

# Supporting Information

for

## **Cyclodextrin-assisted synthesis of tailored mesoporous silica nanoparticles**

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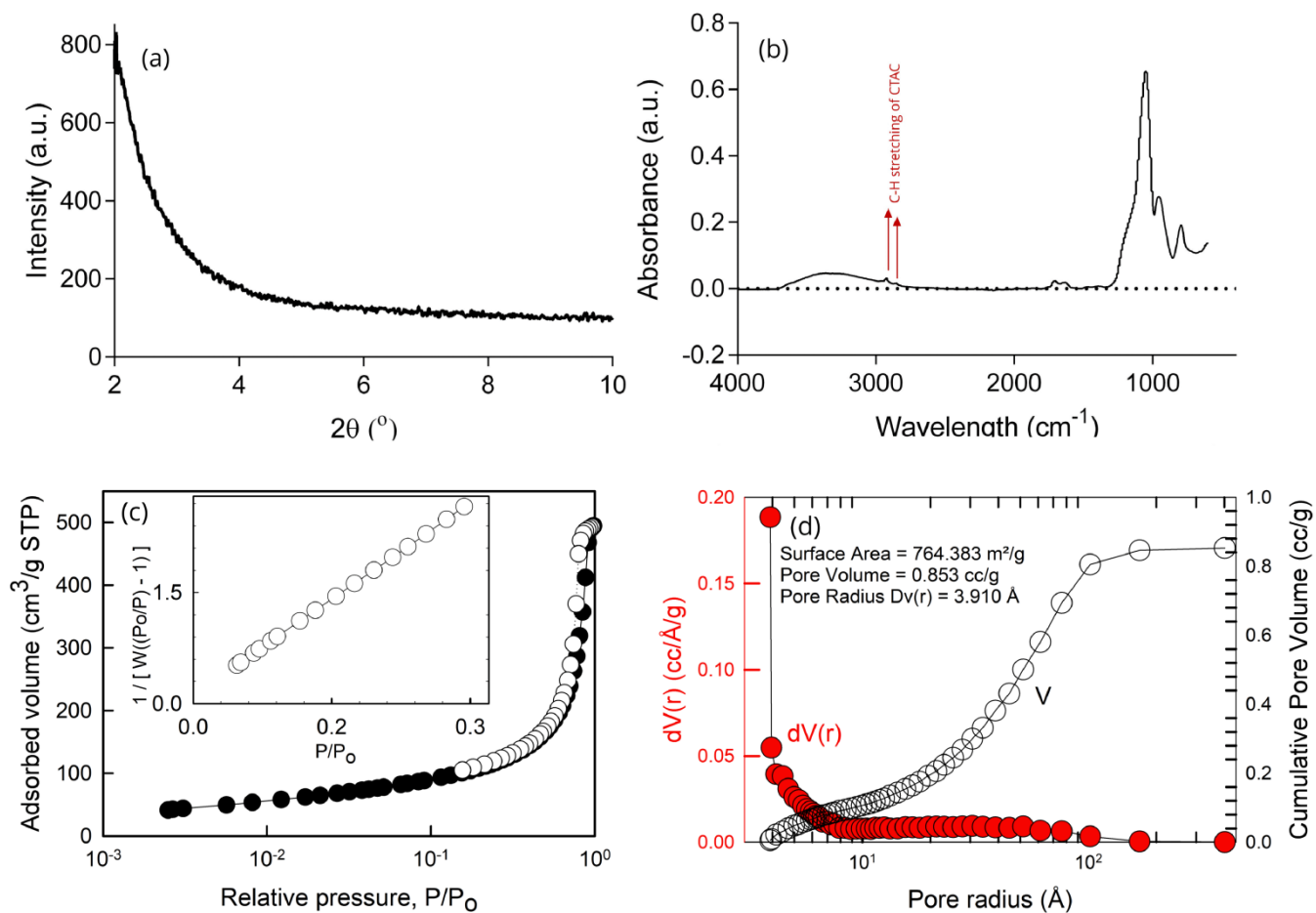
### **Additional experimental data**

