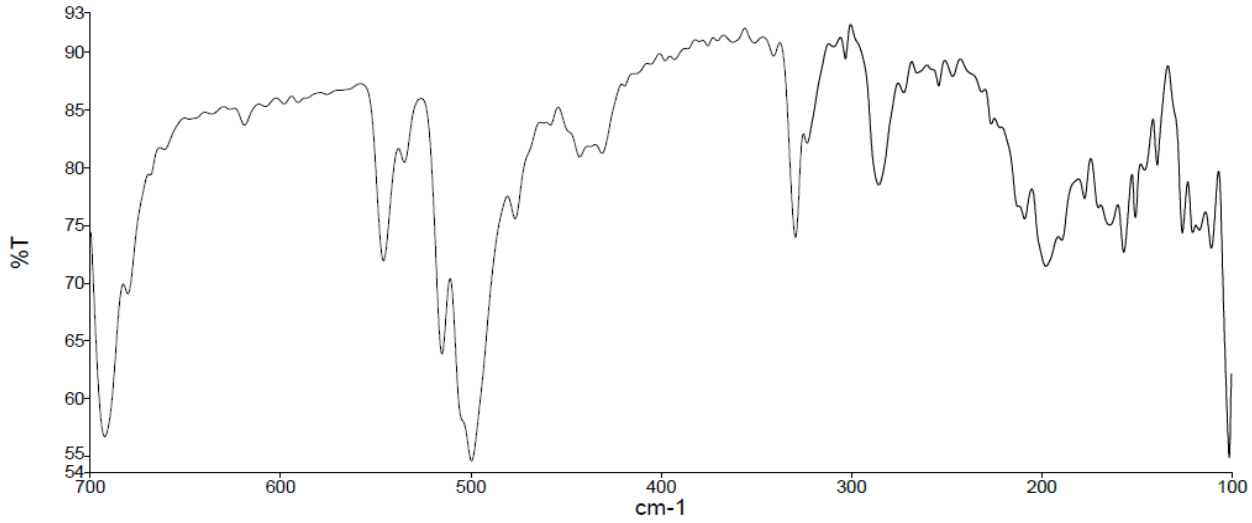


Figure S1. FIR spectrum of compound 8.

^{1}H NMR spectra

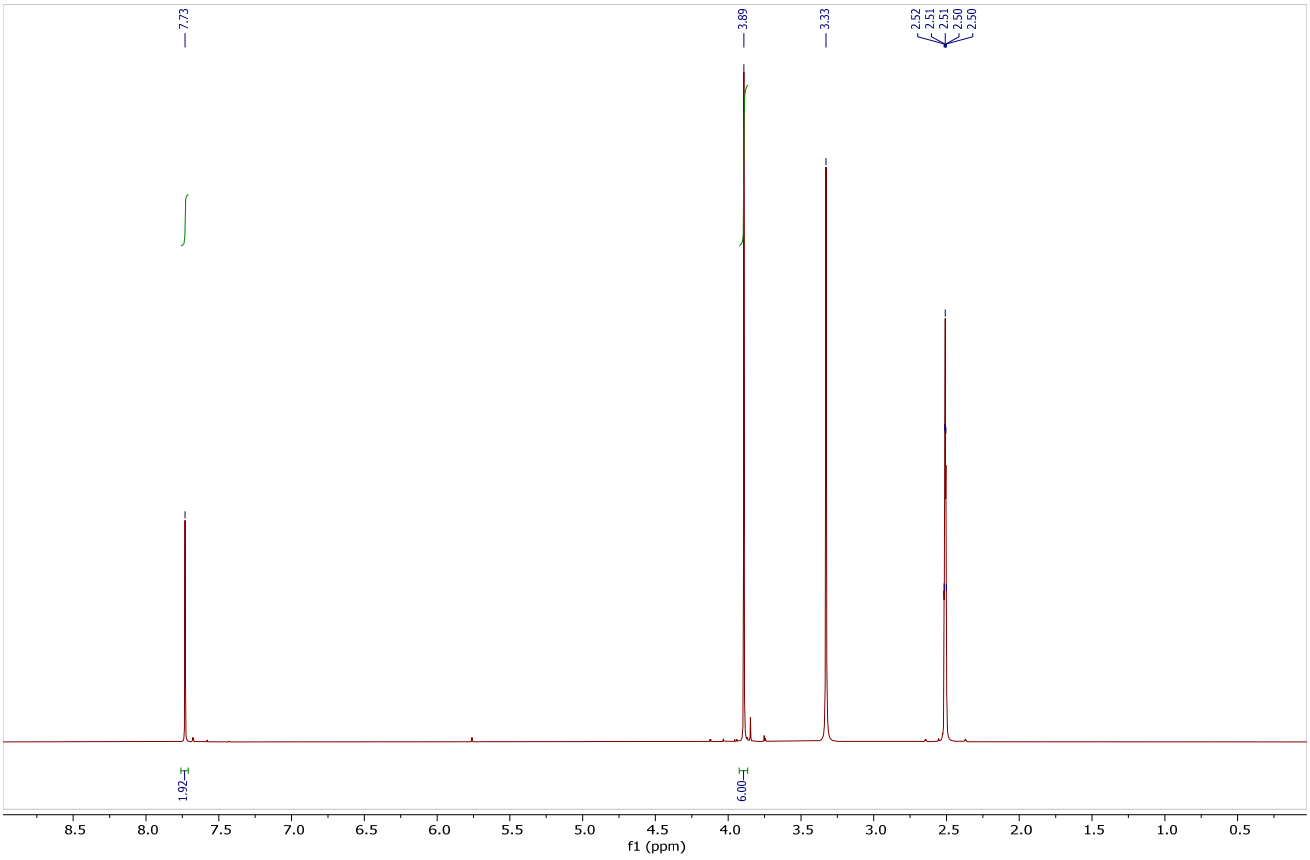


Figure S2. ^{1}H NMR of complex **1** in DMSO.

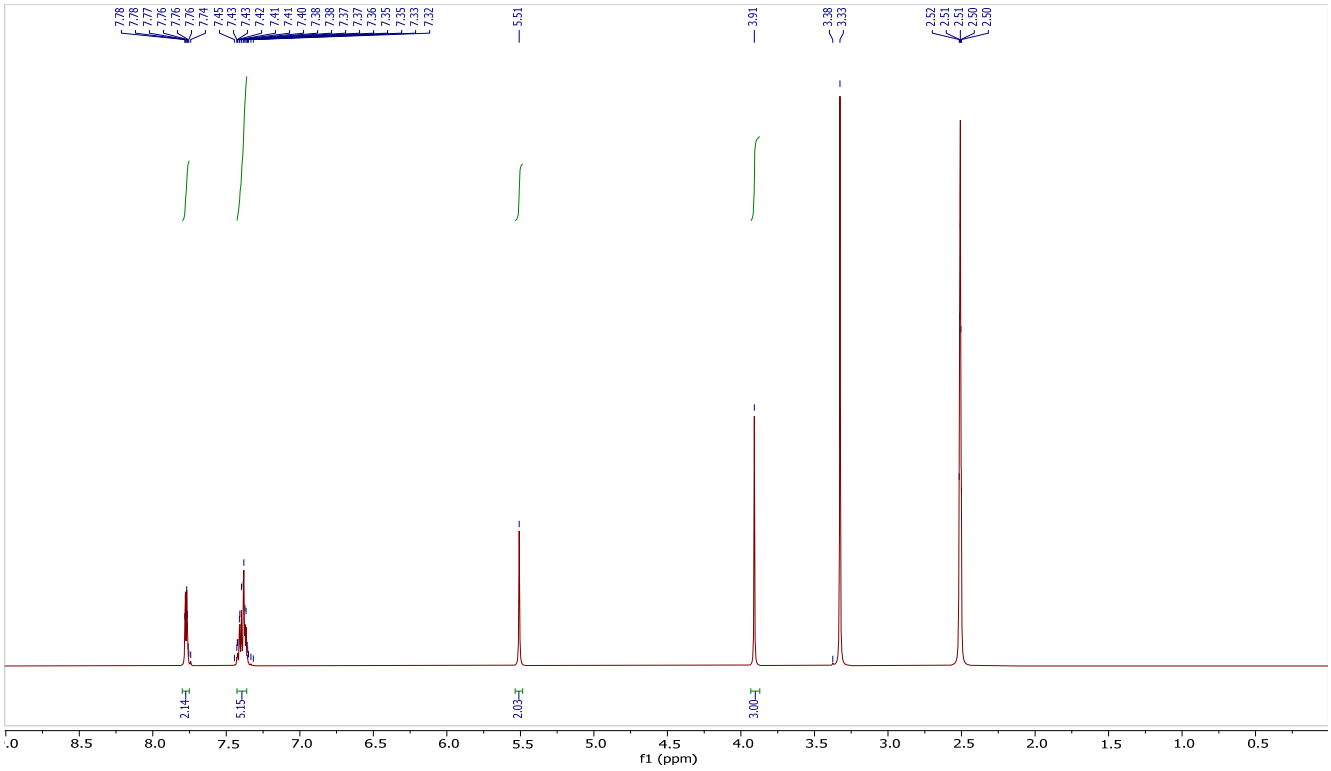


Figure S3. [1]H NMR of complex **2** in DMSO.

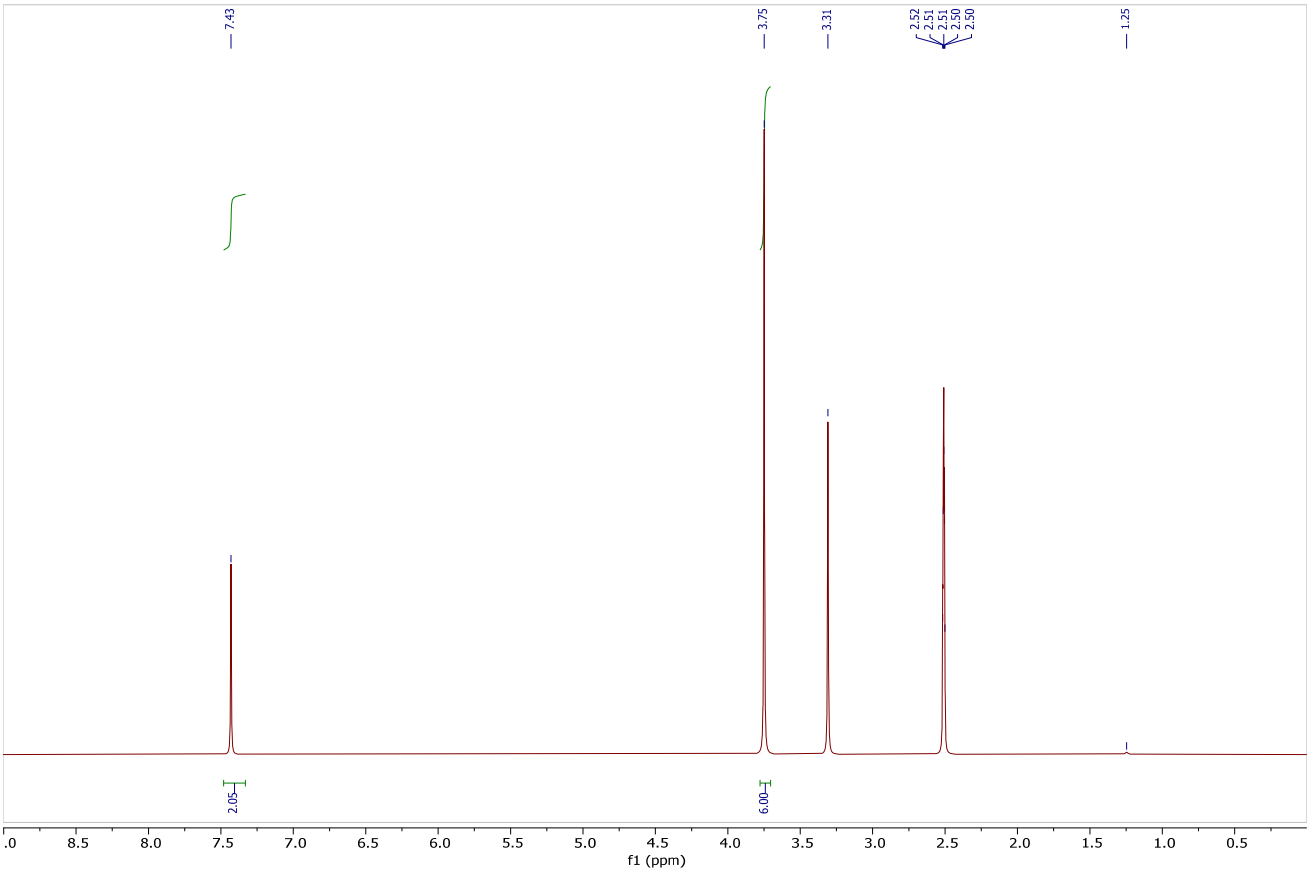


Figure S4. [1]H NMR of complex **3** in DMSO.

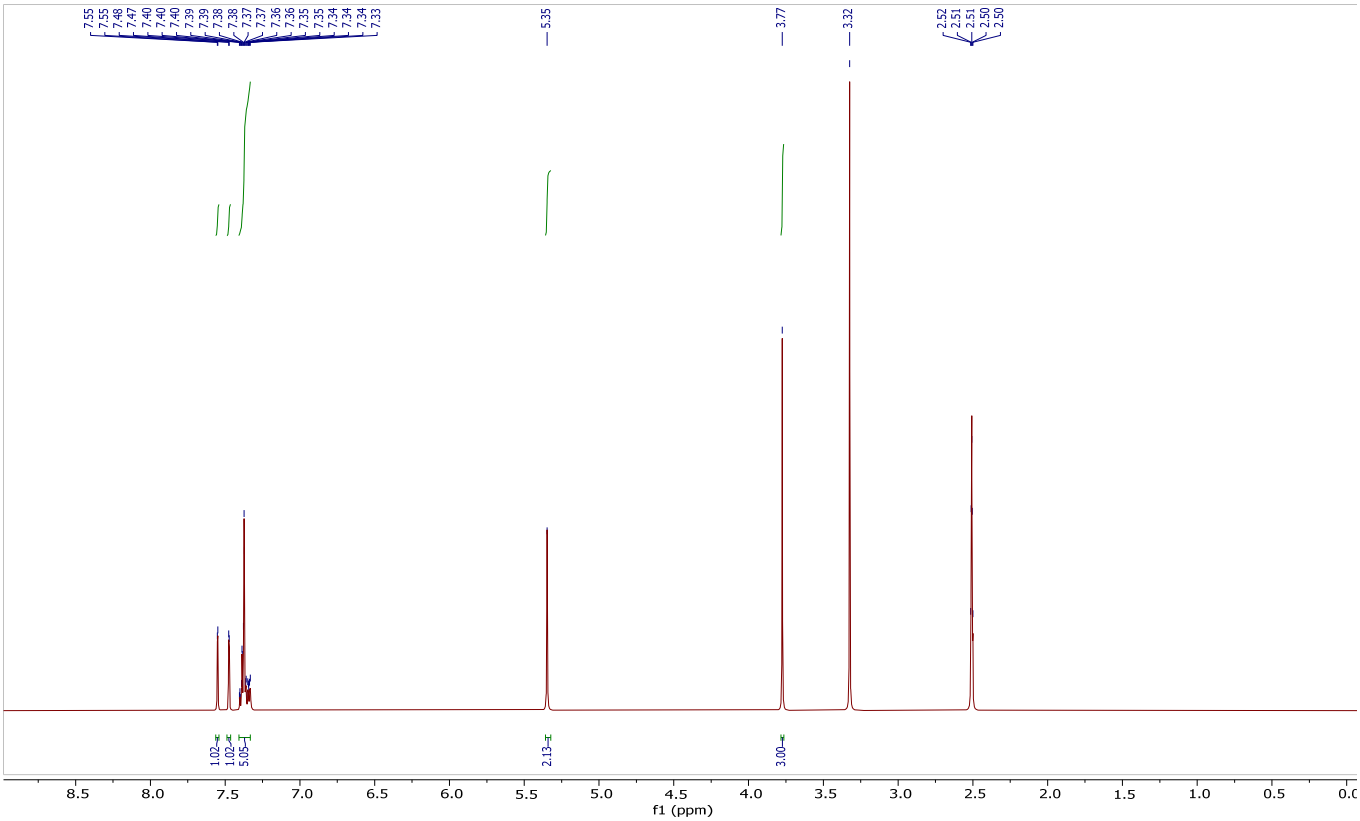


Figure S5. [1]H NMR of complex **4** in DMSO.

