

## Supplementary material for

### Engineering mesoporous silica nanoparticles for improved oral delivery of Vancomycin

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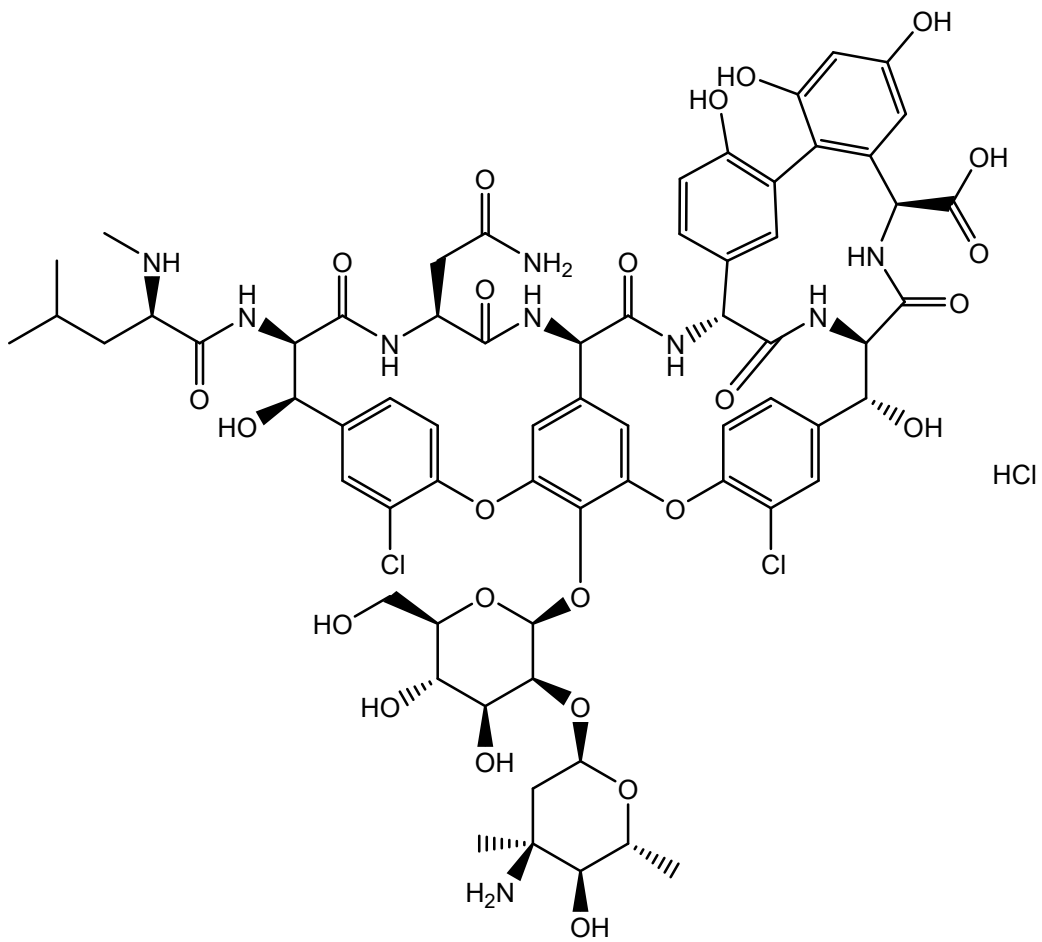
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New South Wales, Australia

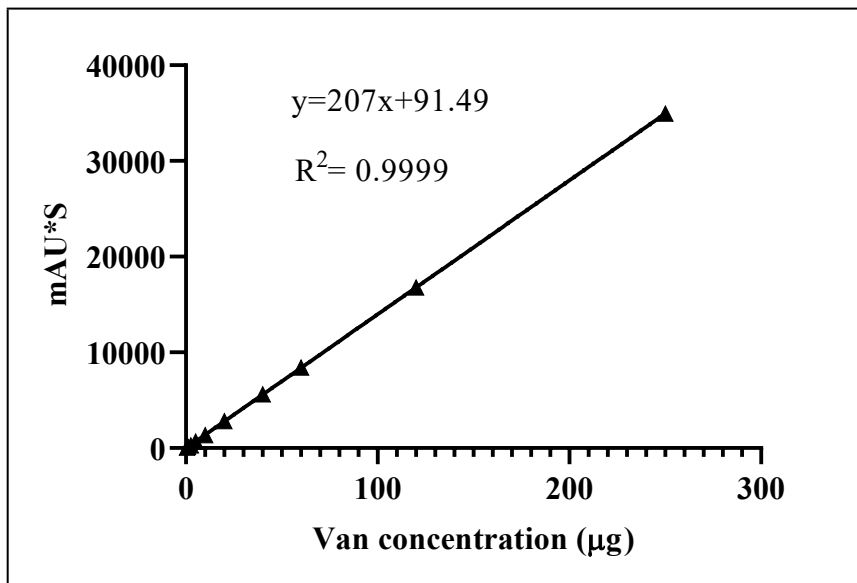
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Queensland 4072 Australia

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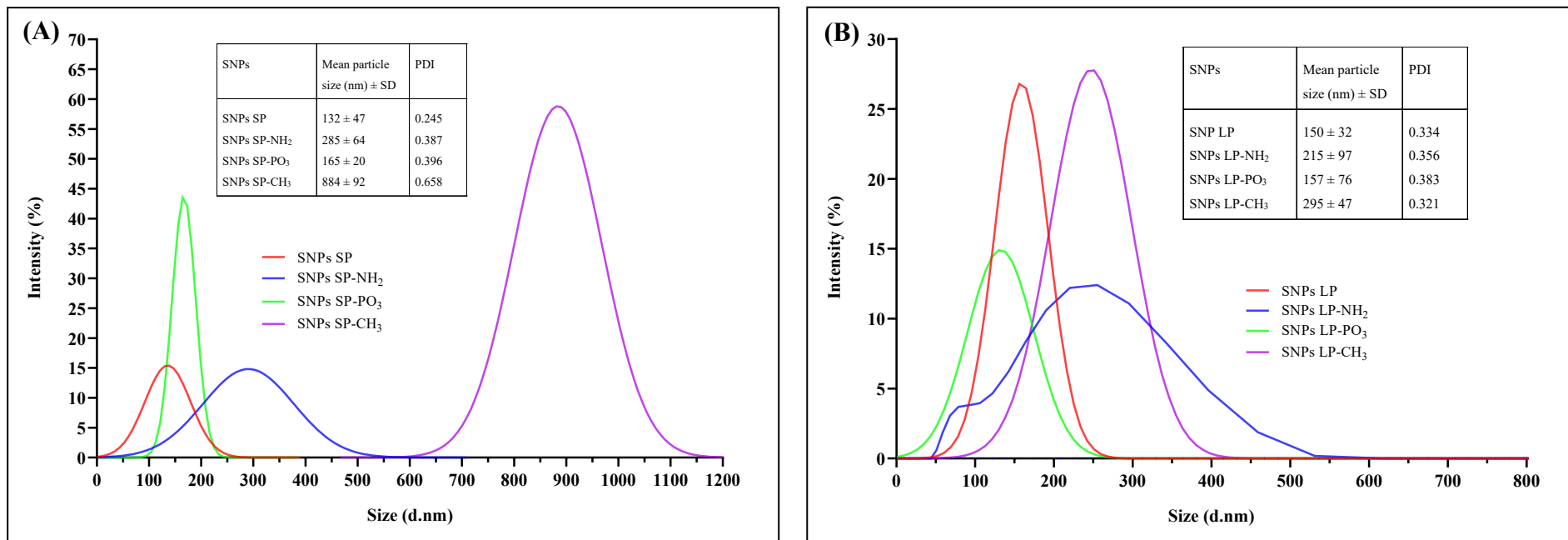
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**Figure S1.** Molecular structure of Vancomycin hydrochloride

