Supporting Information

Tuning the enzyme-like activities of cerium oxide nanoparticles using triethyl phosphite ligand

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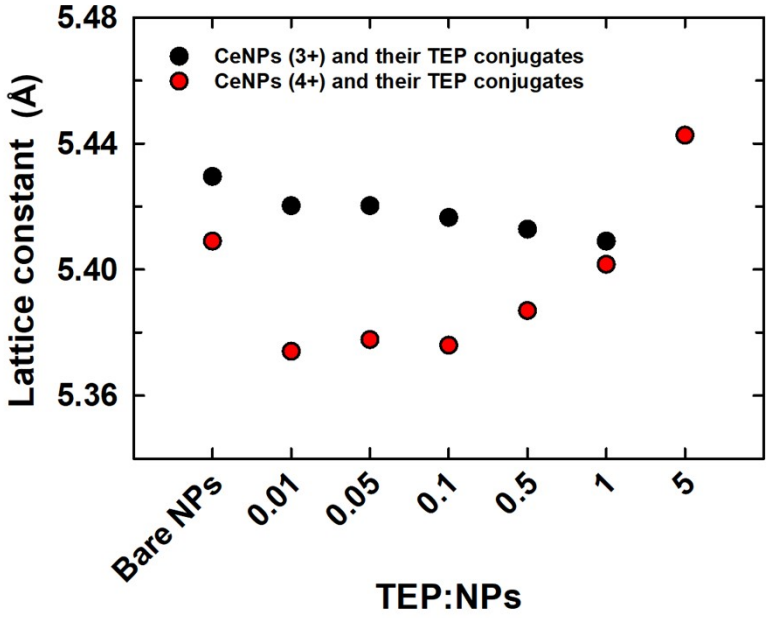
1. Lattice constant of CeNPs in presence and absence of TEP



ESI 1. *The change in the lattice constant as a function of increasing concentration of TEP. (Black dots - CeNPs (3+) and red dots - CeNPs (4+).*