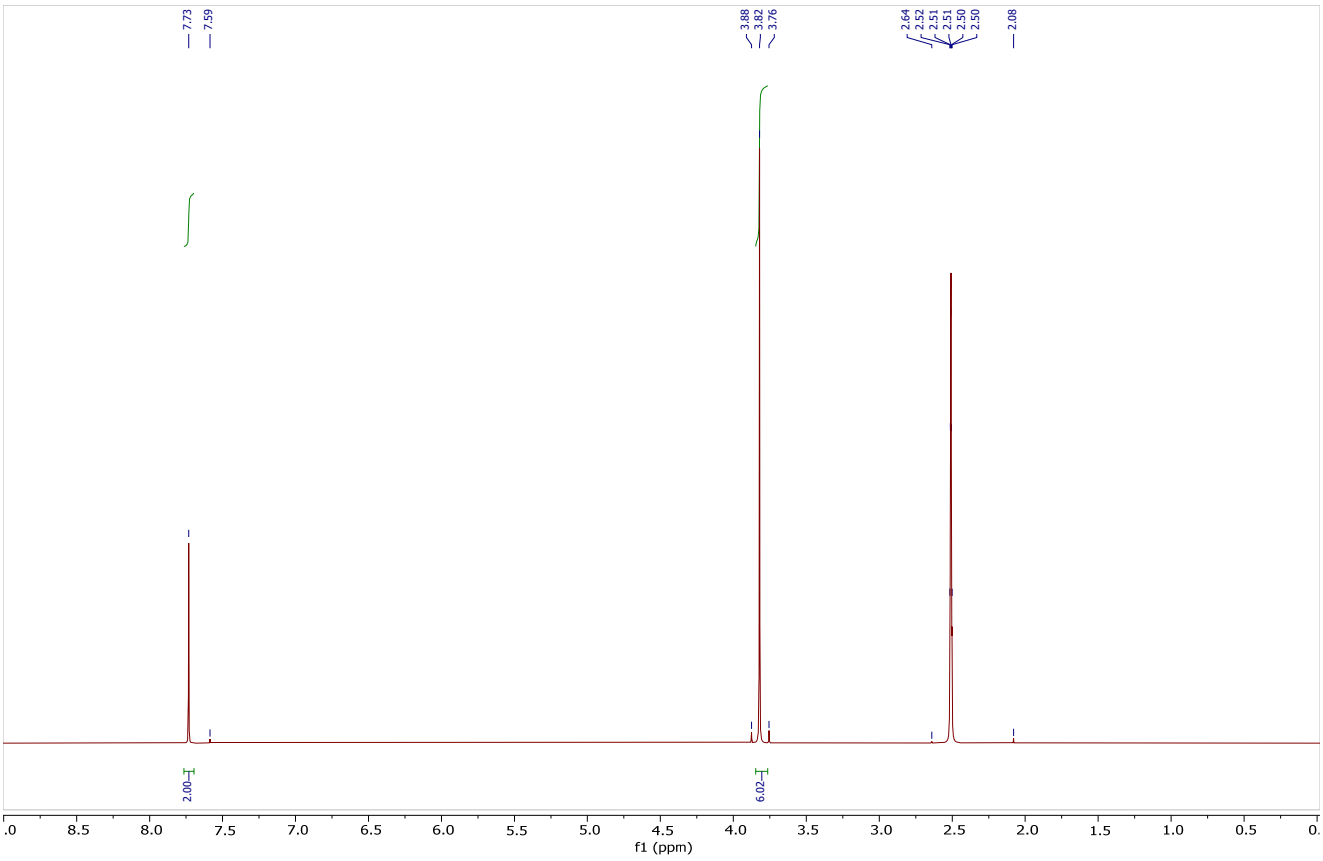


Figure S6. [1]H NMR of complex **5** in DMSO.

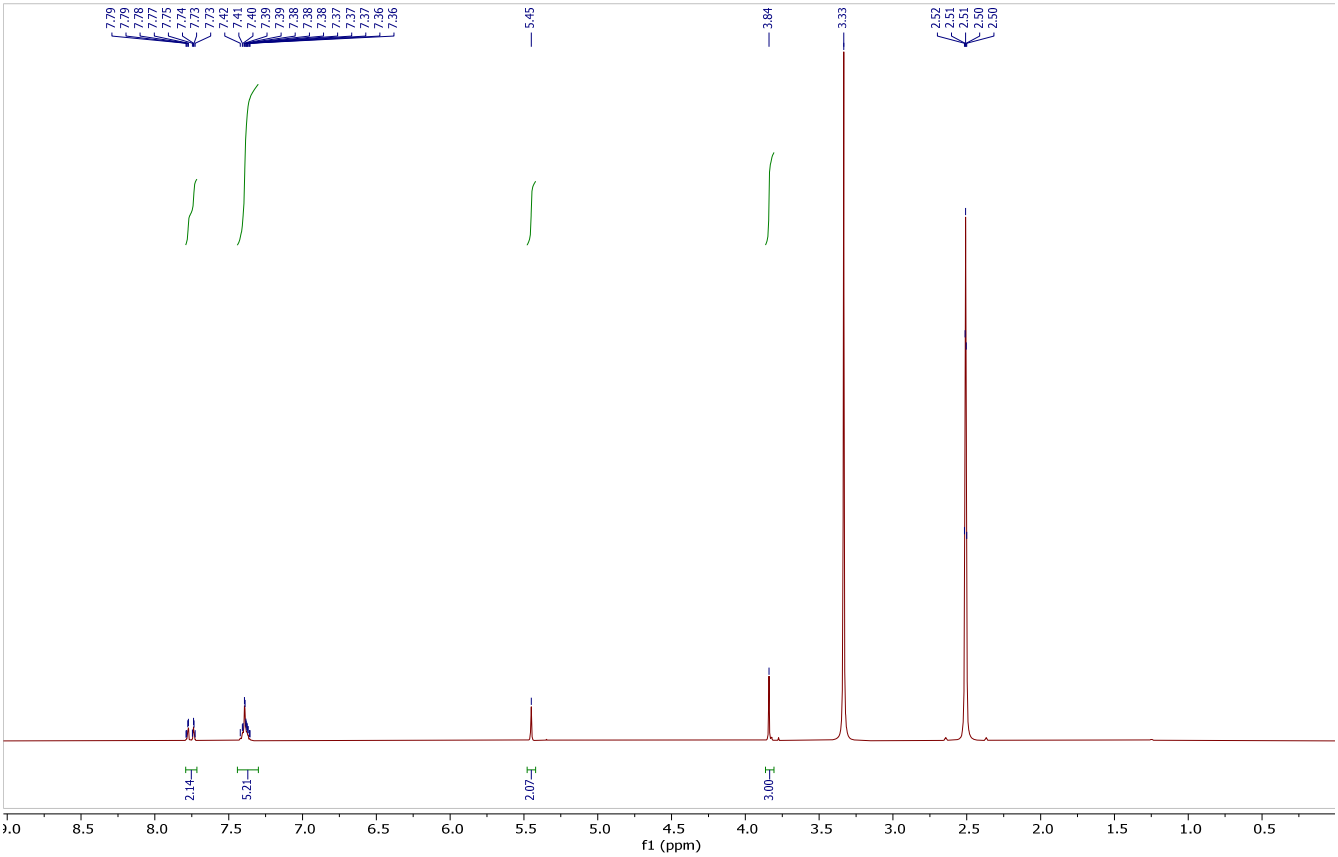


Figure S7. ^{1}H NMR of complex **6** in DMSO.

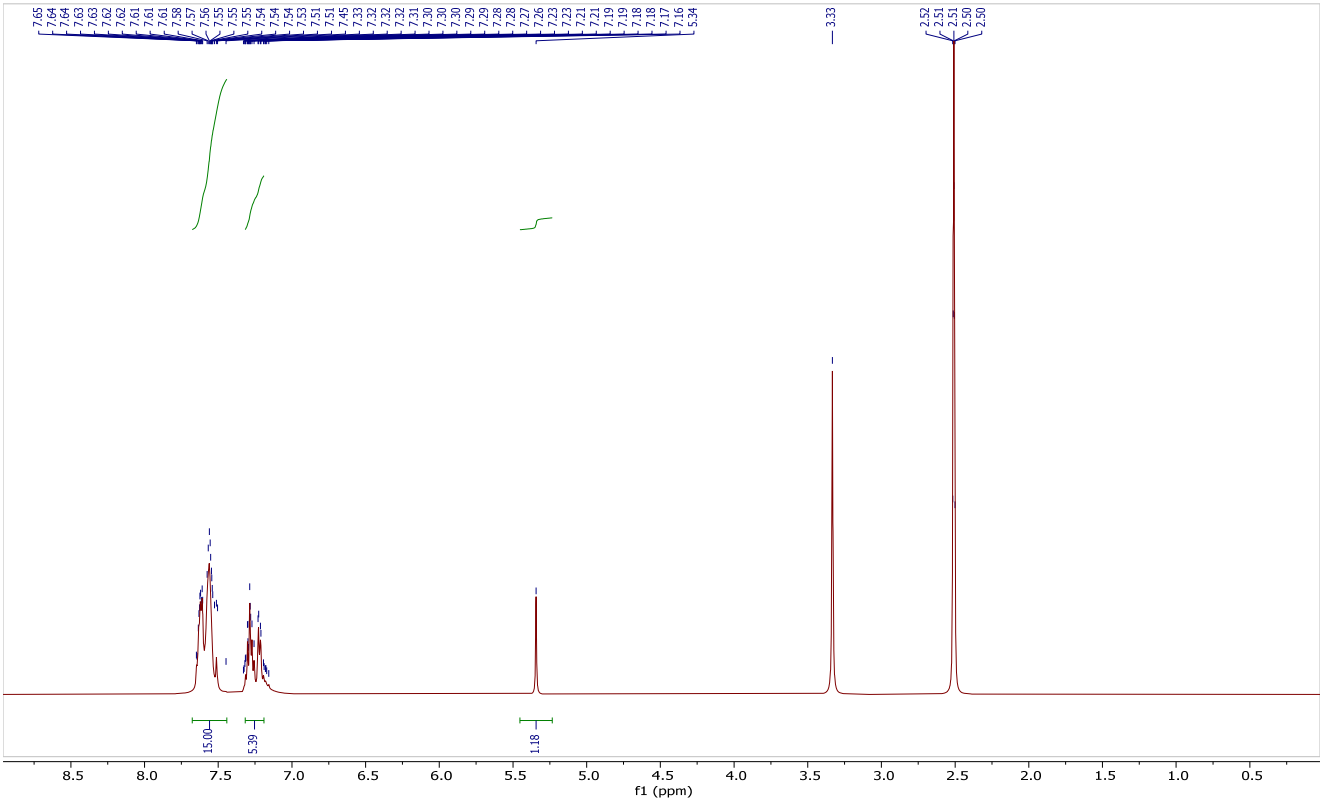


Figure S8. [1]H NMR of complex **7** in DMSO.

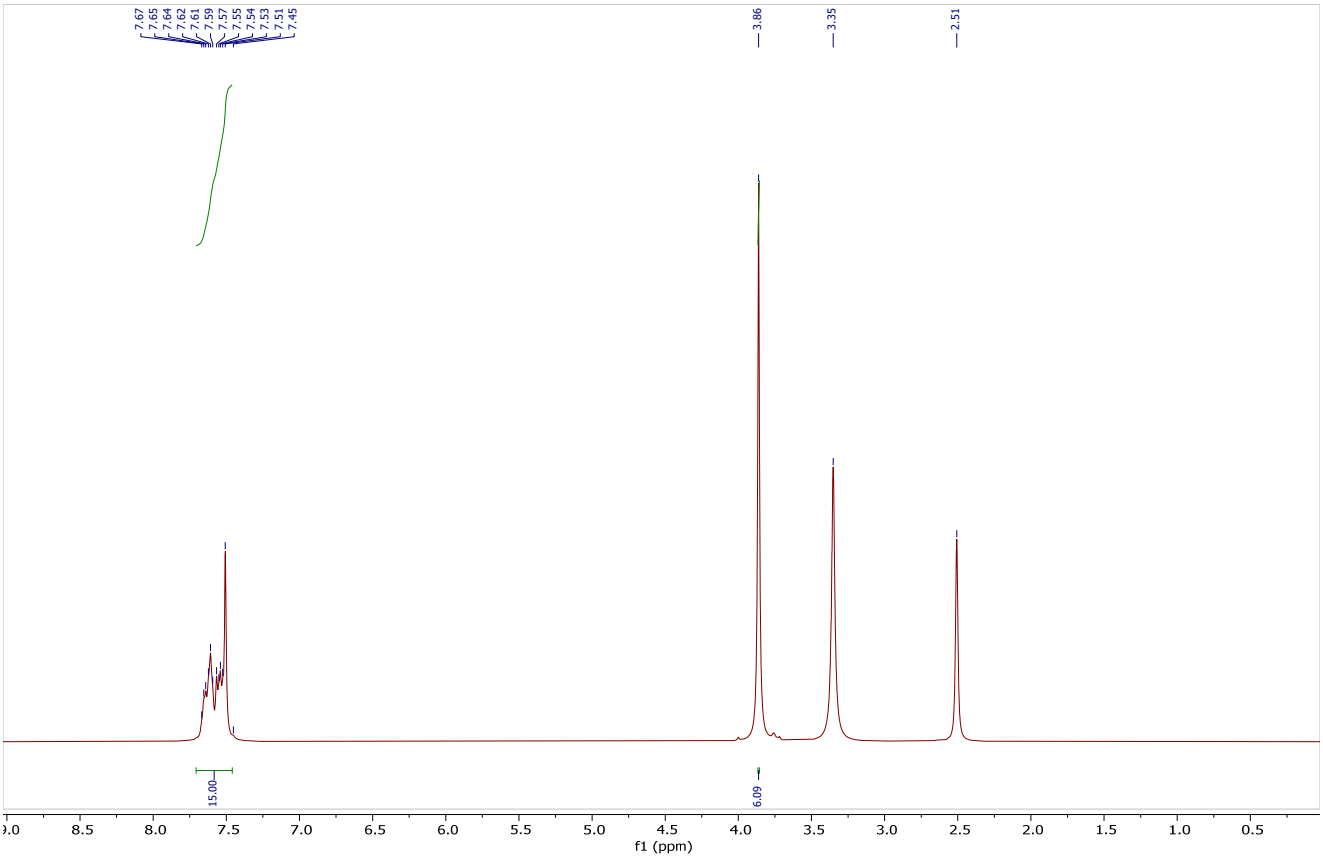


Figure S9. [1]H NMR of complex **8** in DMSO.

