

Environmental fate descriptors for Glycol coated Selenium Nanoparticle: Quantitative Multi Assay Approach

Savita Chaudhary,^{1*} Pooja Chauhan,¹ Rajeev Kumar²

¹*Department of Chemistry and Centre of Advanced Studies in Chemistry, Panjab University,
Chandigarh 160014, India*

²*Department of Environment Studies, Panjab University, Chandigarh 160014, India.*

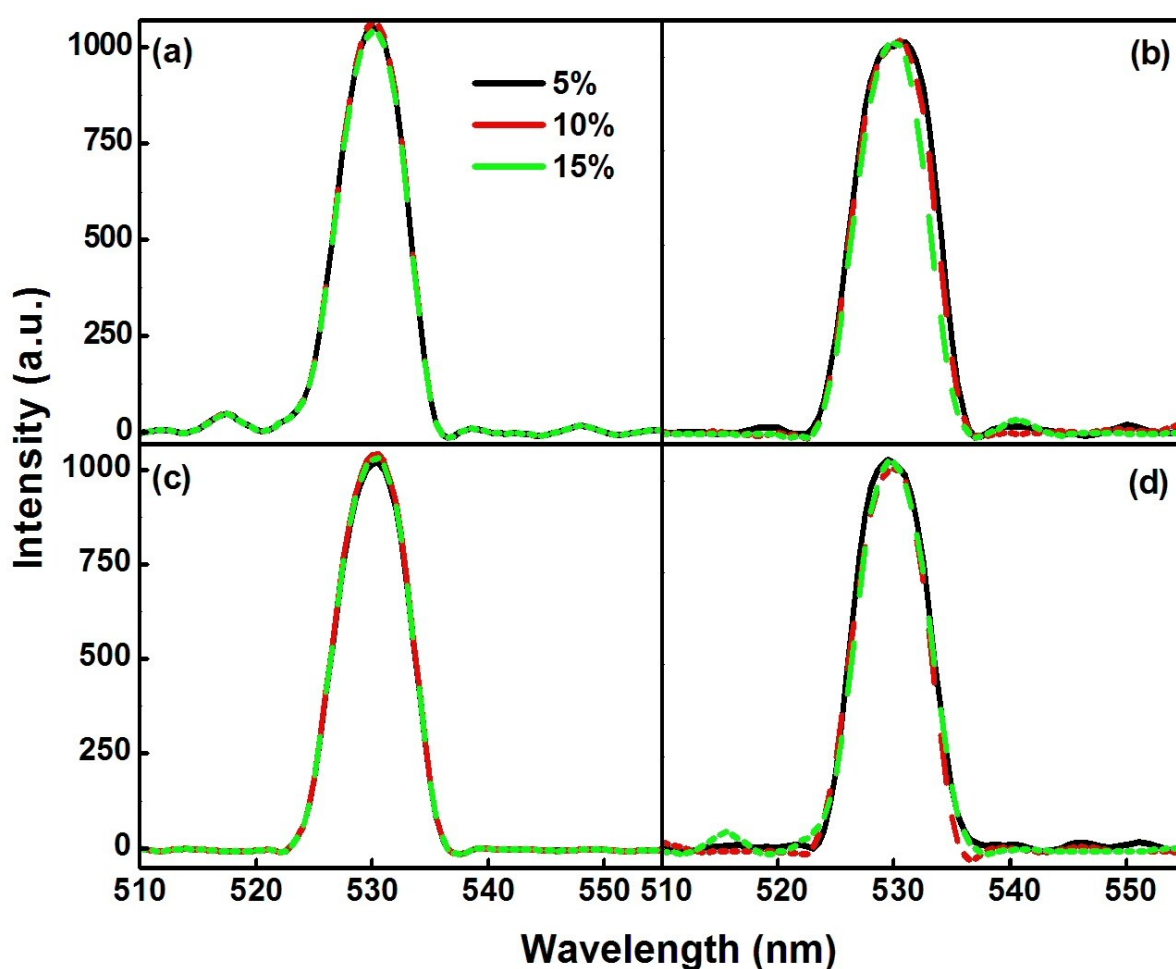


Fig. S1 Fluorescence emission spectrum as function of different concentrations of glycols for (a) EG (b) DEG (c) TEG and (d) PEG coated Se-NPs with [Se] = 0.03M

