

Supplementary Information

A biophysical study of Ru(II) polypyridyl complexes of 2-(4-(pyrimidine-5-yl)phenyl)-1*H*-imidazo[4,5-*f*][1,10]phenanthroline [NPPIP] ligand, its DNA binding affinity and biological activity

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Table-S1: UV-Vis spectral analysis data.

Ligand/Ru-complex	Absorption region, λ_{\max}	Band assigned
NPPIP Ligand	226	$\pi \rightarrow \pi^*$ (INCT)
	263	$n \rightarrow \pi^*$ (INCT)
[Ru(phen)₂NPPIP]⁺²(1)	223	$\pi \rightarrow \pi^*$ (INCT)
	264	$n \rightarrow \pi^*$ (INCT)
	410	MLCT
[Ru(bpy)₂NPPIP]⁺²(2)	225	$\pi \rightarrow \pi^*$ (INCT)
	289	$n \rightarrow \pi^*$ (INCT)
	464	MLCT
[Ru(dmb)₂NPPIP]⁺²(3)	223	$\pi \rightarrow \pi^*$ (INCT)
	290	$n \rightarrow \pi^*$ (INCT)
	470	MLCT

Table-S2: Anti-bacterial zone of Inhibition (mm) and Minimum Inhibitory Concentration (μ L).

S.No.	Gram-positive bacteria						Gram-negative bacteria					
	Staphylococcus			Bacillus			E.Coli			Klebsiella		
	*A	*B	MIC	*A	*B	MIC	*A	*B	MIC	*A	*B	MIC
Complex-1	12	14	25	10	12	25	09	12	25	12	14	50
Complex-2	08	08	75	10	10	75	08	12	50	10	12	50
Complex-3	08	10	75	10	12	25	08	10	75	08	12	50
Standard	16			14			12			12		

*A=75 μ L of the Sample ; *B =100 μ L of the Sample

Table-S3: Anti-fungal zone of Inhibition (*mm) and Minimum Inhibitory Concentration (μ L)..

S.No.	Aspergillus			Candida		
	*A	*B	MIC (μ L)	*A	*B	MIC(μ L)
Complex-1	08	12	25	12	14	50
Complex-2	12	12	50	08	10	75
Complex-3	12	12	75	08	12	25
Standard		12			12	

