Supplementary Information

Synthesis and spectroscopic characterization of diorganotin(IV) complexes of N'–(4–hydroxypent–3–en–2–ylidene)isonicotinohydrazide: Chemotherapeutic potential validation by *in vitro* interaction studies with DNA/HSA, DFT, molecular docking and cytotoxic activity.

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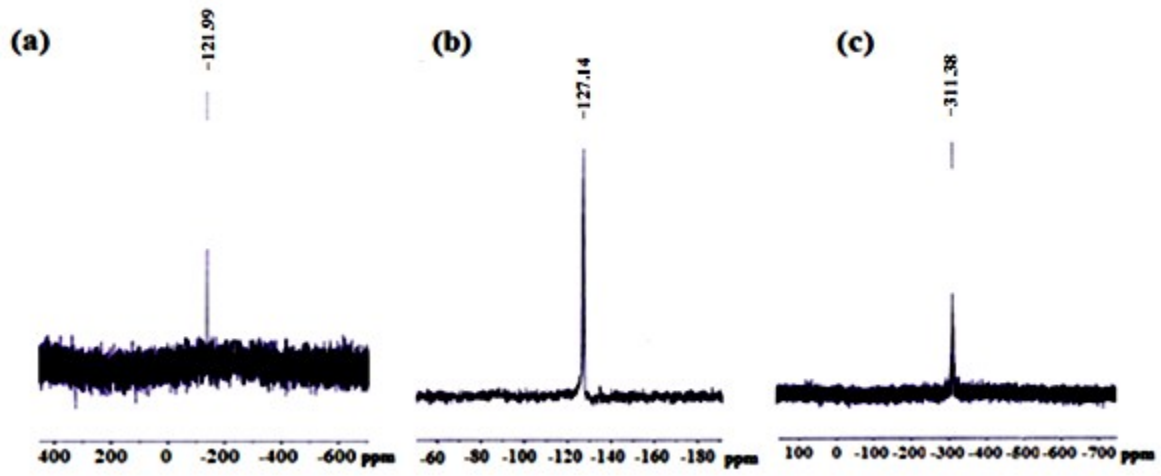
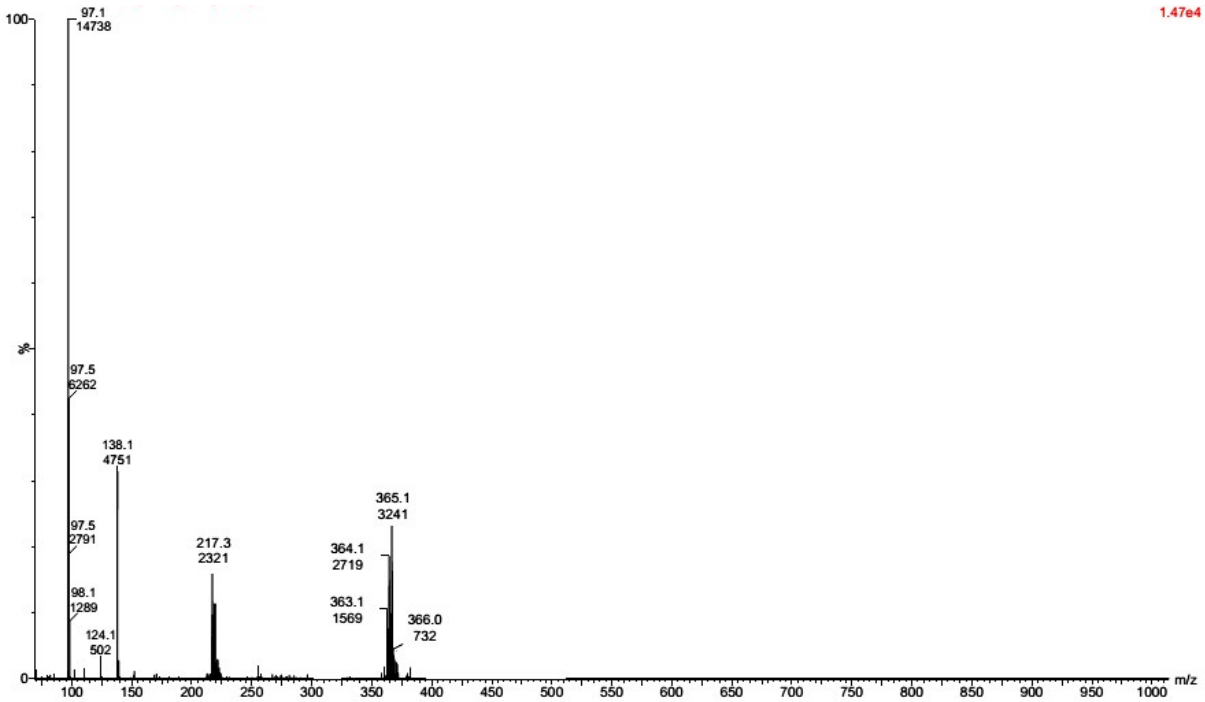
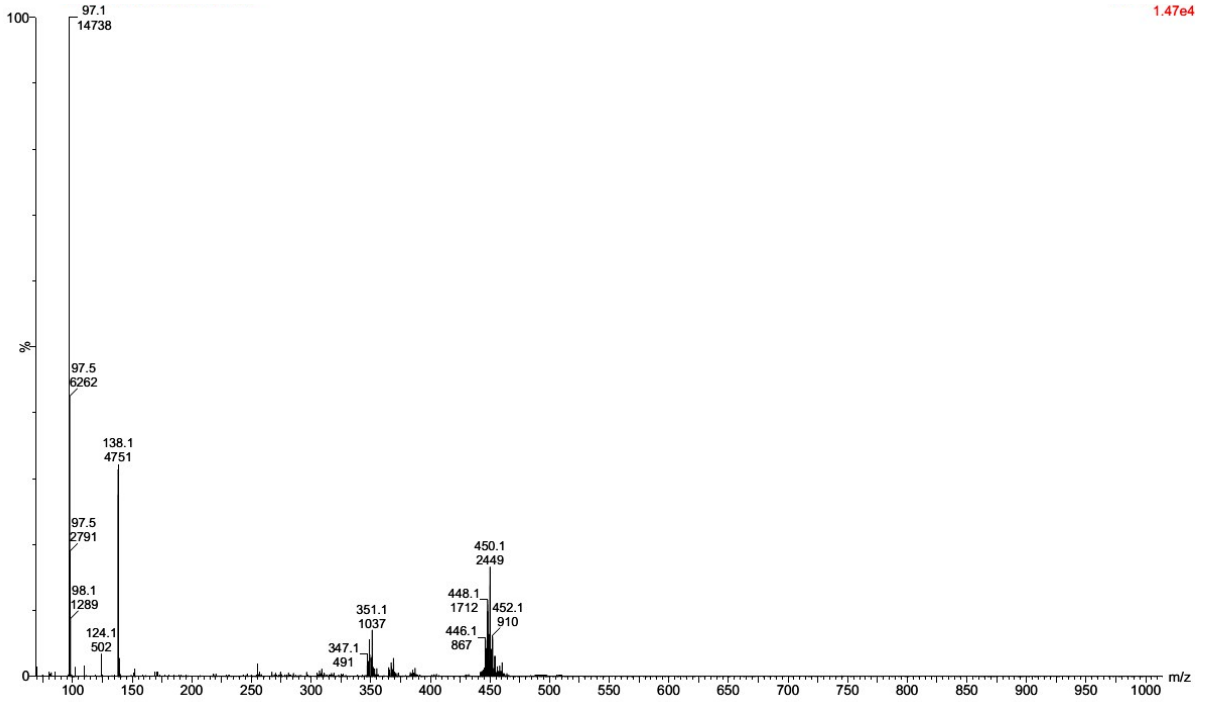


Fig. S1. ^{119}Sn NMR spectra of complexes (a) **1**, (b) **2** and (c) **3**.



(a)



(b)

Fig. S2. ESI MS spectra of diorganotin(IV) complexes (a) **1** and (b) **2**.

