Supplementary Data

A New Usage of Functionalized Oligodeoxynucleotide Probe for Site-Specific Modification of a Guanine Base within RNA

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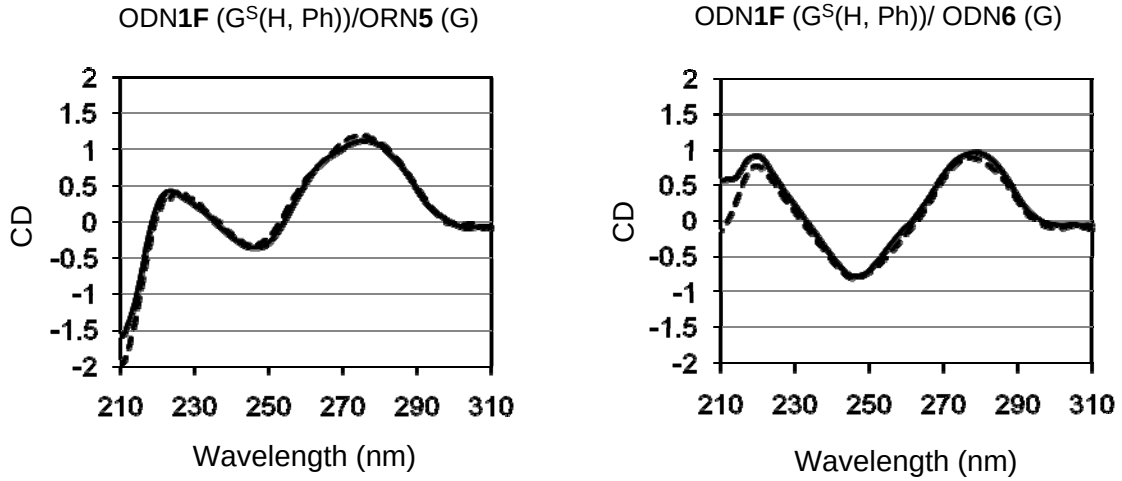
5’-d(CTTT*X*TTCTCCTTTCT)
3’-r(GAAA*Y*AAGAGGAAAGA)

5’-d(CTTT*X*TTCTCCTTTCT)
3’-d(GAAA*Y*AAGAGGAAAGA)

CD spectra



UV melting curves

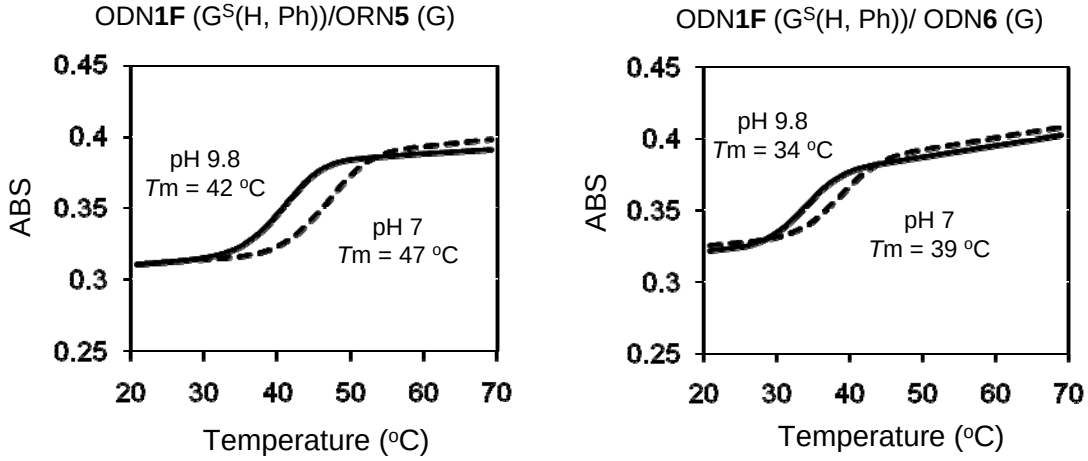
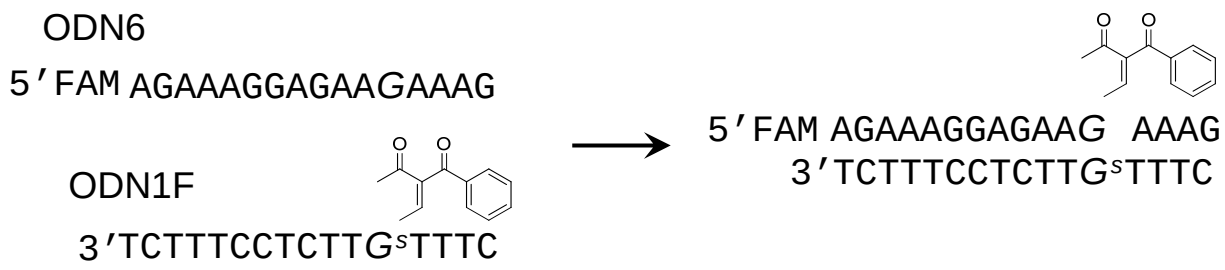


