

Electronic Supplementary Information

Unravelling molecular mechanisms in the fluorescence spectra of Doxorubicin in aqueous solution by femtosecond fluorescence spectroscopy

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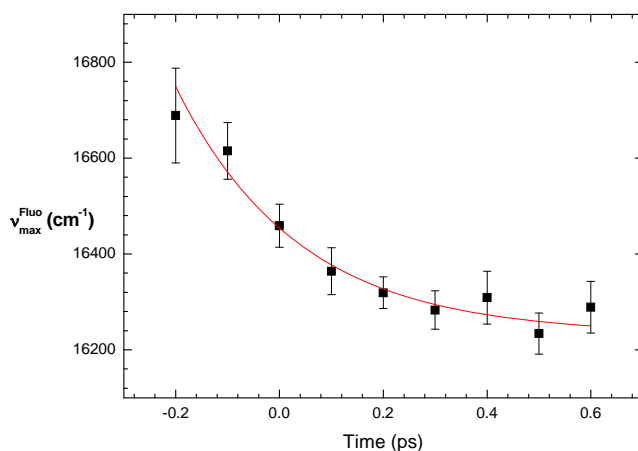


Fig. S1. Time-resolved shift of the fluorescence band of DOX 380 μM DOX in 10 mM Tris buffer at pH 7.4, with 1 mM EDTA and 50 mM NaCl, after excitation at 400 nm. The kinetics trace was fitted to an exponential function with a time constant of 0.24 ± 0.05 ps and an amplitude of 221 ± 42 cm^{-1} .

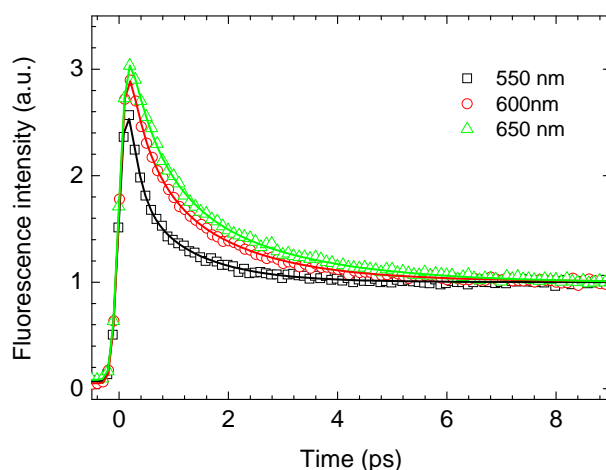


Fig. S2 Typical total fluorescence decay of DOX (800 μM) in D_2O , at 550, 600 and 650 nm, after excitation at 400 nm. The fits with a three-exponential function convoluted with a Gaussian representing the instrumental response function (FWHM 280 fs) are represented by the solid lines.

<i>800 μM DOX / D_2O</i>	<i>a_1</i> <i>τ_1</i>	<i>a_2</i> <i>τ_2</i>	<i>a_3</i> <i>τ_3</i>
550 nm	0.51 \pm 0.02 433 \pm 24 fs	0.24 \pm 0.01 2.6 \pm 0.1 ps	0.25 \pm 0.01 1 ns
600 nm	0.39 \pm 0.01 488 \pm 31 fs	0.35 \pm 0.01 2.22 \pm 0.07 ps	0.26 \pm 0.01 1 ns
650 nm	0.46 \pm 0.01 721 \pm 39 fs	0.33 \pm 0.01 3.1 \pm 0.1 ps	0.20 \pm 0.02 1 ns

Table S11. Time constants and amplitudes obtained from the individual fits of the fluorescence decays measured for 800 μM DOX in D_2O . Decays were fitted using a three-exponential function where the longest time was fixed to 1 ns.

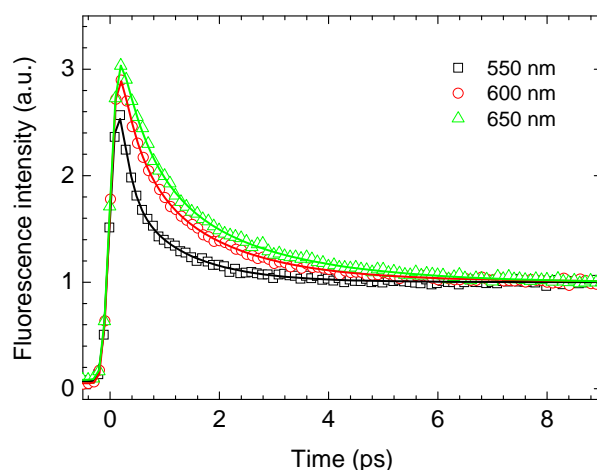


Fig. S3 Typical total fluorescence decay of DOX (800 μM) in H_2O , at 550, 600 and 650 nm, after excitation at 400 nm. The fits with a three-exponential function convoluted with a Gaussian representing the instrumental response function (FWHM 280 fs) are represented by the solid lines.

800 μM DOX / H_2O	a_1 τ_1	a_2 τ_2	a_3 τ_3
550 nm	0.51 \pm 0.05 198 \pm 18 fs	0.24 \pm 0.06 1.09 \pm 0.05 ps	0.25 \pm 0.01 1 ns
600 nm	0.36 \pm 0.04 362 \pm 28 fs	0.36 \pm 0.05 1.53 \pm 0.05 ps	0.28 \pm 0.01 1 ns
650 nm	0.39 \pm 0.04 523 \pm 32 fs	0.35 \pm 0.05 1.97 \pm 0.07 ps	0.26 \pm 0.01 1 ns

Table SI2. Time constants and amplitudes obtained from the individual fits of the fluorescence decays measured for 800 μM DOX in H_2O . Decays were fitted using a three-exponential function where the longest time was fixed to 1 ns.