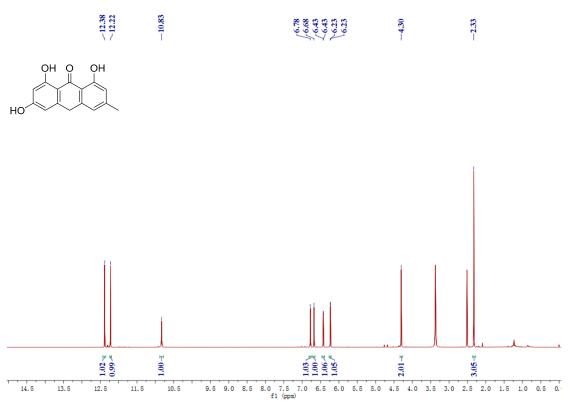
## Supplementary Materials: A facile approach for fabrication of core-shell magnetic molecularly imprinted nanospheres toward hypericin

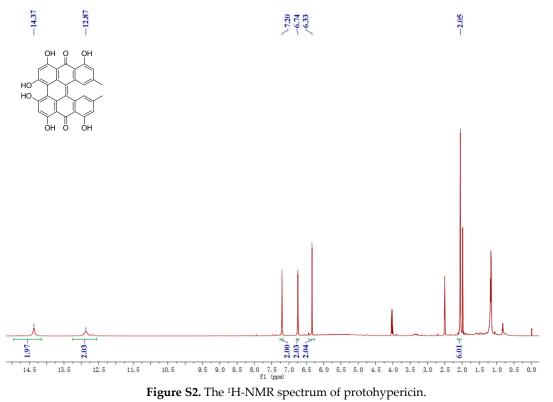
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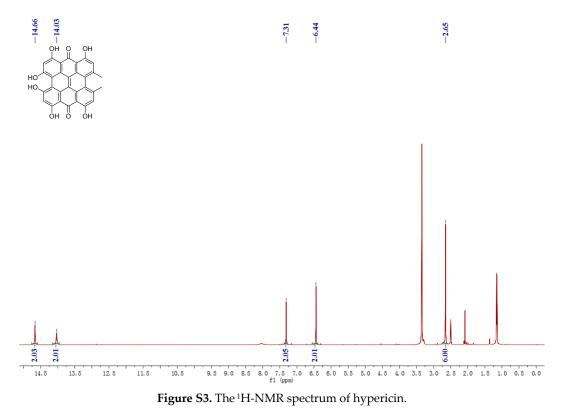




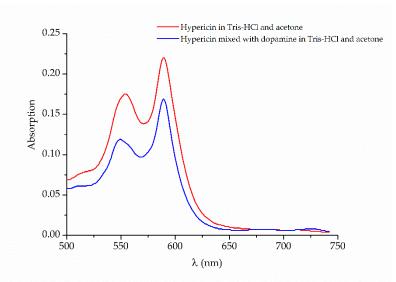
**Emodin anthrone:** <sup>1</sup>H-NMR (500 MHz, DMSO-d<sub>6</sub>) δ 12.38 (s, 1H), 12.22 (s, 1H), 10.83 (s, 1H), 6.78 (s, 1H), 6.68 (s, 1H), 6.44 (d, *J* = 1.8 Hz, 1H), 6.24 (d, *J* = 2.1 Hz, 1H), 4.30 (s, 2H), 2.33 (s, 3H).



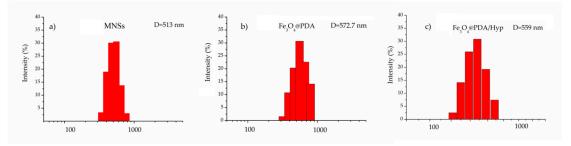
**Protohypericin:** <sup>1</sup>H-NMR (500 MHz, DMSO-d<sub>6</sub>) δ 14.37 (s, 2H), 12.87 (s, 2H), 7.20 (s, 2H), 6.74 (s, 2H), 6.33 (s, 2H), 2.06 (s, 6H).



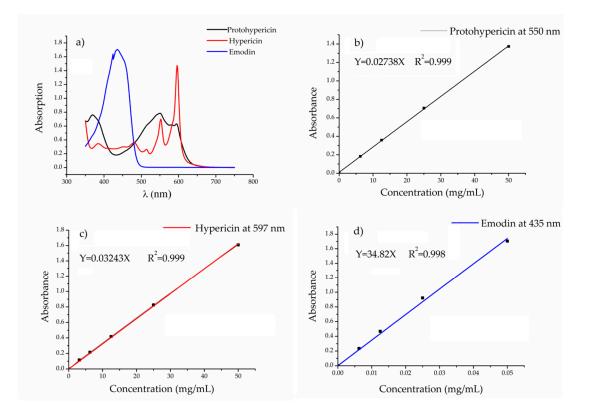
**Hypericin:** <sup>1</sup>H-NMR (500 MHz, CD<sub>3</sub>OD) δ 14.66 (s, 2H), 14.03 (s, 2H), 7.31 (s, 2H), 6.44 (s, 2H), 2.65 (s, 6H).



**Figure S4.** UV-Vis spectra of hypericin in Tris-HCl and acetone (v/v = 6:1, pH = 8.0) with (blue line), or without (red line) the presence of dopamine (2 mg/mL).



**Figure S5.** (a) DLS histogram of MNSs, PDI = 0.44; (b) DLS histogram of Fe<sub>3</sub>O<sub>4</sub>@PDA, PDI = 0.761; (c) DLS histogram of Fe<sub>3</sub>O<sub>4</sub>@PDA/Hyp, PDI = 0.385.



**Figure S6.** (a) UV-Vis spetra of hypericin, protohypericin, and emodin, respectively. (b) Standard curve of hypericin in acetone by UV-spectrophotometer at 597 nm. (c) Standard curve of protohypericin in acetone by UV-spectrophotometer at 550 nm. (d) Standard curve of emodin in acetone by UV-spectrophotometer at 435 nm.

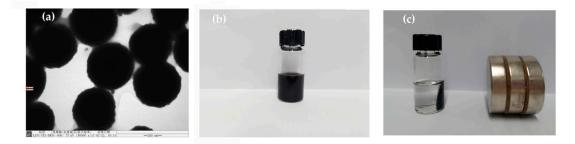


Figure S7. TEM images of MNSs (a) and their response to magnet in 10 s (b and c). Scale bar: 200 nm.

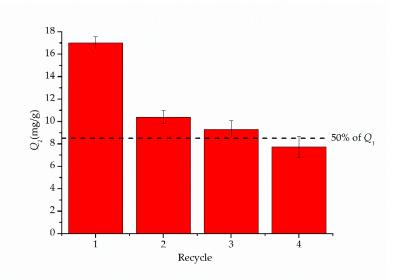


Figure S8. Reusability study of Fe<sub>3</sub>O<sub>4</sub>@PDA/Hyp NSs.