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Supplementary Materials

Multicharged Phthalocyanines as Selective Ligands for G-Quadruplex DNA Structures

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1.1 UV-Vis

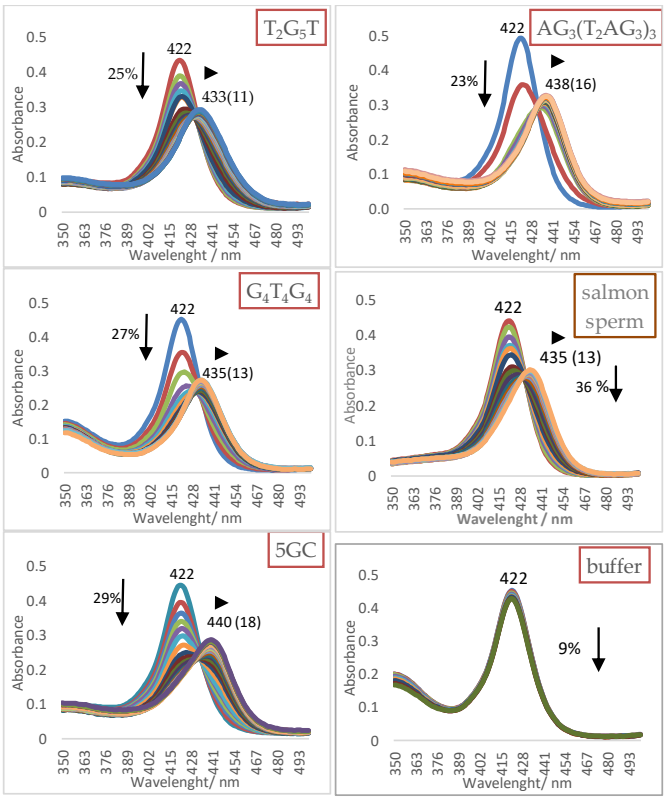

Figure S1. – UV-Vis spectra obtained in the titrations of **TMPyP** with GQ and duplex DNA sequences in PBS.

Table S1. – Spectroscopic data obtained in the titrations of **TMPyP** with different DNA sequences.

TMPyP	Hypochromism/ Hyperchromism (%)	Bathochromism (nm)
(T_2G_5T)	- 25	11
$(G_4T_4G_4)_2$	- 27	13
$AG_3(T_2AG_3)_3$	- 23	16
5GC	- 29	18
Salmon sperm	- 36	13
PBS buffer	- 9	0

Table S2. - Band maxima for **ZnPcs1-4** in PBS and DMSO solutions.

Ligand	Band maximum in PBS (nm)	Band maximum in DMSO (nm)	Band maxima in PBS at the end of the titrations (nm)*
ZnPc1	672	685	691/692
ZnPc2	690	702	706/707
ZnPc3	685	686	686
ZnPc4	677	683	692/693

* The presented value depends on the DNA structure studied.

Table S3. – Name, molar extinction coefficients and band maxima for **ZnPcs1-4** and **TMPyP** in PBS.

Ligand	Name	Molar extinction coefficients	Band maxima (nm)
ZnPc1	2,9(10),16(17),23(24)-tetrakis(4-pyridylsulphanyl) phthalocyaninatozinc(II)	78217	638 / 672
ZnPc2	2,3,9,10,16,17,23,24-Octakis(4-pyridylsulphanyl) phthalocyaninatozinc(II)	70808	658 /690
ZnPc3	2,9(10),16(17),23(24)-Tetrakis(4-methoxypyridinium-1-yl) phthalocyaninatozinc(II)	23956	628 / 685
ZnPc4	2,3,9,10,16,17,23,24-Octakis(4-methoxypyridinium-1-yl) phthalocyaninatozinc(II)	106299	636 / 677
TMPyP	5,10,15,20-tetrakis(N-methylpyridinium-4-yl)porphyrin	226000	422

