Propagation of melting cooperativity along the phosphodiester backbone of DNA

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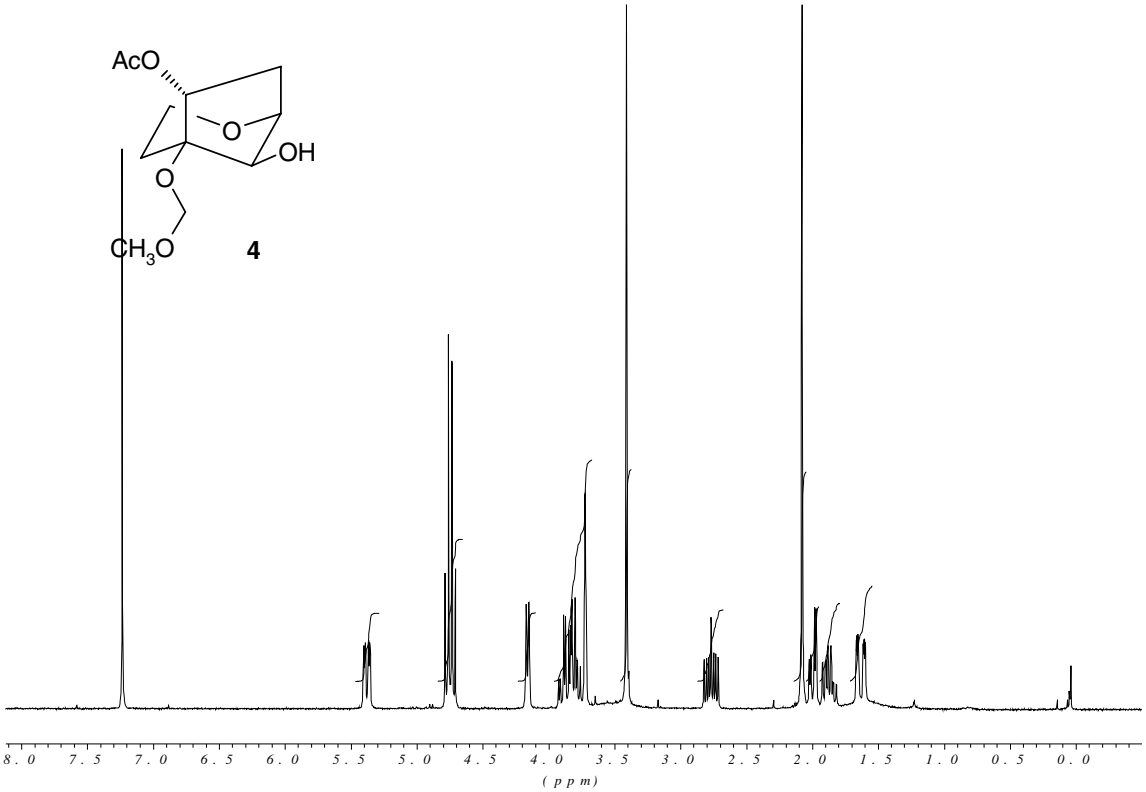
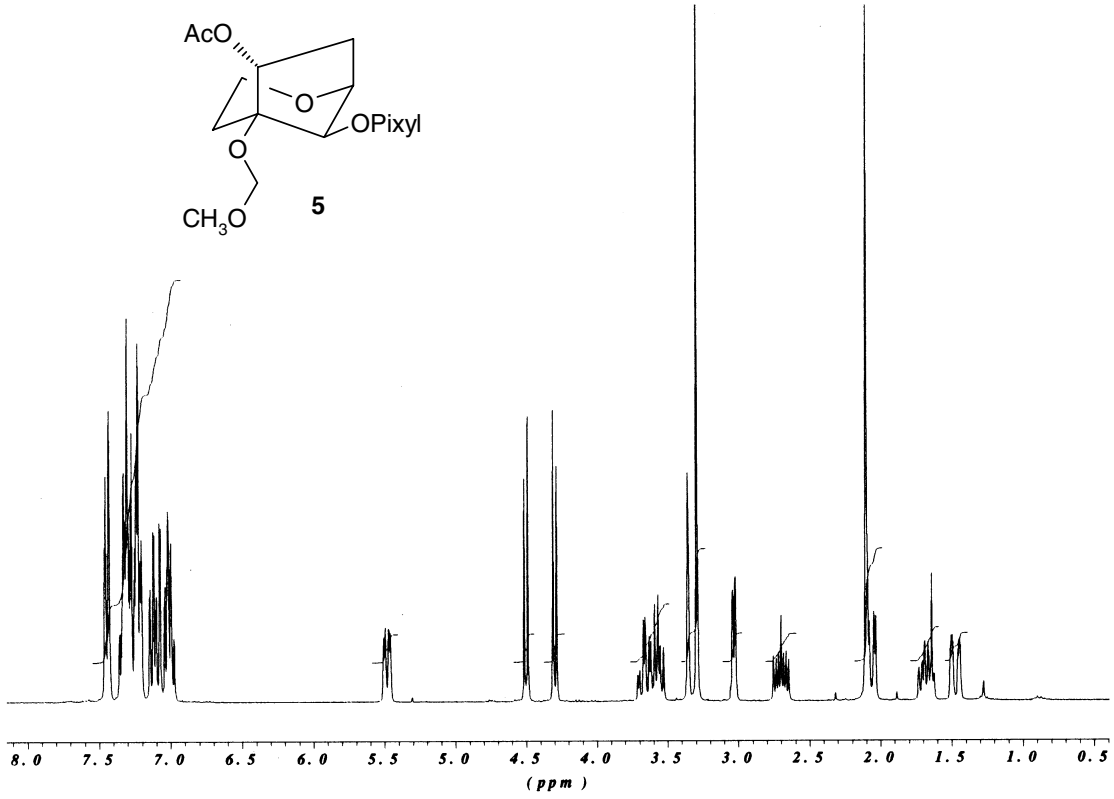
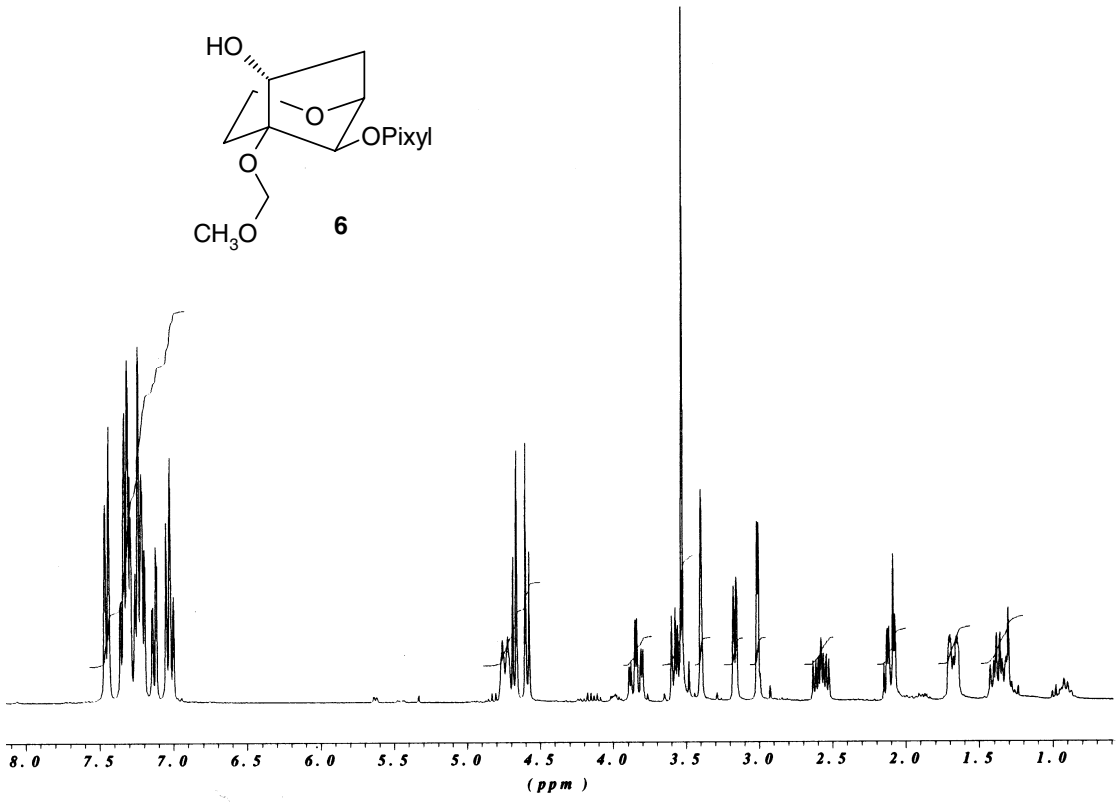
Supporting Information



