The Interacction between Hevein and the Core of N-glycan chains of Glycoproteins. An NMR Study.

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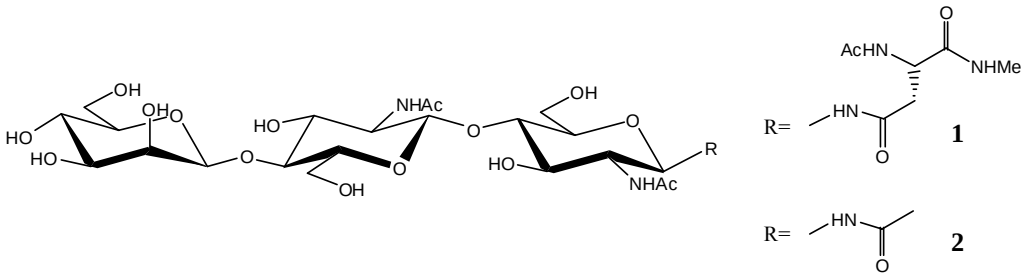
Nowadays, it is well demonstrated that the major role of carbohydrates in biological systems is to be points of molecular recognition.[1]

One of these recognition processes is the chitooligosaccharide binding to hevein domains. Hevein is a small 43 aminoacids protein isolated from the Hevea brasilensis latex.[2]

In the case of the hevein domain from Urtica dioica lectin, which is a superantigen to T cell, it has been shown that it is able to bind the N-glycan chains of mammal glycoproteins.[3]

Considering that the core of these N-glycan chains is formed by the glycopeptide β-Man-1→4-β-GlcNAc-1→4-β-GlcNAc-Asp and that the minimal unit which is recognized by hevein is chitobiose (β-GlcNAc-1→4-β-GlcNAc), we have synthesized (*Univertität Bayreuth*) the model molecules **1** and **2** studied the interaction between them and hevein.



The interaction was followed by NMR titration at different temperatures and the obtained results were compared to those previously obtain for different chitooligosaccarides.

The stability of the complex was studied by docking calculations and solvated molecular dynamics. These results indicate that the complex is stable and the binding corresponds to only one of the binding modes previously decribed for chitooligosascharides.[2]

The calculated model was validated by experimental data extracted from the analisis of NOESY and TOCSY espectra of the complex (500 and 900 MHz).

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This work has been carried out with financial aid of Ministerio de Educación y Ciencia (Spain) and the European Community(FP6 program; RDIS contract number 011952)