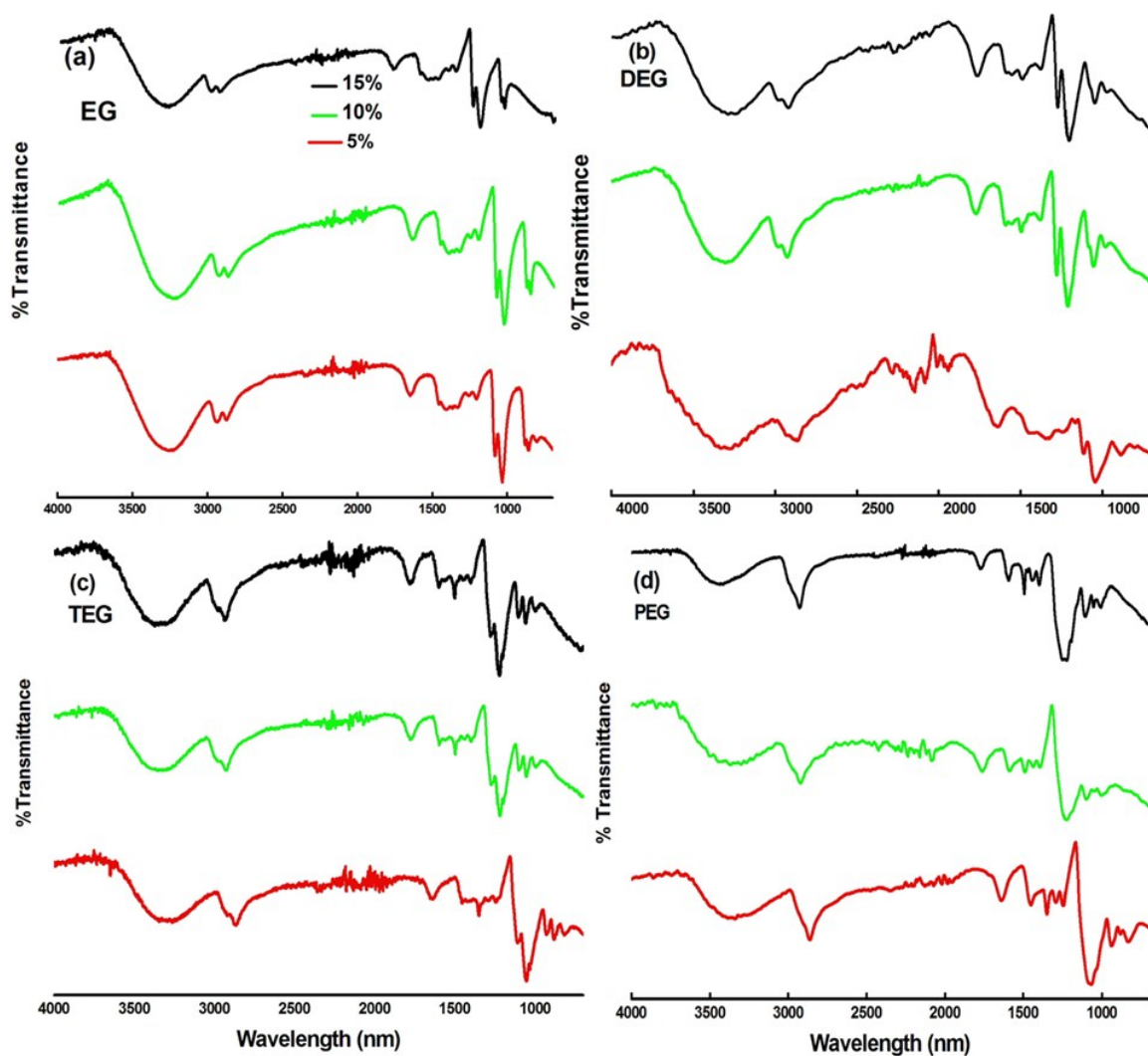


Fig. S2 FTIR spectrum of as function of different concentrations of glycols for (a) EG (b) DEG (c) TEG and (d) PEG coated Se-NPs with $[Se] = 0.03M$

Table S1 Representation of size and PDI values of EG, DEG, TEG and PEG coated SeNPs

Concentration	EG		DEG		TEG		PEG	
	Size (nm)	PDI	Size (nm)	PDI	Size (nm)	PDI	Size (nm)	PDI
5%	54	0.41	105	0.45	122	0.48	102	0.46
10%	22	0.39	68	0.40	51	0.40	70	0.40
15%	8	0.35	21	0.38	32	0.36	20	0.34

