In-Silico Selection of Aptamer: A Review on the Revolutionary Approach to Understand the Aptamer Design and Interaction Through Computational Chemistry

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Abstract

Aptamers are oligonucleotides and peptides with short and medium length around 15-100 nucleotides or amino acids and a molecule of interests due to its specific binding affinities to the vast array of target molecules such as ions, complex proteins and antigens up to cellular surface and cell organelles. Aptamers shows high potential of application in therapeutics and diagnostics. Aptamers are usually obtained through rigorous in-vitro screening procedures known as Systematic Evolution of Ligands by EXponential enrichment (SELEX). There are growing interests in the aptamer screening approach through computational methods such as using molecular docking and molecular modelling (MD) simulations. The approach had been increasingly popular due to minimal use of chemical and reagents, balanced with the reasonable computational costs. In-silico approaches were able to poke the details of aptamer-ligand interactions which is hard to elucidate experimentally. The authors review the successful works in screening and analysing aptamer-target complexes interactions and the effort to design the aptamers through computational simulations. The own personal experience of authors in designing a specific aptamer for Hepatitis B surface antigen through computational screening method was also discussed. In conclusion, the advancement of computational chemistry provides a promising future for the aptamers research. (C) 2019 Elsevier Ltd. All rights reserved.

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