Supplementary Material (ESI) for Polymer Chemistry

Cyclodextrin-based polyurethanes act as specific molecular recognition materials of active pharmaceutical ingredients (APIs)

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Synthetic Procedures

For the syntheses of CDP_2 and CDP_4, diisocyanate (HDI or TDI) was dissolved in DMSO, and DMPA was added. The mixture was stirred at 65°C for 2 h before the addition of the β-CD; the reaction mixture was maintained under stirring for additional 3 h at 65°C. After being cooled to room temperature, the mixture was poured into acetone to yield a white precipitate. The so-produced solids, CDPs, were filtered out and washed with water (3 × 100 mL) and ethanol (3 × 100 mL) to remove unreacted diisocyanate, DMPA and β-CD. Finally, the produced CDPs were dried under vacuum at 90°C for 24 h prior to use. CDP_1 and CDP_3 have been synthesized using the same conditions without DMPA.

Experimental procedures for the HPLC experiments

The sorption of three pharmaceuticals (LVF, ASP or APAP) to the produced CDPs was investigated in water. Appropriate polymer amounts were added to 1.5 mL pharmaceutical solutions and the suspensions were shaked at 25° C for 2 h. The suspensions were then separated by centrifugation at 16000 g for 10 min. 50 µL of supernatant were then collected and injected in the HPLC system (Agilent 1100 Series) equipped with a column (150×4.6 mm)

packed with 3.0 µm PRONTOSIL 120-3-C18-SH (Bischoff-Chromatography, Germany). The mobile phase consisted in a mixture of water:acetonitrile:phosphoric acid (0.025 M), the apparent pH adjusted to 3 with triethylamine (60:20:20, v:v:v).[1] The flow rate of the mobile phase was 1.0 mL/min. The UV detector was set to 246, 330 and 226 nm for APAP, LVF and ASP, respectively. The binding capacity of CDPs was defined as the percentage of pharmaceuticals adsorbed by the CDPs with respect to the starting amount of pharmaceuticals.

Scanning electron micrographs of CDP_1, CDP_2 and CDP_3

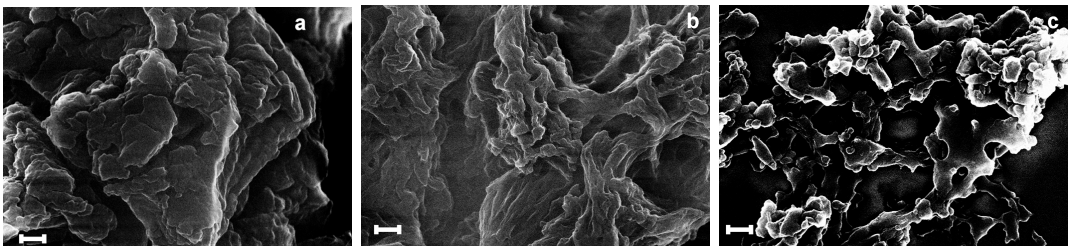
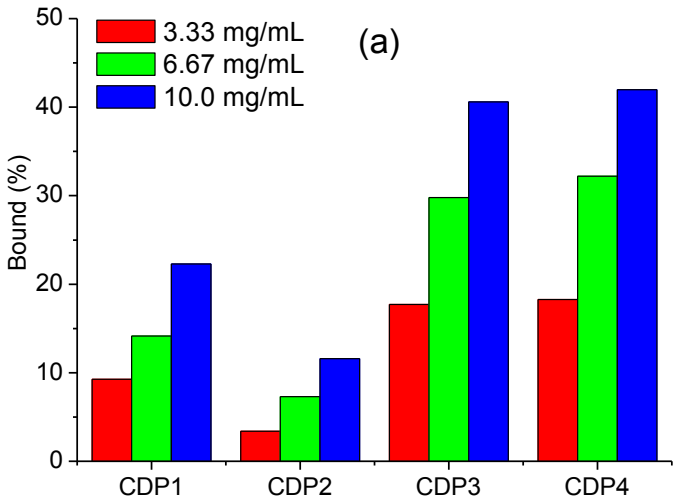


Fig. S1 Scanning electron micrograph of (a) CDP_1; (b) CDP_2; (c) CDP_3. [Scale bar: 200 nm]

Concentration dependant binding experiments



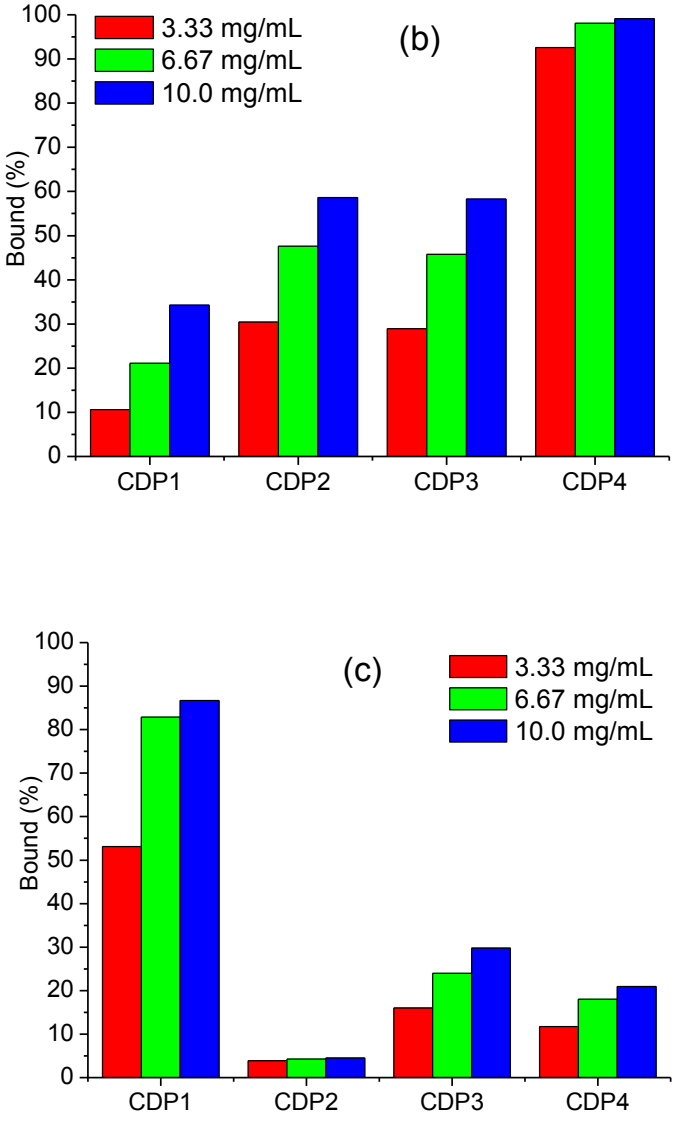


Fig. S2 Sorption of (a) APAP; (b) LVF and (c) ASP onto different concentrations of polymers in water solutions [pharmaceutical solution: 1.0×10^{-4} mol/L, 1.5 mL; contact time: 2 h].

References

1. F. K. Hurtado, D. R. Nogueira, F. Bortolini, L. M. da Silva, E. Zimmermann, M. J. e. Souza, J. de Melo and C. M. B. Rolim, *J. Liq. Chromatogr. Related Technol.*, 2007, **30**, 1981 - 1989.