Electronic Supplementary Material (ESI) for RSC Advances.

Morphology effects on singlet oxygen production and bacterial photoinactivation efficiency by different silica-Protoporphyrin IX nanocomposites

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Supporting equation

$$mol_{(PpIX)}/mg_{(Si)} = \frac{(\frac{Abs_0 - Abs_t}{\varepsilon_{405}}) \times V}{mg_{Si}}$$

(Eq. S1)

Abs$_0$: *absorption values at 405 nm of PpIX starting solution.*

Abs$_t$: *absorption values at 405 nm of the supernatant collected after the anchoring procedure.*

ε_{405}: *PpIX extinction coefficient in DMF at 405 nm.*

V: *volume.*

mg$_{Si}$: *silica weight in milligram added to PpIX solution.*

Supporting figures

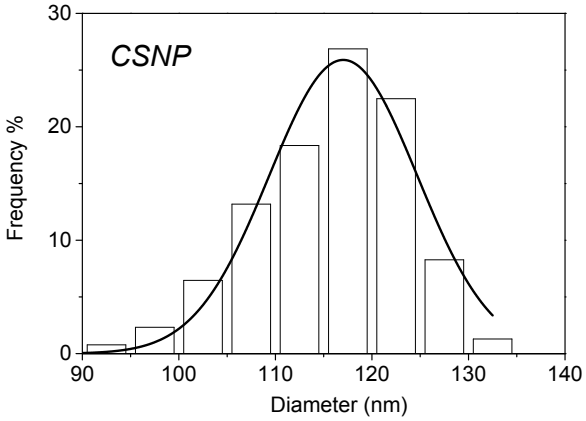

Figure S1. TEM size distribution for CSNP, counting approximately 300 nanoparticles; average diameter 117 nm (σ = 7.1).

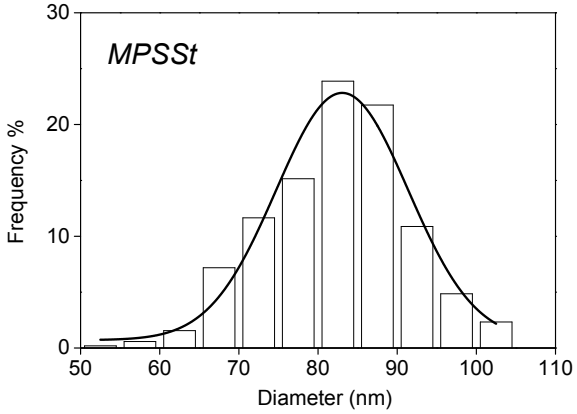

Figure S2. TEM size distribution for MPSSt, counting approximately 300 nanoparticles; average diameter 83 nm (σ = 8.8).

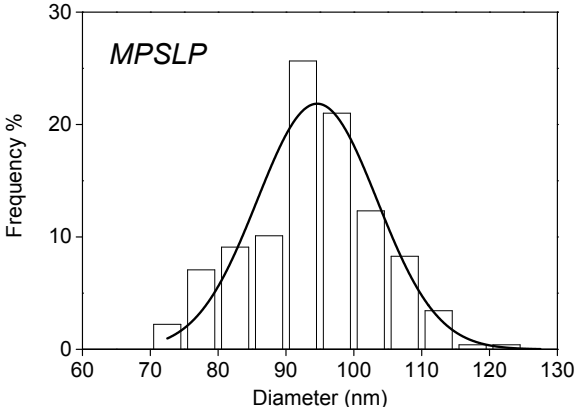

Figure S3. TEM size distribution for MPSLP, counting approximately 300 nanoparticles; average diameter 94 nm (σ = 8.8).

