Supplementary Information

for manuscript entitled

Synthesis of an Oligonucleotide with a Nicotinamide Mononucleotide Residue and its Molecular Recognition in DNA Helices

by

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Contents

1. Mass Spectrum of the Methylimidazolide of NMN^+

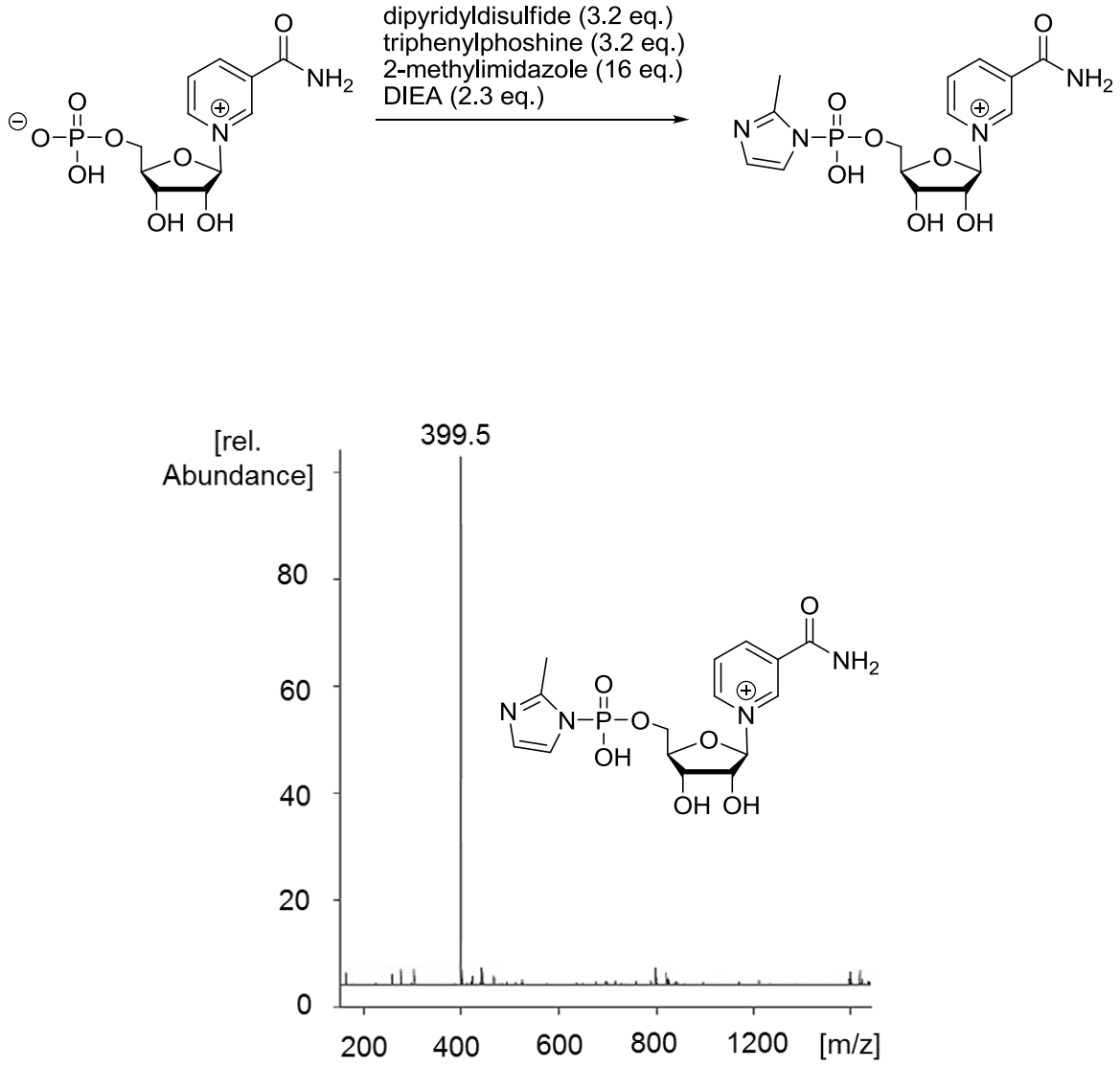

Figure S1. ESI mass spectrum of the purified reaction product after activation of nicotinamide mononucleotide with 2-methylimidazole.

2. Additional Spectra for Compound 1

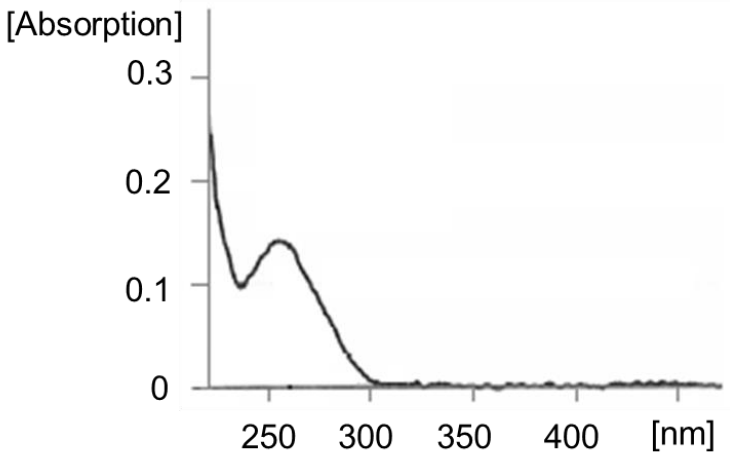

Figure S2. UV-Vis spectrum of OAt-NMN$^+$ (**1**) (aqueous solution, pH 5.5).

