Electronic Supplementary Material (ESI) for RSC Advances.

Electronic supplementary information

Base recognition by L-nucleotides in heterochiral DNAs

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Note added after first publication: This Supplementary Information file replaces that originally published on 6 February 2012. The original version of Table S1 contained some incorrect nucleotide sequences in error. The correct sequences are provided in this updated version.

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1. General methods

Commercially available reagents were used without further purification. L-Nucleotides and their 5'-*O*-dimethoxytrityl-3'-(2-cyanoethyl)-*N,N*-diisopropylphosphoramidite derivatives were synthesized according to a previously reported procedure.[1] HPLC analyses were performed on a Shimadzu LC-10A system. A μBondasphere C18 5μm 100Å column (3.9×150 mm, Waters) was used with a linear gradient of acetonitrile in 50 mM triethylammonium acetate (TEAA, pH 7.0). Matrix-assisted laser desorption/ionization time-of-flight (MALDI TOF) mass spectra were acquired on a Voyager-DE™ STR (Applied Biosystems) with 3-hydroxypicolinic acid as the matrix.

2. Oligonucleotide synthesis and characterization with MALDI-TOF mass spectrometry

Oligodeoxyribonucleotides were synthesized on an Applied Biosystems model 392 automated DNA/RNA synthesizer. Reagents for the synthesis were purchased from Applied Biosystems Japan.

d(AAATCTGCG); m/z calcd for $C_{88}H_{113}N_{35}O_{51}P_8$ ([M+H]$^+$), 2723.82, found: 2723.43;
d(CGCAGATTT); m/z calcd for $C_{88}H_{113}N_{32}O_{53}P_8$ ([M+H]$^+$), 2714.80, found: 2714.51;
d(AA**LA**TCTGCG); m/z calcd for $C_{88}H_{113}N_{35}O_{51}P_8$ ([M+H]$^+$), 2723.82, found: 2724.36;
d(AAATCT**LG**CG); m/z calcd for $C_{88}H_{113}N_{35}O_{51}P_8$ ([M+H]$^+$), 2723.82, found: 2723.53;
d(AAAT**LC**TGCG); m/z calcd for $C_{88}H_{113}N_{35}O_{51}P_8$ ([M+H]$^+$), 2723.82, found: 2723.12;
d(AAA**LT**CTGCG); m/z calcd for $C_{88}H_{113}N_{35}O_{51}P_8$ ([M+H]$^+$), 2723.82, found: 2722.57;
d(CGCAGAATT); m/z calcd for $C_{88}H_{112}N_{35}O_{51}P_8$ ([M+H]$^+$), 2723.82, found: 2723.77;
d(CGCAGAGTT); m/z calcd for $C_{88}H_{112}N_{35}O_{52}P_8$ ([M+H]$^+$), 2739.82, found: 2739.98;
d(CGCAGACTT); m/z calcd for $C_{87}H_{112}N_{33}O_{52}P_8$ ([M+H]$^+$), 2699.79, found: 2699.59;
d(CGAAGATTT); m/z calcd for $C_{89}H_{113}N_{34}O_{52}P_8$ ([M+H]$^+$), 2738.83, found: 2738.04;
d(CGGAGATTT); m/z calcd for $C_{89}H_{113}N_{34}O_{53}P_8$ ([M+H]$^+$), 2754.83, found: 2754.55;
d(CGTAGATTT); m/z calcd for $C_{89}H_{114}N_{31}O_{54}P_8$ ([M+H]$^+$), 2729.82, found: 2729.14;
d(CGCAAATTT); m/z calcd for $C_{88}H_{113}N_{32}O_{52}P_8$ ([M+H]$^+$), 2698.81, found: 2697.01;
d(CGCACATTT); m/z calcd for $C_{87}H_{113}N_{30}O_{53}P_8$ ([M+H]$^+$), 2674.78, found: 2673.62;
d(CGCATATTT); m/z calcd for $C_{88}H_{114}N_{29}O_{54}P_8$ ([M+H]$^+$), 2689.79, found: 2688.94;
d(CGCAGGTTT); m/z calcd for $C_{88}H_{113}N_{32}O_{54}P_8$ ([M+H]$^+$), 2730.80, found: 2729.11;
d(CGCAGCTTT); m/z calcd for $C_{87}H_{113}N_{30}O_{54}P_8$ ([M+H]$^+$), 2690.78, found: 2690.25;
d(CGCAGTTTT); m/z calcd for $C_{87}H_{114}N_{29}O_{55}P_8$ ([M+H]$^+$), 2705.79, found: 2704.63

