Development and DFT calculation of New Ni(II), VO(II), Cr (III) Chelates encompassing Tri-dentate imine for DNA Interaction, Antimicrobial and Anticancer Activities

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Supplementary data

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

Imine ligands and their complexes	λ_{max} (nm)	ε_{max} (dm^3 $mol^{-1}cm^{1}$)	Assignment
ESAP	471	360	$n \rightarrow \pi^*$
	396	1480	$n \rightarrow \pi^*$
	306	1490	$n \rightarrow \pi^*$
ESAPCr	584	113	d - d band
	358	1340	LMCT band
	296	1580	Intraligand band
ESAPNi	519	90	d - d band
	437	274	LMCT band
	414	271	LMCT band
	308	1520	LMCT band
	282	1840	Intraligand band
ESAPV	568	60	d - d band
	434	1220	LMCT band
	399	1110	LMCT band
	300	1900	LMCT band

Table S2: Natural charge, natural population, natural configuration of the central metal ions and coordinated ONO-atoms in the studied complexes using B3LYP/LANL2DZ

Atom	Natural charge	Natural population				Natural configuration
		core	valence	Rydberg	Total	
V	0.8768	17.9723	4.0838	0.0661	22.1231	[core]$4s^{0.2}3d^{3.56}4p^{0.32}4d^{0.06}$
N 8	-0.4589	1.9993	5.4443	0.0153	7.4589	[core]$2s^{1.3}\ 2p^{4.14}3p^{0.01}$
O 15	-0.6386	1.9997	6.6299	0.0088	8.6386	[core]$2s^{1.66}2p^{4.97}3p^{0.01}$
O 16	-0.6748	1.9997	6.6651	0.0100	8.6748	[core]$2s^{1.66}2p^{5.01}3p^{0.01}$
Cr	0.8723	17.9830	5.1015	0.0430	23.1276	[core]$2s^{0.2}3d^{4.57}4p^{0.33}4d^{0.04}$
N 8	-0.5017	1.9993	5.4849	0.0173	7.5017	[core]$2s^{1.32}2p^{4.17}3p^{0.02}$
O 15	-0.6181	1.9998	6.6096	0.0086	8.6181	[core]$2s^{1.67}2p^{4.94}3p^{0.01}$
O 16	-0.5390	1.9998	6.5311	0.0081	8.5390	[core]$2s^{1.66}2p^{4.87}3p^{0.01}$
Ni	0.7757	17.9927	9.2232	0.0082	27.2242	[core]$4s^{0.28}3d^{8.67}4p^{0.07}5p^{0..21}$
N 8	-0.5082	1.9993	5.4924	0.0164	7.5082	[core]$2s^{1.33}2p^{4.17}3p^{0.01}$
O 15	-0.7102	1.9998	6.7021	0.0082	8.7102	[core]$2s^{1.7}2p^{5.0}3p^{0.01}$
O 16	-0.7100	1.9998	6.7009	0.0092	8.7100	[core]$2s^{1.69}2p^{5.01}3p^{0.01}$

Table S3: Natural population of the total electrons in each complex on the sub-shells using B3LYP/LANL2DZ

parameter	ESAPV	ESAPCr	ESAPNi
Effective core	10.0	10.0	10.0
core	49.95	51.96	51.97
valence	114.64	124.64	125.66
Natural minimal basis	174.61	186.61	187.64
Natural Rydberg	0.39	0.38	0.35
total	175	187	188

Table S4: Results of activity index (%) for antimicrobial assay of the prepared Schiff base ligand and its complexes.

Compounds	Activity index (%)					
	Bacteria			Fungi		
	S. aureus	*B. subtilis*	*E. coli*	*A. flavus*	*C. albicans*	*T. rubrum*
ESAP	**31.11**	**31.37**	**30**	**22.58**	**24.32**	**28**
ESAPV	**82.22**	**90.196**	**85**	**80.65**	**75.68**	**80**
ESAPNi	**80**	**86.27**	**82.5**	**77.42**	**75.68**	**76**
ESAPCr	**77.78**	**88.24**	**82.5**	**83.87**	**72.97**	**72**

Table S5 : 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}(µg/µl)		
	MCF-7	HCT-116	HepG-2
ESAP	112±0.29	211±0.42	161±0.32
ESAPCr	52.7±0.31	89.3±0.23	59.6±0.15
ESAPV	27.2±0.27	42.3±0.18	33.6±0.21
ESAPNi	45.6±0.19	69.3±0.32	51.2±0.14
Vinblastine standard	4.12±0.10	13.3±0.19	7.5±0.11

