**Supplementary Material**

**Synthesis, Optical Properties, Anticancer Evaluation and DNA−Binding Spectroscopic Insights of New Bay-Substituted Perylene Derivatives**

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**List of captions:**

**Figure S1.** Mass-spectrum of **4** in DMF.

**Figure S2.** 1H NMR Spectrum of **6** in the solvent mixture CDCl3:CF3COOD (3:1) at room temperature (the impurity peaks shown in the aliphatic range belonged to CF3COOD as shown in Figure S3).

**Figure S3.** 1H NMR Spectrum of Trifluoroacetic Acid−d (the impurity peaks shown in the aliphatic range belonged to CF3COOD).

**Figure S4.** Absorbance and emission spectra (λexc = 485 nm) of **4** and **6** with c-kit with a 2:1 concentration ratio. Intensity, in arbitrary units, a.u., as a function of wavelength, λ, in nm.

**Figure S5.** Absorbance and emission spectra of the electron-donating bay substituents **3** (λexc = 310 nm) and **5** (λexc = 310 nm) in various solvents to check the fluorescence properties. Intensity, in arbitrary units, a.u., as a function of wavelength, λ, in nm.

**Scheme S1.** H-bondinginteraction possibilities of **4**.

**Scheme S2.** H-bondinginteraction possibilities of **6**.

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**Fig. S1.** Mass-spectrum of **4** in DMF.

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**Fig. S2.** 1H NMR Spectrum of **6** in the solvent mixture CDCl3:CF3COOD (3:1) at room temperature (the impurity peaks shown in the aliphatic range belonged to CF3COOD as shown in Figure S2).

**Chart

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**Fig. S3.** 1H NMR Spectrum of Trifluoroacetic Acid−d (the impurity peaks shown in the aliphatic range belonged to CF3COOD).

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**Fig. S4.** Absorbance and emission spectra (λexc = 485 nm) of **4** and **6** with c-kit with a 2:1 concentration ratio. Intensity, in arbitrary units, a.u., as a function of wavelength, λ, in nm.

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**Fig. S5.** Absorbance and emission spectra of the electron-donating bay substituents **3** (λexc = 310 nm) and **5** (λexc = 310 nm) in various solvents to check the fluorescence properties. Intensity, in arbitrary units, a.u., as a function of wavelength, λ, in nm.

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