**Table S1:** The composition and characteristics of the MSNs.

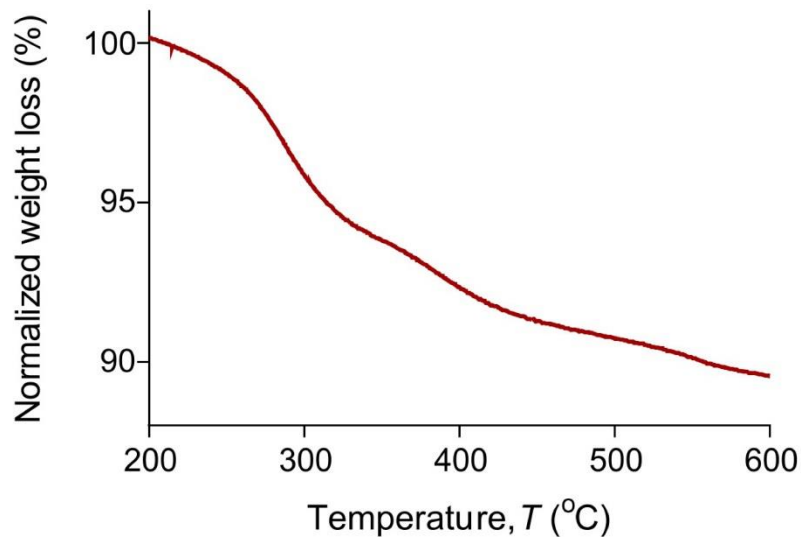
Sample Code	CD-Type	CD (% (w/v))	TEOS (% (v/v))	$r_{\text{CD/CTAC}}$ (w/w)	NaOH 2M (mL)	Water (mL)	Synthesis Temp (°C)	Particle Shape <sup>a</sup>	Particle (nm) <sup>b</sup>
MSN-1	$\beta$	0.50	1	5	0.7	96	80	Spherical - Ellipsoid	351
MSN-2	$\beta$	1	1	10	0.7	96	80	Spherical	750
MSN-3	HP- $\gamma$	0.25	1	1.25	0.7	96	80	Faceted	825
MSN-4	$\beta$	0.25	1	2.50	0.7	96	80	Spherical	273
MSN-5	HP- $\beta$	0.25	1	2.50	0.7	96	80	Faceted	1290
MSN-6	HP- $\gamma$	0.10	1	0.50	0.7	96	80	Spherical- Faceted	139
MSN-7	HP- $\gamma$	0.17	1	0.85	0.7	96	80	Spherical- Faceted	210
MSN-8	HP- $\gamma$	0.40	1	2	0.7	96	80	Spherical	206
MSN-9	HP- $\gamma$	0.60	1	3	0.7	96	80	Spherical	207
MSN-10	HP- $\gamma$	0.10	1	0.25	0.7	96	80	Spherical	83
MSN-11	HP- $\gamma$	0.17	1	0.42	0.7	96	80	Spherical	85
MSN-12	HP- $\gamma$	0.60	1	1.50	0.7	96	80	Spherical	95
MSN-13	$\beta$	0.25	1	1.25	0.7	96	80	Spherical	112

MSN-14	$\beta$	0.75	1	3.75	0.7	96	80	Spherical	125
MSN-15	$\beta$	1.5	1	7.50	0.7	96	80	Bean-like	484
MSN-16	$\beta$	1	1	10	0.7	96	80	Spherical (linked)	1542
MSN-17	$\beta$	1	1	2.50	0.7	96	80	Spherical (monodisperse)	167
MSN-18	$\beta$	1	1	1.66	0.7	96	80	Spherical (linked)	130
MSN-19	$\beta$	1	1	1.25	0.7	96	80	Spherical (linked)	110
MSN-20	—	—	1	0	0.7	96	80	Spherical- Ellipsoid	185

