Supporting Information

Production rate and reactivity of singlet oxygen $^1O_2$ ($^1\Delta_g$) directly photoactivated at 1270 nm in lipid nanocapsules dispersed in water

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Part A-Lipid nanocapsules dispersions in D_2O and H_2O

I- DPIBF consumption rate in lipid nanocapsules dispersions in D_2O and H_2O

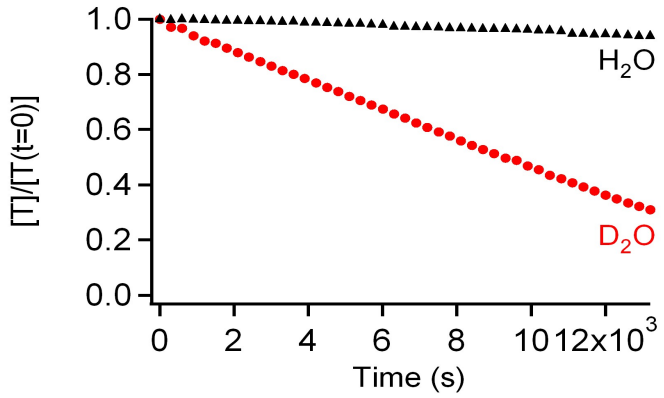

Fig S0. Normalized concentration of DPIBF-loaded LNCs upon 1270 nm irradiation at 1.2 W, for f_{LNC}=0.0017 in H_2O (black triangles) and D_2O (red circles). The slopes of the curve $\Gamma_{app}/([T_0]+\beta_{app})$ are $7.6x10^{-6}$ s^{-1} and $5.3x10^{-5}$ s^{-1} in H_2O and D_2O, respectively. DPIBF initial concentration is $140x10^{-6}$ $mol.L^{-1}$ and $120x10^{-6}$ $mol.L^{-1}$, and dissolved oxygen concentration is $2.04x10^{-4}$ $mol.L^{-1}$ and $2.46x10^{-4}$ $mol.L^{-1}$ in H_2O and D_2O, respectively. Normalized to the same 1270 nm photons flux and considering $\sigma_{d2o} = \sigma_{h2o}$, $k_{r,LNC}=2.44x10^8$ $M^{-1}.s^{-1}$, $k_{d,LNC}=2.56x10^5$ s^{-1} and singlet oxygen lifetime in H_2O and D_2O, the ratio of the two slopes is ~ 4.4 compared to a theoretical value of 4 (see Eq. 1) .

$$\frac{[^3O_2]_{d2o}}{[^3O_2]_{h2o}} x \frac{[T_0]_{h2o}+\beta_{app,h2o}}{[T_0]_{d2o}+\beta_{app,d2o}} \qquad \text{Eq. 1}$$

