Supplemental Materials

The Binding Modes of Cationic Porphyrin-Anthraquinone Hybrids to DNA Duplexes: *In Silico* Study

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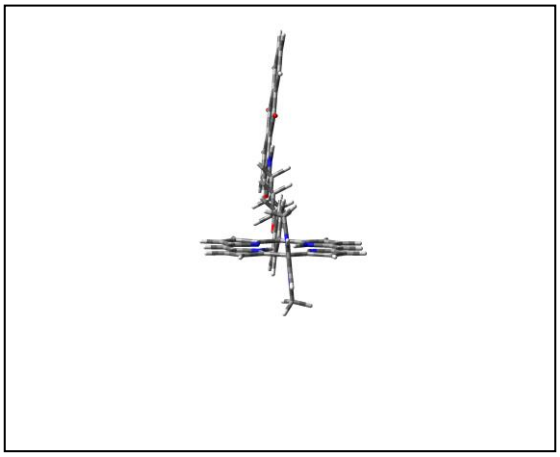
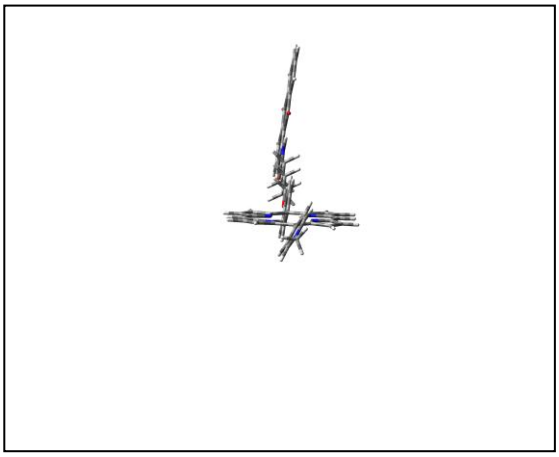
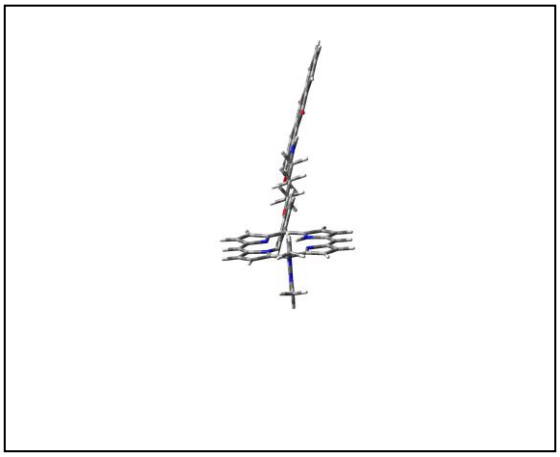


