Supplemental Materials

The Binding Modes of Cationic Porphyrin-Anthraquinone Hybrids to DNA Duplexes:

In Silico Study

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(a) mono-H₂ImP-AQ

b) mono-H₂PyP-AQ,

(c) mono-H₂PzP-AQ

(d) bis-H₂ImP-AQ

(e) bis-H₂PyP-AQ

(f) bis-H₂PzP-AQ

(g) tris-H₂PzP-AQ

Figure S1. The optimized geometry of (a) mono-H₂ImP-AQ, b) mono-H₂PyP-AQ, (c) mono-H₂PzP-AQ, (d) bis-H₂ImP-AQ, (e) bis-H₂PyP-AQ, (f) bis-H₂PzP-AQ, (g) tris-H₂PzP-AQ.

Figure S2. Conformation of bis-H₂PyP-AQ to minor groove of 2DND, binding energy = -14.84 kcal/mol (left) and to 1Z3F, binding energy = -10.52 kcal/mol (right). The π - π interaction was represented by yellow color.

Figure S3. Conformation of mono-H₂PyP-AQ intercalated into base pairs of d(CGATCG)₂ pdb code 1Z3F, binding energy = -10.55 kcal/mol (left); and mono-H₂PyP-AQ intercalated into base pairs of d(TGATCA)₂ pdb code 182D, binding energy = -10.64 kcal/mol (right). Yellow color represent π - π interaction.