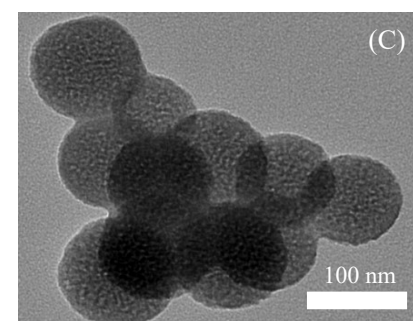
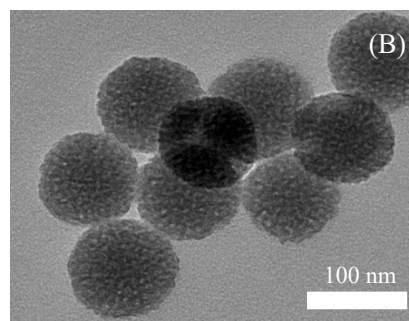
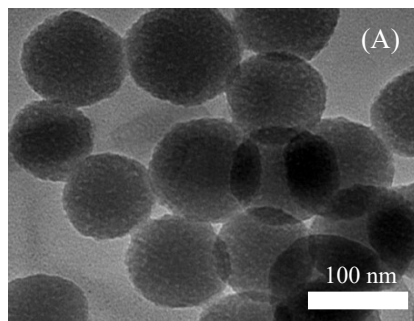


**Figure S2.** Calibration curve of Vancomycin

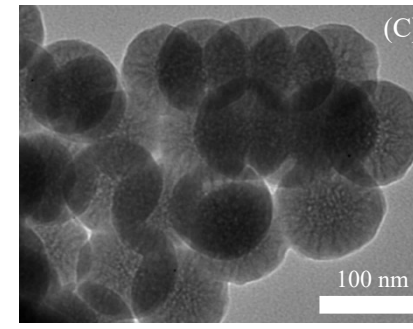
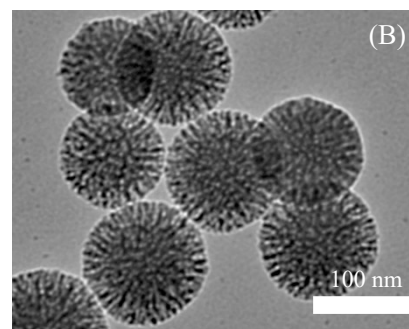
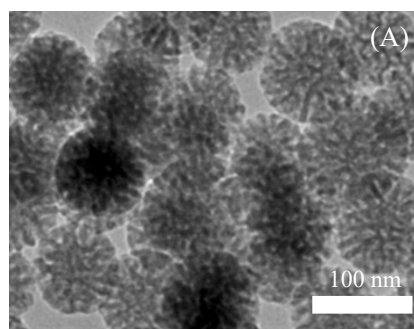


**Figure S3.** Size distribution (by intensity) of SNPs with/without functional groups. (A) SNPs SP and (B) SNPs LP. Each individual peak on the graph represents one measurement

