Supplementary Information

Multifunctional Lignin Bio-Composite for Broad-Spectrum Water Purification

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Formulae and Equations

Equation (1): The maximum uptake of contaminant (q_e) by ZL/ZLC was calculated using the equation given below:

$$Uptake\ (qe) = \frac{(Co - Ce)V}{m}$$

where q_e is the number of contaminant species adsorbed per gram of the adsorbent (mg/g) at equilibrium, C_e is the equilibrium concentration of the contaminant in the bulk solution (mg/L), C_o is the initial concentration (mg/L), V is the volume of solution (L) and m is the mass of the adsorbent (g).

Equation (2): The linearized form of the Langmuir equation used in this work is defined as,

$$\frac{Ce}{qe} = \frac{Ce}{qmax} + \frac{1}{bqmax}$$

where q_e is the amount of adsorption at the surface of the adsorbent (mg/g), C_e is the equilibrium concentration of the solution (mg/L), q_{max} is the maximum surface density at

monolayer coverage and b is the Langmuir adsorption constant (L/mg) related to the free energy of adsorption and $1/q_{max}$ and $1/bq_{max}$ are the Langmuir constants.

Equation (3): The removal % of PFAS was calculated using the equation mentioned below:

$$Removal\ \% = \frac{Co - Ce}{Co} \times 100$$

where C_o and C_e are the initial and equilibrium concentrations of the PFAS, respectively.

Equation (4): A linear form of the Freundlich expression used in this work is defined as,

$$Log\ qe = \frac{1}{n} Log\ Ce + Log\ Kf$$

where q_e is the amount of adsorption at the surface of the adsorbent (mg/g), C_e is the equilibrium concentration of the solution (mg/L), Kf is the Freundlich constant (mg/mg)(L/mg)1/n.

Equation (5): The linear form of pseudo first order kinetic equation is expressed as

$$\log (qe - qt) = log\ qe - \frac{k1}{2.303} t$$

where 'qe' and 'qt' are the amount of contaminant adsorbed at equilibrium and at time 't' respectively, and 'k1' is the equilibrium rate constant of pseudo-first-order adsorption. The slope and intercept of the plot, 'log(qe − qt)' vs. 't' were used to obtain the pseudo-first-order rate constant k1 and equilibrium adsorption density 'qe'.

Equation (6): The linear form of pseudo-second-order kinetics is expressed as:

$$\frac{t}{qt} = \frac{1}{k_2 qe^2} + \frac{t}{qe}$$

where 'qe' and 'qt' are the amount of contaminant adsorbed at equilibrium and at time 't' (mg/mg), respectively, and k_2 is the equilibrium rate constant of pseudo-second-order adsorption. The second-order rate constant 'k_2' and 'qe' values were determined from the slopes and intercepts of the plots.

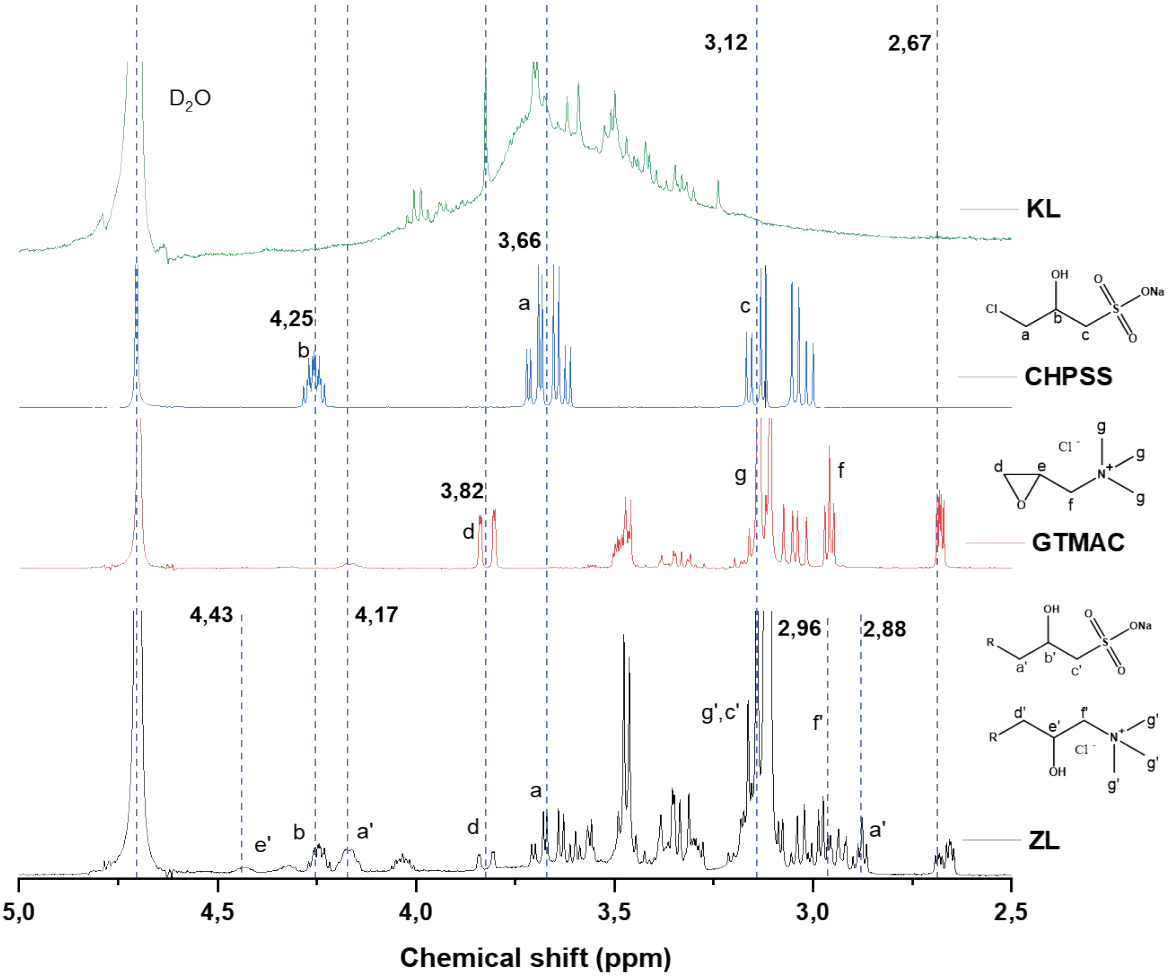


Fig. S1. [1]H NMR spectra of lignin, modifying reagents GTMAC and CHPSS, and modified lignin (ZL).

