High-Performance Hydrogel Based on Modified Chitosan for Removal of Heavy Metal Ions in Borehole: A Case Study from the Bahariya Oasis, Egypt

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Table S1a. Reminder on equations used for modeling uptake kinetics [1-3].

Model	Equation	Parameters	Ref.
PFORE	$$q(t) = q_{eq,1}(1 - e^{-k_1 t})$$	$q_{eq,1}$ (mmol g^{-1}): sorption capacity at equilibrium k_1 (min^{-1}): apparent rate constant of PFORE	[2]
PSORE	$$q(t) = \frac{q_{eq,2}^2 k_2 t}{1 + k_2 q_{eq,2} t}$$	$q_{eq,2}$ (mmol g^{-1}): sorption capacity at equilibrium k_2 (g mmol^{-1} min^{-1}): apparent rate constant of PSORE	[2]
RIDE	$$\frac{q(t)}{q_{eq}} = 1 - \sum_{n=1}^{\infty} \frac{6\alpha(\alpha + 1)\exp\left(\frac{-D_e q_n^2}{r^2}t\right)}{9 + 9\alpha + q_n^2\alpha^2}$$ With q_n being the non-zero roots of $\tan q_n = \frac{3 q_n}{3 + \alpha q_n^2}$ and $\frac{m q}{V C_0} = \frac{1}{1 + \alpha}$	D_e (m^2 min^{-1}) : Effective diffusivity coefficient	[3]

(m (g): mass of sorbent; V (L): volume of solution; C_0 (mmol L^{-1}): initial concentration of the solution).

Table S1b. Reminder on equations used for modeling sorption isotherms [1,4,5].

Model	Equation	Parameters	Ref.
Langmuir	$q_{eq} = \dfrac{q_{m,L}C_{eq}}{1 + b_L C_{eq}}$	$q_{m,L}$ (mmol g^{-1}): Sorption capacity at saturation of monolayer b_L (L mmol^{-1}): Affinity coefficient	[4]
Freundlich	$q_{eq} = k_F C_{eq}^{1/n_F}$	k_F and n_F: empirical parameters of Freundlich equation	[5]
Sips	$q_{eq} = \dfrac{q_{m,S}b_S C_{eq}^{1/n_S}}{1 + b_S C_{eq}^{1/n_S}}$	$q_{m,L}$, b_S and n_S: empirical parameters of Sips equation (based on Langmuir and Freundlich equations)	[1]

Akaike Information Criterion, AIC:

$$AIC = N \ln\left(\frac{\sum_{i=0}^{N}(y_{i,exp.} - y_{i,model})^2}{N}\right) + 2N_p + \frac{2N_p(N_p + 1)}{N - N_p - 1}$$

Where N is the number of experimental points, N_p the number of model parameters, $y_{i,exp.}$ and $y_{i,model}$ the experimental and calculated values of the tested variable.

Table S2. Comparison study of intial and final concntration of metal ions on water sample before and after sorption

	Limited concentration			Initial			Light condition pH3			Light condition pH5			UV emission pH3			UV emission pH5		
	D.W	I.W	L.D.W	D.W	I.W	L.D.W	D.W	I.W	L.D.W	D.W	I.W	L.D.W	D.W	I.W	L.D.W	D.W	I.W	L.D.W
Fe	0.3	5		590	35.4		25.33	1.52		4.3	0.258		10.33	0.62		1.6	0.096	
Zn	5	2	24	2.26	5.65	0.471	0.866	2.165	0.181	0.312	0.78	0.065	0.774	1.935	0.161	0.212	0.53	0.0442
Cd	0.009			33.33			13.33			4.444			10.89			1.111		
Pb	0.005	5	0.1	156	0.156	7.8	42	0.042	2.1	8	0.008	0.4	22	0.022	1.1	2	0.002	0.1

