



Synthesis, Characterization and *in Silico* Study of the New Glycoside-Oxadiazole Hybrid

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ABSTRACT

INTRODUCTION: Carbohydrates constitute an important class of biomolecules and participate in multiple biochemical processes. Because they are biocompatible, they are good candidates to participate in different chemical transformations leading to potential drugs. **OBJECTIVES:** To synthesize, characterize and perform an *in silico* study of the new Glycoside-Oxadiazole hybrid. **METHODS:** The new glycoside-oxadiazole hybrid was synthesized from successive reactions: 1. O-Acylamidoxime reaction followed by cyclodehydration; 2. Glycosylation reaction; and 3. Basic hydrolysis reaction. All reactions were monitored by thin layer chromatography (TLC) and revealed in the H₂SO₄:EtOH system (ratio 95:5). The characterization of the compounds was performed by spectrometric techniques (hydrogen and carbon-13 nuclear magnetic resonance, infrared and high-resolution masses) and polarimetry. The *in silico* study was performed using the *Molinspiration Property Calculator* and *OSIRIS Property Explorer* software's. **RESULTS AND DISCUSSION:** The new Glycoside-Oxadiazole hybrid was obtained with an overall yield of 56% after three reaction steps, while the chemical shift data of the hydrogen and carbon-13 nuclei, the wavenumbers of the bands related to the chemical bonds and the exact mass value confirm the structure of the new hybrid. The *in silico* study of the new Glycoside-Oxadiazole hybrid, through the *Molinspiration* software, indicated that this compound does not violate any Lipinsk rule, since nDLH = 2, nALH = 7, MM = 304.30 g/mol (maximum allowed values: nDLH < 5; nDALH < 10 and MM < 500 daltons). Additionally, from the OSIRES software it was verified that this hybrid did not present risk of mutagenicity, tumorigenicity, irritability and interference in reproduction. **CONCLUSION:** The new Glycoside-Oxadiazole hybrid was synthesized after three reaction steps in moderate overall yield and its structure was confirmed by different spectrometric techniques. The *in silico* study showed that the new hybrid presents good physical, chemical and toxicological properties, which motivate future studies in the synthetic and biological fields.