

Supplementary Material

Discriminating Unalike Single Nucleobase Mismatches using a Molecularly Resolved, Label-free, Interfacial LNA-based Assay

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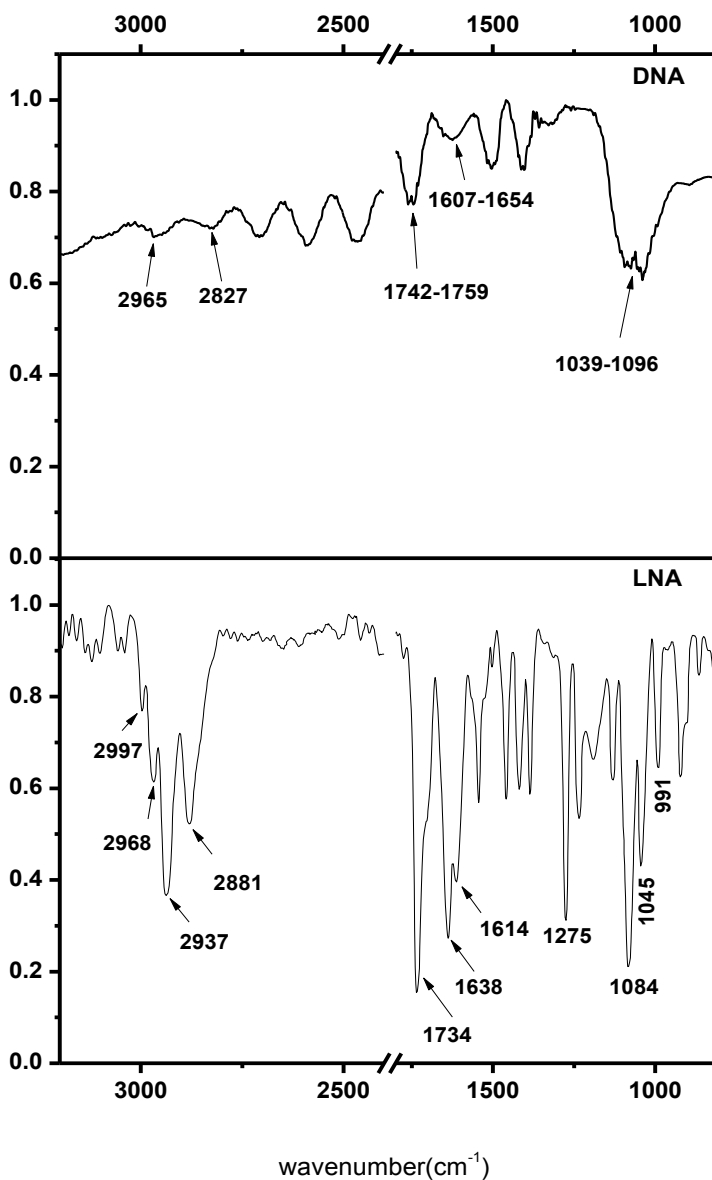


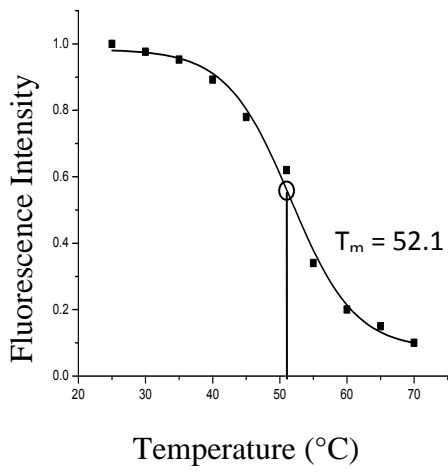
Fig. S1: RAIR spectra of DNA and LNA layers on gold(111) surface acquired for the same probe concentration 0.1 μ M and the same incubation time 4 h.

