Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry. This journal is © The Royal Society of Chemistry 2015

Supporting Information

Double-headed nucleotides introducing thymine nucleobases in the major groove of nucleic acid duplexes

Michael Dalager,^a Nicolai K. Andersen,^a Pawan Kumar,^a Poul Nielsen^{a,*} and Pawan K. Sharma^{b,*}

^aNucleic Acid Center, Department of Physics, Chemistry and Pharmacy, and ^bDepartment of

Chemistry, Kurukshetra University, Kurukshetra-136 119, India.

List of contents:

MALDI-TOF MS of synthesized ONs	S2
CD-spectra	S3-S5
Fluorescence emission spectra	S6-S7
Selected 1D and 2D NMR spectra	S8-S17

MALDI-TOF data

				Ν	Mass ^[b]	
	Sequence	Overall yield ^[a]	Coupling efficiency ^[a]	Calcd.	Found	
ON 2	5'-d(GTG AXA TGC)	69.5%	>95.5%	2963.8	2969.4	
ON 3	5'-d(GTG AYA TGC)	46.2%	>90.8%	2963.8	2969.6	
ON 4	5'-d(GTG AZA TGC)	98.5%	>99%	2939.8	2944.5	
ON 5	5'-d(GTG AWA TGC)	73.2%	>96.1%	2939.8	2936.1	
ON 7	5'-d(GTG TXT TGC)	>99%	>99%	2945.8	2942.1	
ON 8	5'-d(GTG TYT TGC)	95.2%	>99%	2945.8	2943.0	
ON 9	5'-d(GTG TZT TGC)	95.8%	>99%	2921.8	2924.6	
ON 10	5'-d(GTG TWT TGC)	80.3%	>97.3%	2921.8	2922.2	
ON 11	5'-d(GTG XXX TGC)	82.9%	>97.7%	3366.8	3367.2	
ON 12	5'-d(GTG YYY TGC)	81.9%	>97.5%	3366.8	3363.6	
ON 13	5'-d(GTG ZZZ TGC)	69.3%	>95.5%	3294.8	3290.3	
ON 14	5'-d(GTG WWW TGC)	64.9%	>94.7%	3294.8	3294.2	

Table S1. Yields and MALDI-TOF data for modified oligonucleotides.

[a] Yield and coupling efficiency determined from UV-Vis absorption of DMT cation after deblocking. [b] Mass determined by Maldi-TOF mass spectroscopy.

CD-spectra



Figure S1. CD-spectra for ON1-5 with complementary DNA.





Figure S3. CD-spectra for ON1-5 with complementary DNA with an abasic site.





Figure S4. CD-spectra for ON6-10 with complementary DNA.

Figure S5. CD-spectra for ON6-10 with complementary RNA.



Figure S6. CD-spectra for ON6-10 with complementary DNA with an abasic site.





Figure S7. CD-spectra for ON11-14 with complementary DNA.

Figure S8. CD-spectra for ON11-14 with complementary RNA.



Figure S9. CD-spectra for ON11-14 with complementary DNA with an abasic site.



Fluorescence emission spectra



Figure S10. Monomer fluorescence.

Figure S11. Fluorescence emission spectra for single strands and duplexes of ON2-5.





Figure S12. Fluorescence emission spectra for single strands and duplexes of ON7-10.

Figure S13. Fluorescence emission spectra for single strands and duplexes of ON2-5.

