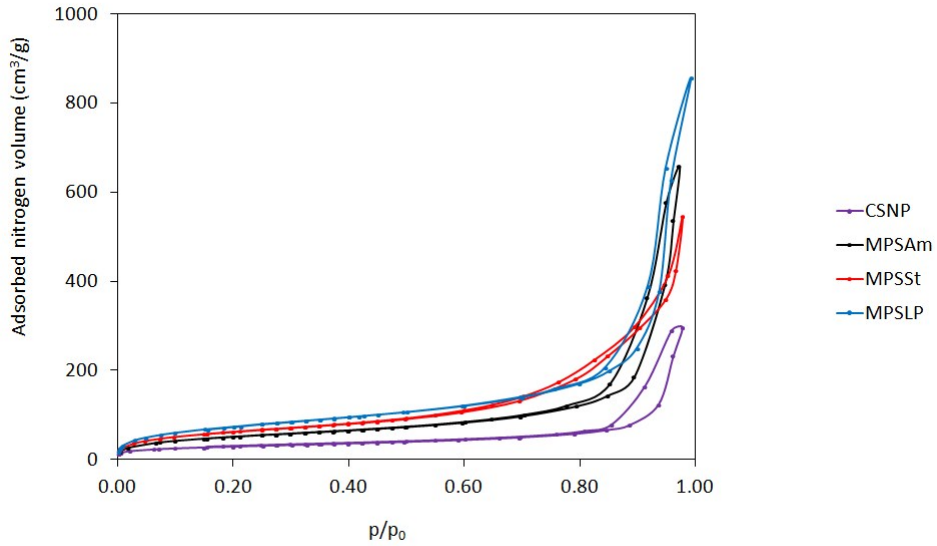

Figure S4. Nitrogen adsorption and desorption isotherms, at 77K, of the indicated samples.

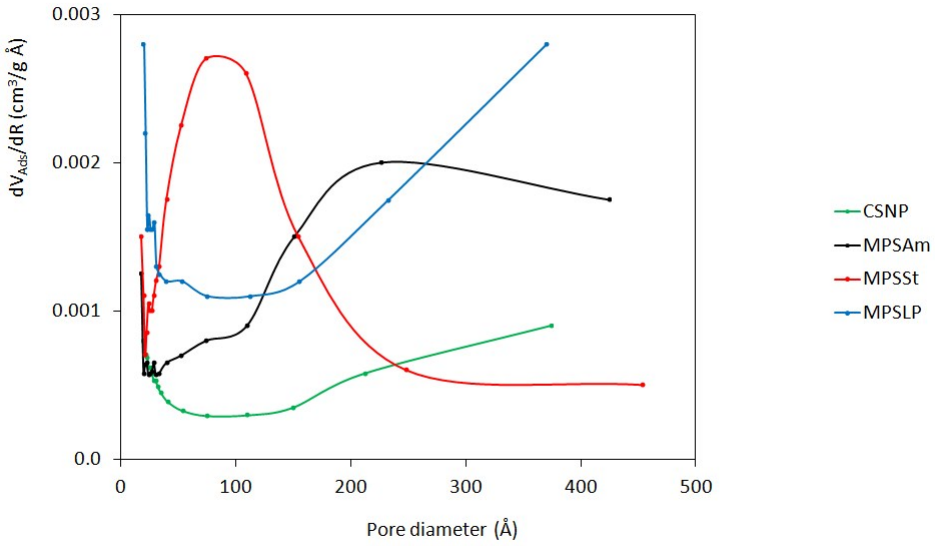

Figure S5. Pore size distribution calculated from nitrogen adsorption data of the indicated samples.

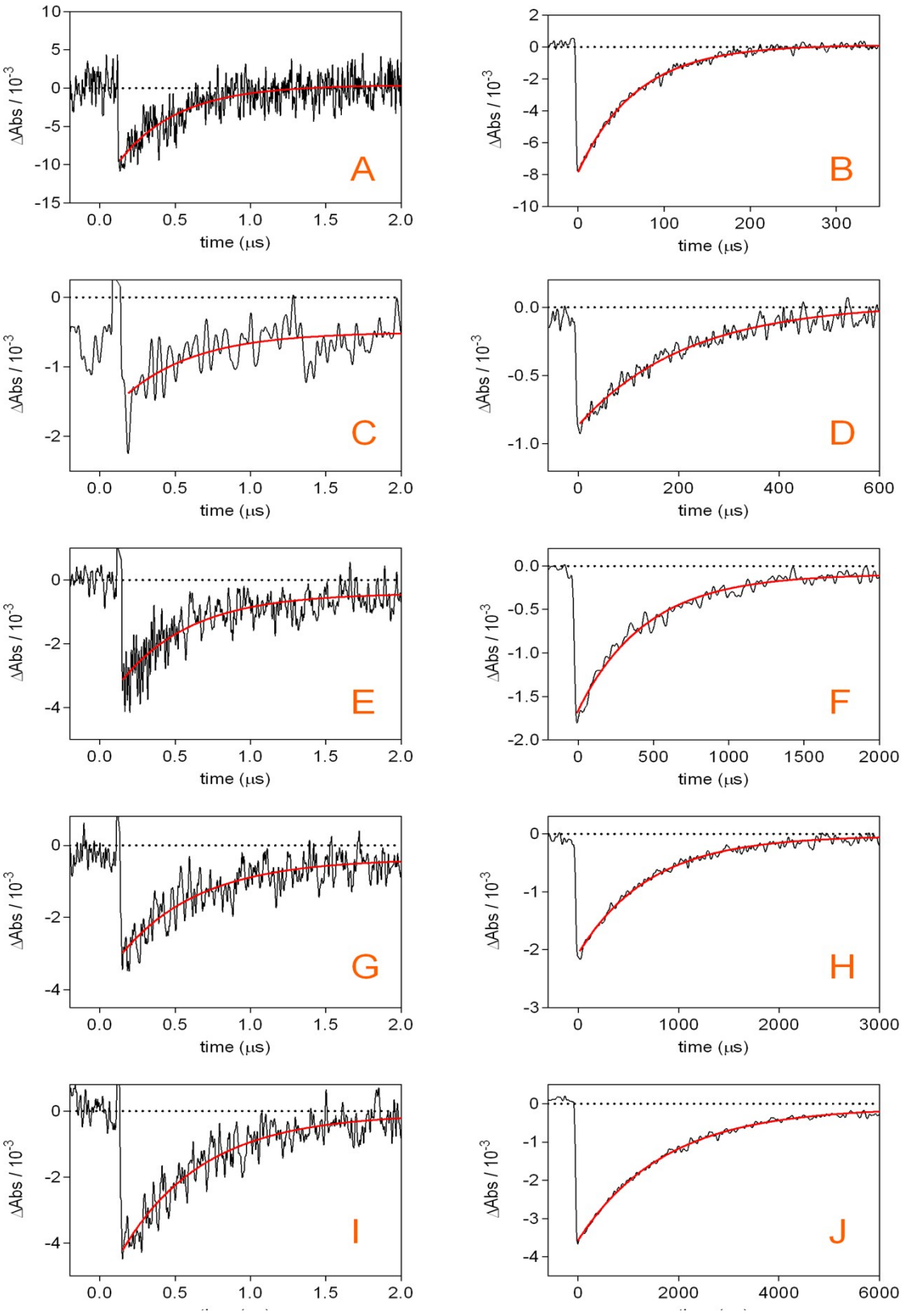
A
B
C
D
E
F
G
H
I
J
ΔAbs / 10-3
time (μs)

Figure S6. Transient absorption signals from PpIX, PpIX-CSNP, PpIX-MPSAm, PpIX-MPSSt and PpIX-MPSLP in air (A,C,E,G,I) and argon-saturated condition (B,D,F,H,J). Observation wavelength 410 nm.

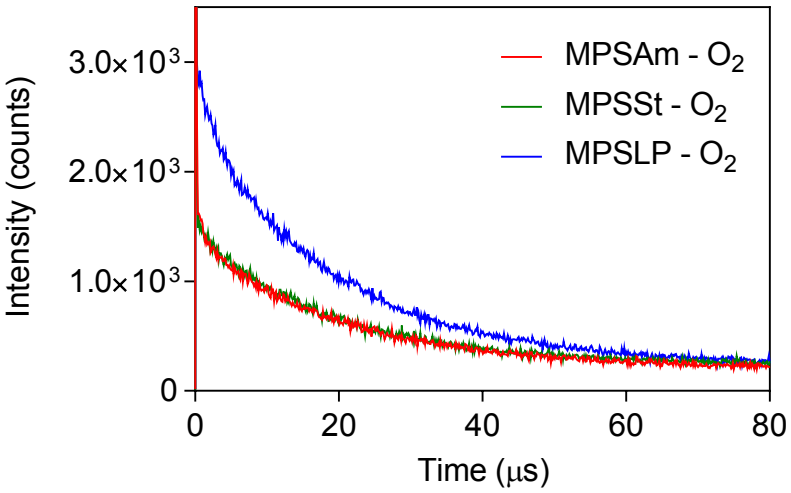

Figure S7. Time-resolved phosphorescence decays at 1270 nm for PpIX-MPSAm, PpIX-MPSSt, PpIX-MPSLP in DMF under oxygen saturated conditions.

