

## Supplementary information

### Exploitation of expired cellulose biopolymers as hydrochars for capturing emerging contaminants from water

Hebatullah H. Farghal<sup>1\*</sup>, Marianne Nebsen<sup>2</sup>, Mayyada M.H. El-Sayed<sup>1\*</sup>

<sup>1</sup>Department of Chemistry, School of Sciences and Engineering, The American University in Cairo, AUC Avenue, P.O. Box 74, New Cairo, 11835, Cairo, Egypt

<sup>2</sup>Analytical Chemistry Department, Faculty of Pharmacy, Cairo University, Kasr-El Aini Street, 11562 Cairo, Egypt

\*Corresponding author: [mayyada@aucegypt.edu](mailto:mayyada@aucegypt.edu)

\*Co-corresponding author: [hebatullahfarghal@aucegypt.edu](mailto:hebatullahfarghal@aucegypt.edu)

#### Physico-chemical properties

$$\rho = m/V \quad [S1]$$

$$\eta_{sp} = \frac{t - t_0}{t_0} \quad [S2]$$

where  $\rho$  is the density of cellulose powder ( $\text{g}/\text{cm}^3$ ),  $m$  is the mass of cellulose powder (g), and  $V$  is the volume occupied by the cellulose powder in the measuring cylinder ( $\text{cm}^3$ ), while  $t$  and  $t_0$  are the flow times for cellulose dissolved in phosphoric acid solution and pure phosphoric acid solvent, respectively (min).

#### Plots for intrinsic viscosity

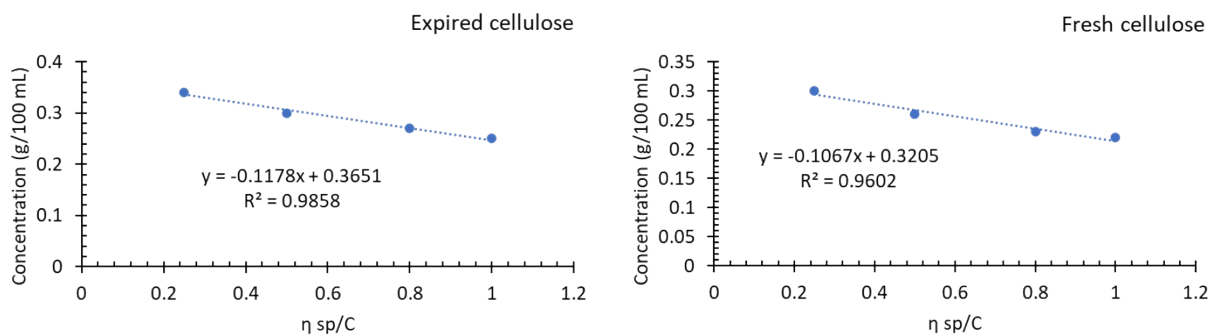


Fig. S1 Plots for intrinsic viscosity of expired and fresh cellulose.

## Characterization

### BET

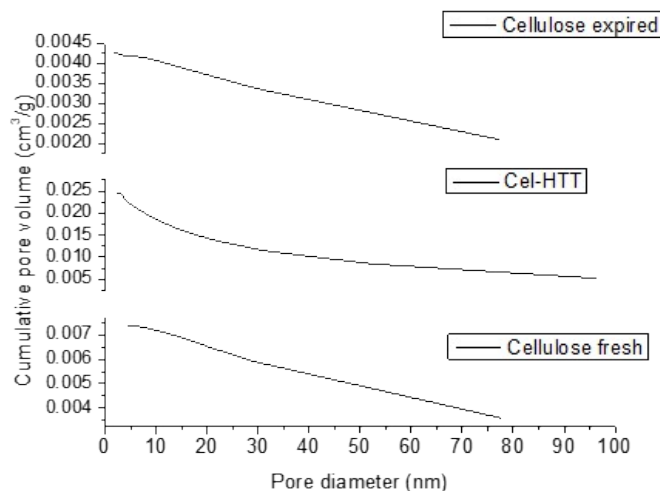


Fig. S2 Pore volume distribution of expired cellulose, Cel-HTT, and fresh cellulose.

