Some New Nano-Sized Cr(III), Fe(II), Co(II), and Ni(II) Incorporating 2-((E)-(pyridine-2-ylimino)methyl)napthalen-1-ol Ligand: Structural Characterization, Electrochemical, Antioxidant, Antimicrobial, Antiviral Assessment and DNA interaction

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Supplementary file

List of Tables

Table S1: Crystal data and structure refinements details for npap ligand.

Formula	$C_{32}H_{24}N_4O_2$
Formula weight	496.57
Crystal system	Monoclinic
Space group	$P12_1/c_1$
Crystal colour/ shape	Yellow/ needle
Temperature	293K
Crystal dimensions (mm)	0.15× 0.20× 0.34
Unit cell dimensions	a = 5.83 (9) Å, b = 17.47 (3) Å, c = 24.29 (4) Å α = 90.00°, β = 91.92 (6) °, γ = 90.00 °
Cell volume (Å)^3	2473.10 (7) Å^3
Formula units/ unit cell	4
D cal (mg m^{-3})	1.33
μ cal (mm^{-1})	0.085
Reflections measured	4173
θ_{max}(°)	16.88
Range of h, k, l	-4< h >4, -13< k >13, -11< l >19
Data collection method	φ and ω scans
S	1.06
R-factor	0.048
weighted R-factor	0.127
Δρmin	- 0.24 e Å^{-3}
Δρmax	0.24 e Å^{-3}
Refinement on	F^2
Weight function	$1/[\sigma^2(F_{obs}^2) + (0.100 \times P)^2 + 0.000 \times P + 0.000 + 0.000 \times \sin\theta]$, $P = 0.333 \times \max(F_{obs}^2,0) + 0.667 \times Fcalc^2$
Parameters refined	181

Table S2: Selected bond lengths (x, y, z) and bond angles (^{o}) of npap ligand.

Label	x(Å)	y(Å)	z(Å)
Bond length (Å)			
O1	0.6674(7)	0.4074(2)	0.28612(17)
C2	0.7862(11)	0.4656(3)	0.2779(2)
C3	0.7239(8)	0.5205(3)	0.2366(2)
C4	0.5328(8)	0.5068(3)	0.2023(2)
N5	0.4060(7)	0.4465(3)	0.20744(19)
C6	0.2184(10)	0.4321(3)	0.1735(3)
C7	0.0970(9)	0.3660(4)	0.1843(2)
C8	-0.0920(11)	0.3462(3)	0.1533(3)
C9	-0.1623(9)	0.3921(4)	0.1111(3)
C10	-0.0384(9)	0.4576(4)	0.1015(2)
N11	0.1531(8)	0.4789(3)	0.1315(2)
C12	0.8631(9)	0.5874(3)	0.2308(2)
Bond angles (^{o})			
C2- O1- H11	165.153°	C30- C31- C32	119.100(5)°
O1 - C2- C19	121.200(6)°	C32- C31- C34	118.300(5)°
C4- C3- C12	121.800(5)°	C32 - C33- C1	119.800(5)°
C3- C4- H41	119.900(13)°	C1- C33- H331	119.600(13)°
C4- N5- C6	122.500(6)°	C31 - C34- H341	119.300(13)°
N5- C6- N11	122.800(5)°	C34 - C35- C36	118.900(6)°
C6- C7- C8	121.300(7)°	C36- C35- H351	120.200(13)°
C8- C7- H71	119.900(13)°	C35- C36- H361	119.600(13)°
C7- C8- H81	120.500(13)°	C30- C37- C36	121.700(5)°
C8- C9- C10	118.200(6)°	C36 -C37- H371	118.900(13)°
C10- C9- H91	121.300(14)°	O20 - C1- C33	119.700(5)°
C9- C10 - H101	118.300(13)°	O1- C2- C3	122.000(6)°

Table S 3. The formation constant (K_f), stability constant (log K_f) and Gibb's free energy$\Delta(G^*)$ values of the synthesized complexes at 298 K.