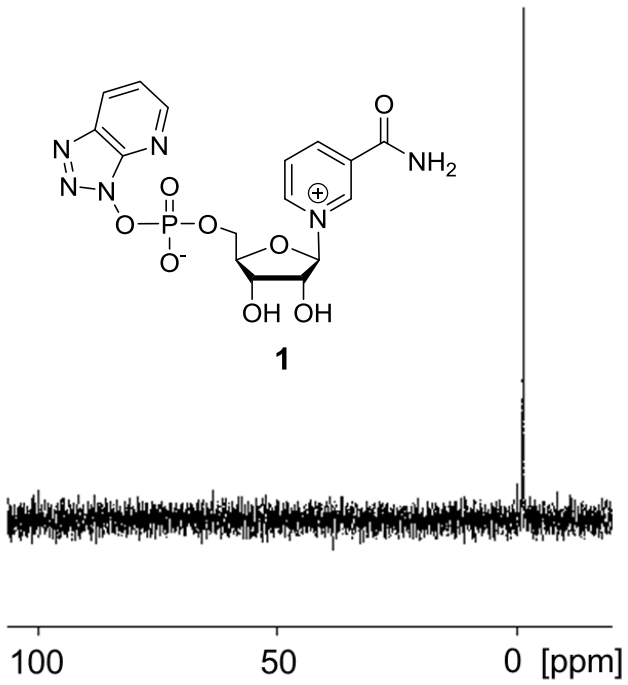

Figure S3. ^{31}P-NMR spectrum of OAt-NMN$^+$ (**1**) in H_2O/D_2O (9:1) at 202 MHz.

3. MALDI-TOF Mass Spectrum of 2

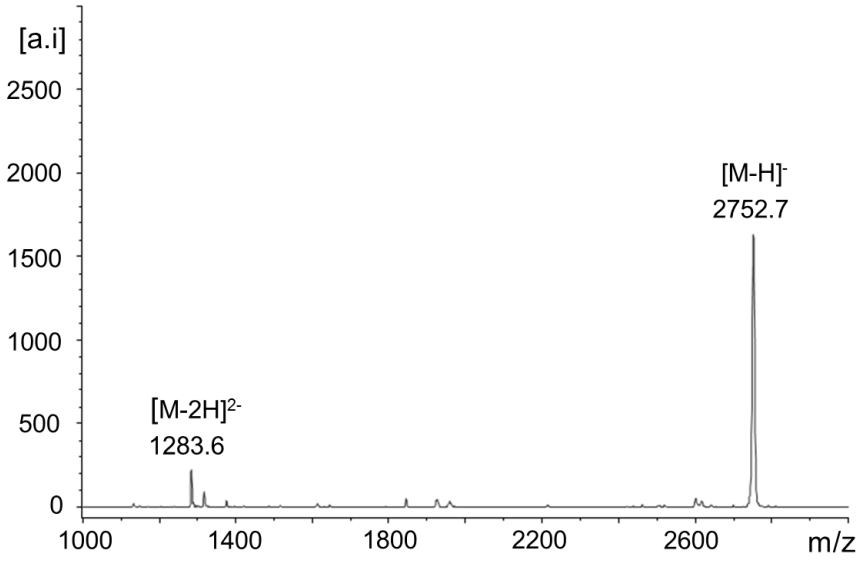

Figure S4. MALDI-TOF mass spectrum of aminoterminal oligonucleotide **2**.

4. Representative UV-Melting Curves

In the following, representative UV-melting curves are shown. See Tables 1 and 2 for details.

Triplexes with Strand 3

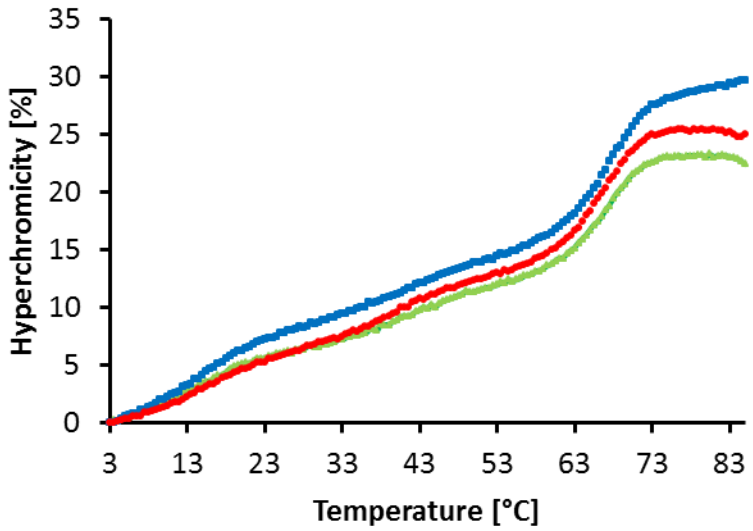

Figure S5. Overlay of three representative melting curves for the triplex of **5a**, **3**, **6a**, and **7**.

