Supplementary Material for

Photoinduced Azobenzene-modified DNA Dehybridization: Insights into Local and Cooperativity Effects from a Molecular Dynamics Study

Nuno Barbosa,[a] Luca Sagresti [a,b] and Giuseppe Brancato[a,b*]

[a] Scuola Normale Superiore, piazza dei Cavalieri 7, I-56126 Pisa, Italy and CSGI.

[b] Istituto Nazionale di Fisica Nucleare, Largo Pontecorvo 3, I-56100 Pisa, Italy

Corresponding authors:

E-mail: giuseppe.brancato@sns.it

Content

Figure S1

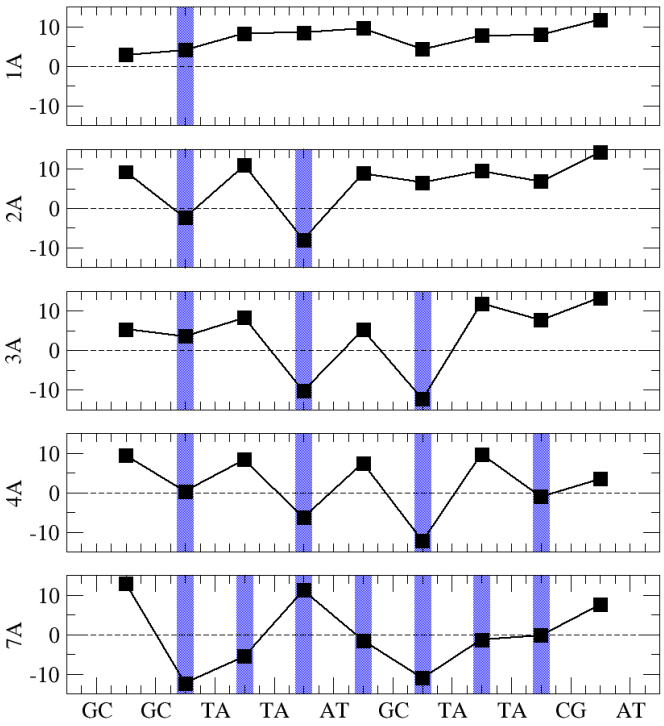

Figure S1 Inclination step parameter (values in degree) as issuing from MD simulations of the **1A**, **2A**, **3A**, **4A** and **7A** all-*trans* azobenzene modified-DNA systems. Shaded areas indicate the azobenzene moiety insertion points along the DNA duplex.

Figure S2

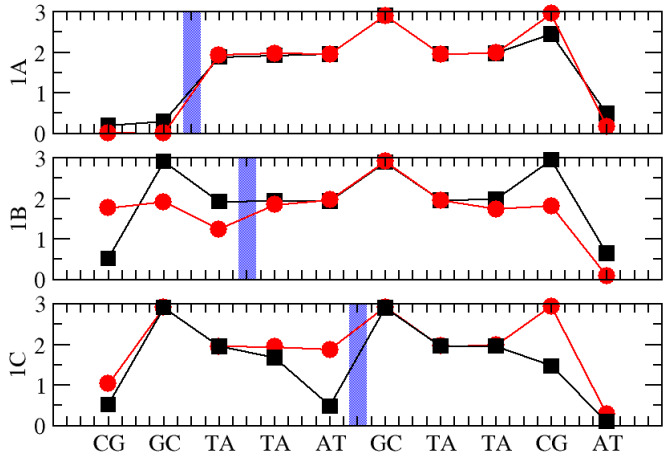

Figure S2 Number of hydrogen bonds between each base pair of the **1A**, **1B**, and **1C** *trans* (black) and *cis* (red) azobenzene modified-DNA systems. Shaded areas indicate the azobenzene insertion points along the DNA duplex.

Figure S3

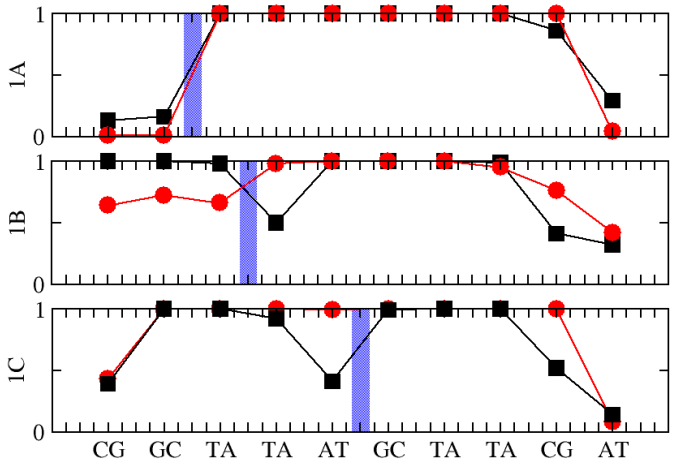

Figure S3 Connection parameter between each base pair of the **1A**, **1B**, and **1C** *trans* (black) and *cis* (red) azobenzene modified-DNA systems. Shaded areas indicate the azobenzene insertion points along the DNA duplex.

