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Towards the development of multisensor for drugs of abuse based on molecular imprinted polymers

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Abstract

The synthetic receptors for cocaine, deoxyephedrine, methadone and morphine were computationally designed and produced using molecular imprinting. The structure and energy of the molecular complexes were analysed by computational techniques. The possible structures of the binding sites in the synthetic receptors have been compared with those of corresponding natural receptors. The composition of imprinted polymers was optimised to allow adequate performance in the same experimental conditions. All selected molecular imprinting polymers (MIPs) demonstrated stronger affinity in comparison with corresponding blank polymers resulting in imprinted factors (I) equal 1.2 (cocaine), 2.5 (deoxyephedrine), 3.5 (methadone) and 3 (morphine) which suggested that the specific binding site for each molecule was successfully created. The studied polymers possessed good selectivity and affinity towards their templates and could be recommended for the integration with sensor devices. From a practical point of view, especially for multisensor requirements, the synthetic receptors based on imprinted polymers could be superior to natural receptors due to their stability, robustness and compatibility with automation processes required for sensor fabrication.

Keywords: Cocaine; Deoxyephedrine; Methadone; Morphine; Molecular imprinting;



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