Supporting Information

Title Robust Surface Coating for a Fast, Facile Fluorine-18 Labeling of Iron Oxide Nanoparticle for PET/MR Dual-modality Imaging†

Ziyan Sun,[a,b‡] Kai Cheng,[b‡] Fengyu Wu,[b,c] Hongguang Liu,[b] Xiaowei Ma,[b] Xinhui Su,[b] Yang Liu,[b] Liming Xia[a]* and Zhen Cheng[b]*

[a.] *Department of Radiology, Tongji Hospital, Tongji Medical College, Huazhong University of Science and Technology, Wuhan,430030, China.*
[b.] *Molecular Imaging Program at Stanford (MIPS), Bio-X Program, Department of Radiology, Stanford University, California, 94305-5344.*
[c.] *Department of Nuclear Medicine, PET/CT Center, Affiliated Hospital of Qingdao University, Qingdao, China.*
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‡These authors contributed equally to this study.
*Email: zcheng@stanford.edu or lmxia@tjh.tjmu.edu.cn

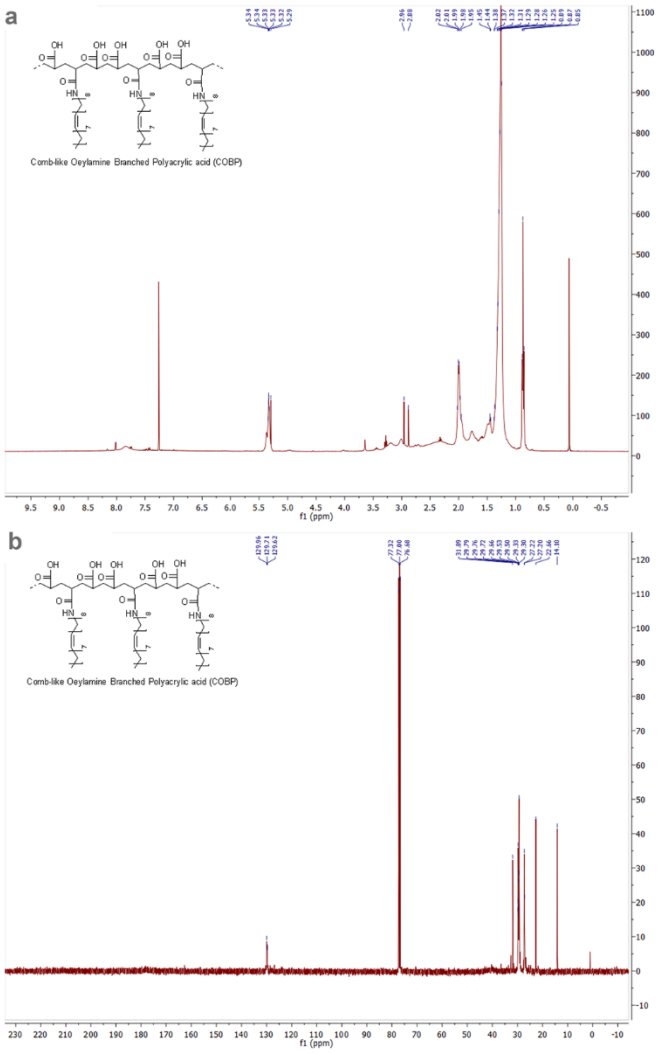

Fig. S1. Characterization of amphiphilic Comb-like Oleylamine Branched Polyacrylic acid (COBP). **a**, ^{1}H NMR spectrum of COBP. **b**, ^{13}C NMR spectrum of COBP.