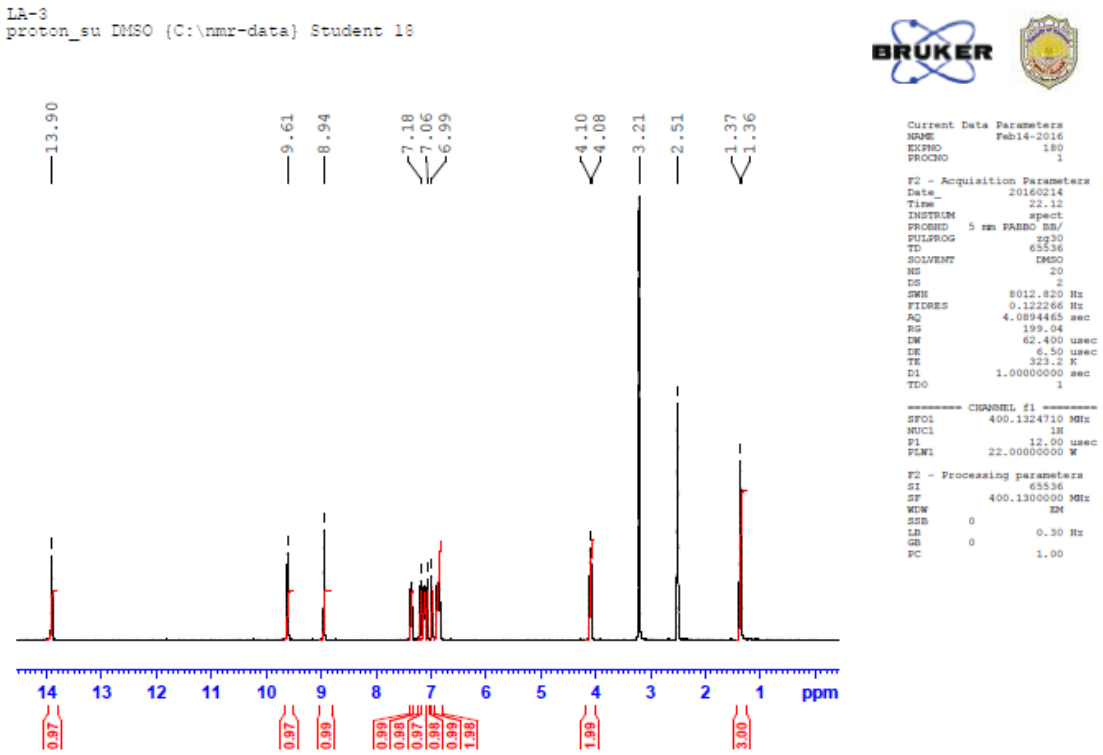

Fig. S1: ^{1}H NMR spectrum of ESAP imine ligand

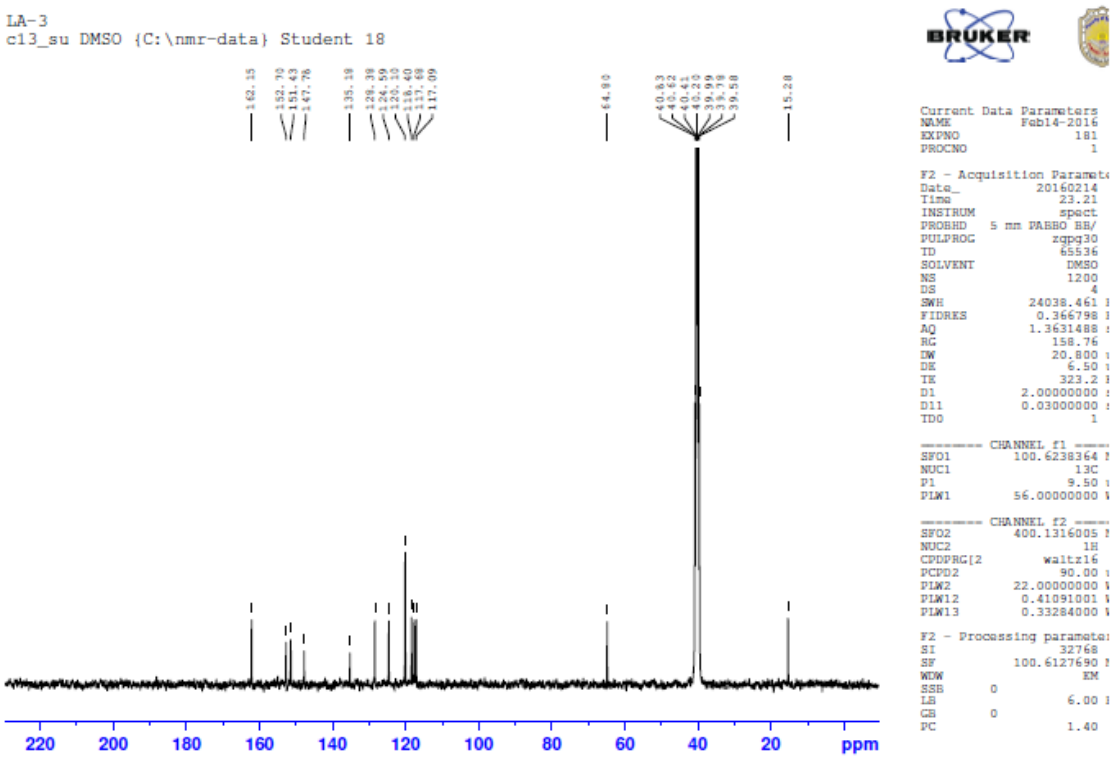

Fig. S2: ^{13}C NMR spectrum of ESAP imine ligand.