*A=75 μ L of the Sample ; *B =100 μ Lof the Sample

Spectral images of Ru(II)NPPIP complexes

Supplementary Data

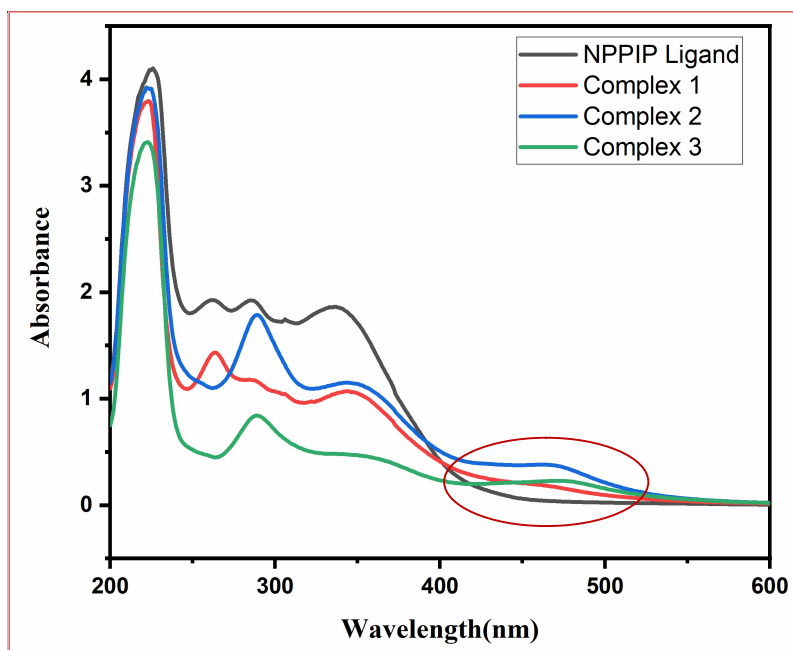


Figure S1: UV-Vis spectrum of NPPIP ligand and its Ru(II) complexes

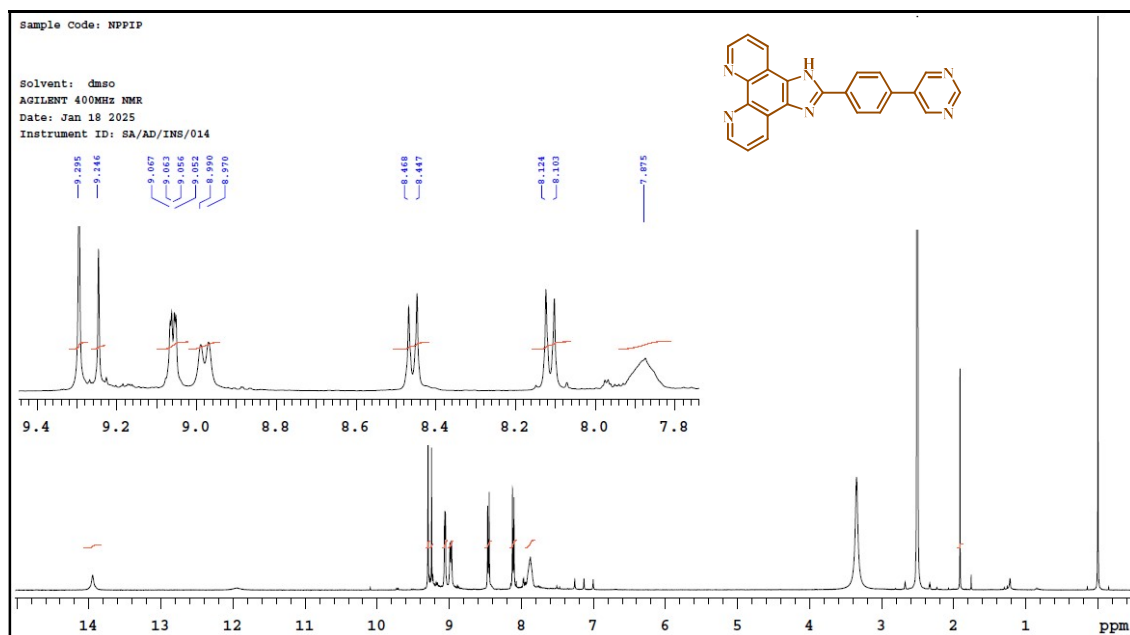


Figure S2: ^1H -NMR spectrum of NPPIP Ligand in DMSO-d_6 , δ -ppm

