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

Project title: Development of a method for nanostructural modification of substrates surface for low molecular weight compounds analysis.

1.1. Project goals

The goal of the project is to develop the method for the preparation of the nanostructurally modified substrates which can be utilized as universal targets/platforms for the profiling of low molecular weight compounds (LWMC).

1.2. Outline

LWMC comprises wide spectrum of compounds such as lipids, sugars, amino acids, flavonoids, antibiotics, etc. Determination of LWMC compounds is required in various research fields including study on the quality of the products in food industry, determination of diseases biomarkers in clinical studies, pollution of environment or search for evidence in forensic science. Separation techniques such as gas or liquid chromatography coupled with mass spectrometry are considered as a "gold standard" in the determination of LWMC in complex matrices. However, these techniques require labor intensive sample preparation and separation parameters optimization. Thus, currently the untargeted approach sample profiling with the use of MALDI or surface enhanced Raman spectroscopy (SERS) become more popular for the detection of marker molecules [1-3]. Such an approach enables determination of characteristic signals from multiple compounds in one run and requires minimum sample preparation.

The utilization of nanoparticles and nanostructured surfaces in the analytical chemistry has shown to enhance the sensitivity of the method [2,3]. Moreover, it allows to eliminate additional compounds utilized in analysis (such as matrix in MALDI) so the data interpretation may be simplified [1-4]. However, till now there is lack of complex solutions on the market for such type of analysis which requires the development of the methods to produce substrates.

Preparation of both NALDI and SERS targets is significant research problem due to reproducibility and stability issues, challenges to study the distribution of nanoparticles on the plate and their relatively low adhesion to the surface of plate. The studies provided in our group has shown that chemical vapor deposition (CVD) technique may help in the production of nanostructured surfaces for analytical chemistry [1]. In general technique has shown to be useful to obtain nanolayers of

silver on the medical devices, such as implants, and thus to prevent the development of bacterial biofilms [5]. In turn, to the best of our knowledge our group was the first that shows the possibility to utilize of this technique to produce substrates for NALDI [1]. What is important the technology enables the production of nanolayers of different coinage metals [6]. Moreover, we have the possibility to use also atomic layer deposition method (ALD), which gives the possibility to obtain even monolayer of nanoparticles, because ALD reactor (Beneq TFS 200) is under Department of Inorganic and Coordination Chemistry supervision. Still, there is a lack of knowledge on the influence of type and amount of utilized precursors on the performance in NALDI and SERS. Thus, the aim of the project is to select the proper conditions to produce nanostructurally modified surfaces which will have the best performance.

Work plan

The work will be realized according to following research tasks:

- optimization of the deposition processes of thin layers of metal and metal oxide nanoparticles (e.g. Ag, Au, TiO_2) on metal surfaces (e.g. stainless steel, brass, metal alloys);
- characterization of obtained nanolayers by means of their structure, morphology, mechanical properties as well as they performance as coatings on targets/platforms in the spectrometric (NALDI-MS) and spectroscopic (SERS, SEIRA) techniques (on standards);
- development of preparation techniques for the extraction of LWMC (lipids, flawonoids, polifenols) from biological matrices (food and food additives, bacteria, clinical samples) with subsequent profiling by spectrometric (MALDI vs NALDI) and/or spectroscopic (RAMAN vs SERS; SEIRA vs FTIR) techniques;
- data processing.

1.3. Literature *(max. 10 listed, as a suggestion for PhD candidate)*

[1] G. Sagandykova, et al. Silver Nanostructured Substrates in LDI-MS of Low Molecular Weight Compounds, Materials, 2022, 15(13), 4660;

[2] P. Pomastowski, et al. Complementarity of Matrix- and Nanostructure-Assisted Laser Desorption/Ionization Approaches, Nanomaterials, 2019, 9(2), 260;

[3] F. Neubrech, et al. Surface-enhanced infrared spectroscopy using resonant nanoantennas, Chem. Rev., 2017, 117, 5110-5145;

[4] E. Maślak, et al. Isolation and Identification of Lactococcus lactis and Weissella cibaria Strains from Fermented Beetroot and Investigation of Their Properties as Potential Starter Cultures and Probiotics, Foods, 2022, 11(15), 2257;

[5] P. Piszczek, A. Radtke; Silver Nanoparticles Fabricated Using Chemical Vapor Deposition and Atomic Layer Deposition Techniques: Properties, Application and Perspectives: Review, Ed. M.S. Seehra, A. D. Bristow, Noble and Precious Metals, InTech, London UK 2018, online ISBN 978-1-78923-293-6, Chapter 9, p 187-213;

[6] A. Grodzicki, et al. Copper (I), silver (I), and gold (I) carboxylate complexes as precursors in chemical vapour deposition of thin metallic films. Coordination Chemistry Reviews, 2005, 241, 2232-2258.

Required initial knowledge and skills of the PhD candidate

PhD candidate:

- should be skilful familiar with the basic methods of synthesis and analytical methods for the characterization of nanomaterials
- have creative thinking
- should have experience in LDI-MS techniques.
- should possess willingness to increase the competence in the field of material engineering and analytical chemistry
- should have very good command of English in writing and speaking, due to planned extensive scientific cooperation
- should be able to work in a team.

1.6 Expected development of the PhD candidate's knowledge and skills: The PhD student will acquire interdisciplinary knowledge in the field of material engineering, methods of instrumental analysis to characterize the structure, morphology, mechanical properties of the materials. Moreover, the PhD student will gain knowledge and skills in field of analytical chemistry and microbiology**.** Additionally, the skills in the interpretation of analytical and statistical data will be developed during PhD study. PhD student also will develop soft skills like ability to organize work, skills in working with scientific literature, preparing the publications and conference presentation.