Literature Report V

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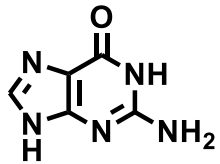
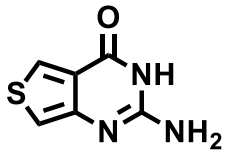
Article

What Makes Thienoguanosine an Outstanding Fluorescent DNA Probe?

Jagannath Kuchlyan,[#] Lara Martinez-Fernandez,[#] Mattia Mori,[#] Krishna Gavvala, Stefano Ciaco, Christian Boudier, Ludovic Richert, Pascal Didier, Yitzhak Tor, Roberto Improta, and Yves Mély*



Guanine



Thienoguanosine

Reporter: Jin Li

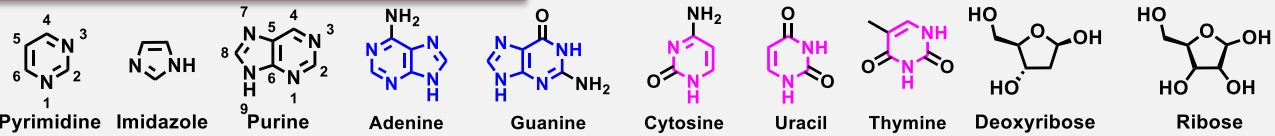
Date: 2020-09-30

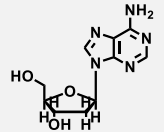
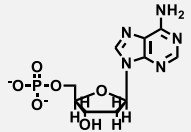
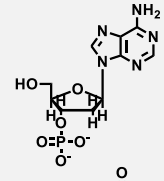
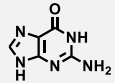
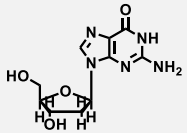
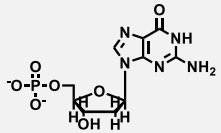
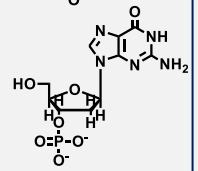
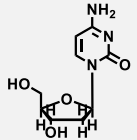
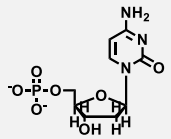
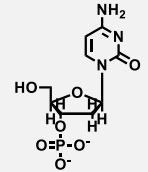
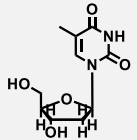
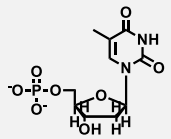
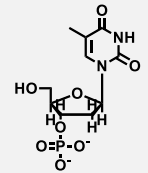
The basic concept

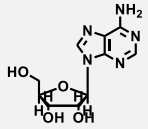
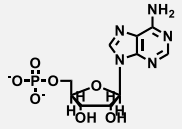
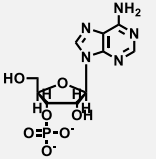
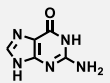
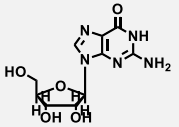
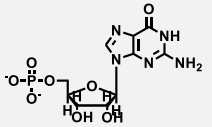
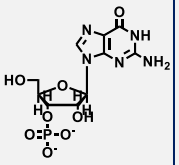
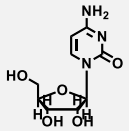
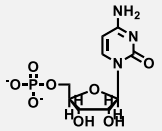
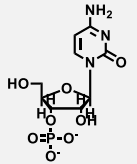
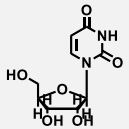
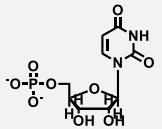
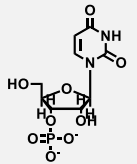
碱基：是嘌呤和嘧啶的衍生物

