

Supplementary Material

SerraNA: a program to determine nucleic acids elasticity from simulation data

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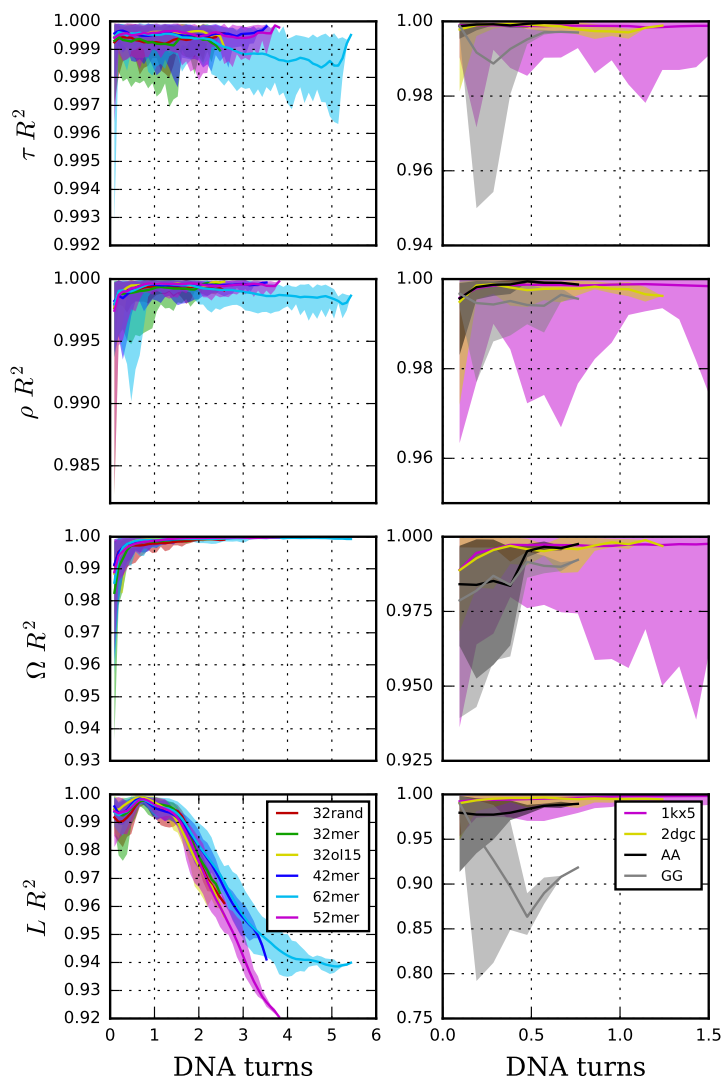


Figure 1: R-squared in linear fits of the quantile-quantile plots between real data against the estimated gaussian distributions for tilt (τ), roll (ρ), twist (Ω) and end-to-end distance (L). Lines correspond to averages and shade areas encompass maximum and minimum values for each sub-fragment length. Canonical relaxed DNAs (first column) can be broadly represented by normal distributions with the exception of (i) bimodal twists, which are only noticeable at the dinucleotide level, and (ii) L in long lengths due to its skewness on the distribution (Figure S2). Quadratic behaviour is significantly altered when DNA is perturbed by different factors (second column) including nucleosome formation (PDB 1kx5) and mismatches (AA and GG) (see Methods). Though, some protein-DNA complexes as the transcription factor GCN4 (PDB 2dgc) can still be described by the harmonic elastic model. Despite the failure of quadratic approximation on these singular DNAs, SerraNA can still provide some insights of how the different types of distortions modify the elasticity of DNA.

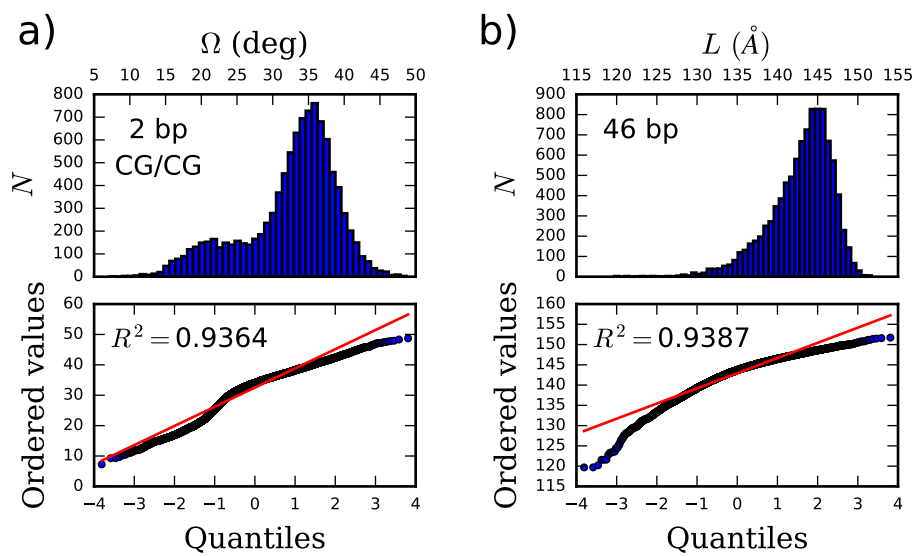


Figure 2: Histograms and quantile-quantile plots for the most non-gaussian cases on canonical relaxed DNAs, including (a) bimodal twist (Ω) for a CG bp step within the 32mer fragment, and (b) skewed end-to-end (L) distribution for the longest analyzed sub-length (46 bp) from the 62mer fragment.

