Supplementary information for

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

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Contents

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 μM). Excitation wavelengths: 310 nm for U^F, 369 nm for U^{FL} and 363 nm for U^{DF}.
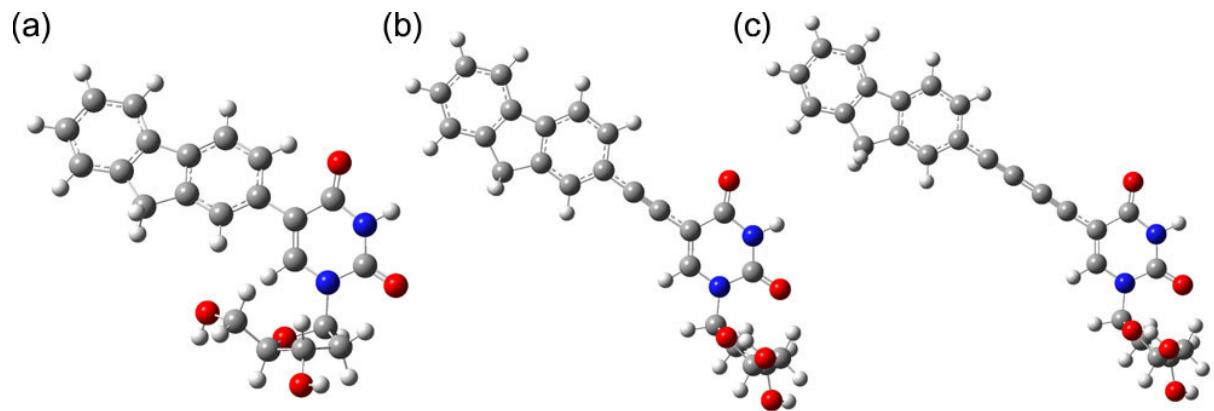
Fig. S2. Ground-state optimized geometries of (a) U^F, (b) U^{FL} and (c) U^{DF}, calculated using density functional theory (DFT) at the B3LYP/6-31 level, in vacuo.
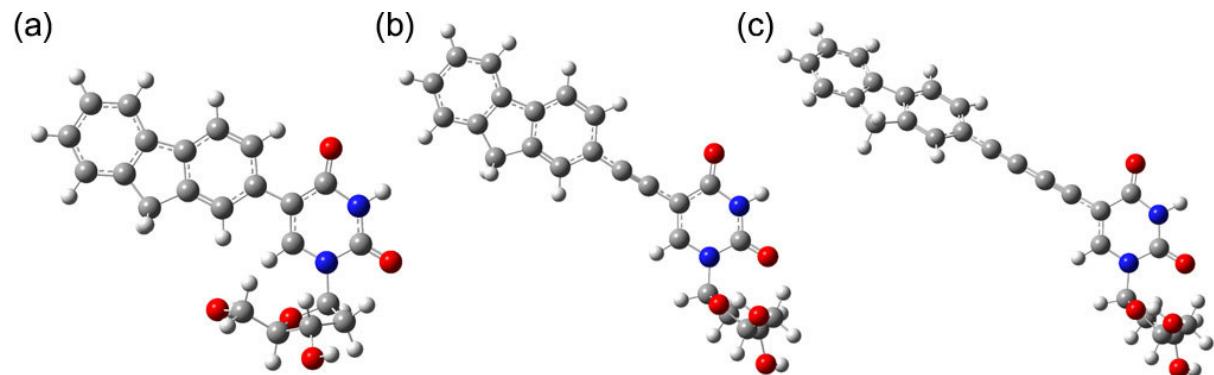

Fig. S3. Excited-state optimized geometries of (a) U^F, (b) U^{FL} and (c) U^{DF}, calculated using density functional theory (DFT) at the B3LYP/6-31 level, in vacuo.