Figure S1. CD spectra and UV melting curves. CD spectra were measured using 2.5 μM duplexes in 50 mM MES buffer (pH 7, broken line) or 50 mM carbonate buffer (pH 9.8, solid line) containing 100 mM NaCl. Melting curves were measured using 1.3 μM duplexs in 50 mM MES buffer (pH 7) or 50 mM carbonate buffer (pH 9.8) containing 100 mM NaCl.

pH dependency (DNA)



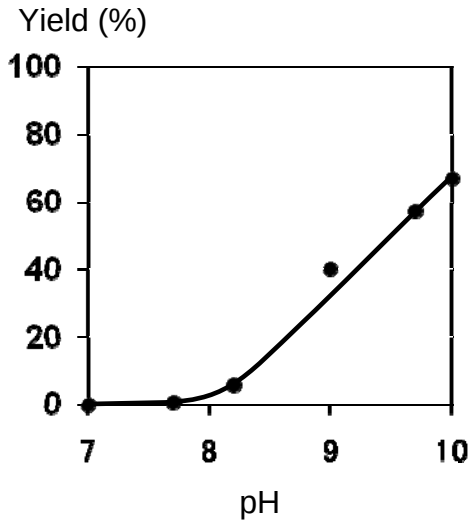
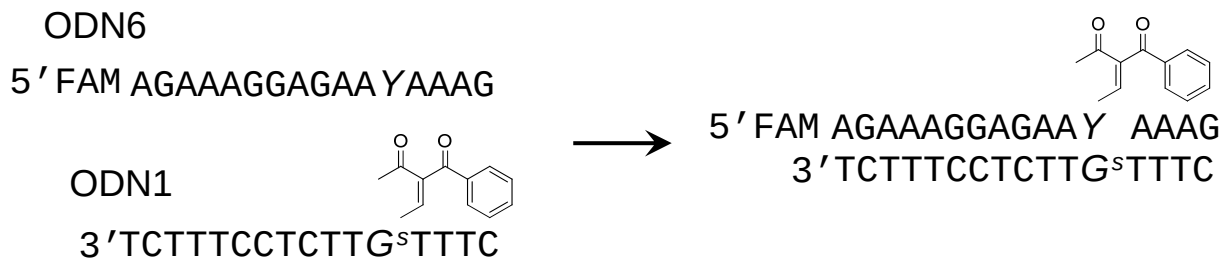
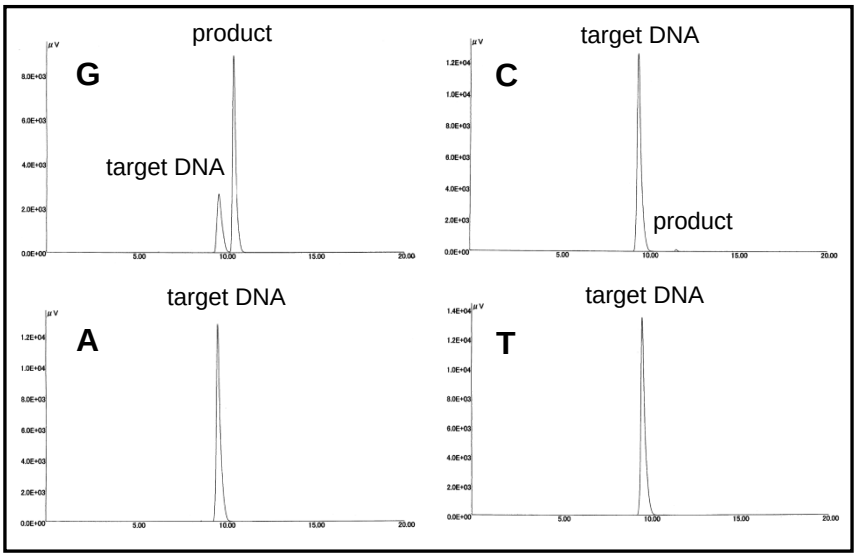


