

Supplementary Information

Crystal structure determination, spectroscopic characterization and biological profile of tailored ionic molecular entity, Sn(IV) iminodiacetic acid–piperazinedium conjugate: *In vitro* DNA/RNA binding studies, Topo I inhibition activity, cytotoxic and systemic toxicity studies

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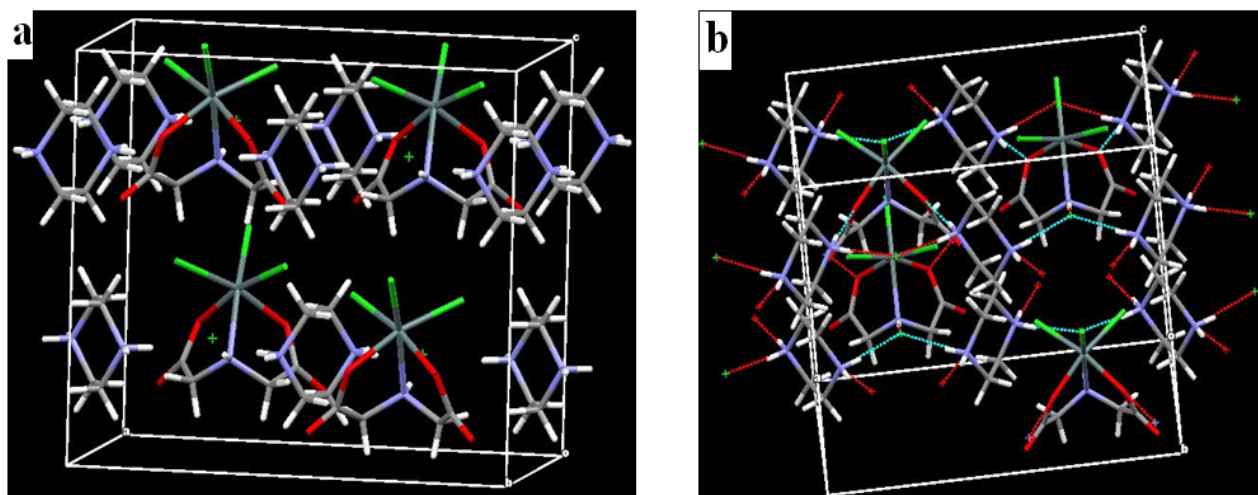


Fig. S1. Packing diagram of the complex 1, (a) without hydrogen bonding interactions and (b) with hydrogen bonding interactions.

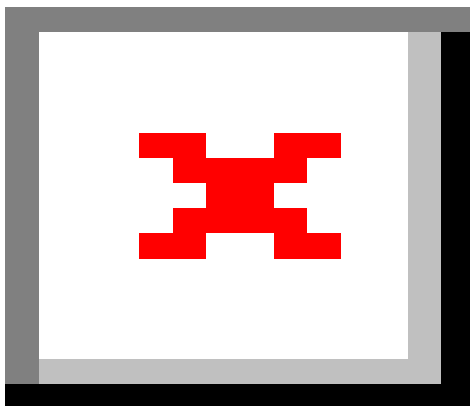


Fig. S2. ^{119}Sn NMR spectra of complex 1

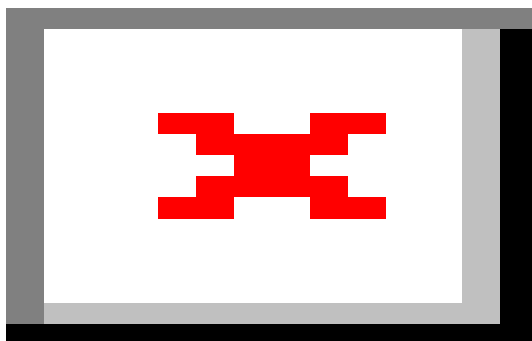


Fig. S3. Electrospray Ionization (ESI) mass spectrum of 1.

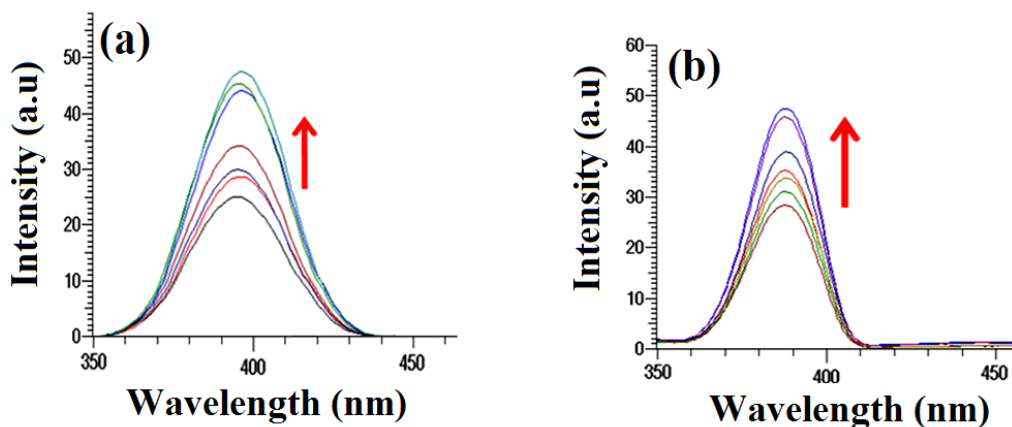


Fig. S4. Emission spectra of complex **1** in Tris-HCl buffer at pH 7.2 upon addition (a) ct-DNA and (b) yeast tRNA. $[DNA], [RNA] = 0.00\text{--}4.00 \times 10^{-5} \text{ M}$, $[Complex \mathbf{1}] = 1.67 \times 10^{-5} \text{ M}$ at 25 °C. Arrows show change in intensity with increasing concentration of DNA/RNA.