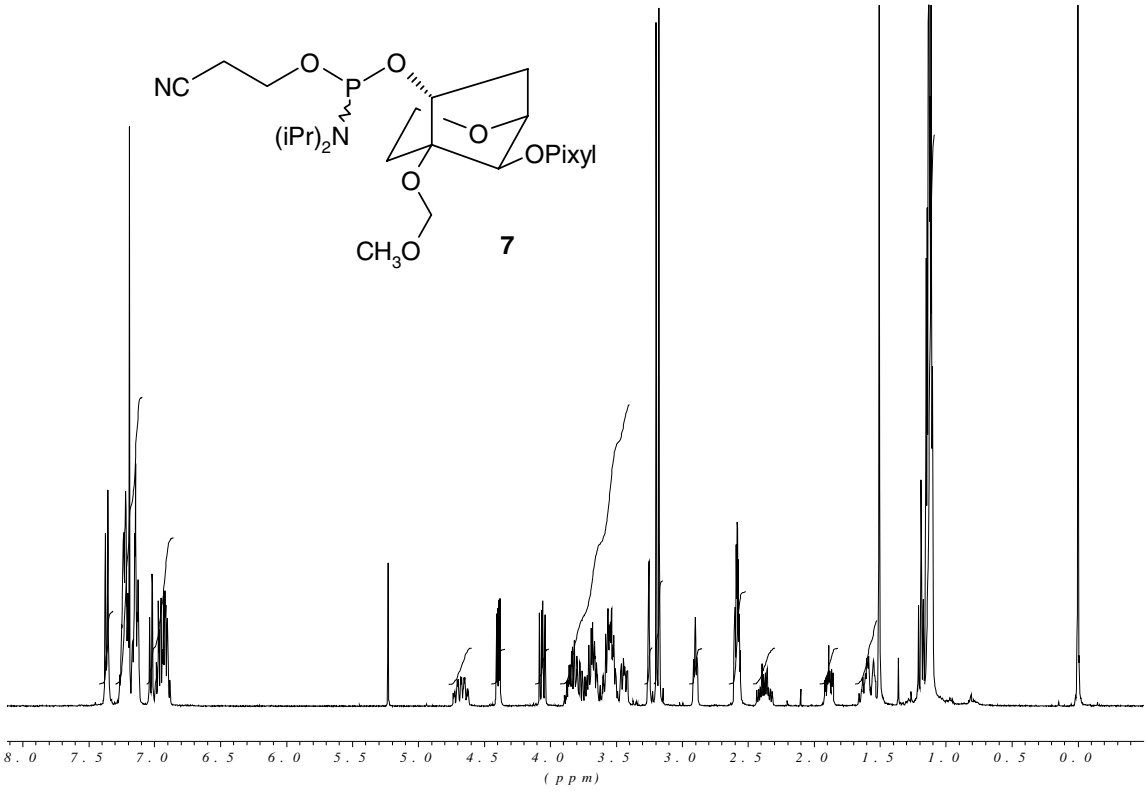
^{1}H NMR spectrum of **4** ($CDCl_3$)



^{1}H NMR spectrum of **5** ($CDCl_3$)



^{1}H NMR spectrum of **6** ($CDCl_3$)



^{1}H NMR spectrum of **7** ($CDCl_3$)

