Supporting Information

Edwards *et al.* 10.1073/pnas.0807699106

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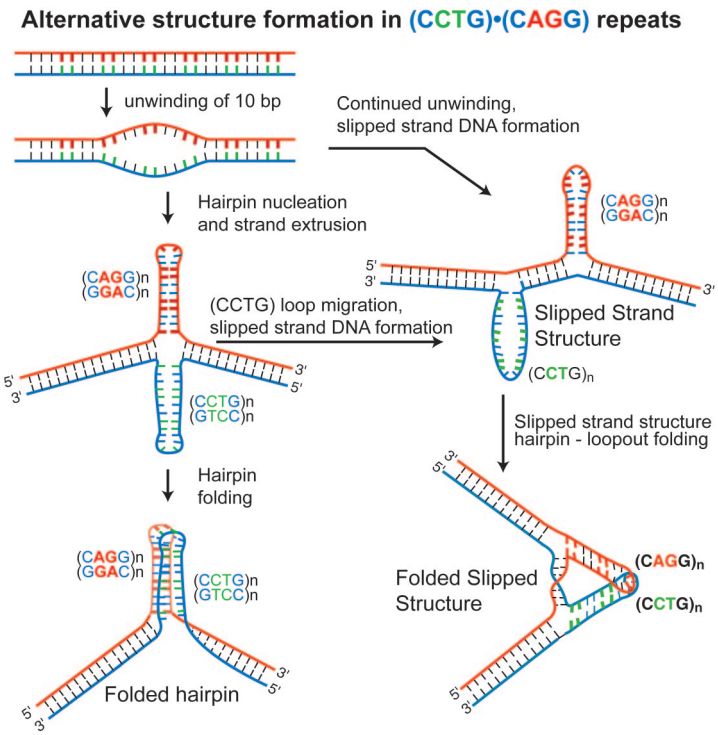

Fig. S1. Alternative structure formation in (CCTG)·(CAGG) repeats. This figure shows possible pathways to alternative DNA structure formation in (CCTG)·(CAGG) repeats as driven by DNA supercoiling. Supercoiling may promote DNA helix unwinding within the (CCTG)·(CAGG) repeats. A 10-bp unwound region is needed to allow nucleation of base pairing within an inverted repeat leading to cruciform extrusion (see ref. 1 for review). Similarly, nucleation may initiate in the (CAGG) strand, as this strand can form a hairpin, while the (CCTG) strand remains unpaired (2). The (CAGG) strand hairpin could be stabilized by 2 C·G base pairs and 2 G·A(*syn*) mispairs, which are stabilized by 2 hydrogen bonds and retain a phosphate–phosphate spacing very similar to that found in canonical A·T or C·G base pairs (3, 4). The hairpins may interact, resulting in a folded hairpin, which has been observed previously in certain inverted repeats (5, 6). This, however, may not be very stable, and it may branch migrate back into a linear form when supercoiling is lost. Alternatively, the (CCTG) loop may migrate, forming a canonical slipped-strand structure. This may be followed by folding and hairpin loop–hairpin loop interaction resulting in a folded slipped-strand structure, as observed previously for (CTG)·(CAG) slipped-strand DNA structures (7).