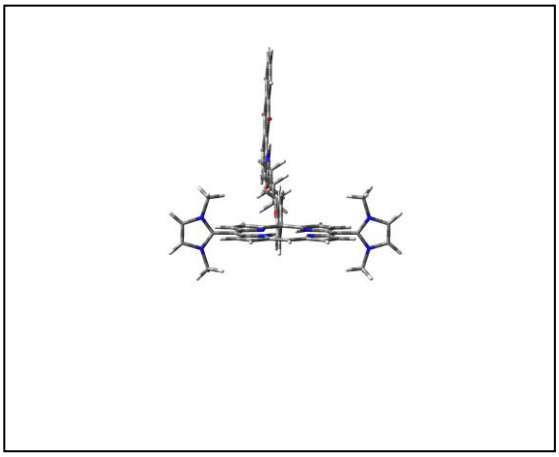
(a) mono-H_2ImP-AQ



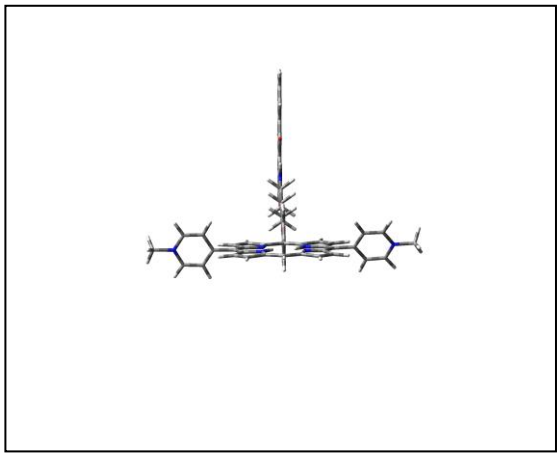
b) mono-H_2PyP-AQ,



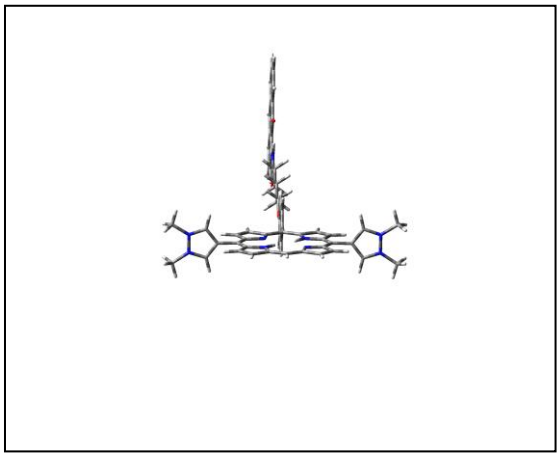
(c) mono-H_2PzP-AQ



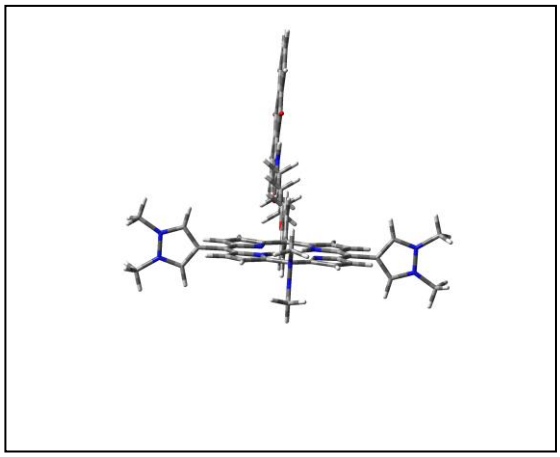
(d) bis-H_2ImP-AQ



(e) bis-H_2PyP-AQ



(f) bis-H_2PzP-AQ



(g) tris-H_2PzP-AQ

Figure S1. The optimized geometry of (a) mono-H_2ImP-AQ, b) mono-H_2PyP-AQ, (c) mono-H_2PzP-AQ, (d) bis-H_2ImP-AQ, (e) bis-H_2PyP-AQ, (f) bis-H_2PzP-AQ, (g) tris-H_2PzP-AQ.