ESI MS spectra

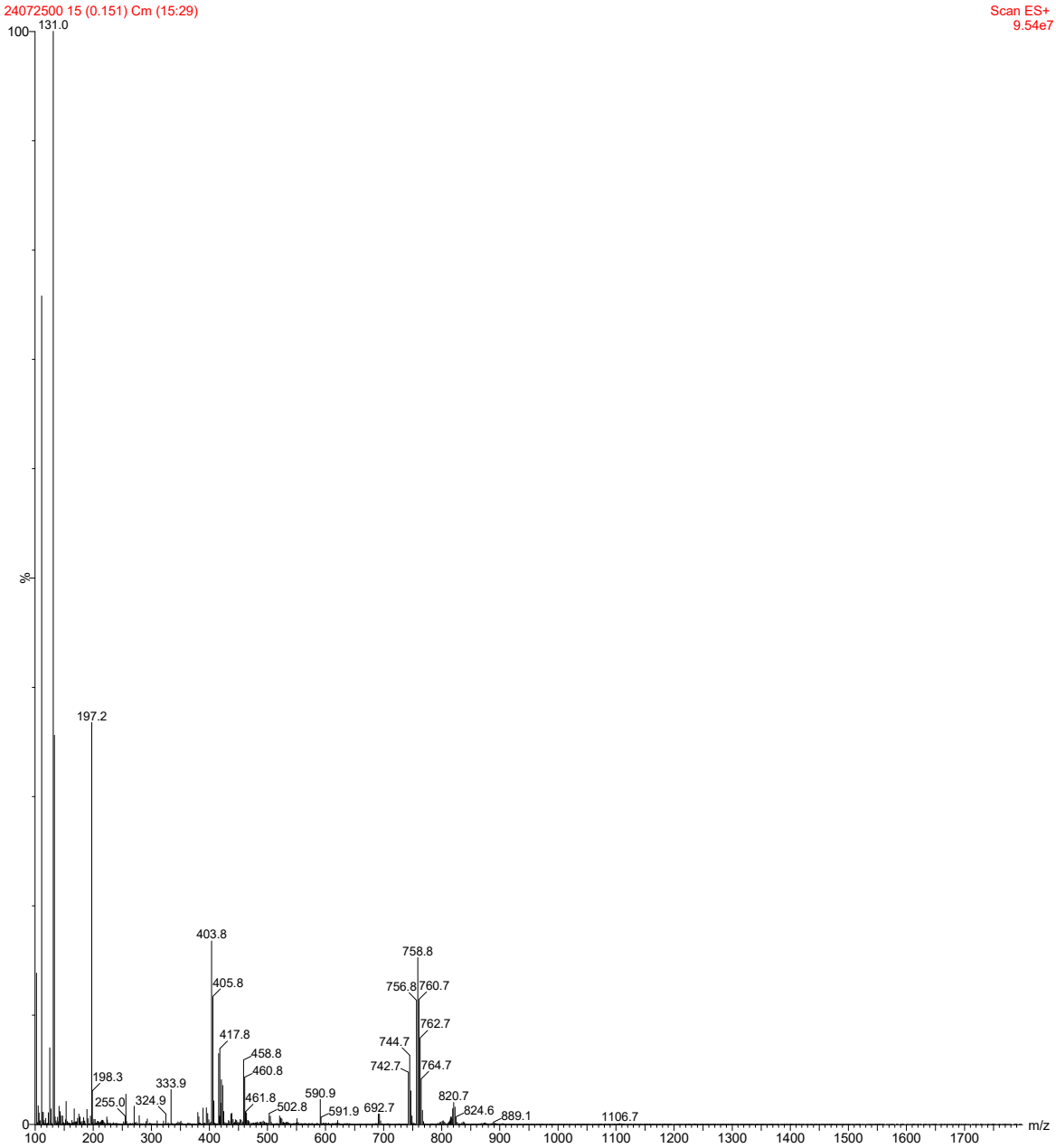


Figure S10. (+) ESI-MS spectrum for compound **1**. Relevant fragments at 334 m/z attributable to $[NHC^{Me}Au + CH_3CN]^+$, at 403.5 m/z attributable to $[NHC^{Me}\text{-}AuCl_3 - Cl + CH_3CN]^+$, at 460.13 m/z attributable to $[(NHC^{Me})_2AuCl_2]^+$.

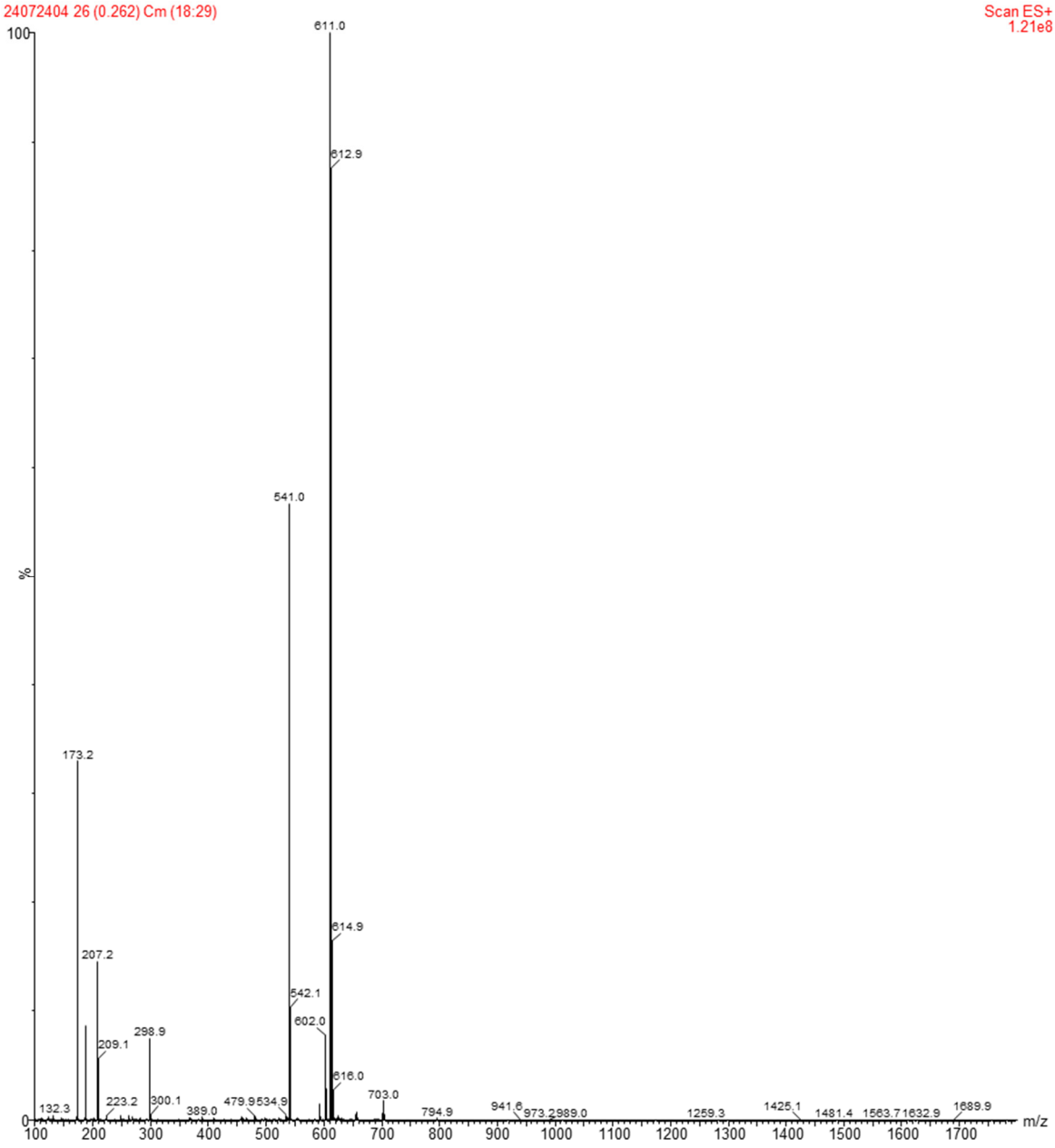


Figure S11. (+)ESI-MS spectrum for compound **2**. Relevant fragment at 541 m/z attributable to $[(NHC^{Bz})_2Au]^+$; 612 m/z attributable to $[(NHC^{Bz})_2AuCl_2]^+$.

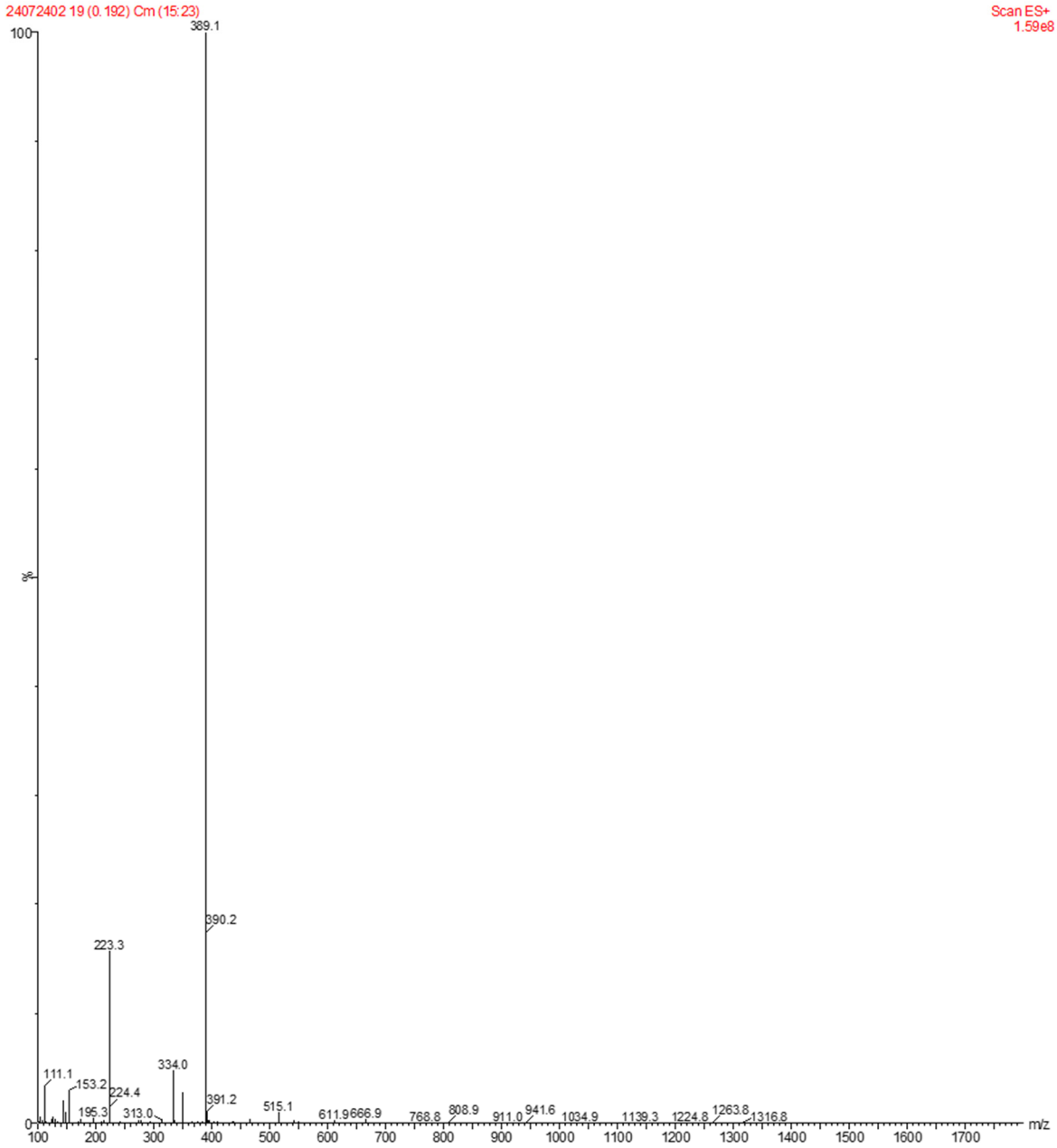


Figure S12. (+)ESI-MS spectrum for compound **3**. Relevant fragments at 389 m/z attributable to $[(NHC^{Me})_2Au]^+$.

