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

Project title: Development of Analytical Methods for Low-Molecular-Weight Bioactive Compounds (Lipids, Derivatives, Flavonoids, Antibiotics) Using SALDI and NALDI Techniques with PVD, CVD, and ALD Substrate Preparation

1.1. Project goals.

The main goal of this PhD project is to develop and optimize analytical methodologies for the qualitative and quantitative assessment of low-molecular-weight bioactive compounds, including lipids, lipid derivatives, flavonoids, and antibiotics, using Surface-Assisted Laser Desorption/Ionization (SALDI) and Nanostructure-Assisted Laser Desorption/Ionization (NALDI) mass spectrometry techniques. A particular focus will be on designing and preparing innovative substrates employing Physical Vapor Deposition (PVD), Chemical Vapor Deposition (CVD), and Atomic Layer Deposition (ALD) methods. These substrates are expected to significantly enhance desorption/ionization efficiency, sensitivity, selectivity, and reproducibility in the analysis of complex biological matrices (Mametov et al., 2024; Arendowski et al., 2024). Ultimately, the project aims to generate high-throughput, matrix-free MS protocols applicable to pharmaceutical, biological, and food science investigations (Czeszewska-Rosiak et al., 2024).

1.2. Outline

The project will integrate advanced materials science with analytical chemistry. The approach involves the fabrication of nanostructured substrates (e.g., metal nanoparticles, metal oxides, composite materials) using PVD, CVD, and ALD techniques, followed by their physicochemical characterization (SEM, AFM, XPS, XRD, UV-Vis) (Mametov et al., 2024). These engineered surfaces will be systematically evaluated for SALDI and NALDI performance with selected standard compounds and real samples. Optimization of laser parameters (e.g., wavelength, pulse energy) will be performed to achieve maximum analytical performance (Arendowski et al., 2024). Finally, the developed methods will be applied to real-world samples such as plant extracts, pharmaceutical formulations, and biological fluids to assess their practical utility (Złoch et al., 2023; Czeszewska-Rosiak et al., 2024).

1.3. Work plan will be realized according to main research task

Substrate preparation and characterization:

- Design and fabrication of nanostructured SALDI/NALDI substrates using PVD, CVD, and ALD on various supports (Si, Al, stainless steel)
- Characterization of surface morphology, roughness, chemical composition, and optical properties using advanced microscopy and spectroscopy techniques.
- Analytical optimization and validation: Evaluation of substrate performance with representative standards of lipids, flavonoids, and antibiotics
- Optimization of laser desorption/ionization parameters and mass spectrometric acquisition settings to improve sensitivity, selectivity, and reproducibility.

- Application to real samples: Analysis of biological and environmental samples, including plant extracts, blood plasma, dairy products, and antibiotic formulations
- Determination of limits of detection (LOD), quantification (LOQ), and method robustness.
- Method dissemination and publication: Development of detailed analytical protocols and application guidelines. Preparation of manuscripts for submission to high-impact peer-reviewed journals and presentations at international scientific conferences

1.4. Literature

Mametov, R., Sagandykova, G., Monedeiro, F. F. S., Florkiewicz, A., Piszczek, P., Radtke, A., & Pomastowski, P. (2024). Metabolic profiling of bacteria with the application of polypyrrole-MOF SPME fibers and plasmonic nanostructured LDI-MS substrates. Scientific Reports, 14, 1–13. https://doi.org/10.1038/s41598-024-56107-0

Czeszewska-Rosiak, G., Złoch, M., Radosińska, M., Florkiewicz, A., Tretyn, A., & Pomastowski, P. (2024). The usefulness of the MALDI–TOF MS technique in the determination of dairy samples' microbial composition: Comparison of the new EXS 2600 system with MALDI Biotyper platform. Archives of Microbiology, 206, 1–11. https://doi.org/10.1007/s00203-024-03885-w

Złoch, M., Maślak, E., Kupczyk, W., & Pomastowski, P. (2023). Multi-instrumental analysis toward exploring the diabetic foot infection microbiota. Current Microbiology, 80, 1–15. https://doi.org/10.1007/s00284-023-03384-z

Arendowski, A., Sibińska, E., Miśta, W., Fijałkowski, P., Złoch, M., Gabryś, D., & Pomastowski, P. (2024). Study of sample preparation influence on bacterial lipids profile in matrix-assisted laser desorption/ionization time-of-flight mass spectrometry. Lipids, 59, 13–26. https://doi.org/10.1002/lipd.12383

1.5. Required initial knowledge and skills of the PhD candidate

PhD candidate should be skilful and intellectually manipulative, familiar with the separation (LDI-MS) and instrumental techniques (FTIR, SERS, UV-VIS, SEM, TEM-EDS). Experienced with the sample preparation and their further analysis using LDI TOF MS as well as skills in the mass spectra recoding. Knowledge in field of protein biochemistry will be highly honoured. Knowledge about work in programs used to identify mass profiles of microorganisms like FlexAnalysis, FlexControl, and MALDI Biotyper will be favoured.

1.6. Expected development of the PhD candidate's knowledge and skills

PhD candidate will gain knowledge and skills in field of analytical chemistry and mass spectrometry. Candidate will get specialized knowledge in nanoparticles synthesis and their physicochemical characterization by instrumental techniques.

Moreover, the interpretation of analytical and statistical data will be developed during PhD study. During the study student will be able to present obtained data in form of high-impact factor publication and posters and oral presentations at domestic and international conferences. As part of the PhD project, it is planned to develop new technological solutions with a high level of invention, legally protected by a patent.