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 TU^{F}T 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 CU^{F}C 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)
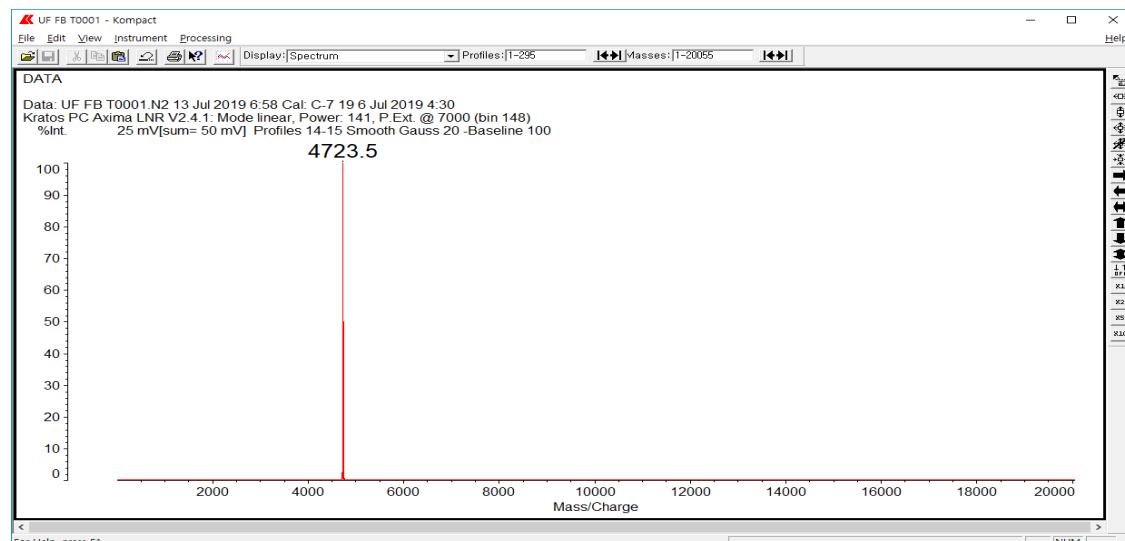
ODN1(U^{DF})
