

Supporting Information

Water Soluble Quantum Dots as Hydrophilic Carriers and Two-Photon Excited Energy Donors in Photodynamic Therapy.

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- Figure S1: Absorbance and Fluorescence Spectra of QD-MPA
- Figure S2: UV-Vis spectrum of **QD-1**
- Figure S3: Photographs of **QD-1**, 1 week, 1 month and 2 months after preparation.
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- Figure S5: Confocal fluorescence image of HeLa cells incubated with DHFA before and after two-photon irradiation
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- Figure S8: TEM and DLS information for QD-1.
- Figure S9: Singlet oxygen production of QD-1 upon at pH6.8 using DPBF assay.
- Figure S10: Determination of FRET efficiency.

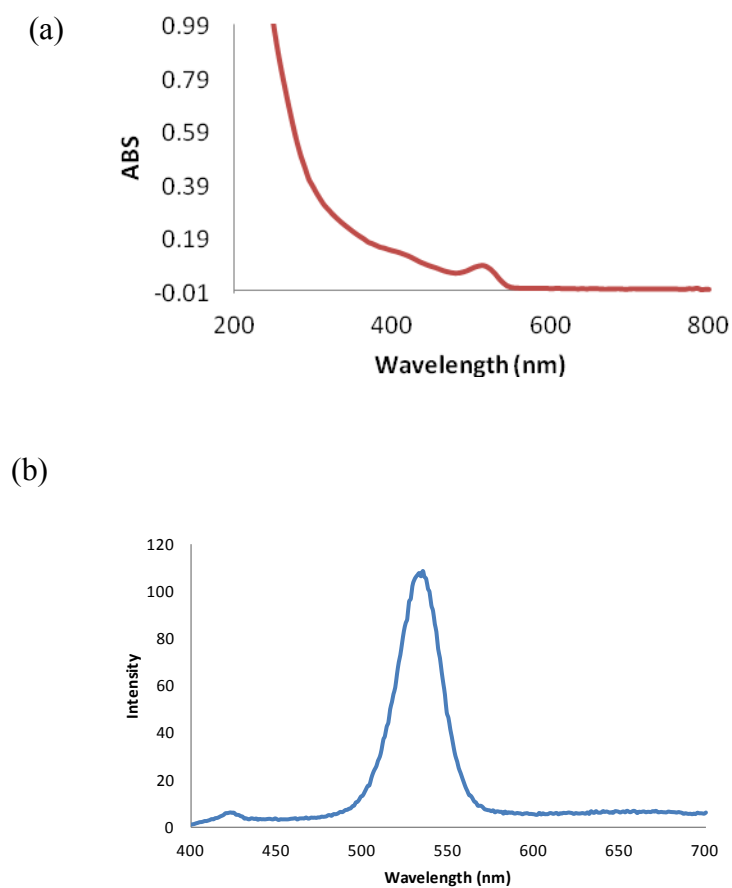


Figure S1 (a) Absorbance and (b) fluorescence spectra of QD-MPA recorded in H₂O.

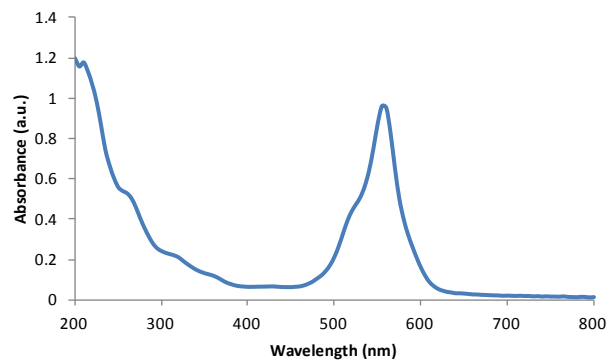


Figure S2 Absorbance spectrum of **QD-1** recorded in PBS solution.

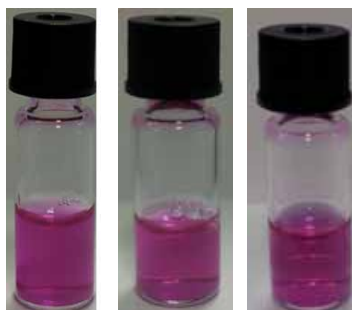


Figure S3 Photograph of **QD-1** solution after 1 week (left vial), 1 month (middle vial) and 2 months (right vial) showing no evidence of aggregation.

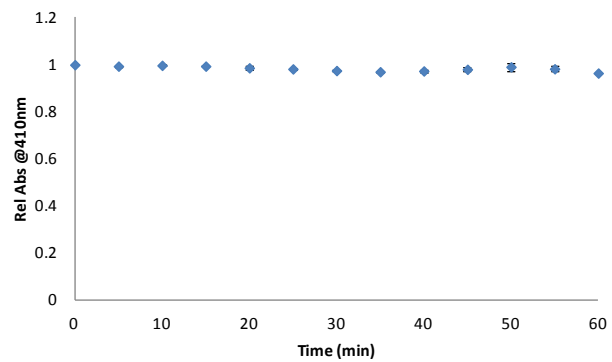


Figure S4 Plot of relative absorbance of DPBF against time for QD-MPA irradiated at 400 nm.

