

# Electronic Supplementary Information

## Sequence-dependent twist-bend coupling in DNA minicircles

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**Table S1. A summary of Gaussian fitting parameters for twist-angle distribution functions of Fig. 3**

| Dinucleotide Steps | $\mu^\dagger$ | $\sigma^\dagger$ | $R^{2\dagger}$ | $\mu^\ddagger$ | $\sigma^\ddagger$ | $R^{2\ddagger}$ |
|--------------------|---------------|------------------|----------------|----------------|-------------------|-----------------|
| AT/AT              | 30.86         | 3.44             | 0.9994         | 29.86          | 3.37              | 0.9999          |
| TA/TA              | 35.42         | 5.38             | 0.9944         | 29.90          | 4.46              | 0.9947          |
| GC/GC              | 32.73         | 4.55             | 0.9996         | 31.77          | 4.31              | 0.9989          |
| CG/CG              | 37.20         | 4.72             | 0.9989         | 34.11          | 4.83              | 0.9997          |
| AC/GT              | 31.61         | 4.07             | 0.9997         | 30.55          | 3.85              | 0.9997          |
| CA/TG              | 35.19         | 4.81             | 0.9993         | 31.06          | 4.73              | 0.9984          |
| AG/CT              | 30.19         | 4.14             | 0.9955         | 30.38          | 4.49              | 0.9956          |
| GA/TC              | 34.55         | 4.84             | 0.9987         | 30.69          | 4.94              | 0.9978          |
| AA/TT              | 33.75         | 4.20             | 0.9991         | 33.32          | 4.60              | 0.9968          |
| GG/CC              | 30.23         | 4.27             | 0.9975         | 28.85          | 3.99              | 0.9976          |

The parameters  $\mu$ ,  $\sigma$  are the mean, standard deviation of the Gaussian distribution function, respectively.  $R^2$  represents the coefficient of determination in fitting.

$\dagger$ Dinucleotide step with the direction of the minor groove facing inward ( $\cos \theta < 0$ ).

$\ddagger$ Dinucleotide step with the direction of the minor groove facing outward ( $\cos \theta > 0$ ).

**Table S2. Average twist angle of circular and linear DNAs**

| Sequence                               | $\langle\Omega^{XY}\rangle^\dagger$ | $\langle\Omega^{YX}\rangle^\ddagger$ | Sequence                               | $\langle\Omega_0^{XY}\rangle^\dagger$ | $\langle\Omega_0^{YX}\rangle^\ddagger$ |
|----------------------------------------|-------------------------------------|--------------------------------------|----------------------------------------|---------------------------------------|----------------------------------------|
| (AT) <sub>45</sub> /(AT) <sub>45</sub> | 30.22 (3.51)                        | 32.84 (5.62)                         | (AT) <sub>12</sub> /(AT) <sub>12</sub> | 30.32 (3.64)                          | 32.99 (4.99)                           |
| (GC) <sub>42</sub> /(GC) <sub>42</sub> | 32.28 (4.40)                        | 35.39 (5.07)                         | (GC) <sub>12</sub> /(GC) <sub>12</sub> | 31.64 (4.23)                          | 35.30 (4.37)                           |
| (AC) <sub>45</sub> /(GT) <sub>45</sub> | 30.49 (4.09)                        | 32.29 (5.18)                         | (AC) <sub>12</sub> /(GT) <sub>12</sub> | 30.87 (3.93)                          | 33.05 (4.47)                           |
| (AG) <sub>45</sub> /(CT) <sub>45</sub> | 30.57 (4.43)                        | 32.59 (5.10)                         | (AG) <sub>12</sub> /(CT) <sub>12</sub> | 30.80 (4.47)                          | 32.54 (4.70)                           |
| (AA) <sub>42</sub> /(TT) <sub>42</sub> | 33.62 (4.37)                        |                                      | (AA) <sub>12</sub> /(TT) <sub>12</sub> | 33.04 (4.26)                          |                                        |
| (GG) <sub>48</sub> /(CC) <sub>48</sub> | 29.67 (4.32)                        |                                      | (CC) <sub>12</sub> /(GG) <sub>12</sub> | 29.35 (3.92)                          |                                        |

$\langle\Omega\rangle$  is the average twist angle in each DNA minicircle, whereas  $\langle\Omega_0\rangle$  is the average twist angle in a linear DNA molecule. The values in parenthesis are the standard deviations.

$^\dagger XY$  represents AT/AT in the cases of sequence (AT)<sub>45</sub>/(AT)<sub>45</sub> and (AT)<sub>12</sub>/(AT)<sub>12</sub>, GC/GC in the cases of (GC)<sub>42</sub>/(GC)<sub>42</sub> and (GC)<sub>12</sub>/(GC)<sub>12</sub>, AC/GT in the cases of (AC)<sub>45</sub>/(GT)<sub>45</sub> and (AC)<sub>12</sub>/(GT)<sub>12</sub>, and AG/CT in the cases of (AG)<sub>45</sub>/(CT)<sub>45</sub> and (AG)<sub>12</sub>/(CT)<sub>12</sub>.

$^\ddagger YX$  represents TA/TA in the cases of sequence (AT)<sub>45</sub>/(AT)<sub>45</sub> and (AT)<sub>12</sub>/(AT)<sub>12</sub>, CG/CG in the cases of (GC)<sub>42</sub>/(GC)<sub>42</sub> and (GC)<sub>12</sub>/(GC)<sub>12</sub>, CA/TG in the cases of (AC)<sub>45</sub>/(GT)<sub>45</sub> and (AC)<sub>12</sub>/(GT)<sub>12</sub>, and GA/TC in the cases of (AG)<sub>45</sub>/(CT)<sub>45</sub> and (AG)<sub>12</sub>/(CT)<sub>12</sub>.