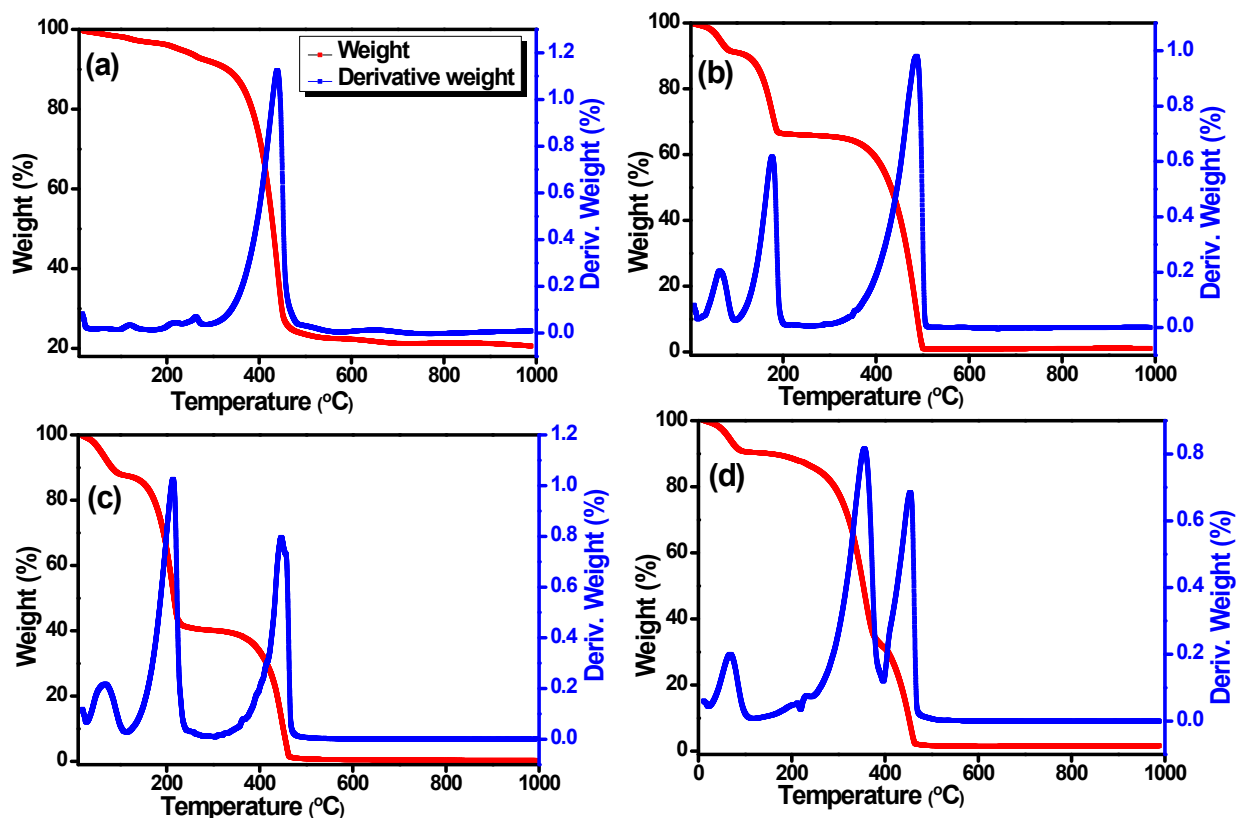


Fig. S3 TGA-DTA thermogram of 15 % (a) EG, (b) DEG, (c) TEG and (d) PEG coated Se-NPs with $[Se] = 0.03M$.

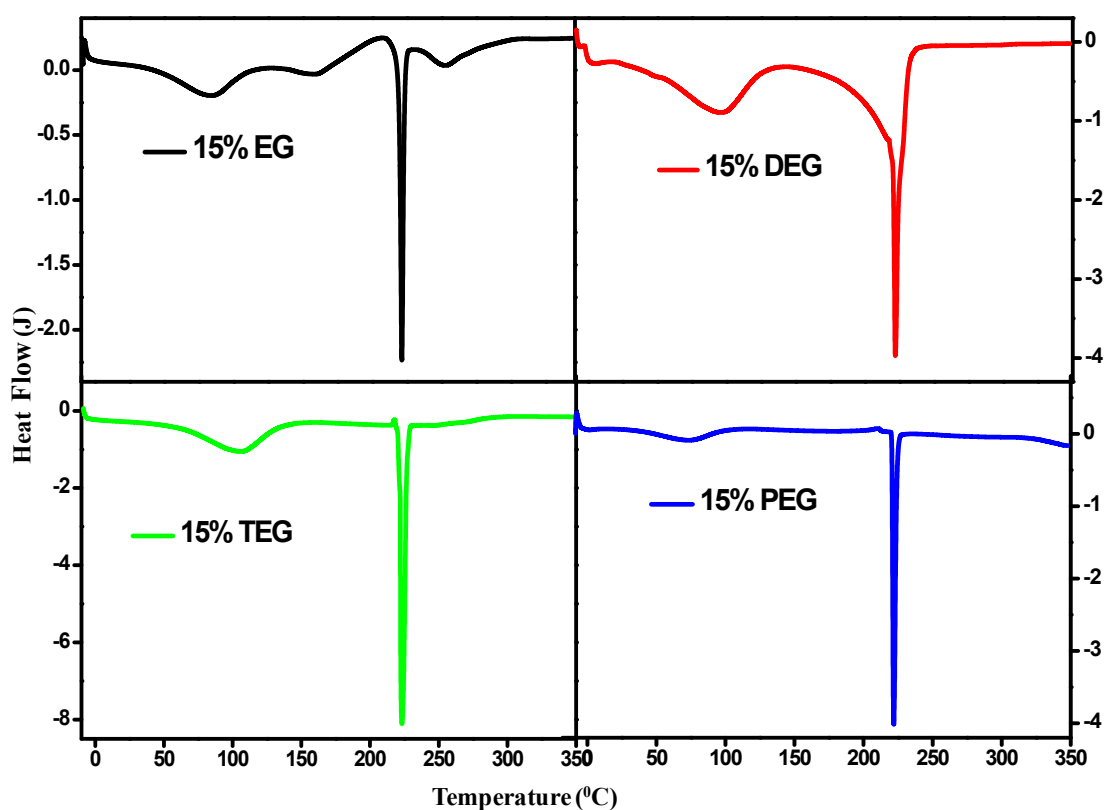


Fig. S4 DSC thermogram of 15% (a) EG, (b) DEG, (c) TEG and (d) PEG coated Se-NPs with $[Se] = 0.03M$.

