Fluorescent Imprinted Nanoparticles for Sensing of chlorogenic acid in coffee extracts

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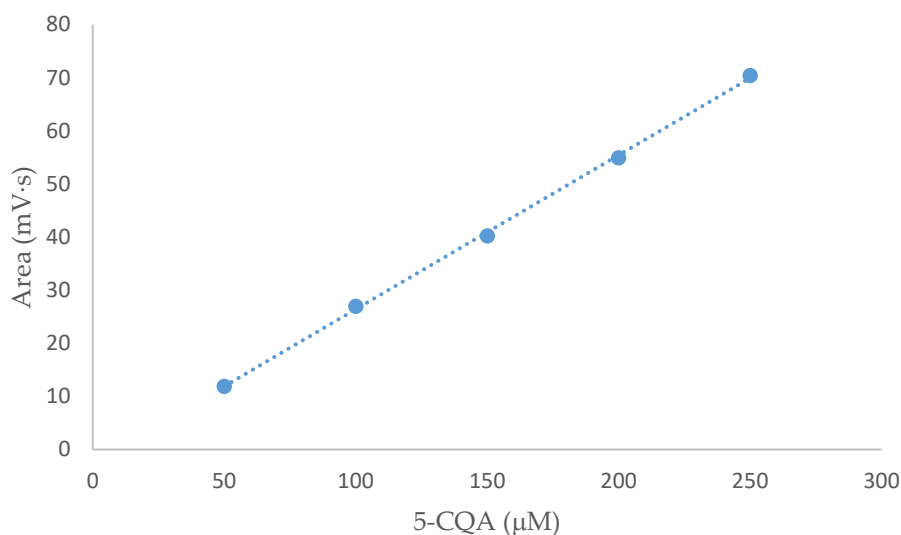
Supplementary Material

Calibration curves

Figure S1. HPLC calibration for 5-CQA, average of triplicate measures. Linear regression for 5-CQA: r^2 0.999, slope 0.29, intc. 2.61. Linear regression for HT: r^2 0.997, slope 47.01, intc. -29.15
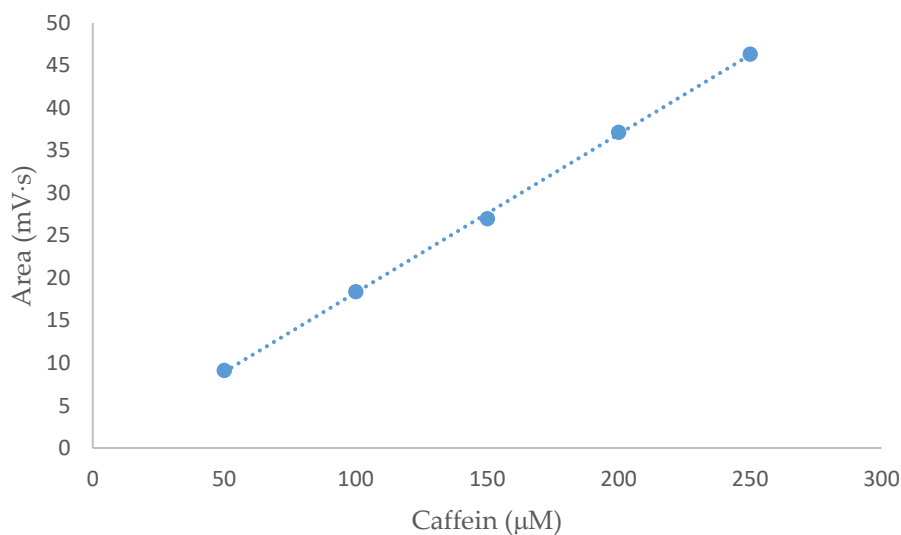

Figure S2. HPLC calibration for caffeine, average of triplicate measures. Linear regression: r^2 0.999, slope 0.19, intc. 0.37

Interactions of functional monomers with the targets: NMR titrations

In figures S3 – S7 are reported the most significant changes in the NMR spectra of 4VP and monomer **7** upon titration with increasing amount of 5-CQA leading to the most relevant effect.
