Computational predictions for inhibitability of *D. citrea* essential oil composition against oligo-1,6-glucosidase

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ABSTRACT

Distichochlamys citrea M.F. Newman, a genus endemic to Vietnam, has been known by folk experiences for its biological potential, including antidiabetics. The essential oil was extracted and characterized by gas chromatography-mass spectrometry for compositional specificity. The data was used as input for computational predictions. Gas chromatography-mass spectrometry analysis revealed the presence of 23 natural components in the essential oil (C1-C23); major constituents: α-citral (C16; 21.20 %), cineole (C7; 16.11 %), β-citral (C14; 16.03 %), geranyl acetate (C20; 15.97 %), geraniol (C15; 10.75 %). Density functional theory calculation suggests C14 and C15 highly promising for intermolecular interactions by on their electronic configurations. Molecular docking simulation predicts the most effective inhibitors against PDB-3AJ7 (oligo-1,6-glucosidase) into the order of ligand-protein complexes: C15-3AJ7 (DS -11.9 kcal.mol-1) ≈ C14-3AJ7 (DS -11.8 kcal.mol^{-1}) > C12-3AJ7 (DS -11.5 kcal.mol^{-1}) > C11-3AJ7 (DS -11.2 kcal.mol^{-1}) > C9-3AJ7 (DS -11.0 kcal.mol^{-1}). All the components are expected to be biocompatible (by QSARIS physical properties) and safe for medicinal use (by ADMET pharmacokinetics and pharmacology). Altogether, the results encourage further consideration of *D. citrea* M.F. Newman essential oil for further wet antidiabetic tests, especially the specification on C14 (aka. β-Citral) and C15 (aka. Geraniol).

Keywords*: Distichochlamys citrea; antidiabetics; density functional theory; molecular docking; QSARIS; ADMET.*