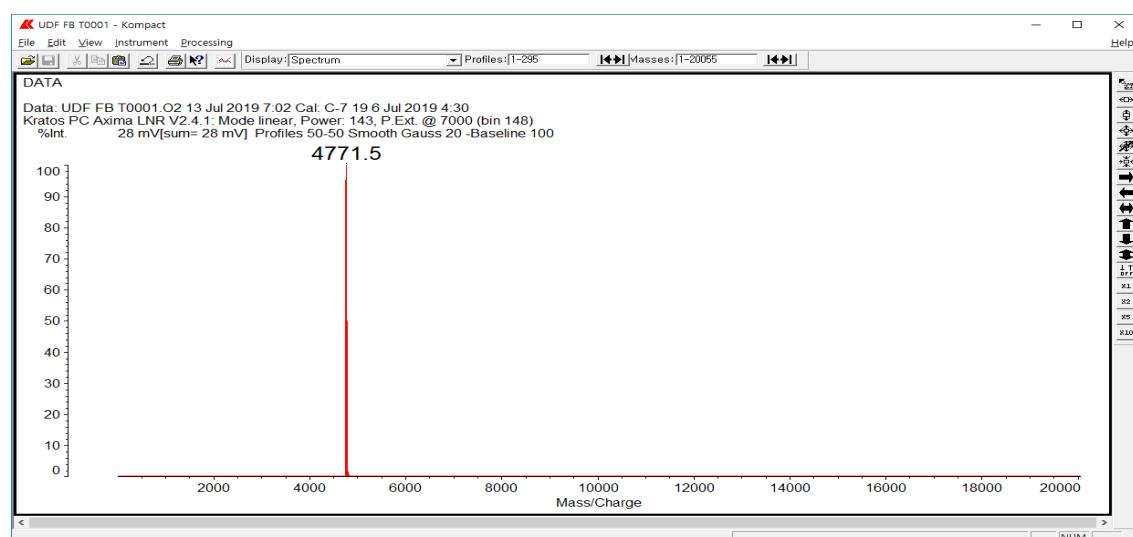
ODN2($\mathbf{U^F}$)
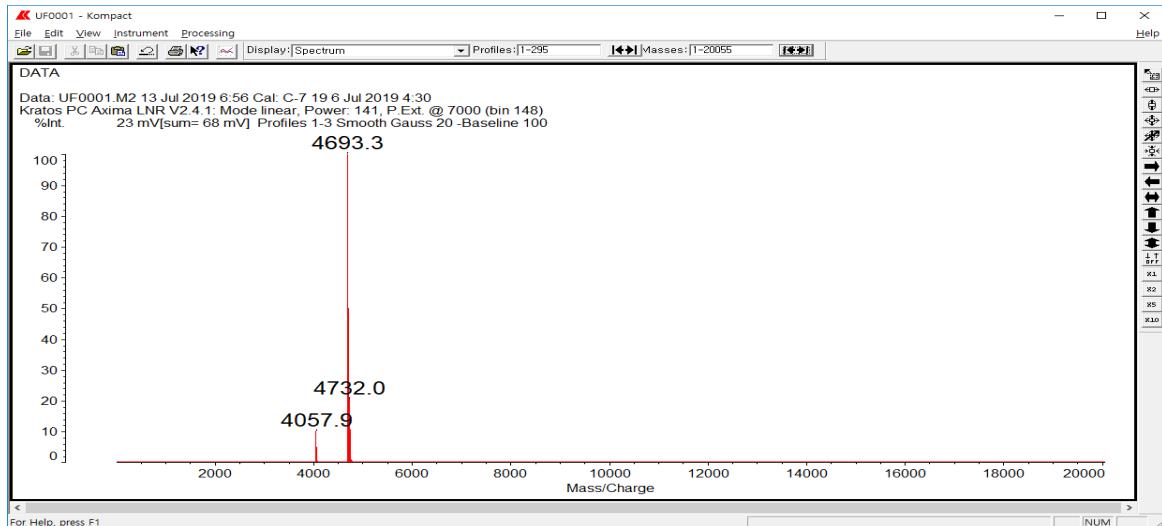
ODN2($\mathbf{U^{DF}}$)
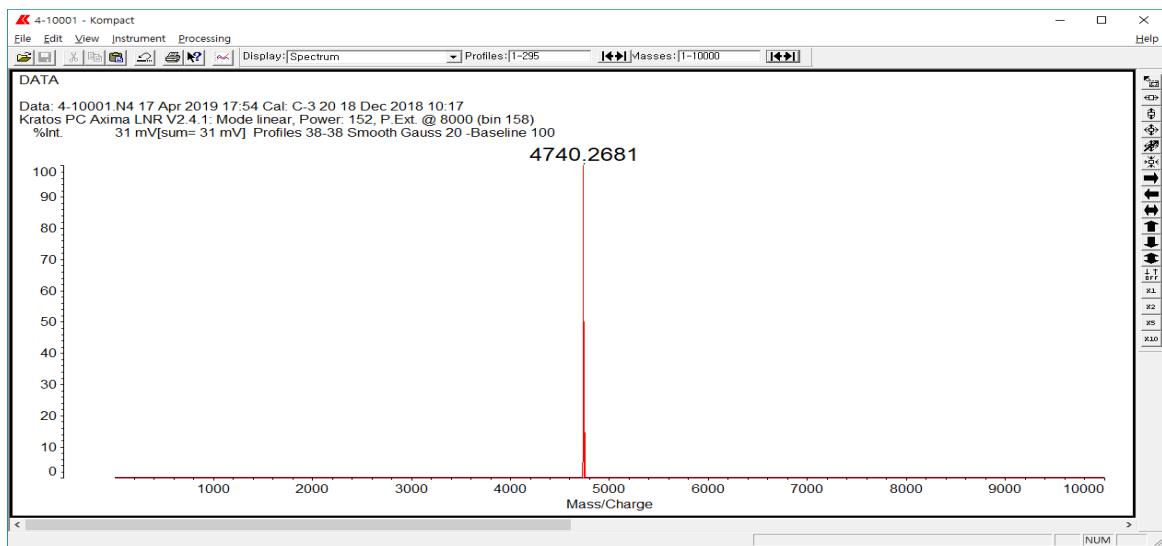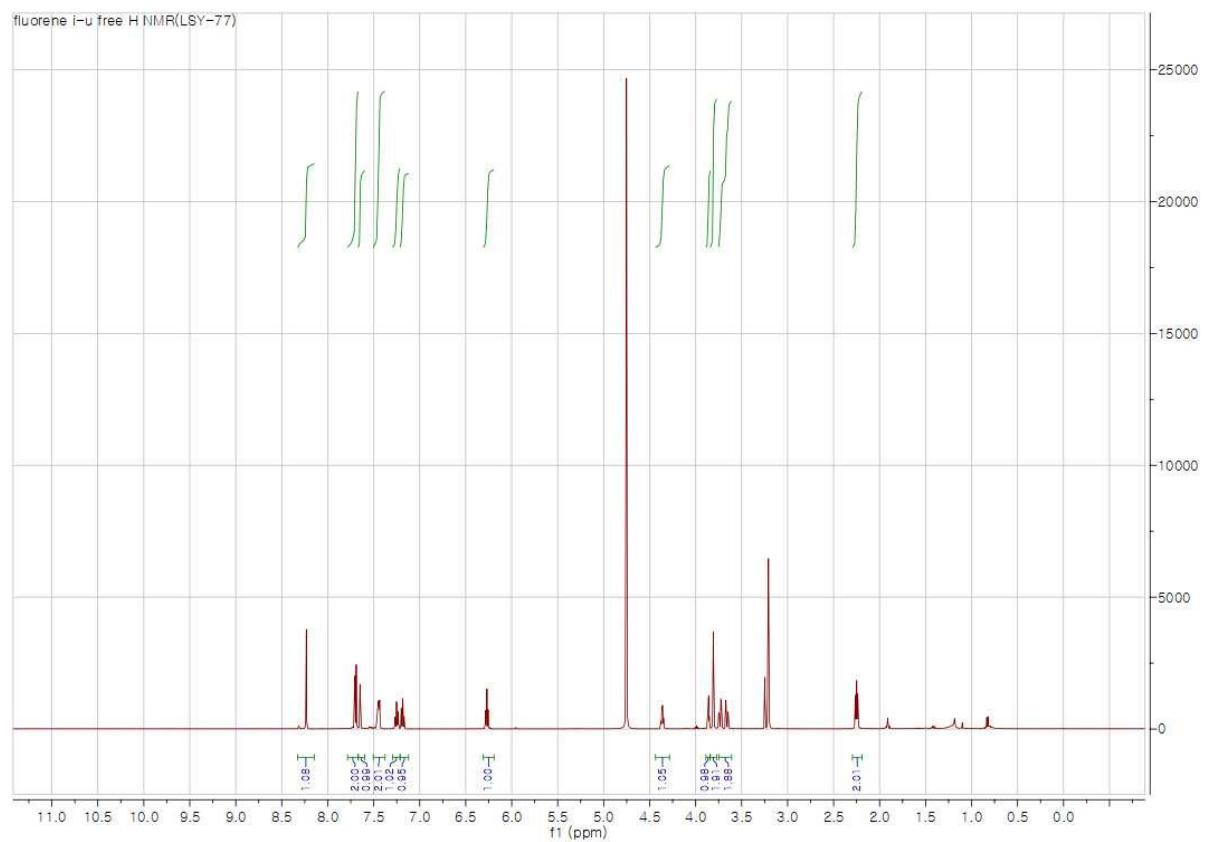
Fig. S4. [^1]H NMR spectrum of **U^F** in CD₃OD.
