

Supporting Informations for

Mixed non-covalent assembled of ethynyl Nile red and ethynyl pyrene along oligonucleotide templates

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Content	Page
1. Materials and methods	2
2. Spectra of titration experiments	2
3. References	4

1. Materials and Methods

DMSO p.a. was purchased from *Carl Roth*. Water was received from Milli-Q system with a resistivity of 18.2 M Ω -cm. Oligonucleotides were purchased from Metabion. The nucleotides ethynyl pyrene deoxyuridine^[1] and nile red deoxyuridine^[2] were synthesized according to literature. Spectroscopic measurements were recorded in water, DMSO or water + 2% DMSO solution at 20 °C using quartz glass cuvettes (10 mm). Samples were corrected by a reference. For the absorption spectra we used a *PerkinElmer Lambda 750* spectrometer equipped with a 6x6 cell changer unit and a peltier system *PTP-6+6*. Fluorescence and excitation spectra were recorded with a *Jobin-Yvon Fluoromax 4* fluorimeter with a step width of 1 nm and an integration time of 0.2 s. All spectra were recorded with an excitation and emission bandpass of 7 nm. A *JASCO J-815* spectropolarimeter equipped with a *Julabo FP35* Refrigerated/Heating Circulator was used to collect the CD data. Each spectrum represented the average of two accumulations recorded between wavelengths of 230 and 800 nm at 0.1 nm intervals with a bandwidth of 1 nm, response time of 8 s and a scan-rate of 20 nm/min. CD data were smoothed using the adaptive smoothing method, which is part of Spectra Analysis software (*JASCO*). All samples were prepared at room temperature. In case of the titrations the Nr- \equiv -dU was added stepwise from a stock solution and incubated for 10 min each step. For the mixture experiments Nr- \equiv -dU and Py- \equiv -dU were premixed in different ratios and then added to the (dA)₂₀ strand. After 10 min incubation the measurements were taken.

2. Spectra of titration experiments

Titration (dA)₁₀

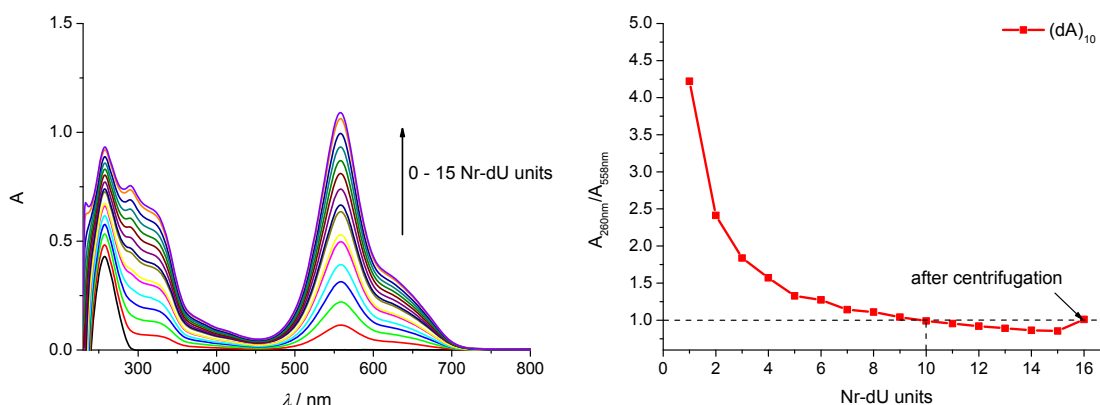


Figure S1: UV/Vis absorption spectra of titration of Nr- \equiv -dU to (dA)₁₀ (2.5 μ M in H₂O + 2 % DMSO)

Titration (dA)₁₄

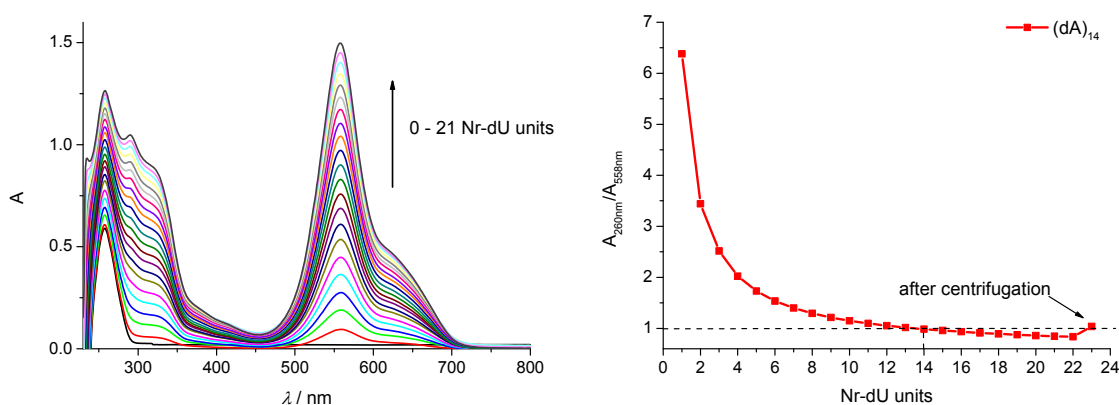


Figure S2: UV/Vis absorption spectra of titration of Nr- \equiv -dU to (dA)₁₄ (2.5 μ M in H₂O + 2 % DMSO)

