SUPPLEMENTARY INFORMATION

Bioconjugated MoS_2 based nanoplatform with increased binding efficiency to cancer cells

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Additive-free MoS_2 liquid phase exfoliation – concentration of the solution

The liquid phase exfoliated solution is green. The saturation of green color depends on the amount of MoS_2 powder (Fig. S1). The concentration of the exfoliated solution was determined by drying up the samples and weighting the dry material. The samples with initial concentrations of crystalline MoS_2 powder 7.5 mg/ml, 5 mg/ml, and 2.5 mg/ml resulted in concentrations

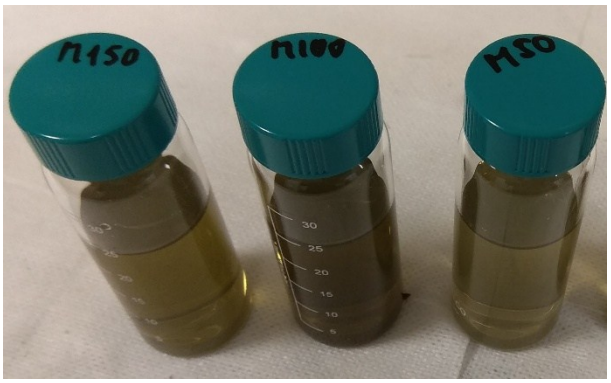

Figure S1 - MoS_2 exfoliated in water with three different initial concentrations of crystalline MoS_2 powder: 7.5 mg/ml (M150), 5 mg/ml (M100) and 2.5 mg/ml (M50).

of the MoS_2 nanosheet solution 84 µg/ml, 124 µg/ml, and 56 µg/ml, respectively.

Transmission electron microscope

TEM measurements were done with a high-resolution transmission electron microscope (HRTEM, ARM200CF, Jeol) on the most concentrated sample to visualize the lateral size of the exfoliated nanosheets. The sample was dropped on standard TEM grids with ultrathin amorphous carbon films. According to these measurements, the average width of the exfoliated nanosheets is 50-100 nm (see Fig S2).

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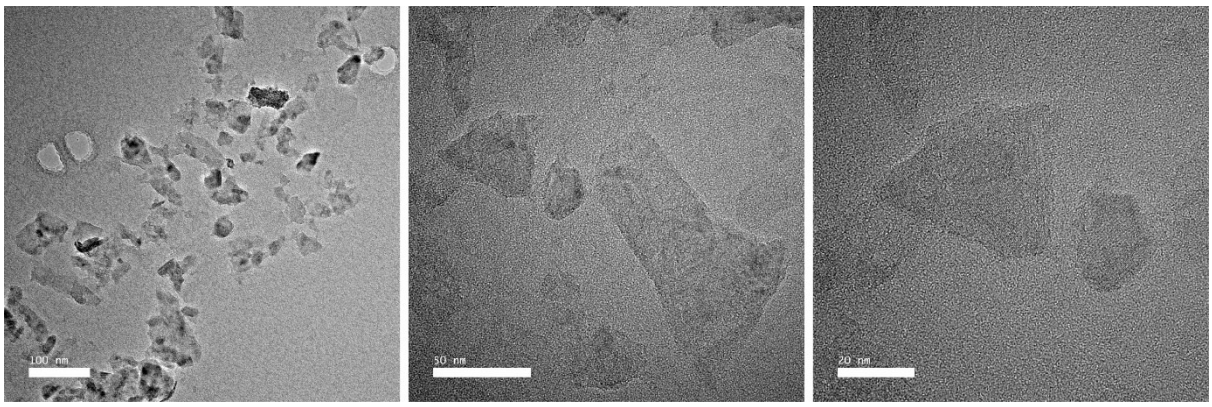

Figure S2 – TEM images of MoS_2 exfoliated in water.

Size distribution of the nanosheets – AFM

The size distribution was estimated from AFM scans (Bruker Multimode). The exfoliated MoS_2 was mixed with 96% ethanol in a ratio of 3:5, then dropcasted onto a cleaned silica wafer. After the solvent evaporation, 10 AFM scans were taken over 2×2 µm area. The images were evaluated by ImageJ software to acquire the lateral size of the nanosheets. 1169 nanosheets were counted on the 10 images. We define the lateral size of a nanosheet as the longest distance between any two points on the nanosheet edge. The mean value of the lateral size is 76.7 nm with a median of 64.4 nm.

