

Chemistry Department

NMR and Molecular recognition

Molecular Structure & interactions NMR group

MSI NMR
group



Filipa Marcelo

(Post-doc researcher)

Filipa Marcelo received her Ph.D. degree (Chemistry) in 2009. After a postdoctoral period working in NMR at CIB-CSIC Madrid, she moved to MSI NMR group focusing her research on NMR and molecular recognition.

Objectives

Carbohydrates in Nature play diverse and key roles, making them attractive subjects for chemical and biological research. Combining NMR binding experiments with molecular modeling protocols, I am interested to investigate the key molecular interactions involving carbohydrates and their biological receptors in the context of molecular recognition events. In particular, I am interested in NMR methodology to study the conformation and dynamics of carbohydrate-protein complexes from a ligand and protein's perspective.

Methodology

Binding studies are accomplished using modern NMR techniques focused on NOE-related and diffusion measurements. Saturation transfer difference (STD-NMR), transferred NOE (trNOESY) and diffusion experiments (DOSY) are the most common techniques employed to investigate carbohydrate-protein molecular interactions from the ligand's perspective. In some cases the solution 3D structure of the protein using a protocol based on NMR spectroscopy is also determined and NMR binding studies from protein's point view carried out. All the NMR data is combined with docking and assisted by molecular mechanics and dynamics simulations.

Expected Results

Characterize the binding epitope of the ligand by STD and its bioactive conformation by trNOESY. Obtain a detailed picture of the receptor 3D structure by NMR assisted by molecular modelling (if not already described). Determine the energetic and dynamics of the interaction process. Define the 3D structure of the carbohydrate-protein complex.



Fig 1. 600 MHz apparatus with cryoprobe head.

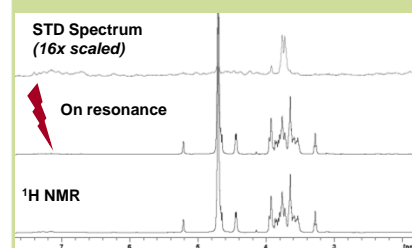


Fig 2. STD spectrum.

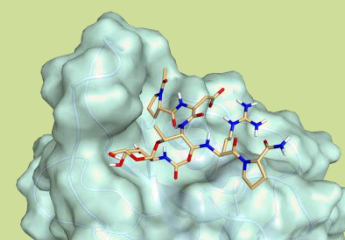


Fig 3. 3D view of the carbohydrate-protein complex.