核苷：戊糖和碱基通过糖苷键连接而成的化合物。

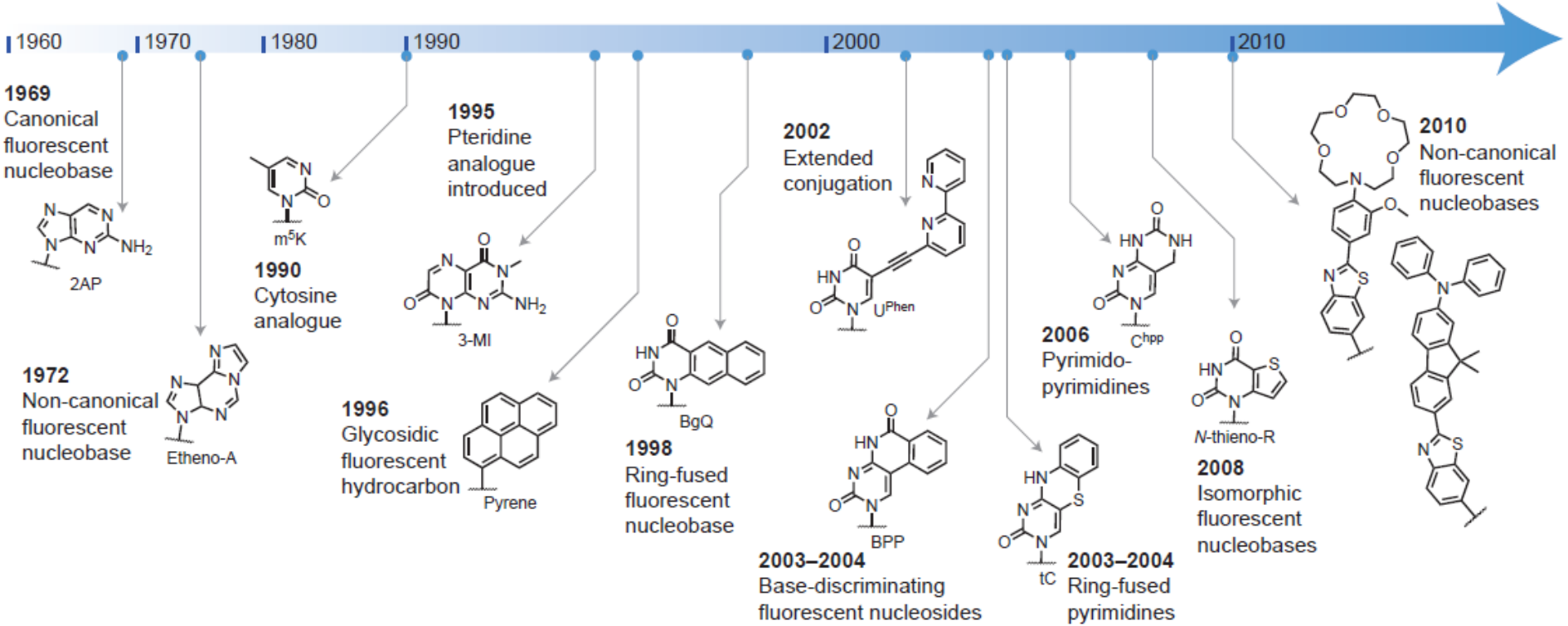
核苷酸：由嘌呤碱或嘧啶碱、核糖或脱氧核糖以及磷酸三种物质组成的化合物



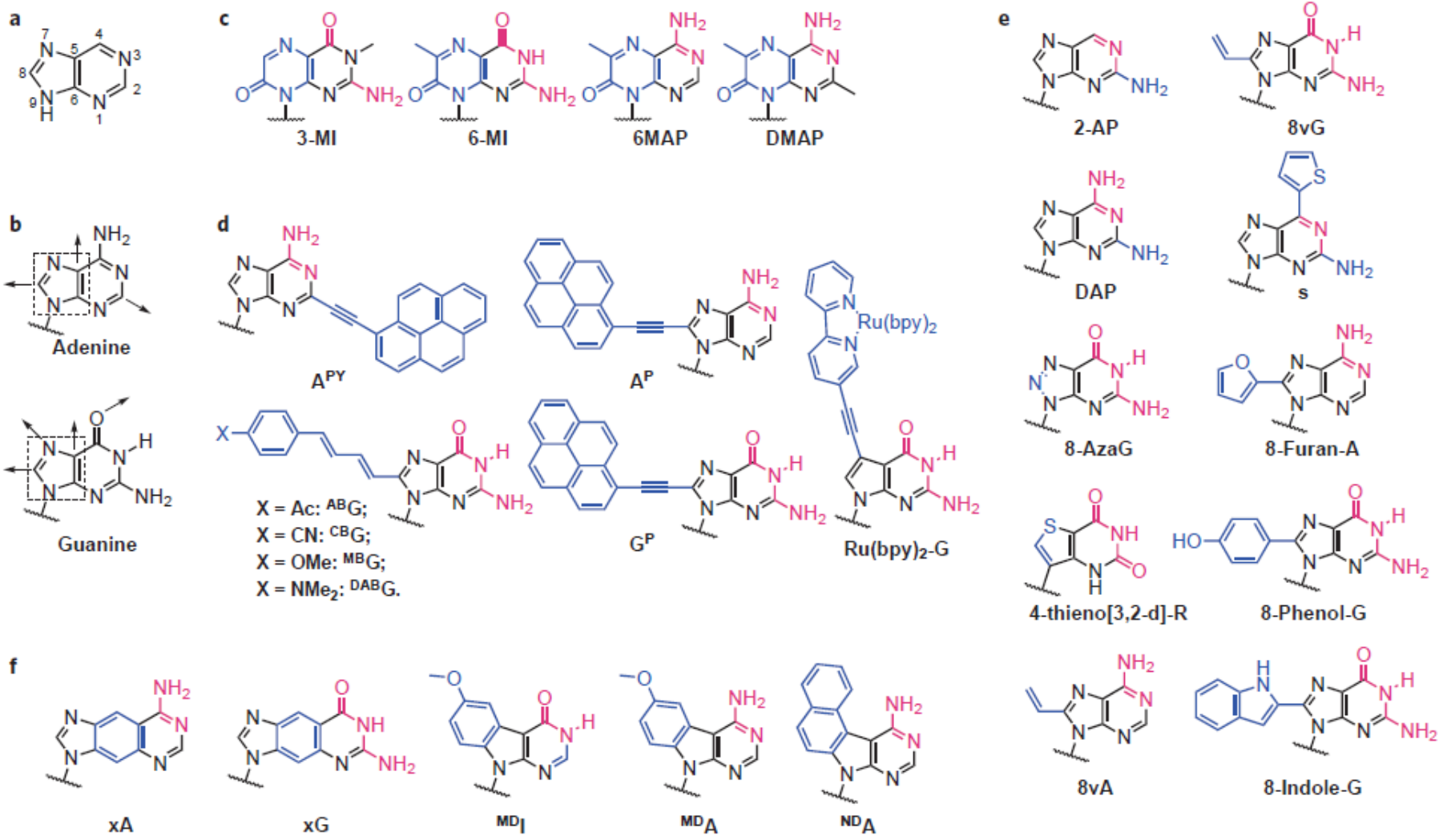
DNA	Base	Deoxyribo-nucleoside	Deoxyribo-nucleotide	Chain Form
Adenine				
Guanine				
Cytosine				
Thymine				

