

ISOLATED CARBOHYDRATES AND CARBOHYDRATE INTERACTIONS

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The interaction between carbohydrates and proteins is a key factor in many biological processes but the factors dictating selective carbohydrate–protein interactions are not easily discerned. Selectivity must depend in part upon the conformational structures of the interacting carbohydrate ligands and their receptors but because of their flexibility and the universality of hydrogen-bonded interactions in aqueous environments, their structures and interactions may also be influenced by explicit hydration, dehydration, or the direct involvement of water at the receptor site. Understanding carbohydrate structural choice and the consequences of carbohydrate interactions with water, with proteins or with both, presents a notoriously complex challenge. Characterizing their *intrinsic* three dimensional structures is a key starting point on the road towards meeting it – a necessary first step on the way to investigating and understanding the consequences of their interactions with other molecules, not least water. The lecture will review recent [1, 2] and current spectroscopic and computational investigations of a range of carbohydrates that are important in Nature, initially isolated in the gas phase and subsequently, interacting with other molecules, particularly water and peptides. They have been selected not just because they *are* ‘do-able’ but because of the physical and biochemical issues they address.

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[1] Sugars in the gas phase: spectroscopy, conformation, hydration, co-operativity and selectivity, J.P.Simons, P.Çarçabal, B.G.Davis, D.P.Gamblin, I.Hünig, R.A.Jockusch, R.T.Kroemer, E.M.Marzluff and L.C.Snoek, Intl. Revs. Phys. Chem., 2005, 24, 489-532.

[2] Good vibrations: probing biomolecular structure and interactions through vibrational spectroscopy in the gas phase, J.P. Simons, Molec. Phys., 2009, **23**, 2435-2458.