

## Supplementary Material

# Adsorptive Features of Magnetic Activated Carbons Prepared by a One-Step Process towards Brilliant Blue Dye

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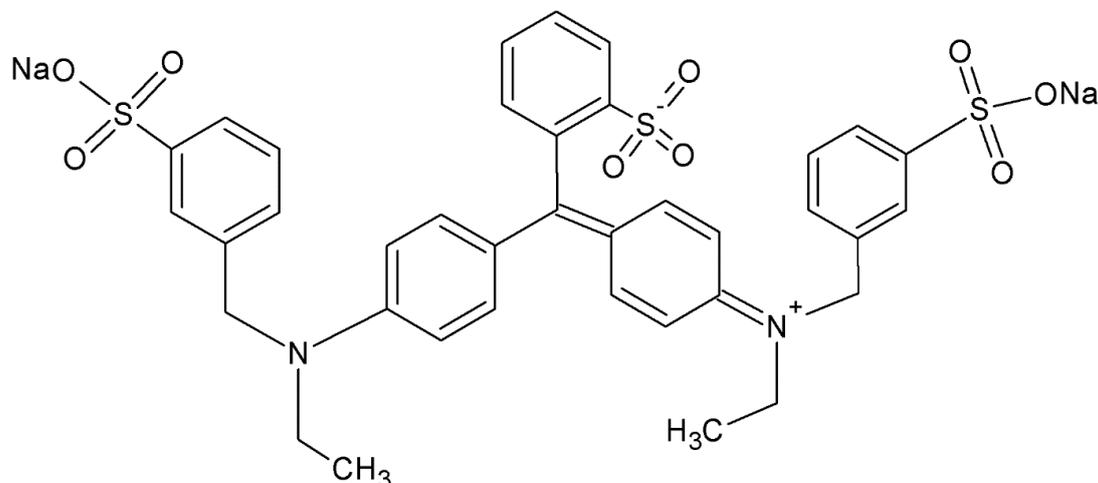
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**Figure S1.** Chemical structure of the brilliant blue dye.

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### S1. Adsorption quantification

All assays were performed in replicate ( $n = 3$ ) and blank tests were also carried out. The adsorption capacity at time  $t$  ( $q_t$ ) and the equilibrium adsorption capacity ( $q_e$ ) were determined by Eq. (1) and (2), respectively:

$$q_t = \frac{V(C_0 - C_t)}{m} \quad (1)$$

$$q_e = \frac{V(C_0 - C_e)}{m} \quad (2)$$

Where  $C_0$  is the initial BB dye concentration ( $\text{mg L}^{-1}$ ),  $C_t$  is the BB dye concentration in the liquid phase at time  $t$  ( $\text{mg L}^{-1}$ ),  $C_e$  is the equilibrium BB dye concentration in the liquid phase ( $\text{mg L}^{-1}$ ),  $m$  is adsorbent mass (g), and  $V$  is the volume of the solution (L).

### S2. Kinetic models

The adsorption kinetic behavior onto the MACs was evaluated by the pseudo-first-order (PFO) and pseudo-second-order (PSO) models [1]. The mathematical equations of these models are shown in Eq. (3) and (4), respectively:

$$q_t = q_1(1 - \exp(-k_1 t)) \quad (3)$$

$$q_t = \frac{t}{(1/k_2 q_2^2) + (t/q_2)} \quad (4)$$

Where  $q_t$  is the adsorption capacity at time  $t$  ( $\text{mg g}^{-1}$ ),  $q_1$  is the adsorption capacity predicted by the pseudo-first-order model ( $\text{mg g}^{-1}$ ),  $q_2$  is the adsorption capacity predicted by the pseudo-second-order model ( $\text{mg g}^{-1}$ ),  $k_1$  is the pseudo-first-order rate constant ( $\text{min}^{-1}$ ), and  $k_2$  is the pseudo-second-order rate constant ( $\text{g mg}^{-1} \text{min}^{-1}$ ).

### S3. Isotherm models

The adsorption equilibrium data were fitted to the Langmuir [2], Freundlich [3], and Sips [4] models, which are presented in the Eq. (5), (6), and (7), respectively:

$$q_e = \frac{q_m K_L C_e}{1 + K_L C_e} \quad (5)$$

$$q_e = K_F C_e^{1/nF} \quad (6)$$

$$q_e = q_s \frac{K_s C_e^{m_s}}{1 + K_s C_e^{m_s}} \quad (7)$$

Where  $q_e$  is equilibrium adsorption capacity ( $\text{mg g}^{-1}$ ),  $C_e$  is the equilibrium BB dye concentration in the liquid phase ( $\text{mg L}^{-1}$ ),  $q_m$  is the maximum adsorption capacity of the Langmuir model ( $\text{mg g}^{-1}$ );  $K_L$  is the Langmuir equilibrium constant ( $\text{L mg}^{-1}$ );  $K_F$  is the Freundlich equilibrium constant ( $(\text{mg g}^{-1}) (\text{mg L}^{-1})^{-1/nF}$ ),  $1/nF$  is the heterogeneity factor,  $q_s$  is the maximum adsorption capacity of the Sips model ( $\text{mg g}^{-1}$ ),  $K_s$  is the Sips equilibrium constant ( $\text{L mg}^{-1}$ ), and  $m_s$  the exponent of the Sips model.

The parameters of the models were estimated through nonlinear regression using the Quasi-Newton estimation method. Statistica 7.0 software (Statsoft, USA) was used in the calculations. The fit quality was evaluated by determination coefficient ( $R^2$ ), adjusted determination coefficient ( $R^2_{adj}$ ), and average relative error (ARE).

## References

1. Ho, Y.S.; McKay, G. A Comparison of Chemisorption Kinetic Models Applied to Pollutant Removal on Various Sorbents. *Process Saf. Environ. Prot.* **1998**, *76*, 332–340, doi:10.1205/095758298529696.
2. Langmuir, I. The adsorption of gases on plane surfaces of glass, mica and platinum. *J. Am. Chem. Soc.* **1918**, *40*, 1361–1403, doi:10.1021/ja02242a004.
3. Freundlich, H.M.F. Über die Adsorption in Lösungen. *Zeitschrift Phys. Chemie* **1907**, *57U*, 385–470, <https://doi.org/10.1515/zpch-1907-5723>.
4. Sips, R. On the Structure of a Catalyst Surface. *J. Chem. Phys.* **1948**, *16*, 490–495, <https://doi.org/10.1063/1.1746922>.