Supporting Information Available

**Modeling the energetics and radius of curvature of the A-tract end loop.**

We have modeled the energy state of the DNA in the loop of a superhelix apex to understand experiments which determine the radius of curvature of the end loop with and without the A-tract. The total length of the plasmid is \( L \), and we allow the length, \( \ell_1 \), of the terminal end loop vary. The radius of the terminal end loop varies as \( R = \ell_1/2 \). The total energy is \( E_{\text{tot}} = E_1(\ell_1) + E_2(L - \ell_1) \), where \( E_1 \) is the energy for the circular end loop and \( E_2 \) includes the energy of the superhelical midsection and the cruciform.

The term \( E_2 \) also includes the twisting energy of the entire structure, \( E_{\text{tw}} \), which is approximately

\[
E_{\text{tw}} = \frac{1}{2} C_{\text{tw}} (L_k - Wr)^2,
\]

where \( Wr \) is the writhe. The properties of \( E_2 \) are complex, but all that we require here is that \( E_2(L - \ell_1) \) becomes smaller as \( \ell_1 \) tends to zero; that is to say that the longer wrapping of the superhelical midsection the larger the writhe which reduces the twisting energy \( E_{\text{tw}} \). This assumes that the twist is a dominant energy of \( E_2 \). This is true for plasmids with large enough \( L_k \), which we assume here to be the case. The energy \( E_1(\ell_1) \) includes the bending energy of the terminal end loop which is assumed to be circular.

Without the A-tract,

\[
E_1(\ell_1) = \frac{1}{2} C \int_{0}^{\ell_1} \kappa(s)^2 ds,
\]

where \( \kappa(s) \) is the curvature along the arc length \( s \) of the loop, and \( C \) is the bending spring constant. For a uniform circular loop this simplifies to

\[
E(\ell_1) = \frac{1}{2} C \frac{2\pi}{R},
\]

where \( 2R = \ell_1 \). We now have two opposing forces in action. The energy \( E_2 \) produces a force driving a decrease in \( \ell_1 \), while \( E_1 \) produces an opposing force increase in \( \ell_1 \). When these forces balance, a mechanical equilibrium exists,

\[
\frac{dE_1(\ell_1)}{d\ell_1} = -\frac{dE_2(L - \ell_1)}{d\ell_1}.
\]

Without the A-tract,
\[
\frac{dE_1(\ell_1)}{d\ell_1} = -\frac{1}{2} C \frac{(2\pi)^2}{\ell_1^2},
\]
and the equilibrium occurs near \( \ell_1 = 65.3 \) nm (R=10.4 nm), taken to be near the peak determined from the angle measurements in Fig. 4B. Adding the A-tract to the terminal loop changes the energy \( E_1 \) dramatically, but is expected to only slightly change \( E_2 \). This is an important concept in understanding the energetics associated with sequence-dependent bending at the loop. The bending energy of the terminal loop with the A-tract is
\[
E_{A_1}^A(\ell_1) = \frac{1}{2} C \int_{\ell_1} (\kappa(s) - \kappa_A(s))^2 ds.
\]
Here \( \kappa_A(s) \) is zero for base pairs outside of the 106-bp A-tract segment, while it is the intrinsic A-tract curvature \( \kappa_A \) when \( s \) is within the A-tract. The intrinsic curvature \( \kappa_A \) is \( 1/R_A \) where the radius of curvature \( R_A = 11.5 \) nm for a 36 nm long A-tract bent by 180°. Evaluating the integral for \( E_A^A(\ell_1) \) yields the result
\[
E(\ell_1) = \frac{1}{2} C \frac{\pi}{R_A}.
\]
Note that \( \ell_2 \) has dropped out. This most curious result (which holds for \( \ell_1 > \ell_2 \)) shows that there is no energy dependence on the arc-length of the circle – any size end loop has the same curvature energy (assuming a circle). As a consequence, a reduction in arc-length of the terminal loop by slithering (non-A-tract) base-pairs from the end loop into the superhelical midsection costs no energy increase to \( E_1 \), even though the loop is shrinking in size. Since \( E_2 \) reduces its energy by increasing its length, the end loop containing the A-tract shrinks until all (or nearly all) non-A-tract base-pairs are removed. Mathematically
\[
\frac{dE_1(\ell_1)}{d\ell_1} \approx 0,
\]
leaving the force
\[
-\frac{dE_2(L-\ell_1)}{d\ell_1}
\]
largely unbalanced. The situation is quite asymmetric when the radius is reduced further so that base-pairs of the A-tract slither into the midsection; then a very large counterforce is generated. The high pitch angle of winding the superhelical coil produces relatively straight segments which will produce a very high energy for an intrinsically bent (A-tract) segment.