

Biocompatible inorganic nanoparticles for [^{18}F]-fluoride binding with applications in PET imaging

ELECTRONIC SUPPLEMENTARY INFORMATION

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Fig. S1: X-ray powder diffractogram of HA1, HA2, HA3 and HA4

Fig. S2: Infrared spectra of HA1, HA2, HA3, HA4 and HA4-PEG

Fig. S3: X-ray powder diffractogram of Mes-SiO₂

Fig. S4: Infrared spectra of Mes-SiO₂ NPs (before and after washing) and CTAC.

Fig. S5: Dynamic Light Scattering (DLS) of the nanoparticles solutions at a concentration of 1 mg/mL for AlhydrogelTM, HA4, HA4Ale, HA4PEG and 0.2 mg/ml for HA1, HA2 and HA3.

Fig. S6: [^{18}F] Fluoride binding to HA2 and HA3 in different media (water, Tris, PBS and cell medium).

Table S1: Effect of competing substances on binding of [^{18}F]-fluoride to hydroxyapatite HA4 and Al(OH)₃.

Fig. S7: Effect of carrier fluoride concentration on binding of [^{18}F]-fluoride to HA2

Fig. S8: Kinetic stability of [^{18}F]-HA4 and Al(OH)₃ in the presence of NaF and alendronate

Fig. S9. Transmission electron micrograph of macrophages after incubation with Al(OH)₃ showing particles sequestered within phagosomes. The right image is close-up of the top right region of the left.

Fig S10: Biodistribution of [^{18}F]-HA2, HA4, HA4-PEG and Al(OH)₃ after intravenous (i.v.) and subcutaneous (s.c.) and intramuscular (i.m.) injections in BALB/c mice