1.2 Fluorimetric Titrations

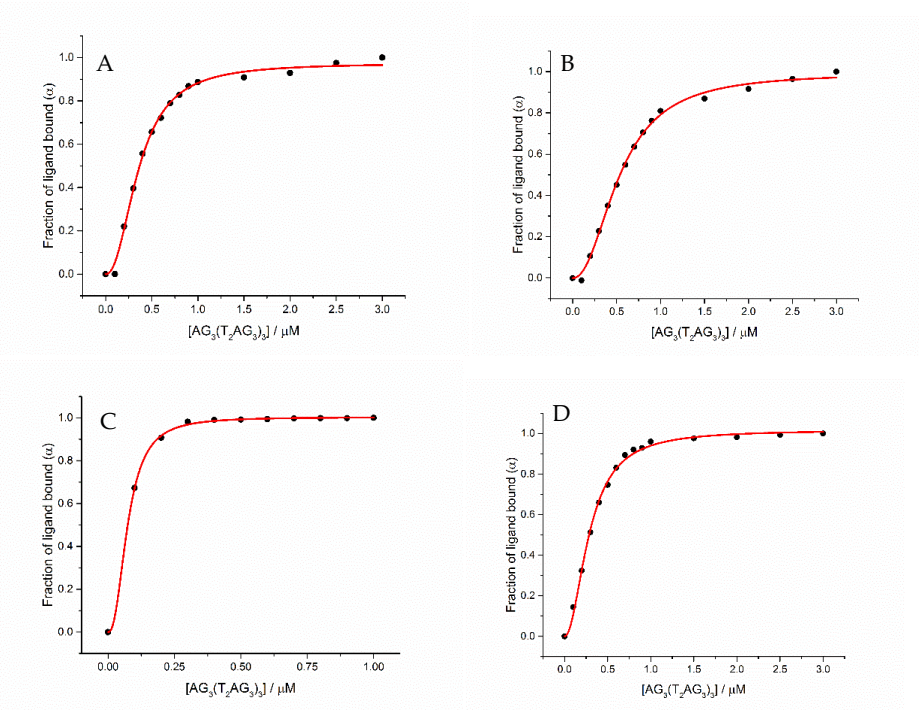

Figure S2. Saturation binding plots of ligands A) **ZnPc1**, B) **ZnPc2**, C) **ZnPc4** and D) **TMPyP** in the presence of increasing concentrations of unimolecular GQ $AG_3(T_2AG_3)_3$ and fitted to Hill binding equation (red curve).

1.3 Circular Dichroism

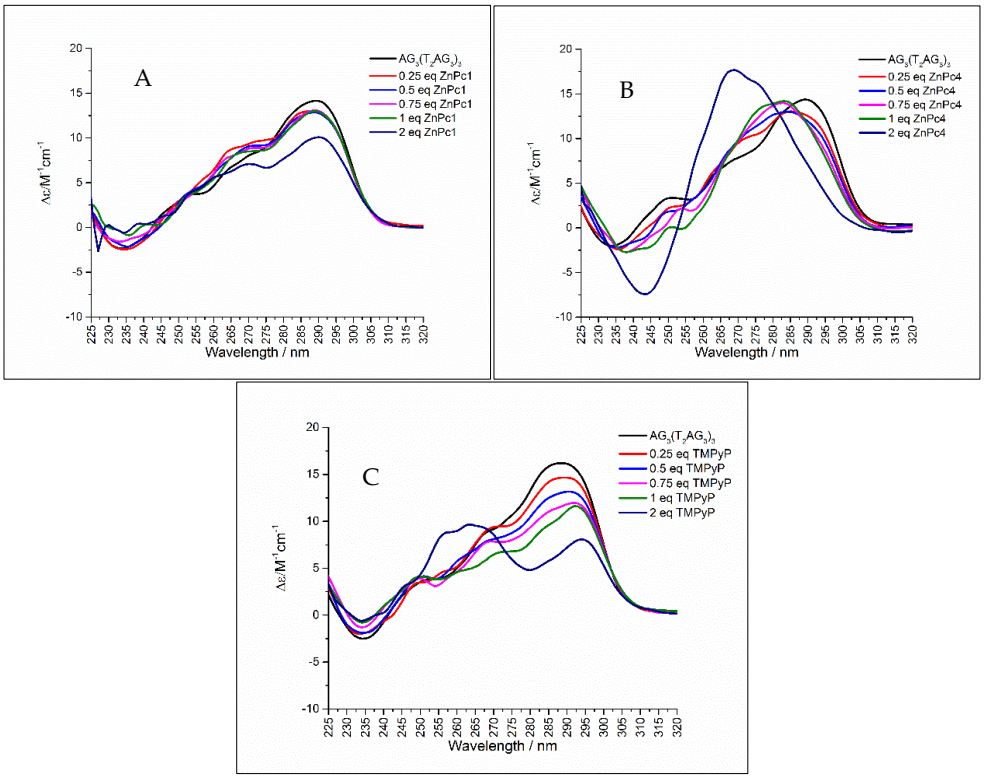

Figure S3. CD spectra obtained for unimolecular GQ $AG_3(T_2AG_3)_3$ in the presence and absence of A) **ZnPc1**, B) **ZnPc4** and C) **TMPyP**.

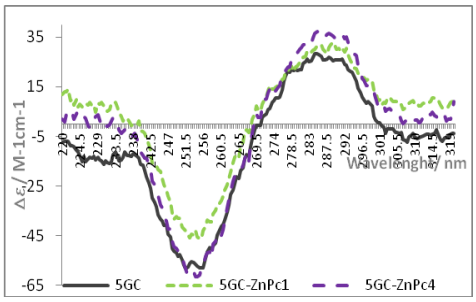

Figure S4. CD spectra obtained for the duplex oligonucleotide 5GC in the presence and absence of **ZnPc1** and **ZnPc4**.

1.4 List of abbreviations

T - thymine; **A** - adenine; **G** - guanine; **Δλ** - wavelenght deviation

DNA - deoxyribonucleic acid; **GQ** - G-Quadruplexes; **Pcs** – phthalocyanines;

TO - thiazole orange; **PBS** – phosphate buffer solution

DC50 - concentration of ligands required to decrease the fluorescence of the probe by 50%

IC50 - concentration of the ligand required to reduce the cell viability by 50%

T_2AG_3 - human telomeric sequence repeat –5′- TTA GGG-3′

T_2G_5T - tetramolecular G-quadruplex sequence - 5′-TTG GGG T-3′

$(G_4T_4G_4)_2$ - bimolecular G-quadruplex sequence - 5'-GGG GTT TTG GGG-3'

$AG_3(T_2AG_3)_3$ - unimolecular G-Quadruplex - 5'-AGG GTT AGG GTTAGG GTT AGGG-3'

5GC - double strand DNA - 5'-GCG CGC GCG C-3'

UV-Vis - UV-Visible spectroscopy; **G4-FID** - G-Quadruplex fluorescent intercalator displacement assay; **CD** - circular dichroism