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PREDICT AND ENHANCE BIOCOMPATIBILITY AND BIODEGRADABILITY OF POLYHYDROXYALKANOATES IMPLANTS USING MACHINE LEARNING ALGORITHMS

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The most promising area of application for biomaterials is medicine, which urgently needs biocompatible materials for producing medical instruments, drug delivery systems, implants, and bio-constructors of organs and tissues in cell and tissue engineering. The interdisciplinary approach used by tissue engineering is aimed at developing tissue and organ replacements – complex structures of functioning cells attached to cell scaffolds. The effectiveness of this approach is largely based on the properties of the material used to construct cell scaffolds the necessary properties of the scaffold are determined by the properties of the starting material and the technology employed to process it. Therefore, the main challenge for production of effective bio constructs is the availability of proper biodegradable and biocompatible material [1].

The discovery of Polyhydroxyalkanoates (PHAs) – thermoplastic, biodegradable, and biocompatible microbial polymers – was a notable event for biotechnology of novel materials. Being UV resistant, non-hydrolyzed in liquid media, and thermoplastic, PHAs are processable from different phase states (solution, emulsion, powder, melt) by available techniques. PHAs have great potential as materials for regenerating damaged skin, repairing the defects of soft tissues, bone engineering, cardiovascular applications, blood vessels, heart valves.

To improve the quality of the PHA films, in this research we will combine both the experimental part by growth the bacteria with different precursors to produce deferent tips of films with different polymers (PHB, PHV, PHHx). extract this polymer treated it to make PHA film.

Examination of the obtained films using atomic force microscopy (AFM) and use the output data from the AFM as an input data in different machine learning and deep learning processes. trying to find correlation between density function theory calculations (DFT), quantitative structure property relationship (QSPR), quantitative structure activity relationship (QSAR), and molecular dynamics simulations (MD).

Use the obtained models to enhance and improve the biocompatibility biodegradability and remove or improve some unwanted features such the high degree of crystallinity and low shock resistance and are rigid and prone to physical ageing. Upon completing of this work, we will be able to predict the qualities and properties that we want only through the molecular structure and apply it directly to produce new types of films according to the need and the properties to be obtained.

References:

1. Volova T. et al. Properties of degradable polyhydroxyalkanoates with different monomer compositions // Int J Biol Macromol. Elsevier, 2021. Vol. 182. P. 98–114.