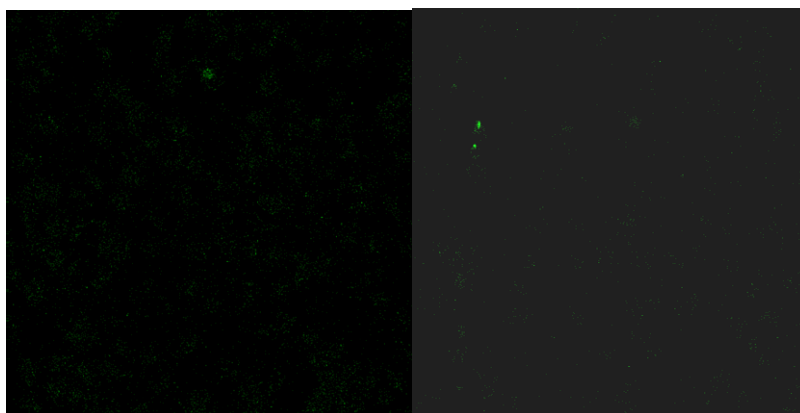


Figure S5 Confocal fluorescence images of HeLa cells incubated with DHFA (a) before and (b) after two-photon irradiation at 800 nm.

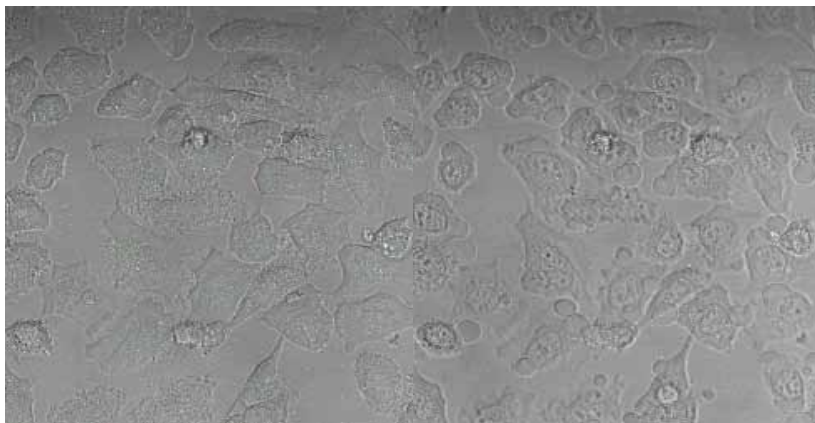


Figure S6 Phase contrast images of HeLa cells incubated with DHFA before (left) and after (right) two-photon irradiation at 800 nm.

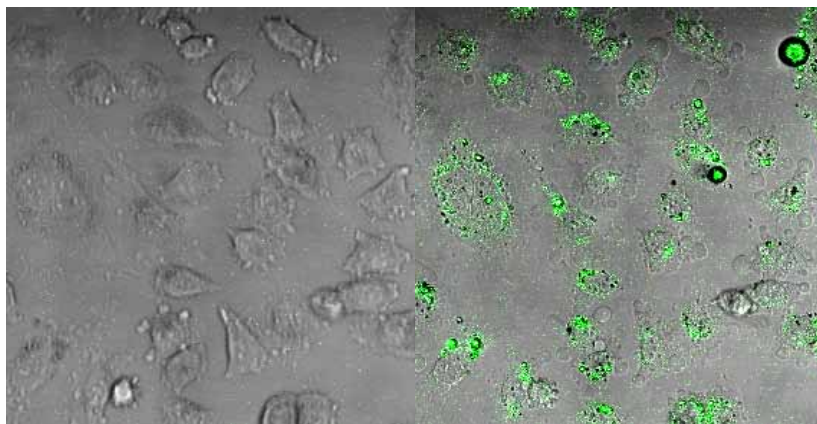
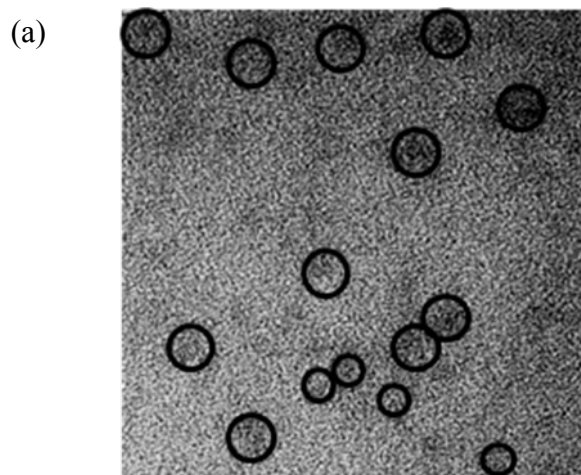


Figure S7 Phase contrast images of HeLa cells incubated with DHFA and **QD-1** before (left) and after (right) two-photon irradiation at 800 nm.



