Abstract:

Biomimetic recognition utilizing molecularly imprinted polymers (MIPs) has proven its potential by providing synthetic receptors for numerous analytical applications including liquid chromatography, solid phase extraction, biomimetic assays, and sensor systems. The inherent advantages of synthetic receptors and functionalized membranes in contrast to biochemical/biological recognition and immobilization schemes include their robustness, synthetic versatility, and potentially lower costs. In principle, molecularly imprinted/templated materials are an ideal molecular capturing matrix tailorable for selective recognition or immobilization of a wide range of molecules. However, tailoring synthetic recognition elements to a target analyte requires thorough analysis and fundamental understanding of the governing molecular processes during the imprinting procedure, with the ultimate goal of rationally designing and predicting optimized synthesis pathways leading to molecular capture, recognition, and immobilization matrices with superior control on their physical geometry and molecular selectivity.
Fundamental understanding of the involved processes via analysis of the governing interactions at a molecular level providing complex stoichiometries, binding affinities, and facilitating pre-screening of optimized functional monomers and component ratios provides the basis for molecular dynamics simulations enabling modeling of the interactions of template molecules with functional monomers and cross-linkers in explicit solvent. While is anticipated that molecular templating based on rational synthetic design will significantly reduce the number of trial & error experiments currently required, it is evident that the complexity of simulating the generation of molecular imprints still requires extensive efforts toward rational design of next-generation synthetic receptors. Of particular interest is the development of biomimetic recognition schemes for selectively binding proteins and large biomolecules, e.g., at the surface of biomedical devices for promoting or preventing adhesion of selected biomolecules, as well as for controlled molecular release. Recent developments on this new frontier in molecular imprinting will be highlighted with selected examples and novel routes toward tailoring polymeric receptors for biomolecular recognition facilitating innovative strategies in medical and pharmaceutical applications.

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