

Synthesis and Photophysical properties of pyrene-labeled 3-deaza-2'-deoxyadenosines comprising a non- π -conjugated linker: Fluorescence quenching-based oligodeoxynucleotide probes for thymine identification

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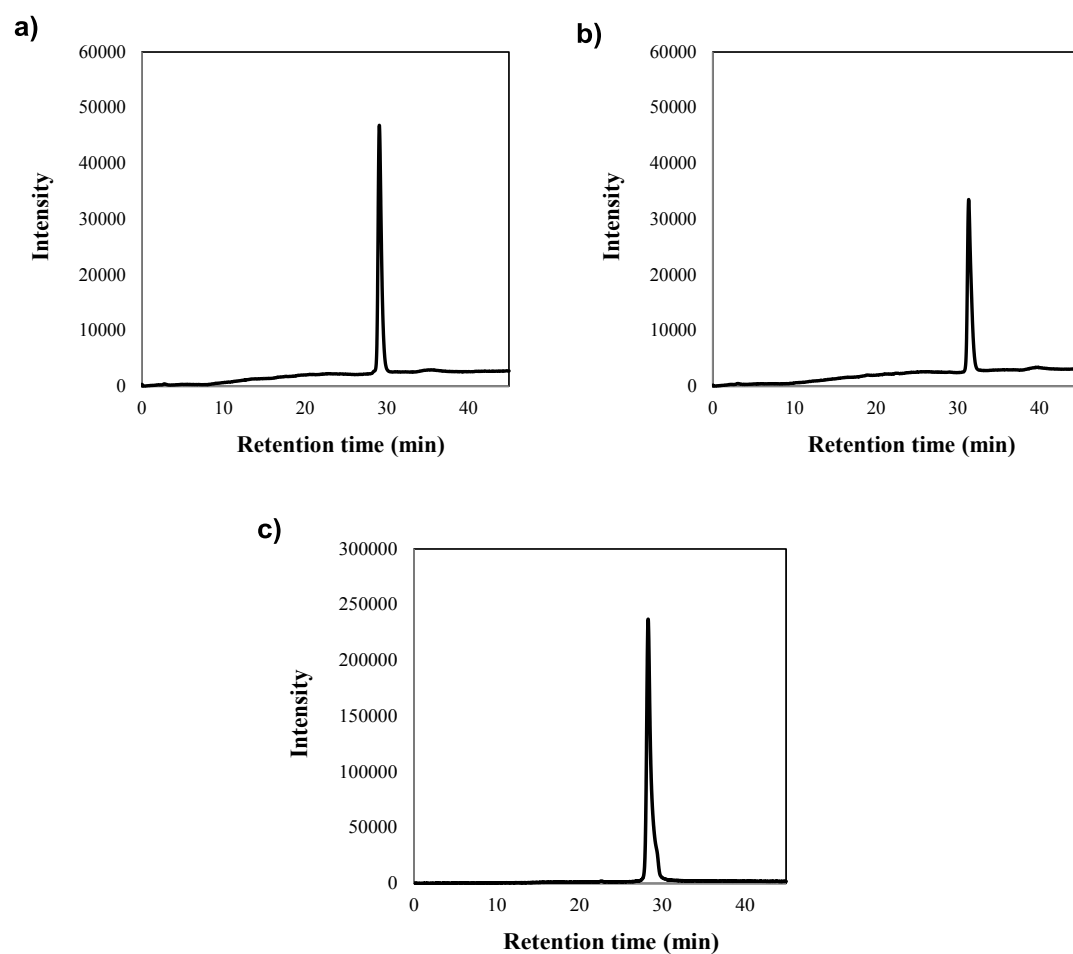


Figure S1. HPLC profiles determined at 260 nm of single-stranded oligonucleotides. (a) ODN1($\text{py}^{\text{3z}}\text{A}$), (b) ODN2($\text{py}^{\text{3z}}\text{A}$), and (c) Probe_(AGT). HPLC analysis was performed on a CHEMCOBOND 5-ODS-H columnm (10×150 nm) eluted with 50 mM ammonium formate buffer containing acetonitrile. Gradient: from 3 to 20 % acetonitrile at a flow rate 2.0 ml/min over 45 min.

Table 1. MALDI-TOF mass spectral data for the ODNs

ODNs	Sequences	MALDI-TOF mass	
		calcd. $[M + H]^+$	found $[M + H]^+$
ODN1	5'-d(CGCAAC ^{py3z} ACAACGC)-3'	4178.96	4178.01
ODN2	5'-d(CGCAAT ^{py3z} ATAACGC)-3'	4208.96	4207.99
Probe _(AGT)	5'-d(GGCTCCC ^{py3z} ATCAGGGA)-3'	4856.90	4857.44

