

Supporting Information

Dual effect of molecular mobility and functional groups of polyrotaxane surfaces on the fate of mesenchymal stem cells

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Experimental Section

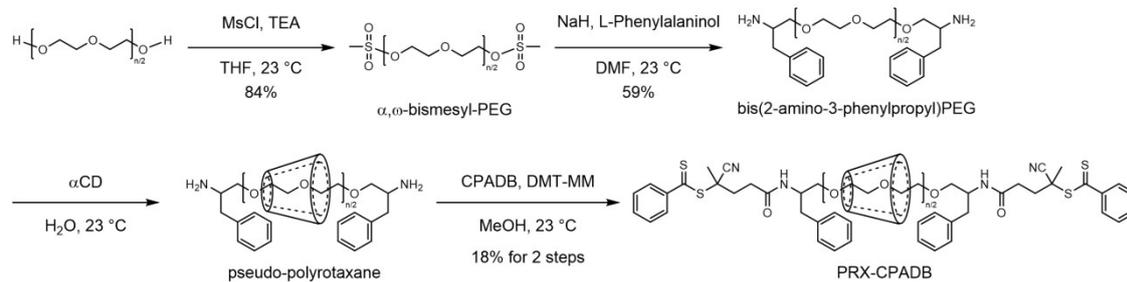
Materials

Hydroxy-terminated PEG ($M_n = 20,000$, PEG-OH) and 4-cyano-4-(phenylcarbonothioylthio)pentanoic acid (CPADB) were purchased from Sigma-Aldrich (St. Louis, MO, USA). Triethylamine (TEA), methanesulfonyl chloride (mesyl chloride or MsCl), sodium hydride (NaH), 4-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-methylmorpholinium chloride n-hydrate (DMT-MM) and tetrahydrofuran (THF) were purchased from FUJIFILM Wako Pure Chemical Corporation (Osaka, Japan). α -CD was purchased from Ensuiko Sugar Refining (Tokyo, Japan). L-Phenylalaninol was obtained from Tokyo Chemical Industry (Tokyo, Japan). N,N-Dimethylformamide (DMF) was purchased from Kanto Chemical (Tokyo, Japan).

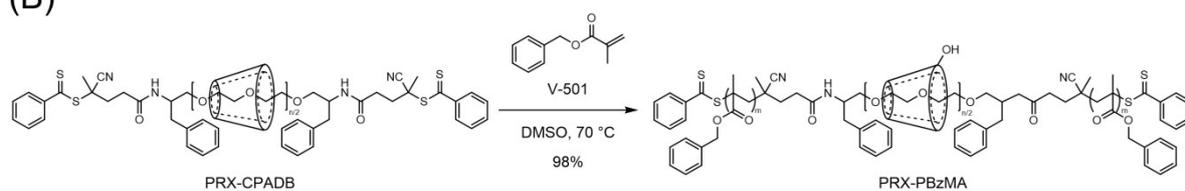
Instruments

Size exclusion chromatography was performed on a Prominence-i LC-2030 Plus (Shimadzu, Kyoto, Japan) equipped with an RID-20A refractive index detector (Shimadzu) and two columns, TSK gel[®] α -4000 and α -2500 (300 mm length, 7.8 mm internal diameter) (Tosoh, Tokyo, Japan). The system was operated at 60 °C at a flow rate of 0.35 mL/min with DMSO containing 10 mM lithium bromide as an eluent. PEG standards were used for calibration.

(A)



(B)



Scheme S1. Synthesis of polyrotaxane with CPADB at both terminals (PRX-CPADB) (A) and polyrotaxane triblock copolymer (PRX-PBzMA) consists of polyrotaxane and poly(benzylmethacrylate) (PBzMA) at both terminals (B).