### Removal studies

$$\%Removal = \frac{C_o - C_e}{C_o} \times 100 \quad [S3]^1$$

$$q_e = \frac{(C_o - C_e) \times V}{m} \quad [S4]^2$$

where  $C_o$  is the initial concentration (mg/L),  $V$  is the volume of the solution (L),  $m$  is the mass of the adsorbent (g),  $C_e$  is the equilibrium concentration (mg/L) and  $q_e$  is the equilibrium adsorption capacity (mg/g).

### Kinetics

$$\log(q_e - q_t) = \log(q_e) - \frac{k_1}{2.303} t \quad [S5]^2$$

$$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{1}{q_e} t \quad [S6]^3$$

$$q = k_{id} t^{0.5} + c \quad [S7]^4$$

where  $k_1$ ,  $k_2$  and  $k_{id}$  are the rate constants for the pseudo-first-order, pseudo-second-order, and intra-particle diffusion models, respectively,  $q_t$  is the adsorption capacity at time  $t$ , and  $C$  is the boundary layer thickness coefficient.

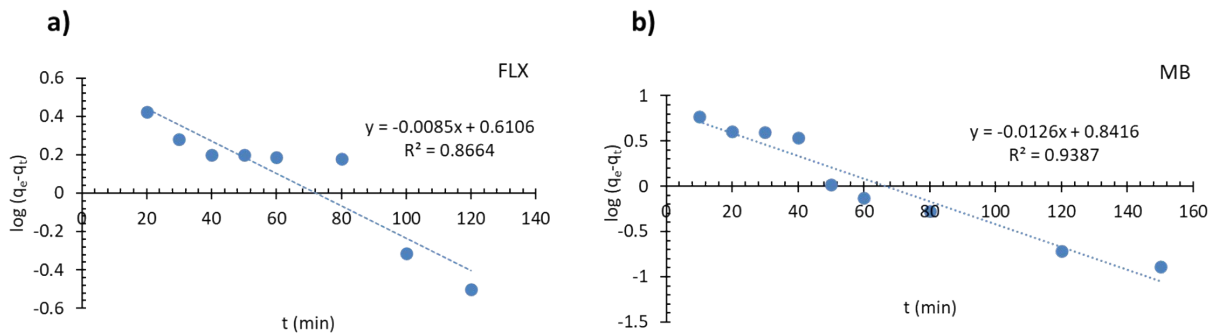


Fig. S3 Pseudo-first-order plots for FLX (a) and MB (b) at 50 ppm and adsorbent dose of 1.33 g/L at pH 7.5.

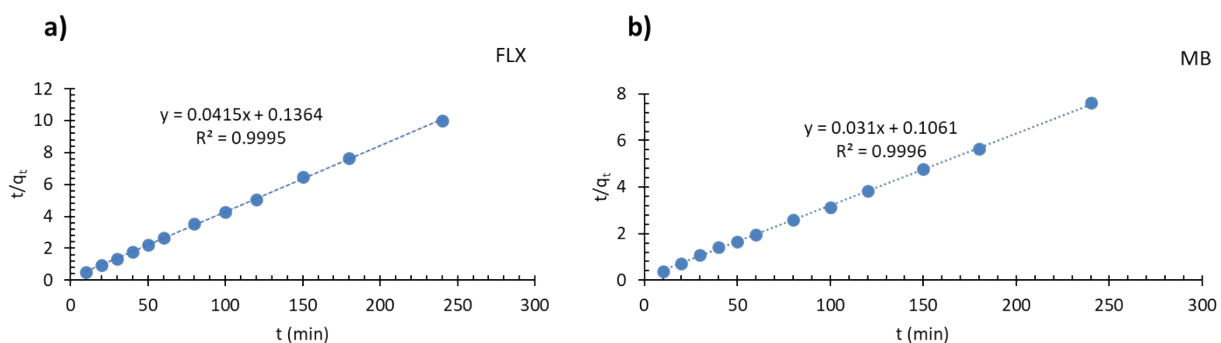


Fig. S4 Pseudo-second-order plots for FLX (a) and MB (b) at 50 ppm and adsorbent dose of 1.33 g/L at pH 7.5.

