Supplementary material for "Dynamics of supercoiled DNA with complex knots: large-scale rearrangements and persistent multi-strand interlocking"

Lucia Coronel [1], Antonio Suma [1,2] and Cristian Micheletti [1]

[1] *SISSA, Trieste, Italy;* [2] *Temple University, Philadelphia, USA*

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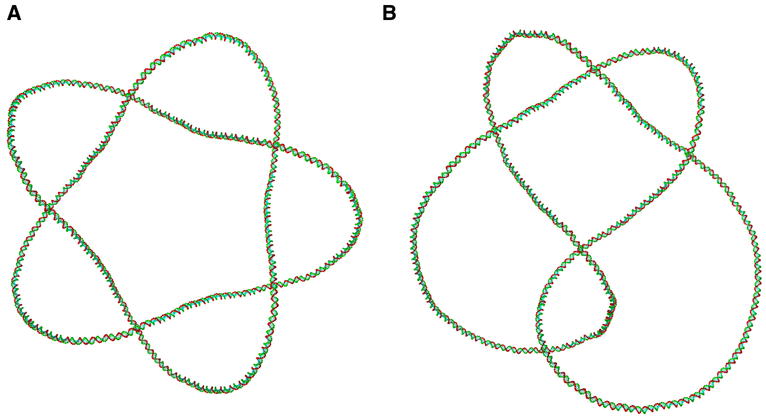

FIG. S1. Initial configurations of the supercoiled double-stranded DNA rings with 5_1 and 5_2 topologies. The two knots are left-handed, i.e. the topological sign of their projected crossings is negative, as indicated.

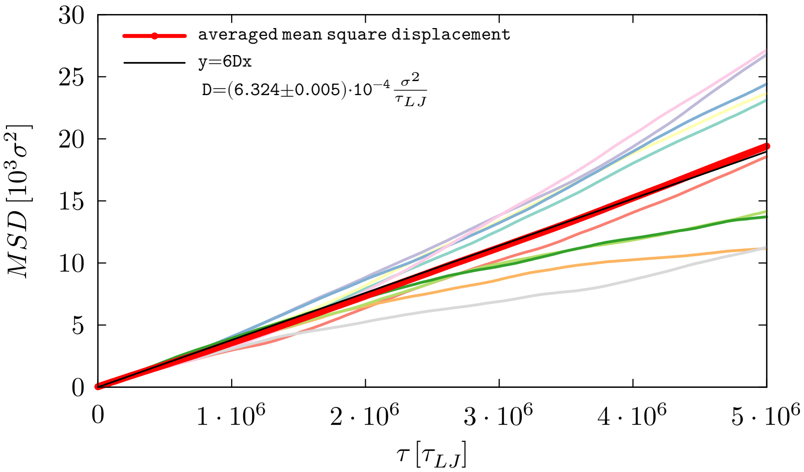

FIG. S2. The thick red line is the mean square displacement (MSD) of the center of mass of 2kb-long supercoiled unknotted rings, at different time lags. This MSD was calculated by averaging the MSD curves of 10 different trajectories (colored thin lines). The diffusion coefficient, computed from the linear best fit (black line), is $D_{theory} \sim (6.324 \pm 0.005) \times 10^{-4}\sigma^2/\tau_{LJ}$.