Table S1: Sequence synthesis and analytical data of oligonucleotides used in this study

Sequence	Scale [µmol]	ESI-MS m/z (calc.)	ESI-MS m/z (found)	Yield OD_{260} (%)	DEAE-HPLC [a]	RP-HPLC [b]
d(GATGAC**1**GCTAGCTAGGAC)	1.3	5685.8	5685.2	42.6 (18)	35% - 60%B in 30min. t_R = 26 min.	0% - 50%B in 30min. t_R = 17 min.
d(GTCCTAGCTAGC**1**GTCATC)	1.3	5587.7	5587.0	21.6 (10)	35% - 60%B in 30min. t_R = 26 min.	0% - 50%B in 30min. t_R = 17 min.
d(GATGAC**1**^{2}GCTAGCTAGGAC)	1.3	5823.8	5823.1	19.7 (8)	35% - 70%B in 30min. t_R = 22 min.	0% - 50%B in 30min. t_R = 17 min.
d(GTCCTAGCTAGC**1**^{2}GTCATC)	1.3	5725.7	5725.1	34.2 (16)	35% - 70%B in 30min. t_R = 21 min.	0% - 50%B in 30min. t_R = 17 min.
d(GATGAC**1**^{3}GCTAGCTAGGAC)	1.3	5960.0	5960.4	40.7 (17)	53% - 75%B in 30min. t_R = 23min.	10% - 35%B in 30min. t_R = 11 min.
d(GTCCTAGCTAGC**1**^{3}GTCATC)	1.3	5863.4	5863.6	56.8 (27)	53% - 75%B in 30min. t_R = 18min.	10% - 35%B in 30min. t_R = 12 min.
d(GATGAC**1**^{6}GCTAGCTAGGAC)	1.3	6377.0	6377.1	67.6 (28)	50% - 75%B in 30min. t_R = 21min.	10% - 35%B in 30min. t_R = 9 min.
d(GTCCTAGCTAGC**1**^{6}GTCATC)	1.3	6278.9	6278.9	65.1 (31)	53% - 75%B in 30min. t_R = 19min.	10% - 35%B in 30min. t_R = 10 min.
d(GATGAC**1**^{9}GCTAGCTAGGAC)	1.3	6790.2	6789.8	19.7 (8)	35% - 80%B in 30min. t_R = 21 min.	0% - 50%B in 30min. t_R = 16 min.
d(GTCCTAGCTAGC**1**^{9}GTCATC)	1.3	6692.1	6691.8	13.6 (6)	35% - 80%B in 30min. t_R = 21 min.	0% - 50%B in 30min. t_R = 18 min.
d(GATGAC**1**^{12}GCTAGCTAGGAC)	1.3	7204.4	7204.2	15.2 (6)	35% - 70%B in 30min. t_R = 26 min.	0% - 50%B in 30min. t_R = 17 min.
d(GTCCTAGCTAGC**1**^{12}GTCATC)	1.3	7106.3	7106.0	21.1 (10)	35% - 80%B in 30min. t_R = 22 min.	0% - 50%B in 30min. t_R = 17 min.
d(GATGAC**1**^{16}GCTAGCTAGGAC)	1.3	7757.6	7757.1	31.8 (13)	55% - 80%B in 30min. t_R = 25 min.	10% - 30%B in 30min. t_R = 9 min.
d(GTCCTAGCTAGC**1**^{16}GTCATC)	1.3	7659.5	7659.5	39.5 (19)	55% - 80%B in 30min. t_R = 24 min.	10% - 30%B in 30min. t_R = 9 min.
d(GATGAC**1**^{20}GCTAGCTAGGAC)	1.3	8308.8	8308.3	12.9 (5)	35% - 70%B in 30min. t_R = 28 min.	0% - 50%B in 30min. t_R = 16 min.
d(GTCCTAGCTAGC**1**^{20}GTCATC)	1.3	8210.7	8210.0	11.4 (5)	35% - 80%B in 30min. t_R = 23 min.	0% - 50%B in 30min. t_R = 17 min.
d(GATGAC**2**GCTAGCTAGGAC)	1.3	5813.5	5813.6	63.4 (27)	53% - 75%B in 30min. t_R = 25min.	10% - 35%B in 30min. t_R = 18 min.
d(GTCCTAGCTAGC**2**GTCATC)	1.3	5714.0	5713.8	54.1 (26)	53% - 75%B in 30min. t_R = 23min.	10% - 35%B in 30min. t_R = 13 min.
d(GATGAC**2**^{2}GCTAGCTAGGAC)	1.3	6078.1	6078.0	41.2 (17)	53% - 75%B in 30min. t_R = 26min.	10% - 35%B in 30min. t_R = 12 min.
d(GTCCTAGCTAGC**2**^{2}GTCATC)	1.3	5980.1	5979.9	44.6 (21)	53% - 75%B in 30min. t_R = 24min.	10% - 35%B in 30min. t_R = 13 min.
d(GATGAC**2**^{3}GCTAGCTAGGAC)	1.3	6344.2	6344.1	26.0 (11)	53% - 75%B in 30min. t_R = 21min.	10% - 35%B in 30min. t_R = 12 min.
d(GTCCTAGCTAGC**2**^{3}GTCATC)	1.3	6246.1	6245.9	43.9 (21)	53% - 75%B in 30min. t_R = 22min.	10% - 35%B in 30min. t_R = 13 min.