Assignment of the primary IR frequencies of that differentiate between DNA and LNA cases

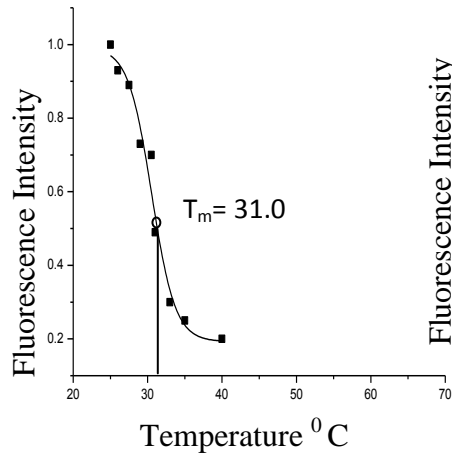
ASSIGNMENT	DNA	LNA
2997 ¹	----	V(C-H)aromatic, present in nucleobases
2965-2968 ¹	Vasym(CH ₃), present in thymine bases	Vasym(CH ₃), present in thymine bases, peak is more intense than in case of DNA
2937 ¹	----	Vasym(CH₂), present in hexyl spacer and locked sugar moieties
2881 ¹	----	Vsym(CH₂)
1734-1743 ^{2,3}	v(C=O) nucleobase, present in thymine and guanine	v(C=O), present in thymine and guanine, peak much sharper and intense
1607-1654 ^{2,3}	v(C=O) nucleobase, present in cytosine and adenine	v(C=O), present in cytosine and adenine, peak much sharper and intense
1614 ⁴	----	δ(-NH₂), v(C=N), present in nucleobases
1544 ⁴	----	v(C=C), v(C=N), present in nucleobases
1458 ⁴	----	purine imidazolic ring vib.
1416 ⁵⁻⁷	----	sugar vib. (C3'- endo)
1275 ⁸	----	thymidine (N3-H bending vib.)
1191 ⁹	----	sugar phosphate backbone vib. and N-type sugar conformation
1039-1096 ¹⁰	v(PO ₂) ⁻ , sugar-phosphate backbone vibration	v(PO ₂) ⁻ , sugar-phosphate backbone vibration, peak much sharper and intense

References:

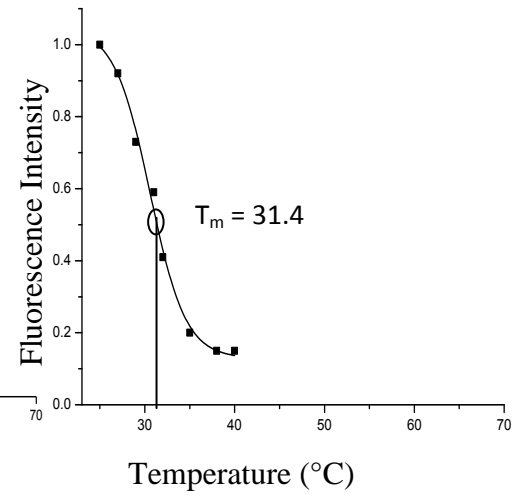
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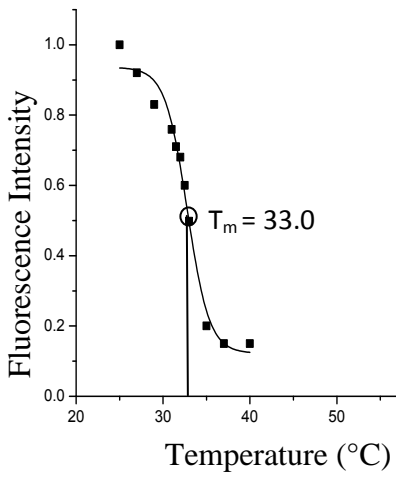
(A)



