# Agrochemicals and Neurological Diseases: A New Method for Searching Biological Process Networks through Molecular Docking Codes

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Brazil is the world's largest pesticide consumer. The use of these products in agriculture is a serious public health problem that generates various diseases such as cancer, congenital malformations, endocrine and immunological diseases. Research on pesticide association with diseases are labour-intensive and time-consuming. The Methodology of this work was to analyse the water of 20 wells located around Vale do Jaguaribe-CE, Brazil. We detected the presence of 13 pesticides in the water samples by HPLC technique. The three highest concentrations were modelled and inserted in biological process networks to verify the change in three common diseases in the studied communities: Alzheimer, Parkinson and long-term depression. As the process of Interactomas is limited only to the tracking of genes and proteins, a new searching technique was developed using construction software and the modelling of molecular docking codes indexed in Protein Data Bank to show the compatibility of connection and its function via Chemical-protein interaction. Within all of the generated networks, it was verified the presence of 39 processes associated with diseases as a whole, and the proteins most connected to the molecules were GRIA1, GRIA2, GRIA3, PARK2 and APP proteins of great influence to the generation of the analysed diseases. To validate the results, the process was repeated showing 99.2% compatibility. This leads to the conclusion that the pesticides found in water are directly related to the formation of neurological diseases. This searching technique of using docking codes can be applied to other studies about diseases that need to find biological processes and prospectively, seek for a treatment by monitoring these pathways.

**Awards Won:**