Figure S4

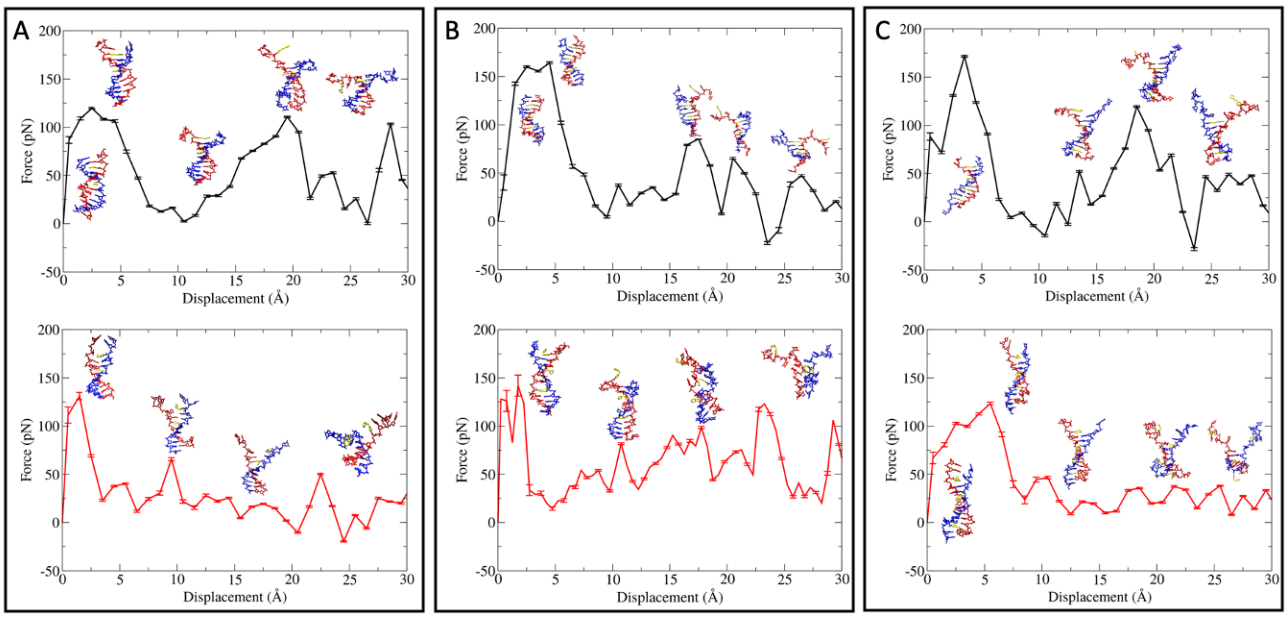

Figure S4 Pulling force as a function of displacement from SMD simulations of the (A) **2A**, (B) **3A** and (C) **4A** all-*trans* (top, black) and all-*cis* (bottom, red) azobenzene modified-DNA systems. Insets, representative molecular configurations from corresponding MD trajectories: the two DNA strands are in blue and red, azobenzene unit in yellow.

Figure S5

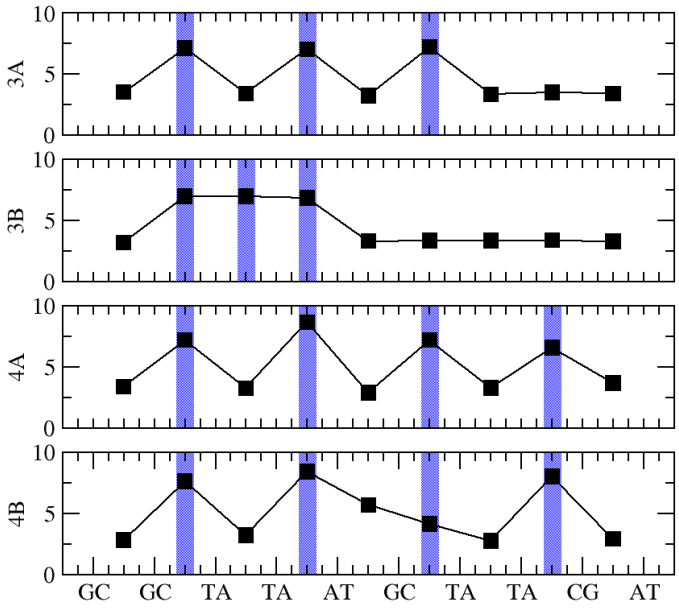

Figure S5 Rise parameter (values in Å) as issuing from MD simulations of the **3A**, **3B**, **4A**, and **4B** all-*trans* azobenzene modified-DNA systems. Shaded areas indicate the azobenzene insertion points along the DNA duplex.

