Supporting Materials

Disulfide-Modified Mesoporous Silica Nanoparticles for Biomedical Applications

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Equation S1:

DOX drug loading efficiency was calculated from the following equation[1,2]:

$$Drug\ Loading\ Efficiency\ (\%) = \frac{1000MV(C_0 - C_e)}{m} * 100\%$$

where V is the volume of the supernatant, C_0 and C_e are the initial and equilibration concentration of DOX in the MSN samples, M is the molar mass of DOX, and m is the mass of MSN samples.
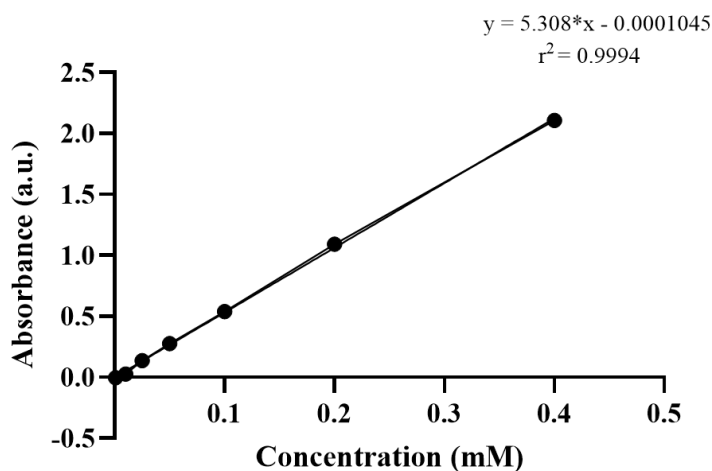

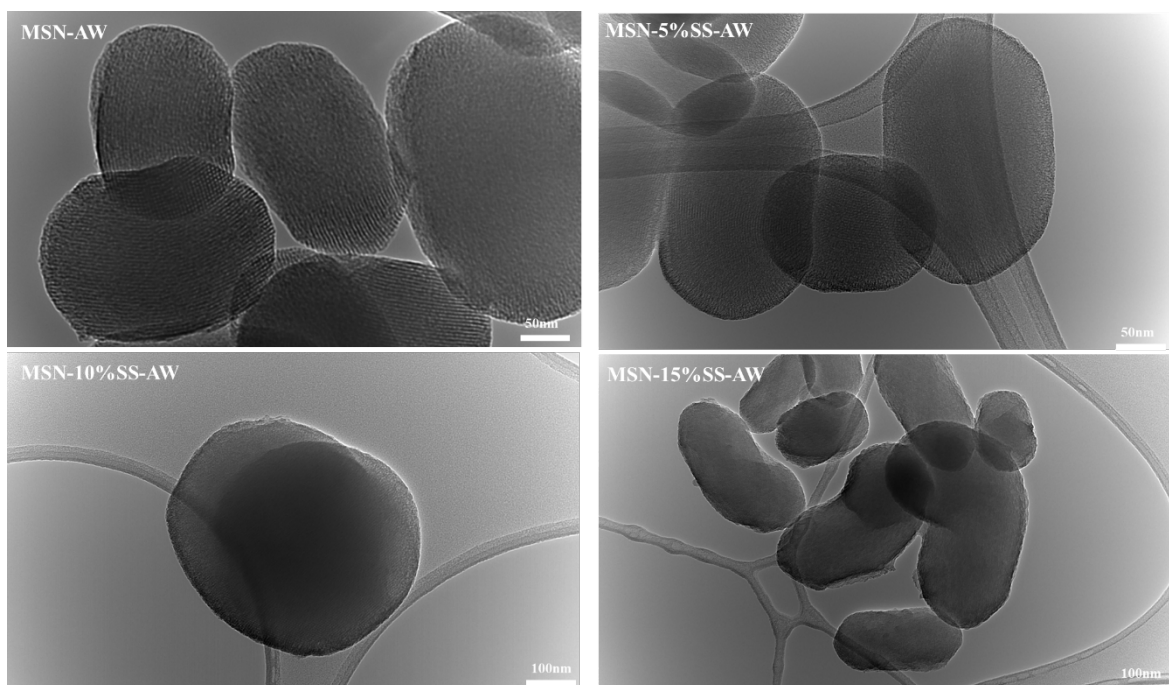Figure S1: Doxorubicin calibration curve at 480nm wavelengths

