

Supplementary Material

Photophysical properties, complexometry, and aggregation-induced emission of a 2-donor-substituted 3-ethynylquinoxaline

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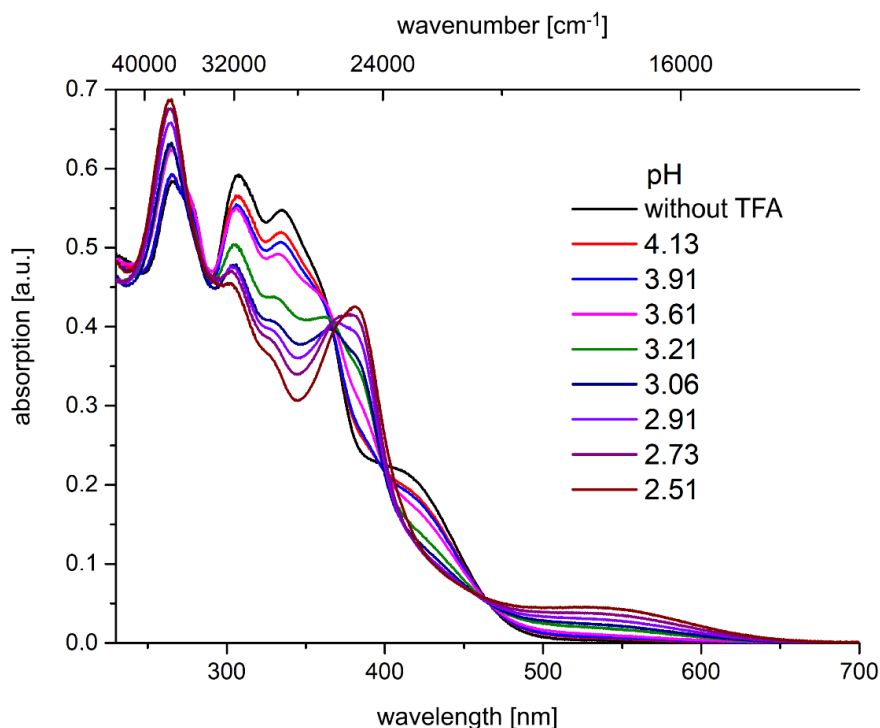
1 UV/Vis spectra for the determination of the pK_a of MEQDMA- H^+ 

Figure S1. UV/Vis titration experiment of **MEQDMA** in the presence of TFA (recorded in CH_2Cl_2 , $T = 293$ K, $c(\text{MEQDMA}) = 10^{-5}$ M).

