

Supplementary material

Specific Buffer Effects on the Formation of BSA Protein Corona Around Amino-Functionalized Mesoporous Silica Nanoparticles

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Table S1. Physicochemical characterization of MSN-NH₂ through nitrogen physisorption and SAXS.

sample	S _{BET} (m ² g ⁻¹)	d _{BJH} (nm)	Pore volume (cm ³ g ⁻¹)	Lattice parameter (nm)
MSN-NH₂	675	2.6	0.72	4.05

Table S2. Hydrodynamic size (d_H), polydispersity index (PdI) and zeta potential (ζ) of MSN samples in MilliQ water.

sample	d _H (nm)	PdI	ζ (mV)
MSN-NH₂	163 ± 16	0.255	+16.6 ± 0.3

Table S3. Buffer species used in the present work and their respective pK_a values.

Buffer	Acid/base equilibrium	pK _a
Tris		8.06
BES		7.09
Cacodylate		6.30
Phosphate		7.22
Citrate		6.40

Table S4. Zeta potentials (ζ) of BSA in buffer solutions at pH 7.15 and different concentrations (10, 50, 100 mM).

Buffer	ζ / mV		
	10 mM	50 mM	100 mM
Tris	-13.4 ± 0.6	-3.7 ± 0.8	-5 ± 1
BES	-15.2 ± 0.9	-5.4 ± 0.6	-5.4 ± 0.3
Cacodylate	-20 ± 2	-8.7 ± 0.4	-6 ± 1
Phosphate	-22 ± 1	-13 ± 1	-6.2 ± 0.5
Citrate	-19 ± 1	-11.3 ± 0.8	-8.2 ± 0.1

Table S5. Zeta potentials (ζ) of MSN-NH₂ in buffer solutions at pH 7.15 and different concentrations (10, 50, 100 mM).

Buffer	ζ / mV		
	10 mM	50 mM	100 mM
Tris	17 ± 1	10 ± 1	9 ± 1
BES	9 ± 0.6	-5.0 ± 0.1	-4.6 ± 0.2
Cacodylate	9 ± 1	-4.3 ± 0.6	-5.5 ± 0.2
Phosphate	-1.7 ± 0.4	-7.1 ± 0.2	-9.9 ± 0.8
Citrate	-14 ± 0.7	-14 ± 2	-8.6 ± 0.7

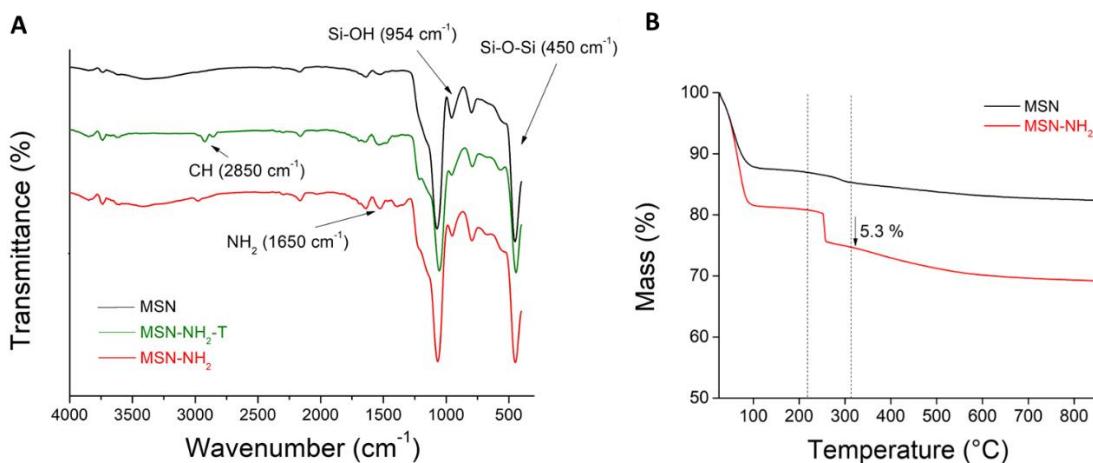


Figure S1. FTIR spectra (A) and TGA analysis (B) of MSN and MSN-NH₂ samples

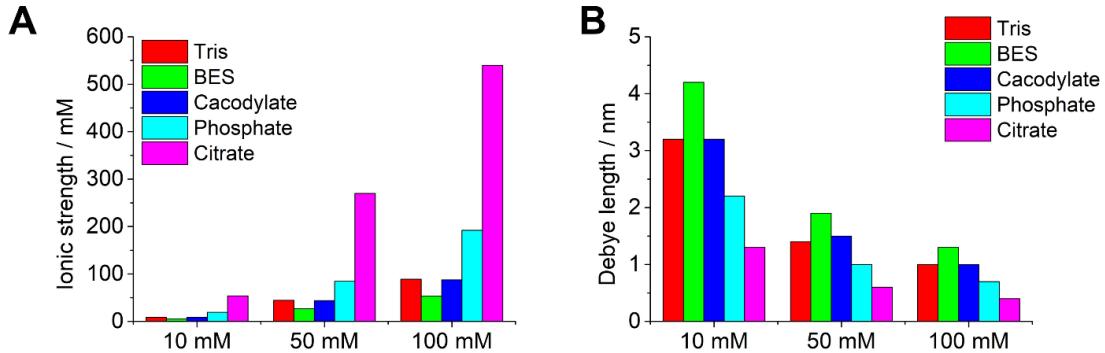


Figure S2. Ionic strength (A) and Debye length (B) for each buffer solution.