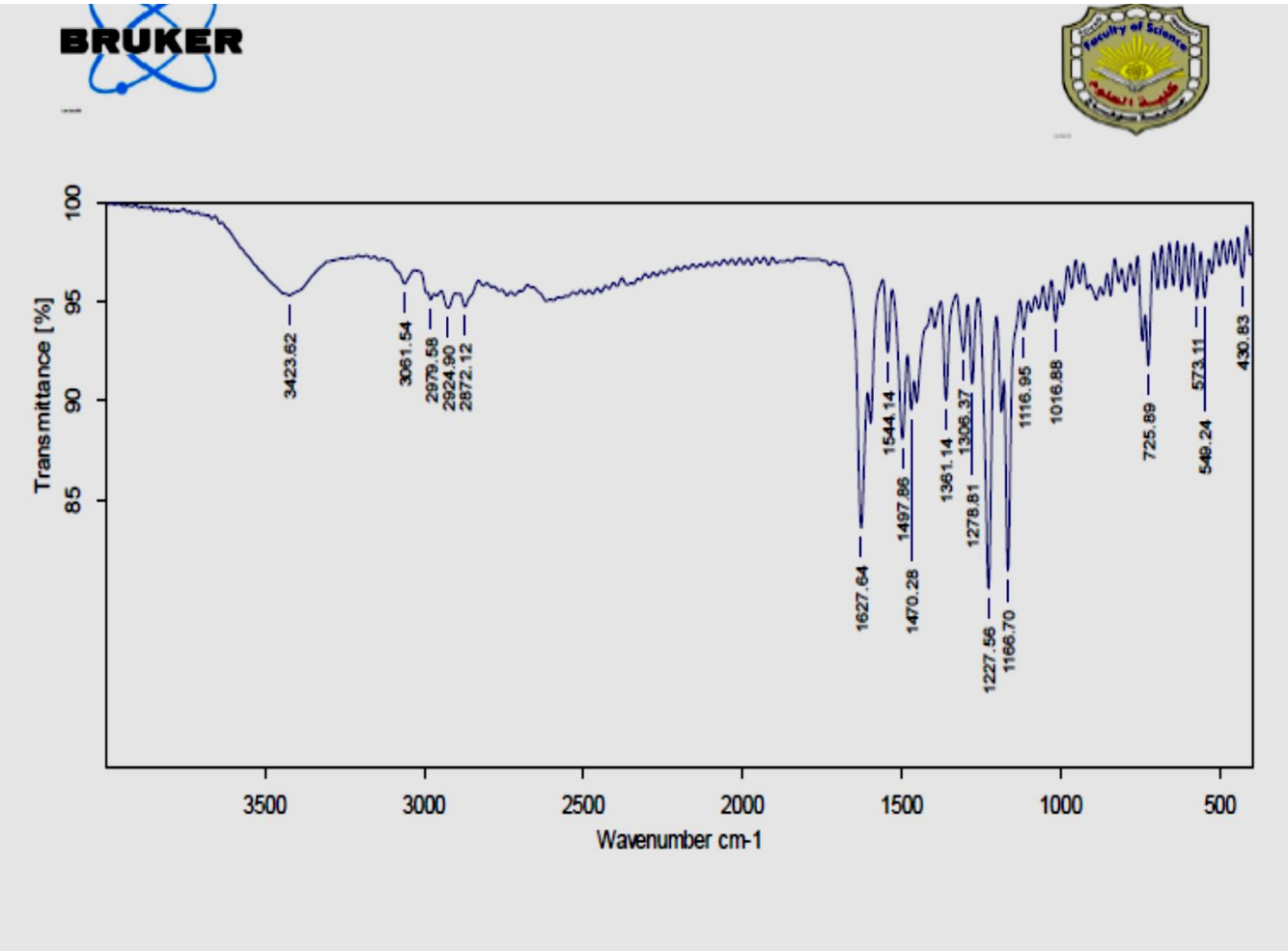

Fig. S3: FT-IR spectrum of ESAP imine ligand.

