Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Binding symmetric porphyrins to c-MYC promoter Pu24I G-quadruplex: toward more specific ligand recognition by flanking bases

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Supporting Information

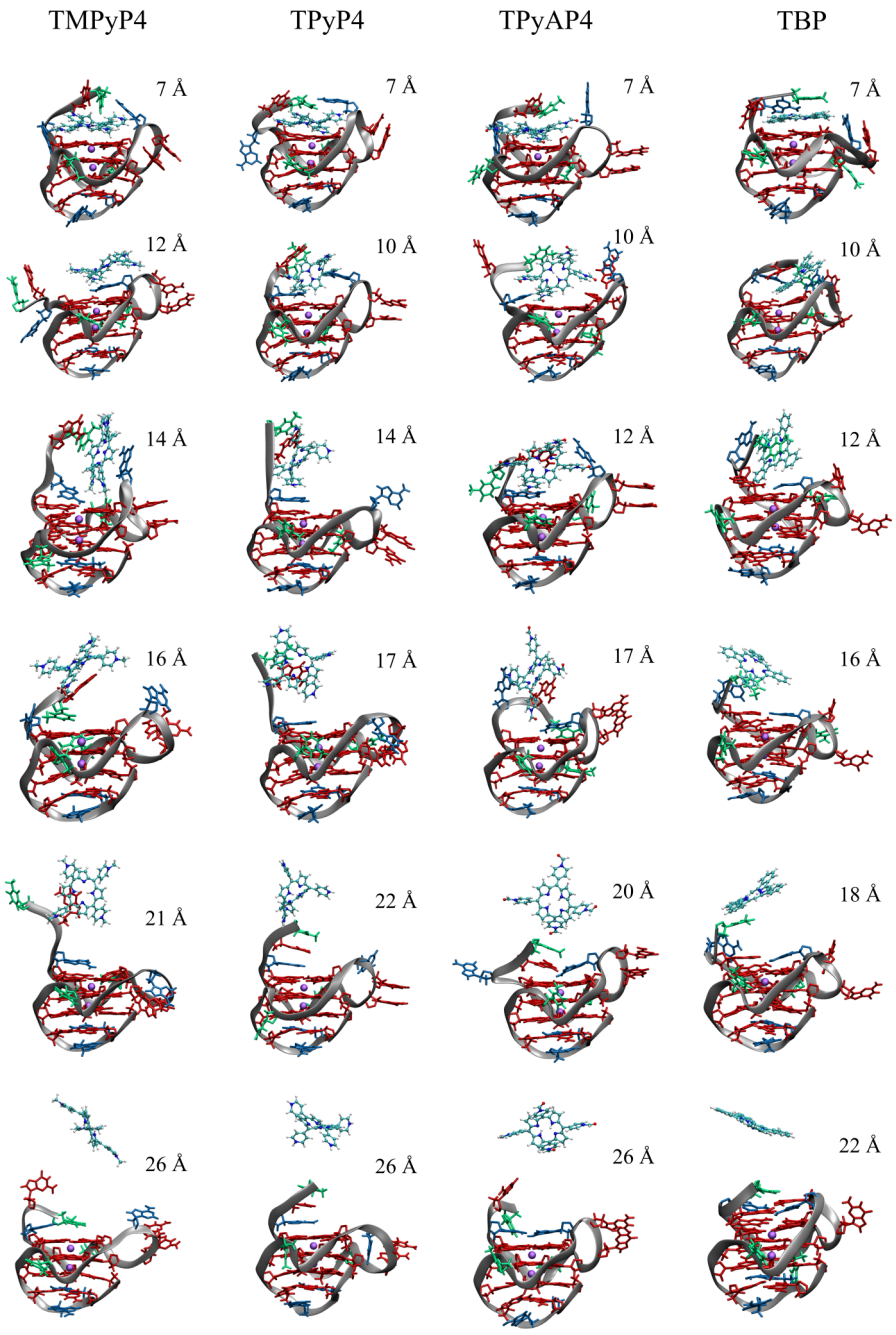

Figure S1: Selected structures from ABF simulations and their ligand–G-quadruplex distances. Colour code is the same as in Figure 2.