Figure S2. The pH dependency of the transfer reaction with DNA substrate. The transfer reactions were performed by using 1.5 μM of *S*-functionalized ODN**1F** (G^S(Me, Ph)) and 1.0 μM of the target ODN**6** (G) in 50 mM phosphate or carbonate buffer (pH > 9) at 25°C for 1h, and followed by HPLC (Column: SHISEIDO C18, 4.6 x 250 mm; Solvent: A: 0.1 M TEAA Buffer, B: CH_3CN, B: 10% to 30% /20 min, linear gradient; Flow rate: 1.0 ml/min; monitored by fluorescence detector at 518 nm with emission at 494 nm).

Base selectivity (DNA)





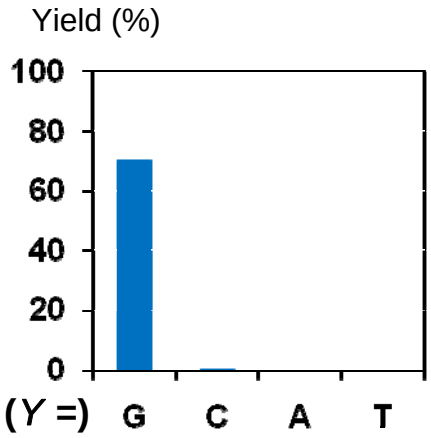
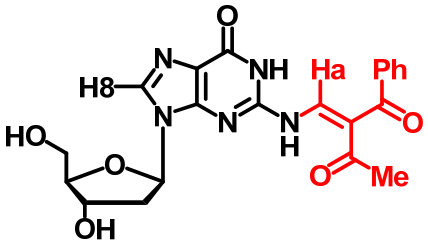
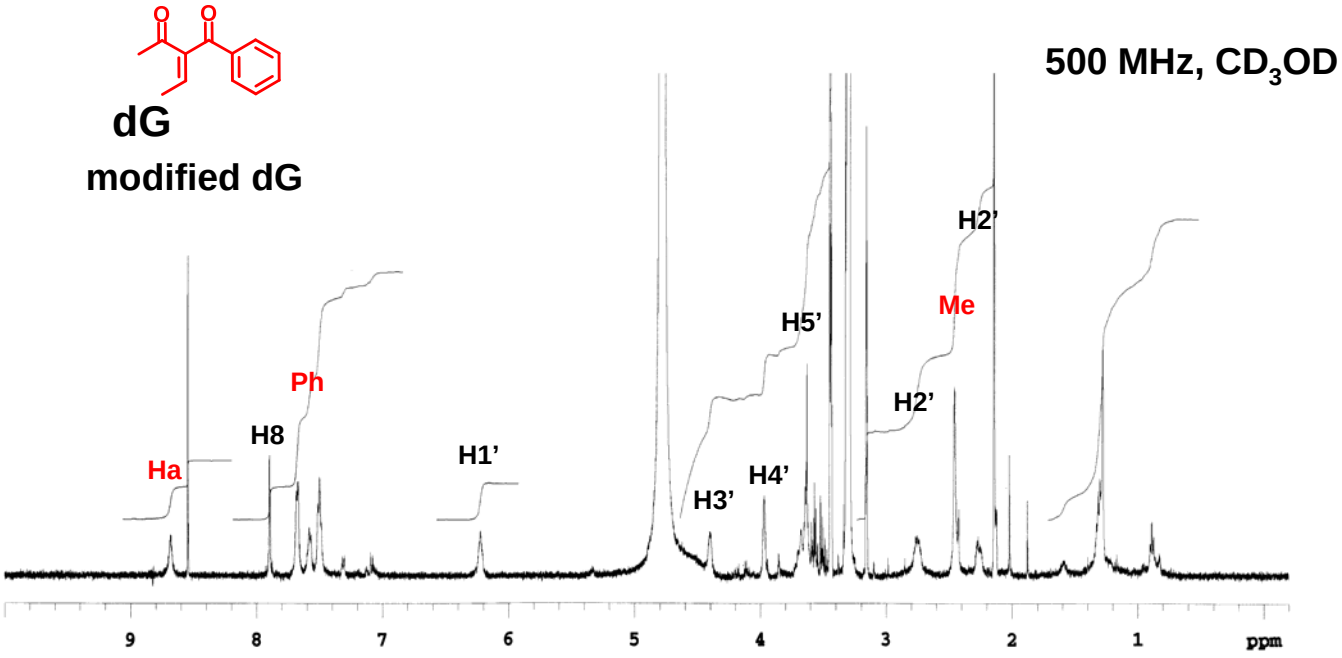


