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Chemical Characterization, Crystallography and Acute Toxicity Evaluation of Two Boronic-Carbohydrate Adducts

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Abstract : Boronic acids are able to create diester bonds with carbohydrates because of their hydroxyl groups; in nature, there are some organoborates with these characteristics, such as the calcium fructoborate, formed by the union of two fructose molecules and a boron atom, synthesized by plants. In addition, it has been observed that, in animal cells only the compounds with cis-diol functional groups are capable of linking to boric or boronic acids. The formation of these organoboron compounds could impair the physical and chemical properties of the precursors, even their acute toxicity. In this project, two carbohydrate-derived boron-containing compounds from D-fructose and D-arabinose and phenylboronic acid are analyzed by different spectroscopy techniques such as Raman, Infrared with Fourier Transform Infrared (FT-IR), Nuclear Magnetic Resonance (NMR) and X-ray diffraction crystallography to describe their chemical characteristics. Also, an acute toxicity test was performed to determine their LD50 using the Lorke's method. It was confirmed by multiple spectra the formation of the adducts by the generation of the diester bonds with a β-D-pyranose of fructose and arabinose. The most prominent findings were the presence of signals corresponding to the formation of new bonds, like the stretching of B-O bonds, or the absence of signals of functional groups like the hydroxyls presented in the reagents used for the synthesis of the adducts. The NMR spectra yielded information about the stereoselectivity in the synthesis reaction, observed by the interaction of the protons and their vicinal atoms in the anomeric and second position carbons; but also, the absence of a racemic mix by the finding of just one signal in the range for the anomeric carbon in the 13C NMR spectra of both adducts. The acute toxicity tests by the Lorke's method showed that the LD50 value for both compounds is 1265 mg/kg. Those results let us to propose these adducts as highly safe agents for further biological evaluation with medical purposes.

Keywords : acute toxicity, adduct, boron, carbohydrate, diester bond
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