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Investigation of antitumor potential of Ni(II) complexes with tridentate PNO acylhydrazones of 2-(diphenylphosphino)benzaldehyde and monodentate pseudohalides

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Keywords: Nickel(II) complexes, Girard's T reagent, Phosphine ligands, Cytotoxicity, DNA interactions

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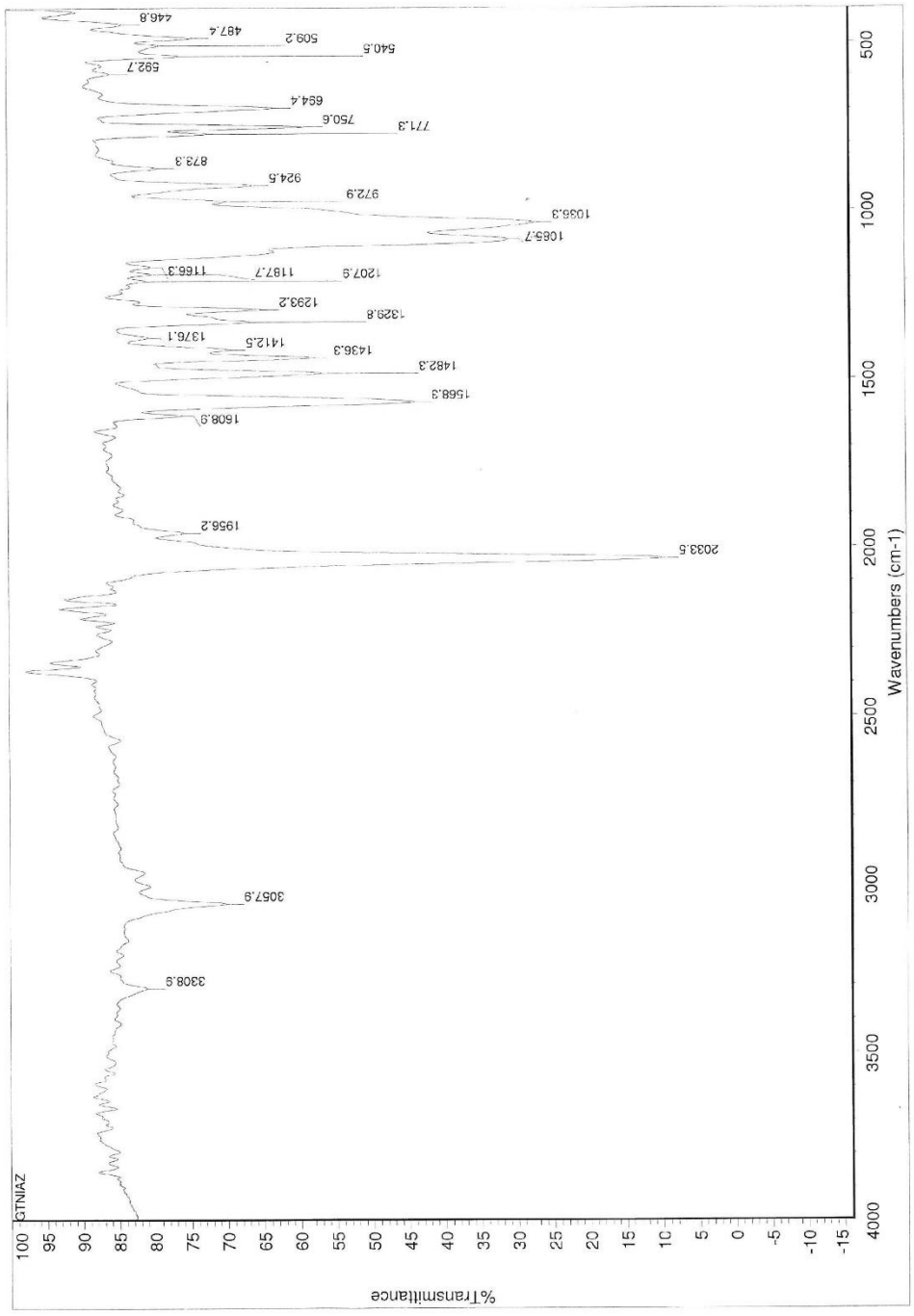

Fig. S1. IR spectrum of [Ni**L**N_3]BF_4.

