

## Supplementary figures and data

# Ceria nanoparticles immobilized with self-assembling peptide for biocatalytic applications

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### **Abbreviations**

**CeNP:** ceria nanoparticles.

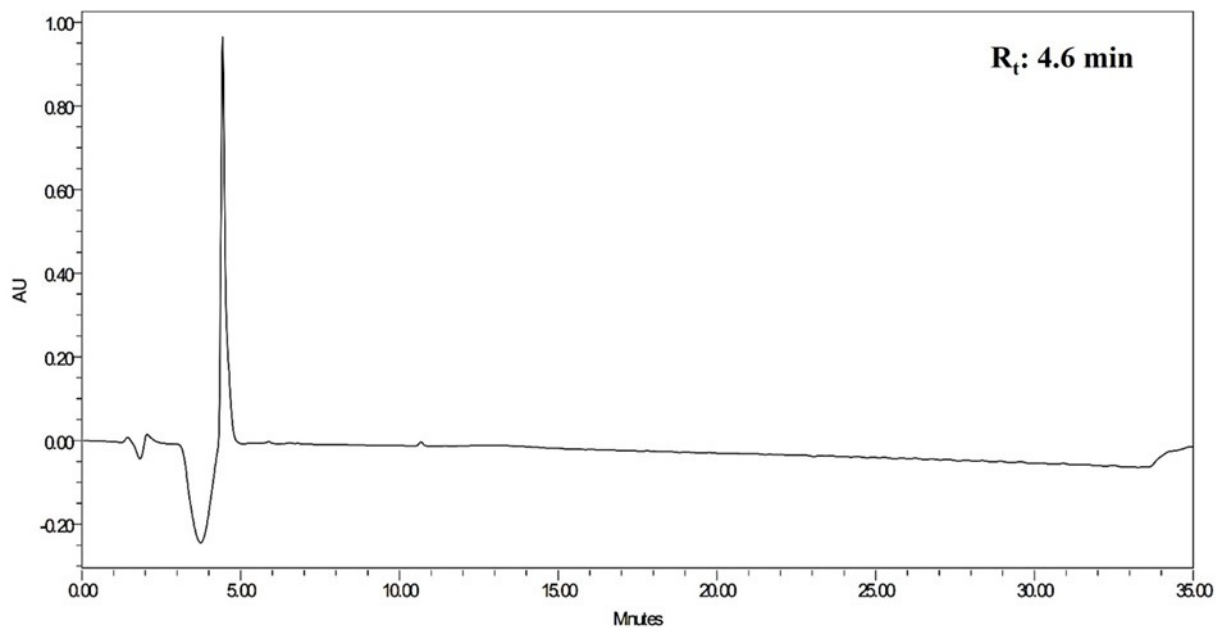
**PA:** peptide amphiphile.

