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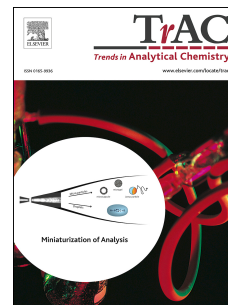
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1 **Computational modeling of molecularly imprinted polymers as a green approach to the**  
2 **development of novel analytical sorbents**

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17

18 **Abstract**

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

31

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

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