Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

A Bimodal Fluorescent and Photocytotoxic Naphthalene Diimide for Theranostic Applications

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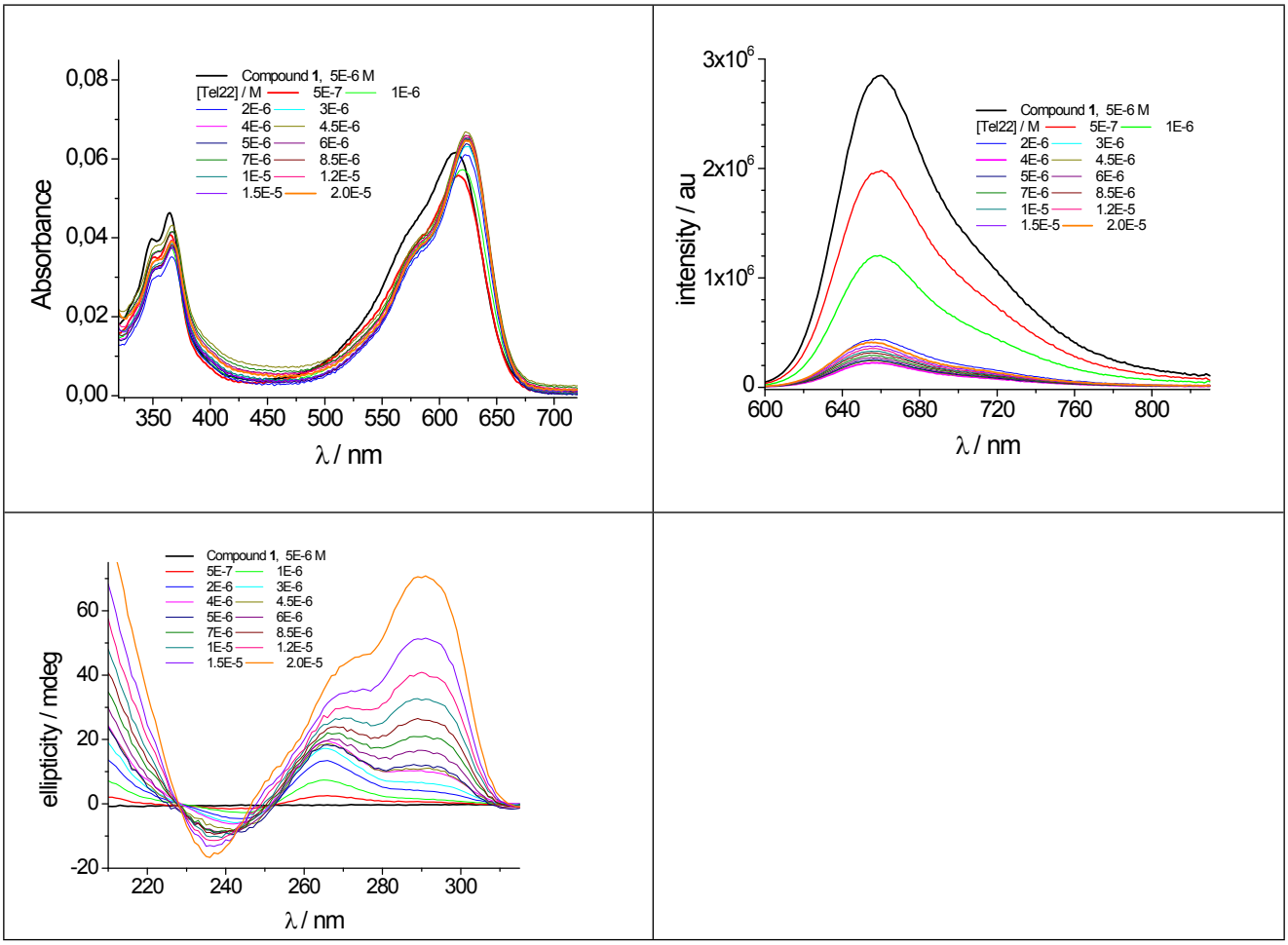
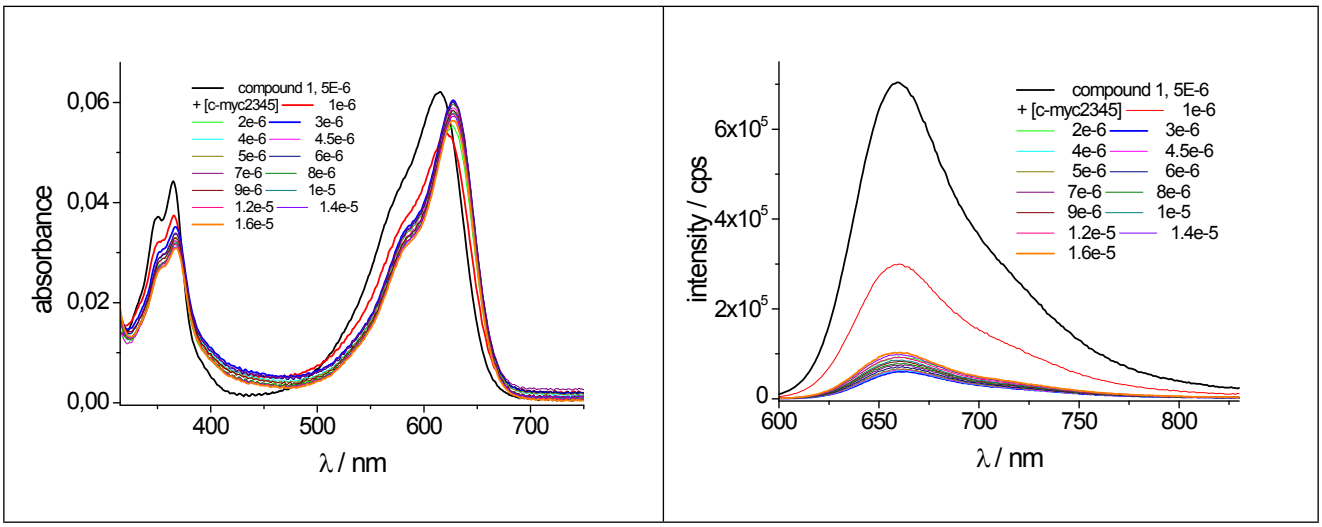
Supplementary Information

