

Supporting Information

Hybridization-sensitive fluorescent DNA probe with self-avoidance ability

Shuji Ikeda, Takeshi Kubota, Mizue Yuki, Hiroyuki Yanagisawa, Shizuho Tsuruma and Akimitsu Okamoto*

Table S1. Photophysical Properties of Doubly Thiazole Orange-Labeled Probes Hybridized with the Complementary DNA Strands.^a

Probe sequences	Complementary	Absorption/nm (ϵ)		λ_{em}/nm (λ_{ex}/nm)	Quantum yields	$I_{hybrid}/I_{nonhybrid}$ (λ/nm)	T_m (°C) ^b
GAGTTCD ₅₁₄ CTACTA	No addition	509 (51,000)	481 (54,000)	531 (516)	0.076		
	TAGTAGAGAAGCTC	509 (76,000)		530 (515)	0.36	6.0 (530)	61
IAITTED ₅₁₄ ETAETA	No addition	508 (54,000)	479 (78,000)	535 (516)	0.020		
	TAGTAGAGAAGCTC	509 (77,000)	481 (67,000)	532 (514)	0.19	15 (532)	39
IAITTCDD ₅₁₄ CTAETA	No addition	508 (55,000)	479 (110,000)	535 (515)	0.023		
	TAGTAGAGAAGCTC	510 (110,000)		531 (514)	0.37	38 (531)	51
ATTATGD ₅₁₄ CAGACT	No addition	509 (57,000)	482 (46,000)	533 (515)	0.14		
	AGTCTGACATAAT	510 (78,000)		529 (515)	0.38	3.9 (529)	62
ATTATID ₅₁₄ EAI AET	No addition	508 (52,000)	480 (60,000)	536 (515)	0.030		
	AGTCTGACATAAT	510 (71,000)	482 (55,000)	529 (515)	0.19	11 (529)	41
ATTATID ₅₁₄ CAIAET	No addition	506 (74,000)	480 (95,000)	537 (516)	0.017		
	AGTCTGACATAAT	510 (110,000)		529 (514)	0.39	24 (529)	46
AGCTTCD ₅₁₄ CCTTAA	No addition	508 (70,000)	481 (75,000)	536 (515)	0.057		
	TTAAGGAGAAGCT	510 (110,000)		530 (515)	0.38	8.6 (530)	62
AIETTED ₅₁₄ EETTAA	No addition	509 (69,000)	479 (90,000)	534 (516)	0.033		
	TTAAGGAGAAGCT	509 (92,000)	482 (76,000)	532 (514)	0.22	7.3 (532)	41
AIETTCDD ₅₁₄ CETTAA	No addition	507 (63,000)	479 (99,000)	535 (517)	0.033		
	TTAAGGAGAAGCT	510 (110,000)		531 (514)	0.41	20 (531)	52

^a 0.4 μ M hybrid, 50 mM sodium phosphate buffer (pH = 7.0), 100 mM sodium chloride, except T_m measurements. ^b 2.0 μ M hybrid, 50 mM sodium phosphate buffer (pH = 7.0), 100 mM sodium chloride.

Table S2. Photophysical Properties of Doubly Thiazole Orange-Labeled Probes Hybridized with the Complementary RNA Strands.^a

Probe sequences	Complementary	Absorption/nm (ϵ)		$\lambda_{\text{em}}/\text{nm}$ ($\lambda_{\text{ex}}/\text{nm}$)	Quantum yields	$I_{\text{hybrid}}/I_{\text{nonhybrid}}$ (λ/nm)	T_m ($^{\circ}\text{C}$) ^b
AGATCCD ₅₁₄ GACAGA	UCUGUCAGGAUCU	511 (110,000)		530 (515)	0.48	1.7 (530)	62
AIATEED ₅₁₄ IAEAIA	UCUGUCAGGAUCU	509 (40,000)	480 (39,000)	531 (515)	0.12	3.5 (531)	35
AIATECD ₅₁₄ IAEAIA	UCUGUCAGGAUCU	509 (110,000)		531 (515)	0.39	18 (531)	44
TCTTGCD ₅₁₄ CGAAGT	ACUUCGAGCAAGA	512 (120,000)		529 (517)	0.49	3.8 (529)	63
TETTIED ₅₁₄ EIAAIT	ACUUCGAGCAAGA	509 (74,000)	479 (98,000)	531 (518)	0.11	8.2 (531)	37
TETTICD ₅₁₄ CIAAIT	ACUUCGAGCAAGA	511 (110,000)		530 (516)	0.40	35 (530)	46
GAGTTCD ₅₁₄ CTACTA	UAGUAGAGAACUC	511 (87,000)		531 (516)	0.39	7.1 (531)	54
IAITTED ₅₁₄ ETAETA	UAGUAGAGAACUC	510 (69,000)	481 (56,000)	532 (517)	0.26	15 (532)	36
IAITTC ₅₁₄ CTAETA	UAGUAGAGAACUC	510 (98,000)		531 (516)	0.42	38 (531)	47
ATTATGD ₅₁₄ CAGACT	AGUCUGACAUAAU	512 (82,000)		529 (516)	0.38	3.8 (529)	59
ATTATID ₅₁₄ EIAIET	AGUCUGACAUAAU	509 (69,000)	481 (61,000)	531 (516)	0.13	5.0 (531)	32
ATTATID ₅₁₄ CAIET	AGUCUGACAUAAU	511 (77,000)		529 (516)	0.25	10 (529)	36
AGCTTCD ₅₁₄ CCTTAA	UUAAGGAGAAGCU	510 (84,000)		532 (514)	0.39	6.5 (532)	61
AIETTED ₅₁₄ EETTAA	UUAAGGAGAAGCU	511 (79,000)		535 (517)	0.27	9.7 (535)	40
AIETTC ₅₁₄ CETTAA	UUAAGGAGAAGCU	509 (95,000)		535 (515)	0.41	22 (535)	51

^a 0.4 μM hybrid, 50 mM sodium phosphate buffer (pH = 7.0), 100 mM sodium chloride, except T_m measurements. ^b 2.0 μM hybrid, 50 mM sodium phosphate buffer (pH = 7.0), 100 mM sodium chloride.