Probing the Intracellular Bio-Nano Interface in Different Cell Lines with Gold Nanostars

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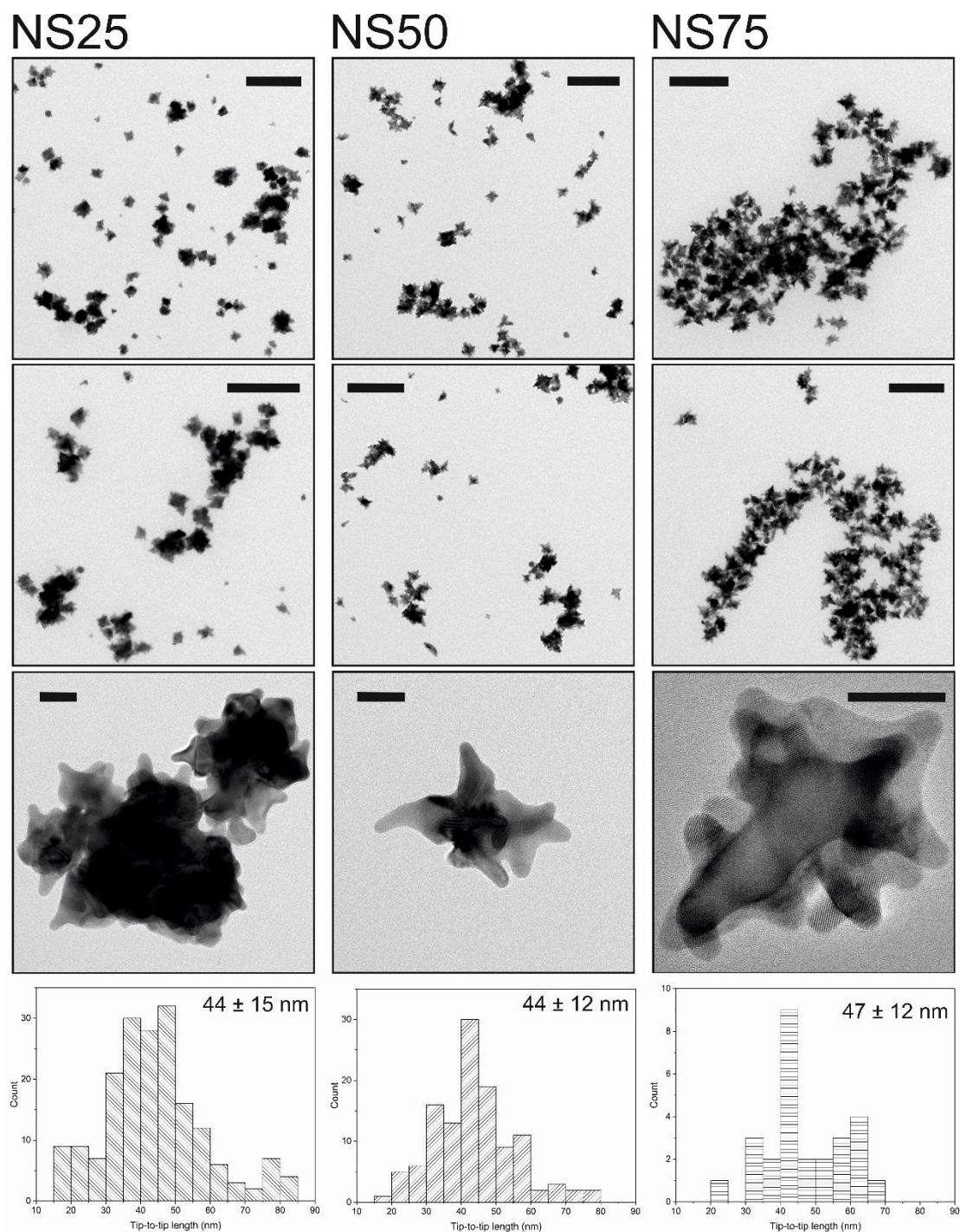* Correspondence: janina-kneipp@chemie.hu-berlin.de