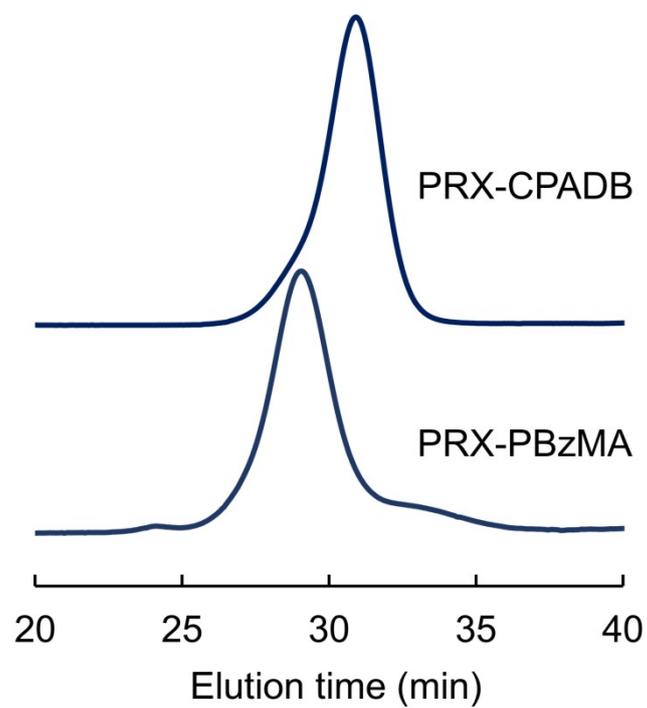
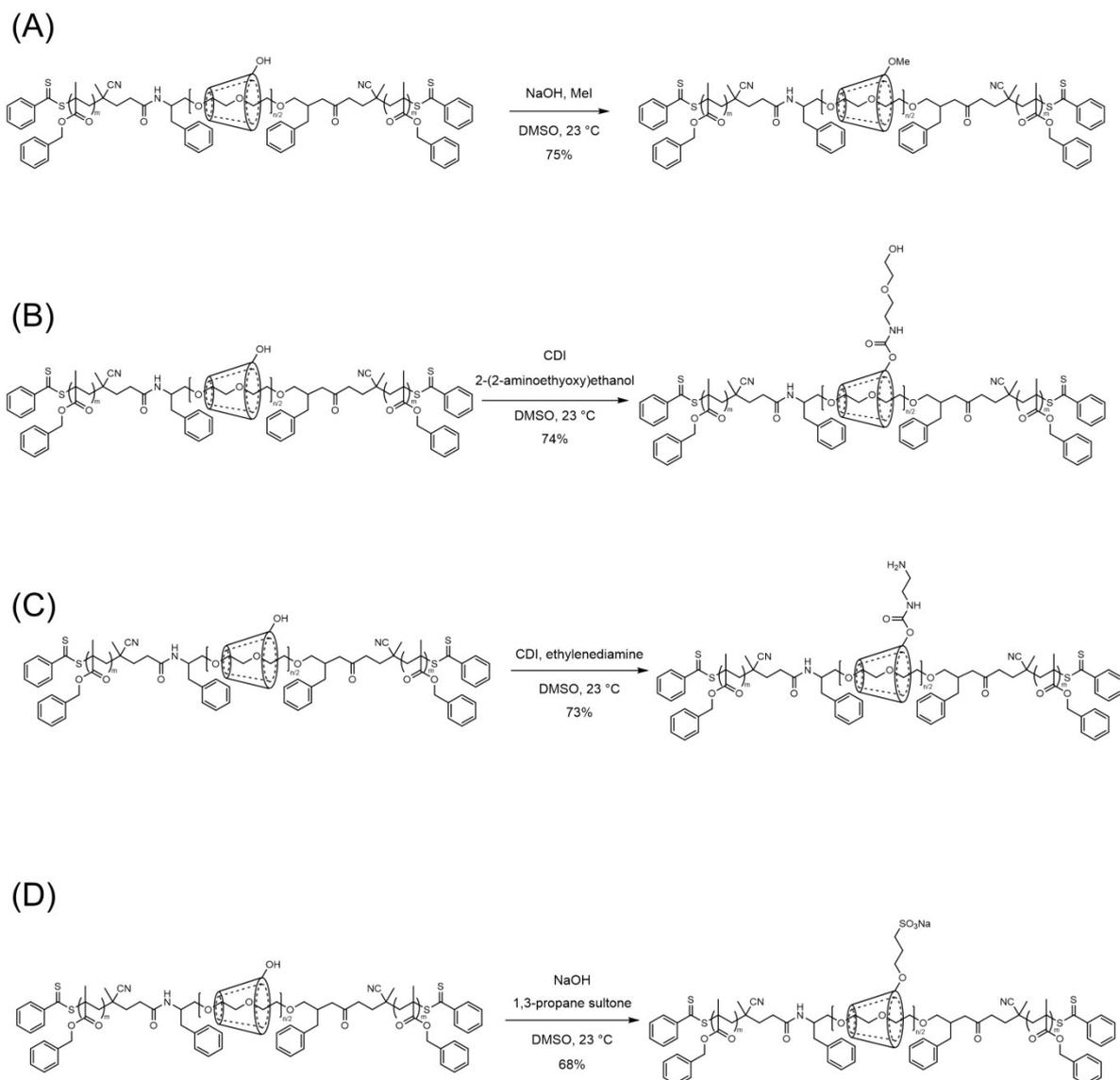


