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The effects of protecting and acyl groups on the conformation of benzyl α-L-rhamnopyranosides: An in silico study

Farzana Islam[a], Md. Rezaur Rahman[b], Mohammed M. Matin[1,a]

[a]Bioorganic and Medicinal Chemistry Laboratory, Department of Chemistry, Faculty of Science, University of Chittagong, Chittagong, 4331, Bangladesh.

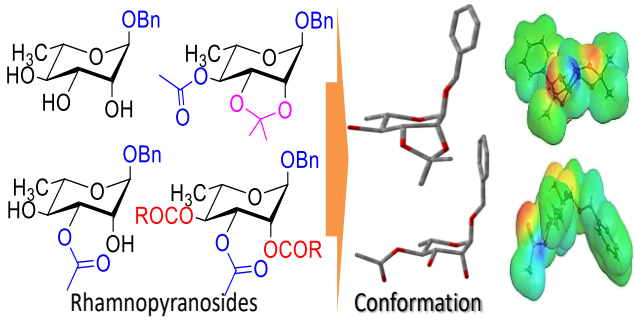
[b]Department of Chemical Engineering and Energy Sustainability, Faculty of Engineering, Universiti Malaysia Sarawak, Jalan Datuk Mohammad Musa, Kota Samarahan, 94300, Malaysia

Abstract:

Carbohydrate fatty acid (CFA) esters especially rhamnopyranoside esters having both the hydrophilic and lipophilic nature showed broader applications including anticancer activities. It was reported that appropriate conformation is needed for better activities and conformational distortion reduced antimicrobial functionality. In this context, two different esters series of benzyl α-L-rhamnopyranosides, one with 2,3-O-acetonide group and the other one without acetonide group, were subjected for the density functional theory (DFT) optimization. The optimized structures with 2,3-O-acetonide rhamnopyranoside clearly showed distortion from the regular $^1C_4$ chair conformation while rhamnopyranoside esters without 2,3-O-acetonide functionality exhibited almost regular $^1C_4$ chair conformation. Also, the number and position of acyl group(s) present in the benzyl rhamnopyranoside imposes a small effect on their pyranose chair conformation. Thermodynamic properties including frontier molecular orbitals (FMO) and molecular electrostatic potential (MEP) of both the series of rhamnopyranosides are also discussed which indicated that 4-O-acyl rhamnopyranosides are more reactive than the 3-O-acyl analogues.

Keywords: *Conformational study; DFT optimization; MEP; Rhamnopyranoside; Sugar esters (SEs); Thermodynamic properties.*

Graphical Abstract



Highlights

- Acetonide protected rhamnopyranosides are highly distorted from $^1C_4$ chair conformation.
- Acyl group at C-4 position of rhamnopyranoside imposes more electrophilicity than at C-3 position.
- The number and chain length of acyl group(s) in rhamnopyranoside affect very little on its chair conformation.

1. Introduction

The most ubiquitous biomolecules named carbohydrates play the pivotal role in many biological processes. However, many natural carbohydrate compounds showed poor binding affinities [1] which led their structural modification to improves applicability in various fields including drug candidates [2-4]. Structural modification with

[1] Corresponding Authors

e-mail: mahbubchem@cu.ac.bd; mmmatin2004@yahoo.co.in