II-Effect of 1270 nm irradiation on LNCs

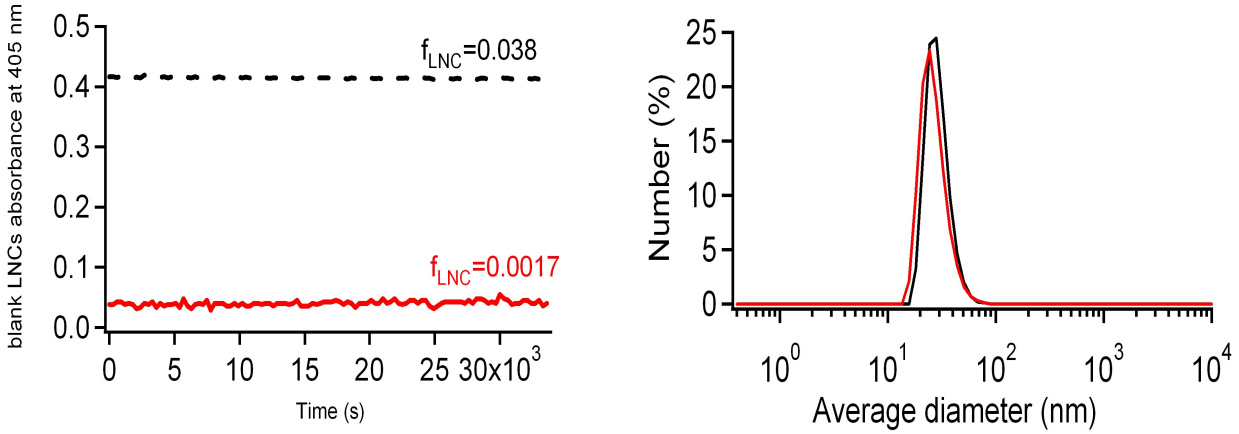

Fig S1. **(a)** Blank LNCs absorbance at 405 nm upon 1270 nm irradiation. Blank LNCs dispersed in D_2O have been irradiated at 1270 nm at a power of 1.0 W for f_{LNC}=0.0017 (red straight line) and f_{LNC}=0.038 (black dashed line). No decrease of absorbance is observed for the lower and upper range of f_{LNC}. **(b)** Average diameter of DPIBF-loaded LNCs in D_2O ($[T_0]=120x10^{-6}$ $mol.L^{-1}$, f_{LNC}=0.0017) before (black line) and after (red line) 8 h 1270 nm irradiation at 1.0 W. Measurements have been performed using dynamic ligth scattering with a Zetasizer® Nano ZS (Malvern Instrument S.A., Worcestershire, U.K). LNCs average diameters are quiet identical before and after irradiation.

III-Formation of two oxidation productsduring 1270 nm irradiation

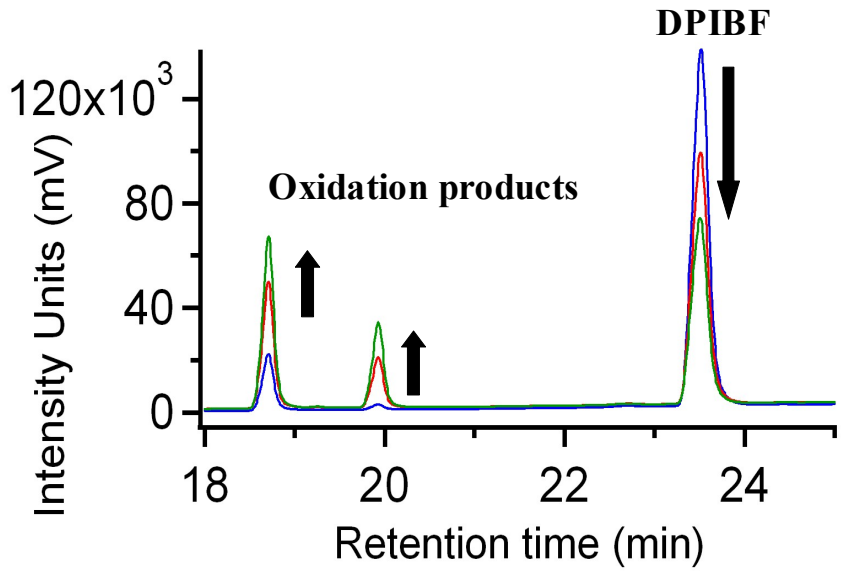

Fig S2. HPLC chromatograms of DPIBF-loaded LNCs in D_2O with $[T_0]=120x10^{-6}$ mol.L^{-1} for $f_{LNC}=0.006$ before and after 1270 nm irradiation at 1.0 W (detection at 215 nm). Non irradiated (blue line), 1 h (red line) and 2 h (green line) irradiated dispersions have been analysed. 28 % and 47% of DPIBF is degraded for 1 h and 2 h irradiation, respectively. Two products of oxidation are formed and their proportions increase with irradiation time.