**pNPA:** *para*-nitrophenyl acetate.

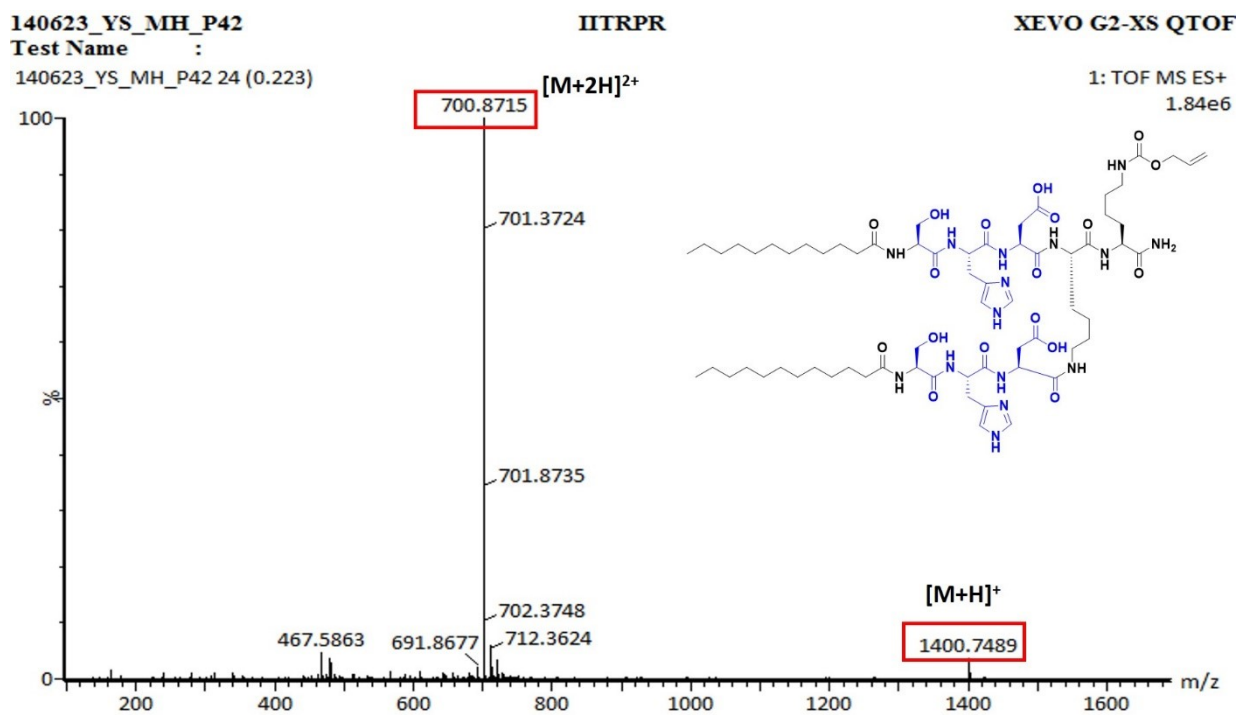
**pNPP:** *para*-nitrophenyl phosphate.

**TC:** thiolated ceria nanoparticles.

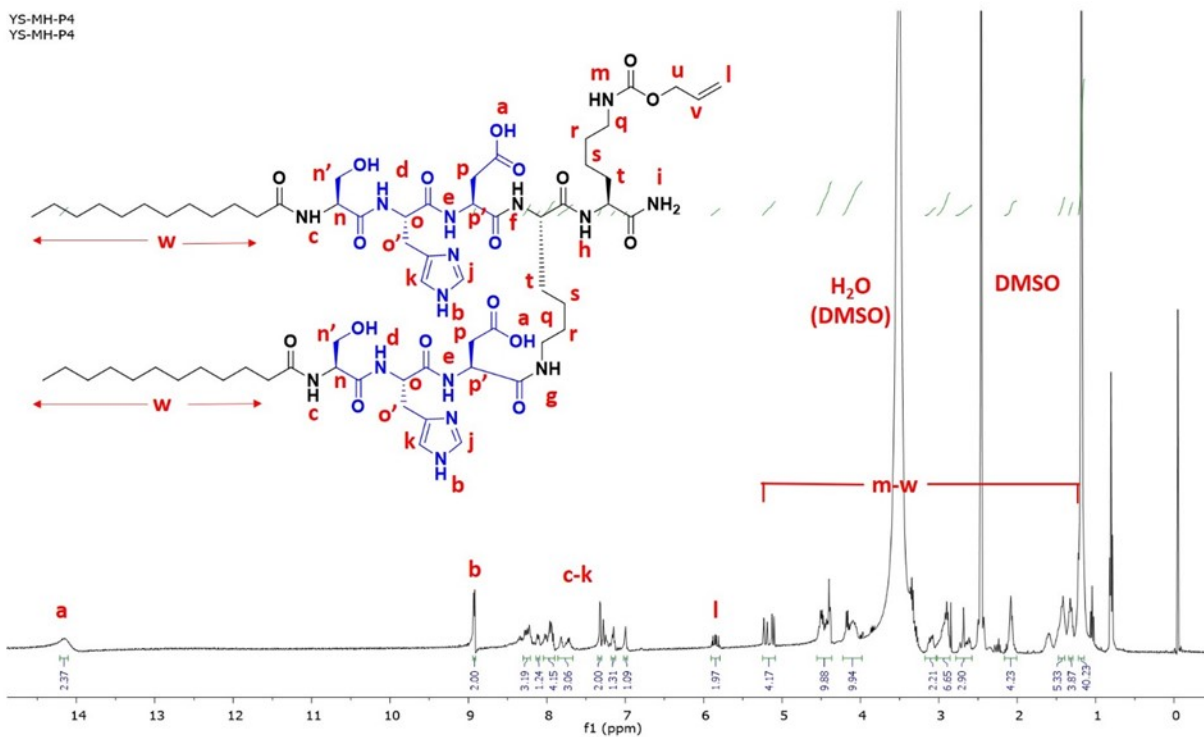
**TCP:** peptide conjugated ceria nanoparticles.



