Electronic Supplementary Information (ESI)

Surface functionalization of polymer substrates with biomimetic apatite using polymer-binding peptides

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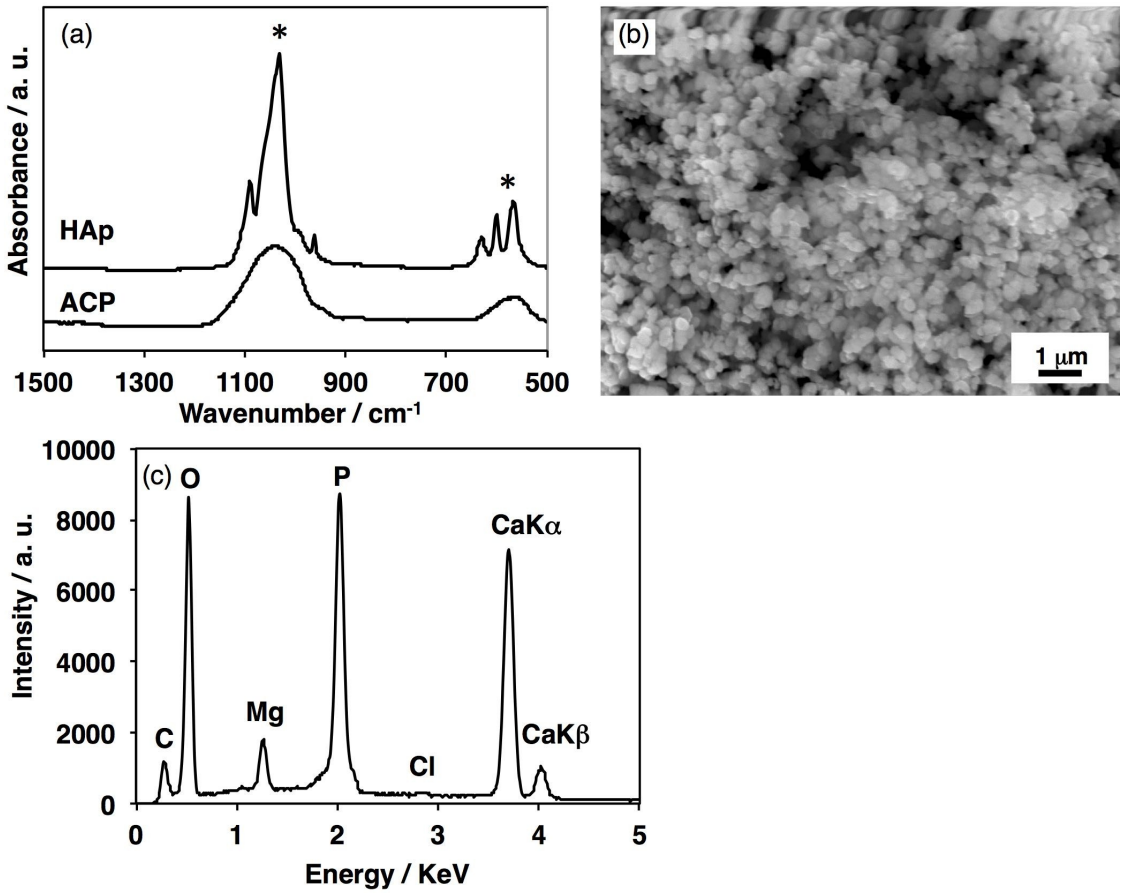

Fig. S1 Characterization of amorphous calcium phosphate (ACP) nanoparticles. (a) FT-IR spectra of sintered hydroxyapatite (HAp) nanoparticles (SHAp, SofCera Corp.) and ACP nanoparticles (1500–500 cm^{-1}), (b) SEM image of ACP nanoparticles, (c) EDX spectrum of ACP nanoparticles. In FT-IR spectra, the asterisk (*) shows the peak at 1100–1050 cm^{-1}, assignable to stretching vibrations of PO_4^{3-} groups, and peak at 600–540 cm^{-1}, to deformation vibrations of PO_4^{3-} groups. FT-IR spectra can reveal the crystallinity of the HAp, and broad peaks detected in ACP supported their low crystllinity. (N. Pleshko, A. Boskey and R. Mendelsohn, *Biophys. J.*, 1991, **60**, 786–793.)