D.W. drinking water

I.W. Irrigation water
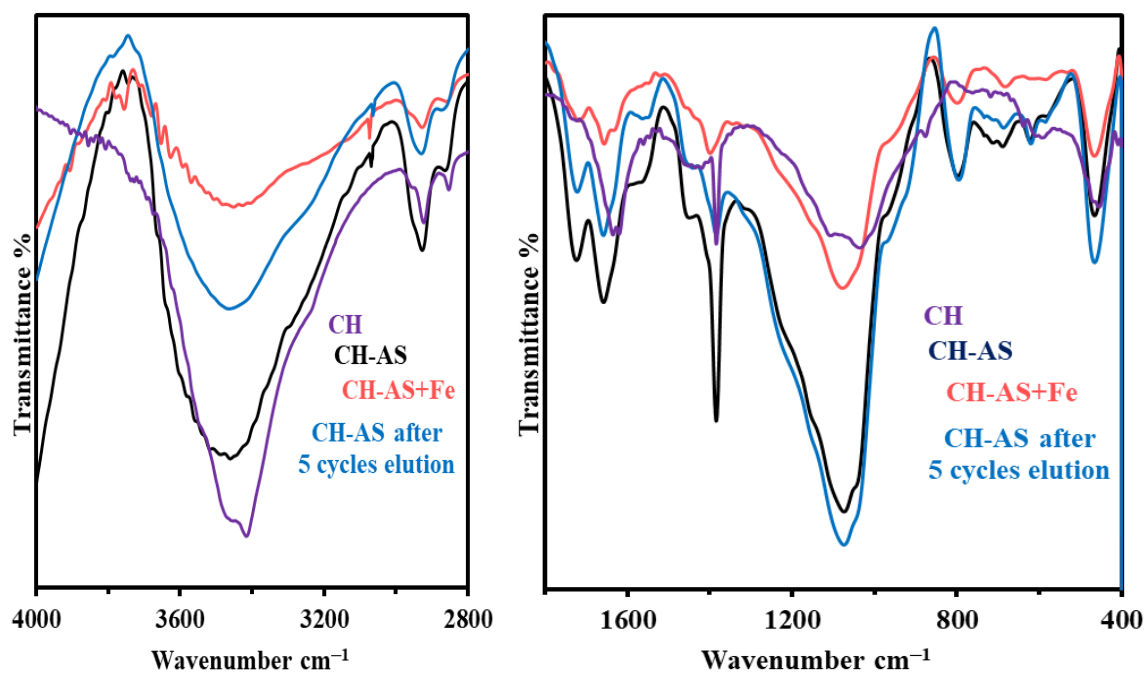
L.D.W. Livestock drinking water