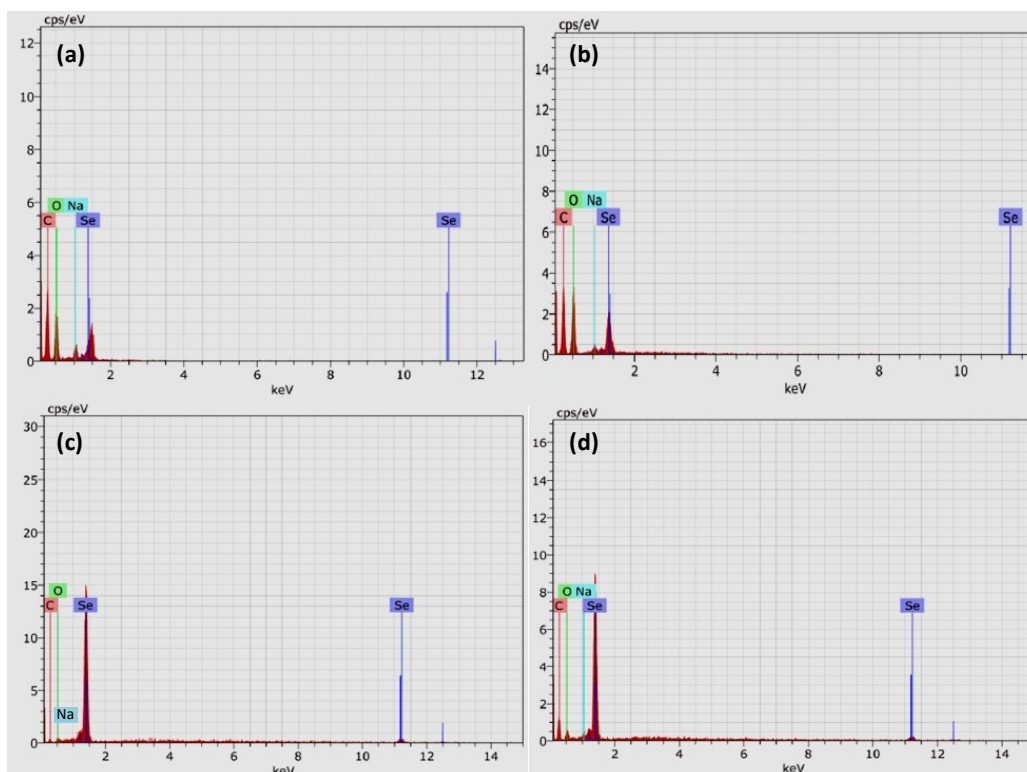


Fig. S5 EDX analysis of 15% (a) EG, (b) DEG, (c) TEG and (d) PEG coated Se-NPs with $[\text{Se}] = 0.03\text{M}$.

