Electronic Supplementary Information

Avenue to X-ray-induced photodynamic therapy of prostatic carcinoma with octahedral molybdenum cluster nanoparticles

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Content

Figure S1. Transmission electron micrographs of **1NPs**.

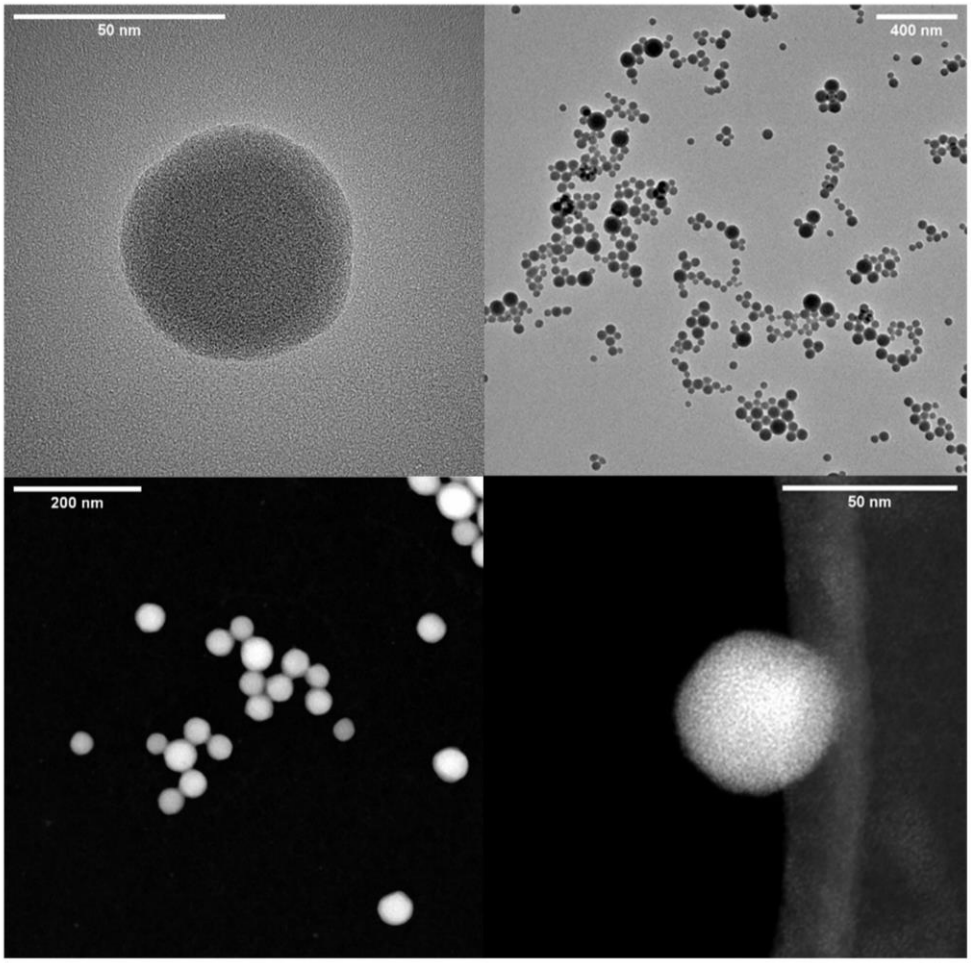

Figure S2. Powder XRD pattern in the transmission mode (Cu Kα) of dried **1NPs** deposited on a Mylar® foil.

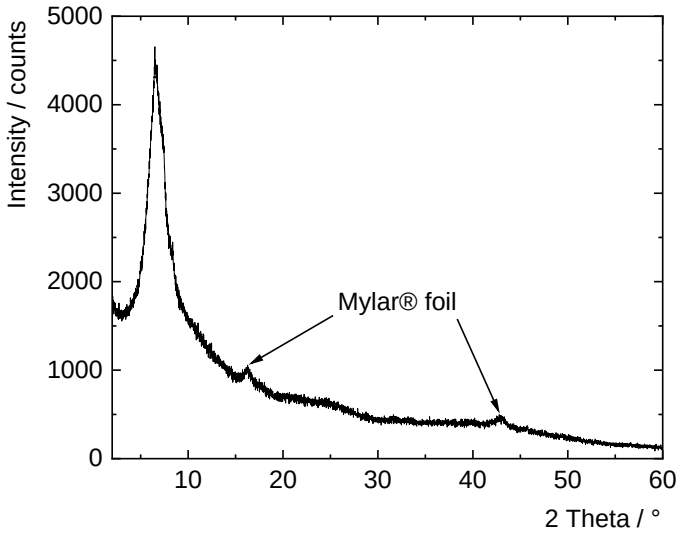

Table S1. Average size by number and zeta potential of **1NPs** in deionized water and PBS obtained by dynamic light scattering.

