Electronic Supplementary Information

Octahedral Molybdenum Clusters as Radiosensitizers for X-ray Induced Photodynamic Therapy

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Content

Figure S1. FTIR spectra of starting compound **1** (a) and **1NPs** (b).

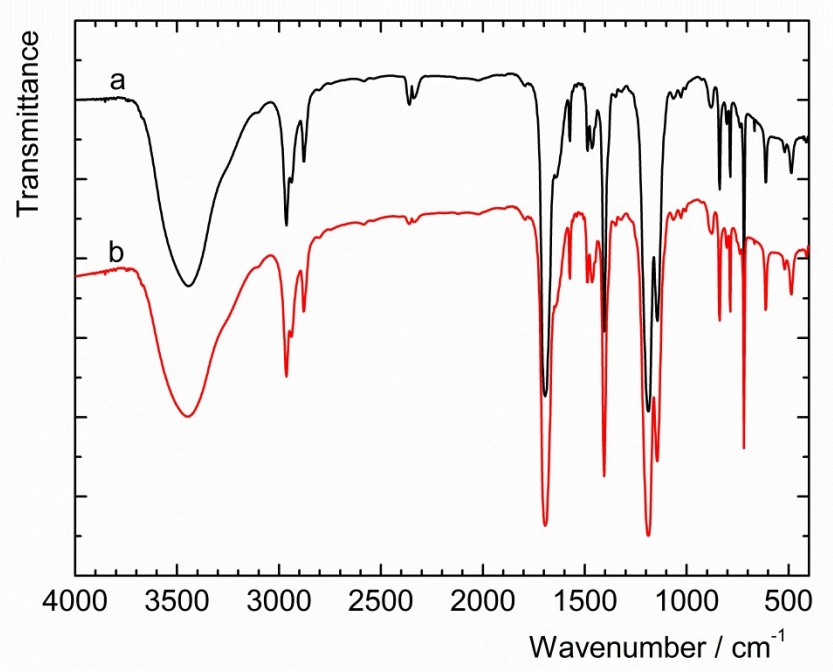


Figure S2. Powder X-ray diffraction pattern of starting compound **1** (a) and **1NPs** (b).

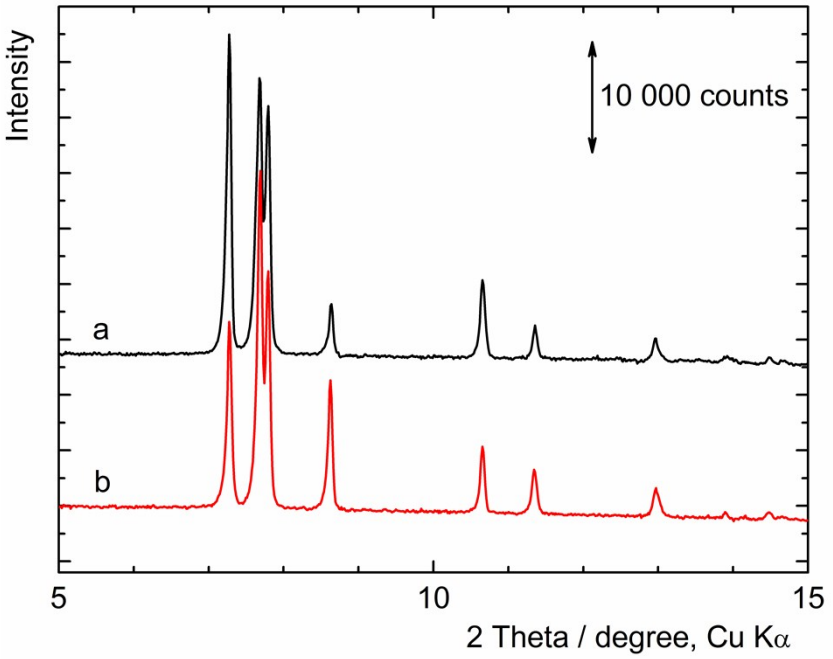
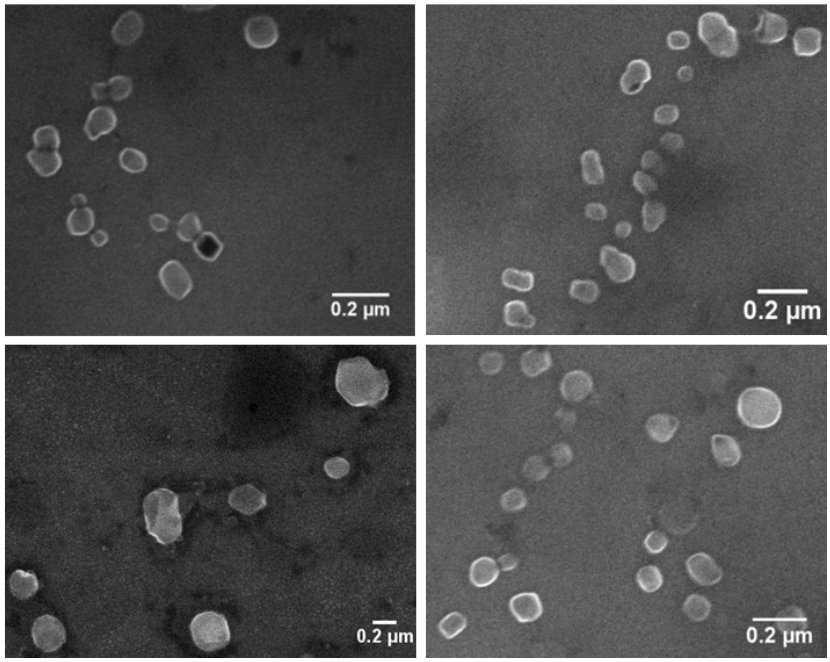


