

Synthesis, Structural Characterization, DNA Interaction, Antimicrobial Evaluation and Anticancer Activity of two novel quari-dentate VO(II) and Mn (II) Mononuclear Complexes

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Supplementary data

Table S1: Molecular electronic spectra, λ_{\max} (nm) and ϵ_{\max} ($\text{dm}^3 \text{mol}^{-1} \text{cm}^{-1}$) of the prepared imine ligands and their complexes in DMF at 298 K against DMF as a blank.

Imine ligands and their complexes	λ_{\max} (nm)	ϵ_{\max} ($\text{dm}^3 \text{mol}^{-1} \text{cm}^{-1}$)	Assignment
ESPN	349	1190	n \rightarrow *
	308	1460	\rightarrow *
ESPNMn	527	360	d - d band
	295	2190	\rightarrow *
ESPNV	421	870	d - d band
	324	1960	LMCT band
	310	1940	LMCT band

Table S2: The formation constant (K_f), stability constant (pK) and Gibbs free energy (G^*) values of the synthesized complexes at 298K.

Complex	Type of complex	K_f	Log K_f	G^* (KJmol⁻¹)
ESPNMn	1:1	8.27×10^4	4.92	-28.05
ESPNV	1:1	1.32×10^4	4.12	-23.51

Table S3: Results of activity index (%) for antimicrobial assay of the prepared Schiff base ligand and its complexes.

Compounds	Activity index (%)					
	Bacteria			Fungi		
	<i>S. aureus</i>	<i>B. subtilis</i>	<i>E. coli</i>	<i>A. flavus</i>	<i>C. albicans</i>	<i>T. rubrum</i>
ESPN	35.56	35.29	35	29.03	29.73	32
ESPNMn	86.67	92.16	87.5	83.87	78.38	84
ESPNV	91.11	94.12	90	87.09	89.19	92

Table S4 : Cytotoxic activity (IC_{50}) of ESPN imine ligand and its complexes against Colon carcinoma cells, (HCT-116 cell line) and hepatic cellular carcinoma cells, (HepG-2),

Compounds	$IC_{50}(\mu\text{g}/\mu\text{l})$		
	MCF-7	HCT-116	HepG-2
ESPN	84.6	103	91.5
ESPNMn	65.8	87	73.4
ESPNV	35.8	56.2	46.3
Vinblastine standard ^a	4.12	13.3	7.5

