

**Three Novel Ni(II), VO(II) and Cr (III) Mononuclear Complexes Encompassing Potentially Tri -dentate imine ligand: Synthesis, Structural Characterization, DNA Interaction, Antimicrobial Evaluation and Anticancer Activity**

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**Supplementary data**

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

<b>Imine ligands and their complexes</b>	<b><math>\lambda_{\max}</math> (nm)</b>	<b><math>\epsilon_{\max}</math> (<math>\text{dm}^3 \text{mol}^{-1} \text{cm}^{-1}</math>)</b>	<b>Assignment</b>
<b>HNAP</b>	480	1990	INCT
	400	1290	$n \rightarrow \pi^*$
	311	1230	$\pi \rightarrow \pi^*$
<b>HNAPCr</b>	518	230	d - d band
	472	1090	LMCT band
	446	1100	LMCT band
	316	1150	LMCT band
<b>HNAPNi</b>	524	403	d - d band
	473	1080	LMCT band
	447	1100	LMCT band
	318	1150	LMCT band
<b>HNAPV</b>	504	570	d - d band
	457	1450	LMCT band
	327	1210	LMCT band

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

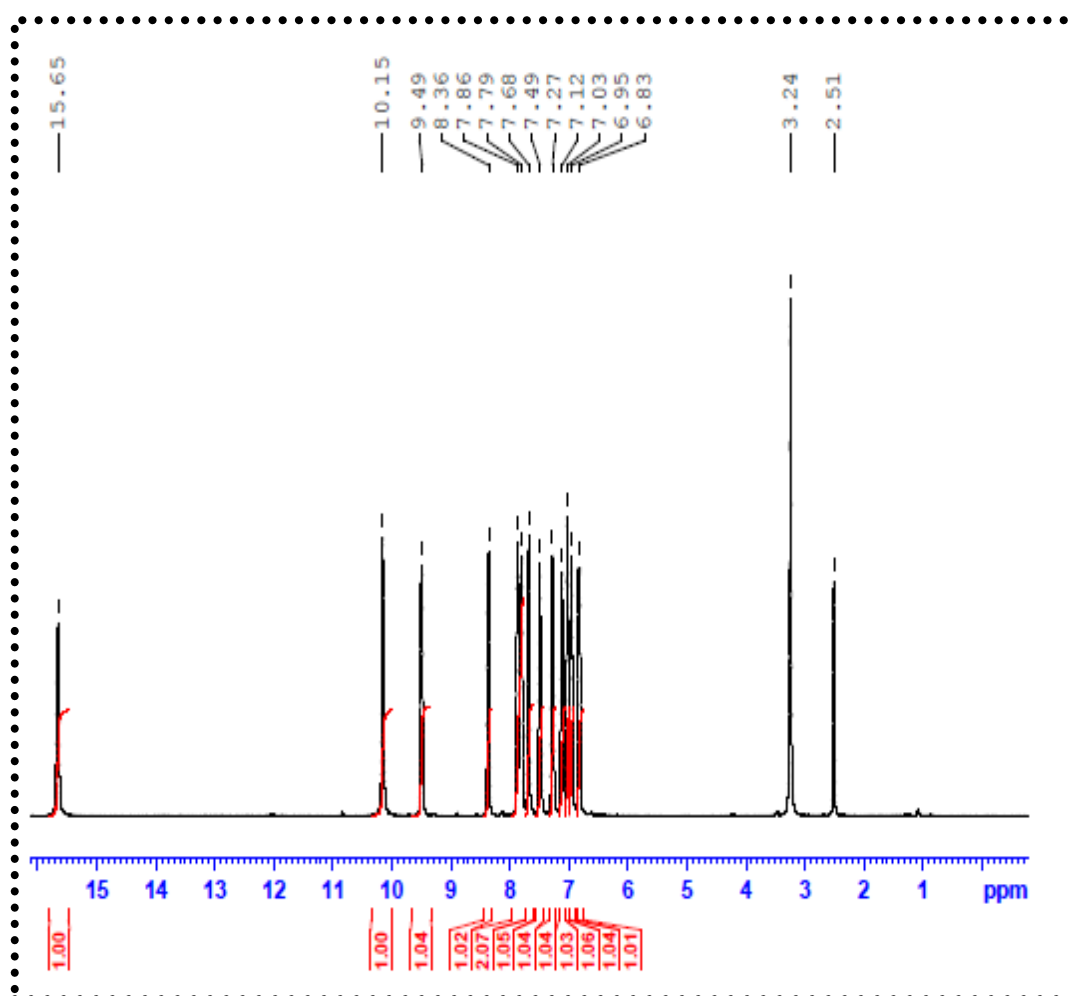
<b>Complex</b>	<b>Type of complex</b>	<b><math>K_f</math></b>	<b>Log <math>K_f</math></b>	<b><math>\Delta G^*</math> (<math>\text{KJmol}^{-1}</math>)</b>
<b>HNAPCr</b>	<b>1:1</b>	<b><math>2.64 \times 10^4</math></b>	<b>4.42</b>	<b>-25.22</b>
<b>HNAPNi</b>	<b>1:1</b>	<b><math>1.06 \times 10^4</math></b>	<b>4.03</b>	<b>-22.96</b>
<b>HNAPV</b>	<b>1:1</b>	<b><math>1.16 \times 10^4</math></b>	<b>4.06</b>	<b>-23.19</b>