Titration (dA)₁₆

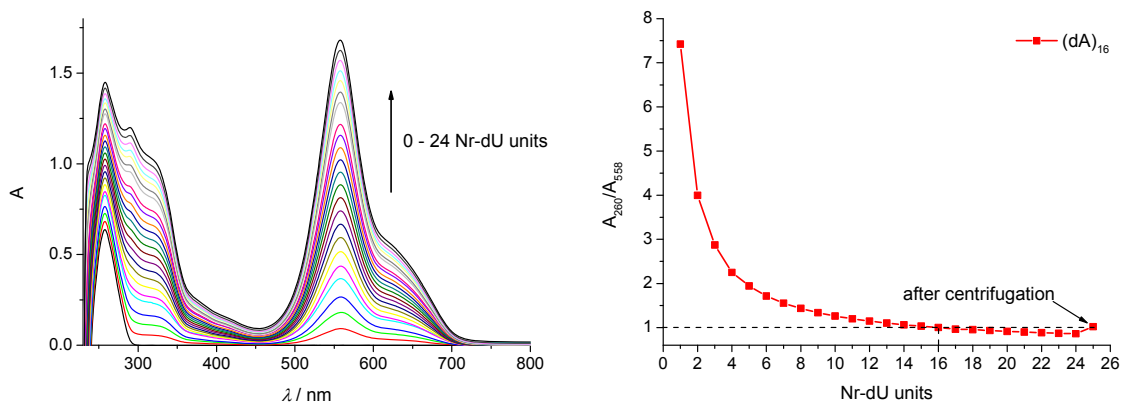


Figure S3: UV/Vis absorption spectra of titration of Nr-≡-dU to (dA)₁₆ (2.5 μ M in H₂O + 2 % DMSO)

Titration (dA)₂₀

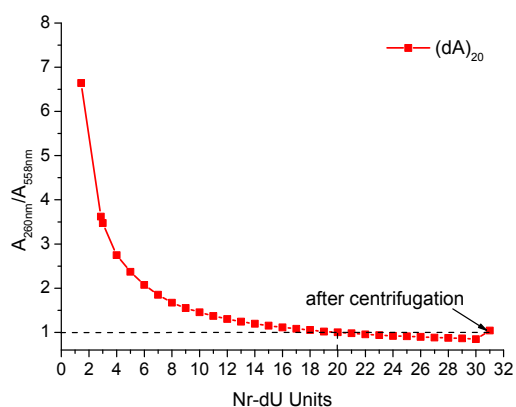


Figure S4: Ratio of A_{260nm}/A_{558nm} of Nr-≡-dU to (dA)₂₀ (1,25 μ M in H₂O + 2 % DMSO)

Emission $\lambda_{exc} = 558$ nm

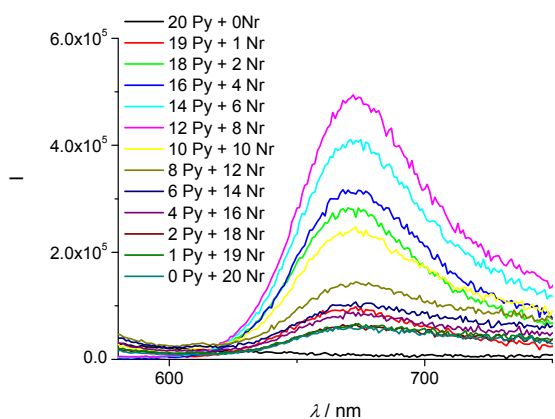


Figure S5: Fluorescence of the assembled Py-≡-dU:Nr-≡-dU mixtures along (dA)₂₀ (1,25 μ M in H₂O + 2% DMSO).

References

- [1] A. D. Malakhov, E. V. Malakhova, S. V. Kuznitsova, I. V. Grechishnikova, I. A. Prokhorenko, M. V. Skorobogaty, V. A. Korshun, Y. A. Berlin, *Russ. J. Bioorg. Chem.* **2000**, 26, 34-44.
- [2] R. Varghese, P. K. Gajula, T. K. Chakraborty, H.-A. Wagenknecht, *Synlett* **2009**, 3253-3257.