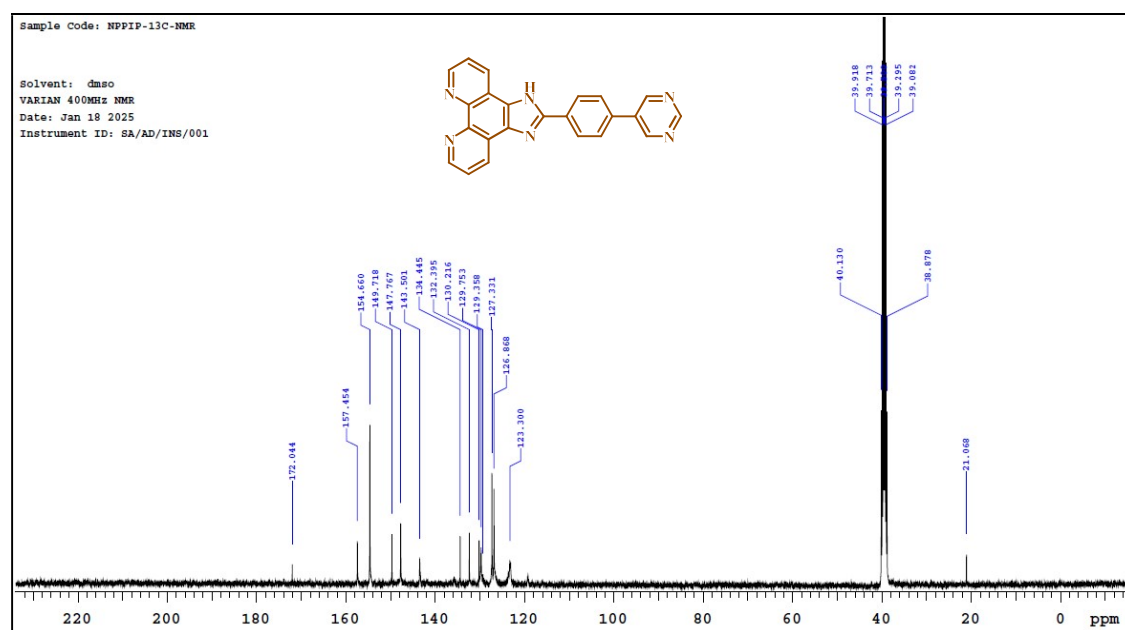


Figure S3: ^{13}C -NMR spectrum of NPPIP ligand in DMSO-d_6 , δ -ppm

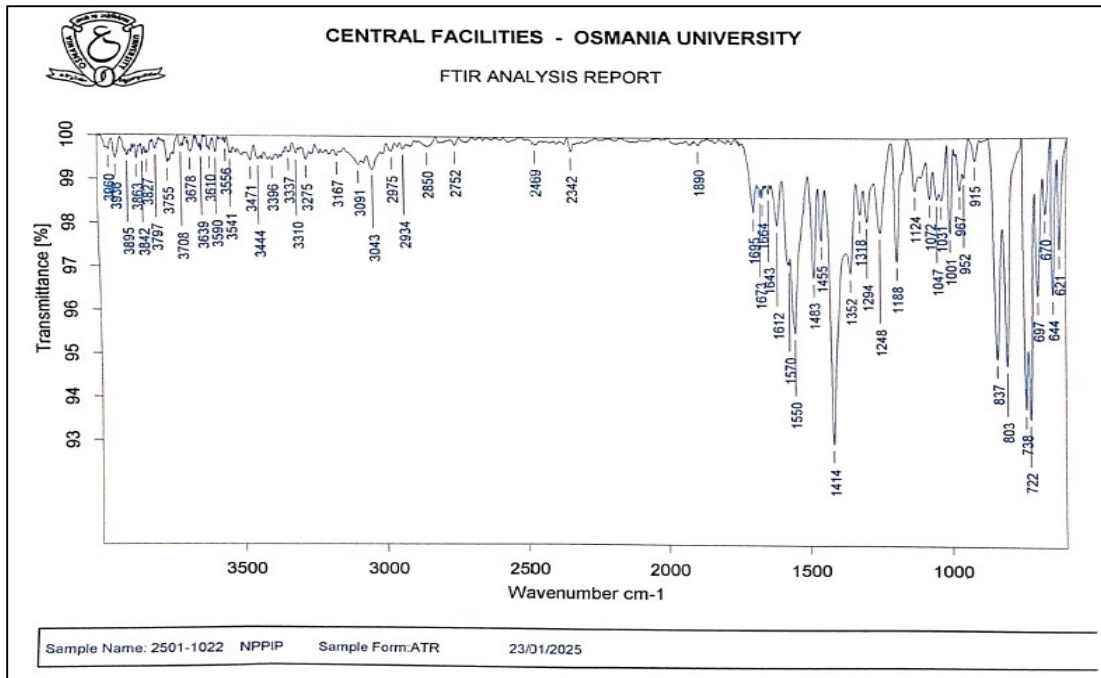


Figure S4: FT-IR (KBr, cm⁻¹) Spectrum of NPIP Ligand

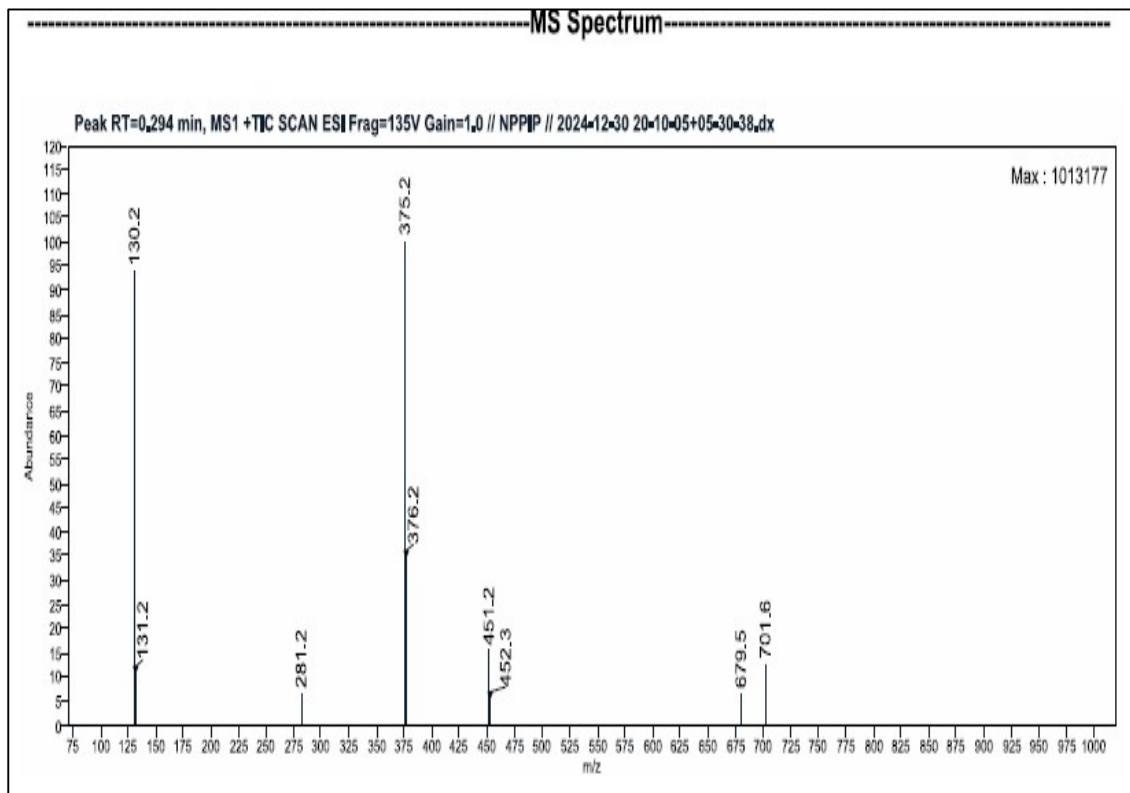


Figure S5: Mass spectrum of NPIP Ligand