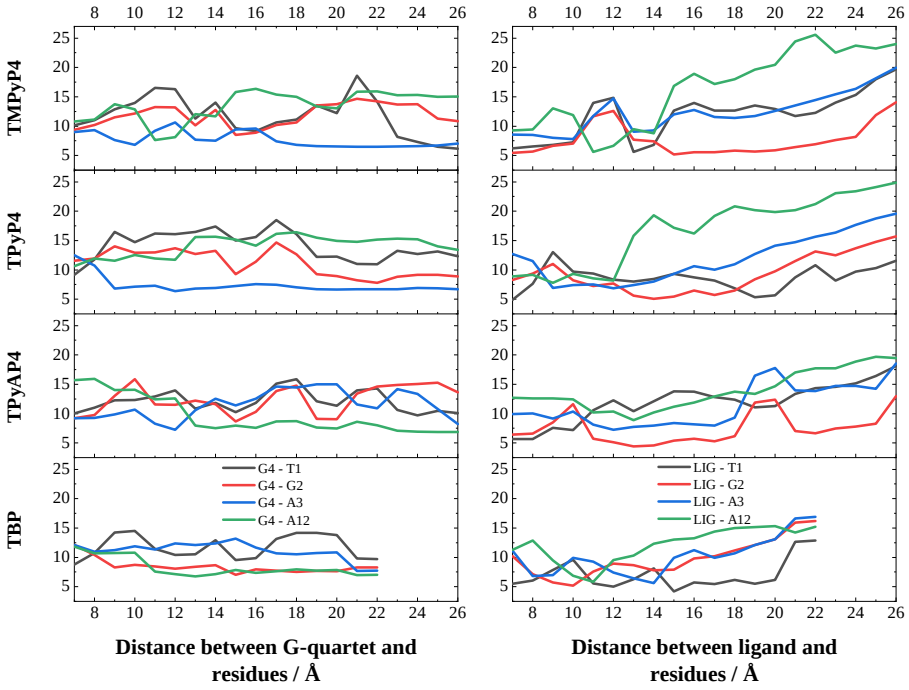

Figure S2: Average distances between selected bases and the top G-quartet (left) or a ligand (right) along a path of minimum free energy. The distances were computed from the coordinate origin.

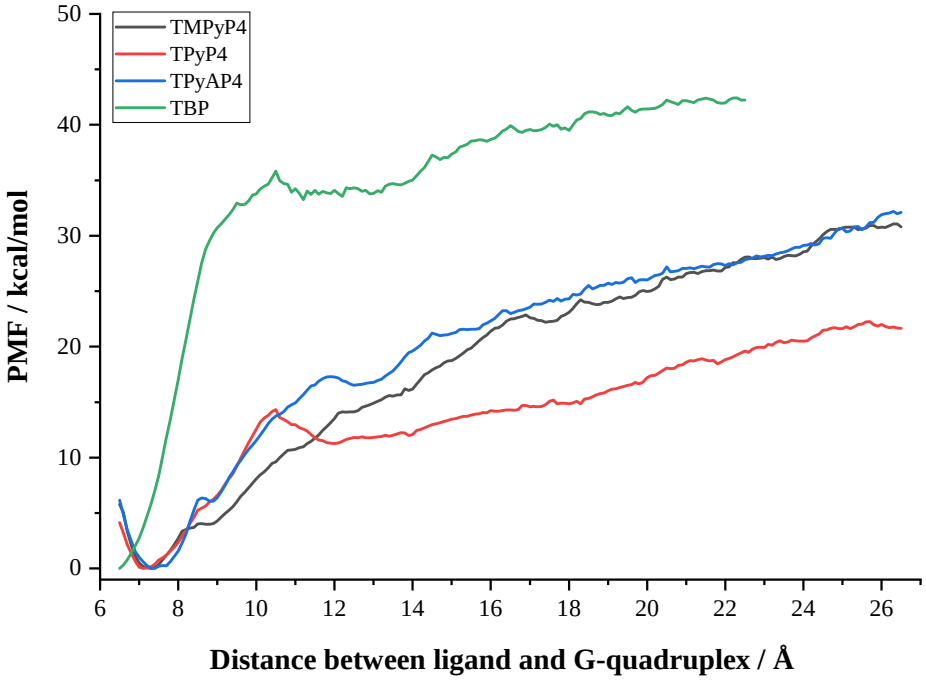

Figure S3: Potential of mean force along a minimum energy path. The distances were computed from the coordinate origin.