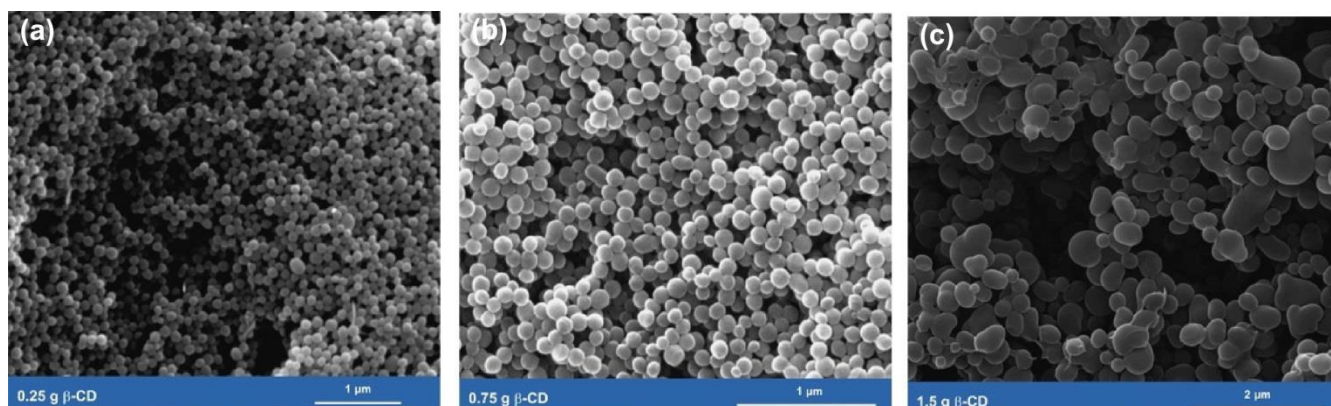
<sup>a</sup>The particle shape was evaluated through SEM or TEM analysis. <sup>b</sup>Particle size was determined through SEM or TEM images over single particles.



