

# Integrated Study of Antiretroviral Drugs Adsorption onto Calcined Layered Double Hydroxide Clay: Experimental and Computational Analysis

Lehlogonolo S. Tabana<sup>\*a</sup>, Gbolahan J. Adekoya<sup>b</sup> and Shepherd M. Tichapondwa<sup>a</sup>

<sup>a</sup>Department of Chemical Engineering, Sustainable Environmental and Water Utilisation Processes Division, University of Pretoria, Pretoria, South Africa.

<sup>b</sup>Institute of NanoEngineering Research (INER) & Department of Chemical, Metallurgical and Materials Engineering, Faculty of Engineering and the Built Environment, Tshwane University of Technology, Pretoria, South Africa

tabana.ls@tuks.co.za

## Supplementary data

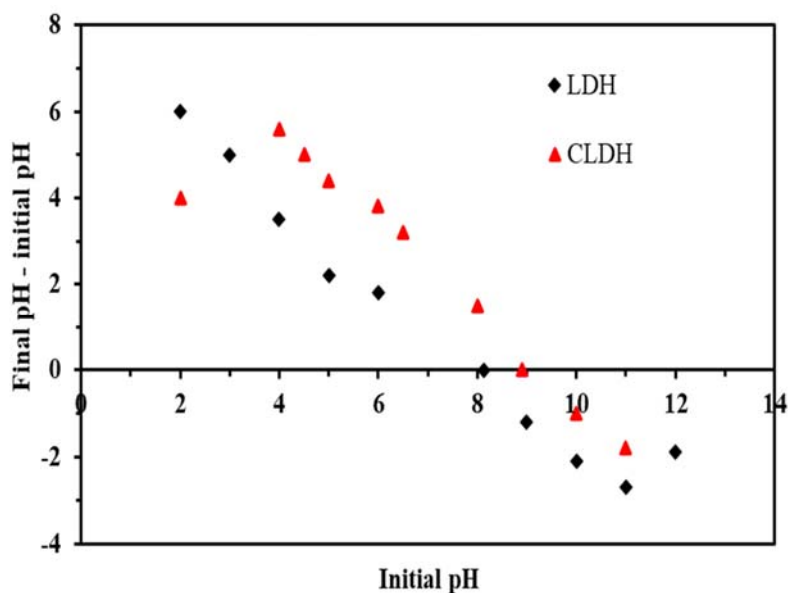


Figure S1: Point of zero charge for LDH and CLDH

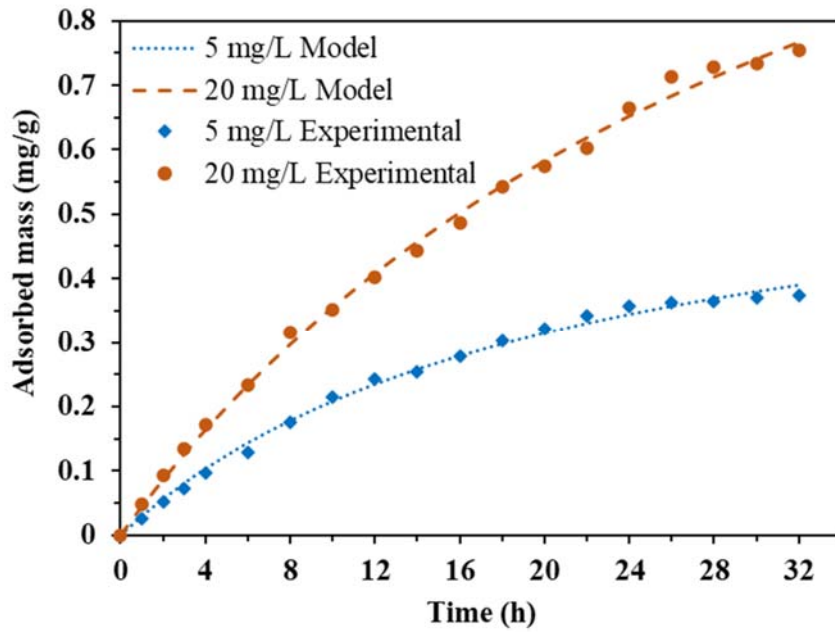


Figure S2: PSO kinetics model for EFV at initial concentrations of 5 and 20 mg/L, pH 5, T=25 °C and a dosage of 10 g/L

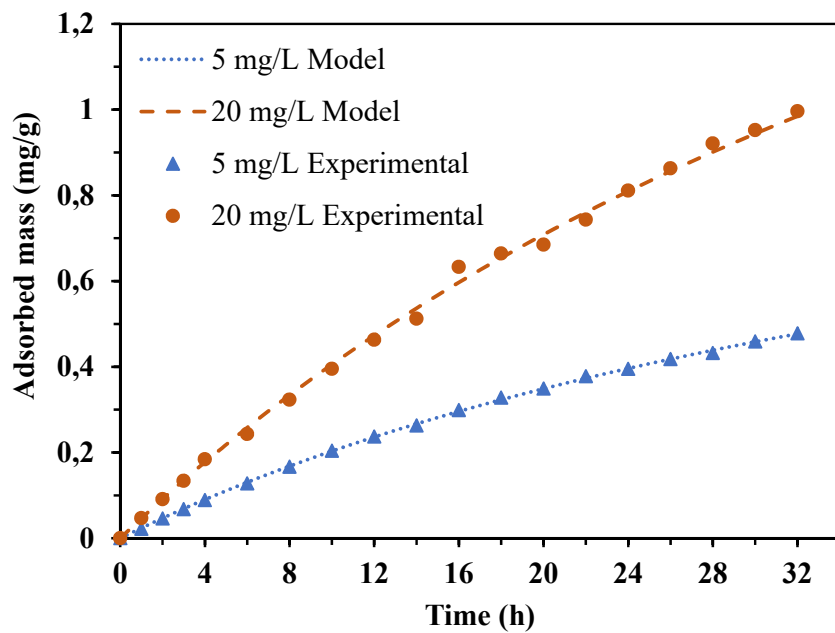


Figure S3: PSO kinetics model for NVP at initial concentrations of 5 and 20 mg/L, pH 5, T=25 °C and a dosage of 10 g/L

Table S 1: PFO kinetic models' parameters

Concentration	Parameter	Efavirenz	Nevirapine
5 mg/L	$k_l$ ( $\text{h}^{-1}$ )	0.107	0.115
	$q_e$ (calculated)(mg/g)	0.413	0.528
	$q_e$ (experimental)(mg/g)	0.362	0.42
	$R^2$	0.92	0.90
10 mg/L	$k_l$ ( $\text{h}^{-1}$ )	0.104	0.126
	$q_e$ (calculated)(mg/g)	0.719	1
	$q_e$ (experimental)(mg/g)	0.629	0.748
	$R^2$	0.93	0.95
20 mg/L	$k_l$ ( $\text{h}^{-1}$ )	0.137	0.105
	$q_e$ (calculated)(mg/g)	0.789	0.996
	$q_e$ (experimental)(mg/g)	0.64	0.824
	$R^2$	0.95	0.93