Fig. S1: X-ray powder diffractogram of HA1, HA2, HA3 and HA4

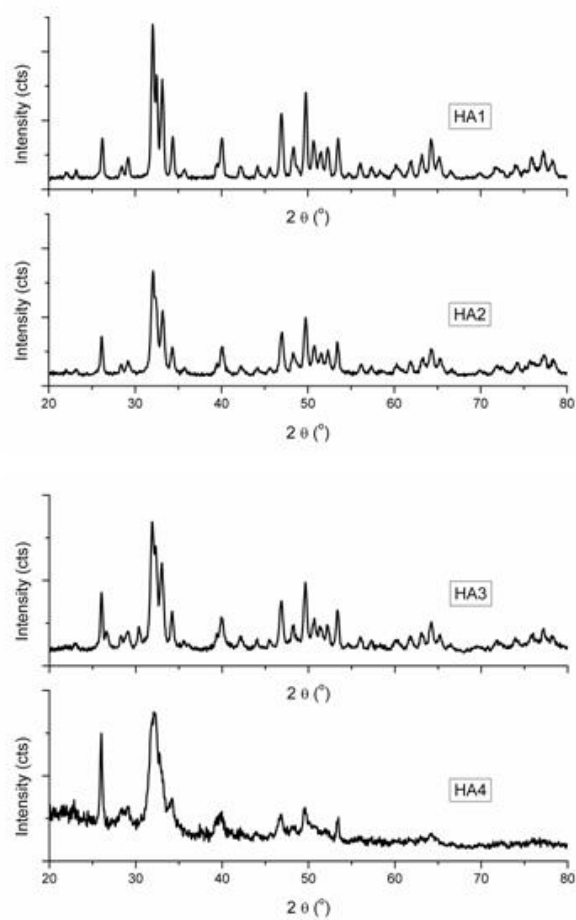


Fig. S2: Infrared spectra of HA1, HA2, HA3, HA4 and HA4-PEG

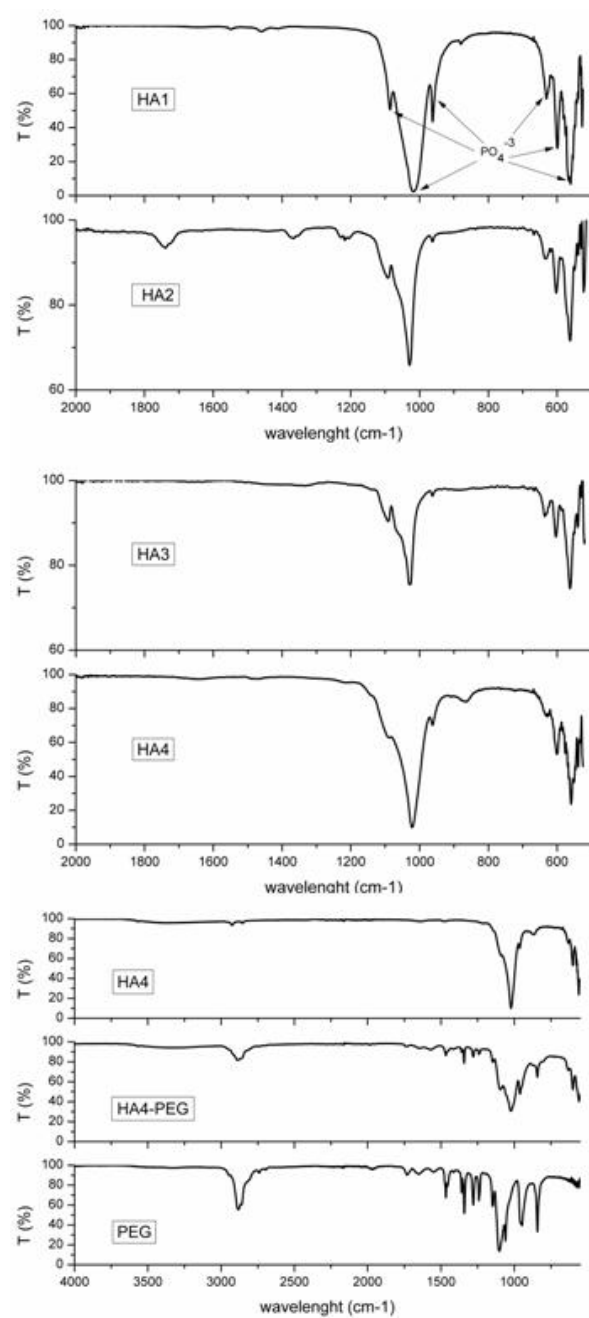


Fig. S3: X-ray powder diffractogram of Mes-SiO₂

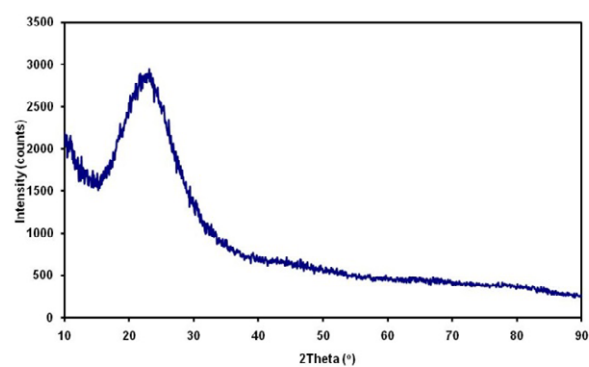


Fig. S4: Infrared spectra of Mes-SiO₂ NPs (before and after washing) and CTAC.

