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Abstract

Exploring Carbendazim–Aptamer Interactions via In Silico Modeling and Molecular Dynamics Simulations †

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Carbendazim (CBZ), a systemic fungicide, has been found in a variety of food and feed products, agricultural soil, and water bodies, raising concerns about its possible environmental and organismal effects. While aptamers have been identified as a viable detection approach, the fundamental mechanics of ligand binding in this context have not been thoroughly investigated. In this study, CBZ-specific aptamers (CZ1, CZ2, CZ5, CZ6, CZ12, and CZ13) with known sequences were used to evaluate the binding interactions of CBZ and the aptamer. The analysis entails an all-atom molecular dynamics (MD) simulation in an aqueous environment after ensemble molecular docking. Because this aptamer lacked 3D structural information, it was rebuilt using an in-house workflow. Multiple CBZ molecules were found in a putative binding area of the anticipated 3D aptamer structure. The aptamer-CBZ complex was subjected to a 100 ns MD simulation, which allowed for the investigation of component interactions. The internal loop of the aptamer was found to include CBZ-specific bases. A prominent interaction between the aptamer and CBZ for all the studied aptamers (CZ1, CZ2, CZ5, CZ6, CZ12, and CZ13) involved H-bonds, and a hydrophobic interaction between T-shaped Pi-Pi and Pi-alkyl was observed throughout the MDS. The binding energies (BE, kJ/mol) recorded for the aptamer-CBZ complexes CZ1, CZ2, CZ5, CZ6, CZ12, and CZ13 were -136.66 ± 2.27, -93.81 ± 1.92, -67.53 ± 4.25, -86.16 ± 1.75, -52.29 ± 3.86, and -90.03 ± 1.96 respectively. This study advances our understanding of ligand–aptamer interactions. The established workflow makes it easier to create and explore new fascinating ligand–aptamer complexes.

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