**Table S3. List of PDB files of nucleosomal DNAs from the Protein Data Bank**

|      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|
| 1AOI | 3A6N | 3MGS | 4KGC | 5B32 | 5XF6 | 6IY3 | 6NE3 | 6SEE | 6Y5E |
| 1EQZ | 3AFA | 3MNN | 4KUD | 5B33 | 5XM0 | 6J99 | 6NJ9 | 6SEF | 6YOV |
| 1F66 | 3AN2 | 3MVD | 4LD9 | 5B40 | 5XM1 | 6JM9 | 6NN6 | 6SEG | 6Z6P |
| 1ID3 | 3AV1 | 3O62 | 4R8P | 5CP6 | 5Y0C | 6JMA | 6NOG | 6T79 | 6ZHX |
| 1KX3 | 3AV2 | 3REH | 4WU8 | 5CPI | 5Y0D | 6JOU | 6NQA | 6T7A | 6ZHY |
| 1KX4 | 3AYW | 3REI | 4WU9 | 5CPJ | 5Z23 | 6JR0 | 6O1D | 6T7B | 7A08 |
| 1KX5 | 3AZE | 3REJ | 4X23 | 5CPK | 5Z30 | 6JR1 | 6O96 | 6T7C | 7AT8 |
| 1M18 | 3AZF | 3REK | 4XUJ | 5DNM | 5Z3L | 6JXD | 6OM3 | 6T7D | 7BXT |
| 1M19 | 3AZG | 3REL | 4XZQ | 5DNN | 5Z3O | 6JYL | 6PA7 | 6T90 | 7BY0 |
| 1M1A | 3AZH | 3TU4 | 4YM5 | 5E5A | 5Z3U | 6K1I | 6PWE | 6T93 | 7C0M |
| 1P34 | 3AZI | 3UT9 | 4YM6 | 5F99 | 5Z3V | 6K1J | 6PWF | 6T9L | 7CCQ |
| 1P3A | 3AZJ | 3UTA | 4YS3 | 5GSU | 5ZBX | 6K1K | 6PWV | 6TEM | 7CCR |
| 1P3B | 3AZK | 3UTB | 4Z5T | 5GT0 | 6BUZ | 6K1P | 6PWW | 6UGM | 7D1Z |
| 1P3F | 3AZL | 3W96 | 4Z66 | 5GT3 | 6C0W | 6KE9 | 6PWX | 6UH5 | 7D20 |
| 1P3G | 3AZM | 3W97 | 4ZUX | 5GTC | 6DZT | 6KIU | 6PX1 | 6UPH | 7DBP |
| 1P3I | 3AZN | 3W98 | 5AV5 | 5GXQ | 6E0C | 6KIV | 6R0C | 6UPK | 7JO9 |
| 1P3K | 3B6F | 3W99 | 5AV6 | 5KGF | 6E0P | 6KIW | 6R1T | 6UPL | 7JOA |
| 1P3L | 3B6G | 3WA9 | 5AV8 | 5MLU | 6ESF | 6KIX | 6R1U | 6USJ | 7JZV |
| 1P3M | 3C1B | 3WAA | 5AV9 | 5NL0 | 6ESG | 6KIZ | 6R25 | 6V2K | 7K5X |
| 1P3O | 3C1C | 3WKJ | 5AVB | 5OMX | 6ESH | 6KVD | 6R8Y | 6V92 | 7K5Y |
| 1P3P | 3KUY | 3WTP | 5AVC | 5ONG | 6ESI | 6KW3 | 6R8Z | 6VEN | 7K60 |
| 1S32 | 3KWQ | 3X1S | 5AY8 | 5ONW | 6FQ5 | 6KW5 | 6R90 | 6VYP | 7K61 |
| 1U35 | 3KXB | 3X1T | 5B0Y | 5T5K | 6FQ6 | 6KXV | 6R91 | 6VZ4 | 7K63 |
| 1ZLA | 3LEL | 3X1U | 5B0Z | 5WCU | 6FQ8 | 6L9H | 6R92 | 6WZ5 | 7K6P |
| 2CV5 | 3LJA | 3X1V | 5B1L | 5X0X | 6GEJ | 6LE9 | 6R94 | 6WZ9 | 7K6Q |
| 2F8N | 3LZ0 | 4J8U | 5B1M | 5X0Y | 6GEN | 6M4D | 6RYR | 6X0N | 7KTQ |
| 2FJ7 | 3LZ1 | 4J8V | 5B24 | 5X7X | 6IPU | 6M4G | 6RYU | 6X59 |      |
| 2NQB | 3MGP | 4J8W | 5B2I | 5XF3 | 6IQ4 | 6M4H | 6S01 | 6X5A |      |
| 2Nzd | 3MGQ | 4J8X | 5B2J | 5XF4 | 6IRO | 6MUO | 6SE0 | 6XJD |      |
| 2PYO | 3MGR | 4J2N | 5B31 | 5XF5 | 6IY2 | 6MUP | 6SE6 | 6Y5D |      |

We have downloaded all PDB files obtained from the Protein Data Bank, using a search keyword of nucleosome. A subset of these structures was selected based on the following criteria: (i) mono-nucleosomal DNA, (ii) the absence of additional proteins other than histone proteins, and (iii) the compatibility with the analysis software Curves+. For nucleosomes with DNA of more than 147 base pairs, the base pairs in the linker region were removed.

**Table S4. A summary of circular DNAs with constituent dinucleotide steps and the number of base pairs**

| Seq   | $N_{bp}$ | $L_{k_0}$      | $\sigma$ | kink | ellipticity    | $\langle \Omega \rangle$ | $\langle \Omega^{XY} \rangle^+$ | $\langle \Omega^{YX} \rangle^{\#}$ | $\langle \Omega^{XY} \rangle^+$ | $\langle \Omega^{YX} \rangle^{\#}$ | $\langle \Omega_{out}^{XY} \rangle^+$ | $\langle \Omega_{in}^{YX} \rangle^{\#}$ | $\langle \Omega_{out}^{YX} \rangle^{\#}$ |
|-------|----------|----------------|----------|------|----------------|--------------------------|---------------------------------|------------------------------------|---------------------------------|------------------------------------|---------------------------------------|-----------------------------------------|------------------------------------------|
| AT/AT | 88       | 7.74<br>(0.01) | 0.034    | 0    | 1.14<br>(0.00) | 32.27<br>(0.00)          | 30.55<br>(0.01)                 | 34.00<br>(0.01)                    | 30.99<br>(0.01)                 | 36.81<br>(0.01)                    | 30.14<br>(0.01)                       | 36.81<br>(0.01)                         | 31.38<br>(0.01)                          |
| AT/AT | 90       | 7.91<br>(0.01) | 0.011    | 0    | 1.15<br>(0.00) | 31.53<br>(0.00)          | 30.22<br>(0.01)                 | 32.84<br>(0.01)                    | 30.70<br>(0.01)                 | 35.63<br>(0.02)                    | 29.77<br>(0.01)                       | 35.63<br>(0.02)                         | 30.25<br>(0.01)                          |
| AT/AT | 92       | 8.09<br>(0.01) | -0.011   | 1    | 1.21<br>(0.01) | 30.86<br>(0.01)          | 29.90<br>(0.01)                 | 31.80<br>(0.01)                    | 30.41<br>(0.01)                 | 34.26<br>(0.06)                    | 29.45<br>(0.03)                       | 34.26<br>(0.06)                         | 29.60<br>(0.05)                          |
| AT/AT | 94       | 8.26<br>(0.01) | -0.032   | 0    | 1.17<br>(0.00) | 30.18<br>(0.01)          | 29.34<br>(0.01)                 | 31.01<br>(0.01)                    | 29.96<br>(0.01)                 | 33.58<br>(0.02)                    | 28.77<br>(0.01)                       | 33.58<br>(0.02)                         | 28.61<br>(0.01)                          |
| AT/AT | 96       | 8.44<br>(0.01) | -0.052   | 1    | 1.50<br>(0.01) | 30.98<br>(0.03)          | 29.85<br>(0.02)                 | 32.14<br>(0.05)                    | 30.08<br>(0.02)                 | 34.02<br>(0.05)                    | 29.63<br>(0.03)                       | 34.02<br>(0.05)                         | 30.46<br>(0.06)                          |
| GC/GC | 84       | 7.81<br>(0.00) | 0.024    | 1    | 1.20<br>(0.02) | 33.83<br>(0.02)          | 32.28<br>(0.02)                 | 35.39<br>(0.04)                    | 32.73<br>(0.01)                 | 36.91<br>(0.01)                    | 31.85<br>(0.03)                       | 36.91<br>(0.01)                         | 33.95<br>(0.08)                          |
| GC/GC | 86       | 8.00<br>(0.00) | 0.001    | 1    | 1.59<br>(0.10) | 33.22<br>(0.05)          | 31.74<br>(0.02)                 | 34.69<br>(0.08)                    | 32.05<br>(0.03)                 | 35.80<br>(0.05)                    | 31.44<br>(0.05)                       | 35.80<br>(0.05)                         | 33.61<br>(0.20)                          |
| GC/GC | 88       | 8.18<br>(0.00) | -0.022   | 2    | 1.29<br>(0.04) | 32.44<br>(0.06)          | 31.24<br>(0.04)                 | 33.66<br>(0.08)                    | 31.72<br>(0.03)                 | 35.04<br>(0.05)                    | 30.77<br>(0.05)                       | 35.04<br>(0.05)                         | 32.33<br>(0.14)                          |
| GC/GC | 90       | 8.37<br>(0.00) | -0.044   | 2    | 1.22<br>(0.01) | 31.84<br>(0.07)          | 30.77<br>(0.04)                 | 32.93<br>(0.11)                    | 31.30<br>(0.04)                 | 34.24<br>(0.08)                    | 30.25<br>(0.05)                       | 34.24<br>(0.08)                         | 31.65<br>(0.14)                          |

