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Analysis of the properties of Picloram and proposal of a compound as its replacement

Jorge Eliecer Buitrago Salazar*, Olga Lucia Ramos Sandoval, Dario Amaya Hurtado

Universidad Militar Nueva Granada, Facultad de Ingeniería en Mecatrónica, Bogotá, Colombia; Grupo de Aplicaciones Virtuales – GAV.

Abstract: Pesticides such as Picloram, are considered toxic to humans and the environment, which is necessary search new substancesless toxics. With the analysis of the structure and some molecular descriptors, it is possible to propose new compounds, in which it can reduce the toxicity in humans without affect its power as herbicide. This paper presents the results of the molecular structure of the new compounds, starting with the Picloram. The characteristics of absorption, metabolism and toxicity of each possible replacement were evaluated. From which, a less toxic compound containing specific characteristics of an organochlorine herbicide was obtained. From the 10 compounds tested, 2 were selected, in order to carry out the proposals for replacement the pesticide. The compound 4-amino-6-chloropyridine-2-carboxylic acid (substance I) got less simulated toxicity. In the toxicity for some species, an increase of 8.36 % on average in the lethal dose was founded.
Keywords -Organochlorine Herbicide, Picloram, ADMET Properties, Toxicity.

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