Figure S1. TEM micrographs (first, second and third row) and tip-to-tip length distribution based on TEM data (last row) of gold nanostars synthesized with 25 mM HEPES (NS25, left column), 50 mM HEPES (NS50, middle column) and 75 mM HEPES (NS75, right column). Scale bars first and second row: 200 nm; third row: 20nm. The size distribution average and standard deviation were obtained from 187 particles for NS25, 126 particles for NS50 and 26 particles for NS75.
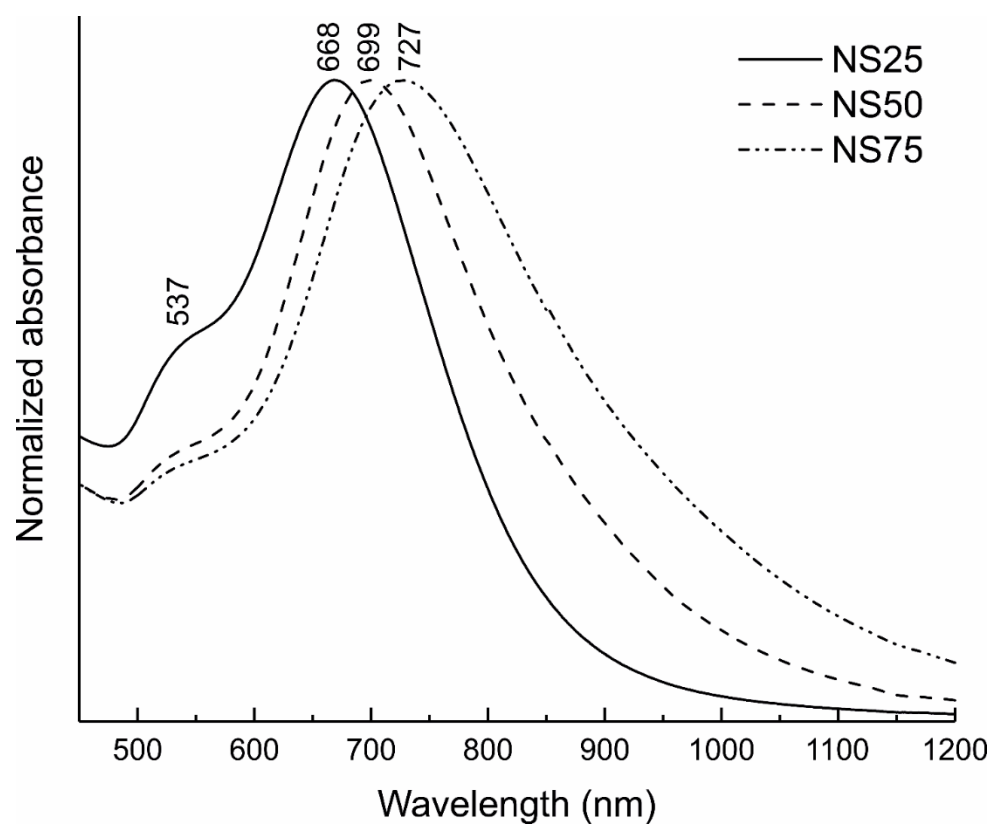
Figure S2. UV-vis-NIR spectra of gold nanostars synthesized with 25 mM HEPES (NS25), 50 mM HEPES (NS50) and 75 mM HEPES (NS75). Plasmon resonance maxima are labeled. The 537 nm band is common to all spectra.