Figure S3. Selected SEM images of **1NPs** (A) and size distribution obtained by dynamic light scattering in fresh (B) and seven days old (C) dispersions in phosphate-buffered saline.

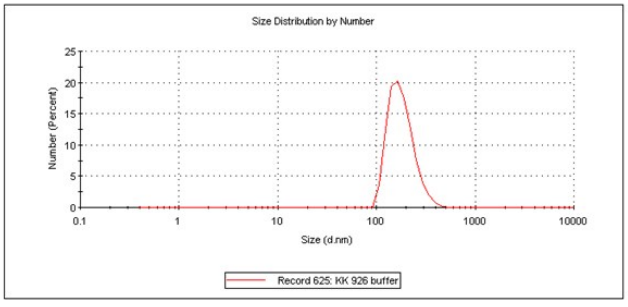
A



B

		Size (d.nm):	% Number:	St Dev (d.nm):
Z-Average (d.nm): 219.8	Peak 1:	182.0	100.0	56.23
PdI: 0.124	Peak 2:	0.000	0.0	0.000
Intercept: 0.961	Peak 3:	0.000	0.0	0.000

Result quality : Good



C

		Size (d.nm):	% Number:	St Dev (d.nm):
Z-Average (d.nm): 236.2	Peak 1:	195.9	100.0	58.14
PdI: 0.168	Peak 2:	0.000	0.0	0.000
Intercept: 0.980	Peak 3:	0.000	0.0	0.000

