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Nanostructured polymeric membranes for solid-phase extraction of bisphenol A from aqueous samples

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Nanostructured rationally-designed polymeric membranes capable of highly-selective recognition of bisphenol A (BPA) were synthesized according to the technique of molecular imprinting and used for pre-concentration of diluted BPA aqueous samples. Free-standing molecularly-imprinted polymer (MIP) membranes were obtained using the method of *in situ* polymerization in a combination with the method of computational modeling. Binding energies BPA-functional monomer were estimated using Silicon Grafics Octane workstation running SYBYL 6.8 software. It has been shown that itaconic, methacrylic, and 2-acrylamido-2-methyl-1-propanesulfonic acids as well as diethylaminoethylmethacrylate were the best monomers, capable of formation of BPA-selective binding sites in the structure of the MIP membranes. The monomers interact with BPA with binding energies –40.8 kcal/mol, –38.1 kcal/mol, –36.7 kcal/mol, and –28.1 kcal/mol, respectively. Good correlation between binding energies "BPA-functional monomer" and capability of the MIP membranes to bind BPA selectively was demonstrated. Negligible binding of BPA close structural analogues by the MIP membranes was shown. Dependence of BPA adsorbtion on composition of the analyzed sample (pH, NaCl concentration, etc.) was investigated. The structure of the selective membranes was studied using BET and SEM methods. Application of the MIP membranes in solid-phase extraction provided efficient (up to 100 times) pre-concentration of the diluted BPA samples.

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