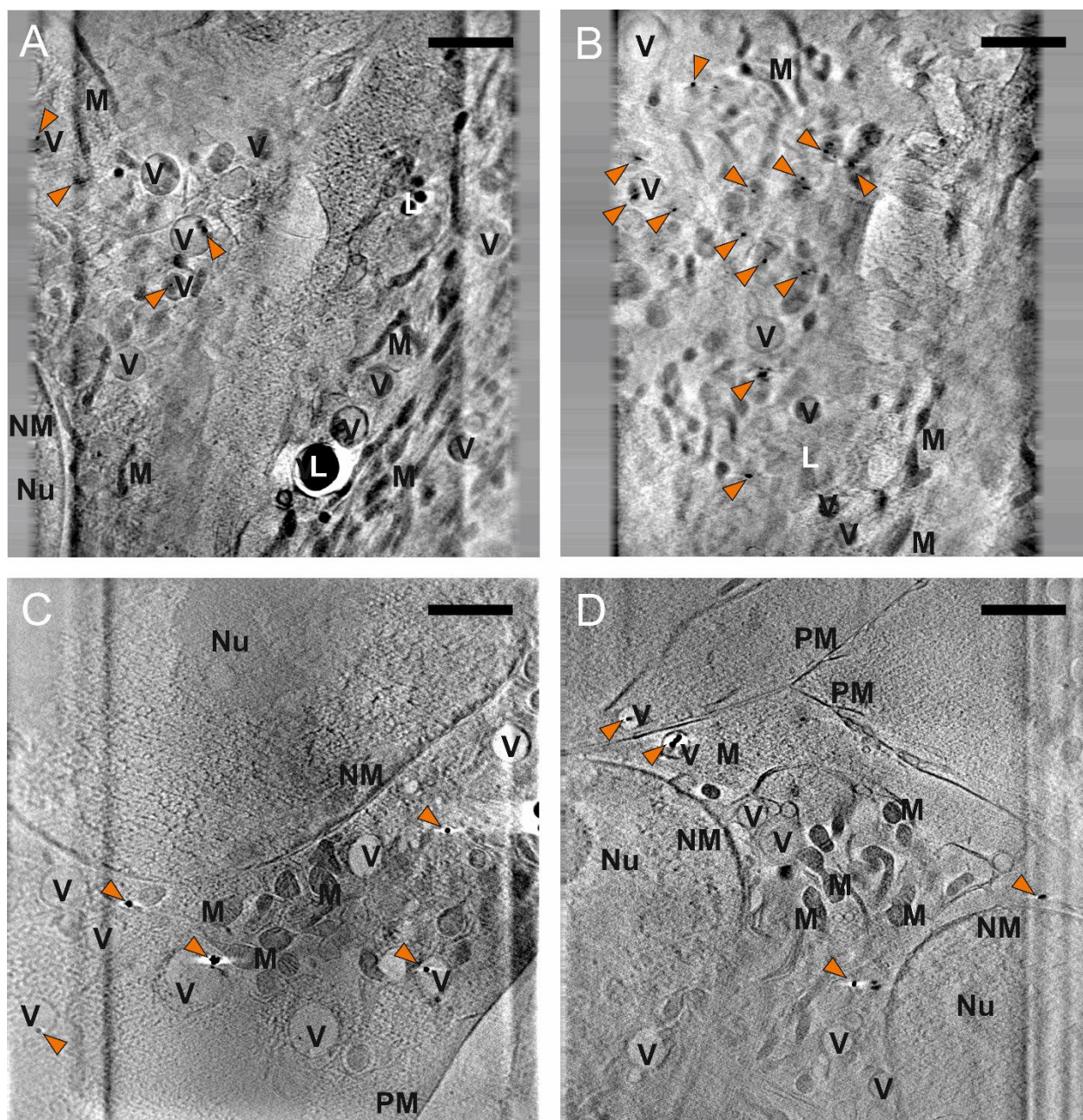**Figure 3.** Slices of X-ray tomographic reconstruction (further examples) of 3T3 (**A** and **B**) and J774 (**C** and **D**) cells incubated for 3 h with gold nanostars synthesized with 25 mM HEPES (NS25). The orange arrows indicate single particles or aggregates of nanostars. Abbreviations: Nu nucleus; NM nuclear membrane; PM plasma membrane; V vesicles; M mitochondria; L lipid droplets. Scale bars: 2 μm.

