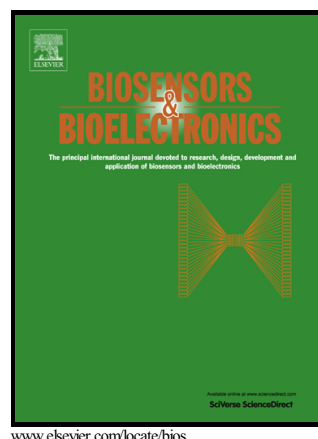


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Nicotine molecularly imprinted polymer: synergy of coordination and hydrogen bonding

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Abstract

Two new bis(2,2'-bithienyl)methane derivatives, one with the zinc phthalocyanine substituent (ZnPc-S16) and the other with the 2-hydroxyethyl substituent (EtOH-S4), were synthesized to serve as functional monomers for biomimetic recognition of nicotine (Nic) by molecular imprinting. Formation of a pre-polymerization complex of the Nic template with ZnPc-S16 and EtOH-S4 was confirmed by both the high negative Gibbs free energy gain, $\Delta G = -115.95$ kJ/mol, calculated using the density functional theory at the B3LYP/3-21G(*) level, and the high stability constant, $K_s = 4.67 \times 10^5$ M⁻¹, determined by UV-vis titration in chloroform. A solution of this complex was used to deposit a Nic-templated molecularly imprinted polymer (MIP-Nic) film on an Au electrode of a quartz crystal resonator of EQCM by potentiodynamic electropolymerization. The imprinting factor was as high as ~9.9. Complexation of the Nic molecules by the MIP cavities was monitored with X-ray photoelectron spectroscopy (XPS), as

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