

Supplementary Materials

The combination of computational and biosensing technologies for selecting aptamer against prostate specific antigen

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S1. Materials and Methods

S1.1 Computational process by using the genetic algorithm.

The Genetic Algorithm Toolbox for MATLAB[®] was downloaded from this link: <http://codem.group.shef.ac.uk/index.php/ga-toolbox>. The toolbox was developed at the Department of Automatic Control and Systems Engineering of The University of Sheffield, UK and the software version was v1.2. After unzipping the download file, users have to correct the filename extension of these files from M to m. After this modification, the function named as `xovsp`, which is a low-level crossover function, can be used to generate new sequences based on the input sequence data. The `XOVR` parameter in this function was set by using the default value. Bases A, T, G, and C for sequences were numbered 00, 01, 10, and 11, respectively. Here, we use four short-length DNA sequences to illustrate the processes.

1. Original sequences:

CTGGTGTTTA, GTGTTGCCCG, AATATCAACT, ACTTAATGAT

2. Convert sequences according to the codes

11011010011001010100, 10011001011011111110, 00000100011100001101,
00110101000001100001

3. Run the Matlab function: `xovsp`

Four new sequences will be produced for each run.

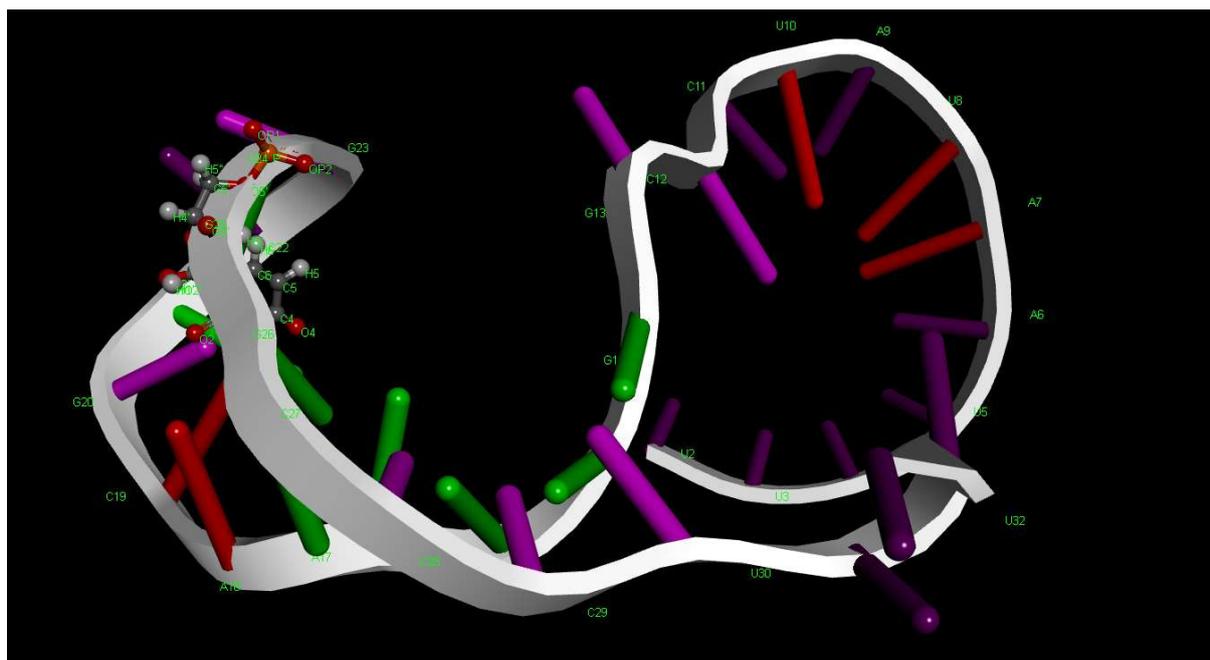
```
OldChrom = [ 1 1 0 1 1 0 1 0 0 1 1 0 0 1 0 1 0 1 0 0;  
             1 0 0 1 1 0 0 1 0 1 1 0 1 1 1 1 1 1 1 1 0;  
             0 0 0 0 0 1 0 0 0 1 1 1 0 0 0 0 1 1 0 1;  
             0 0 1 1 0 1 0 1 0 0 0 0 0 1 1 0 0 0 0 1];  
NewChrom = xvosp(OldChrom);
```