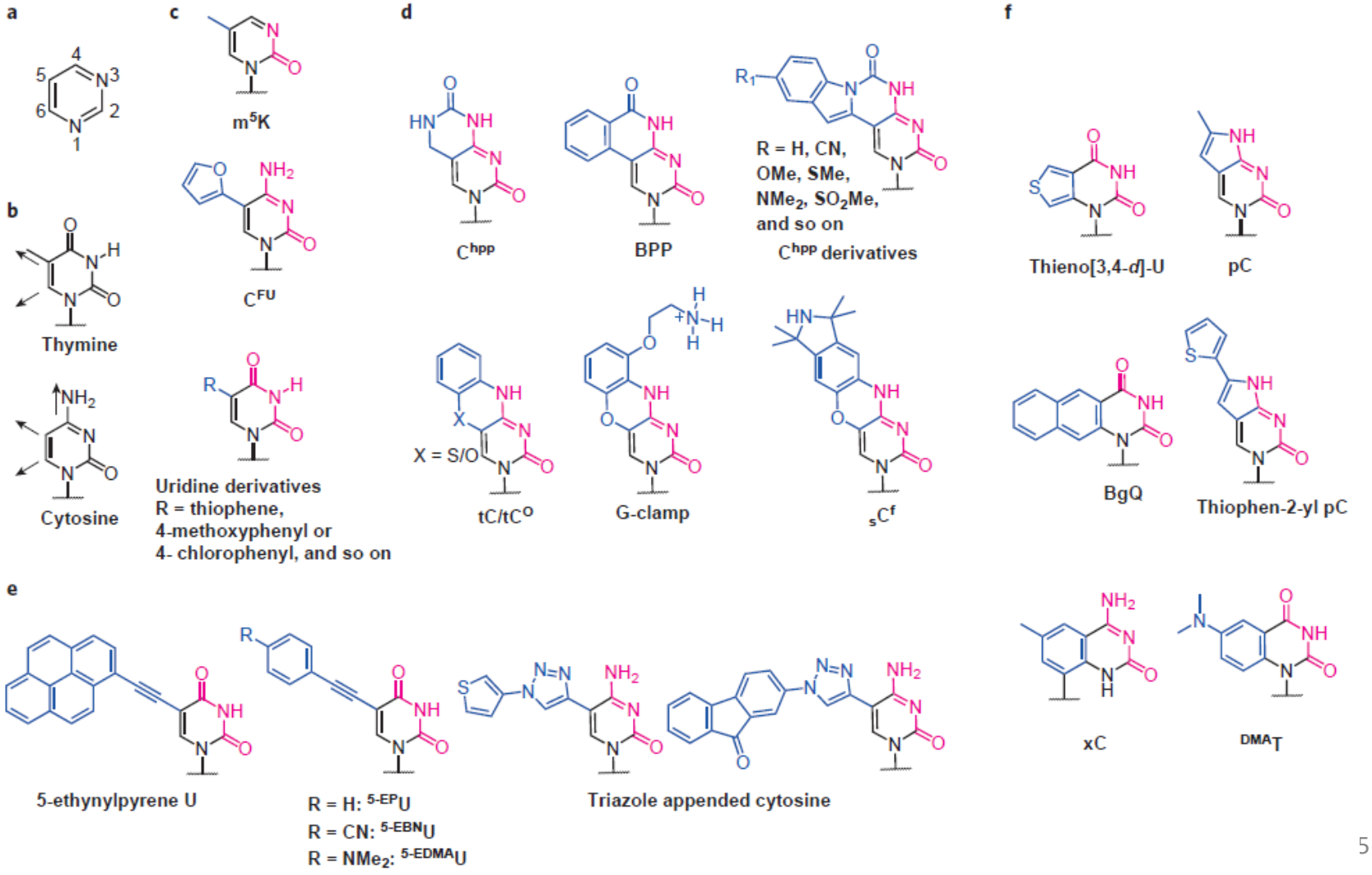
RNA	Base	Ribo-nucleoside	Ribo-nucleotide	Chain Form
Adenine				
Guanine				
Cytosine				
Uracil				