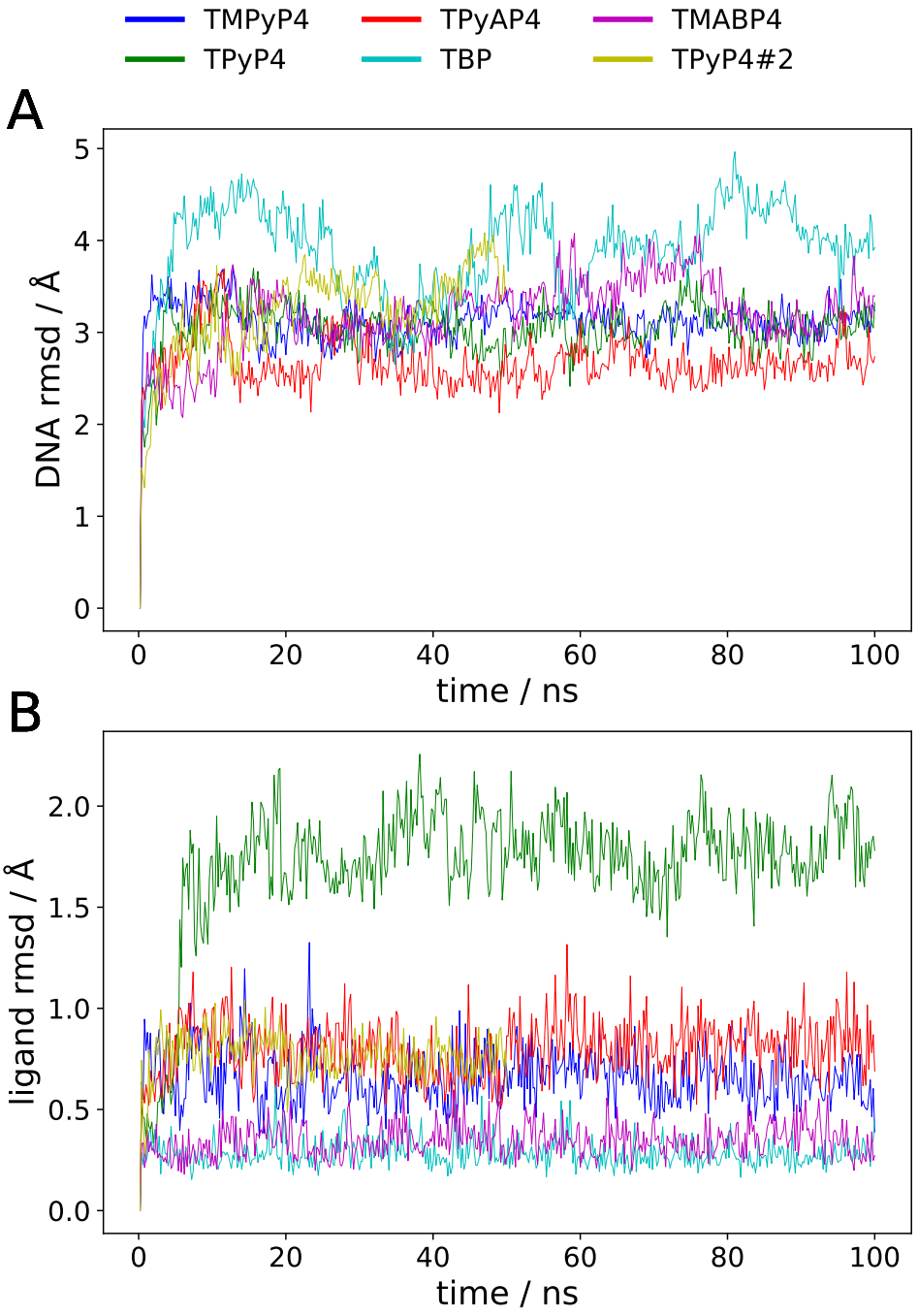

Figure S4: RMSD of A) G-quadruplex and B) ligands in simulations with different ligands.

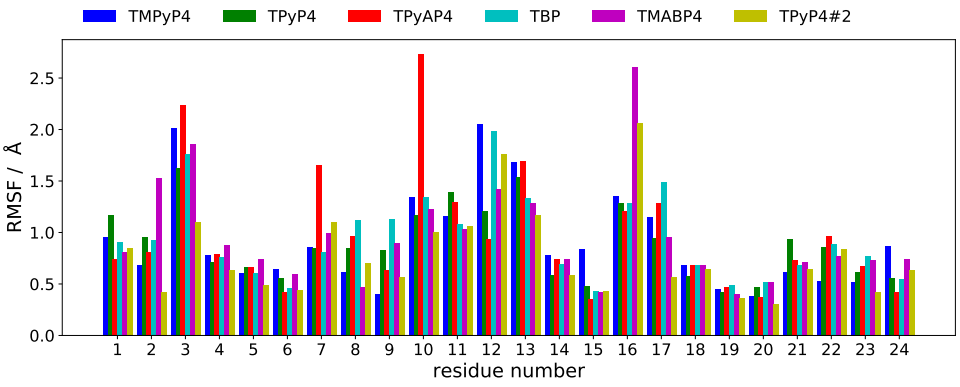

Figure S5: RMSF of G-quadruplex's residues in complexes.