4. The data of `NewChrom`:

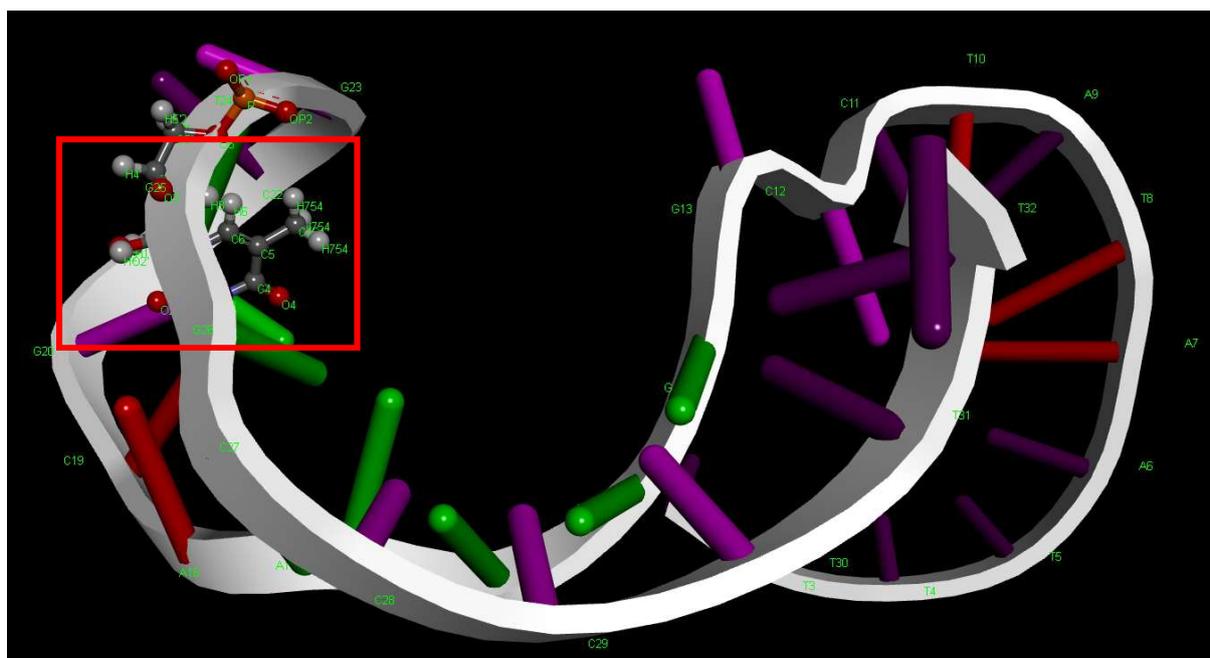
```
1 1 0 1 1 0 0 1 0 1 1 0 1 1 1 1 1 1 1 0  
1 0 0 1 1 0 1 0 0 1 1 0 0 1 0 1 0 1 0 0  
0 0 0 0 0 1 0 1 0 0 0 0 0 1 1 0 0 0 0 1  
0 0 1 1 0 1 0 0 0 1 1 1 0 0 0 0 1 1 0 1
```

5. By using a self-written C# program for the conversion of data to sequence information, four new sequences are obtained.

CTGTTGCCCG, GTGGTGTTTA, AATTAATGAT, ACTATCAACT



(A)



(B)

Figure S1. Model of the 3D Structure of PSAG28. (A) This RNA model is generated by using the RNAComposer web server and viewed in the Accelrys Discovery Studio (DS). (B) The structure of uracil was edited by DS software to become the structure of thymidine. Please note the structure inside the inserted red rectangle. The hydrogen atom at the C5 position was changed to CH₃.