Figure S4. Slices of X-ray tomographic reconstruction of HCT-116 cells (**A** and **B**) incubated for 3 h with gold nanostars synthesized with 25 mM HEPES (NS25). The orange arrows indicate single particles or aggregates of nanostars. Abbreviations: Nu nucleus; NM nuclear membrane; V vesicles; M mitochondria. Scale bars: 2 μm.
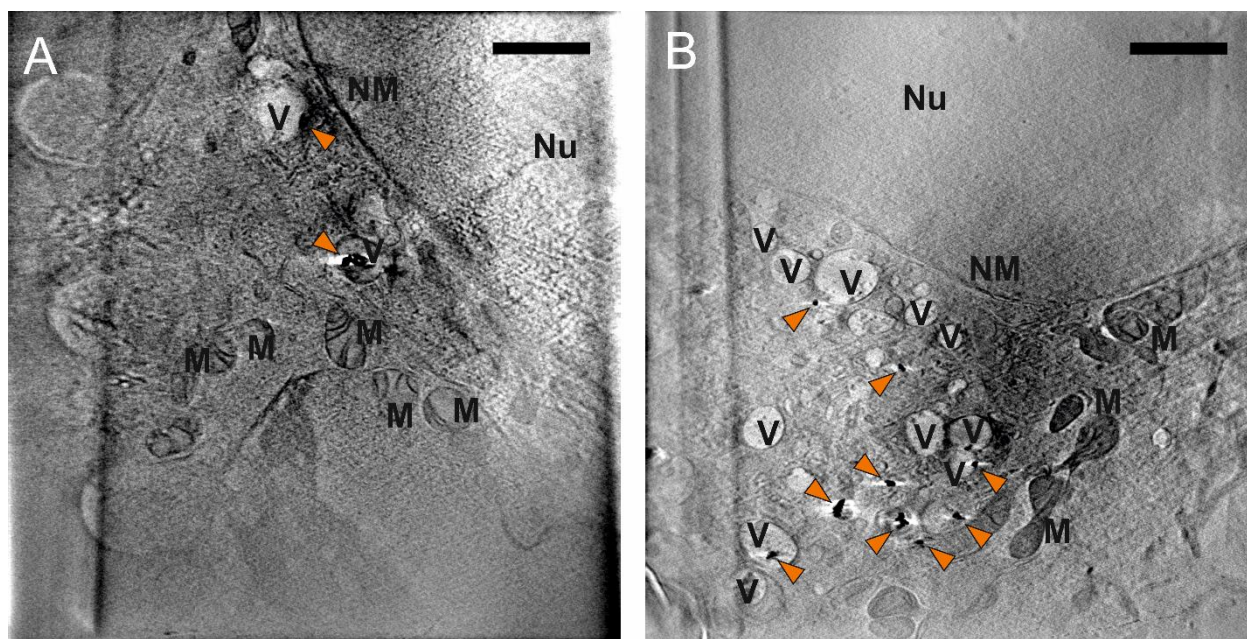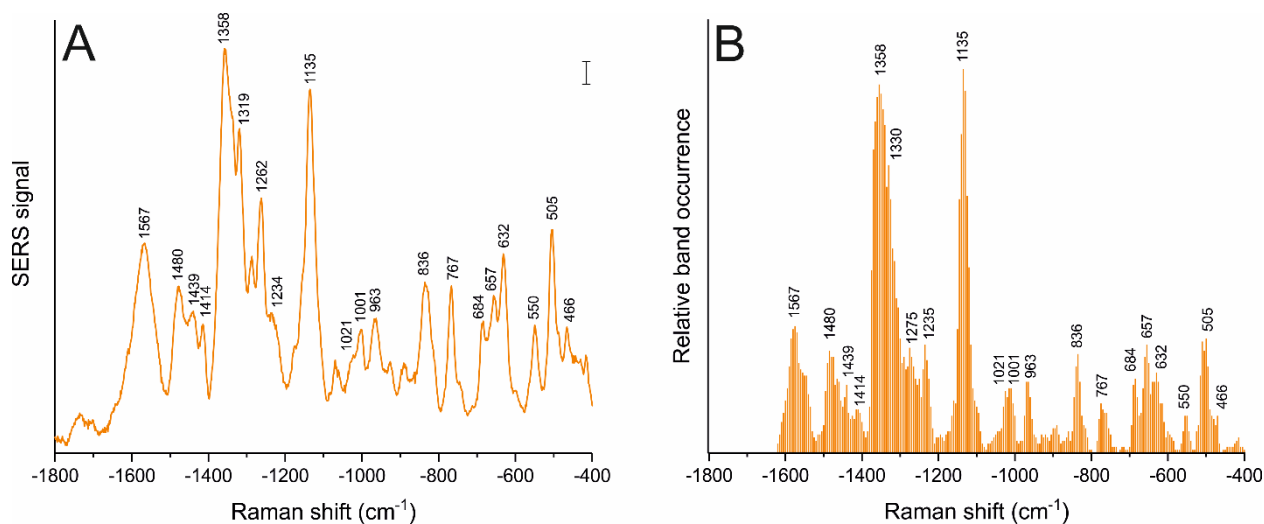

