

Electronic Supplementary Information

Title: *In Silico* before *In Vivo*: how to Predict the Heating Efficiency of Magnetic Nanoparticles within the Intracellular Space

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Table S1. Saturation magnetization M_s , coercive field H_c , average particle core diameter $\langle d \rangle$, average hydrodynamic diameter in water $\langle d_H \rangle_{\text{water}}$, and in DMEM $\langle d \rangle_{\text{DMEM}}$, of the magnetic nanoparticles used in this work.

Sample	M_s Am²/kg	H_c kA/m	$\langle d \rangle$ nm	$\langle d_H \rangle_{\text{water}}$ nm	$\langle d_H \rangle_{\text{DMEM}}$ nm
PEI-MNPs	51.9	5.6	25±5	73±25	3094±730
PAA-MNPs	51.6	5.6	32±6	155±25	1305±381

Table S2. SPA values ($H_0 = 24$ kA/m, $f = 560$ kHz) of *as prepared* magnetic nanoparticles in water, protein-rich medium (DMEM) and *in vitro*. Also de values of exponent λ obtained from the fit of the power law $SPA(H) = \Phi H^\lambda$ are tabulated.

Sample	WATER		DMEM		Cells	
	SPA (W/g _{Fe3O4})	λ	SPA (W/g _{Fe3O4})	λ	SPA (W/g _{Fe3O4})	λ
PEI-MNPs	274±37	3.6(3)	185±16	4.3(3)	157±19	4.0(3)
PAA-MNPs	413±42	4.8(3)	378±47	6.2(4)	217±12	3.9(3)

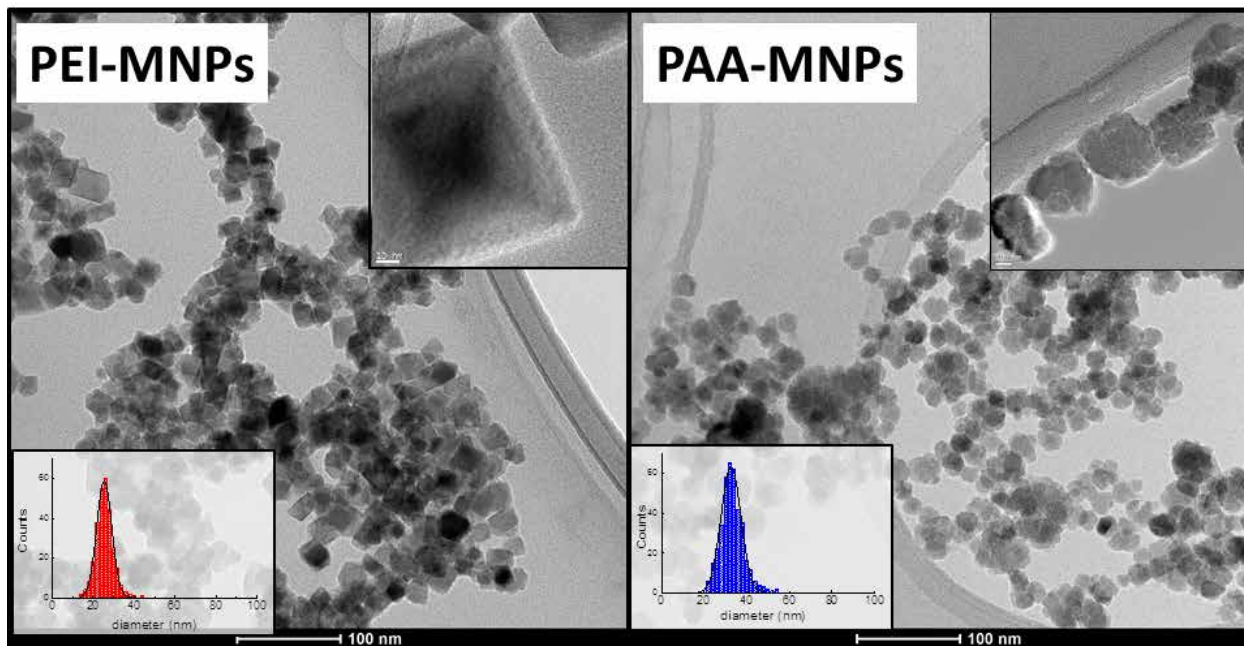


Figure S1. TEM images of the two magnetic particles used in this work. Left panel: PEI-MNPs, magnified area and resulting particle size histogram fitted with a Gaussian function. Right panel: PAA-MNPs, magnified area and resulting particle size histogram.