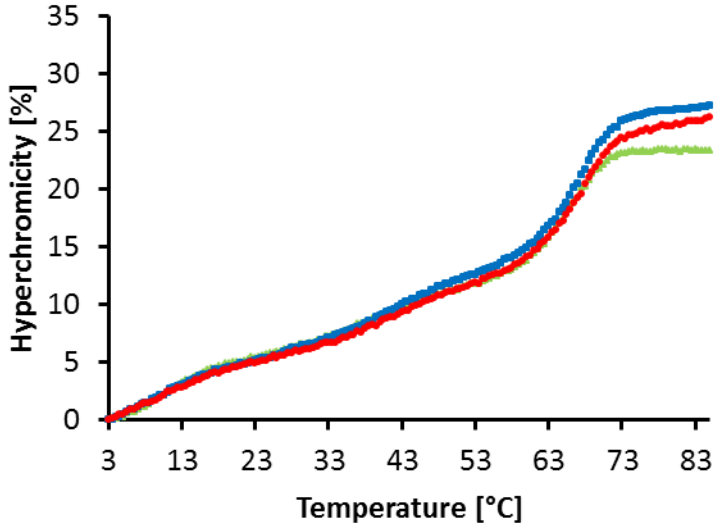

Figure S6. Overlay of three representative melting curves for the triplex of **5a**, **3**, **6c**, and **7**.

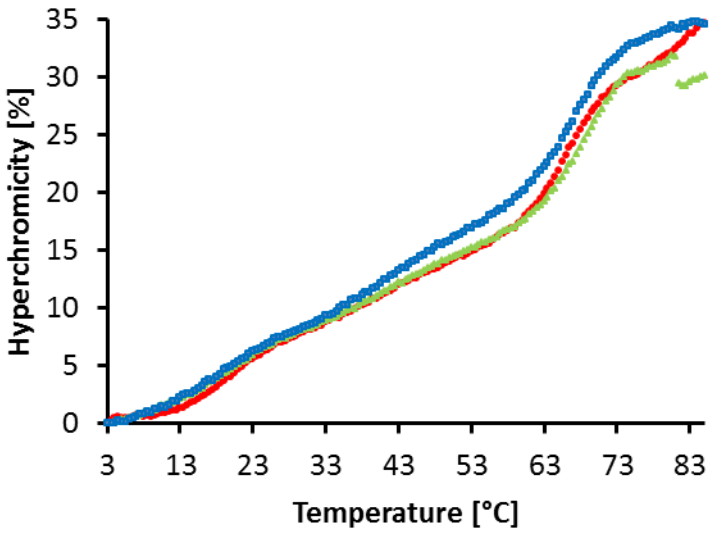

Figure S7. Overlay of three representative melting curves for the triplex of **5a**, **3**, **6g**, and **7**.

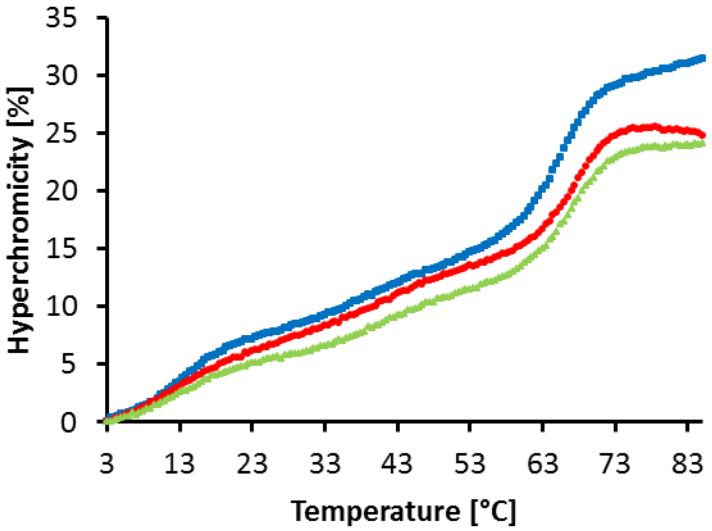

Figure S8. Overlay of three representative melting curves for the triplex of **5a**, **3**, **6t**, and **7**.

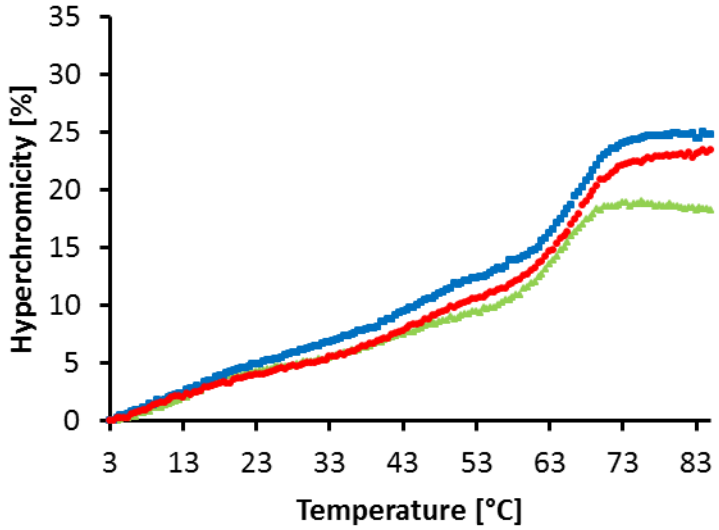

Figure S9. Overlay of three representative melting curves for the triplex of **5c**, **3**, **6a**, and **7**.