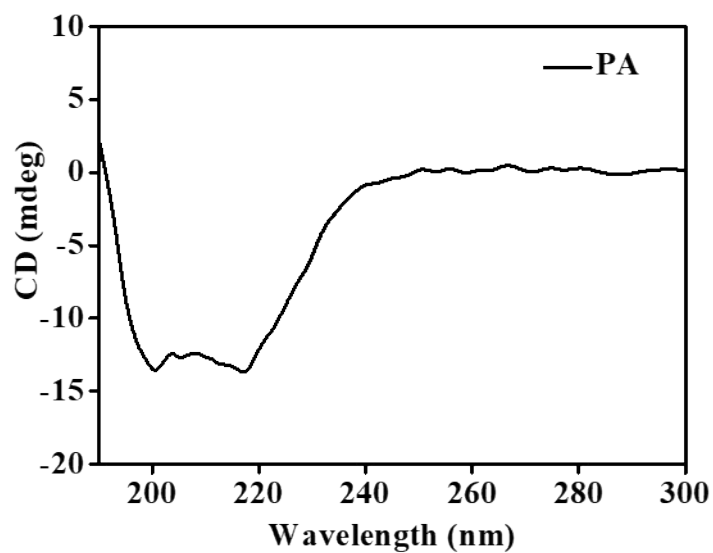
**Fig. S1** RP-HPLC profile of peptide amphiphile (PA).



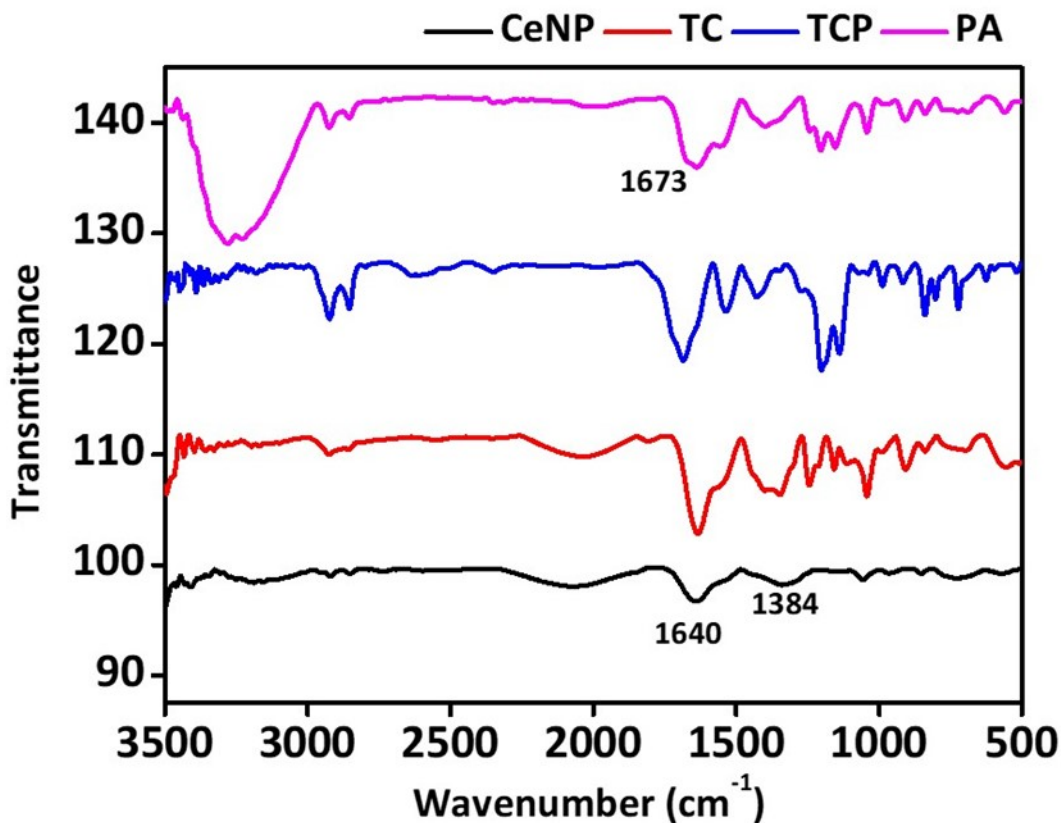
**Fig. S2** Mass spectrum of peptide amphiphile (PA).