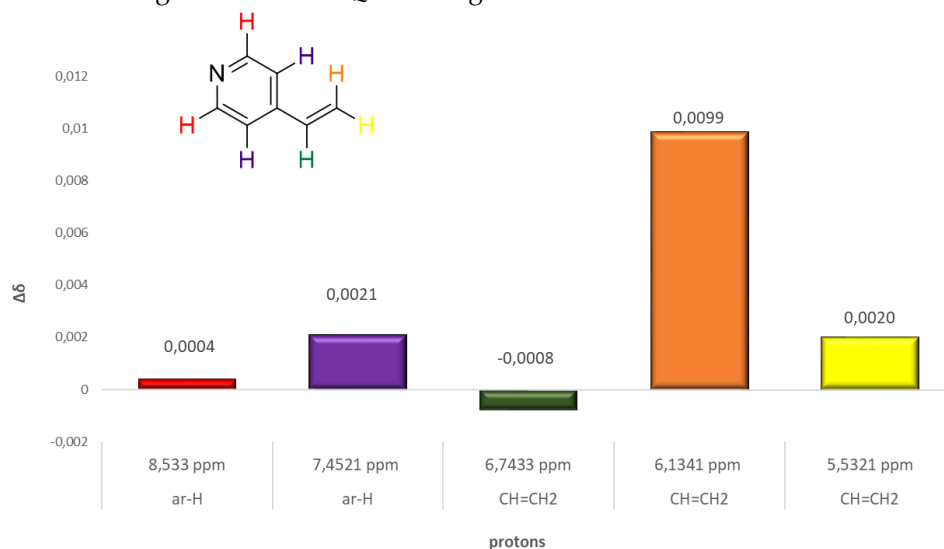

Figure S3. Histogram of the chemical shift variations in the ^{1}H-NMR spectrum of 4VP upon addition of 10 equivalents of 5-CQA
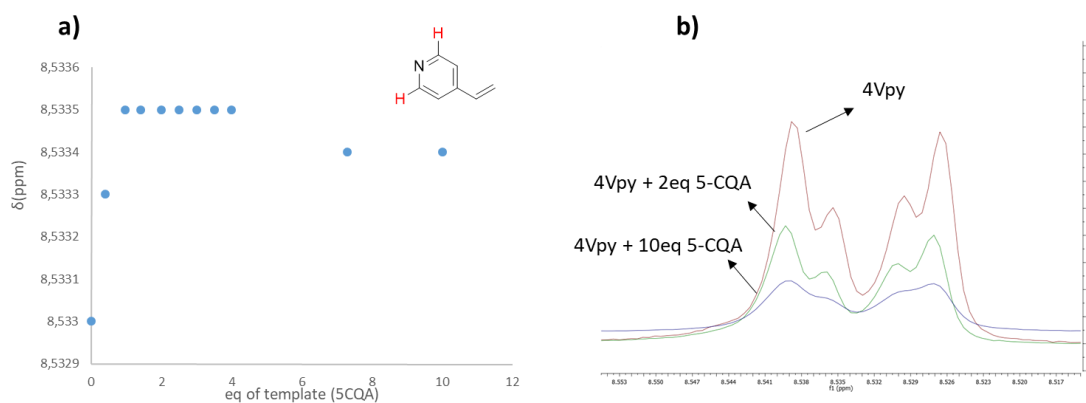

Figure S4. a) Chemical shift variation of aromatic proton of 4-vinypiridine (4Vpy) upon interaction with template molecule (5-CQA). b) progressive shift of the proton aromatic protons adjacent to the nitrogen atom of the pyridine ring in the ^{1}H-NMR spectra. Pure 4VPy (red), addition of 2eq of 5-CQA (green) and 10eq (blue).