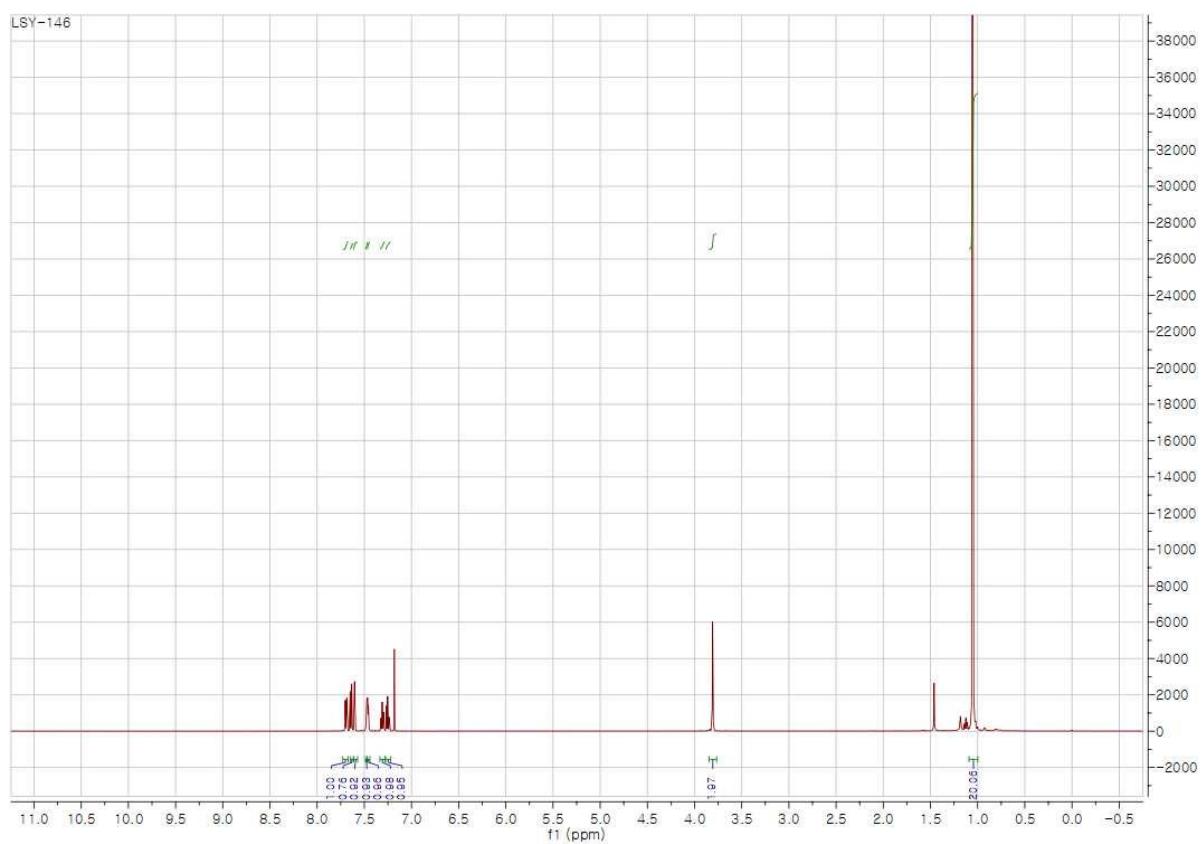
Fig. S5. ^{1}H NMR spectrum of **5** in CDCl$_3$.