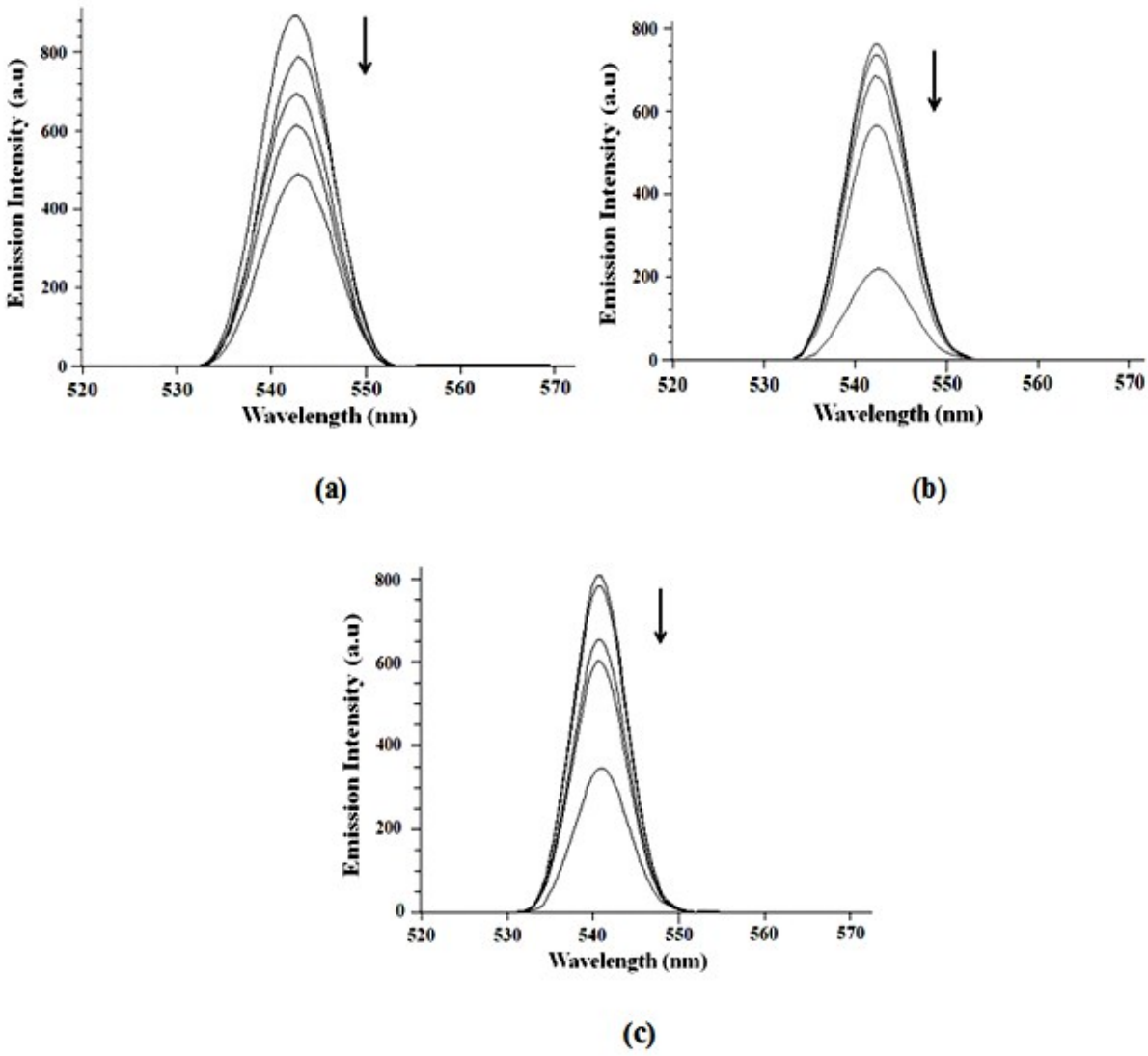


Fig. S3. Fluorescence spectra of complexes (a) **1**, (b) **2** and (c) **3** in Tris–HCl buffer (pH 7.2) with increasing concentration of complexes in presence of fixed concentration of EB–DNA ([DNA]/[EB]=1). Arrow indicates the change in intensity upon increasing concentration of complexes.