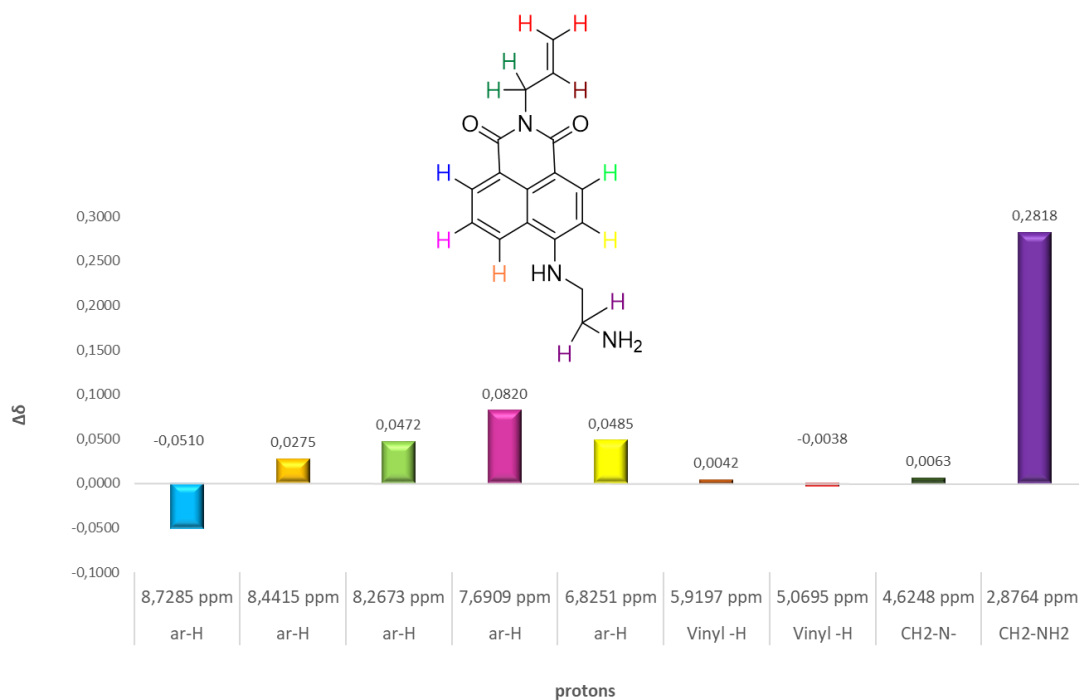
Figure S5. Histogram of the chemical shift variations in the ^{1}H-NMR spectrum of **7** upon progressive additions of 10eq of 5-CQA
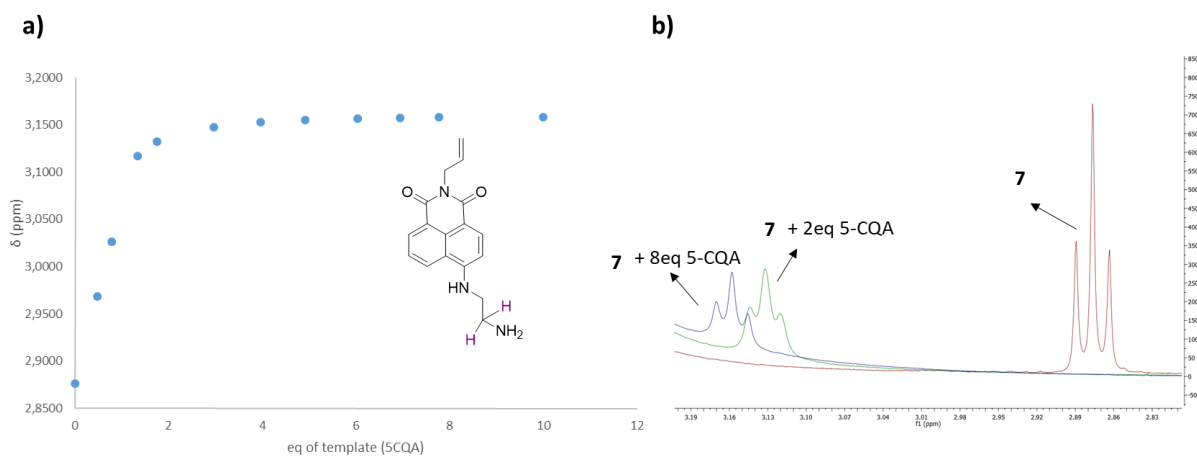

Figure S6. a) Chemical shift variation of CH_2NH_2 protons of monomer **7** upon interaction with 5-CQA; b) progressive shift of protons CH_2NH_2 in the ^{1}H-NMR spectra.
