Electronic Supplementary Information

Molecularly imprinted magnetic materials prepared from modular and clickable nanoparticles

Changgang Xu,[‡] Xiantao Shen,[‡] and Lei Ye^{*}

Division of Pure and Applied Biochemistry, Lund University, Box 124, 221 00 Lund, Sweden

[‡]These authors contributed equally to this work.

*Corresponding to: Lei Ye, Tel. + 46 46 2229560; Fax + 46 46 2224611; Email: <u>lei.ye@tbiokem.lth.se</u>

1. Quantification of Fe₃O₄ in Fe₃O₄@SiO₂@N₃ nanoparticles

Iron (III) can be easily measured in the presence of ammonium thiocyanate as indicator [1]. Here, this method was used to determine the content of Fe₃O₄ in Fe₃O₄@SiO₂@N₃ nanoparticles. In brief, 80 mg of Fe₃O₄@SiO₂@N₃ nanoparticles were mixed with 1 g of NaOH in 10 mL of hot water (70 °C). After the mixture was shaken for 5 min, 5 mL of concentrate HCl (37%) was added, and the mixture was kept at 70 °C for 20 min to give clear solution. To precipitate silicic acid, 2 mL of animal gelatin solution (10 g L⁻¹) was added, and the mixture was shaken at 70 °C for 5 min. The hot mixture was filtered, and the precipitate on the filter paper was washed with 0.5% HCl solution until no color remained. The final volume of the filtrate was adjusted to 100 mL with water. To convert Fe (II) to Fe (III), 80 mg of ammonium persulfate was added into 40 mL of the solution, 1 mL sample was taken and mixed with 1 ml of ammonium thiocyanate (20 g L⁻¹). The UV-Vis absorbance at 480 nm was measured to determine the concentration of Fe (III) complex. To obtain a standard curve, $Fe(NO_3)_3$ •9H₂O was used as standard for Fe (III), which was treated in the same procedure as used for $Fe_3O_4@SiO_2@N_3$ nanoparticles.

Figure S1 is the standard curve for the measurement of Fe (III) using ammonium thiocyanate as indicator. The absorbance of the diluted sample obtained from the magnetic $Fe_3O_4@SiO_2@N_3$ nanoparticles was 0.566 ± 0.002 .



Figure S1. Standard curve for the measurement Fe (III) using ammonium thiocyanate as indicator.

2. Kinetics of propranolol binding

The kinetics of radioligand propranolol binding on mipCS@Fe₃O₄ and mipCS particles was investigated. Figure S2 shows that for the two types of imprinted particles, the time to reach equilibrium binding is almost the same (less than 50 min). The kinetic binding results indicate that coating the mipCS with the Fe₃O₄ nanoparticles (*via* the click reaction) did not affect the template binding kinetics.



Figure S2. Kinetic binding data for propranolol on mipCS (0.5 mg) and mipCS@Fe₃O₄ (1.25 mg) particles. The initial propranolol concentration was 246 pM.



3. TEM image of propranolol-imprinted core-shell particles (mipCS)

Figure S3. TEM image of mipCS nanoparticles.

[1] C. Liteanu, I. Lukács and C. Strusievici, Anal. Chim. Acta., 1961, 24, 200-202.