nConformational characterization of saponins conformation in pyridine

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Saponins are glycosides produced by plants, consisting of a polycyclic aglycone (a triterpene or a steroid), added by a sugar chain. This biomacromolecules might present antinociceptive and antitumoral actions, as well as antiinflammatory, antiviral and antithrombotic activities. In this context, Erucasaponin A and Stellatoside B, triterpene saponins extracted from the cactaceous plant *Stenocereus eruca,* are the subject of this project, which aims to evaluate the capability of computational methodologies in describing and predicting the conformation of glycoconjugates in non-aqueous solvents, that is, pyridine, and compared the obtained results to our previous data in aqueous solutions. Accordingly, parameters for pyridine were obtained from HF/6-31G**, while the glycosidic linkages of the studied saponins were described by energy contour plots, rotating the Φ and Ψ angles from 0° to 360°, in steps of 30° using the GROMACS simulation package and GROMOS96 force field, added by a series of carbohydrate parameters previously described by the group. The employed methodology allowed us to characterize the major conformations of the saponins glycosidic linkages in a pyridine solution, as well as the flexibility pattern of each of its constituent linkages. Additionally, the so obtained parameters for both pyridine and compounds conformation were accordingly validated through previous experimental data as NOESY distances. Therefore, the obtained results agrees with previous works indicating that MD simulations are also capable to handle part of the π interactions in molecular systems and may further contribute in the comprehension of the structure and function of biologically active compounds.

Keywords: *saponin; Stenecereus eruca; molecular dynamics; pyridine; building blocks*
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