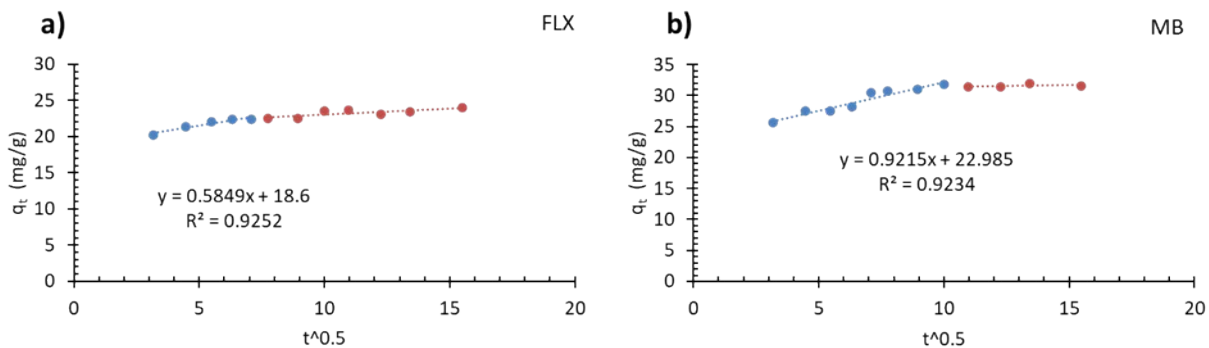


Fig. S5 Intra-particle diffusion plots for FLX (a) and MB (b) at 50 ppm and adsorbent dose of 1.33 g/L at pH 7.5.

### Equilibrium isotherms

$$q_e = K_f C_e^{1/n} \quad [S8]^5$$

$$\frac{C_e}{q_e} = \frac{C_e}{q_m} + \frac{K_d}{q_m} \quad [S9]^6$$

where  $K_f$  and  $n$  are Freundlich constants,  $K_d$  is the Langmuir desorption constant (L/g) and  $q_m$  is the maximum adsorption capacity (mg/L).

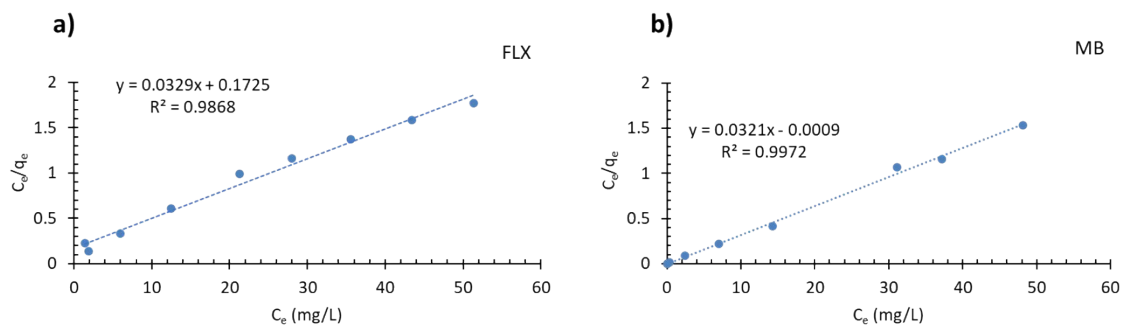


Fig. S6 Langmuir isotherm plots for FLX (a) and MB (b) at 10-90 ppm and adsorbent dose of 1.33 g/L at pH 7.5.

