APPLICATION OF COMPUTATIONAL METHODS IN THE DESIGN OF MOLECULARLY IMPRINTED POLYMERS

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Molecularly imprinted polymers (MIPs) are synthetic receptors capable of selectively recognising a specific target. MIPs are made by polymerisation of functional monomers in the presence of the analyte that forms a polymer film decorated with tailor-made cavities for the target (template) molecules [1]. The process of MIP synthesis has the challenging steps as follows: a) Selection of best monomer(s), crosslinking agent(s), and solvent; b) Polymerisation; c) Template removal to make complementary binding sites; d) Sensitivity and selectivity studies through rebinding step. On one hand, extensive and costly procedures, and on the other hand, methods such as molecular mechanics, molecular dynamics, Monte Carlo, quantum mechanics, and statistical simulations have made these leveraging computational methods widely used in the stepwise process of MIP preparation [2].

Calculations are performed for the selection of the best reagents in the pre-polymerisation mixture such as monomer(s), crosslinking agent, and solvent system, and their relevant optimal ratios. It is found that the simulation of polymerisation facilitates optimisation of this step and models the polymeric structure of MIPs making it plausible to analyse the resulting binding sites. The selectivity and sensitivity of MIPs are evaluated by computations showing the mechanism of recognition of specific targets and the binding affinities. The reviewed papers proved the significance of computational methods for a greener approach and their widespread applicability in the MIP design.

[1] Pilvenyte, G. et al. Molecularly imprinted polymers for the recognition of biomarkers of certain neurodegenerative diseases. Journal of Pharmaceutical and Biomedical Analysis 228, 115343 (2023).

[2] Mohsenzadeh, E. et al. Application of computational methods in the design of molecularly imprinted polymers (review). TrAC Trends in Analytical Chemistry 171, 117480 (2024).