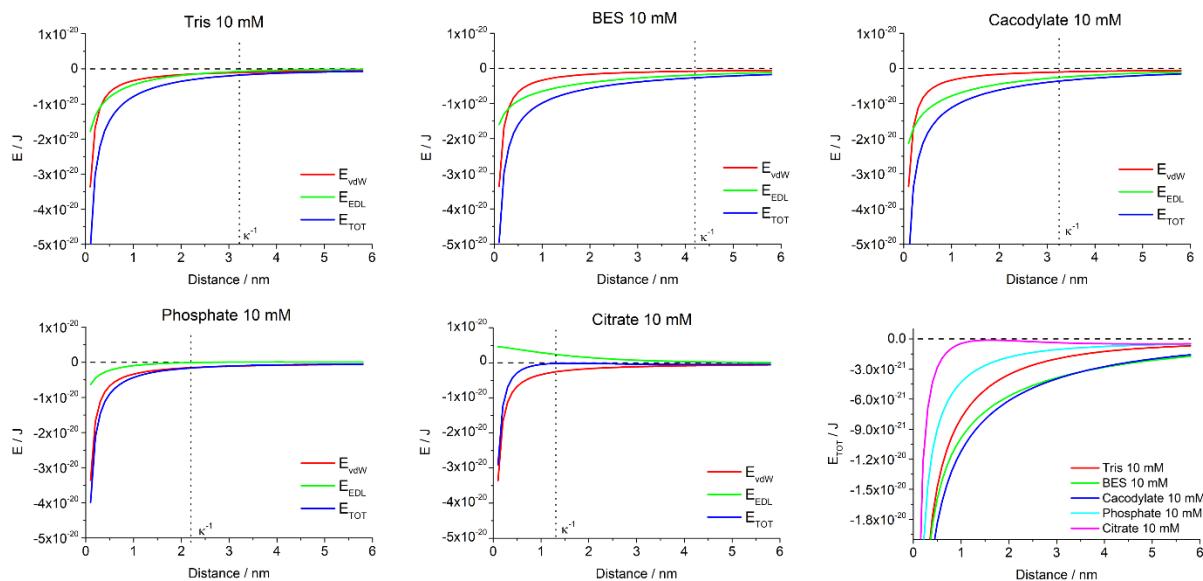


Figure S3. Interaction energies between BSA and MSN-NH₂ vs distance for 10 mM buffer concentration. van der Waals energy (E_{vdW}), electric double layer energy (E_{EDL}) and total energy (E_{TOT}).

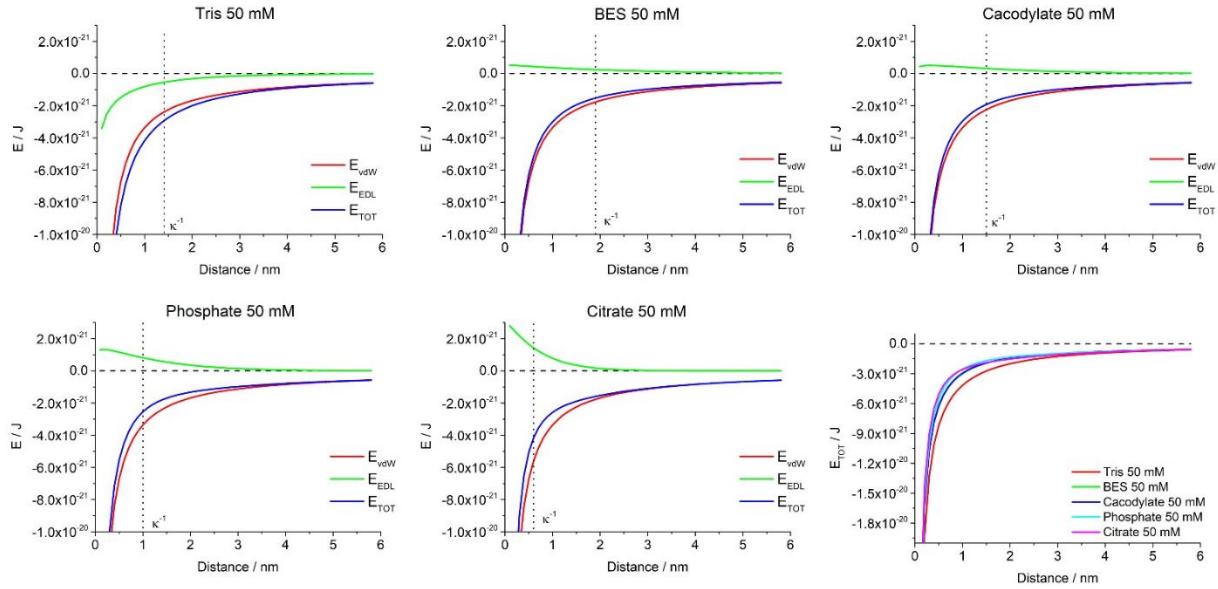


Figure S4. Interaction energies between BSA and MSN-NH₂ vs distance for 50 mM buffer concentration. van der Waals energy (E_{vdW}), electric double layer energy (E_{EDL}) and total energy (E_{TOT}).

