

The aim of the project is to carry out simultaneously a comprehensive spectroscopic study and to investigate the antimicrobial and antioxidant activity of the selected compounds (which possess antimicrobial properties and naturally occur in *Oregano vulgaris*) and their complexes with metals. We would like to receive answers to questions about which elements of the molecular structure of examined compounds (e.g. the length of conjugated unsaturated bonds systems, the aromaticity, the acceptor-donor properties, the polarity of the molecule, the dipole moment) have the greatest influence on their biological activity. The formation of complexes of biologically active substances with metals, including lanthanides (metals that possess antibacterial activity and are used in medicine and agriculture), through the changes in the distribution of a charge in the ligand and/or synergistic effect, can cause a change in the mechanism of their interaction with cellular membranes, and consequently increase their biological activity. Moreover, complexation of ligands with metals may change the lipophilic character of these compounds, what favours their permeation through the lipid layers of the membranes and therefore enhance their activity. The studies will be performed in a systemic way, namely by using complementary research techniques for carefully selected (on the basis of the chemical structure) series of ligands and metals. The structure of the natural ligands, components of oregano, and their complexes with metals will be investigated by spectroscopic methods. In order to determine the structure and calculate the electron charge distribution, aromaticity, bound state, etc., the theoretical quantum chemistry methods will be applied. For the investigation of antioxidant activity of investigated compounds spectrophotometric methods will be used. Microbiological tests will be carried out on the microorganisms that cause foodborne diseases: gram-negative bacteria: *Escherichia coli* (EC), *Salmonella spp.*, *Campylobacter spp.*; gram-positive bacteria: *Staphylococcus aureus* (SA), *Bacillus subtilis* (BS). On the basis of the performed studies the compounds with the highest biological activity will be typed. In the next step of the research the toxicity of selected compounds will be examined, the IC50 values will be determined for the additional bacterial strains. The cytotoxicity of the selected compounds, potential preservatives, will be performed on human cell lines derived from the gastrointestinal system. The outcome of these studies will be the selected group of compounds, save for humans, which could be further investigated for food preservation.

The statistical methods will be used in order to find out the correlation between the selected parameters of chemical structures of the compounds and their microbial activity and toxicity. On this basis, the general relationships between the molecular structure and the biological activity of chemical compounds naturally present in plants will be formulated. In the future, this will allow the design of new substances with antimicrobial activity, that potentially could be used as food preservatives. An attempt will be made to determine the mechanisms of interaction of the selected compounds with the surface of biological and model membranes. We will try to find out if the analysed compounds, that are microbiologically active, permeate inside the cells of microorganisms by biological membranes or destroy them. The modern food industry could not exist without food additives, including preservatives, they are used even in organic products. The usage of preservatives allows to prolong the shelf-life of food products by protecting them against the formation of harmful substances that could be dangerous for the health of the consumers. According to the Federation of Food Banks, 2 million tonnes of food is thrown away in Poland each year, mainly due to its deterioration. The National Institute of Hygiene communicated that there is a growing number of reported cases of foodborne diseases, the majority of them are of bacterial origin. Plants possess many bioactive substances such as phenols, flavonoids, quinones, coumarins, phenolic acids, tannins, flavones and flavonols, terpenes and alkaloids, that protect them against microorganisms. The essential oil and extracts from oregano exhibit antibacterial and antifungal properties. The complexes of natural ligands with metals may exhibit stronger preservation properties than the free ligands. Better understanding of the influence of molecular structure on biological activity of studied compounds, as well as the interactions between metal complexes and model biological membranes and cells of microorganisms, will open new possibilities of designing preservatives and their applications in food processing. The obtained results will help to search for new substances with antimicrobial properties, not by 'trial-and-error-approach', but to design them rationally. We expect that some of the tested compounds may have better properties than commonly applied food preservatives. Moreover the new substances based on natural ligands that are complexed with macro- and microelements will be safer for human health than those ones currently used in the food industry.