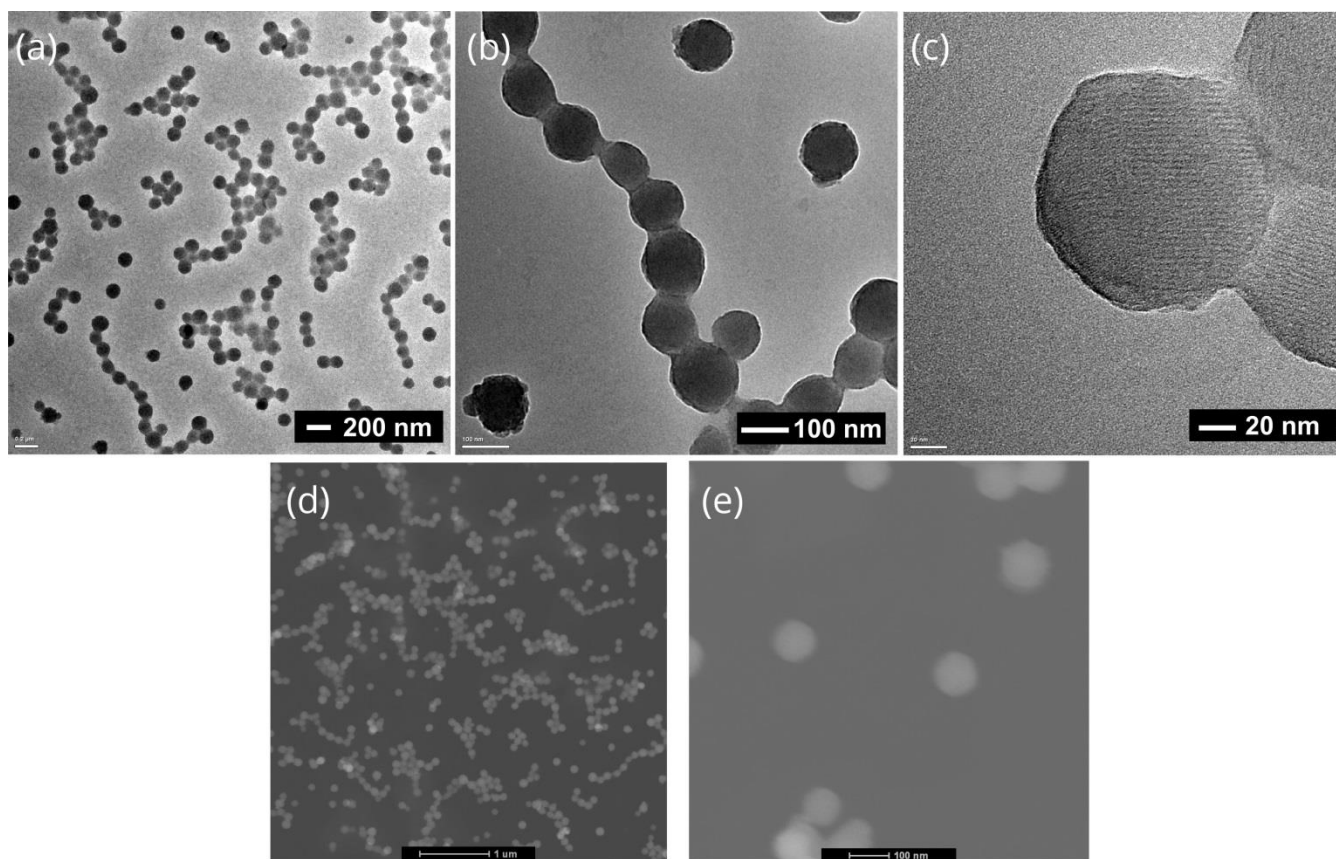
**Figure S1:** (a) XRD pattern and (b) FTIR spectrum of MSN-3.  $c_{\text{HP-}\gamma\text{-CD}} = 0.25\%$  (w/v) and  $r_{\text{CD}/\text{CTAC}} = 1.25$ . (c) The nitrogen adsorption–desorption isotherms and (d) BJH pore-size distribution of MSN-3. Inset shows the multi-point BET plot.



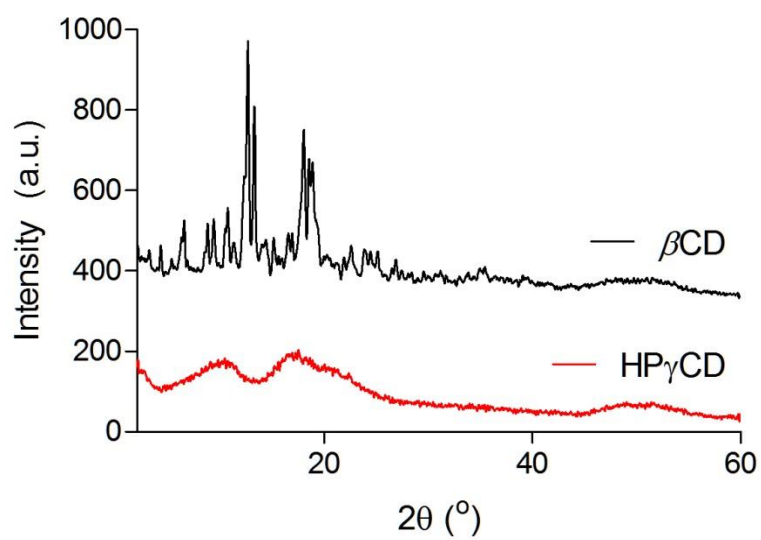
**Figure S2:** TGA of MSN sample produced at 0.25% (w/v) of HP- $\gamma$ -CD (MSN-3).  $c_{CD} = 0.25\%$  (w/v),  $r_{(CD/CTAC)} = 1.25$  and  $T = 80$  °C.