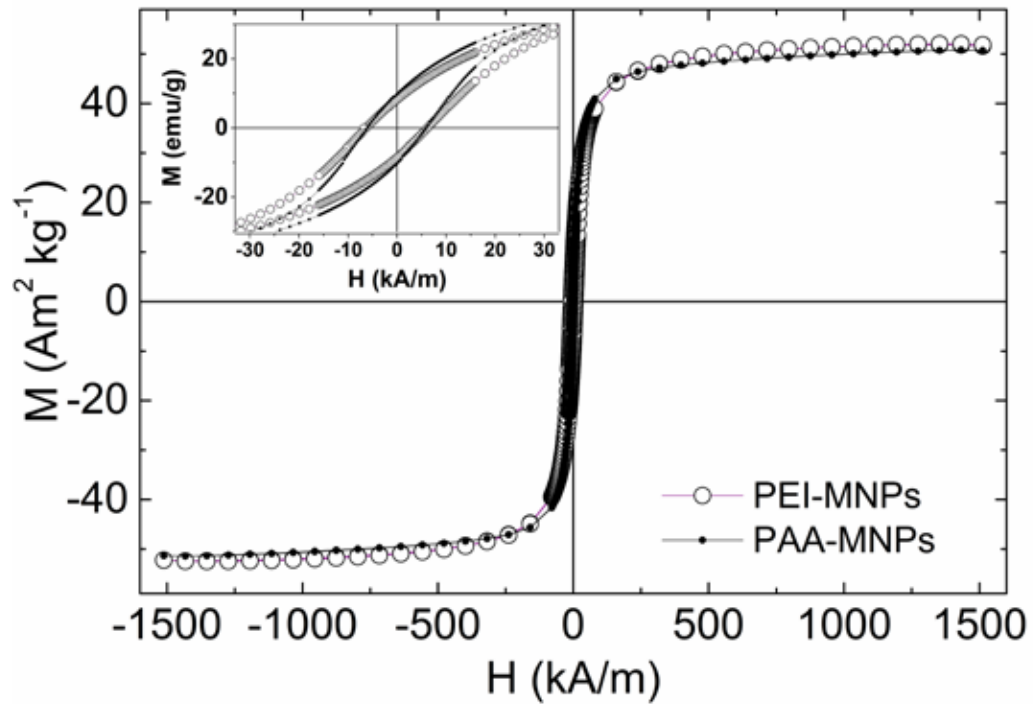


Figure S2. Room-temperature magnetization curves as a function of applied field for poly(ethyleneimine)-coated nanoparticles (open circles) and poly(acrylic acid)-coated nanoparticles (solid circles).