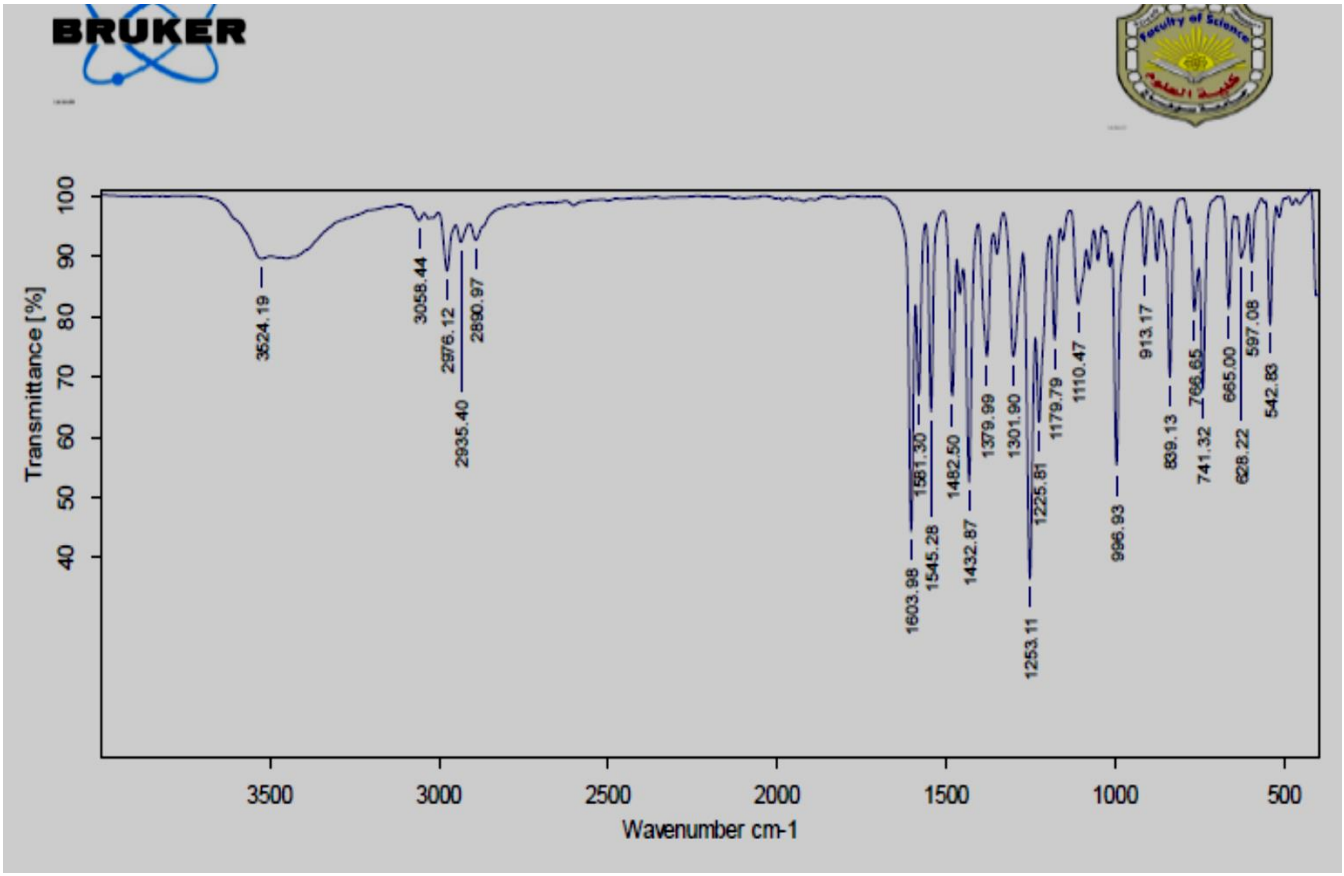

Fig. S4: FT-IR spectrum of ESAPV complex.

