Electronic Supplementary Information

Molecularly Imprinted Antibiotic Receptor on Magnetic Nanotube

for Detection and Removal of Environmental Oxytetracycline

Jixiang Wang ^{1, 2, 3, #}, Xiaolei Li ^{1, #}, Rong Zhang ⁵, Bingjie Fu ¹, Mingcan Chen ¹, Mengxue Ye ¹, Wanyu Liu ¹, Jingjing Xu ^{1, *}, Guoqing Pan ^{4, *}, and Hongbo Zhang ^{2, 3, *}

¹ Sino-European School of Technology of Shanghai University, Shanghai University, CN-200444 Shanghai, P. R. China.

² Pharmaceutical Sciences Laboratory, Åbo Akademi University, FI-20520 Turku, Finland.

³ Turku Bioscience Centre, University of Turku and Åbo Akademi University, FI-20520 Turku, Finland.

⁴ Institute for Advanced Materials, School of Materials Science and Engineering, Jiangsu University, Zhenjiang 212013, Jiangsu, China.

⁵ Department of Interventional Radiology, Shanghai Jiao Tong University Affiliated Sixth People's Hospital, CN-200233 Shanghai, P. R. China.

* Correspondence: jingjing_xu@shu.edu.cn (J. Xu); panguoqing@ujs.edu.cn (G. Pan); hongbo.zhang@abo.fi (H. Zhang).

[#] These authors contributed equally to this work.

Synthesis of Allyl Rhodamine B

For the synthesis of allyl rhodamine B (ARhB), 2.4g RhB, 0.73g 3-bromopropylene, 2.65g Na₂CO₃, trace hydroquinone and iodine were dissolved in 60mL dry DMF, stirred evenly and heated. Under N₂ atmosphere, the reaction was carried out at 71°C in the dark for 25h. Then impurities were removed from the mixture, and DMF was evaporated by distillation under reduced pressure. The ARhB (yield: ~70%) was obtained after separation and purification through a chromatography column (dichloromethane/methanol, 40/1, v/v).

Synthesis of 4-(2-acrylamidoethylcarbamoyl)-3-fluorobenzeneboronic acid

For 4-(2-acrylamidoethylcarbamoyl)-3-fluorophenylboronic acid (AFPBA) synthesis, 5g 4-carboxy-3-fluorophenylboronic acid was added to 50mL thionyl chloride and refluxed for 6h under argon atmosphere. After evaporating thionyl chloride under vacuum, the remaining solid and 9.4g N-carboxybenzyloxy-1,2diaminoethane hydrochloride were dissolved in 90mL THF and placed in an ice water bath. Then, 28mL trimethylamine was slowly added with stirring at room temperature for 6h. After washing with dilute hydrochloric acid, the organic layer was evaporated, producing a white solid. Afterward, the produced white solid was dissolved in 400mL ethanol followed by 10% Pd/C (1 g) addition. They were hydrogenated at 40°C for 3h. Then, the mixture was filtered and evaporated using a rotary evaporator, then dissolved in 150 mL of sodium carbonate aqueous solution (100 mM, pH=10) in an ice bath. 4.0 mL of acryloyl chloride was slowly added with stirring for 6h at room temperature. Afterward, the mixture was acidified to pH 2 with HCl. At the end, the final AFPBA was recrystallized in acetone and dried in a vacuum (yield: ~45%).

Characterization of ARhB

¹H NMR (400 MHz, CD_2Cl_2) δ 8.30 (m, 1H), 7.83 (s, 1H), 7.75 (m, 1H), 7.45-7.00 (m, 3H), 6.89 (dt, J = 9.5, 2.5 Hz, 2H), 6.80 (dd, J = 22.1, 2.5 Hz, 2H), 5.73 (d, J = 10.4, 5.8 Hz, 2H), 5.60-5.33 (m, 1H), 5.24-5.06 (m, 2H), 4.52 (ddd, J = 8.5 Hz, 2H), 3.83 – 3.33 (m, 8H), 1.73-1.22 (m, 12H).



Figure S1. ¹H NMR spectra of ARhB.

Characterization of AFPBA

¹H NMR (400 MHz, DMSO) 8.40 (s, 2H, B(OH)₂), 8.21 (m, 1H, -CO-NH-), 7.70-7.49 (3H, Ar-H), 6.21 (m, 2H, -CH=CH₂), 5.60 (d, 1H, -CH=CH₂), 3.22-2.51 (m, 4H, -NHCH₂CH₂NH-).



Figure S2. ¹H NMR spectra of AFPBA