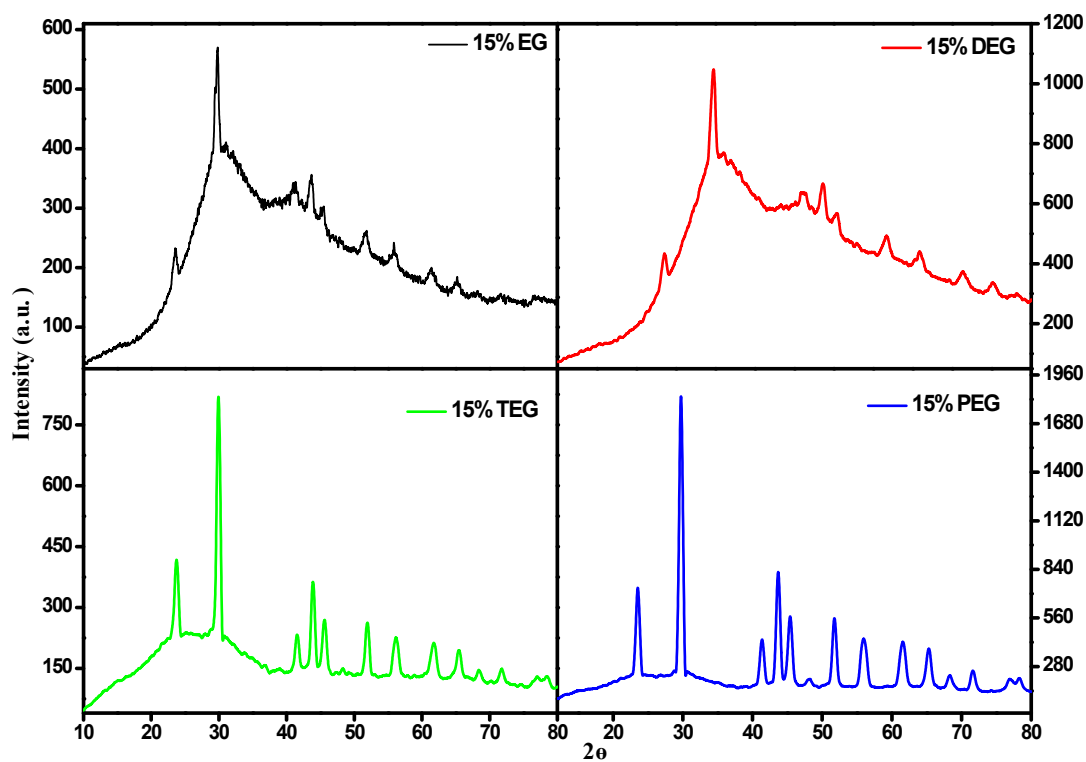


Fig. S6 XRD spectra of 15% (a) EG, (b) DEG, (c) TEG and (d) PEG coated Se-NPs with $[\text{Se}] = 0.03\text{M}$.

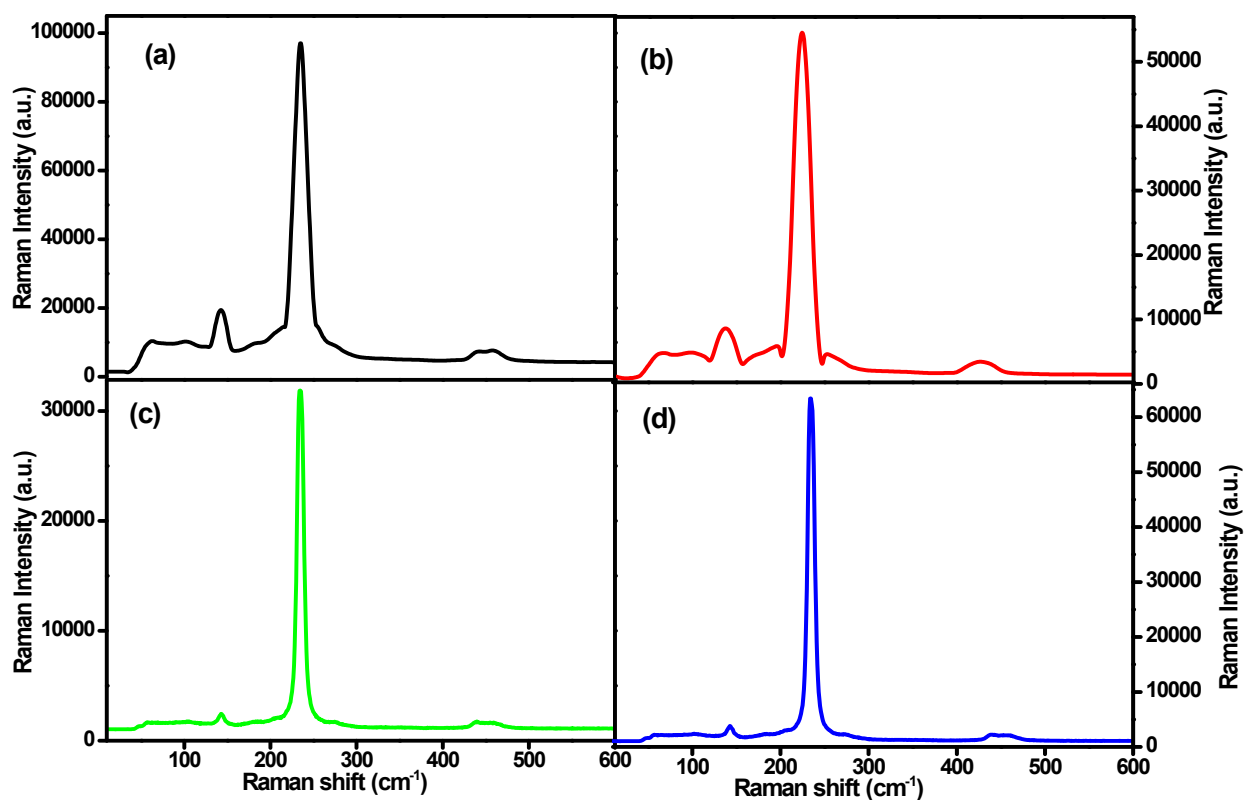


Fig. S7 Raman spectra of 15% (a) EG, (b) DEG, (c) TEG and (d) PEG coated Se-NPs with $[\text{Se}] = 0.03\text{M}$.