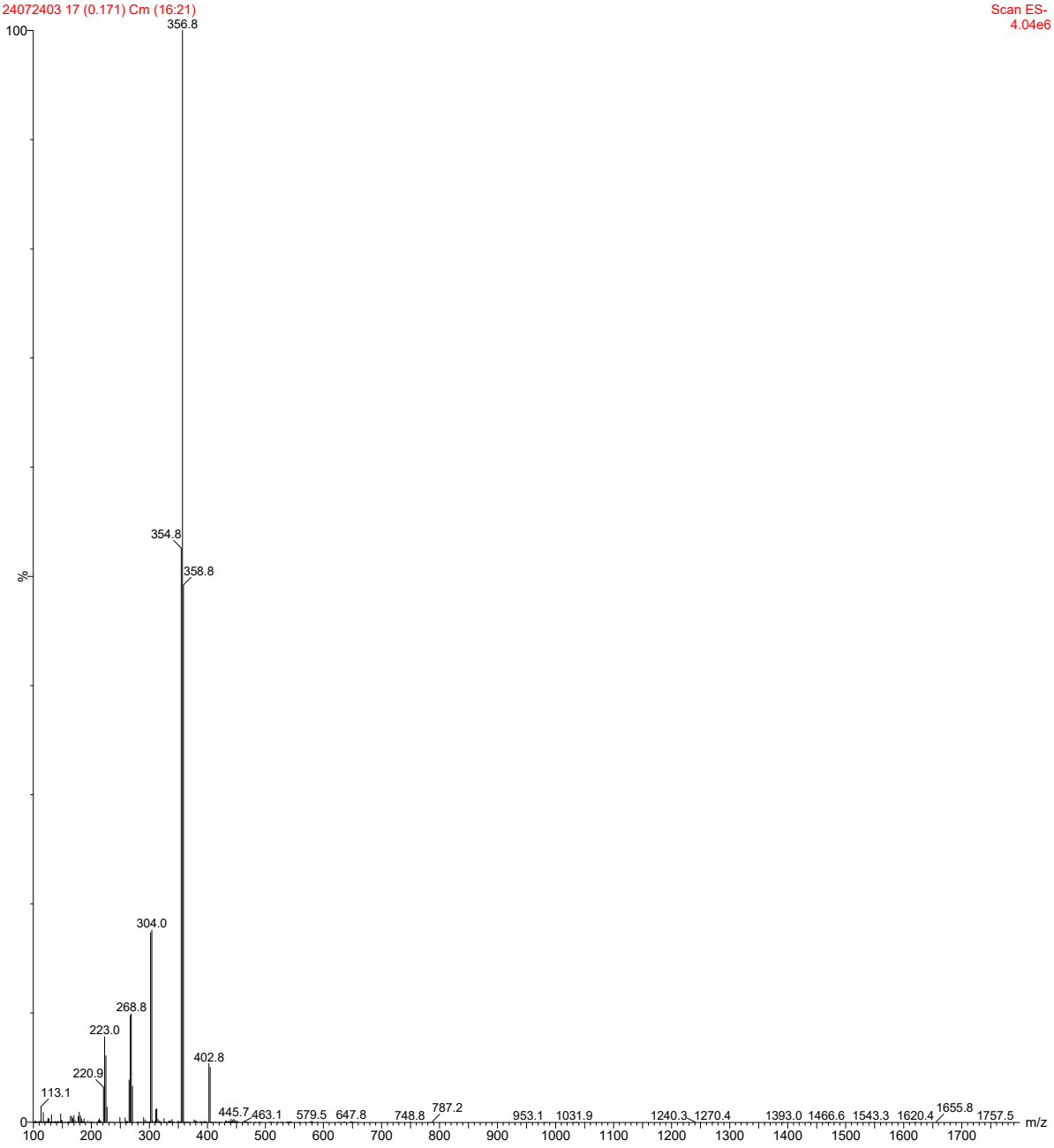


Figure S13. (-)ESI MS for compound **3**. Relevant fragment at 356.8 m/z attributable at $[AuBr_2]^-$.

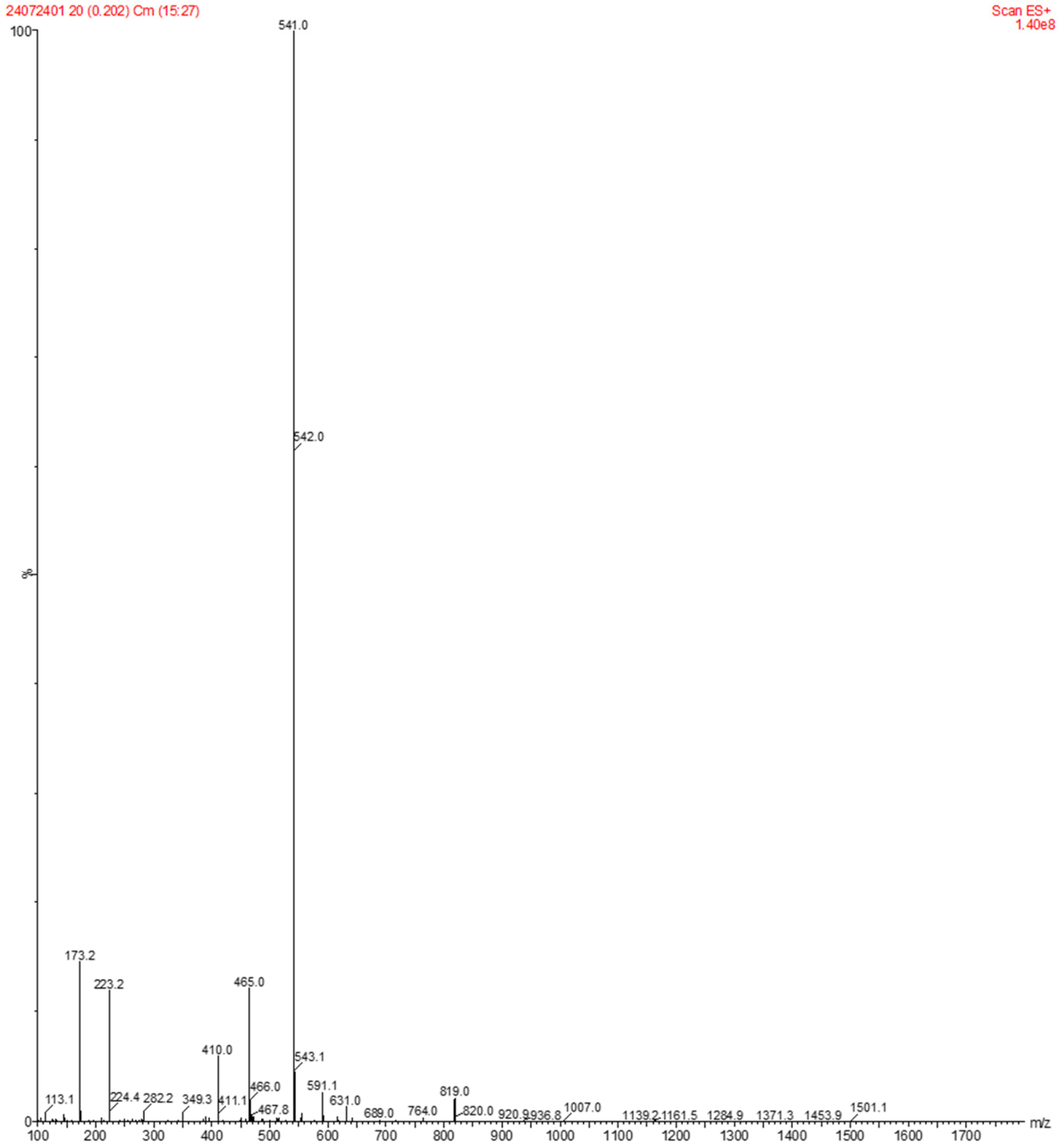


Figure S14. (+)ESI-MS spectrum for compound **4**. Relevant fragments at 541 m/z attributable to $[(NHC^{Bz})_2Au]^+$.

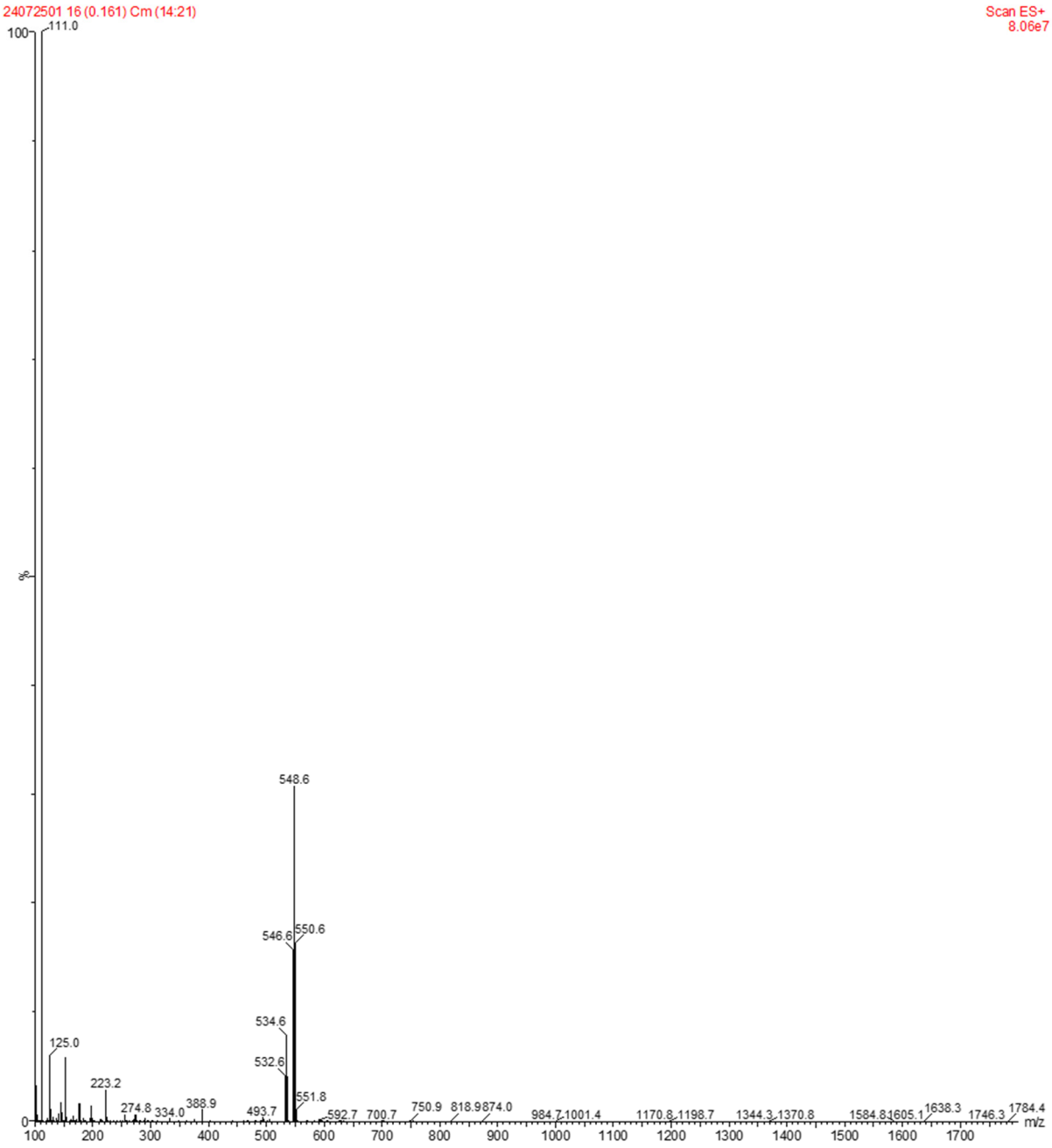


Figure S15. (+)ESI-MS spectrum for compound **5**. Relevant fragments at 549 m/z attributable to $[(NHC^{Me})_2AuBr_2]^+$.

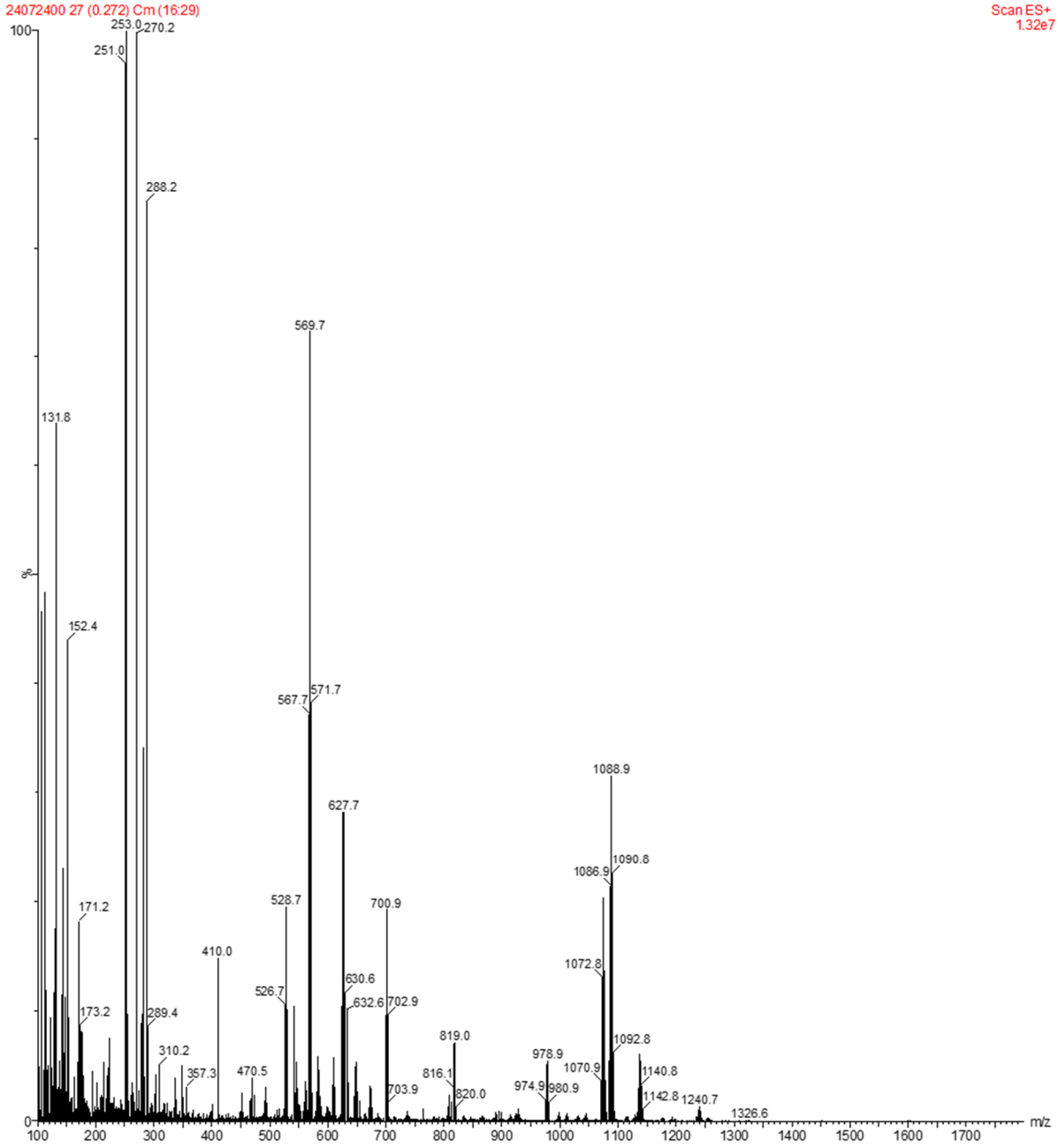


Figure S16. (+)ESI-MS spectrum for compound **6**. Relevant fragments at 528.7 m/z attributable to $[(NHC^{Bz})AuBr_2]^+$, and at 1072.6 m/z attributable to $[(NHC^{Bz})_2Au_2 + Br + 2CH_3CN]^+$.