Result quality : Good

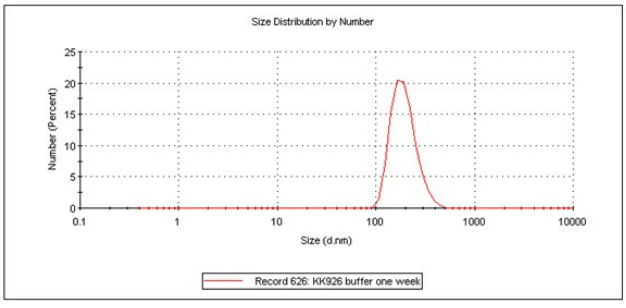
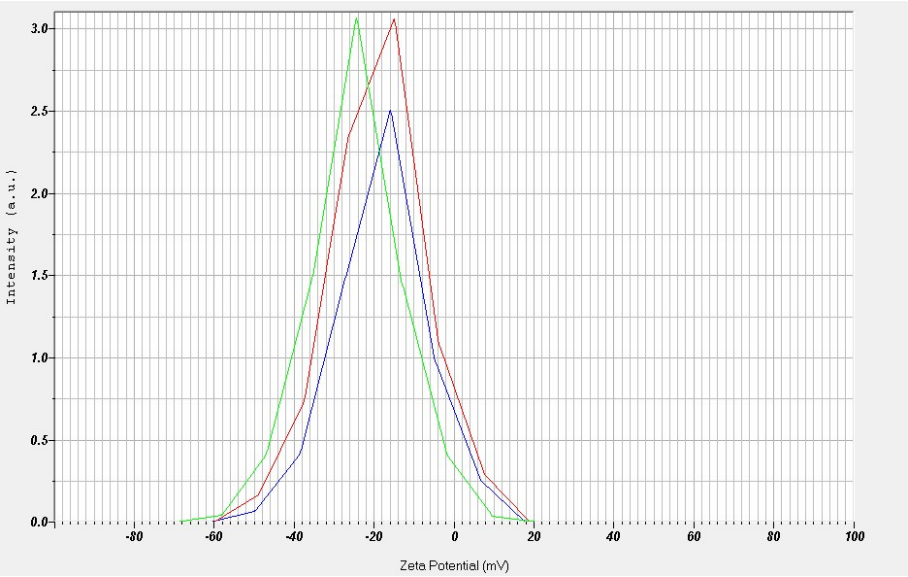


Figure S4. Zeta potentials of **1NPs** in phosphate-buffered saline including data from three measurements.



Measurement	Zeta Potential / mV
1	-24.4
2	-18.9
3	-17.9
Average	-20.4
S. D.	3.5

Figure S5. Concentration-dependent uptake of **1NPs**. HeLa cells were loaded with the indicated concentrations of **1NPs** for 120 minutes and the fluorescence with excitation/emission wavelengths 405/655-685 nm associated with the cells was recorded with the fluorescence-activated cell sorting. Mock cells are in grey, the growing concentration of nanoparticles is represented by darkening of the tones of green: 0.3, 0.6, 1.5, 3, and 6 μM.

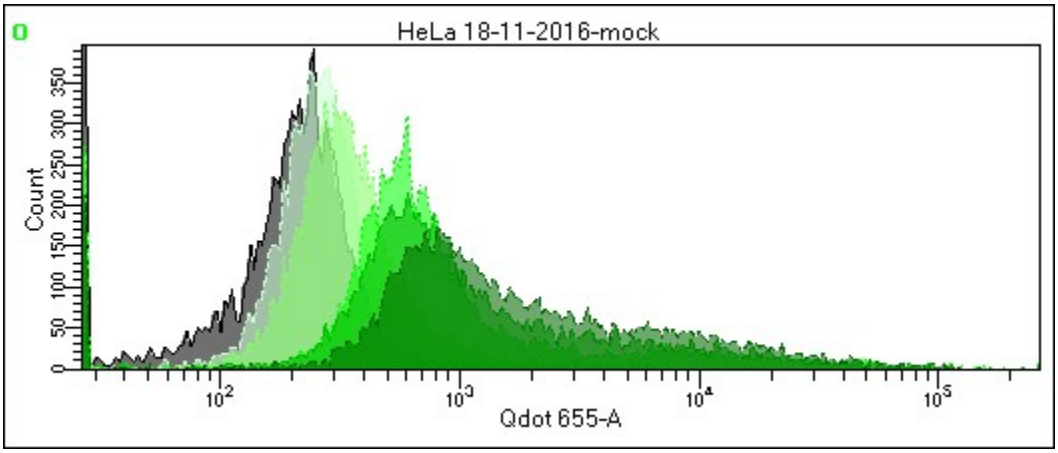


Figure S6. Time-dependent uptake of **1NPs**. HeLa cells were loaded with **1NPs** at concentration of 6 μM for the indicated time period and the fluorescence with excitation/emission wavelengths 405/655-685 nm associated with the cells was recorded with the fluorescence-activated cell sorting. Mock cells are in grey, the increasing uptake time is represented by the darkening of the tones of green: 30, 60, 90 and 120 min.

