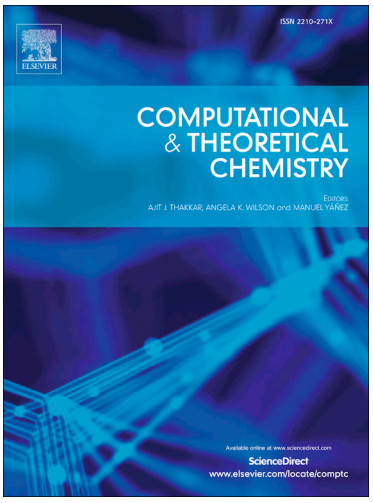

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Computer-aided Design of Molecularly Imprinted Polymers for Recognition of Atrazine

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Abstract Density functional theory (DFT) method was performed to preliminarily select monomers and solvents for the preparation of atrazine molecularly imprinted polymers (MIPs). The probabilities of forming non-covalently bonded complexation between the template and five commonly used monomers were evaluated by electronic interaction energy. These monomers involved acrylic acid, methacrylic acid, 2-(trifluoromethyl) acrylic acid, acrylamide and 4-vinylpyridine. The most stable conformations of atrazine-monomer complex were selected and the electronic interaction energies of each interaction site were analyzed. Solvent effect was studied using the Polarizable Continuum Model (PCM) for the following five solvents: acetonitrile, dichloromethane, methanol, tetrahydrofuran and toluene. Thermodynamics analysis implied that less polar medium and lower temperature is favourable for pre-polymerization process. A method was provided to properly choose function monomer or co-monomers, solvents and pre-polymerization conditions in the preparation process of MIPs, which will be useful to the synthesis of MIPs for detecting atrazine.

Keywords Molecularly imprinted polymers; Molecular modeling; Density functional theory; Atrazine;

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