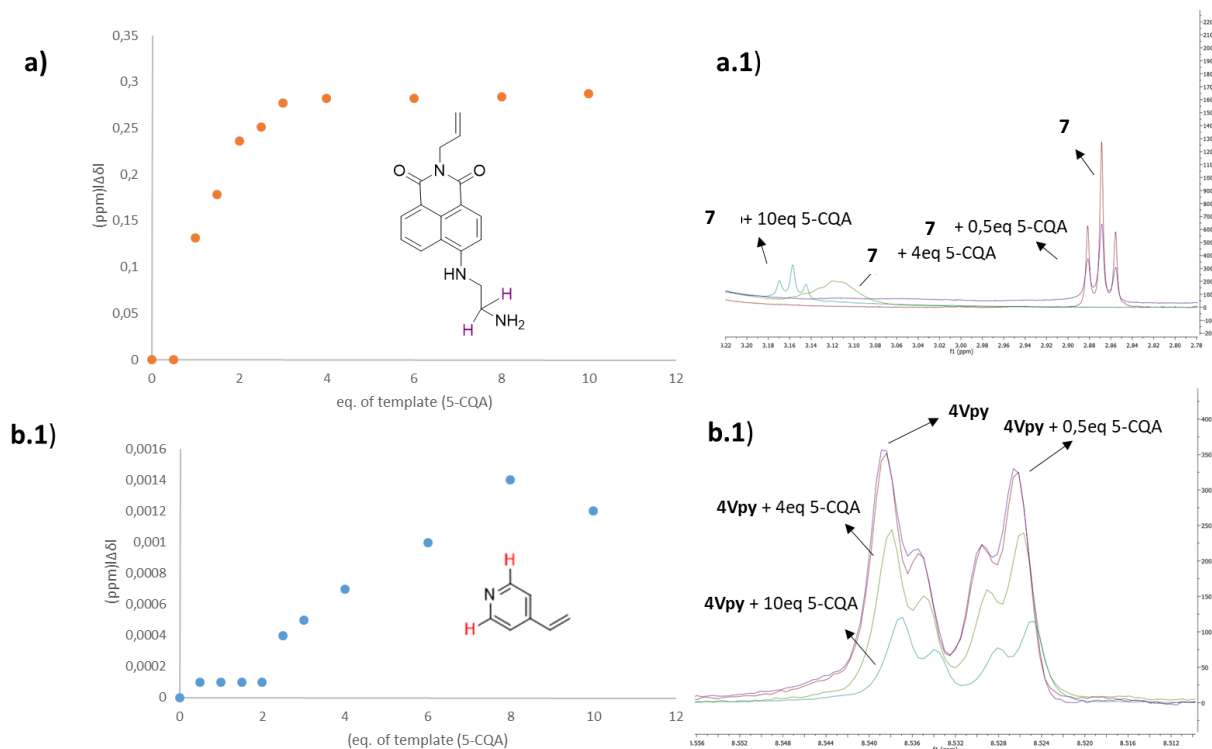
Figure S7: **a)** Chemical shift variation of CH_2NH_2 protons of monomer **7** upon interaction of a monomers mix with template molecule (5-CQA). **a.1)** progressive shift of the protons CH_2NH_2 in the ^1H-NMR spectra: **7** (red), addition of 0.5eq of 5-CQA (purple), 4eq (green) and 10q (blue). **b)** Chemical shift variation of aromatic proton of 4VP upon interaction of a mixture of monomers and the template molecule (5-CQA). **b.1)** progressive shift of the proton Ar-**H** in the ^1H-NMR spectra. 4VP (red), addition of 0.5eq of 5-CQA (purple), 4eq (green) and 10q (blue).