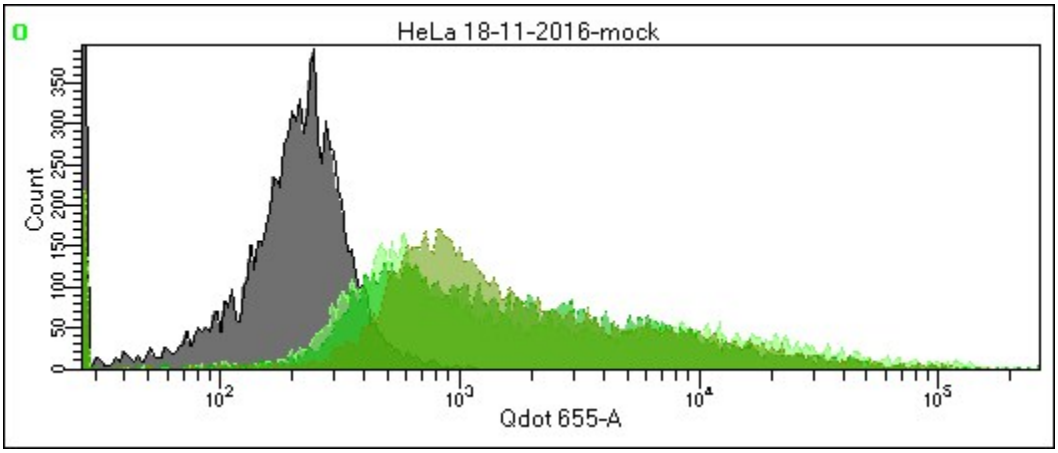


Figure S7. Bright field image of HeLa cells merged with a confocal image of **1NPs** (red) after 2 h incubation. White bar represents 100 μm.

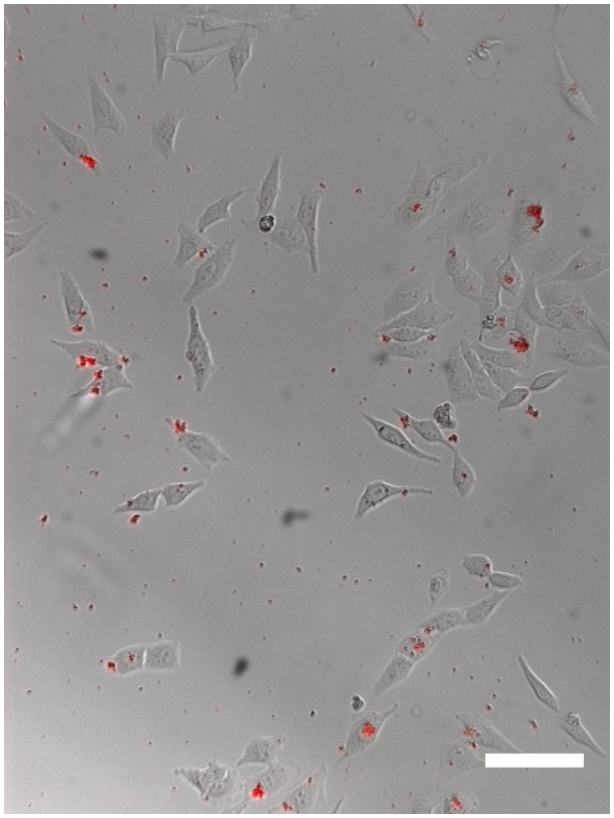


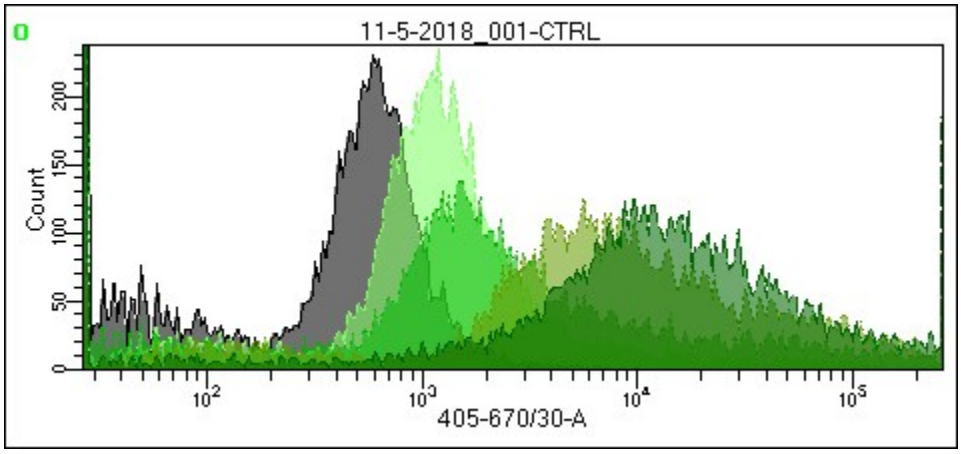
Figure S8. Uptake and photodynamic effects of **1NPs** on MRC fibroblast cells.