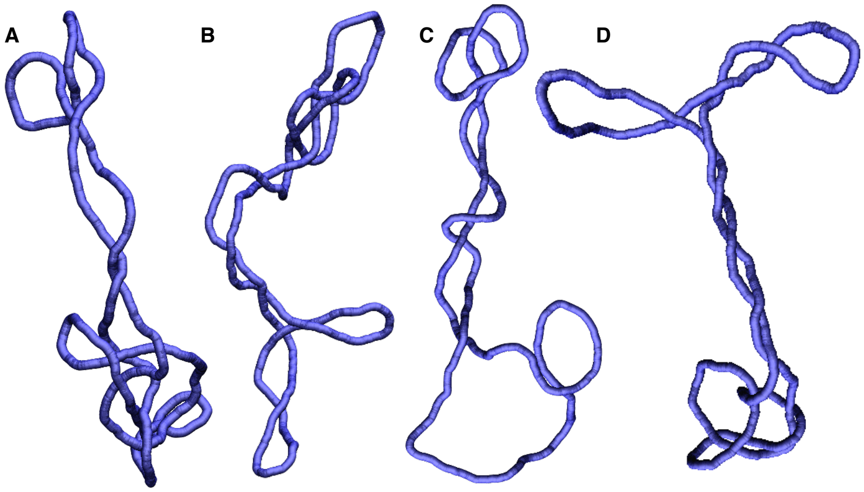

FIG. S3. Examples of supercoiled conformations for which no plectonemes are identified by the algorithm described in the main text due to excessively large apical loops or non well-formed superhelical regions. The topologies of the shown conformations are as follows: 5_1 for panels A and B, 0_1 for panel C and 5_2 for panel D.

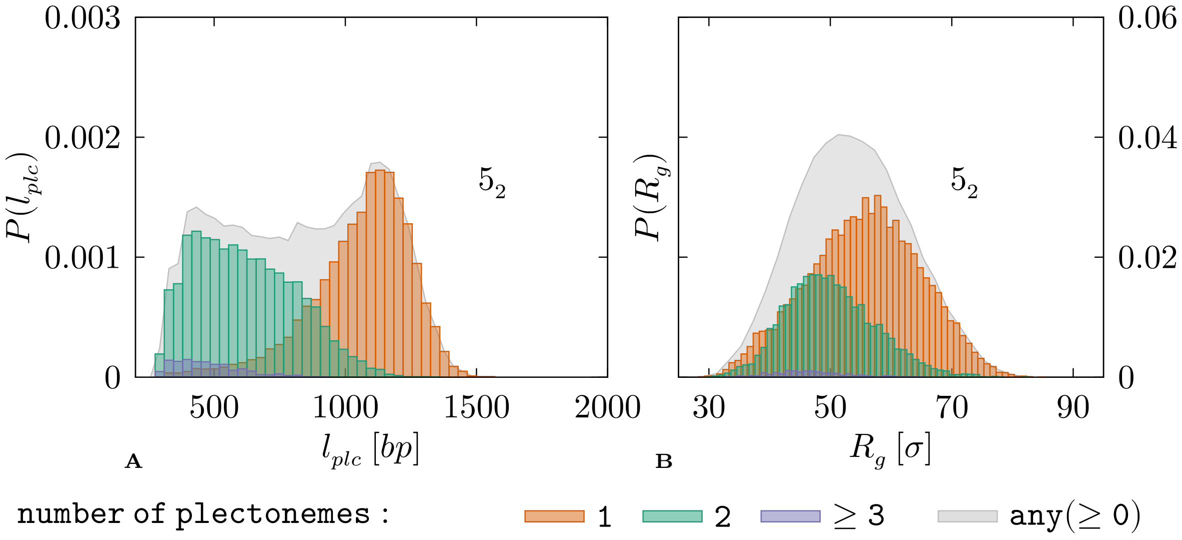

FIG. S4. Normalised probability distributions of (**A**) the plectoneme's lengths, l_{plc}, and of (**B**) the gyration radius, R_g for 2kbp-long supercoiled rings with 5_2-knots.