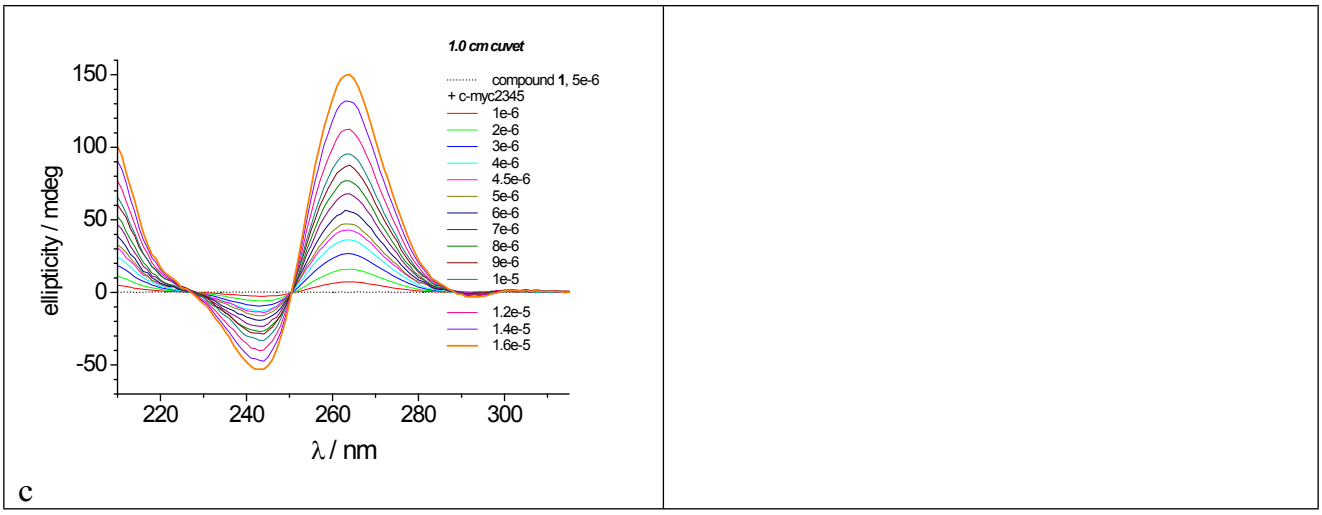
Content

SI Figure 1: Titration of compound 1 with Tel22: absorption, fluorescence and circular dichroism spectra of 1 with increasing amounts of Tel22. Mixtures have been heated for 20 minutes at 50°C.

