Investigating Hydrogen bond donating ability of deoxygenated and deoxyfluorinated carbohydrates

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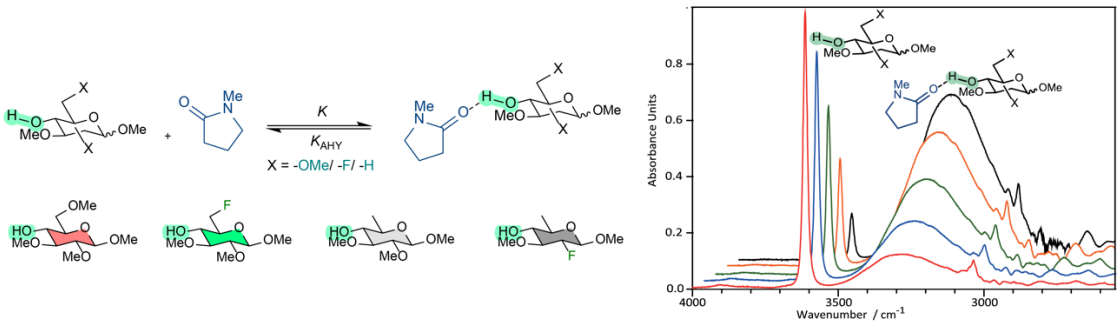
The Hydrogen bond (HB) is one of the main interactions between carbohydrates and proteins. There is little detailed knowledge of HB properties of individual alcohol groups in carbohydrates. Based on our previous work on HB donating (HBD) properties of alcohol groups in model compounds [1], this work aims to chart the HBD properties of alcohols in important sugars, and how this is influenced by substitutions such as deoxygenations and deoxyfluorinations.

The HBD capacity is measured as the equilibrium constant between an alcohol and a standard acceptor (*N*-methylpyrrolidinone, NMP), and achieved by FTIR through the absorption bands of the free and hydrogen-bonded O–H bonds. [2]

This IR-based method is only suitable for monohydroxylated compounds. Hence, initial series of model substrates have been synthesised with the 4-OH group unprotected. For some compounds, both anomers were investigated. Furthermore, the influence of deoxygenation and deoxyfluorination at the 6- and 2-positions was investigated.

The data show that despite the presence of intramolecular OH•••OMe hydrogen bonding, the alcohol groups of carbohydrates display a hydrogen bond donating capacity similar to that of isolated alcohols, and that there are marked differences upon changing stereochemistry or introducing remote deoxygenation and deoxyfluorinaton. These results will be valuable for the interpretation of binding data of carbohydrates and glycomimetics to proteins.



Determination ohydrogen-bond (HB) donating ability of an alcohol by infrared (IR) spectroscopy

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Bibliographic references:

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