Supplementary Materials:

Configuration transitions of free circular DNA system induced by nicks

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Table SI: Quantitative results of nicked circular DNA.

Nicked DNA	Flat circular form	Intersecting form	Ratio (%)	Mean of ratio (%)	*s.e.m* of ratio (%)
pUC19 (0 nicks)	275	85	76.4:23.6	75.4:24.6	0.52
	283	96	74.7:25.3		
	261	87	75:25		
pUC19 (2 nicks)	359	75	82.7:17.3	82.4:17.6	0.61
	348	78	81.7:18.3		
	322	67	82.8:17.2		
pUC19 (4 nicks)	438	50	89.8:10.2	90:10	0.62
	414	44	90.4:9.6		
	417	47	89.9:10.1		
pUC19 (6 nicks)	311	29	91.5:8.5	90.6:9.4	0.32
	315	33	90.5:9.5		
	329	37	89.9:10.1		

Electrophoretic Analysis

The assay of nicking reactions were analyzed using 10% (w/v) an agarose electrophoresis gel in 0.5× TBE (pH 8.3) running buffer under the condition of room temperature for 2 h at 10 V/cm. Two DNA maker were applied in this experiment including the 200 bp ladder DNA marker and λ DNA-HindIII digest DNA marker,

which were bought from TIANGEN BIOTECH (BEIJING) CO., LTD. The sample of nicked DNA in electrophoretic assay were performed by pUC19 vector DNA and Nb.BsrDI according to the suggested protocol from NEB.

Then the efficiency of the nicking reactions were revealed by running their samples on an electrophoresis gel, which is shown in Figure S1. The electrophoresis chambers indicated by letters shown in Figure S1, illustrate the different samples, including 200 bp ladder DNA marker (A), pUC19 plasmid vector with two nicks (B), pUC19 plasmid vector (C) and λ DNA-HindIII digest DNA marker (D), respectively. The result infers that the efficiency of nicking reactions are approximately 100%.

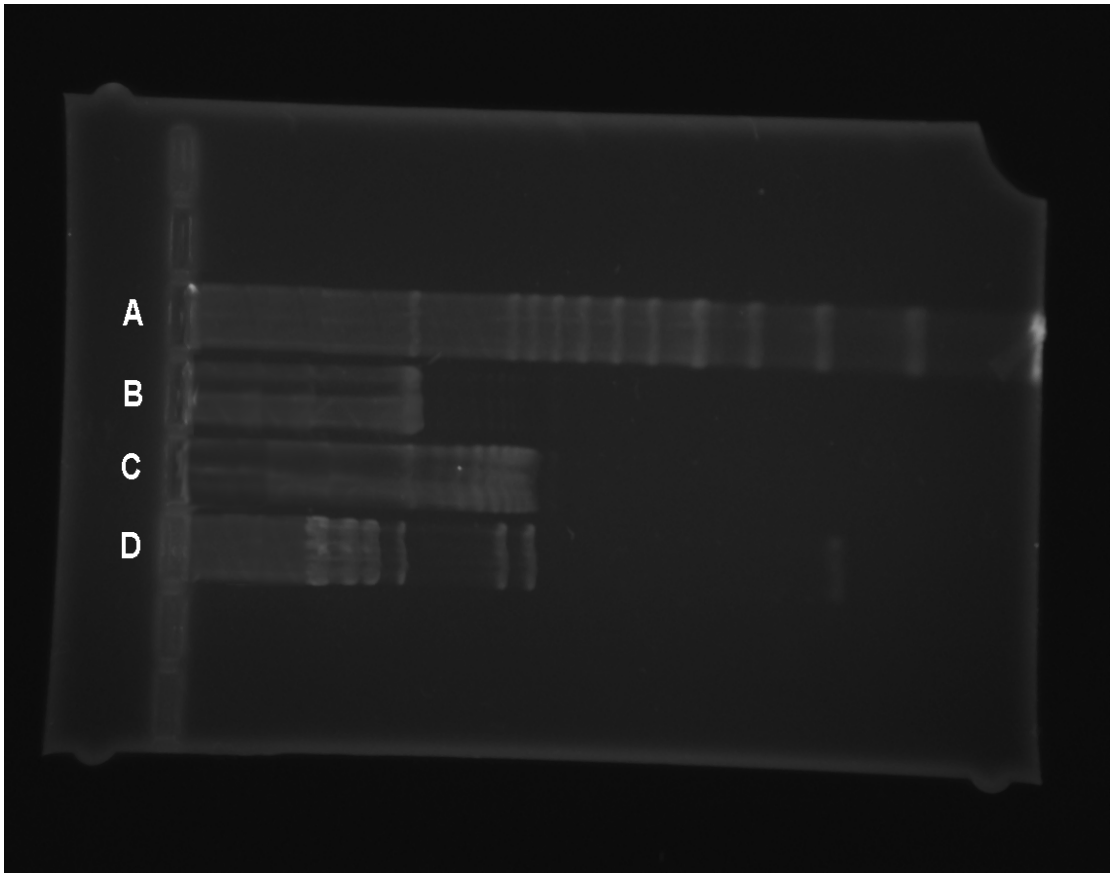

Figure S1. The result of nicking reactions is demonstrated by an agarose gel. (A) 200 bp ladder DNA marker; (b) pUC19 plasmid vector with two nicks; (C) pUC19 plasmid vector; (D) λDNA-HindIII digest DNA marker.

Algorithm Section

The worth of torsional energy can be released by the nicks, which can be calculated according to the effective length and nicking angles.

According to the Figure 5, under conditions of two nicks, the total length of the plasmid vector can be expressed by

$$2s + d_{2nicks} + effL_{2nicks} = Length_{total} \quad (1)$$

and under the condition of four nicks, the total length can be represented by

$$6s + d_{4nicks} + effL_{4nicks} = Length_{total} \quad (2)$$

Here, s means the release length by a nick; d_{2nicks} and d_{4nicks} respectively means the distant length between two neighbor nicks, which should be less than double release length by a nick; $effL_{2nicks}$ and $effL_{4nicks}$ means the length that cannot be released by nicks under conditions of two nicks and four nicks, respectively; $Length_{total}$ means the length of plasmid vector that equals to 2686 base pairs for pUC19 circular DNA in this experiment.

And then, according to the Figure 5, we can calculate that the d_{2nicks} and d_{4nicks} equal to 176 bp with 264 bp, respectively. Furthermore, the quantitative result demonstrates that the occurrence of the intersecting state with two nicks (18%) is approximately twice that with four nicks (10%). It can infer that $effL_{2nicks}$ equals to $1.8*effL_{4nicks}$. Finally, the worth of torsional energy released by the nicks can be calculated by means of equations (1) with (2).