Aguinaldo R de Souza et al., Med chem 2016, 6:7(Suppl)
http://dx.doi.org/10.4172/2161-0444.C1.021

Determination of the rotational barrier of divanillin enantiomers by density functional theory (DFT) calculations and docking computer simulation of the complex with bovine serum albumin (BSA)

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Divanillin (6,6'-Dihydroxy-5,5'-dimethoxy-[1,1'-biphenyl]-3,3'-dicarboxaldehyde) is an antioxidant and a reactive poly-functional molecule (CAS Number 2092-49-1), linear formula [HOC6H2(OCH3)(CHO)-]2, CAS Number 2092-49-1, and molecular weight 302.28. The numerous beneficial health properties of vanillin have been extended to Divanillin due to the various functional groups present in the molecule and due to its specific molecular properties. We performed a comprehensive, theoretical (DFT), experimental (ECD), and docking computer simulation of the interaction of Divanillin with bovine serum albumin (BSA) to understanding the preferential sites of interaction between these two bio-molecules. The rotational barrier of Divanillin enantiomers was calculated using with the M06-2X method with the 6-31G(d) basis set, where the solvent, water, was included through the Polarized Continuum Medium (PCM). The docking was obtained by Molecular Mechanics models for Divanillin and BSA. In accordance with the theoretical and experimental results Divanillin bound to a specific site of BSA in a conformation where the torsion angle between selected atoms is equal to 130 degrees due to the hydrogen-bound found between the hydroxyl groups of Divanillin and the protein pocket.

Biography

Aguinaldo Robinson de Souza has completed his PhD from University of São Paulo (USP) and postdoctoral studies from University of California at San Diego. He is a Professor at São Paulo State University – UNESP at Bauru/SP/Brazil. He has published more than 40 papers in reputed journals and participated in several scientific congress

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