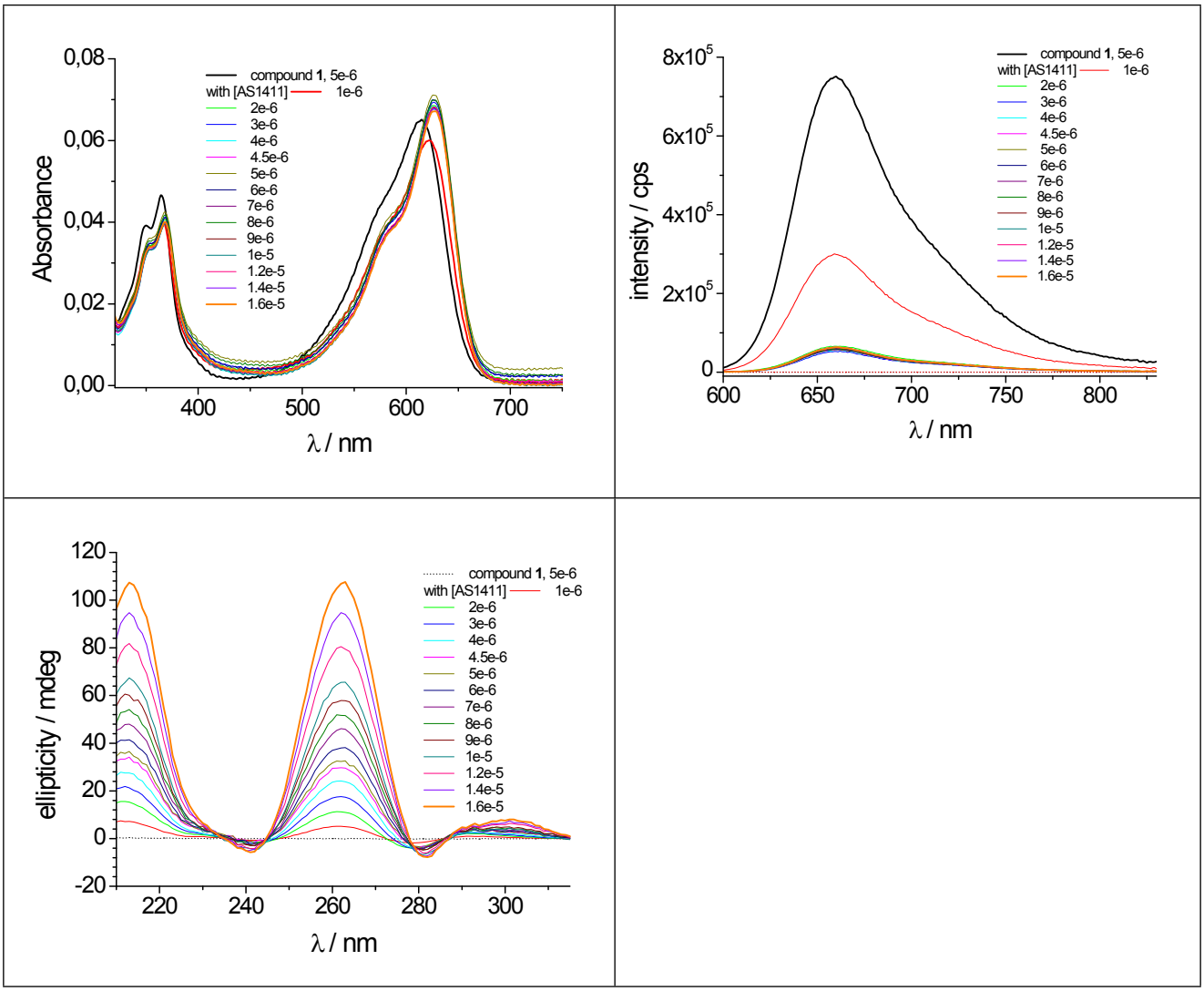


SI Figure 2: Titration of compound 1 with *c-myc*2345: absorption, fluorescence and circular dichroism spectra of 1 with increasing amounts of *c-myc*2345.