Figure S3. Selectivity to the guanine base in the DNA substrates. The transfer reactions were performed by using 1.5 μM of *S*-functionalized ODN**1F**(G^S(Me, Ph)) and 1.0 μM of the target ODN**6** (Y) in 50 mM carbonate buffer containing 100 mM NaCl at pH 10 for 2h, and followed by HPLC (Column: SHISEIDO C18, 4.6 x 250 mm; Solvent: A: 0.1 M TEAA Buffer, B: CH_3CN, B: 10% to 30% /20 min, linear gradient; Flow rate: 1.0 ml/min; monitored by fluorescence detector at 518 nm with emission at 494 nm).



Hydrolysate of the modified DNA



Synthesized compound

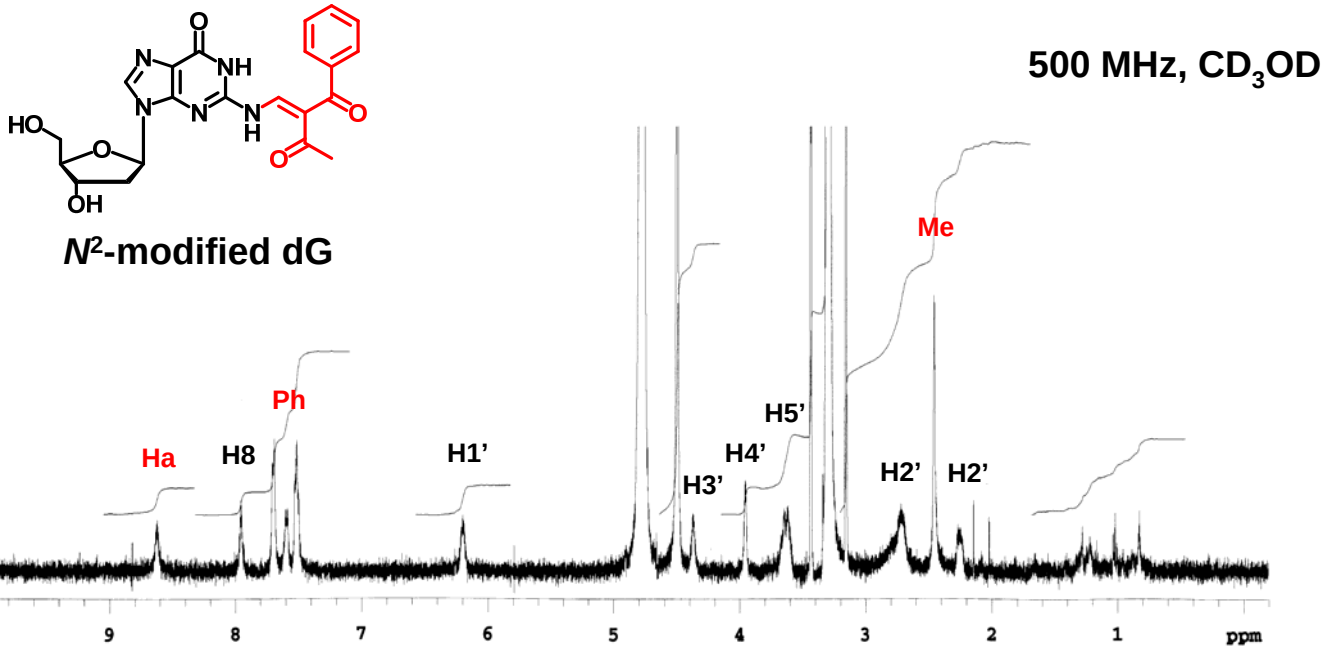
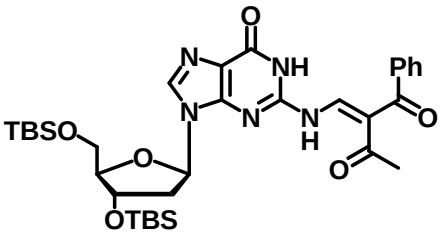


