Isothiocyanate-Functionalized Mesoporous Silica Nanoparticles as Building Blocks for the Design of Nanovehicles with Optimized Drug Release Profile

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Size / nm	TEM	DLS	PDI	Z-pot / mV
MSN-(NH_2)	50	129	0.19	-1.7
	100	142	0.07	-12
MSN-(NCS)	50	152	0.09	-1.4
	100	190	0.19	-11

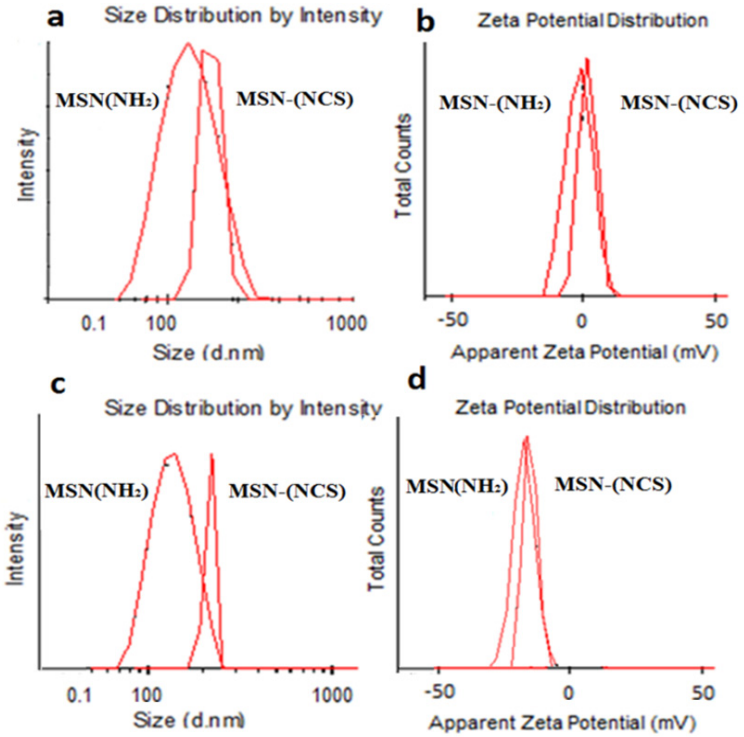

Figure S1. Dynamic light scattering (DLS) size and Zeta-potential values of MSN-(NH_2) and MSN-(NCS) of 50 nm (a, b) and 100 nm (c, d).

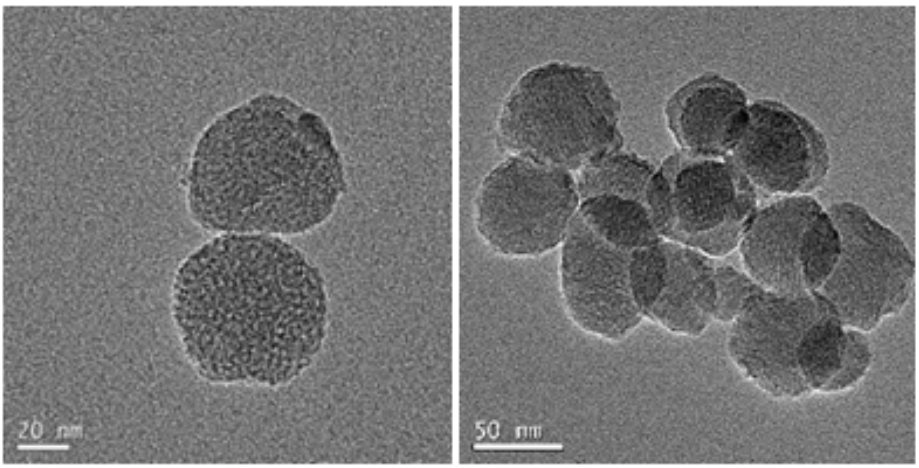

Figure S2. Representative TEM images of 50 nm MSN-(NCS).