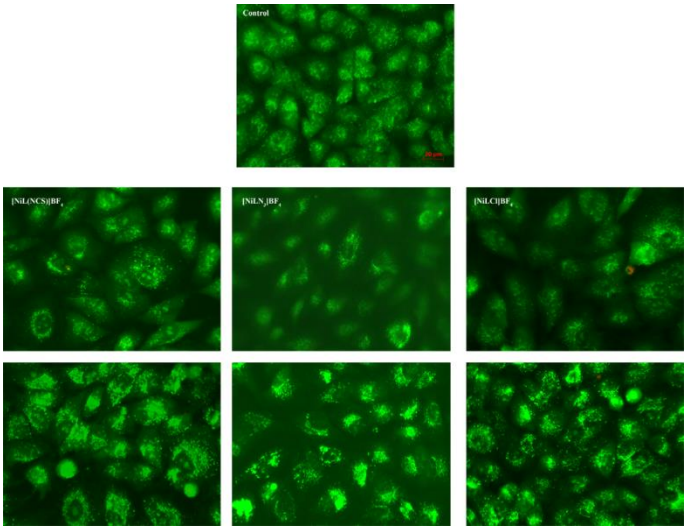

Fig. S2. Photomicrographs of acridine orange/ethidium bromide-stained control A549 cells and A549 cells exposed for 24h (upper images) and 48 h (lower images) to complexes $[NiL(NCS)]BF_4$ and $[NiLCl]BF_4$. Applied concentrations of complexes corresponded to 0.5 × IC_{50} values determined for 48 h.

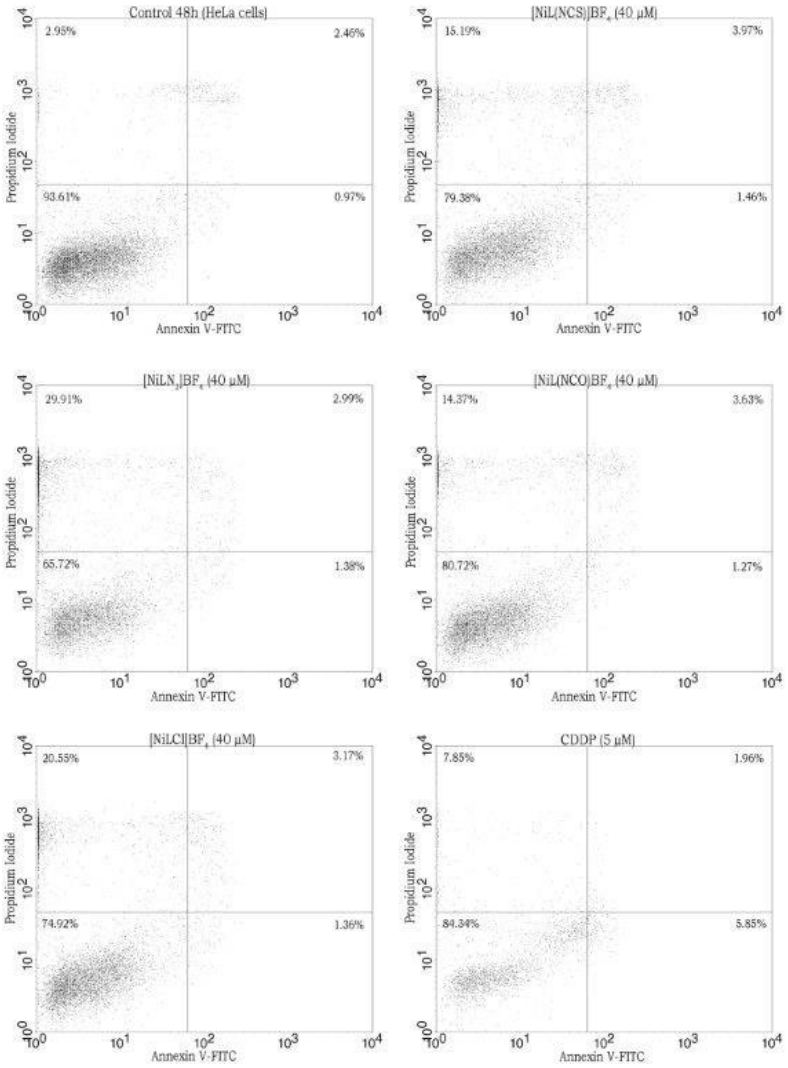

Fig. S3. Dot plot diagrams obtained by flow-cytometric analysis of treated HeLa cells after dual staining with Annexin V-FITC and PI. Annexin V-FITC/PI staining was performed after 48 h of HeLa cells exposure to nickel complex ([NiL(NCS)]BF_4 [NiL(N_3)]BF_4 [NiL(NCO)]BF_4, [NiLCl]BF_4) and CDDP with 40 µM concentration for nickel complexes and 5 µM concentration for cisplatin. Representative dot plots are given, presenting live cells at lower-left quadrant, FITC(-)/PI(-); early apoptotic cells at lower-right quadrant, FITC(+)/PI(-); late apoptotic or necrotic cells at upper-right quadrant, FITC(+)/PI(+); and dead cells at upper-left quadrant, FITC(-)/PI(+).