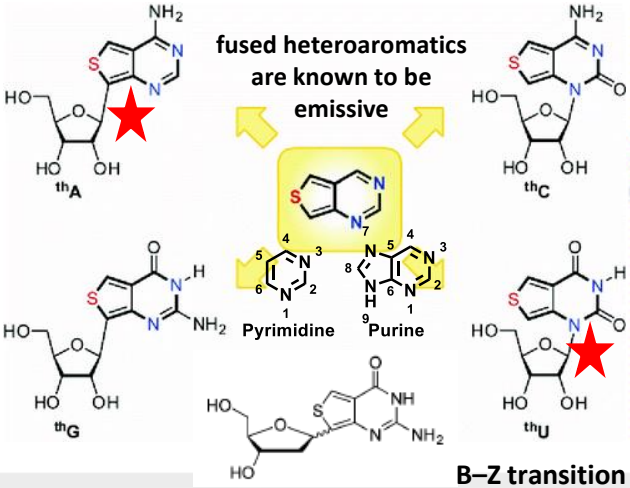
Fluorescent nucleobase development

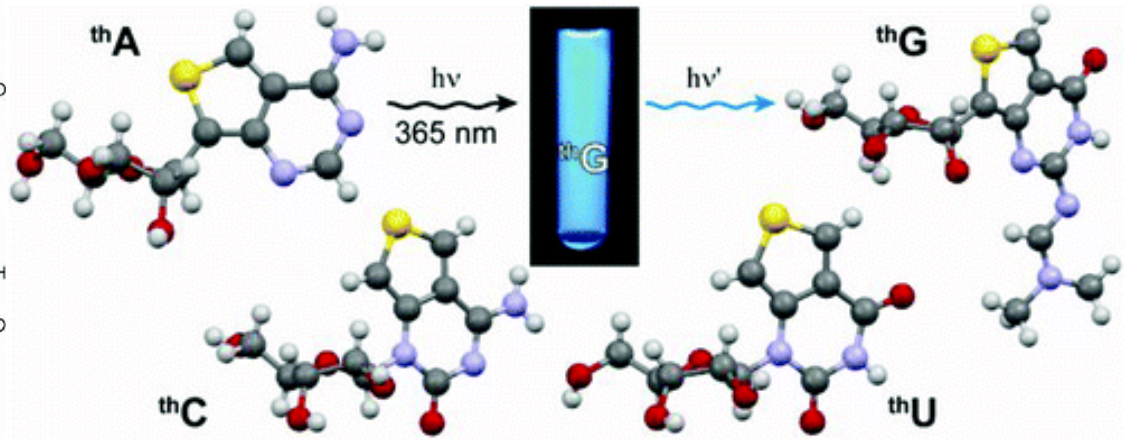


Nat. Chem., **2017**, 9, 1043;


a
b
Adenine
Guanine
c
3-MI
6-MI
6MAP
DMAP
d
A^{PY}
A^{P}
G^{P}
Ru(bpy)2-G
X = Ac: ABG;
X = CN: CBG;
X = OMe: MBG;
X = NMe2: DABG.
e
2-AP
8vG
DAP
s
8-AzaG
8-Furan-A
4-thieno[3,2-d]-R
8-Phenol-G
8vA
8-Indole-G
f
xA
xG
MDI
MDA
NDA


a
b
Thymine
Cytosine
c
m5K
CFU
Uridine derivatives
R = thiophene,
4-methoxyphenyl or
4- chlorophenyl, and so on
d
Chpp
BPP
R = H, CN,
OMe, SMe,
NMe2, SO2Me,
and so on
Chpp derivatives
X = S/O
tC/tCO
G-clamp
sCf
e
5-ethynylpyrene U
R = H: 5-EPU
R = CN: 5-EBNU
R = NMe2: 5-EDMAU
Triazole appended cytosine
f
Thieno[3,4-d]-U
pC
BgQ
Thiophen-2-yl pC
xC
DMAT





	sugar pucker	rmsd (Å)[a] ribose	rmsd (Å)[a] base	solvent	λ_{abs} (ε)	λ_{em} (Φ)	$\Phi\varepsilon$	τ	Stokes shift	polarity sensitivity[c]
thA	C3′-endo	0.0521	0.157	water	341 (7.44)	420 (0.21)	1562	3.9	5950	68.9
				dioxane	345 (7.83)	411 (0.14)	1096	3.2	5080	
thC	C2′-endo	0.294	0.045	water	320 (4.53)	429 (0.41)	1857	15.2	8300	27.3
				dioxane	326 (4.21)	422 (0.01)	42	5.0	7550	
thG	C2′-endo	0.0525	0.158	water	321 (4.15)	453 (0.46)	1909	14.8	9580	107.2
				dioxane	333 (4.53)	424 (0.50)	2265	13.0	6890	
thU	C1′-exo	0.240	0.047	water	304 (3.16)	409 (0.41)	1296	11.5	8860	80.8
				dioxane	304 (3.50)	378 (0.04)	140	1.0	6690	

