Evaluation of Phenyltrimethylammonium (PTMA) as a Probe for Sorption of Cationic Organic Compounds to Soils and Sediments

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The presence of polyfunctional ionogenic compounds (PICs) such as personal care products (PCPs), pharmaceuticals, and pesticides have been detected in our natural water supplies. It is necessary to study the environmental fate of these compounds because they have caused harm to aquatic life and pose potential threats to other natural ecosystems and human health. One environmental process that influences contaminant fate is sorption—the transfer of chemicals from water to soil interfaces. Although (PIC) sorption has been studied qualitatively, the predictive tools to determine the extent of sorption (equilibrium sorption constant, K_d) have yet to be developed. Cation exchange—one type of sorption mechanism—occurs when a cationic amine (NH_3^+) group on a PIC replaces a naturally occurring metal cation (e.g., Ca^{2+}) on a negatively charged soil site. Mackay and Vasudevan (2012) proposed the use of mechanism specific probe compounds and the use of scaling factors to extrapolate the probes K_d values to K_d values of larger compounds (e.g., pharmaceuticals) that sorb via the same mechanism.

Previous work done by Katie Carter (Class of 2016) and Reaha Gotyeche (Class of 2014) evaluated Benzylamine as a probe compound for cation exchange and compared Benzylamine sorption, through linear regressions, with sorption to the pharmaceuticals: Tramadol (chronic pain reliever) and Desipramine (anti-depressant) on 30 different well-characterized soils. This study evaluates the potential of Phenyltrimethylammonium (PTMA), a quaternary amine, as an alternate probe for cation exchange. The reasons for examining PTMA is that it has permanent positive charge (no pKa), is a solid at room temperature and is cheaper than Benzylamine. An initial concentration of $5x10^{-5}$ M of PTMA was equilibrated with the 30 different soils for 18-24 hours, centrifuged at 3400 rpm at 4 degrees Celsius, filtered, and then analyzed through high performance liquid chromatography (HPLC) to obtain the concentration of PTMA left in the solution (C_w). Using the C_w, the concentration of PTMA sorbed by the soil was calculated and then used to establish a K_d (sorption equilibrium constant, C_s/C_w) value for each soil. The K_d values of PTMA on the 30 soils range from 0.26 L/kg to 1539.19 L/kg.

Our results to date suggest that PTMA may be a better probe than Benzylamine: Linear regressions of $\log K_d$PTMA vs. $\log K_d$Trammadol ($R^2=0.891$)(Figure 1) and $\log K_d$PTMA vs. $\log K_d$Desipramine ($R^2=0.874$)(Figure 2), showed a better correlation than the regressions previously done with $\log K_d$Benzylamine vs. $\log K_d$Tramadol ($R^2=0.625$) and $\log K_d$Benzylamine vs. $\log K_d$Desipramine ($R^2=0.85$). LogK_dPTMA however, vs. log of effective cation exchange capacity values (ECEC)—a measure of available cation exchange sites—($R^2=0.486$)(Figure 3) showed weaker correlation than $\log K_d$Benzylamine vs. logECEC ($R^2=0.535$). Future work will include desorption studies and a more detailed evaluation of differences in PTMA and Benzylamine sorption.

Figure 1: Log (K_dPTMA) vs. Log (K_dTramadal)

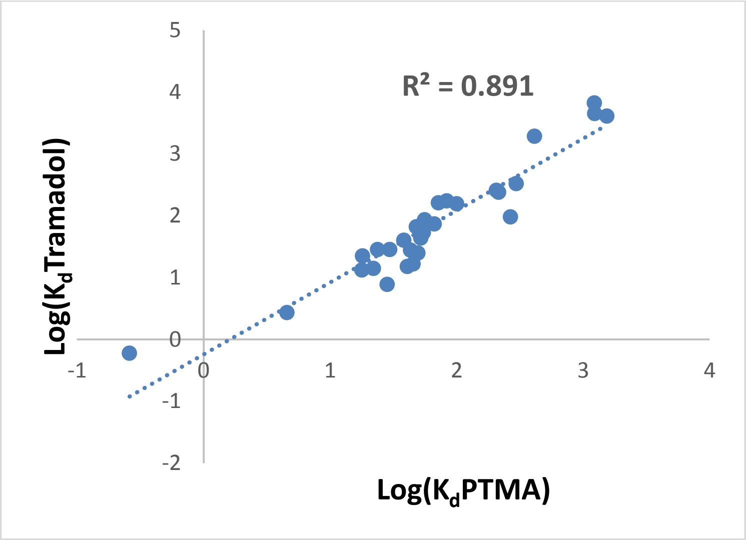


Figure 2: Log (K_dPTMA) vs. Log (K_dDesipramine)

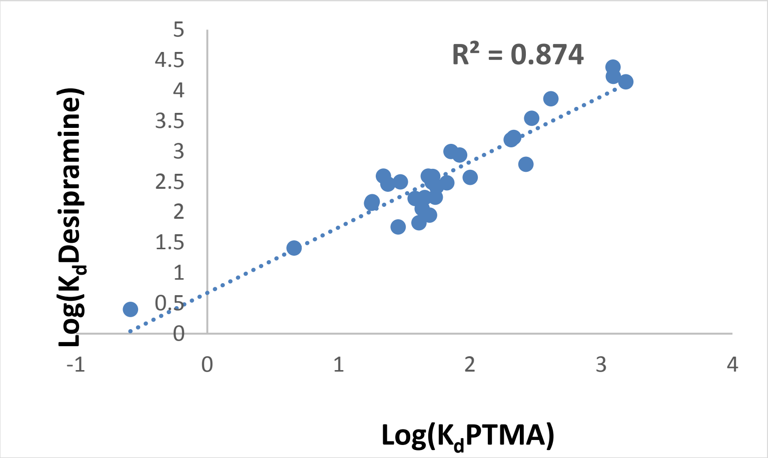
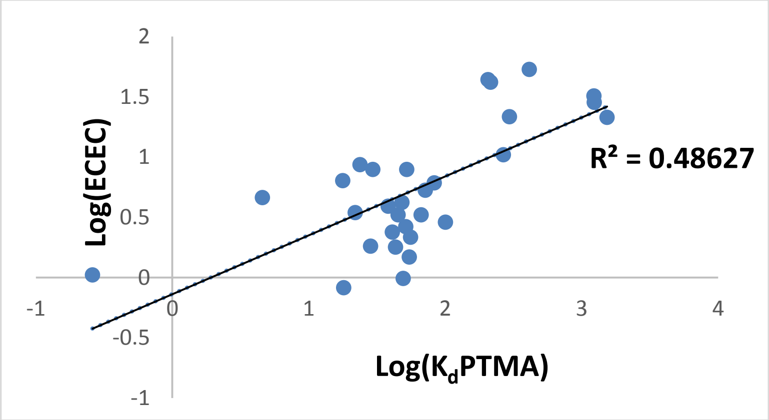


Figure 3: Log (K_dPTMA) vs. Log (ECEC)



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