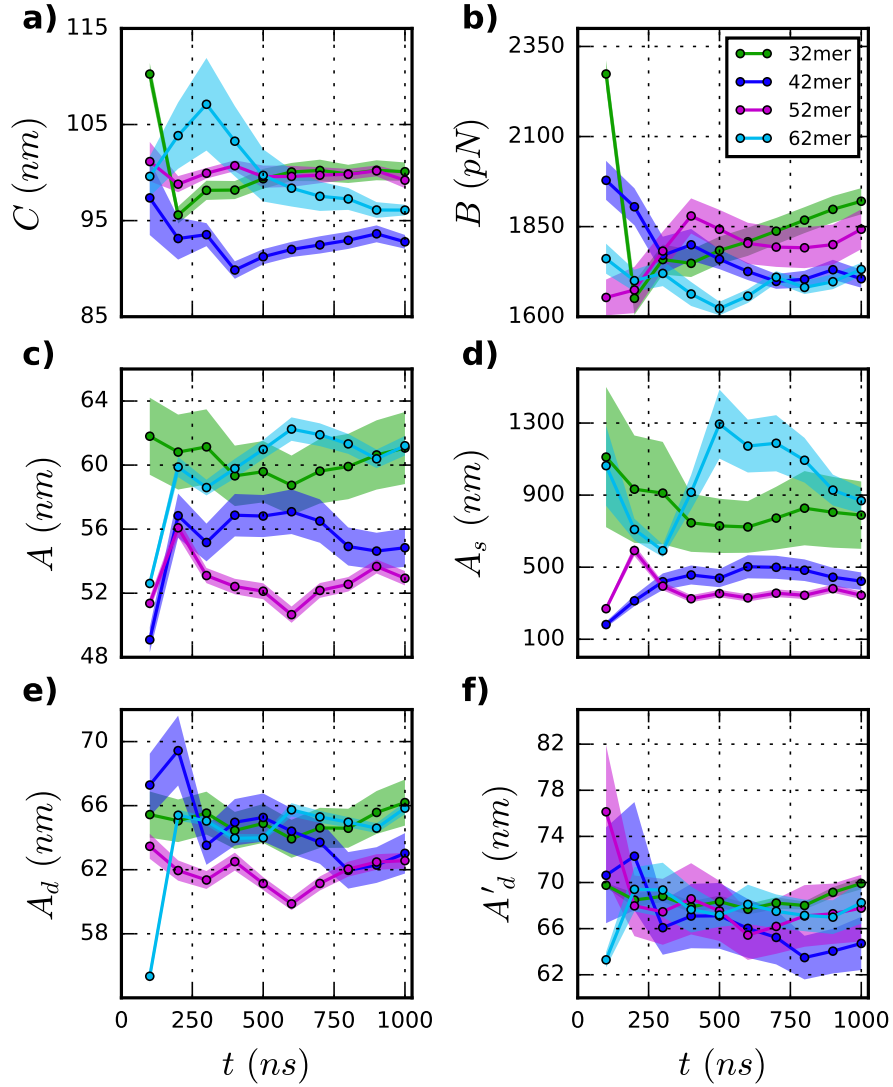


Figure 3: Elastic constants for twist C , stretch B , persistence length A , static persistence length A_s , dynamic persistence length A_d and a second prediction of the dynamic persistence length A'_d for increasing extensions (in ns) of the trajectories over DNA fragments containing 32 (green), 42 (blue), 52 (purple) and 62 (cyan) bp long. Shaded areas represent standard deviations in the case of C and A'_d , and uncertainty values with 70% of confidence level for variables obtained through linear fits (B, A, A_s and A_d).

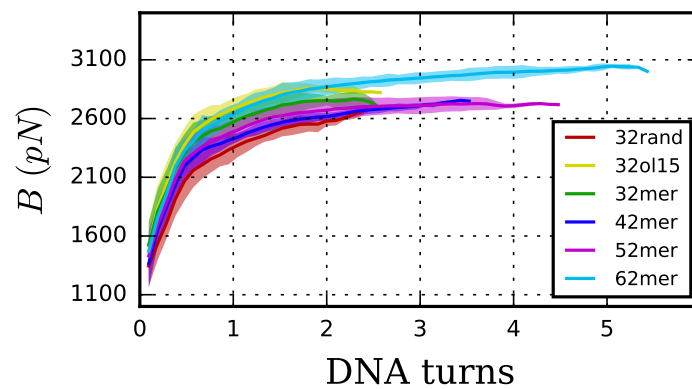


Figure 4: Stretch Modulus B at different lengths using contour length instead of end-to-end distance and including simulations for a 32bp random sequence (32rand) and the 32mer using par-mOL15 force field (32ol15) (see Methods).