d(GATGAC**2**^{6}GCTAGCTAGGAC)	0.2	7144.8	7144.9	3.1 (9)	60% - 95%B in 30min. t_R = 21 min.	10% - 40%B in 30min. t_R = 14 min.
d(GTCCTAGCTAGC**2**^{6}GTCATC)	0.2	7046.7	7046.3	2.5 (7)	60% - 95%B in 30min. t_R = 19 min.	10% - 40%B in 30min. t_R = 14 min.
d(GATGAC**2**^{9}GCTAGCTAGGAC)	0.2	7943.3	7943.3	1.7 (5)	60% - 95%B in 30min. t_R = 24 min.	10% - 40%B in 30min. t_R = 15 min.
d(GTCCTAGCTAGC**2**^{9}GTCATC)	0.2	7845.2	7845.4	6.1 (18)	60% - 95%B in 30min. t_R = 20 min.	10% - 40%B in 30min. t_R = 14 min.
d(GATGAC**2**^{12}GCTAGCTAGGAC)	0.2	8741.9	8741.4	2.2 (6)	70% - 100%B in 30min. t_R = 19 min.	10% - 40%B in 30min. t_R = 16 min.
d(GTCCTAGCTAGC**2**^{12}GTCATC)	0.2	8643.8	8643.3	2.2 (7)	60% - 95%B in 30min. t_R = 24 min.	10% - 40%B in 30min. t_R = 15 min.
d(GATGAC**2**^{16}GCTAGCTAGGAC)	1.3	9807.7	9807.1	5.34 (2)	53% - 80%B in 30min. t_R = 26min.	10% - 30%B in 30min. t_R = 12 min.
d(GTCCTAGCTAGC**2**^{16}GTCATC)	1.3	9709.6	9708.8	26.0 (12)	55% - 88%B in 30min. t_R = 19min.	10% - 30%B in 30min. t_R = 12 min.

a) Nucleogen DEAE 60-7, Macherey & Nagel; **A**: 20mM KH_2PO_4 in H_2O/CH_3CN 4:1, pH 6.0; **B**: 20mM KH_2PO_4, 1M KCl in H_2O/CH_3CN 4:1, pH 6.0

b) Aquapore RP-300; Brownlee; **A**: 0.1M triethylammoniumacetate in H_2O, pH 7.0; **B**: 0.1M triethylammoniumacetate in H_2O/CH_3CN 1:4, pH 7.0