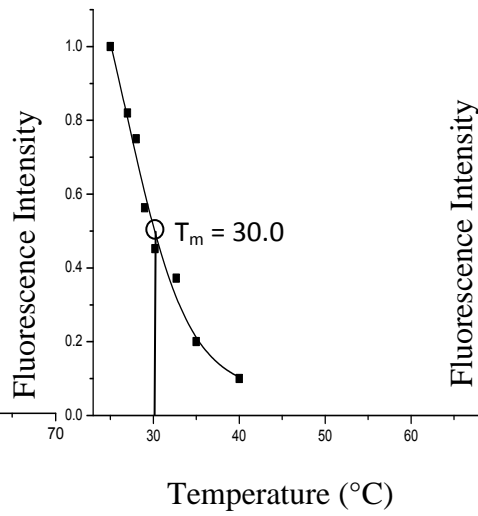
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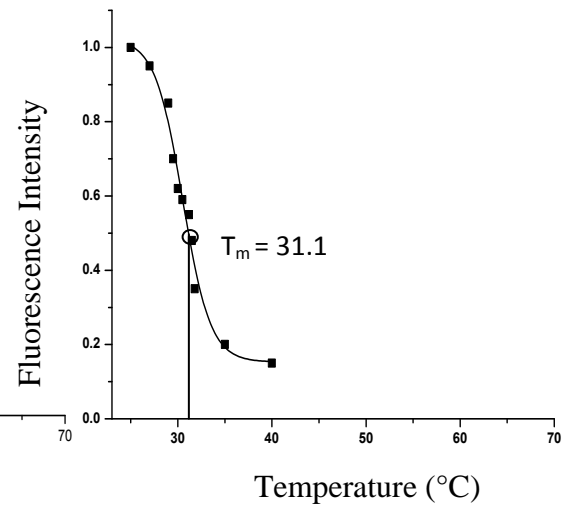
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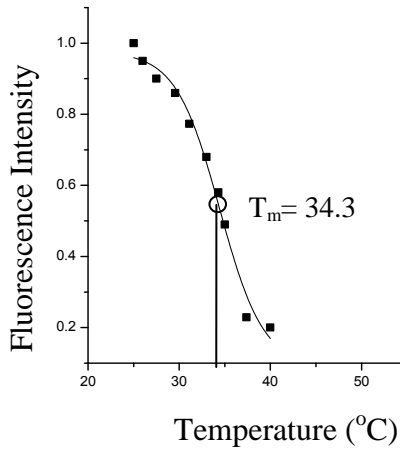
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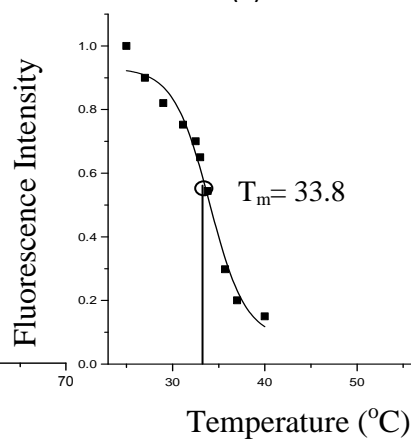
(E)



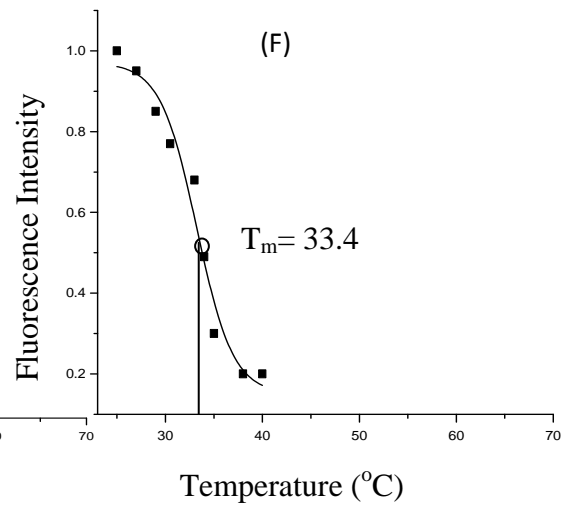
(F)



(G)



(H)



(I)