Figure S1. FTIR characterization of CH, CH-AS, after loading by Fe(III) and after 5th cycles of sorption desorption (scale 400-1800 and 2800-4000 cm^{-1}).
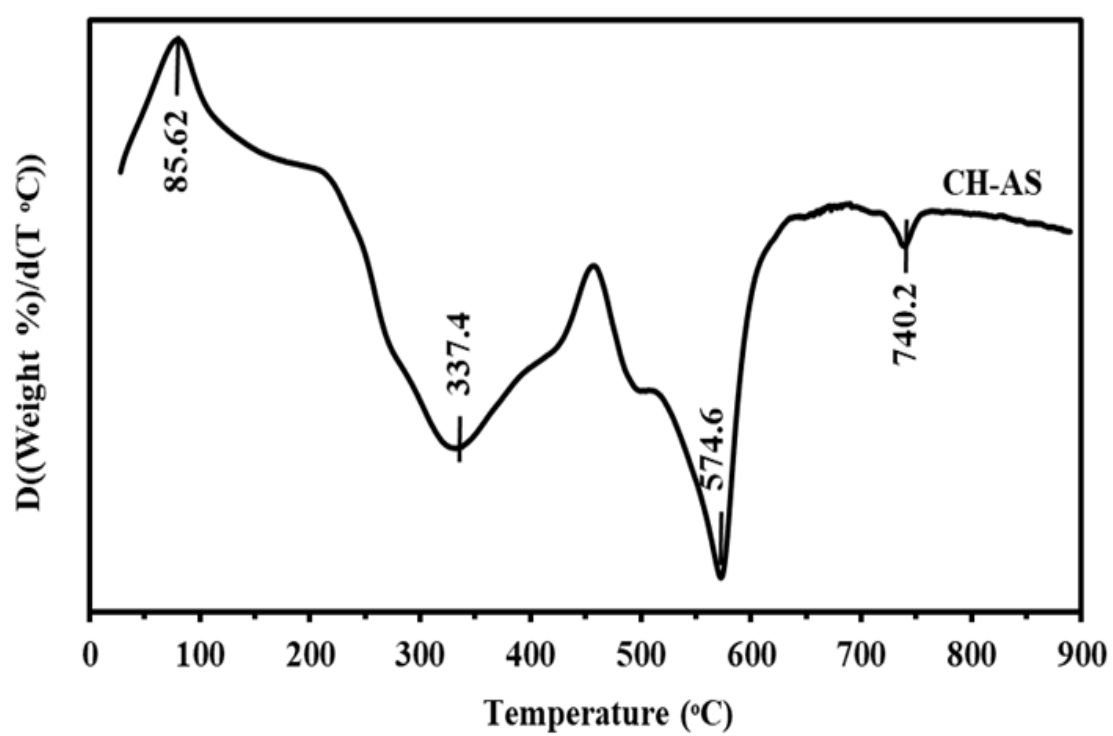
Figure S2. DrTGA of the functionalized chitosan composite.
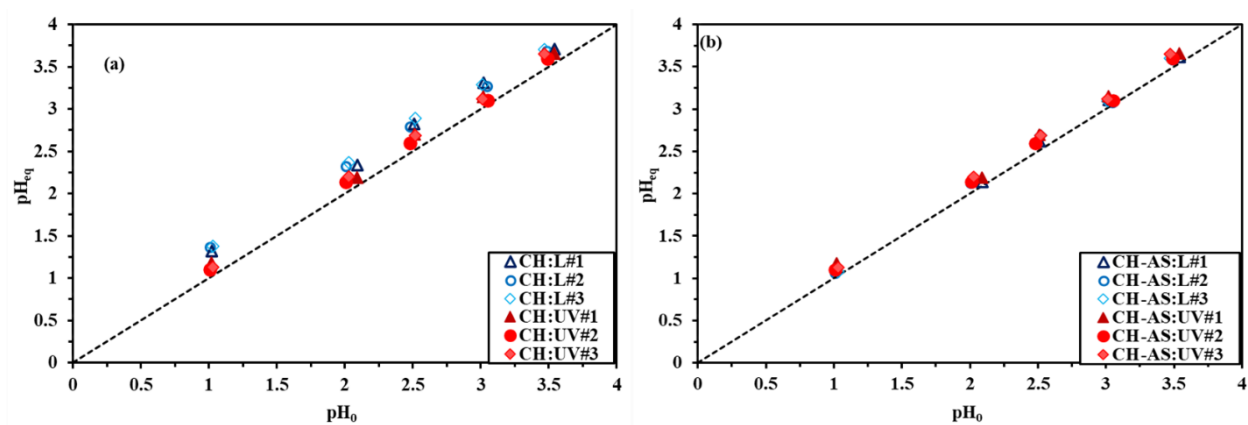
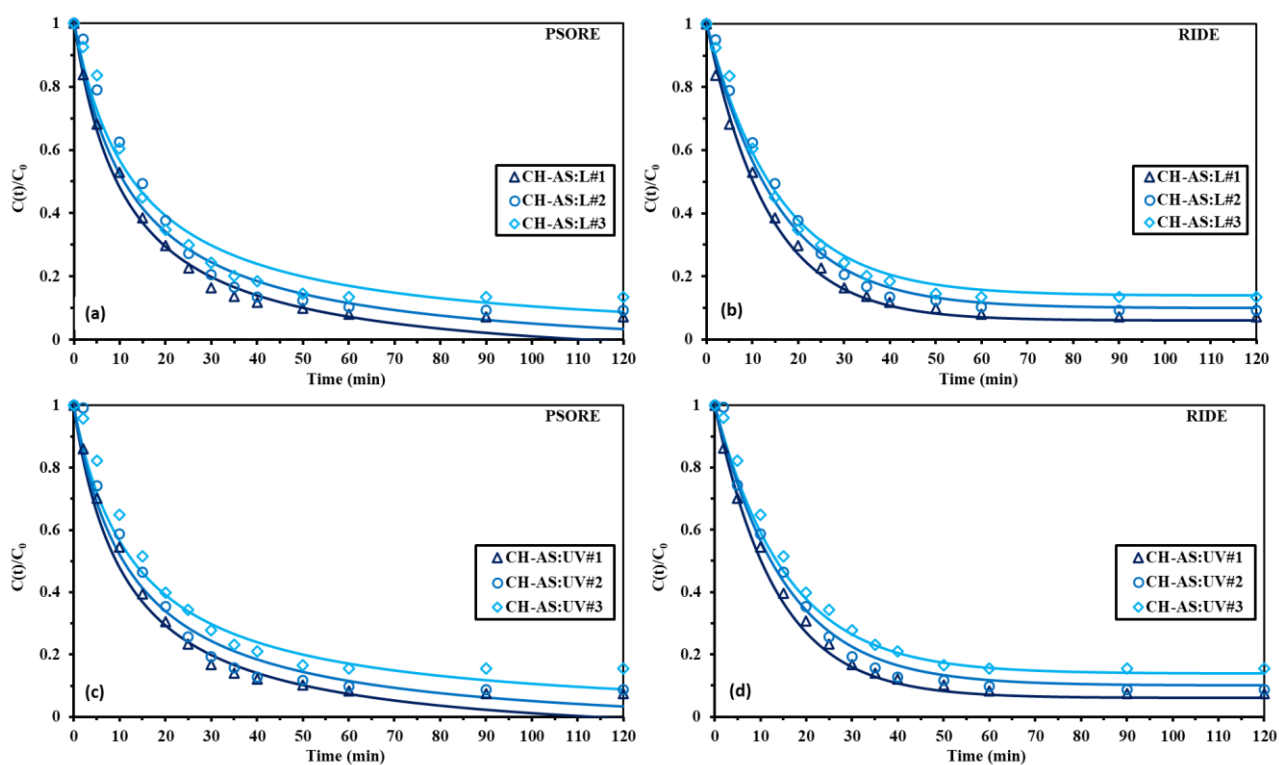**Figure S3.** pH variation of the CH (a) and CH-AS (b) in the presence of Light and UV.

