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THE NMR INVESTIGATIONS OF D-GLUCOFURANOSIDURONO-6,3-LACTONES CONFORMATIONS

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Despite of their ubiquity in biological structures, furanosides have received much less attention than pyranosides as regards the conformational analysis. This is because different conformations of five-membered rings have quite similar energies, whereas six-membered rings are normally present in a single low-energy chair conformation. Therefore, conformations of pyranosides in solution are easily identified by NMR techniques, which is not the case with furanosides. These are equilibrating rapidly on the NMR scale and averaging of coupling constants occurs. However, when a tetrahydrofuran ring is conformationally restricted by a rigid second skeleton, it is possible to predict its conformation.¹

Previously, we found that methyl 2,5-di-O-acetyl- β -D-glucofuranosidurono-6,3-lactone and 1,2,5-tri-O-acetyl- β -D-glucofuranurono-6,3-lactone adopt a 1T_2 -like conformation, both in the crystal structure and in solution. It seems to us that the characteristic 1H NMR spectra of these β -D-glucofuranosidurono-6,3-lactones may be indicative of a 1T_2 -like conformation. To verified this thesis we synthesized a series of D-glucofuranosidurono-6,3-lactones with different aglycones. The NMR studies of obtained β -D-glucofuranosidurono-6,3-lactones confirm our assumptions. Additionally, we obtained the NMR data, indicative for α -D-glucofuranosidurono-6,3-lactones in a 1T_2 -like conformation.

References:

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