

A theoretical analysis of the relationship between the electronic structure of indole derivatives and their phytotoxicity against *Lactuca sativa* seeds

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Allelopathic effects of a chemical compound strongly depends on the target species, dose or concentration employed, structure of the molecule and physical properties, such as water solubility, lipophilicity and others. In this work, we present the results of a preliminary quantum-chemical analysis of the possible relationships between the electronic structure of a series of indole derivatives and the percentage of germination inhibition (I) of *Lactuca Sativa* seeds. The results allow predicting phytotoxicity activity of these compounds, the structural features of an ideal indole derivative, as well as some structural characteristics of the active site.