Electronic Supplementary Information

Threoninol as a Scaffold of Dyes (Threoninol-nucleotide) and Their Stable Interstrand Clustering in Duplexes

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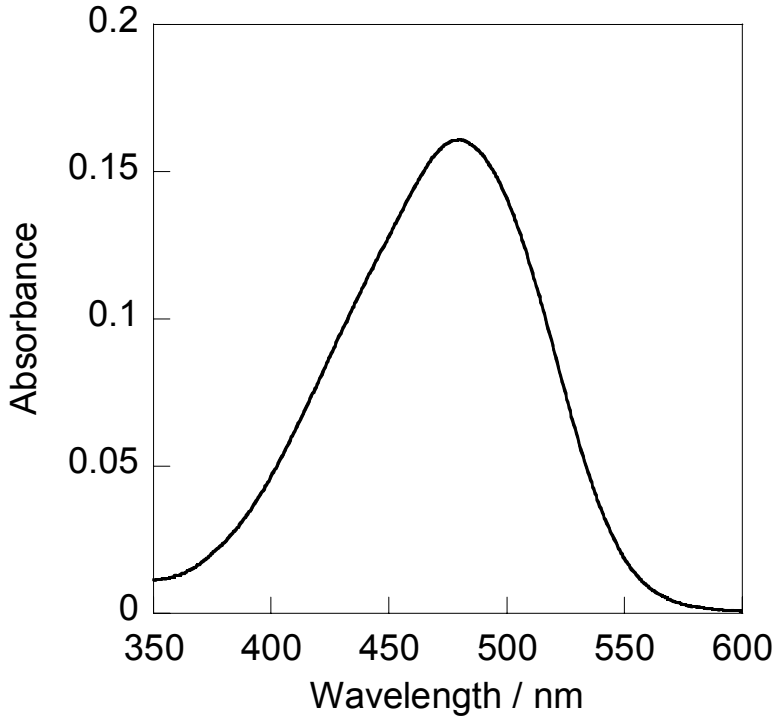
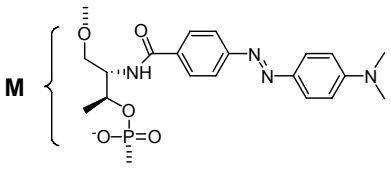


Figure S1. UV-Vis spectra of **M1b** at pH 7.0 (10 mM phosphate buffer), 0 ^{o}C, in the presence of 100 mM NaCl.

M1b: 5'-GAT-TGC-**M**-GAT-ACC-3'

M represents Methyl Red moiety as shown below.



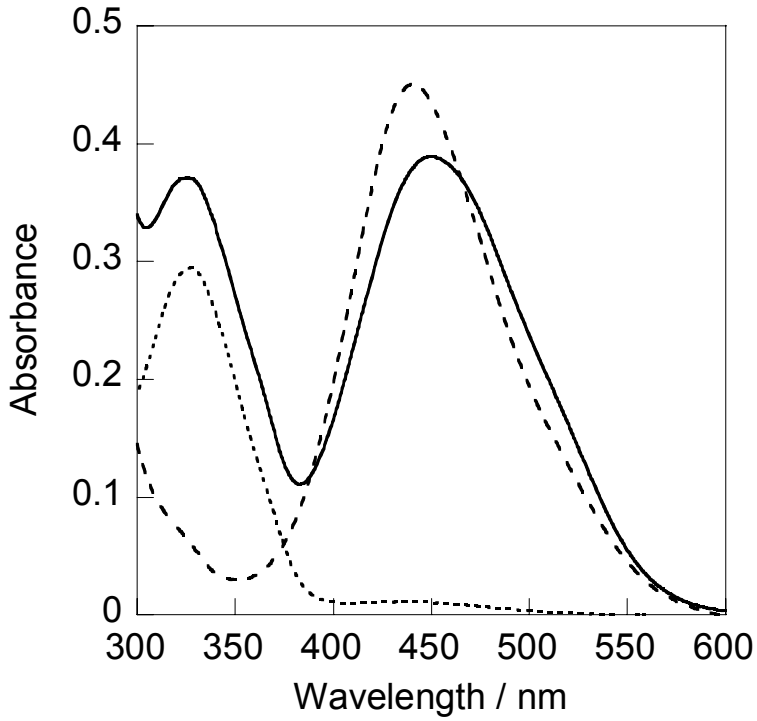
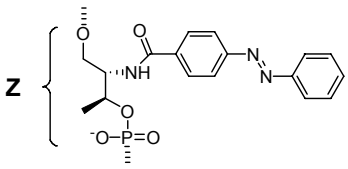


Figure S2. UV-Vis spectra of hetero cluster of Methyl Red and azobenzene (**Z3a**/**M3b;** solid line) , single-stranded **Z3a** (dotted line) and **M3b** (broken line) at 0 ^{o}C, pH 7.0 (10 mM phosphate buffer) in the presence of 100 mM NaCl.