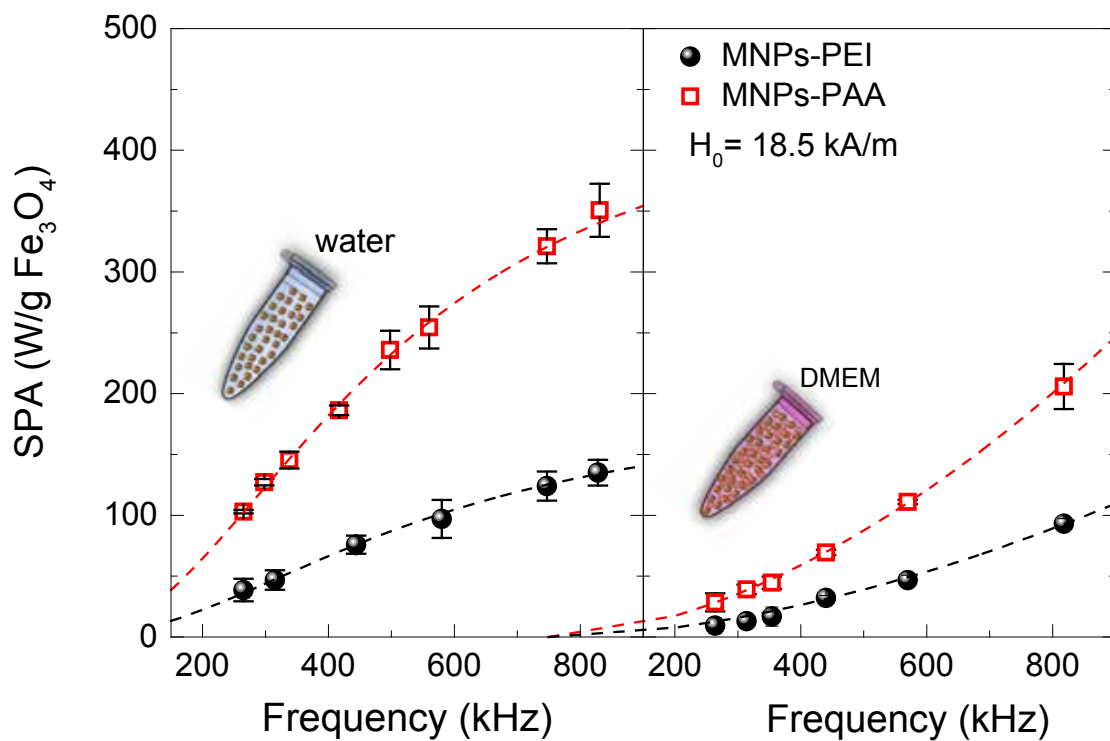


Figure S3. SPA vs. frequency (f) measured at a fixed amplitude $H_0 = 18.5$ kA/m.
 Dashed lines are the best-fit curves determined using the relation $SPA(f) = A \left(\frac{Bf^2}{1+(Bf)^2} \right)$.