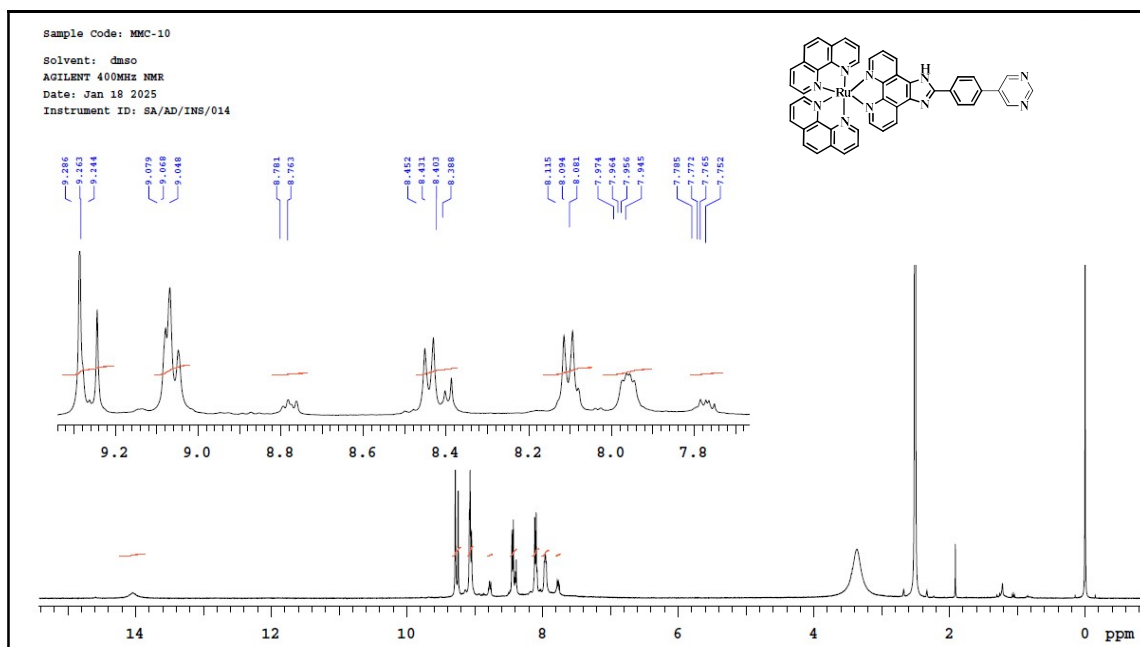


Figure S6: $^1\text{H-NMR}$ spectrum of $[\text{Ru}(\text{phen})_2\text{NPPIP}]^{+2}$ complex in DMSO-d_6 , δ -ppm

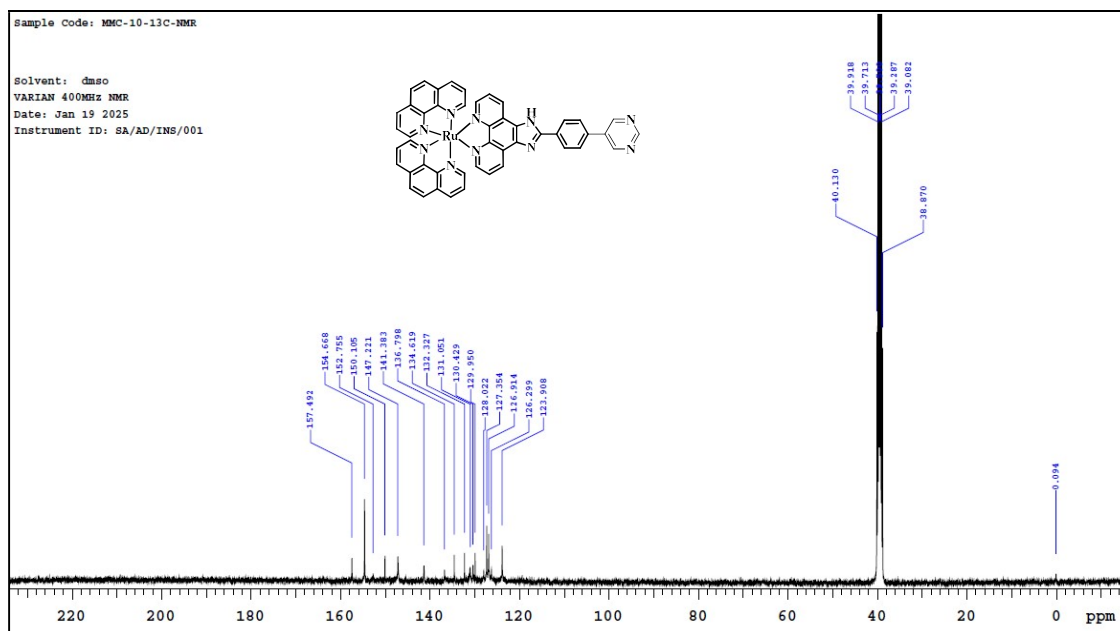


Figure S7: $^{13}\text{C-NMR}$ spectrum of $[\text{Ru}(\text{phen})_2\text{NPPIP}]^{+2}$ complex in DMSO-d_6 , δ -ppm