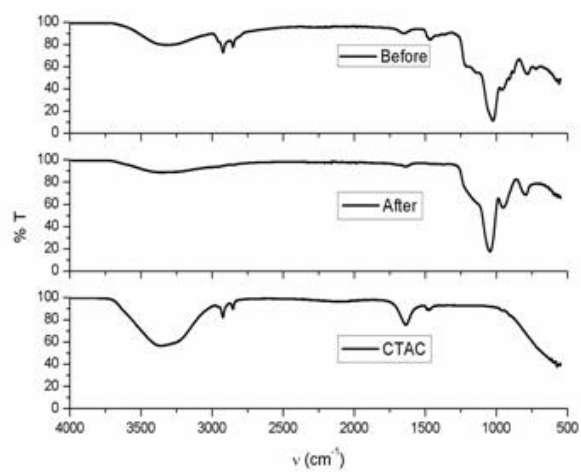


Fig. S5: Dynamic Light Scattering (DLS) of the nanoparticles solutions at a concentration of 1 mg/mL for AlhydrogelTM, HA4, HA4Ale, HA4PEG and 0.2 mg/ml for HA1, HA2 and HA3.

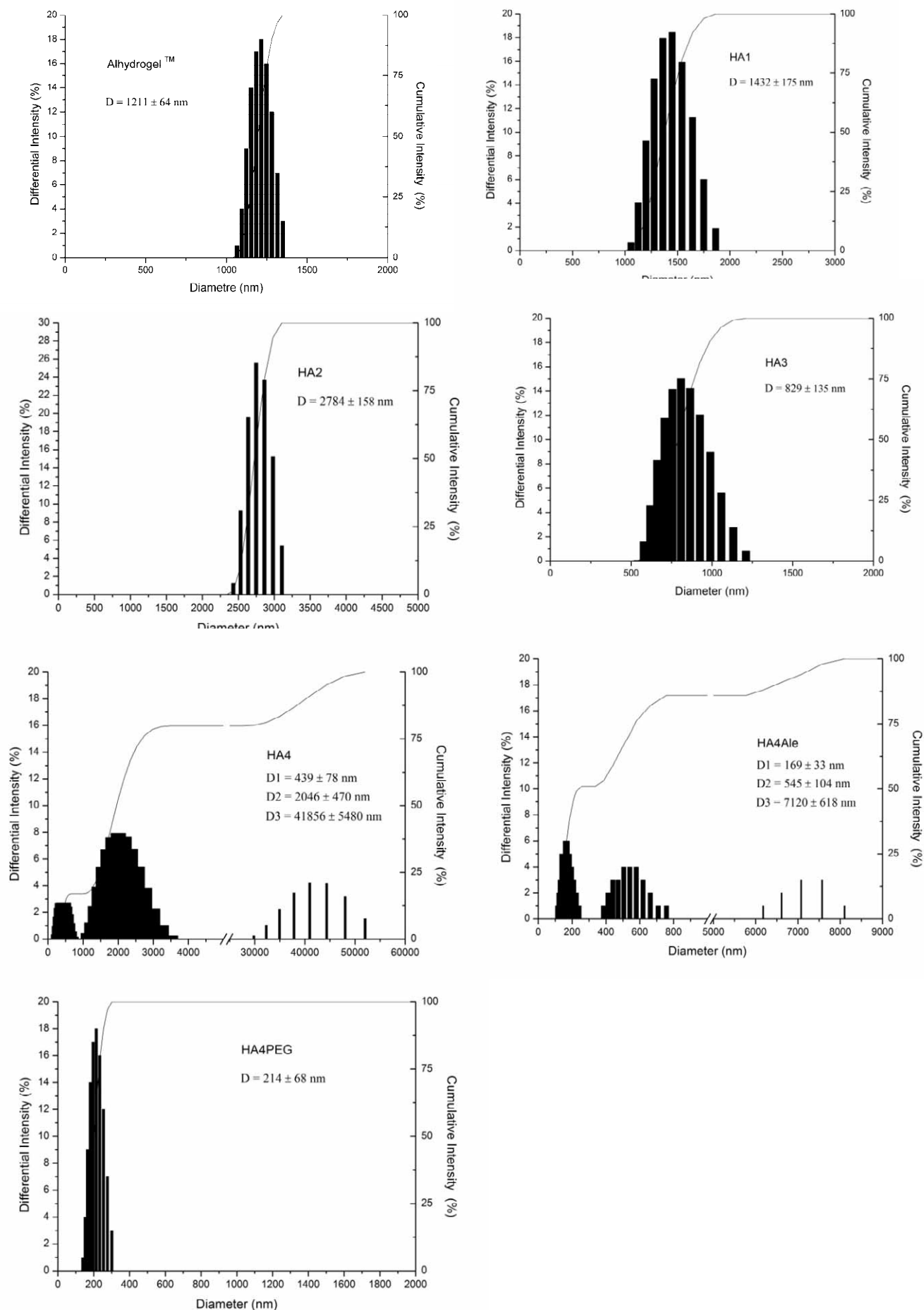


Fig. S6: [^{18}F] Fluoride binding to HA2, and HA3 in different media (water, Tris, PBS and cell medium).

