

Article

Reconstructing the Free Energy Profiles Describing the Switching Mechanism of a pH-Dependent DNA Nanodevice from ABMD Simulations

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SUPPLEMENTARY DATA

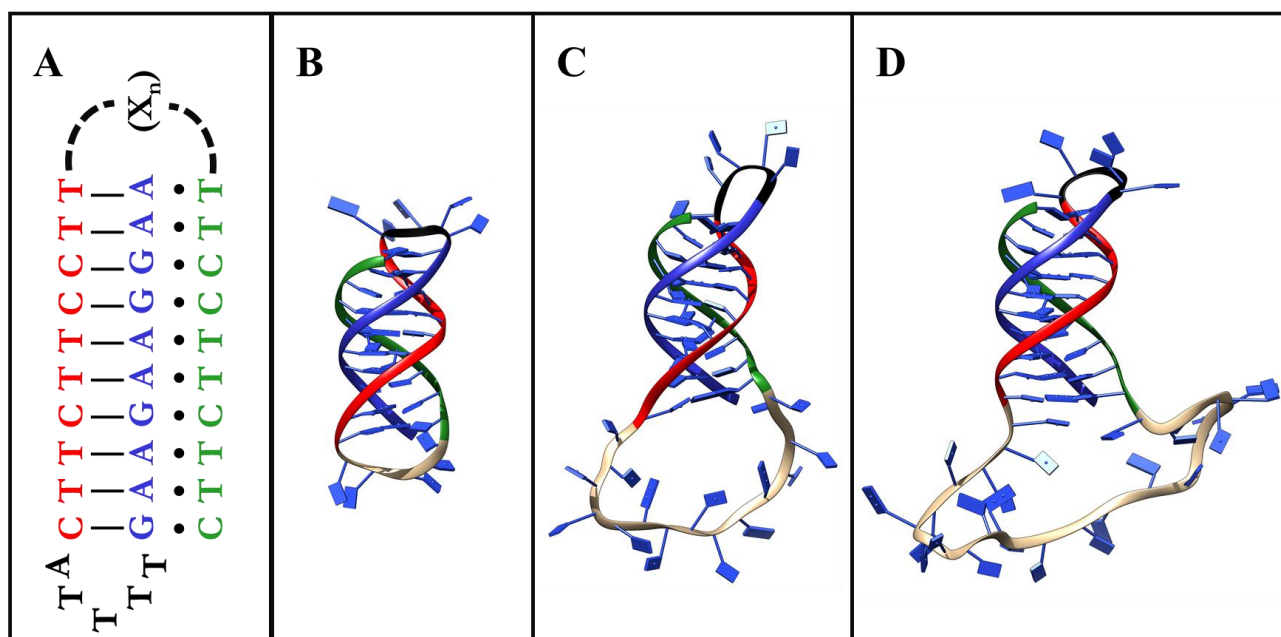


Figure S1. Schematic (A) and cartoon (B–D) representations of the simulated tetraprotic DNA nanoswitches. The red and blue colors indicate the two strands forming the double helix region, while the black indicates the conserved five-base loop and the green indicates the TFO. The black dashed line in A and the tan-colored ribbon in B–D represent the 5 (B), 15 (C) and 25 (D) base variable loop. The pictures were produced using the UCSF Chimera 1.12 program [43].