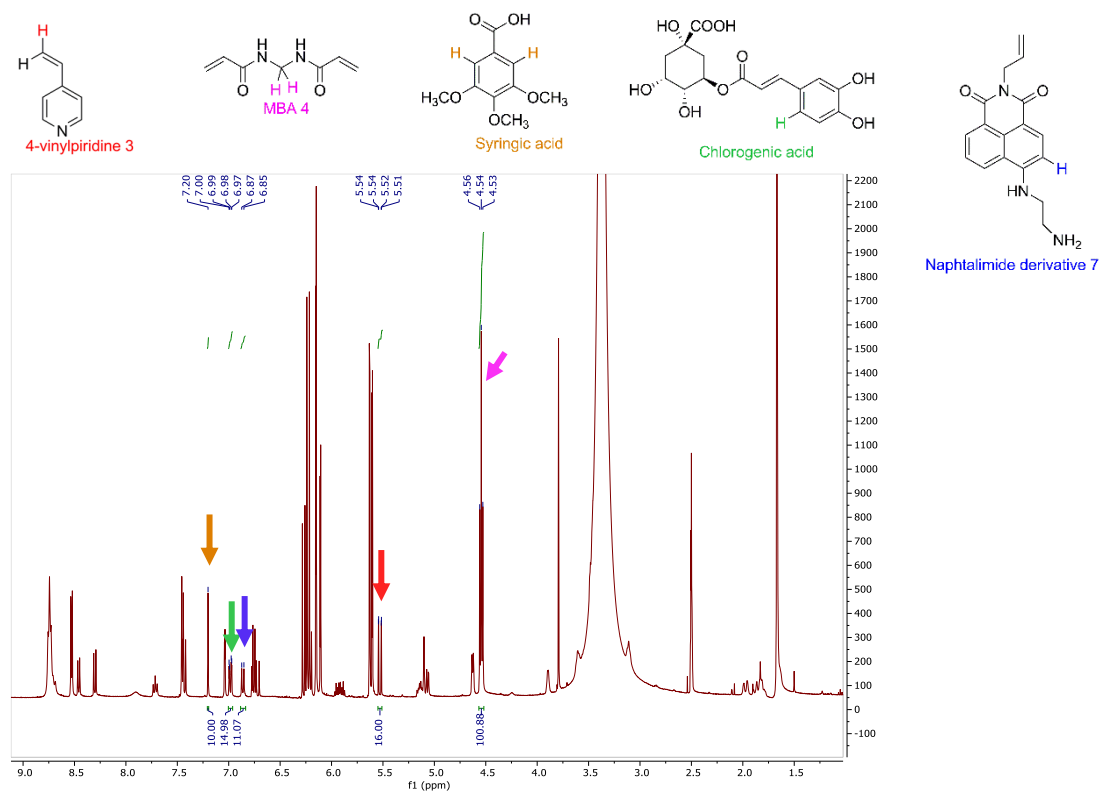
Figure S8: Mixture of monomers 4VP **3** and naphtalimide derivative **7**, cross-linker MBA **4**, syringic acid (internal standard) and 5-CQA in DMSO–d₆ before polymerization
