Clay Nanopore Trapping of Structurally-Different Fluoroquinolone Antimicrobials: Adsorbate Conformations and Interactions

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Smectite clay nanopores are implicated in the retention of antimicrobials within soils and sediments. Cation exchange has been considered the primary mechanism of adsorption but recent studies proposed a dual role of chemical structures and acid-base chemistry in facilitating favorable interactions within smectite clay nanoparticles. Using the smectite clay montmorillonite, we employed X-ray diffraction, nuclear magnetic resonance (NMR), and molecular dynamics simulations to investigate interlayer adsorption of two structurally-different fluoroquinolone (FQ) antimicrobials: ciprofloxacin (a first-generation FQ) and moxifloxacin (a third-generation FQ). Consistent with favorable cation-exchange of positively-charged FQ species, we found that adsorption was greater at pH 5 than at pH 7. However, the clay exhibited higher adsorption capacity for moxifloxacin than for ciprofloxacin. This preference was shown by X-diffraction and ^{23}Na-NMR data to be accompanied by enhanced interlayer trapping of moxifloxacin. Molecular dynamics simulations coupled with ^{1}H-^{13}C NMR signatures shed light on the specific FQ structural features responsible for preferential retention and different intercalation behavior within the clay nanopores.

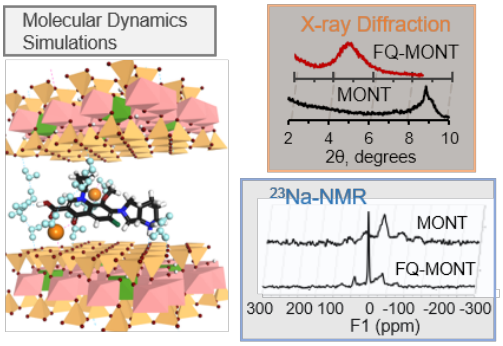

Figure 1. Montmorillonite-trapped fluoroquinolone probed by molecular simulations and multiple spectroscopic analyses.