УНИВЕРЗИТЕТ У НОВОМ САДУ
ТЕХНОЛОШКИ ФАКУЛТЕТ НОВИ САД

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Title of the project:
Chemometric approach to the concept of sustainable development in the field of continuous design of anticancer compounds towards prostate cancer cells

Project number:
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The Provincial Secretariat for Higher Education and Scientific Research of AP Vojvodina

Duration of the project:
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802.747,00 RSD

Logo or acronym:
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Research area of the project:
Natural sciences

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Key words:
Chemometrics, QSAR modeling, Biologically active compounds, Steroids

Project summary:
The research conducted within this project is based on computational modeling of anticancer compounds using adequate computer programs for molecular design and on chemometric analysis of their anticancer activity and chromatographic behavior. Chemometrics, as a relatively young scientific discipline, is applicable in the analysis, interpretation and processing of data from various scientific disciplines.

Within this project, the correlations between the chemical structure and anticancer activity of molecules against prostate cancer cells PC-3 (with emphasis on different steroid derivatives) were investigated, as well as the correlation of different physicochemical properties of molecules with structural descriptors and predictors of pharmacological activity. QSAR (Quantitative Structure-Activity Relationships) and QSRR (Quantitative Structure-Retention Relationships) analyzes of steroid derivatives with anticancer activity were performed using various mathematical and statistical methods, such as: linear regression (LR), multiple linear regression (MLR), analysis principal components (PCA), hierarchical cluster analysis (HCA), principal components regression (PCR), partial least squares regression (PLS), artificial neural networks (ANN). The quality of the obtained mathematical models was confirmed on the basis of the values of certain statistical parameters. The internal validation was used for model validation, as well as a much more rigorous external validation procedure, which involves the use of an external group of molecules that was not used to define the model.
The obtained results enable the prediction of anticancer activity of structurally similar steroid derivatives and thus enable the selection of derivatives with significant anticancer activity, and can be applied as certain guidelines for further synthesis of potential new therapeutics. Also, the obtained QSRR relations significantly contribute to the definition of the chromatographic lipophilicity of steroid derivatives, as one of the key factors for the distribution of molecules in the biological system.

Graphical abstract or graphical presentation of project results: