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Supplementary Information

Square Planar Mononuclear Ni(II) Complexes of Functionalized 2,2':6',2''-Terpyridines: BSA/DNA Binding and Anticancer Activity

Rakesh R Panicker, Martin Luther John, Daphne Morrison N, Pralayakaveri Yogendra Varma, Dharani S, Chayan Pandya, A. S. Vijai Anand, Joydip Mondal, Akella Sivaramakrishna*

Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore 632014, Tamil Nadu, India

E-mail: asrkrishna@vit.ac.in

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Figure S1. ¹H NMR Spectrum of compound L1



Figure S2. ¹³C NMR Spectrum of compound L1





Figure S3. IR Spectrum of compound L1

Figure S4. ESI-Mass Spectrum of compound L1





Figure S5. ¹H NMR Spectrum of compound L2

Figure S6. ¹³C NMR Spectrum of compound L2



Figure S7. IR Spectrum of compound L2



Figure S8. ESI-Mass Spectrum of compound L2



Figure S9. ¹H NMR Spectrum of compound L3



Figure S10. ¹³C NMR Spectrum of compound L3



Figure S11. IR Spectrum of compound L3



Figure S12. ESI-Mass Spectrum of compound L3



Figure S13. ¹H NMR Spectrum of compound L4



Figure S14. ¹³C NMR Spectrum of compound L4



Figure S15. IR Spectrum of compound L4



Figure S16. ESI-Mass Spectrum of compound L4



Figure S17. IR Spectrum of compound NiL1



Figure S18. ESI-Mass Spectrum of compound NiL1



Figure S19. IR Spectrum of compound NiL2



Figure S20. ESI-Mass Spectrum of compound NiL2



Figure S21. IR Spectrum of compound NiL3



Figure S22. ESI-Mass Spectrum of compound NiL3



Figure S23. IR Spectrum of compound NiL4



Figure S24. ESI-Mass Spectrum of compound NiL4



Figure S25. UV-Visible Spectra of compound L1 and NiL1



Figure S26. UV-Visible Spectra of compound L2 and NiL2



Figure S27. UV-Visible Spectra of compound L3 and NiL3



Figure S28. UV-Visible Spectra of compound L4 and NiL4



Figure S29. Stability studies of L1-L4 (In order a-d) using UV–Visible absorption spectral data (1×10^{-5} M) in 0.1 mM glutathione (GSH)



Figure S30. Stability studies of NiL1-NiL4 (In order a-d) using UV–Visible absorption spectral data $(1 \times 10^{-5} \text{ M})$ in 0.1 mM glutathione (GSH)



Figure S31. Stability studies of L1-L4 (In order a-d) using UV–Visible absorption spectral data (1×10^{-5} M) under MTT conditions (*i.e.* 5% DMSO in phosphate buffer)



Figure S32. Stability studies of NiL1-NiL4 (In order a-d) using UV–Visible absorption spectral data $(1 \times 10^{-5} \text{ M})$ under MTT conditions (*i.e.* 5% DMSO in phosphate buffer)



Figure S33. Stability studies of L1-L4 (In order a-d) using UV–Visible absorption spectral data $(1 \times 10^{-5} \text{ M})$ in water



Figure S34. Stability studies of NiL1-NiL4 (In order a-d) using UV–Visible absorption spectral data $(1 \times 10^{-5} \text{ M})$ in water



Figure S35. Frontier molecular orbitals of the complexes L1 (a), L2 (b), L3 (c) and L4 (d)



Figure S36 The ESP mapped on the surface of the ligand L1 (a), L2 (b), L3 (c) and L4 (d) by the DFT-B3LYP method

Table S1 Binding energy values of the synthesized ligands and complexes with BSA, 1m17-3 and DNA (AT Rich, GC Rich and Mixed)

. No	Compound	BSA	1m17-3	DNA		
				AT Rich	GC Rich	Mixed
1	L1	-10.1	-9.3	-7.6	-7.1	-8.7
2	L2	-10.3	-9.7	-8.0	-7.8	-8.6
3	L3	-10.6	-10.5	-8.0	-8.1	-8.7
4	L4	-9.0	-10.6	-7.3	-7.3	-6.5
5	NiL1	-8.8	-9.7	-8.1	-7.6	-7.8
6	NiL2	-10.3	-10.5	-8.2	-8.3	-8.7
7	NiL3	-10.4	-9.6	-8.6	-8.9	-9.2
8	NiL4	-9.0	-9.8	-7.3	-7.4	-8.2



Figure S37 Molecular docking interactions of ligands with BSA



Figure S38 Molecular docking interactions of ligands with Im-17-3



Figure S39. Molecular docking interactions of ligands with DNA (AT Rich)



Figure S40. Molecular docking interactions of ligands with DNA (GC Rich)



Figure S41. Molecular docking interactions of ligands with DNA (Mixed)



Figure S42. Molecular docking interactions of complexes NiL1 (a), NiL2 (b), NiL4 (c) with DNA (AT Rich)



