

Article

Inhibition of Aldose Reductase by Ginsenoside Derivatives via a Specific Structure Activity Relationship with Kinetics Mechanism and Molecular Docking Study

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Abstract: This present work is designed to evaluate the anti-diabetic potential of 22 ginsenosides via the inhibition against rat lens aldose reductase (RLAR), and human recombinant aldose reductase (hERAR), using α -glyceraldehyde as a substrate. Among the ginsenosides tested, ginsenoside Rh2, (20S) ginsenoside Rg3, (20R) ginsenoside Rg3, and ginsenoside Rh1 inhibited RLAR significantly, with IC_{50} values of 0.67, 1.25, 4.28, and 7.28 μ M, respectively. Moreover, protopanaxadiol, protopanaxatriol, compound K, and ginsenoside Rh1 were potent inhibitors of hERAR, with IC_{50} values of 0.36, 1.43, 2.23, and 4.66 μ M, respectively. The relationship of structure–activity exposed that the existence of hydroxyl groups, linkages, and their stereo-structure, as well as the sugar moieties of the ginsenoside skeleton, represented a significant role in the inhibition of hERAR and RLAR. Additional, various modes of ginsenoside inhibition and molecular docking simulation indicated negative binding energies. It was also indicated that it has a strong capacity and high affinity to bind the active sites of enzymes. Further, active ginsenosides suppressed sorbitol accumulation in rat lenses under high-glucose conditions, demonstrating their potential to prevent sorbitol accumulation *ex vivo*. The findings of the present study suggest the potential of ginsenoside derivatives for use in the development of therapeutic or preventive agents for diabetic complications.

Keywords: ginsenosides; diabetic complication; aldose reductase; enzyme kinetics; molecular docking; sorbitol accumulation

1. Introduction

According to the World Health Organization, approximately 200 million people—5.9% of the adult population worldwide—suffer from diabetes, a very common disease that has assumed epidemic proportions. As a result, it is expected that by 2025, the disease will have a significant impact on human health [1,2]. Diabetes mellitus (DM) is a complex and chronic metabolic disease characterized by hyperglycemia, a condition in which a

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