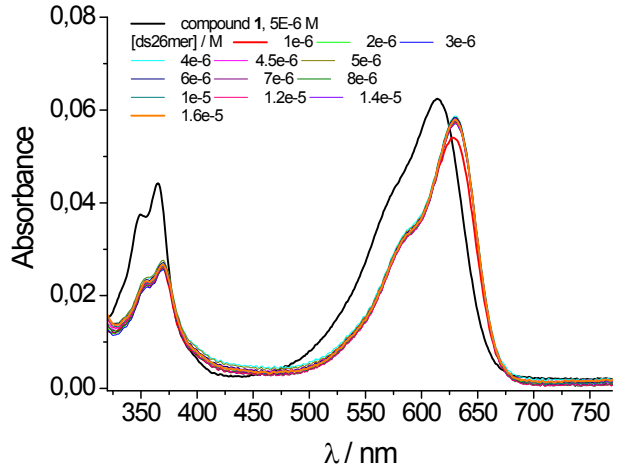


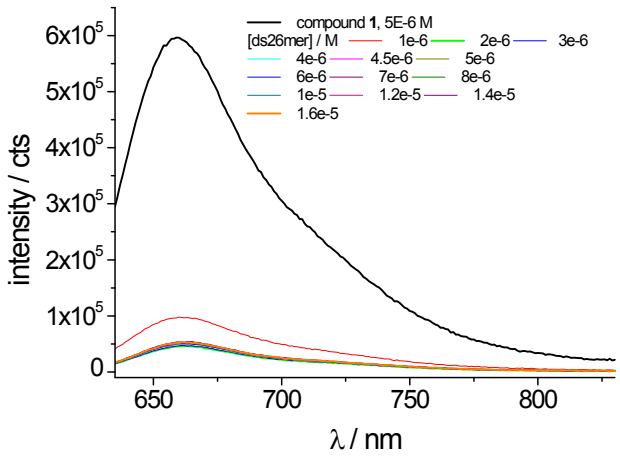


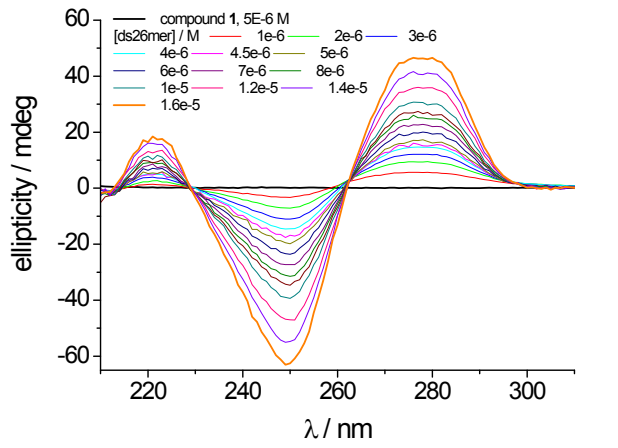
SI Figure 3: Titration of compound 1 with AS1411: absorption, fluorescence and circular dichroism spectra of 1 with increasing amounts of AS1411.

