

Supplementary Material

Adsorption of Pharmaceuticals onto Smectite Clay Minerals. A Combined Experimental and Theoretical Study

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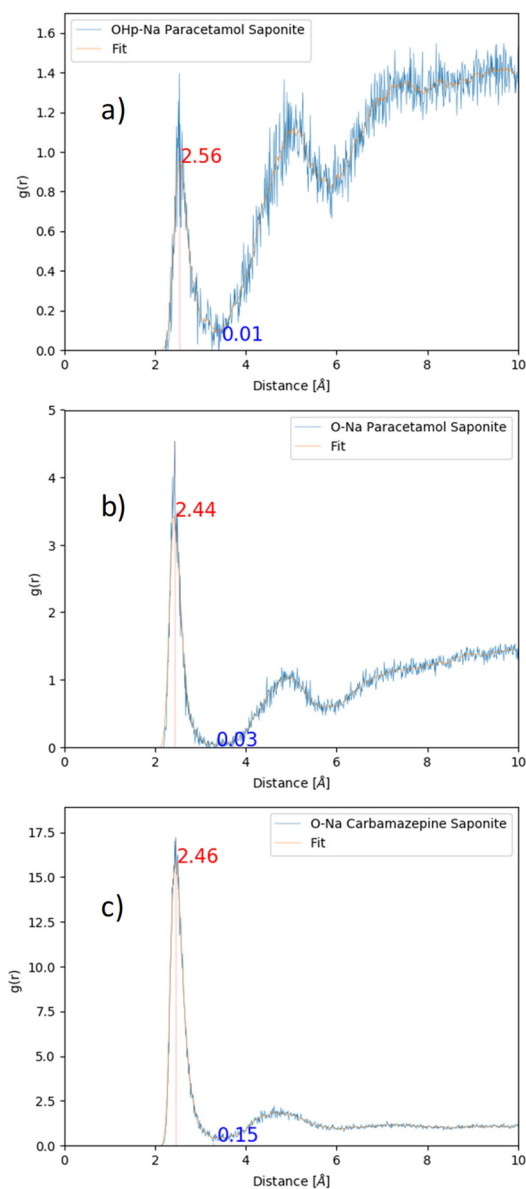


Figure S1. Radial distribution functions for (a) hydroxyl oxygen atom of paracetamol and sodium cations, (b) carboxyl oxygen atom of paracetamol and sodium cations, (c) carboxyl oxygen of carbamazepine and sodium cations. In red the distance at which the rdf's maximum is found and in blue the coordination number computed over the whole simulation.

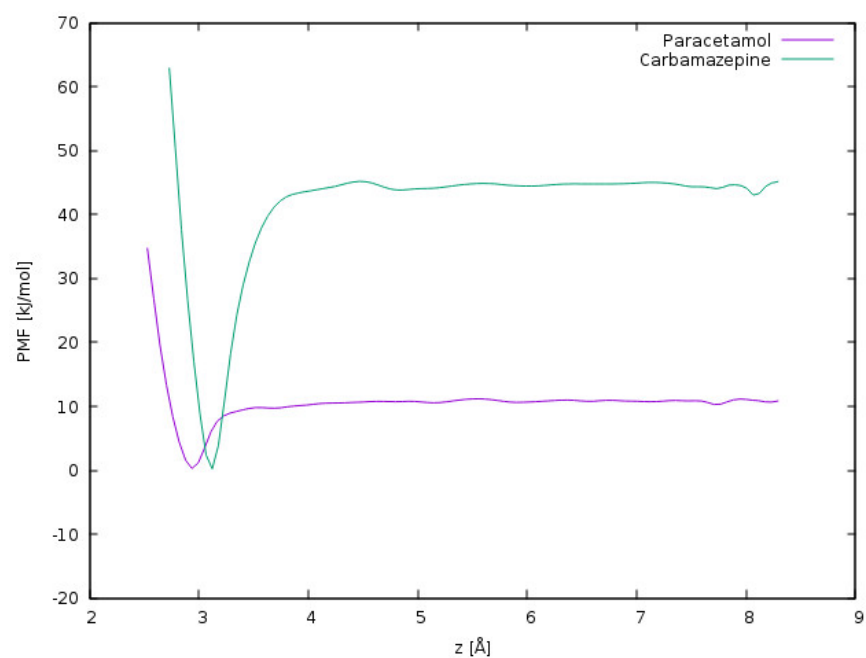


Figure S2. Potential of Mean Force (kJ mol^{-1}) computed for paracetamol (purple curve) and carbamazepine (green curve).