

Supplementary Materials

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S.1 Batch adsorption equations

The adsorption capacity at any time (q_t , mg g⁻¹), adsorption capacity at the equilibrium (q_e , mg g⁻¹), and removal percentage (R , %) values were calculated by the Equations (S2), (S3) and (S4), respectively:

$$q_t = (C_0 - C_t) \frac{V}{m} \quad (S1)$$

$$q_e = (C_0 - C_e) \frac{V}{m} \quad (S2)$$

$$R = \frac{(C_0 - C_t)}{C_0} 100 \quad (S3)$$

Where: C_0 is the initial adsorbate concentration in the liquid phase (mg L⁻¹), C_e is the equilibrium concentration of the adsorbate in the liquid phase (mg L⁻¹), C_t is the adsorbate concentration in the liquid phase at any time (mg L⁻¹), m is the mass of adsorbent (g), and V is the volume of solution (L).

S.2 Isotherm models

The Langmuir model (Equation (4)), Freundlich model (Equation (S5)), and Koble-Corrigan model (Equation (S7)) are presented as follows:

$$q_e = q_L \frac{K_L C_e}{1 + K_L C_e} \quad (S4)$$

$$q_e = K_F C_e^{1/n_f} \quad (S5)$$

$$q_e = \frac{K_{RP} C_e}{1 + a_{RP} C_e^{n_{RP}}} \quad (S6)$$

$$q_e = \frac{A_{KC} (C_e)^{n_{KC}}}{1 + K_{KC} (C_e)^{n_{KC}}} \quad (S7)$$

$$q_{KC} = \frac{A_{KC}}{K_{KC}} \quad (S8)$$

Where: q_L is the maximum adsorption capacity of Langmuir model (mg g^{-1}), K_L is the Langmuir constant (L mg^{-1}); K_F is the Freundlich constant ($(\text{mg g}^{-1}) (\text{mg L}^{-1})^{-1/n}$); $1/n_f$ (dimensionless) is the heterogeneity factor; K_{RP} is the Redlich-Peterson constant (L mg^{-1}), a_{RP} is the affinity coefficient (L mg^{-1})^{n_{RP}}, n_{RP} is the Redlich-Peterson exponent; A_{KC} is the Koble-Corrigan constant ($(\text{mg g}^{-1})(\text{L mg}^{-1})^{n_{KC}}$), K_{KC} is the Koble-Corrigan equilibrium constant ($(\text{L mg}^{-1})^{n_{KC}}$), n_{KC} is the Koble-Corrigan exponent (dimensionless), q_{KC} is the Koble-Corrigan adsorption equilibrium (mg g^{-1}).

S.3 Thermodynamic estimation

The Gibbs free energy (ΔG^0 , kJ mol^{-1}), enthalpy change (ΔH^0 , kJ mol^{-1}), and entropy change (ΔS^0 , $\text{kJ mol}^{-1} \text{K}^{-1}$) were calculated by the following Equations:

$$K_e = \frac{K_L M_W \gamma^{PROP}}{\Gamma} \quad (S9)$$

$$\Delta G^0 = -RT \ln(K_e) \quad (S10)$$

$$\Delta G^0 = \Delta H^0 - T \Delta S^0 \quad (S11)$$

$$\ln(K_e) = \frac{\Delta S^0}{R} - \frac{\Delta H^0}{RT} \quad (S12)$$

where: K_e is the equilibrium constant (dimensionless), γ^{PROP} is the activity coefficient of the drug in solution (dimensionless, assuming $\gamma^{PROP} = 1$); Γ is the unitary activity coefficient of 1 mol L^{-1} ; T is the temperature (K); R is the universal gas constant ($8.31 \times 10^{-3} \text{ kJ mol}^{-1} \text{K}^{-1}$).

S.4 Kinetic models

For describing the kinetics of adsorption the following models were adjusted to the experimental data: Pseudo-first order, Pseudo-second order, General order, Elovich, and Avrami

$$q_t = q_1 (1 - e^{-k_1 t}) \quad (S13)$$

$$q_t = \frac{t}{\left(\frac{1}{k_2 q_2^2}\right) + \left(\frac{t}{q_2}\right)} \quad (S14)$$

$$q_t = \left(q_e - \frac{q_n}{\left[k_N \cdot (q_n)^{n-1} \cdot t \cdot (n-1) + 1 \right]^{1/(1-n)}} \right) \quad (S16)$$

Where k_1 (min^{-1}), k_2 ($\text{g mg}^{-1} \text{min}^{-1}$), and k_N [$(\text{min}^{-1})(\text{g mg}^{-1})^{n-1}$] are the kinetics constants of pseudo-first-order, pseudo-second-order, and general order models, respectively; q_1 , q_2 , and q_n are the theoretical values for the adsorption capacity at the equilibrium for each

model (mg g^{-1}); n is the general order of General Kinetic model (dimensionless), t is contact time (min).

The linear driving force model (LDF) was also selected, where the adsorption rate can be expressed as:

$$\frac{d\bar{q}}{dt} = k_{\text{LDF}} \left(q_L \frac{K_L C_0 - D_0 \bar{q}}{1 + K_L C_0 - D_0 \bar{q}} - \bar{q} \right) \quad (\text{S17})$$

Furthermore, the diffusivity for a homogeneous particle can be estimated from the LDF kinetic lumped parameter:

$$D_s = \frac{R_p^2 k_{\text{LDF}}}{15} \quad (\text{S18})$$

R_p is the adsorbent particle radius, and D_s is the surface diffusivity ($\text{cm}^2 \text{s}^{-1}$).