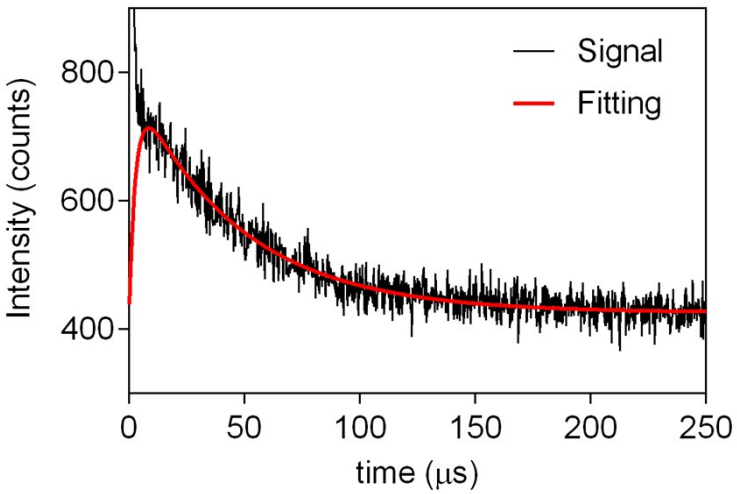

Figure S8. Time-resolved phosphorescence decay at 1270 nm for PpIX-MPSLP in D_2O.

Supporting tables

Table S1. Surface area, mesopore volume, ζ-potential values and relative PpIX quantity per mg of silica, for silica samples.

Sample	Surface area (m^2/g)	Mesopore volume (cm^3/g)	ζ-potential of SiO_2-NH_2 (mV)	Concentration ($nmol_{PpIX}/mg_{silica}$)	ζ- potential of SiO_2-NH_2PpIX (mV)
CSNP	102	0.13	34.3 ± 0.8	1.01 ± 0.04	30.2 ± 0.9
MPSAm	184	0.52	23.4 ± 0.6	0.74 ± 0.03	27.0 ± 0.2
MPSSt	228	0.48	12.3 ± 0.5	0.60 ± 0.02	15.1 ± 0.2
MPSLP	272	0.44	- 0.32 ± 0.13	0.64 ± 0.02	- 5.2 ± 0.2

The specific surface area was determined by the Brunauer, Emmett and Teller (B.E.T.) technique [S. Brunauer, P. H. Emmett and E. Teller, J. Am. Chem. Soc., 60 (1938) 309–319]; mesopore volume was calculated by the BJH method [E. P. Barrett, L. G. Joyner and P. P. Halenda, J. Am. Chem. Soc., 73 (1951) 373–380].

Table S2. PpIX triplet lifetimes in different systems, in air and argon-saturated environment.

System	Air	Argon
$PpIX_{solution}$	0.4 μs	70 μs
PpIX-CSNP	0.3 μs	200 μs
PpIX-MPSAm	0.4 μs	450 μs
PpIX-MPSSt	0.4 μs	720 μs
PpIX-MPSLP	0.4 μs	1.7 ms

Table S3. Fitting parameters obtained from the analysis of singlet oxygen phosphorescence decays sensitized by mesoporous suspensions under oxygen-saturated condition.

Conjugate	$S_{0,1}$ (%)	$S_{0,2}$ (%)	$\tau_{\Delta 1}$ / μs	$\tau_{\Delta 2}$ / μs
PpIX-MPSAm	93%	7%	21.0	3.1
PpIX-MPSSt	92.1%	7.9%	19.2	1.6
PpIX-MPSLP	82%	18%	19.8	2.2

Table S4. Silica and PpIX concentration of each system used in bacterial inactivation.

System	Silica concentration (mg/mL)	PpIX concentration (μM)
PpIX-CSNP	2	2.0
PpIX-MPSAm	2	1.5
PpIX-MPSSt	2	1.2
PpIX-MPSLP	2	1.3