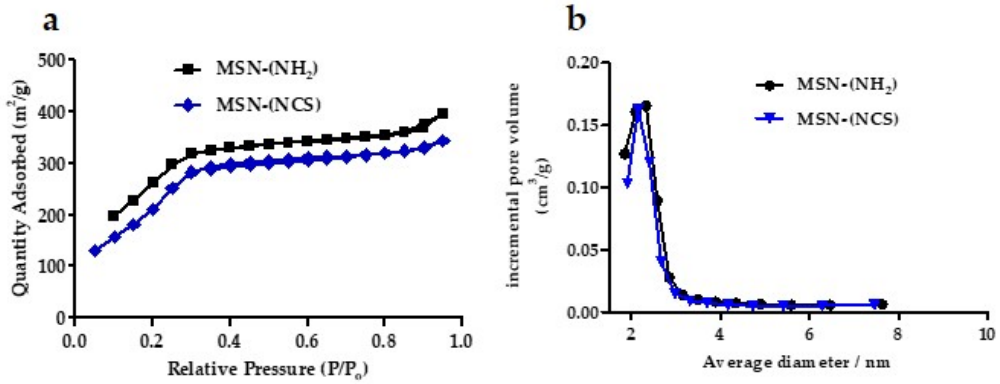

Figure S3. N_2 adsorption-desorption and BJH pore size distribution plots of of MSN-(NH_2) and MSN-(NCS) of 50 nm (a, b).

Table S2. N_2 adsorption-desorption and BJH pore size distribution values of MSN-(NH_2) and MSN-(NCS) of 50 nm.

	MSN-(NH_2)	**MSN-(NCS)**
BET surface area (m^2/g)	1120.90	849.20
BJH pore volume (cm^3/g)	0.72	0.53
Pore size (nm)	2.30	2.20

II. Functionalization test of MSN-(NCS) and MSN-(N_3)

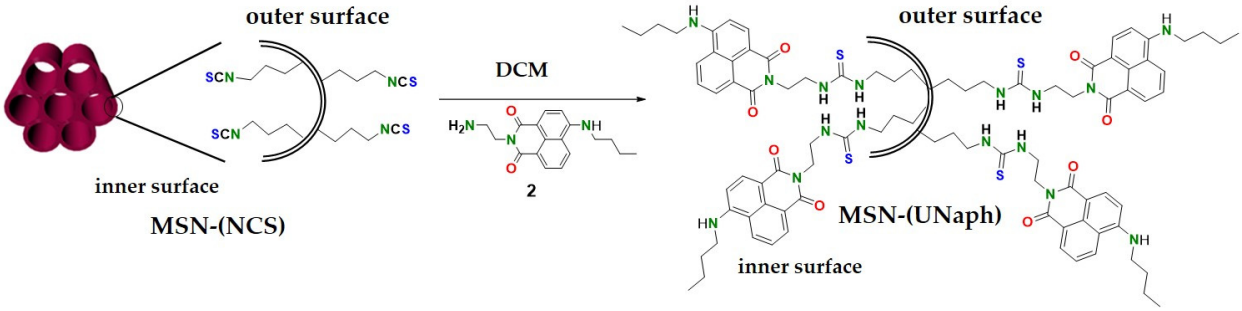

Figure S4. MSN-NCS functionalization with 4-(*n*-butylamino)-*N*-(2-aminoethyl)-1,8-naphthalimide.

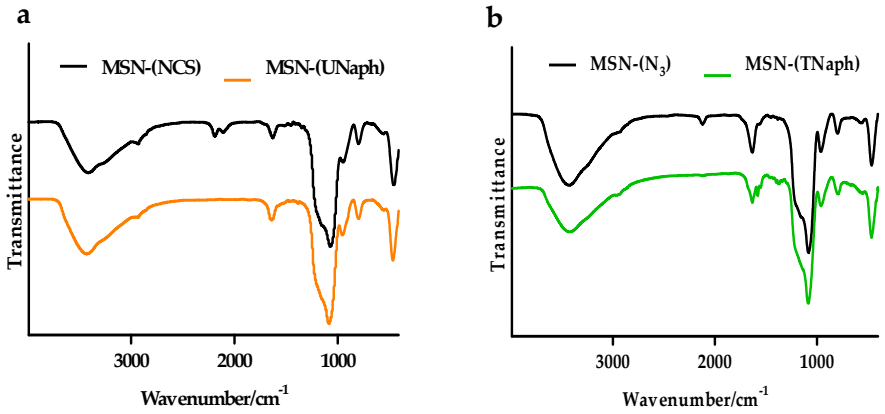

Figure S5. FTIR spectra of MSN-(NCS) (a) and MSN-(N_3) (b) reacted with 4-(*n*-butylamino)-*N*-(2-aminoethyl)-1,8-naphthalimide.