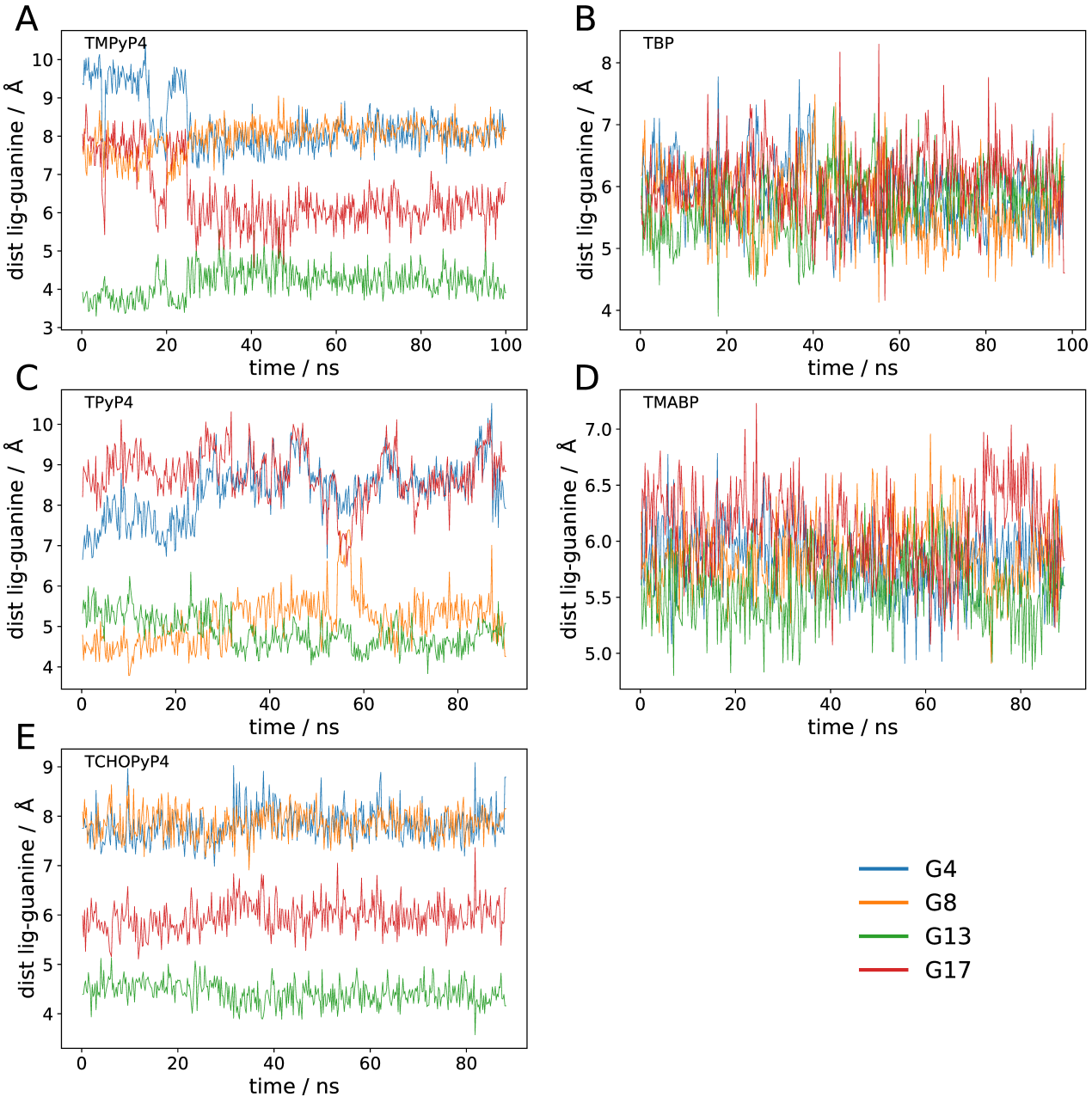

Figure S6: Distances between the geometric centers of the ligands and each guanine from the top G-quartet.