
USING STRUCTURAL ACTIVITY RELATIONSHIPS TO DERIVE ENVIRONMENTAL STANDARDS FOR PESTICIDES WITH SPARSE TOXICITY DATA



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ABSTRACT

A site near Marseilles, France, produced and/or imported fungicides from 1956 until early 2000, including ofurace [2-chloro-N-(2,6-dimethylphenyl)-N-(tetrahydro-2-oxo-3-furanyl)acetamide] from 1981 until early 2000. Ofurace produced on site was marketed in various formulations including a folpet/ofurace liquid suspension concentrate. Ofurace in site soils ranged from 0.01-0.41 mg/kg and in surface water at concentrations ranging from 0.15 μ g/L to 12.61 μ g/L. Groundwater concentrations ranged from 1.24 μ g/L to 6,569 μ g/L. However, there are no specific values for fungicides/pesticides in the French guidance manual, except for a generic fungicide/pesticide value of 0.5 μ g/l for groundwater. This paper describes how structural activity relationships were used to develop defensible comparison standards for soils, surface water, and groundwater.

Structural activity relationships (SARs) are useful in developing criteria when limited toxicological information is available regarding a specific chemical compound and are a widely accepted method that relate chemical compounds with similar physio-chemical characteristics by applying mathematical relationships. The available data for ofurace included molecular weight, Log P (K_{ow}), solubility, and limited LD₅₀ and EC₅₀ values for rabbits, rats, partridge, trout, golden orfe, daphnia, and bees. These same descriptors were collected and compiled for other acetanilide herbicides of similar structure for use in estimating the toxicity of ofurace by SAR correlations.

The SAR analyses show that ofurace is consistently less toxic than metolachlor, another acetanilide fungicide for which the U.S. EPA has developed a constituent-specific drinking water standard of 5,500 μ g/l, a value far greater than the French generic fungicide/pesticide 0.5 μ g/l standard for groundwater. Based on an SAR approach, and consistent with the metolachlor data, a criterion for groundwater of 5,500 μ g/l, and for soil of 310 g/kg would be appropriate for ofurace.

Key words: ofurace, structural activity relationships, comparison standards