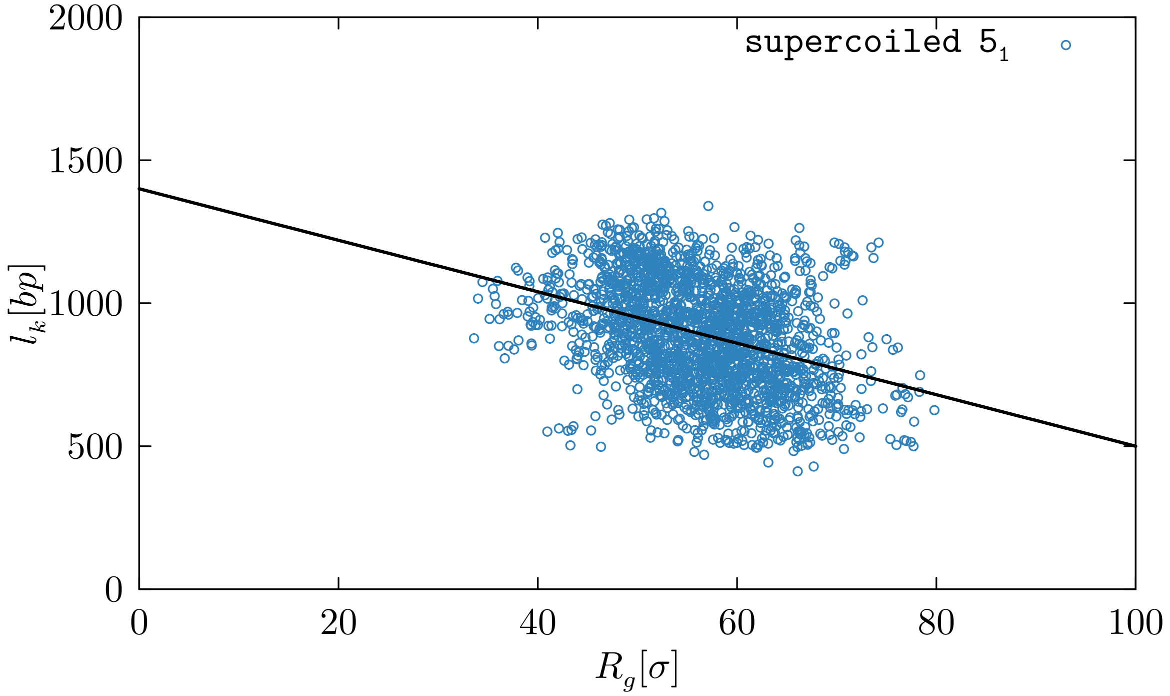

FIG. S5. Scatter plot of knot length, l_k, versus gyration radius, R_g, for 2kbp-long supercoiled rings tied in 5_1 knots. The best linear fit (black line) has correlation coefficient $r = -0.36$.

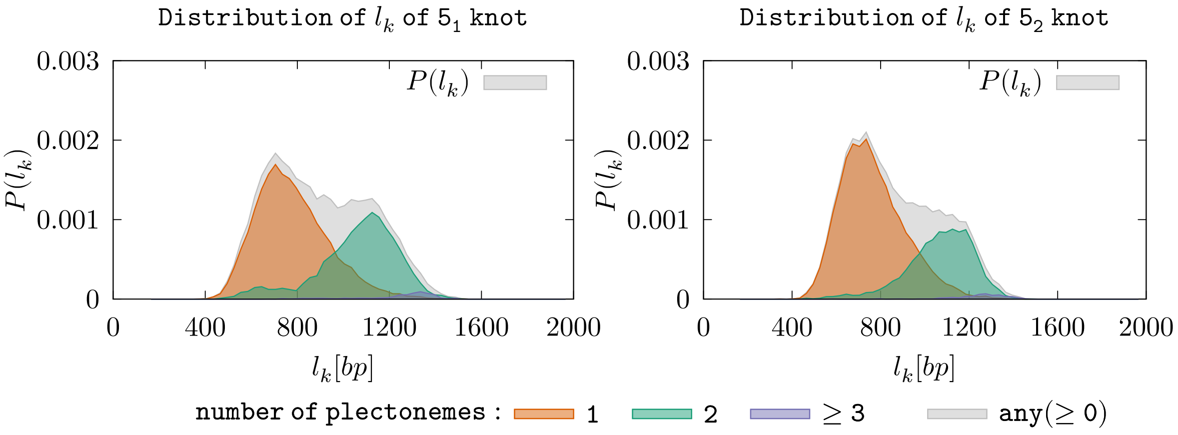

FIG. S6. Normalised probability distribution of the knot length, l_k for 2kbp-long supercoiled 5_2-knotted DNA rings.