3. Melting experiments

The concentrations of oligonucleotide solutions were calculated by using the equation and coefficients described by Bore.[2] The coefficients of the heterochiral oligomer were assumed to be the same as those of the corresponding homochiral oligomer. Duplex solutions (6 mM) in 10 mM $MgCl_2$, 100 mM NaCl, and 70 mM MOPS (pH 7.1) were heated at 90 ºC and cooled gradually to room temperature. Melting curves were measured at least twice at 270 nm on a JASCO V-560 spectrophotometer equipped with a programmable temperature control unit. The temperature was raised at a rate of 0.5ºC/min and T_m values were obtained from the first-derivative plots of the melting curves.

4. Table S1. Melting temperature of mismatched homo- and heterochiral duplexes.[a]

complementary strand		homo- and heterochiral strand			
		d(AA**DA**TCTGCG)		d(AA**LA**TCTGCG)	
d(CGCAGA**X**TT)	X = A	27.6 ± 0.0	(-14.5)	26.0 ± 0.4	(-7.6)
	X = G	31.8 ± 0.4	(-10.3)	29.2 ± 0.2	(-4.4)
	X = C	27.3 ± 0.3	(-14.8)	27.7 ± 0.5	(-5.9)
	X = T	42.1 ± 0.3	F.M.	33.6 ± 0.2	F.M.
		d(AAATCT**DG**CG)		d(AAATCT**LG**CG)	
d(CG**X**AGATTT)	X = A	22.1 ± 0.1	(-20.0)	19.3 ± 0.3	(-13.3)
	X = G	22.5 ± 0.1	(-19.6)	31.6 ± 0.4	(-1.0)
	X = C	42.1 ± 0.3	F.M.	32.6 ± 0.4	F.M.
	X = T	25.0 ± 0.2	(-17.1)	22.4 ± 0.4	(-10.2)
		d(AAAT**DC**TGCG)		d(AAAT**LC**TGCG)	
d(CGCA**X**ATTT)	X = A	16.4 ± 0.0	(-25.7)	13.8 ± 0.2	-24.4
	X = G	42.1 ± 0.3	F.M.	38.2 ± 0.2	F.M.
	X = C	13.6 ± 0.2	(-28.5)	9.9 ± 0.1	(-28.3)
	X = T	18.2 ± 0.2	(-23.9)	13.7 ± 0.1	(-24.5)
		d(AAA**DT**CTGCG)		d(AAA**LT**CTGCG)	
d(CGCAG**X**TTT)	X = A	42.1 ± 0.3	F.M.	33.9 ± 0.1	F.M.
	X = G	31.3 ± 0.1	(-10.8)	25.7 ± 0.5	(-8.2)
	X = C	22.2 ± 0.2	(-19.9)	20.7 ± 0.5	(-13.2)
	X = T	26.4 ± 0.2	(-15.7)	26.9 ± 0.1	(-7.0)

[a]Samples contained 6 µM duplex in 10 mM $MgCl_2$, 100 mM NaCl, and 70 mM MOPS (pH 7.1). Melting points are the average of at least two measurements ± standard deviation. Melting point differences from the fully matched (F. M.) duplex are shown in parenthesis.

5. References.

1. H.Urata, E. Ogara, K. Shinohara, Y. Ueda, and M. Akagi, *Nucleic Acids Res*., 1992, **20**, 3325
2. P.N Bore, Optical properties of nucleic acids, in: G.D. Fasman (Ed.), *Handbook of Biochemistry and Molecular Bioligy, third ed, Nucleic acid, vol. 1, CRC Press, Boca Raton, FL*, 1975, p589