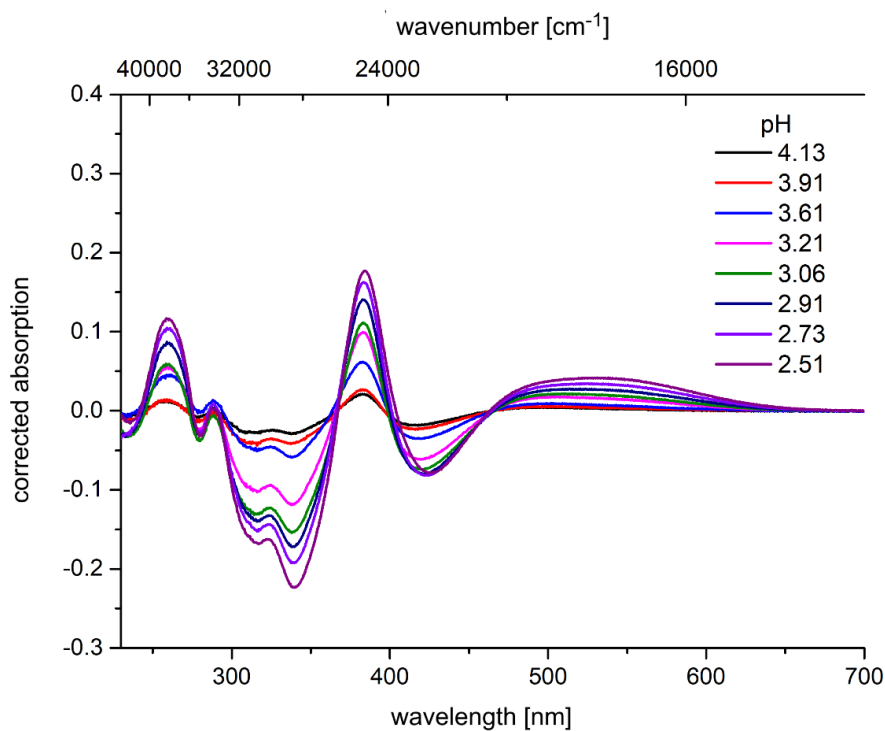


Figure S2. Difference spectra of the corrected absorbance versus wavelength in the presence of TFA in CH_2Cl_2 (see Figure S1) (recorded in CH_2Cl_2 , $T = 293$ K, $c(\text{MEQDMA}) = 10^{-5}$ M).

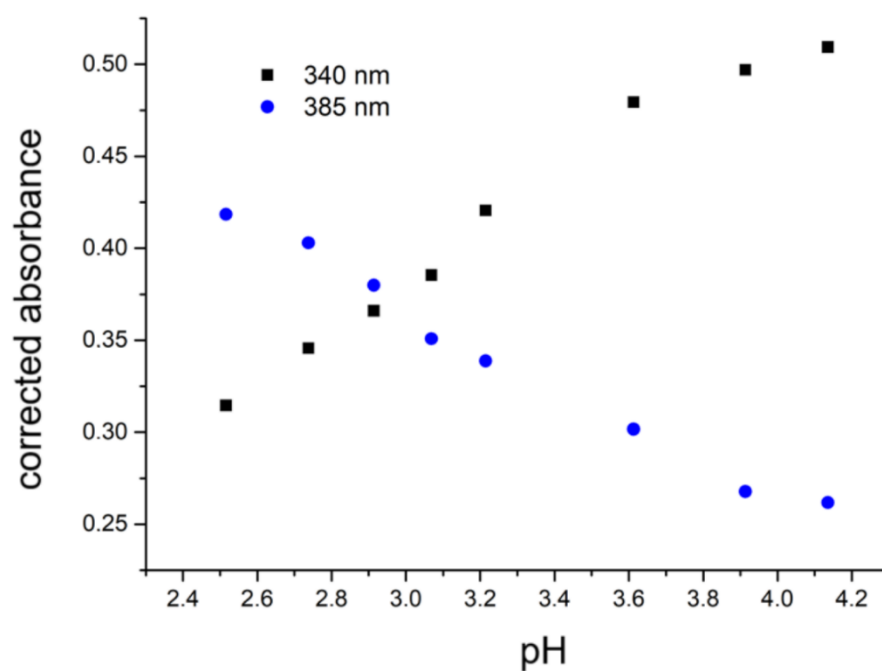


Figure S3. Plot of the corrected absorbance against the pH of the solution (recorded in CH_2Cl_2 , $T = 293 \text{ K}$, $c(\text{MEQDMA}) = 10^{-5} \text{ M}$).