Figure S6

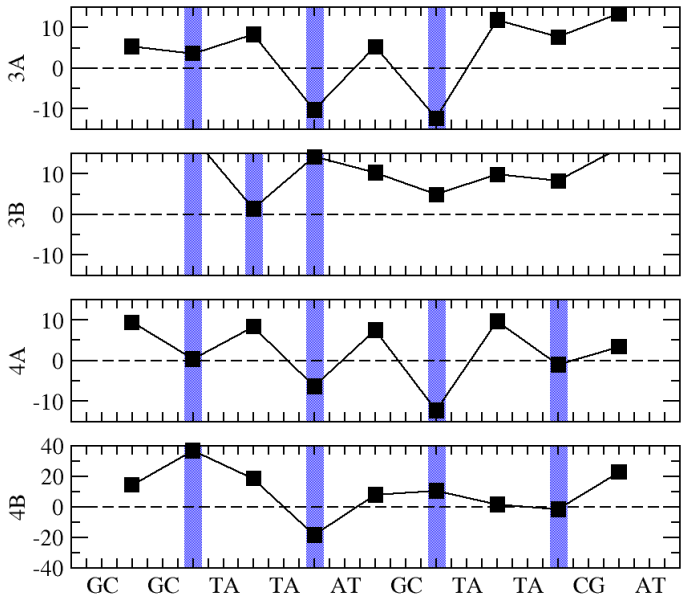

Figure S6 Inclination parameter (values in degree) as issuing from MD simulations of the **3A**, **3B**, **4A**, and **4B** all-*trans* azobenzene modified-DNA systems. Shaded areas indicate the azobenzene insertion points along the DNA duplex.

Figure S7

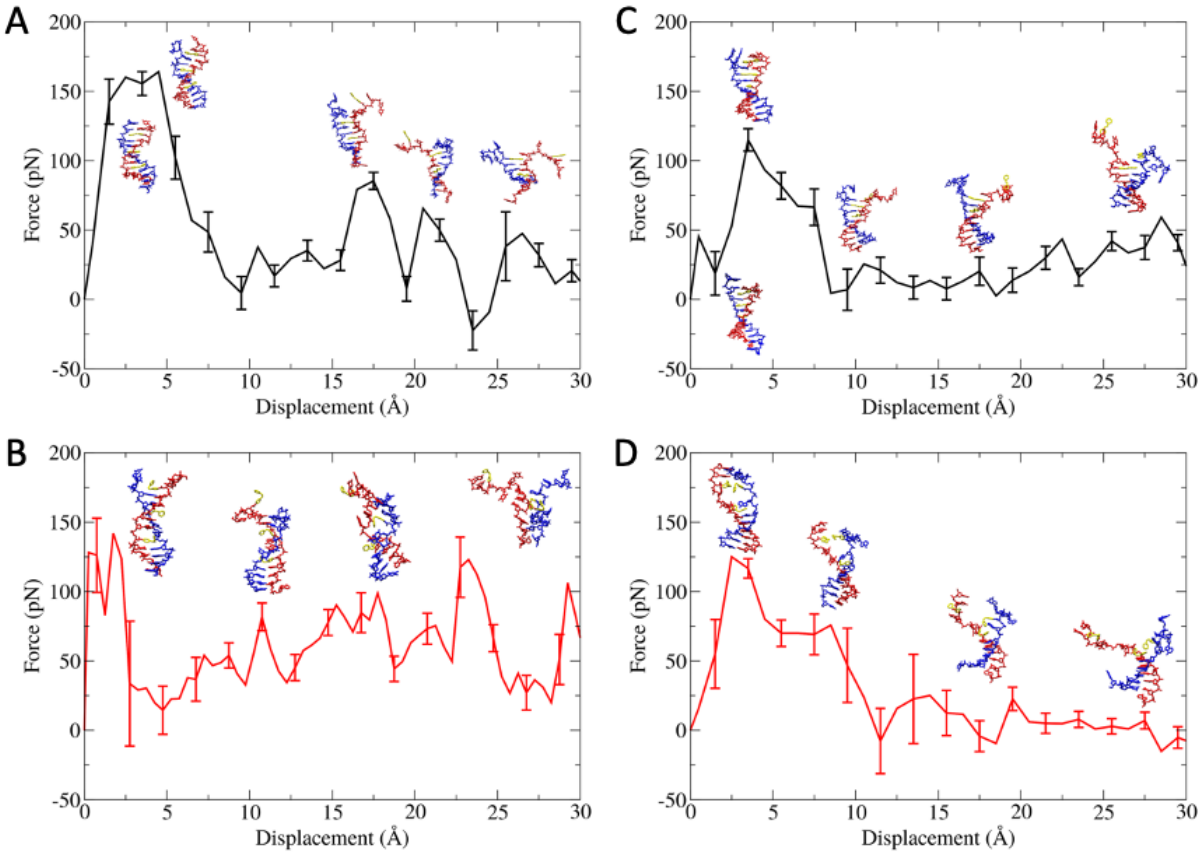

Figure S7 Pulling force as a function of displacement from SMD simulations of the (A, B) **3A** and (C, D) **3B** all-*trans* (top, black) and all-*cis* (bottom, red) azobenzene modified-DNA systems. Insets, representative molecular configurations from corresponding MD trajectories: the two DNA strands are in blue and red, azobenzene unit in yellow.