**Table S4 - continued from previous page**

| Seq   | $N_{bp}$ | $L_{k_0}$      | $\sigma$ | kink | ellipticity    | $\langle \Omega \rangle$ | $\langle \Omega^{XY} \rangle^{\dagger}$ | $\langle \Omega^{YX} \rangle^{\#}$ | $\langle \Omega_{in}^{XY} \rangle^{\dagger}$ | $\langle \Omega_{in}^{YX} \rangle^{\#}$ | $\langle \Omega_{out}^{XY} \rangle^{\dagger}$ | $\langle \Omega_{out}^{YX} \rangle^{\#}$ |
|-------|----------|----------------|----------|------|----------------|--------------------------|-----------------------------------------|------------------------------------|----------------------------------------------|-----------------------------------------|-----------------------------------------------|------------------------------------------|
| AC/GT | 88       | 7.81<br>(0.01) | 0.024    | 0    | 1.15<br>(0.00) | 32.11<br>(0.00)          | 31.05<br>(0.01)                         | 33.17<br>(0.01)                    | 31.57<br>(0.02)                              | 35.27<br>(0.02)                         | 30.54<br>(0.01)                               | 31.16<br>(0.01)                          |
| AC/GT | 90       | 7.99<br>(0.01) | 0.001    | 0    | 1.16<br>(0.00) | 31.39<br>(0.00)          | 30.49<br>(0.01)                         | 32.29<br>(0.01)                    | 31.06<br>(0.01)                              | 34.42<br>(0.02)                         | 29.95<br>(0.01)                               | 30.26<br>(0.02)                          |
| AG/CT | 88       | 7.74<br>(0.01) | 0.033    | 0    | 1.14<br>(0.00) | 32.20<br>(0.00)          | 31.22<br>(0.01)                         | 33.19<br>(0.01)                    | 30.85<br>(0.01)                              | 34.80<br>(0.01)                         | 31.59<br>(0.01)                               | 31.59<br>(0.01)                          |
| AG/CT | 90       | 7.92<br>(0.01) | 0.011    | 0    | 1.14<br>(0.00) | 31.58<br>(0.01)          | 30.57<br>(0.01)                         | 32.59<br>(0.01)                    | 30.50<br>(0.01)                              | 34.38<br>(0.02)                         | 30.63<br>(0.01)                               | 30.86<br>(0.01)                          |

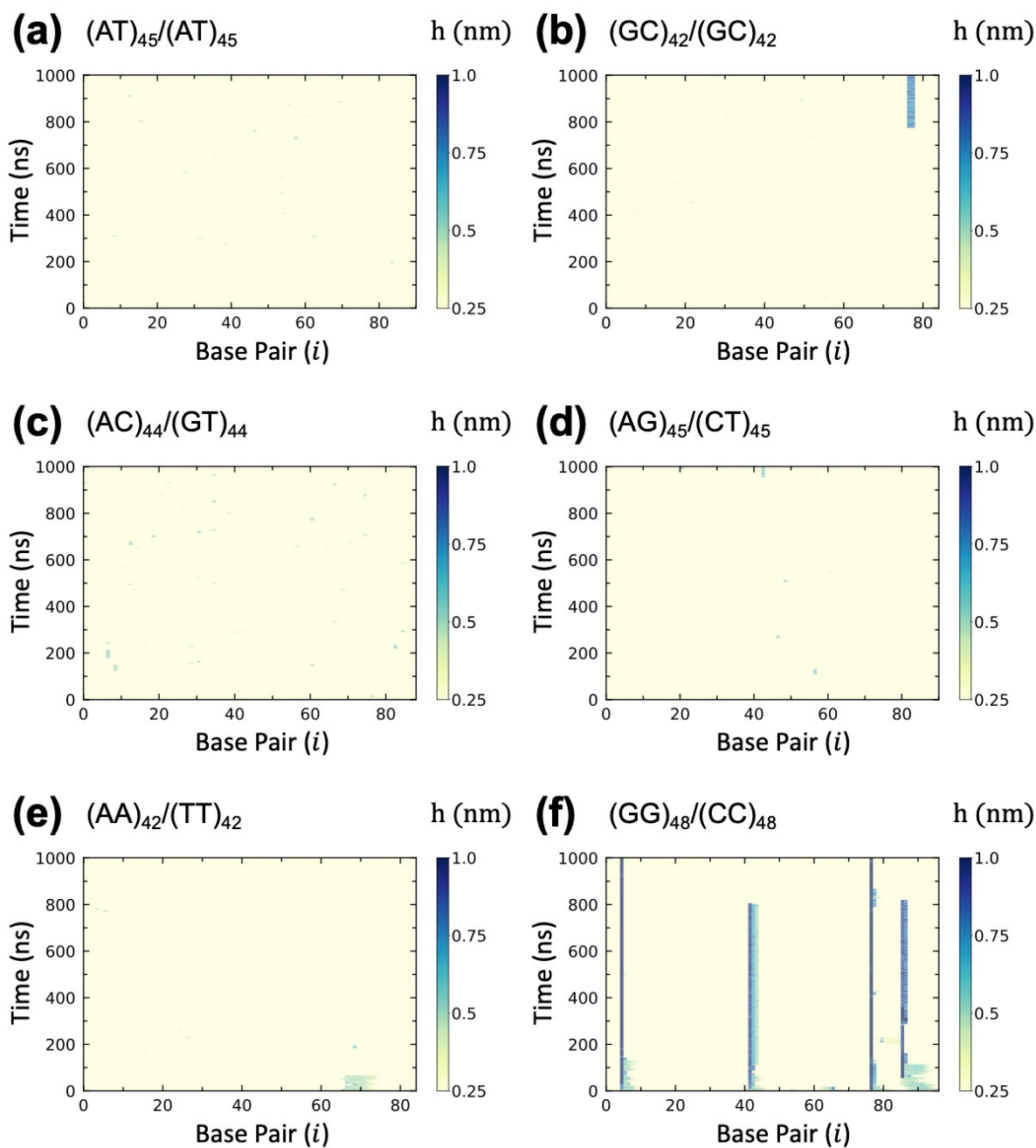
**Table S4 - continued from previous page**

| Seq   | $N_{bp}$ | $L_{k_0}$      | $\sigma$ | kink | ellipticity       | $\langle\Omega\rangle$ | $\langle\Omega_{in}\rangle$ | $\langle\Omega_{out}\rangle$ |
|-------|----------|----------------|----------|------|-------------------|------------------------|-----------------------------|------------------------------|
| AA/TT | 84       | 7.71<br>(0.01) | 0.038    | 1    | 1.13<br>(0.00)    | 33.62<br>(0.00)        | 33.81<br>(0.01)             | 33.44<br>(0.01)              |
| AA/TT | 86       | 7.89<br>(0.01) | 0.014    | 3    | 1.18<br>(0.01)    | 33.13<br>(0.02)        | 33.45<br>(0.01)             | 32.84<br>(0.03)              |
| AA/TT | 88       | 8.08<br>(0.01) | -0.010   | 3    | 1.15<br>(0.01)    | 32.36<br>(0.02)        | 33.05<br>(0.02)             | 31.72<br>(0.04)              |
| AA/TT | 90       | 8.26<br>(0.01) | -0.032   | 3    | 1.30<br>(0.01)    | 32.04<br>(0.01)        | 32.43<br>(0.04)             | 31.74<br>(0.05)              |
| GG/CC | 88       | 7.17<br>(0.00) | 0.115    | 2    | 2.59<br>(0.07)    | 31.14<br>(0.12)        | 31.16<br>(0.15)             | 31.12<br>(0.10)              |
| GG/CC | 90       | 7.34<br>(0.00) | 0.090    | 2    | Not<br>calculable | 30.96<br>(0.03)        | 31.18<br>(0.04)             | 30.76<br>(0.02)              |
| GG/CC | 94       | 7.66<br>(0.00) | 0.044    | 4    | 1.30<br>(0.01)    | 30.10<br>(0.01)        | 30.78<br>(0.02)             | 29.52<br>(0.04)              |
| GG/CC | 96       | 7.83<br>(0.00) | 0.022    | 4    | 1.19<br>(0.01)    | 29.67<br>(0.02)        | 30.44<br>(0.03)             | 29.04<br>(0.03)              |