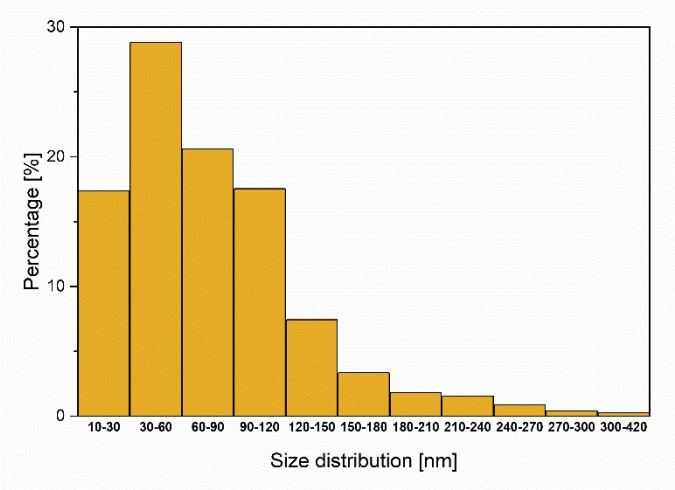

Figure S3 – Size distribution of the exfoliated MoS_2 nanosheets based on AFM images.

Number of MoS_2 monolayers in the exfoliated sheets – confocal Raman microscopy

The number of MoS_2 monolayers[1,2] was estimated relying on the peaks E^1_{2g} and A_{1g} of 50 Raman spectra taken on different sheets of the dropcasted sample. The mean distance between the peaks is 24.7 cm^{-1}, the standard deviation being 0.9 cm^{-1}. According to this, the estimated number of MoS_2 monolayers in the exfoliated sheets is 5.

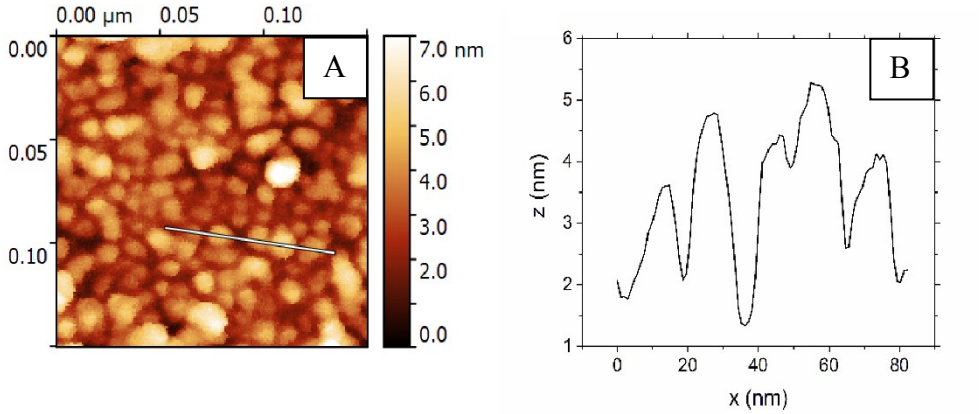

Figure S4 - AFM image of a Langmuir layer of MoS_2 nanosheets (A), cross-sectional line profile (B) of the line marked on image A.

AFM image of single layer of MoS_2 nanosheets

AFM scan (Bruker Multimode) of a single layer of MoS_2 nanosheets prepared by Langmuir-Schaefer deposition method[3,4] is shown in Fig. S4 A. The AFM image shows a closely packed layer of individual few-layer MoS_2 nanosheets, while the cross-sectional line profile in Fig. S4 B illustrates the height profile and further validates that the MoS_2 nanosheets are not aggregated. The average height of the Langmuir layer corresponds to the number of MoS_2 monolayers in the exfoliated nanosheets estimated by the Raman measurement above.

Stability of the nanoplatform solutions

Zeta potential (indicative of the surface charge of the nanosheets) was measured on Zetasizer Nano ZS 90 (Malvern Panalytical) to determine how the different ways of the functionalization improve the stability of the MoS_2 solution. The following aqueous solutions were used: MoS_2 with LA-PEG-biotin 2000 Da (P2), LA-PEG-biotin 2000 Da and LA-sulfobetaine mixtures 1:4 (SB5), 1:24 (SB25) molecule wise. The results (Table S1) observed are between -24 and -35 mV, which indicates high stability of the solutions tested, the pure MoS_2 solution included.