Solvent	Average size by number / nm	Dh / nm	PDI	Zeta potential / mV
Deionized water	55 ± 19 nm	103	0.19	-46 ± 13
PBS	69 ± 16 nm (94 %)	343	0.40	-35 ± 11
	269 ± 110 nm (6 %)			

Figure S3. Size distributions by number (left) and by intensity (right) of **1NPs** in deionized water (top) and PBS (bottom) obtained by dynamic light scattering.

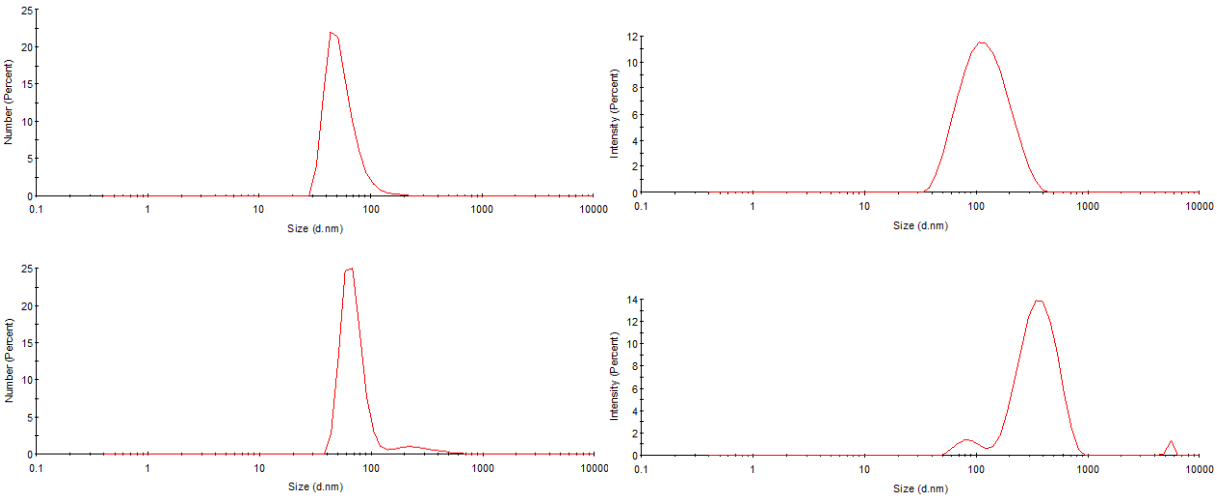

Figure S4. Zeta potential distributions of **1NPs** in deionized water (left) and PBS (right) obtained by dynamic light scattering.