2. Zeta potential of CeNPs in the presence and absence of TEP.

ESI 2. *Zeta potential of CeNPs in the presence and absence of TEP.*

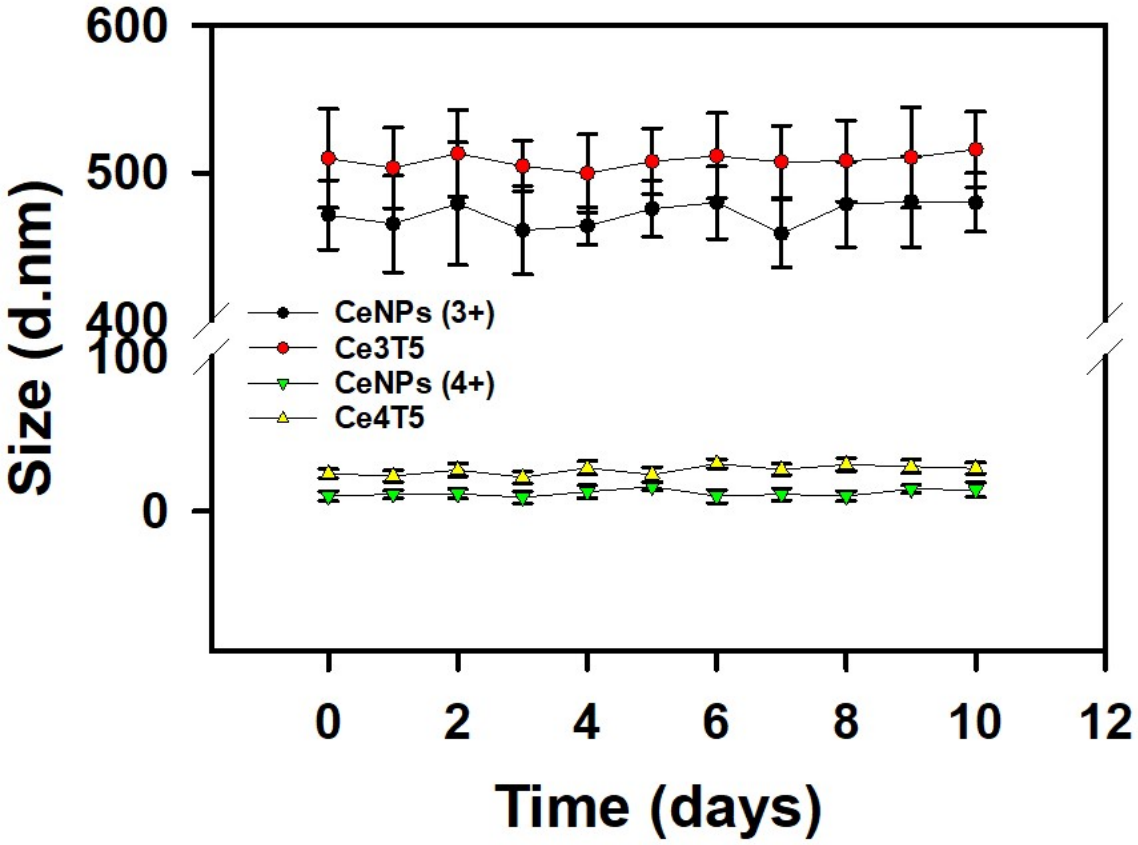
NPs	Size (nm)	PDI	Zeta Potential (mV)
CeNPs (3+)	464.2 ± 53.2	0.467	+38.4 ± 2.0
CeNPs (4+)	9.8± 4.1	0.351	+46.8 ± 4.1
Ce3T1	479.5± 67.8	0.608	+31.1 ± 3.5
Ce3T2	484.6± 94.8	0.568	+24.3 ± 2.7
Ce3T3	480.4± 77.5	0.597	+17.5 ± 3.5
Ce3T4	495.2± 56.9	0.421	+11.3 ± 3.9
Ce3T5	501.5± 97.5	0.588	+3.8 ± 1.1
Ce3T6	526.1± 87.1	0.569	+0.17 ± 2.0
Ce4T1	12.67± 17.5	0.287	+43.8 ± 3.0
Ce4T2	11.43± 8.4	0.381	+39.1 ± 5.1
Ce4T3	15.47± 10.7	0.321	+31.2 ± 3.9
Ce4T4	17.39± 12.5	0.402	+23.3 ± 4.4
Ce4T5	24.27 ± 15.7	0.364	+12.2 ± 3.5
Ce4T6	38.81± 22.5	0.318	+9.78 ± 3.3

3. EDX(S) analysis of TEP interacted CeNPs.

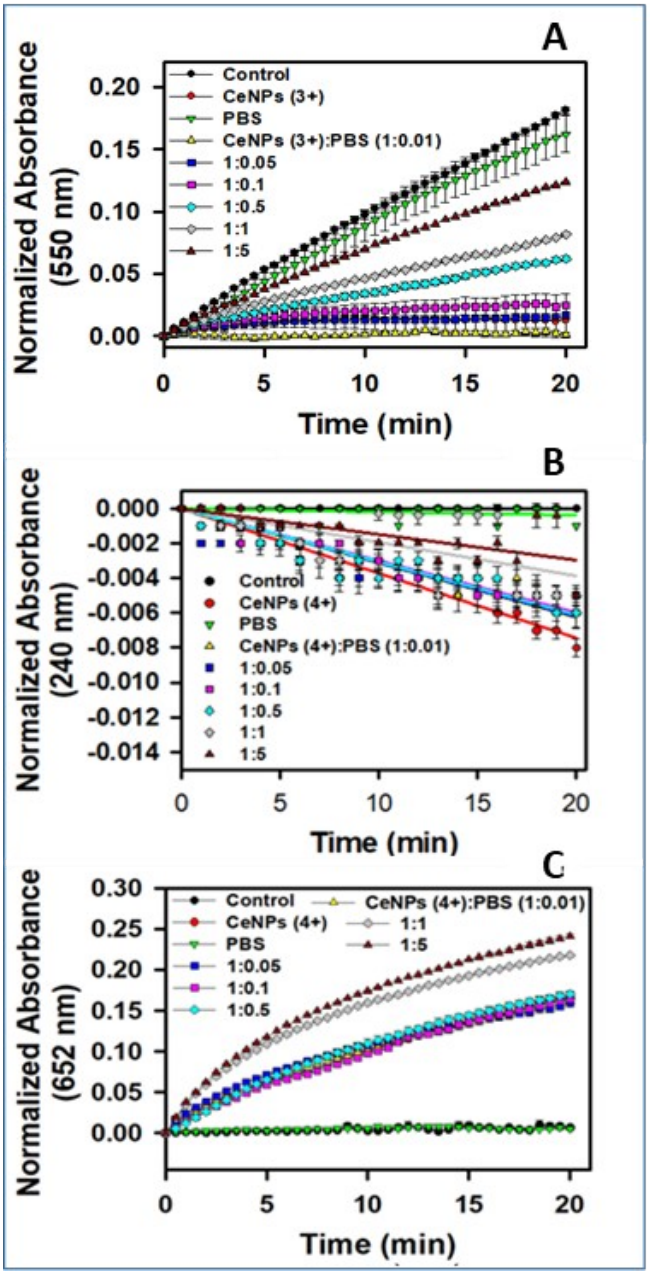
ESI 3. *EDX(S) analysis of TEP interacted CeNPs for elemental mapping of Ce, O, and P*