J. Am. Chem. Soc. **2011**, 133, 14912; *Chem. Commun.*, **2014**, 50, 1573;

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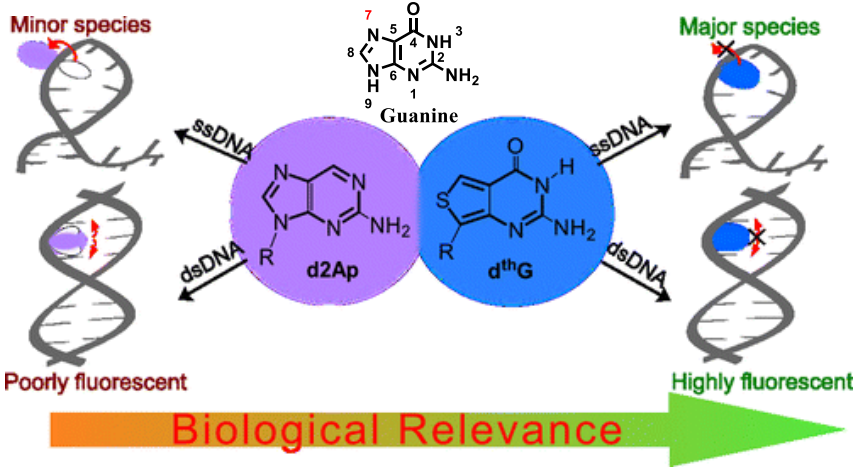
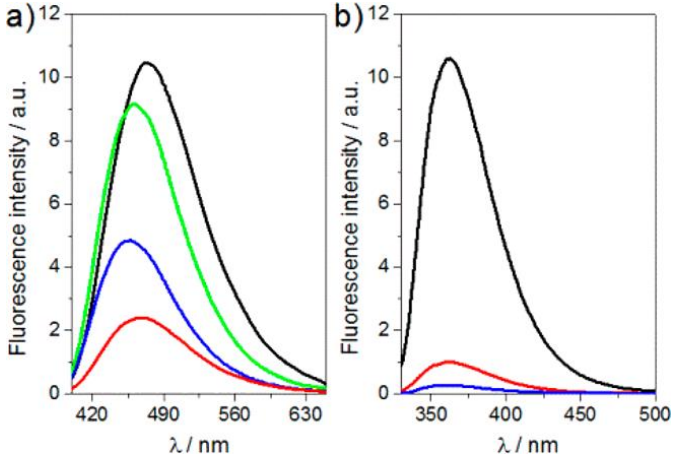
Conquering 2-Aminopurine's Deficiencies: Highly Emissive Isomorphic Guanosine Surrogate Faithfully Monitors Guanosine Conformation and Dynamics in DNA

Marianna Sholokh,[†,§] Rajhans Sharma,[†] Dongwon Shin,[‡] Ranjan Das,[∥] Olga A. Zaporozhets,[§] Yitzhak Tor,[*,‡] and Yves Mély[*,†]





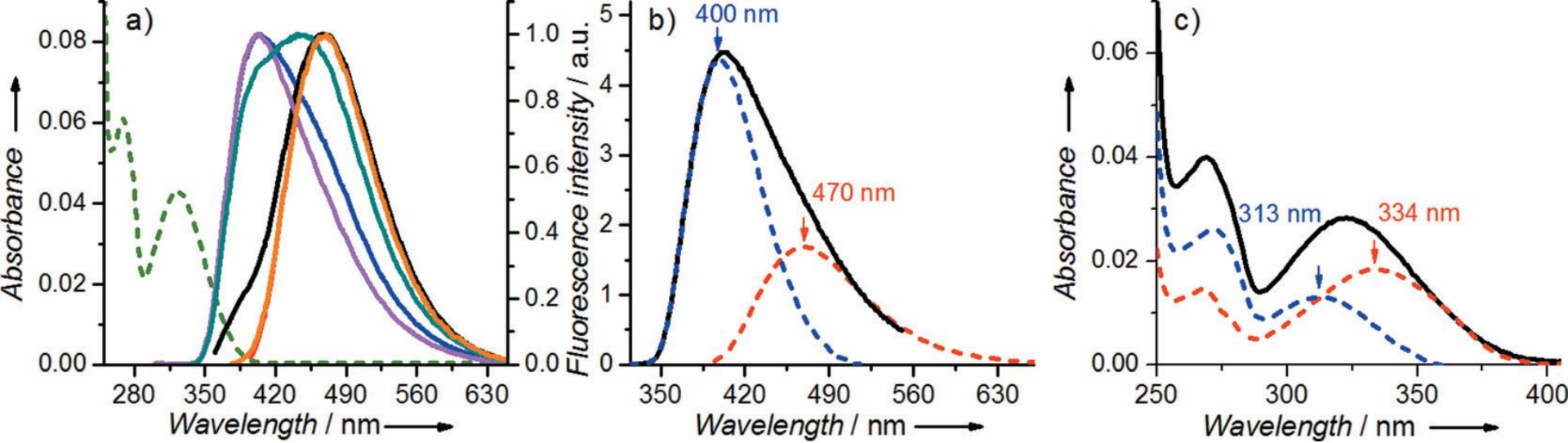
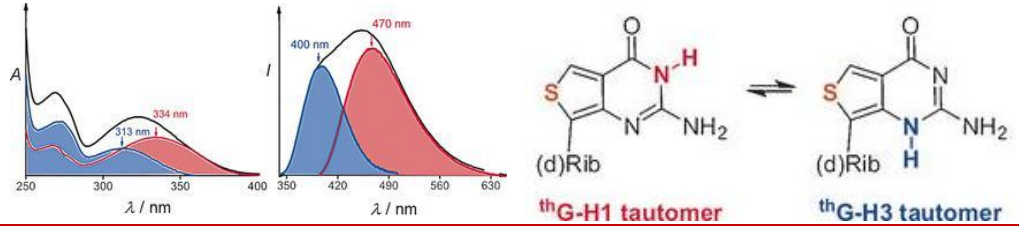