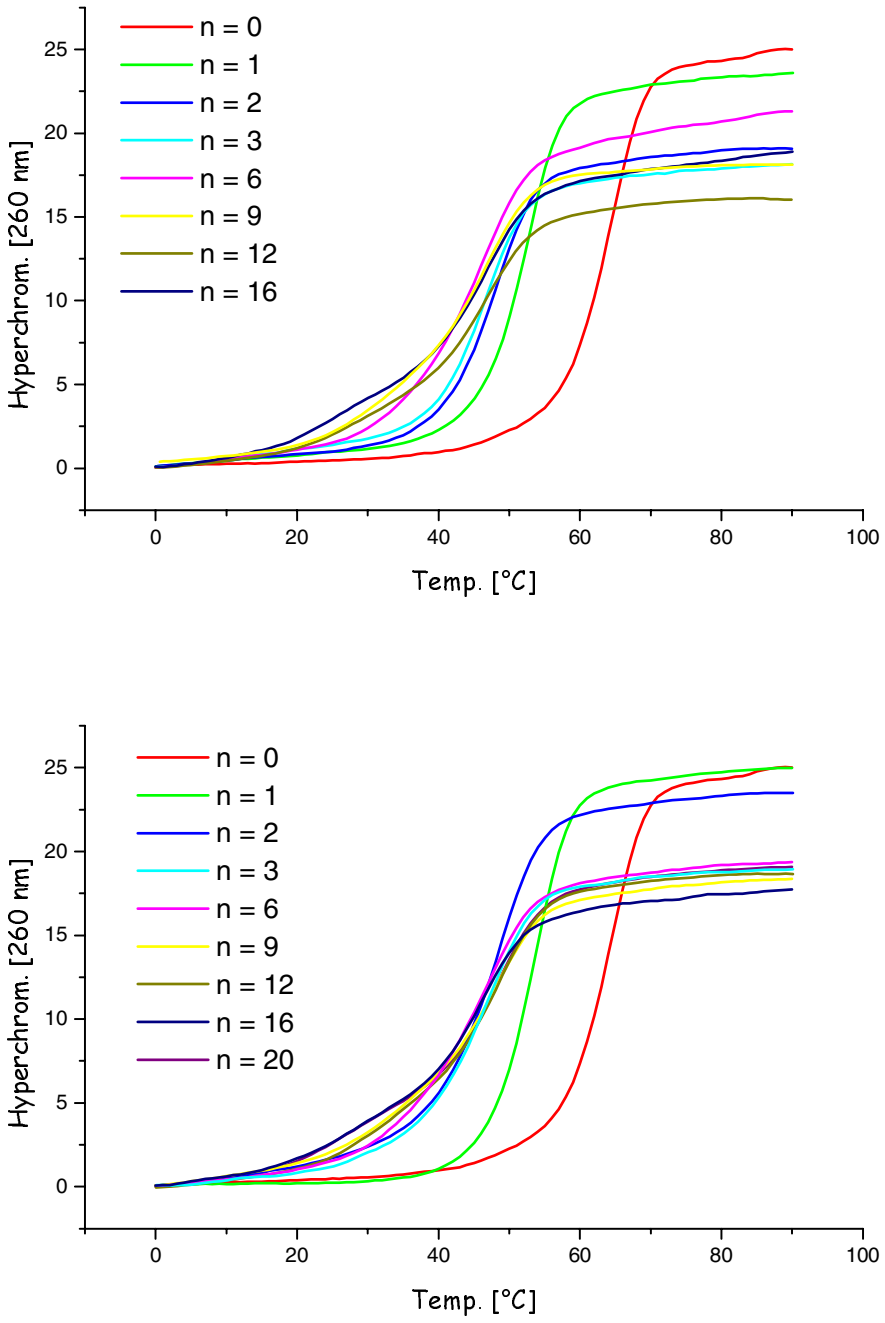


Figure S1: UV-melting curves of the symmetric duplexes with the propanediol anucleosidic linker (X = **1**) bottom; and the bicyclic linker (X = **2**), top. C = 1.8-2.0 µM in 10 mM NaH_2PO_4, 150 mM NaCl, pH 7.0. Sequence context as in Figure 1 of the printed paper.