	Ce	**O**	**P**
CeNPs (4+)	26.20	65.36	
Ce4T1	25.22	64.68	0.46
Ce4T2	32.11	60.51	0.97
Ce4T3	27.29	62.77	1.34
Ce4T4	20.68	65.72	5.37
Ce4T5	20.20	55.49	7.29
Ce4T6	4.69	68.08	19.88

4. Stability study of CeNPs in presence and absence of TEP



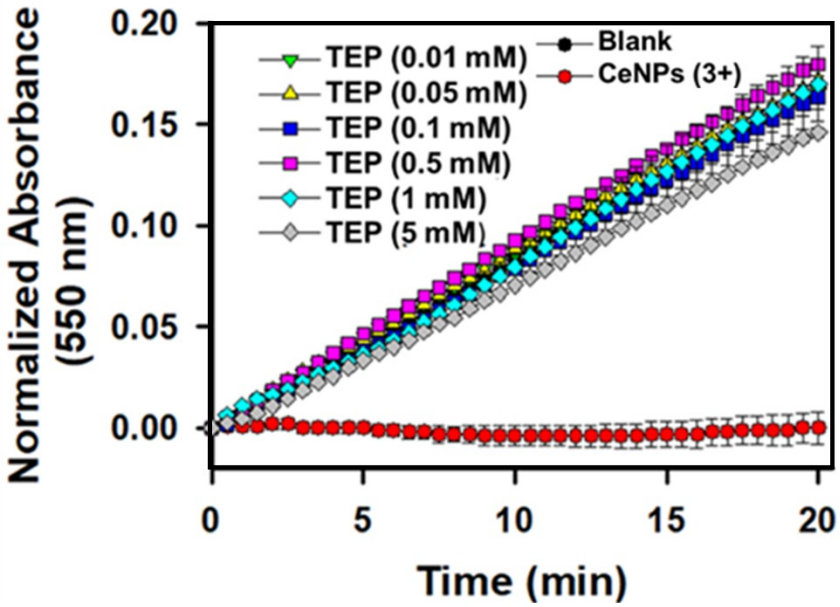
ESI 4. *The changes in the hydrodynamic size of bare and TEP incubated CeNPs as a function of time. TEP conjugated (1 mM :1 mM) and bare CeNPs (1 mM) were stored in a glass vial and the changes in the size of CeNPs were observed for 10 days. CeNPs were found stable after TEP binding. The data is represented as SE obtained from three (n=3) independent experiments.*



ESI 5. *Enzyme-like activities of CeNPs in presence of PBS. (A) SOD-like activity of CeNPs (3+), (B) Catalase-like activity of CeNPs (4+) and (C) Oxidase-like activity of CeNPs (4+) after incubation with different concentrations of PBS. The data is represented as SE obtained from three (n=3) independent experiments.*