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

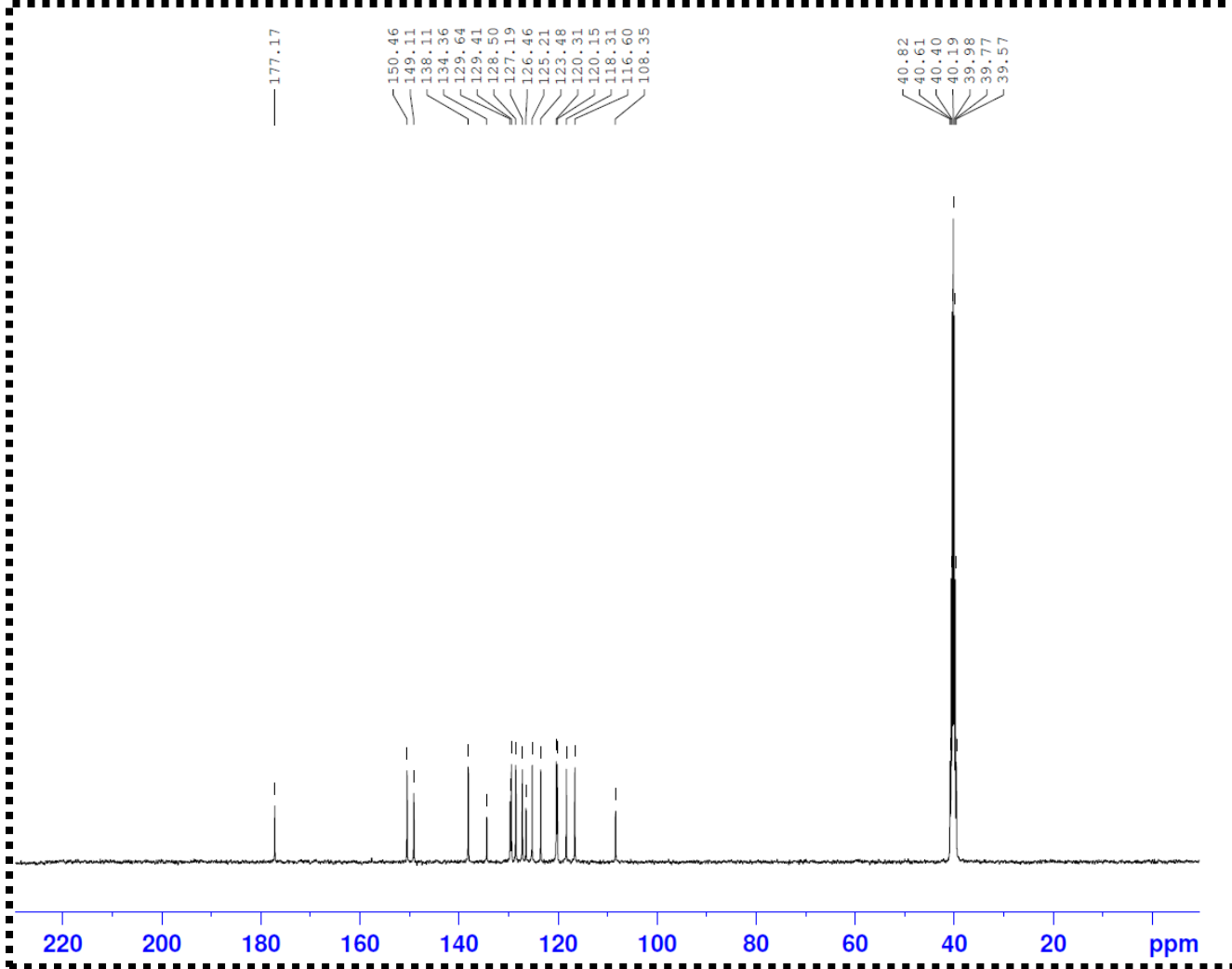
Compounds	Activity index (%)					
	Bacteria			Fungi		
	<i>S. aureus</i>	<i>B. subtilis</i>	<i>E. coli</i>	<i>A. flavus</i>	<i>C. albicans</i>	<i>T. rubrum</i>
HNAP	26.67	25.49	25.00	19.35	18.92	20.00
HNAPV	68.89	72.55	70.00	70.97	72.97	68.00
HNAPNi	64.44	62.75	65.00	48.39	45.95	44.00
HNAPCr	71.11	76.47	75.00	64.52	64.86	60.00