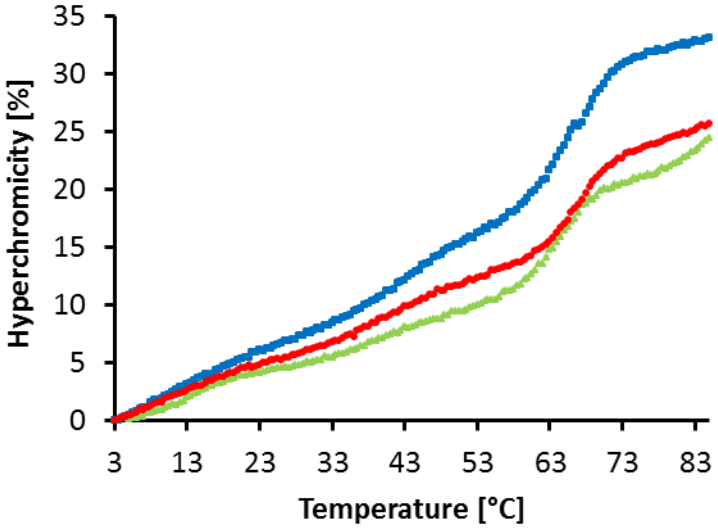

Figure S10. Overlay of three representative melting curves for the triplex of **5c**, **3**, **6c**, and **7**.

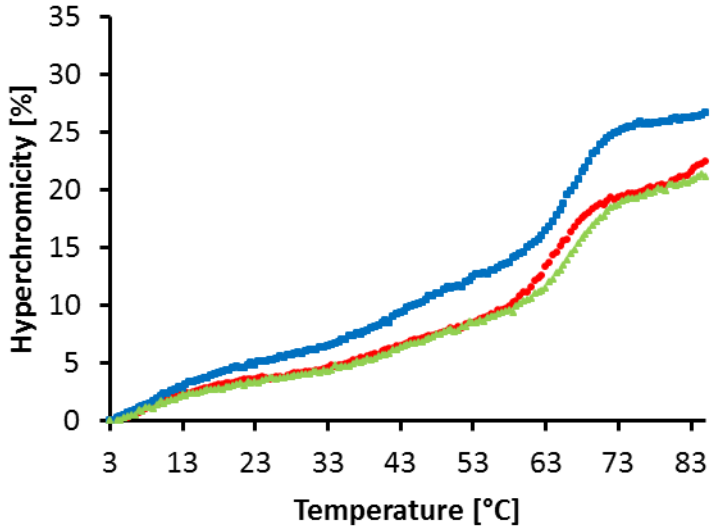

Figure S11. Overlay of three representative melting curves for the triplex of **5c**, **3**, **6g**, and **7**.

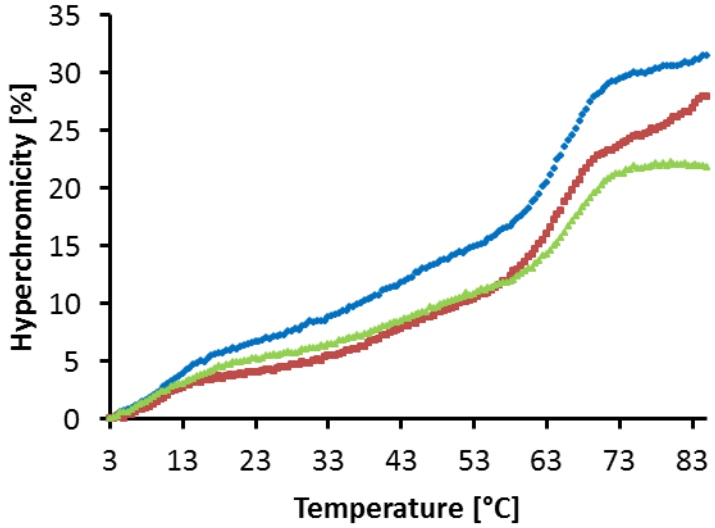

Figure S12. Overlay of three representative melting curves for the triplex of **5c**, **3**, **6t**, and **7**.

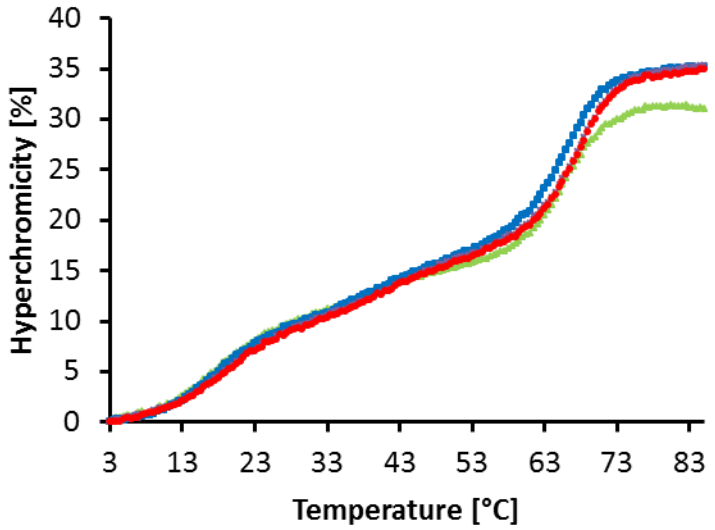

Figure S13. Overlay of three representative melting curves for the triplex of **5g**, **3**, **6a**, and **7**.

