

# Ligand 5,10,15,20-Tetra(*N*-methyl-4-pyridyl)porphine (TMPyP4) Prefers the Parallel Propeller-Type Human Telomeric G-Quadruplex DNA over Its Other Polymorphs

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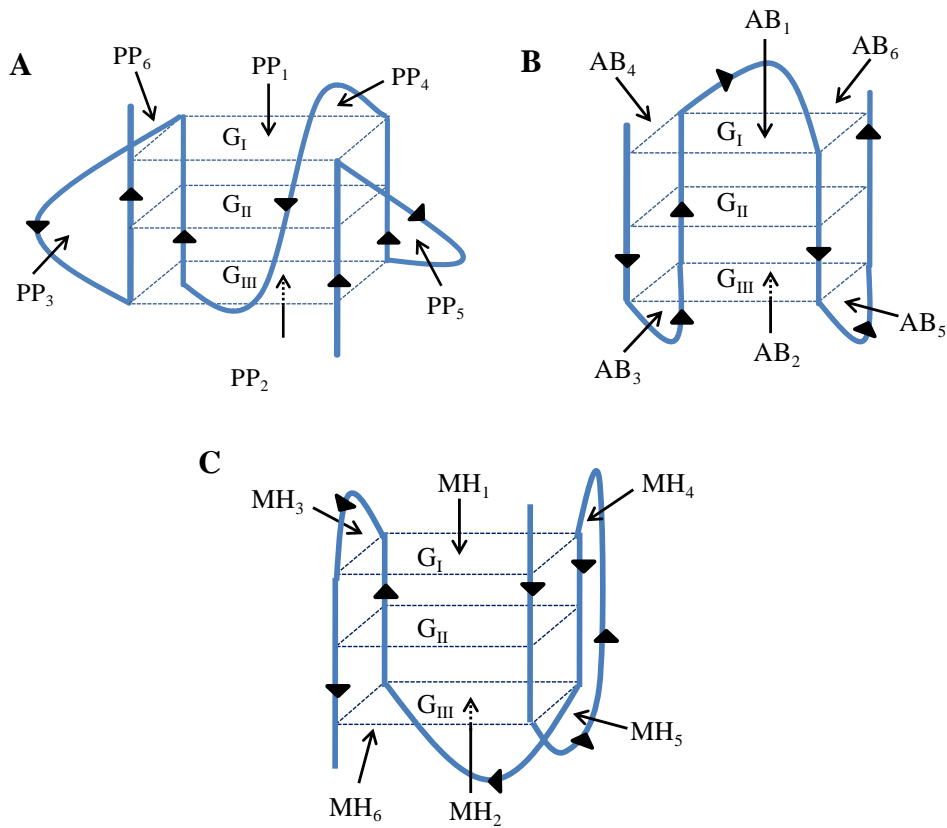
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**Supporting Information**

**Table S1.** A comparative study of the “blind” docking of TMPyP4 to different G-quadruplex DNA.

	Number of Runs	Clustering	L.B.E.	M.B.E.	Site of Binding
PP <sub>0</sub>	150	61	-7.70	-7.46	End-stacking
AB <sub>0</sub>	150	73	-5.90	-5.77	Groove binding
MH <sub>0</sub>	150	145	-5.48	-5.35	Groove binding

PP<sub>0</sub>, AB<sub>0</sub>, MH<sub>0</sub> = complexes formed due to blind docking of TMPyP4 to PP, AB, and MH, respectively, L.B.E. = lowest binding energy in kcal mol<sup>-1</sup>, M.B.E. = mean binding energy in kcal mol<sup>-1</sup>.



**Figure S1.** Probable binding positions of the 22-mer human telomeric G-quadruplex DNA. (A) binding sites of parallel propeller-type (PP) G-quadruplex DNA: PP<sub>1</sub>, PP<sub>2</sub> = two end-stacking positions, PP<sub>3</sub>-PP<sub>6</sub> = four groove binding positions; (B) binding sites of antiparallel basket-type (AB) G-quadruplex DNA: AB<sub>1</sub>, AB<sub>2</sub> = two end-stacking positions, AB<sub>3</sub>-AB<sub>6</sub> = four groove binding positions; (C) binding sites of mixed hybrid-type (MH) G-quadruplex DNA: MH<sub>1</sub>, MH<sub>2</sub> = two end-stacking positions, MH<sub>3</sub>-MH<sub>6</sub> = four groove binding positions. G<sub>I</sub>, G<sub>II</sub>, and G<sub>III</sub> are the three G-tetrads in the native G-quadruplex DNA.

**Table S2.** Hydrogen bond occurrence<sup>a</sup> during the final molecular dynamics simulation for 50 ns for different G-quadruplex DNAs.

	PP		AB		MH	
	N2-H21...N7	N1-H1...O6	N2-H21...N7	N1-H1...O6	N2-H21...N7	N1-H1...O6
G2	95.4	99.1	99.3	98.7	99.6	99.9
G3	99.5	92.6	99.4	81.5	99.8	97.2
G4	99.1	98.9	99.7	100.0	98.7	99.7
G8	97.9	98.8	98.4	99.6	96.1	99.6
G9	99.3	96.3	99.3	97.8	99.9	96.4
G10	98.3	98.8	99.3	98.7	99.6	99.8
G14	98.8	99.3	99.5	99.7	99.6	99.8
G15	99.5	95.1	100.0	97.0	100.0	95.3
G16	98.3	98.8	96.1	99.8	99.7	99.8
G20	99.6	99.9	99.9	100.0	99.9	99.7
G21	99.8	97.1	98.8	85.9	99.9	98.5

PP = parallel propeller-type, AB = antiparallel basket-type, and MH = mixed hybrid-type quadruplex DNA. GX = guanine bases in the 22-mer sequence used where X = residue number. <sup>a</sup>All the values are shown in percentages.