Complex	Type of complex	K_f	$\log K_f$	ΔG^* (KJ mol $^{-1}$)
npapCr	1:1	$5.53 \pm 0.02 \times 10^5$	5.74	- 32.76
npapFe	1:2	$1.79 \pm 0.02 \times 10^{10}$	10.25	- 58.49
npapCo	1:1	$1.42 \pm 0.02 \times 10^5$	5.15	- 29.40
npapNi	1:1	$5.38 \pm 0.02 \times 10^5$	5.73	- 32.96

Table S 4. Minimum inhibition concentration (MIC) in mg/ ml for antimicrobial assay of the prepared compounds.

	Bacteria			Fungi		
compounds	***P. aeruginosa***	***E. coli***	***S. aureus***	***A. flavus***	***C. albicans***	***T. rubrum***
npap	9	8	8	9	7	9
npapFe	3	5	5	5	3	4
npapCr	2	4	4	3	5	4
npapCo	4	5	6	5	6	6
npapNi	5	4	5	4	3	6

p. aeruginosa= pseudomonas aeruginosa, E. coli= Escherichia coli, S. aureus = Staphylococcus aureus, A. flavus = Aspergillus flavus, C. albicans = Candida albicans, T. rubrum = Trichophyton rubum.

List of Figures

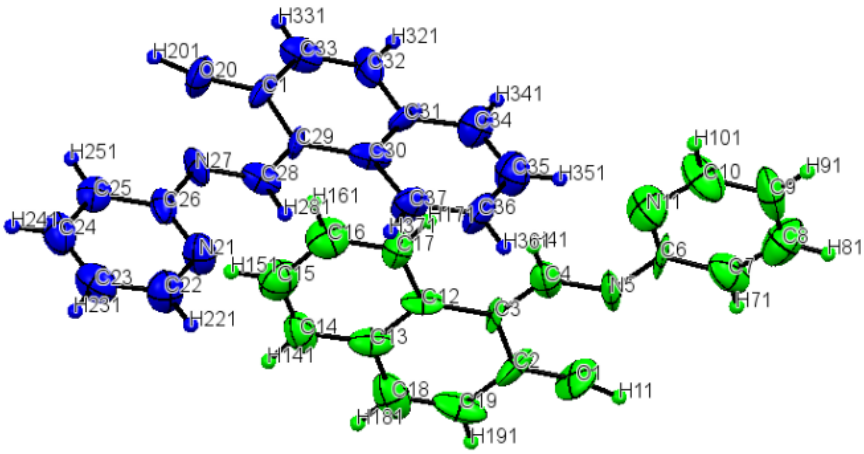

Fig. S1. An ORTEP drawing of the npap Schiff base ligand with the atom- numbering scheme.

