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New Approaches to Synthesis and Binding Elucidation of Hydrophilic Molecularly Imprinted Monoliths

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Academic dissertation

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Abstract

The demands in clinical, food, and environmental sciences are growing rapidly. Molecular imprinting technology must therefore be developed to handle increasingly complex sensing, purification, and separation tasks. The key to success in this area lies in (i) producing the materials with appropriate morphology and surface chemistry, as well as (ii) using the right tools to elucidate their binding mechanisms.

The thesis focuses on designing, manufacturing, characterizing, and evaluating monolithic scaffolds to use as molecularly imprinted polymers (MIPs) targeting hydrophilic analytes in aqueous media.

Paper I presents the manufacturing procedure of monolithic MIP using step-growth polymerization of melamine and formaldehyde. A terminally functionalized block copolymer is synthesized and used as an imprinting template and porogen simultaneously. The use of the prepared MIP monolith in liquid chromatography-tandem mass spectroscopy, combined with multivariate data analysis and modeling, demonstrated the ability to selectively target desired analytes, in this case, phosphopeptides from a digest of twelve proteins.

The synthesis procedure of melamine-based monolithic MIPs was further tuned to manufacture affinity materials targeted at compounds with glycan (sialyllactose) and herbicides (glyphosate) motifs. The temperature of polymerization not only influenced the binding capacity but also impacted the morphology of the monolith backbone. The cauliflower-like topology, formed by thermal polymerization, was changed to spaghetti-like features when a freeze-thaw polymerization process was used. In addition to the bound-free isotherm method for capacity evaluation, the interaction pattern and orientation of the targeted analytes with the monolithic MIPs were probed at the molecular scale by spectroscopic approaches, such as liquid phase NMR combined with solid-state STD NMR in *Paper II* and Paper *IV,* and liquid phase NMR as well as FTIR in *Paper III*.

Keywords: Monolithic sorbents, molecularly imprinted polymer, step-growth polymerization, cryo-polymerization, freeze-thaw processes, nuclear magnetic resonance, saturation-transfer difference, Fourier transform infrared spectroscopy, projection to latent structures, melamine, Pluronics, polypeptides, sialyllactose, glyphosate.

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