**Supplementary materials**

**Mestranol moieties clicked to Zn(II) phthalocyanine for controllable photosensitized oxidation of cholesterol**

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1. **Apparatus**

FT-IR spectra were recorded on a Perkin Elmer Spectrum 100 FT-IR spectrometer. MALDI-MS of phthalocyanines were obtained in dihydroxybenzoic acid as MALDI matrix using nitrogen laser accumulating 50 laser shots using Bruker Microflex LT MALDI-TOF mass spectrometer. 1H-NMR spectra were recorded in DMSO-d6 solution on a Bruker Advance 600 MHz spectrometer. Absorption spectra in the UV-visible region were recorded with a Perkin Elmer Lambda 25 UV-Vis spectrophotometer. Fluorescence excitation and emission spectra were recorded on a Perkin Elmer fluorimeter using 1 cm path length cuvettes and room temperature. Fluorescence lifetimes were measured by a time correlated single photon counting (TCSPC) method using FLUOROLOG-3 apparatus (Horiba Jobin Yvon, Edison, NJ) equipped with a nano LED and a standard air cooled R928 PMT detector. Photo-irradiations were done by using a light emitting diode 635 nm (100 W). Power density was controlled with POWER MAX5100 power meter.

1. **Photophysical investigations**
   1. ***Fluorescence quantum yields***

Fluorescence quantum yield (ΦF) of phthalocyanine-mestranol conjugates were determined by the comparative method using equation 1,

 (1)

where F and FStd are the ranges under the fluorescence emission curves of phthalocyanine- conjugates (**4, 5**) and the standard, respectively. A and AStd are the respective absorbances of phthalocyanine- conjugates (**4, 5**) and the standard at the excitation wavelengths, respectively. n and nstd are the refractive index of solvents used for phthalocyanine- conjugates (**4, 5**) and the standard, respectively. Unsubstituted ZnPc (ΦF = 0.2 in DMF) was used as the standard. Both the samples and the standard were excited at the same wavelength. The absorbance of the solutions at the excitation wavelength was around 0.05.

1. **Photochemical studies**
   1. ***Singlet oxygen quantum yield***

Singlet oxygen quantum yields (ΦΔ) of phthalocyanine-mestranol conjugates (**4, 5**) were carried out using the self-prepared experimental set-up as shown below. Usually, the solutions with concentration approx. 10−5 M, mixed with DPBF as a singlet oxygen quencher (60 mM) were irradiated with LED 635 nm using the software of the Ocean Optics Inc. (QE 65000). Singlet oxygen quantum yield (ΦΔ) was determined in air by the relative method in DMF using unsubstituted ZnPc as a reference. DPBF was used as a chemical quencher for singlet oxygen. Equation 2 was employed for the calculations:

 (2)

where is the singlet oxygen quantum yield for the standard unsubstituted ZnPc ( = 0.56 in DMF [7]). R and RStd are the DPBF photobleaching rates in the presence of phthalocyanine-BODIPY conjugates (8-10) and the standard, respectively. Iabs and   
 are the rates of light absorption by samples (8-10) and the standard, respectively. Solutions of the sensitizer and the standard (10−5 M) containing DPBF were prepared in the dark and irradiated in the Q band region using the photo-irradiation setup. DPBF degradation at 417 nm was monitored. A light intensity of 6.7 × 1015 photons s−1 cm−2 was used for ΦΔ determinations.

* 1. ***Photodegradation quantum yield***

Photodegradation quantum yield (Φd) measurement of phthalocyanine conjugates (**4, 5**) was studied using the experimental set-up. Photodegradation quantum yield was calculated using equation 3.

 (3)

where C0 and Ct are phthalocyanine- conjugates (**4, 5**) concentrations before and after irradiation respectively, V is the reaction volume, NA is Avogadro’s constant, S is the irradiated cell area and t is the irradiation time. Iabs is the overlap integral of the radiation source light intensity and the absorption of phthalocyanine- conjugates (**4, 5**). A light intensity of 2.24 × 1016 photons s−1 cm−2 was employed for Φd determinations.

1. **Photosensitized oxidation studies**

A well-documented set-up which contains a spectrometer of Ocean Optics QE 65000 (USA), a personal computer with a specialized software and two light sources was used in the present study. Briefly, there are replaceable light sources of LED 665 nm and LED 635 nm, optical fibers and lenses which are arranged to be convenient for studies in solutions in different dishes (Fig. 1). The parameters of the light sources such as the power and the distance to the spot of irradiation (object), time of irradiation (*texc*), light intensity (*I*) are basic parameters for determination of the light dose (*D*) which calculation was made accordance to the equation: *D* *=* *I.texc*. The power density of the used LED 665 nm on its maximum was measured at 10 cm for light spot of 25 cm2 (ELO Ltd., Sofia, Bulgaria).

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**Fig 1.** Experimental set-up used in photosensitized oxidation studies.