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## **ACCEPTED MANUSCRIPT**

New potentiometric sensor based on molecularly imprinted nanoparticles for cocaine detection

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#### **ABSTRACT**

Here we present a potentiometric sensor for cocaine detection based on molecularly imprinted polymer nanoparticles (nanoMIPs) produced by the solid-phase imprinting method. The composition of polymers with high affinity for cocaine was optimised using molecular modelling. Four compositions were selected and polymers prepared using two protocols: chemical polymerisation in water and UV-initiated polymerisation in organic solvent. All synthesised nanoparticles had very good affinity to cocaine with dissociation constants between 0.6 nM and 5.3 nM. Imprinted polymers produced in organic solvent using acrylamide as a functional monomer demonstrated the highest yield and affinity, and so were selected for further sensor development. For this, nanoparticles were incorporated within a PVC matrix which was then used to prepare an ion-selective membrane integrated with a potentiometric transducer. It was demonstrated that the sensor was able to quantify cocaine in blood serum samples in the range of concentrations between 1 nM and 1 mM.

Keywords: cocaine, molecular modelling, nanoMIPs, solid-phase imprinting, potentiometric sensor

#### 1. Introduction

Cocaine is one of the most widely-used recreational drugs in the world with the number of its users estimated between 13.8 - 20.7 million for the population aged between 15 to 64 (World Drug Report, 2015). It is known that cocaine addiction can cause serious side-effects in users, including anxiety, organ damage and cardiac arrest, in addition to wider societal and economic impacts (Wren et al., 2014; Emrani et al., 2016). Therefore, the development of

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