# Computationally designed sensing elements for BPA analysis using smartphone

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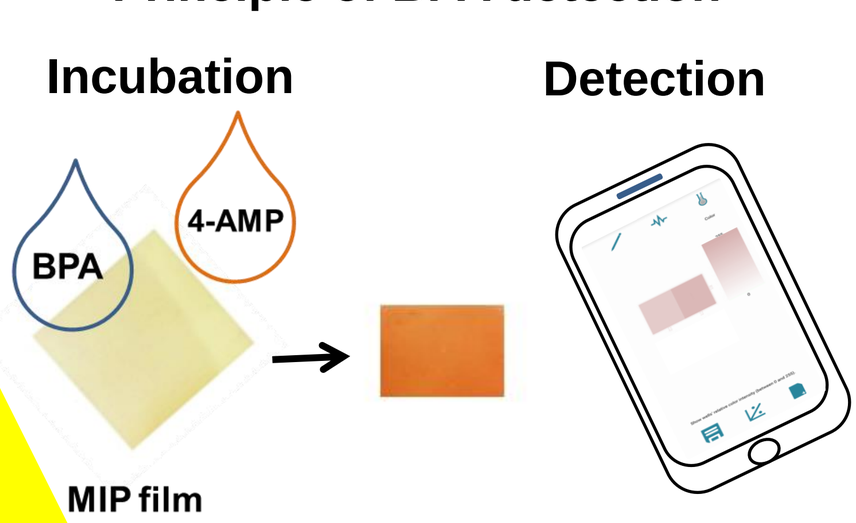
## Abstract

The novel, user-friendly, colourimetric biosensor for bisphenol A (BPA) was introduced. The BPA-sensitive molecularly imprinted polymers (MIP) films were designed and used as sensing elements of smartphone-based biosensor for BPA analysis. Using computational modelling method, we demonstrated the successful design of BPA-sensitive artificial binding sites, which were formed in the structure of the proposed MIP-based sensing elements. The MIP films were synthesized using the method of *in situ* polymerization with BPA as a template, ethylene glycol methacrylate phosphate (EGMP) as a functional monomer, the tri(ethylene glycol) dimethacrylate/ oligourethaneacrylate (TGMA/OUA) mixture as the main component of the polymeric network. The colourimetric detection of BPA, selectively adsorbed by the artificial binding sites in the EGMP-based thin MIP films' structure, is based on the 4-aminoantipyrine (4-AMP) method. The sensor responses associated with BPA binding to the MIP films surface were registered by the smartphone camera (Meizu 16, 20 MP, F/1,8) and the captured images were analyzed with the smartphone application Spotxel® Reader (Sicasys Software GmbH, Germany) within real-time. The pink-coloured intensity of MIP films was proportional to BPA concentration in the analyzed samples. Some parameters of analyzed samples including pH, buffer and salt concentration, affecting sensor performance were tested and optimized. A dynamic linear range of 10 μM to 1000 μM was obtained. The detection limit of the designed biosensor was calculated equal to 10 μM. The smartphone-based biosensor with computationally designed MIP film sensing elements can successfully identify and quantify BPA in samples of natural and waste waters contaminated with BPA.

## Principle of BPA detection




## Results

### Computational modeling of MIP films capable of selective recognition of BPA

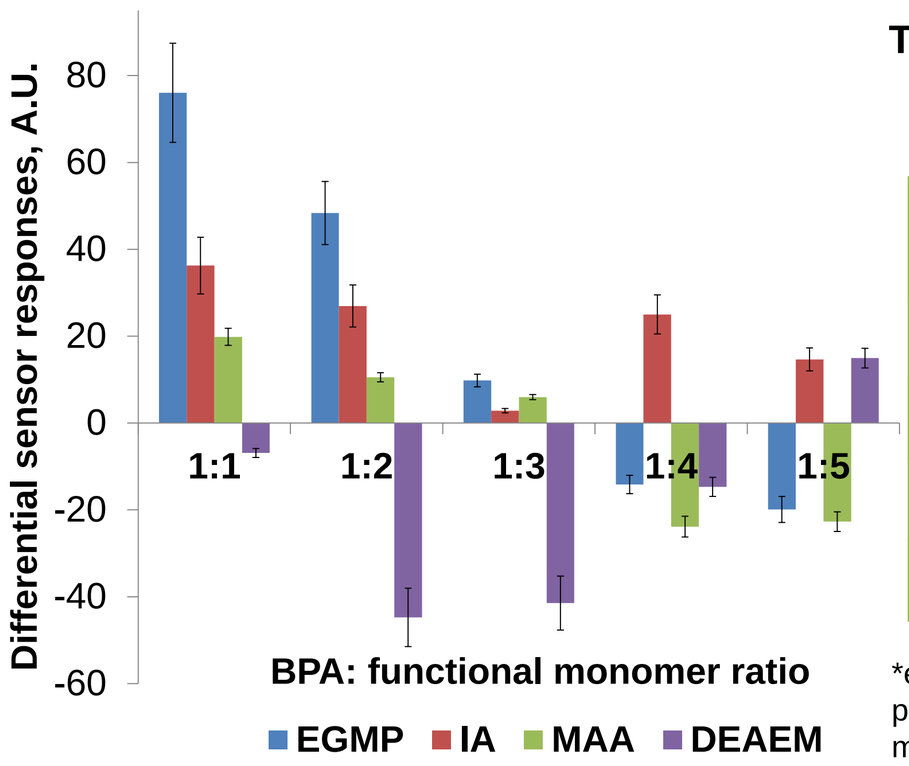



**Table 1.** Binding energies between functional monomers* and BPA

| FM | Binding energy, kcal mol$^{-1}$ |
|---|---|
| -EGMP | -48.62 |
| -IA | -40.84 |
| -MAA | -38.07 |
| DEAEM | -28.1 |

