



## Supporting Information

for

### **Photophysics and photochemistry of NIR absorbers derived from cyanines: key to new technologies based on chemistry 4.0**

Bernd Strehmel, Christian Schmitz, Ceren Kütahya, Yulian Pang, Anke Drewitz and Heinz Mustroph

*Beilstein J. Org. Chem.* **2020**, *16*, 415–444. [doi:10.3762/bjoc.16.40](https://doi.org/10.3762/bjoc.16.40)

### **Information of the electrochemical measurements and the determination of photophysical data**

## Materials

The NIR-absorbers were available either as catalog products or samples from FEW Chemicals GmbH. Solvents used were purchased as spectroscopic grade purity from Sigma Aldrich.

## UV–vis–NIR data

Spectra of the dissolved sensitizers in the monomers were measured with a Cary 5000 from Agilent. Measurements were carried out in 1 × 1 cm quartz cuvettes.

## Fluorescence measurements

Fluorescence measurements were pursued in 1 × 1 cm quartz cuvettes. Data were taken with a NIR-fluorescence spectrometer FS920 von Edinburgh Instruments equipped with a Hamamatsu PMT R2658P photomultiplier and double monochromators. A Xe-450W lamp served as excitation source. Sulforhodamine 101 ( $c = 0.1$  M) in HCl/ethanol exhibiting a quantum yield of 1 served as reference. The absorbers were measured with respect to the reference under identical conditions to determine the fluorescence quantum yield. Four samples were prepared for each absorber ( $OD < 0.1$ ,  $d = 1$  cm)) choosing three distinct excitation wavelengths while the emission of the solvent was subtracted as background. Samples were measured at 22 °C. The fluorescence spectrometer worked in both the emission and excitation side in the correction mode. The fluorescence quantum yield is given in percent data with respect the reference.

## Cyclic voltammetry

The oxidation potential of the sensitizers was recorded by cyclic voltammetry (Zennium from Zahner-Elektrik GmbH and a VERSASTAT4-400 from AMETEK served as potentiostats) in acetonitrile ( $c_{\text{absorber}} = 10^{-3}$  M) with tetrabutylammonium hexafluorophosphate from Sigma Aldrich (0.1 M) as supporting electrolyte against ferrocene as an external standard. The data were taken with a scanning rate of 0.015 V·s<sup>-1</sup> using platinum disc as a working electrode and Ag/AgCl as reference electrode.