Functionalised SNPs SP

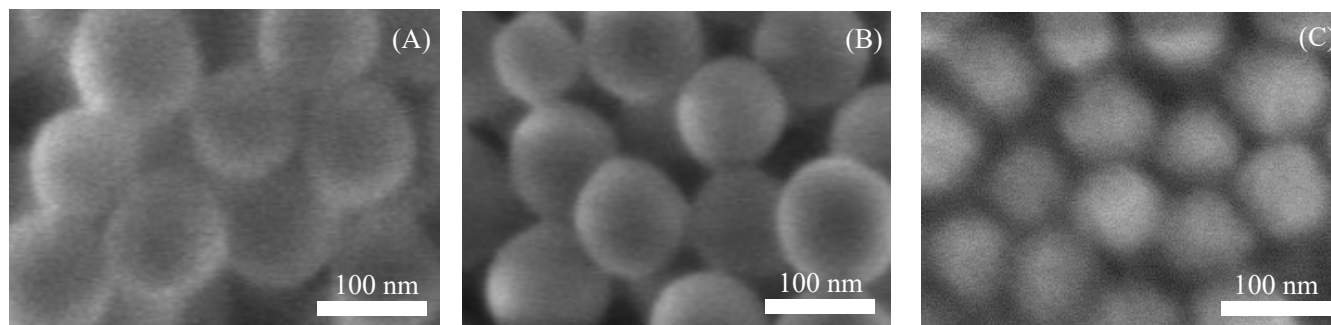


Functionalised SNPs LP

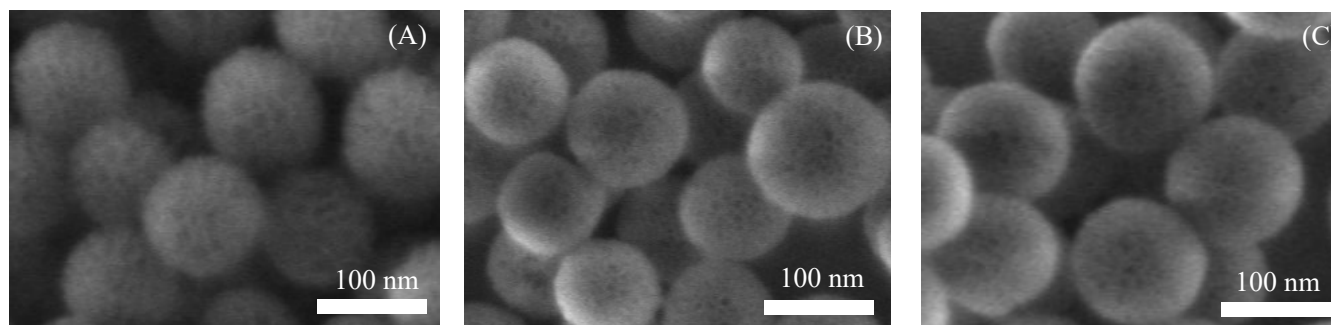


**Figure S4.** TEM images of (A) SNPs-NH<sub>2</sub>, (B) SNPs-PO<sub>3</sub> and (C) SNPs-CH<sub>3</sub>

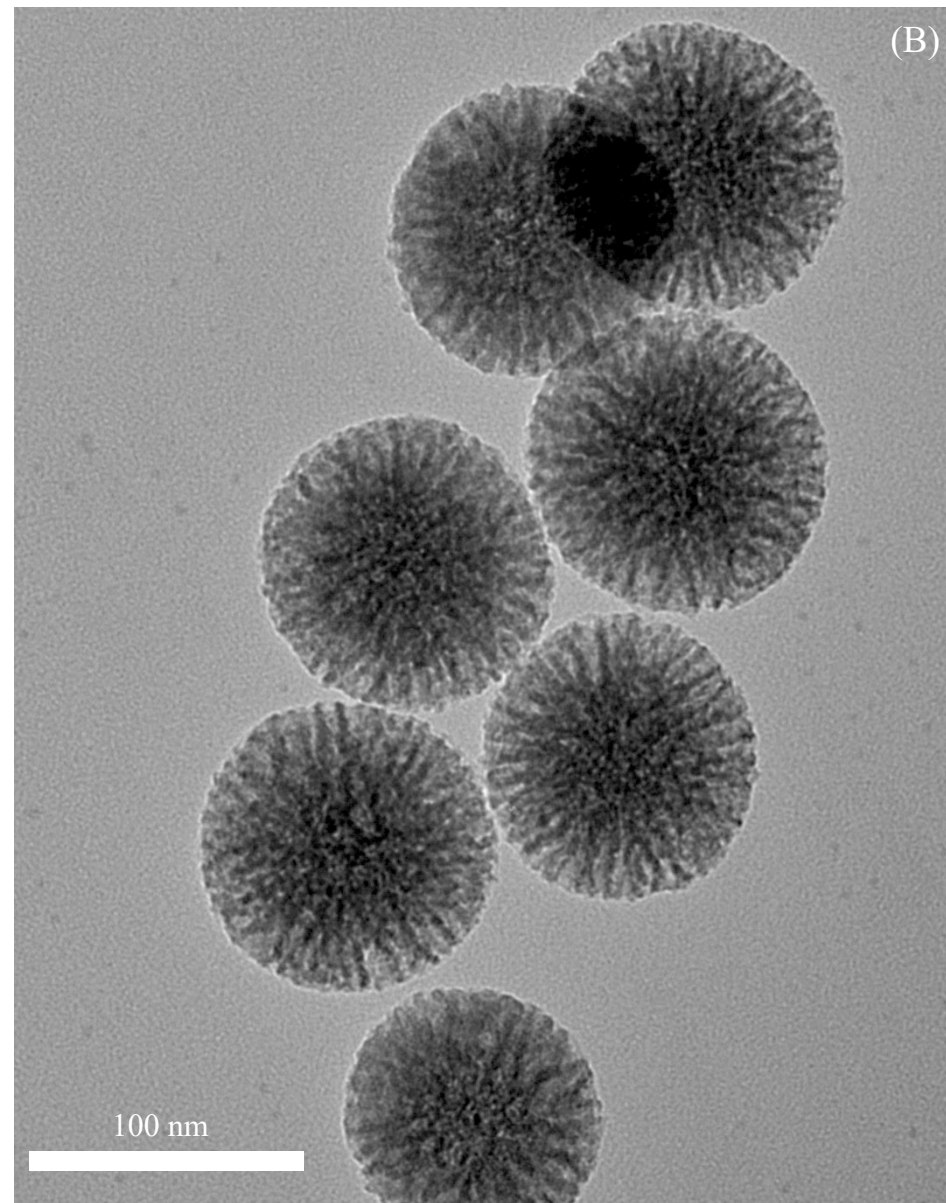
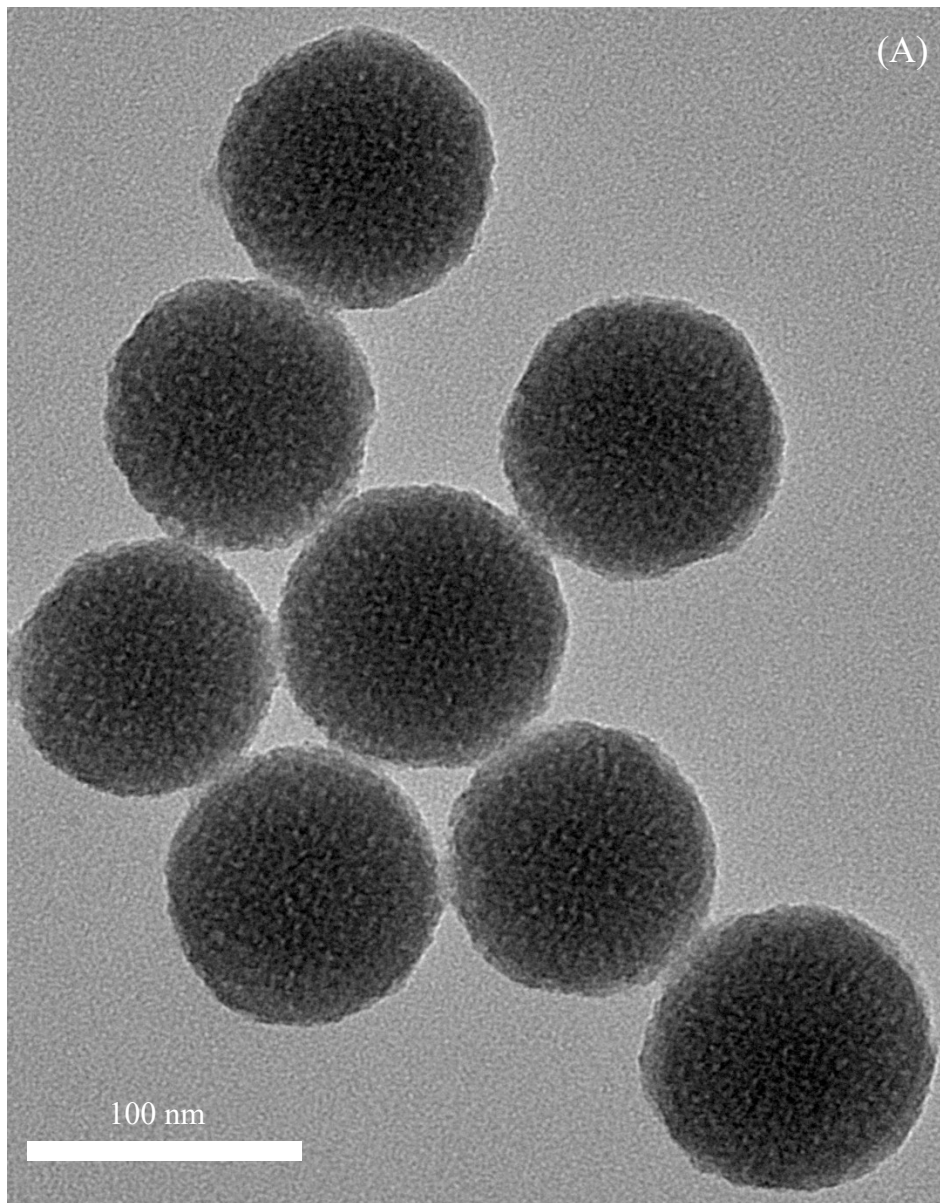
Functionalised SNPs SP



