

6th International Conference on

Bioinformatics & Systems Biology

August 22-23, 2016 Philadelphia, USA

Selection of RNA aptamers to the target CHS3 chitin trafficking signal as antifungal drugs *in silico*

Mohammad Vahed, Hiroki Takahashi, Majid Vahed and Tyuji Hoshino
Chiba University, Japan

Saccharomyces cerevisiae (*S. cerevisiae*) is one of the emerging fungal pathogens with an opportunistic characteristic. This concept implies that under normal conditions, these organisms are not capable of producing infection but when the frequently moderated and localized of them change, they are able to produce fungal disease in the worst scenarios. Opportunistic *S. cerevisiae* strains show a specific resistant to human immune and low differences including genes and proteins between mammalian and fungal cells, more difficult to discover antifungals drugs by exploiting to kill the fungal organism with fewer adverse effects to the host. Chitin synthase is one such promising target as it is absent in plants and mammals. Our works was *in silico* approach to create a list of RNA sequences with potential binding affinities to a chitin trafficking signals. The Chs3 crystallography structure was extracted from the PDB code: 4GNS. *In silico* screening process was done and selection of RNA sequences pool used by the Vienna RNA package based on secondary structure was analyzed. The sequences that passed the selection criteria were forwarded to the next step of generation of three-dimensional (3D) structures. Computational prediction of RNA tertiary structures was used the Rosetta package. The lowest energy structures for each sequence were placed into a library of RNA molecules to perform ensemble docking. Screening the library of RNA molecules with computational docking is a common tool used for high-throughput virtual screenings of the entire RNA library.

Biography

Mohammad Vahed is doctoral studies from Chiba University School of Medicine. He is researcher on Mycology at fungal pathogens. He research in bioinformatics and computational biology.

pc_vahed@yahoo.com

Notes: