

Accurate diagnosis is pivotal in effective healthcare management and containment of antimicrobial resistance. This thesis explores the potential of molecularly imprinted polymers (MIPs), also known as synthetic receptors or artificial antibodies, as a groundbreaking solution for pathogen detection, aiming to address the limitations of traditional diagnostic methods. In an era where rapid and precise diagnosis of infectious diseases is imperative, MIPs emerge as a stable, cost-effective, and versatile alternatives to conventional antibodies. Differentiating between bacterial and viral infections remains a significant challenge due to overlapping symptoms. Diagnostics based on the identification of whole microorganisms can be a biosafety issue, laborious, time-consuming and costly, thus alternative strategies for early clinical diagnosis include biomarker-based detection. By selectively targeting specific biomarkers, MIPs offer a promising avenue to enhance healthcare outcomes through the development of a comprehensive and multiplexed diagnostic platform for a wide array of infectious diseases. This study focusses on designing synthetic receptors for pathogen specific biomarkers like pyocyanin characteristic of *P. aeruginosa* infections, viral coat proteins specific to SARS-CoV-2 and host biomarkers like Myxovirus Resistance proteins expressed in viral infections. To achieve precise structuring of recognition sites within the polymer matrix for biomarkers, this thesis emphasises on rational design and advanced synthesis techniques. For protein-based biomarkers, an epitope imprinting approach complemented by *in silico* screening of polymerization components has been used to fabricate chemically stable and cost-effective synthetic receptors for correct identification of bacterial and viral etiologies. Herein, introducing a novel multi monomer simultaneous docking approach for MIP design highlights the binding mechanics and the intermediates of monomers during the polymerization steps. It serves as a critical bridge between theoretical concepts and practical applications, significantly enhancing our understanding of MIPs' molecular engineering. The adaptability, specificity, and the capacity to imprint a wide spectrum of molecules, regardless of size, paves the way for innovative solutions that can enhance disease diagnosis, treatment, and monitoring, ultimately improving patient care and public health.