2 Fluorescence spectra for the determination of the $\text{p}K_a$ of MEQDMA-H^+

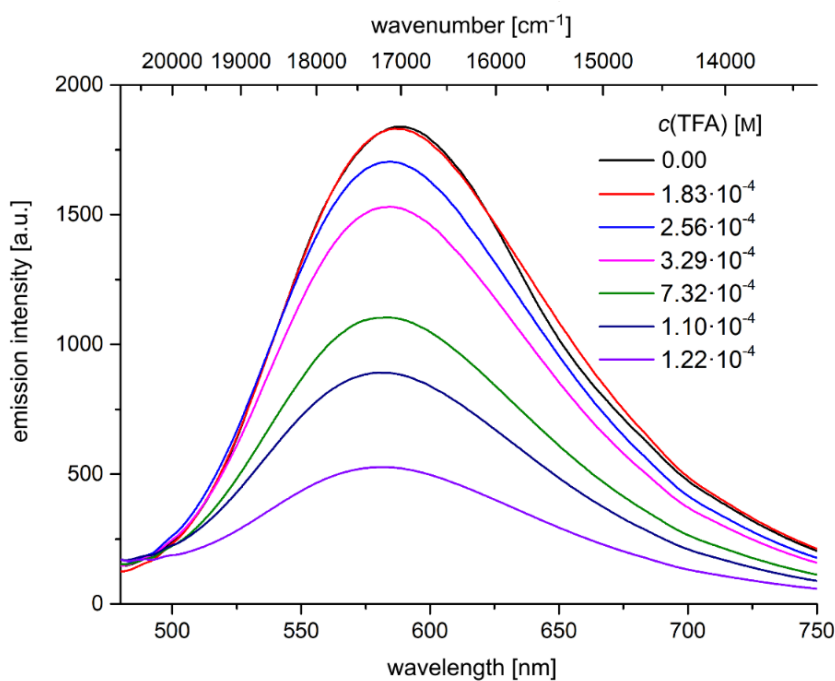


Figure S4. Fluorescence titration experiment of **MEQDMA** with TFA (recorded in CH_2Cl_2 , $T = 293 \text{ K}$, $c(\text{MEQDMA}) = 10^{-5} \text{ M}$).

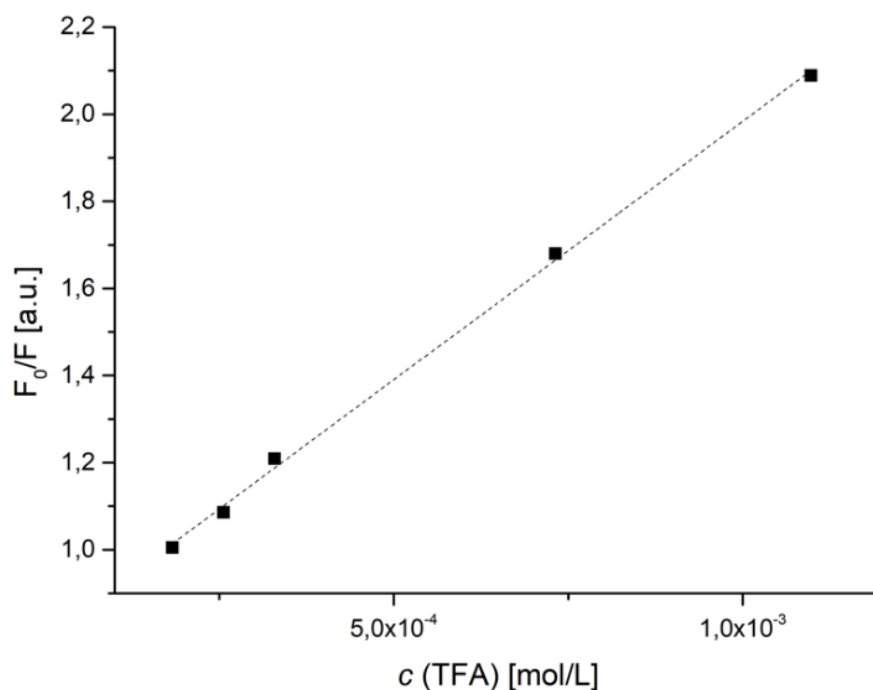


Figure S5. The plot of $F_0 \cdot F^{-1}$ against the concentration of TFA to determine the Stern-Volmer constant K_{SV} of **MEQDMA**.

$$\frac{F_0}{F} = 0.7972 + 1186.58 [H^+] \quad (r^2 = 0.99)$$

The results obtained from the experiment are summarized in Table S1. The outlier value at a concentration of $1.22 \cdot 10^{-3} \text{ mol} \cdot \text{L}^{-1}$ was not considered.

Table S1. Summary of the resulting and calculated data from the linear correlation

Parameter	
y-axis intercept	0.79
K_{SV} (slope)	1186.58
$c(H^+)$	$6.71 \cdot 10^{-4} \text{ M}$
pKa	3.1
r^2	0.99