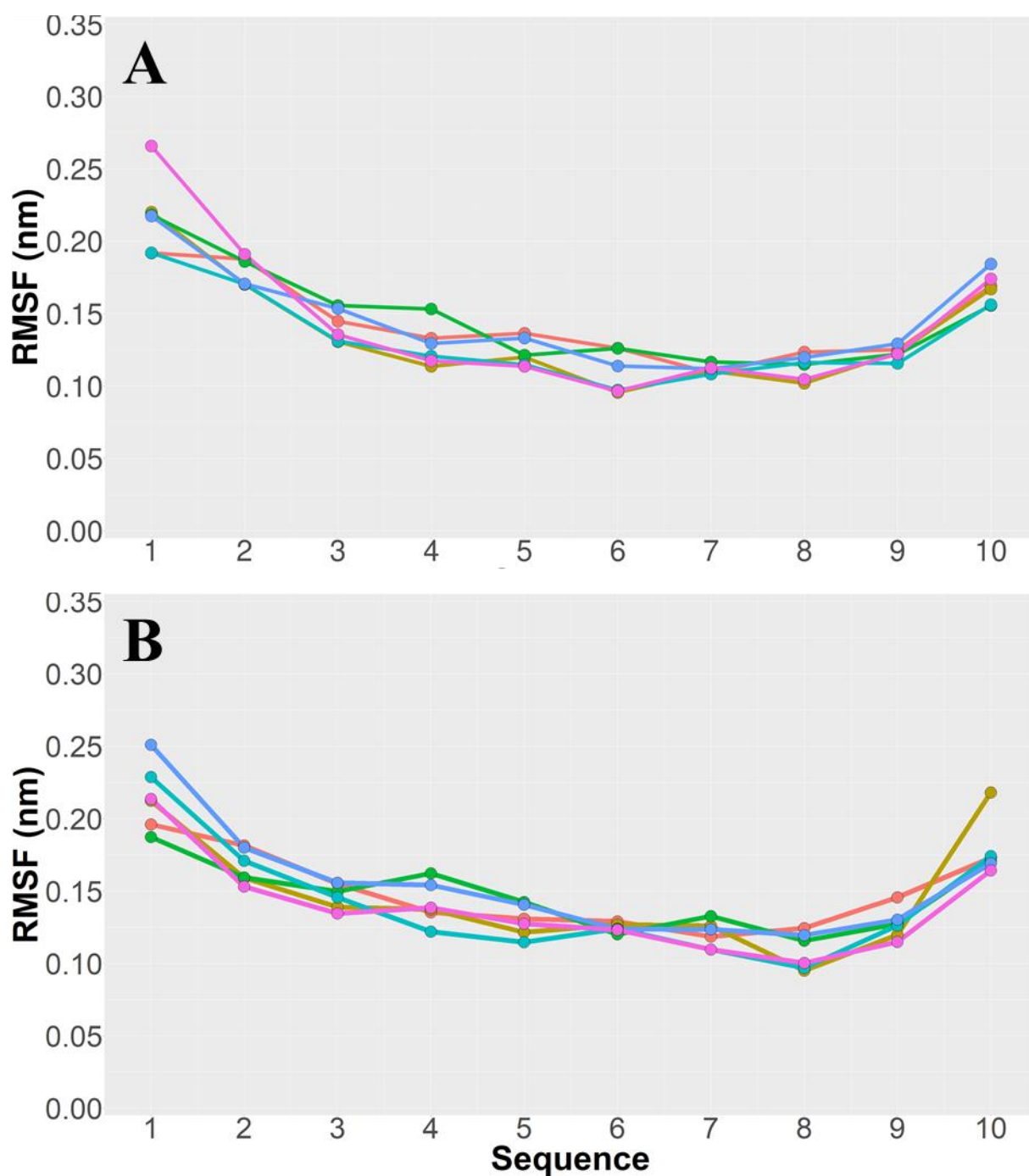


Figure S2. (A) Per-nucleotide RMSF values calculated for the DH of the three diprotic switches. The pink and orange lines with filled circles specify the two strands of the DIPRO5 system, while the green and cyan and the lavender and violet lines represent the DIPRO15 and DIPRO25 strands, respectively. **(B)** Per-nucleotide RMSF values calculated for the DH of the three tetraprotic switches. The pink and orange lines with filled circles represent the two strands of the TETRA5 system, while the green and cyan and the lavender and violet lines represent the TETRA15 and TETRA25 strands, respectively.

Table S1. DNA DH geometrical parameters, calculated for the tree switches, in comparison with the standard B-DNA values (standard deviations are indicated in parentheses).