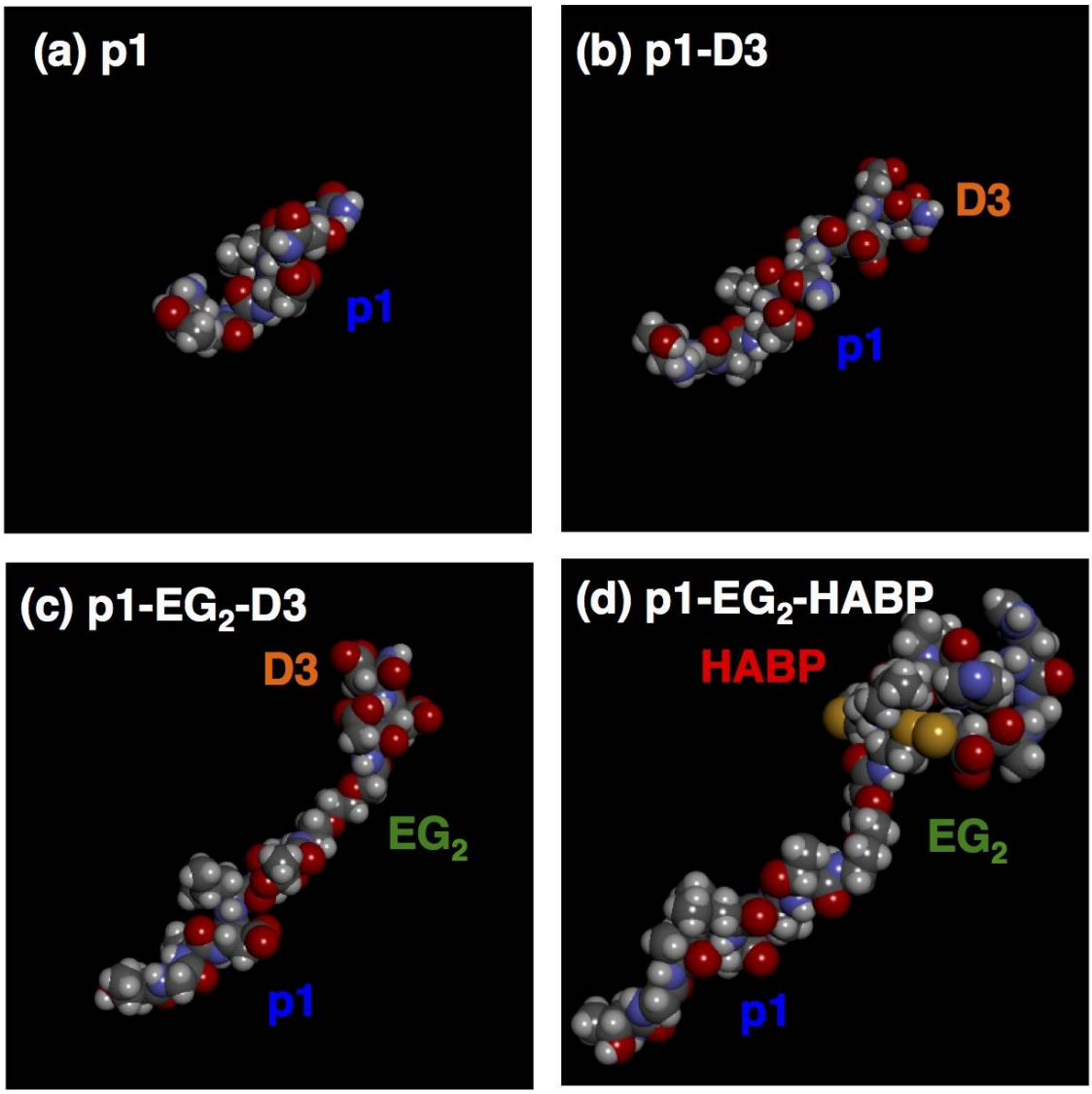

Fig. S2 Representative Snapshots of peptides calculated from a molecular dynamics simulation. (a) p1, (b) p1-D3, (c) p1-EG_2-D3, and (d) p1-EG_2-HABP (oxidized form). Molecular dynamics simulation was calculated using Discovery Studio 4.0 (Dassault Systèmes, France). Firstly, peptides surrounded by water with periodic boundary conditions were minimized using steepest descent algorithm at max step of 1000 and root mean square (RMS) gradient of 1.0, followed by second minimization using conjugate gradient algorithm at max step of 1000 and RMS gradient of 0.1. Then, objects were heated from 50 K to 300 K and equilibrated at 300 K for 10 ps. After that, structures of peptides were captured at each 2 ps for 10 ps.

Table S1 Sequences of synthesized peptides and their respective molecular mass.

Peptide	Sequence	Adduct composition	Calculated	Observed
p1	TGADLNT	$[M+H]^+$	690.72	690.06
		$[M+Na]^+$	712.71	712.12
		$[M+K]^+$	728.68	728.12
p1-D3	TGADLNTDDD	$[M+H]^+$	1035.43	1035.55
		$[M+Na]^+$	1057.41	1057.13
		$[M+K]^+$	1073.48	1073.64
p1-EG_2-D3	TGADLNT$(EG)_2$DDD	$[M+Na]^+$	1202.48	1202.90
		$[M+K]^+$	1218.45	1218.90
p1-EG_2-HABP	TGADLNT$(EG)_2$CMLPHHGAC	$[M+H]^+$	1784.78*	1785.23

*For p1-EG_2-HABP peptide, calculated mass of reduced form was shown.