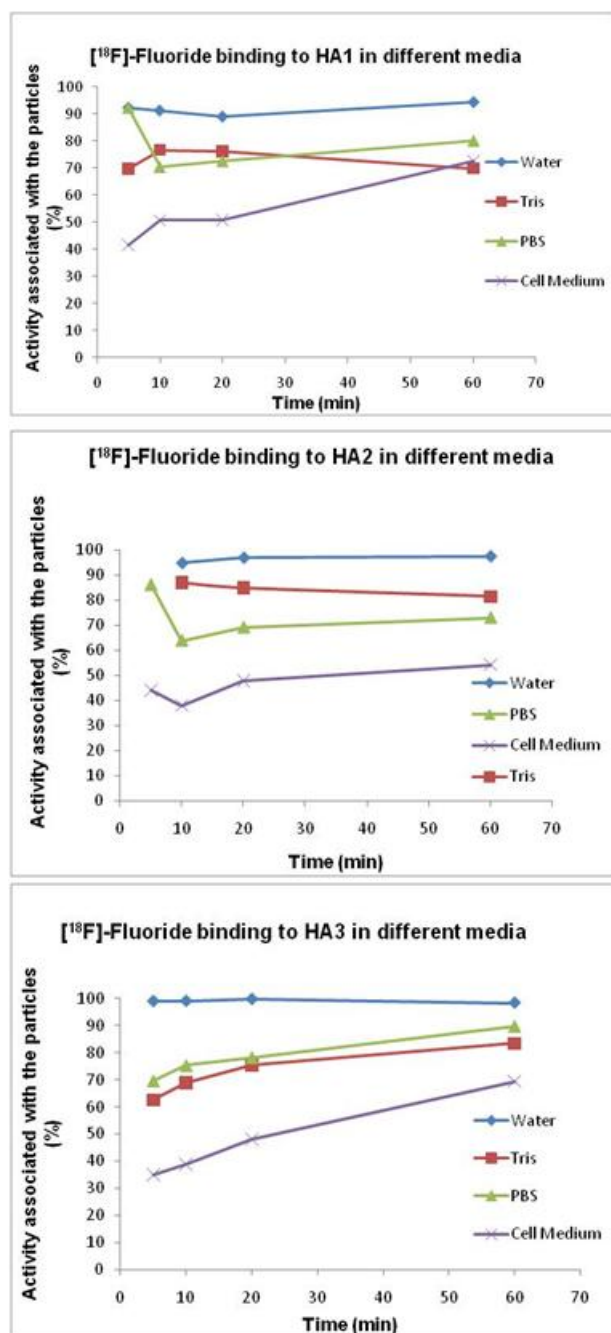


Table S1: Effect of competing substances on binding of [^{18}F]-fluoride to hydroxyapatite HA4 and $\text{Al}(\text{OH})_3$. HMP is sodium hexametaphosphate; BP is the bisphosphonate Alendronate; CTAB is cetyltrimethylammonium bromide; phosphate is phosphate buffered saline.