Table S1 – Zeta potential measurement of MoS2 and functionalized MoS2 with LA-PEG-biotin 2000 Da (P2), LA-PEG-biotin 2000 Da and LA-sulfobetaine mixtures 1:4 (SB5), 1:9 (SB10) in aqueous solution.

Sample	Measurement no.	Zeta potential (mV)
MoS_2	1.	-26.1
	2.	-25
	3.	-24.3
	4.	-23.7
	5.	-23.8
MoS_2 – P2	1.	-33.9
	2.	-35.8
	3.	-33.2
	4.	-32.4
	5.	-34.2
MoS_2 – P2SB5	1.	-31.8
	2.	-32.7
	3.	-33.1

	4.	-32.9
	5.	-32.7
MoS_2 – P2SB10	1.	-34.5
	2.	-33.8
	3.	-35.4
	4.	-34.6
	5.	-35.2

Confocal Raman imaging - MRC5

The identified cellular compartments in the case of MRC5 fibroblasts and MoS_2 nanoplatforms together with the decomposed Raman spectra are shown in Fig. S5 B-C. The MoS_2 is easily detectable by the two main modes, the $E_{2g}{}^1$ and A_{1g} as in the case of the JIMT-1 cells. The increased tryptophan signal at 750 cm^{-1} suggests lysosome activity similarly as it was in the JIMT-1 cells.

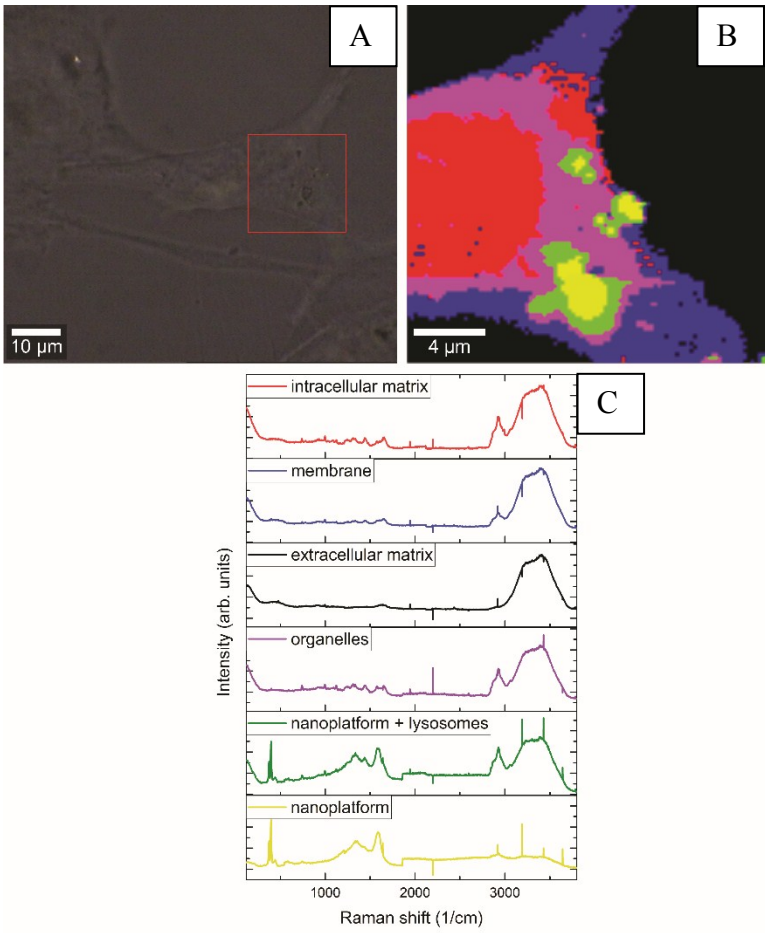

Figure S5 - Label-free Raman localization of MoS_2 nanoplatforms (sample MP2-M75): optical image of the MRC5 cells (A), reconstructed Raman image (B) and corresponding Raman spectra (C) with the same color codes (phosphate buffer saline - black, cell membrane – blue, intracellular matrix – red, lysosomes and organelles – purple, MoS_2 nanoplatform – yellow, nanoplatform with clear lysosome peak - green).

Bibliography

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