Stable "snow lantern-like" aggregates of silicon nanoparticles suitable as a drug delivery platform

Supporting information

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1. Theoretical surface area estimation from particle size

Surface area calculations for a spherical particle were done using the density of Si, ρ = 2.329 g/cm^3, in the following expression

$$A = 4\pi r^2 = \left(\frac{4}{3}\pi r^3\right)\frac{3}{r} = V\ \frac{3}{r} = \left(\frac{m}{\rho}\right)\frac{3}{r} = \left(\frac{m}{\rho}\right)\frac{6}{d} \quad (1)$$

where A is the surface area, V is the volume, r is the radius, d is the diameter, m is the mass and ρ is the density of a sphere. An expression for area per mass (as measured by nitrogen adsorption) is then

$$\frac{A}{m} = \frac{6}{\rho\, d} \quad (2)$$

An expression for the sphere diameter, when the area per mass is known, is then

$$d = \left(\frac{A}{m}\right)^{-1}\frac{6}{\rho} \quad (3)$$

2. Results

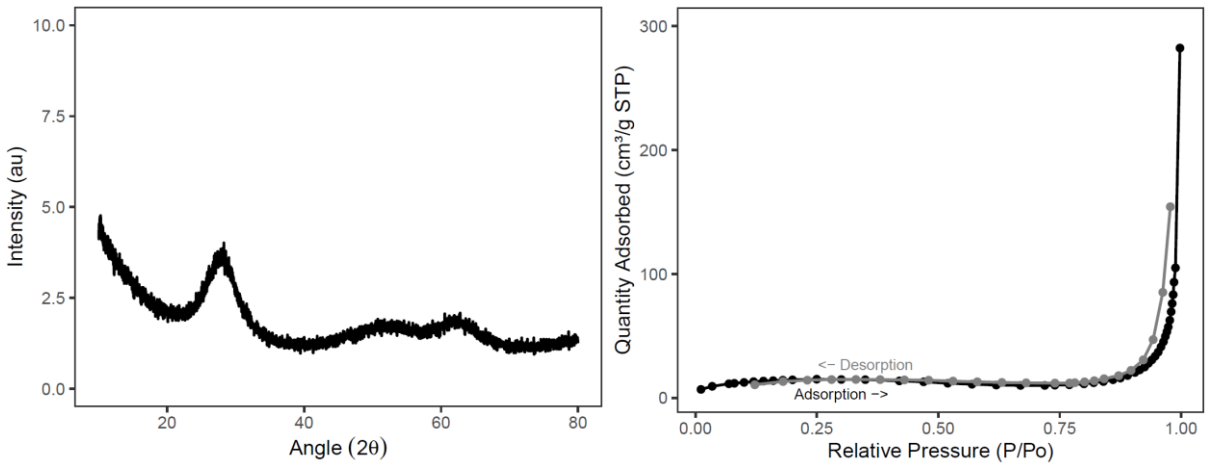


Figure SI1. X-ray diffraction data (left) and nitrogen sorption isotherm data (right) of the cCVD Si aggregate snow-lantern particles showing mesoporous material with amorphous halos and no sharp crystalline peaks.

Diameter (nm)	**Surface area (m^2/g)**
500	5
200	13
100	26
50	52
43	60
40	65
30	86
20	129
10	258
5	516

Table SI1. Theoretical surface area calculations of spherical particles of the given diameters, calculated from A/m = 6/(ρxd), with the density of Si = 2.329 g/cm^3, where A/m is equivalent to the surface area per mass (m^2/g).