Figure S5. (A) SERS average spectra and **(B)** relative band occurrence for 3T3 cells incubated with gold nanostars synthesized with 25 mM HEPES (NS25) for 6 h. Scale bar in A: 5 cps.
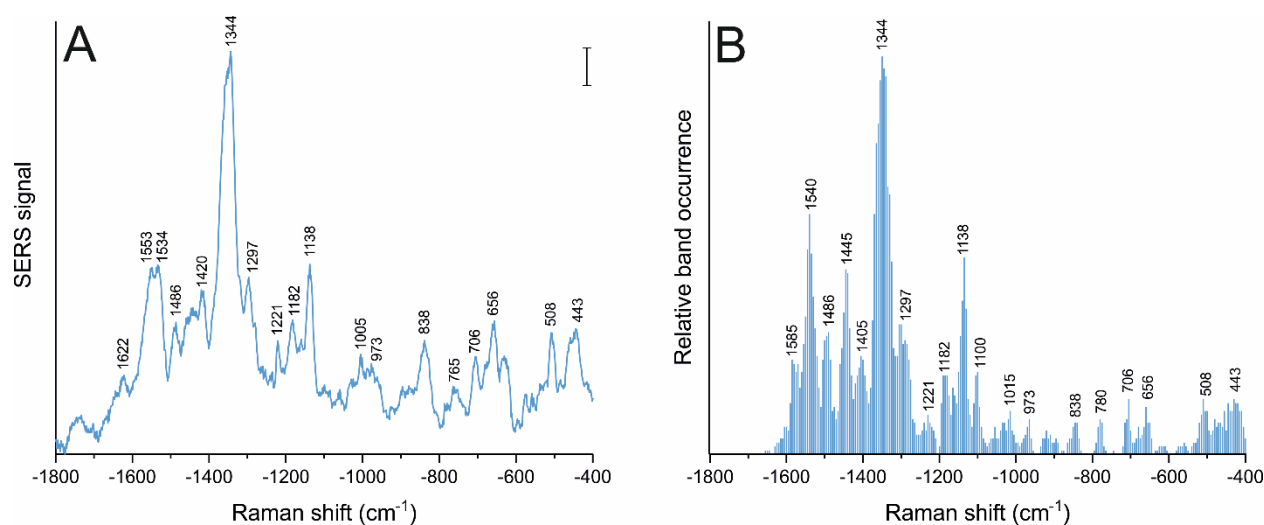
Figure S6. (A) SERS average spectra and **(B)** relative band occurrence for HCT-116 cells incubated with gold nanostars synthesized with 25 mM HEPES (NS25) for 6 h. Scale bar in A: 5 cps.

Table S1. Raman shifts and their tentative assignments in the spectra displayed in Figures S5 and S6. Band assignments and S6. Band assignments based on references[1–9].

Raman shift (cm⁻¹)		Tentative band assignment	
3T3	*HCT-116*		
	443	Protein S-S str	
466		C-S str	
505	508	Protein S-S str	Trp, tryptophan;
550		S-S str	Tyr, tyrosine;
632		C-S str	Phe, phenylalanine;
657	656	Cys C-S str, Tyr C-C twist, Phe	Cys, cysteine;
684		Cys C-S str, Tyr C-C twist	Pro, proline;
	706	COO⁻ def, C-S str	Val, valine;
767	765	Trp indol br	T, thymine;
	780	O-P-O str; C, U, T ring br	C, cytosine;
836	838	Tyr ring br, Phe, Cα-N and C-C str, O-P-O str	U, uracil;
			A, adenine;
963	973	Lipids C-C str, Pro, Val	G, guanine;
1001	1005	Phe ring br	str, stretching;

1021	1015	Ribose C-O str	def, deformation;
	1100	Phe; C-N str	twist, twisting;
1135	1138	Protein backbone C-C str; C-N str	br, breathing;
	1182	Tyr C-H bend; Phe	bend, bending;
	1221	Amide III; Trp ring	wag, wagging;
1234		Amide III, CH_2 wag, O-P-O str	sciss, scissoring
1262		Amide III	
1275		Amide III; $CH/CH_2/CH_3$ def	
	1297	Amide III, A and C, $CH/CH_2/CH_3$ def	
1319		Amide III, G, lipids CH_2/CH_3 def	
1330		Amide III; CH_2/CH_3 def	
	1344	CH def	
1358		Protein $CH/CH_2/CH_3$ def; Trp	
1414	1405	COO^- str	
	1420	A, G, CH_3CH_2 twist	
1439	1445	CH_2/CH_3 def	
1480	1486	Amide II, NH_3^+	
	1540	Amide II, lipid CH_2 sciss	
1567		Amide II; Trp, Tyr, COO^- str	
	1585	C=C str, COO^- str; Phe	
	1622	Trp	

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