

ANALYSIS OF DIFFERENCE OF HOMO-LUMO ENERGY TO COMPREHENSION OF INTERACTION BETWEEN THE HUMAN DNA AND THE GLYPHOSATE

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Abstract

The indiscriminate usage of agrochemicals, no matter if it is for the employee quantity or for using forbidden products, leads inevitably to two recurrent problems on literature: the human and environmental contamination. Among the others impacts that affect the humans, like quick and chronic intoxication, it is relevant to talk about carcinogenic potential of these products, and their carcinogenics. In this study, we analyze o Glyphosate Agrochemical, widely used in the field in Brazil and outside, but that currently is under inspection of National Health Surveillance Agency of Brazil (ANVISA). In this way, the objective of this study was evaluating the difference of energy between the DNA electronic orbitals and of Glyphosate Agrochemicals, the named Homo-Lumo (H-L) energy difference to assert the interaction between them. About the DNA, this calculus is concentrated on Guanine, since it has a high level of electronegativity, compared to the others nitrogen bases. To realize the calculus, we make a molecular drawing and simulation of conformational analysis to molecular geometric optimization on *HyperChem* 8.0. After this, we made the second optimization using the DFT method under the B3LYP functional and the 6-311++g(d,p) bases on Gaussian09. This result was displayed on Chemcraft 1.6 software, where is possible to identify the as orbital energies and their differences used in this works. Finally, we observed that energy difference calculated to Glyphosate is 4,07 eV, a value that, even without been conclusive, put this agrochemical next to de carcinogenic substances.