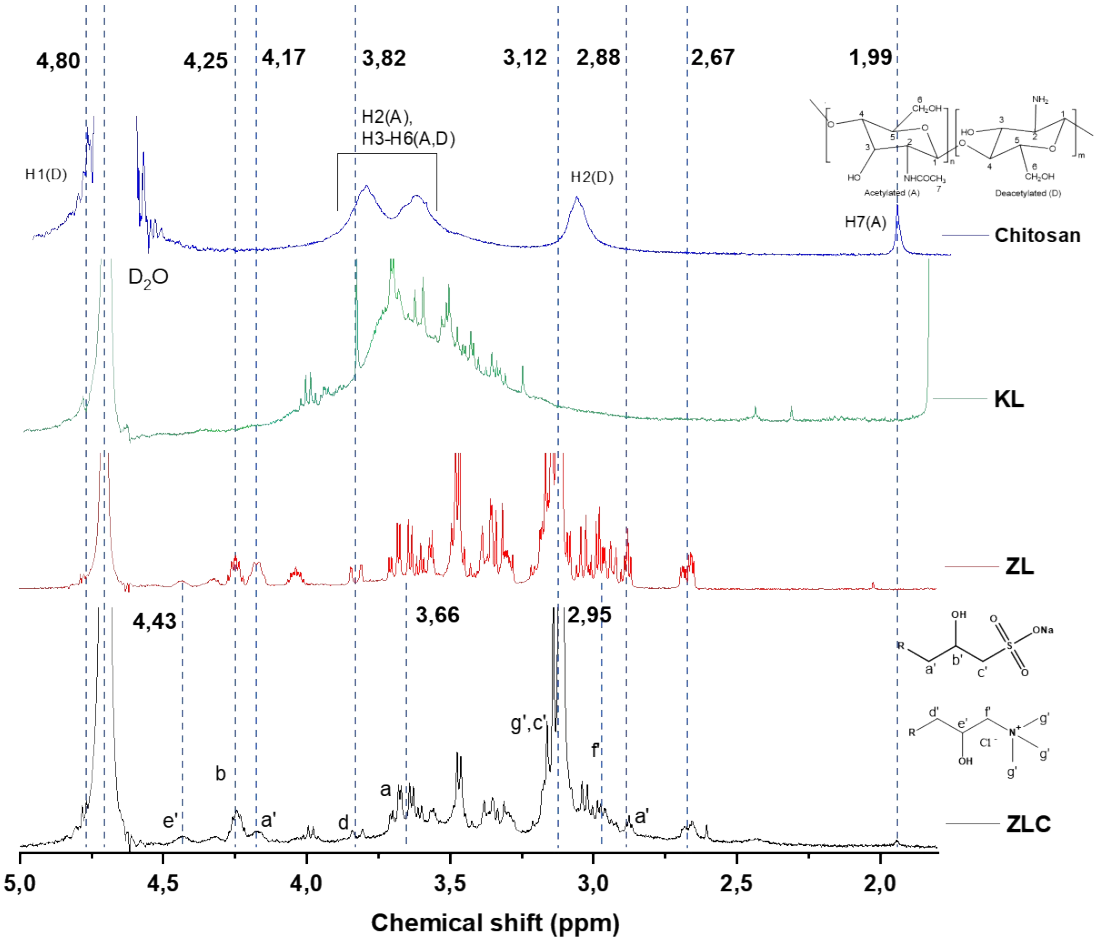


Fig. S2. [1]H NMR spectra showing chitosan and lignin reagents, followed by modified lignin (ZL) and ZLC composite.

Fig. S3. Photographic images of ZL, ZLC granules, and powdered ZLC in dried form.

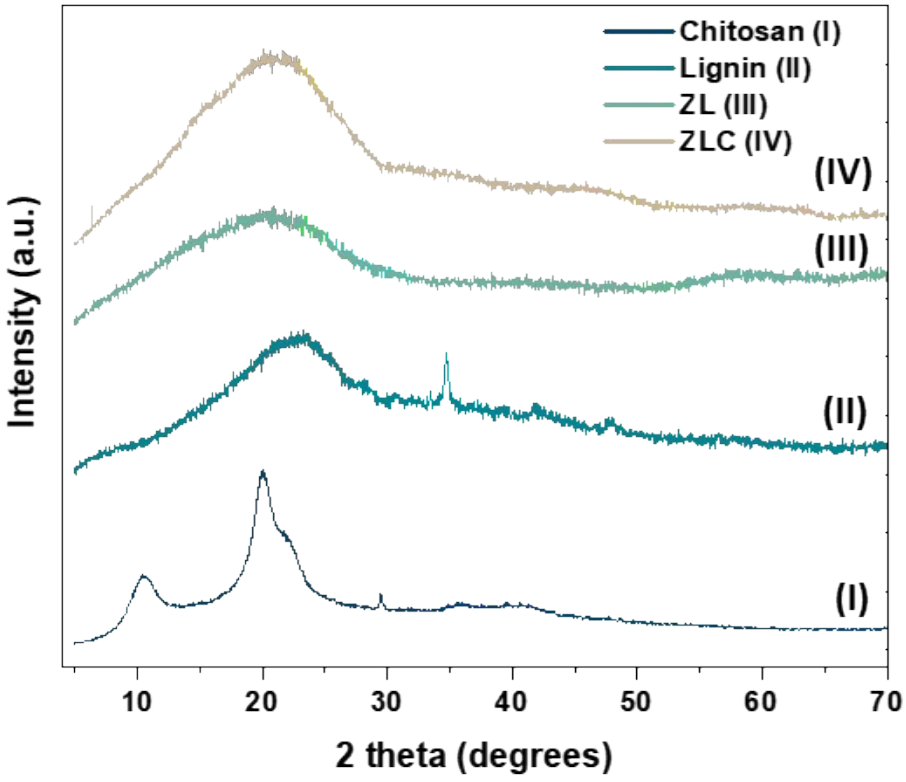


Fig. S4. pXRD patterns of chitosan, lignin, as-synthesized ZL, and ZLC materials.