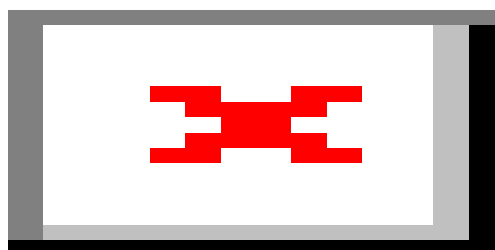


Fig. S5. CD spectra of (a) ct-DNA in absence and presence of **1** and (b) yeast tRNA in absence and presence of **1**. $[Complex \mathbf{1}] = [DNA] = [RNA] = 10^{-4} \text{ M}$.

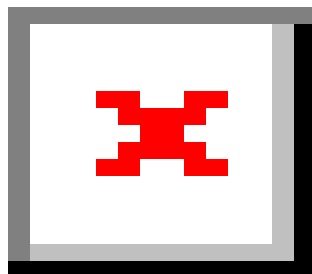


Fig. S6. Effect of increasing amount of **1** (red) and EB (green) on the relative viscosities (η/η_0) of ct-DNA in Tris-HCl buffer at pH 7.2. The concentration of ct-DNA was 0.10 mM, and the molar ratios of complex **1** or EB to DNA were 0.2, 0.4, 0.6, 0.8 and 1.0, respectively.

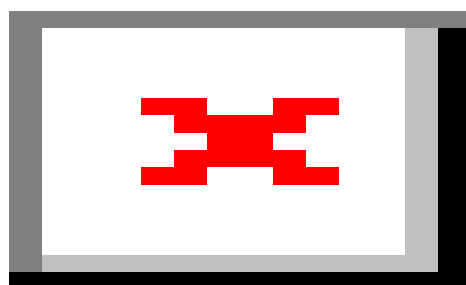


Fig. S7. FT-IR spectra and difference spectra [(ct-DNA/tRNA + **1**) solution-**1** solution] in the region of 1800-800 cm^{-1} for (a) free ct-DNA and in presence of **1** (b) free yeast tRNA and in presence of **1**.

Tables:**Table S1.** Selected bond lengths (Å) and angles (°) for complex **1**.

Bond lengths	(Å)
Sn(1) – Cl(1)	2.367 (8)
Sn(1) – Cl(2)	2.351 (1)
Sn(1) – O(1)	2.089 (2)
Sn(1) – N(1)	2.221 (3)
O(1) – C(2)	1.303 (3)
O(2) – C(2)	1.203 (3)
N(1) – C(1)	1.484 (4)
N(2) – C(3)	1.464 (5)
N(2) – C(4)	1.478 (3)
N(2)–H(2A)	0.920(2)
N(2)–H(2B)	0.921(2)

Bond Angles	(°)
Cl1–Sn1–Cl2	99.73(3)
Cl1–Sn1–O1	89.56(6)
Cl1–Sn1–N1	91.07(9)
Cl1–Sn1–O1	168.43(6)
Cl1–Sn1–Cl1	95.30(3)
Cl2–Sn1–O1	89.74(6)
Cl2–Sn1–N1	163.88(9)
Cl2–Sn1–O1	89.74(6)
Cl2–Sn1–Cl1	99.73(3)
Sn1–O1–C2	118.9(2)
O1–Sn1–N1	78.3(1)
O1–Sn1–O1	83.82(7)
N1–Sn1–O1	78.3(1)
N1–Sn1–Cl1	91.07(9)
O1–Sn1–Cl1	89.56(6)
Sn1–N1–C1	108.0(2)
O1–C2–C1	116.4(2)
O2–C2–C1	120.6(3)
Sn1–O1–C2	118.9(2)

Table S2. % Control growth against different concentration ($\mu\text{g/ml}$) of **1** and ADR of various human carcinoma cell lines: U373MG (CNS), PC3 (Prostate), Hop62 (Lung), HL60 (Leukemia), HCT15 (Colon), SK-OV-3 (Ovarian), HeLa (Cervix) and MCF7 (breast).

