Electronic Supplementary Material (ESI) for RSC Advances. This journal is © The Royal Society of Chemistry 2020

Supplementary information for

The linkers in fluorene-labeled 2'-deoxyuridines affect fluorescence discriminating phenomena upon duplex formation

So Young Lee,^a Seung Woo Hong,^a Hyeonuk Yeo^{*b} and Gil Tae Hwang^{*a}

^a Department of Chemistry and Green-Nano Materials Research Center, Kyungpook National University, Daegu 41566, Republic of Korea

^b Department of Chemistry Education, Kyungpook National University, Daegu 41566, Republic of Korea

Contents

Fig. S1. (a) Absorption and (b) emission spectra of U^F , U^{FL} and U^{DF} in MeOH at 25 °C	S2
Fig. S2. Ground-state optimized molecular structures of (a) U^F , (b) U^{FL} and (c) U^{DF}	S3
Fig. S3. Excited-state optimized molecular structures of (a) U^F , (b) U^{FL} and (c) U^{DF}	S3
Table S1. MALDI-TOF mass spectral data of ODNs containing U^F and U^{DF}	S4
Fig. S4. ¹ H NMR spectrum of U ^F in CD ₃ OD	S6
Fig. S5. ¹ H NMR spectrum of 5 in CDCl ₃	S 7
Fig. S6. ¹ H NMR spectrum of 6 in CDCl ₃	S 8
Fig. S7. ¹ H NMR spectrum of U^{DF} in DMSO- d_6	S9
Fig. S8. ¹ H NMR spectrum of 7 in CDCl ₃	S10
Fig. S9. ¹ H NMR spectrum of 8 in CDCl ₃	S11
Fig. S10. ¹ H NMR spectrum of 9 in CDCl ₃	S12
Fig. S11. ¹ H NMR spectrum of 10 in DMSO- d_6	S13



Fig. S1. (a) Absorption and (b) emission spectra of U^F , U^{FL} and U^{DF} in MeOH at 25 °C (each at a concentration of 3 μ M). Excitation wavelengths: 310 nm for U^F , 369 nm for U^{FL} and 363 nm for U^{DF} .



Fig. S2. Ground-state optimized geometries of (a) U^F , (b) U^{FL} and (c) U^{DF} , calculated using density functional theory (DFT) at the B3LYP/6-31 level, in vacuo.



Fig. S3. Excited-state optimized geometries of (a) U^F , (b) U^{FL} and (c) U^{DF} , calculated using density functional theory (DFT) at the B3LYP/6-31 level, in vacuo.

Table S1. MALDI-TOF mass spectral data of ODNs containing U^{F} and U^{DF}

ODN	Sequence	m/z found (calcd) for $[M + H]^+$
ODN1(U ^F)	5'-d(TGG ACT TUFT TCA ATG)-3'	4723.5 (4723)
ODN1(U ^{DF})	5'-d(TGG ACT TU ^{DF} T TCA ATG)-3'	4771.5 (4771)
ODN2(U ^F)	5'-d(TGG ACT CUFC TCA ATG)-3'	4693.3 (4693)
ODN2(U ^{DF})	5'-d(TGG ACT CU ^{DF} C TCA ATG)-3'	4740.3 (4741)

ODN1(U^F)



ODN1(U^{DF})







ODN2(U^{DF})





Fig. S4. ¹H NMR spectrum of U^F in CD₃OD.



Fig. S5. ¹H NMR spectrum of 5 in CDCl₃.



Fig. S6. ¹H NMR spectrum of 6 in CDCl₃.



Fig. S7. ¹H NMR spectrum of U^{DF} in DMSO-*d*₆.



Fig. S8. ¹H NMR spectrum of 7 in CDCl₃.



Fig. S9. ¹H NMR spectrum of 8 in CDCl₃.



Fig. S10. ¹H NMR spectrum of 9 in CDCl₃.



Fig. S11. ¹H NMR spectrum of 10 in DMSO- d_6 .