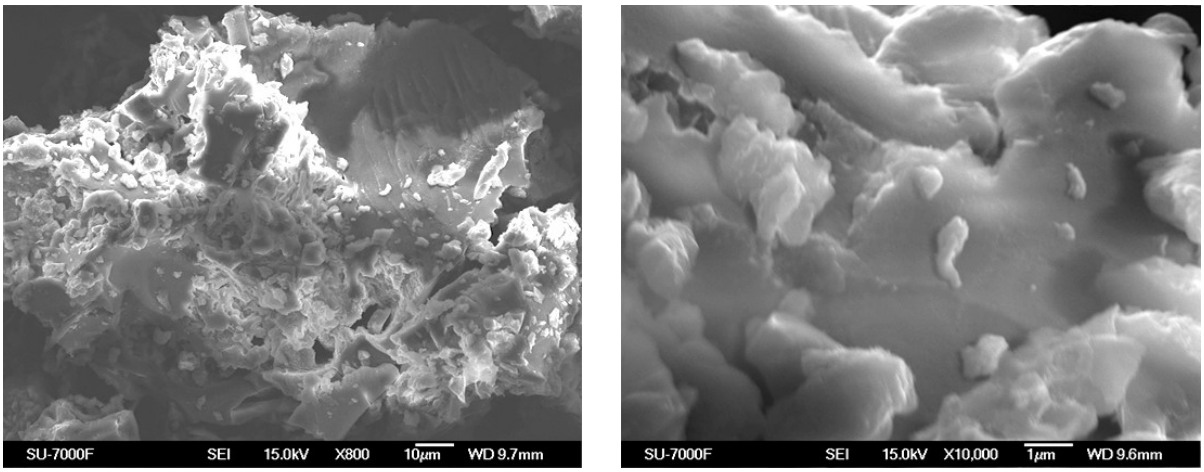


Fig. S5. SEM images of ZLC cross-section at higher magnification.

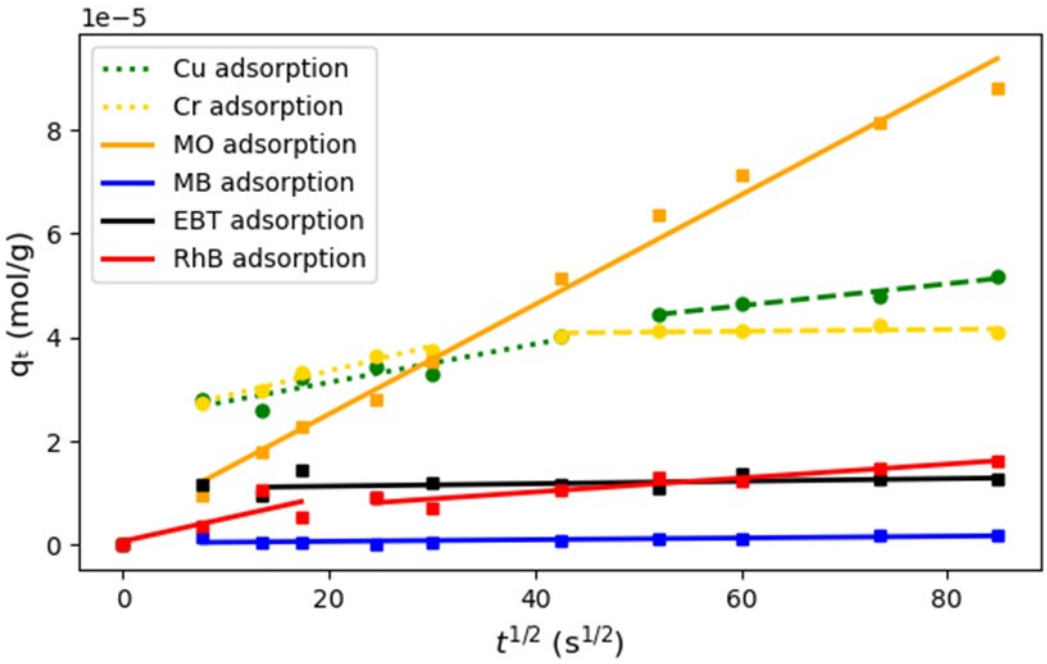


Fig. S6. Kinetics of contaminant adsorption on ZLC fitted with the intraparticle diffusion model.

For metal ions, adsorption proceeded through three stages: a rapid surface interaction within the first minute, followed by diffusion into the pores (completed within the first hour for Cr(VI)), and finally equilibrium. For Cu(II), diffusion was slower, but the decrease in adsorption rate after 2 h indicated that equilibrium was approaching. Overall, most adsorption occurred rapidly, confirming that surface interactions dominate the process. Dyes were adsorbed more slowly than metal ions. The intraparticle diffusion model showed a single linear region, and equilibrium was not reached within 2 h. This slower behavior may result from their larger molecular size and possible aggregation, which hinder diffusion into micropores, or from alternative interaction modes possible for dyes (e.g., π–π or van der Waals forces).