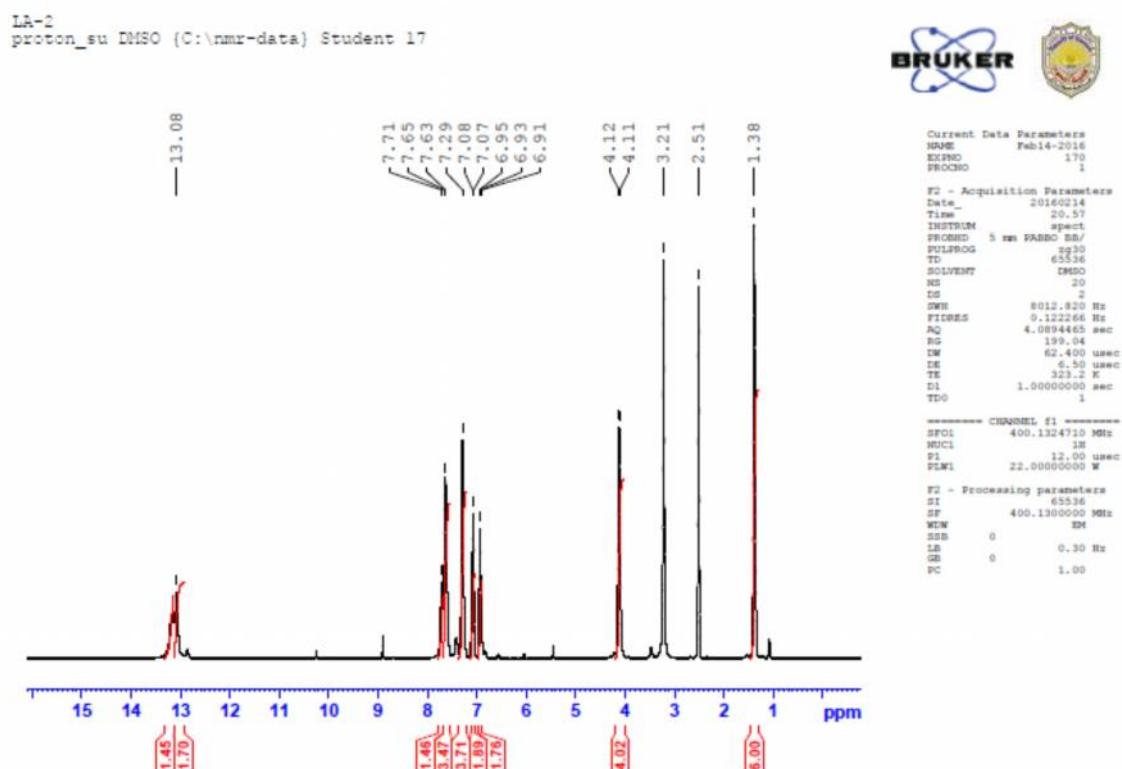


Fig. S1: ^1H NMR spectrum of HNAP imine ligand

LA-2
c13_su DMSO (C:\nmr-data) Student 17

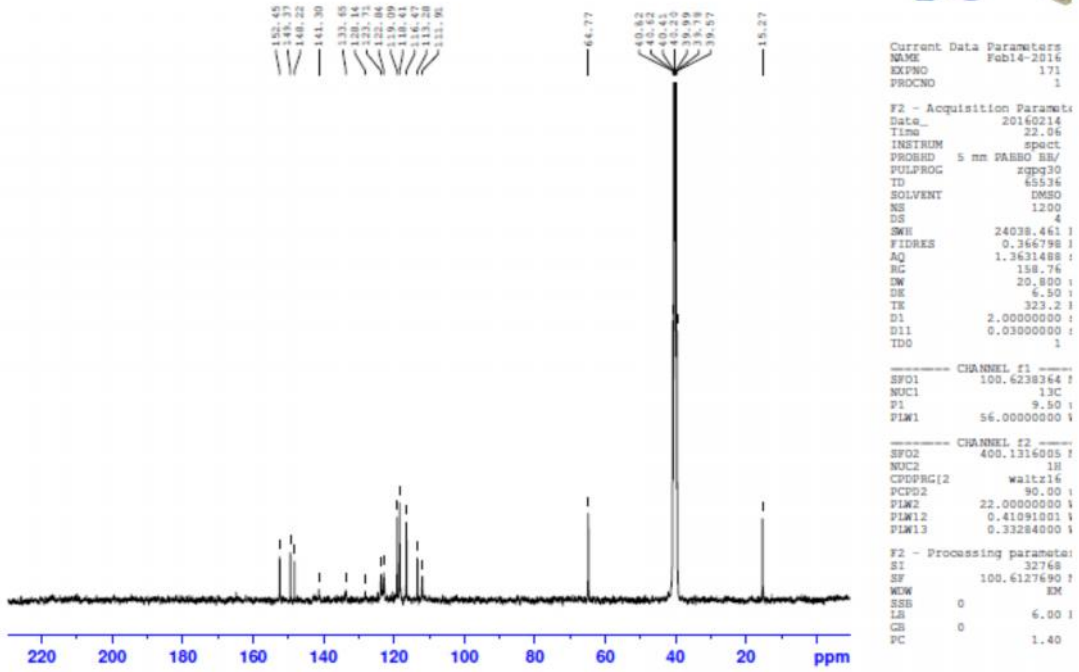


Fig. S2: ^{13}C NMR spectrum of HNAP imine ligand.

