MIMÉTICOS: UMA ROTA PARA ELETRODOS DESCARTÁVEIS NA QUANTIFICAÇÃO DE PESTICIDAS?

Mimetics: A route for disposable electrodes in the quantification of pesticides?

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Abstract: The quantification of pesticides in foodstuffs is a strategic subject due to the hazardous effect of such substances in human health. The governmental ANVISA proposed a long-term project, called PARA, aiming to monitor the amount of pesticides residues in several types of fruits and legumes, in the whole country. However, difficulties concerning the analytical techniques (GC and HPLC, mostly) costs and long time necessary for analysis imposes a severe drawback to the objectives of such program, in fact, the last available report from such measurements was published in 2014, being not useful for daily control of such contaminants. The use of biosensors may be a more convenient analytical method due to its low price and short time of analysis. However, the reproducibility of such measurements is yet low enough to limit the available publications almost only to development of new materials and systems. This is a clearly indication that the use of disposable electrodes (like those of diabetes control) may be helpful. However, enzymes (mainly acetylcholinesterase, the most used for organophosphorous and carbamates quantifications) are quite expensive and unstable to be employed in such biosensors. So, mimetics are the natural route for such devices. In this presentation, the development of organic molecules that can hydrolase acetylcholine (the enzyme substrate) in the Group of Electrochemical Materials and Electroanalytical Methods, IQSC - USP is discussed. The studies begun with the synthesis and characterization of the 4-[(1E)ethanohydrazonoil]benzoic acid in the esterase of acetycholine. The organic molecule is easy to synthesize, cheap and presented the reaction site similar to the active site of the enzyme. So, it showed some activity in the hydrolyzes, although the reaction rate was much slower than the corresponding enzyme. Studies continued with several hydrazones but with very similar results. To improve the reaction rate, a new class of mimetic molecules was synthesized through the modification of the functional groups of the polyacrylamide polymer with carboxylic and hydroxamic acids. The resulting polymer, the polyhydroxamicalcanoato (PHA), showed reaction sites with geometric distances very close to the enzyme acetylcholinesterase and very improved capability to hydrolase the ester acetylcholine with much higher reaction rates. The reactivity of PHA was also inhibited by the presence of carbamates and organophosphorous pesticides, indicating the possibility to use it as a low-cost mimetic in dischargeable electrochemical biosensors. The interactions between the active centers of the polymer and the target molecules (acetylcholine and pesticides) were analyzed by theoretical studies.

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