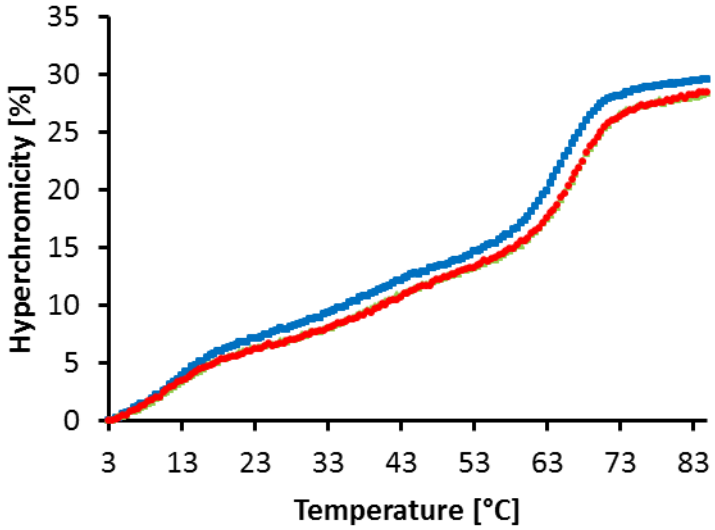

Figure S14. Overlay of three representative melting curves for the triplex of **5g**, **3**, **6c**, and **7**.

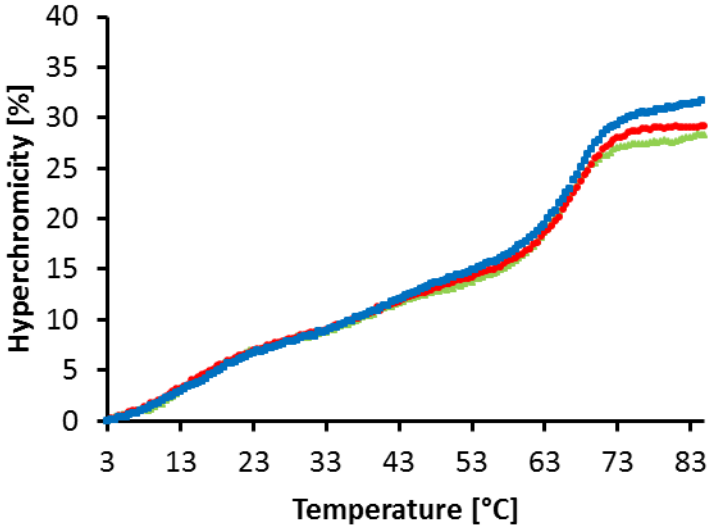

Figure S15. Overlay of three representative melting curves for the triplex of **5g**, **3**, **6g**, and **7**.

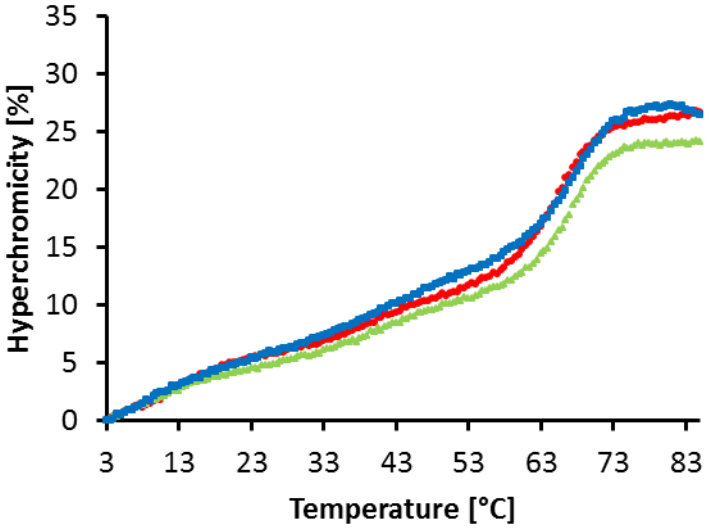

Figure S16. Overlay of three representative melting curves for the triplex of **5g**, **3**, **6t**, and **7**.

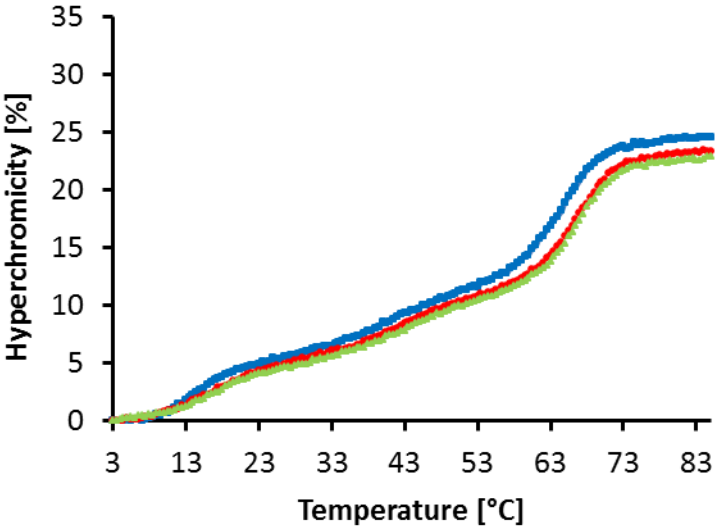

Figure S17. Overlay of three representative melting curves for the triplex of **5t**, **3**, **6a**, and **7**.