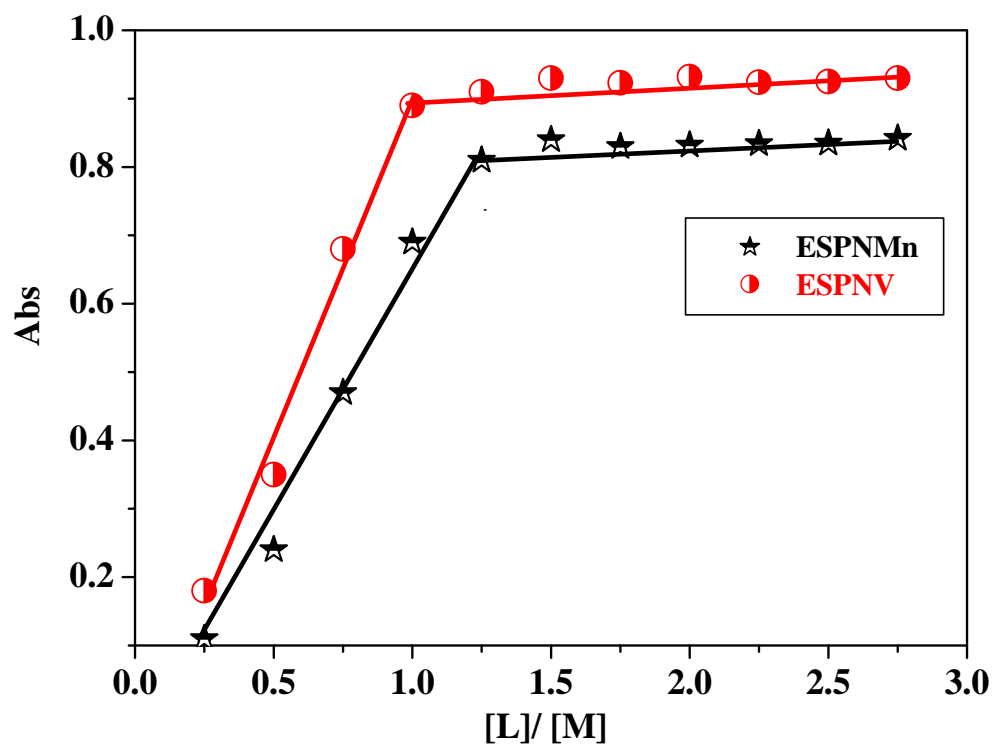


Fig. S3: Molar ratio plots for the studied complexes in aqueous–ethanolic mixture at $[M] = 10^{-3}M$ and $[ESPN] = 10^{-3} M$.

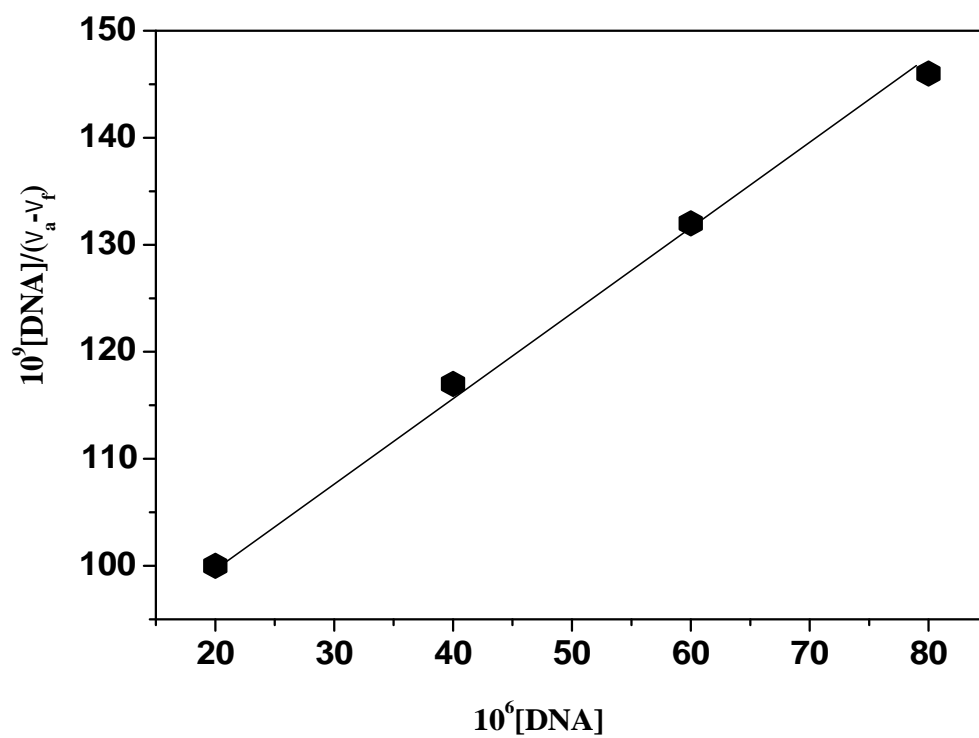


Fig. S4: Plot of $[\text{DNA}] / (V_a - V_f)$ versus $[\text{DNA}]$ for the titration of DNA with ESPNMn complex.