How To Design for a Tailored Subcellular Distribution of Systemic Agrochemicals in Plant Tissues

Foliar-applied systemic agrochemicals require entrance into the plant vascular system or into specific subcellular compartments to reach their target in planta or to be imbibed by piercing/sucking pests. An inappropriate subcellular localization, like accumulation of aphicides in vacuoles, might lower the compound's efficiency due to reduced exposure to the target. Permeabilities and mass distributions of 16 compounds covering a broad range of properties were measured across a pH gradient in a PAMPA ("parallel artificial membrane permeability assay") system, providing experimental evidence for ion trapping of acids and bases in basic and acidic compartments, respectively. The results validated a predictive model which was then expanded to simulate a standardized plant cell (cytosol and vacuole) with a vascular system (phloem and xylem). This approach underlined that the absolute mass distribution across aqueous phases is defined by membrane retention, whereas the relative mass distribution is determined by the species (neutral, acidic, basic) of compounds. These processes depend largely on pK(a) and log K-ow of the test compounds, which subsequently determine the partitioning of the substances in plant cell compartments. The validated model can be used as a tool in agrochemistry research to tailor the subcellular distribution by chemistry design and to interpret biology results.

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