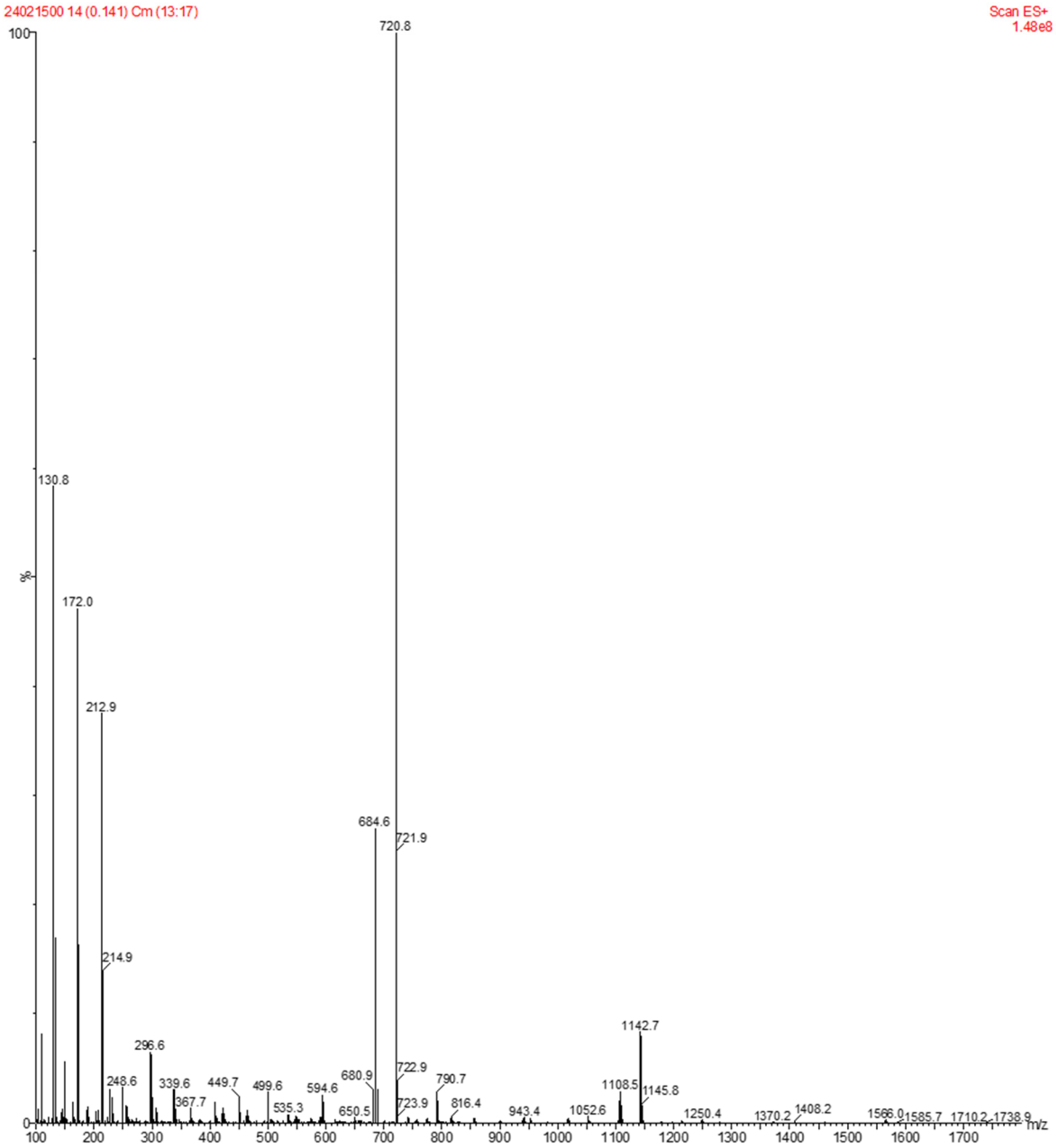


Figure S17. (+)ESI-MS spectrum for compound **7**. Relevant fragments at 684 m/z attributable to $[ImCl_2AuPPh_3]^+$ and at 721.8 m/z attributable to $[(PPh_3)_2Au]^+$.

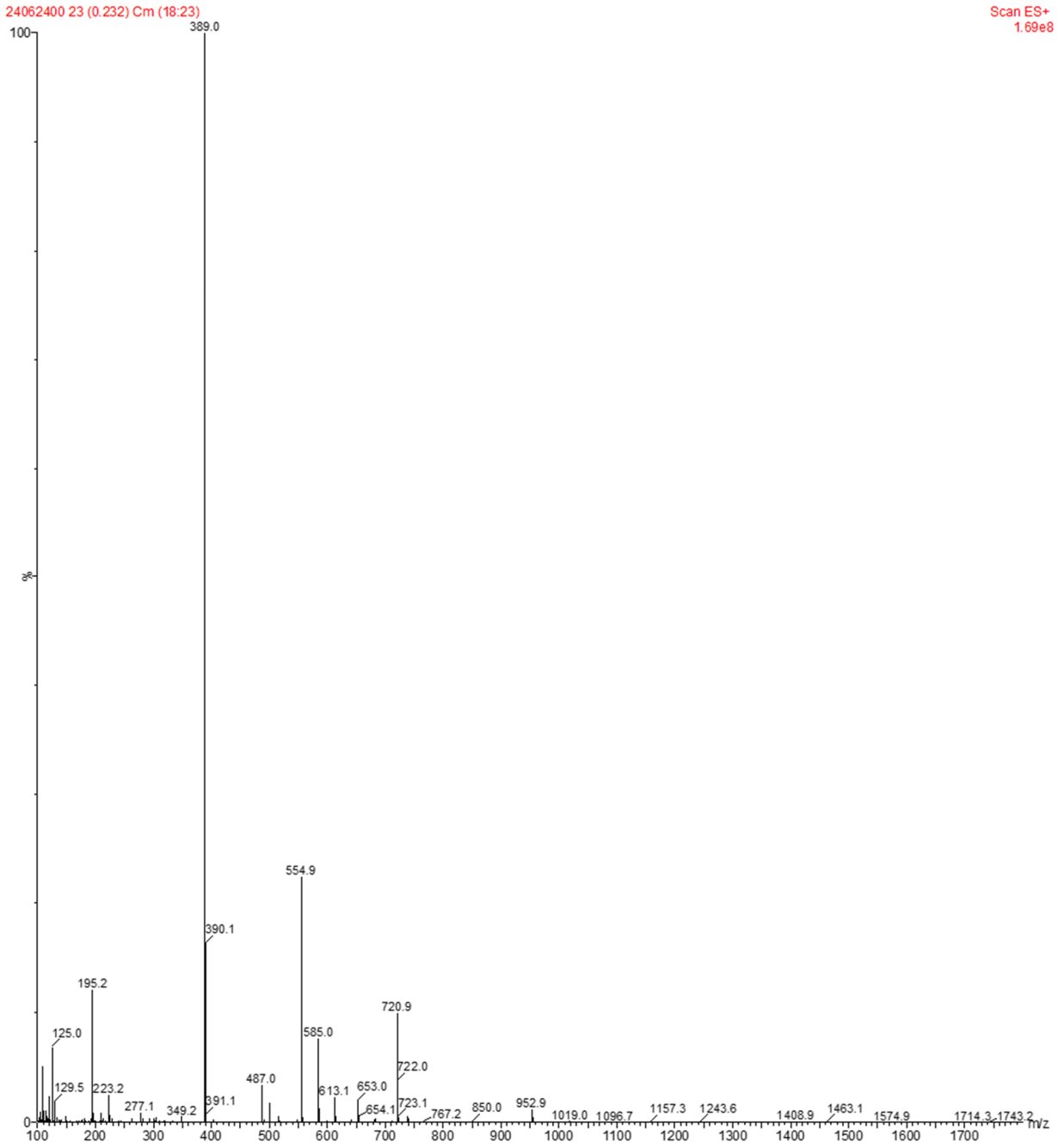


Figure S18. (+)ESI-MS spectrum for compound **8**. Relevant fragments at 554.9 m/z attributable to [NHC^{Me}-$AuPPh_3$]+ and at 721 m/z attributable to $[(PPh_3)_2Au]^+$.

Stability studies

The stability of the samples 1-8 in DMSO solution was assayed by UV-visible spectroscopy. Spectra were acquired using the Shimadzu UV-2700i spectrophotometer, equipped with the Shimadzu CPS-100 Peltier, at 293 K. Unless diversely specified, 100 μM DMSO solutions of the 1-8 compounds were prepared and spectra were acquired each 10 minutes for a total of 60 minutes. The spectra obtained are reported as following.

