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In silico screening of aptamers configuration against hepatitis B surface antigen (Article) (Open Access)

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Abstract

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Aptamer has been long studied as a substitute of antibodies for many purposes. However, due to the exceeded length of the aptamers obtained in vitro, difficulties arise in its manipulation during its molecular conjugation on the matrix surfaces. Current study focuses on computational improvement for aptamers screening of hepatitis B surface antigen (HBsAg) through optimization of the length sequences obtained from SELEX. Three original aptamers with affinity against HBsAg were truncated into five short hairpin structured aptamers and their affinity against HBsAg was thoroughly studied by molecular docking, molecular dynamics (MD) simulation, and Molecular Mechanics Poisson-Boltzmann Surface Area (MMPBSA) method. The result shows that truncated aptamers binding on HBsAg "a" determinant region are stabilized by the dynamic H-bond formation between the active binding residues and nucleotides. Amino acids residues with the highest hydrogen bonds hydrogen bond interactions with all five aptamers were determined as the active binding residues and further characterized. The computational prediction of complexes binding will include validations through experimental assays in future studies. Current study will improve the current in vitro aptamers by minimizing the aptamer length for its easy manipulation. © 2019 Mohamad Zulkeflee Sabri et al.

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