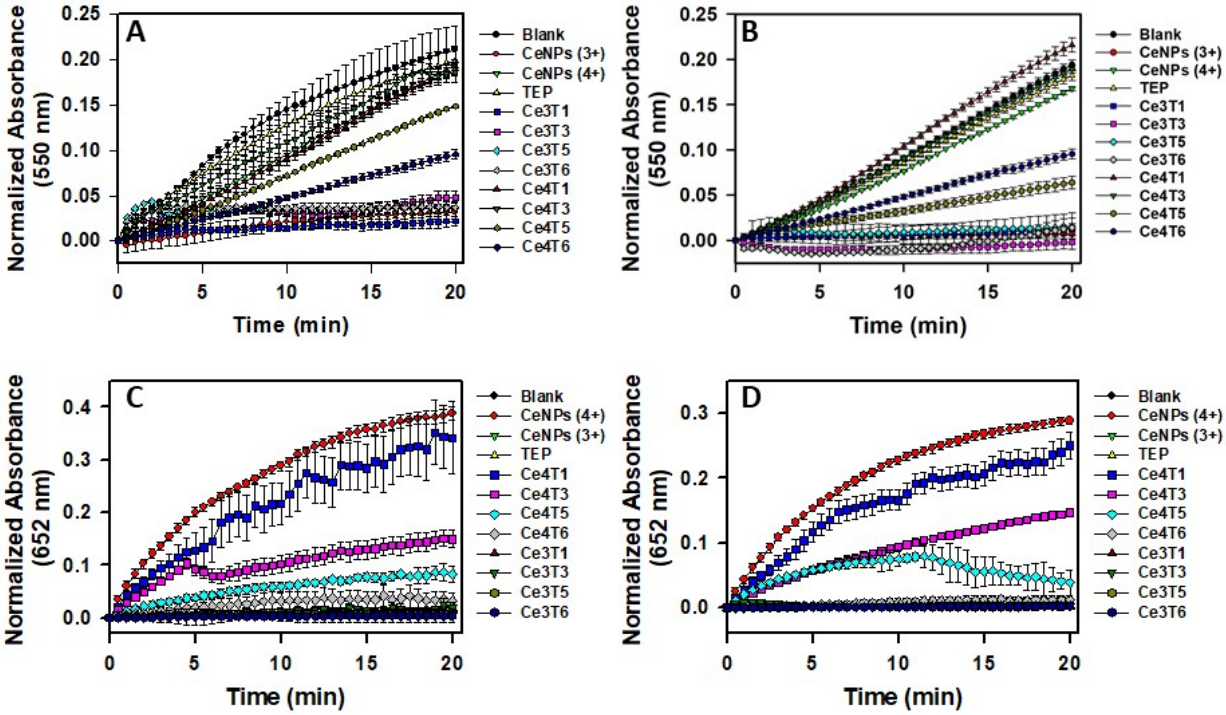
5. Enzyme-like activities of CeNPs in presence of PBS

6. Analysis of the effect of TEP on the activity of xanthine oxidase



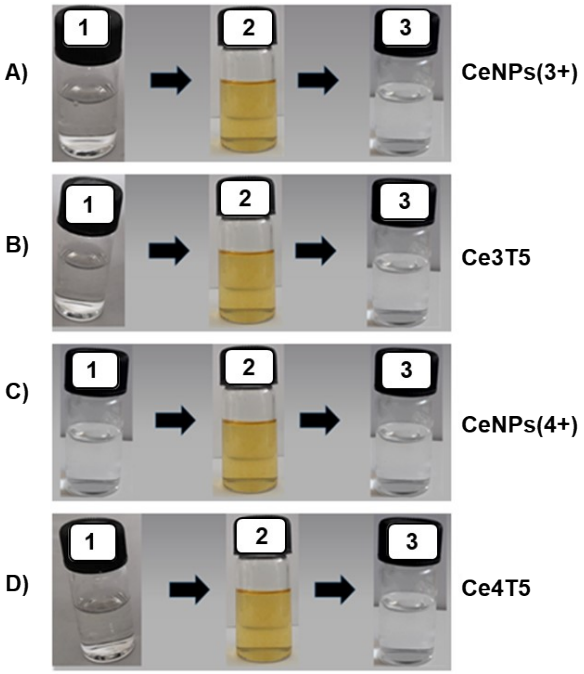
ESI 6. *SOD-like activity in presence of various concentrations of TEP. The effect of different concentrations (0.01-5 mM) of TEP on the activity of xanthine oxidase was followed by measuring the reduction of cytochrome C in presence of superoxide anions. The data is represented as SE obtained from three (n=3) independent experiments.*