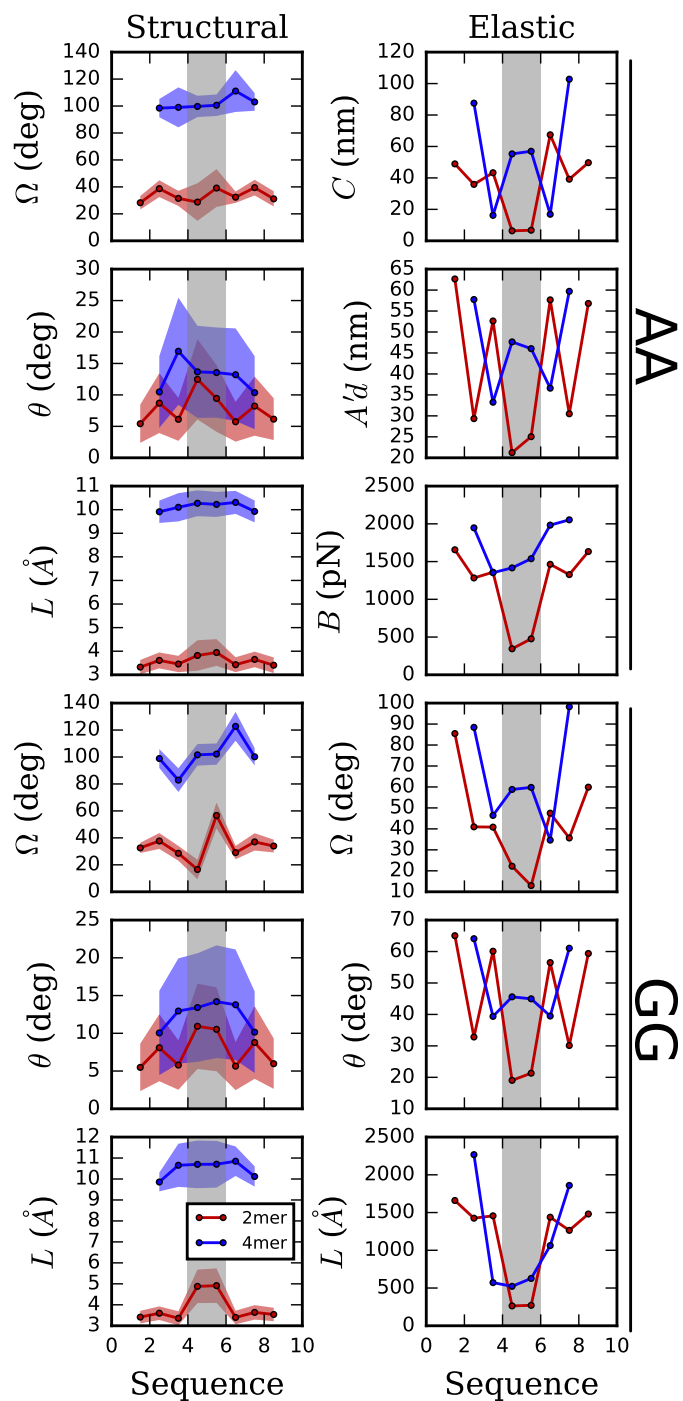


Figure 5: Structural (left) and elastic (right) profiles along the molecule for dimer and tetramer sub-lengths of trajectories containing an AA (top) and GG (bottom) mismatch, the localization of which is indicated by grey shade.

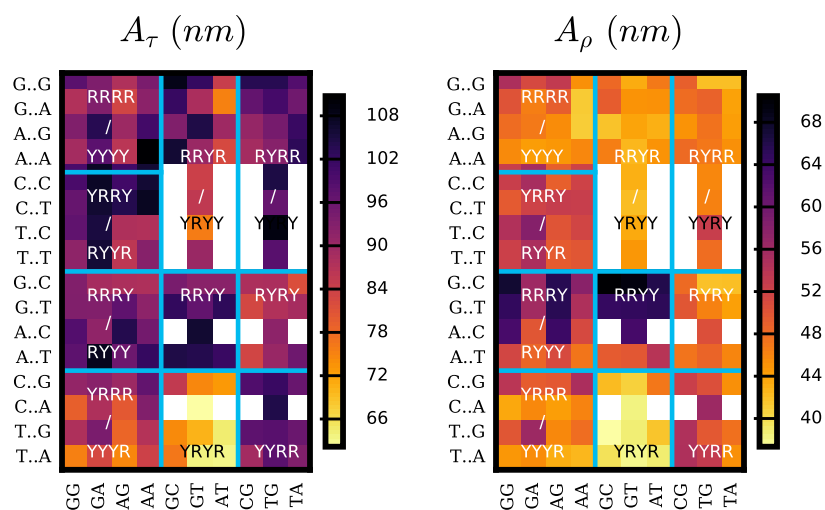


Figure 6: Roll and tilt persistence lengths (A_ρ and A_τ , respectively) at the 4 bp length for the 136 tetranucleotide sequences from ABC simulation database. Vertical axis represent the flanking base-pairs and the horizontal axis represents the middle base-steps. Horizontal and vertical lines organize sequences according purine (R) or pyrimidine (Y) type. Sequence duplication is excluded through the use of white squares.

