SUPPLEMENTARY MATERIALS

Synthesis, characterization, DNA interaction, molecular docking, α-amylase and α-glucosidase inhibition studies of a water soluble Zn(II) phthalocyanine

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Abbreviations

H_2O_2 : Hydrogen peroxide

AA : Ascorbic acid

ME : 2-Mercaptoethanol

DMSO : Dimethyl sulfoxide

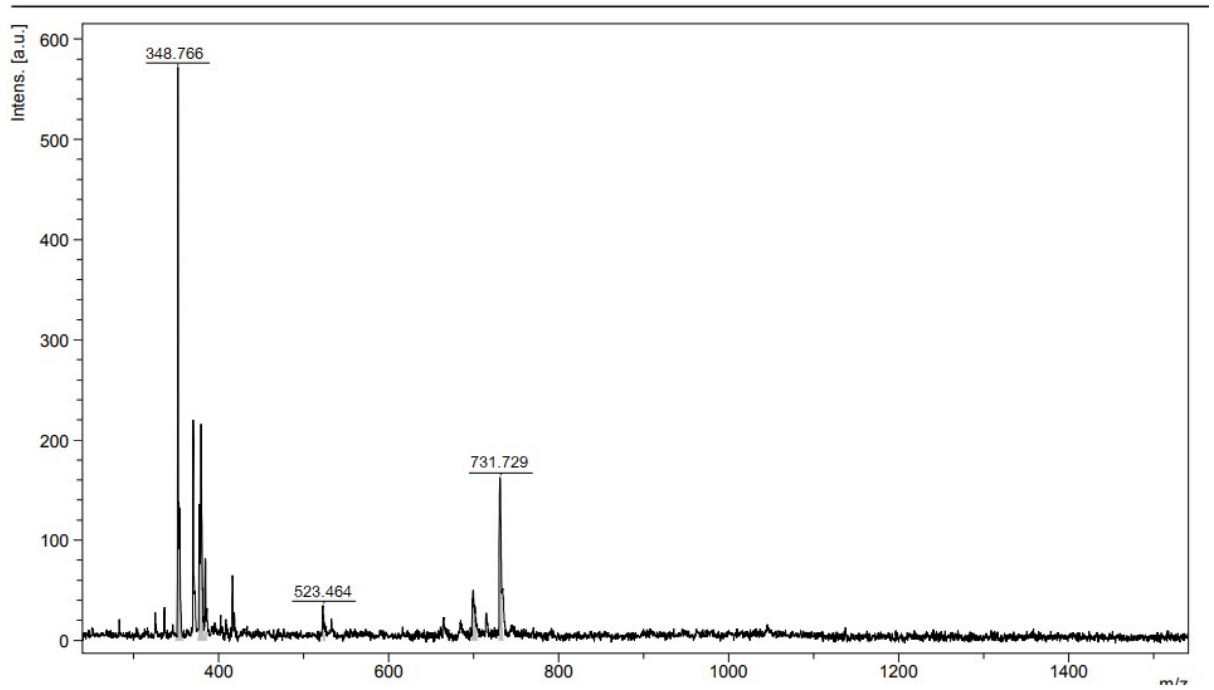
NaN_3 : Sodium azide

SOD : Superoxide dismutase

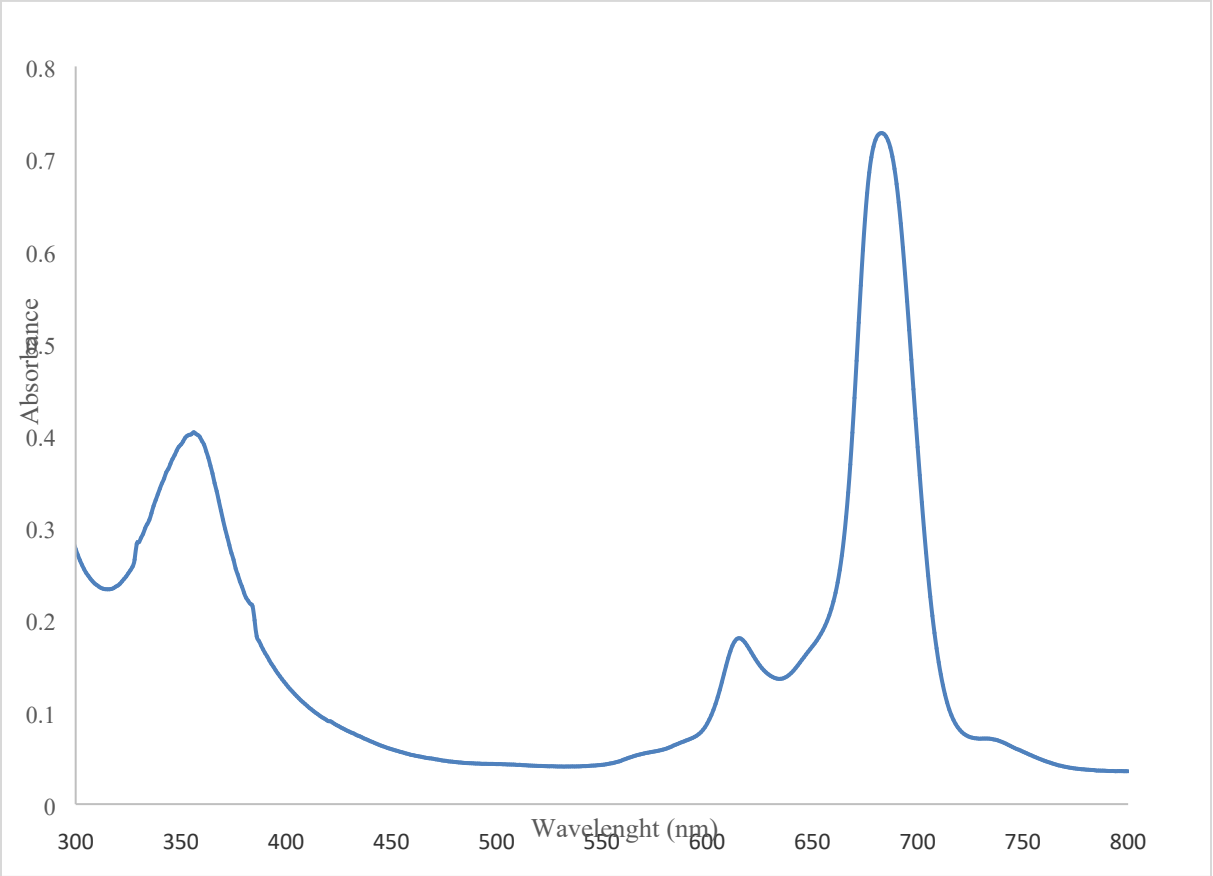
2. Materials and Methods

2.1. Materials

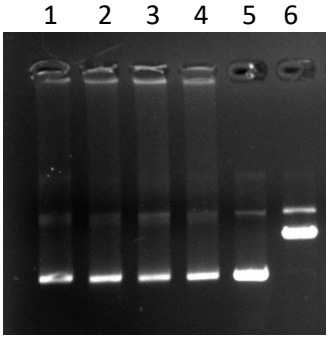
The reagents and chemicals were purchased from Merck and Sigma-Aldrich and used without further purification. The IR spectra were recorded on a Perkin Elmer 1600 FT-IR spectrophotometer using KBr pellets. Spectrophotometric tests were performed using Perkin Elmer Lambda 25 UV–Vis Spectrometer. Deoxyribonucleic acid sodium salt from calf thymus (CT-DNA) was purchased from Sigma-Aldrich. pBR322 was obtained from Prof. Dr. Ali Osman Beldüz (Karadeniz Technical University, Faculty of Science, Department of Biology, Trabzon, Türkiye). Plasmid DNA and CT-DNA concentrations were measured by using Thermo Scientific NonoDrop™ 2000 Microvolume Spectrophotometer. The denaturation profiles of CT-DNA and CT-DNA- ZnPc-2 solutions were evaluated using a Cary 100 Bio UV/VIS spectrophotometer equipped with a Peltier thermostatted 6×6 multicell changer and a temperature controller with an in situ temperature probe (Varian).



