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Multispectral, molecular docking and molecular dynamic simulation studies of DNA binding of a β-ionone-derived ester

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Abstract

β-Ionone is the end-ring counterpart of β-carotenoids, which are widely found in fruits and vegetables. In this research, interaction between DNA and a β-Ionone-derived ester, *(E)-4-(2,6,6-trimethylcyclohex-1-enyl) but-3-en-2-ylpyrazine-2-carboxylate* (4-TM. P), have been elucidated by various methods, such as ultraviolet-visible spectroscopy, fluorescence assays, viscosity measurements, molecular docking, and dynamic simulation. Analyses of multi-spectroscopy and viscosity assays strongly implies the groove binding of 4-TM. P to Ct-DNA. The fluorescence emission spectra of 4-TM. P values for the different Ct-DNA concentrations at 298 K showed an interaction between 4-TM. P and Ct-DNA, leading to quenching of the intrinsic fluorescence of 4-TM. P. Moreover, a fluorescence enhancement indicated a static process characterized by complex formation between 4-TM. P and Ct-DNA. The viscosity measurements demonstrated the binding mechanism between 4-TM. P and Ct-DNA because it offers unequivocal evidence of their interaction. Molecular docking simulation using AutoDock4.2 revealed that 4-TM. P was placed at the minor groove of the B-DNA, confirming the above experimental results. The dynamic stability of the complex was also confirmed using molecular dynamic simulation analyses.

Keywords: β-Ionone, DNA interaction, Docking, Dynamic simulation.