$N_{bp}$  is the number of base pairs.  $\langle\Omega\rangle$  is the average twist angle in each DNA minicircle, whereas  $\langle\Omega_0\rangle$  is the average twist angle in a linear DNA molecule with 24 base pairs of the same repeating nucleotides. The linking number  $L_k$  is the number of helical turns in the DNA minicircles. The fractional linking number  $L_{k_0}$  is the number of helical turns predicted based on the average twist angle  $\langle\Omega_0\rangle$  of the corresponding linear molecules. The superhelical density is defined as  $\sigma = (L_k - L_{k_0})/L_{k_0}$  with non-zero values indicating deviation of the DNA minicircles from the ideal structure free from torsional stress. A kink is defined in terms of base-pair dissociation that lasts for some duration in the course of the 1- $\mu$ s simulation. Ellipticity is measured by fitting the 2D-projection of the helical axis to the equation of an ellipse. The values in parenthesis are the error estimated by batch means method.

<sup>†</sup>XY represents AT/AT, GC/GC, AC/GT, and AG/CT in the case of sequence (AT)<sub>n</sub>/(AT)<sub>n</sub>, (GC)<sub>n</sub>/(GC)<sub>n</sub>, (AC)<sub>n</sub>/(GT)<sub>n</sub>, and (AG)<sub>n</sub>/(CT)<sub>n</sub>, respectively.

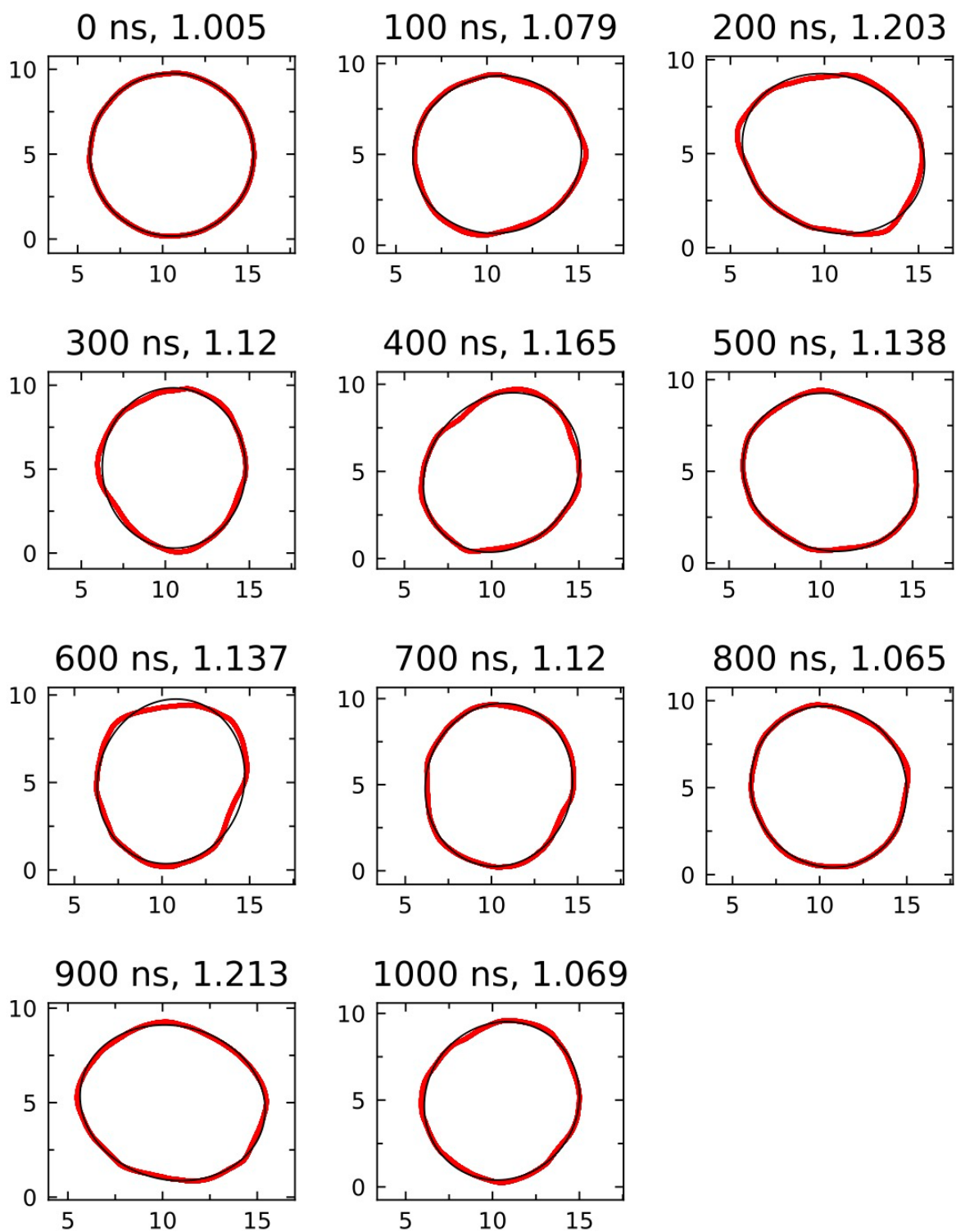
<sup>‡</sup>YX represents TA/TA, CG/CG, CA/TG, and GA/TC in the case of sequence (AT)<sub>n</sub>/(AT)<sub>n</sub>, (GC)<sub>n</sub>/(GC)<sub>n</sub>, (AC)<sub>n</sub>/(GT)<sub>n</sub>, and (AG)<sub>n</sub>/(CT)<sub>n</sub>, respectively.