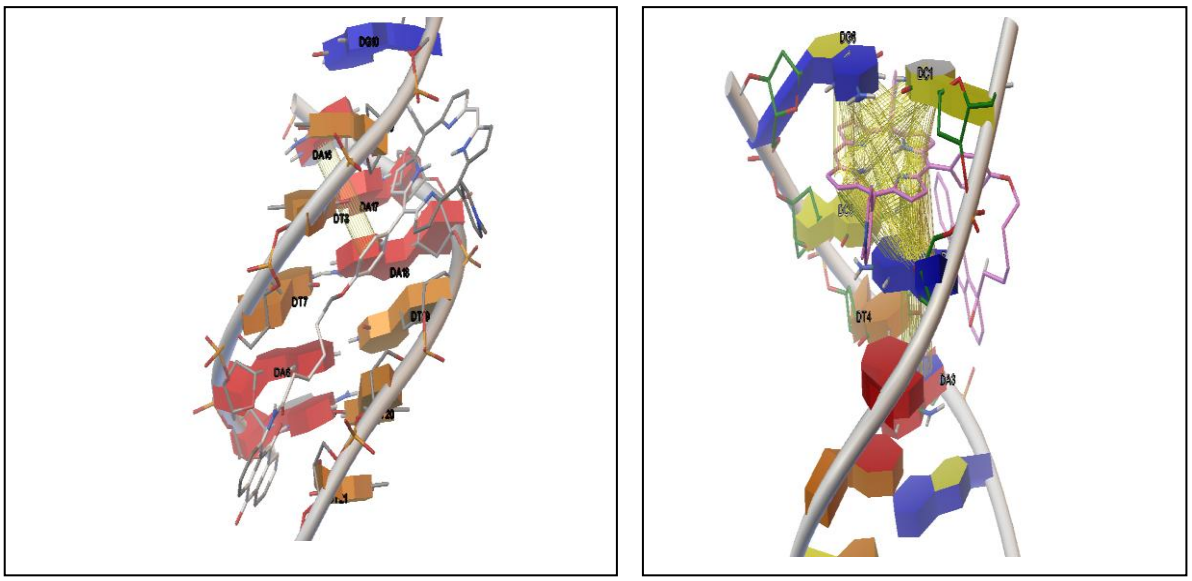


Figure S2. Conformation of bis-H_2PyP-AQ to minor groove of 2DND, binding energy = −14.84 kcal/mol (left) and to 1Z3F, binding energy = −10.52 kcal/mol (right). The π-π interaction was represented by yellow color.

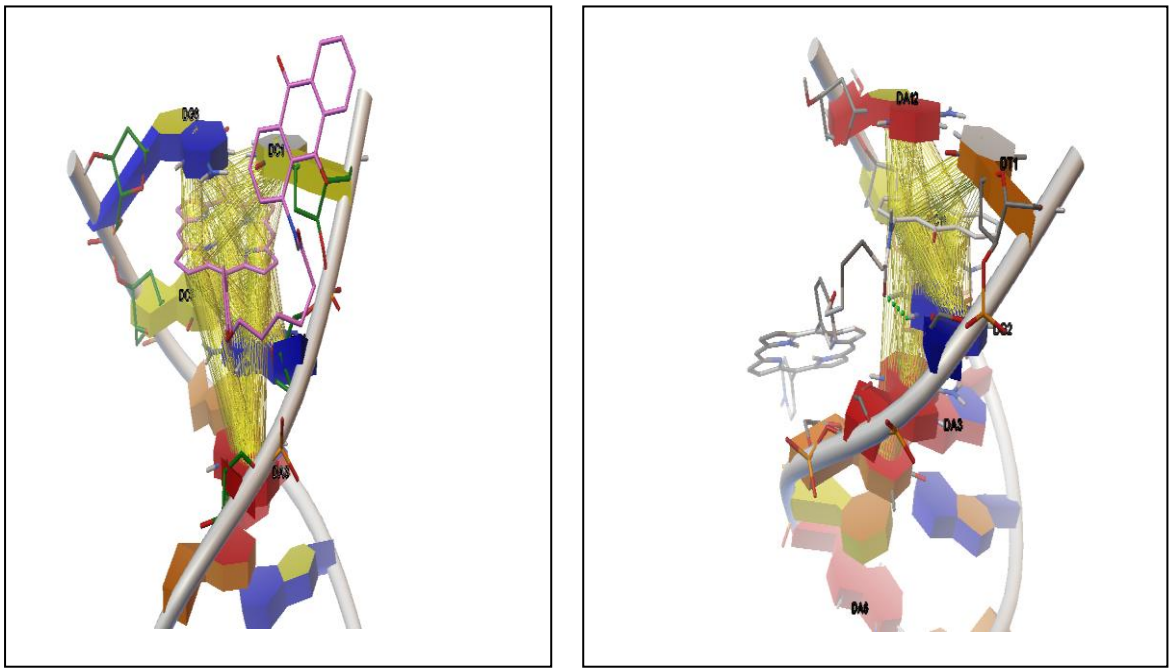


Figure S3. Conformation of mono-H_2PyP-AQ intercalated into base pairs of d(CGATCG)$_2$ pdb code 1Z3F, binding energy = −10.55 kcal/mol (left); and mono-H_2PyP-AQ intercalated into base pairs of d(TGATCA)$_2$ pdb code 182D, binding energy = −10.64 kcal/mol (right). Yellow color represent π-π interaction.