Figure S1. Size exclusion chromatography (SEC) charts of a polyrotaxane capped with CPADB at both terminals (PRX-CPADB) and polyrotaxane triblock copolymer (PRX-PBzMA) consists of polyrotaxane and poly(benzylmethacrylate) (PBzMA) at both terminals.



Scheme S2. Synthesis of methyl group-modified polyrotaxane triblock polymer (CH₃-PRX) (A), hydroxyl group-modified polyrotaxane triblock polymer (OH-PRX) (B), amino group-modified polyrotaxane triblock polymer (NH₂-PRX) (C) and sulfo group-modified polyrotaxane triblock polymer (SO₃H-PRX) (D).

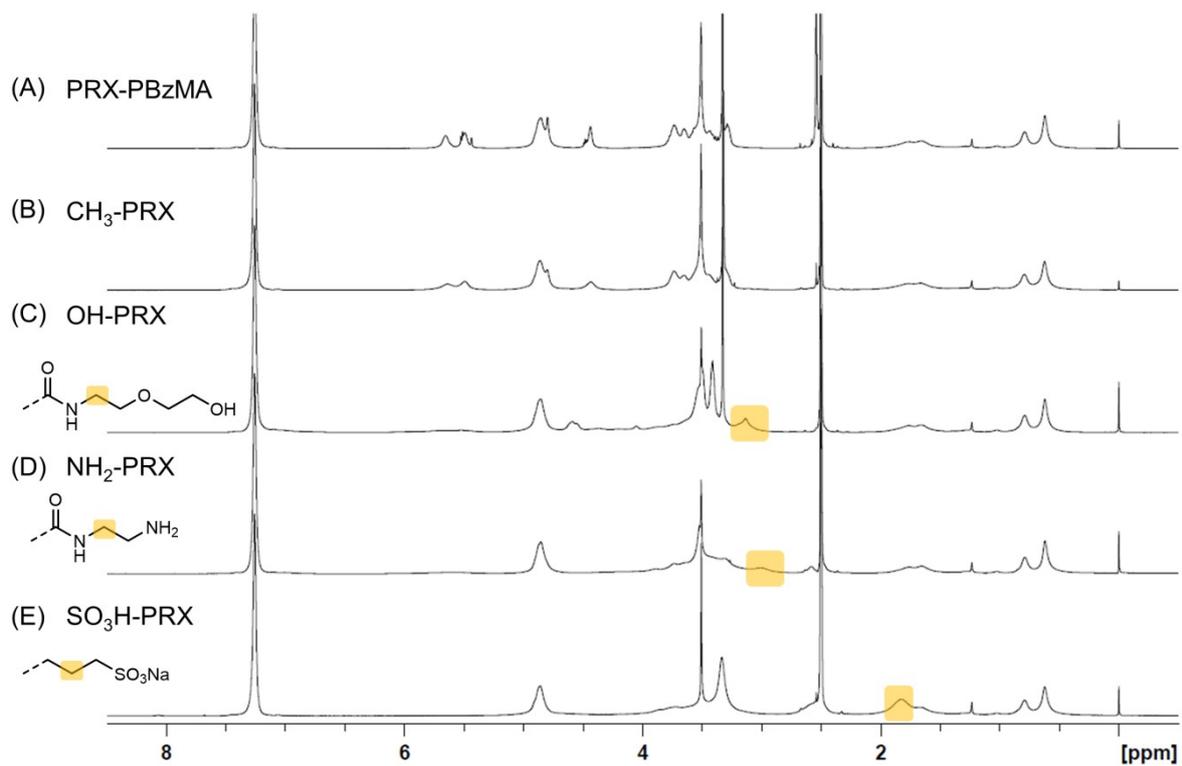


Figure S2. ¹H NMR spectra of polyrotaxane triblock copolymer (PRX-PBzMA) (A), methyl group-modified polyrotaxane triblock polymer (CH₃-PRX) (B), hydroxyl group-modified polyrotaxane triblock polymer (OH-PRX) (C), amino group-modified polyrotaxane triblock polymer (NH₂-PRX) (D) and sulfo group-modified polyrotaxane triblock polymer (SO₃H-PRX) (E) in DMSO-*d*₆.