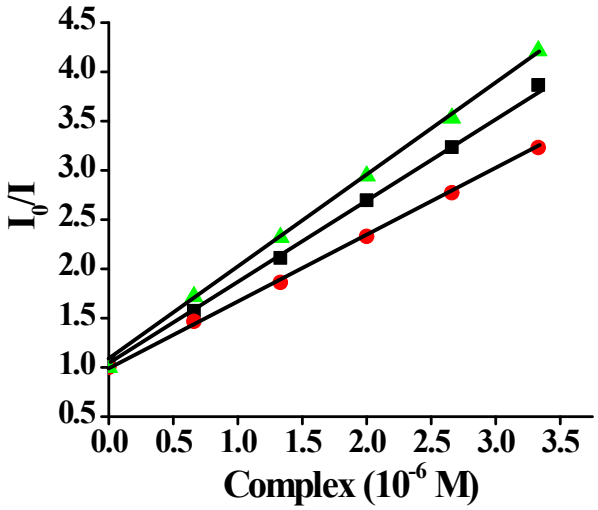
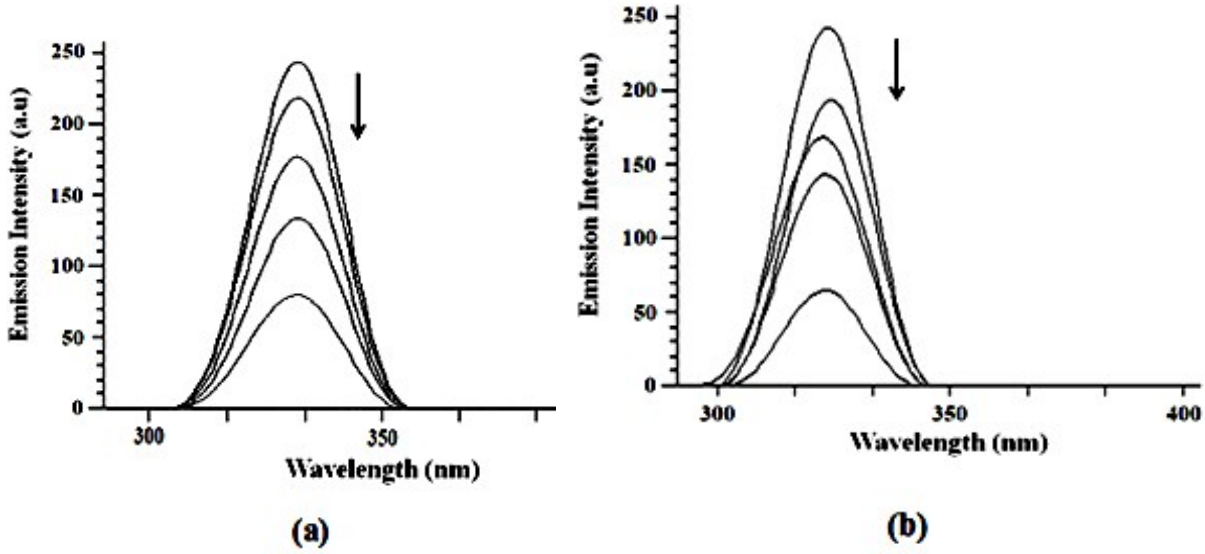
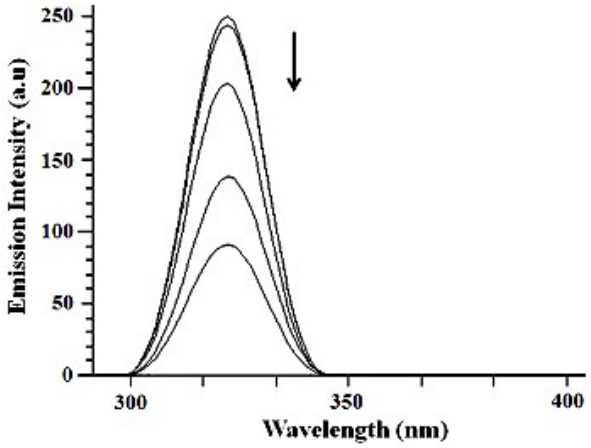


Fig. S4. Stern–Volmer plot of the EB–DNA fluorescence titration for complexes **1** (red), **2** (green) and **3** (black).





(c)

Fig. S5. Effect of different concentration of NaCl on the fluorescence spectra of complexes (a) **1**, (b) **2** and (c) **3**. Arrow indicates the gradual decrease of emission intensity as a function of NaCl concentration.

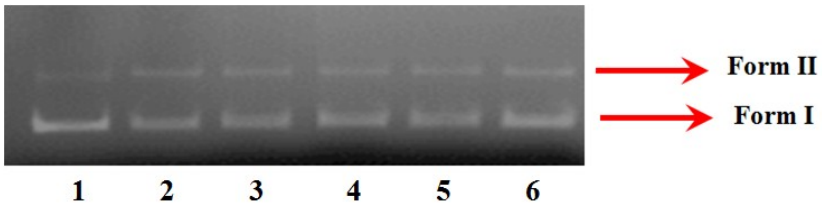


Fig. S6. Agarose gel electrophoresis patterns for the cleavage of pBR322 plasmid (300 ng) as a function of increasing concentration of **2** at 310 K after 45 min of incubation at different concentrations; Lane 1: DNA control; Lane 2: 2 μM of **2** + DNA; Lane 3: 4 μM of **2** + DNA; Lane 4: 6 μM of **2** + DNA; Lane 5: 8 μM of **2** + DNA; Lane 6: 10 μM of **2** + DNA.