3 Difference UV/Vis spectra and Job plots of $\text{Sc}(\text{OTf})_3$ and MEQDMA in ethyl acetate and acetonitrile.

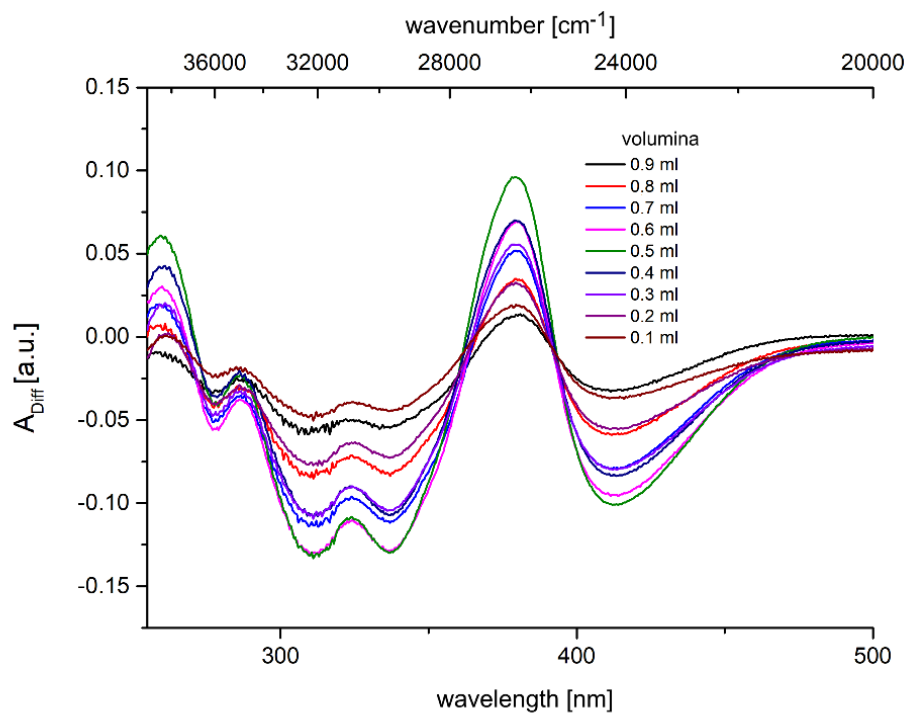


Figure S6. Differential spectra of **MEQDMA** and in presence of various volumina of $\text{Sc}(\text{OTf})_3$ in ethyl acetate (recorded at $T= 293$ K).

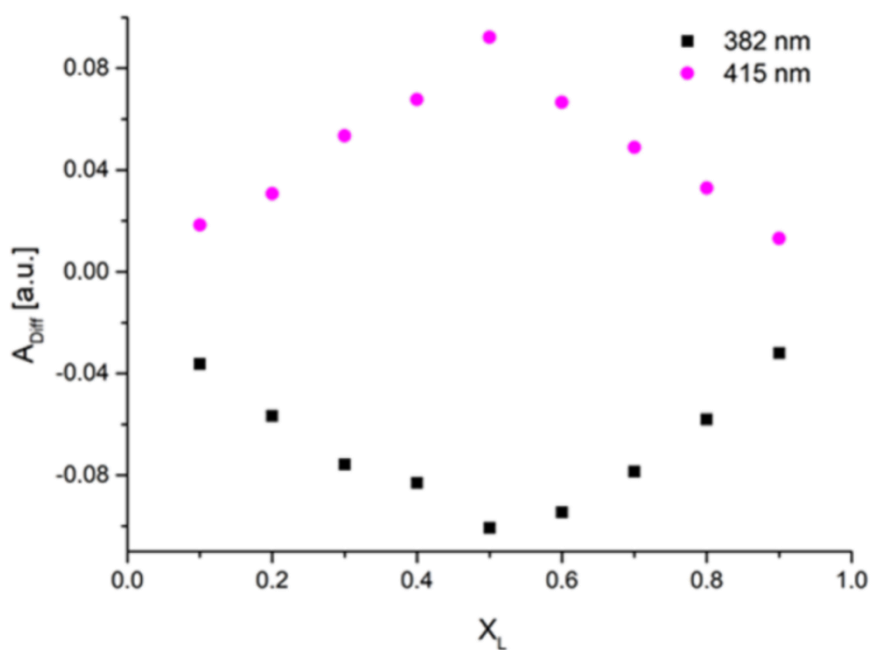


Figure S7. Job plots of **MEQDMA** and in presence of mole fractions X_L of $\text{Sc}(\text{OTf})_3$ in ethyl acetate (recorded at $T= 293$ K).