Figure S4. ^{1}H-NMR measurements


O
N
NH
Ph
N
N
N
H
O
TBSO
O
O
OTBS

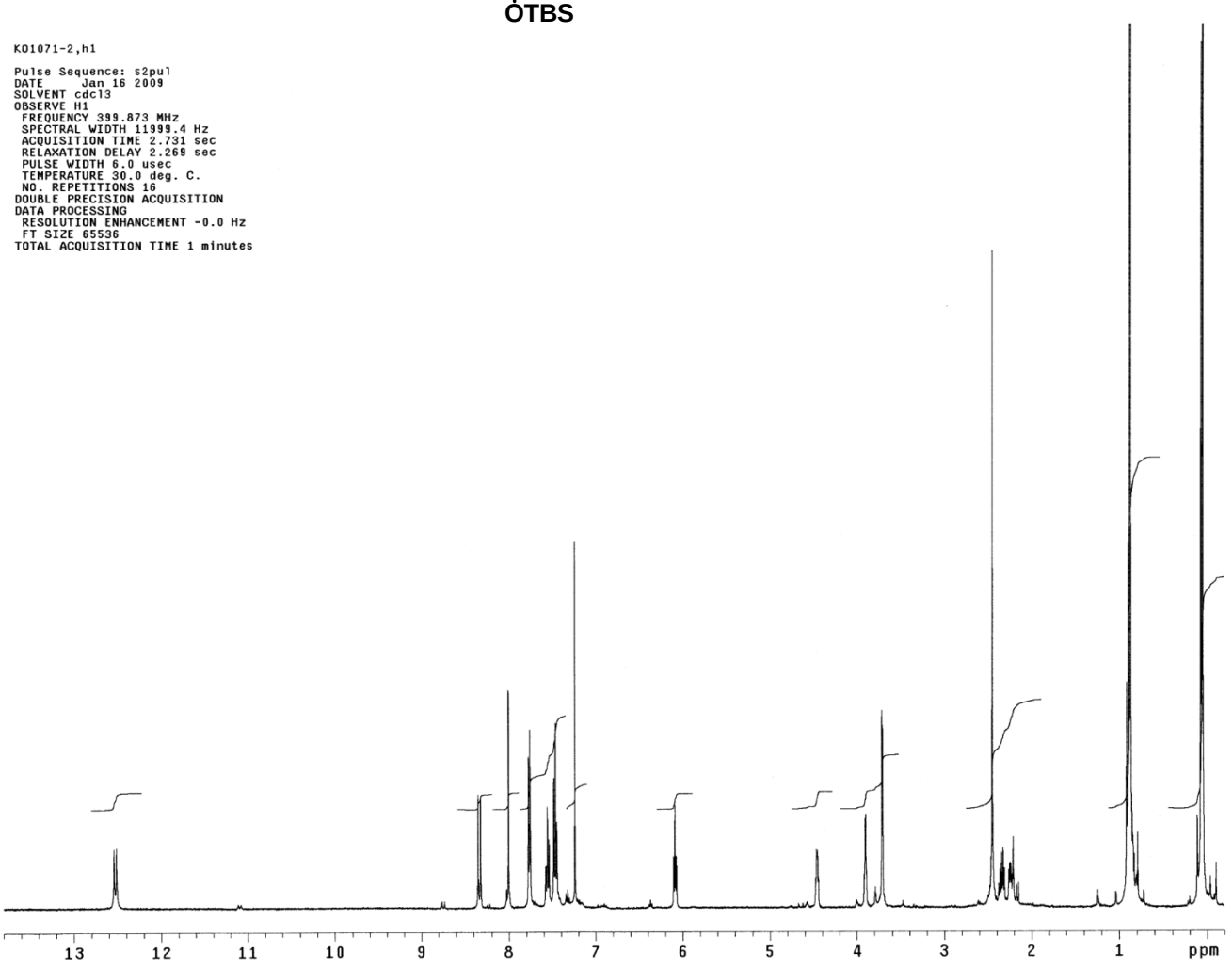

KO1071-2,h1
Pulse Sequence: s2pul
DATE Jan 16 2009
SOLVENT cdcl3
OBSERVE H1
FREQUENCY 399.873 MHz
SPECTRAL WIDTH 11999.4 Hz
ACQUISITION TIME 2.731 sec
RELAXATION DELAY 2.269 sec
PULSE WIDTH 6.0 usec
TEMPERATURE 30.0 deg. C.
NO. REPETITIONS 16
DOUBLE PRECISION ACQUISITION
DATA PROCESSING
RESOLUTION ENHANCEMENT -0.0 Hz
FT SIZE 65536
TOTAL ACQUISITION TIME 1 minutes
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm

Table S1. UV Melting temperatures of the duplexes formed with.

ODN	Complementary strand	Y =	pH	Tm (°C)
ODN**1**-G^{S}	ORN**5**	rG	9.8	39
ODN**1F**-G^{S}(H, Ph)	ORN**5**	rG	9.8	42
ODN**1F**-G^{S}(H, Ph)	ORN**5** (FAM)	rG	9.8	43
ODN**1F**-G^{S}(H, Ph)	ORN**5** (FAM)	rC	9.8	42
ODN**1F**-G^{S}(H, Ph)	ORN**5** (FAM)	rA	9.8	44
ODN**1F**-G^{S}(H, Ph)	ORN**5** (FAM)	rU	9.8	43
ODN**1F**-G^{S}(H, Ph)	ORN**5**	rG	7	47
ODN**1**-G^{S}(H, Ph)	ORN**5** (FAM)	rG	7	49