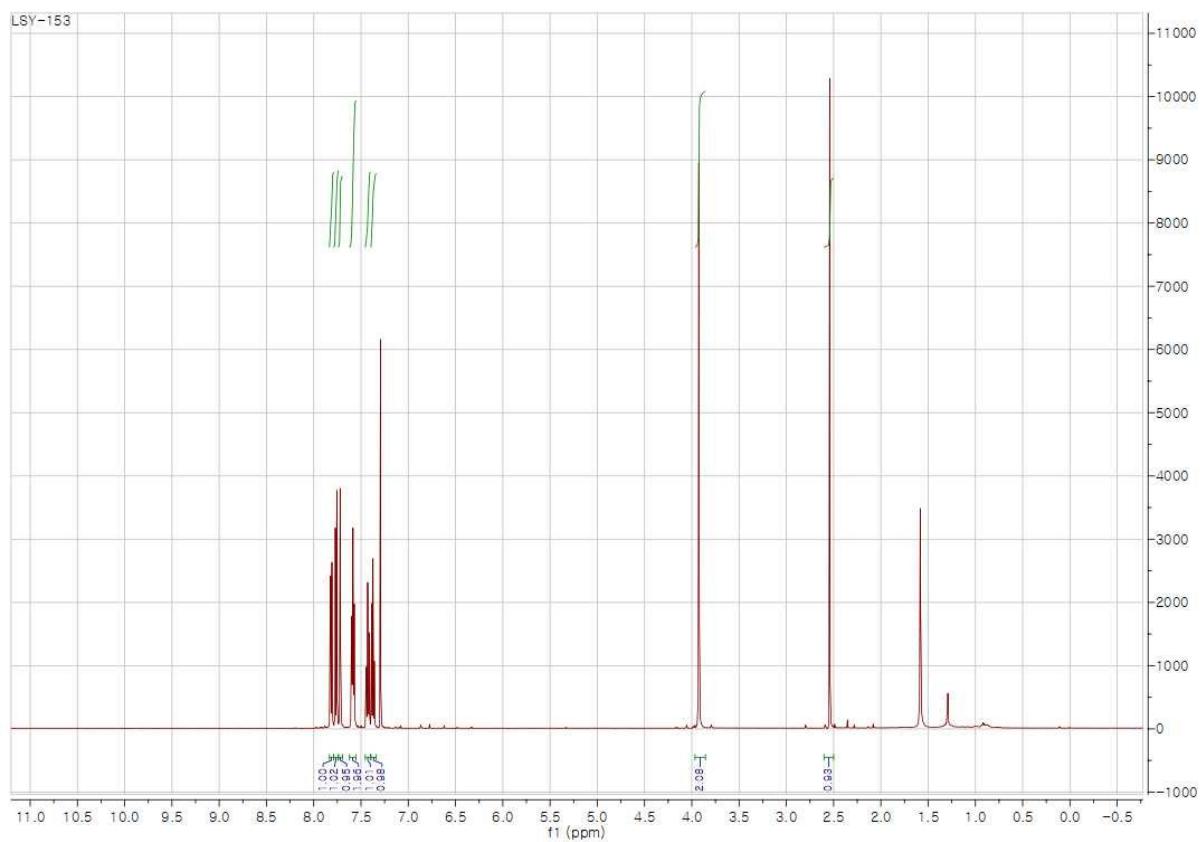
Fig. S6. ^{1}H NMR spectrum of **6** in CDCl$_3$.