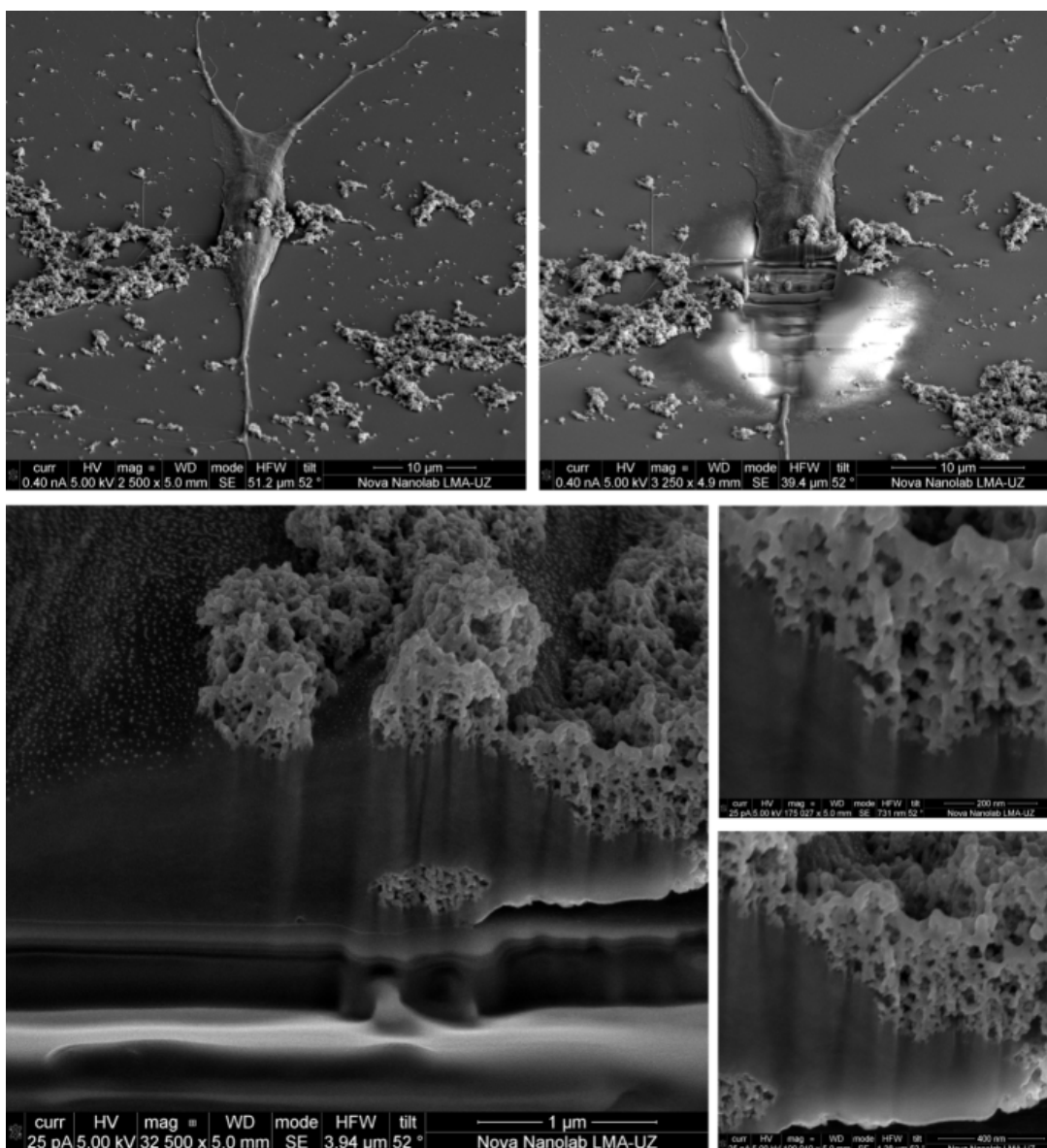


Figure S4. FIB-SEM Dual Beam images of SH-SY5Y cells incubated with PEI-MNPs ($100 \mu\text{g}\cdot\text{ml}^{-1}$) for 24 hours. Lower panels: cross section images showing a detail of the dense cluster structures observed inside the cells and across the cell membrane.

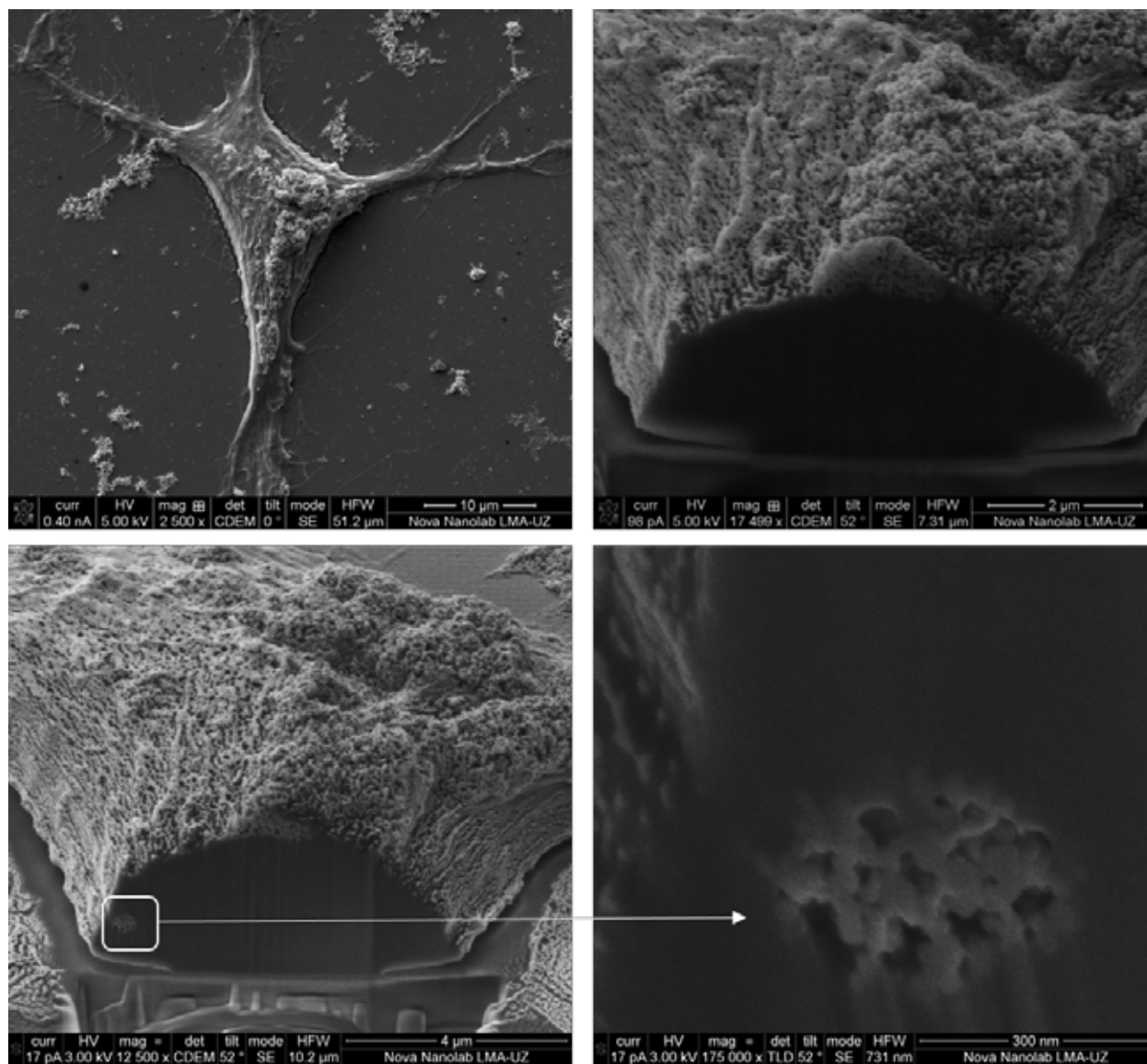


Figure S5. FIB-SEM images of SH-SY5Y cells incubated with PAA-MNPs ($100 \mu\text{g}\cdot\text{ml}^{-1}$) for 24 hours. The lower panels show a cross-sectioned cell (left) and a magnification of the NPs clusters (right)