ODN**1F**-G^{S}(H, Ph)	ORN**5** (FAM)	rC	7	49
ODN**1F**-G^{S}(H, Ph)	ORN**5** (FAM)	rA	7	49
ODN**1F**-G^{S}(H, Ph)	ORN**5** (FAM)	rU	7	48
ODN**1F**-G^{S}(H, Ph)	ODN**6** (FAM)	dG	9.8	35
ODN**1F**-G^{S}(H, Ph)	ODN**6** (FAM)	dC	9.8	37
ODN**1F**-G^{S}(H, Ph)	ODN**6** (FAM)	dA	9.8	35
ODN**1F**-G^{S}(H, Ph)	ODN**6** (FAM)	dT	9.8	35
ODN**1F**-G^{S}(H, Ph)	ODN**6**	dG	9.8	34
ODN**1F**-G^{S}(H, Ph)	ODN**6**	dHx	9.8	33
ODN**1F**-G^{S}(H, Ph)	ODN**6**	d2AP	9.8	34
ODN**1F**-G^{S}(H, Ph)	ODN**6**	dG	7	39
ODN**1F**-G^{S}(H, Ph)	ODN**6**	dHx	7	38
ODN**1F**-G^{S}(H, Ph)	ODN**6**	d2AP	7	39
ODN**2F**-G^{S}(H, Ph)	ORN**7** (FAM)		9.8	45
ODN**2F**-G^{S}(H, Ph)	ORN**8** (FAM)		9.8	45
ODN**3F**-G^{S}(H, Ph)	ORN**7** (FAM)		9.8	42
ODN**3F**-G^{S}(H, Ph)	ORN**9** (FAM)		9.8	45
ODN**4F**-G^{S}(H, Ph)	ORN**10** (FAM)	rG	9.8	36
ODN**4F**-G^{S}(H, Ph)	ORN**10**(FAM)	rC	9.8	37
ODN**4F**-G^{S}(H, Ph)	ORN**10**(FAM)	rA	9.8	36
ODN**4F**-G^{S}(H, Ph)	ORN**10** (FAM)	rU	9.8	36