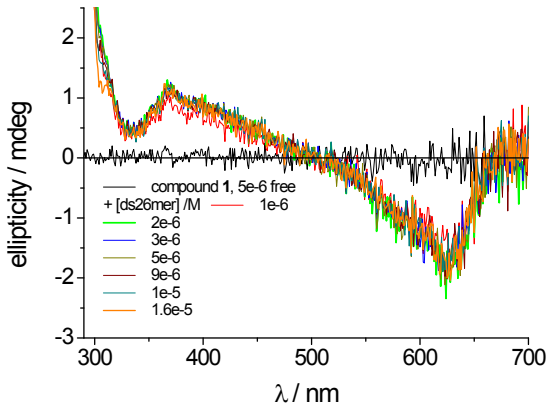


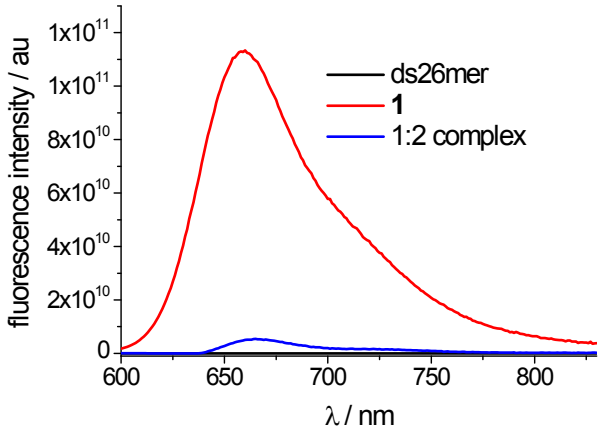
SI Figure 4: Titration of compound 1 with ds26mer: absorption, fluorescence and circular dichroism spectra in the UV and in the visible of 1 with increasing amounts of ds26mer.





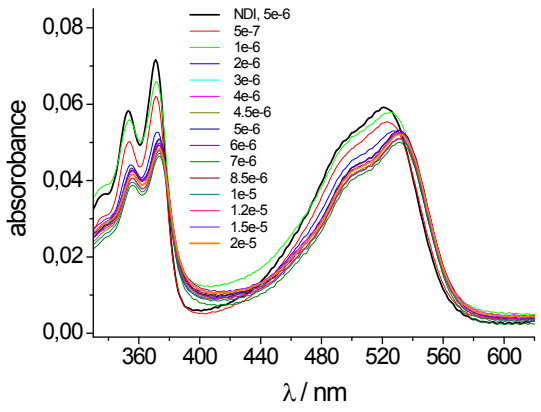


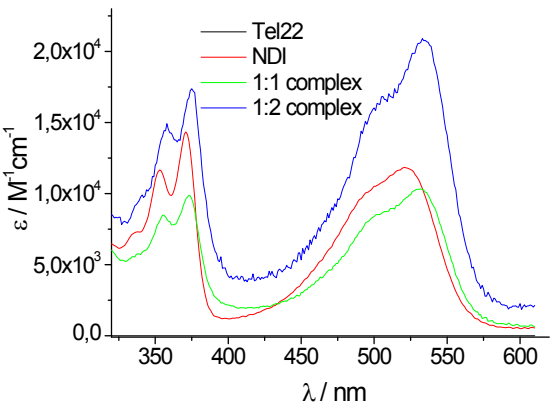




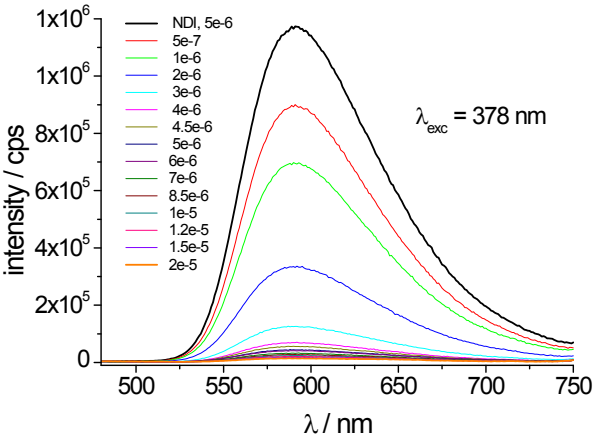
Calculated fluorescence spectra of compound **1** and the 1:2 complex obtained with the binding constant, $\log(K_{12}/M^{-2}) = 13.59 \pm 0.17$

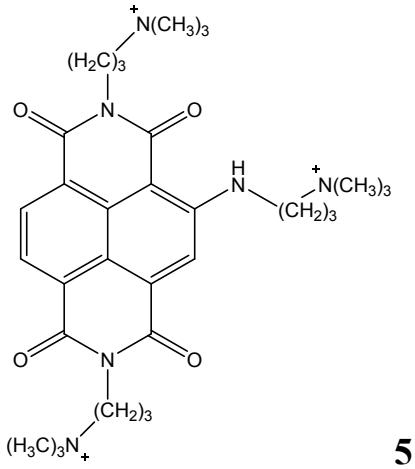
SI Figure 5: Titration of tri-substitued compound 5 with Tel22: absorption, fluorescence and circular dichroism spectra of 1 with increasing amounts of mixtures have been heated for 20 minutes at 50°C





Absorption spectra calculated with the binding constants $\log(K_{11}/M^{-1}) = 6.7$ and $\log(K_{12}/M^{-2}) = 12.6 \pm 0.1$.