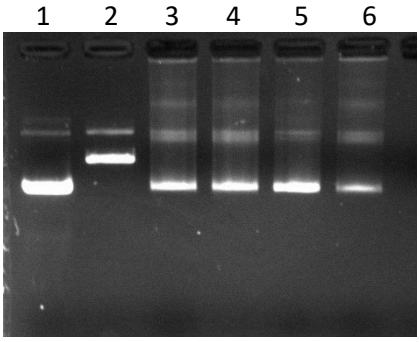
Supplementary Figure 1. MALDI-TOF spectrum of **ZnPc-2**



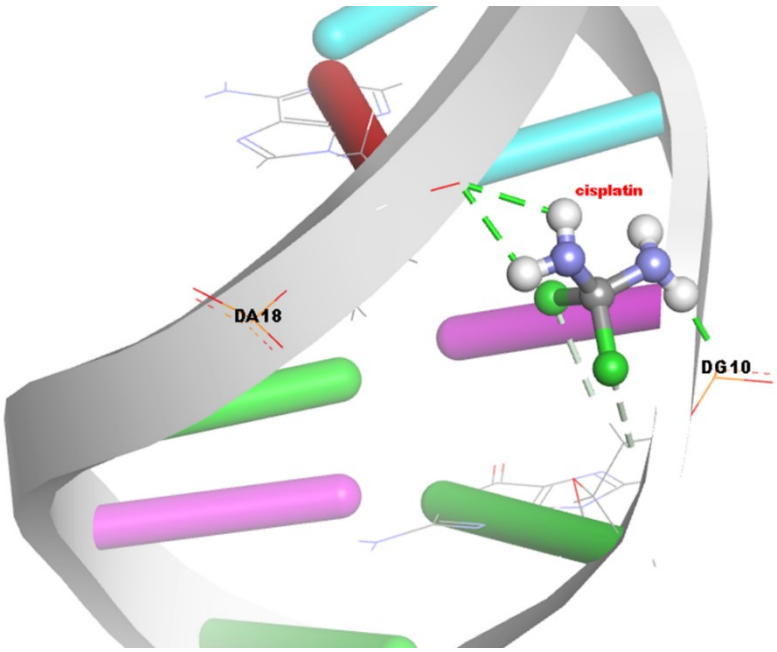
Supplementary Figure 2. UV-Vis spectrum of **ZnPc-2** in DMSO



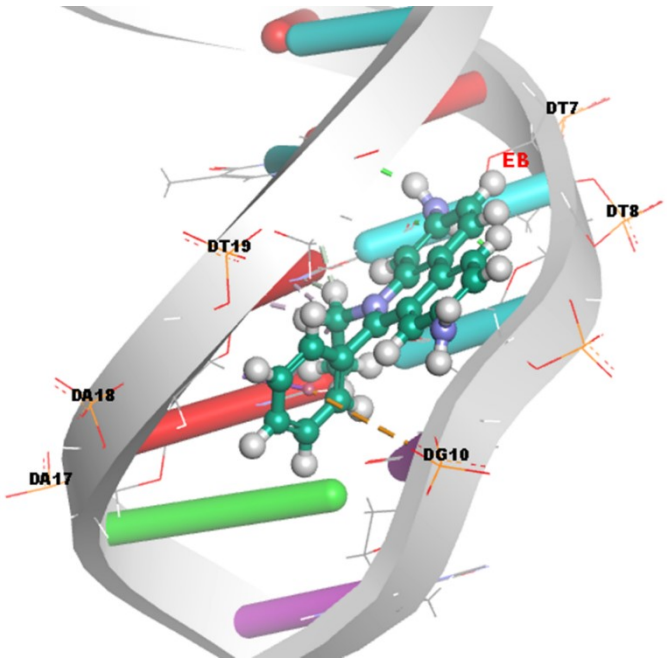
Supplementary Figure 3. pBR322 DNA cleavage activity of ZnPc-2 complex in the presence of some reducing/oxidizing agents. Lane 1; pBR322 (240 ng) + ZnPc-2(10 μM), Lane 2; pBR322 (240 ng) + ZnPc-2 (10 μM) + H_2O_2 (1 mM), Lane 3; pBR322 (240 ng) + ZnPc-2 (10 μM) + AA (1 mM), Lane 4; pBR322 (240 ng) + ZnPc-2 (10 μM) + ME (1 mM), Lane 5; pBR322 (240 ng), Lane 6; pBR322 (240 ng)-*Eco*RI.



