

Pesticides

Pesticides are chemicals that are especially chosen for their ability to affect “unwanted organisms” whether it may be animals, plants, fungi or microorganisms without affecting non-target organisms. Thus, pesticides are biological active substances or preparations containing one or more substances with a broad range of biocidal activity and often with a specific mode of action.

Modes of action

It has been observed that chemicals of analogous structures have similar modes of action on the target organism. Dividing such chemicals into chemical classes therefore means that predictions of the mode of action are possible. Pesticides may act by contact or systemic mode of action. A contact action means that the pesticide by contact with the target organisms affects the surface or penetrates the surface to reach the target site. A systemic mode of action means that a pesticide is taken up by an organism and then acts after the uptake (e.g. insecticides taken up by eating or sucking insects from the plants the insecticide has entered).

Below some of the major chemical classes used in pesticides are presented.

Aryloxyalkanoic acids

Aryloxyalkanoic acids (phenoxy acids) are selective systemic hormone type herbicides that are absorbed by the leaves and roots and translocated throughout the plant but concentrates in the meristematic regions where it inhibits growth.

Azoles

Azoles are fungicides acting as steroid demethylation inhibitor.

Carbamates

Carbamates may be herbicides or insecticides. As herbicides, carbamates are systemic herbicides, which are absorbed by the roots, leaves and stem, and translocated to active growth sites (meristems) where it inhibits elongation of roots and aerial parts. Some carbamates are insecticides with contact and stomach action and act as cholinesterase inhibitor.

Dinitroanilines

Dinitroanilines are selective soil herbicides, which are absorbed by the roots. Dinitroanilines affect seed germination and prevent plant growth by inhibition of root and shoot development.

Organophosphorous

Organophosphorous substances are usually insecticides with contact and stomach action and act as cholinesterase inhibitor affecting the nervous system. Organophosphorous herbicides do exist as selective herbicides, which are absorbed through the roots.

Pyrethroids

Pyrethroids are usually non-systemic insecticides with contact action. They cause paralysis initially (“knock-down effect”) and may lead to death later. Usually, they are non-phytotoxic.

Sulfonylureas

Sulfonylureas are selective systemic herbicides, which are absorbed by the leaves and roots and translocated throughout the plant. Sulfonylureas inhibit the acetolactate synthesis. Plant growth is inhibited followed by the development of chlorotic patches, which spread acropetally and then basipetally

Triazines

Triazines are selective systemic herbicides, which are absorbed by the leaves and roots and then translocated acropetally in the xylem to accumulate in apical meristems. Triazines inhibit photosynthesis and interfere with other enzymatic processes.

Triazoles

Triazoles are non-selective systemic herbicides, which are absorbed by the leaves and roots and then translocated in both the phloem and the xylem. Triazoles inhibit the chlorophyll formation and re-growth from buds.

QSAR and pesticides

Most QSARs are based on simple chemical structures and the use on more complex organic molecules which is often the case with pesticides, should be performed with this in mind. However, some studies have been using the QSAR models on pesticides. Generally, most aspects of pesticides are very well documented compared with other chemicals and this should improve the input data quality. However, data on metabolites and degradation products are usually missing and validated QSAR models may present estimates on whether a metabolite or degradation product should be considered for more study or not.

Evaluation of the validity of the latest accepted QSARs is performed by comparing experimental values and the QSAR model estimates using specified models.

The QSAR estimations on physico-chemical proportions are performed by programmes developed by Syracuse Research Corporation: MPBPVP, WSKOW, KOWWIN, HENRY, and PCKOCWIN. The programmes are stand-alone programmes but can be run together using the Estimation Programs Interface (EPIWIN) as an interface.

Reference

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