A) Concentration-dependent uptake of **1NPs** in fibroblasts. Fibroblasts were loaded with the indicated concentrations of **1NPs** for 120 minutes and the fluorescence with excitation/emission wavelengths 405/655-685 nm associated with the cells was recorded with the fluorescence-activated cell sorting. Mock cells are in grey, the growing concentration of nanoparticles is represented by darkening of the tones of green: 0.6, 1.5, 3, and 6μM.

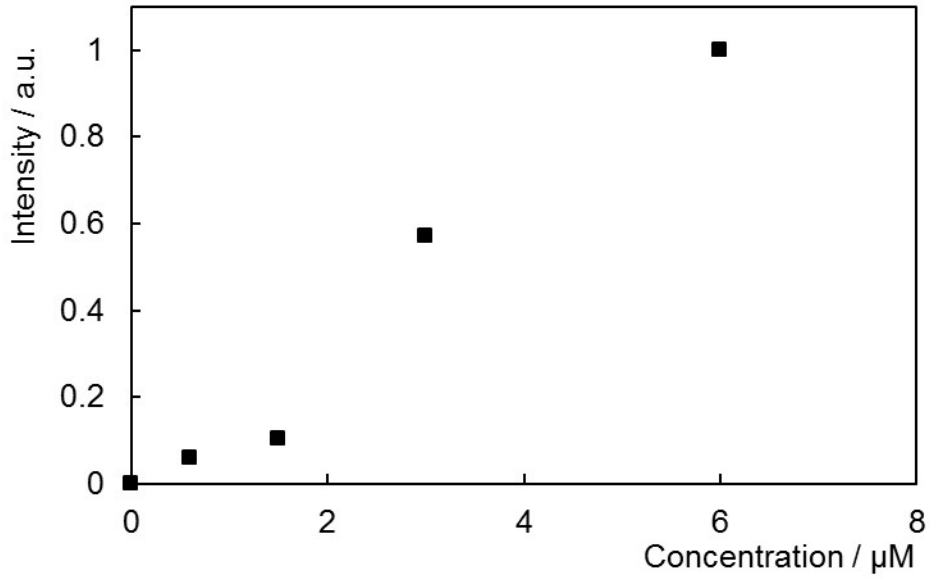
B) Relative uptake of **1NPs.** Dose-dependent uptake of **1NPs** after 2h incubation as follows from flow cytometry analysis. The axis y represents the fluorescence intensity of cells.

C) Dark toxicity and phototoxicity of **1NPs**. MRC fibroblast cells were loaded with **1NPs** using indicated concentrations for 2 h and irradiated with 460 nm light (20 mW cm^{-2}) for 15 minutes. The bars labeled as 0 belong to control experiments, i.e., the cells irradiated in the absence of **1NPs**.