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

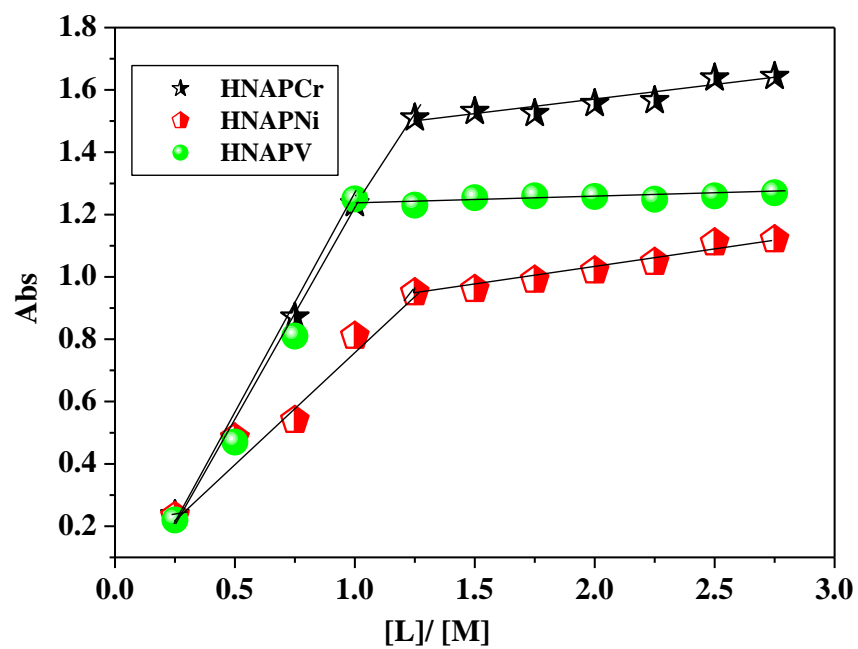
Compounds	$IC_{50}(\mu\text{g}/\mu\text{l})$		
	MCF-7	HCT-116	HepG-2
HNAP	103.00	207.0	133.90
HNAP Cr	55.30	98.40	68.60
HNAP Ni	37.40	55.30	44.20
HNAP V	14.00	25.40	19.30



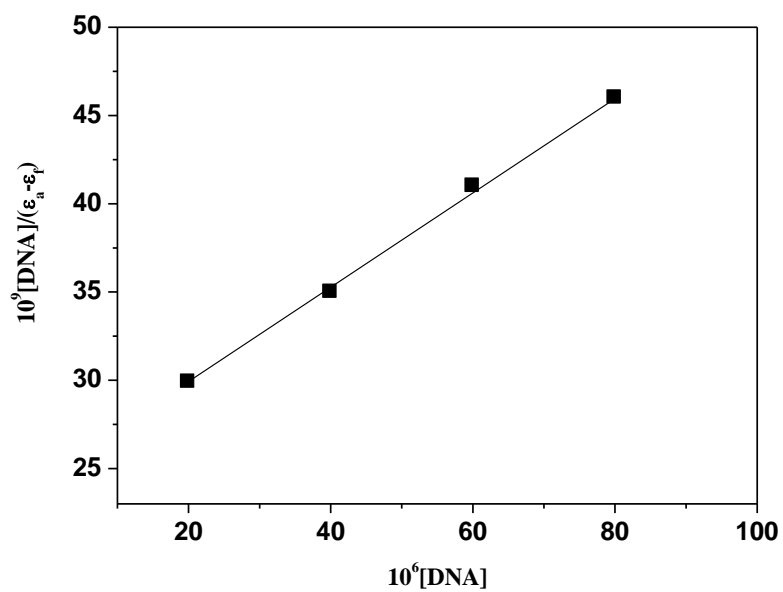
**Fig. S1:**  $^1\text{H}$  NMR spectrum of HNAP imine ligand



**Fig. S2:**  $^{13}\text{C}$  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  $[HNAP] = 10^{-3}M$ .



**Fig. S4:** Plot of  $[\text{DNA}] / (\epsilon_a - \epsilon_f)$  versus  $[\text{DNA}]$  for the titration of DNA with HNAPCr complex.