

## Modeling of molecular recognition processes in Glycobiology. Some examples.

Sonsoles Martín-Santamaría,<sup>a,\*</sup> Maria Morando,<sup>b</sup> Karla Ramírez-Gualito,<sup>a,b</sup> Virginia Roldós<sup>b</sup>  
<sup>a</sup>Dep. de Química, Facultad de Farmacia, Universidad San Pablo CEU, Urb. Montepríncipe, Madrid-28668, Spain; <sup>b</sup>CIB-CSIC, C/ Ramiro de Maeztu 9, Madrid-28040, Spain  
e-mail: [smsantamaria@ceu.es](mailto:smsantamaria@ceu.es)

In the last decades, molecular modeling has been widely used for the understanding of relevant molecular recognition events. The knowledge of target-ligand interactions at atomic level has proven to have many beneficial applications for human health, as drug design, among others. We report here some examples that account for the application of molecular modeling tools to the study of a) carbohydrate-carbohydrate, and b) protein-carbohydrate interactions.

a) Weak  $\text{Ca}^{2+}$ -mediated carbohydrate-carbohydrate interactions have been studied for sugar-decorated gold nanoparticles as the “macromolecule” and the same carbohydrate as the ligand (Figure 1). 3D models of trisaccharide- $\text{Ca}^{2+}$ -trisaccharide complexes based on results from MD simulations are presented, in agreement with experimental observations. The obtained complexes provide a working model on the cell-cell recognition process that mediates interactions in certain types of marine sponges.[1]

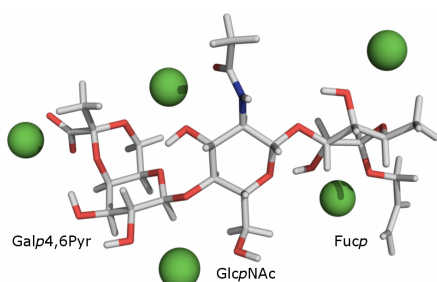


Figure 1

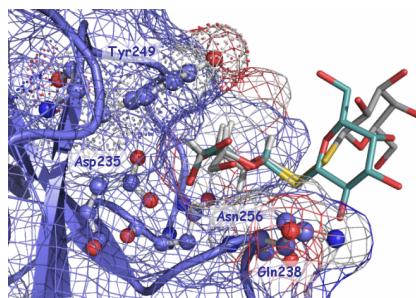


Figure 2

b) Docking and MD simulation techniques have been applied to the study of specific interactions of human galectin-1 and lactose mimetics (Figure 2).[2] Human galectin-1 is involved in cell recognition and adhesion processes, and has proven to play a pivotal role in metastasis. Insights into galectin binding can be very valuable for the understanding of the interaction mechanism of these compounds, and for further design of selective binders able to modulate galectins functions.[3] It has been shown that intermolecular hydrogen bonds as well as van der Waals and CH- $\pi$  interactions are the key forces involved in the process. The role of water has also been evaluated.

- [1] a) Carvalho de Souza, A.; Vliegthart, J. F. G.; Kamerling, J. P. *Org. Biomol. Chem.* **2008**, 6, 2095-2102. b) Santos, J. I.; Carvalho de Souza, A.; Cañada, J.; Martín-Santamaría, S.; Kamerling, J. P.; Jiménez-Barbero, J. *ChemBioChem*, **2009**, 10, 511-519.  
[2] Camby, I.; Le Mercier, M.; Lefranc, F.; Kiss, R. *Glycobiology*, **2006**, 16, 137R-157R.  
[3] Gabius, H.-J. Ed. *The Sugar Code. Fundamentals of glycosciences*, Wiley-VCH, Weinheim, **2009**.