Figure S43. Molecular docking interactions of complexes NiL1 (a), NiL2 (b), NiL4 (c) with DNA (GC Rich)



Figure S44. Molecular docking interactions of complexes NiL1 (a), NiL2 (b), NiL4 (c) with DNA (Mixed)



Figure S45. UV-Visible absorbance response of L1 (1.0 x 10⁻⁵) at pH 7.2 in 5 mM Tris-HCl-NaCl buffer solution in the presence of incremental addition of CT-DNA



Figure S46. UV-Visible absorbance response of **NiL1** (1.0 x 10⁻⁵) at pH 7.2 in 5 mM Tris-HCl-NaCl buffer solution in the presence of incremental addition of CT-DNA



Figure S47. UV-Visible absorbance response of L2 (1.0 x 10⁻⁵) at pH 7.2 in 5 mM Tris-HCl-NaCl buffer solution in the presence of incremental addition of CT-DNA



Figure S48. UV-Visible absorbance response of **NiL2** (1.0 x 10⁻⁵) at pH 7.2 in 5 mM Tris-HCl-NaCl buffer solution in the presence of incremental addition of CT-DNA



Figure S49. UV-Visible absorbance response of L3 (1.0 x 10⁻⁵) at pH 7.2 in 5 mM Tris-HCl-NaCl buffer solution in the presence of incremental addition of CT-DNA



Figure S50. UV-Visible absorbance response of **NiL3** (1.0 x 10⁻⁵) at pH 7.2 in 5 mM Tris-HCl-NaCl buffer solution in the presence of incremental addition of CT-DNA



Figure S51. UV-Visible absorbance response of L4 (1.0 x 10⁻⁵) at pH 7.2 in 5 mM Tris-HCl-NaCl buffer solution in the presence of incremental addition of CT-DNA



Figure S52. UV-Visible absorbance response of **NiL4** (1.0 x 10⁻⁵) at pH 7.2 in 5 mM Tris-HCl-NaCl buffer solution in the presence of incremental addition of CT-DNA



Figure S53 Binding parameters of interaction of the ligand (L1) with BSA



Figure S54 Binding parameters of interaction of the ligand (NiL1) with BSA



Figure S55 Binding parameters of interaction of the ligand (L2) with BSA



Figure S56 Binding parameters of interaction of the ligand (NiL2) with BSA



Figure S57 Binding parameters of interaction of the ligand (L3) with BSA



Figure S58 Binding parameters of interaction of the ligand (NiL3) with BSA



Figure S59 Binding parameters of interaction of the ligand (L4) with BSA



Figure S60 Binding parameters of interaction of the ligand (NiL4) with BSA



Figure S61 Fluorescence spectral response of the EtBr-DNA at pH 7.2 in the presence of L1



Figure S62 Fluorescence spectral response of the EtBr-DNA at pH 7.2 in the presence of NiL1



Figure S63 Fluorescence spectral response of the EtBr-DNA at pH 7.2 in the presence of L2



Figure S64 Fluorescence spectral response of the EtBr-DNA at pH 7.2 in the presence of NiL2



Figure S65 Fluorescence spectral response of the EtBr-DNA at pH 7.2 in the presence of L3



Figure S66 Fluorescence spectral response of the EtBr-DNA at pH 7.2 in the presence of NiL3



Figure S67 Fluorescence spectral response of the EtBr-DNA at pH 7.2 in the presence of L4



Figure S68 Fluorescence spectral response of the EtBr-DNA at pH 7.2 in the presence of NiL4



Figure S69. Sigmoidal plot for finding the IC_{50} Values of the Ni(II) complexes NiL1-NiL4 (In order a-d) and using the standard drug Cisplatin (e) using Hep-G2 cell line. f) Sigmoidal plot for the Vero cell line.

 Table S2. Crystallographic data refinement details of the ligand L4 and the Ni(II) complex

 NiL4

Identification	T 4	N;I 4
Identification	1.4	11124
code		
Empirical	$C_{26}H_{16}CIN_3O_2S$	$C_{28}H_{22}Cl_3N_3NiO_4S$
formula		
Formula weight	469.93	661.60
(g/mol)		
Temperature/K	300.00	300.00
Crystal system	Triclinic	Monoclinic
Space group	P-1	$P2_1/n$
a (Å)	8.238(2)	7.4934(11)
b (Å)	10.517(3)	26.809(4)
c (Å)	13.479(4)	14.499(2)
α (Å)	96.239(10)	90
β (Å)	102.378(10)	92.652(5)
γ (Å)	99.049(10)	90
Volume/ Å ³	1114.1(5)	2909.7(7)
Z	2	4
P (calc)g/cm ³	1.401	1.510
θ for data	4.674 to 56.54	4.14 to 52.736
collection		
Reflections	49070	36563
collected		
Independent	5464	5934
reflections		
GOF on F ²	1.058	1.036
R1 [I>2σ]	0.0453	0.0551
wR2 [F ²]	0.0867	0.1193