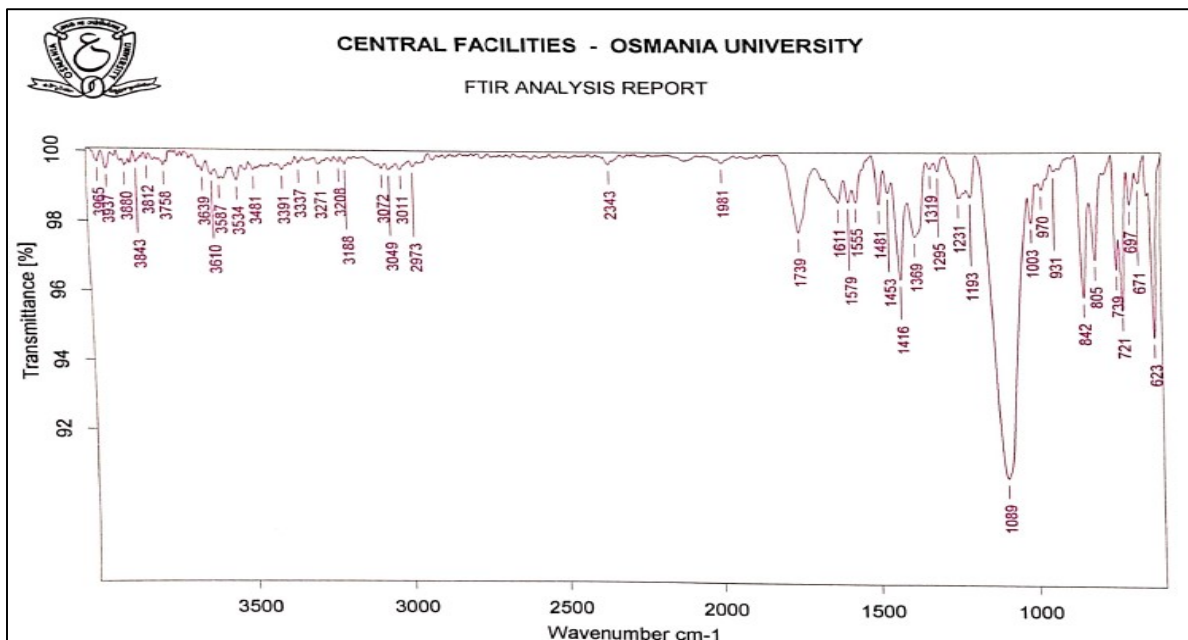


Figure S8: FT-IR (KBr, cm⁻¹) spectrum of [Ru(phen)₂NPIP]²⁺ complex

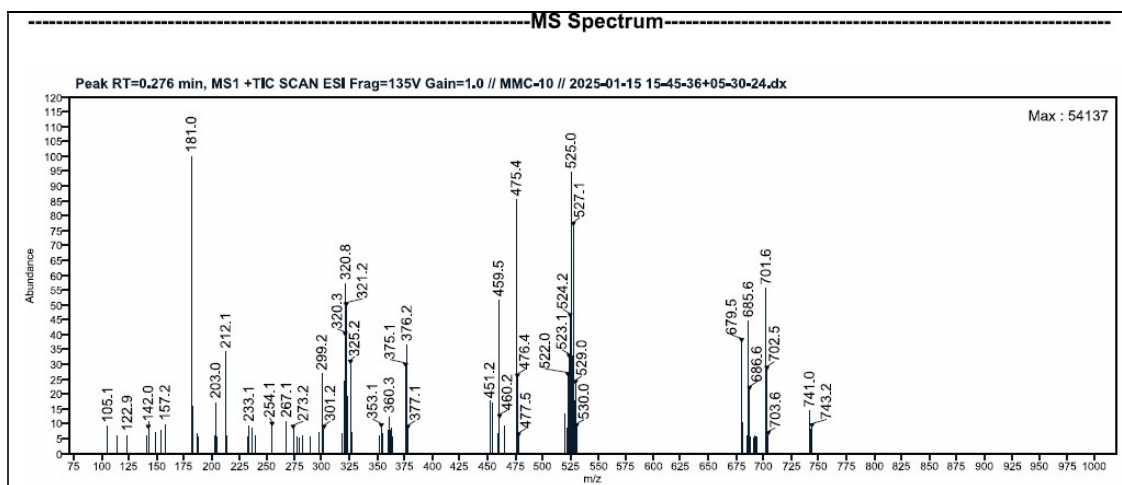


Figure S9: Mass Spectrum of [Ru(phen)₂NPIP]²⁺ complex

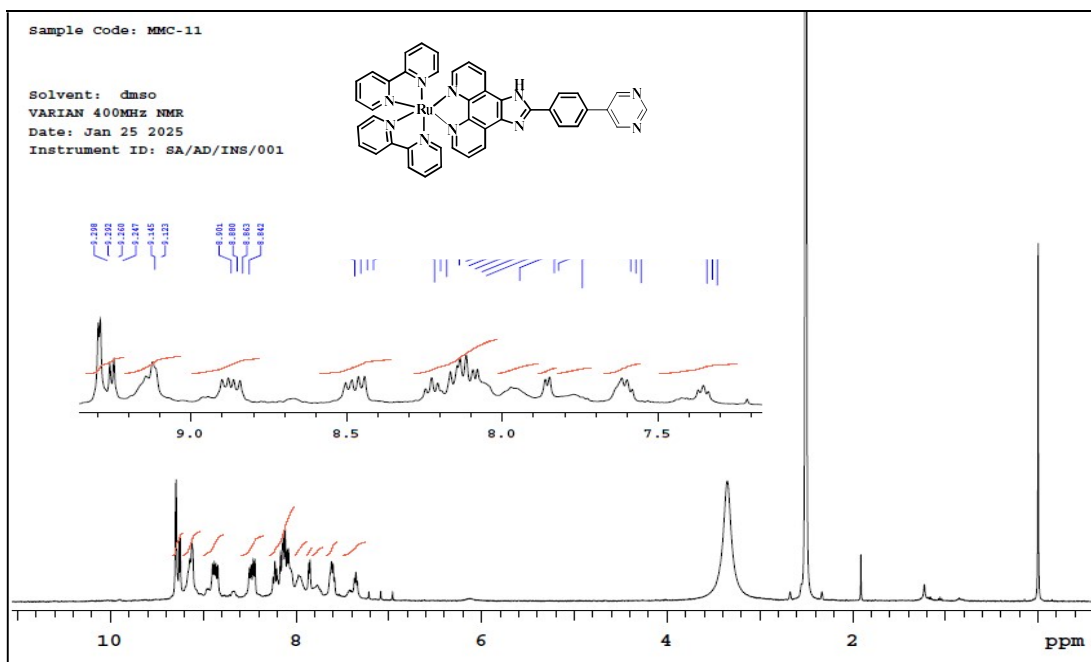


Figure S10: ¹H-NMR spectrum of [Ru(bpy)₂NPPIP]⁺² complex in DMSO-d₆, δ-ppm