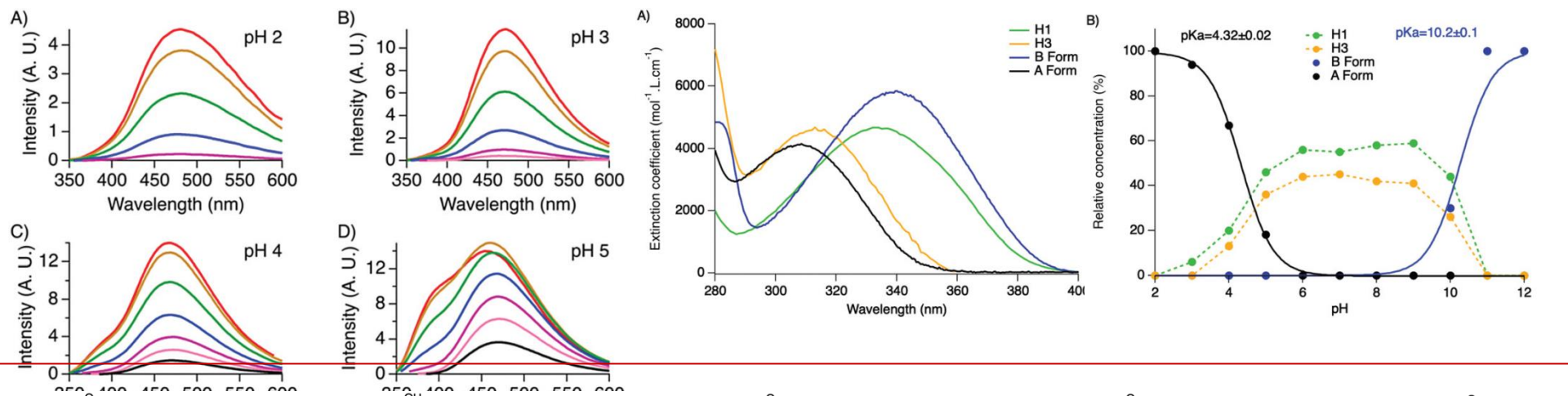
Figure. Absorption and emission spectra of thG in TRIS-HCl buffer 25 mm, pH 7.5, 30 mm NaCl, 0.2 mm $MgCl_2$.

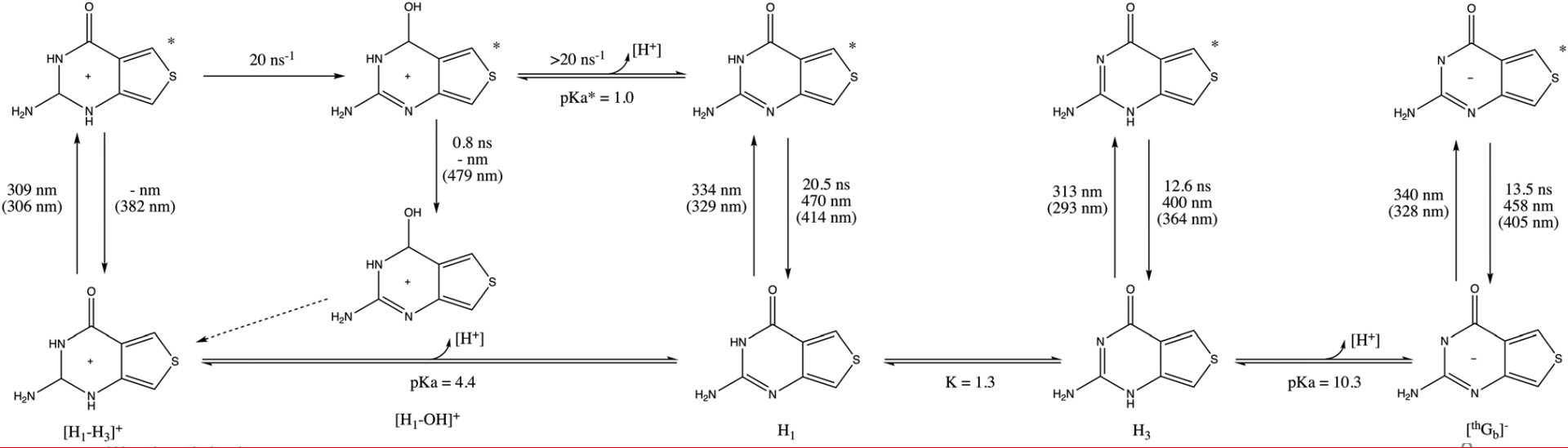
a) Absorption (green dashed line) and emission spectra of thG at different excitation wavelengths: λ=283 nm (magenta line); λ =298 nm (blue); λ =320 nm (green); λ =345 nm (black); and λ =360 nm (orange). The emission spectra were normalized at their maxima. The normalized emission spectrum at λ exc=380 nm fully overlaps that at λ exc=360 nm and is not shown.

b) Deconvoluted emission spectrum of thG, obtained at λ ex=283 nm.

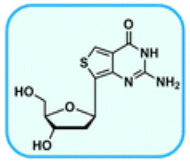
c) Deconvolution of the absorption spectrum of thG (black line) in its two ground-state forms (colors as in b).

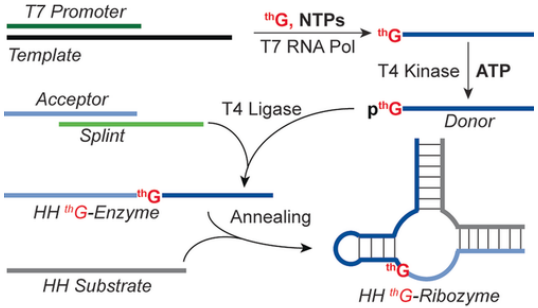




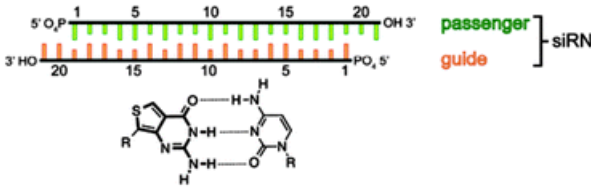


Phys. Chem. Chem. Phys., **2020**, 22, 7381;

