

Probing interactions of carbohydrates with biomolecules and water by vibrational spectroscopy

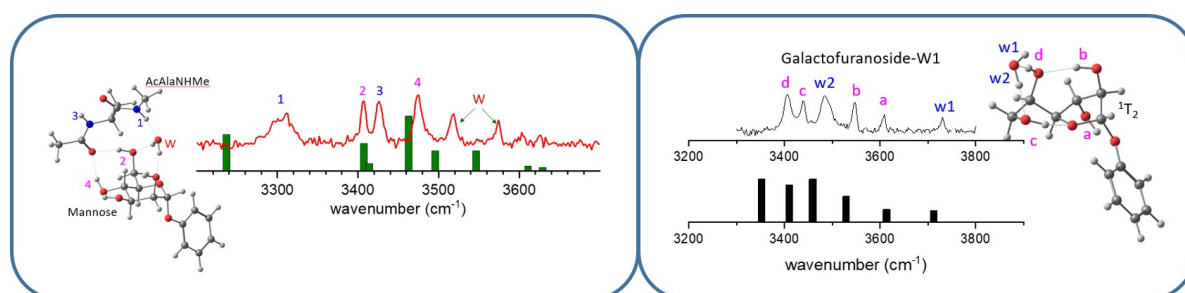
Pierre CARCABAL [1]

[1] Institut des Sciences Moléculaires d'Orsay, CNRS, FRANCE

pierre.carcabal@universite-paris-saclay.fr

Carbohydrates are especially efficient as vectors of molecular information encoded in their structural and conformational diversity and flexibility that enables communicating selectively with other biomolecules. This molecular communication proceeds *via* subtle non-covalent interaction networks engaged by the carbohydrates. These networks are dominated by electrostatic Hydrogen Bonding and the full range of non-covalent interactions is at play, including polarization and dispersion. In the gas phase, applying to carbohydrates experimental mass resolved and conformer selective vibrational spectroscopy and modeling,¹ we have extensively studied the conformational and structural preferences of non-covalent complexes between carbohydrates molecules, water² and also peptide models.³ The vibrational resolution achieved in cold gas phase measurements (Figure), allows identifying each molecular group involved in the interactions and evaluating their strength. It is possible to remove any solvent perturbation, before reintroducing water effects by studying size-controlled hydrated complexes.

In this presentation we will survey the most recent results obtained on the structural preferences of monosaccharides such as furanoside cycle stabilization with and without the perturbation of water molecules (on the right in the figure), or mannopyranosides engaged in direct interaction with peptide models in non-covalent complexes where water comes to play a cementing role, intercalated between the interacting molecules (on the left in the figure).



Vibrational spectra of complexes formed by one water molecule and (left) a mannoside and a peptide model, and (right) a Galactofuranoside.

Bibliographic references:

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2. P. Çarçabal, R.A. Jockusch, I. Hünig, R.T. Kroemer, L.C. Snoek, J.P. Simons, I. Compagnon, J. Omens (2005), *J. Amer. Chem. Soc.* (127) 11414-11425.
3. E. J. Cocinero, P. Çarçabal, J. P. Simons and B. G. Davies (2011), *Nature* (469) 76–79.