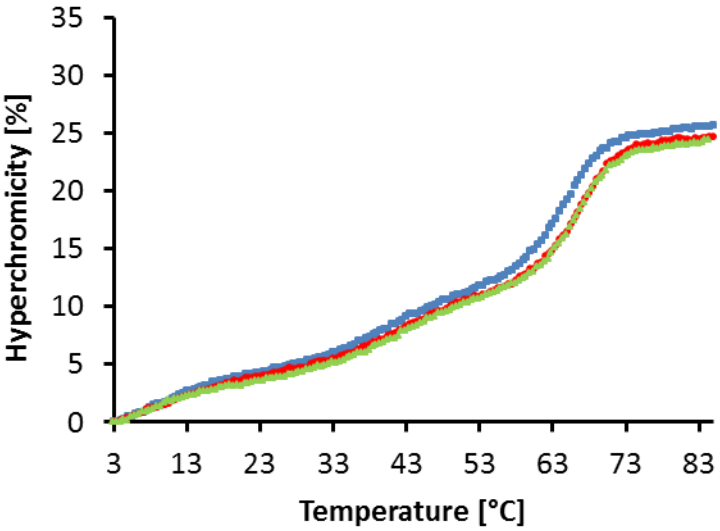

Figure S18. Overlay of three representative melting curves for the triplex of **5t**, **3**, **6c**, and **7**.

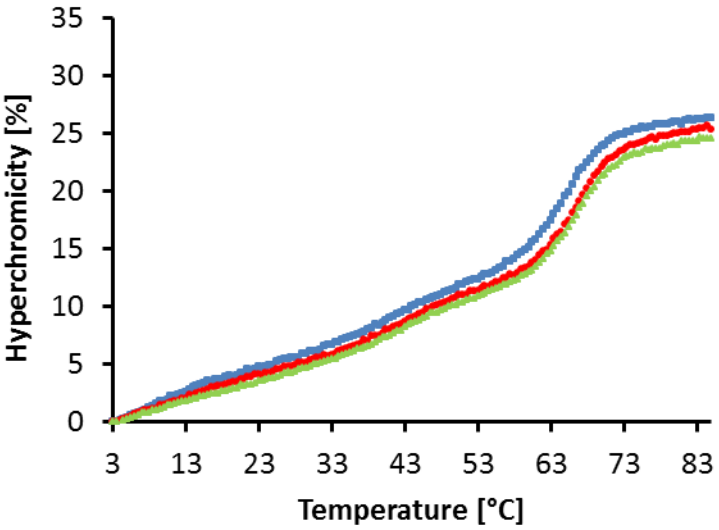

Figure S19. Overlay of three representative melting curves for the triplex of **5t**, **3**, **6g**, and **7**.

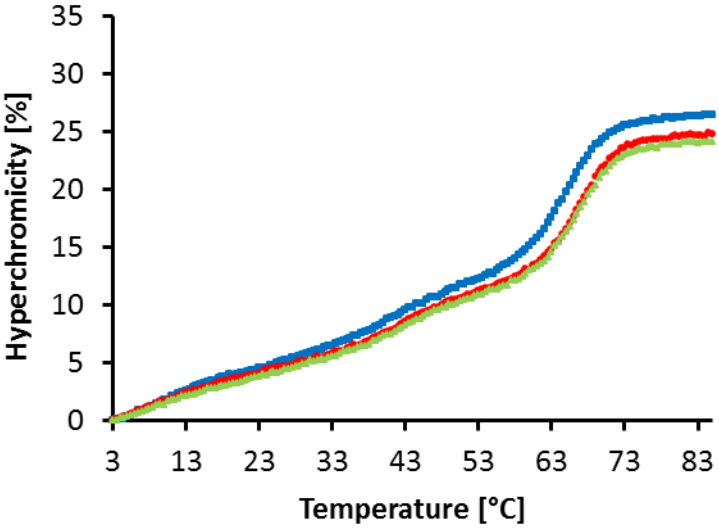

Figure S20. Overlay of three representative melting curves for the triplex of **5t**, **3**, **6t**, and **7**.

Triplexes with Strand 4

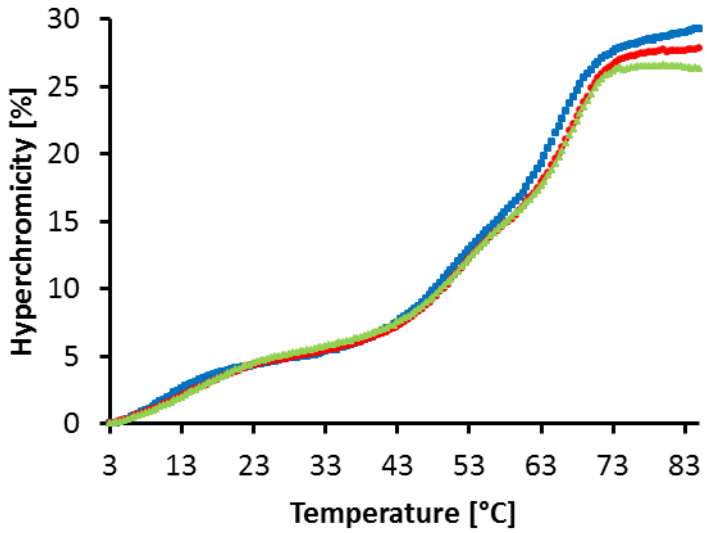

Figure S21. Overlay of three representative melting curves for the triplex of **5a**, **4**, **6a**, and **7**.