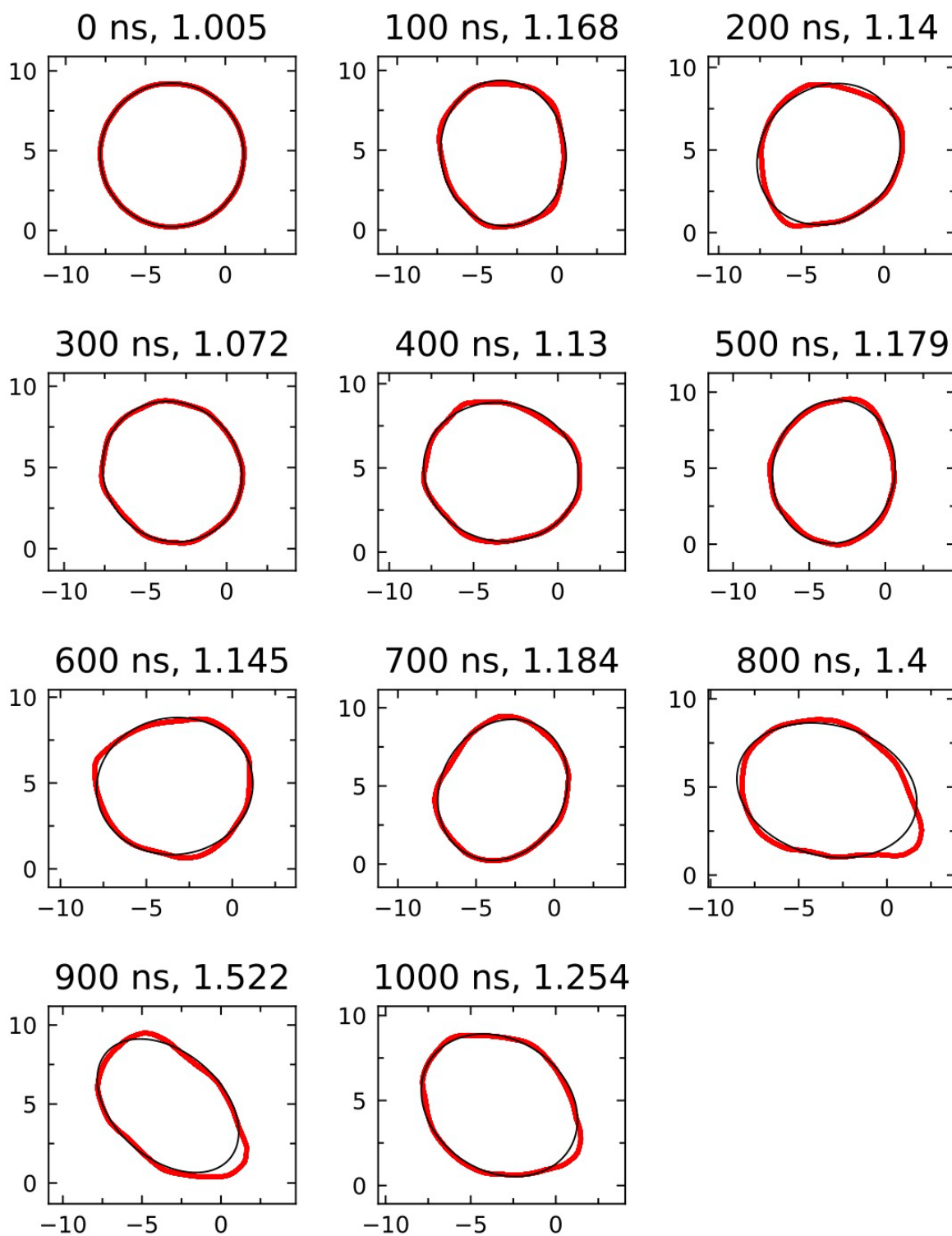
**Fig. S1. Determination of kink formation based on the hydrogen bond distance between complementary bases in DNA minicircles.** Time evolution of hydrogen bond distances,  $h$ , of all base pairs in DNA minicircles. The value of  $h$  was calculated as a distance between the N1 atom of adenine and the H3 atom of thymine for adenine-thymine (AT) complementary base pairs and between the H1 atom of guanine and the N3 atom of cytosine for guanine-cytosine (GC) complementary base pairs. The color in the scale bar on the right indicates the value of  $h$  in unit of nm. The kink formation is determined by the value of  $h$  greater than 0.29 nm.