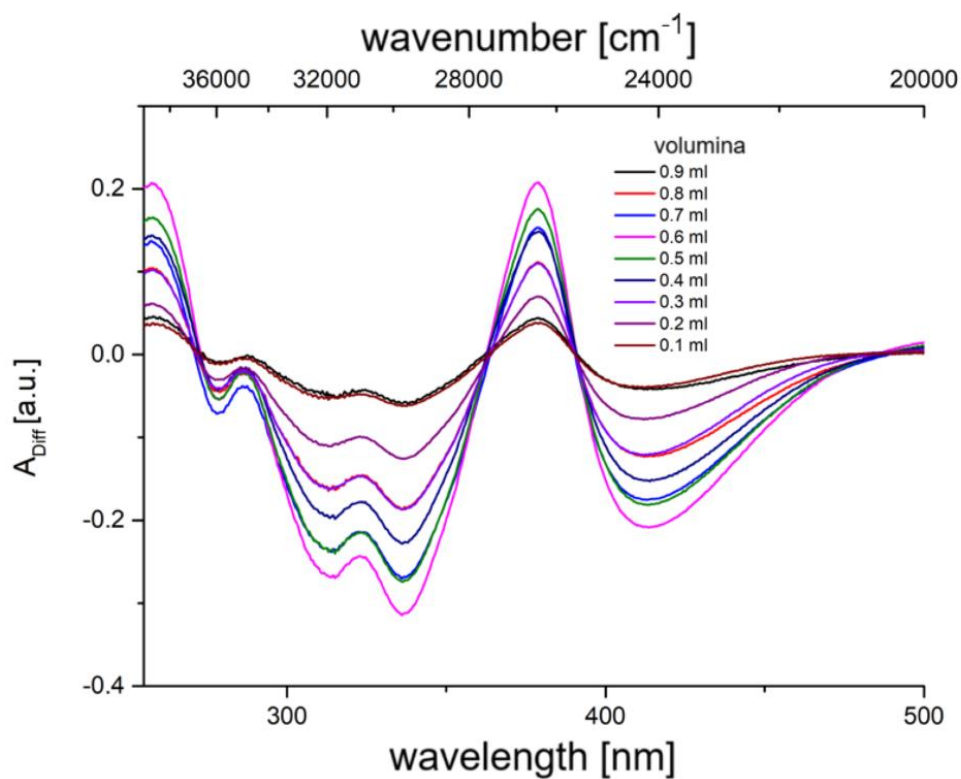


Figure S8. Differential spectra of **MEQDMA** and in presence of various volumina of $\text{Sc}(\text{OTf})_3$ in acetonitrile (recorded at $T= 293$ K).