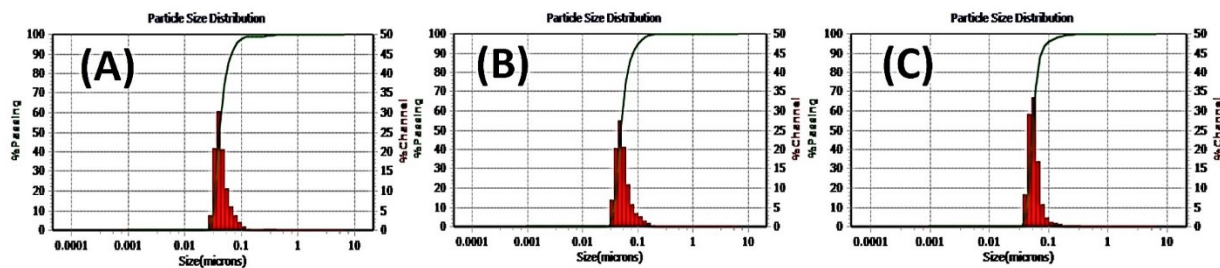
**Fig. S3** <sup>1</sup>H NMR spectrum of peptide amphiphile (PA).



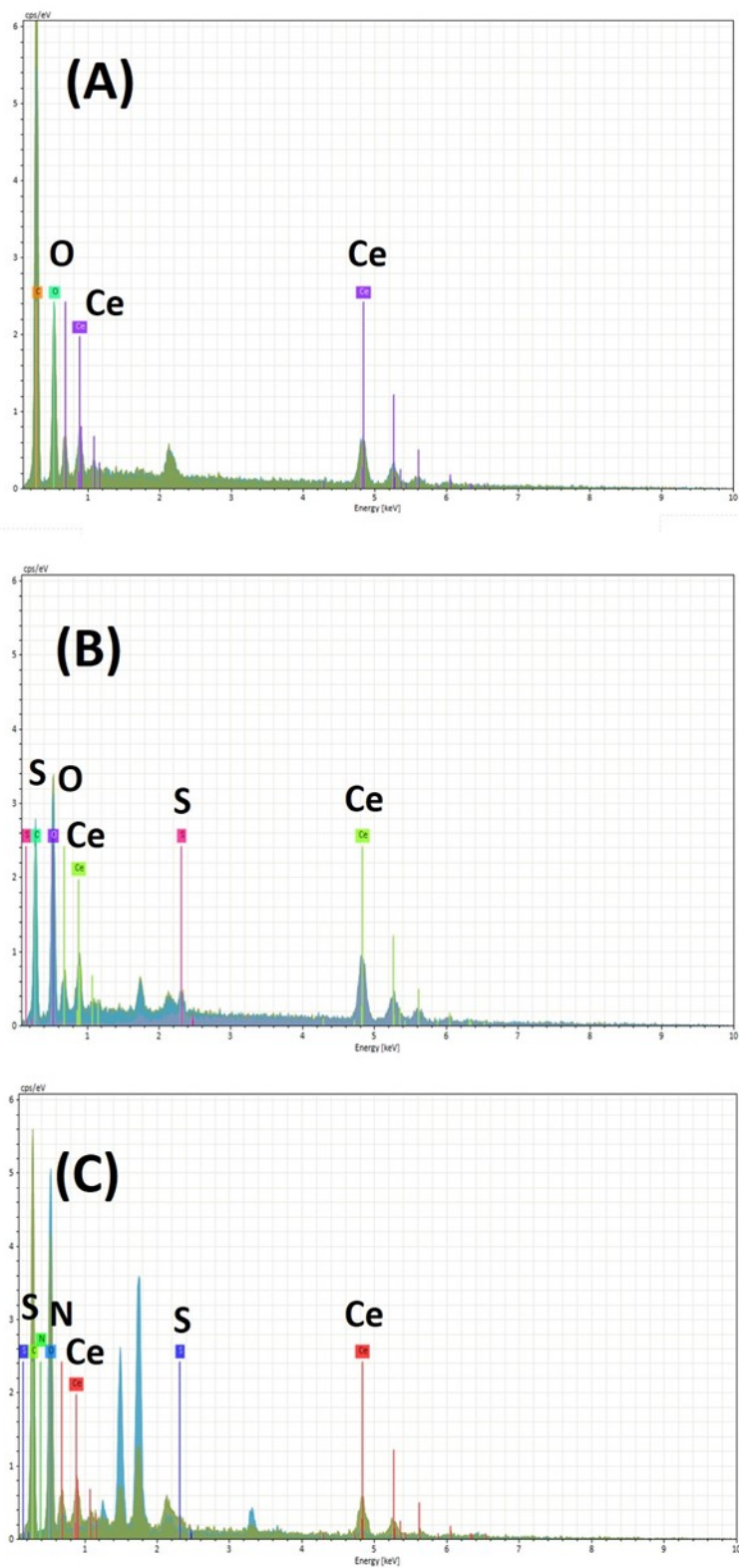
**Fig. S4** Circular Dichroism (CD) spectrum of peptide amphiphile (PA).