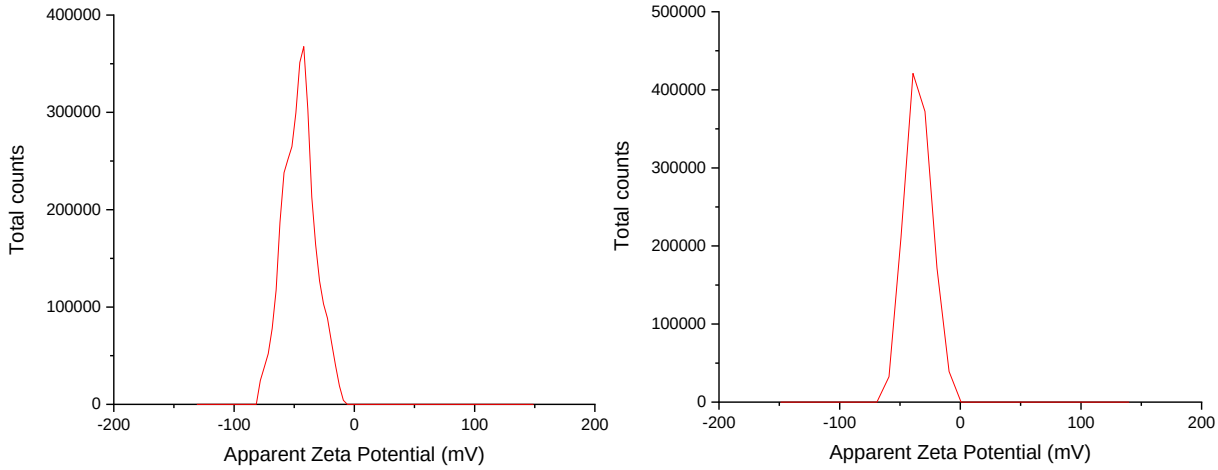

Figure S5. Normalized luminescence emission spectra of **1NP**s in argon-saturated PBS, fresh (black) and after 3 days (red).

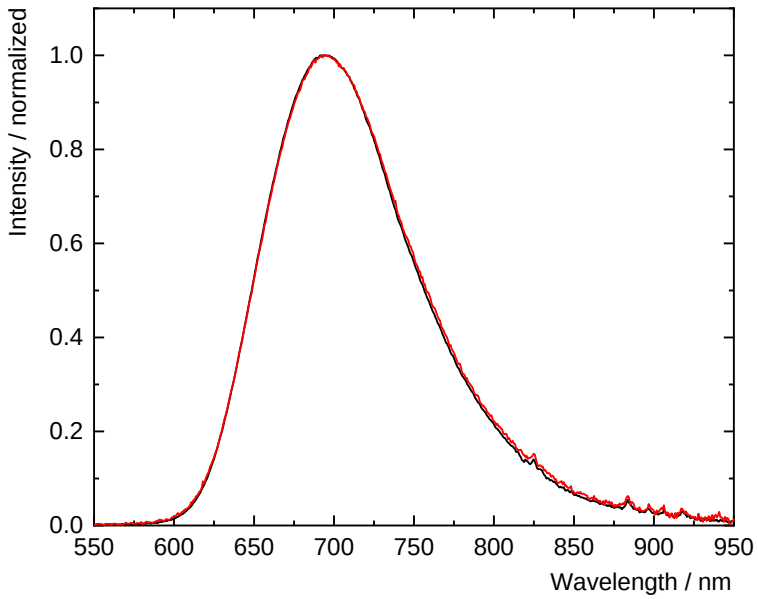

Figure S6. Phototoxicity of **1NPs** towards TRAMP-C2 cells: 4 h incubation with **1NPs**, then irradiation with 460 nm light (15 min, 9 mW cm^{-2}), and measured after next 24 h with the resazurin assay. With exception of experiments under standard conditions, i.e., at pH 7.4 (C, black bars), cells were pretreated with 12 mM lactate (L), pH adjusted to 6.8 by the addition of HCl (A), or 12 mM lactate at pH 6.8 (LA) in the full medium for 48 h. Experiments were performed in (**A**) normoxia (20% O_2) and (**B**) in hypoxia (5% O_2). Significance was set at $p < 0.05$ (* $p < 0.05$ compared to C, # $p < 0.05$ when comparing A and LA).

