**Dissertation abstract**

Author: mgr Dominika Rapacz-Kinas

Title: *Molecularly imprinted polymers as sensors selective to S–metolachlor*

The present doctoral dissertation *Molecularly imprinted polymers as sensors selective to S–metolachlor* comprises a series of seven thematically related scientific publications, thereby filling a gap in the field of molecularly imprinted polymers with affinity for S–metolachlor. A review of the literature revealed a lack of attention devoted to the design of "*smart*" sorbents in the field of synthesising molecularly imprinted polymers selective to herbicides, in accordance with the concept of "*green molecular imprinting*".

Continuous civilisational and technological development constantly contributes to increasing environmental pollution and deteriorating water quality. Harmful substances such as medicines, heavy metals, herbicides and detergents may be present in water. These compounds are very often found in trace amounts, even in ng × $L^{-1}$, which means that traditional analytical methods may not be sensitive enough and, as a result, the water sample tested may appear to be clean. Therefore, the stage of preparing the sample for analysis is crucial. In recent years, molecularly imprinted polymers have been widely used in analytical chemistry due to their highly selective ability to bind molecules of a selected analyte. These synthetic sorbents mimic naturally occurring enzymes, and their mechanism of action can be described using the well–known lock and key model. During synthesis, specific binding sites are created on the surface of the polymer matrix, which are complementary in shape, size and functional groups to the target analyte molecule, just as a specific key fits into the right lock.

Considering the high costs of analysis, associated with the need for expensive measuring equipment and highly qualified personnel, as well as the difficulties in determining the actual concentration of a given compound, the aim of the doctoral dissertation was to synthesise molecularly imprinted polymers that are selective for S–metolachlor, obtained in accordance with the concept of so–called "*green chemistry*". As part of this work, four types of materials were obtained: block molecularly imprinted polymers that react to changes in temperature or pH, and core–shell sorbents with a layer of molecularly imprinted polymer that respond to changes in temperature or pH. The most important task was to develop the composition of the reaction mixture. The selection of appropriate functional monomers with affinity for the template molecule, enabling the formation of stable pre–polymerisation complexes, as well as the selection of a cross–linking agent and reaction initiator and the determination of the molar ratio of the reagents were key tasks. The choice was difficult because it was limited to chemical compounds soluble in water, which was used as a porophore. In addition, despite the widespread use of S–metolachlor in weed control sprays, its limited solubility in water posed a major challenge in preparing the appropriate concentration of the template.

In order to characterise the synthesised materials, sorption kinetics and isotherms were studied, and the data obtained were fitted to appropriate models. Sorption and desorption

conditions were optimised, both in static and dynamic modes, on solid phase extraction columns. In order to verify the effectiveness of the polymers, the sorption process was successfully carried out on real samples, also taken from a river and a pond located near corn fields. The sorbents were analysed using various research techniques, including infrared spectroscopy, scanning electron microscopy, thermogravimetric analysis, dynamic light scattering, porosimetry and water absorption.

The results obtained in the doctoral thesis constitute a significant contribution to the development of research on the synthesis and characterisation of "*smart*" polymers with a molecular imprint selective for S–metolachlor. The design of reaction conditions in accordance with the concept of "*green chemistry*" – without energy loss and in an aqueous medium – as well as the creation of self–cleaning materials capable of repeated use, is in line with the principles of "*greenification*" concerning "*green*" molecular imprinting and contributes to the promotion of environmentally friendly and sustainable technologies. Further research plans will be expanded to include new sorbents with specific selectivity towards specific herbicides to create multifunctional SPE columns.