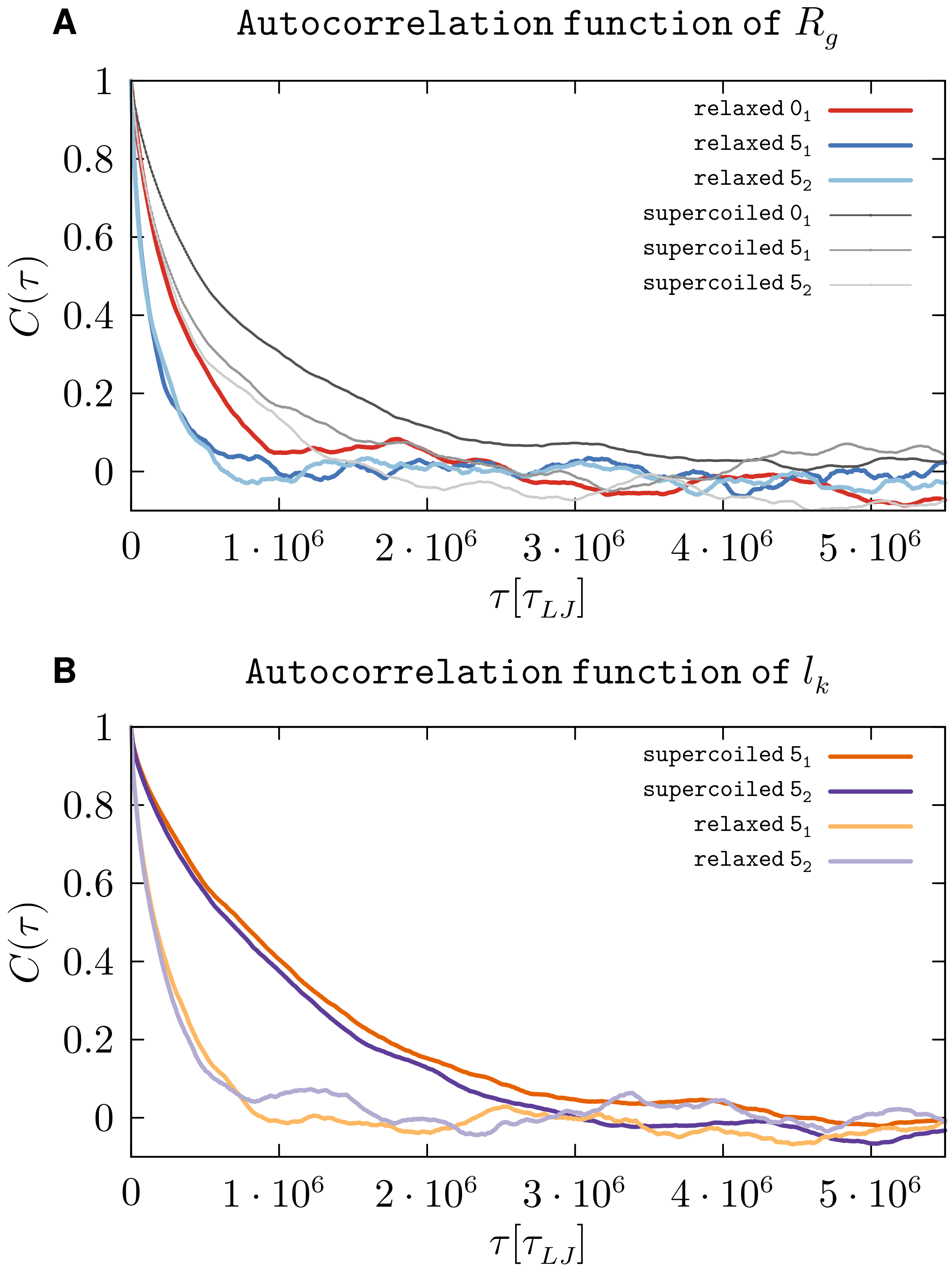

FIG. S7. Autocorrelation functions of (**A**) the radius of gyration, R_g, and (**B**) the knot length, l_k for 2kbp-long rings with various topologies (both supercoiled and torsionally-relaxed).