(b)

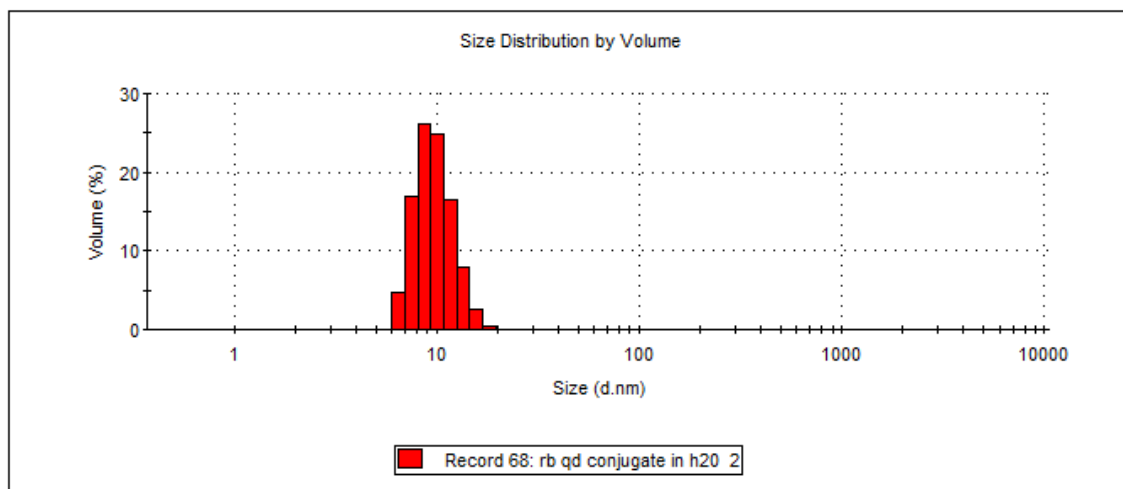


Figure S8 (a) TEM image and (b) DLS trace of **QD-1**.

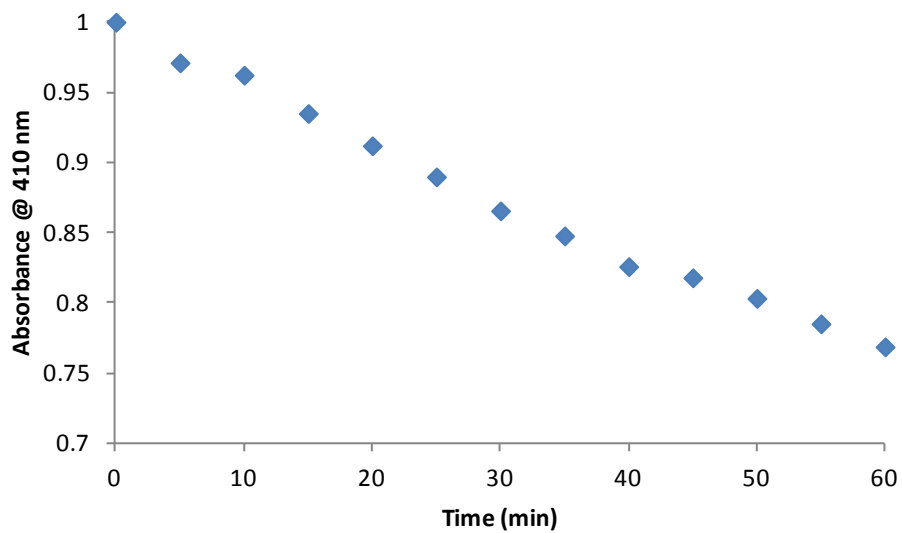


Figure S9 Plot of DPBF absorbance at 410 nm against time for a solution **QD-1** buffered at pH 6.8

Determination of FRET efficiency.

We have calculated the FRET efficiency using the following equation derived for Donor-Acceptor pairs with only one acceptor. (Tsay et al, J. Am. Chem. Soc, 2007, 129, 6865)

$$E = R_0^6 / R_0^6 + r^6$$

where: R_0 = the Förster radius i.e. the QD-PS separation distance at which energy transfer is 50% and r = actual donor acceptor distance.

Assuming multiple acceptors present on the one donor molecule the equation becomes: (Clapp et al., J. Am. Chem. Soc 2004, 126, 301)

$$E = nR_0^6 / nR_0^6 + r^6$$

where n = number of acceptors per QD.

R_0 can be calculated from the following equation:

$$R_0^6 = 8.785 \times 10^{-5} K^2 QD^0 J/n^4$$

where K^2 is the orientation factor between donor and acceptor molecules which has been established by Clapp et al as 2/3 for QD-dye conjugates, QD^0 is the quantum yield of the QD in the absence of acceptor, and n is the index of refraction, usually taken as 1.4. J is the overlap integral between the fluorescence spectrum of the donor and the molar absorption spectrum of the acceptor.

J can be calculated from the following equation:

$$J = \int F_D(\lambda) \varepsilon_A(\lambda) \lambda^4 d\lambda$$

where: F_D is the peak-normalized fluorescence spectrum of the donor and ε_A is the absorption spectrum of the acceptor.

Using these equations, an R_0 value of 43.9 Å was calculated leading to a FRET efficiency of 73.0% for 1 acceptor per QD molecule and 99.4% for 64 acceptors as determined for QD-1.