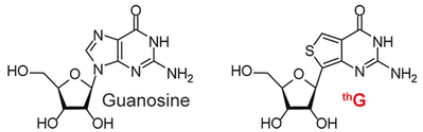




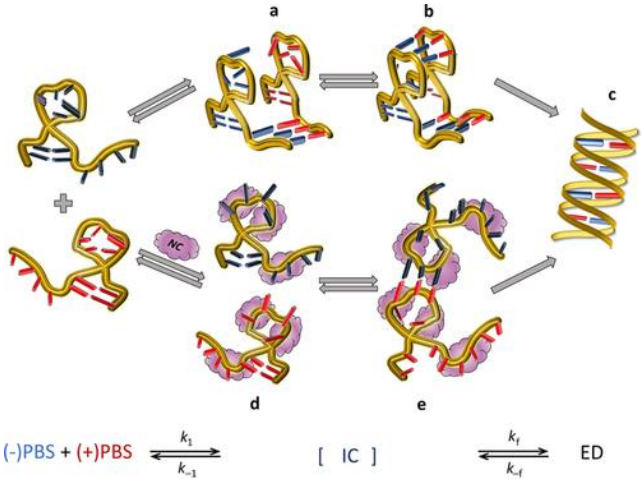
Highly Emissive Deoxyguanosine Analogue Capable of Direct Visualization of B–Z Transition



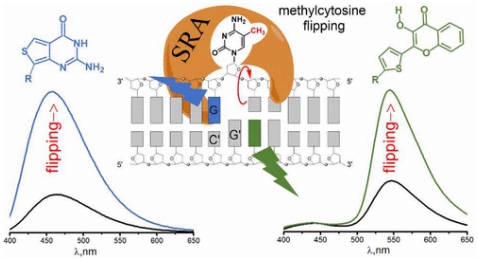
Cellular activity of siRNA oligonucleotides containing synthetic isomorphic nucleoside surrogates



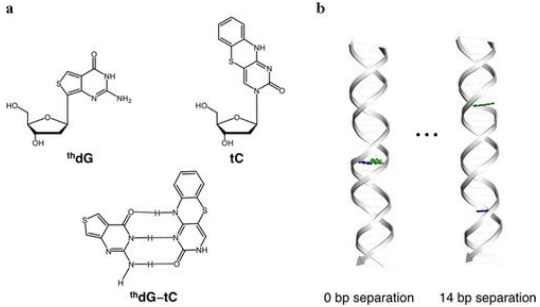
Polymerase-MediatedSite-Specific Incorporation of a Synthetic



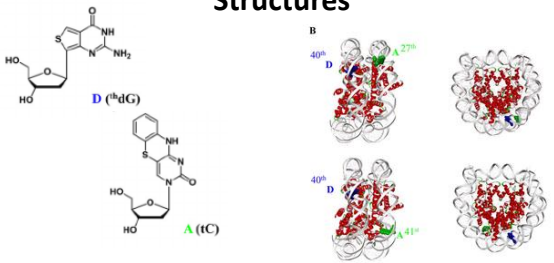
Environmentally Sensitive Fluorescent Nucleoside Analogues for Surveying Dynamic Interconversions of Nucleic Acid Structures



Dynamics of Methylated Cytosine Flipping by UHRF1

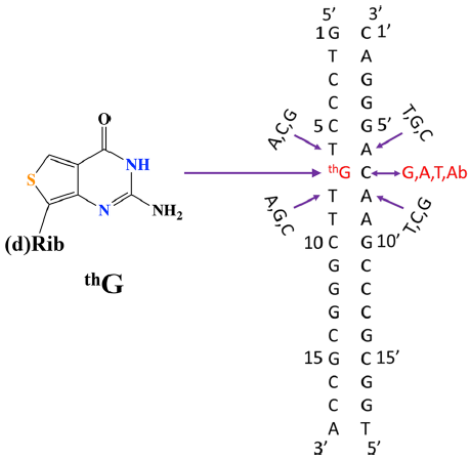


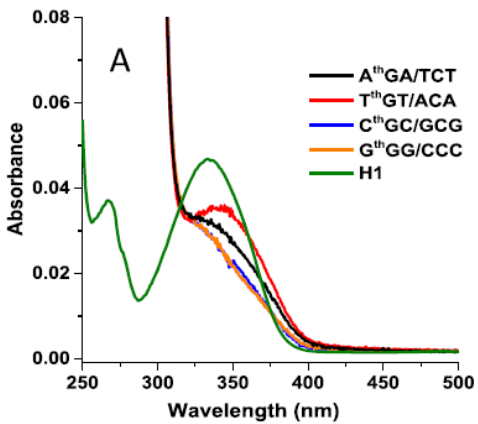
Development of a Vivid FRET System Based on a Highly Emissive dG–dC Analogue Pair



Approach to the Investigation of Nucleosome Structure by Using the Highly Emissive Nucleobase thdG–tC FRET Pair

Chem. Commun., **2014**,**50**, 1573; *Chem. Commun.*, **2015**,51, 1662; *J. Am. Chem. Soc.* **2017**, 139, 2520; *Angew. Chem. Int. Ed.* **2017**, 56,1303; *Chem.Eur.J.***2017**, 23,7607; *Chem. Eur.J.***2018**, 24,13850; *Chem. Eur.J.***2018**, 24,17091