7. Enzyme-like activities of CeNPs in different pH conditions



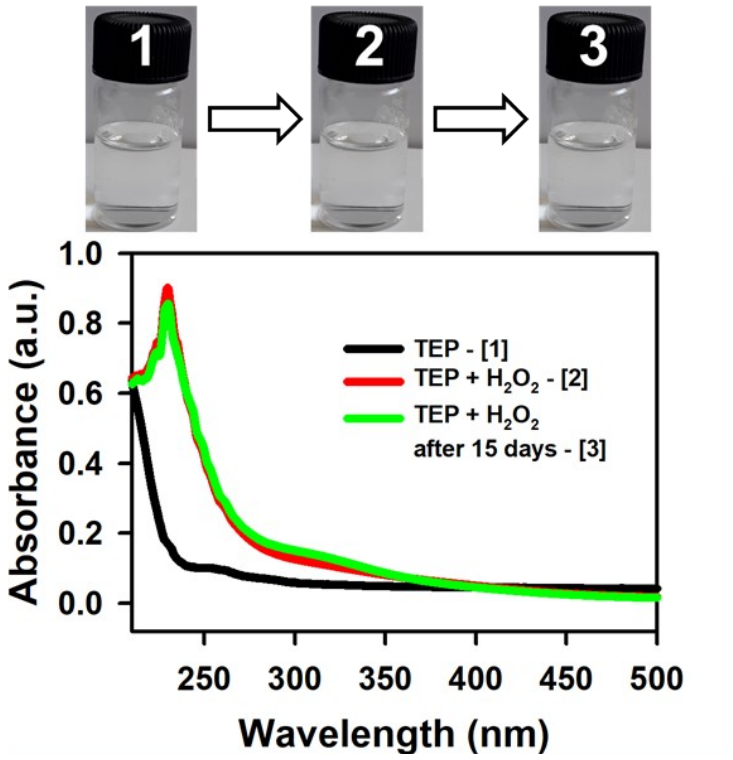
ESI 7. *Enzyme-like activities of bare and TEP incubated CeNPs in different pH conditions. (A) SOD-like activity of CeNPs after incubating in citrate buffer (pH=3) for 24 hours, (B) SOD-like activity of CeNPs after incubating in Tris buffer (pH=7) for 24 hours, (C) Oxidase-like activity of CeNPs after incubating in citrate buffer (pH=3) for 24 hours, and (D) Oxidase-like activity of CeNPs after incubating in Tris buffer (pH=7) for 24 hours. The data is represented as SE obtained from three (n=3) independent experiments.*

8. Analysis of surface regeneration of CeNPs:



ESI 8. *Autocatalytic activity of CeNPs before and after TEP interaction [colour transition of respective samples before H_2O_2 addition (1), after H_2O_2 addition (2) and after 15 days of incubation (3)].*

