

PROVING THE ROLE OF WATER MOLECULES IN SUGAR-PEPTIDE INTERACTIONS

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Sugars are one of the most important families of biomolecules. They act as mediators of molecular recognition processes. Among the possible biomedical applications, one example is the addition of mannosides to photosensitizers used in PhotoDynamic Therapy, targeting Mannose Receptor (MR) proteins on pathogenic cells. A precise description of the structural basis of Mannose-MR local and direct interplay, which can be provided by gas phase spectroscopy, critically lacks to design PSs with improved selectivity.

In the gas phase, combining experimental mass resolved and conformer selective double resonance vibrational spectroscopy and theoretical chemistry studies,^a we have already been able to observe several complexes between sugars and peptide models.^{b,c} We can now also observe such complexes with a controlled number of water molecules. Our most recent results on complexes of mannose with different peptide models, either hydrated or not, allow resolving the nature of the interactions between the molecules, for each donor and acceptor molecular group involved in the non-covalent bonds governing the complexes. These results evidence the adaptability of the sugar moiety to its peptide receptor. In particular, the study of the complexes formed with few water molecules may highlight the role of water in molecular recognition processes in an unprecedented manner.

^aCocinero E.J.; Çarçabal P., *Top. Curr. Chem.*, 2015, 364, pp. 299-333.

^bCocinero E.J.; Çarçabal P.; Vaden T.D.; Simons J.P.; Davis B.G., *Nature*, 2011, 469, 76-79.

^cCocinero E.J.; Çarçabal P.; Vaden T.D.; Davis B.G.; Simons J.P., *J. Amer. Chem. Soc.*, 2011, 133, 4548-4557.