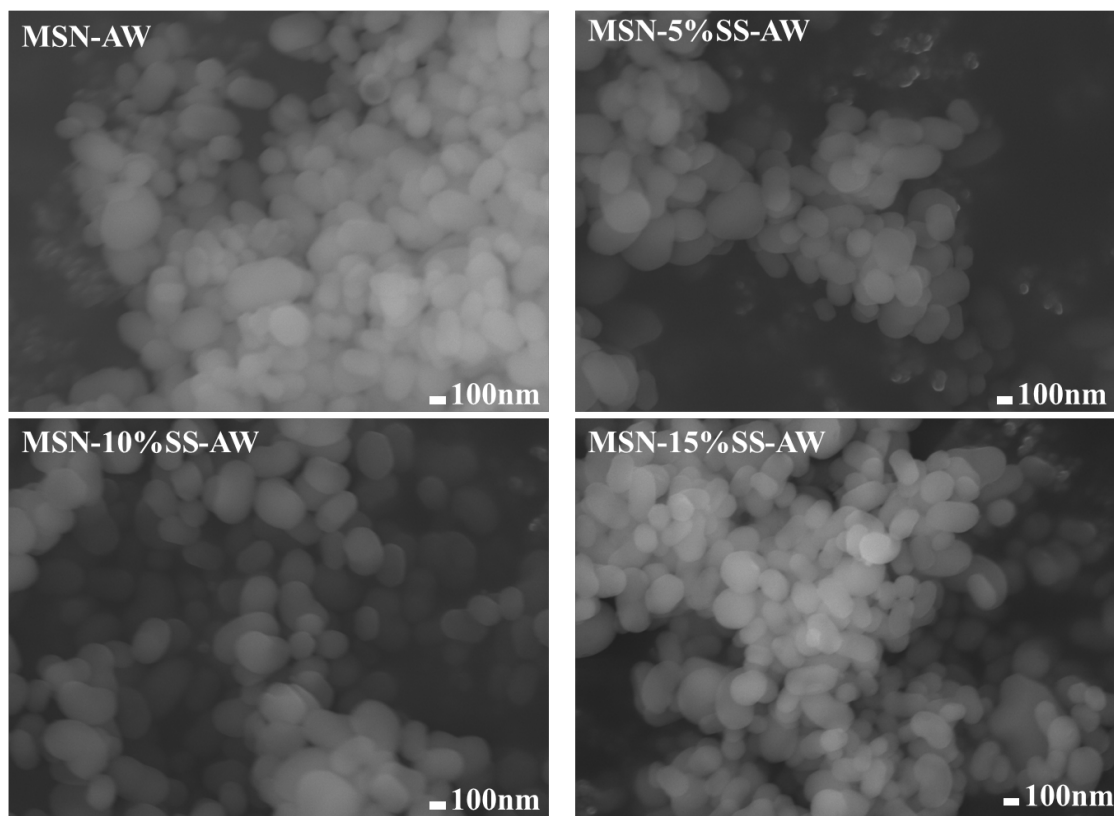Figure S2: TEM Surface Morphology Comparison of MSN-disulfide

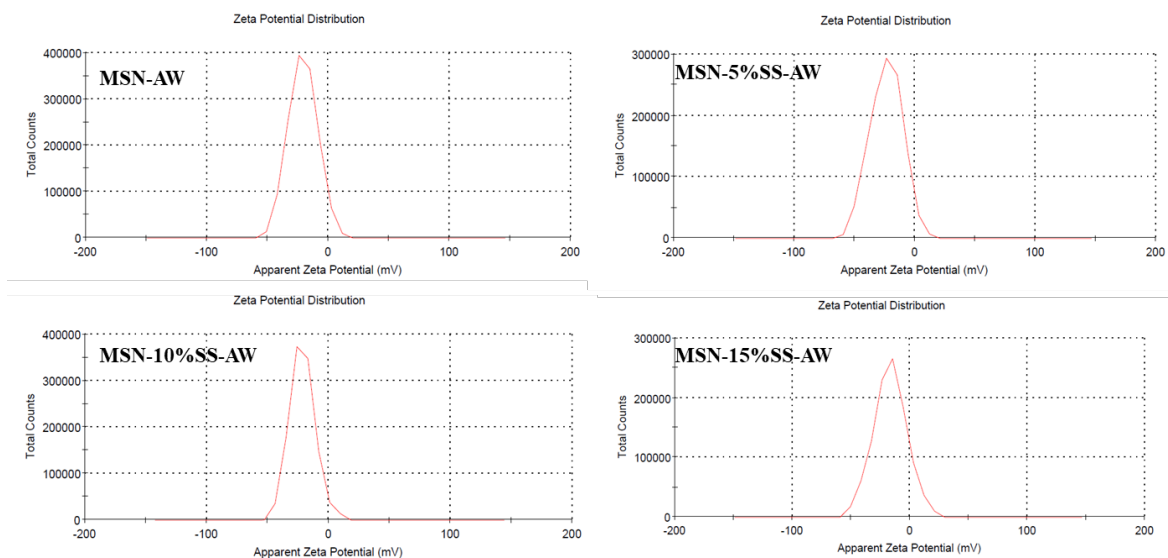Figure S3: SEM Surface Morphology Comparison of MSN-disulfide

Figure S4: Zeta potential Comparison of MSN-AW to disulfide-MSN

Material	Zeta Potential (mV)
MSN-AW	-20.8 ± 11.8
MSN-5%SS	-23.6 ± 13.4
MSN-10%SS	-21.5 ± 10.4
MSN-15%SS	-16.6 ± 14.4

Table S1: MSN Zeta Potential among various disulfide concentrations.