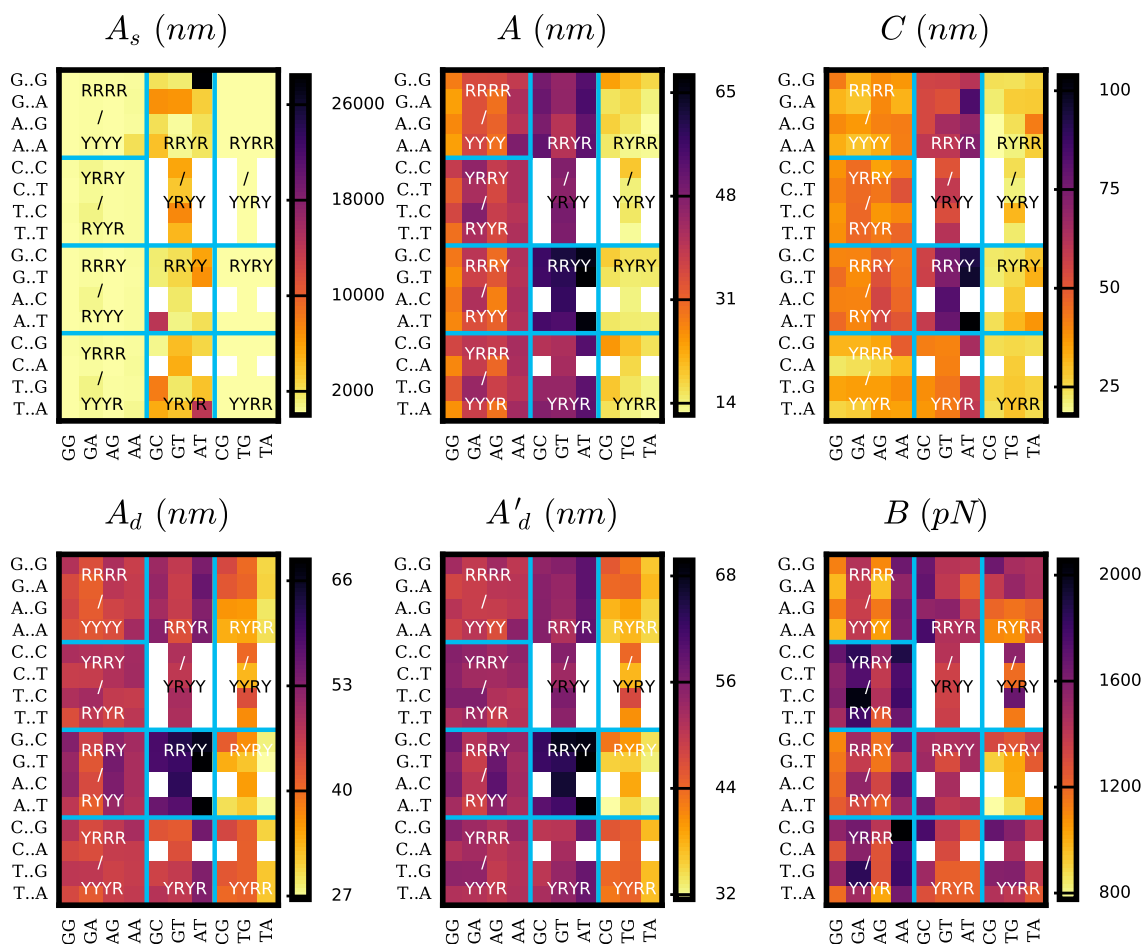


Figure 7: Elastic constants at the dinucleotide length for the whole set of 136 tetra-nucleotide sequences from ABC simulation database. Total persistence length together with its static and dynamic components (A , A_s and A_d , respectively) are calculated using the directional decay at dimer level. Twist (C), stretch modulus (B) and the second estimation of dynamic persistence length (A'_d) are obtained directly from the inverse-covariance matrix for dinucleotides. Vertical axis indicates middle steps, and horizontal axis flanking bases. Horizontal and vertical lines organize sequences according purine (R) or pyrimidine (Y) type. Sequence duplication is excluded through the use of white squares.

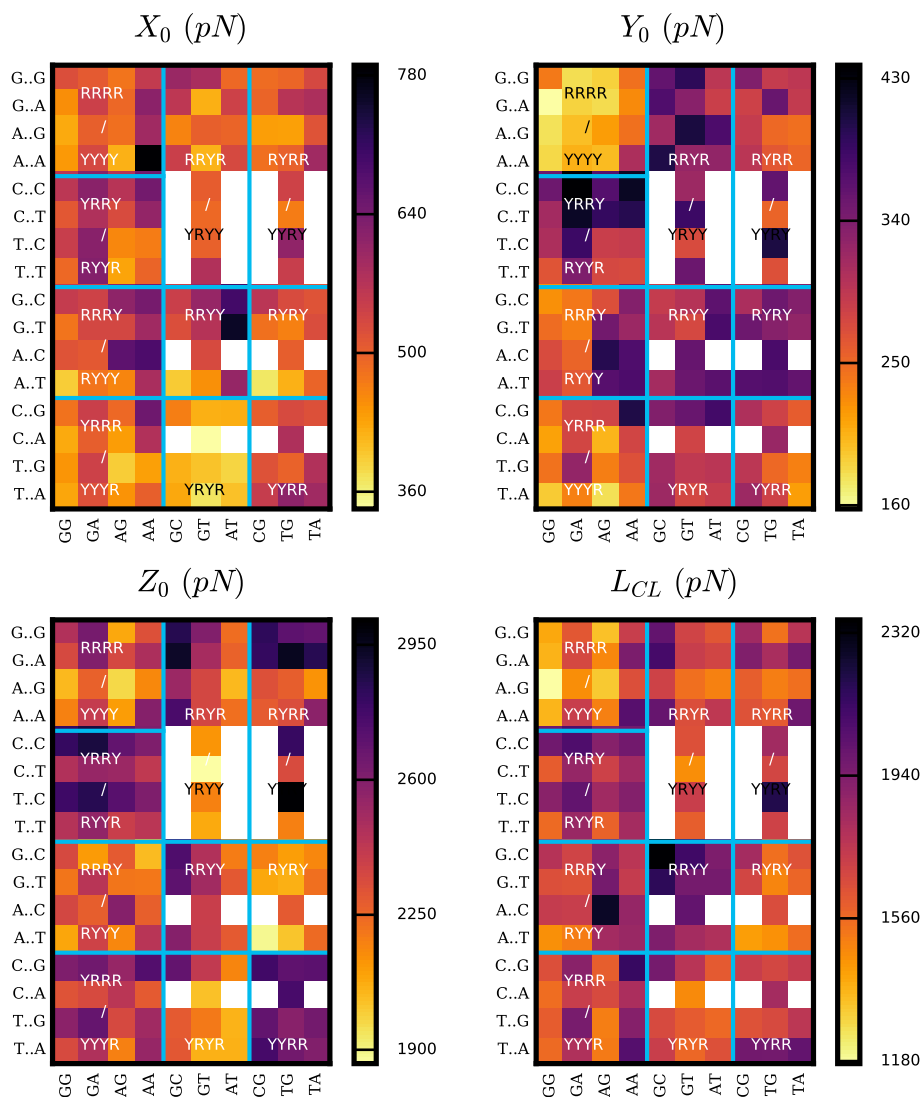


Figure 8: Added shift X_0 , slide Y_0 , rise Z_0 and contour length L_{CL} elastic constants at the 4 bp length for the 136 tetranucleotide sequences from ABC simulation database. Vertical axis represent the flanking base-pairs and the horizontal axis represents the middle base-steps. Horizontal and vertical lines organize sequences according purine (R) or pyrimidine (Y) type. Sequence duplication is excluded through the use of white squares.

Table 1: Two versions of dynamics persistence length (A'_d and A''_d) estimated from unconstrained MD trajectories over linear DNA fragments and calculated following equation 9 and 11, respectively, as in Table 1 in the main manuscript.

