Electronic Supporting Information on

Biocompatible Tailored Zirconia Mesoporous Nanoparticles with High Surface Area for Theranostic Applications

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The XRPD spectra in Figure S1A show the pattern of MZNs sample Z1, taken as an example, before and after a thermal treatment at 350°C. This temperature has been chosen to verify a possible phase transformation after the exothermic peak. In the MZNs pattern, the two evident halos, visible around 30° and 55°, are characteristics of the amorphous zirconia oxide. No diffraction peaks were detectable in the whole diffraction range.[§] In the MZNs_350°C diffraction pattern, the tetragonal-zirconia reflections and a slight amount of monoclinic phase, confirm that a calcination process at about 350°C could promote the phase transition. No significant changes are found among different samples after calcination process as reported in Figure S1B.

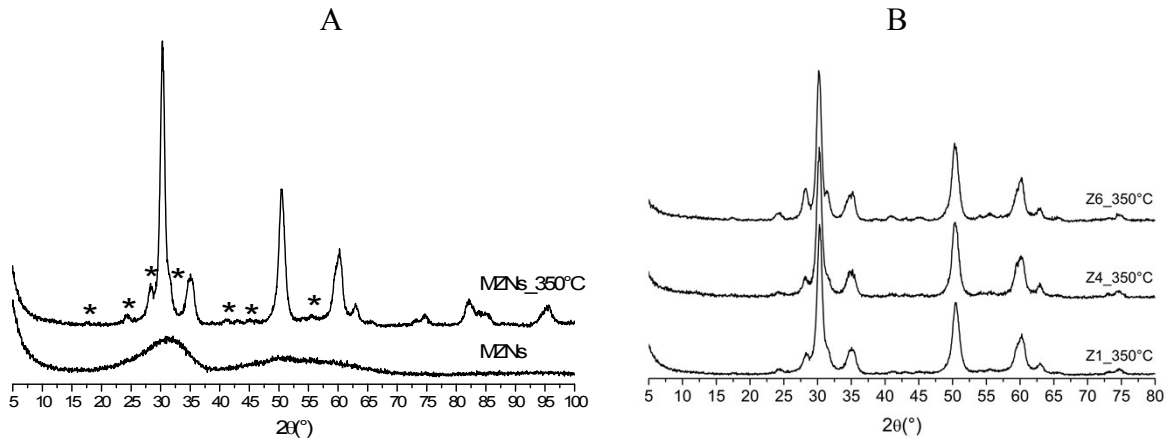

Figure S1 A) A representative XRPD pattern of the MZNs (Z1) after purification process *via* vacuum extraction, and after heating at 350°C. The marked peaks (*) were related to monoclinic zirconia phase. B) XRPD patterns of different samples after calcination.

Figure S2 reports the comparison between the IR spectra of the MZNs before the vacuum extraction and the surfactant and it evidences the amine presence into the pore network. The peaks below 3000 cm^{-1} are characteristic of the alkyl chains (stretching vibrations) of the surfactant tails. After the extraction (see the blue spectrum) these vibrations disappear, underlining the good process efficiency.

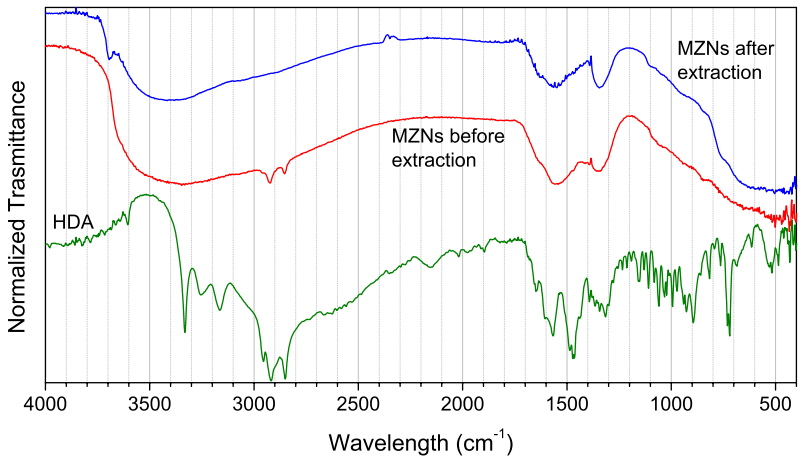

Figure S2 IR spectra of MZNs before and after purification process. HDA spectrum is also reported.

In Figure S3 the adsorption-desorption curves of MZNs samples Z1 after heating at 350°C is proposed. An evident change respect to the sample after vacuum extraction (Figure 6) could be found. The BET surface decreases from 240m^2/g to 80m^2/g after heating. The increment of the pore size should be attributed to the coalescence of the MZNs during the heating, so this distribution is not connected to the pore network inside the particles but it is due to the space between the NPs.

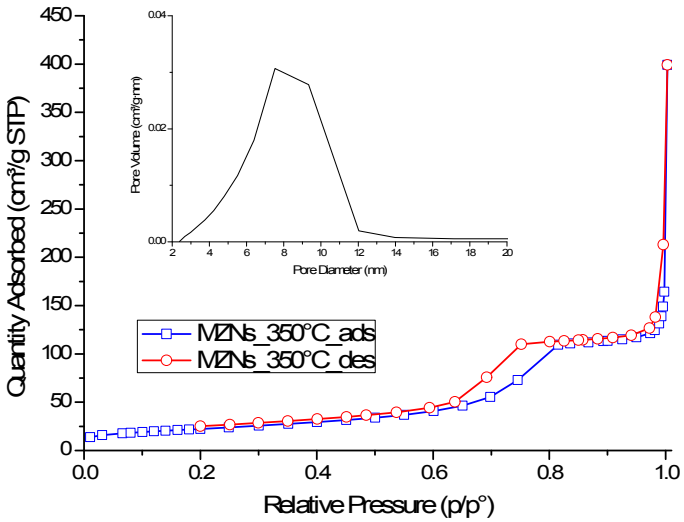

Figure S3 Nitrogen adsorption-desorption curves of MZNs sample Z1 after heating at 350°C. The inset of each graph shows the pore distribution curve.

§ Zeng, Y.W.; Fagherazzi, G.; Pinna, F.; Polizzi, S.; Riello, P.; Signoretto, M. Short-Range Structure of Zirconia Xerogel and Aerogel, Determined by Wide Angle X-Ray Scattering. *J. Non-Cryst. Solids* **1993**, *155*, 259-266.