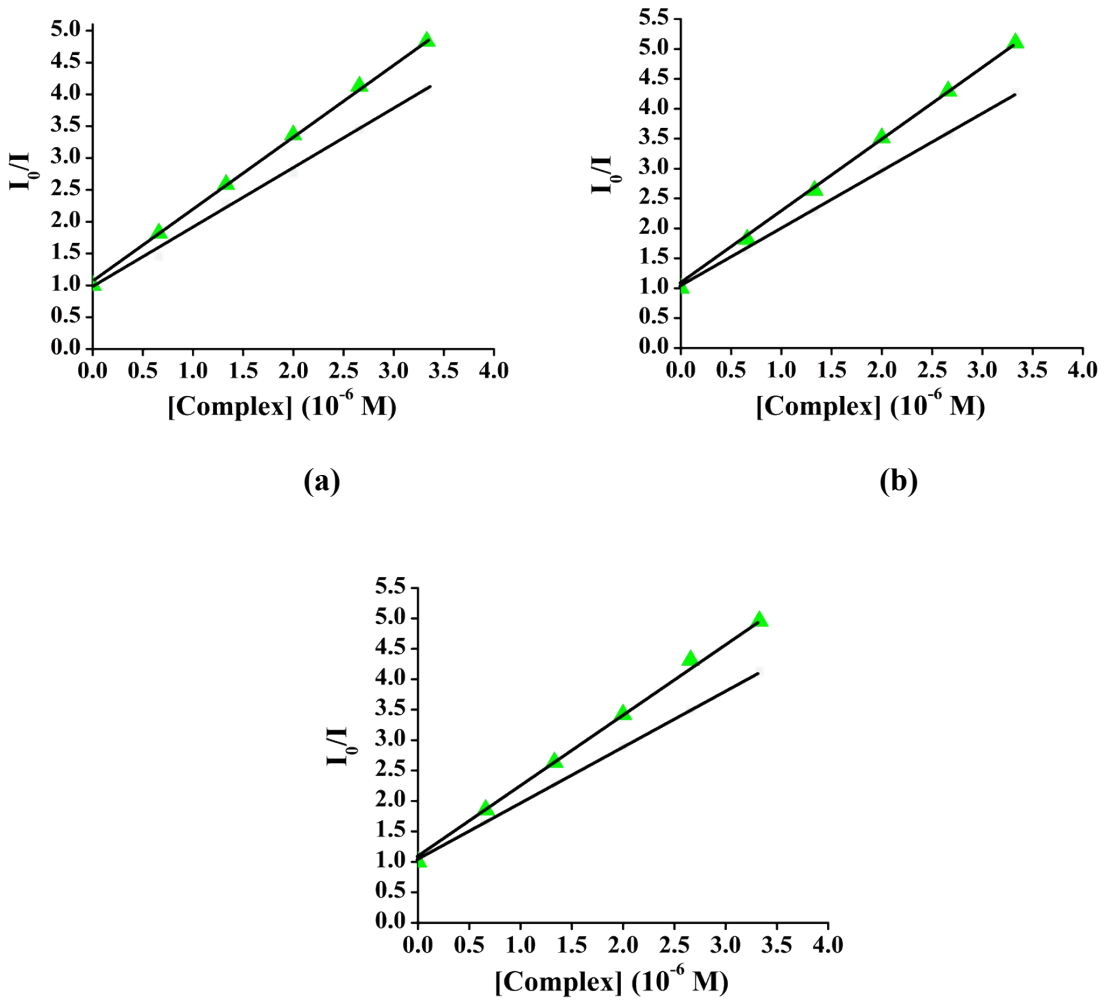


Fig. S7. Stern–Volmer plots of complexes (a) **1**, (b) **2** and (c) **3** at 298 (green), 310 K (black).

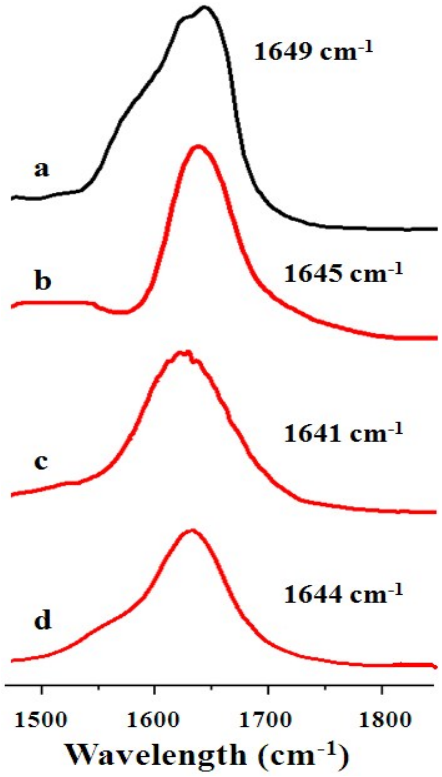


Fig. S8. FT IR difference spectra of the amide band of (a) HSA alone (1 x 10^{-3} M), (b) **1** + HSA, (c) **2** + HSA, and (d) **3** + HSA (1 x 10^{-3} M).