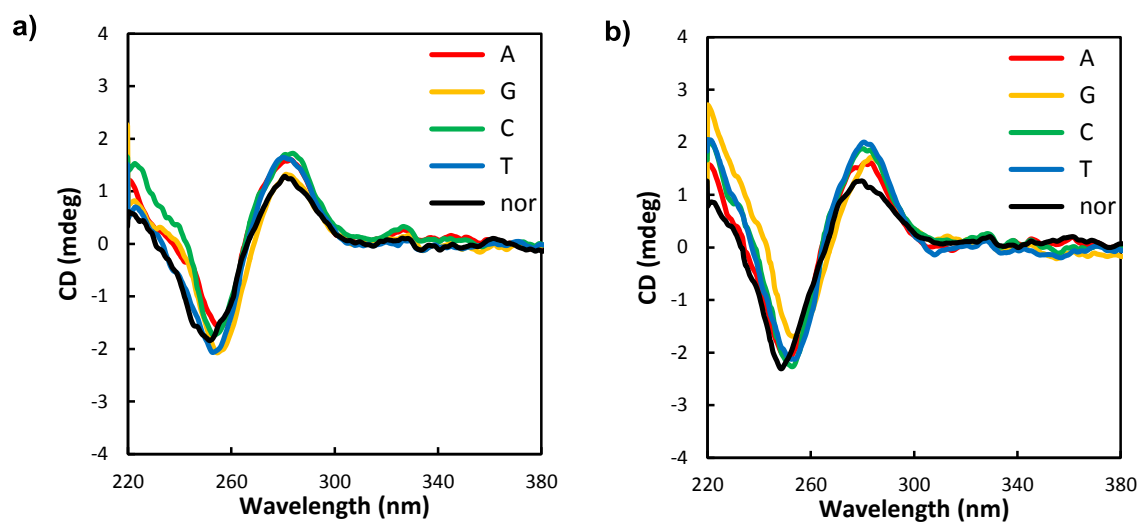


Figure S2. CD spectra of (a) 2.5 μM ODN1(py^{3z}A) hybridized with complementary strand 2.5 μM cODN1(N) and (b) 2.5 μM ODN2(py^{3z}A) hybridized with complementary strand 2.5 μM cODN2(N) (50 mM sodium phosphate, 0.1 M sodium chloride, pH 7.0, rt). "nor" denotes the corresponding unmodified duplex: a) ODN1(A)/cODN1(T), b) ODN2(A)/cODN2(T).

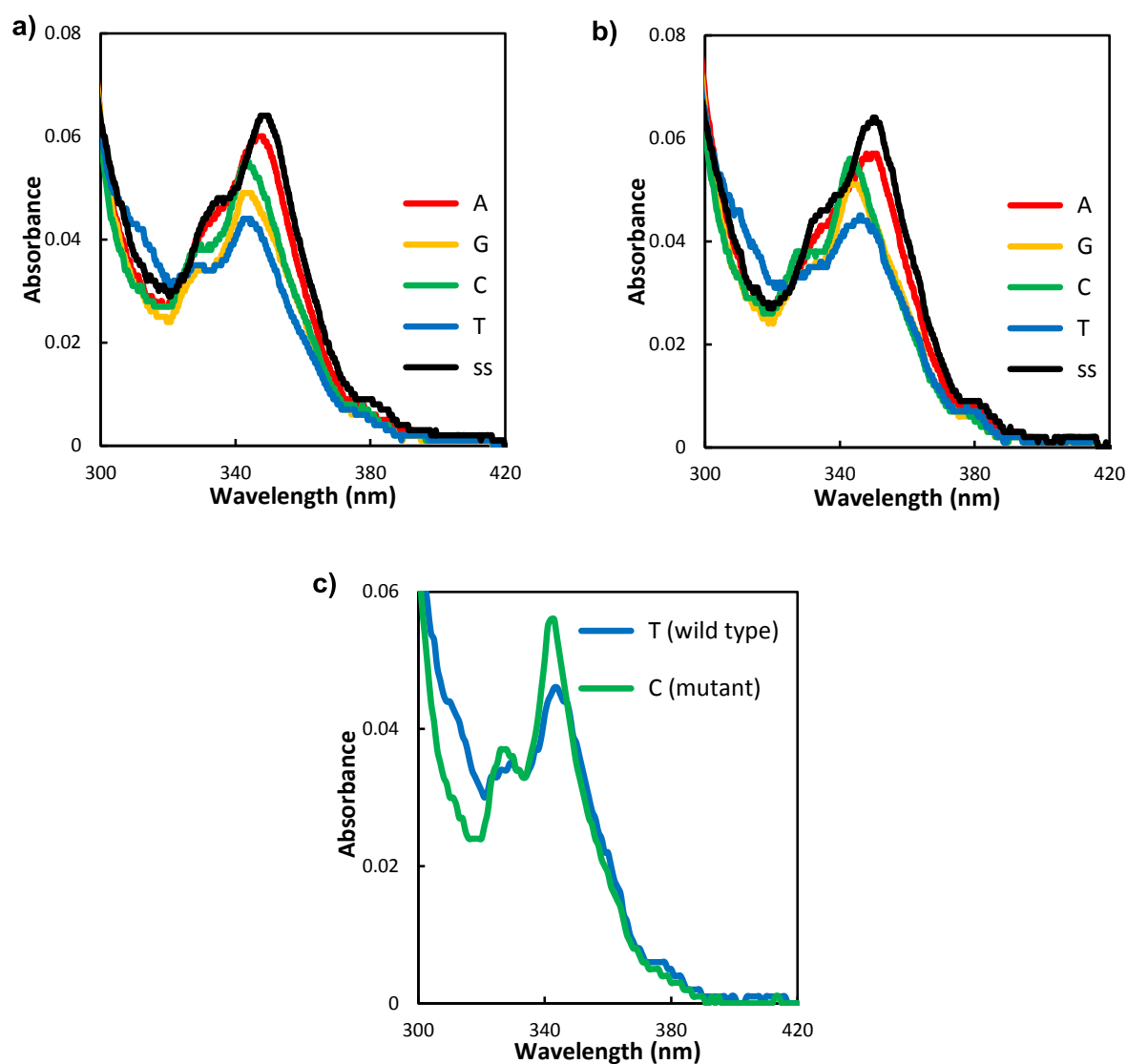


Figure S3. Absorption spectra of (a) ODN1(py^{3z}A), (b) ODN2(py^{3z}A) and (c) Probe_(AGT) hybridized with their complementary ODNs (50 mM sodium phosphate, 0.1 M sodium chloride, pH 7.0, rt). "ss" denotes single-stranded ODN(^{3n7z}A). ODN and cODN concentrations both amounted to 2.5 μ M.