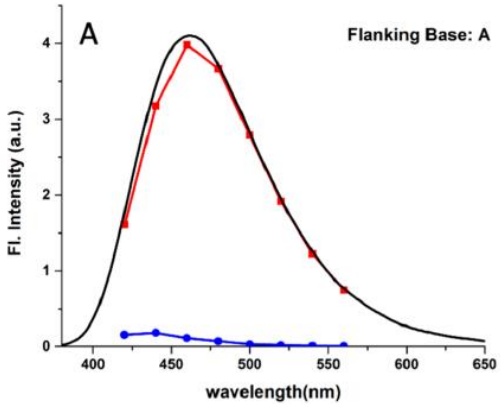


Table 1. Photophysical Data of thG-Labeled (−)/(+) PBS Matched Duplexes[a]

(−)PBS	(+)PBS	hypochromism (%)[b]	QY[c]	τ_1 (ns)[d]	α_1[e]	f_1[e]	τ_2 (ns)[d]	α_2[e]	f_2[e]	$\langle\tau\rangle$ (ns)	k_r ($10^7 \times S^{-1}$)	k_{nr} ($10^7 \times S^{-1}$)
AthGA	TCT	32	0.18	1.7	0.17	0.03	11.9	0.83	0.97	10.1	1.8	8.1
TthGT	ACA	29	0.15	2.4	0.14	0.04	11.1	0.86	0.96	9.9	1.5	8.6
CthGC	GCG	41	0.16	3.4	0.31	0.13	10.6	0.69	0.87	8.4	1.9	10.0
GthGG	CCC	41	0.15	4.4	0.39	0.19	12.3	0.61	0.81	9.2	1.6	9.2
thG H1 in water[f]			0.51				20.5				2.49	2.39
thG H1 in MeOH[f]			0.42				14.5				2.9	4.0

[a]Standard Deviation (SD) = [b]±2%; [c]±0.02. [d]±0.1−0.3 ns. [e]±0.01−0.05. [f]Data from Martinez-Fernandez et al, 2019.[5] Excitation wavelength was 360 nm. The amplitudes, α_i, are calculated from the integrated areas under the DAS of each lifetime component normalized with respect to the total emitted intensity. The fractional intensities were calculated by $f_i = \alpha_i\tau_i/\langle\tau\rangle$. The radiative and nonradiative rate constants were calculated by $k_r = QY/\langle\tau\rangle$ and $k_{nr} = 1/\langle\tau\rangle - k_r$, respectively.

Table 5. Photophysical Properties of thG-Labeled (−)/(+) PBS Mismatched Duplexes[a]

(−)PBS	(+)PBS	hypochromism (%)	QY	τ_1 (ns)	α_1	f_1	τ_2 (ns)	α_2	f_2	$\langle\tau\rangle$ (ns)	k_r ($10^7\times s^{-1}$)	k_{nr} ($10^7\times s^{-1}$)
GthGG	CTC	37	0.10	2.4	0.43	0.16	9.3	0.57	0.84	6.3	1.6	14.2
GthGG	CAC	13	0.17	4.4	0.39	0.18	12.9	0.61	0.82	9.6	1.8	8.7
GthGG	CGC	32	0.23	2.5	0.29	0.05	19.8	0.71	0.95	14.8	1.5	5.2
GthGG	CAbC	28	0.15	4.0	0.49	0.25	11.6	0.51	0.75	7.9	1.9	10.8
CthGC	GTG	24	0.15	2.1	0.42	0.10	13.5	0.58	0.90	8.7	1.7	9.8
CthGC	GAG	15	0.34	2.7	0.19	0.03	18.8	0.81	0.97	15.7	2.2	4.2
CthGC	GGG	30	0.21	3.5	0.26	0.08	14.8	0.74	0.92	11.8	1.8	6.7
CthGC	GAbG	26	0.12	4.7	0.68	0.42	14.5	0.32	0.58	7.8	1.5	11.2
AthGA	TTT	33	0.37	2.3	0.31	0.04	27.3	0.69	0.96	19.6	1.9	3.2
AthGA	TAT	12	0.48	2.8	0.22	0.03	28.6	0.78	0.97	22.9	2.1	2.3
AthGA	TGT	28	0.42	2.3	0.17	0.02	26.9	0.83	0.98	22.7	1.8	2.6
AthGA	TAbT	28	0.47	2.4	0.18	0.02	25.0	0.82	0.98	20.9	2.2	2.5
TthGT	ATA	25	0.35	3.0	0.27	0.04	26.8	0.73	0.96	20.4	1.7	3.1
TthGT	AAA	25	0.42	3.0	0.24	0.04	23.8	0.76	0.96	18.8	2.2	3.1
TthGT	AGA	31	0.33	5.5	0.25	0.09	19.4	0.75	0.91	15.9	2.1	4.2
TthGT	AAbA	23	0.25	3.4	0.28	0.07	16.9	0.72	0.93	13.1	1.9	5.7

[a]All reported values are the means for two to four experiments. The standard errors of the mean of the reported values are 8% for the QY, 10% for hypochromism, ±0.1−0.3 ns for τ_1, ±0.2−0.8 ns for τ_2, <0.05 for the amplitudes (α_i) and fractional intensities (f_i). The radiative and nonradiative rate constants were calculated as described in Table 1.

Thanks for your attention!