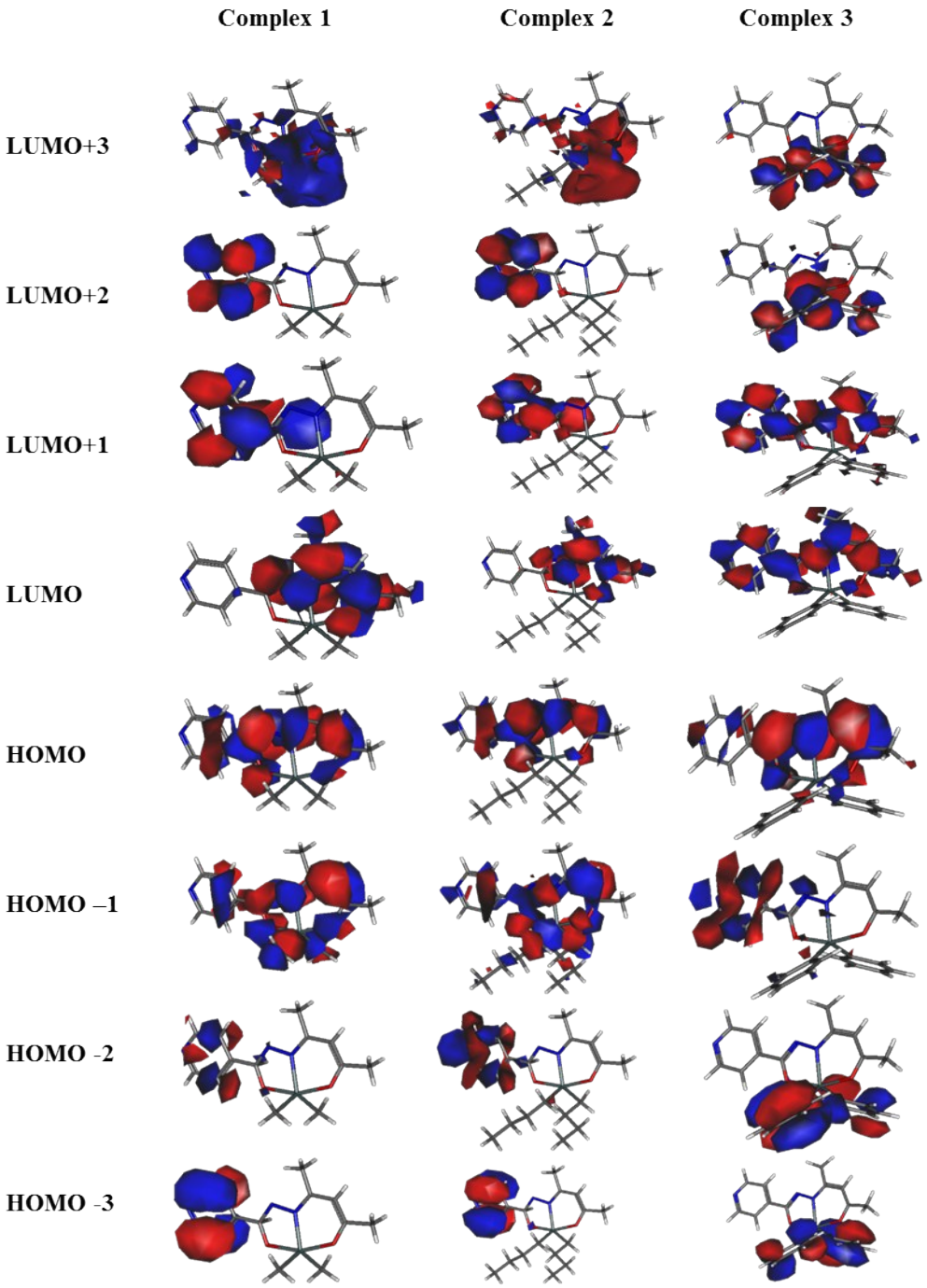


Fig. S9. Molecular orbital diagram for HOMOs and LUMOs for complex **1**–**3**.

Table S1: Selected bond lengths (Å) and angles (°) for complex **3.**

Bond Length

C1 N2 1.306(6)	C1 O1 1.311(6)	C1 C2 1.480(7)
C2 C3 1.391(7)	C2 C6 1.404(7)	C3 C4 1.388(7)
C4 N3 1.341(7)	C5 N3 1.336(7)	C5 C6 1.378(7)
C7 N1 1.326(6)	C7 C8 1.424(7)	C7 C11 1.498(7)
C8 C9 1.360(7)	C9 O2 1.302(6)	C9 C10 1.500(7)
C12 C17 1.385(7)	C12 C13 1.399(7)	C12 Sn1 2.112(5)
C13 C14 1.387(7)	C14 C15 1.389(8)	C15 C16 1.391(8)
C16 C17 1.381(7)	C18 C19 1.399(7)	C18 C23 1.408(7)
C18 Sn1 2.115(5)	C19 C20 1.383(7)	C20 C21 1.398(8)
C21 C22 1.384(8)	C22 C23 1.374(7)	N1 N2 1.398(5)
N1 Sn1 2.129(4)	O1 Sn1 2.130(3)	O2 Sn1 2.100(3)