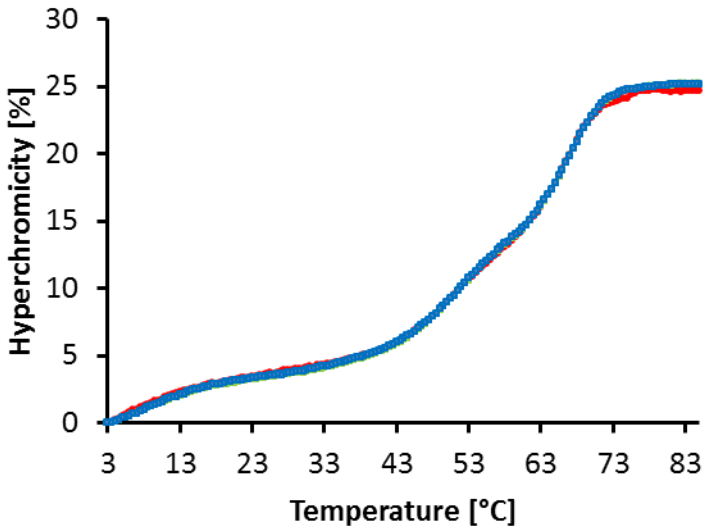

Figure S22. Overlay of three representative melting curves for the triplex of **5a**, **4**, **6c**, and **7**.

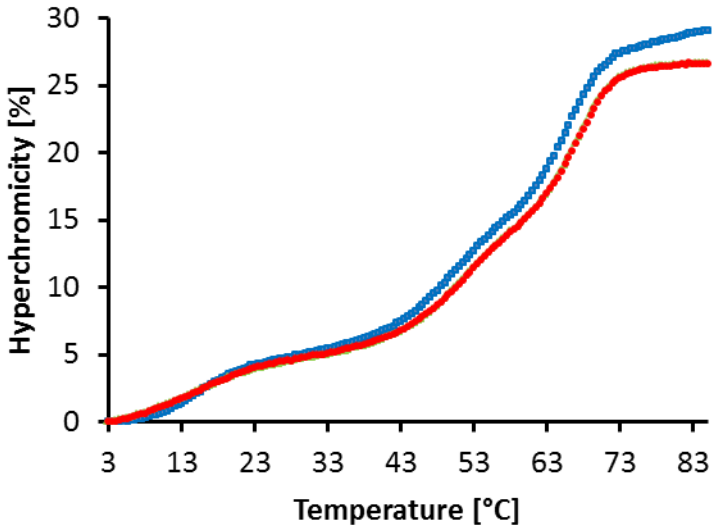

Figure S23. Overlay of three representative melting curves for the triplex of **5a**, **4**, **6g**, and **7**.

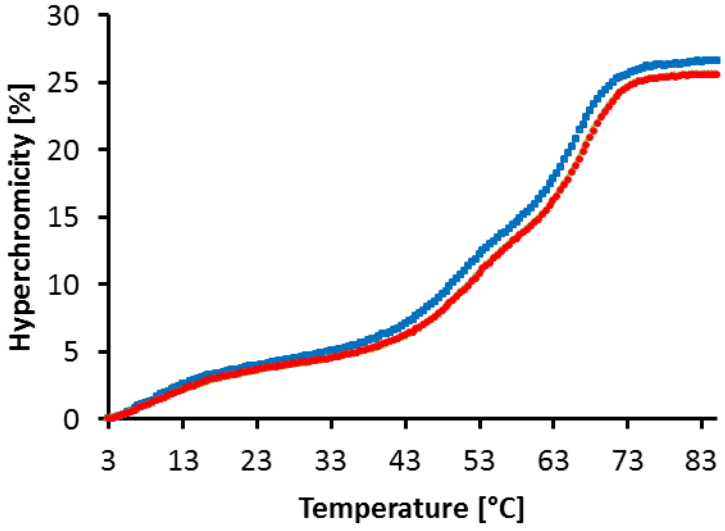

Figure S24. Overlay of three representative melting curves for the triplex of **5a**, **4**, **6t**, and **7**.

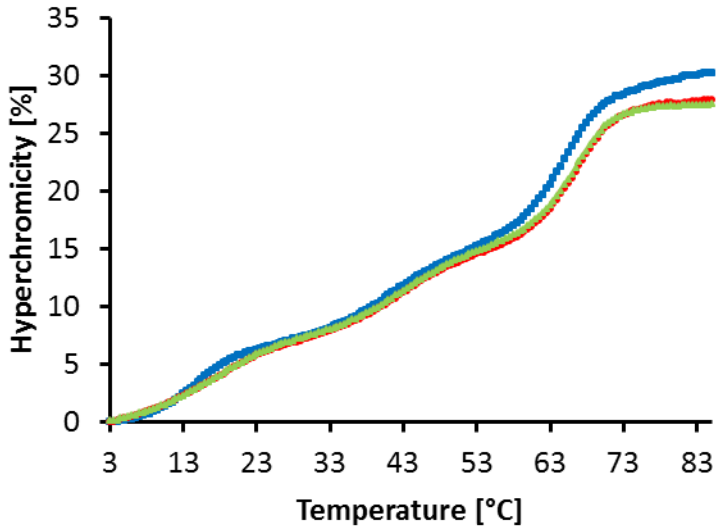

Figure S25. Overlay of three representative melting curves for the triplex of **5c**, **4**, **6a**, and **7**.