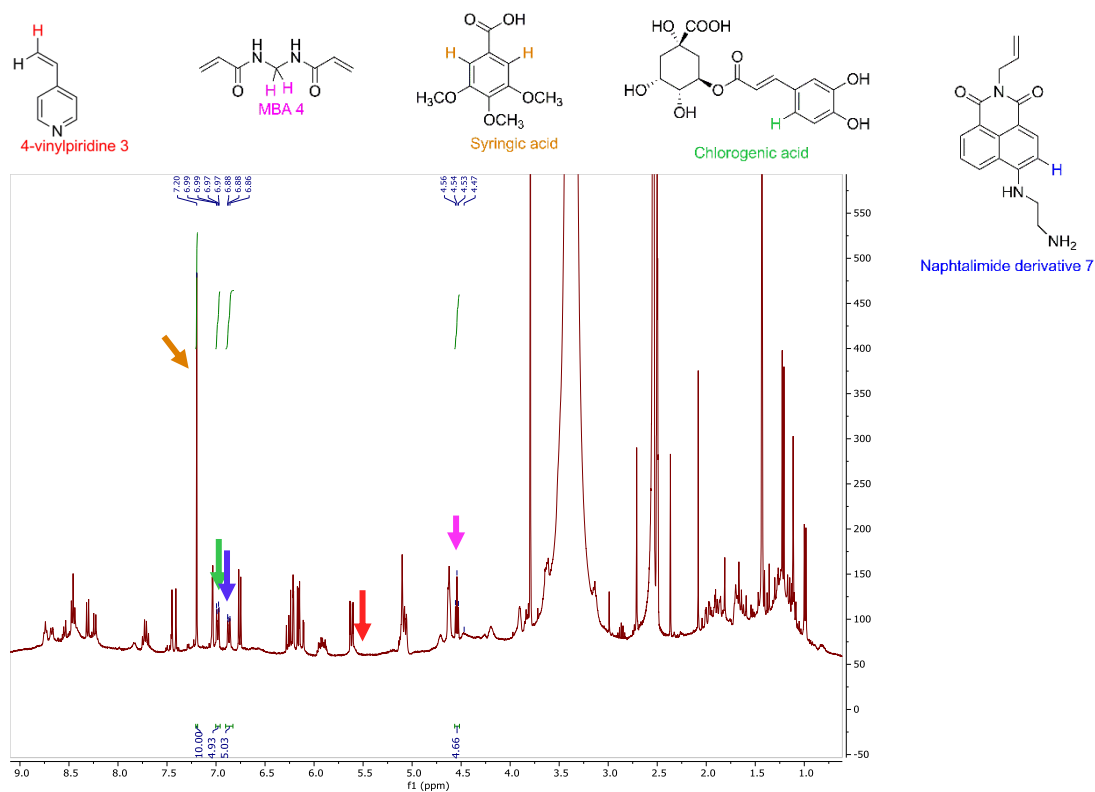

Figure S9: Mixture of monomers 4VP **3** and naphtalimide derivative **7**, cross-linker MBA **4**, syringic acid (internal