Material	Inhibitor	Log [Inhibitor]	%binding	Stdev
HA4	NaCl	0	79.1	2.1
HA4	NaCl	-0.3	79.7	2.2
HA4	NaCl	-1	78.1	4.6
HA4	HMP	-1	18.3	1.7
HA4	HMP	-2	19.1	0.3
HA4	HMP	-3	49.9	0.8
HA4	HMP	-4	87.8	0.2
HA4	HMP	-5	88.9	0.4
HA4	Citrate	-1	57.4	0.3
HA4	Citrate	-2	72.7	0.2
HA4	Citrate	-3	88.5	0.3
HA4	Citrate	-4	93.1	0.6
HA4	Citrate	-5	93.2	0.4
HA4	BP	-2	78.7	0.6
HA4	BP	-3	80.6	0.2
HA4	BP	-4	87.4	0.6
HA4	BP	-5	85.8	0.5
HA4	BP	-6	92.7	0.9
HA4	BP	-7	93.3	0.7
HA4	CTAB	-1	93.2	0.2
HA4	CTAB	-2	88.6	2.8
HA4	CTAB	-3	91.1	1.8
HA4	CTAB	-4	88.7	2.7
HA4	CTAB	-5	88.9	1.9
HA4	Tris	-1	62.82	0.4
HA4	phosphate	-1	92.39	0.7
$\text{Al}(\text{OH})_3$	NaCl	0	98.6	0.8
$\text{Al}(\text{OH})_3$	NaCl	-0.3	97.8	0.6
$\text{Al}(\text{OH})_3$	NaCl	-1	98.5	0.1
$\text{Al}(\text{OH})_3$	HMP	-1	7.5	1.6
$\text{Al}(\text{OH})_3$	HMP	-2	8.7	0.3
$\text{Al}(\text{OH})_3$	HMP	-3	77.2	0.5
$\text{Al}(\text{OH})_3$	HMP	-4	89.8	0.4
$\text{Al}(\text{OH})_3$	Citrate	-1	10.4	0.7
$\text{Al}(\text{OH})_3$	Citrate	-2	20.1	0.8
$\text{Al}(\text{OH})_3$	Citrate	-3	39.5	0.9
$\text{Al}(\text{OH})_3$	Citrate	-4	87.4	0.5
$\text{Al}(\text{OH})_3$	Citrate	-5	90.2	0.5
$\text{Al}(\text{OH})_3$	BP	-1	68.8	0.3
$\text{Al}(\text{OH})_3$	BP	-2	69.4	0.5
$\text{Al}(\text{OH})_3$	BP	-3	80.5	1.2
$\text{Al}(\text{OH})_3$	BP	-4	86.8	1.6

Al(OH) ₃	BP	-5	88.0	1.1
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Fig. S7: Effect of carrier fluoride concentration on binding of [¹⁸F]-fluoride to HA2

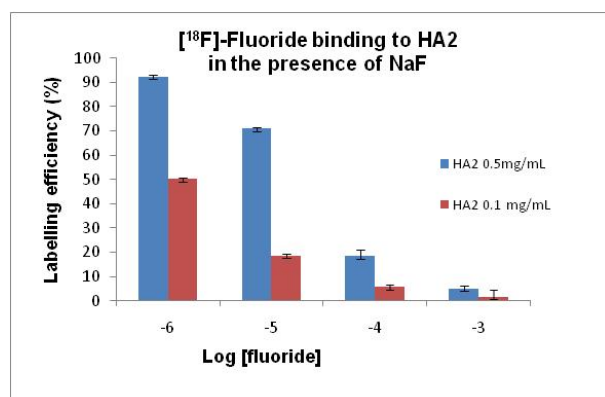


Fig. S8: Kinetic stability of [¹⁸F]-HA4 and Al(OH)₃ in the presence of NaF and alendronate