9. Analysis of the effect of H_2O_2 on TEP

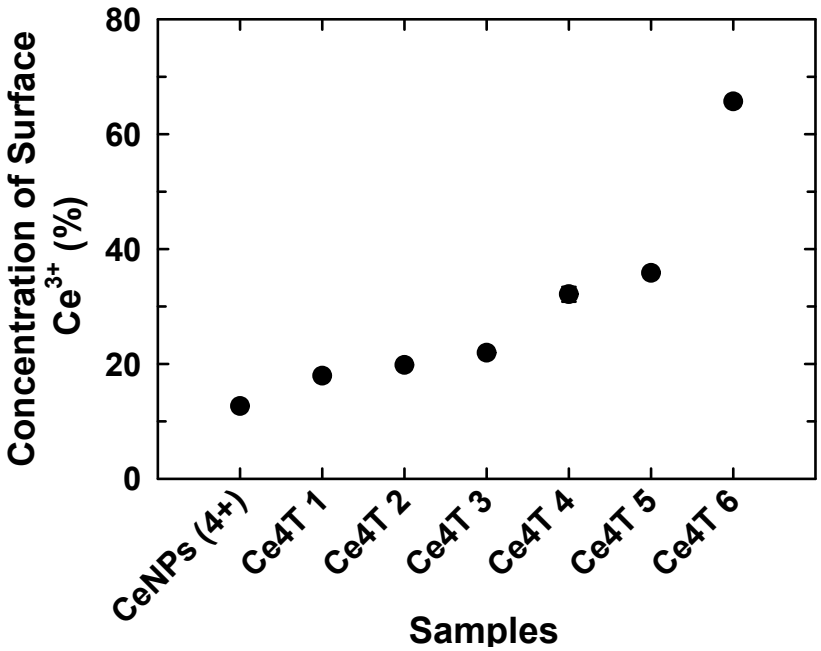


ESI 9. *UV-Vis absorbance of TEP, after addition of H_2O_2, after incubation of 15 days. The subset images show the color of the suspension of TEP (bottle 1), after H_2O_2 addition (bottle 2), after incubation of 15 days (bottle 3).*

10. XPS analysis of bare and TEP conjugated CeNPs

ESI 10a. *XPS analysis of TEP interacted CeNPs for quantifying the concentration of surface Ce^{3+} ions*

Assigned Peak	Charge state	Referenced peak position	CeNPs (4+)		Ce4T1		Ce4T2		Ce4T3		Ce4T4		Ce4T5		Ce4T6	
			FWHM	Peak %	FWHM	Peak %	FWHM	Peak %	FWHM	Peak %	FWHM	Peak %	FWHM	Peak %	FWHM	Peak %
v	Ce^{4+}	882	2.0	18.26	2.0	16.57	2.0	14.15	2.0	15.31	2.2	13.99	2.2	15.19	2.2	9.75
v''	Ce^{4+}	888	4.4	16.16	4.3	14.87	4.2	13.76	4.2	13.43	4.5	13.78	4.5	12.70	3.0	2.15
v'''	Ce^{4+}	898	2.0	19.26	2.0	18.11	2.0	17.34	2.0	17.61	2.0	14.10	2.2	14.56	2.5	9.52
u	Ce^{4+}	901	1.8	11.20	1.8	9.87	2.0	10.68	1.8	9.18	2.0	7.96	2.0	7.51	2.5	9.39
u''	Ce^{4+}	907	4.4	8.82	4.5	9.54	4.5	10.18	4.5	8.99	4.5	7.96	3.5	4.86	3.5	2.31
u'''	Ce^{4+}	916	2.2	13.89	2.3	13.74	2.5	14.28	2.3	12.94	2.5	11.01	2.3	9.10	2.5	2.06
v^0	Ce^{3+}	880	2.0	0.76	2.0	1.22	2.0	1.14	2.0	1.83	2.2	2.07	2.0	2.64	2.0	7.97
v'	Ce^{3+}	884	2.5	7.75	2.9	9.63	3.5	12.09	3.5	13.12	3.5	16.41	3.5	18.91	3.5	34.02
u^0	Ce^{3+}	899	2.0	0.00	2.0	1.59	2.0	0.87	2.0	1.33	2.0	2.59	2.0	2.29	1.6	4.35
u'	Ce^{3+}	903	2.4	3.91	2.6	4.85	3.0	5.52	3.0	6.28	3.5	10.12	3.5	12.25	3.5	18.49
Total Ce^{3+} (%)			12.42		17.29		19.62		22.56		31.19		36.09		64.83	



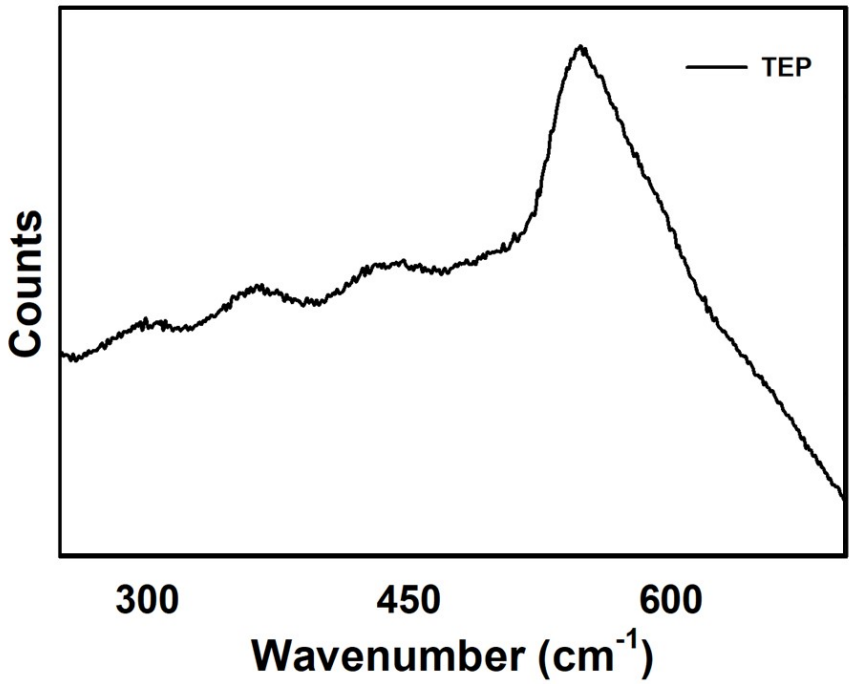
ESI 10b. *The concentration of Ce^{3+} ions (%) in CeNPs (4+) and TEP conjugated CeNPs (4+) depicting an increase in Ce^{3+} concentration with increasing TEP concentration.*