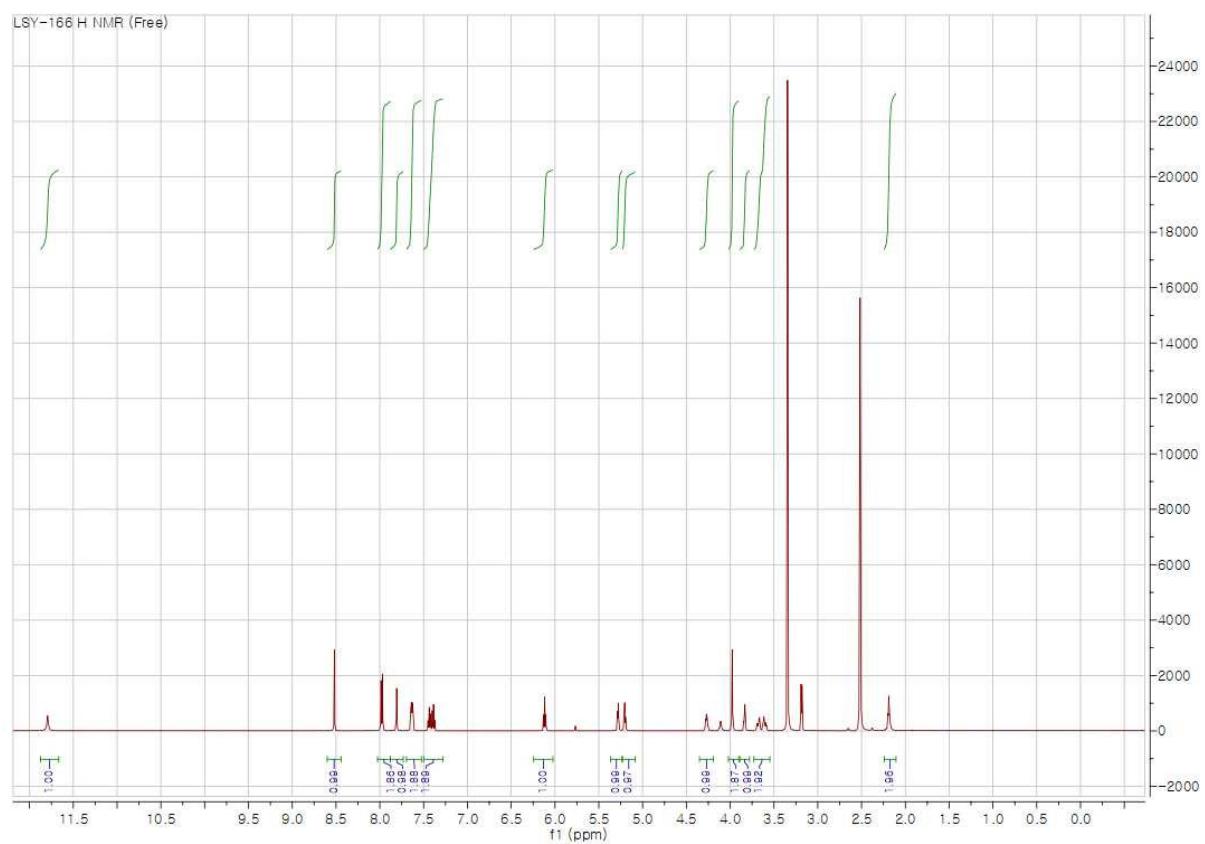
**Fig. S7.** ^{1}H NMR spectrum of $\mathbf{U^{DF}}$ in DMSO-d_6.
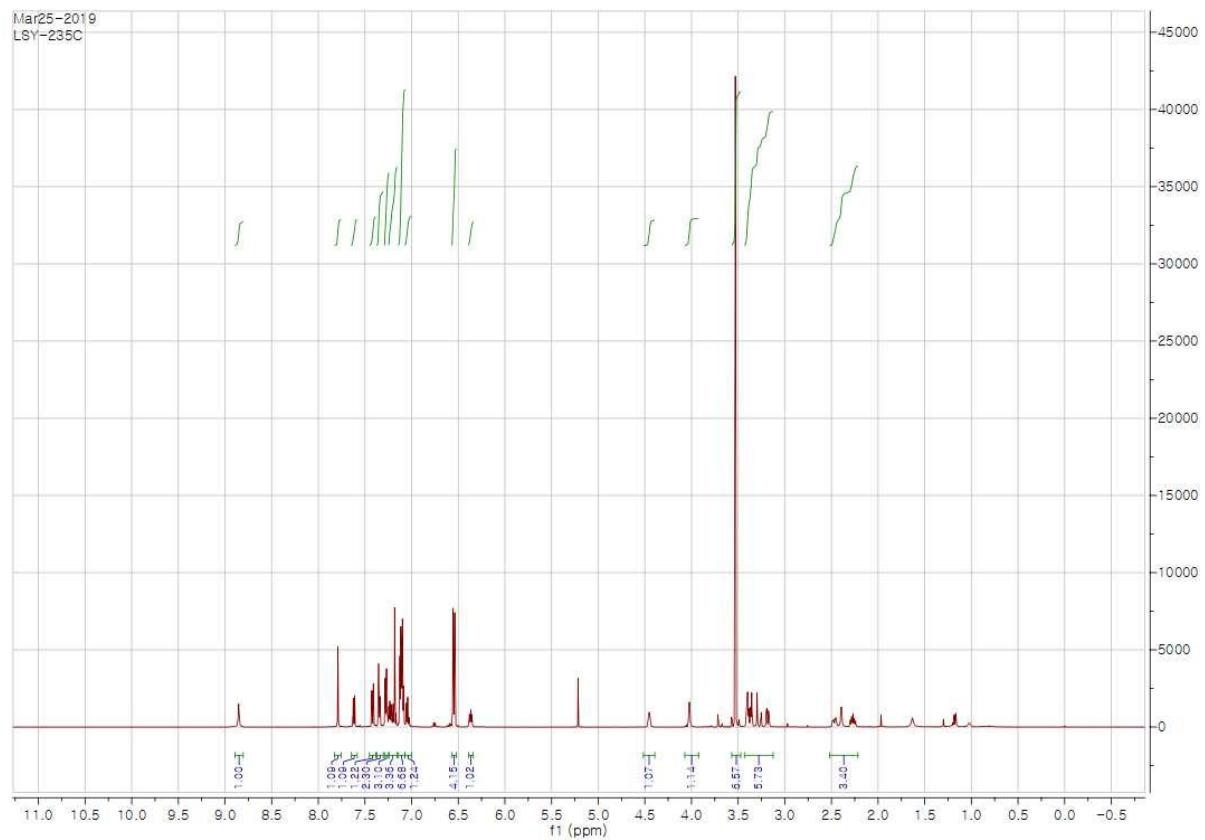
**Fig. S8.