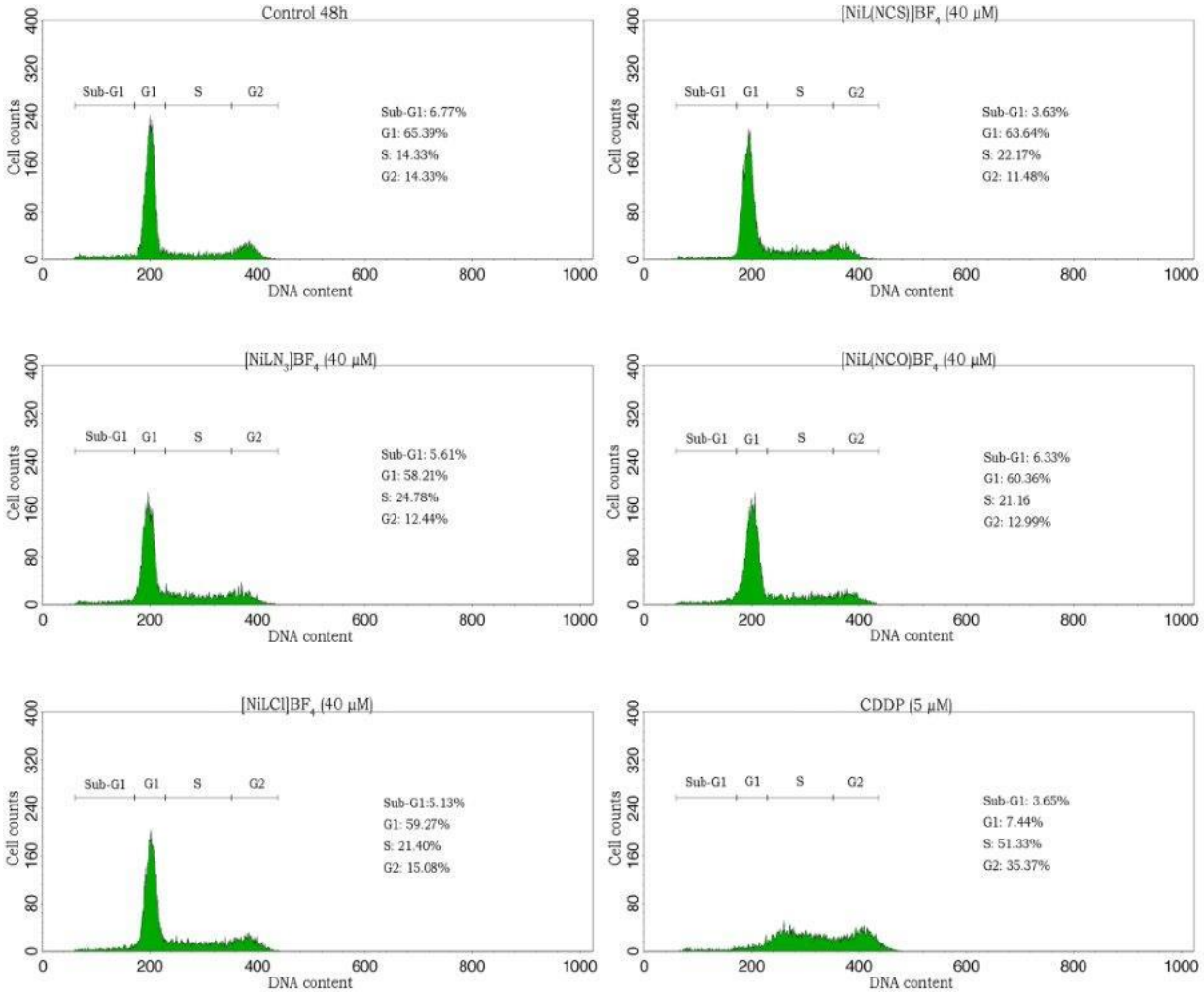

Fig. S4. Effect of the Ni(II) complexes ([Ni**L**(NCS)]BF_4, [Ni**L**(N_3)]BF_4, [Ni**L**(NCO)]BF_4 and [Ni**L**Cl]BF_4) and cisplatin (CDDP) on cell cycle progression of HeLa cells following 48 h incubation with 40 µM concentration for nickel (II) complexes and 5 µM concentration for cisplatin. Histograms presented are representative of three independent experiments.