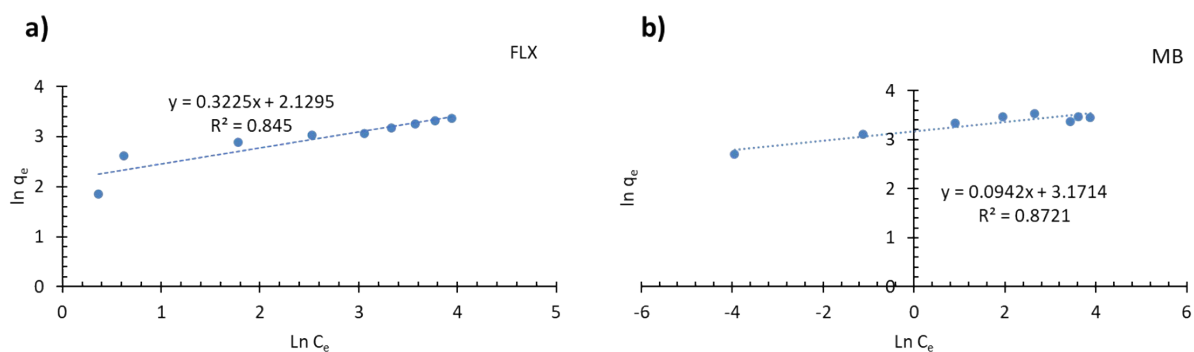


Fig. S7 Freundlich isotherm plots for FLX (a) and MB (b) at 10-90 ppm and adsorbent dose of 1.33 g/L at pH 7.5.

### Adsorption mechanism

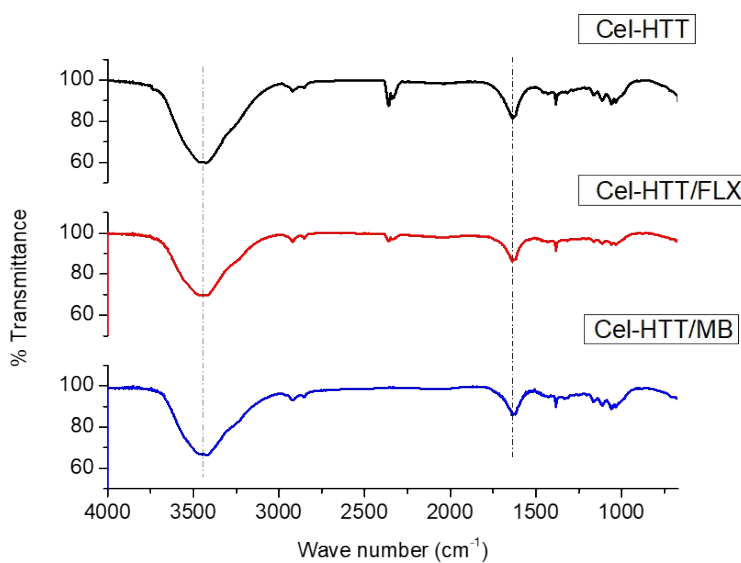


Fig. S8 FTIR measurements before and after adsorption of FLX and MB on Cel-HTT.

## References

1. M. Omraei, H. Esfandian, R. Katal and M. Ghorbani, *Desalination*, 2011, **271**, 248-256.
2. X. Huang, N.-y. Gao and Q.-l. Zhang, *Journal of Environmental Sciences*, 2007, **19**, 1287-1292.
3. J.-P. Simonin, *Chemical Engineering Journal*, 2016, **300**, 254-263.
4. A. E. Ofomaja, *Bioresource technology*, 2010, **101**, 5868-5876.
5. I. N. Najm, V. L. Snoeyink, M. T. Suidan, C. H. Lee and Y. Richard, *Journal-American Water Works Association*, 1990, **82**, 65-72.
6. A. Idris and K. Saed, *Environmentalist*, 2003, **23**, 329-334.