Z3a: 5'-GGT-ATC-**ZZZ**-GCA-ATC-3'
M3b: 5'-GAT-TGC-**MMM**-GAT-ACC-3'

Z represents azobenzene moiety as shown below.



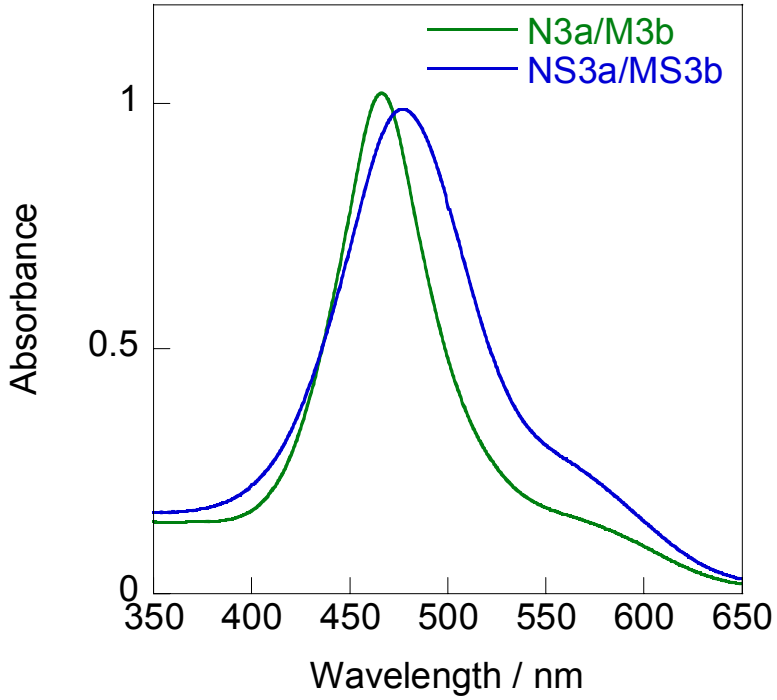


Figure S3. UV-Vis spectra of **N3a**/**M3b** and **NS3a**/**MS3b** at 0 °C. Solution conditions are as follows: [ODN] = 5 μM, [NaCl] = 100 mM, pH 5.0 (10mM MES buffer)

N3a: 5'-GGT-ATC-**NNN**-GCA-ATC-3'
NS3a: 5'-GGT-ATC-**NSNSNS**-GCA-ATC-3'
M3b: 5'-GAT-TGC-**MMM**-GAT-ACC-3'
MS3b: 5'-GAT-TGC-**MSMSMS**-GAT-ACC-3'

N and **S** represent Naphthyl Red and Spacer moieties as shown below, respectively.

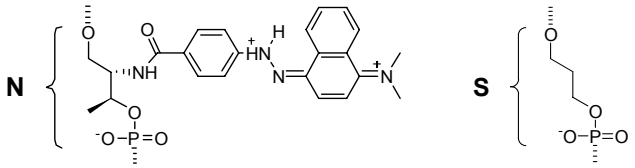


Table S1. Effects of the number of Methyl Red/adenine pairs on the melting temperature (T_m) and absorption maximum and half-line-width of π-π* transition of Methyl Red.[a)]

Sequences	T_m / °C	λ_{max} / nm [b)]	Half-line width [b)] / cm^{-1}
A1a/**M1b**	39.7	485	3946
A2a/**M2b**	35.0	462	4452
A3a/**M3b**	32.4	456	4381
A4a/**M4b**	29.5	442	4487
A5a/**M5b**	24.8	441	4751
A6a/**M6b**	16.4	422	4890
T5a/**M5b**	27.9	441	4852
C5a/**M5b**	27.9	442	4845
G5a/**M5b**	27.9	437	4891

a) Solution conditions: [ODN] = 5 μM, [NaCl] = 100 mM, pH 7.0 (10 mM phosphate buffer)
b) UV-Vis spectrum was measured at 0 °C.

A*n*a: 5'-GGT-ATC-A_n-GCA-ATC-3' (*n* = 1-6)
M*n*b: 5'-GAT-TGC-$\mathbf{M}_n$-GAT-ACC-3' (*n* = 1-6)
T5a: 5'-GGT-ATC-T_5-GCA-ATC-3'
C5a: 5'-GGT-ATC-C_5-GCA-ATC-3'
G5a: 5'-GGT-ATC-G_5-GCA-ATC-3'

M represents Methyl Red moiety as shown in Figure S1.