11. RAMAN data comparison of bare CeNPs (4+) and TEP with TEP interacted CeNPs

ESI 11a. *RAMAN data for comparing the shift in the peak position of the F_{2g} peak of bare CeNPs (4+) after incubation with different concentrations of TEP*

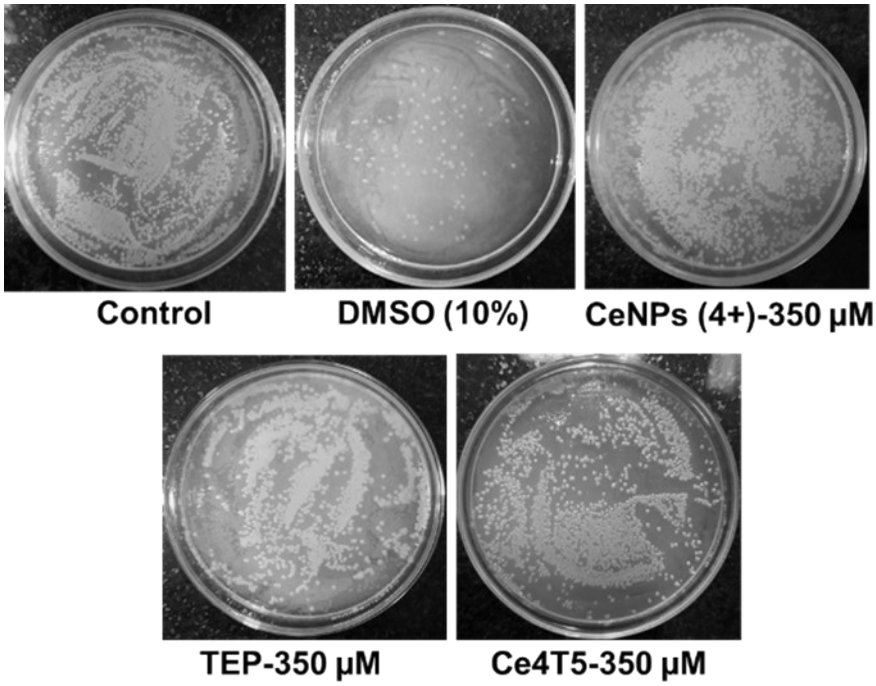
Sample	Peak Wavenumber (cm^{-1})	Peak Wavenumber STD.(cm^{-1})
CeNPs (4+)	448.43	2.07
Ce4T1	448.01	0.75
Ce4T3	446.74	1.16
Ce4T4	444.62	2.04
Ce4T5	440.37	2.95
TEP	499.00	0.57

(4+) and RAMAN spectra of pure TEP.



ESI 11b. *Raman spectra of pure TEP in the range of 250-700 cm^{-1}. The RAMAN spectra of TEP shows the characteristic vibrational band at ~ 548 cm^{-1} and a shoulder that extends to more than 600 cm^{-1}.*

12. Antibacterial activity of bare CeNPs (4+), TEP and TEP interacted CeNPs (4+).



ESI 12. *Antibacterial activity of bare CeNPs (4+), TEP, Ce4T 5, and DMSO against E. coli. The number of colonies formed on an agar plate is shown in presence of different treatments.*