Artificial Neural Network Development to Predict Plant Uptake and Translocation of Chlorinated Contaminants: Implications on Risk and Remediation

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Anthropogenic activities have led to a legacy of fugitive pollutants in our biosphere that affected the quality of food and water, fundamental cornerstones of human welfare. Plants serve as the foundation of human food, and the potential exposure through food contamination is growing in concern due to the emergence of new chemicals, many chlorinated compounds, in the environment and the shortening of the water cycle as water reuse as irrigation waters increases for example. The chlorinated contaminants could be uptaken by plants and be translocated to all parts of plants, including edible leafy tissues or fruit. Understanding of plant uptake is also essential in phytoremediation and in site assessment and plume delineation through phytoforensic approaches. The transpiration stream concentration factor (TSCF) was introduced demonstrate efficient transport from subsurface sources, soil, groundwater and vapor. Efforts have introduced mathematical relationships, which relate the TSCF to octanol/water partition coefficient (Log Kow). Such approaches are predictive, but lack accurate prediction of TSCF. Recent studies have demonstrated that plant uptake exhibits similarity to other transport through other bio-membranes, with impacts of chemical properties: molecular weight, hydrogen bond donors and acceptors, and lesser impacts of polar surface area and rotatable bonds. In this study, multi-layer perceptron artificial neural network (MLPANN) was introduced as an tool to predict the uptake and translocation of chlorinated compounds in plants, based upon the listed chemical properties. TSCFs of chlorinated compounds was also compared with non-chlorinated compounds to examine if chlorination significantly impacts uptake and translocation of emerging environmental contaminants.

The MLPANN modeling approach was performed using writing real code in the MATPAB software. A comprehensive selection of TSCF data for both chlorinated and non-chlorinated compounds was compiled from published literature. The compound properties including Log Kow, molecular weight, H-bond donor, H-bond acceptor, rotatable bonds, polar surface area, and Henry's constant were obtained from chemical structure databases execute MLPANN modeling. Sensitivity analysis was performed to compare the chlorine compounds with non-chlorine compounds in the terms of plant uptake and translocation.

The results of this study indicate that the MLPANN models can predict plant uptake and translocation of chlorinated compounds with good accuracy. This intelligent modeling approach is more precise than the traditional mathematical relationships. Thus, this intelligent predictor can be used to estimate the capacity of chlorinated compounds for uptake and translocation in plants even before conducting a real experiment. The sensitivity analysis shows that the important parameters for the modeling of chlorine compound is different from non-chlorine compounds.