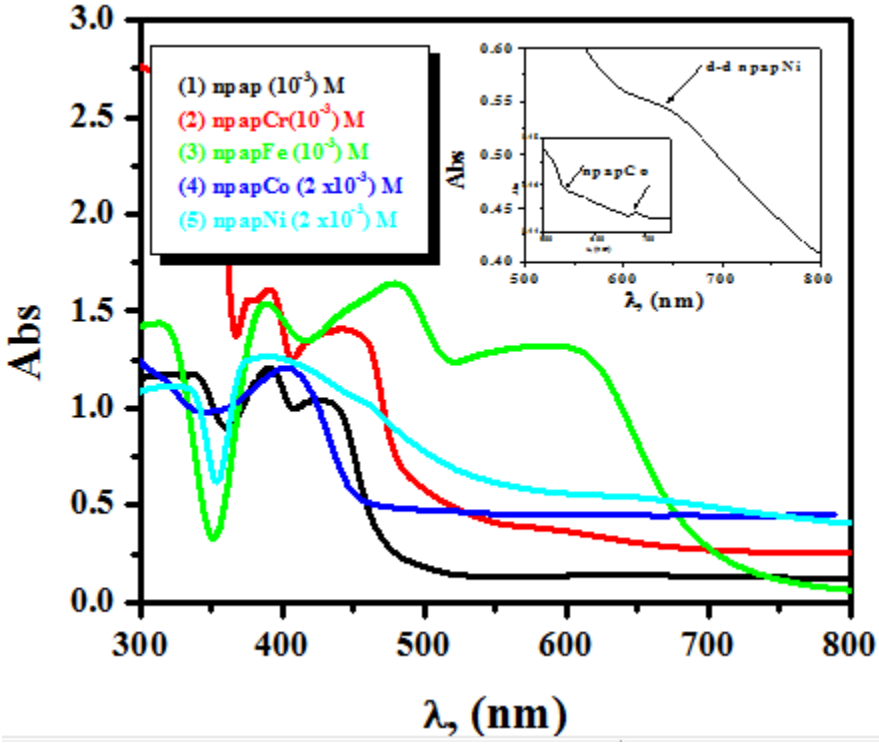

Fig. S2. Molecular electronic spectra of (1) [npap] = (2) [npapCr] = (3) [npapFe] = 10^{-3} mol dm^{-3}, (4) [npapCo] = (5) [npapNi] = 2×10^{-3} mol dm^{-3} in DMF at 298 K.

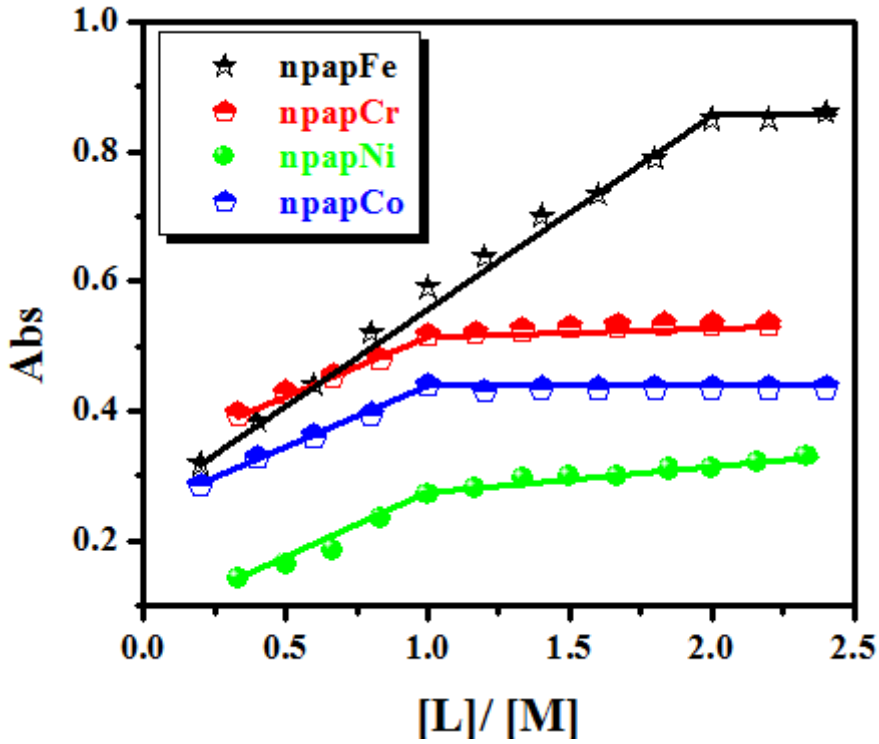

Fig. S 3. Molar ratio plots for the studied complexes in aqueous–ethanolic mixture at [M] = [Fe] = [Cr] = [Co] = [Ni] = 10^{-3} mol dm^{-3}, [npap]= 10^{-3} mol dm^{-3} at 298 K.