(Z)-3-(dicyanomethylene)-4-((5-fluoro-3,3-dimethyl-1-(3-phenylpropyl)-3Hindol-1-ium-2-yl) methylene)-2-(((E)-5-fluoro-3,3-dimethyl-1-(3-phenylpropyl) indolin-2-ylidene) methyl) cyclobut-1-en-1-olate

Stefanie Casa¹, Guliz Ersoy Ozmen¹ and Maged Henary^{1,2} *

¹ Department of Chemistry, Petit Science Center, Georgia State University, 100 Piedmont Avenue SE, Atlanta, GA, 30303, USA

² Center for Diagnostics and Therapeutics, Petit Science Center, Georgia State University, 100 Piedmont Avenue SE, Atlanta, GA, 30303, USA

* Correspondence: mhenary1@gsu.edu

Table of Contents

Figure S1. ¹H NMR spectrum of Compound 5.

Figure S2. ¹⁹F NMR spectrum of Compound **5**.

Figure S3. ¹³C NMR spectrum of Compound **5**.

Figure S4. HRMS of Compound 5.

Figure S5. Structure of SQ

Figure S6. Absorbance of dye 5 in ethanol with increasing concentration (left) and molar

extinction coefficient of dye 5 in ethanol (right).

Figure S7. Absorbance of dye **5** in acetonitrile with increasing concentration (left) and molar extinction coefficient of dye **5** in acetonitrile (right).

Figure S8. Absorbance of dye **5** in dimethyl sulfoxide with increasing concentration (left) and molar extinction coefficient of dye **5** in dimethyl sulfoxide (right).

Figure S9. Absorbance of dye **5** in toluene with increasing concentration (left) and molar

extinction coefficient of dye 5 in toluene (right).



Figure S1. ¹H NMR spectrum of Compound **5**



Figure S2. ¹⁹F NMR spectrum of Compound **5**



Figure S3. ¹³C NMR spectrum of Compound **5**



Figure S4. HRMS of Compound 5



SQ

Figure S5. Structure of SQ



Figure S6. Absorbance of dye **5** in ethanol with increasing concentration (left) and molar extinction coefficient of dye **5** in ethanol (right).



Figure S7. Absorbance of dye **5** in acetonitrile with increasing concentration (left) and molar extinction coefficient of dye **5** in acetonitrile (right).



Figure S8. Absorbance of dye **5** in dimethyl sulfoxide with increasing concentration (left) and molar extinction coefficient of dye **5** in dimethyl sulfoxide (right).



Figure S9. Absorbance of dye **5** in toluene with increasing concentration (left) and molar extinction coefficient of dye **5** in toluene (right).

Quantum Yield Calculations

The fluorescence quantum yield of the dye was calculated using Equation 1. R is the reference, which is Rhodamine 800, S refers to the sample. Φ shows the quantum yield, A is the absorbance at the excitation wavelength, F is the area under the fluorescence intensity curve and n shows the refractive index of the solvent. The area of fluorescence intensity curve was calculated using Origin Lab Pro 8.5. The 1 mM dye and reference stock solutions were prepared in DMSO.

$$\Phi_{\rm S} = \Phi_{\rm R} * \frac{A_R}{A_S} * \frac{F_S}{F_R} * \left(\frac{n_S^2}{n_R^2}\right) \tag{1}$$