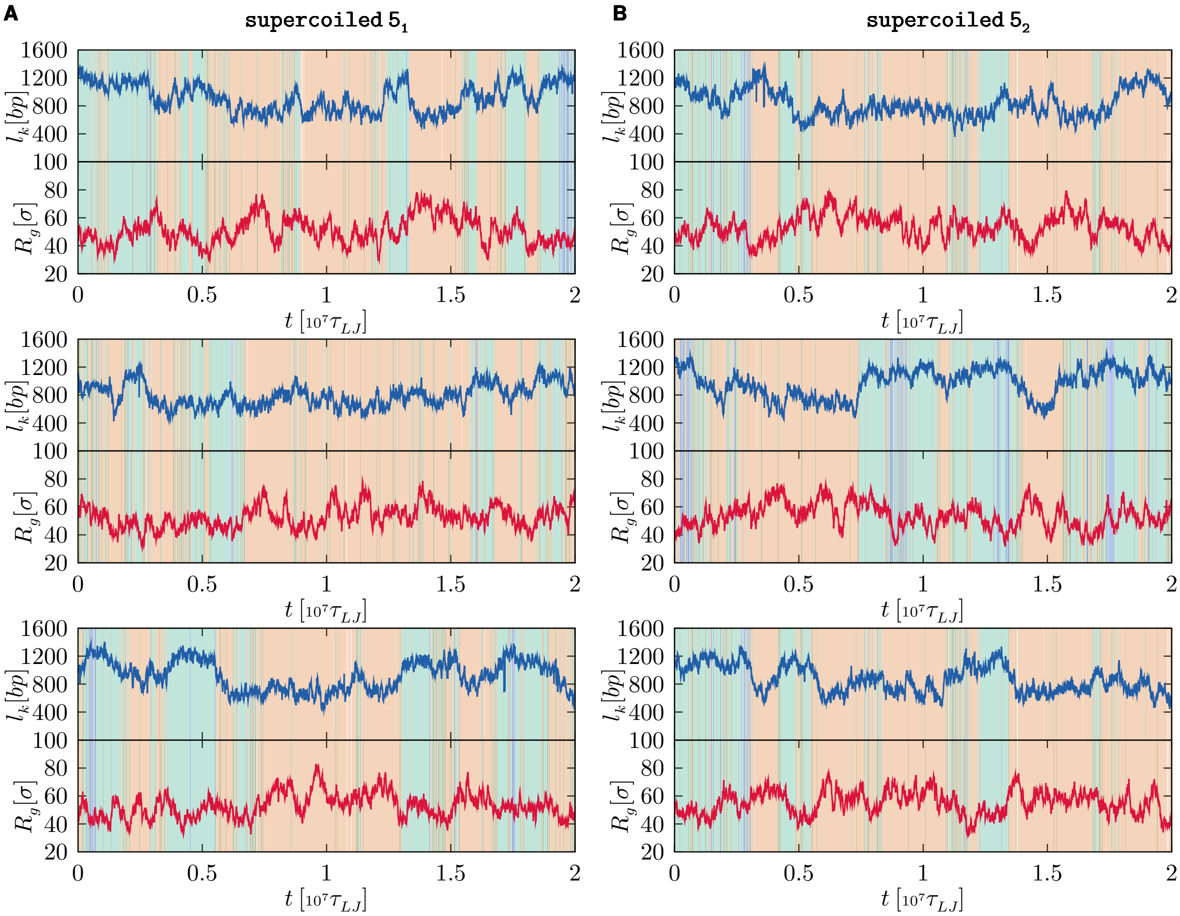

FIG. S8. Temporal traces of the length of the knotted region, l_k, and the gyration radius, R_g, for 2kbp-long supercoiled rings with (**A**) 5_1 and (**B**) 5_2 topologies. The color-coded background reflects the number of plectonemes present: orange for 1 plectoneme, green for 2 plectonemes, as in the legend of Fig. S2.