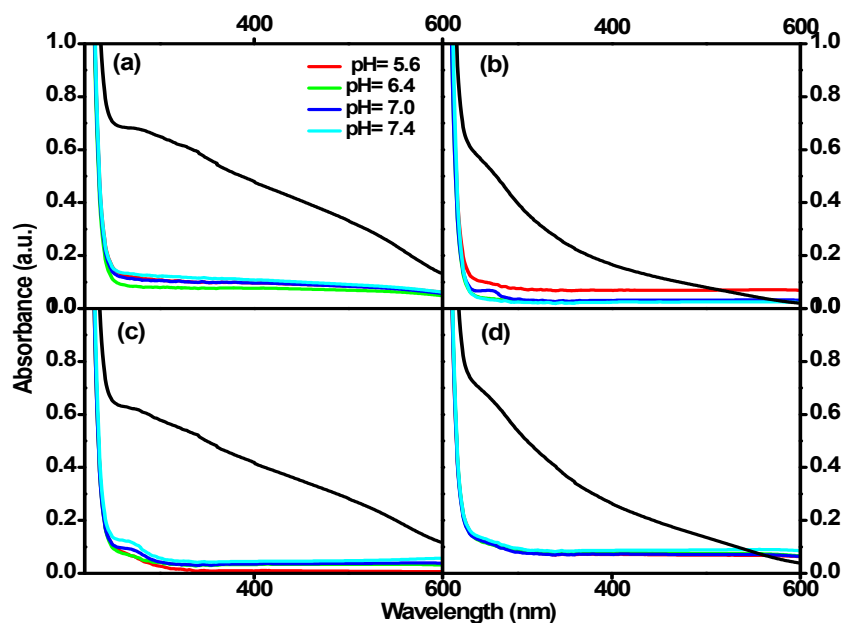


Fig. S8 *In-vitro* stability of 15% (a) EG, (b) DEG, (c) TEG and (d) PEG coated Se-NPs with $[\text{Se}] = 0.03\text{M}$ in presence of different phosphate buffer pH solutions (pH= 5.6, 6.4, 7 and 7.5).