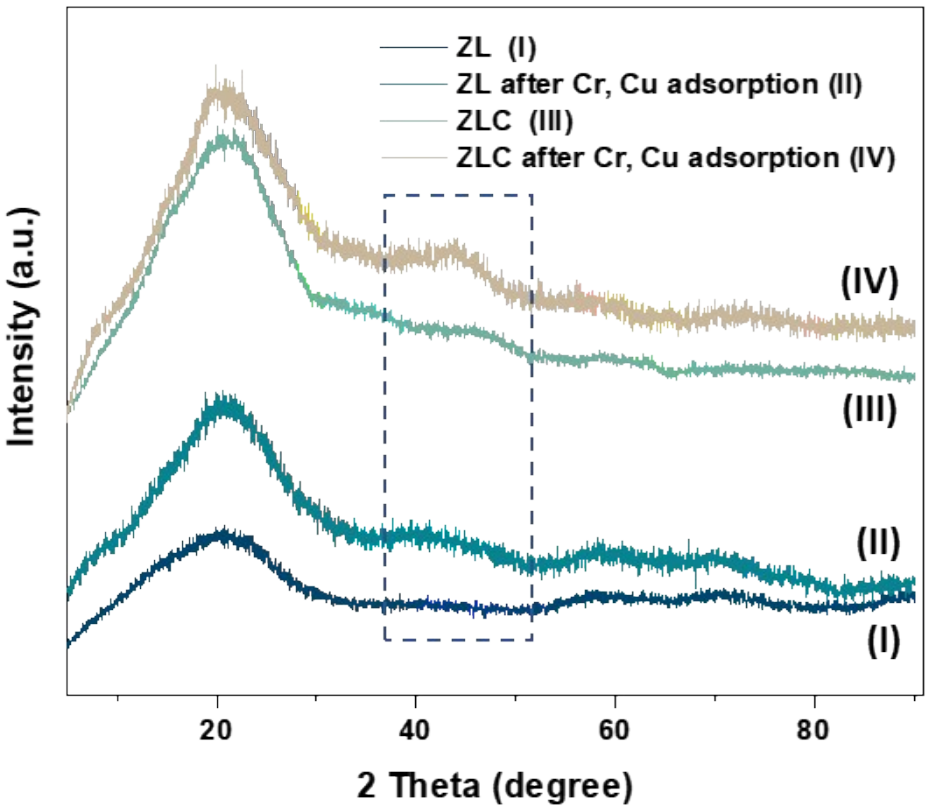


Fig. S7. pXRD patterns of ZL and ZLC before and after adsorption of Cr and Cu ions.

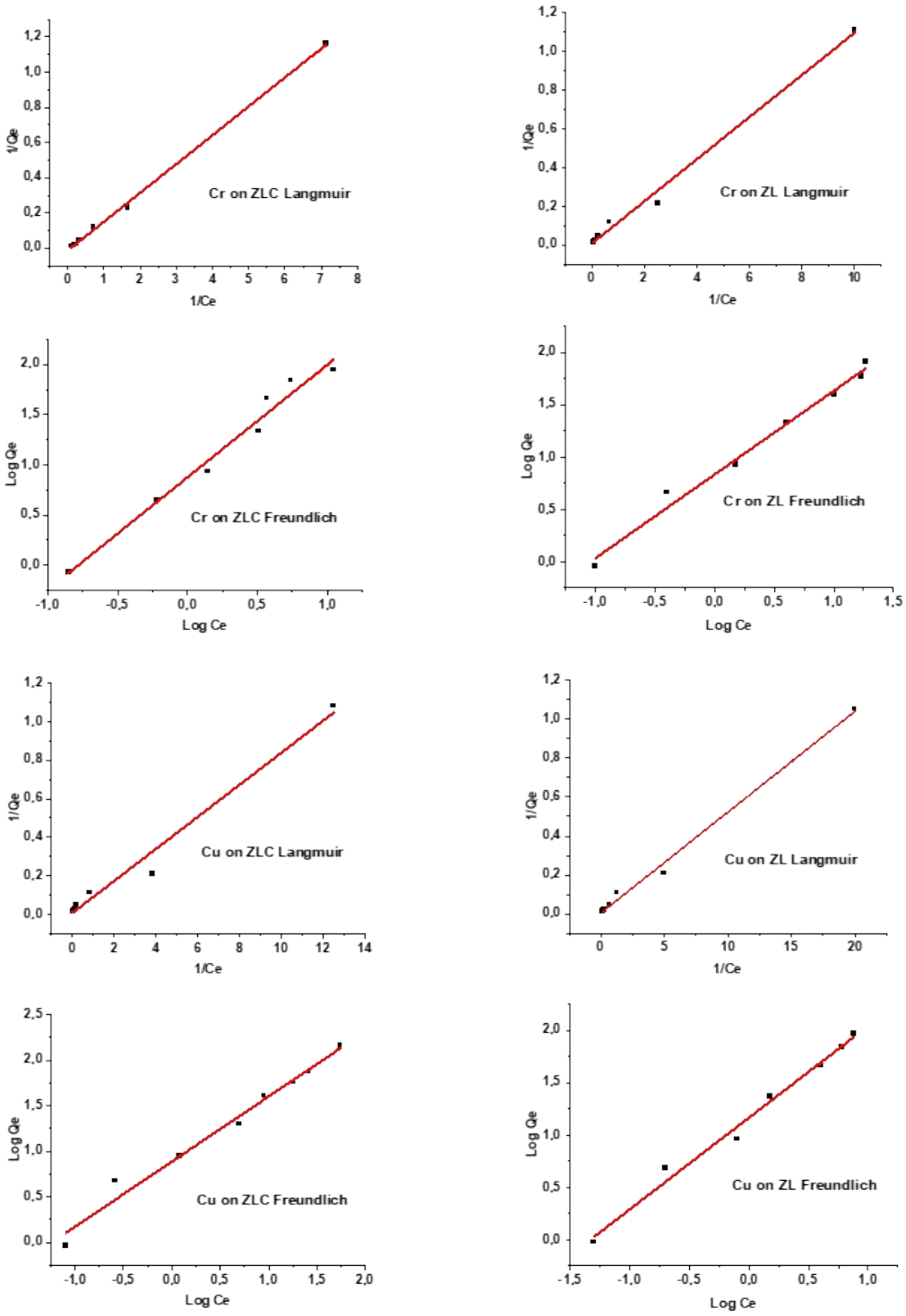
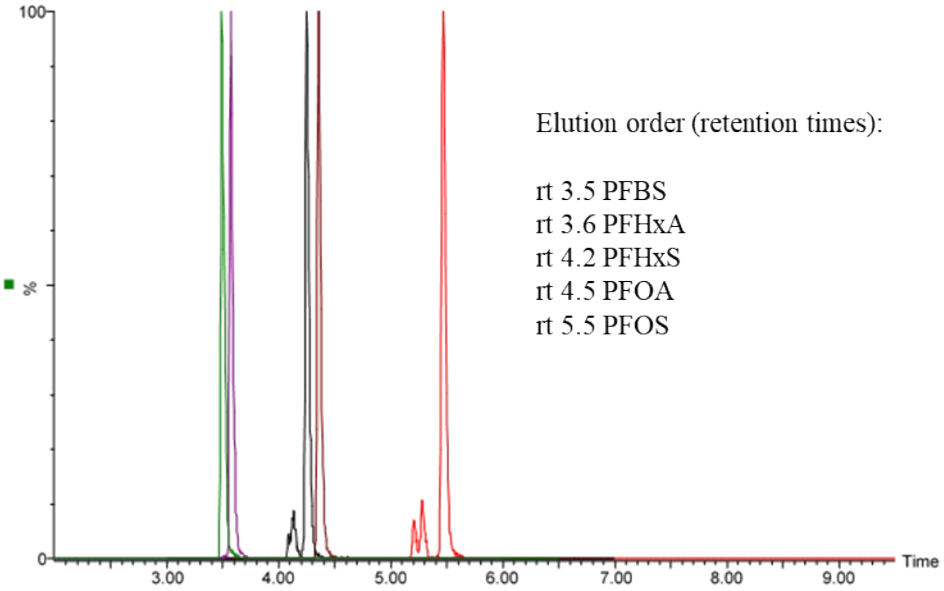