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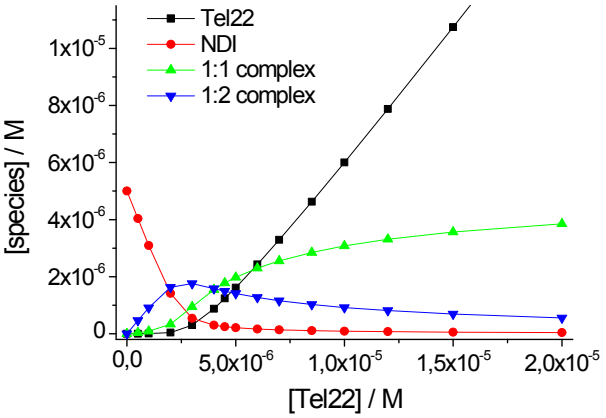
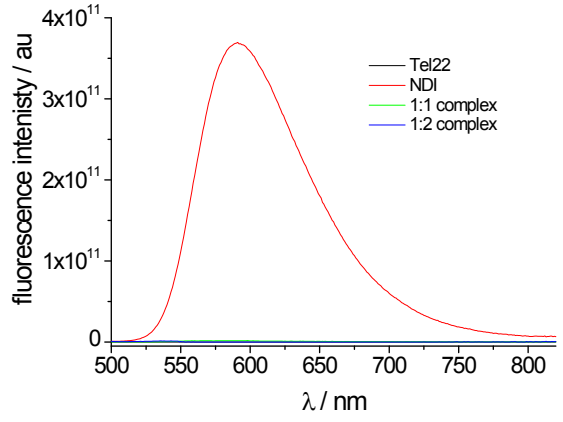
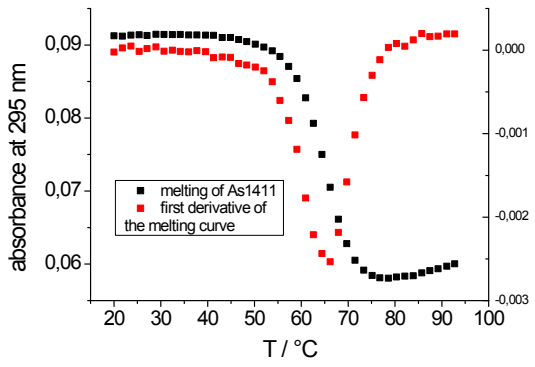


Species distribution with increasing Tel22 concentration; binding constants are $\log(K_{11}/M^{-1}) = 6.7 \pm 0.02$, $\log(K_{12}/M^{-2}) = 13.3 \pm 0.01$.

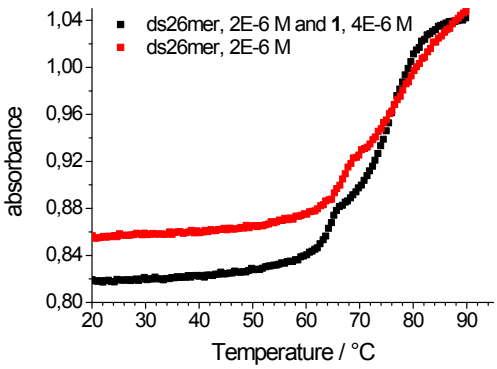


Fluorescence spectra calculated with the binding constants $\log(K_{11}/M^{-1}) = 6.7 \pm 0.02$ and $\log(K_{12}/M^{-2}) = 13.3 \pm 0.01$.

