

Title : Aptamer biosensor design for the detection of endocrine-disrupting chemicals small organic molecules using novel bioinformatics methods

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Abstract: Endocrine-disrupting chemicals (EDCs) are substances that can disrupt the normal functioning of hormones . Using aptamers, which are biological recognition elements, biosensors can quickly and accurately detect EDCs in environmental samples. However, the elucidation of aptamer structures by conventional methods is highly challenging due to their complexity. This has led to the development of three-dimensional aptamer structures based on different models and techniques. To do this, we developed a way to predict the 3D structures of the SS DNA needed for this sequence by starting with an aptamer sequence that has biosensor properties specific to bisphenol-A (BPA), one of the chemicals found in water samples that can interfere with hormones. In addition, we will elucidate the intermolecular mechanisms and binding affinity between aptamers and endocrine disruptors using bioinformatics techniques such as molecular docking, molecular dynamics simulation, and binding energies. The outcomes of our study are to compare modeling programs and force fields to see how reliable they are and how well they agree with results found in the existing literature, to understand the intermolecular mechanisms and affinity of aptamer-based biosensors, and to find a new way to make aptamers that takes less time and costs less.

Keywords: Endocrine-Disrupting Chemicals (EDCs), Aptamer-Based Biosensors, Bisphenol-A (BPA), 3D Structure Prediction, Molecular Docking

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