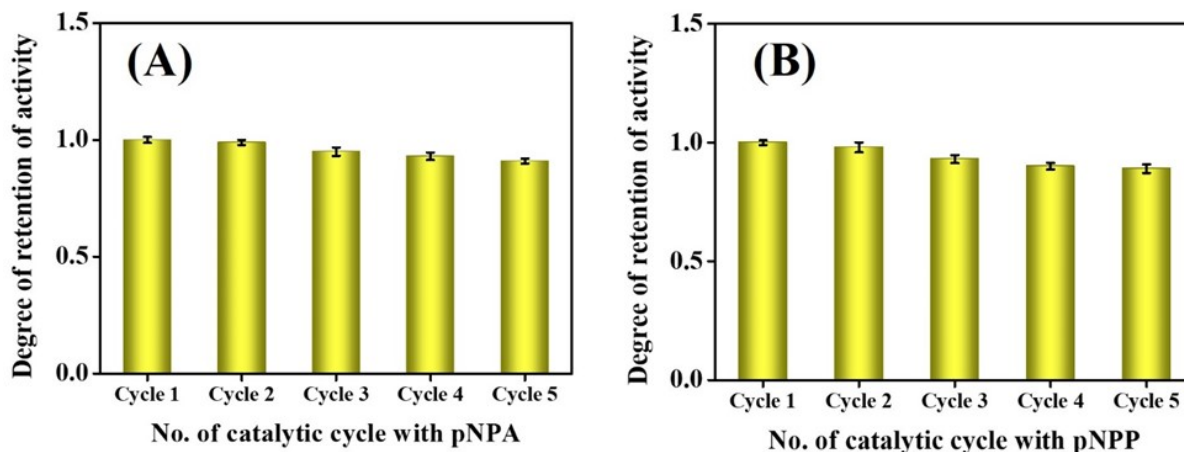
**Fig. S5** FT-IR spectra of ceria nanoparticles (CeNP), thiolated ceria nanoparticles (TC), peptide conjugated ceria nanoparticles (TCP), and peptide amphiphile (PA).



