Virtual Screening of the Active Components of Garcinia mangostana Linn. Potentially Inhibiting the Interaction of Advanced Glycation End-products and their Receptor

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Abstract

BACKGROUND: Mangosteen (Garcinia mangostana L.) is a plant that contains various secondary metabolite compounds, one of which is xanthone. Xanthone in mangosteen has a variety of beneficial biological and medical effects, one of which is an antioxidative, anti-inflammatory, and antiapoptotic agent.

AIM: The aim of the study was to perform the selection of any xanthone in mangosteen pericarp that have potentially inhibit the interaction of AGEs and RAGE.

METHODS: The analysis was made in silico by docking method using software Hex 8.0. The docking was done between AGEs-RAGE, also between nine active compounds of G. mangostana with RAGE. The active compounds analyzed here were including α-mangostin, β-mangostin, γ-mangostin, mangostanol, garcinone D, 1,6-Dihydroxy-3,7-dimethoxy-2-(3-methylbut-2-enyl)-xanthone, gartanin, 1-isomangostin, and 3-isomangostin. Further analysis was performed to see the interactions formed between ligands with their receptors using software LigPlus+ and Discovery Studio 4.1.

RESULTS: 1-isomangostin, 3-isomangostin, γ-mangostin, mangostanol, D-garcinone, and gartanin have potentially could inhibit the interaction and activity of imidazole in RAGE through a competitive binding mechanism.

CONCLUSIONS: The inhibition of imidazole-RAGE activity by the mangosteen active components may inhibit the pathobiology of AGEs-RAGE axis.