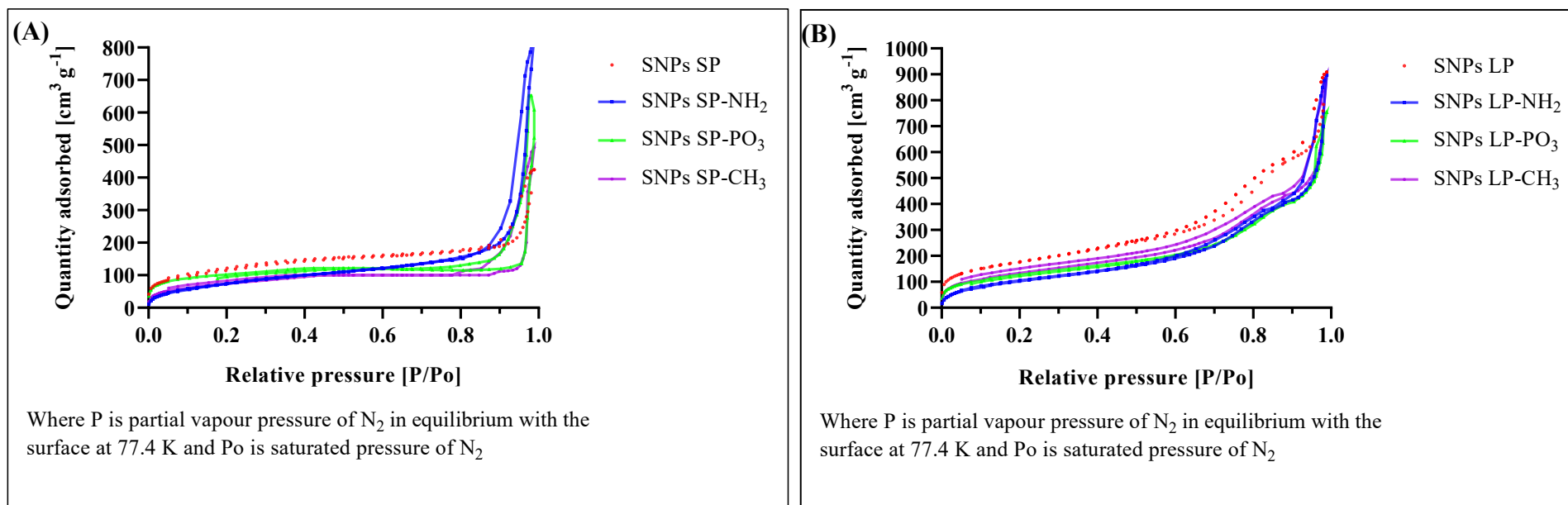
Functionalised SNPs LP



**Figure S5.** SEM images of (A) SNPs-NH<sub>2</sub>, (B) SNPs-PO<sub>3</sub> and (C) SNPs-CH<sub>3</sub>

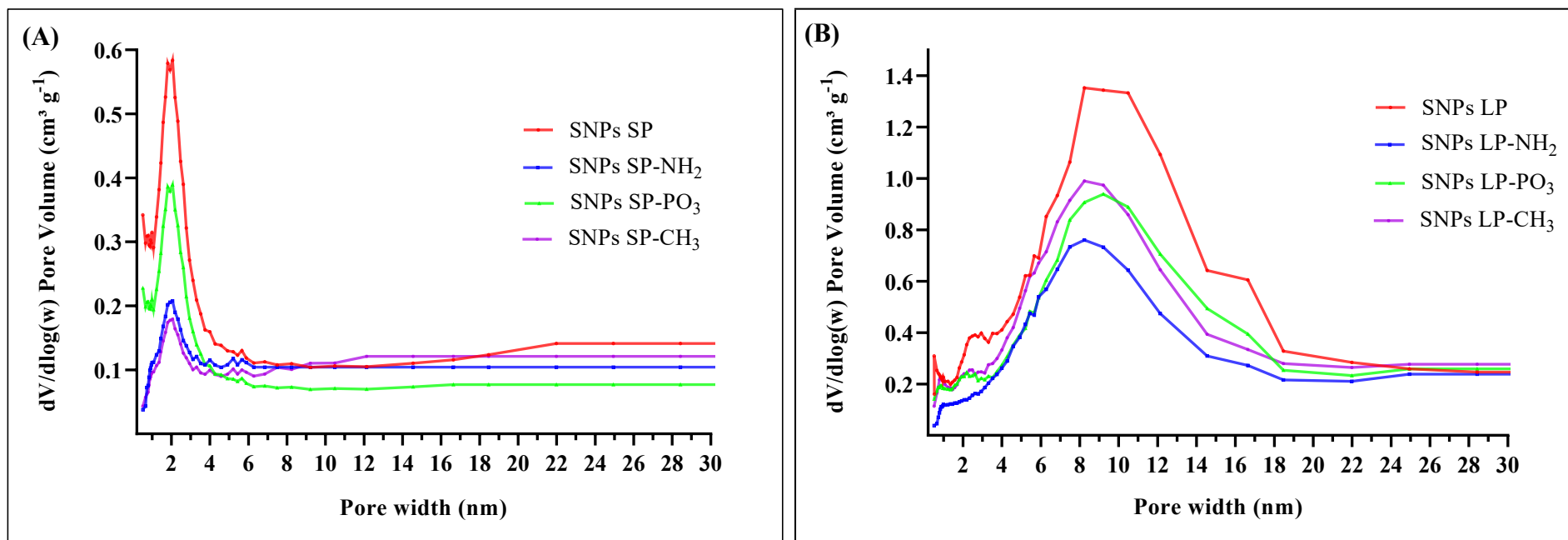


**Figure S6.** TEM images of (A) SNPs SP and (B) SNPs LP showing SNPs rough outer surfaces

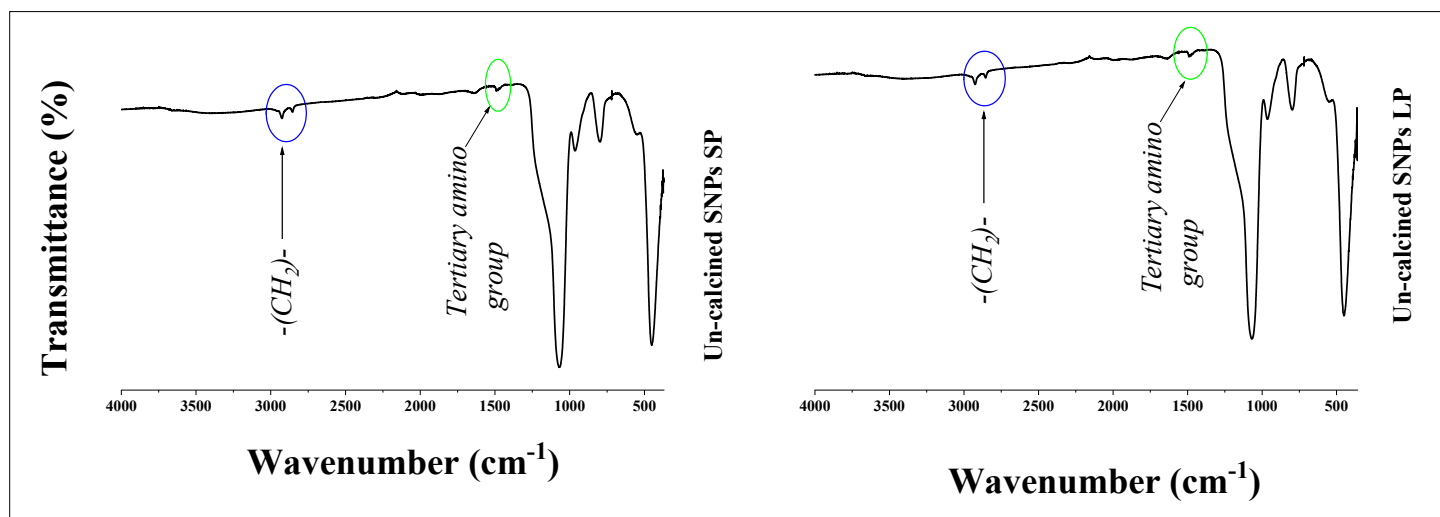


**Figure S7.**  $\text{N}_2$  adsorption/desorption isotherms of (A) SNPs SP and (B) SNPs LP with/without functional groups

