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Streszczenie rozprawy doktorskiej pt. „Zastosowanie polimerów z odciskiem molekularnym na bazie poli(2-oksazolin) do selektywnej adsorpcji połączonej z ilościowym oznaczaniem wybranych analitów" w języku angielskim

Molecularly imprinted polymers (MIP) are a class of polymeric materials capable of selective recognition of specific chemical compounds (analytes). Due to the presence of specific molecular cavities formed during their synthesis, which are complementary in shape, size, and type of interactions to the target analytes, MIPs find broad applications in selective adsorption, separation processes, chemical sensors, and environmental analysis.

In general, MIPs have been designed based on well-known polymers, such as poly(methacrylates), poly(acrylates), or polystyrene. This doctoral thesis presents an innovative approach to MIPs design, using poly(2-oxazolines) as the main structural component for creating selective molecular recognition materials. Poly(2-oxazolines) represent a promising class of functional polymers, characterized by high structural tunability, biocompatibility, and significant application potential. The use of this polymer class in molecular imprinting required the development of an innovative synthesis strategy based on a multi-step approach, including prepolymer preparation, controlled functionalization, and final cross-linking to form the MIP structure.

The aim of this work was to develop poly(2-oxazolines)-based MIPs capable of selective recognition and adsorption of environmentally analytes. The research hypothesis assumed a relationship between the polymer structure and its adsorption properties, allowing the identification of factors promoting the formation of selective molecular cavities and the design of materials with high application potential.

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Within this study, I synthesized monomers and prepolymers based on selected poly(2-oxazolines): poly(2-(3-butenyl)-2-oxazoline) (Poly(ButenOx)) and poly(2-allylamidopropyl-2-oxazoline) (Poly(AllylamidOx)), containing terminal double bonds in their side chains. These structures enabled the use of the "click" thiol-ene reaction as a tool for selective functionalization. Although the thiol-ene reaction is well-known and widely used in polymer chemistry, its application in poly(2-oxazoline) systems as a step for prepolymer functionalization for MIP synthesis represents a novel methodological approach. The synthesis process included partial functionalization of prepolymers *via* UV-initiated thiol-ene reactions in the presence of thiol compounds with diverse donor groups. Subsequently, the remaining unmodified double bonds were cross-linked using difunctional thiols to obtain a stable, networked polymer structure. Cross-linking was performed both in the presence of template analytes to obtain MIPs and in their absence to produce reference non-imprinted polymers (NIP). Environmental analytes of potential ecological and health concern were selected as template molecules based on literature data and regulatory documents. These were compounds subject to usage restrictions under institutions such as the European Union and the Scientific Committee on Consumer Safety (SCCS). Using these analytes as templates enabled the formation of selective molecular cavities tailored for the recognition of environmentally relevant compounds.

The resulting MIPs and NIPs were comprehensively characterized structurally, physicochemically, and functionally. Adsorption properties were investigated through isotherms, kinetics, and thermodynamics, as well as assessment of selectivity and reusability studies. Furthermore, the analytical performance, including linearity, and limits of detection (LOD), was determined using flowing atmospheric-pressure afterglow mass spectrometry (FAPA-MS). The efficiency of the developed MIPs and NIPs was further verified using real environmental samples, including river water and selected food samples. Techniques such as UV-Vis spectroscopy, HPLC, and the novel FAPA-MS method were employed, along with material characterization methods including FTIR, TG, and SEM.

The results confirmed that the developed synthesis strategy enables rational design of poly(2-oxazoline)-based MIPs with controlled molecular recognition properties and high adsorption selectivity. This work represents a significant step toward a systematic understanding of molecular imprinting mechanisms in this class of polymers and provides a foundation for designing advanced sensor materials with high application potential in environmental analysis.