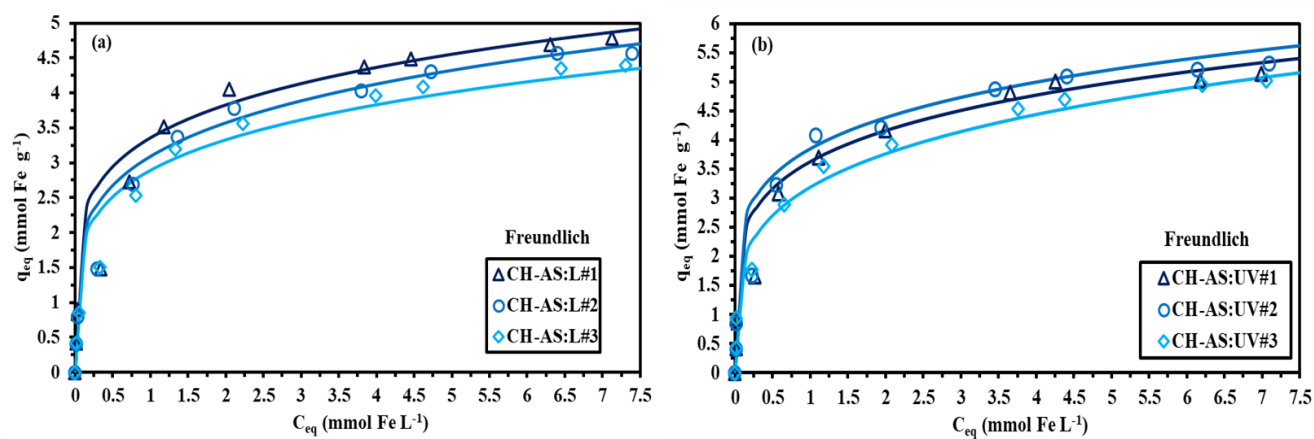**Figure S4.** Uptake kinetics; PSORE (a and c) and RIDE (b and d) at light and UV emission.

