**Development, Structural investigation, DNA Binding, Antimicrobial Screening and Anticancer Activities of Two Novel Quari-dentate VO(II) and Mn (II) Mononuclear Complexes**

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**Supplementary data**

**Table S1:**Characteristic IR bands of the prepared ESPN imine ligand and its complexes

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Comp. | υ(OH)/H2O | υSt (-C=N) | υph(C-O) | υph(V=O) | υ (M-O) | υ (M-N) |
| ESPN | 3478 (m) | 1615 (s) | 1230 (m) | - | - | - |
| ESPNV | 3418 (s) | 1602 (s) | 1193 (m) | 943 | 564 (s) | 463 (w) |
| ESPNMn | 3419 (s) | 1600 (s) | 1194 (m) | - | 551 (m) | 436 (m) |

**vs = very strong, s= strong, m= medium, b= broad, w= weak, ar= aromatic, py= pyridine, ph= phenolic, asy= asymmetric,sy= symmetric.**

**Table S2:** Molecular electronic spectra, λmax (nm) and εmax (dm3 mol-1cm-1) of

the prepared imine ligands and their complexes in DMF at 298 K

against DMF as a blank.

|  |  |  |  |
| --- | --- | --- | --- |
| **Imine ligands and their complexes** | **λmax (nm)** | **εmax**  **(dm3 mol-1cm1)** | **Assignment** |
| **ESPN** | 349 | 1190 | n π\* |
| 308 | 1460 | π π\* |
| **ESPNMn** | 527 | 360 | d - d band |
| 295 | 2190 | π π\* |
| **ESPNV** | 421 | 870 | d - d band |
| 324 | 1960 | LMCT band |
| 310 | 1940 | LMCT band |

**Table S3:** The formation constant (Kf), stability constant (**Log Kf**) and Gibbs free energy∆(G\*) values of the synthesized complexes at 298K.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| ***∆G\****  **(KJmol-1)** | **Log Kf** | **Kf** | **Type of complex** | **Complex** |
| **-28.05** | **4.92** | **8.27×104** | **1:1** | **ESPNMn** |
| **-23.51** | **4.12** | **1.32×104** | **1:1** | **ESPNV** |

**Table S4:** Results of antimacrobial bioassay of the prepared ESPN imine ligand and its complexes

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Compounds** | SD±Inhibition zone (mm) | | | | | | | | | | | |
|  | *Escherichia coli(-ve)* | | *Bacillus subtilis (+)* | | *Staphylococcus*  *aureus (+ve)* | | *Candida*  *albicans* | | *Aspergillus*  *flavus* | | *Trichophyton*  *rubrum* | |
| Conc. (mg/ml) | 10 | 20 | 10 | 20 | 10 | 20 | 10 | 20 | 10 | 20 | 10 | 20 |
| ESPN | 7±0.81 | 14±0.13 | 9±0.52 | 18±0.90 | 8±0.70 | 16±0.60 | 7±0.33 | 11±0.42 | 5±0.91 | 9±0.22 | 4±0.19 | 8±0.96 |
| ESPNMn | 16±0.02 | 35±0.33 | 22±0.39 | 47±0.66 | 19±0.54 | 39±0.91 | 19±0.39 | 29±0.92 | 12±0.11 | 26±0.90 | 11±0.91 | 21±0.68 |
| ESPNV | 17±0.17 | ±0.7836 | 22±0.88 | ±0.1248 | 21±0.03 | ±0.74 41 | 21±0.91 | 33±.70 | 13±0.30 | 27±0.22 | 12±0.51 | 23±0.11 |
| Gentamycin | 20±0.71 | 40±0.33 | 26±0.15 | 51±0.72 | 25±0.93 | 45±0.11 | --- | --- | --- | --- | --- | --- |
| Fluconazol | --- | --- | --- | --- | --- | --- | 24±0.55 | 37±0.62 | 16±0.49 | 31±0.88 | 15±0.71 | 25±0.90 |

**Table S5:**Results of activity index (%) for antimicrobial assay of the prepared Schiff base ligand and its complexes.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Compounds | Activity index (%) | | | | | |
| Bacteria  *E. coli B. subtilis S. aureus* | | | Fungi  *A. flavus C. albicans T. rubrum* | | |
| 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 |

**TableS6:** Spectral parameters for the interaction of the prepared imine complexes.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Complex** | **λmax**  **free**  **(nm)** | **λmax bound**  **(nm)** | **∆n** | **Chromism (%)a** | **Type of**  **Chromism** | **Binding Constant**  **104 (Kb)b** | **∆G\***  **KJmol-1** |
| **ESPNMn** | 584 | 552 | 32 | 77.25 | Hypo | 8.52 | -28.13 |
| 397 | 389 | 8 | 24.37 | Hypo |
| 237 | 236 | 1 | 16.91 | Hypo |
| **ESPNV** | 416 | 398 | 18 | 55.83 | Hypo | 4.65 | -26.63 |
| 324 | 312 | 12 | 18.49 | Hypo |

a Chromism (%) = (Abs free- Absbound)/ Absfreeb Binding constant Kb = mol-1 dm3

**Table** S7 : Cytotoxic activity (IC50) of ESPN imine ligand and its complexes against Colon carcinoma cells, (HCT-116 cell line) and hepatic cellular carcinoma cells, (HepG-2),

|  |  |  |  |
| --- | --- | --- | --- |
| **Compounds** | **IC50(µg/µl)** | | |
|  | **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 standarda** | **4.12** | **13.3** | **7.5** |

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**Fig. S1**: 1H NMR spectrum of ESPN imine ligand

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**Fig. S2**: 13C NMR spectrum of ESPN imine ligand.



**Fig. S3**: IR spectrum of ESPN imine ligand



**Fig. S4**: IR spectrum of ESPNMn complex

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**Fig. S5:** Molecular electronic spectra of ESPNMn complex and its ligand in DMF at 298 K.

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**Fig. S6: TGA of the prepared ESPNMn complex.**

|  |
| --- |
|  |

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**Fig. S7:** Molar ratio plots for the studied complexes in aqueous–ethanolic mixture at [M] = 10-3M and [ESPN] = 10-3 M.



**Fig. S8:** Plot of [DNA] / (εa - εf) versus [DNA] for the titration of DNA with ESPNMn complex.