Fig. S8. Isotherm fits for linearized Langmuir and Freundlich models for Cr and Cu adsorption on ZL and ZLC.

Spiked PFAS in H2O

(a)

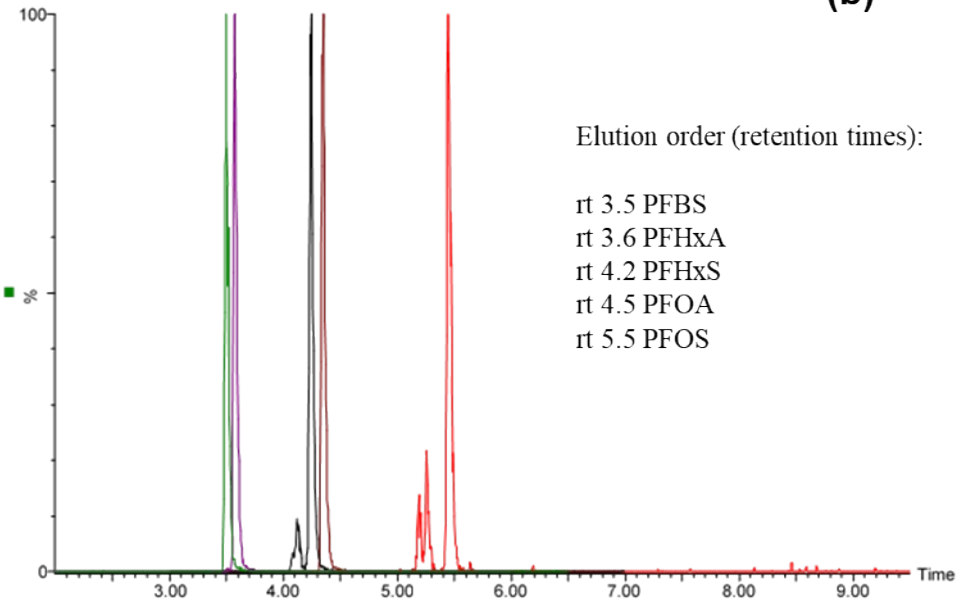


Elution order (retention times):

rt 3.5 PFBS
rt 3.6 PFHxA
rt 4.2 PFHxS
rt 4.5 PFOA
rt 5.5 PFOS

500 mg/l ZLC

(b)



Elution order (retention times):

