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In silico Design of RNA Aptamers for therapy, diagnosis, and drug delivery

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Aptamers, the single-stranded nucleic acid analogs of antibodies, hold a great promise in molecular diagnostics, therapeutics, and drug targeting, due to their sensitivity and high selectivity toward target molecules. Antibodies have significant disadvantages in their production, such as their costly synthesis, batch-to-batch variation, cross-reactivity, and the possibility of contamination. On the other hand, aptamers are easily synthesized and modified, with a high reproducibility. Owing to their smaller size than antibodies, aptamers have high biocompatibility, low immunogenicity and toxicity, and better transport and tissue penetration properties.

Bioinformatic tools are comprised of a broad range of methods for aptamer design. Molecular modeling involves the prediction of the secondary structure of RNA from its primary nucleotides sequence, then, building a 3D tertiary structure based on this secondary structure. The predicted 3D model can then be used in docking simulations to investigate different poses of the RNA-protein interaction and select the complexes with the lowest binding energies.

In the study, the tyrosine kinase domain of the NT-3 growth factor receptor was used as a target to demonstrate the potential of the bioinformatics methods as promising tools in the area of aptamer design and selection, by employing a complete set of in silico strategies for the development of aptamers, using a simple sequence-based procedure. As a result, a 69-nt aptamer was optimized to have a relatively stable structure and acceptable binding score to the target domain. Despite being simple, this method may contribute to the process of aptamer design in the future to reduce the number of sequences in the initial SELEX pool, by generating more sequences with similar nucleotides distribution or introducing minor mutations, or through coupling with other more sophisticated approaches.

Recent Publications

1. Novel Design of RNA Aptamers as Cancer Inhibitors and Diagnosis Targeting the Tyrosine Kinase Domain of the NT-3 Growth Factor Receptor Using a Computational Sequence-Based Approach.

Biography

Muhammad Ashraf is a graduate student with a BSc in Applied Biotechnology, who is interested in Bioinformatics and Pharmaceutical Biotechnology. He is focused on employing computational techniques to design and screen for new types of drugs and targeted therapies such as natural extracts from plants and microbes, RNA aptamers, and short peptides instead of conventional chemotherapies. Such products would have lower side effects and higher specificity toward their targets. In this manner, He has published a paper about RNA aptamers and currently working on another regarding natural products. He is always open to new ideas and projects to explore and work on with the aim of making a contribution to the progress in Pharmaceutical Biotechnology.

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