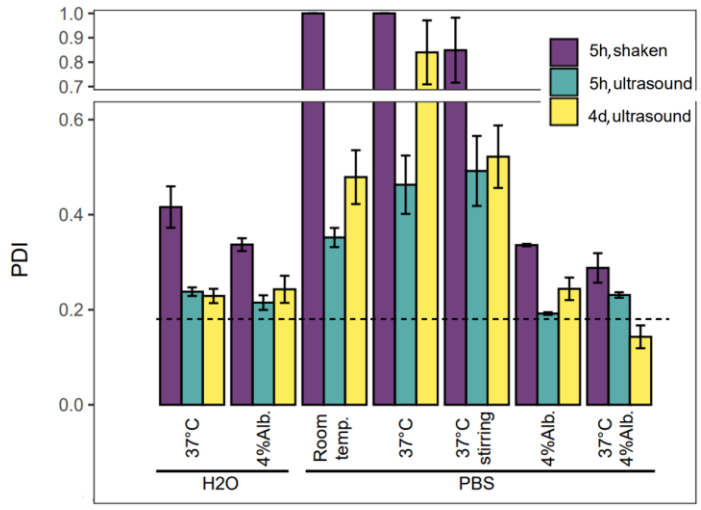


Figure SI2. Colloidal stability of cCVD Si particles. Polydispersity index (PDI) of cCVD particles in different solutions, measured by DLS after hand shaking or ultrasonication treatment after 5 hours or 4 days incubation. Dashed line indicates control sample in water (diameter = 210 nm and PDI = 0.2). Alb. = human serum albumin.

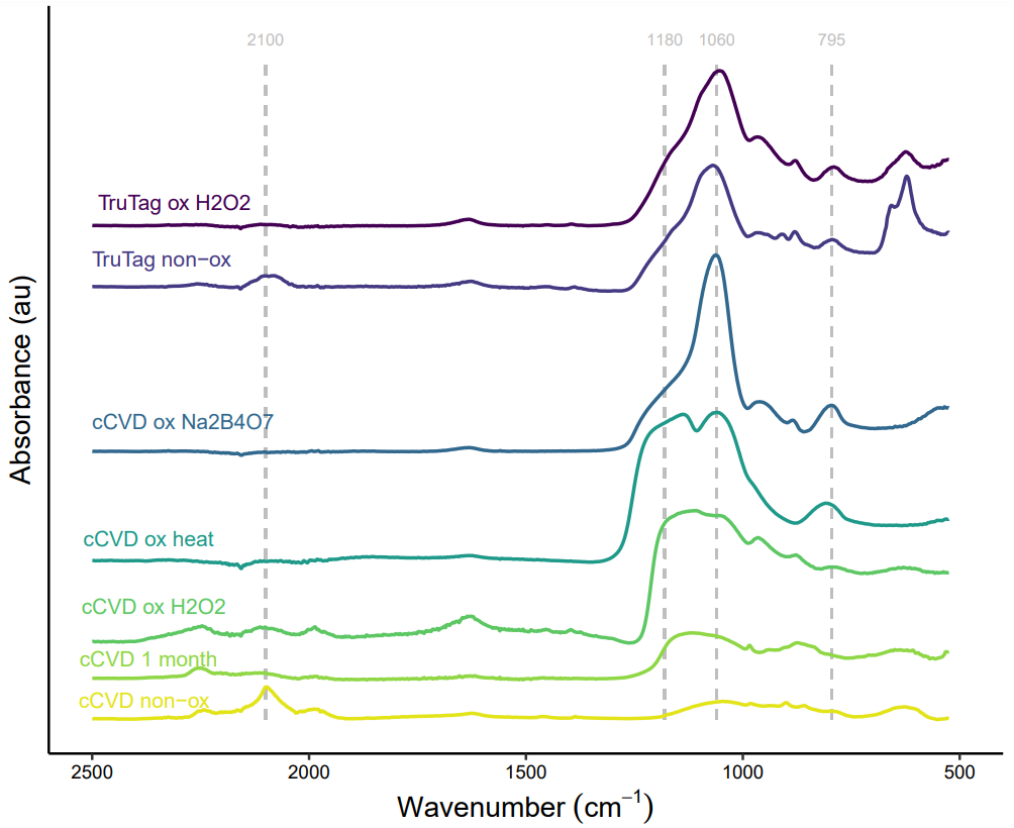


Figure SI3. FTIR spectra of cCVD and TruTag Si particles, non-oxidized (non-ox) and oxidized (ox) samples using the indicated oxidation techniques.

