Developing a Free Energy Parameter Model for the Prediction and Mapping of the Uptake of Hazardous Organic Pollutants by Plant Cuticle Membranes

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This project presents a novel end-to-end solution for predicting, mapping, and mitigating the absorption of hazardous organic pollutants by the plant cuticle membrane. The plant cuticle is vegetation's first line of defense against environmental threats such as hydrophobic or volatile organic contaminants. These atmospheric pollutants enter the cuticle through contact with various mediums—industrial air, wastewater pollutants, pesticides, herbicides, and contaminated soil—and pose a threat to the humans and animals who consume the plant. For phase 1, a predictive free energy parameter model (Abraham Free Energy Model) was chosen by developing quantitative structure-property relationships between the characteristics of the plant cuticle membrane and absorbed organic contaminants. The properties in which the model takes into account are molar refractivity, polarizability, 3-D structure, dispersion, and hydrogen-bond acidity/basicity. Using the concept of chemical-free energy, the model uses structural factors to predict the ratio of absorbed containment. For phase 2, the model was tested on experimental databases of 25 diverse plant species. To construct the databases used in the study, solubility data pertaining to the concentration of hydrophobic contaminants adsorbed by the isolated cuticular membranes (CM) and by the polymer matrix membranes (MX) was mined from published literature and data released by the Environmental Protection Agency. To test the accuracy of the model, a regression analysis was performed using indicator variables. A root-mean-square error (RMSE) of about 0.22 and an R squared value of 0.987 were determined, indicating that the proposed model is much more accurate than previous methods used.