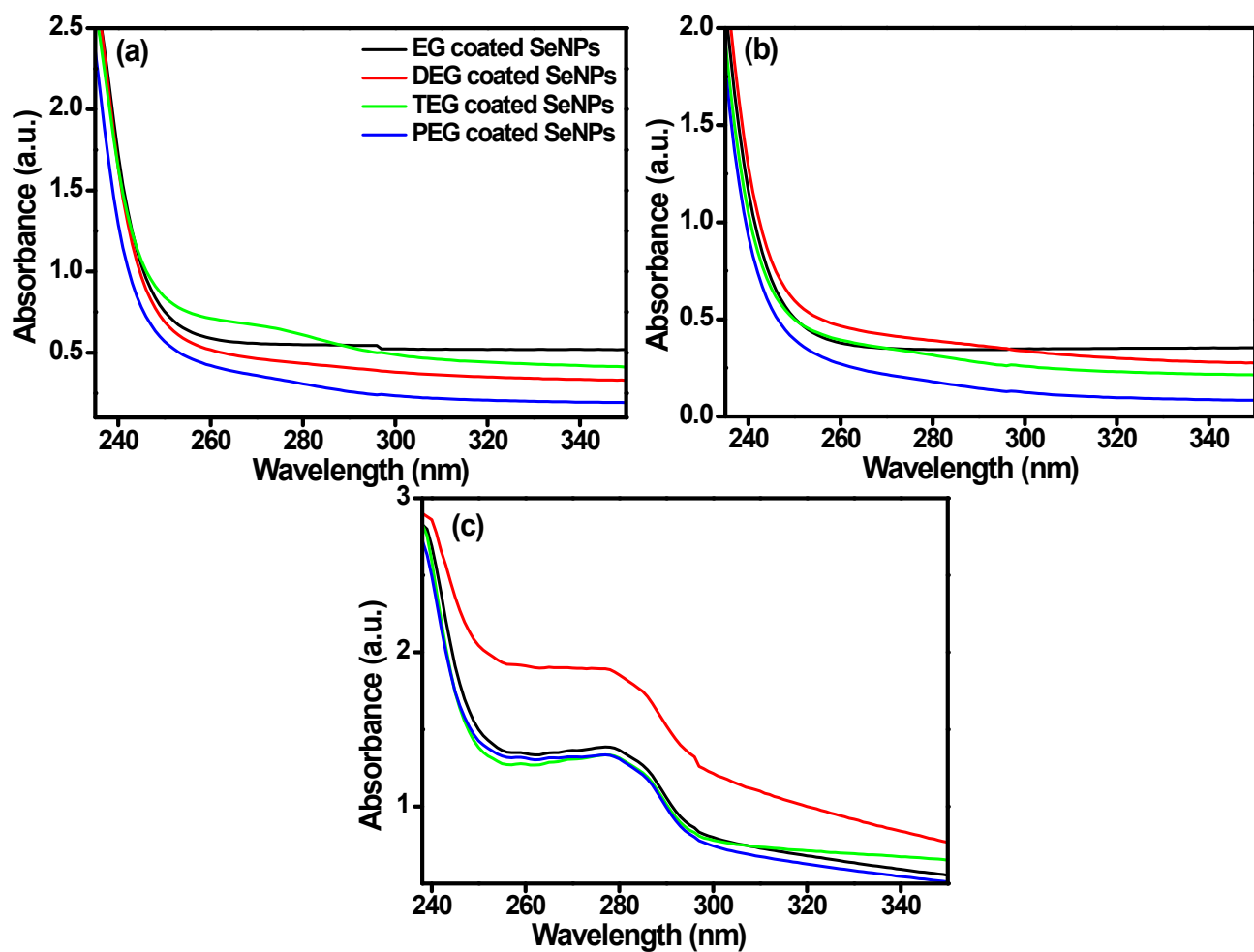


Fig. S9 *In-vitro* stability of 15% EG, DEG, TEG and PEG coated Se-NPs with $[Se] = 0.03M$ in presence of (a) PBS, (b) DMEM and (c) Serum.

Table S2 Representation of average diameter (nm) and polydispersity index of 15% EG, DEG, TEG and PEG coated Se-NPs (0.03M) in presence of (a) PBS, (b) DMEM and (c) Serum.

S.No.	Nanoparticles	PBS		DMEM		Serum	
		Avg. Diameter (nm)	PDI	Avg. Diameter (nm)	PDI	Avg. Diameter (nm)	PDI
1	EG coated Se-NPs	447.0	0.26	362.0	0.27	362.5	0.27
2	DEG coated Se-NPs	319.4	0.30	309.0	0.66	307.8	0.54
3	TEG coated Se-NPs	307.0	0.54	337.0	0.60	333.0	0.61
4	PEG coated Se-NPs	604.0	0.30	425.0	0.40	419.0	0.31

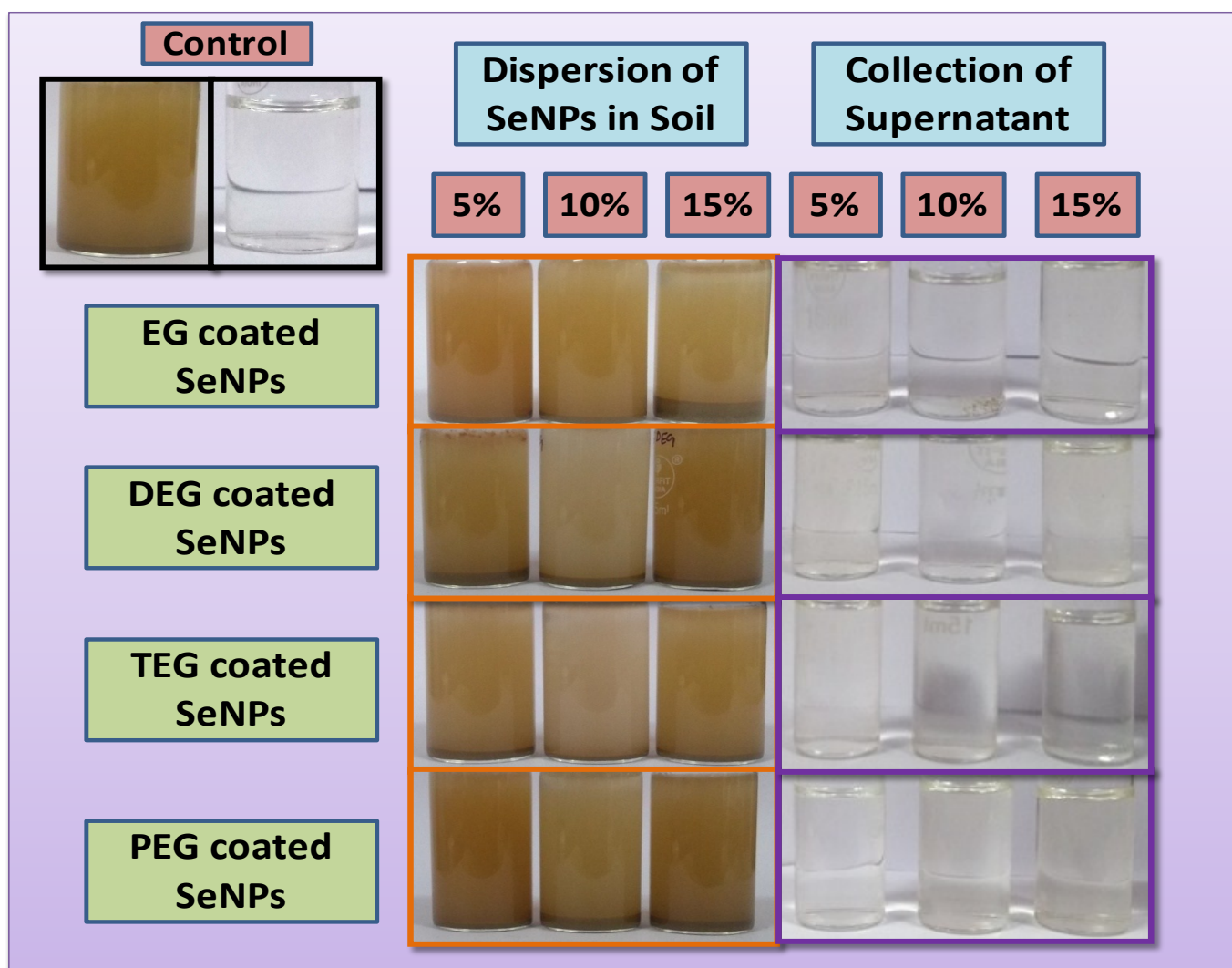


Fig. S10 Sorption study performed over 5, 10 and 15% different glycol coated Se-NPs where concentration of Se was kept fixed at 0.03M.