rt 3.5 PFBS
rt 3.6 PFHxA
rt 4.2 PFHxS
rt 4.5 PFOA
rt 5.5 PFOS

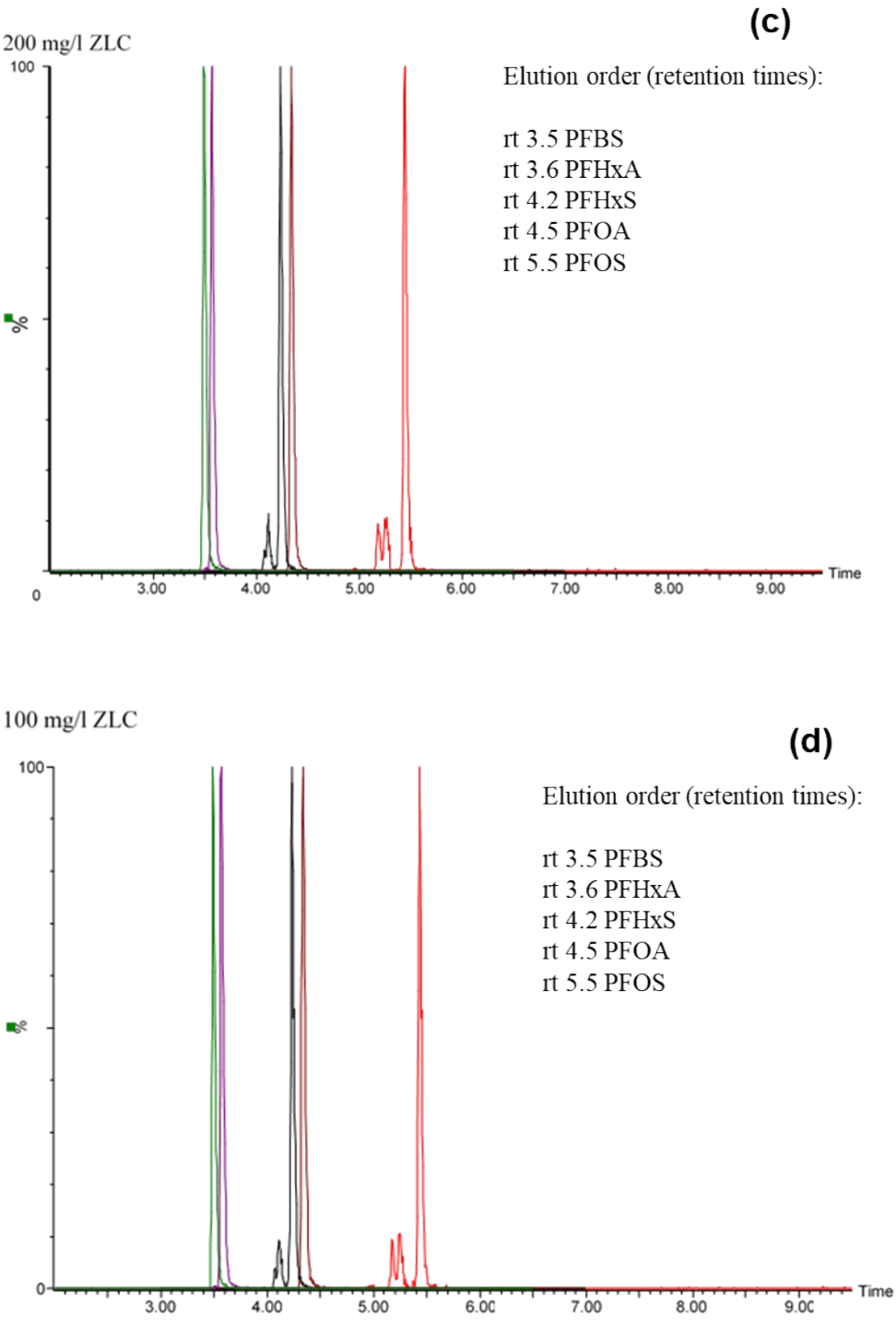


Fig. S9. LC-MS/MS graphs showing elution time of various PFAS molecules in case of (a) PFAS stock solution, (b) PFAS treated 500 mg/L ZLC, (c) 200 mg/L ZLC, and (d) 100 mg/L ZLC.

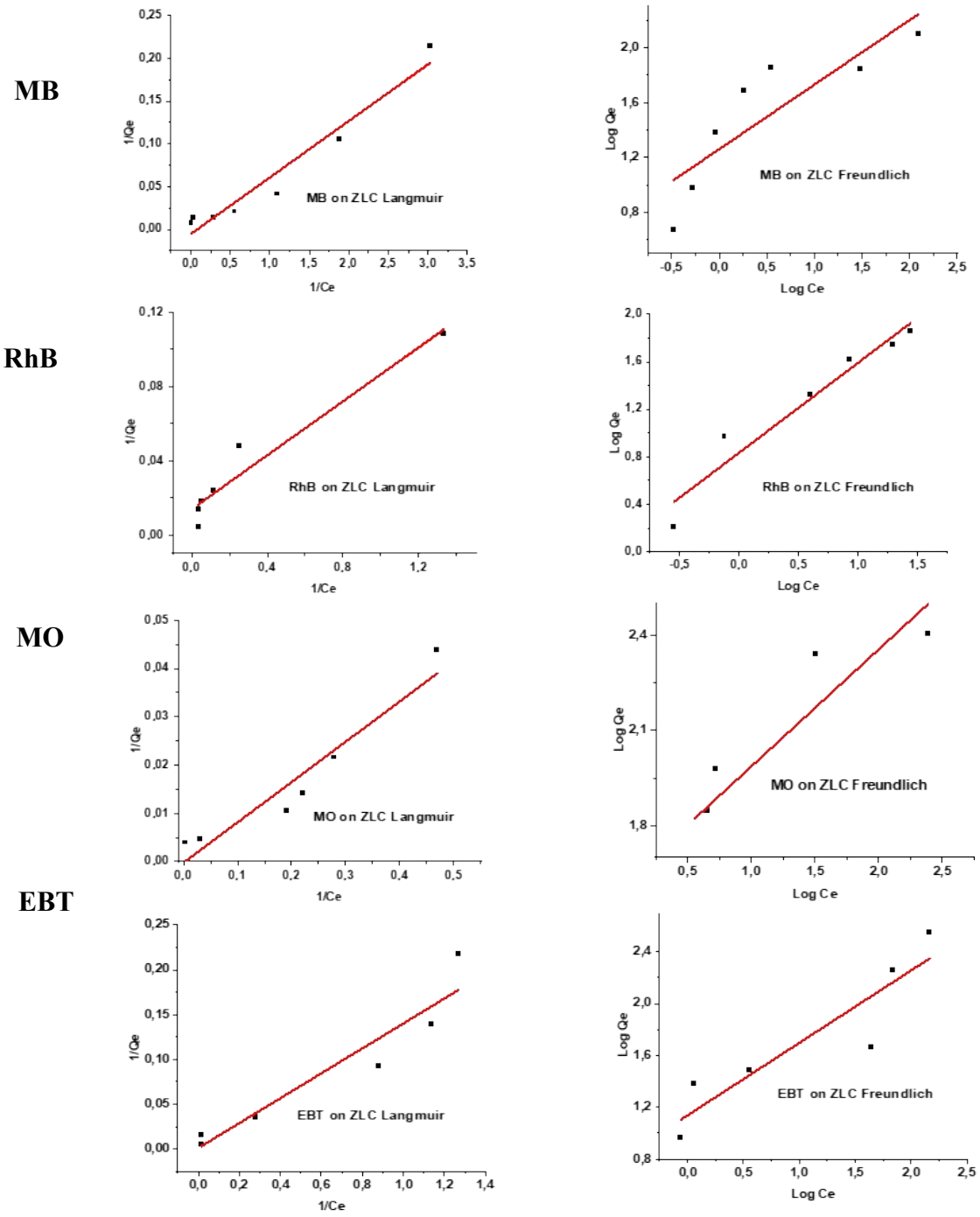


Fig. S10. Isotherm fits for linearized Langmuir (left) and Freundlich (right) models for the adsorption of dyes on ZL and ZLC.