A



B


Intensity / a.u.
1
0.8
0.6
0.4
0.2
0
0
2
4
6
8
Concentration / μM

C

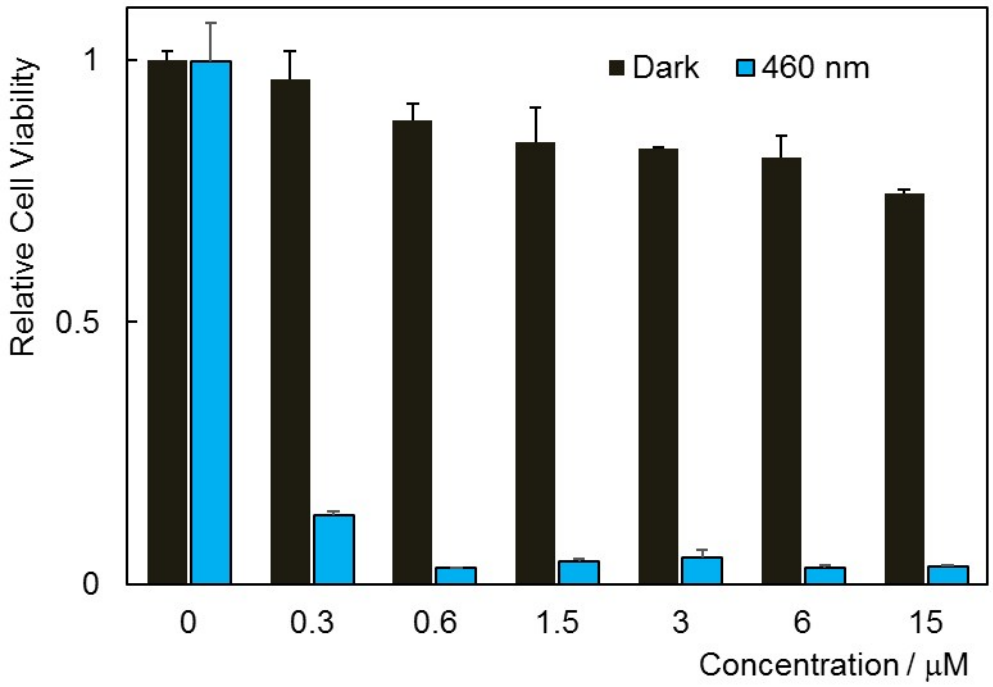
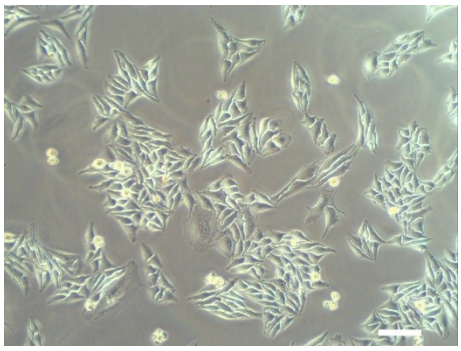
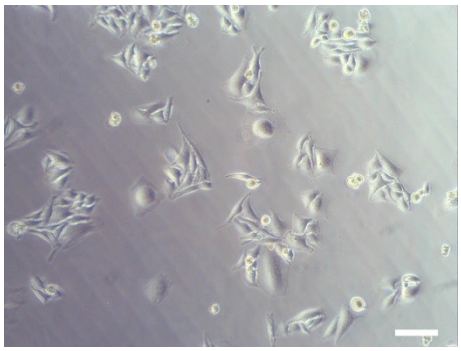

Relative Cell Viability
1
0.5
0
Dark
460 nm
0
0.3
0.6
1.5
3
6
15
Concentration / μM

Figure S9. Bright field image of the HeLa cell colony-forming assay. Control (A), irradiated by 4 Gy (B), and irradiated by 4 Gy after incubation with 3 μM **1NPs** (C). HeLa cells were seeded at 10x lower density and cultured for 4 days. White bar represents 100 μm.

A



B



C

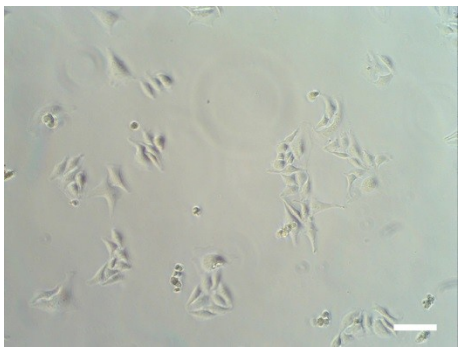


Figure S10. Percentage of necrotic (A) and apoptotic (B) HeLa cells 48 h after X-ray irradiation was determined with FACS analysis. The cells were treated with 3 μM **1NPs** for 2 hours and subsequently irradiated with X-rays to receive the indicated dose (black bars). The empty bars are for control experiments performed in the absence of **1NPs**.