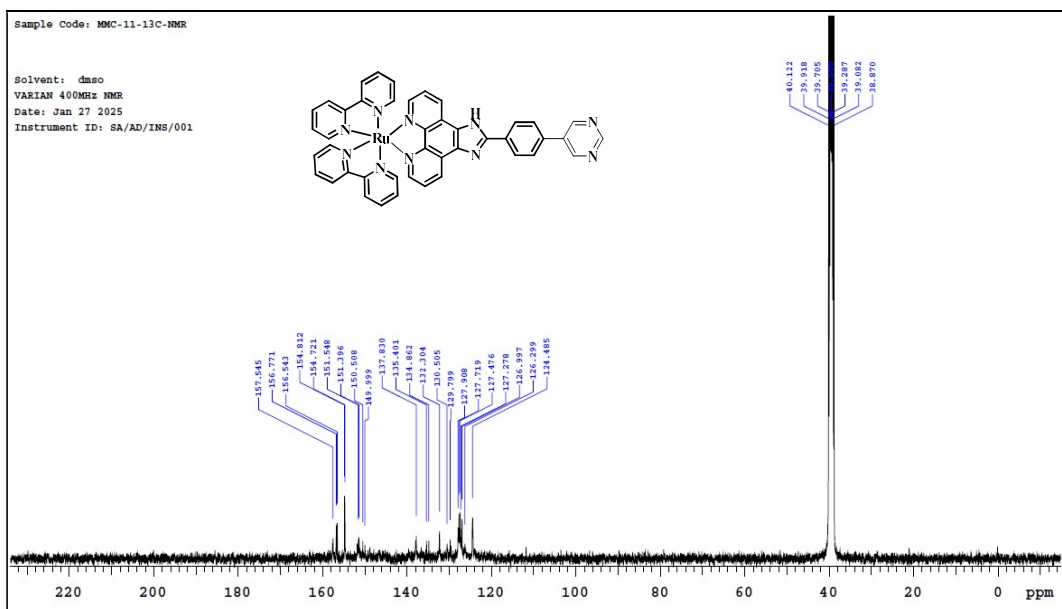


Figure S11: ^{13}C -NMR spectrum of $[\text{Ru}(\text{bpy})_2\text{NPPIP}]^{+2}$ complex in DMSO-d_6 , δ -ppm

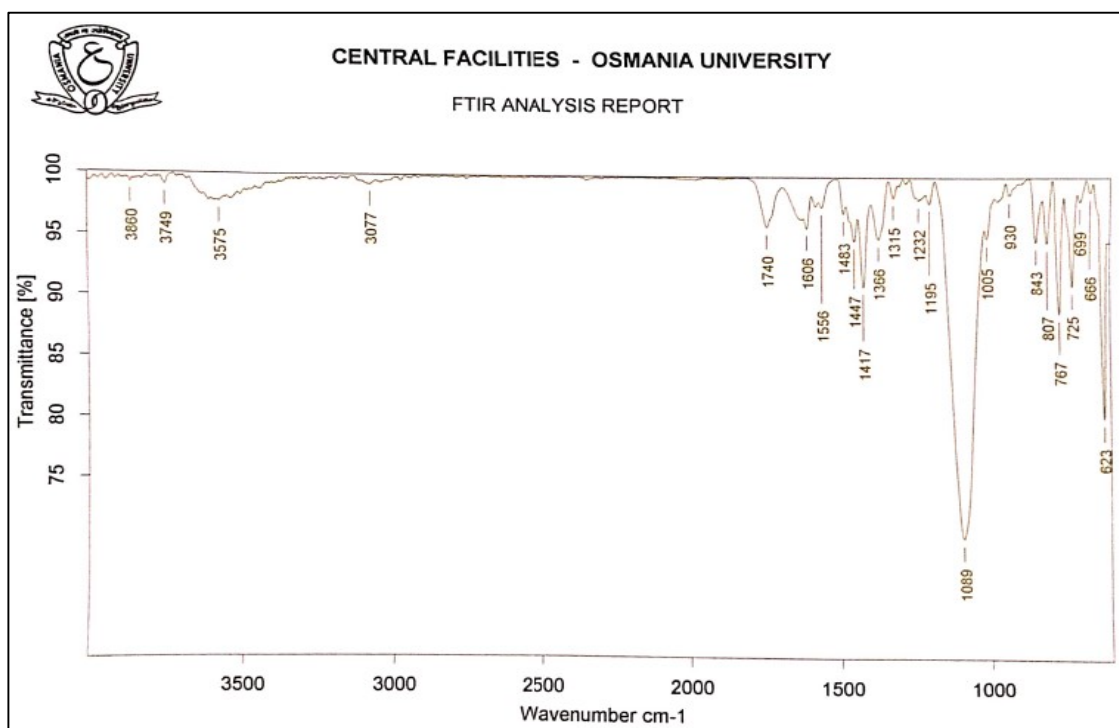


Figure S12: FT-IR (KBr, cm^{-1}) Spectrum of $[\text{Ru}(\text{bpy})_2\text{NPPIP}]^{+2}$ complex

