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Sensor systems for sulfamethoxazole detection based on nanostructured rationally-designed polymer membranes

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Optical biosensor systems for selective detection of sulfamethoxazole were developed on the basis of nanostructured molecularly imprinted polymer (MIP) membranes. Free-standing MIP membranes were synthesized using the principle of molecular imprinting. Functional monomers for the formation of sulfamethoxazole-selective binding sites in the structure of the MIP membranes were identified by the method of molecular dynamics (computational modeling). Binding energies sulfamethoxazole-functional monomer were estimated using Silicon Grafics Octane workstation running SYBYL 6.8 software. It has been shown that 2-acrylamido-2-methyl-1-propanesulfonic, itaconic, and methacrylic acids were the best candidates for formation of sulfamethoxazole-selective sites in the MIP membranes. The monomers interact with sulfamethoxazole with binding energies –50.3 kcal/mol, –35.1 kcal/mol, and –29.5 kcal/mol, respectively. Good correlation between binding energies "sulfamethoxazole-functional monomer" and capability of the MIP membranes to bind the pharmaceticals selectively was demonstrated. Negligible binding of sulfamethoxazole close structural analogues (sulfathiazole and sulfanilamide) by the MIP membranes was shown. The membranes with the optimized composition were used as a basis of a colorimetric sensor system. Sulfamethoxazole adsorbed by the membranes' surface was revealed after the color reaction with sodium nitroprusside and potassium ferricyanide in alkaline media, leading to formation of a brown-colored product. The main working characteristics of the sensor system were analyzed.

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