	A'_d	A''_d
32rand	68.3 ± 1.0	68.04 ± 1.0
32mer	69.9 ± 0.5	69.2 ± 0.6
42mer	64.7 ± 2.3	64.4 ± 2.4
52mer	67.8 ± 2.9	67.1 ± 3.0
62mer	68.2 ± 1.8	67.9 ± 1.9
Average	67.8 ± 1.7	67.3 ± 1.8

Table 2: Persistence length A , its static A_s and dynamic A_d components and twist C and stretch modulus B of RRRR tetranucleotide sequences.

Sequence	A (nm)	A_d (nm)	A_s (nm)	C (nm)	B (pN)
GGGG	19.0 ± 0.6	65.4 ± 2.6	26.9 ± 1.1	79.1 ± 6.4	1541 ± 47
GGGA	24.0 ± 0.7	57.9 ± 1.1	41.0 ± 2.2	65.8 ± 2.0	1411 ± 34
AGGG	18.0 ± 0.5	59.3 ± 1.7	25.8 ± 0.7	63.7 ± 3.1	1188 ± 26
AGGA	23.5 ± 2.2	57.2 ± 0.8	40.3 ± 6.3	61.0 ± 0.8	1358 ± 39
GGAG	31.9 ± 0.6	60.7 ± 1.1	67.6 ± 3.9	69.3 ± 2.1	1863 ± 6
GGAA	36.7 ± 0.6	55.5 ± 0.7	108.1 ± 2.7	74.5 ± 4.9	1844 ± 44
AGAG	25.5 ± 2.1	60.5 ± 1.0	44.5 ± 6.4	66.9 ± 4.8	1637 ± 78
AGAA	35.4 ± 5.0	55.0 ± 4.3	101.8 ± 26.9	66.7 ± 1.7	1863 ± 136
GAGG	23.3 ± 1.6	60.6 ± 0.9	37.9 ± 3.8	58.6 ± 1.6	1652 ± 122
GAGA	27.7 ± 0.8	57.6 ± 0.5	53.4 ± 3.0	60.1 ± 1.7	1603 ± 38
AAGG	21.2 ± 1.0	56.8 ± 0.5	34.0 ± 2.7	59.2 ± 4.5	1311 ± 23
AAGA	27.4 ± 4.7	56.6 ± 2.6	54.7 ± 14.7	51.8 ± 8.4	1581 ± 84
GAAG	34.9 ± 1.3	55.4 ± 0.5	95.6 ± 10.6	61.3 ± 1.4	2028 ± 109
GAAA	46.9 ± 0.1	52.3 ± 0.1	454.1 ± 20.1	61.5 ± 2.0	2127 ± 24
AAAG	33.7 ± 0.4	54.6 ± 1.1	87.8 ± 0.1	56.8 ± 3.0	1754 ± 47
AAAA	55.8 ± 7.0	61.6 ± 3.4	970.0 ± 506.1	74.6 ± 6.6	2241 ± 88
Average	30.3 ± 9.9	57.9 ± 3.2	140.2 ± 236.0	64.4 ± 7.0	1688 ± 288

Table 3: Persistence length A , its static A_s and dynamic A_d components and twist C and stretch modulus B of YRRY tetranucleotide sequences.

Sequence	A (nm)	A_d (nm)	A_s (nm)	C (nm)	B (pN)
TGGT	19.6 ± 0.8	61.1 ± 3.8	28.8 ± 1.0	72.9 ± 5.4	1700 ± 109
TGGC	28.4 ± 2.2	65.5 ± 2.4	50.4 ± 5.4	69.9 ± 2.1	2139 ± 82
CGGT	23.0 ± 0.5	62.7 ± 2.5	36.4 ± 0.6	69.0 ± 4.5	2072 ± 88
CGGC	32.7 ± 0.6	66.2 ± 2.3	64.9 ± 2.6	65.8 ± 2.7	2468 ± 82
TGAT	28.5 ± 1.6	68.7 ± 3.4	48.8 ± 3.2	82.3 ± 2.5	2153 ± 118
TGAC	42.3 ± 1.7	70.1 ± 1.9	106.7 ± 6.6	81.0 ± 0.4	2470 ± 39
CGAT	33.6 ± 0.7	68.1 ± 0.7	66.5 ± 2.9	68.3 ± 2.8	2421 ± 44
CGAC	41.5 ± 1.2	69.0 ± 2.7	104.2 ± 1.7	74.1 ± 1.4	2754 ± 65
TAGT	24.0 ± 1.9	57.2 ± 2.8	41.4 ± 4.3	68.0 ± 4.9	1771 ± 62
TAGC	33.1 ± 0.8	57.4 ± 0.9	78.1 ± 3.7	65.4 ± 1.9	2119 ± 49
CAGT	30.9 ± 1.1	66.9 ± 1.8	57.6 ± 3.2	78.2 ± 1.8	2097 ± 26
CAGC	35.5 ± 1.7	62.8 ± 2.4	81.8 ± 5.4	70.2 ± 2.0	2329 ± 70
TAAT	31.6 ± 2.5	57.4 ± 2.3	70.7 ± 9.0	69.5 ± 2.0	1923 ± 68
TAAC	38.8 ± 3.6	56.8 ± 2.4	124.0 ± 23.3	72.0 ± 2.6	2171 ± 16
CAAT	36.6 ± 2.5	67.4 ± 2.9	80.2 ± 7.9	80.5 ± 2.4	2147 ± 81
CAAC	44.6 ± 1.6	65.5 ± 2.4	139.7 ± 5.9	81.5 ± 0.9	2347 ± 125
Average	32.8 ± 6.9	63.9 ± 4.5	73.8 ± 30.7	73.0 ± 5.7	2193 ± 261

Table 4: Persistence length A , its static A_s and dynamic A_d components and twist C and stretch modulus B of RRRY tetranucleotide sequences.