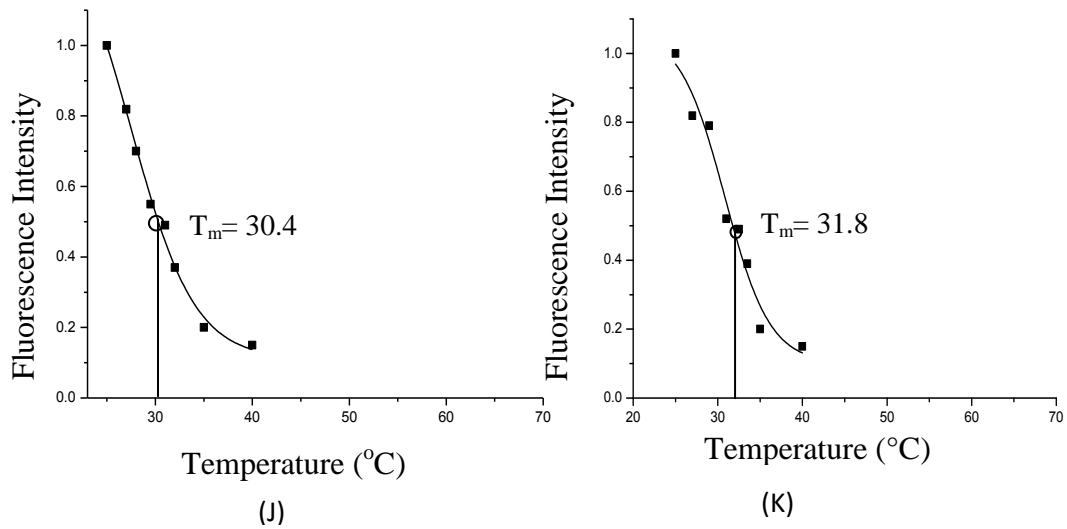


Fig. S2: Representative plots for on-surface melting temperature of LNA-DNA duplex (A) for fully matched LNA-DNA duplex, $T_m = 52.1$ °C; and [B-G] for single mismatch at the central position (B) G: G, $T_m = 31$ °C; (C) G: T, $T_m = 31.4$ °C; (D) T: G, $T_m = 33$ °C; (E) A: G, $T_m = 30$ °C; (F) A: C, $T_m = 31.1$ °C; (G) C: A, $T_m = 34.3$ °C; (H) C: T, $T_m = 33.8$ °C; (I) C: C, $T_m = 33.4$ °C; (J) A: A, $T_m = 30.4$ °C; (K) T: T, $T_m = 31.8$ °C.

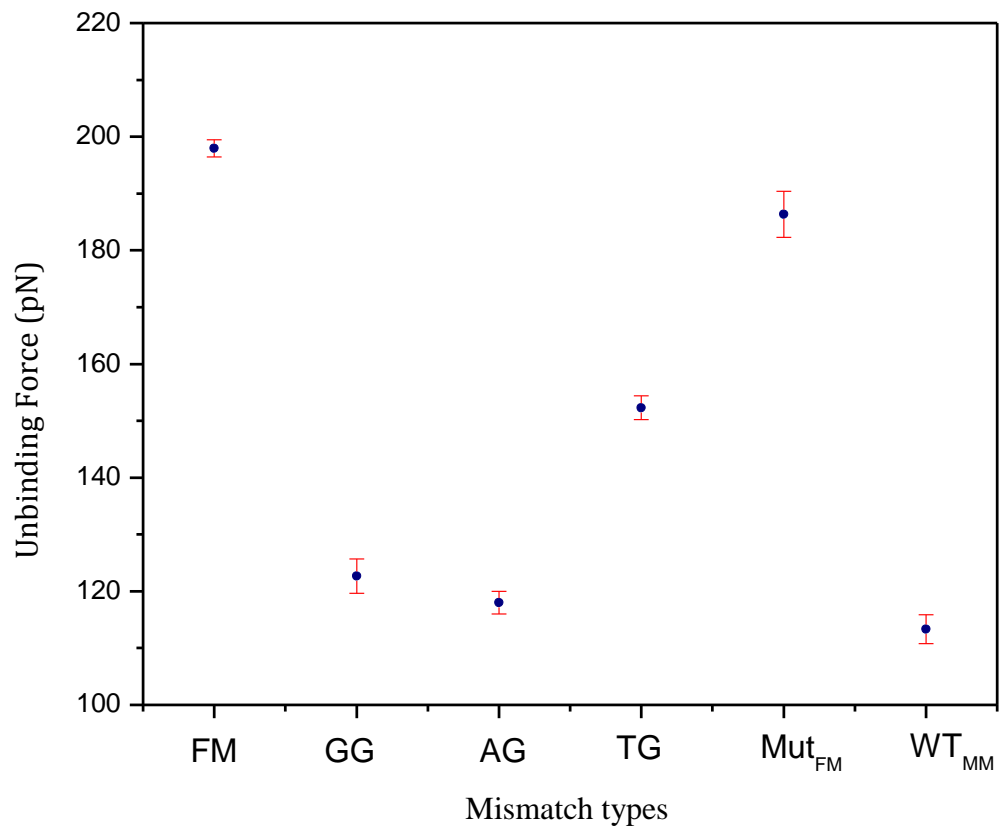


Fig. S3: Unbinding force values for fully matched as well as the mismatched combinations presented including the standard errors from mean.