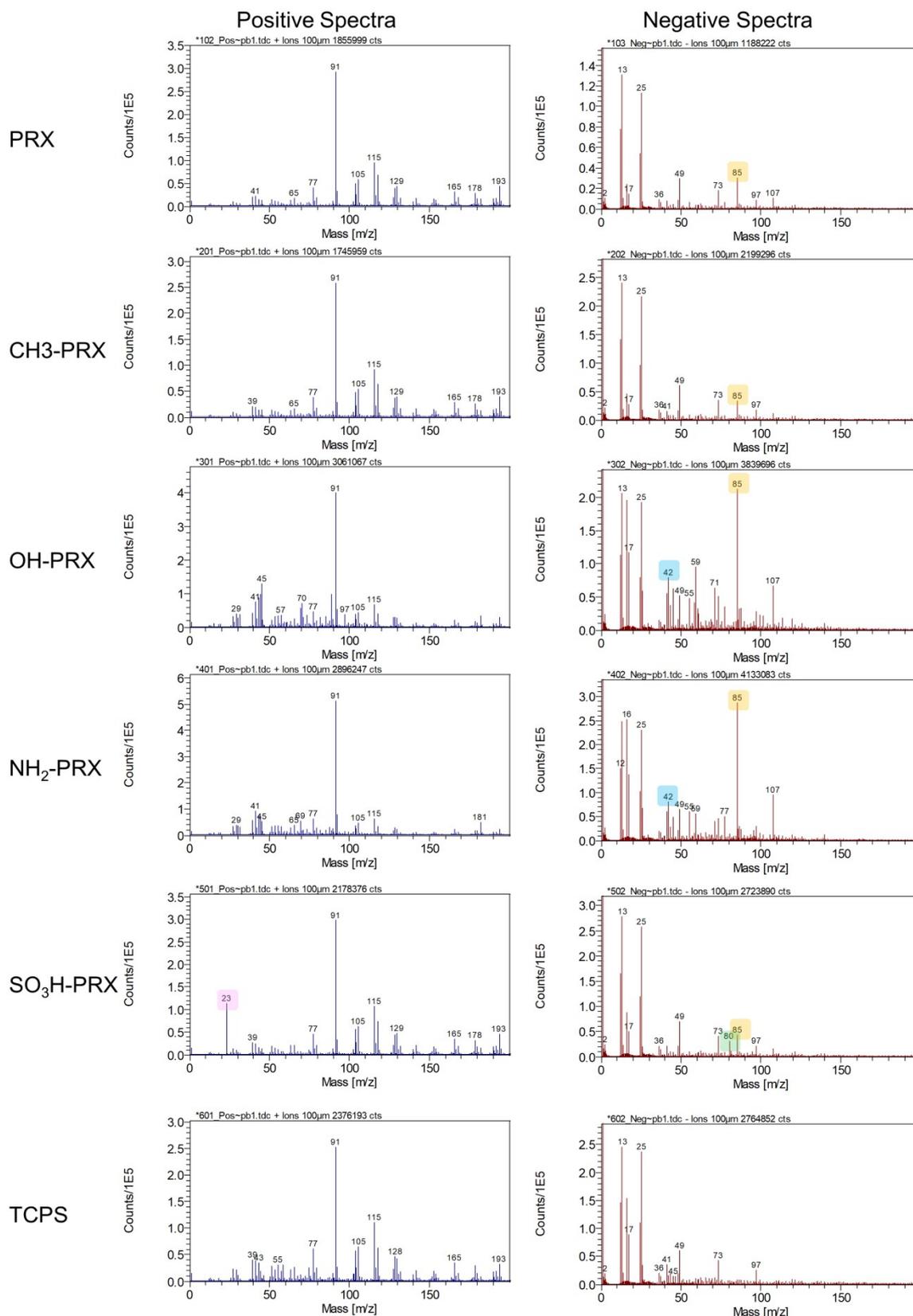


Figure S3. TOF-SIMS spectra of PRX, CH₃-PRX, OH-PRX, NH₂-PRX, SO₃H-PRX and TCPS surfaces.