Sequence	A (nm)	A_d (nm)	A_s (nm)	C (nm)	B (pN)
GGGT	29.7 ± 1.3	60.8 ± 0.2	58.5 ± 5.3	58.4 ± 1.2	1682 ± 113
GGGC	35.9 ± 2.2	64.9 ± 2.2	80.5 ± 7.8	61.5 ± 2.0	1861 ± 105
AGGT	33.5 ± 1.7	56.7 ± 2.0	82.3 ± 7.8	60.5 ± 0.1	1498 ± 82
AGGC	36.5 ± 0.7	63.3 ± 1.4	86.5 ± 4.7	61.0 ± 3.0	1833 ± 71
GGAT	36.4 ± 0.6	57.6 ± 0.4	99.1 ± 5.8	63.9 ± 0.7	1670 ± 69
GGAC	41.9 ± 2.1	56.0 ± 0.9	169.0 ± 25.4	55.8 ± 0.0	1938 ± 46
AGAT	33.7 ± 0.4	57.6 ± 0.4	81.5 ± 3.3	74.0 ± 1.8	1589 ± 28
AGAC	41.6 ± 1.3	56.1 ± 0.3	163.2 ± 22.0	57.1 ± 0.5	1923 ± 52
GAGT	50.0 ± 2.2	64.5 ± 1.2	233.9 ± 55.2	63.2 ± 2.6	2219 ± 34
GAGC	37.4 ± 0.8	62.8 ± 2.3	93.5 ± 9.3	59.2 ± 2.4	2072 ± 24
AAGT	43.3 ± 1.6	57.6 ± 2.0	174.5 ± 6.7	62.8 ± 1.6	1993 ± 15
AAGC	40.8 ± 0.6	69.5 ± 1.4	99.1 ± 0.8	79.8 ± 3.1	2551 ± 52
GAAT	51.0 ± 2.4	57.0 ± 2.0	484.7 ± 69.6	54.8 ± 4.2	1981 ± 25
GAAC	52.5 ± 2.7	58.7 ± 3.1	496.5 ± 18.6	56.7 ± 2.2	2155 ± 97
AAAT	53.9 ± 0.2	59.2 ± 0.9	613.0 ± 78.7	62.5 ± 1.0	2185 ± 8
AAAC	50.4 ± 0.7	59.7 ± 1.6	327.7 ± 17.1	57.1 ± 2.4	2203 ± 47
Average	41.8 ± 7.4	60.1 ± 3.7	209.0 ± 170.6	61.8 ± 6.4	1960 ± 264

Table 5: Persistence length A , its static A_s and dynamic A_d components and twist C and stretch modulus B of YRRR tetranucleotide sequences.

Sequence	A (nm)	A_d (nm)	A_s (nm)	C (nm)	B (pN)
TGGG	17.1 ± 0.3	59.8 ± 1.0	24.0 ± 0.5	60.6 ± 1.7	1673 ± 67
TGGA	18.0 ± 1.0	52.5 ± 0.8	27.6 ± 2.4	62.0 ± 0.8	1695 ± 82
CGGG	21.5 ± 1.4	65.4 ± 0.8	32.2 ± 2.9	56.6 ± 2.5	1974 ± 40
CGGA	21.9 ± 0.7	54.5 ± 0.6	36.6 ± 2.0	51.6 ± 1.9	2000 ± 44
TGAG	33.2 ± 1.0	65.5 ± 2.2	67.3 ± 2.2	72.7 ± 2.7	2335 ± 100
TGAA	28.0 ± 0.5	54.9 ± 1.8	57.5 ± 3.1	69.0 ± 1.1	2044 ± 28
CGAG	27.6 ± 0.7	61.9 ± 0.8	50.0 ± 2.3	69.3 ± 1.5	2377 ± 65
CGAA	31.6 ± 0.6	57.6 ± 2.2	70.2 ± 1.0	54.3 ± 1.3	2357 ± 100
TAGG	20.1 ± 0.7	52.6 ± 1.9	32.7 ± 1.2	59.8 ± 3.9	1663 ± 43
TAGA	16.8 ± 0.3	49.5 ± 0.6	25.5 ± 0.8	74.1 ± 3.3	1593 ± 40
CAGG	23.0 ± 1.3	60.9 ± 1.6	36.9 ± 2.9	63.5 ± 2.1	1996 ± 23
CAGA	22.4 ± 0.3	54.3 ± 0.4	38.1 ± 0.8	60.5 ± 2.4	1958 ± 83
TAAG	32.2 ± 1.5	55.8 ± 1.5	76.5 ± 6.9	67.5 ± 1.8	2186 ± 49
TAAA	35.0 ± 0.9	51.4 ± 2.2	110.4 ± 9.5	75.7 ± 1.8	2161 ± 63
CAAG	35.1 ± 1.6	66.9 ± 2.1	73.7 ± 4.9	81.2 ± 5.1	2566 ± 110
CAAA	34.6 ± 0.1	58.0 ± 0.7	85.5 ± 1.3	65.1 ± 3.2	2060 ± 87
Average	26.1 ± 6.5	57.6 ± 5.2	52.8 ± 24.6	65.2 ± 7.9	2040 ± 276

Table 6: Persistence length A , its static A_s and dynamic A_d components and twist C and stretch modulus B of RRYR /YRY Y tetranucleotide sequences.