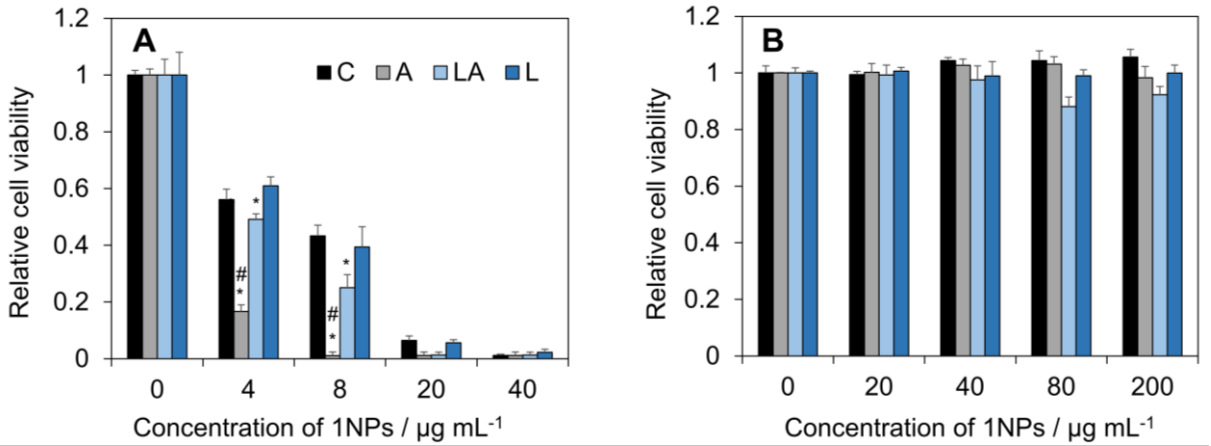

Table S2. Blood count of mice treated with **1NPs**. All but "Healthy mice" bear TRAMP-C2 tumors. Mice treated with **1NPs** received 200 μg.

	Control	**1NPs**	Healthy
WBC	14±4	10±3	10±1
Neu	4±3	1.6±0.5	1.2±0.2
Lym	9±3	8±3	8±1
Mon	0.7±0.2	0.7±0.2	0.4±0.2
Eos	0.2±0.1	0.2±0.1	0.5±0.3
Bas	0.04±0.04	0.01±0.02	0.03±0.04
RBC	11±1	10.3±0.6	10.7±0.8
HGB	163±16	156±8	162±10
HCT	0.57±0.05	0.54±0.03	0.54±0.04
MCV	52.6±0.5	52.3±0.5	50.0±0.3
MCH	15.2±0.2	15.1±0.2	15.2±0.2
MCHC	288±1	289±2	304±4
RDW-CV	0.14±0.01	0.14±0.01	0.13±0.01
RDW-SD	30±2	30±2	27±1
PLT	970±170	900±330	770±230
MPV	5.4±0.1	5.5±0.2	5.5±0.1
PDW	14.7±0.1	14.7±0.2	14.8±0.1
PCT	5±1	5±2	4±1

Abbreviation: WBC (white blood cells), Neu (neutrophils), Lym (lymphocytes), Mon (monocytes), Eos (eosinophils), Bas (basophils), RBC (red blood cells), HGB (hemoglobin), HCT (hematocrit), MCV (mean corpuscular volume), MCH (mean corpuscular hemoglobin), MCHC (mean corpuscular hemoglobin concentration), RDW-CV / RDW-SD (red blood cell distribution width), PLT (platelets), MPV (mean platelet volume), PDW (platelet distribution width), PCT (procalcitonin).

Table S3. Selected splenocytes populations of mice treated with **1NPs** (percentages of the CD45-positive cells are given). Analyzed by flow cytometry for percentage of important selected immune cell populations: CD45, CD4, CD8, Gr-1+/CD11b+ and activated CD8+ immune cells (CD69+). All but "Healthy mice" bear TRAMP-C2 tumors. Mice treated with **1NPs** received 200 μg.

	Control	**1NPs**	Healthy
$CD4^+$	15±1	19±2	23±6
$CD8^+$	9±2	11±2	10±2
$Gr\text{-}1^+/CD11b^+$	5±4	1.4±0.7	0.7±0.3
$CD69^+$	6±2	3±2	3.1±0.5

Table S4. Concentration of Mo (μg g^{-1} of wet weight) in selected tissue / material from control mice (not treated with **1NPs**) and mice injected subcutaneously with 200 μg of **1NPs.**

	Control	4 h after **1NPs** injection	3 weeks after **1NPs** injection
Entry	0.10±0.01	350±130*	7.7±4.0*
Kidney	0.50±0.01	0.4±0.2	0.50±0.02
Urine	1.9±1.0	1.5±0.6	0.6±0.5
Lung	0.10±0.01	0.10±0.02	0.20±0.02
Liver	1.10±0.08	1.30±0.07*	1.80±0.08*
Gallbladder	1.00±0.03	1.20±0.02*	1.30±0.06*
Stool	0.9±0.2	1.9±0.5*	1.9±0.4*
Feed	1.90±0.03	-	-

*Statistically different from the control group ($p < 0.05$).

Figure S7. Staining of tissue with **1NPs** after subcutaneous injection (red arrow).