THE COMPUTATIONAL APPROACH FOR RATIONAL MONOMER SELECTION IN MOLECULARLY IMPRINTED POLYMER SYNTHESIS

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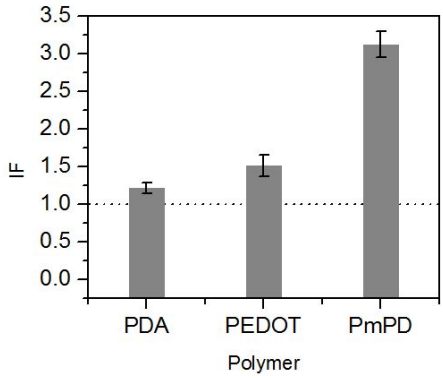
Molecular imprinting has become a promising approach for synthesis of polymeric materials, with a predetermined selectivity and specificity for a given analyte, so called molecularly imprinted polymers (MIPs). The basic principle of molecular imprinting consists of prepolymerization complex formation between template and functional monomers and followed by polymerization and template removal. As the result specific cavities are formed in the polymer matrix, which are capable of rebinding the templates. It is important to estimate non-covalent interactions between the monomer and template especially for a macromolecular template because strength of these interactions in the prepolymerization mixture influences directly on the selectivity of MIPs, and consequently on its performance[1].



A computational approach allowing the selection of a more favorable functional monomer for a protein-MIP synthesis has been developed. Molecular docking (MD) combined with quantum chemical calculations (QCCs) were used for modelling and comparing the monomer arrangement and the strength of non-covalent interactions between a model protein template molecule, Immunoglobulin G (IgG), and one of three electropolymerizable functional monomers: m-phenylenediamine (mPD), dopamine (DA), and 3.4-ethylenedioxythiophene (EDOT). It was revealed that mPD tended to be arranged more uniformly around IgG participating in multiple H-bond interactions with its polar residues and therefore, could be considered as more advantageous for a synthesis of a MIP for IgG recognition (IgG-MIP). These theoretical predictions were verified by the experimental results and found to be in good agreement showing higher binding affinity of the PmPD-based IgG-MIP towards IgG as compared with the IgG-MIPs generated from the other two monomers, what is reflected by the highest imprinting factor (IF).

References

1. A. G. Ayankojo, A. Tretjakov, J. Reut, R. Boroznjak, A. Öpik, J. Rappich, A. Furchner, K. Hinrichs, V. Syritski (2016). Molecularly imprinted polymer integrated with surface acoustic wave technique for detection of sulfamethizole. Analytical Chemistry, 88 (2), 1476−1484, 10.1021/acs.analchem.5b04735.

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