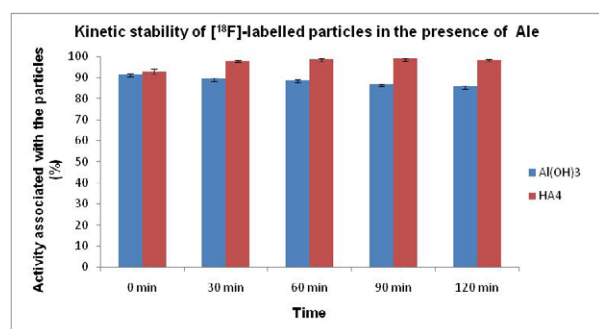
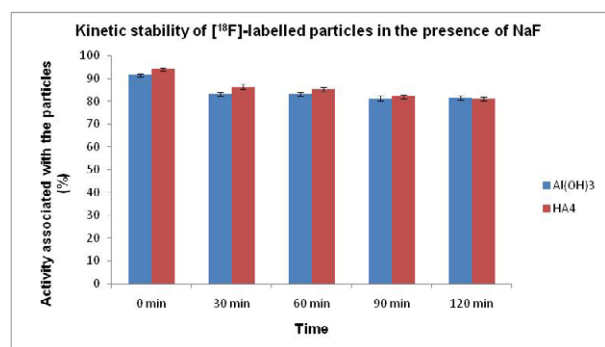


Fig. S9. Transmission electron micrograph of macrophages after incubation with $\text{Al}(\text{OH})_3$ showing particles sequestered within phagosomes. The right image is close-up of the top right region of the left.

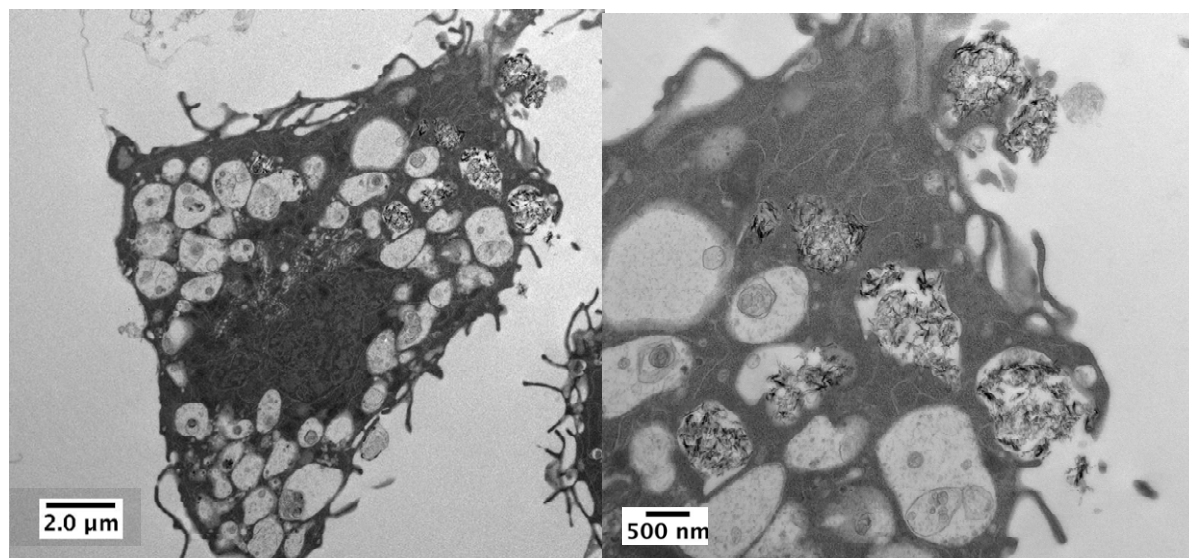


Fig S10: Biodistribution of [^{18}F]-HA2, HA4, HA4-PEG and $\text{Al}(\text{OH})_3$ after subcutaneous (s.c.) and intramuscular (i.m.) injections and intravenous (i.v.) injection in BALB/c mice.

