Computational Prediction of Molecular Targets responsible for Antioxidant Activity of D-pinitol in Caenorhabditis elegans

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Abstract

D-pinitol (3-O-methyl-D-inositol), a form of vitamin B inositol is a sugar-like molecule used for natural healing purposes for various diabetic-associated conditions. It is found in various plants like legumes, leafy vegetables, and citrus fruits, but is not found in animals and humans. In the present investigation, we have predicted possible biological molecular targets for D-pinitol using reverse docking approaches. In the process, we have identified that D-pinitol have affinity for most of the enzymes directly/indirectly associated with the free radical scavenging processes, indicating that D-pinitol might use as a potential antioxidant. The prediction was further in vivo validated on C. elegans, a multicellular model system using chemotaxis, thermo-tolerance and ROS scavenging activities assay. A strong correlation was observed in the computational prediction and in vivo antioxidant activities assays of D-pinitol in a dose-dependent manner. The findings broaden our current perspectives in understanding the antioxidative properties of D-pinitol.

References

- Singh RK, Pandey BL, Tripathi M, Pandey VB. Anti-inflammatory effect of (+)-pinitol.
Computational Prediction of Molecular Targets responsible for Antioxidant Activity of D-pinitol in Caenorhabditis elegans

Index Terms

Computer Science  Artificial Intelligence

Keywords

Caenorhabditis Elegans  D-pinitol  Anti-oxidative Activity  Reverse Docking Approach