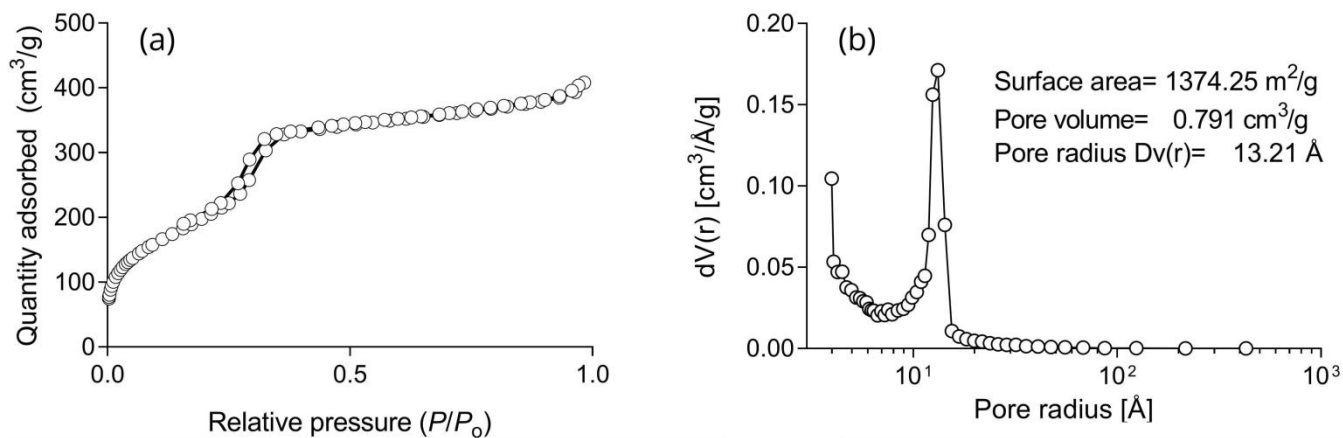
**Figure S3:** SEM images of the nanoparticles produced at various  $\beta$ -CD concentrations; MSN-13 ( $c_{\beta\text{-CD}} = 0.25\%$  (w/v) and  $r_{CD/CTAC} = 1.25$ ) (a), MSN-14 ( $c_{\beta\text{-CD}} = 0.75\%$  (w/v) and  $r_{CD/CTAC} = 3.75$ ) (b) and MSN-15 ( $c_{\beta\text{-CD}} = 1.5\%$  (w/v) and  $r_{CD/CTAC} = 7.50$ ) (c).



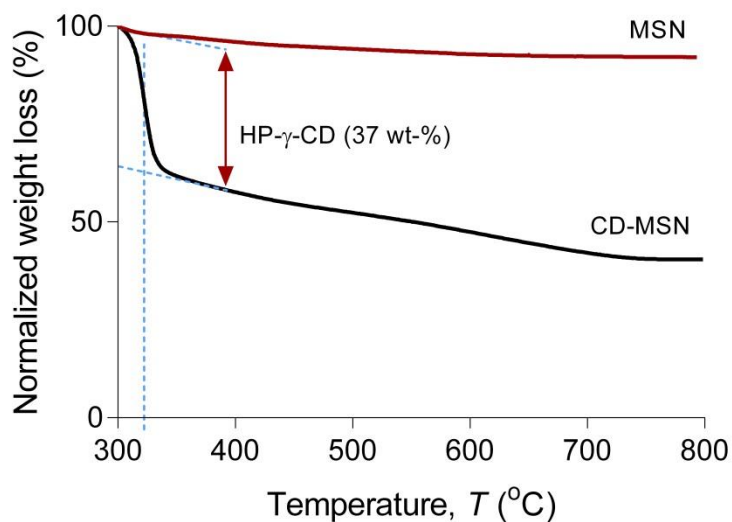
**Figure S4:** TEM (a–c) and STEM (d, e) images of MSNs (MSN-13).  $c_{\beta\text{-CD}} = 0.25\%$  (w/v) and  $r_{\text{CD}/\text{CTAC}} = 1.25$ .