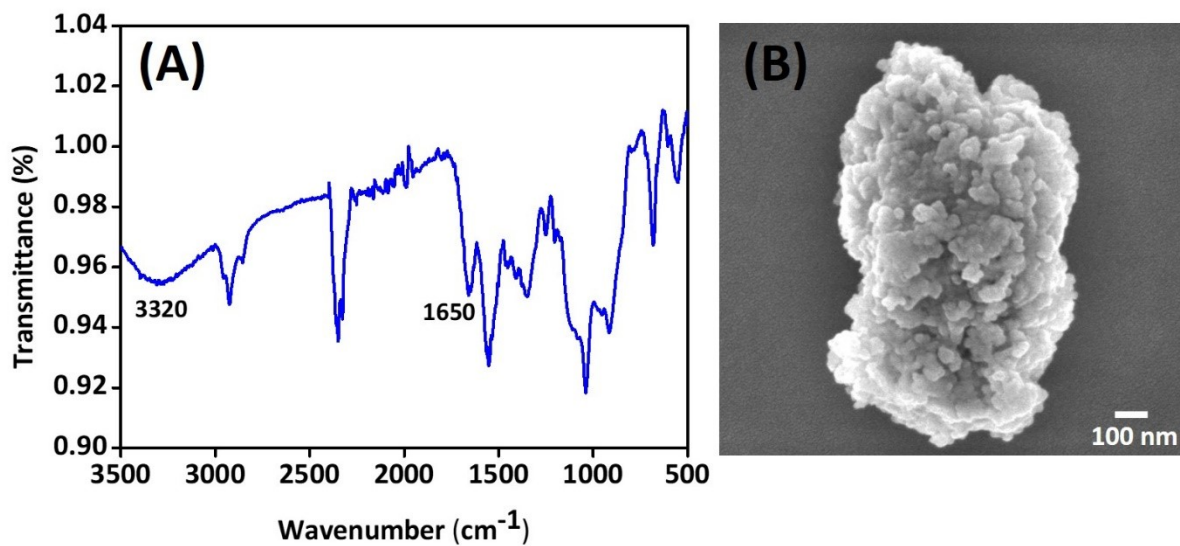
**Fig. S6** Particle size distribution ( $n = 3$ ) using dynamic light scattering (DLS). (A) Ceria nanoparticles (CeNP), (B) Thiolated ceria nanoparticles (TC), and (C) Peptide conjugated ceria nanoparticles (TCP).



**Fig. S7** EDX spectra of: (A) ceria nanoparticles (CeNP), (B) thiolated ceria nanoparticles (TC), and (C) peptide conjugated ceria nanoparticles (TCP).



**Fig. S8** Recyclability ( $n = 3$ ) of peptide conjugated ceria nanoparticles (TCP): (A) hydrolysis of *para*-nitrophenyl acetate (pNPA), and (B) hydrolysis of *para*-nitrophenyl phosphate (pNPP). Experiments were performed in triplicates and data are presented as average  $\pm$  SD.



**Fig. S9** Characterization of peptide conjugated ceria nanoparticles (TCP) after fifth catalytic cycle. (A) FT-IR spectra, and (B) FESEM image. Scale bar: 100 nm.