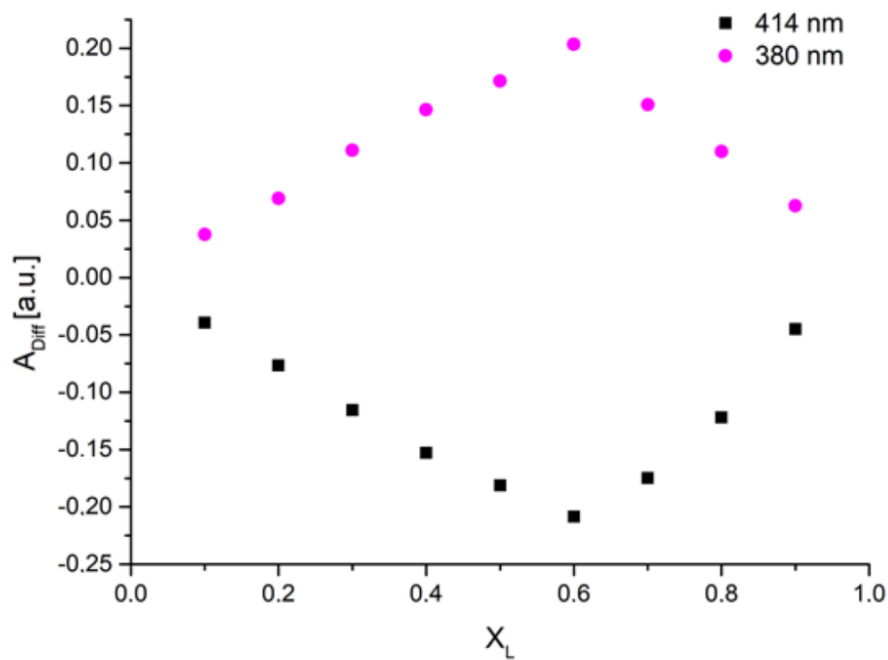


Figure S9. Job plots of **MEQDMA** and in presence of mole fractions X_L of $\text{Sc}(\text{OTf})_3$ in ethyl acetate (recorded at $T= 293$ K).

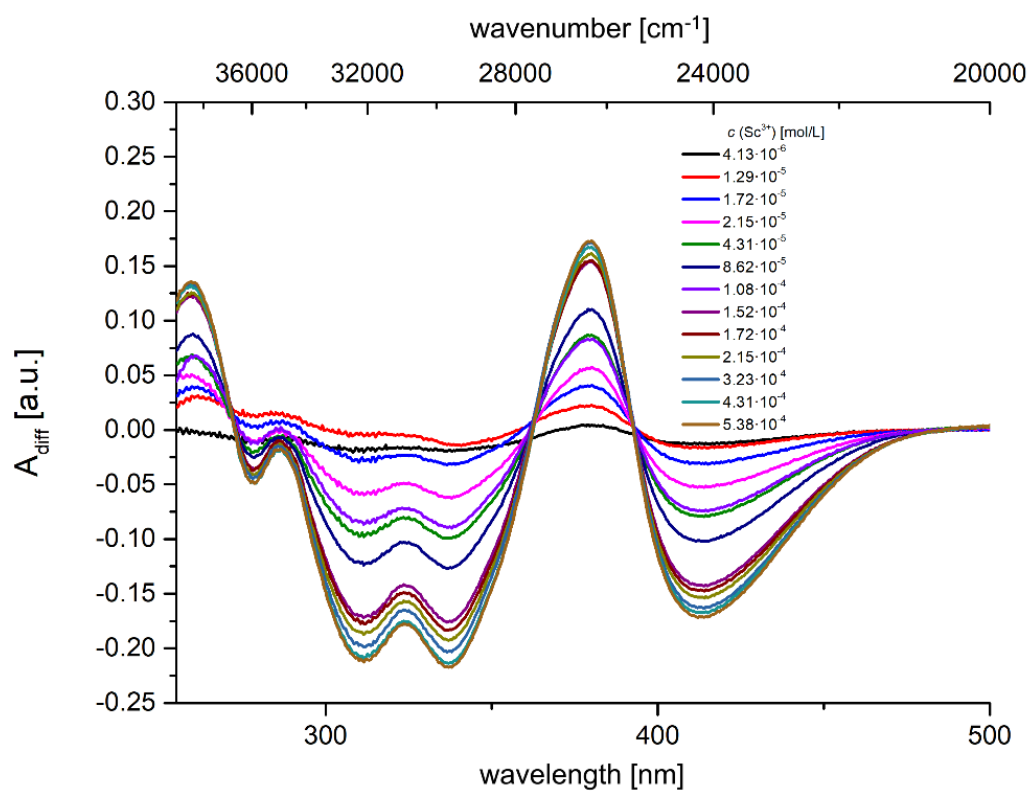


Figure S10. Difference spectra of the titration experiment of **MEQDMA** and various concentrations of Sc(OTf)₃ in ethyl acetate.