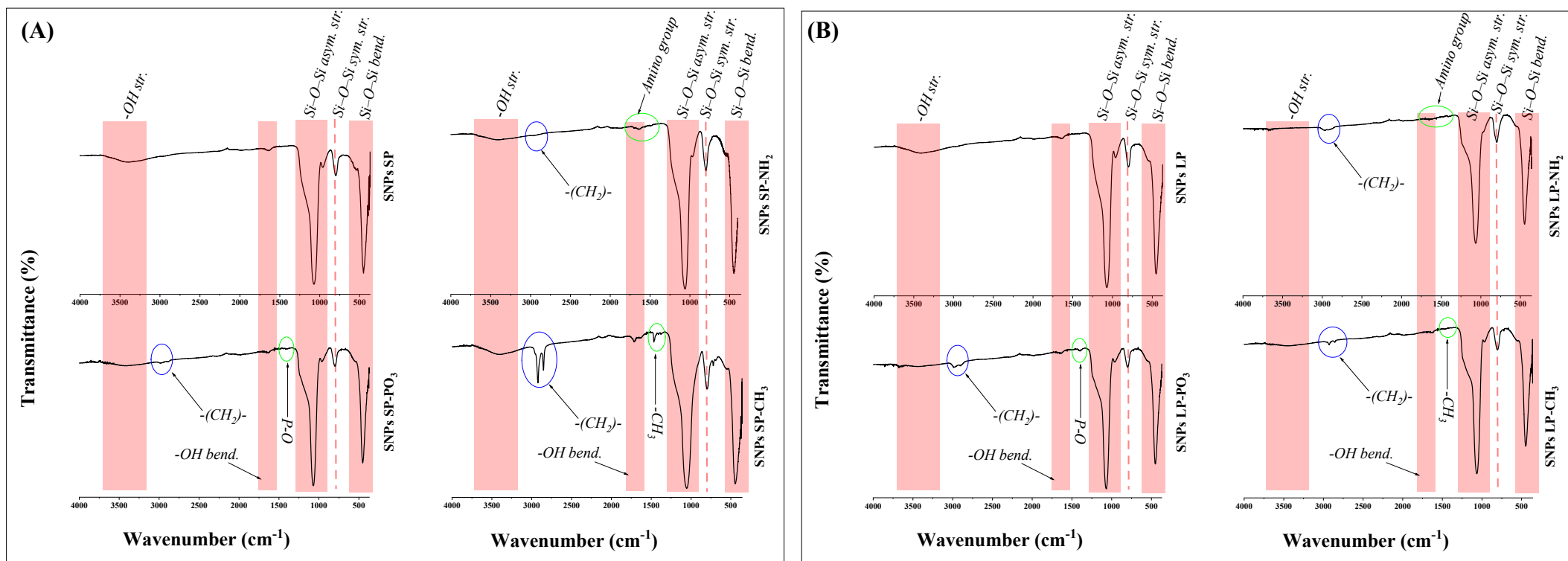




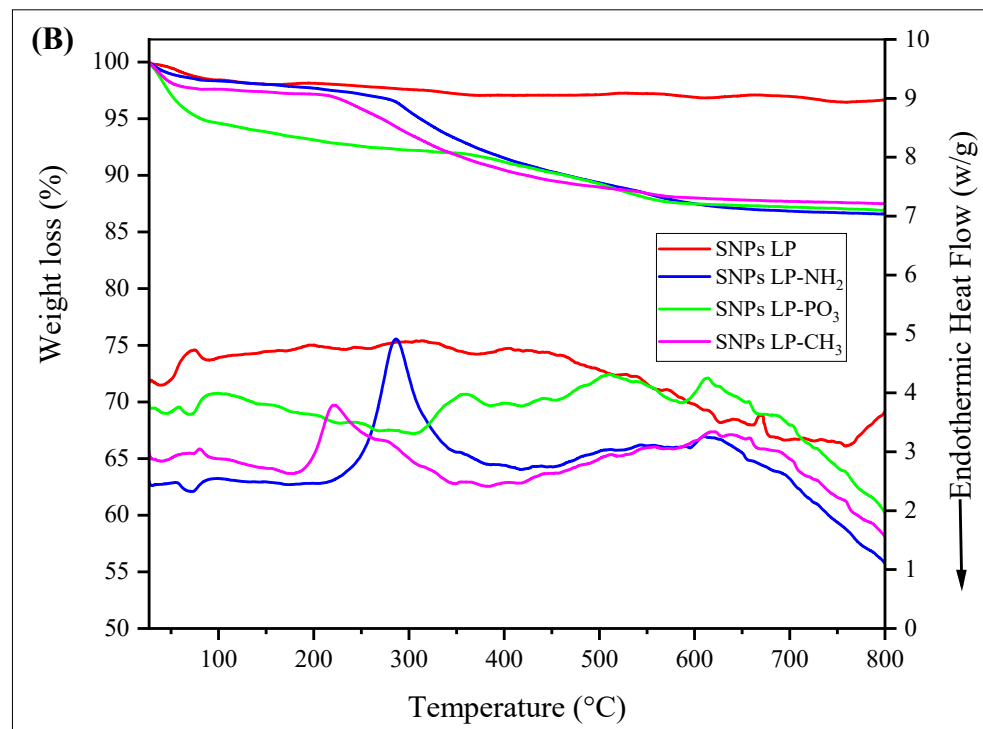
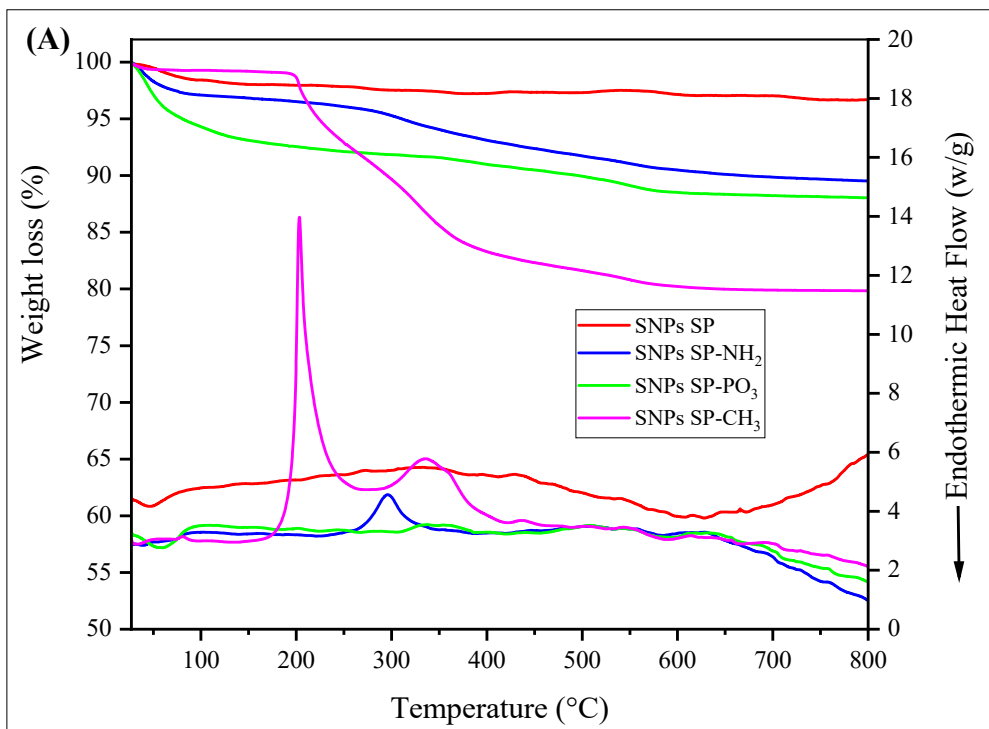
**Figure S8.** Pore size distributions (BJH Adsorption  $dV/d\log(w)$  Pore Volume) of (A) SNPs SP and (B) SNPs LP with/without functional groups



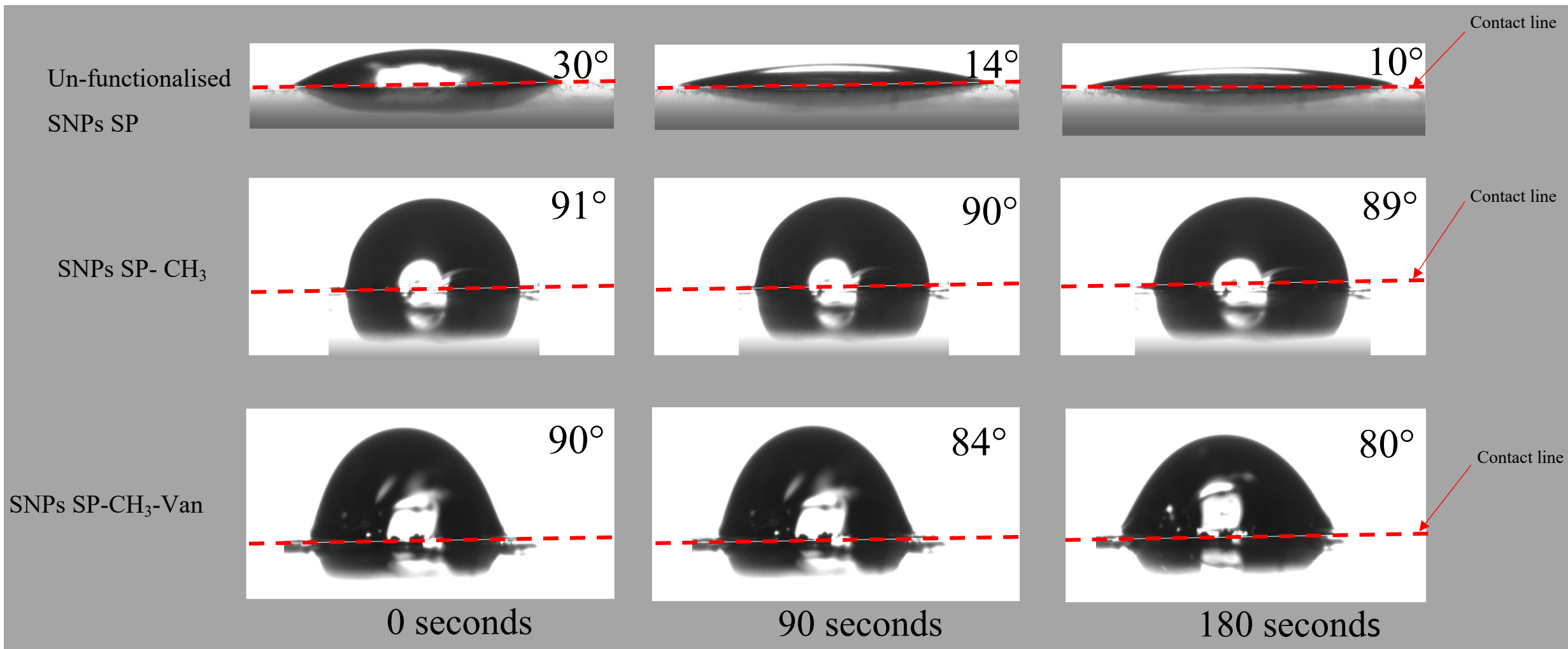
**Figure S9.** FTIR spectra of un-calcined SNPs (before calcination) showing the alkyl and tertiary amino groups characteristic of CTAC and TEA



