## SUPPORTING INFORMATION

## Table S1

Relative Ca and P amounts in two systems obtained by XRF studies and the crystallite size obtained from Scherrer equation

Element	CMC added system		CTS added system	
	Mass %	Atomic	Mass %	Atomic
	percentage %		percentage %	
15 P	26.29	40.81	46.68	34.40
20 Ca	69.08	63.25	61.40	55.05
Ca/P ratio	1.55		1.60	
Crystallite size (nm)	9.57		11.78	



Fig. S1 a Multi-point BET plot of CMC@HAp



Fig . S1 b. Multi-point BET plot of CTS@HAp



Fig. S2 Effect of initial Pb(II) ion concentration on the sorption capacity (q) of CMC@HAp and CTS@HAp

![](_page_3_Figure_0.jpeg)

Fig. S3 The effect of pH on the sorption capacity of the HAp systems a. CMC@HAp (0.010 g in 200 ppm solution) and b. CTS@HAp (0.010 g in 500 ppm solution) for the adsorption of Lanaset dye

![](_page_4_Figure_0.jpeg)

Fig. S4 Effect of contact time on the adopttion capacity of a. CMC@HAp (0.020 g, 200 ppm of lanaset dye) and b. CTS@HAp (0.020 g and 500 ppm of lanaset dye) for the adsorption of the Lanaset dye

![](_page_5_Figure_0.jpeg)

Fig. S5 Effect of contact time on the adoprtion capacity of Lanaset dye by neat HAp

![](_page_6_Figure_0.jpeg)

Fig. S6 The amount of remaining Dye after adsorption by a. CMC@HAp and b. CTS@HAp in the presence of varying concentration of Acid yellow 220 over a period of 2 hours at room temperature ( i= 500 ppm, ii= 400 ppm, iii= 300 ppm, iv= 200 ppm, v= 100 ppm, vi= 50 ppm)

![](_page_7_Figure_0.jpeg)

![](_page_7_Figure_1.jpeg)

Fig. S7 Adsorption isotherm of Azo dye removal by neat HAp explained by (a) Freundlich model, (b) Langumir model

## Table S2 Free energies of optimized monomer and dimer systems

A 2017C20.00C 2017041.770 210.0721740	
A -391/630.806 -391/941.//8 -310.9/21/49	
B -5260683.913 -5260818.159 -134.2462458	

Table S3

Free energies of optimized three monomer and two trimer systems

Binding Mode	G <sub>System</sub> before binding (kJ mol <sup>-1</sup> )	G <sub>System</sub> after binding (kJ mol <sup>-</sup> <sup>1</sup> )	Free energy change (∆G) (kJ mol <sup>-1</sup> )
Α	-6720418	-6720708.18	-290.180187
В	-10866285.2	-10866349.3	-64.09780563

The complete energy profiles for these binding processes were not modelled. However, it is possible to compare the relative spontaneities of the two binding modes using the calculated Gibbs free energy change ( $\Delta G$ ) values. Results show that in both monomer and trimer systems, binding mode A is energetically more favorable by a significant factor. In fact, as the number of units in the polymer increases, the difference between the two binding modes appears to increase. Therefore, it can be concluded that a Ca<sup>2+</sup> ion prefers to bind to a single chitosan monomer unit under aqueous conditions.

![](_page_9_Figure_0.jpeg)

Fig. S8 Ca<sup>2+</sup> ion binding with single Chitosan monomer unit

![](_page_10_Figure_0.jpeg)

Fig. S9 Ca<sup>2+</sup> ion binding with two Chitosan monomer units

![](_page_10_Figure_2.jpeg)

Fig. S10 Ca<sup>2+</sup> ion binding with three chitosan monomer units

![](_page_11_Figure_0.jpeg)

Fig. S11 Ca<sup>2+</sup> ion binding with 6 chitosan monomer units