S.5 Statistical evaluation

The determination coefficient (R^2) (Equation (S18)), adjusted determination coefficient (R^2_{adj}) (Equation (S19)), average relative error (ARE) (Equation (S20)), and mean square error (MSR) (Equation (S21)), Bayesian indicator criterion (BIC) are given by the following Equations:

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_{\text{exp}} - y_{\text{pred}})^2}{\sum_{i=1}^n (y_{\text{exp}} - \bar{y}_{\text{exp}})^2} \quad (\text{S19})$$

$$R^2_{\text{adj}} = 1 - (1 - R^2) \frac{(n-1)}{(n-p-1)} \quad (\text{S20})$$

$$\text{ARE} = \frac{100\%}{n} \sum_{i=1}^n \left| \frac{y_{\text{exp}} - y_{\text{pred}}}{y_{\text{exp}}} \right| \quad (\text{S21})$$

$$\text{MSR} = \frac{1}{n-p} \sum_{i=1}^n (y_{\text{exp}} - y_{\text{pred}})^2 \quad (\text{S22})$$

$$\text{BIC} = n \ln \left(\frac{\text{RSS}}{n} \right) + p \ln(n) \quad (\text{S23})$$

where: y_{exp} is the experimental value; y_{pred} is the predicted value; n is the number of experimental values; p is the number of parameters according to the model.

S.6 Figures

This section presents all the Figures called in the manuscript.

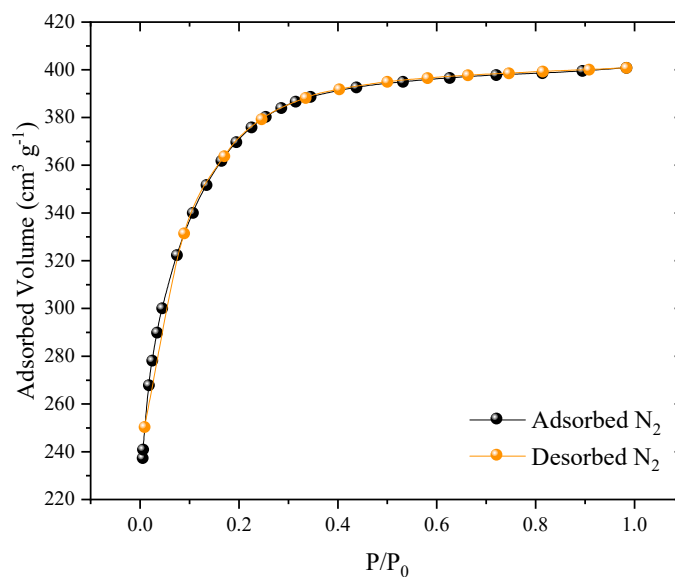


Figure S1. N₂ adsorption and desorption isotherms for the activated carbon.

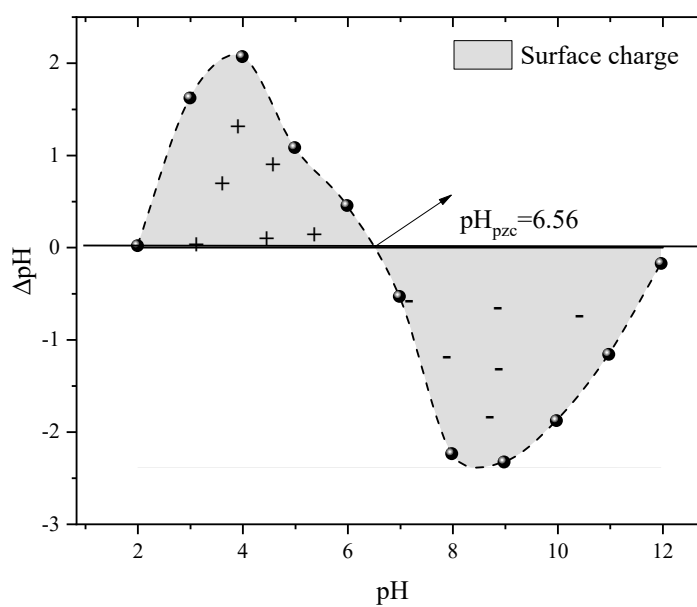


Figure S2. Variation of the solution pH as function of the initial solution pH and representation of pH_{pzc} and surface charges

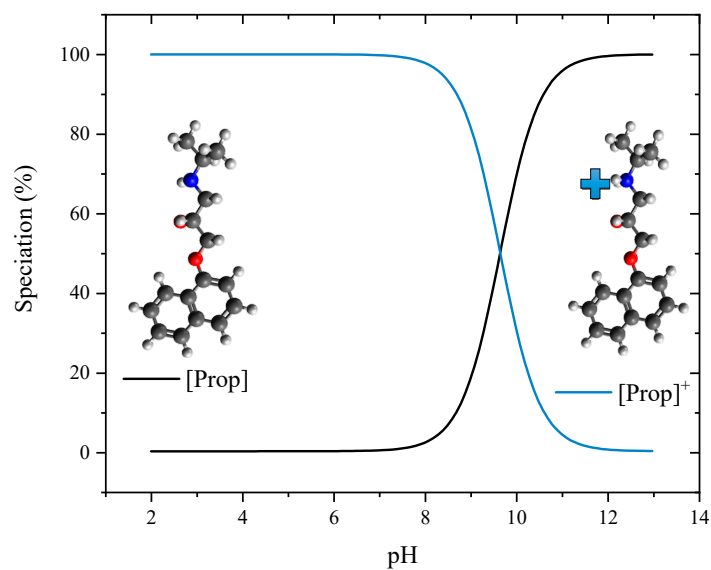


Figure S3. Speciation diagram for the propranolol, according to the pH, prediction obtained from the MarvinSketch software.

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