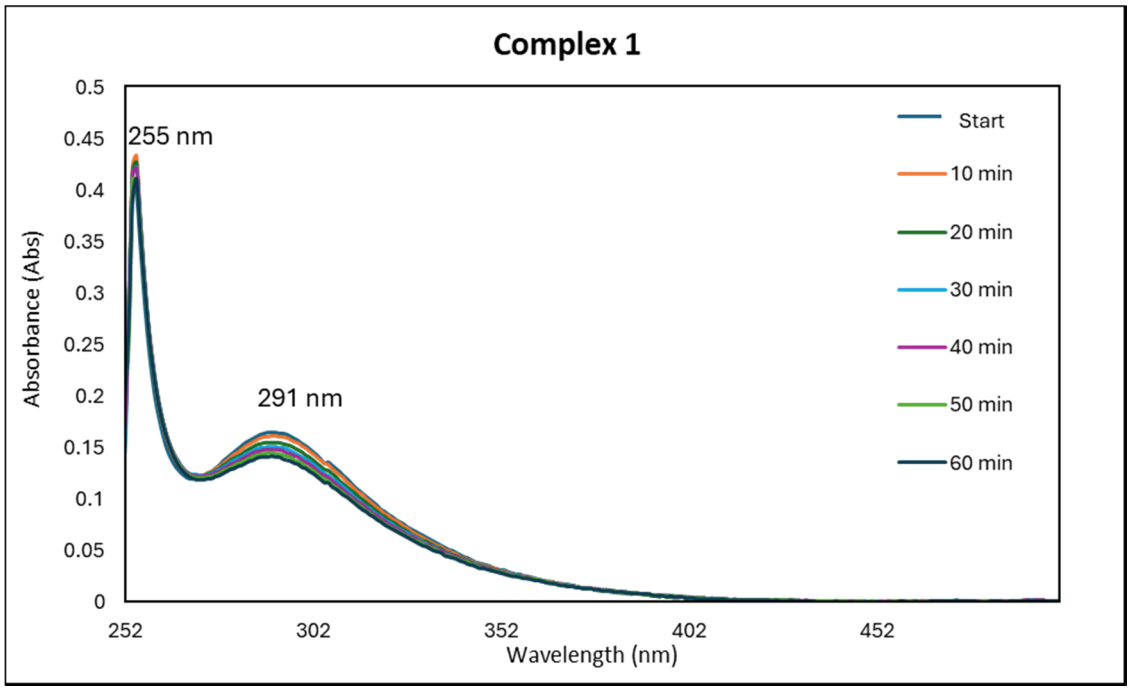


Figure S19. UV-Visible Spectra acquired for complex **1.**

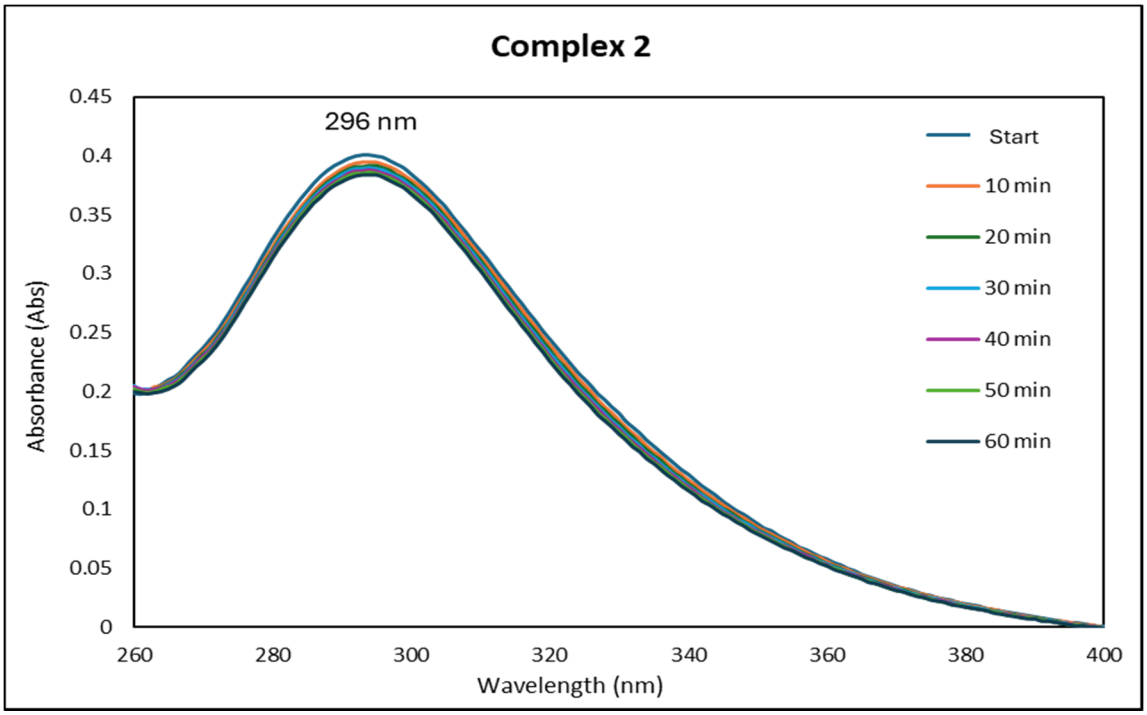


Figure S20. UV-Visible Spectra acquired for complex **2.**

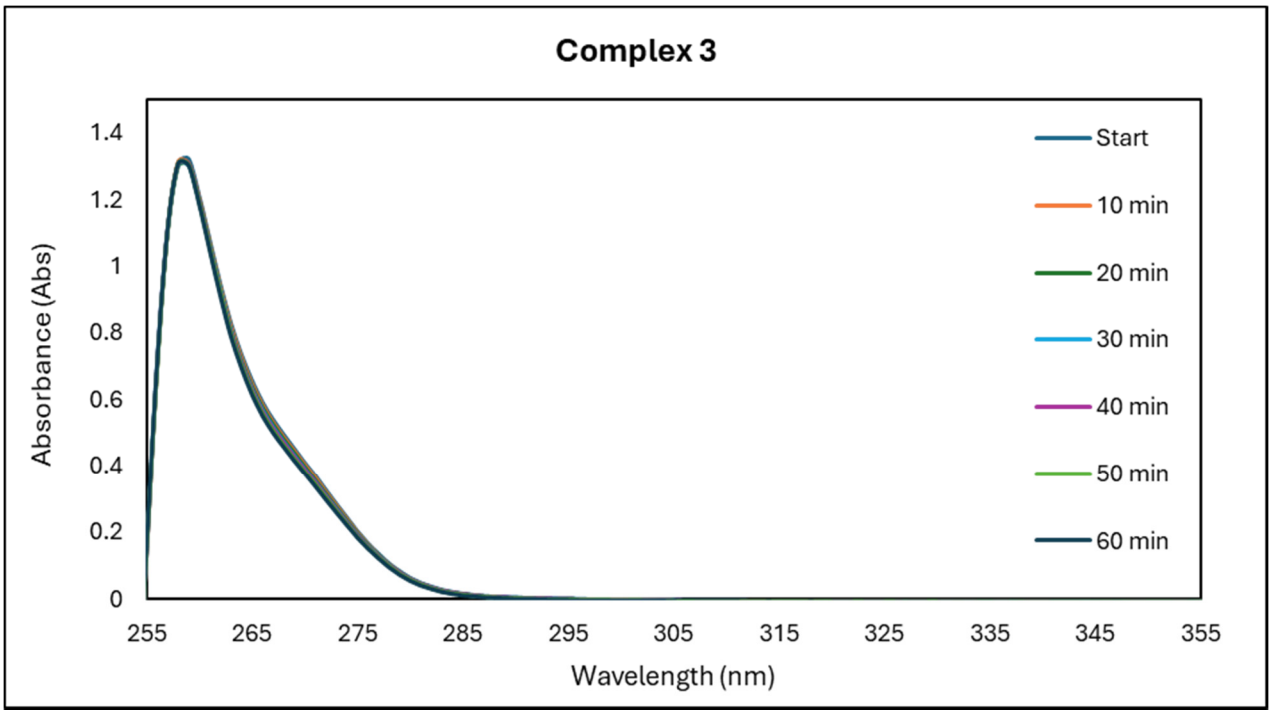


Figure S21. UV-Visible Spectra acquired for complex **3.**

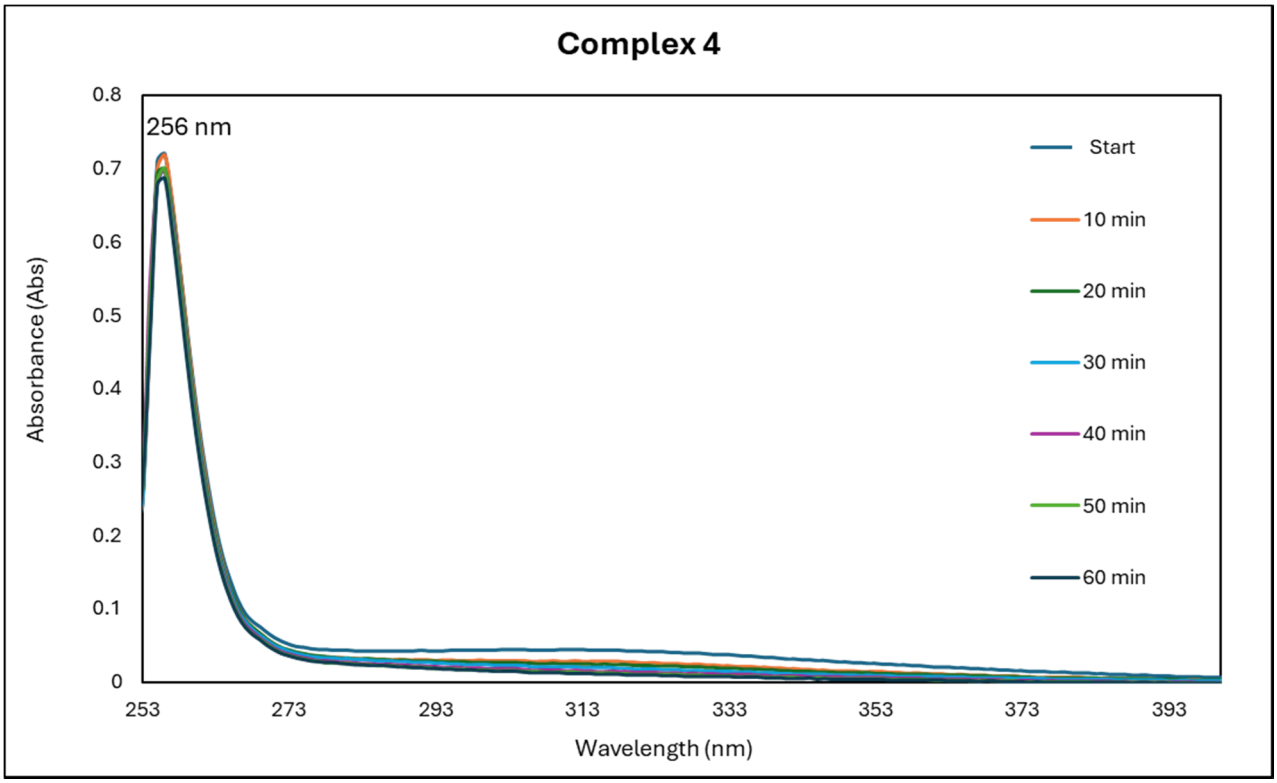


Figure S22. UV-Visible Spectra acquired for complex **4.**

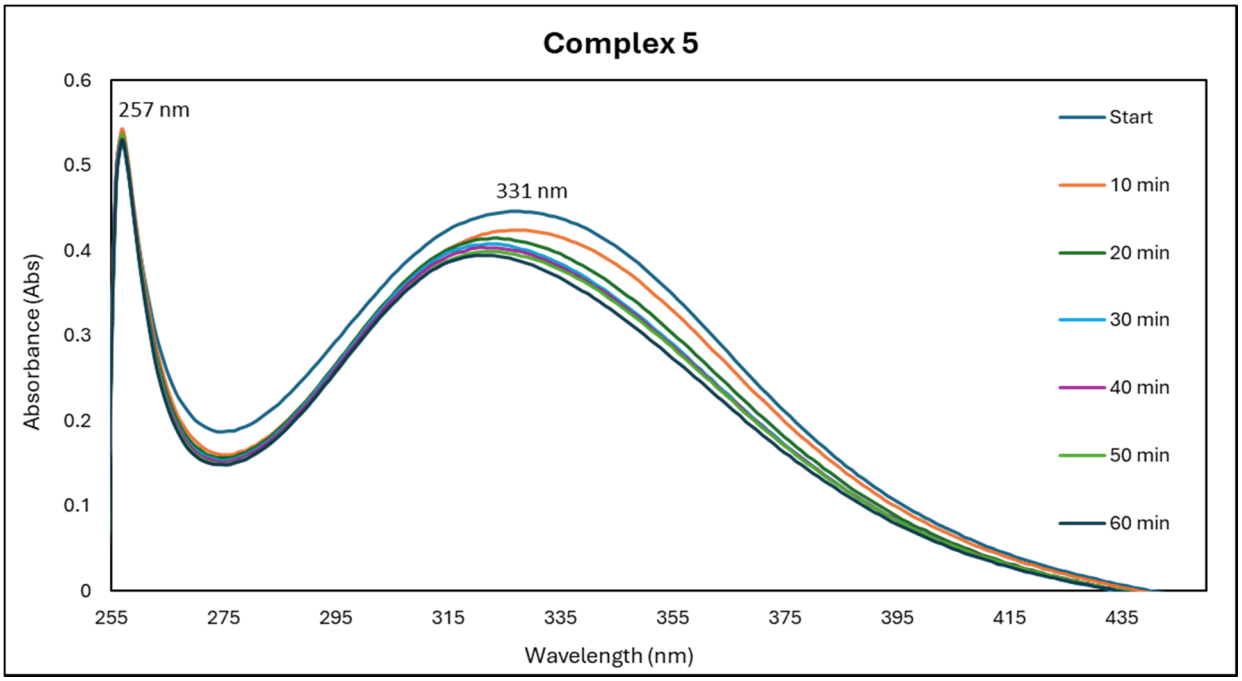


Figure S23. UV-Visible Spectra acquired for complex **5.**

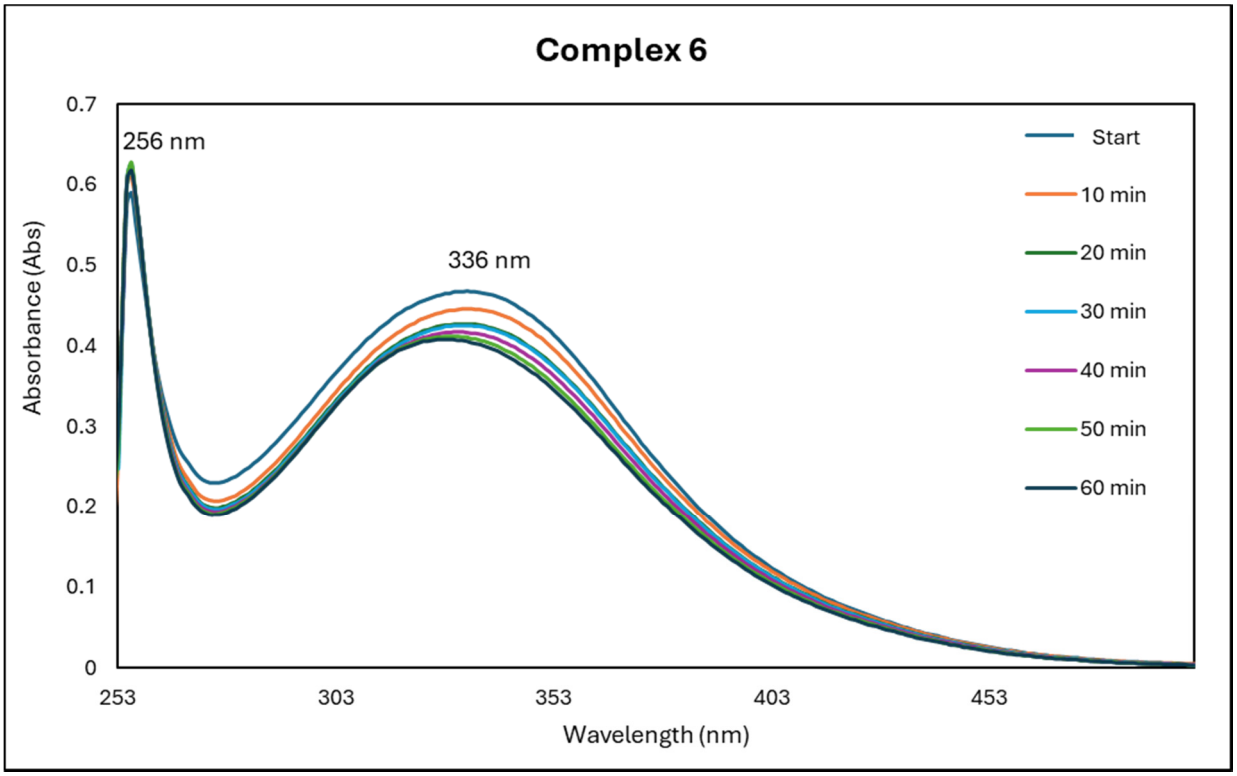


Figure S24. UV-Visible Spectra acquired for complex **6.**

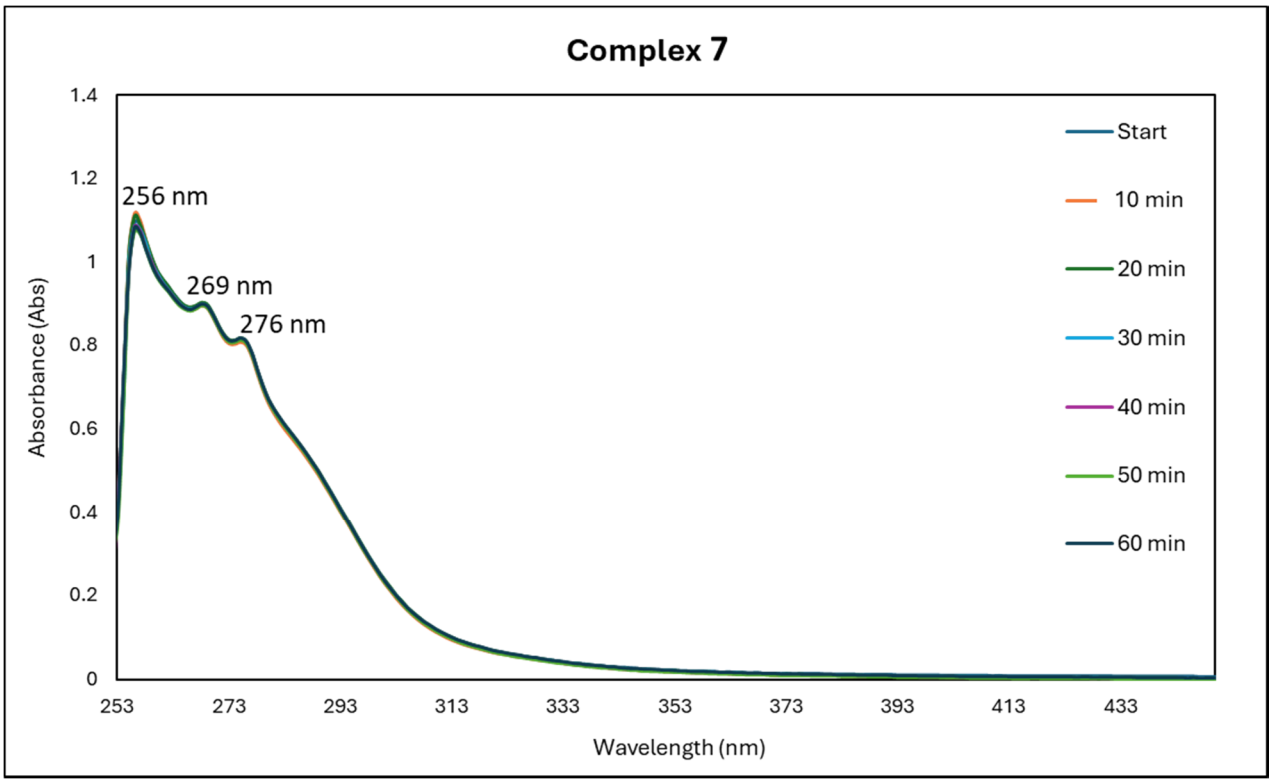


Figure S25. UV-Visible Spectra acquired for complex **7.**

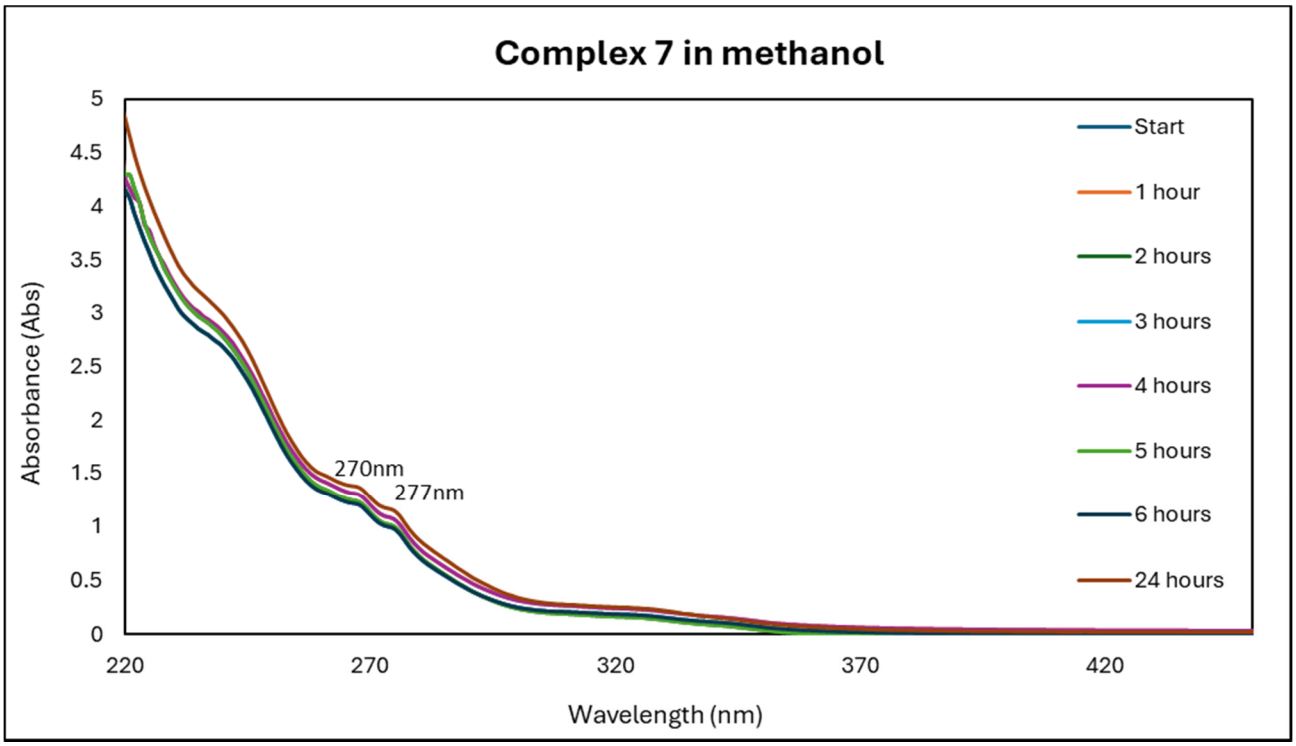


Figure S26. UV-Visible Spectra acquired in 24 hours in methanol for complex **7.**