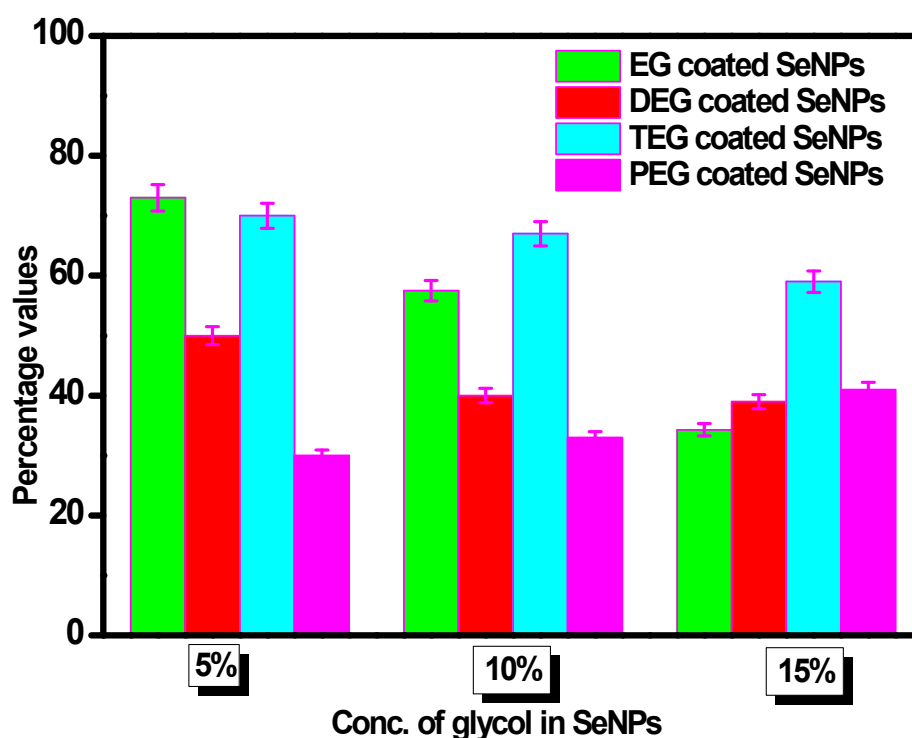


Fig. S11 Transformation of 5, 10 and 15% different glycol coated Se-NPs (0.03M Se) in aqueous solution.

Table S3 Representation of antimicrobial activity and aggregation, dissolution study of bare, surfactant coated and glycol coated Se-NPs.

Nanoparticles	Antimicrobial activity (Zone of inhibition)	Aggregation & dissolution study ¹
Bare Se-NPs	2.8cm	High aggregation tendency at all pH ranging from 2 to 12 in visible light simultaneously size distribution varies non-linearly with increase in ionic strength of solution
CTAB capped Se-NPs	2.1cm	Size of respective nanoparticles were found to be varied at all pH ranges which suggest the unstable nature of nanoparticles
SDS capped Se-NPs	1.6cm	The respective sample exhibits similar sizes at all pH ranges which does not show selectivity of these nanoparticles
Brij-58 capped Se-NPs	0.1cm	The aggregation tendency reduced to minimum in this case and exhibits small size particles.
EG coated Se-NPs	0cm	The minimum size of nanoparticles was obtained at pH=10, which suggest that developed nanoparticles favours slightly basic nature.
DEG coated Se-NPs	0cm	Clear dispersion was obtained at all pH which reflects the prevention of agglomeration tendency and stability of nanoparticles.
TEG coated Se-NPs	0cm	Same kind of behaviour was obtained when compared with

		EG and DEG coated Se-NPs
PEG capped Se-NPs	0cm	Same as TEG

From table S3, it can be concluded that the bare (naked) Se-NPs exhibits highly toxic nature. Chaudhary et al. also investigated the efficiency of bare Se-NPs over various environmental species such as fungus, plants, human DNA and algae, where result of all these studies reflects the toxic behaviour of bare Se-NPs.¹

References

S. Chaudhary, P. Chauhan, R. Kumar and K.K. Bhasin, Toxicological responses of surfactant functionalized Selenium nanoparticles: A quantitative multi-assay approach, *Sci. total Environ.*, 2018, **643**, 1265-1277.