Human CNS Cancer Cell Line U373MG																
% Control Growth																
Drug Concentrations ($\mu\text{g/ml}$)																
Experiment 1				Experiment 2				Experiment 3				Average Values				
	10	20	40	80	10	20	40	80	10	20	40	80	10	20	40	80
Complex 1	82.8	81.4	49.0	44.1	86.3	41.7	37.9	35.1	83.5	40.3	34.0	33.3	84.2	54.5	40.3	37.5
ADR	75.9	57.7	50.4	32.6	82.1	58.1	56.3	44.8	58.8	56.7	54.2	36.1	72.3	57.5	53.7	37.9

Human Prostate Cancer Cell Line PC3																
% Control Growth																
Drug Concentrations ($\mu\text{g/ml}$)																
Experiment 1				Experiment 2				Experiment 3				Average Values				
	10	20	40	80	10	20	40	80	10	20	40	80	10	20	40	80
Complex 1	-33.0	-35.3	-37.4	-42.5	-35.0	-43.0	-44.0	-45.9	-56.8	-56.7	-59.3	-62.2	-41.6	-45.0	-46.9	-50.2
ADR	-30.7	-35.1	-36.8	-39.0	-51.2	-61.1	-63.6	-66.4	-59.6	-63.0	-67.2	-68.6	-47.2	-53.1	-55.9	-58.0

Human Lung Cancer Cell Line Hop62																
% Control Growth																
Drug Concentrations ($\mu\text{g/ml}$)																
Experiment 1				Experiment 2				Experiment 3				Average Values				
	10	20	40	80	10	20	40	80	10	20	40	80	10	20	40	80
Complex 1	-81.1	-81.6	-82.6	-77.5	-81.5	-86.5	-86.6	-87.8	-81.4	-84.4	-84.7	-85.3	-81.3	-84.2	-84.6	-83.5
ADR	-3.7	-13.7	-53.2	-65.1	-28.2	-35.9	-62.5	-72.8	-25.8	-28.8	-57.8	-69.4	-19.2	-26.1	-57.8	-69.1

Human Leukemia Cell Line HL60																
% Control Growth																
Drug Concentrations ($\mu\text{g/ml}$)																
Experiment 1				Experiment 2				Experiment 3				Average Values				
	10	20	40	80	10	20	40	80	10	20	40	80	10	20	40	80
Complex 1	-22.3	-22.8	-27.3	-32.7	-26.9	-33.5	-34.0	-47.5	-28.4	-33.3	-40.4	-46.0	-25.9	-29.9	-33.9	-42.1
ADR	-8.2	-16.7	-27.9	-36.0	-13.5	-26.8	-27.5	-34.2	-13.1	-18.2	-28.8	-34.2	-11.6	-20.6	-28.1	-34.8

Human Colon Cancer Cell Line HCT15																
% Control Growth																
Drug Concentrations ($\mu\text{g/ml}$)																
Experiment 1				Experiment 2				Experiment 3				Average Values				
10	20	40	80	10	20	40	80	10	20	40	80	10	20	40	80	
Complex 1	-29.6	-39.0	-42.0	-59.1	-29.6	-41.2	-45.7	-58.2	-45.6	-46.2	-52.4	-86.5	-35.0	-42.2	-46.7	-67.9
ADR	-14.2	-6.4	-18.3	-19.5	-2.7	-9.1	-9.5	-14.5	-15.3	-20.6	-21.5	-21.6	-10.7	-12.0	-16.4	-18.6

Human Ovarian Cancer Cell Line SK-OV-3																
% Control Growth																
Drug Concentrations ($\mu\text{g/ml}$)																
Experiment 1				Experiment 2				Experiment 3				Average Values				
10	20	40	80	10	20	40	80	10	20	40	80	10	20	40	80	
Complex 1	-71.4	-82.5	-83.9	-84.8	-68.8	-78.8	-82.2	-84.6	-64.2	-78.2	-85.5	-85.6	-68.1	-79.8	-83.9	-85.0
ADR	20.9	13.0	-14.1	-17.7	8.5	8.2	-22.0	-28.2	11.7	6.8	-22.2	-25.3	13.7	9.3	-19.5	-23.7

Human Cervix Cancer Cell Line HeLa																
% Control Growth																
Drug Concentrations ($\mu\text{g/ml}$)																
Experiment 1				Experiment 2				Experiment 3				Average Values				
10	20	40	80	10	20	40	80	10	20	40	80	10	20	40	80	
Complex 1	-0.3	-5.0	-21.4	-29.6	-52.4	-62.1	-74.1	-76.9	-47.3	-57.2	-72.1	-81.0	-33.4	-41.4	-55.9	-62.5
ADR	1.3	1.3	-7.1	-11.2	-75.7	-78.8	-80.0	-81.2	-71.3	-76.2	-78.6	-79.0	-48.6	-51.2	-55.2	-57.2

Human Breast Cancer Cell Line MCF7																
% Control Growth																
Drug Concentrations ($\mu\text{g/ml}$)																
Experiment 1				Experiment 2				Experiment 3				Average Values				
10	20	40	80	10	20	40	80	10	20	40	80	10	20	40	80	
Complex 1	-39.0	-48.0	-52.9	-55.3	-47.8	-57.2	-57.3	-58.6	-38.6	-49.7	-56.1	-54.5	-41.8	-51.6	-55.4	-56.1
ADR	-18.8	-24.2	-48.0	-58.3	-28.8	-31.9	-50.2	-65.9	-20.3	-22.2	-53.7	-63.4	-22.7	-26.1	-50.6	-62.6