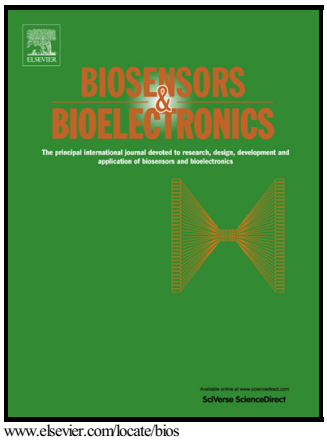

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Nicotine molecularly imprinted polymer: synergy of coordination and hydrogen bonding

Tan-Phat Huynh,[a,b,1] Chandra B. KC,[b,1] Marta Sosnowska,[a,b] Janusz W. Sobczak,[a] Vladimir N. Nesterov,[b] Francis D'Souza,[b,*] and Wlodzimierz Kutner[a,c,*]

[a]*Institute of Physical Chemistry (IPC PAS), Kasprzaka 44/52, 01-224 Warsaw, Poland*

[b]*Department of Chemistry, University of North Texas, Denton, 1155, Union Circle, #305070 TX 76203-5017, USA*

[c]*Faculty of Mathematics and Natural Sciences, School of Sciences, Cardinal Stefan Wyszynski University in Warsaw, Woycickiego 1/3, 01-938 Warsaw, Poland*

[1]These authors equally contributed to this work.

*Corresponding author. Email: wkutner@ichf.edu.pl; Francis.Dsouza@unt.edu

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, ΔG = -115.95 kJ/mol, calculated using the density functional theory at the B3LYP/3-21G(*) level, and the high stability constant, $K_s = 4.67\times10^5$ 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