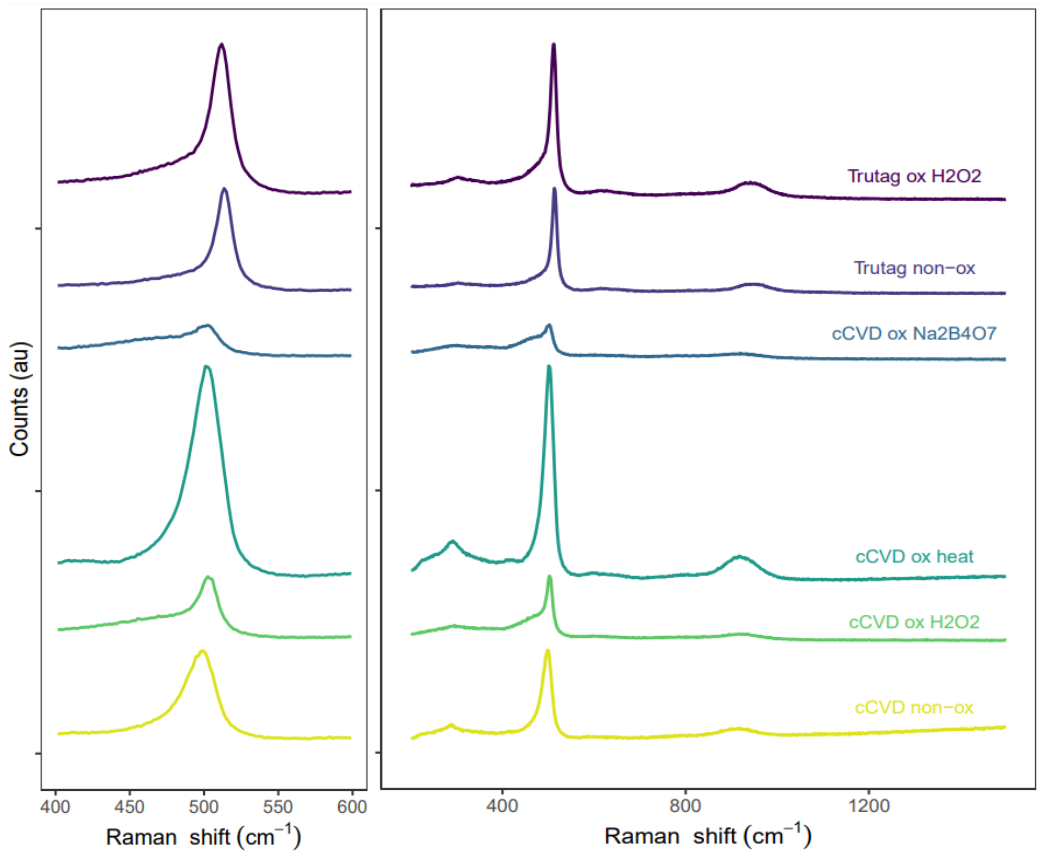
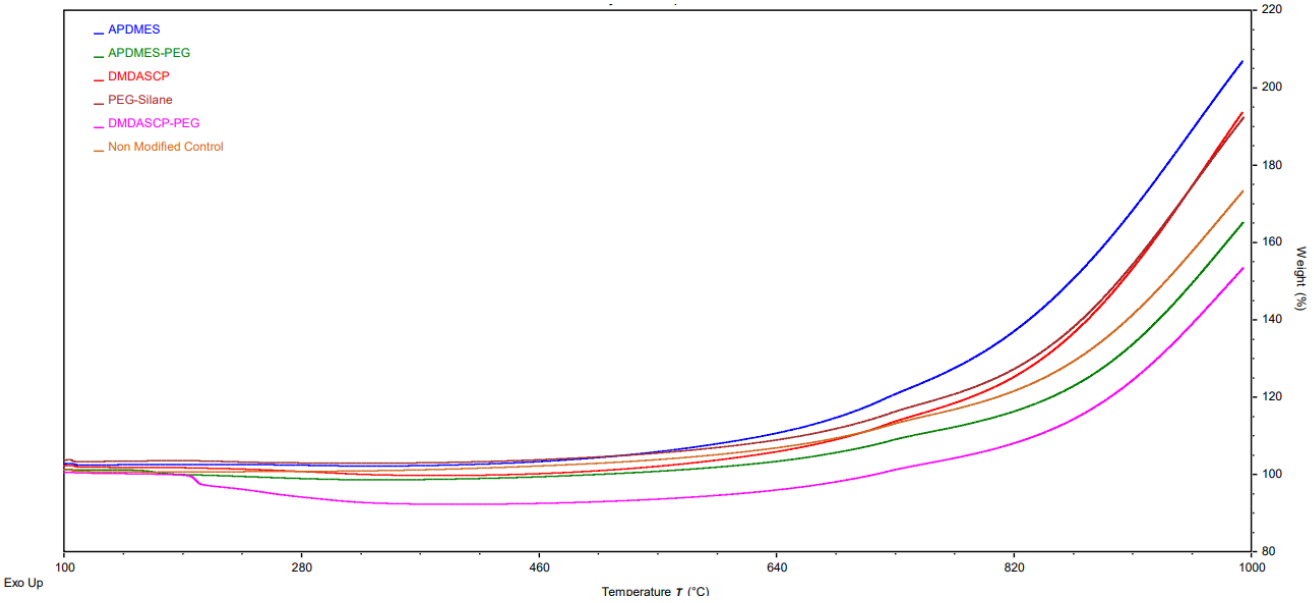


Figure SI4. Raman spectra comparing cCVD and TruTag Si particles, non-oxidized (non-ox) and oxidized (ox) samples using the indicated oxidation techniques.



