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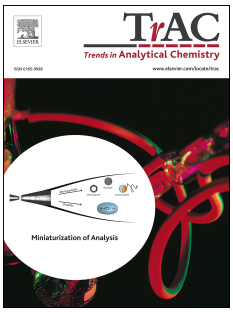

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Computational modeling of molecularly imprinted polymers as a green approach to the development of novel analytical sorbents

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Abstract

The development of novel molecularly imprinted polymers (MIP) sorbents for specific chemical compounds require a lot of tedious and time-consuming laboratory work. Significant quantities of solvents and reagents are consumed in the course of the verification of appropriate configurations of polymerization reagents. Implementation of molecular modeling in the MIP sorbent development process appears to provide a solution to this problem. Appropriate simulations and computations facilitate the determination of the nature of interaction between the reagents and thus the selection of the best configuration of chemicals for the preparation of the sorbent. The article presents literature information on major computer software used for molecular modeling, its application in the development of MIP sorbents, as well as the advantages resulting from the implementation of computer-assisted techniques. The appropriate choice of polymerization reagents and conditions allows for a significant reduction of the adverse environmental impact of the entire laboratory process.

Key Words: molecularly imprinted polymers; computational modeling; green analytical sorbents; green analytical chemistry; basic laboratory studies