*ethylene glycol methacrylate phosphate (EGMP), itaconic (IA), methacrylic (MAA) acids, diethylamino-ethylmethacrylate (DEAEM)

**Fig. 1.** Dependence of BPA sensor responses* on the type of a functional monomer used for MIP films synthesis.
*Differential sensor response – difference in BPA fluorescence on MIP and blank membranes. 10% aqueous acetonitrile solutions (100 μM) of BPA were used for the adsorption experiments.

### Typical calibration plot of the MIP-film-based smartphone sensor system for BPA detection

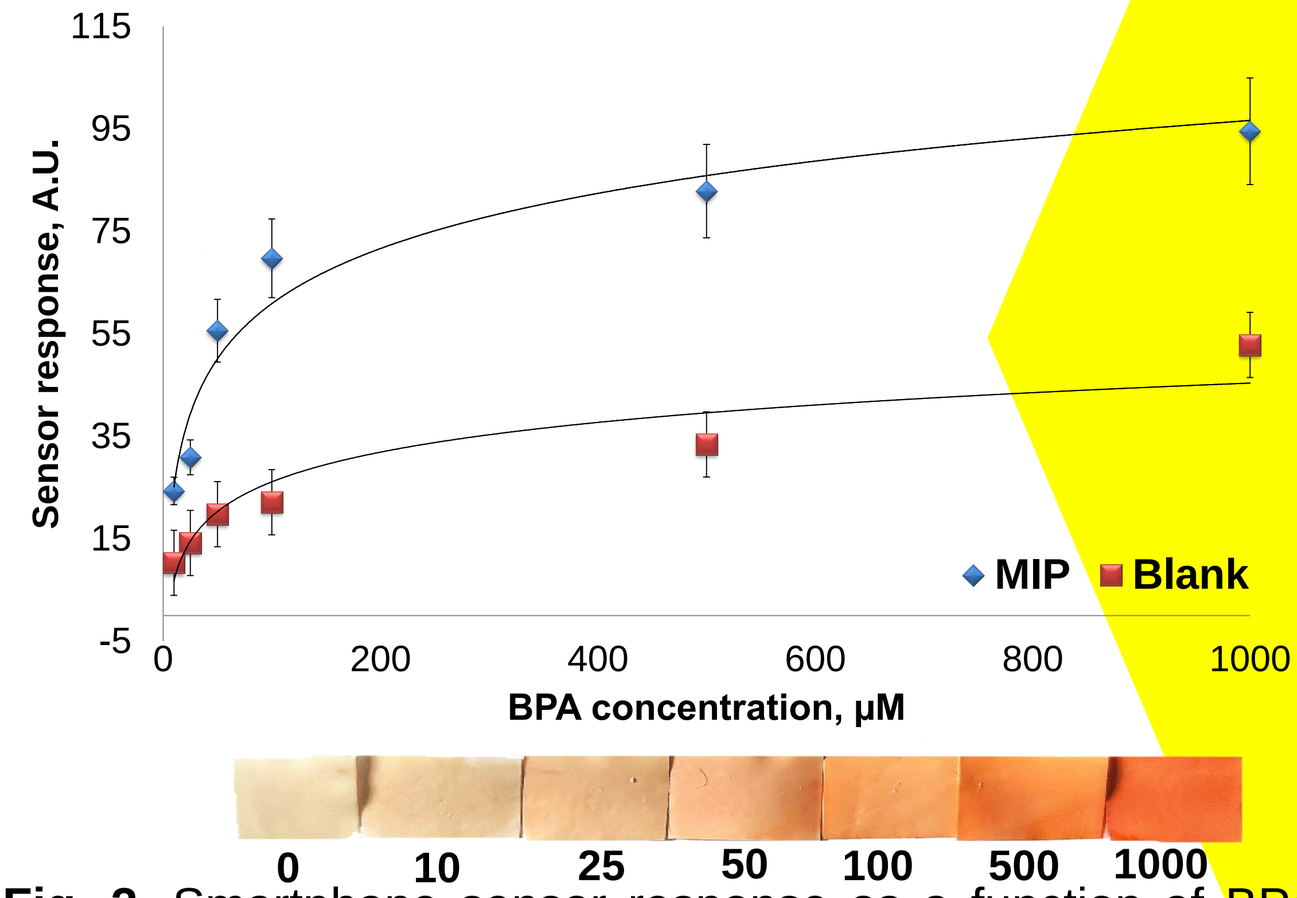



**Fig. 2**. Smartphone sensor response as a function of BPA concentration generated by Spotxel® Reader smartphone application.
* An inset shows photos of fluorescence of the EGMP-based MIP and blank films (BPA: functional monomer ratio 1:1) after incubation in solutions containing different amounts of BPA.

## Acknowledgement

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