standard) and 5-CQA in DMSO–d₆ after polymerization
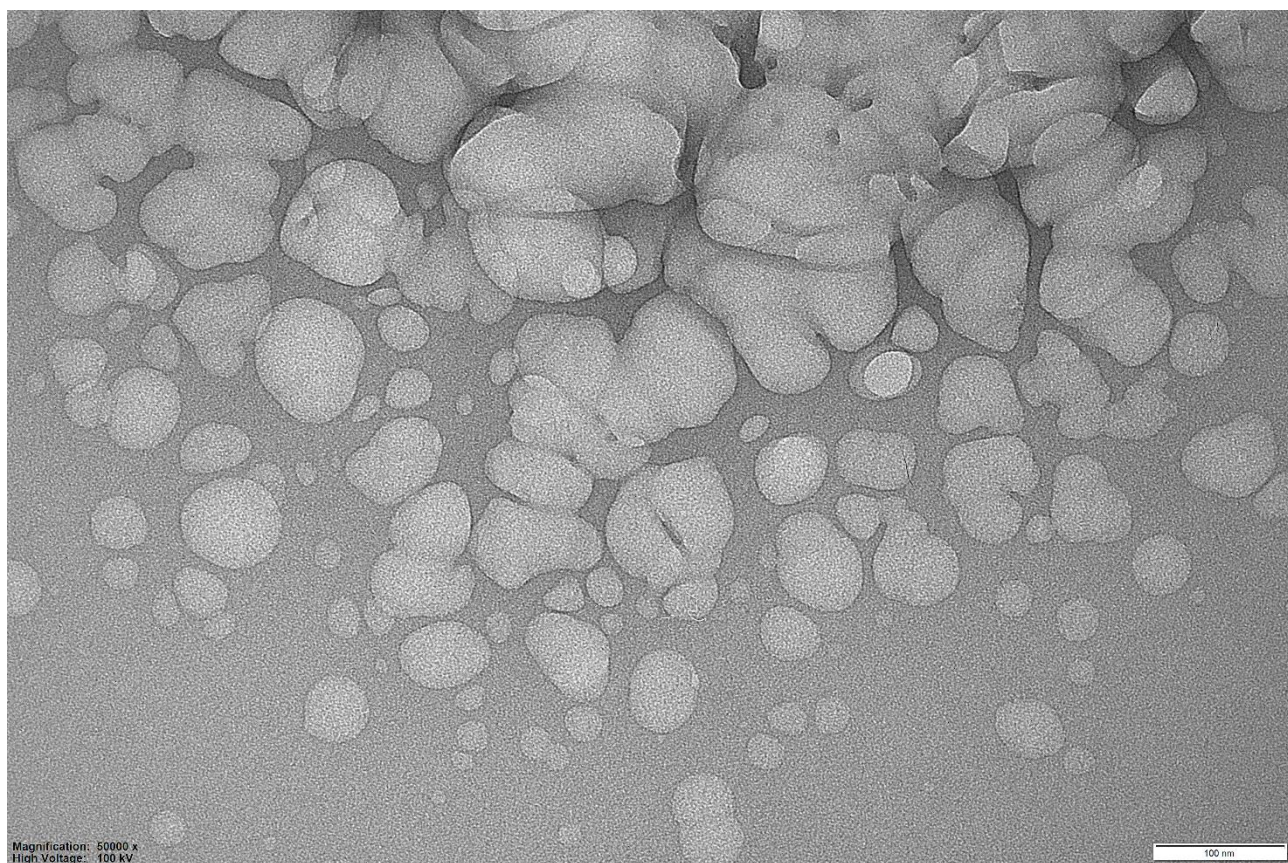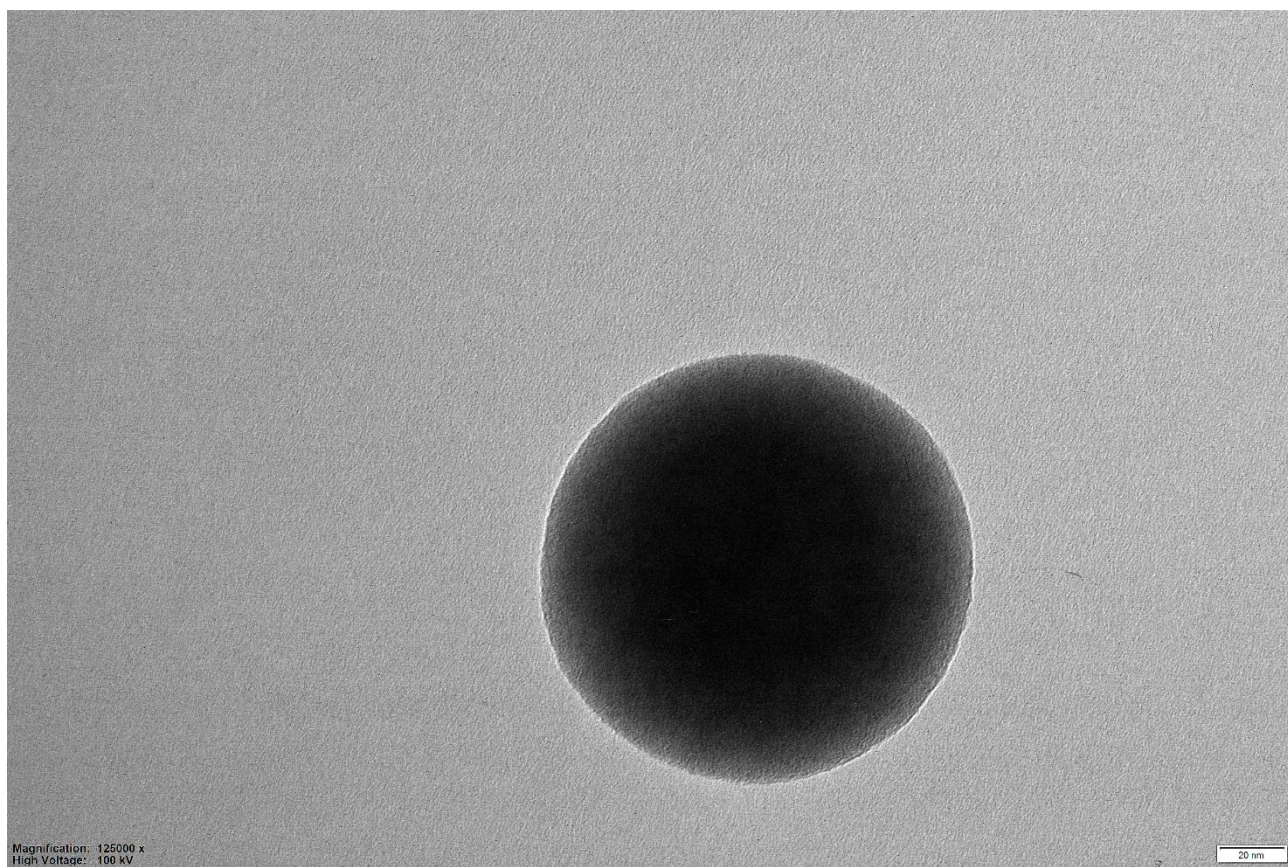
Figure S10: TEM image of fMIP03

Figure S11: TEM image of fMIP03