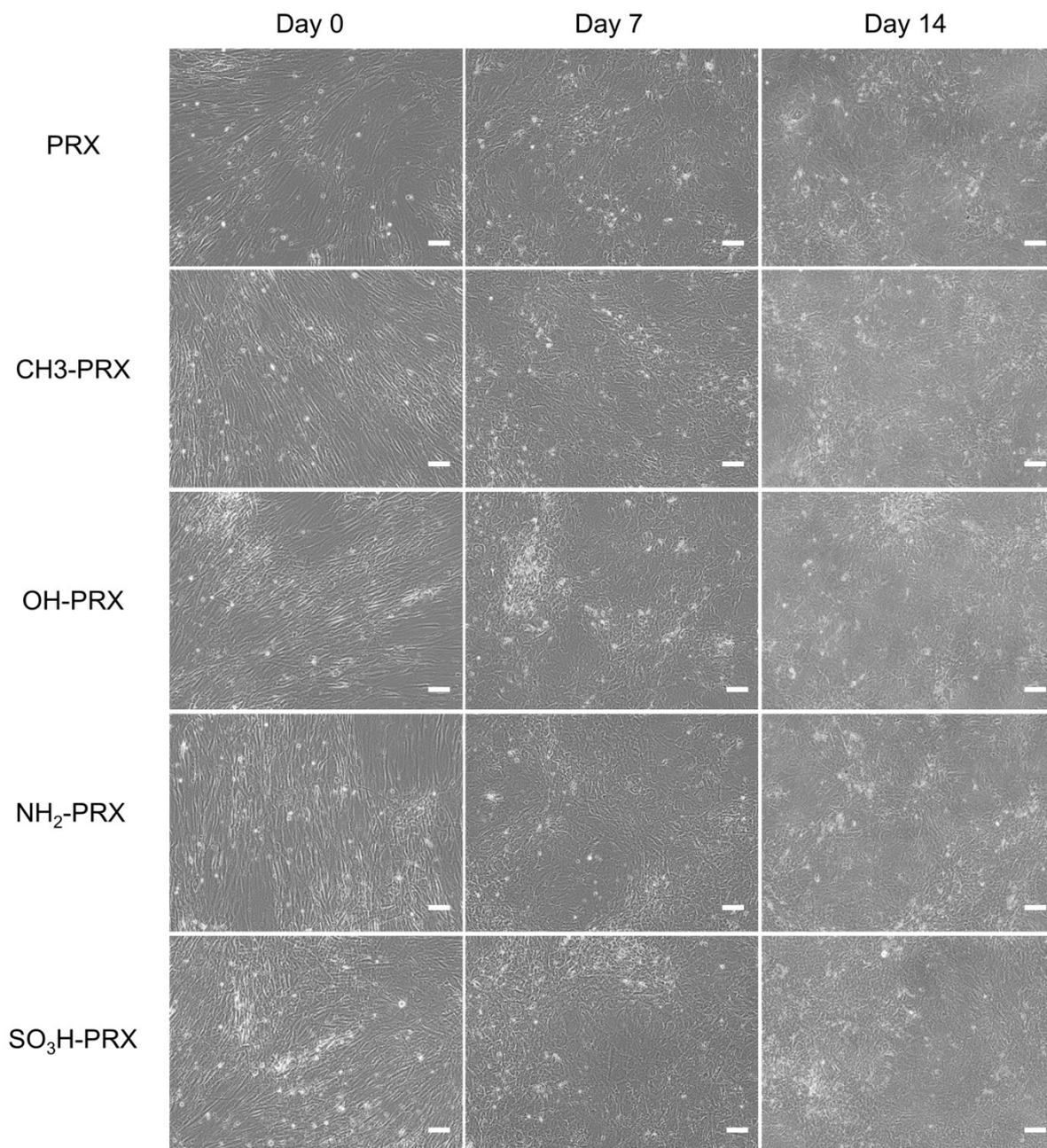


Figure S4. Phase-contrast microscopic images of osteoblast differentiation of hMSCs cultured on PRX, CH₃-PRX, OH-PRX, NH₂-PRX and SO₃H-PRX surfaces. The hMSCs were seeded at a density of 2.4×10^4 cells/cm² and expanded for 5 d. Osteoblast differentiation was subsequently induced in culture for 14 d. Scale bar: 100 μ m.

