Electronic Supplementary Information

Electrochemical sensing of cocaine in real samples based on electrodeposited biomimetic affinity ligands

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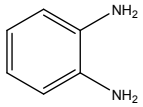
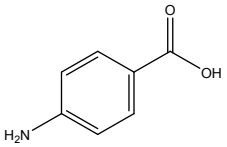
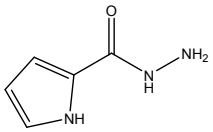
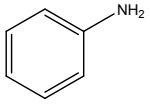
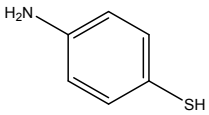
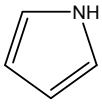
Table S1. Hierarchy of relative binding energies for cocaine-electropolymerizable monomers screening.

Monomer	**Chemical structure**	**Binding energy (**kJ mol^{-1}**)**
Orto-phenylene-diamine		-190.12
Para-aminobenzoic acid		-114.99
Pyrrole carbohydrazide		-110.71
Aniline		-104.39
Thioaniline		-98.28
Pyrrole		-57.97

The results of the computational modelling show that orto-phenylene-diamine and para-aminobenzoic acid are the best candidates for molecular imprinting having the highest affinity for cocaine binding and thus ensuring a high probability of imprinting success during polymerization. Experimental work performed with the two monomers in our previous work[37] showed that, eventhough orto-phenylene-diamine shows a higher binding score, from the application point of view in electrochemical sensors para-aminobenzoic acid shows better results in terms of cocaine peak current intensity, having a higher conductivity. Thus, para-amino-benzoic was selected as monomer for further experiments.