1. PHD PROJECT DESCRIPTION (4000 characters max., including the aims and work plan, all in English)

Project title: Determination of macro and microelements and main phytocomponents in teas and herbs for drinks as markers of geographical origin and application for their authenticity

1.1. Project goals

Project is focused on determination of macro and micro metals in teas and herbs drinks available on the European market by Inductively Coupled Plasma Mass Spectrometry (ICP MS). SEM-EDX analysis and imaging in order to find the ionic speciation in leaves and correlation with metals distribution. The second goals is identification and determination of the main phytocomponents in teas and herbs by IR and Raman imaging of the solid materials. The results of analyses will be used to develop a reliable multivariate classification model of production using statistical methods applied in quantitative chemical analysis. Pattern recognition methods such as principal component analysis (PCA), linear discriminant analysis (LDA), and artificial neural networks (ANN), will be ere applied to differentiate the tea and herbs types.

1.2. Outline

The demand for health foods is increasing, hence new analytical tools for their authentication are compulsory. The project focuses on biomarkers by analytical approaches for authentication of tea and herbs used for preparation of herbal extracts. The authenticity of tea, herbs and their mixtures as a healthy product or dietary supplements has become important issue also for food industry. Because the supply chains become complex, hence there is a problem of the quality and adulteration of the original products. Moreover the tea and herbs produced in different regions varies greatly. One of analytical method for testing the geographical origin of tea and herbs can be SEM EDX with the ICPMS as reference method. SEM-EDX can be used as a screening technique of the solid samples for mineral and elemental analysis with applications in the traceability of tea and herbs. The novelty of SEM EDX can be related to the mapping of elemental composition to as low as carbon atomic number. The SEM EDX mapping correlation will be used for the speciation of ionic composition of solid samples and correlation with ICPMS . Pattern recognition methods such as principal component analysis (PCA), linear discriminant analysis (LDA), and artificial neural networks (ANN), will be applied to differentiate the samples types. It is unlikely that the authentication of tea and other food products can be attained by the measurement of a multiple markers and elucidation of chemical or physical profiles supported by multivariate statistical analysis. Therefore in the project the methods of molecular spectroscopy will be applied for the development of robust classification models. As solution in the project IR and Raman imaging of the main phytochemical components will be examined in tea and herbs used for the production of "herbs teas". The main components will be identified and determined by chromatographic techniques HPLC,

GC-MS and data will be used for the imaging of the bands from these components in IR and Raman spectra. Data from IR and Raman imaging will be correlated with SEM EDX using mentioned above pattern recognition methods. The novelty of the project will be on new analytical method for determination of mineral and organic components in tea and herbs and correlation with origin and food safety using chemometric methods.

1.3. Work plan 1. Literature studies are foreseen in first 3 months of the project.

2) Extraction of natural compounds from tea and herbs samples and identification of phytocomponents by chromatographic methods, **3)** determination of compounds specific to tea and herbs by HPLC **4) determination of** elements in studied plants using destructive and non-destructive techniques using ASA, ICP-MS, SEM-EDX and their correlation for the origin, **5)** analysis of phytocomponents in tea and herbs by IR and Raman imaging spectroscopy, 6) application of chemometric methods to discrimination of analyzed plants, **6)** Development of chemical composition model for the studied plant materials based on the content of phytocomponents and macro and micro-elements, and correlation with the geographical origin.

1.4. Literature

1. Lim C. M, Carey M., Williams P. N., Koidis A.. Rapid classification of commercial teas according to their origin and type using elemental content with X-ray fluorescence (XRF) spectroscopy, Cur Res. in Food Sci. 2021, 4, , 45-52.
2. Fernández-Cáceres P. L., Martín M. J., Pablos F., González G. A., Differentiation of Tea (*Camellia sinensis*) Varieties and Their Geographical Origin According to their Metal Content, J. Agric. Food Chem. 2001, 49, 10, 4775–4779,
3. Fernández, P. L., Pablos, F., Martin, M. J., González, A. G., Multi-element analysis of tea beverages by inductively coupled plasma atomic emission spectrometry, .Food Chemistry, 2002, 76, 483–489.
4. Filipiak-Szok A., Kurzawa M., Szłyk E., Determination of toxic metals by ICP-MS in Asiatic and European medicinal plants and dietary supplements, J Trace El Med and Biol, 2015, 30, 54-58.

1.5. Required initial knowledge and skills of the PhD candidate: knowledge of analytical chemistry, in particular instrumental techniques used in qualitative and quantitative analysis such as: ICP MS , SEM EDX, AAS, XRF, IR, Raman, chromatographic techniques (HPLC, TLC, GC-MS), basic knowledge of

chemometry, basic skills in laboratory work, knowledge of speaking and writing in English.

1.6. Expected development of the PhD candidate's knowledge and skills It is expected that the PhD candidate will learn new techniques of extraction and purification of natural compounds from plants. He/she will be able to use modern techniques for the characterization of the extracts and elements analysis.