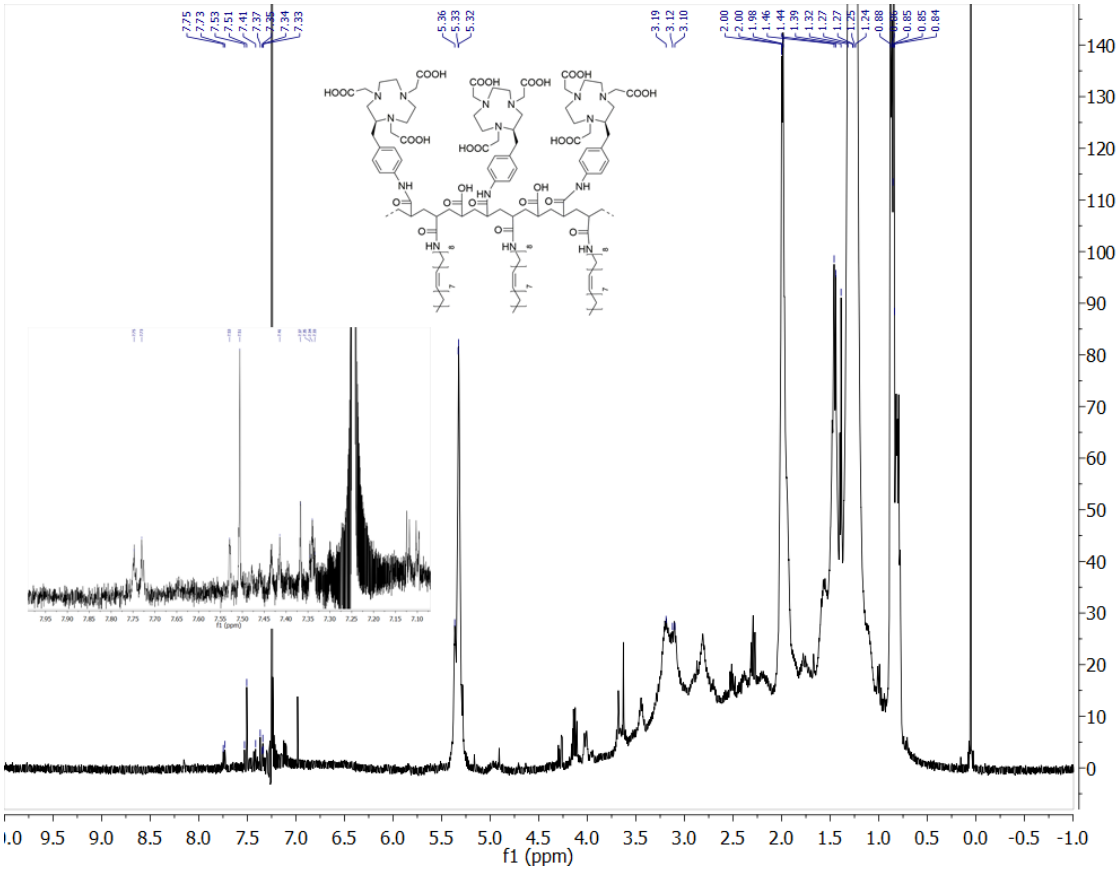

Fig. S2. ^{1}H NMR spectrum of NOTA-COBP.

