**Área: MAT**

# Adsorption of caffeine and metabolites on $Na^+$-exchanged bentonite

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## Highlights

The major metabolites' effect on caffeine's adsorption rates was systematically investigated. Only for caffeine, adsorption was favorable, and the maximum adsorption capacity was 20 ± 3 mg/g.

## Resumo/Abstract

Clay minerals are potential candidates for caffeine removal because they are environmentally friendly and abundant in nature. In this work, commercially available bentonite was exchanged with $Na^+$ and characterized by X-ray diffractometry, electron scanning microscopy, Zeta-potential measurements, and specific surface area. Adsorption of caffeine was fast and reached equilibrium within contact times < 15 min, suggesting the interaction occurs predominantly in surface groups at the edge of the clay mineral. Adsorbent mass, ionic force, and medium pH were also investigated.

Adsorption isotherms (25.0 ± 0.5°C) (Fig. 1) of caffeine and the metabolites theobromine, paraxanthine, and theophylline were constructed for each compound individually (Fig. 1A) or in mixtures of the four compounds (Fig. 1B) and treated by the Langmuir and Freundlich models. Only for caffeine, adsorption was favorable and fitted to the Langmuir equation, enabling the estimation of a maximum adsorption capacity of 20 ± 3 mg/g, independent of the presence of the metabolites.

The affinity order was: caffeine >>> theobromine > paraxanthine ~ theophylline. The less efficient adsorption of the metabolites was particularly evident in alkaline solutions, where the anionic forms of theobromine, paraxanthine, and theophylline predominate. This resulted in reduced adsorption due to electrostatic repulsion and steric hindrance, as supported by both experimental data and molecular modeling. The sodium bentonite was then applied to remove the analytes from beverages and synthetic urine, finding removal percentages of caffeine > 87%.

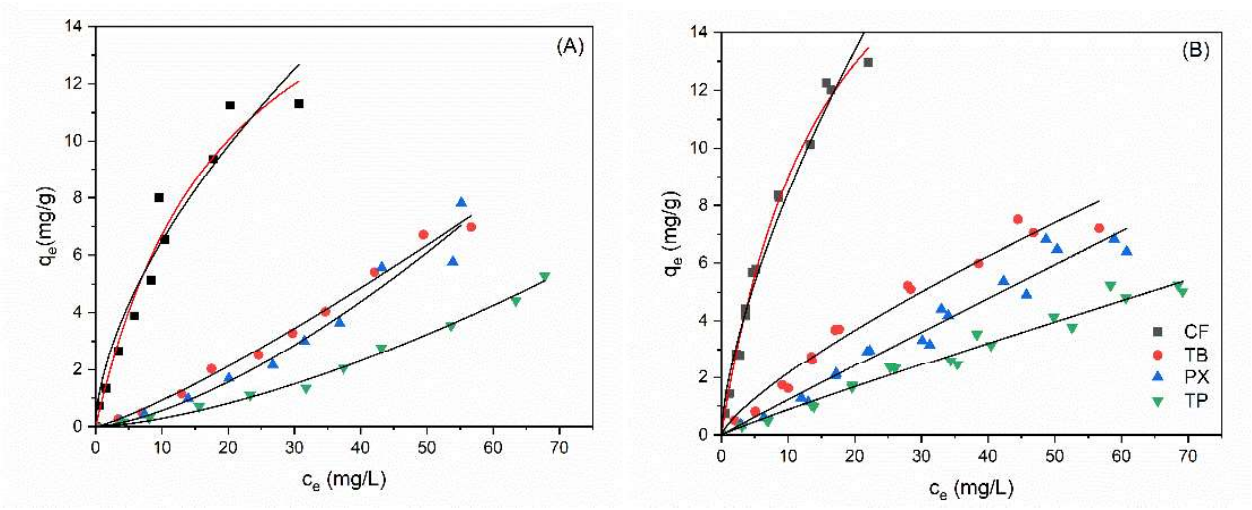


Fig. 1. Adsorption isotherms (25.0 ± 0.5°C) of CF, TB, PX, and TP onto Na-BT fitted by Langmuir (Caffeine, red line) and Freundlich (black lines) models, for (A) each analyte separately, and for (B) a mixture containing all four compounds.

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