AChE: Acetylcholinesterase; OP: Organophosphate; S-Ach: S-acetylthiocholine

Fig. S10 Mechanism of pesticide detection.<sup>1</sup>

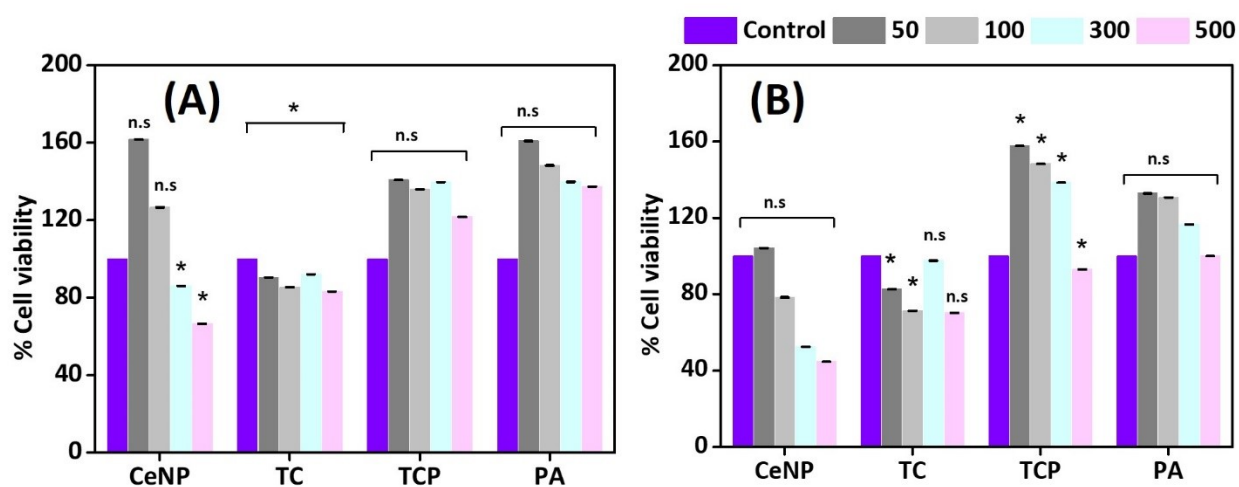
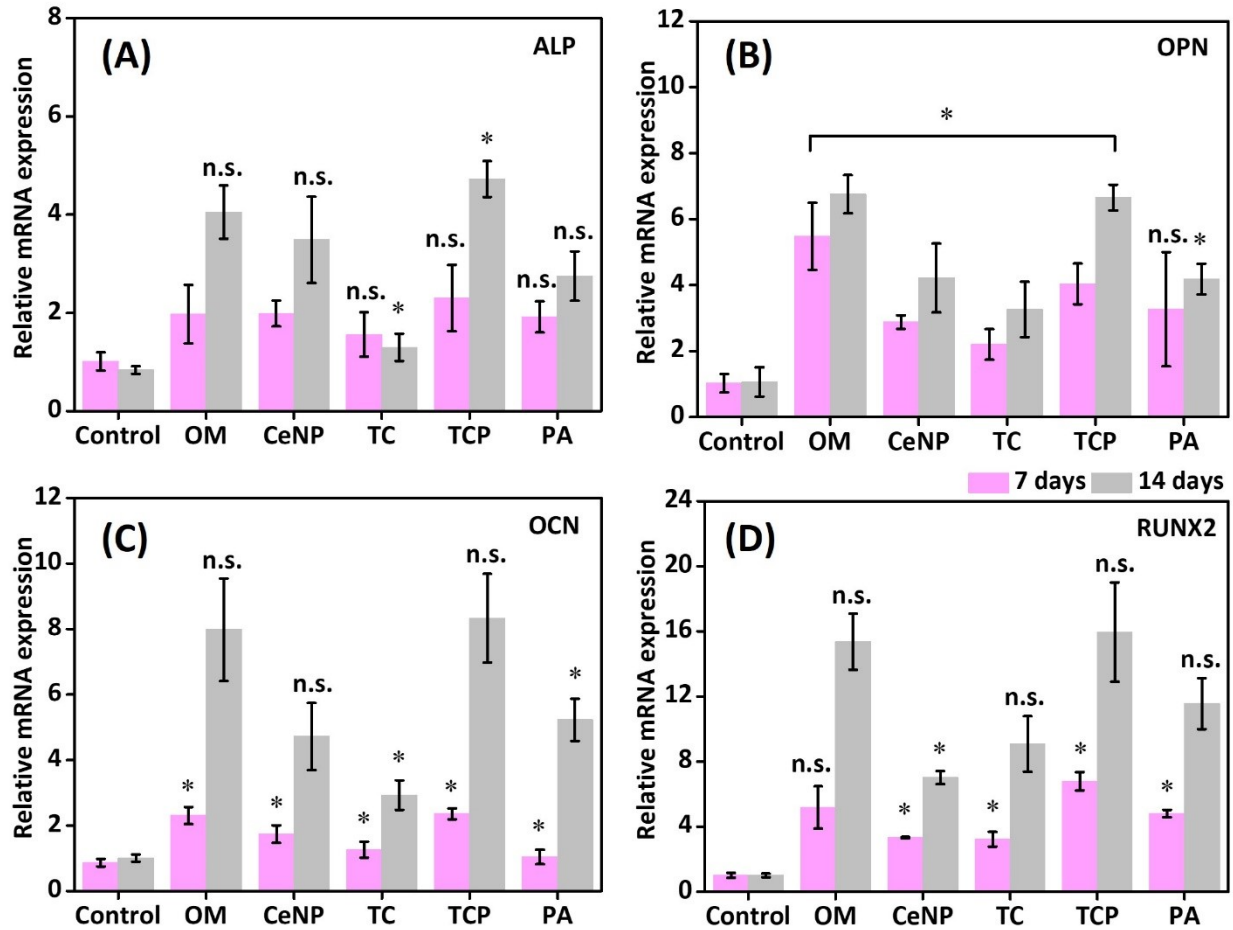