Table S2. MALDI-TOF.MS Data of all ODN and ORN compounds used in this study.

DNA or RNA	5' Label	X or Y	Calcd ([M-H]$^-$)	Found
ODN**1**		X = G^S	4767.8	4766.5
ODN**1F**		X = G^S(Me, Ph)	4939.7	4941.5
ODN**1F**		X = G^S(Me, Pyrene)	5063.9	5064.4
ODN**1 F**		X = G^S(H, Ph)	4897.8	4898.8
ODN**2**		X = G^S	4742.7	4742.8
ODN**2 F**		X = G^S(Me, Ph)	4914.7	4914.2
ODN**2 F**		X = G^S(Me, Pyrene)	5038.8	5037.8
ODN**2F**		X = G^S(H, Ph)	4872.7	4872.9
ODN**3**		X = G^S	4742.7	4742.4
ODN**3F**		X = G^S(Me, Ph)	4914.7	4914.0
ODN**3F**		X = G^S(Me, Pyrene)	5038.8	5038.4
ODN**3F**		X = G^S(H, Ph)	4872.7	4872.7
ODN**4**		X = G^S	6719.1	6719.1
ODN**4 F**		X = G^S(Me, Ph)	6891.1	6890.5
ODN**4** F		X = G^S(H, Ph)	6849.1	6849.0
ORN**5**		Y = rG	5297.8	5297.8
ORN**5**	FAM	Y = rG	5835.9	5835.9
ORN**5**	FAM	Y = rC	5795.9	5795.1
ORN**5**	FAM	Y = rA	5819.9	5819.5
ORN**5**	FAM	Y = rU	5796.9	5796.5
ORN**5**		Y = rG(Me, Ph)	5469.8	5469.6
ORN**5**		Y = rG(Me, Pyrene)	5593.9	5593.8
ODN**6**	FAM	Y = dG	5579.1	5579.5
ODN**6**	FAM	Y = dC	5539.1	5538.7
ODN**6**	FAM	Y = dA	5563.1	5563.5
ODN**6**	FAM	Y = dT	5554.1	5553.7
ODN**6**		Y = dG	5041.9	5091.6
ODN**6**		Y = dHx	5026.9	5026.7
ODN**6**		Y = d2AP	5026.0	5025.4
ODN**6**		Y = dG(Me, Ph)	5214.0	5213.6
ODN**6**		Y = d2AP(Me, Ph)	5198.0	5198.3
ORN**7**	FAM		5851.9	5851.3
ORN**8**	FAM		5811.9	5811.3
ORN**9**	FAM		5811.9	5811.2
ORN**10**	FAM	Y = rG	9145.1	9145.4
ORN**10**	FAM	Y = rC	9105.1	9105.9
ORN**10**	FAM	Y = rA	9129.1	9129.0
ORN**10**	FAM	Y = rU	9106.1	9106.3