4 Aggregation-induced emission spectra of MEQDMA in isopropanol/water and acetonitrile/water

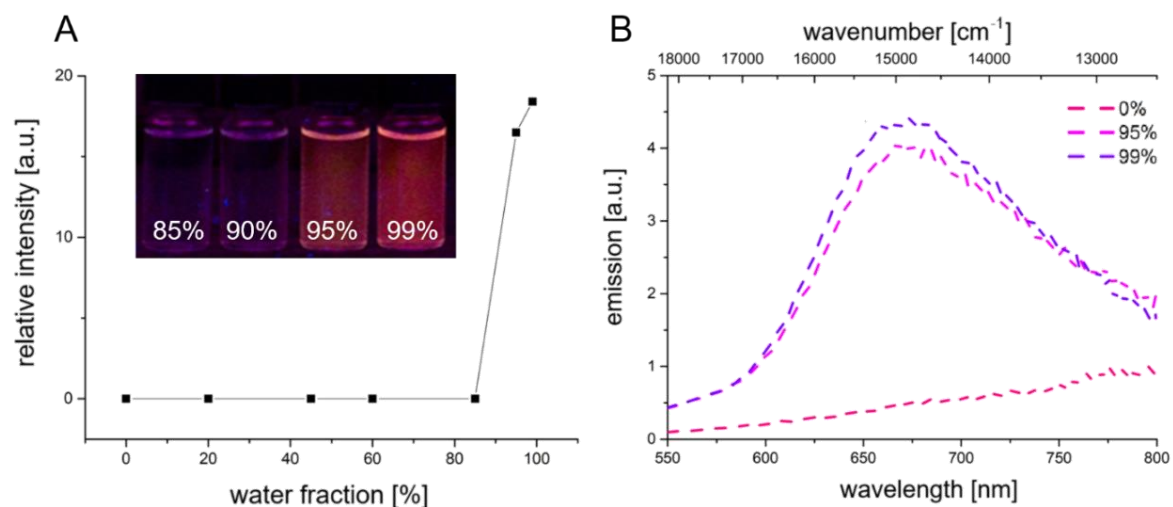


Figure S11. A: Emission intensity (inset: visualization of **MEQDMA** at 85, 90, 95 und 99% water content, $\lambda_{exc} = 365$ nm) and B: emission spectra (right) of **MEQDMA** in isopropanol/water mixtures upon increasing water content (recorded at $T = 298$ K, $c = 10^{-5}$ M, $\lambda_{exc} = 413$ nm).

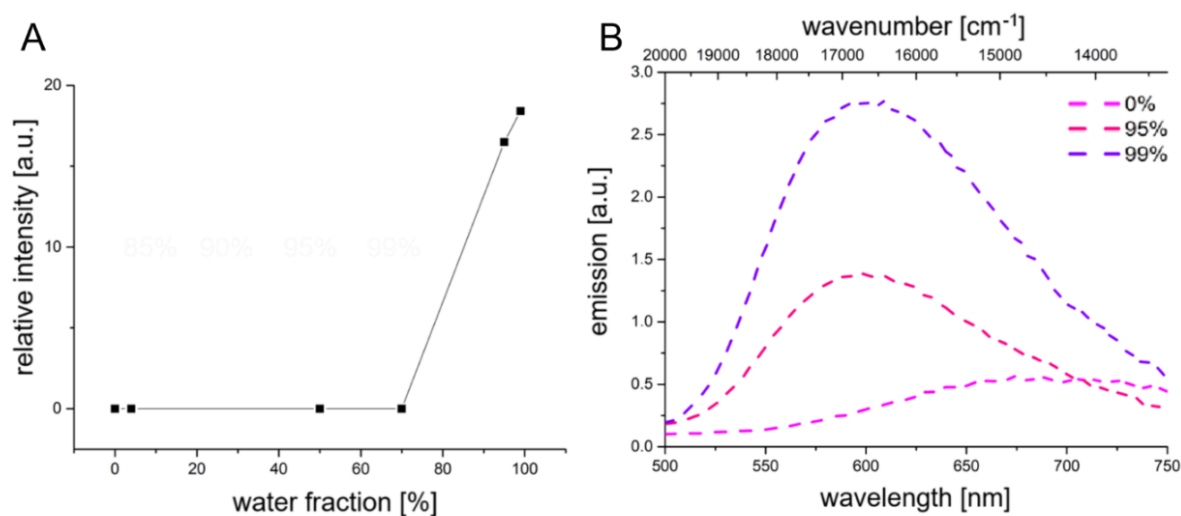


Figure S12. A: Emission intensity and B: emission spectra (right) of **MEQDMA** in acetonitrile/water mixtures upon increasing water content (recorded at $T = 298$ K, $c = 10^{-5}$ M, $\lambda_{exc} = 413$ nm).