Supplementary Figure 4. Agarose gel electrophoresis pattern for the cleavage of pBR322 by ZnPc-2 in the presence of standard radical scavengers. Lane 1; pBR322 (240 ng), Lane 2; pBR322 (240 ng)-*Eco*RI, Lane 3; pBR322 (240 ng) + ZnPc-2 (10 μM), Lane 4; pBR322 (240 ng) + ZnPc-2 (10 μM) + DMSO (10 mM), Lane 5; pBR322 (240 ng) + ZnPc-2 (10 μM) + NaN_3 (10 mM), Lane 6; pBR322 (240 ng) + ZnPc-2 (10 μM) + SOD (10 U).



Supplementary Figure 5. Docking conformation and interactions of cisplatin with DNA.



Supplementary Figure 6. Docking conformation and interactions of ethidium bromide (EB) with DNA.

Supplementary Table 1. Interactions types and distances of the compound **ZnPc-2** against DNA, ethidium bromide (EB) and cisplatin as positive compounds of the target, respectively.

Distance Å	Bonding	Binding site of target (DNA)	Binding site of ligand (ZnPc-2)
5.5407	Electrostatic	A:DC9:OP1	:ZnPc-2:Zn
3.9480	Electrostatic	B:DT20:OP1	:ZnPc-2:Zn
4.3635	Electrostatic	A:DG10:OP1	:ZnPc-2:N
3.8554	Electrostatic	B:DT19:OP1	:ZnPc-2:N
5.5173	Electrostatic	B:DT20:OP1	:ZnPc-2:N
5.4063	Electrostatic	B:DC21:OP2	:ZnPc-2:N

5.2324	Electrostatic	A:DT8:OP1	:ZnPc-2:N
5.0046	Electrostatic	B:DC21:OP1	:ZnPc-2:N
2.3451	Hydrogen Bond	B:DT20:H5'2	:ZnPc-2:N
2.3603	Hydrogen Bond	B:DA18:O3'	:ZnPc-2:H32
2.3184	Hydrogen Bond	B:DA18:O3'	:ZnPc-2:H35
1.7864	Hydrogen Bond	B:DT19:OP1	:ZnPc-2:H37
2.1986	Hydrogen Bond	A:DG10:OP1	:ZnPc-2:H40
1.9822	Hydrogen Bond	A:DT7:O3'	:ZnPc-2:H74
3.7922	Electrostatic	B:DT20:OP1	:ZnPc-2
4.4550	Electrostatic	B:DT20:OP2	:ZnPc-2
4.7454	Electrostatic	B:DT20:OP2	:ZnPc-2
2.3418	Hydrophobic	B:DT19:H4'	:ZnPc-2
Distance Å	**Bonding**	**Binding site of target (DNA)**	**Binding site of ligand (EB)**
2.1297	Hydrogen Bond	B:DT19:O2	:EB:H19
2.3222	Hydrogen Bond	A:DT7:O2	:EB:H20
2.2932	Hydrogen Bond	A:DT8:O4'	:EB:H20
2.0460	Hydrogen Bond	B:DA18:N3	:EB:H12
2.6319	Hydrogen Bond	B:DT19:O4'	:EB:H12
4.0589	Electrostatic	A:DG10:OP1	:EB
2.6028	Hydrophobic	B:DA18:H4'	:EB
4.6736	Hydrophobic	A:DC9	:EB:C21
4.2178	Hydrophobic	B:DA17	:EB:C21
4.7243	Hydrophobic	B:DA18	:EB:C21
4.3887	Hydrophobic	B:DA18	:EB:C21
Distance Å	**Bonding**	**Binding site of target (DNA)**	**Binding site of ligand (cisplatin)**
1.8182	Hydrogen Bond	A:DG10:OP1	cisplatin:H6
2.4486	Hydrogen Bond	B:DA18:O3'	cisplatin:H8
2.4875	Hydrogen Bond	B:DA18:O3'	cisplatin:H9
2.6658	Hydrogen Bond	A:DG10:H5'1	cisplatin:Cl5
2.6813	Hydrogen Bond	A:DG10:H5'2	cisplatin:Cl2