Fig. S11 Cytocompatibility of mesenchymal stem cells (MC3T3-E1) in presence of different concentrations (50, 100, 300, and 1 µg/mL) of nanomaterials, ceria nanoparticles (CeNP), thiolated ceria nanoparticles (TC), peptide conjugated ceria nanoparticles (TCP), and peptide amphiphile (PA), using MTT assay. (A) 7<sup>th</sup> day. (B) 14<sup>th</sup> day. Experiments were performed in triplicates and data are presented as average  $\pm$  SD ( $n = 3$ ), and \* $p < 0.05$  indicates statistically significant data and ns non-significant data.





**Fig. S12** Gene expression studies of osteogenic markers, ALP, OPN, OCN, and RUNX2 in mesenchymal stem cells (MC3T3-E1) cultured in osteogenic media (OM) and nanomaterials for 7 and 14 days. Untreated cells were considered as negative control and those treated with OM as positive control. Data are presented as mean  $\pm$  SD,  $n = 3$ , and \* $p < 0.05$  indicates statistically significant data and ns indicates non-significant data.

**Table. S1** Physical properties of ceria nanoparticles (CeNP), thiolated ceria nanoparticles (TC), and peptide conjugated ceria nanoparticles (TCP).

<b>Sample</b>	<b>Surface area (m<sup>2</sup>/g)</b>	<b>Pore volume (cm<sup>3</sup>/g)</b>	<b>Mean pore diameter (nm)</b>
CeNP	1120	5.3094	19.034
TC	105	0.3961	15.113
TCP	76	0.2878	15.172

**Table. S2** Ratio of Ce<sup>3+</sup>/Ce<sup>4+</sup> estimated using Ce 3d XPS spectrum of peptide conjugated ceria nanoparticles (TCP).

Peaks	Binding energy (eV)	Area
i	882.1	18840
ii	884.9	16200
iii	888.5	13500
iv	898	17280
v	900.6	12890
vi	903	10350
vii	907	15670
viii	916.3	15750
ii, iv, vi	Ce <sup>3+</sup>	43830
i, viii, v, vii, viii	Ce <sup>4+</sup>	76650
	Ce <sup>3+</sup> /Ce <sup>4+</sup>	0.57
	Ce <sup>3+</sup> /(Ce <sup>3+</sup> +Ce <sup>4+</sup> )	37%

## Reference

1. S. Qian and H. Lin, *Anal. Chem.*, 2015, **87**, 5395–5400.