Figure S5. Sorption isotherms for unfitting the experimental data of Fe(III) sorption by Freundlich at light (a) and UV effect (b).
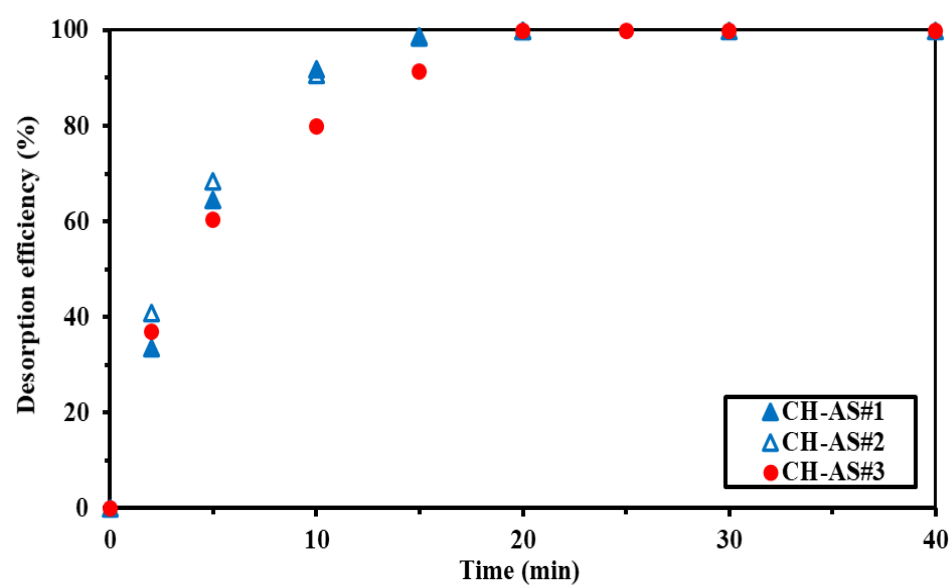
Figure S6. Desorption kinetics of the functionalized sorbent for three repeated experiments.
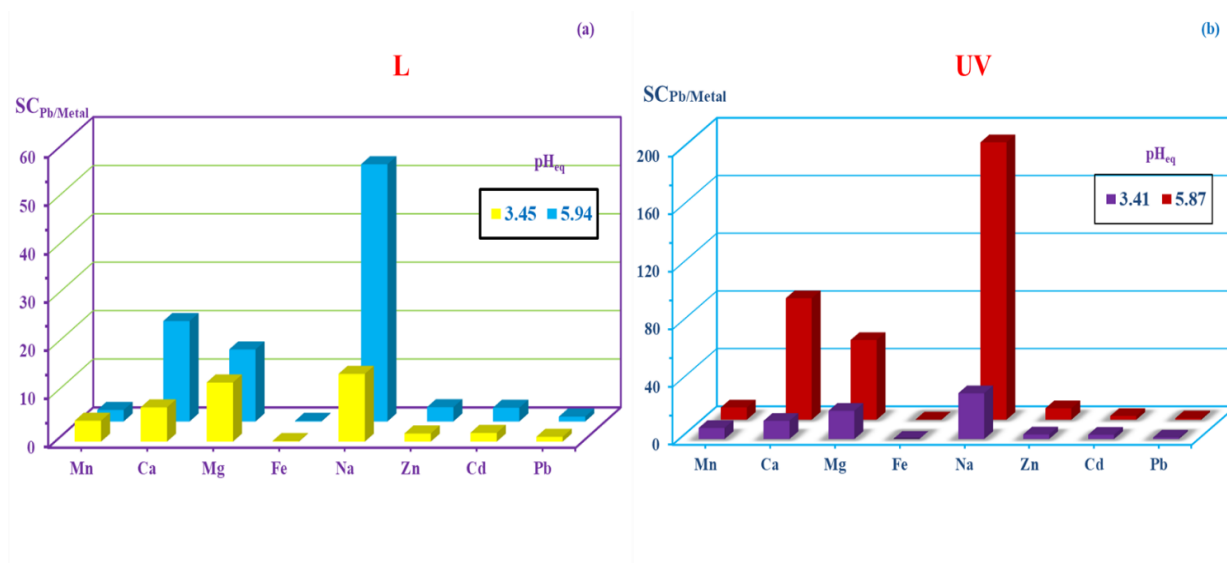
Figure S7. Selectivity coefficient for functionalized sorbent for Pb(II) vs. associated metal ions at light (a) and UV (b).

References

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