** ^{1}H NMR spectrum of **7** in CDCl₃.
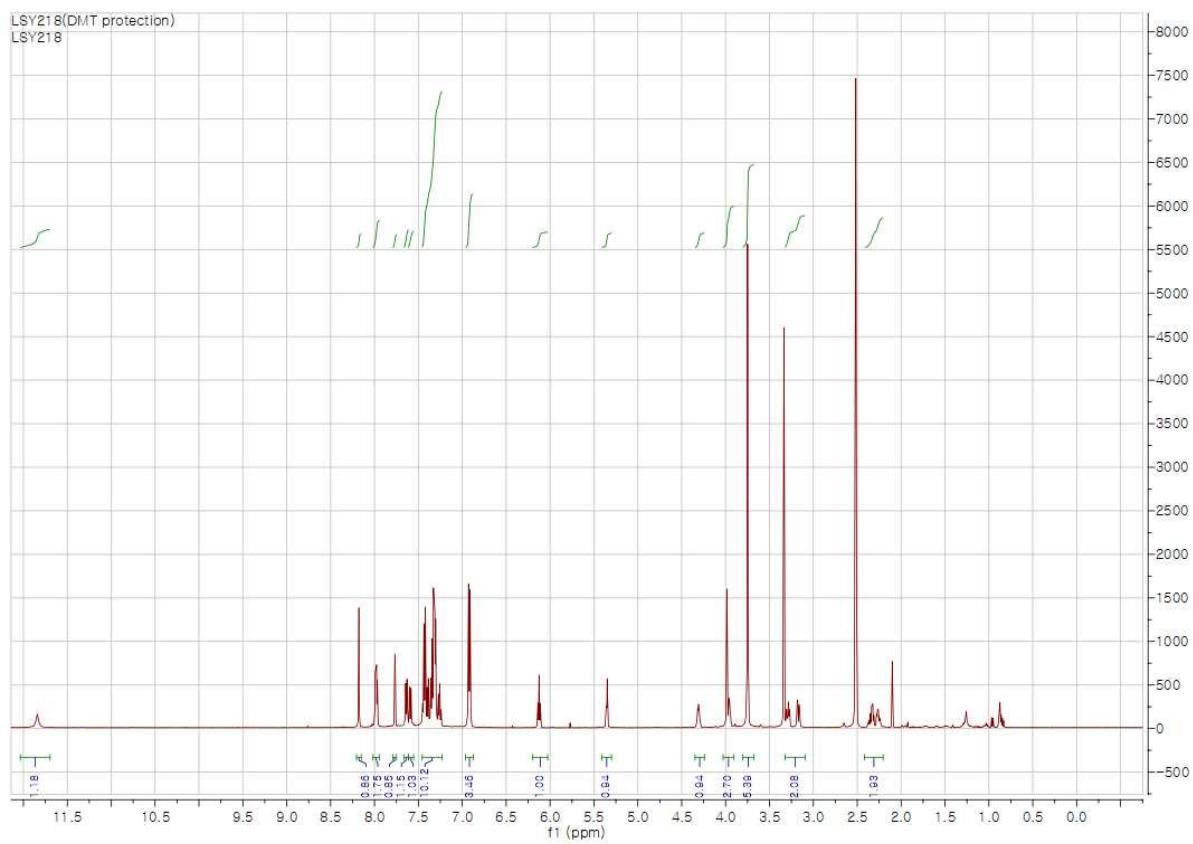
**Fig. S9.** ^{1}H NMR spectrum of **8** in CDCl$_3$.
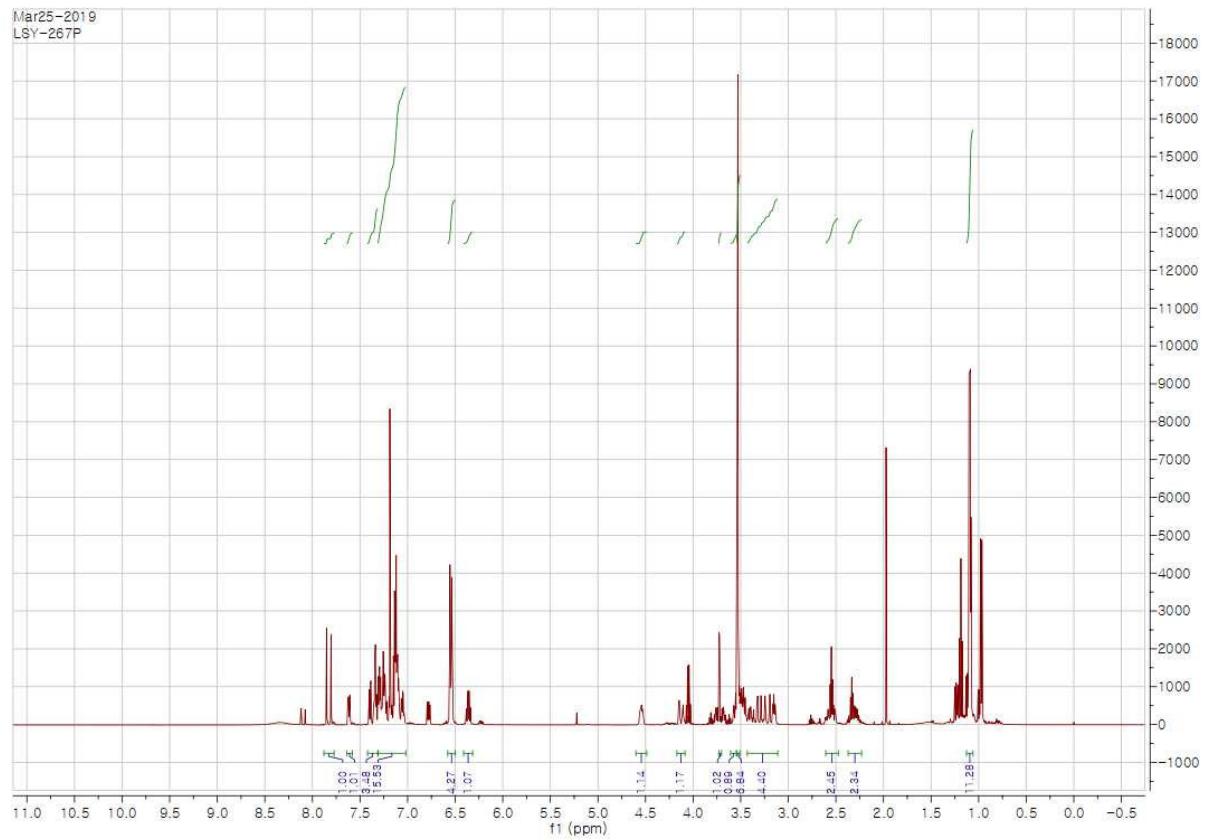
