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Synthesis, Antifungal Activity, and Molecular Docking Studies of Some New Di-*O*-Isopentanoyl Glucopyranosides

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Extensive research over the past decades has shown that sugar ester (SE)-type biomolecules bring long-chain fatty acids with sugar moieties into the plant cells and play various important roles in food, surfactants, innovative green materials, and biological properties. Thus, in this study, dimolar isopentanoylation of methyl α-D-glucopyranoside (compound 4) furnished methyl-2,6-di-*O*-isopentanoyl-α-D-glucopyranoside (compound 5), indicating selectivity at C-2 and C-6 positions. The obtained compound (5) was further acylated to give 3,4-di-*O*-acyl esters (compounds 5-8) in good yields. *In vitro* antifungal activities of these compounds exhibited moderate to good zone of inhibition. To rationalize these results, molecular docking studies of compounds 4-8 were performed on lanosterol 14-α-demethylase (CYP 51). The attachment of acyl ester chain(s) to the glucopyranoside ring added more lipophilicity and affected their fungal inhibition by binding to the lanosterol 14-α-demethylase enzyme. In particular, the isopentanoyl group showed a stronger binding affinity with lauroyl groups, as in compound 8, than with the fluconazole group, indicating the higher efficiency of SEs.

Keywords: Antimicrobial, Glucose esters, HMBC, Selective acylation, Lanosterol 14-α-demethylase

INTRODUCTION

Sugar esters (SEs), also known as sugar fatty acid esters, are generally prepared by esterification between sugar/sugar alcohols and non-polar fatty acids/acyl halides [1]. Glycosidic and ester bonds with alkyl fatty acid chain showed amphiphilicity and biodegradability under aerobic and anaerobic conditions [2], indicating that SEs are environment friendly, biocompatible, non-toxic, tasteless, odorless, non-irritating, and cost-effective [3-5]. SEs-type biomolecules bring long-chain fatty acids with sugar moieties into the plant cells and play various important roles, including the gelatinization of starch, formation of emulsions, *etc*. [6]. These properties allow SEs to have broad-spectrum applications in the food, cosmetics, beverage, surfactant, chemical, and pharmaceutical sectors [7-8]. Encouragingly, many natural and synthetic SEs have been reported to have antibacterial [9], antifungal [10-11], and pesticide [12-13] properties. Recently, SEs have been used in the preparation of biocompatible materials. For instance, SEs have been found to improve the performance of high-amylose starch-based wood adhesives (HASWA) by increasing the thermal stability of starch and blocking the aggregation of latex particles [14]. In addition, several SEs have been found to resist wood decay in aspen and pine wood. Biomaterials prepared by the combination of SEs and chitosan showed superior wound healing properties *in vivo* compared to the available wound healing products (Healosol®) [15]. These wound healing properties were found to depend on the degree of substitution of the SEs

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