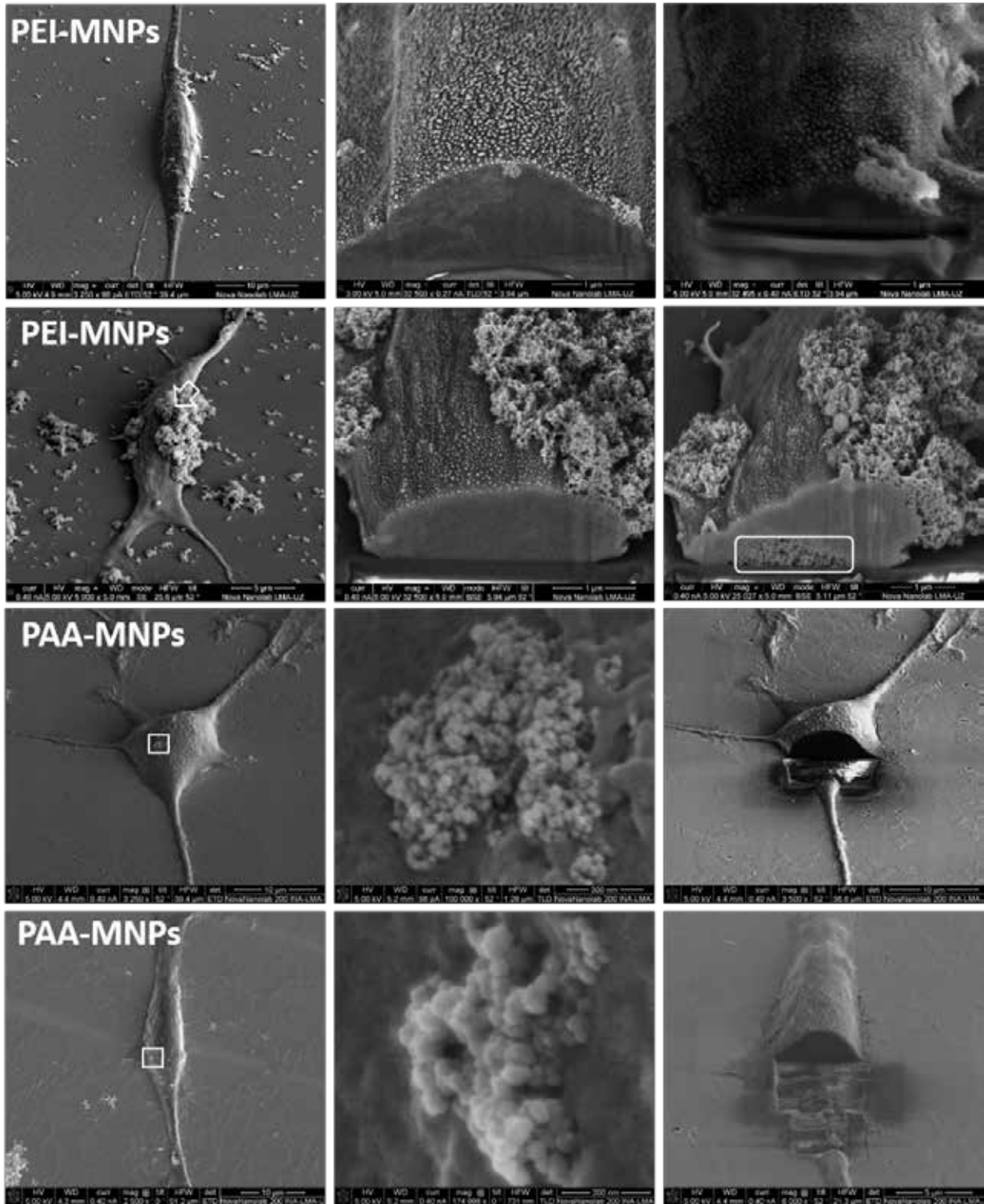


Figure S6. FIB-SEM images of SH-SY5Y cells incubated with PEI-MNPs and PAA-MNPs for 24 hours.