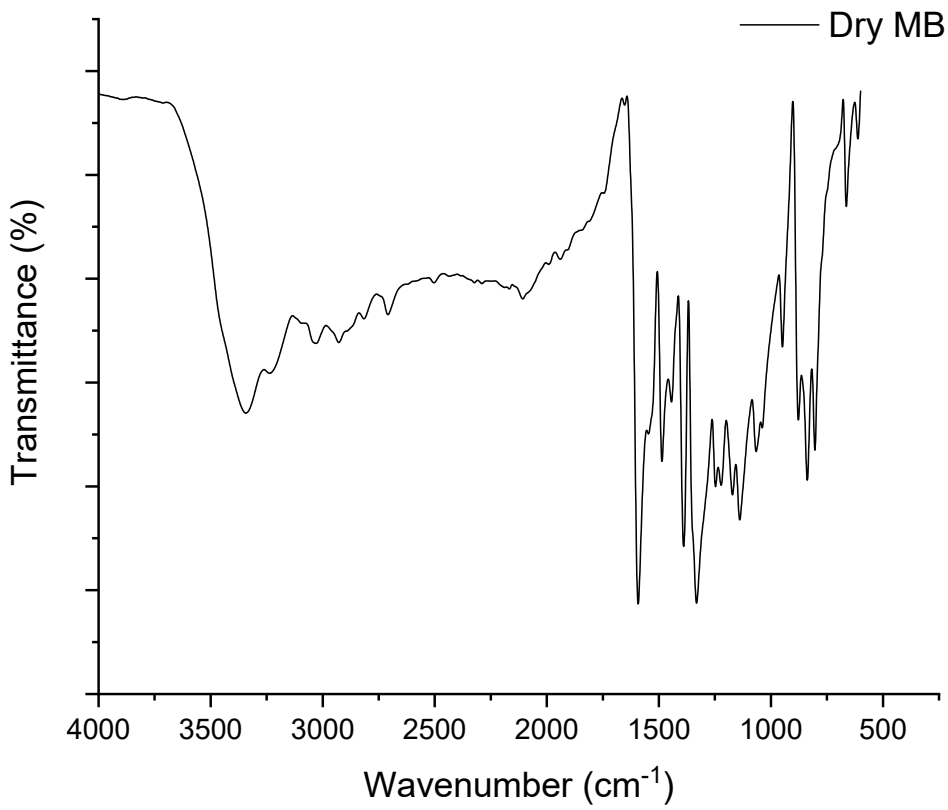


Fig. S11. FT-IR spectrum of dry MB dye**.**

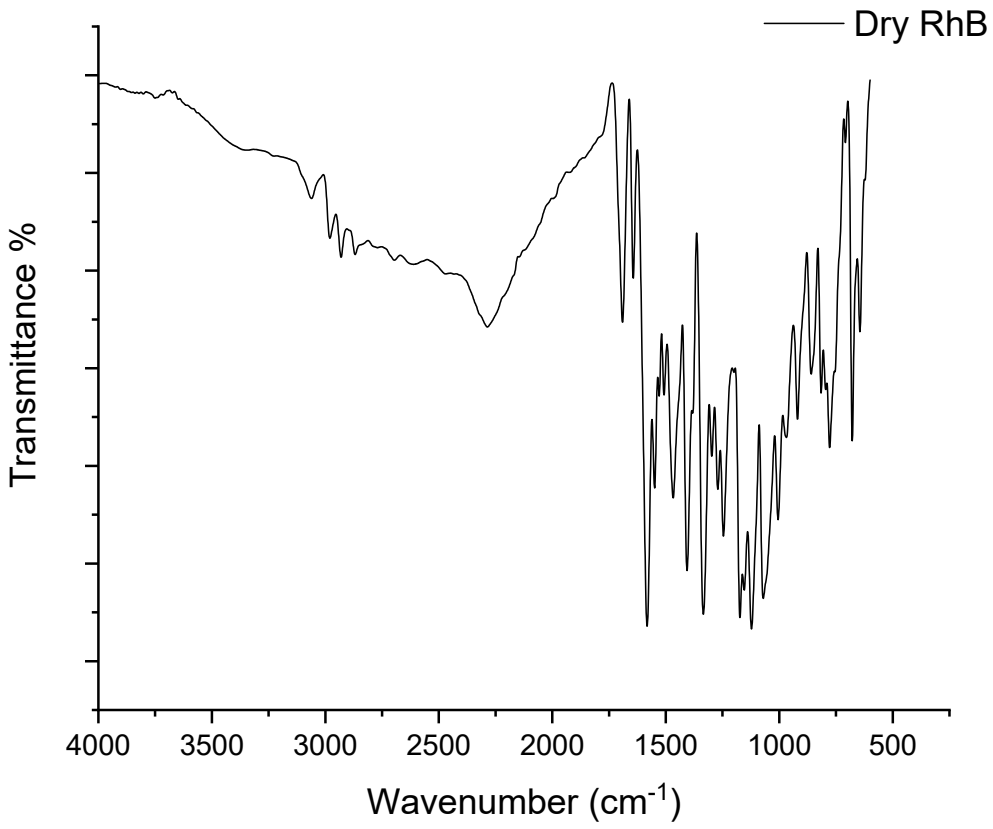


Fig. S12. FT-IR spectrum of dry RhB dye**.**

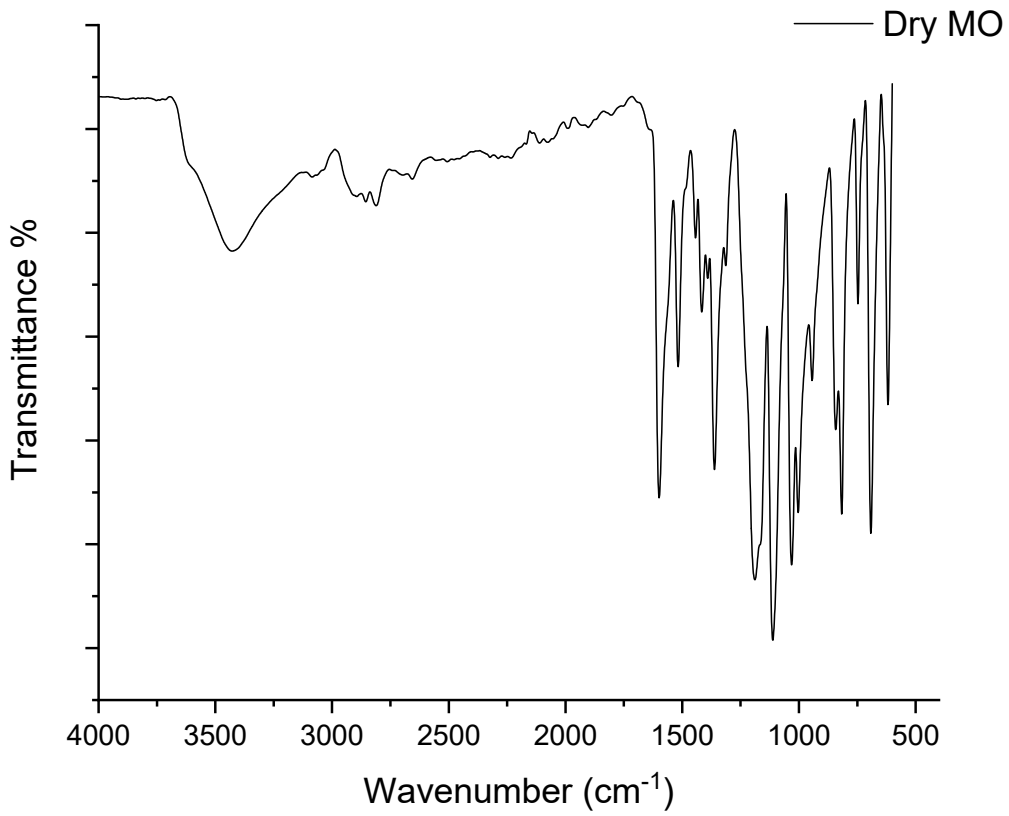


Fig. S13. FT-IR spectrum of dry MO dye**.**

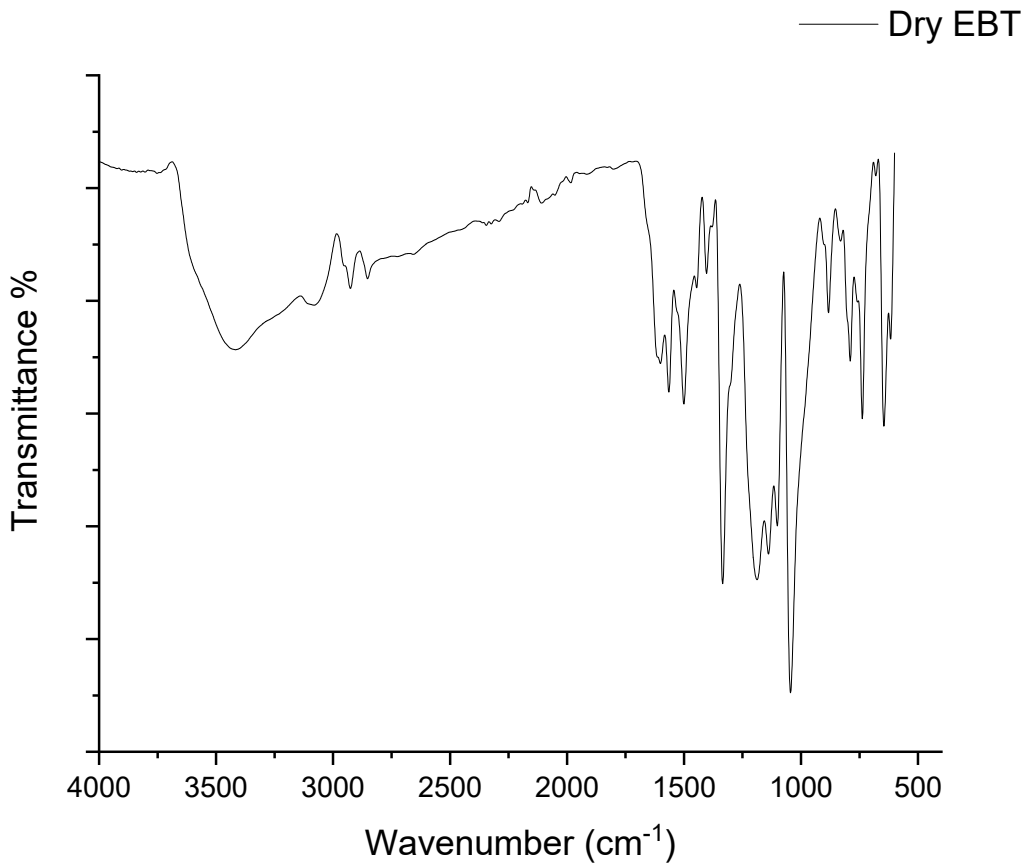


Fig. S14. FT-IR spectrum of dry EBT dye**.**

Table S1. Kinetic parameters for linearized pseudo-first and second-order models for the adsorption of contaminants on ZLC.

Units:

K (pseudo first order model) = sec^{-1}

K (pseudo first order model) = L mol^{-1} sec^{-1}

Qe = mol L^{-1}

Species	**Model**	**K**	**Qe**	**R^2**
Methylene Blue	pseudo 1st order	2.00E-04	1.20E-06	0.93
	pseudo 2nd order	5.99	9.13E-5	0.96
Rhodamine B	pseudo 1st order	3.00E-05	1.49	0.78
	pseudo 2nd order	20.15	7.04E-05	0.98
Methyl Orange	pseudo 1st order	4.00E-09	5.37E-05	0.84
	pseudo 2nd order	11.35	5.42E-05	0.98
Erichrome Black T	pseudo 1st order	4.00E-5	7.40E-02	0.05
	pseudo 2nd order	388.85	2.50E-08	0.98
Cu	pseudo 1st order	2.00E-4	6.94E-05	0.97
	pseudo 2nd order	49.32	6.37E-05	0.99
Cr	pseudo 1st order	8.00E-4	4.24E-05	0.92
	pseudo 2nd order	572.50	4.29E-05	0.99

Table S2. Physicochemical parameters of field waters from a mining area.

Parameter	Sample 1 (µg/L)	Sample 2 (µg/L)
pH	8.3	8,6
Dissolved Organic Carbon DOC	1500	13000
Total Suspended Solids TSS	2200	2440
NO_3-N	2000	3400
NH_4-N	1650	1000
SO_4	1039000	1200000
Cu(II)	11.3	2.4
Cr(VI)	0.18	0.34
Ca(II)	374000	474000
Al(III)	338	12
Na(I)	26000	48800
K(I)	14000	85000