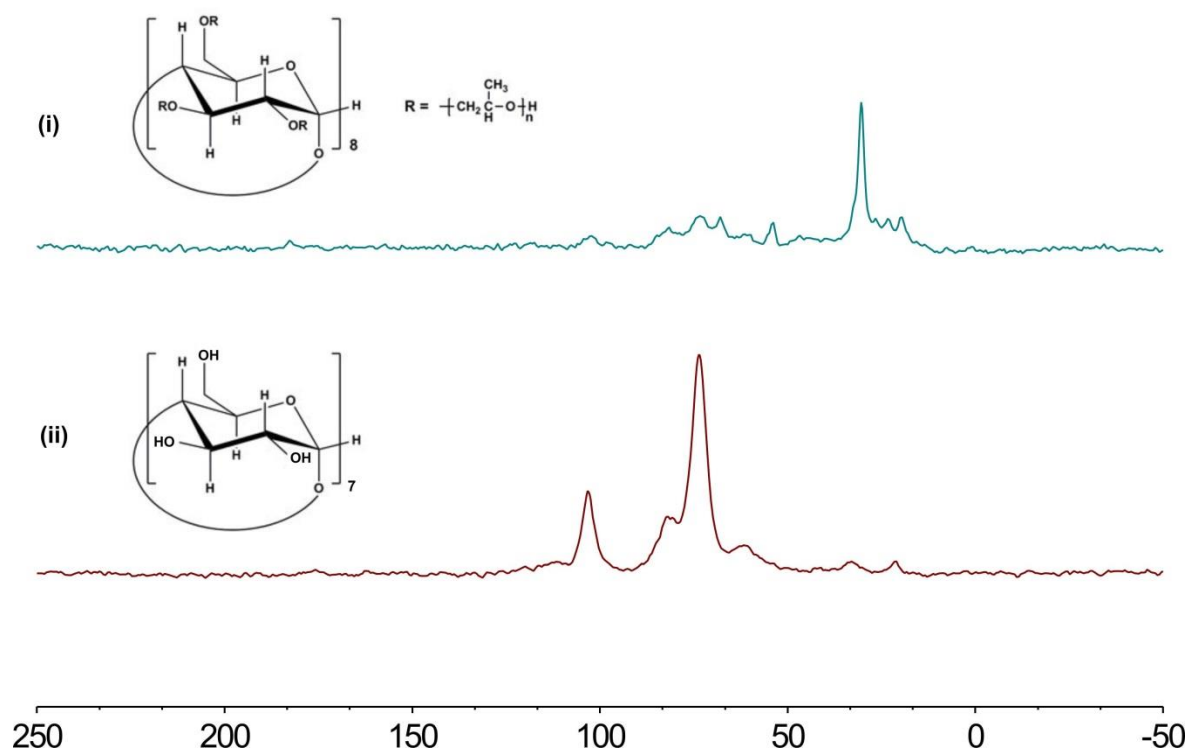
**Figure S5:** XRD patterns of as-received  $\beta\text{-CD}$  and  $\text{HP-}\gamma\text{-CD}$ .



**Figure S6:** BET analyses for MSNs. (a) Nitrogen adsorption–desorption isotherm measured at 77 K and (b) BJH pore size analysis of the pristine MSNs (0.2% (w/v) CTAC) (MSN-20).



**Figure S7:** TGA curves of MSNs (MSN-9 and MSN-20) prepared in the presence and absence of CD. The dotted line corresponds to the burning of the embedded CD.  $c_{\text{CTAC}} = 0.2\%$  (w/v) and  $c_{\text{HP-}\gamma\text{-CD}} = 0.6\%$  (w/v).



**Figure S8:** Solid-state  $^{13}\text{C}$  NMR spectra of MSNs; (i)  $c_{\text{HP-}\gamma\text{-CD}} = 0.25\%$  (w/v) (MSN-3) and (ii)  $c_{\beta\text{-CD}} = 1.5\%$  (w/v) (MSN-15).