IV-DPIBF and oxidation products leakage outside LNCs

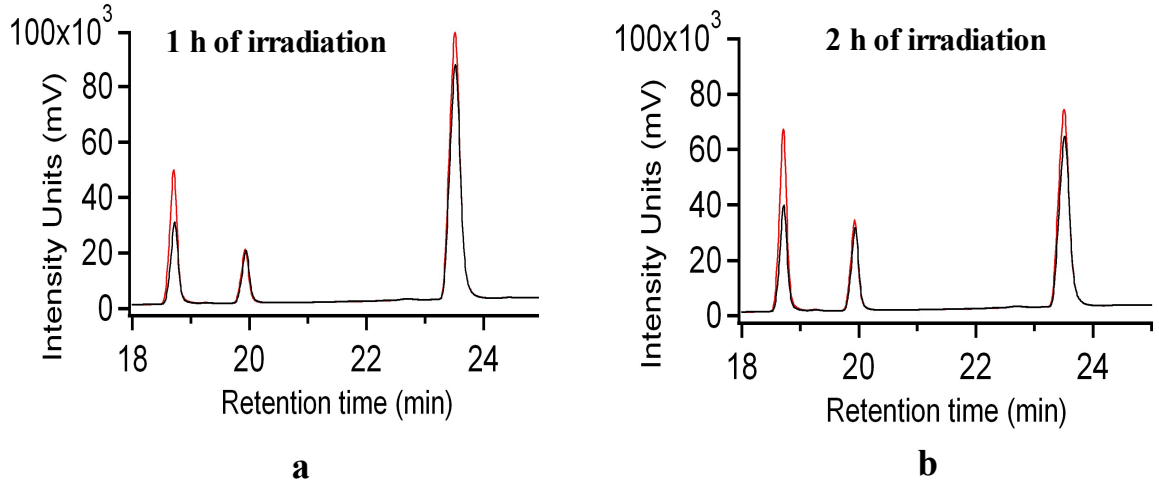

Fig.S3.HPLC chromatograms of DPIBF-loaded LNCs in D_2O for $f_{LNC}=0.006$ with $[T_0]=120x10^{-6}$ mol.L^{-1} after 1 h **(a)** or 2 h **(b)** 1270 nm irradiation at 1.0 W (detection at 215 nm). Irradiated dispersions (red line) and filtrated dispersions (black line) of LNCs have been analysed. Approximatively 90% of DPIBF is found inside LNCs after 1 h or 2 h irradiation. The most hydrophobic oxidation product is found predominantly inside LNCs (at 95%). The most hydrophilic one is found at 60% inside LNCs.

Part B-Solutions of RTC in D_2O

V-Effect of oxidation product on $^1O_2$ production rate

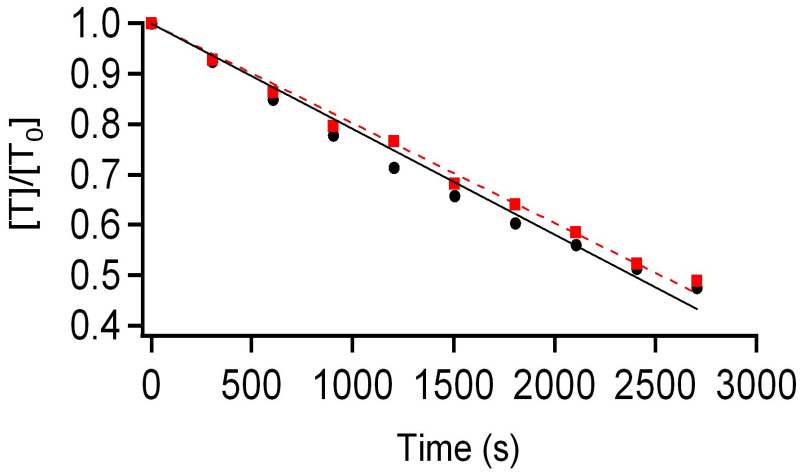

Fig S4. Normalized RTC concentration in D_2O saturated with oxygen with $[T_0]=100x10^{-6}$ mol.L^{-1} upon 1270 nm irradiation experiment at 1.1 W (red squares). Once all RTC has been degraded, the same amount of RTC is newly dissolved in the solution containing the oxidation products. Then this solution is irradiated a second time at the same IR power (black circles). The slopes of the curve are $1.98x10^{-4}$ s^{-1} ± 2% compared to $2.1x10^{-4}$ s^{-1} ± 2% for the first and the second experiment, respectively.

VI-Effect of dissolved oxygen concentration on $^1O_2$ production rate

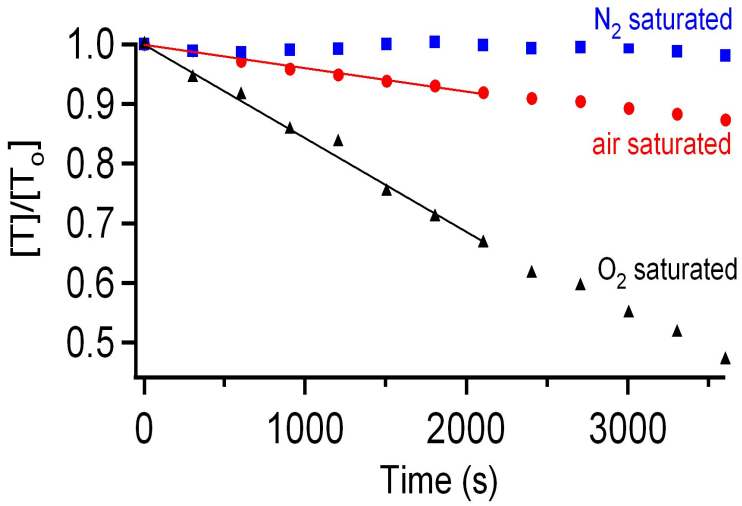

Fig S5. Normalized RTC concentrations in D_2O with $[T_0]=105x10^{-6}$ mol.L^{-1}saturated with air (red circles), oxygen (black triangles) and nitrogen (blue squares) have been irradiated at 1270 nm at the power of 1.0 W. No RTC disappearance is observed for the solution saturated with N_2. Singlet oxygen production rates are $6.76x10^{-9}$ $M^{-1}.s^{-1}$ and $3.43x10^{-8}$ $M^{-1}.s^{-1}$ in solutions saturated with air and oxygen respectively, then $^1O_2$ production rate is increased by ~ 5 when the solution is saturated with oxygen.