Title: Molecularly imprinted hybrid polyoxazoline materials as scavenging molecular probes used for rapid analysis with ambient mass spectrometry

1. The goal of the project

The project's goal is to synthesize hybrid polyoxazoline-based molecularly imprinted materials and their use as scavenging molecular probes for subsequent quantification using an ambient mass spectrometry system. The scavenging molecular probes are solid materials that are composed of inorganic material that is responsible for their shape and available surface area, whereas the polyoxazolines are polymer forming an outer layer on the inorganic material. They are responsible for forming interactions with targeted chemical compounds (called analytes), which they selectively adsorb from their surrounding area, which usually is a highly diluted environmental sample. Considering that a small amount of these selective adsorbents is used for a process, so-called preconcentration occurs, which means that the concentration of analytes in the solid material is much higher than in the starting solution. This effect significantly impacts the whole analytical procedure, as it dramatically improves the analytical method's detection limits, selectiveness, and applicability range. After adsorption, the obtained hybrid materials can be directly analyzed using ambient mass spectrometry, an analytical tool that allows rapid analysis, is very versatile, and allows direct analysis of solid materials. The project aims to find a correlation between the structure of the polyoxazoline-based hybrid molecularly imprinted materials and their usefulness in detecting and quantifying the target analytes. Moreover, the project will be focused on improving the already existing detection limit of the targeted analytes, including hazardous compounds such as explosives, drugs of abuse, prescription drugs, and herbicides.

2. Research description

The research will be conducted within five work packages (WPs). In the first WP, a series of functional poly(2-oxazoline)s will be obtained possessing various side-chain functionalities and various groups at the end of the main chain. In the second WP, these functional poly(2-oxazoline)s will be attached to inorganic surfaces, including silica, Fe_3O_4 magnetic nanoparticles, clay, and graphitic carbon. To perform grafting of the polymers, the surface of inorganic materials will have to be chemically modified to introduce groups that can efficiently react with end-chain functionalities. The third WP includes molecular imprinting, a synthetic strategy allowing to obtain surfaces selective towards particular analytes. In the fourth WP, an in-depth investigation of the interactions formed between materials and analytes will be performed, along with the examination of the adsorption mechanism. During the last WP, a final quantitative analysis of the real-life samples will be performed along with complete method validation.

3. Reason for conducting the research

Molecularly imprinted materials are specially designed materials that possess very high selectivity towards targeted compounds, thus they are often called artificial antibodies. Investigation of these materials' properties and their application in analytical sciences is of the utmost importance. It allows for tracking the concentration and fate of hazardous compounds in the environment. Detecting these substances in very low concentrations allows to correlate their levels with their influence on the environment and allows for tracking their sources and eliminating them. The proposed materials will be new to science, thus finding a correlation between their structure and their adsorption properties will allow other researchers to better design synthesis and properties of their materials.

4. The most important expected effects

The most important expected effect of the project realization will be finding new materials that can be used for selective extraction and quantification of hazardous compounds in real-life samples. The developed method will include using obtained materials and an experimental mass spectrometry setup that allows rapid sample screening. The second expected effect is finding the correlation between the materials' structure and their adsorption properties, which will increase knowledge in materials chemistry, which will be profitable for other scientists.