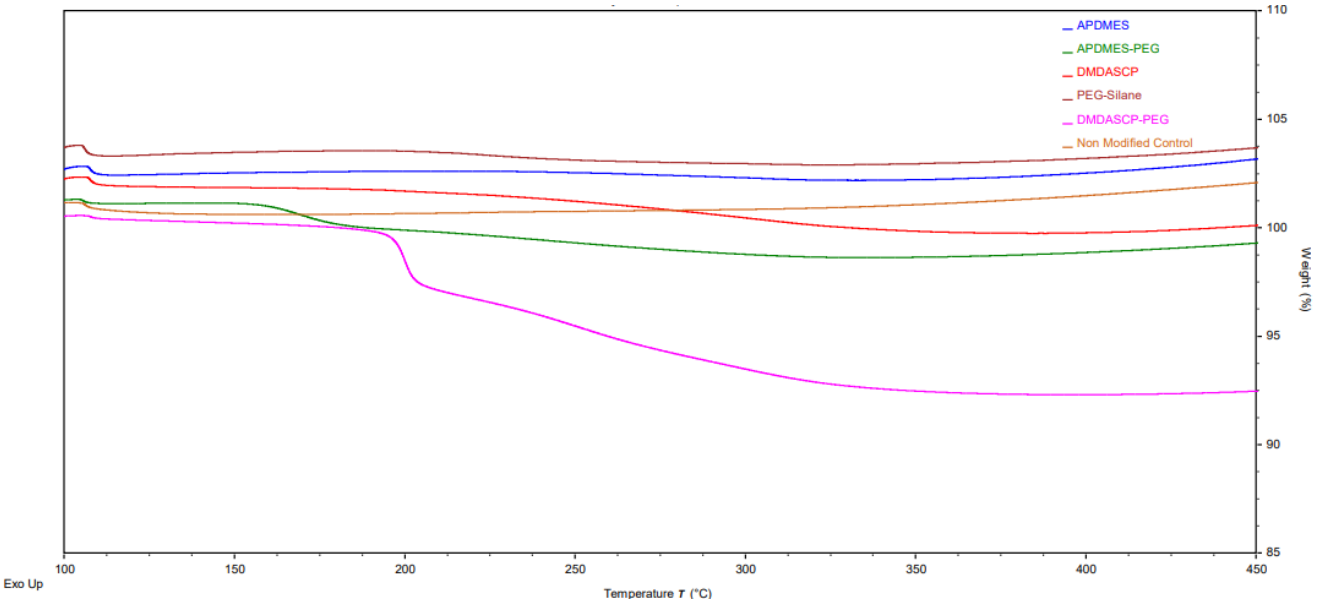


Figure SI5. TGA data from the H_2O_2-oxidized cCVD Si particle samples with different organic surface modifications, as indicated. The top panel shows the full temperature range (100-1000°C), and the bottom panel shows the same data in the temperature range of 100-450°C.

Surface modification	**Linker content (wt%)**	**PEG content (wt%)**	**Calculated linker density (µmol/ m^2)**	**Calculated PEG density (µmol/ m^2)**
DMDASCP-PEG	5.1	2.8	4.72	0.10
APDMES-PEG	1.8	1.1	1.90	0.04
DMDASCP	1.9	-	1.70	-
APDMES	0.4	-	0.42	-
mPEG-silane	-	0.4	-	0.01

Table SI2. Organic content (weight%) of different modified samples calculated from the TGA curves of Figure SI5. The grafting densities (no. of molecules per surface area) were calculated from the molecular weight of each organic component, the weight% of linker or PEG (from TGA) for each sample and the Si particle surface area of 59.8 m^2/g (Table 1).