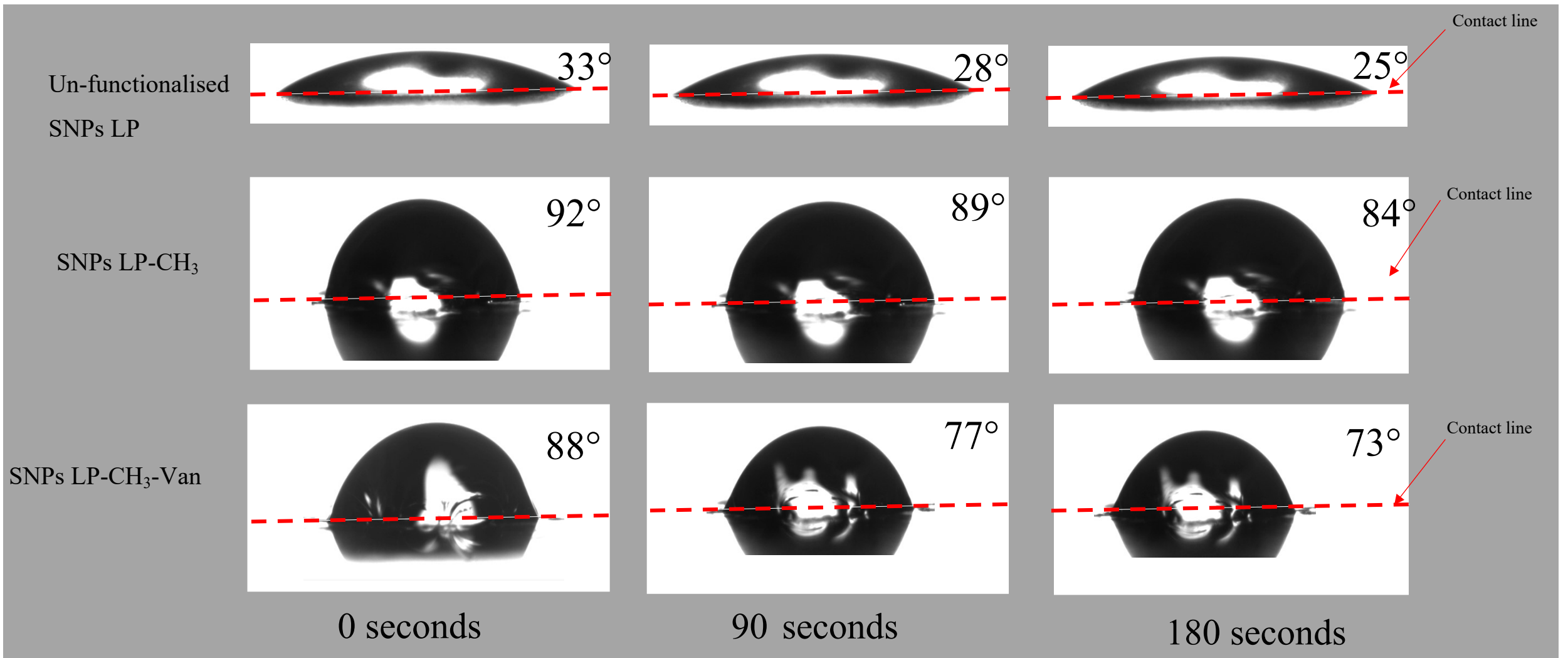
**Figure S10.** FTIR of functionalized (A) SNPs SP and (B) SNPs LP



**Figure S11.** TGA and DSC of functionalised (A) SNPs SP and (B) SNPs LP



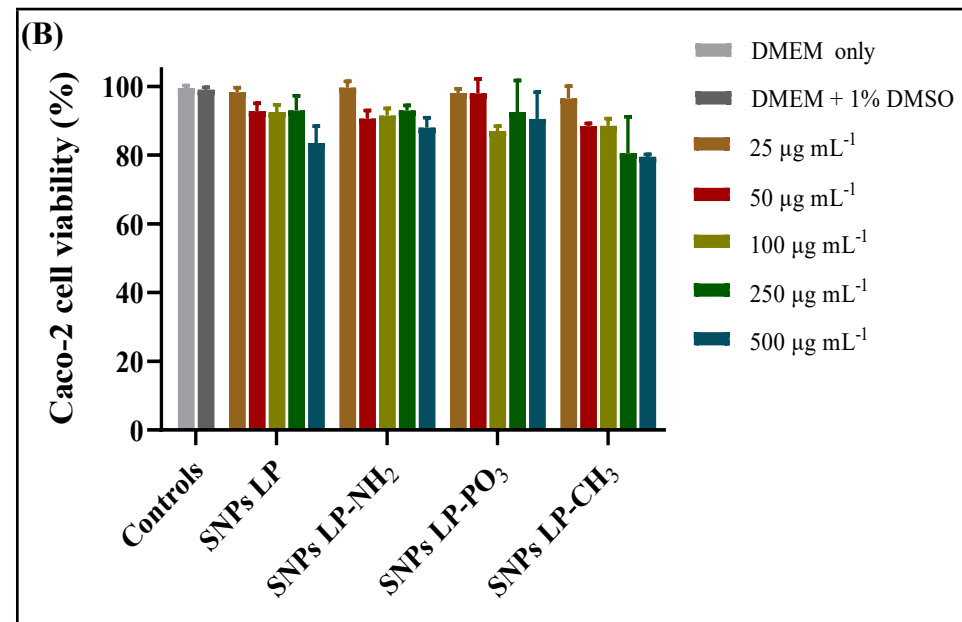
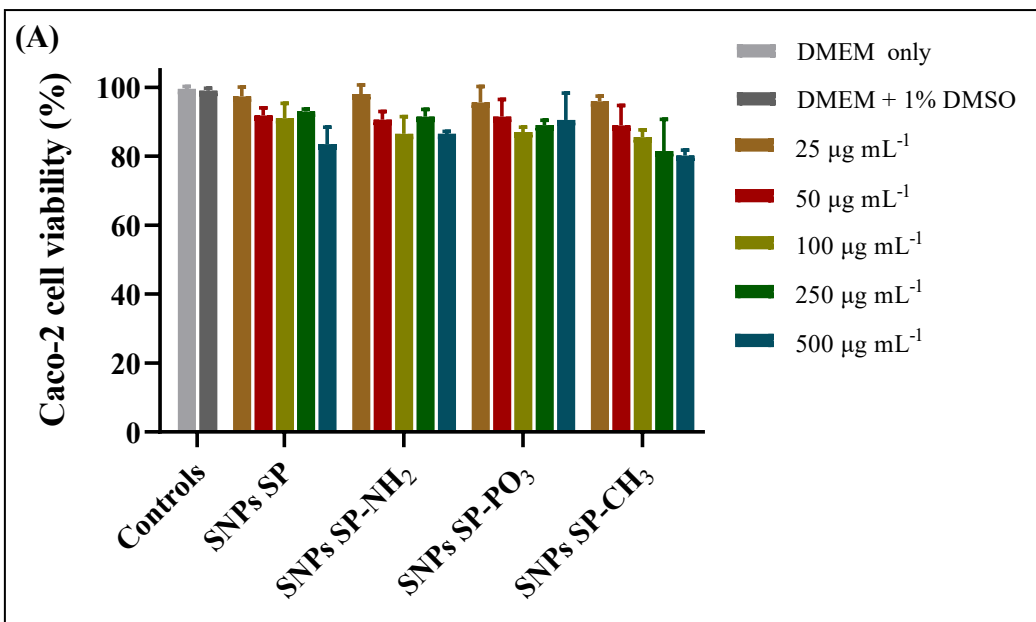
**Figure S12.** Images of water droplet interacting with the surface of SNPs SP with/without functional groups. Contact angles for Van-loaded SNPs SP-CH<sub>3</sub> show that SNPs SP-CH<sub>3</sub> do not lose their hydrophobic characteristics once loaded with Van loading.