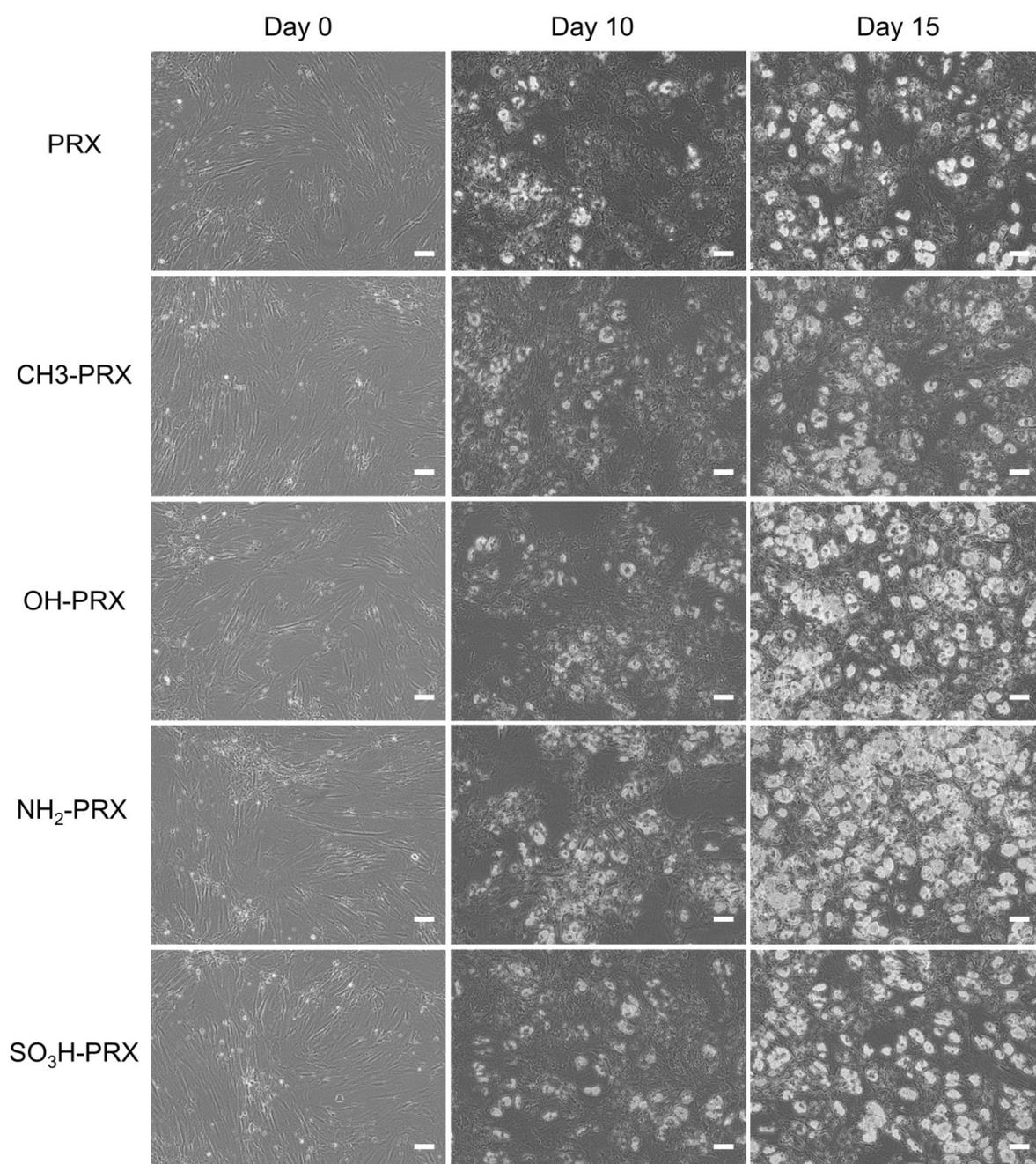


Figure S5. Phase-contrast microscopic images of adipocyte differentiation of hMSCs cultured on PRX, CH₃-PRX, OH-PRX, NH₂-PRX and SO₃H-PRX surfaces. The hMSCs were seeded at a density of 1.0×10^4 cells/cm² and expanded for 5 d. Adipocyte differentiation was subsequently induced in culture for 15 d. Scale bar: 100 μ m.