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DEVELOPMENT OF AN ELECTROCHEMICAL *CYCLOOXYGENASE* BIOSENSOR TO EVALUATE TARGET-DRUG VIABILITY AND INTERACTIONS

Resumo: The process for drug development is costly. The 1st stage, discovery, and development, is carried out throughout trial-and-error tests, involving cultures of animal cells and tissues [1]. The drug development market moved 79.6 billion US$ in 2018 and has been expanding steadily since 2010 [2], with non-steroidal anti-inflammatory drugs (NSAIDs) being the most relevant. In order to facilitate drug development, a biosensor was developed to study the interaction between non-steroidal anti-inflammatory drugs and their target enzyme, cyclooxygenase-2 (COX). For this purpose, a glassy carbon electrode modified with mouse liver homogenate is used to characterize the electrochemical behavior of COX, present in the homogenate. The enzyme showed three reduction processes, all involving one electron and one proton. The 3rd process was attributed to the reduction of Iron IV to III, in the active center of the enzyme, which in the presence of peroxide, originates a catalytic cycle, and represents the peroxidase function of the enzyme. According to Smith and Marnett [3] in the absence of endoperoxide, responsible for the self-activation of the enzyme through the presentation of its metallic site, an enzyme can be inactivated. Thus, a protocol was developed using differential pulse voltammetry to evaluate the signal of the 3rd enzyme reduction process in the presence of its substrate, hydrogen peroxide, and of its substrate in the presence of several NSAIDs. Note that acetylsalicylic acid (AAS), dipyrone (MTM) and ibuprofen (IBU) showed a percentage of flux with the enzyme of 64, 74 and 84%, respectively. In order to distinguish the type of follow-up (by allosteric or by redox interaction) EPR and Hematin (enzyme active site mimetic) were used. The astonishing results that the AAS and the IBU presented a lower slope signal than those obtained by the voltammetric method. In this way, the inflammation caused by AAS and IBU was caused by allostery, while MTM presented a redox. Therefore, the developed sensor allowed discerning the type of trend caused, as well as providing a semi-quantitative value of the trend trend. The values obtained may be used in QSAR studies (quantitative relationship between chemical structure and biological activity), which should facilitate the development of new drugs in academia and industry.

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