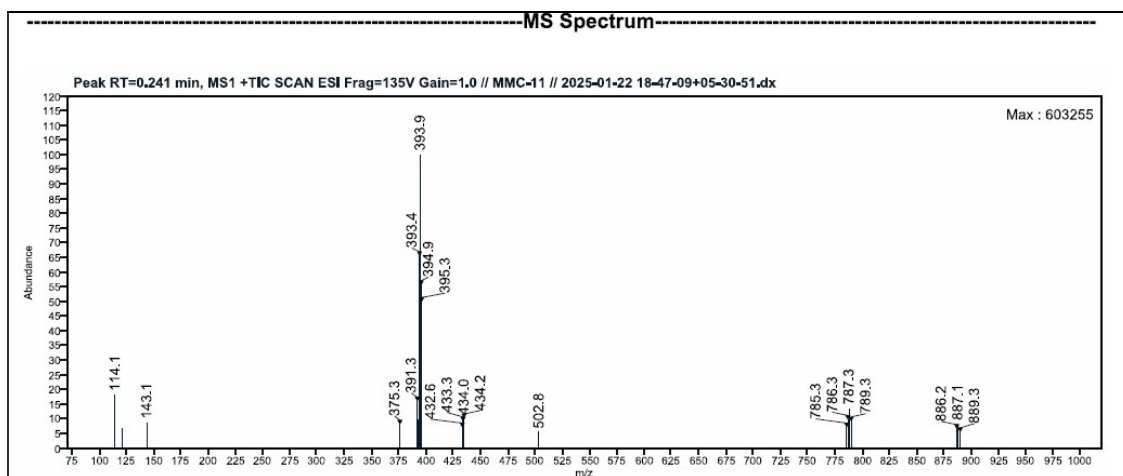


Figure S13: Mass Spectrum of $[\text{Ru}(\text{bpy})_2\text{NPPIP}]^{+2}$ complex

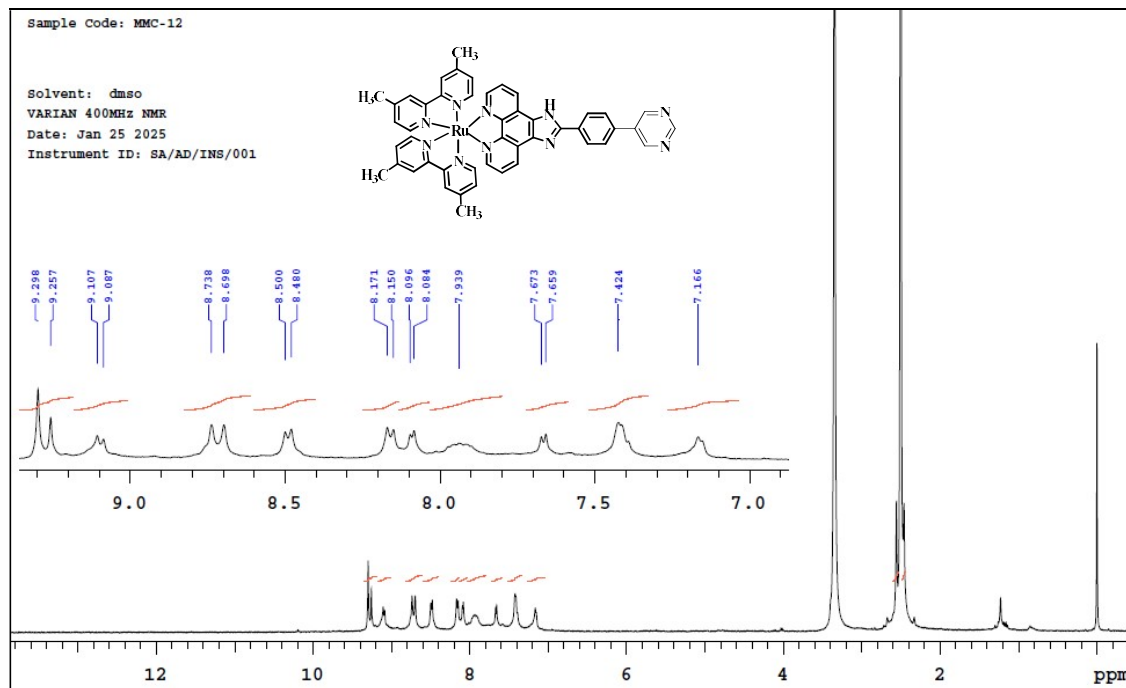


Figure S14: ^1H -NMR Spectrum of $[\text{Ru}(\text{dmb})_2\text{NPPIP}]^{+2}$ complex in DMSO-d_6 , δ -ppm

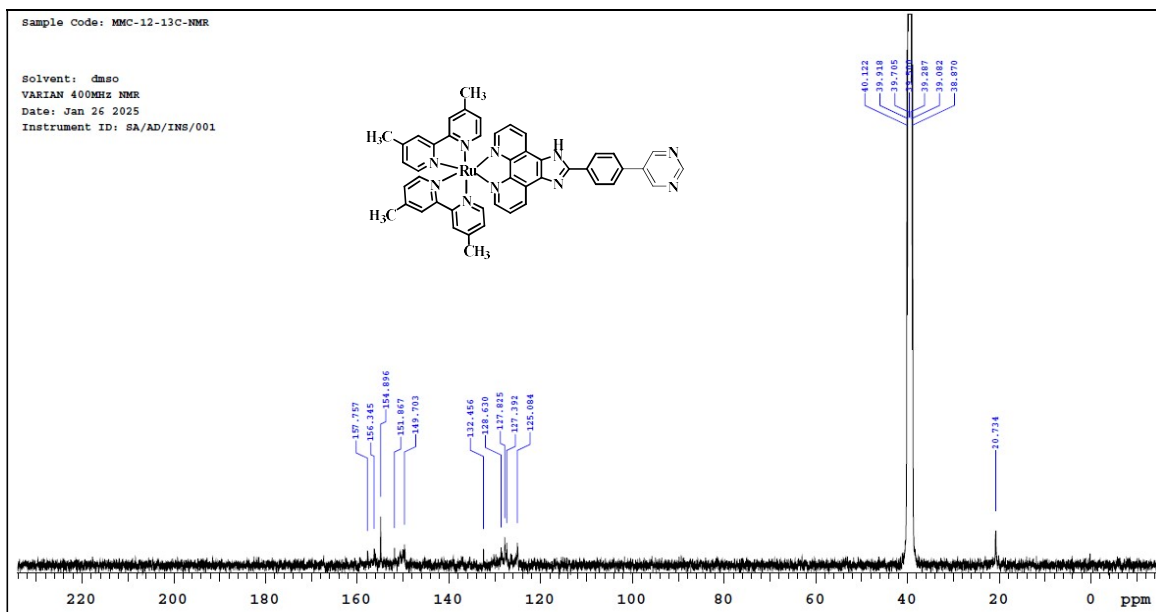


Figure S15: ^{13}C -NMR Spectrum of $[\text{Ru}(\text{dmb})_2\text{NPPIP}]^{+2}$ complex in DMSO-d_6 , δ -ppm