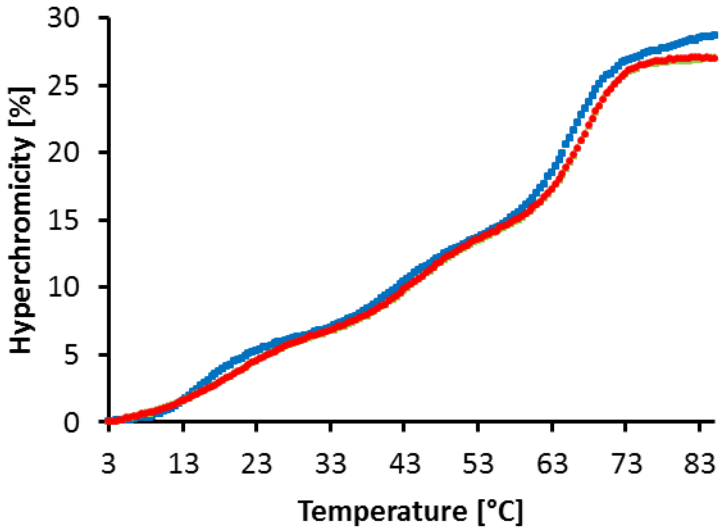

Figure S26. Overlay of three representative melting curves for the triplex of **5g**, **4**, **6a**, and **7**.

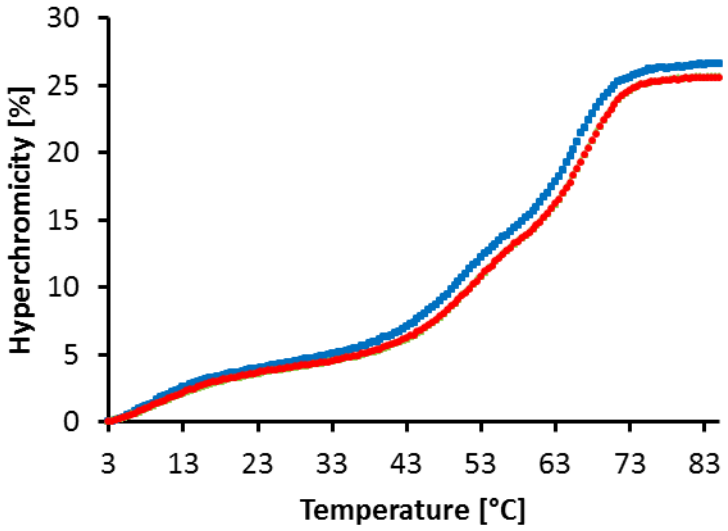

Figure S27. Overlay of three representative melting curves for the triplex of **5t**, **4**, **6a**, and **7**.

5. Melting Points Obtained by Graphical Analysis

In the following, triplex melting points (T_m1) are listed that were obtained by an alternative mode of analysis, namely graphical determination. For this, melting curves were printed, upper and lower baselines for the triplex transition were drawn manually, with a ruler, and the intercept of the 50% line of hyperchromicity and the actual melting curve was determined graphically. See Tables 1 and 2 for melting points obtained by numerical analysis (maximum of first derivative) from the same data.

Table S1. UV-Melting points [°C] of triplexes containing strand **3** with Watson-Crick partner strand **5a**, **5c**, **5g** or **5t** and Hoogsteen partner strand **6a**, **6c**, **6g** or **6t**, in the presence of downstream-binding strand **7**, as obtained by graphical analysis.[a]

	5a	**5c**	**5g**	**5t**
6a	13.8 ± 0.7	12.3 ± 0.5	19.6 ± 0.4	15.8 ± 0.6
6c	10.9 ± 0.1	15.3	12.0 ± 0.6	10.5 ± 0.5
6g	19.5 ± 0.2	10.3 ± 0.3	13.9 ± 0.1	12.5
6t	13.4 ± 0.7	10.7 ± 0.1	11.5 ± 0.4	11.3

[a] One standard derivation (SD) is given, when more than two measurements were made. Otherwise the average value of two measurements is given. For conditions, see Table 1 of the main text.

Table S2. UV-Melting points [°C] of triplexes containing strand **4** with Watson-Crick partner strand **5a**, **5c**, **5g** or **5t** and Hoogsteen partner strand **6a**, **6c**, **6g** or **6t**, in the presence of downstream-binding strand **7**, as obtained by graphical analysis.[a]

	5a	**5c**	**5g**	**5t**
6a	13.5 ± 0.4	16.5 ± 0.4	16.8 ± 0.1	< 10
6c	< 10			
6g	15.9 ± 0.3			
6t	< 10			

[a] One standard derivation (SD) is given, when more than two measurements were made. Otherwise the average value of two measurements is given. For conditions, see Table 2 of the main text.