**Figure S13.** Images of water droplet interacting with the surface of SNPs LP with/without functional groups. Contact angles for Van-loaded SNPs LP-CH<sub>3</sub> show that SNPs LP-CH<sub>3</sub> do not lose their hydrophobic characteristics once loaded with Van loading.

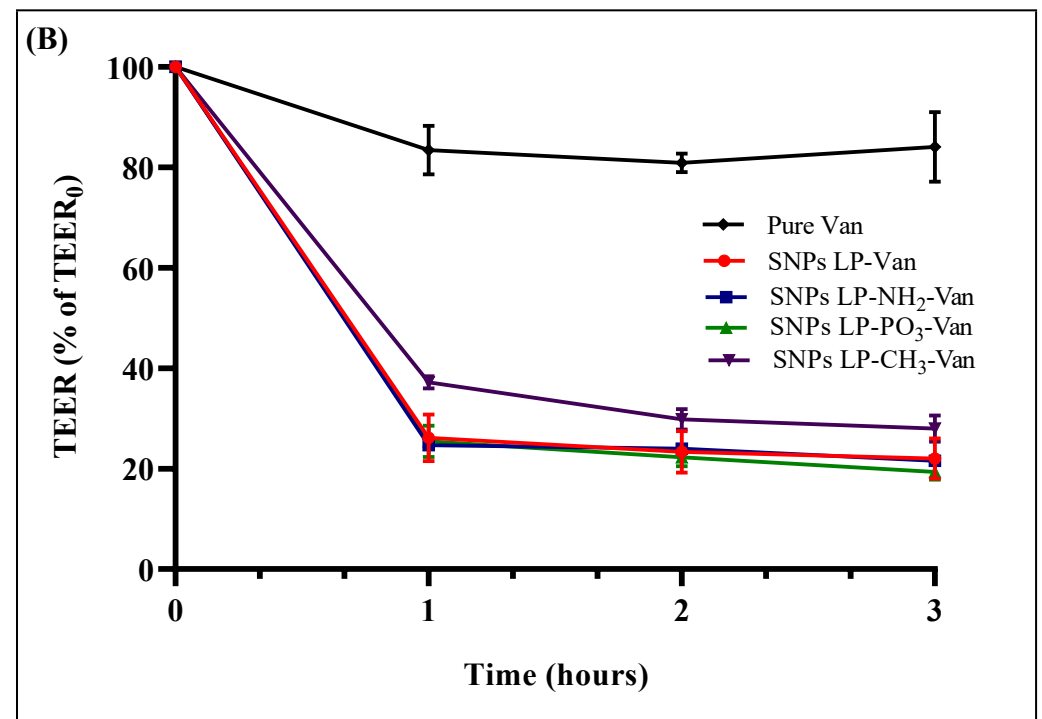
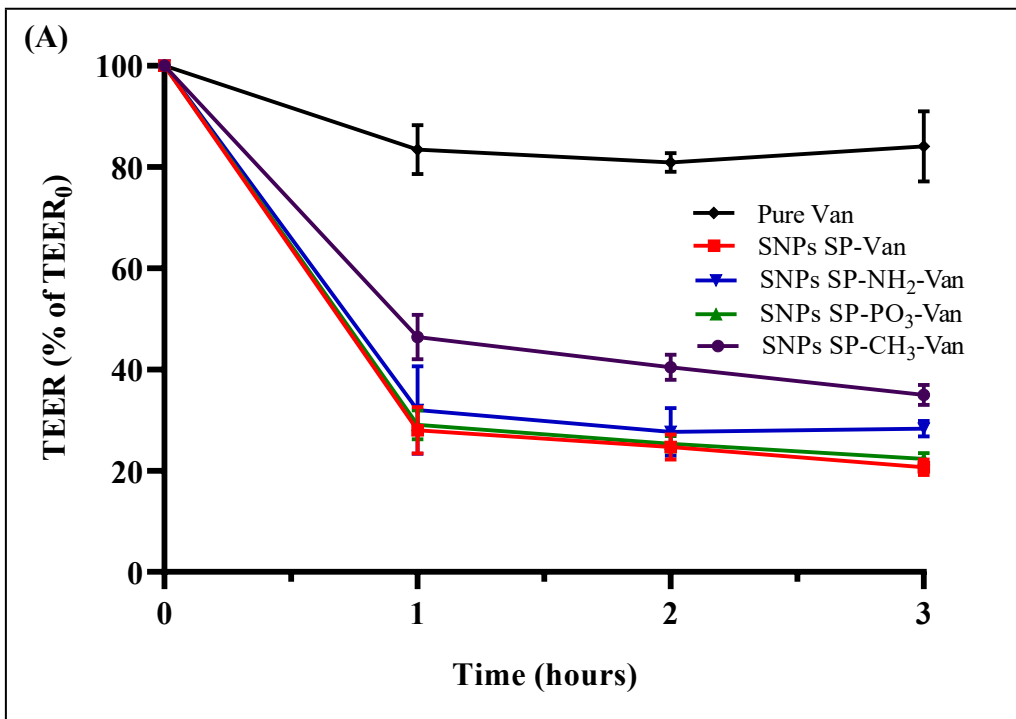
**Table S14.** Binding energies and concentrations (at %) of different elements on the surface of un-functionalised and functionalised SNPs

Peak detail	Binding energy (eV)	Concentration (at %)							
		SNPs SP				SNPs LP			
		SNPs SP	SNPs SP-NH <sub>2</sub>	SNPs SP-PO <sub>3</sub>	SNPs SP-CH <sub>3</sub>	SNPs LP	SNPs LP-NH <sub>2</sub>	SNPs LP-PO <sub>3</sub>	SNPs LP-CH <sub>3</sub>
C 1s	282	-	17.63	7.49	58.33	-	19.84	8.74	15.76
N 1s	397	-	2.39	-	-	-	3.69	-	-
O 1s	531	70.71	56.05	67.82	28.53	70.98	54.36	67.62	60.79
Si 2p	102	29.29	23.93	24.69	13.15	29.02	22.10	23.65	23.44



**Figure S15.** In vitro cytotoxicity assays of (A) SNPs SP and (B) SNPs LP. The values are presented as means  $\pm$  SDs of  $n = 3$





**Figure S16.** TEER values of (A) Van-loaded SNPs SP and (B) Van-loaded SNPs LP during 3 h of transport experiment. TEER values are presented as means  $\pm$  SDs (n=3) considering the TEER values of un-treated Caco-2 cells (Caco-2 cell monolayers with only HBSS or HBSS+1% DMSO without SNPs).