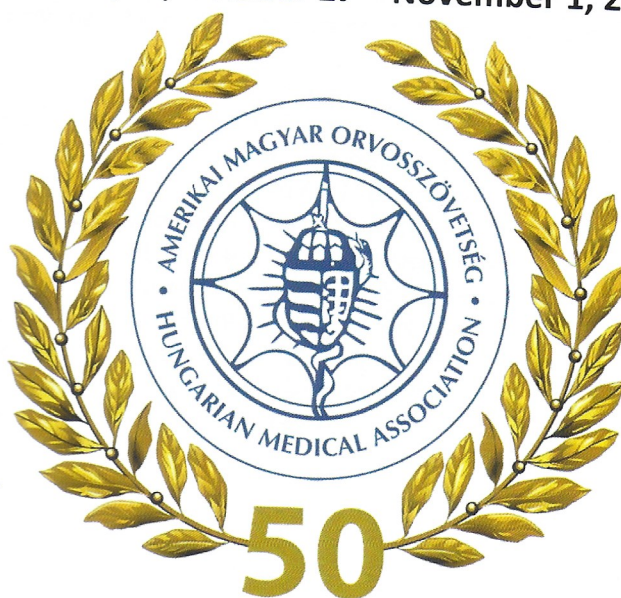


CURRENT DEVELOPMENTS IN BIOMEDICAL AND CLINICAL SCIENCES

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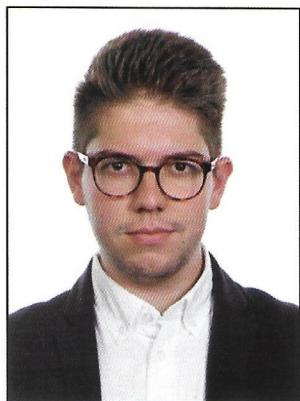
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INVESTIGATION OF THE ROLE OF ARYLSULFATASE B IN THE PATHOGENESIS OF PROSTATE CANCER BY PREDICTION OF PROTEIN-PROTEIN INTERACTIONS WITH ARTIFICIAL INTELLIGENCE

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I am a sixth year medical student at the University of Medicine, Pharmacy, Science, and Technology of Targu Mures and my main areas of interest are molecular biology, oncogenetics, cardiogenetics, as well as bioinformatics and structural biology.

Aim: The low expression of arylsulfatase B (ARSB) has been identified as a useful biomarker in predicting prostate cancer prognosis and recurrence, as supported by previous studies. The binding of proteins together and the formation of functional complexes between them represent an essential part of numerous physiological processes. While the experimental study of protein-protein interactions can present significant challenges, the mapping of these interactions in silico using artificial intelligence has the potential to yield valuable insights. The aim of this research is to examine the function of ARSB and its potential involvement in prostate tumorigenesis, while utilizing data from bioinformatics databases and employing artificial intelligence-based interaction predictions.

Methods: The initial phase of our investigation entailed an examination of the ARSB interaction network through the utilization of the STRING online database, where the confidence value for the strength of the connection was set to 0.400. Subsequently, a one-by-one analysis of the proteins comprising the most optimal interaction pathway was conducted using two machine learning bioinformatics tools. These software tools employ different techniques for interaction prediction, with the PEPPI system utilizing the amino acid sequence of proteins and the HDock Server tool employing the tertiary structures.

Results: The strongest interaction pathway between ARSB and proteins involved in prostate cancer development was represented by GUSB (0.778) and HSP90AB1 (0.626) proteins. The PEPPI system predicted the most likely interaction of the HSP90AB1 protein with ERBB2 ($\log(\text{LR}) = 0.995$), TP53 ($\log(\text{LR}) = 0.965$) and EGFR ($\log(\text{LR}) = 0.874$) proteins. In contrast, the HDock Server tool showed the highest confidence values for interaction of the HSP90AB1 protein with BRAF (0.9141), EGFR (0.9020), and TP53 (0.8750) proteins.

Conclusions: The PEPPI system predicts ERBB2, whereas the HDock Server predicts the BRAF protein as the most probable interaction partner for the HSP90AB1 protein. It is noteworthy that both bioinformatics tools indicated a considerable interaction probability between the HSP90AB1 protein and the EGFR, as well as the TP53 proteins. Our findings demonstrate the advantages of employing artificial intelligence in the field of molecular biology and highlight how this technology can also help to elucidate the potential role of ARSB in prostate cancer development.

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