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ABSTRACTS

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APPLICATION OF
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Key words: cellular automata
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References:

1. V.I. Zorkalcev, I.V. Mokry,
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2. O.L. Bandman (2010) Cell
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PARALLELIZATION OF ALGORITHM OF PREDICTION OF miRNA BINDING SITES IN mRNA ON THE CLUSTER COMPUTING PLATFORM

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Key words: parallelized algorithm, cluster computing platform, Java MPI, miRNA, mRNA

Motivation and Aim: The problem of a prediction of binding sites of microRNAs (miRNAs) with messenger RNAs (mRNAs) had increased after discovery of an important role of miRNAs in regulation of gene expression. There are data about the value of free energy of hydrogen bond between nucleotides in water solution [1]. However, there are a wide range of free energy value of this bond and it is difficult to choose a correct data. It is important to know the relative relations of free energy of hydrogen bond between nucleotides as they are necessary at formation of secondary and tertiary structures of RNAs. Some programs which predict miRNA binding sites were created, however, many of them had unreasonable limitations for search of binding sites. It was established that binding sites are localized only in 3'UTRs. Other programs were based on identification of binding sites with the obligatory requirement to have complementary interactions. Many such programs predict a large number of false positive sites and they are not allow to reveal the binding sites located in 5'UTRs and CDSs. Aim of this research is creation of the program which has not aforementioned disadvantages and with high reliability revealed binding sites of miRNAs with mRNAs.

Methods and Algorithms: Scanning genes is a process of consecutive comparison of nucleotide sequence of mRNA with miRNA with possibility of adding one gap in miRNA sequence in positions with the 3-rd on n-2-th, where by n – nucleotide number (length) of miRNA. The binding sites are selected according to the value of free energy of compared sequences. It is considered the best that option which is closer (in a percentage ratio) of free energy for coincidence of miRNA with binding site on the basis of complementarity.

Results: The developed algorithm scans of mRNA with miRNA with one possible gap in miRNA sequence, calculates a maximum of free energy and analyzes a coincidence of miRNA and binding site of mRNA on the basis of complementarity properties. The algorithm is base of MirTarget program. The program determines a free energy of miRNA hybridization with mRNA and the schemes of their interactions. It calculates of the nucleotide bounds of binding sites, level of reliability and the mRNA parts, where the sites are located since the first nucleotide. The algorithm can be parallelized on the computational cluster with use of MPJ tools.

Conclusion: The MirTarget program has advantages which are not present in known programs predicting of miRNA binding sites with mRNAs.

Availability: The program works on the computing cluster of al-Farabi Kazakh National University (http://ursa.kaznu.kz/).

References:

K.M. Guckian, B.A. Schweitzer, R.F. Ren, C.J. Sheils, P.L. Paris. (1996) Experimental measurement of aromatic stacking in the contex to duplex DNA, Vol. 118: 8182–83. J.Am.Chem.Soc.