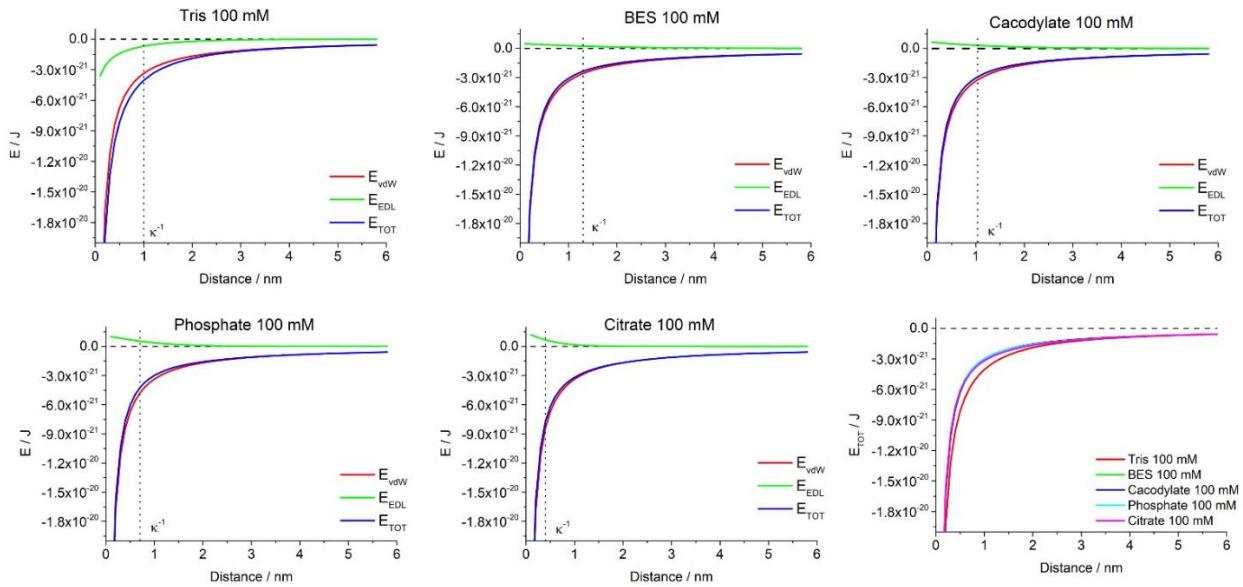


Figure S5. Interaction energies between BSA and MSN-NH₂ vs distance for 100 mM buffer concentration. van der Waals energy (E_{vdW}), electric double layer energy (E_{EDL}) and total energy (E_{TOT}).

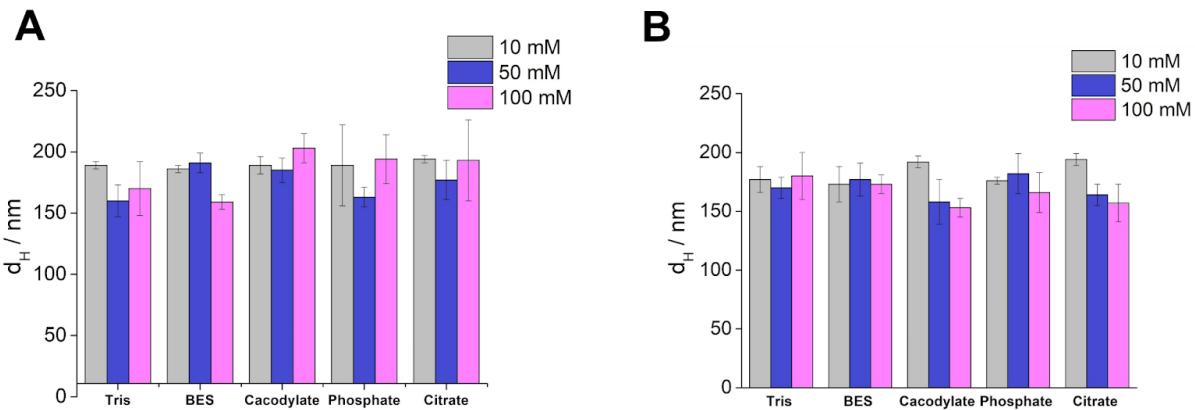


Figure S6. Hydrodynamic size of the BSA corona adsorbed onto the MSN-NH₂, following the 24-hours long incubation step in (A) buffers and (B) MilliQ water with pH adjusted to 7.15.