Fig. S10. ¹H NMR spectrum of **9** in CDCl₃.
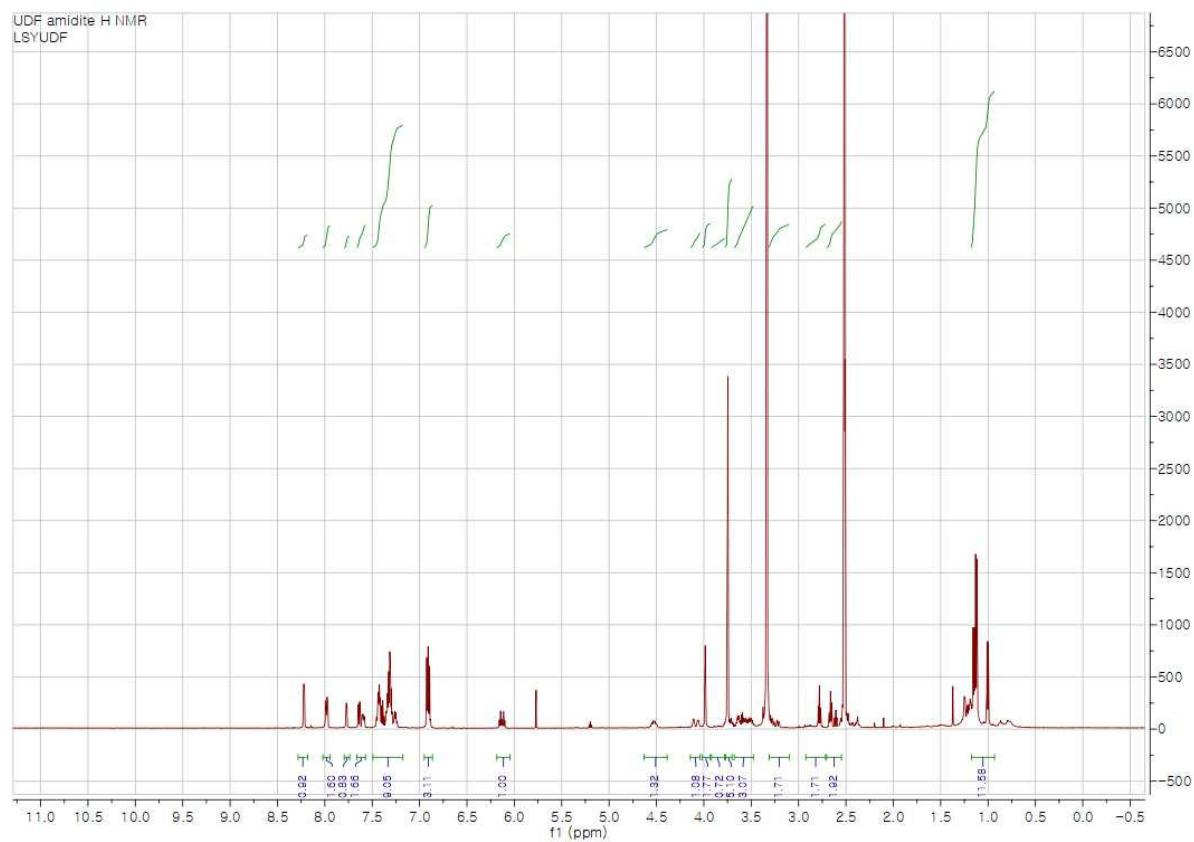
Fig. S11. ^{1}H NMR spectrum of **10** in DMSO-d_6.

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