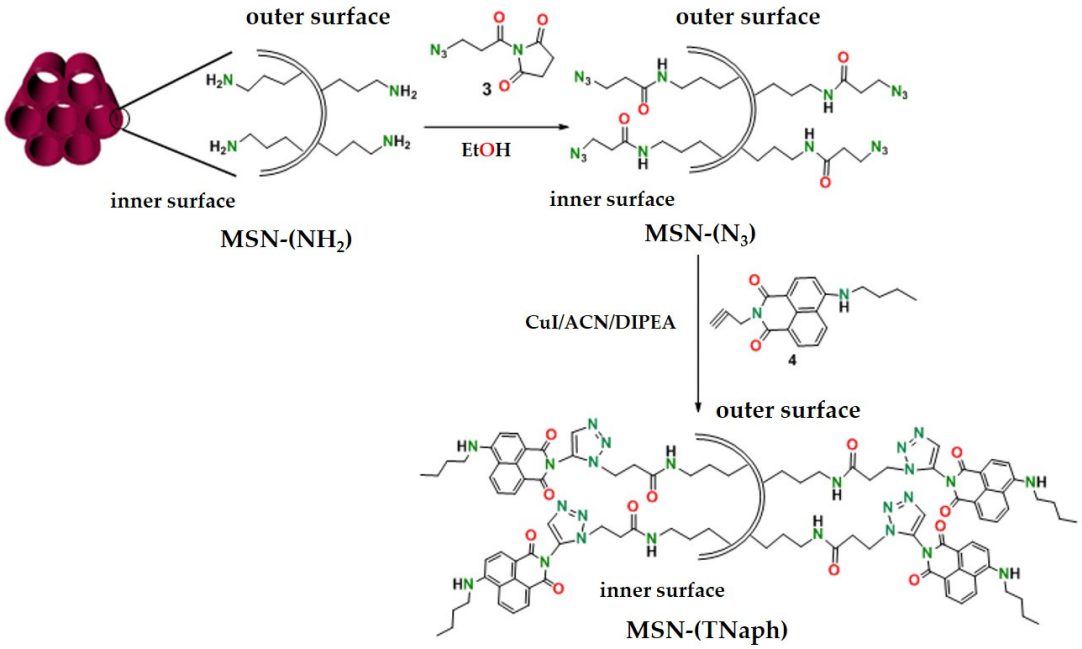

Figure S6. MSN-(N_3) functionalization with 4-(*n*-Butylamino)-*N*-(2-propargyl)-1,8-naphthalimide.

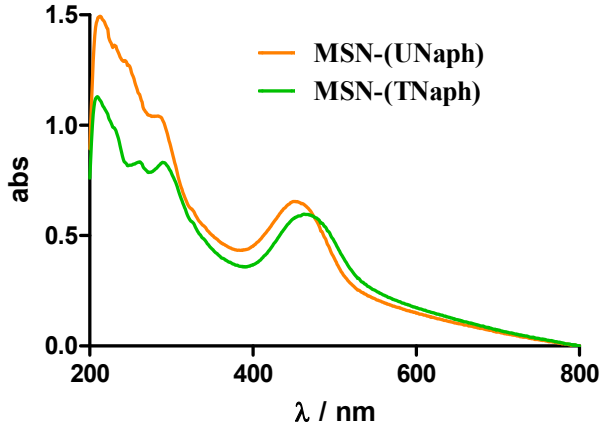

Figure S7. Absorption spectra of MSN-(UNaph) and MSN-(TNaph).

III. Characterization of regioselective bifunctionalized MSN-$(NH_2)_i(NCS)_o$

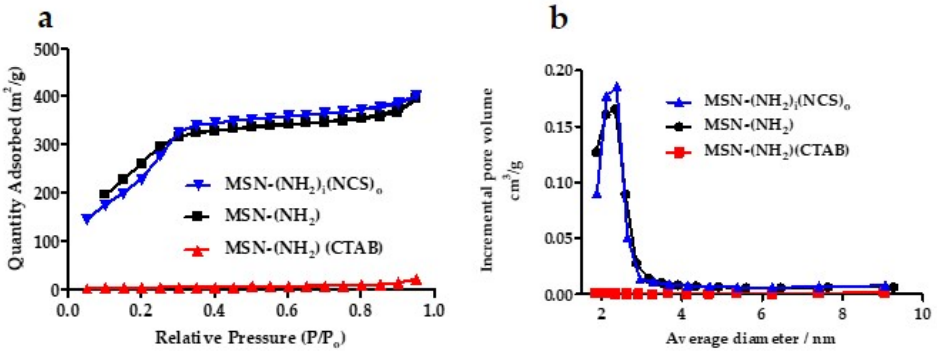

Figure S8. N_2 adsorption-desorption surface area (a) and BJH pore size distribution plots (b) of MSN-(NH_2) (CTAB), MSN-(NH_2) and MSN-$(NH_2)_i(NCS)_o$ of 50 nm.