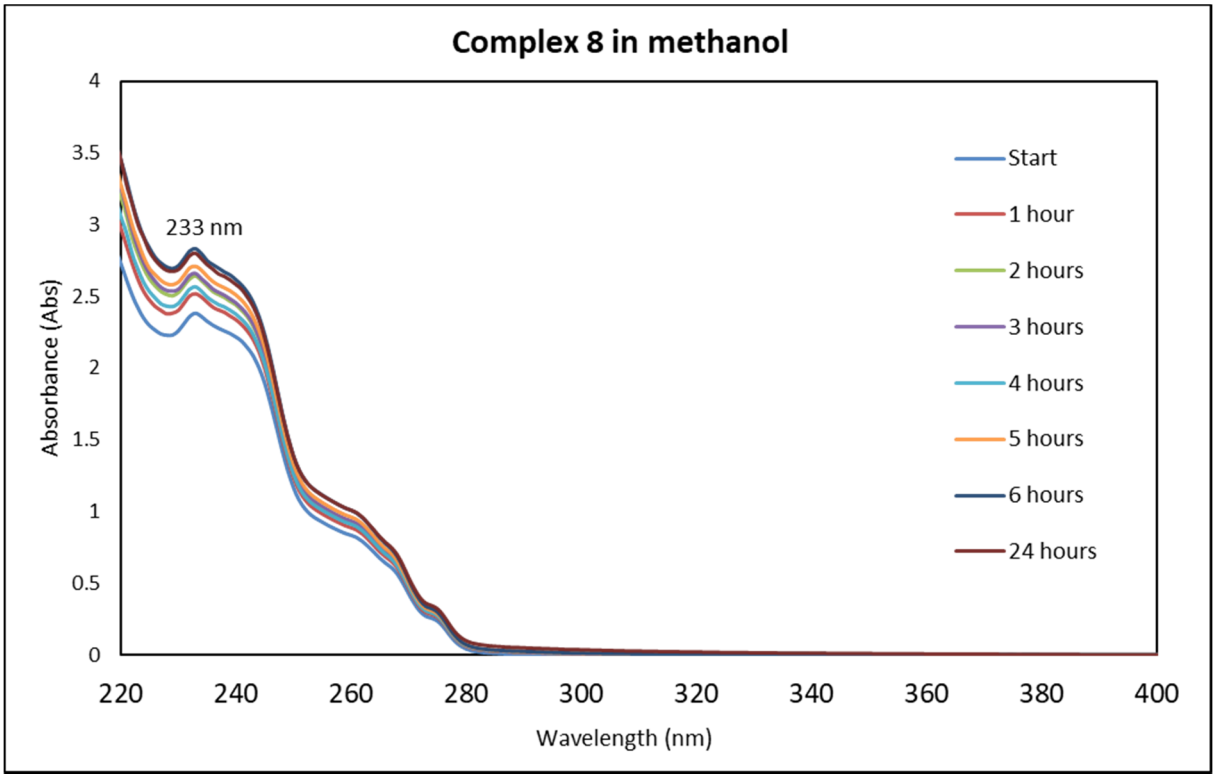


Figure S27. UV-Visible Spectra acquired in 24 hours in methanol for complex **8.**

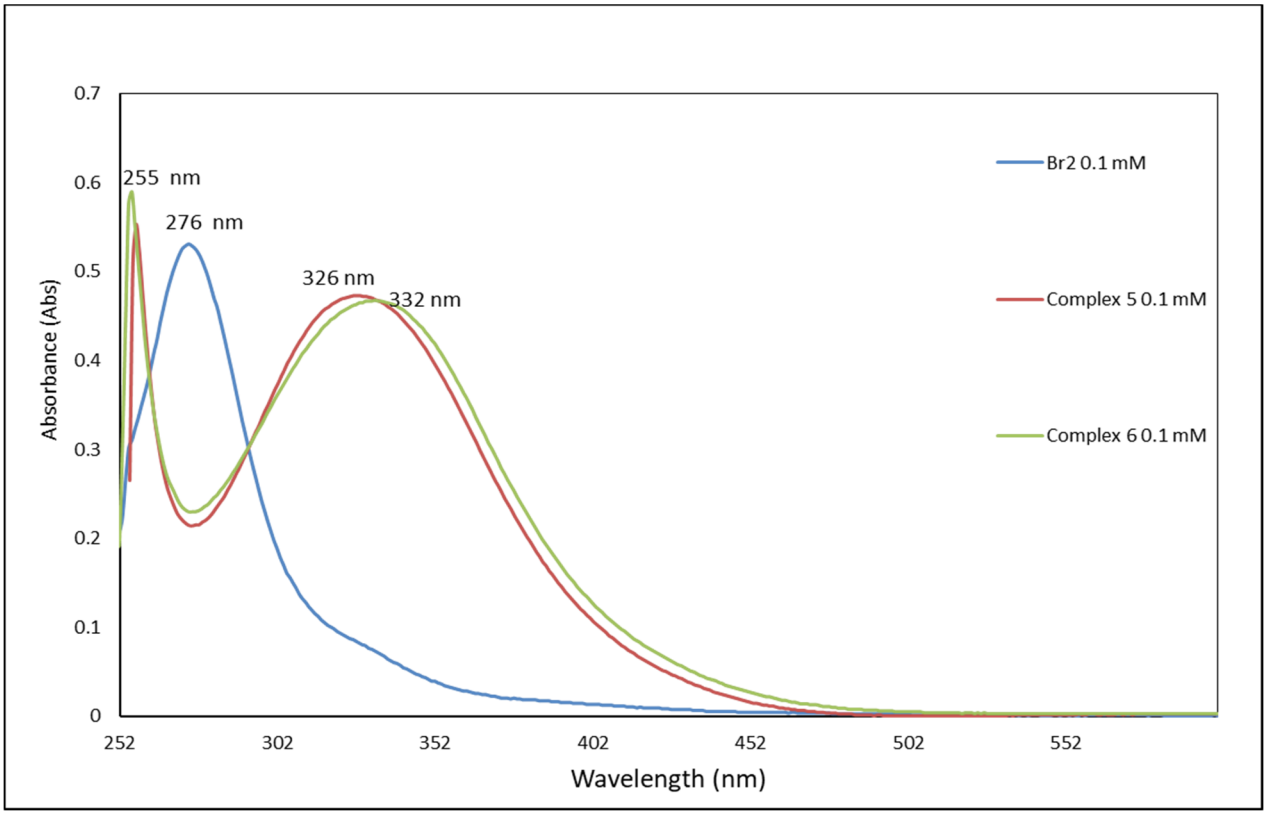


Figure S28. UV-visible spectra of 0.1 mM solutions of compounds 5 and 6 and of bromine in DMSO.

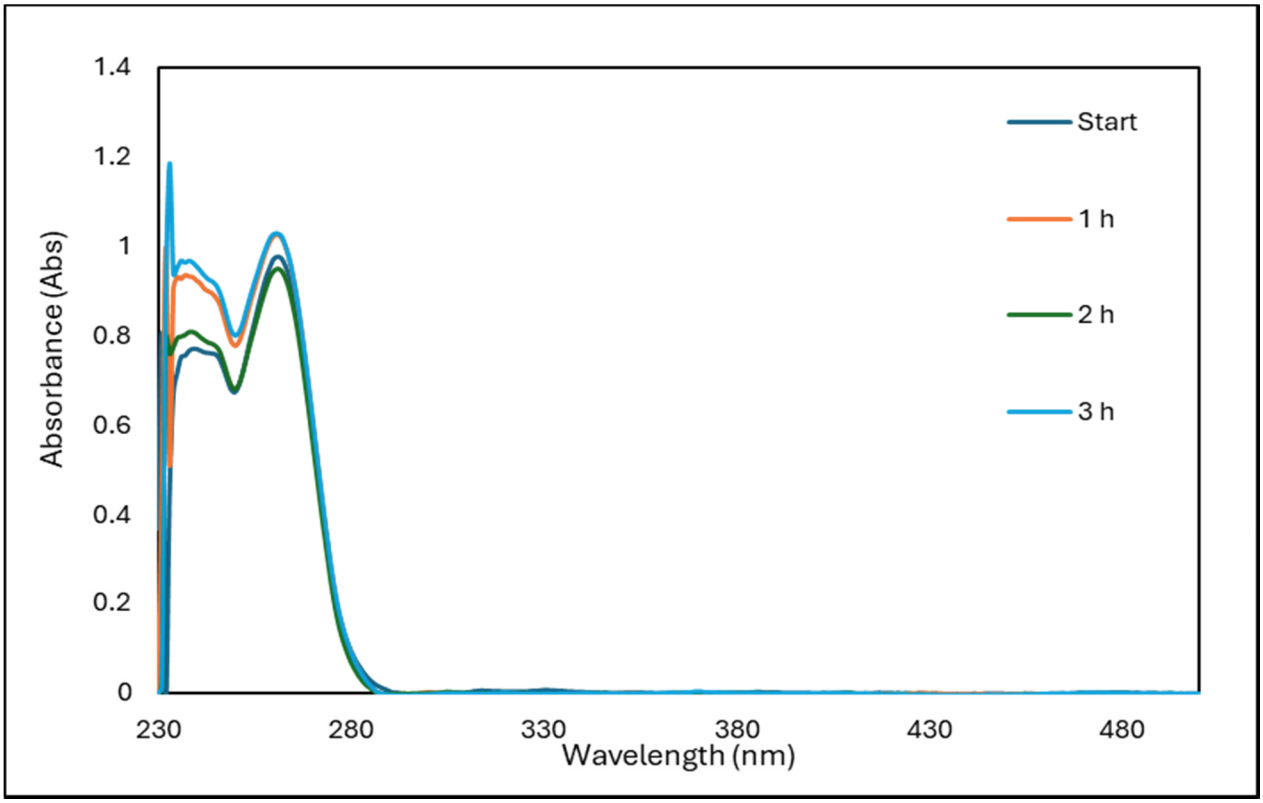


Figure S29. 1 mg of complex 8 was dissolved in 1 mL of DMSO (1.69 mM). The compound was diluted in a solution of phosphate buffer 10 mM (ca) at pH 7.4. UV-Visible spectra were recorded over 3h at 25°C.

Cell Lines Mutations data set

Table S1. Legenda of Table 2S.

Mutation Data	
NS	Nonsense substitution
MS	Missense substitution
Del-IF	Deletion - In frame
Del-FS	Deletion - Frameshift
Ins-IF	Insertion - In frame
Ins-FS	Insertion - Frameshift
Del-WG	Whole gene deletion
NS-ext	Nonstop extension
FS	Frameshift
SS	Splice Site Mutation
TSS	Translation Start Site Mutation
NSt	Nonstop Mutation
RNA	RNA Mutation
Som	somatic variant

Possibly som or Likely som	somatic in other cancers
Hom	Homozygous mutation
Het	Heterozygous mutation
Gazdar	Mutation reported by Adi Gazdar (Shigematsu Cancer Res (2005) 65:1642, Shigematsu JNCI (2005) 97:339, Yamamoto Cancer Res (2008) 68:6913)
NCI-Navy	Mutation reported in the original NCI-Navy paper (Phelps J Cell Biochem Suppl (1996) 24:32)
Genes likely involved in cancer (Cancer Gene Census, Sanger)	
Mutated	

Table S2. Lung cancer cell lines mutations data set.