SI Figure 6: Melting of AS1411 and ds26mer alone and in the presence of 1

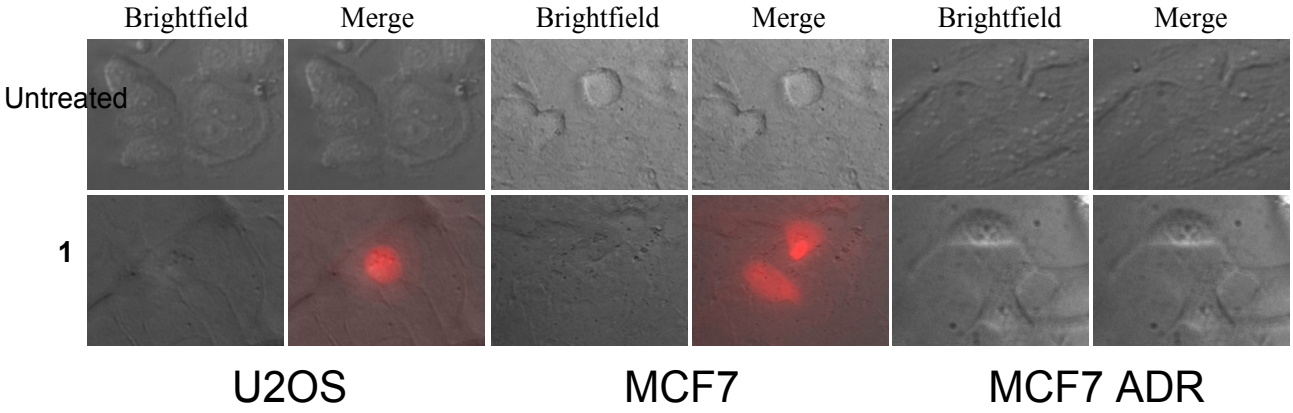


Absorbance changes at 295 nm of 2.0×10^{-6} M AS1411 solution in 10 mM K^+ PB of pH 7.4 with 100 mM KCl at 295 nm (■) and its first derivative with temperature (■).



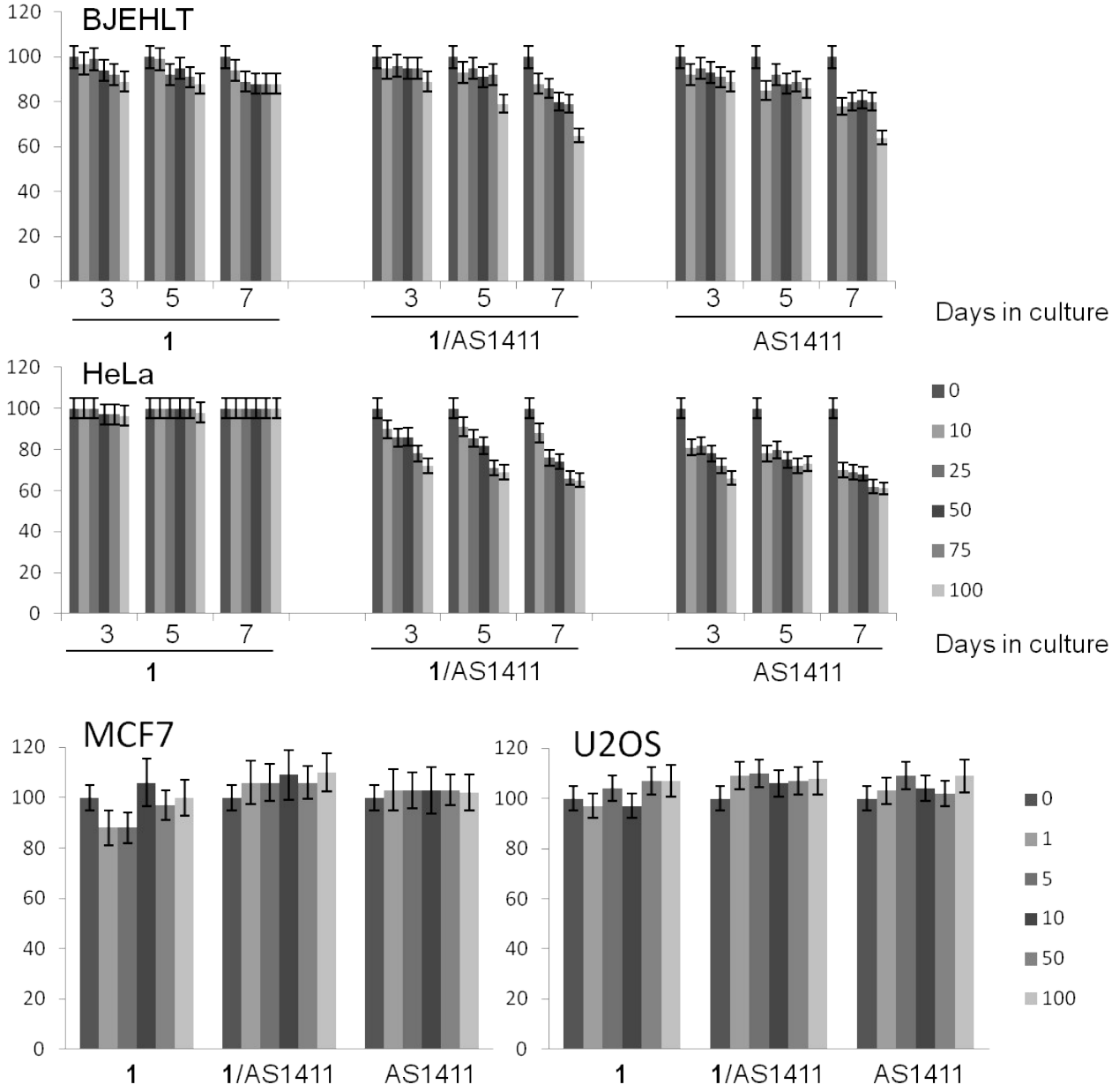
Absorbance changes of ds26mer (2.0×10^{-6} M) solution (red) and a mixture (black) of ds26mer (2.0×10^{-6} M) and **1** (4.0×10^{-6} M) in 10 mM K^+ PB of pH 7.4 with 100 mM KCl at 250 nm.

