MEMBRANE-THIRAM INTERFACE DESCRIBED BY SOLUBILITY

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ABSTRACT: In the present study, the carcinogenicity of a fungicide particularly used in seed defense, Thiram (C6H12N2S4) is discussed, the interest in this compound is due to the fact that it is among the compounds under reassessment in the National Agency of Sanitary Surveillance (ANVISA), the official body responsible for regulating these products in Brazil. And for this analysis, we used the information found through the Partition Logarithm Coefficient (LogP), this variable describes the interaction of the pesticide with the cell membrane and its tendency to transpose it based on solubility. In this work, after the molecular structure design, the LogP property was calculated in the ALOGPS 2.1 software environment, for comparison with other values already established in the relevant literature. The results showed low interaction between the membrane and the pesticide, suggesting a low invasiveness for Thiram.

Key words: Carcinogenic, Anvisa, Agrotoxic