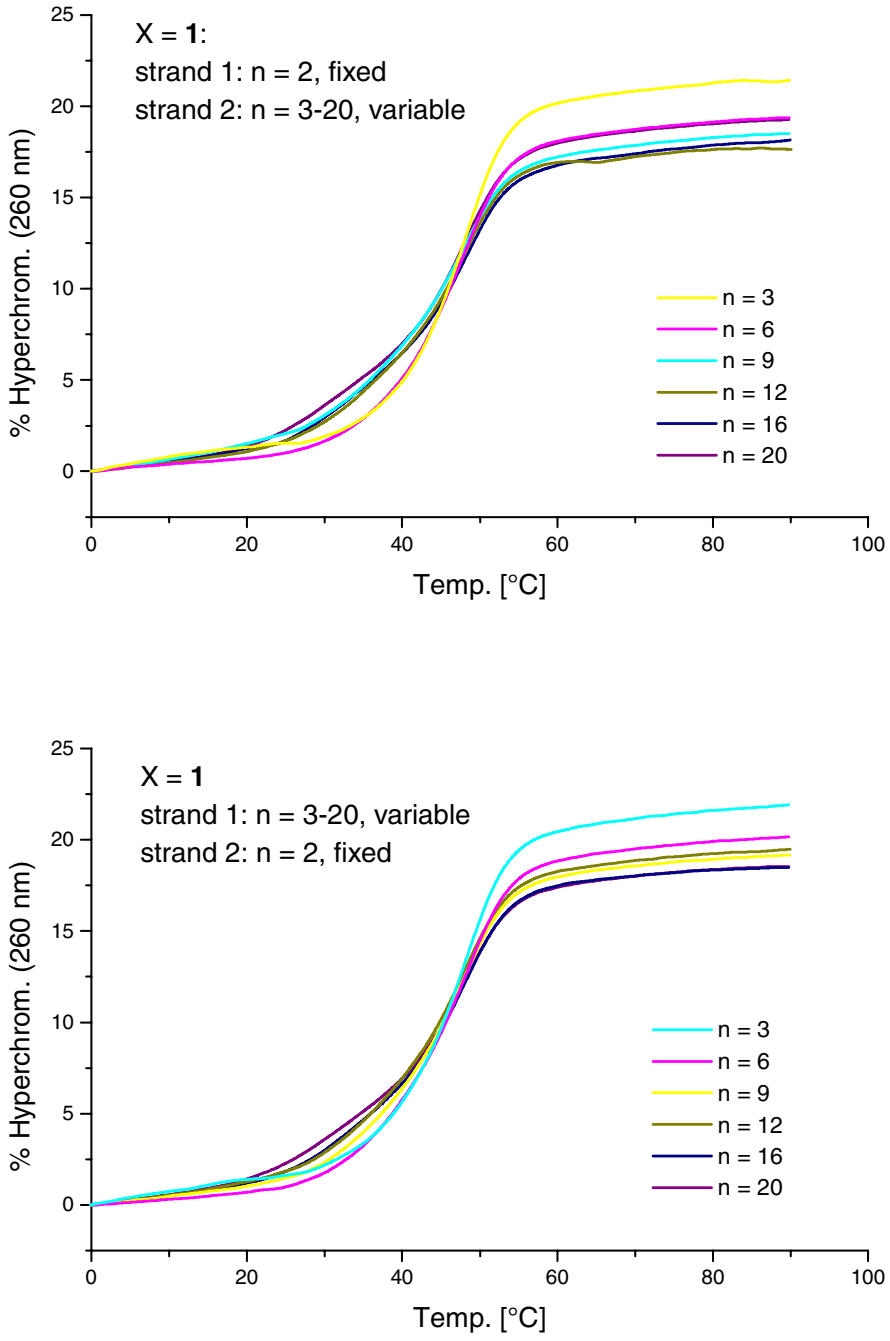


Figure S2: UV-melting curves of the asymmetric duplexes with the propanediol anucleosidic linker (X = **1**). C = 1.8-2.0 μM in 10 mM NaH_2PO_4, 150 mM NaCl, pH 7.0. Sequence context as in Figure 1 of the printed paper.

