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Compatibility of benzimidazole and benzothiazole derivatives towards poly-A.poly-T DNA

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Benzimidazole (BNIMZ) and benzothiazole (BNTZA) based compounds are studied to understand their binding features with poly-A.poly-T DNA sequence and their mode of binding is also explored. According to thermal denaturation data, BNTZA slightly favors DNA stability with a 2.9°C advantage over BNIMZ. The DNA conformational stability of the B-DNA form was recorded with and without ligands by circular dichroism. The estimated docking scores support the findings from the UV denaturation investigation, and we observed that BNTZA had a higher docking score than BNIMZ. With the help of 50 ns MD simulations, additional conformational analyses have been performed. Both compounds effectively bind to the minor-grooves of AT-rich DNA sequence with a favorable binding free energy in accordance with the RMSD analysis, and pucker distribution of deoxyribose sugars. Future oligonucleotide therapies may be benefited because of the current discovery.

Keywords: Benzimidazole, Benzothiazole, AT-rich DNA, Thermal denaturation, Molecular Docking, Molecular Dynamics simulation