SI Figure 7: Qualitative analysis of 1 uptake.



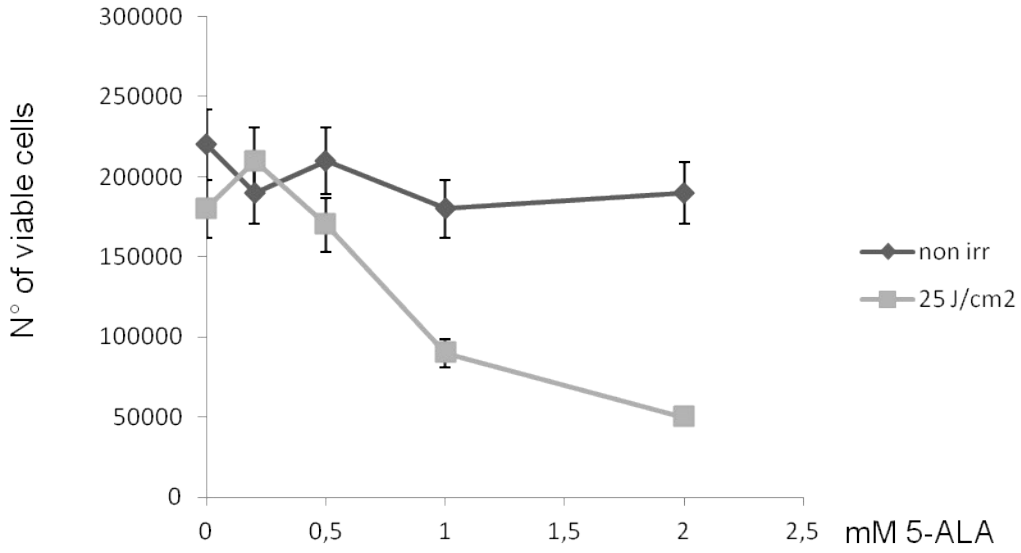
The indicated cell lines were exposed to 5 μM of **1** for 12 hours and then analyzed with an inverted fluorescence microscope at 40X magnification. Pictures show images of brightfield alone or merged with fluorescence acquisition (Excitation filter 515-560 nm, Suppression filter LP 590 nm). One representative out of three independent experiments is shown.

SI Figure 8: Cytotoxic effect of 1, AS1411 and combination 1/ AS1411.



The indicated cell lines were chronically exposed to the indicated micromolar doses of **1** alone or complexed with AS1411 in a 1:2 molar ratio. Viability of cells was determined after 7 days treatment by MTT assay, or at different time points where indicated, and expressed as percentage of cell viability compared to untreated samples. Histograms show the mean values of three independent experiments. Bars indicate means ±SD.

SI Figure 9. Light induced 5-ALA cytotoxicity.



BJEHLT fibroblasts were treated with the indicated doses of 5-ALA for 12 hours and then exposed or not to light, 630 nm as described in the Experimental Section. Cell were then detached and counted at the indicated time points after irradiation to determine the number of viable cells. Curves report the number of viable cells in each condition. Histograms show the mean values of three independent experiments. Bars indicate means ±SD.