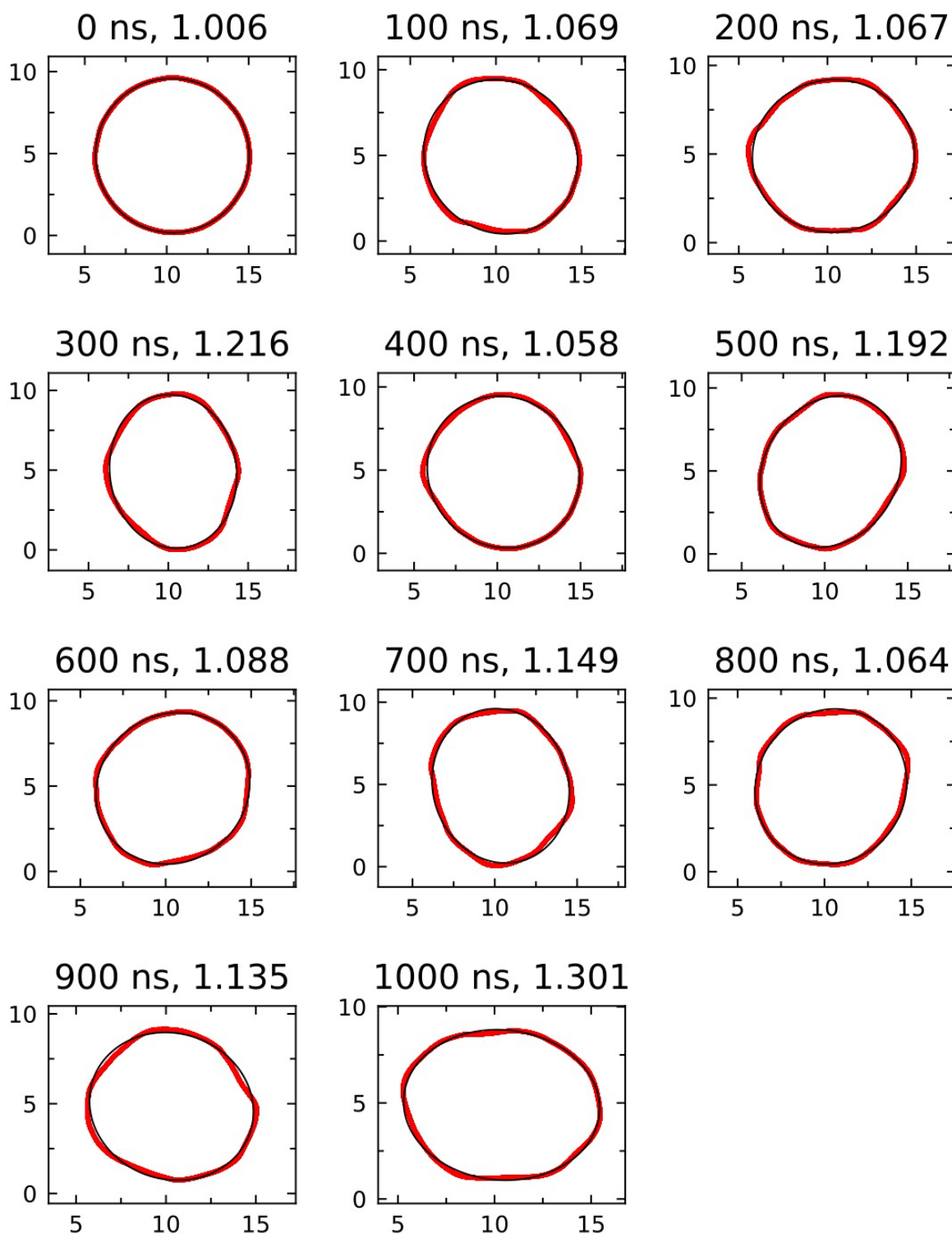
**(a)**  $(AT)_{45}/(AT)_{45}$



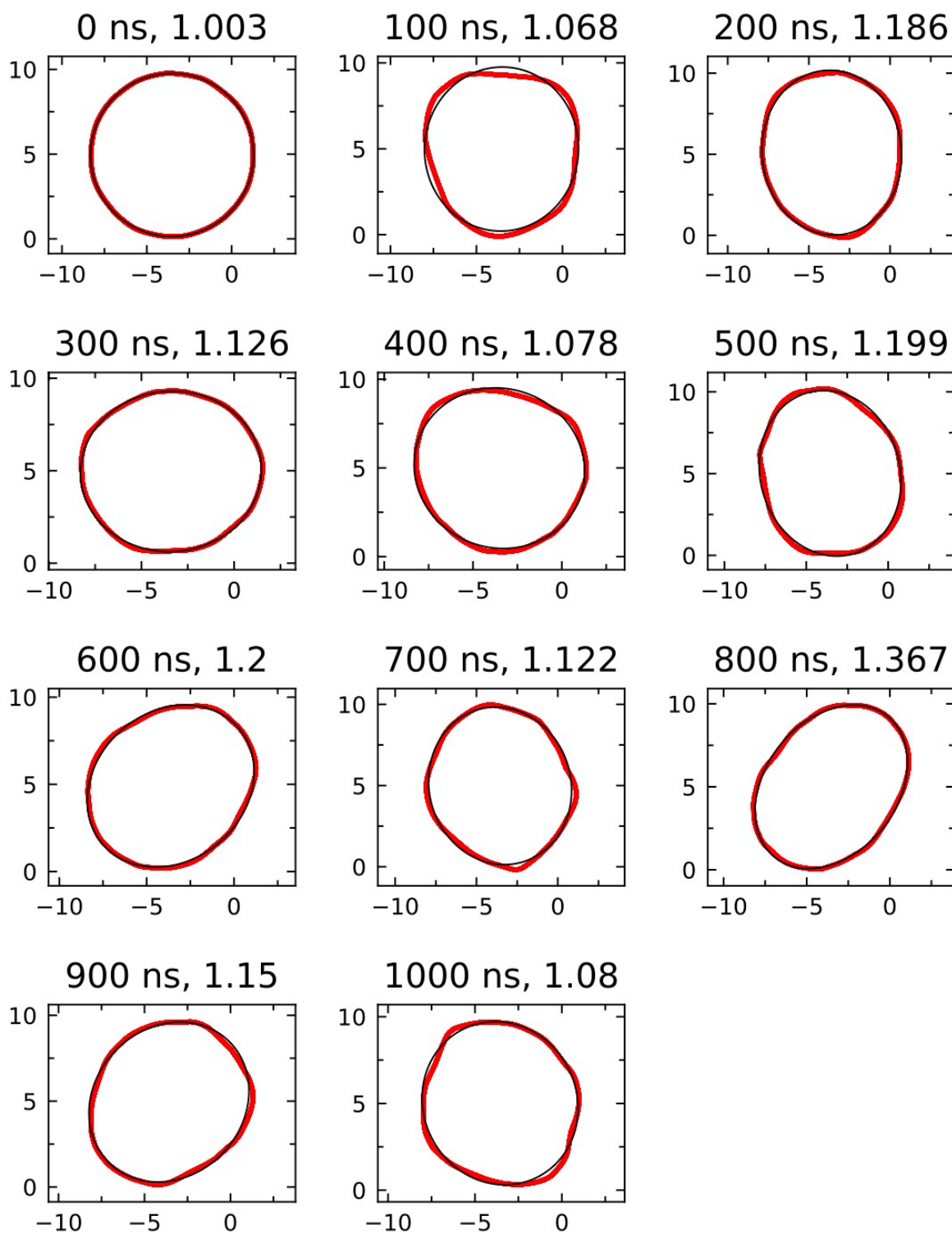
**(b)  $(GC)_{42}/(GC)_{42}$**



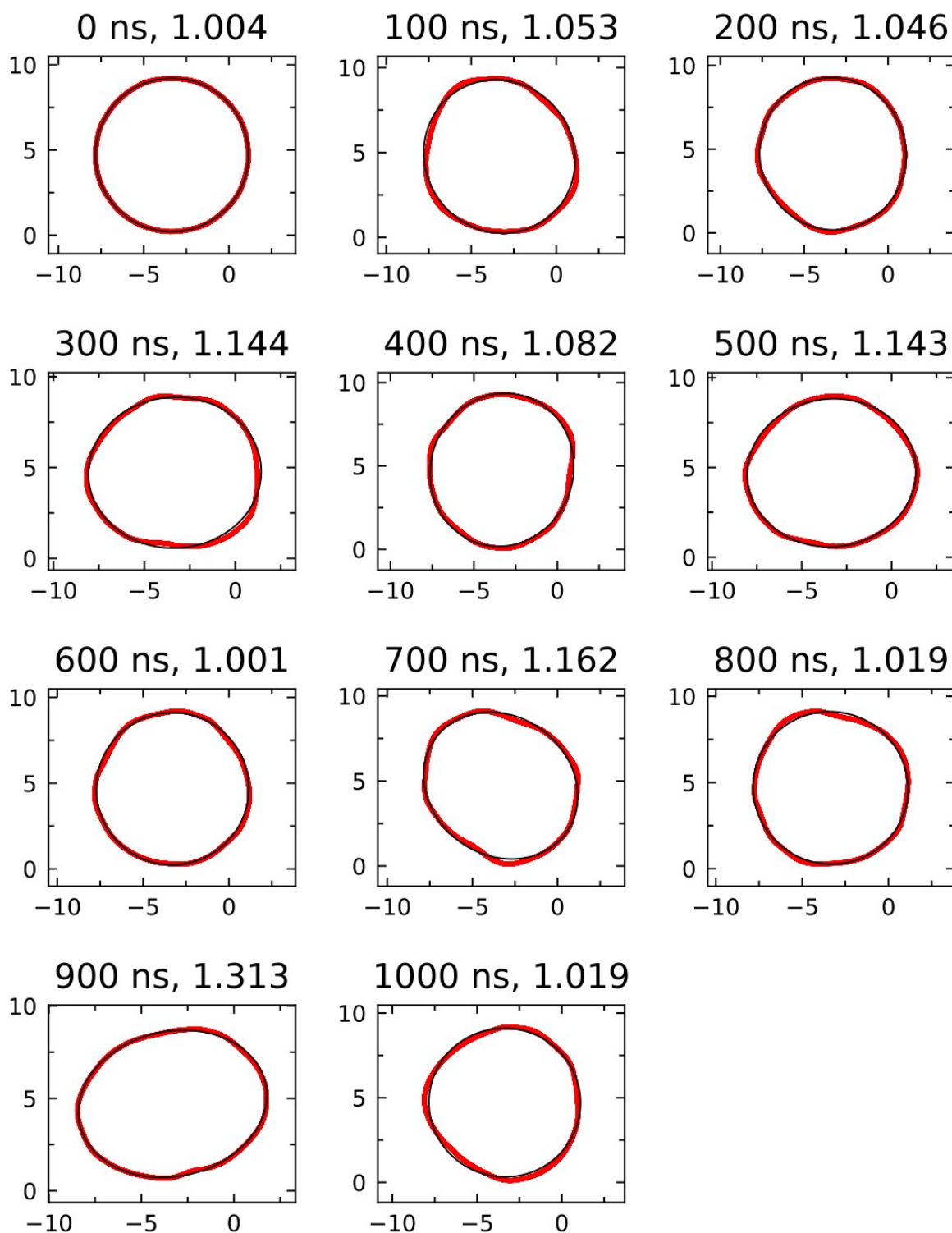
**(c)  $(AC)_{44}/(GT)_{44}$**



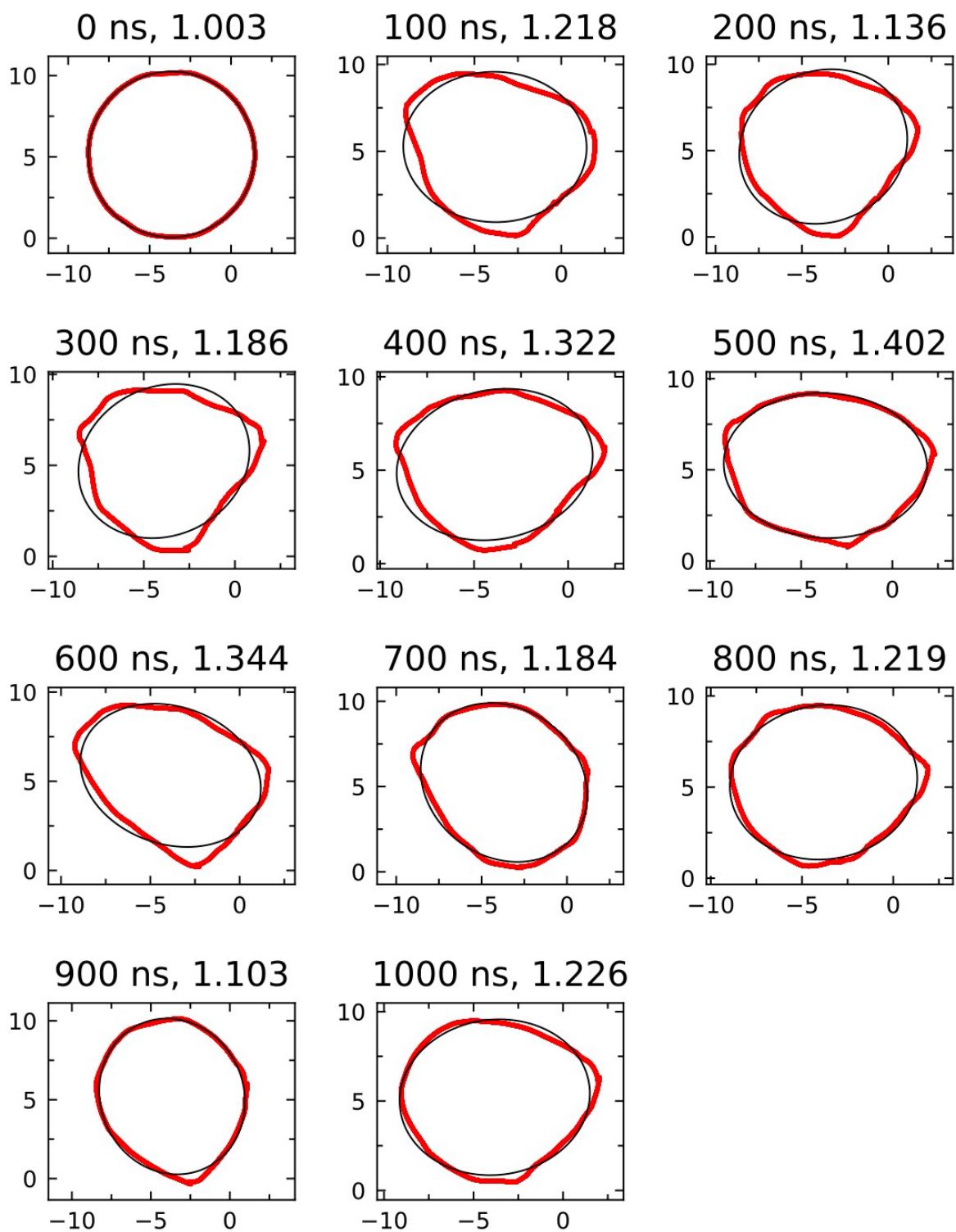
**(d)  $(AG)_{45}/(CT)_{45}$**



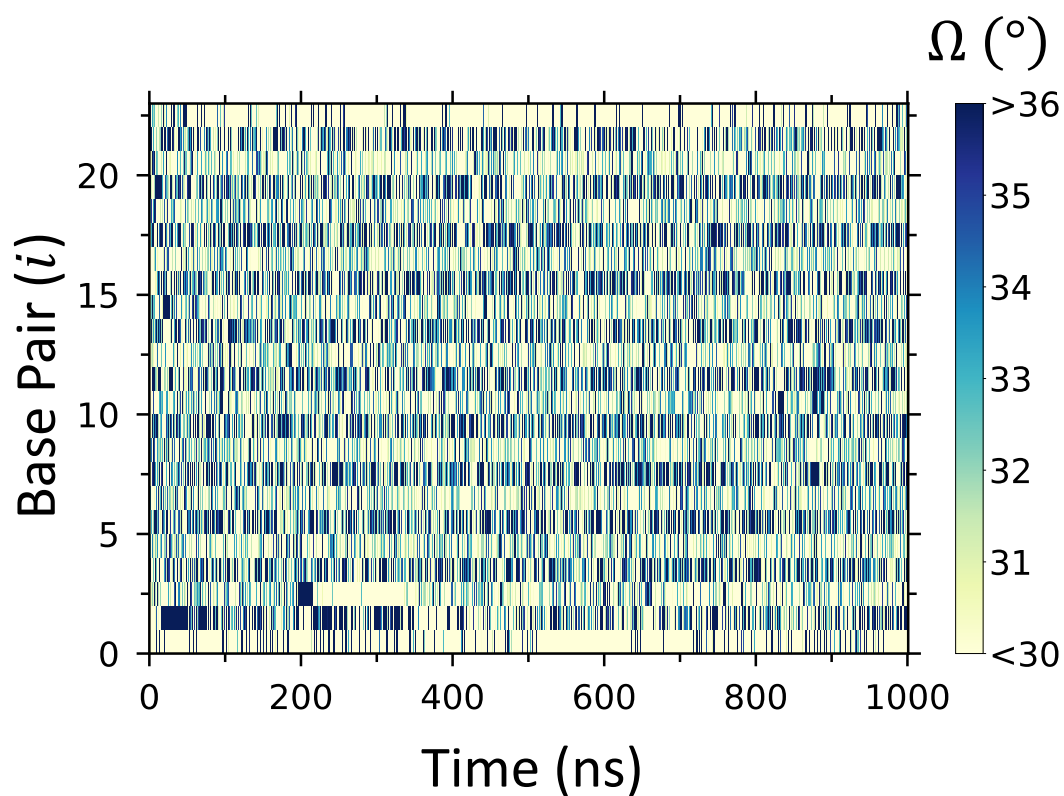
**(e)  $(AA)_{42}/(TT)_{42}$**



**(f)  $(GG)_{48}/(CC)_{48}$**

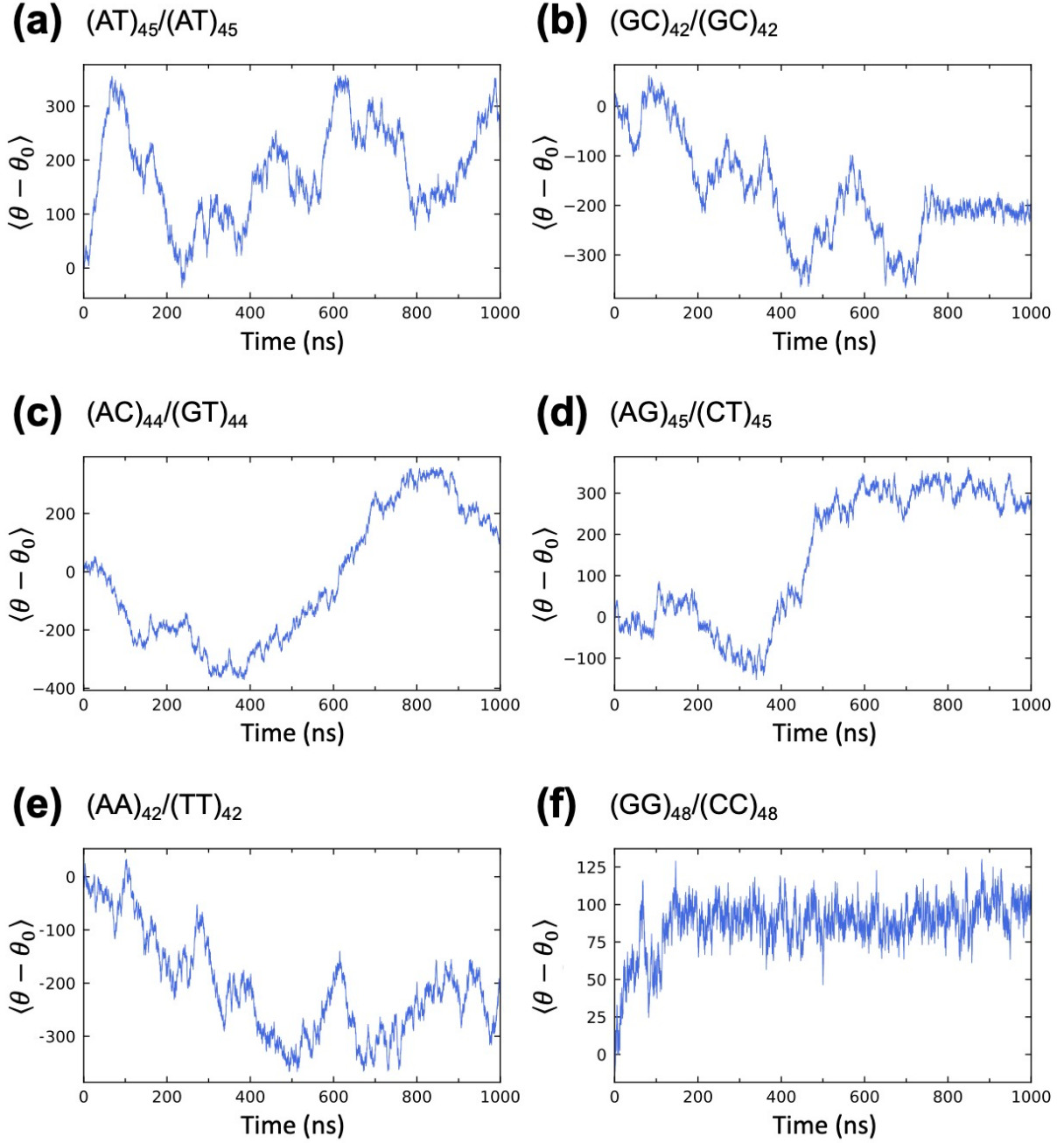


**Fig. S2. Ellipticity of DNA minicircles as a function of time. (a)**  $(AT)_{45}/(AT)_{45}$ , **(b)**  $(GC)_{42}/(GC)_{42}$ , **(c)**  $(AC)_{44}/(GT)_{44}$ , **(d)**  $(AG)_{45}/(CT)_{45}$ , **(e)**  $(AA)_{42}/(TT)_{42}$ , and **(f)**  $(GG)_{48}/(CC)_{48}$ . Ellipticity is defined as the ratio of the major axis to the minor axis of the ellipse. The ellipse is obtained by fitting the 2D-projection of the helical axis