ACTIVITY REPORT 2024

For the implementation of the Postdoctoral Project **PD 90/2020**

Advanced chemometric methods applied for authentication and traceability of Transylvanian agriproducts – *AGRICHEM*
Stage 3. Chemometric models validation and testing, using blind sample, for traceability and authentication purposes
(January-September 2024)

Summary of the stage

Beyond authenticity, which focuses on identifying and determining the origin of samples, traceability refers to the quantitative assessment and qualitative discrimination of components in complex arrays. In the present case, traceability aimed at detecting counterfeiting of labeled products and evaluating the composition of heterogeneous or multivarietal mixtures. A common authenticity-traceability problem concerned the prediction of the geographic origins of monovarietal samples. It is generally handled by linear discriminant analysis or other pattern recognition methods.

Content of the scientific and technical report (RST)

1. ICP-MS and IRMS analysis of unknown samples
2. Traceability of unknown samples using chemometric models
3. Identification of possible false declaration regarding the origin of agriproducts
4. Results dissemination.

For this stage of testing the unknown samples, 11 juice samples and 10 mushrooms were analyzed (elemental and isotopic content). The results obtained after the application of the classification and prediction analysis are presented.

The experimental results of blind samples obtained after the IRMS and ICP-MS analysis, were joined in a single data file, which constituted the working matrix for the subsequent chemometric processing. The chemometric models obtained in previously stages of the projects, were applied for the blind sample's prediction. In the case of juices, the LDA was applied for three different matrices. For the first case (three categories of samples, apples, oranges and other fruits) the classification percent were not very high, for the second case consisted only of two categories (apples, oranges) the percent were higher around 90%, while for the last data set only apples (commercially and freshly squeezed) a percent of 100% was reached. The same tendency of classification was obtained by applying ANNs, where the blind samples were predicted to be apples juices.

In the case of mushrooms, the same algorithm was applied, the working matrix was used for LDA and ANNs chemometric processing. LDA did not manage to classify all blind

mushrooms, the percent did not exceed 90%. But, ANNs successfully classified samples the samples in percent of 100%.

As an important conclusion of testing blind samples, a very important aspect is represented by the characteristics of the initial set. It should encompass as much as possible all the characteristics of the blind samples. Also, the larger, more comprehensive the initial set of samples that is used in creating the classification model, the higher the vote classification percentages will be, that is, the identifications will be more accurate and the results more robust

In the case of the unknown samples tested at this stage, both mushrooms and fruit juices, no false statements were identified. The prediction and assignments made for the unknown samples, using the classical (LDA) and advanced (ANN) chemometric methods, led in all cases to 100% predictions.

Results dissemination for this stage:

1. Update of web page https://www.itim-cj.ro/PNCDI/agrichem/#
2. Two presentations to economic environment, presenting the importance of the research topic in the field of food quality and safety, highlighting the results obtained, for the analyzed samples, in identifying the best differentiation markers for fruit and mushroom juices from spontaneous flora.
3. **Oral presentation entitled „FT-IR analysis followed by chemometric approach for rapid screening of wild mushrooms”**, authored by **Ioana Feher**, Veronica Floare Avram, Florina Covaciu, Olivian Marincas, Romulus Puscas, Dana Alina Magdas la Conferinţa ***12th International Conference, Agriculture & Food, 12-15 August 2024, Burgas, Bulgaria***
4. **Working visits and experience exchange,** in 12 April 2024, Mr. dr. Michael S. Bloom, professor at George Mason University, Virginia, S.U.A., “Department of Global and Community Health College of Public Health”, participated in a working visit to INCDTIM Cluj-Napoca, in order to identify complementary research themes for future collaborations.

5. **Poster presentation entitled "Advanced chemometric methods for fruits juices differentiation",** authored by **I Feher,** A Dehelean, G Cristea, R Puscas, D A Magdas and C Sârbu, at ***12th International Conference, Agriculture & Food, 12-15 August 2024, Burgas, Bulgaria***
6. **Poster presentation entitled "WILD MUSHROOMS EVALUATION THROUGH ELEMENTAL PROFILE FOLLOWED BY ADVANCED CHEMOMETRIC APPROACH",** authored by **Ioana FEHER,** Adriana DEHELEAN, Gabriela CRISTEA, Veronica FLOARE AVRAM, Florina COVACIU, Romulus PUSCAS, and Dana-Alina MAGDAS, at ***23rd International Conference "Life Sciences for Sustainable Development", 26-28 September 2024, Cluj-Napoca, Romania***
7. **Stage report** of the project.
8. **Final report** of the project.

Data

25.09.2024

Project coordinator

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