Gene	A549	H157	H460	H1355	H1792	HCC44	H1395	H522	H661	H1993
TP53		[CAG to TAG (stop)](NCI-Navy)	WT	[c.853G>A; p.E285K; MS; hom; som; CLP](COSMIC-V73), [GAG to AAG(miss)](NCI-Navy)	[c.672+1G>A; p.?; hom; som; CLP](COSMIC-V73), [GT to AT(spl don)](NCI-Navy)	[c.128G>T; p.R43L; MS; hom; possibly som; CLP](COSMIC-V73), [c.245G>T; p.R82L; MS; hom; possibly som; CLP](COSMIC-V73), [c.281C>G; p.S94*; NS; hom; possibly som; CLP](COSMIC-V73), [c.524G>T; p.R175L; MS; hom; som; CLP](COSMIC-V73)	WT	[c.175delC; p.P59fs*>32; Del-FS; hom; pred neutral; som](COSMIC-V73), [c.292delC; p.P98fs*56; Del-FS; hom; pred neutral; som](COSMIC-V73), [c.571delC; p.P191fs*56; Del-FS; hom; pred neutral; som](COSMIC-V73), [c.572delC; p.P191fs*56; Del-FS; het; pred neutral; som; CLP](COSMIC-V73), [CCT to CT,?1bp](NCI-Navy)	[AGT to ATT](NCI-Navy), [c.194G>T; p.R65L; MS; het; possibly som; CLP](COSMIC-V73), [c.248G>T; p.S83I; MS; het; possibly som; CLP](COSMIC-V73), [c.365G>T; p.S122I; MS; het; possibly som; CLP](COSMIC-V73), [c.473G>T; p.R158L; MS; het; som; CLP](COSMIC-V73), [c.644G>T; p.S215I; MS; het; som; CLP](COSMIC-V73), [c.77G>T; p.R26L; MS; het; possibly som; CLP](COSMIC-V73)	[c.726C>G; p.C242W; MS; hom; som; CLP](COSMIC-V73), [TGC to TGG](NCI-Navy)
KRAS	[c.34G>A; p.G12S; MS; possibly som](COSMIC-V73), [Mut](Gazdar)	[12CGT](Gazdar), [c.34G>C; p.G12R; MS; som](COSMIC-V73)	[61CAT](Gazdar), [c.183A>T; p.Q61H; MS; som](COSMIC-V73)	[13TGC](Gazdar), [c.37G>T; p.G13C; MS; possibly som](COSMIC-V73)	[12TGT](Gazdar), [c.34G>T; p.G12C; MS; possibly som](COSMIC-V73)	[12TGT](Gazdar), [c.34G>T; p.G12C; MS; hom; som; CLP](COSMIC-V73)	WT	WT	WT	WT
RB1	WT					WT				WT
STK11	[c.109C>T; p.Q37 stop](Gazdar), [c.109C>T; p.Q37*; NS; possibly	[c.ex 2,3 del; p.E98-G155 del., stop at normal but trancated](Gazdar)	[c.109C>T; p.Q37*; NS; hom; possibly som](COSMIC-V73)	[c.143-4 AG>T; p.K48I (fs), stop at 50 aa](Gazdar)	WT		[c.156-169 1G del.; p.E57K (fs), stop at 63 aa](Gazdar), [c.169delG; p.E57fs*7; Del-FS; hom;	WT	WT	[c.595 G>T; p.E199 stop](Gazdar), [c.595G>T; p.E199*; NS; hom; som;

	som](COSMIC-V73)						pred neutral; possibly som](COSMIC-V73)			CLP](COSMIC-V73)
CDKN2A	[c.1_471del471; p.0?; Del-WG; hom; possibly som](COSMIC-V73)	[c.205G>T; p.E69*; NS; hom; possibly som](COSMIC-V73)	WT		[c.330G>A; p.W110*; NS; het; pred neutral; som; CLP](COSMIC-V73)	[c.457+1G>T; p.?; possibly som](COSMIC-V73)				
EGFR	WT	WT	WT		WT	WT	WT	WT	WT	WT
PIK3CA	WT	WT	[c.1633G>A; p.E545K; MS; het; possibly som](COSMIC-V73), [E545K](Gazdar)	WT	WT	WT	WT	WT	WT	WT
PTEN	WT	[c.751G>T; p.G251C; MS; possibly som](COSMIC-V73)	WT					WT		
SMARCA4	[c.2184_2206del23; p.Q729fs*4; Del-FS; hom; pred neutral; possibly som](COSMIC-V73)	WT			WT	WT	[c.809_810delCC; p.P270fs*16; Del-FS; hom; pred neutral; som](COSMIC-V73)			
BRAF	WT	WT	WT	WT	WT	WT	[c.1406G>C; p.G469A; MS; hom; possibly som](COSMIC-V73), [G468A](Gazdar)	WT	WT	WT
NRAS	WT	WT	WT	WT	WT		WT	WT	WT	WT
KDR	WT		[c.3910G>T; p.G1304C; MS; het; som](COSMIC-V73)	WT	WT					
MLL2								WT		
CTNNB1	WT	WT	WT		WT	WT	WT	WT	WT	WT
ATM	WT					WT	[c.7996A>G; p.T2666A; MS; hom; som](COSMIC-V73)			
CREBBP					WT		WT			
NFE2L2	WT									
EP300							WT		WT	WT
NTRK3				WT			WT			WT
PDGFRA							WT			WT
NOTCH2	WT			WT			WT			
APC										
MYH11			[c.2271C>A; p.D757E; MS; het; som](COSMIC-V73), [c.2292C>A; p.D764E; MS; het; som](COSMIC-V73)	WT	WT					
TPR							WT			WT
FUBP1							WT		WT	
WHSC1						WT	WT			
MSH2	[c.965G>A; p.G322D; MS; possibly	WT	WT	[c.1054G>C; p.D352H; MS; het;						

	som](COSMIC-V73)			som](COSMIC-V73)						
ARID1A			[c.6403_6408delATTCTG; p.I2135_L2136del; Del-IF; het; pred neutral; som](COSMIC-V73)	WT	WT					
TNFAIP3			[c.406C>T; p.R136C; MS; het; som](COSMIC-V73)	WT						
U2AF1					WT					
HLF							WT		WT	
KDM6A	WT	WT	WT	WT	WT		WT	WT	WT	WT
SF3B1		WT		WT	WT		WT		WT	WT
HRAS	WT	WT	WT	WT	WT		WT	WT	WT	WT
VHL		WT	WT		WT		WT	WT	WT	WT
MLL3	WT					WT				WT
CARD11				WT			WT		WT	
ROS1							WT			
KIAA1549						WT				WT
MYH9							WT			
PRDM16					[c.1574G>A; p.R525Q; MS; het; possibly som; CLP](COSMIC-V73)	WT		WT		
IKZF1							WT		WT	
NUP214			WT			WT	[c.4738G>T; p.E1580*; NS; het; som](COSMIC-V73)			
CBLB							WT			
PIK3R1	WT		WT				WT	WT		
RET						WT	WT	WT		WT
FBXW7			WT				WT			
NOTCH1	WT			WT			WT		WT	
GNAS							WT			
NUMA1							WT			
DNMT3A							WT			
RAD21			[c.353A>T; p.D118V; MS; het; som](COSMIC-V73)	WT						
CDH1							WT			
ARID2			WT	WT				WT		
RALGDS							WT			
POT1							WT			
GOLGA5			[c.595A>G; p.K199E; MS; het; som](COSMIC-V73)	WT		WT				
NACA				WT			WT			
RAF1							WT			
GPC3							[c.490G>C; p.D164H; MS; hom; som](COSMIC-V73)			
BCOR				[c.377C>T; p.P126L; MS; hom; possibly som; CLP](COSMIC-V73)	WT	[c.2266G>T; p.E756*; NS; hom; som](COSMIC-V73)				
ZNF521							WT		WT	

SETD2							WT			
PML							WT			
PALB2							WT			
RNF43										
ERBB2	WT	WT	WT	WT	WT	WT	WT	WT	WT	WT
EML4	WT	WT	WT	WT	WT	WT	WT		WT	WT
MAX	WT		WT			WT	WT	WT	WT	WT
NF2		WT	WT		WT		WT	WT	WT	WT
TRRAP					WT		WT			
MET	WT		WT				WT	WT		WT
MAP2K1	WT				WT		WT	WT		WT
PTPRC							WT			
ARHGEF12	WT		WT				WT			
HIP1	[c.830G>A; p.S277N; MS; het; som](COSMIC-V73)			WT						
FANCD2							WT			
NUP98					WT		WT			
PDGFRB							WT			
KDM5A							WT			
WRN							WT			
TSHR			WT			WT				WT
PDE4DIP			WT				WT		WT	
MEN1										
FGFR2						WT	WT			
USP6							WT			WT
CDH11			WT				WT	WT	WT	
CBLC							WT			
TRIP11	WT						WT	[c.3083G>A; p.R1028Q; MS; het; som](COSMIC-V73)	WT	
ATRX							WT		WT	WT
PICALM							WT	WT		WT
ETV1						WT	WT		WT	
LRIG3					WT		WT			
MLH1					[c.52C>T; p.R18C; MS; het; possibly som; CLP](COSMIC-V73)	WT				
NSD1										
ABL2						WT	WT			
XPO1							WT			
DICER1							WT			
TCF12							WT			
NTRK1							WT			
PPP2R1A	WT		[c.192G>T; p.E64D; MS; hom; som](COSMIC-V73)	WT						
LIFR			[c.1477C>T; p.L493F; MS; het; pred neutral; som](COSMIC-V73)	WT	WT					
TRIM33							WT			
TCEA1							WT			
BUB1B							WT		WT	WT
LCP1							WT	[c.1412C>A; p.A471E; MS; hom; som](COSMIC-V73)		
COL1A1							WT		WT	
PTPN11							WT			
EBF1										
ITK							WT			

IDH1						WT	WT		
ATIC					WT	WT			
NCOA2					WT	WT			
ELN				WT				WT	
TRAF7						WT			
SUZ12						WT			
MYB						WT			
BRIP1						WT			
FBXO11						WT			
NCOA1						WT			
FOXP1					WT	WT			
MAP2K4						WT			
ATP2B3					WT	WT			
LPP						WT			
TERT	WT					WT			
MSH6						WT			
EZH2			WT			WT			
THRAP3						WT		WT	
KDM5C						WT			
STAT5B						WT			
FGFR3				WT		WT			
MLLT3						WT		WT	
PCSK7						WT	WT		
TMPRSS2						WT			
ERG						WT			
MLLT1						WT			
PBRM1									
IL7R									
RUNX1					WT	WT			
EIF4A2						WT			
GMPS						WT			
BMPR1A						WT			
FH	[c.1391G>T; p.G464V; MS; het; som](COSMIC-V73)			WT					
BCL3						WT			
EXT1						WT			
CAMTA1									
FANCC				WT		WT			
MLF1						WT			
ETV4						WT			
GATA2						WT			
WIF1						WT			
HOOK3									
HNRNPA2B1					WT			WT	
ELF4						WT			
SUFU	[c.1232C>T; p.T411M; MS; het; possibly som; CLP](COSMIC-V73)			WT					
PDGFB						WT			
RARA						WT			
DDX5						WT			
LHFP						WT			
TSC1									
CCND1						WT			
SOCS1						WT			
NR4A3									
CDC73									
C15orf55			[c.1001C>A; p.P334Q; MS; hom; som](COSMIC-V73)	WT					
TET2									
FAM46C									
SDC4									
SETBP1	WT		WT	WT	WT	WT	WT	WT	WT
AKT1	WT	WT	WT		WT	WT	WT	WT	

FCGR2B											WT					
CLTCL1					WT						WT					
AKAP9							WT				WT			WT		
FANCA											WT					WT
MAP2K2	WT			WT			WT				WT		WT			WT
KTN1											WT		WT			
NF1				WT	WT						WT					
ALK											WT					
MLLT4											WT					
SMARCB1	WT		WT								WT					
CARS											WT					WT
BCR										WT	WT					
PCM1																
PER1											WT					
JAK2											WT					WT
BRCA2											WT		WT			
CBFA2T3										WT	WT					WT
NFIB										WT	WT					
GPHN											WT					
TSC2				WT												
DDX10											WT					
GAS7				WT							WT					
AXIN1										WT	WT					
ERCC2					WT						WT			WT		
CHN1										WT	WT					
FLT3											WT					
WHSC1L1											WT			WT		
EPS15					WT						WT		WT	WT		
KIT											WT					WT
ERCC3					WT						WT					
CACNA1D	WT													WT		
SRGAP3											WT					
CHEK2	WT			WT							WT			WT		
BLM											WT					
MED12	WT										WT					
RANBP17					WT											WT
TCF3	WT			WT							WT					
TOP1					WT						WT					
BCL6				WT							WT					
PBX1											WT					
STAG2											WT					
BCL11A											WT					
PMS2											WT					
PAX5											WT					
NPM1											WT					
NIN											WT					
CIITA											WT					
BRCA1											WT					
STAT3											WT					
BRD4					WT						WT					WT
MLLT10					WT						WT					
ARNT											WT					
PMS1				WT							WT					
CLTC					WT						WT					WT
ETV6											WT					WT
FIP1L1											WT					
ERCC5											WT					
MLL																
JAK3					WT						WT					
ABL1											WT					
SYK											WT		WT			
CNOT3																
MDM4	WT										WT					
ERCC4											WT					
CDKN2C	WT										WT					
DDX6											WT					WT
BCL9					WT						WT					
BRD3											WT					
IRF4											WT					
IL6ST											WT					
TFRC											WT					
SH3GL1											WT					

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SS18L1			WT	
TTL			WT	
SS18			WT	
PAFAH1B2			WT	
CCND2			WT	
PHF6			WT	
TFG			WT	
CDK4	WT	WT	WT	
CD274			WT	
CCDC6			WT	
XPA		WT	WT	
SDHC			WT	
HEY1			WT	
BCL2			WT	
FANCG			WT	
CBFB			WT	
RPN1			WT	
HOXA11			WT	
TFEB			WT	
TAL1			WT	
ELK4			WT	
HOXD13			WT	
RPL22			WT	
TFE3			WT	
DNM2				WT
MYCN			WT	
RBM15			WT	
TLX3			WT	
KLF4			WT	
PLAG1			WT	
NT5C2				
REL			WT	WT
FOXA1			WT	
LMO1			WT	
GATA1			WT	
BCL10			WT	
FANCF			WT	
SDHB			WT	
TNFRSF17			WT	
IL2			WT	
MDS2			WT	
LMO2			WT	
HOXC11			WT	
BTG1			WT	
WT1				
CYLD				
FGFR1			WT	
CRTC3				
MUC1			WT	
SLC34A2				
TIF1			WT	
NONO			WT	
YWHAE			WT	
MAFB			WT	
CDX2			WT	
RPL10			WT	
TLX1			WT	
FSTL3			WT	
ATF1			WT	
MDS1			WT	
HOXC13			WT	
MYC			WT	
OLIG2			WT	
NKX2-1			WT	
HOXA13			WT	
HOXD11			WT	
P2RY8			WT	
MAF			WT	
PIM1			WT	
HOXA9			WT	
DDIT3			WT	
ATP1A1				

CHIC2		WT	
LYL1		WT	
CCNB1IP1		WT	
MTCP1		WT	
SOX2		WT	
SDHD		WT	
POU5F1		WT	
HMGA1		WT	
COX6C		WT	
OMD		WT	
FEV		WT	
JUN		WT	
TCL6		WT	
TAF15		WT	
BAP1			
CSF3R			
CIC			
TCF7L2			WT
ASXL1			
CREB3L2			
MITF			
SSX1	WT		
CREB3L1			WT
EXT2			
SBDS			WT
MKL1			
RUNDC2A			
WWTR1			
VTI1A			
PPARG			
EWSR1			
FNBP1			
EZR			
PHOX2B			
CD79B			
NFKB2			
LASP1			WT
NCOA4			
MN1			
CREB1			
HERPUD1			
KCNJ5			
CD74			
SLC45A3			
MYCL1			
CALR			
ZNF198			
FAM22A			
RPL5			
ZNF278			
SH2B3			
MYD88			
FHIT			WT
C2orf44			
PRF1			
CHCHD7			
CD79A			
H3F3A			
CANT1			
H3F3B			
TAL2			
HIST1H3B			
HIST1H4I			
CEBPA			
CRLF2			