Table S3. N_2 adsorption-desorption and BJH pore size distribution values of MSN-(NH_2) (CTAB), MSN-(NH_2) and MSN-$(NH_2)_i(NCS)_o$ of 50 nm.

	MSN-NH_2(CTAB)	MSN-(NH_2)	MSN-$(NH_2)_i(NCS)_o$
BET surface area (m^2/g)	78.60	599.80	554.50
BJH pore volume (cm^3/g)	0.25	0.55	0.45
Pore size (nm)	--	2.60	2.60

Table S4. Dynamic light scattering (DLS) size and Z-potential values of MSN-(NH_2) and MSN-$(NH_2)_i(NCS)_o$ of 50 nm and 100 nm.

Size / nm	TEM	DLS	PDI	Z-pot / mV
MSN-(NH_2)	50	129	0.19	-1.7
	100	142	0.07	-12
MSN-$(NH_2)_i(NCS)_o$	50	141	0.29	-1.7
	100	173	0.04	-13

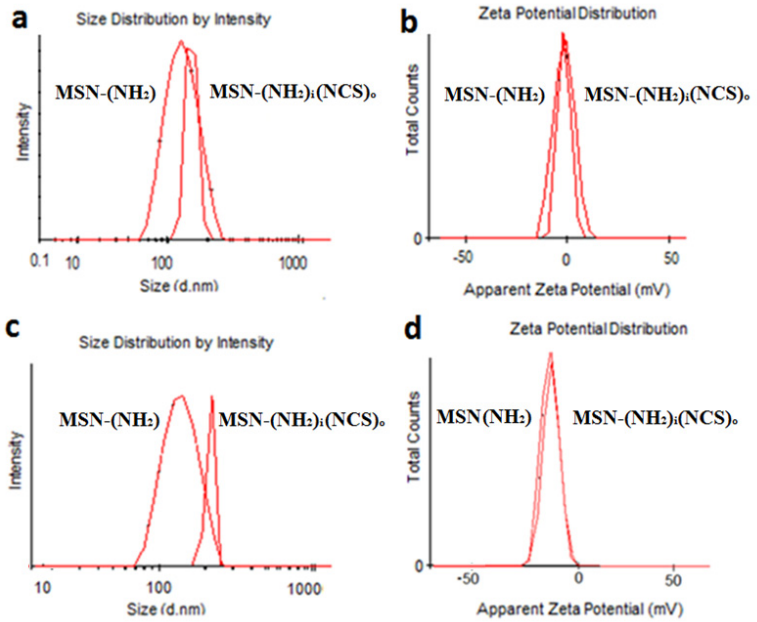

Figure S9. Dynamic light scattering (DLS) size and Z-potential measures of MSN-(NH_2) and MSN-$(NH_2)_i(NCS)_o$ of 50 nm (a, b) and 100 nm (c, d).

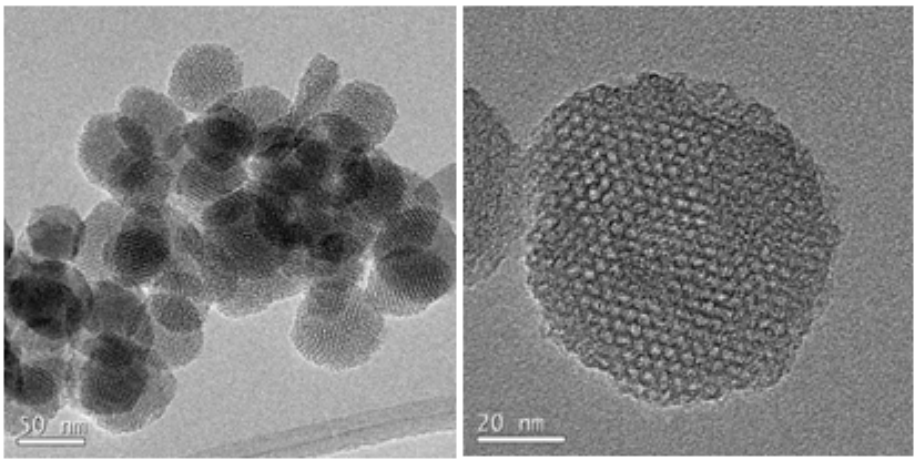

Figure S10. TEM images of 50 nm MSN-$(NH_2)_i(NCS)_o$.

$$\%\ Ataluren\ relaesed = \frac{mg\ Ataluren\ released}{mg\ Ataluren\ charged} \cdot 100$$

Equation S1. % Release Ataluren.