Sequence	A (nm)	A_d (nm)	A_s (nm)	C (nm)	B (pN)
GGTG	30.4 ± 0.1	57.6 ± 0.8	64.1 ± 0.7	66.0 ± 2.0	2076 ± 68
GGTA	29.2 ± 0.1	52.6 ± 0.6	65.8 ± 0.4	61.1 ± 0.9	1783 ± 53
AGTG	29.2 ± 0.7	59.5 ± 1.3	57.5 ± 2.4	66.0 ± 3.2	1996 ± 74
AGTA	22.7 ± 2.1	51.7 ± 1.5	40.6 ± 5.7	56.5 ± 3.2	1854 ± 13
TGTT	22.8 ± 0.1	58.9 ± 0.1	37.2 ± 0.2	52.5 ± 1.9	1832 ± 28
TGTC	26.1 ± 1.5	53.4 ± 0.7	51.3 ± 6.0	48.8 ± 1.3	2035 ± 114
CGTT	24.6 ± 0.1	57.2 ± 0.1	43.1 ± 0.3	41.1 ± 0.3	1931 ± 10
CGTC	26.6 ± 2.5	57.0 ± 0.6	50.7 ± 8.4	43.8 ± 1.8	2309 ± 108
GGCG	31.5 ± 0.3	65.2 ± 0.3	61.1 ± 0.9	56.3 ± 0.6	2462 ± 27
GGCA	28.1 ± 0.0	63.4 ± 1.3	50.4 ± 0.9	57.8 ± 0.3	2293 ± 41
AGCG	22.2 ± 3.1	56.6 ± 4.6	38.8 ± 12.4	60.5 ± 3.1	2171 ± 149
AGCA	19.8 ± 1.1	63.1 ± 3.6	29.0 ± 1.6	66.1 ± 6.9	2266 ± 46
GATG	25.8 ± 3.5	56.2 ± 0.4	49.0 ± 11.4	52.4 ± 2.9	2142 ± 191
GATA	20.9 ± 0.5	48.5 ± 0.2	36.7 ± 1.4	65.4 ± 1.3	1678 ± 74
AATG	24.5 ± 0.7	56.0 ± 0.2	43.6 ± 2.3	48.7 ± 1.1	1714 ± 43
AATA	25.8 ± 0.5	52.2 ± 1.7	50.9 ± 0.3	56.2 ± 0.8	1799 ± 6
Average	25.6 ± 3.3	56.8 ± 4.4	48.1 ± 10.2	56.2 ± 7.7	2021 ± 229

Table 7: Persistence length A , its static A_s and dynamic A_d components and twist C and stretch modulus B of RRYT tetranucleotide sequences.

Sequence	A (nm)	A_d (nm)	A_s (nm)	C (nm)	B (pN)
GGTT	38.4 ± 0.4	65.8 ± 0.8	92.4 ± 0.9	54.5 ± 0.1	2255 ± 24
GGTC	44.5 ± 0.1	65.6 ± 0.5	138.4 ± 3.3	65.1 ± 1.2	2493 ± 1
AGTT	48.2 ± 0.7	60.8 ± 0.9	232.1 ± 3.2	56.4 ± 0.4	2179 ± 12
AGTC	50.2 ± 5.8	68.3 ± 1.5	205.5 ± 65.0	62.3 ± 1.9	2533 ± 59
GGCT	42.1 ± 0.3	65.2 ± 0.6	118.9 ± 3.9	55.7 ± 2.3	2527 ± 28
GGCC	44.1 ± 0.4	65.3 ± 0.0	136.3 ± 4.0	60.7 ± 1.6	2677 ± 18
AGCT	41.5 ± 1.8	58.8 ± 1.4	141.7 ± 12.7	55.4 ± 0.5	2314 ± 67
GATT	59.4 ± 0.5	70.7 ± 0.3	370.7 ± 11.9	65.2 ± 2.6	2413 ± 49
GATC	58.1 ± 0.4	65.9 ± 0.3	495.3 ± 17.6	66.7 ± 0.9	2339 ± 15
AATT	61.7 ± 1.0	64.9 ± 0.7	1267.1 ± 144.2	57.9 ± 0.9	2209 ± 16
Average	48.8 ± 7.8	65.1 ± 3.2	319.8 ± 337.9	60.0 ± 4.4	2394 ± 154

Table 8: Persistence length A , its static A_s and dynamic A_d components and twist C and stretch modulus B of YRYR tetranucleotide sequences.

Sequence	A (nm)	A_d (nm)	A_s (nm)	C (nm)	B (pN)
TGTG	17.5 ± 0.9	47.4 ± 2.1	28.0 ± 3.1	54.7 ± 4.5	1847 ± 136
TGTA	17.5 ± 0.4	43.3 ± 0.9	29.3 ± 0.9	64.6 ± 4.3	1682 ± 40
CGTG	19.9 ± 0.1	51.3 ± 0.8	32.7 ± 0.5	54.5 ± 1.5	2173 ± 51
CGTA	19.0 ± 0.5	44.0 ± 1.0	33.6 ± 2.0	50.9 ± 3.5	1749 ± 52
TGCG	18.9 ± 0.3	48.8 ± 0.9	30.7 ± 0.9	50.8 ± 1.8	2095 ± 53
TGCA	15.1 ± 0.1	49.7 ± 0.3	21.7 ± 0.2	69.7 ± 1.1	1850 ± 30
CGCG	25.6 ± 0.7	56.4 ± 1.9	47.1 ± 2.6	52.1 ± 1.0	2660 ± 63
TATG	17.7 ± 0.8	43.9 ± 0.3	29.8 ± 2.3	60.6 ± 0.2	1676 ± 12
TATA	17.6 ± 0.8	41.1 ± 0.8	31.0 ± 2.8	70.1 ± 4.1	1672 ± 30
CATG	16.3 ± 0.5	53.2 ± 0.9	23.6 ± 0.9	60.4 ± 0.2	1887 ± 38
Average	18.5 ± 2.7	47.9 ± 4.6	30.8 ± 6.5	58.9 ± 7.0	1929 ± 293

Table 9: Persistence length A , its static A_s and dynamic A_d components and twist C and stretch modulus B of RYRR/YYRY tetranucleotide sequences.