to the equation of an ellipse. The numbers on top of each figure are the simulation time at which the DNA conformation was taken and the ellipticity calculated for the conformation.

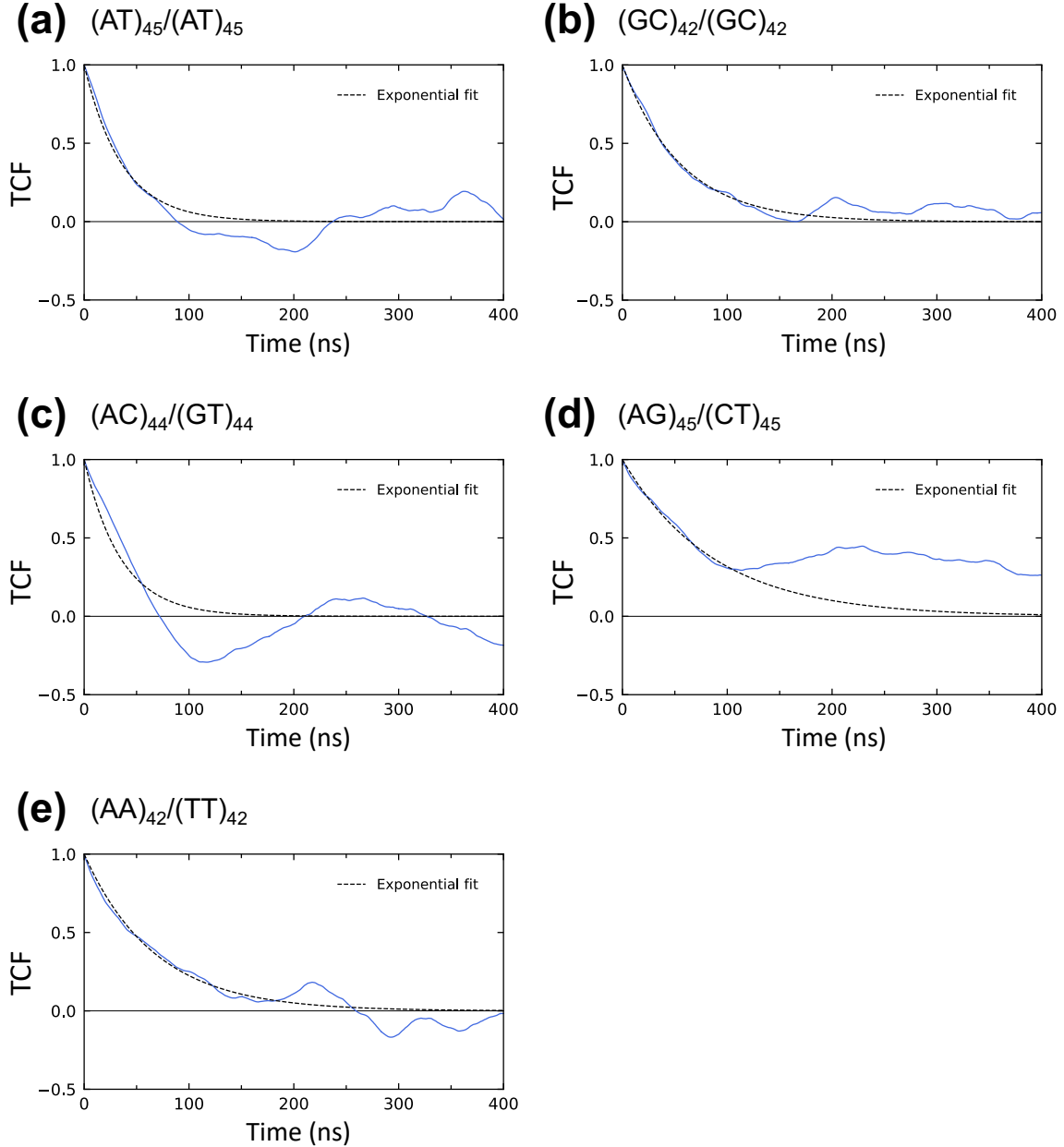


**Fig. S3. Time evolution of twist angles of all nucleotide steps in a linear DNA molecule.** The figure shows the case of  $(AT)_{12}/(AT)_{12}$ . At each time,  $\Omega$  was calculated for each dinucleotide step and the value was assigned to a base pair with the lower index number. The y-axis is the index number for the base pairs.





**Fig. S4. Time evolution of DNA poloidal orientation as a function of time.** Values of  $\theta(t)$  for each base pair were calculated at each time step and subtracted by the initial value  $\theta_0 = \theta(t = 0)$ , so that all DNA poloidal orientations start from 0 at the beginning. Then the orientations at each time step were averaged over all base pairs of DNA minicircles, resulting in the time evolution of  $\langle \theta - \theta_0 \rangle$  for (a)  $(AT)_{45}/(AT)_{45}$ , (b)  $(GC)_{42}/(GC)_{42}$ , (c)  $(AC)_{44}/(GT)_{44}$ , (d)  $(AG)_{45}/(CT)_{45}$ , (e)  $(AA)_{42}/(TT)_{42}$ , and (f)  $(GG)_{48}/(CC)_{48}$ .



**Fig. S5. Time correlation functions (TCF) of DNA poloidal orientations  $\langle \theta - \theta_0 \rangle$ , as presented in Fig. S4, for sequences of (a)  $(AT)_{45}/(AT)_{45}$ , (b)  $(GC)_{42}/(GC)_{42}$ , (c)  $(AC)_{44}/(GT)_{44}$ , (d)  $(AG)_{45}/(CT)_{45}$ , and (e)  $(AA)_{42}/(TT)_{42}$ . Solid lines are time correlation functions and dashed lines represent exponential fittings of the data. We obtained relaxation times of  $\tau = 36, 55, 35, 87,$  and  $67$  ns from the exponential fittings of (a), (b), (c), (d), and (e).**