Equation S2:

Interplanar spacing (d_{100}) was calculated by using Bragg's Law[3]

$$d_{100} = \frac{\lambda}{2} * sin\theta_{100}$$

where (d_{100}) is the interplanar distance (Å), λ is the wavelength of the Cu Kα radiation, and θ is the position of the peak (degrees). The pore size (a_0) can be calculated through Bragg's Law, such as:

$$a_0 = \frac{2}{\sqrt{3}} d_{100}$$

Material	d_{100} (Å)	d_{110} (Å)	d_{200} (Å)
MSN-AS	4.78	3.21	2.37
MSN-5%SS	4.82	3.02	2.33
MSN-10%SS	4.59	2.65	2.31
MSN-15%SS	4.59	2.65	2.28

Table S2: MSN-AS nanocarrier using lattice parameter analysis via XRD

Material	d_{100} (Å)	d_{110} (Å)	d_{200} (Å)
MSN-AW	4.84	2.77	2.37
MSN-5%SS-AW	4.74	2.71	2.34
MSN-10%SS-AW	4.53	2.63	2.27
MSN-15%SS-AW	4.58	2.64	2.29
MSN-10%SS-DOX	0.96	-	-

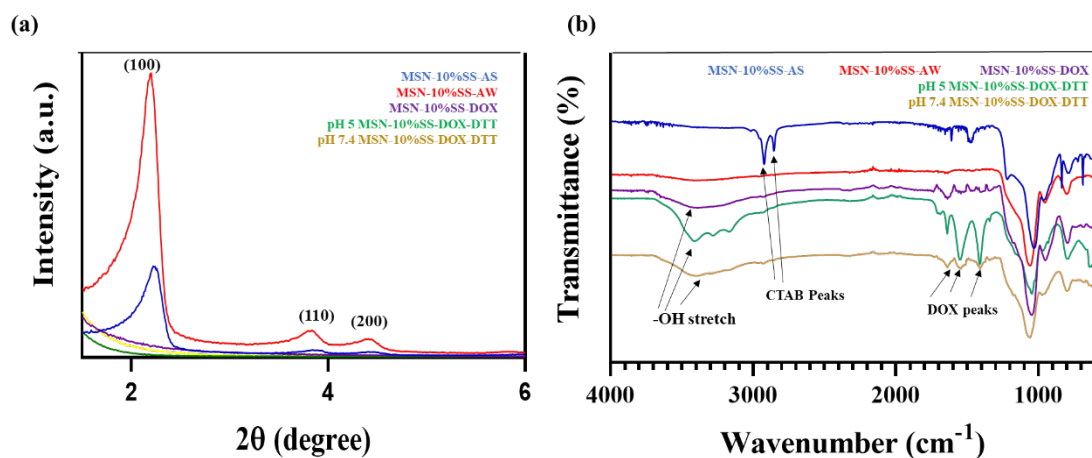Table S3: MSN-AW nanocarrier using lattice parameter analysis via XRD

Figure S4: (a) XRD analysis between MSN-AS, MSN-AW, MSN-DOX, and MSN-DOX-DTT to show deformed structure after pore filling, and (b) FTIR analysis between MSN-AS, MSN-AW, MSN-DOX, and MSN-DOX-DTT.

References:

1. Mao, C.; Xiang, Y.; Liu, X.; Cui, Z.; Yang, X.; Li, Z.; Zhu, S.; Zheng, Y.; Yeung, K.W.K.; Wu, S. Repeatable Photodynamic Therapy with Triggered Signaling Pathways of Fibroblast Cell Proliferation and Differentiation To Promote Bacteria-Accompanied Wound Healing. *ACS Nano* **2018**, *12*, 1747-1759, doi:10.1021/acsnano.7b08500.
2. Liu, M.; Radu, D.R.; Selopal, G.S.; Bachu, S.; Lai, C.Y. Stand-Alone CuFeSe(2) (Eskebornite) Nanosheets for Photothermal Cancer Therapy. *Nanomaterials (Basel)* **2021**, *11*, doi:10.3390/nano11082008.
3. Jaroniec, M.; Kruk, M.; Shin, H.J.; Ryoo, R.; Sakamoto, Y.; Terasaki, O. Comprehensive characterization of highly ordered MCM-41 silicas using nitrogen adsorption, thermogravimetry, X-ray diffraction and transmission electron microscopy. *Microporous and Mesoporous Materials* **2001**, *48*, 127-134, doi:https://doi.org/10.1016/S1387-1811(01)00335-3.