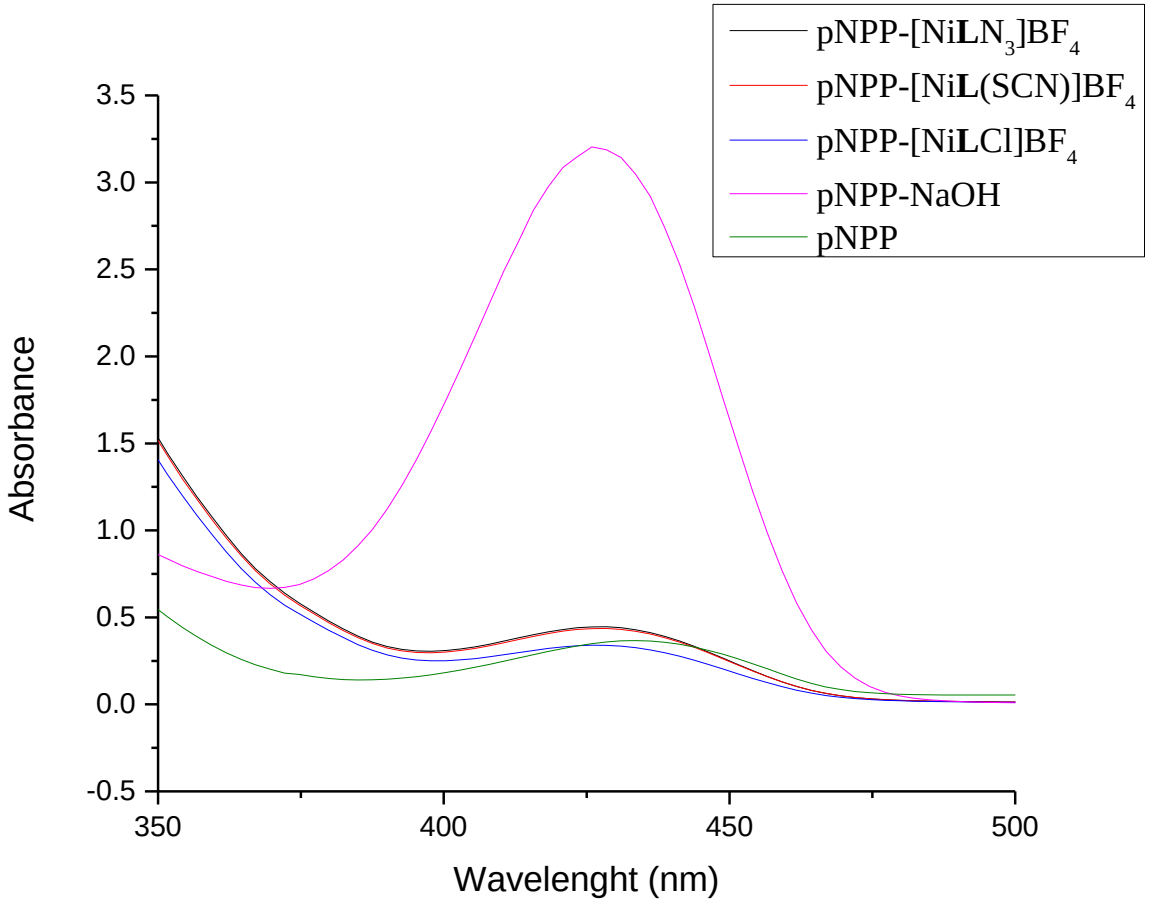

Fig. S5. Wavelength scan for hydrolysis of pNPP in the absence and presence of Ni(II) complexes and NaOH in 97.5 % DMSO. [pNPP] = 1×10^{-3} M; [Ni(II) complexes] = 5×10^{-5} M (in the NaOH control [NaOH] = 5×10^{-5} M).

Table S1. Hydrogen bonding geometry for [Ni**L**N_3]BF_4.

D – H ⋯ A	*d*(D – H)/ Å	*d*(H ⋯ A)/ Å	*d*(D ⋯ A)/ Å	<(DHA)/ º	Symmetry transformation for acceptors
C1–H1A···F1	0.96	2.34	3.229(8)	154	x, 1/2-y, -1/2+z
C1–H1B···F3	0.96	2.48	3.358(9)	152	1/2-x ,-y, -1/2+z
C2–H2A···F3	0.96	2.44	3.367(8)	163	x, 1/2-y, -1/2+z
C14–H14···N6	0.93	2.61	3.358(8)	138	1/2+x, y, 1/2-z