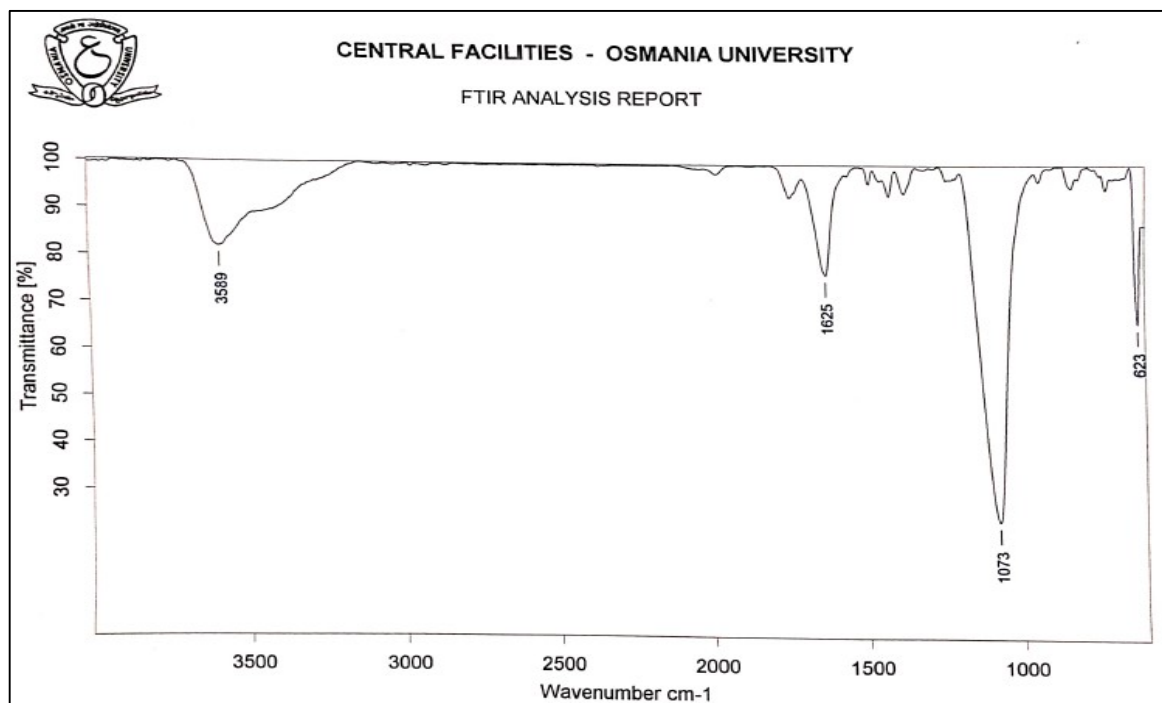


Figure S16: FT-IR (KBr, cm^{-1}) Spectrum of $[\text{Ru}(\text{dmb})_2\text{NPPIP}]^{+2}$ complex

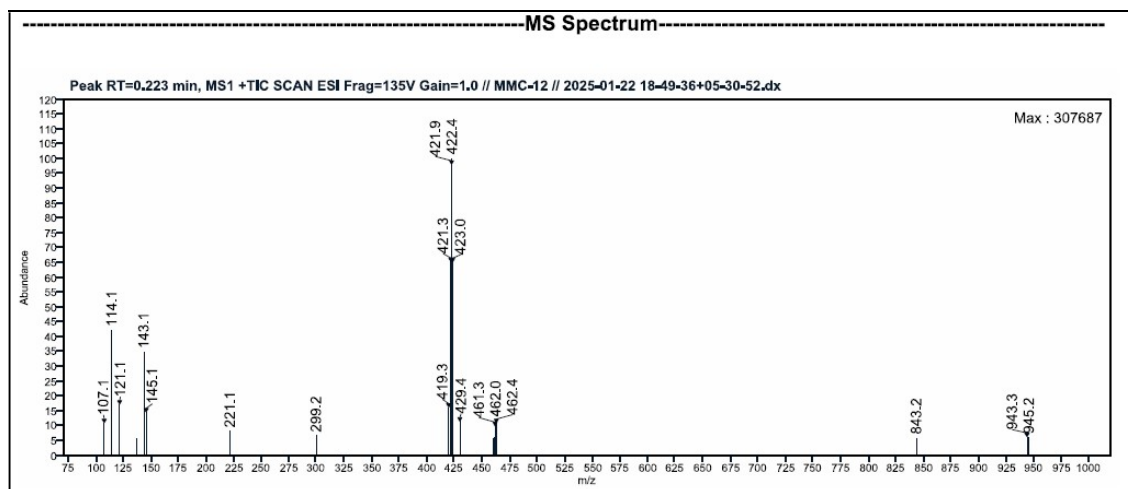


Figure S17: Mass spectrum of $[\text{Ru}(\text{dmb})_2\text{NPIP}]^{+2}$ complex