Bond Angles

N2 C1 O1 125.6(4)	N2 C1 C2 117.2(4)	O1 C1 C2 117.2(4)
C3 C2 C6 117.5(5)	C3 C2 C1 121.9(5)	C6 C2 C1 120.6(4)
C4 C3 C2 118.3(5)	N3 C4 C3 124.7(5)	N3 C5 C6 123.9(5)
C5 C6 C2 119.3(5)	N1 C7 C8 122.5(4)	N1 C7 C11 118.5(4)
C8 C7 C11 119.0(4)	C9 C8 C7 127.9(5)	O2 C9 C8 125.4(5)
O2 C9 C10 114.7(5)	C8 C9 C10 119.9(5)	C17 C12 C13 118.5(5)
C17 C12 Sn1 121.4(4)	C13 C12 Sn1 120.2(4)	C14 C13 C12 120.9(5)
C13 C14 C15 119.3(5)	C14 C15 C16 120.5(5)	C17 C16 C15 119.3(5)
C16 C17 C12 121.5(5)	C19 C18 C23 118.5(5)	C19 C18 Sn1 120.8(4)
C23 C18 Sn1 120.6(4)	C20 C19 C18 121.1(5)	C19 C20 C21 119.1(5)
C22 C21 C20 120.5(5)	C23 C22 C21 120.2(5)	C22 C23 C18 120.5(5)
C7 N1 N2 116.0(4)	C7 N1 Sn1 128.7(3)	N2 N1 Sn1 115.2(3)
C1 N2 N1 111.5(4)	C5 N3 C4 116.2(5)	C1 O1 Sn1 111.6(3)
C9 O2 Sn1 128.7(3)	O2 Sn1 C12 94.47(17)	O2 Sn1 C18 93.46(16)
C12 Sn1 C18 124.22(18)	O2 Sn1 N1 85.49(14)	C12 Sn1 N1 121.87(16)
C18 Sn1 N1 113.76(17)	O2 Sn1 O1 160.46(13)	C12 Sn1 O1 94.83(16)
C18 Sn1 O1 95.45(16)	N1 Sn1 O1 75.01(14)	

Table S2. Selected bond angles for complexes **1** – **3**.

Bond angles	Calculated Complex **1**	Calculated Complex **2**	Calculated Complex **3**
C9 O2 Sn1	131.64	131.99	130.36
C12 Sn1 C18	120.37	123.21	130.60
C18 Sn1 N1	103.35	120.36	108.42
C18 Sn1 O1	105.64	101.99	95.31
C7 N1 Sn1	126.86	127.99	128.18
O2 Sn1 C12	88.01	92.86	95.58
O2 Sn1 N1	81.34	82.41	84.82
O2 Sn1 O1	149.88	156.77	158.34
N1 Sn1 O1	74.56	74.77	74.12
N2 N1 Sn1	115.58	115.54	114.85
C1 O1 Sn1	118.96	117.15	113.64
O2 Sn1 C18	97.22	92.86	95.31
C12 Sn1 O1	105.64	97.58	93.91

Table S3. Energy levels (eV) of MOs for complexes **1–3**, calculated in their ground state in the gas phase.

	Complex **1** (eV)	Complex **2** (eV)	Complex **3** (eV)	DNA (eV)
LUMO+3	−0.3570 (120)	−0.5983 (127)	−0.2566 (96)	
LUMO+2	−0.2310 (119)	−0.9066 (126)	−0.2111 (95)	
LUMO+1	−0.6557 (118)	−1.0051 (125)	−0.6435 (94)	
LUMO	−1.4351 (117)	−2.0460 (124)	−1.5039 (93)	1.14
HOMO	−4.6917 (116)	−5.7361 (123)	−4.7836 (92)	−1.27
HOMO−1	−6.2667 (115)	−6.9370 (122)	−6.4194 (91)	−1.33
HOMO−2	−6.7780 (114)	−7.0131 (121)	−6.7759 (90)	−1.69
HOMO−3	−6.9933(113)	−7.0265 (120)	−7.0058 (89)	−1.79