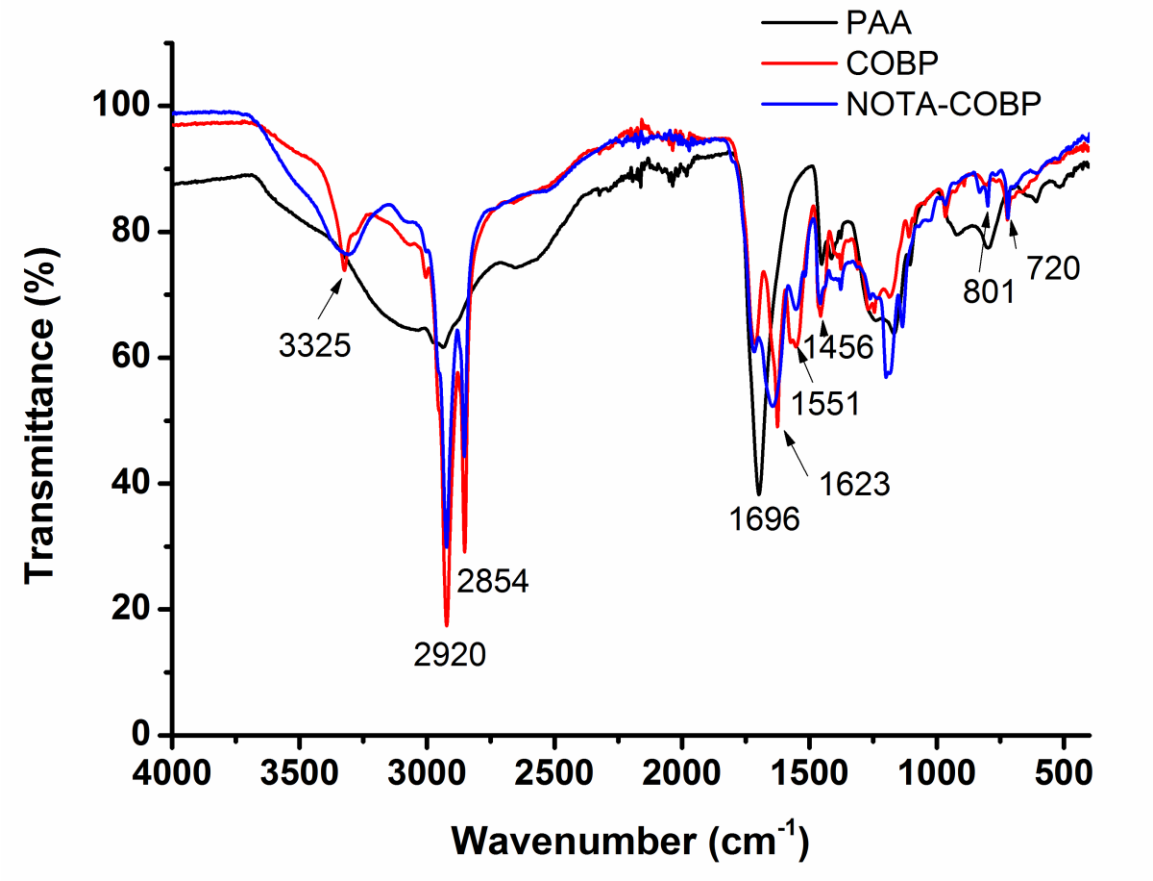

Fig. S3. FTIR spectra of PAA (black line), COBP (red line) and NOTA-COBP (blue line).

Discussion: The Fourier transform infrared spectroscopy (FTIR) analysis of COBP revealed two strong alkyl stretching peaks at 2920 and 2845 cm^{-1}, demonstrating the presence of grafted oleylamine groups. The N-H stretching vibration signal at 3325 cm^{-1} appeared on the FTIR spectrum of COBP, indicating the existence of amide bonds. The C=O amide I and II bonds were found at 1623 and 1551 cm^{-1}, respectively, which indicated that oleylamine was successfully grafted on the PAA. For the FTIR spectrum of NOTA-COBP, two peaks at 801 and 720 cm^{-1} were observed and attributed to the bending vibration of benzene ring of NOTA linker, which confirmed the conjugation of NOTA molecules and PAA.

Cytotoxicity assay

Cytotoxicity of NOTA-COBP-IONPs (NOTA-IONPs) was evaluated by using a cell viability assay (MTT, (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyl tetrazolium bromide (Sigma-Aldrich, St. Louis, MO)). Briefly, NIH-3T3 cells were plated into a 96-well plate at a concentration of 6×10^3 cells/well in DMEM with 10% fetal bovine serum (FBS) at 37°C and 5% CO_2, and 24 h later, the cells were incubated with NOTA-IONPs with different concentrations in DMEM for 24 and 48 h. The cell viability assays were carried out according to the manufacturer's instruction. After treatment, MTT compound (5 mg/ml in PBS) was diluted 1:100 with DMEM medium into each well. After 3 h incubation, culture supernatants were carefully removed, and the purple reduced MTT product was redissolved in 100 μL of DMSO in 10 min. The concentration of the reduced MTT in each well was determined spectrophotometrically at 570 nm with a reference wavelength of 650 nm using a microplate reader (TECAN Infinite M100). All samples were done in tetraplicate and all experiments were repeated 3~5 times. MTT absorbance values were normalized to 100%; experimental values (treated) were expressed as percentage of the control. Significant differences between sets of values for control and test groups were assessed by Student's t-test.

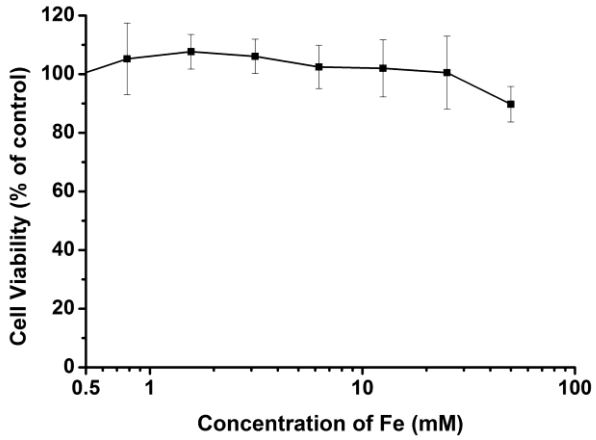

Fig. S4. *In vitro* cell viability of NIH-3T3 cells incubated with NOTA-IONPs at different iron concentrations for 24 h at 37°C.