## Reg. No: 2018/31/D/ST5/01057; Principal Investigator: dr Michał Kazimierz Niemczak

Ionic liquids are a unique group of chemical compounds that has been the subject of intensive research of many scientific as well as industrial facilities for more than two decades. They may be defined as organic ionic compounds, which are liquids at temperatures below the temperature of 100 °C. The high popularity of ionic liquids results from their unique multifunctional properties allowing for their application as electrolytes, media of chemical and enzymatic reaction, disinfecting agents, antistatic agents softeners or surface active compounds. The insertion of the pesticidal anion into the structure of ionic liquids opened up a new possibility for their application. Correspondingly, new active substances capable of eliminating harmful or unwanted organisms in both crops as well as stored grain, have been introduced to the world literature. Among the last years, we may find reports describing successful attempts to synthesize ionic liquids exhibiting: herbicidal properties (herbicidal ionic liquids); fungicidal properties (fungicidal ionic liquids), with antifeedant properties (deterrent ionic liquids).

The course of realization of the project entitled *"Research on the synthesis, physicochemical characteristics and biological activity of the esterified forms of glycine betaine as multifunctional ionic liquids for effective pest control"* the effective methods for the preparation of new ionic liquids, designed as proecological, multifunctional agents for protection of cultivated plants and harvested crops, will be developed. The synthesis will be divided into two steps, whereas a betaine will be the key reagent. This naturally occurring amino acid derivative of glycine is commonly known as the one of the main by-products of the sugar industry. In the first step, a betaine will be subjected to O-alkylation reaction with a suitable alkylating agent introducing a specific function/property to the cation. Next, the anion exchange reactions in the obtained esterified forms of betaine will be performed, where the halide anion will be replaced by selected anions, demonstrating the significant effect of the length of the carbon chain in the molecule of ionic liquid on the biological activity, it is assumed to synthesize homologous series that differ in the length of alkyl groups in both, the cation as well as the anion. The structures of the obtained products will be confirmed by the use of ultraviolet (UV), infrared (IR) and nuclear magnetic resonance (NMR) spectroscopies. In addition, the influence of the structure of ions present in the new salts on the location of particular signals on the collected spectra will be determined.

The next stage involves measurements of basic physicochemical properties of the synthesized ionic liquids, such as viscosity, refractive index, density and solubility in selected common solvents characterized by different polarity indices in the Snyder's scale. Differential scanning calorimetry will be used to determine three phase transition temperatures: glass transition, melting point and crystallization temperature, in the obtained products. Furthermore, by using thermogravimetric analysis their thermal stability will be examined and compared with the stability of starting reactants.

Subsequently, the biological (herbicidal, fungicidal, deterrent) activity will be tested for selected esterified forms of glycine betaine, and then the obtained results will be compared with the commonly used commercial preparations. The experiments will be focused on providing information if the biological activity in all compounds tested is maintained; as well as selecting the structures characterized by the highest efficiency that surpasses the utilized reference preparations. Another very important aspect of the project will concern the determination of the impact of these new compounds on the environment through tests revealing their toxicity, biodegradation rate, volatility and risk of permeation into groundwater. Due to the fact that ionic liquids offer the opportunity of tailoring their properties by changing the chemical structure of the cation and anion, the final stage will be focused on the establishment of quantitative correlations between diverse molecular or biological properties and chemical structure of the products obtained in the course of a project. All these findings will allow for a significant improvement of knowledge regarding designability of ionic liquids.

To sum up, designed for syntheses, ionic liquids comprising esterified analogues of betaine in the cation, are substances with a potentially reduced impact on the ecosystem. Additionally, they will be cheap in production, which results from the good availability and low prices of sources of the cation as well as the anion. As a result of the presence of ionic bonds in the molecule, these compounds will be characterized by a negligible vapor pressure, which eliminates the risk of poisoning *via* inhalation and makes them very attractive active ingredients for effective pest control.