SUPPLEMENTARY INFORMATION

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| a) |
| b) |
| c) |
| d) |
| **Figure Sx.** (a) Initial structures of the drug-free CA21×6 DNA circle showing how a given stretch in a DNA strand (spheres) will face opposite directions with respect to the center of the ring (left and right) depending on the definition of the first nucleotide in the input sequence built by the MCDNA server. Convergence of both systems is achieved after the molecular dynamics simulations and shown as a cluster of 30 equilibrated structures (middle). Average roll (b), twist (c), and tilt (d) values obtained from two separate replicas for every base pair step in the drug-free doubly nicked CA21×6 circle (red) and in the same structure containing an offset of 5 bp (gray). Initial opposite values are shown as dashed lines. Phased peaks of positive roll are identified with arrows. |

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| **Figure Sx.** Arcs of varying curvature…circles of different diameters and number of oligomers. a) Internally tangent covalently closed DNA circles of increasing lengths (CA21×6−CA21×11), as provided by the MCDNA web server (https://mmb.irbbarcelona.org/MCDNA/help/method). Note the superposition of the first monomeric units and their identical groove orientations. b) arcs. c) Roll variation |