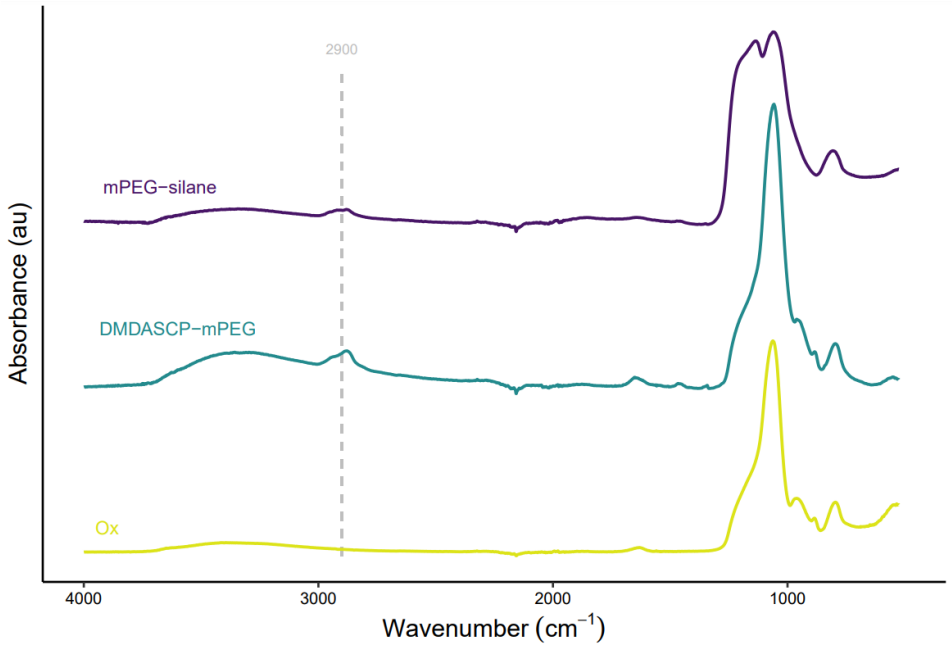


Figure SI6. FTIR spectra of cCVD Si particles modified by H_2O_2-oxidation (ox) and with DMDASCP-mPEG or mPEG-silane.

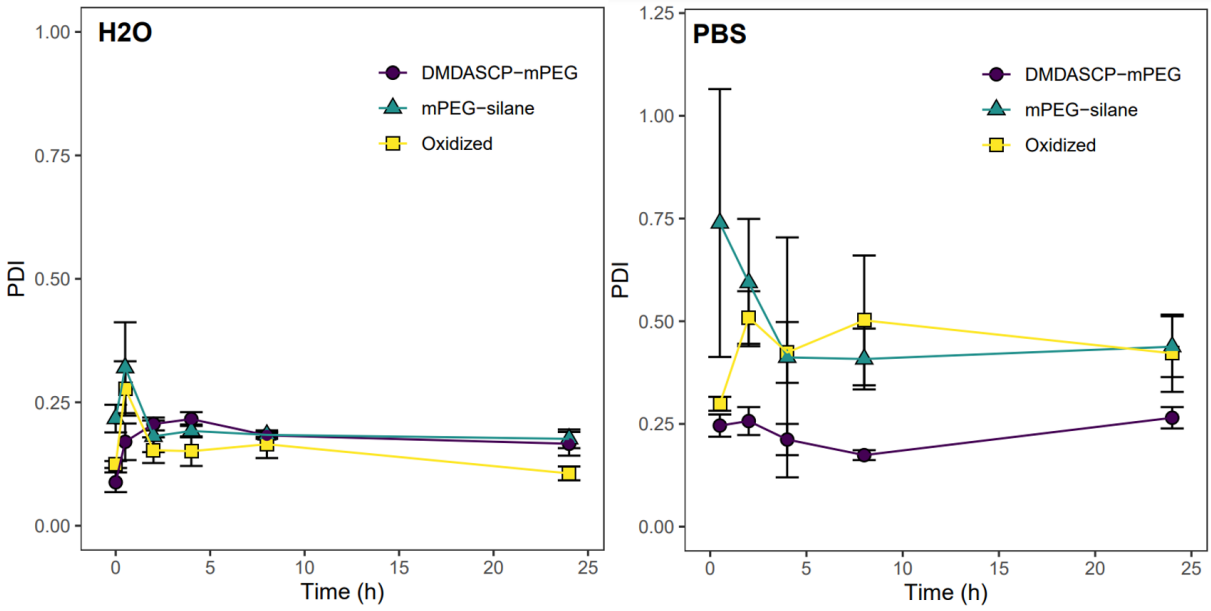


Figure SI7. Colloidal stability of pristine and PEGylated particles in water (left) and PBS (right) over 24 hours. Polydispersity index as measured by DLS. The data are shown as the average of three measurements with error bars showing standard deviations.

