

## Biosensor applications of functional polymers

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The conformation of biological molecules on surfaces or in solution environments strongly effects the successful implementation of biosensing platforms for the detection of target molecules as possible conformational changes lead to decreased sensing signals. To date, artificial protein binders have been developed using linear peptides with an unknown structure in epitope imprinting process. Despite successful outcomes obtained to some extent, most of these works lack of providing either high affinity, selectivity or sensitivity.

We aim to address these problems by performing molecular dynamic calculations for the design of high affinity artificial protein binding surfaces for cancer biomarker recognition [1]. Computational simulations are employed to identify particularly stabile secondary structure elements. These epitopes are used for subsequent molecular imprinting, where surface imprinting approach is applied to obtain functional materials. The molecular imprints generated with the calculated epitopes of greater stability show better binding properties than those of lower stability. The average binding strength of imprints created with stabile epitopes is found to be around fourfold higher for the selected biomarker models [1]. The artificial protein binders can recognize the target molecules even in a complex medium including non-specific molecules at a high concentration [1-4]. Moreover, certain amino acid modifications of the computationally selected epitope templates (e.g. addition of histidine to the peptide chain or cysteine modification on both terminal of the elongated peptide to form self-assembled monolayer bridges) further improve the performance of artificial protein binders in biosensor applications [2-4].

Our novel and rational selection can be used for establishing epitope-based molecularly imprinted polymer (MIP) sensors for protein molecules by eliminating unsuitable epitopes and ranking the best candidates based on their stability analysis obtained from molecular dynamic simulations [1-4]. The integrated approach has shown a good potential to contribute to some limitations of medical diagnostic field. Research disciplines that require recognition receptors can apply this technique for designing stable and efficient receptors.

### References

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