Studies on DNA-binding and anti-cancer activity of Ru(II) polypyridyl complexes by using (2-(4-(diethoxymethyl)-1H-imidazo[4,5-f] [1,10] phenanthroline)) intercalative ligand

Vuradi Ravi Kumar\textsuperscript{a}, Kamakshi Dandu\textsuperscript{b}, Yata Praveen Kumar\textsuperscript{a}, M. Vinoda Rani\textsuperscript{c}, Mallepally Rajender Reddy\textsuperscript{a}, Nagamani Chintakuntla\textsuperscript{a}, Ch. Ravi\textsuperscript{d}, Suman S Thakur\textsuperscript{b}, Ch. Mohan Rao\textsuperscript{b} and S. Satyanarayana\textsuperscript{a}\textsuperscript{*}

\textsuperscript{a} Department of Chemistry, Osmania University, Hyderabad, India, 500007.
\textsuperscript{b} Centre for Cellular and Molecular Biology, Hyderabad, India, 500007.
\textsuperscript{c} Department of Physics, Osmania University, Hyderabad, India, 500007
\textsuperscript{d} Department of Chemistry, JNTU, Hyderabad, Telangana State, India.

\textsuperscript{*}Address for correspondence:

Prof. S. Satyanarayana,
Department of Chemistry, Osmania University, Hyderabad, Telangana, India, 500007,
E-mail: ssnsirasani@gmail.com.
Table of Contents

Content........................................................................................................................................... Page

Figure S1. Absorption spectra of complexes 1 & 3 in Tris–HCl buffer upon addition of CT-DNA. Arrow shows hypochromatic and bathochromic shifts upon increase of DNA concentration. Inserted plot, [DNA]/(ε_b–ε_f) versus [DNA] for the titration of DNA with Ru(II) complexes, which gives intrinsic binding constant (K_b)........................................................................................................................................... 3

Figure S2. Fluorescence of complexes 1&3 in Tris–HCl buffer upon addition of CT-DNA. Arrow shows the intensity change upon the increase of DNA concentration. Inset: Scatchard plot of above complex, which gives binding constant (K_b)........................................................................................................................................... 3

Figure S3. HEK 293 cells were treated with complexes 1, 2 and 3 with different concentrations for 48h and untreated cells were used as control and then cell viability was evaluated by MTT assay. IC_{50} value for complex 1,2 and 3 are 124±8.5 µM, 145±3 µM and 157±9 µM respectively….. 4

Figure S4. ^1H- NMR Spectra of Ligand (DEPIP).................................................................................... 5

Figure S5. ^1H-NMR Spectra of Complex-2 ([Ru(bpy)_2(depip)]^{2+} .................................................. 5

Figure S6. ^1H-NMR Spectra of Complex-3 ([Ru(dmb)_2(depip)]^{2+} .................................................. 6

Figure S7. ^13C -NMR Spectra of Ligand (DEPIP) .................................................................................. 6

Figure S8. ^13C -NMR Spectra of Complex-2 [Ru(bpy)_2(depip)]^{2+} .................................................. 7

Figure S9. Mass Spectra of Ligand (DEPIP)........................................................................................... 7

Figure S10. Mass Spectra of Complex-1 ([Ru(phen)_2depip]^{2+}).......................................................... 8

Figure S11. Mass Spectra of Complex-2 ([Ru(bpy)_2depip]^{2+}).......................................................... 8

Figure S12. Mass Spectra of Complex-3 ([Ru(dmb)_2depip]^{2+})......................................................... 9

Figure S13. IR Spectra of Ligand (DEPIP)............................................................................................ 9

Figure S14. IR Spectra of Complex-2 ([Ru(bpy)_2(depip)]^{2+} .............................................................. 10
Figure S1. Absorption spectra of complexes 1&3 in Tris–HCl buffer upon addition of CT-DNA. Arrow shows hypochromic and bathochromic shifts upon increase of DNA concentration. Inserted plot, [DNA]/(ε_b−ε_f) versus [DNA] for the titration of DNA with Ru(II) complexes, which gives intrinsic binding constant (K_b).

Figure S2. Fluorescence of complexes 1&3 in Tris–HCl buffer upon addition of CT-DNA. Arrow shows the intensity change upon the increase of DNA concentration. Inset: Scatchard plot of above complex, which gives binding constant (K_b).
Figure S3. HEK 293 cells were treated with complexes 1, 2 and 3 with different concentrations for 48h and untreated cells were used as control and then cell viability was evaluated by MTT assay. IC\textsubscript{50} value for complex 1, 2 and 3 are 124±8.5 µM, 145±3 µM and 157±9 µM respectively.
Figure S4. H-NMR Spectra of Ligand (DEPIP)

Figure S5. H-NMR Spectra of Complex-2 (RBDEPIP)
Figure S6. H-NMR Spectra of Complex-3 (RDDEPIp)

Figure S7. $^{13}$C-NMR Spectra of Ligand (DEPIp)
Figure S8. $^{13}$C-NMR Spectra of Complex-2 (RBDEPIP)

Figure S9. Mass Spectra of Ligand (DEPIP)
Figure S10. Mass Spectra of Complex-1 ([Ru(phen)$_2$depip]$^{2+}$)

Figure S11. Mass Spectra of Complex-2 ([Ru(bpy)$_2$depip]$^{2+}$)
**Figure S12.** Mass Spectra of Complex-3 ([Ru(dmb)₂depip]^{2-})

**Figure S13.** IR Spectra of Ligand (DEPIP)
Figure S14. IR Spectra of Complex-2 ([Ru(bpy)$_2$depip]$^{2+}$)