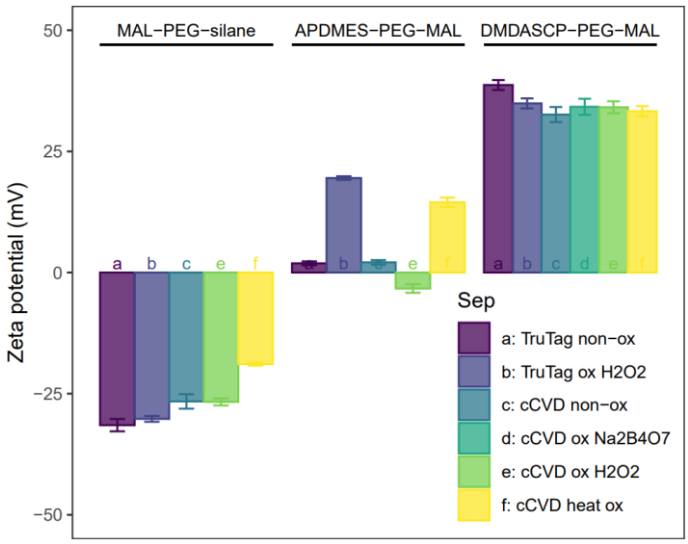


Figure SI8. Zeta potential of PEG-MAL modified cCVD and TruTag Si particles oxidized by different methods.

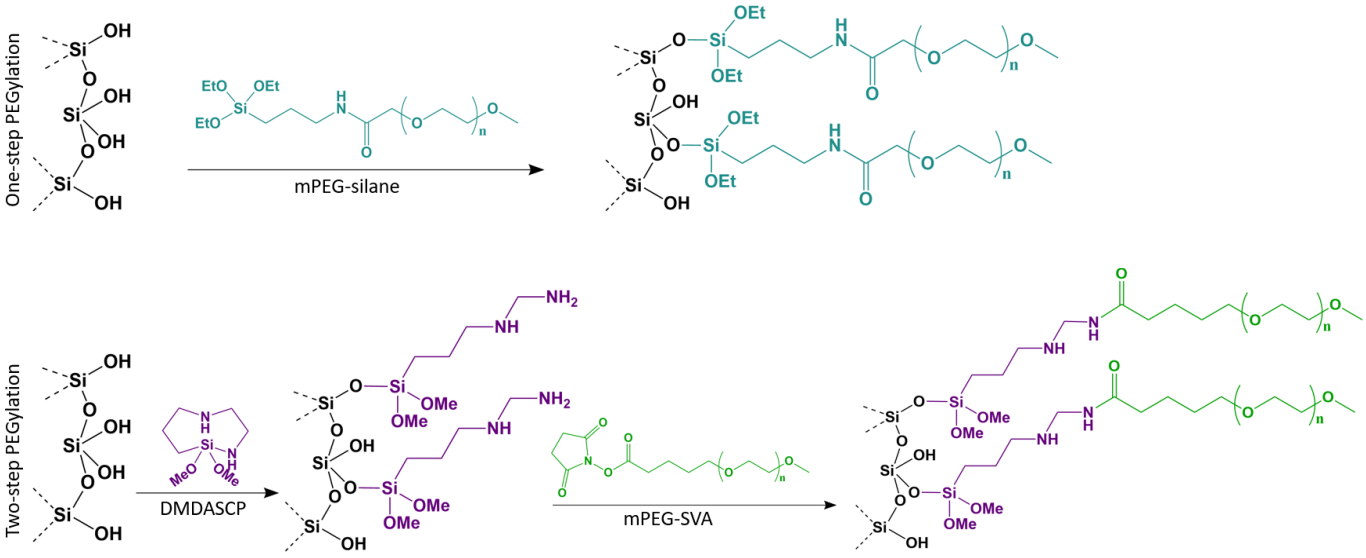


Figure SI9. Schematic illustration of the one-step (mPEG-silane) and two-step (DMDASCP-mPEG) PEGylation routes.