

	OUTPUT (into EXCEL file)	VARIABLE (in "isd3.m" file)	UNIT	DEFINITION	VARIABLE IN LINE
NANOPARTICLES	LiquidMediaParticleNumber	output.t_partNumL		Number of particles in liquid media vs. time	1078
	CellDepositedParticleNumber	output.t_PartNumC		Number of particles deposited on cells vs. time	1079
	TotalParticleNumber	output.t_partNumTot		Total number of particles in the system vs. time	1080
	LiquidMediaParticleConc	output.t_partConcL	[µg/mL]	Mass concentration of particles in liquid media vs. time	1207
		output.tx_partConcL	[µg/mL]	Mass concentration of particles in liquid media vs. time and x	1191
	CellDepositedParticleConc	output.t_partConcC	[µg/mL]	Mass concentration of particles deposited on cells vs. time	1278
	LiquidMediaParticleMass	output.t_partMassL	[µg]	Mass of particles in liquid media vs. time	1201
	CellDepositedParticleMass	output.t_partMassC	[µg]	Mass of particles deposited on cells vs. time	1277
	LiquidMediaParticleSurfArea	output.t_partSAL	[cm ²]	Surface area of particles in liquid media vs. time	1235
	CellDepositedParticleSurfArea	output.t_partSAC	[cm ²]	Surface area of particles deposited on cells vs. time	1279
IONS	LiquidMediaFreeIonConc	output.t_ionConcFreeL	[µg/mL]	Mass concentration of ions in free state in liquid media vs. time	1286
	LiquidMediaProteinBoundIonConc	output.t_ionConcBndL	[µg/mL]	Mass concentration of ions in protein-bound state in liquid media vs. time	1287
	LiquidTotalIonConc	output.t_ionConcTotL	[µg/mL]	Total concentration of ions in liquid media vs. time	1288
	CellIonConc	output.t_ionConcC	[µg/mL]	Mass concentration of ions deposited in cells vs. time	1289
	LiquidMediaFreeIonMass	output.t_ionMassFreeL	[µg]	Mass of ions in free state in liquid media vs. time	1292
	LiquidMediaProteinBoundIonMass	output.t_ionMassBndL	[µg]	Mass of ions in protein-bound state in liquid media vs. time	1293
	LiquidTotalIonMass	output.t_ionMassTotL	[µg]	Total mass of ions in liquid media vs. time	1294
	CellIonMass	output.t_ionMassC	[µg]	Total mass of ions in cells vs. time	1295
	totalConc	output.t_totalConc	[µg/mL]	Total concentration (particles + ions) in liquid media and in cells vs. time	1298

Table S3. List of the outputs generated by ISD3 particokinetic model and saved in a EXCEL file. The mass concentration of nanoparticles in liquid media vs. time and height x (i.e. output.tx_partConcL) is used for extracting the predicted Ag. NP concentration computed at half height of the cuvette (dashed line, Fig. 3). The target cell doses computed over 24 h (Fig. 4 and 5) are obtained from the variables named output.t_partConcC and output.t_ionConcC which are saved into the EXCEL file as “CellDepositedParticleConc” and “CellIonConc”, respectively.