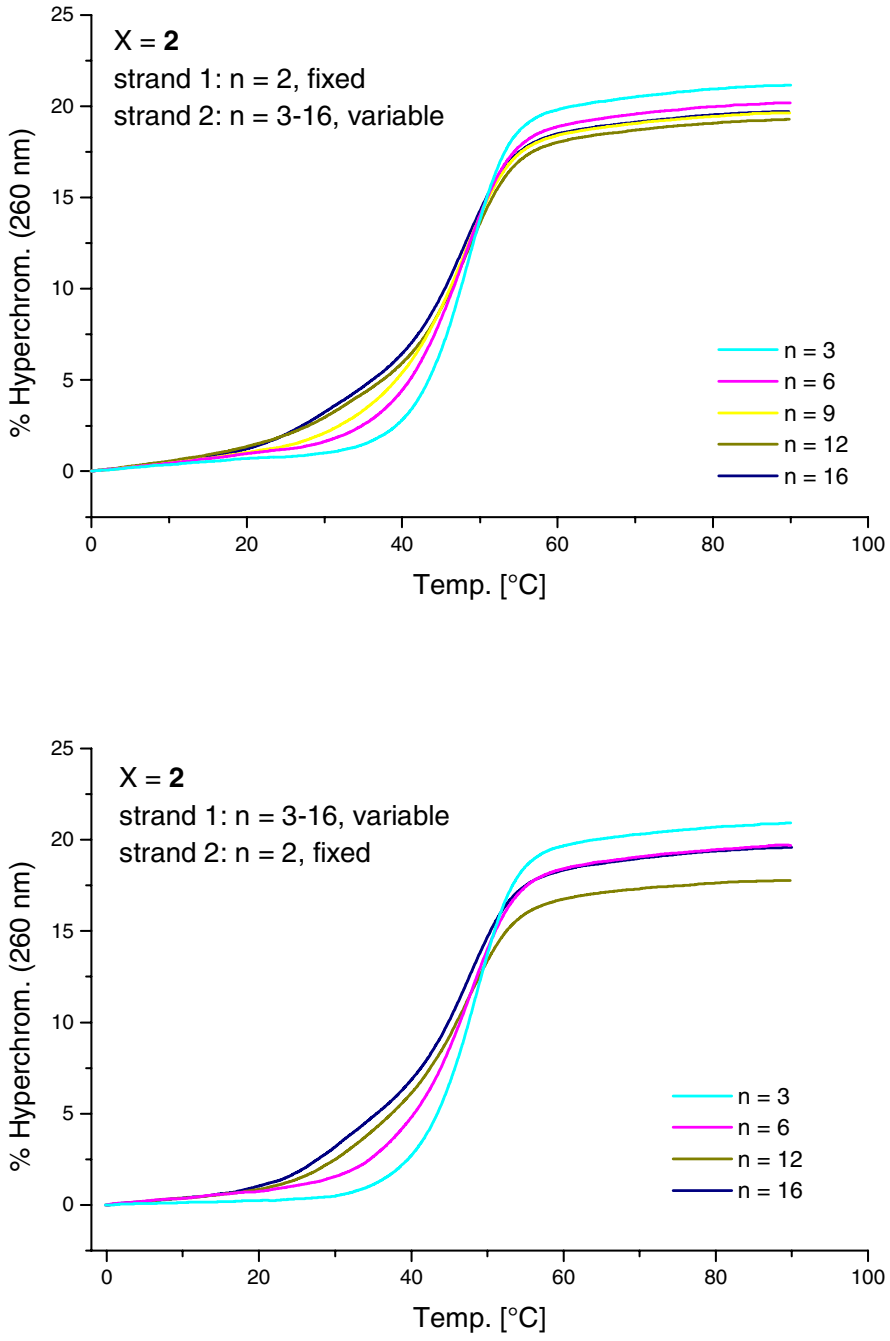


Figure S2: UV-melting curves of the asymmetric duplexes with the bicyclic linker (X = **2**). C = 1.8-2.0 µM in 10 mM NaH_2PO_4, 150 mM NaCl, pH 7.0. Sequence context as in Figure 1 of the printed paper.