Sequence	A (nm)	A_d (nm)	A_s (nm)	C (nm)	B (pN)
GTGG	30.0 ± 0.6	56.0 ± 1.7	64.9 ± 0.6	85.1 ± 1.6	2271 ± 131
GTGA	46.1 ± 0.6	61.5 ± 0.2	184.6 ± 7.5	92.2 ± 1.8	2645 ± 14
ATGG	20.7 ± 1.4	59.9 ± 1.2	31.7 ± 3.7	79.3 ± 0.8	1746 ± 203
ATGA	26.6 ± 1.2	59.1 ± 1.1	48.7 ± 4.1	83.3 ± 0.6	1875 ± 54
TTGT	29.6 ± 1.4	61.3 ± 2.1	57.3 ± 3.5	74.4 ± 5.4	1898 ± 31
TTGC	43.6 ± 2.1	67.8 ± 1.3	122.6 ± 13.1	93.4 ± 1.7	2829 ± 164
CTGT	24.0 ± 0.7	59.9 ± 0.4	40.1 ± 1.9	81.7 ± 2.5	1889 ± 52
CTGC	37.9 ± 0.4	62.1 ± 2.4	97.7 ± 4.1	82.2 ± 6.3	2497 ± 87
GTAG	34.9 ± 2.2	54.9 ± 3.0	96.1 ± 7.4	81.1 ± 4.5	2147 ± 148
GTAA	40.3 ± 2.6	54.0 ± 1.3	161.7 ± 28.9	84.9 ± 1.4	2378 ± 111
ATAG	19.7 ± 0.5	55.9 ± 0.5	30.4 ± 1.2	97.3 ± 2.7	1504 ± 23
ATAA	32.0 ± 3.2	54.4 ± 1.0	79.7 ± 16.8	83.8 ± 3.5	1919 ± 58
GCGG	32.6 ± 0.1	65.2 ± 2.1	65.5 ± 2.4	69.3 ± 6.4	2659 ± 116
GCGA	30.2 ± 0.1	62.5 ± 0.3	58.5 ± 0.8	87.1 ± 1.2	2503 ± 66
ACGG	21.7 ± 0.8	60.0 ± 0.9	34.0 ± 2.0	74.4 ± 1.3	2050 ± 116
ACGA	26.9 ± 0.9	62.0 ± 1.5	47.4 ± 2.0	62.0 ± 1.4	2111 ± 48
Average	31.1 ± 7.7	59.8 ± 3.8	76.3 ± 44.6	82.0 ± 8.7	2183 ± 363

Table 10: Persistence length A , its static A_s and dynamic A_d components and twist C and stretch modulus B of RYRY tetranucleotide sequences.

Sequence	A (nm)	A_d (nm)	A_s (nm)	C (nm)	B (pN)
GTGT	29.6 ± 1.3	55.7 ± 0.7	63.2 ± 5.4	72.6 ± 1.9	1599 ± 47
GTGC	35.1 ± 0.2	53.9 ± 0.8	100.8 ± 4.3	70.7 ± 1.7	2014 ± 38
ATGT	31.0 ± 0.4	56.4 ± 0.6	69.0 ± 0.8	83.8 ± 3.7	1455 ± 54
ATGC	29.4 ± 1.0	59.8 ± 1.7	58.5 ± 6.0	79.7 ± 3.4	1785 ± 106
GTAT	30.6 ± 0.7	50.3 ± 0.0	78.4 ± 4.6	91.0 ± 0.1	1550 ± 22
GTAC	31.5 ± 0.2	49.0 ± 0.1	88.0 ± 2.2	82.2 ± 3.1	1792 ± 78
ATAT	31.6 ± 0.9	51.9 ± 1.1	81.0 ± 4.9	97.5 ± 3.8	1448 ± 22
GCGT	34.0 ± 0.5	56.7 ± 0.7	85.0 ± 1.8	58.6 ± 1.2	2047 ± 37
GCGC	46.4 ± 1.7	57.7 ± 0.8	239.7 ± 31.4	59.9 ± 1.5	2642 ± 90
ACGT	30.9 ± 1.7	54.9 ± 0.7	71.2 ± 8.5	65.8 ± 1.6	1569 ± 41
Average	33.0 ± 4.8	54.6 ± 3.2	93.5 ± 50.2	76.2 ± 12.3	1790 ± 349

Table 11: Persistence length A , its static A_s and dynamic A_d components and twist C and stretch modulus B of YYRR tetranucleotide sequences.

Sequence	A (nm)	A_d (nm)	A_s (nm)	C (nm)	B (pN)
TTGG	26.7 ± 0.8	59.6 ± 2.7	48.5 ± 1.1	88.0 ± 5.0	2313 ± 81
TTGA	32.1 ± 0.7	64.6 ± 2.1	64.0 ± 1.5	93.7 ± 1.2	2466 ± 86
CTGG	30.8 ± 1.5	61.6 ± 1.6	61.7 ± 4.6	87.3 ± 1.3	2529 ± 66
CTGA	36.0 ± 2.0	67.1 ± 2.4	78.5 ± 10.5	94.4 ± 2.4	2597 ± 107
TTAG	32.9 ± 1.3	57.2 ± 1.6	77.3 ± 4.2	84.4 ± 2.0	2245 ± 70
TTAA	33.7 ± 0.9	55.7 ± 0.6	85.5 ± 4.3	80.4 ± 1.9	2276 ± 55
CTAG	34.5 ± 1.3	56.8 ± 1.9	87.7 ± 4.1	78.7 ± 8.1	2365 ± 97
TCGG	26.3 ± 0.3	66.0 ± 1.5	43.7 ± 0.9	83.3 ± 3.0	2546 ± 132
TCGA	29.6 ± 1.4	65.4 ± 0.3	54.4 ± 4.5	81.1 ± 2.4	2698 ± 45
CCGG	27.4 ± 0.6	65.0 ± 0.8	47.3 ± 1.5	83.0 ± 2.3	2755 ± 61
Average	31.0 ± 3.2	61.9 ± 4.1	64.9 ± 15.6	85.4 ± 5.1	2479 ± 168

Table 12: Averages and standard deviations of tetranucleotide elastic constants.

Parameter	Average
A (nm)	31.8 ± 1.0
A_d (nm)	58.8 ± 5.9
A'_d (nm)	64.3 ± 7.1
A_s (nm)	108.1 ± 158.9
C (nm)	68.0 ± 12.0
B (pN)	2054 ± 354