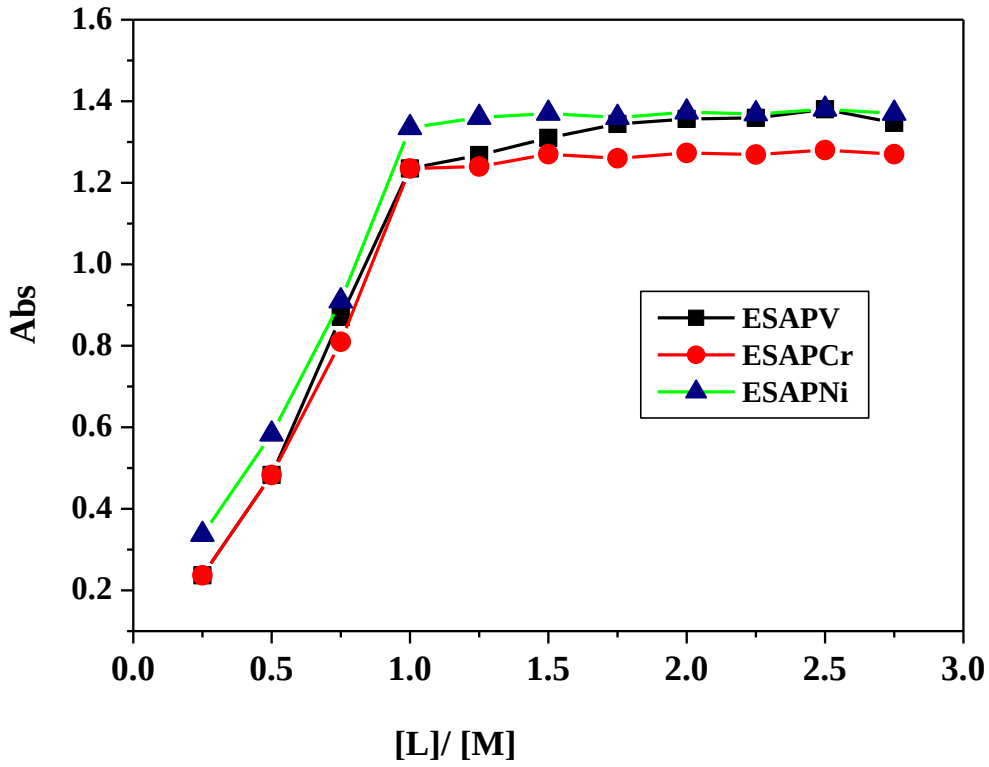

Fig. S5: Molar ratio plots for the studied complexes in aqueous–ethanolic mixture at [M] = 10^{-3}M and [ESAP] = 10^{-3} M.

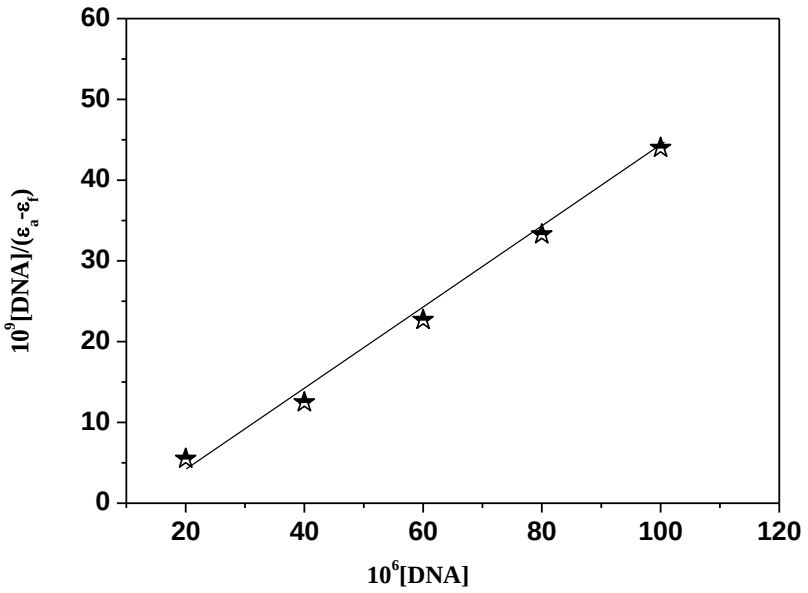

Fig. S6: Plot of [DNA] / (ε_a - ε_f) versus [DNA] for the titration of DNA with ESAPV complex.