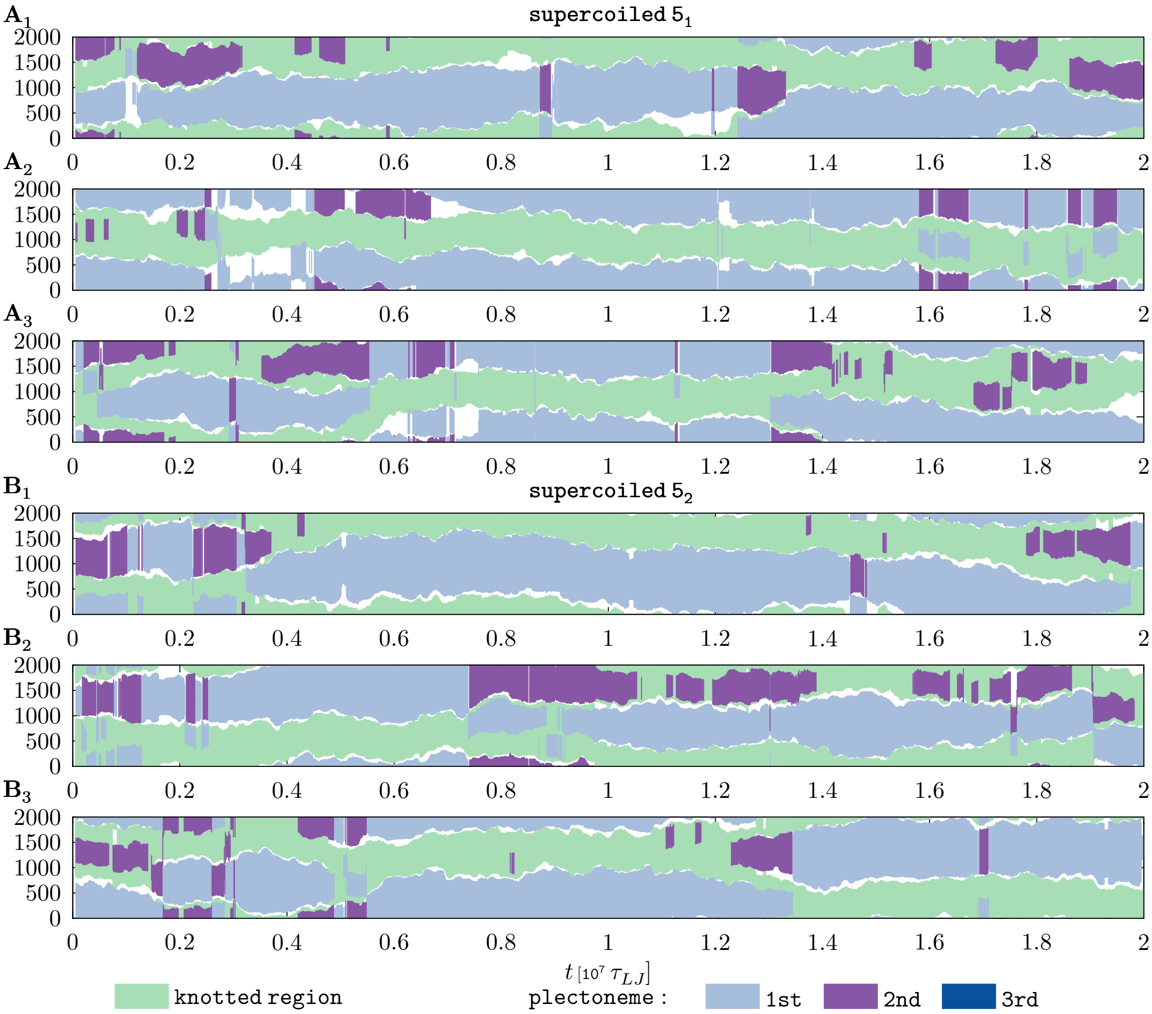

FIG. S9. Kymographs showing the contour motion of the knotted and plectonemically-wound regions. Data are for different trajectories of 2kbp-long supercoiled rings with 5_1 or 5_2-knots, as indicated. Notice the persistence of the boundaries between the knotted and the main plectonemically-wound region.