	B-DNA	DIPRO5	DIPRO15	DIPRO25
Buckle	0.30	1.36 (± 16.27)	3.24 (± 15.83)	3.01 (± 16.36)
Inclination	-0.10	1.73 (± 7.33)	2.26 (± 7.73)	2.42 (± 8.49)
Opening	1.00	2.20 (± 6.71)	2.69 (± 7.52)	4.67 (± 14.29)
Propeller	-13.70	-9.52 (± 11.46)	-6.79 (± 16.39)	-4.35 (± 28.60)
Rise	3.36	3.38 (± 0.48)	3.41 (± 0.49)	3.54 (± 0.83)
Roll	0.30	0.80 (± 6.96)	0.96 (± 7.70)	-0.04 (± 12.27)
Shear	-0.04	0.10 (± 0.38)	0.01 (± 1.10)	-0.03 (± 0.85)
Shift	-0.02	-0.08 (± 0.90)	-0.04 (± 0.88)	0.11 (± 1.37)
Slide	0.14	-0.83 (± 0.78)	-0.80 (± 0.98)	-0.94 (± 1.13)
Stagger	0.21	-0.02 (± 0.57)	-0.11 (± 0.73)	-0.38 (± 1.69)
Stretch	-0.17	0.02 (± 0.14)	-0.05 (± 0.48)	0.28 (± 1.16)
Tilt	-0.20	-0.46 (± 6.17)	-0.30 (± 6.34)	-0.23 (± 7.24)
Tip	-1.00	0.55 (± 5.43)	0.14 (± 5.32)	-1.67 (± 12.22)
Total bend	6.80	14.69 (± 8.46)	14.17 (± 7.79)	18.98 (± 9.22)
Twist	35.80	32.86 (± 7.93)	33.12 (± 8.77)	31.14 (± 11.88)
X-disp	0.27	-1.68 (± 1.15)	-1.64 (± 1.34)	-1.47 (± 1.58)
Y-disp	0.11	0.09 (± 0.76)	-0.07 (± 0.81)	-0.13 (± 1.31)

Table S2. DNA DH geometrical parameters, calculated for the tree tetraprotic switches, in comparison with the standard B-DNA values (standard deviations are indicated in parentheses).

	B-DNA	TETRA5	TETRA15	TETRA25
Buckle	0.30	4.33 (\pm 14.73)	4.15 (\pm 14.31)	3.29 (\pm 16.77)
Inclination	-0.10	2.83 (\pm 6.11)	1.99 (\pm 8.30)	3.21 (\pm 6.88)
Opening	1.00	3.39 (\pm 0.54)	2.21 (\pm 6.04)	2.53 (\pm 6.28)
Propeller	-13.70	-8.71 (\pm 12.91)	-6.69(\pm 11.94)	-7.39 (\pm 12.38)
Rise	3.36	3.40 (\pm 0.51)	3.35 (\pm 0.54)	3.36 (\pm 0.51)
Roll	0.30	1.74 (\pm 8.32)	1.00 (\pm 7.45)	1.61 (\pm 7.72)
Shear	-0.04	-0.14 (\pm 1.20)	0.07 (\pm 0.37)	0.07 (\pm 0.36)
Shift	-0.02	-0.16 (\pm 1.17)	-0.06 (\pm 0.93)	-0.12 (\pm 0.93)
Slide	0.14	-0.69 (\pm 1.01)	-0.76 (\pm 0.93)	-0.79 (\pm 0.99)
Stagger	0.21	0.15 (\pm 0.87)	-0.02 (\pm 0.59)	-0.06 (\pm 0.61)
Stretch	-0.17	0.03 (\pm 0.28)	0.03 (\pm 0.59)	0.02 (\pm 0.14)
Tilt	-0.20	-0.61 (\pm 6.92)	-0.78 (\pm 6.87)	-1.06 (\pm 6.29)
Tip	-1.00	-0.92 (\pm 7.98)	0.87 (\pm 5.55)	2.12 (\pm 5.29)
Total bend	6.80	18.82 (\pm 10.11)	14.71 (\pm 8.67)	13.42 (\pm 7.01)
Twist	35.80	32.93 (\pm 8.37)	32.72 (\pm 8.84)	31.80 (\pm 8.06)
X-disp	0.27	-1.49 (\pm 1.32)	-1.48 (\pm 1.09)	-1.76 (\pm 1.25)
Y-disp	0.11	0.16 (\pm 1.02)	-0.01 (\pm 0.89)	0.03 (\pm 0.86)