Sequence Determination of Oligo- and Polysaccharides from NMR using a WWW-interface to the Computer Program CASPER

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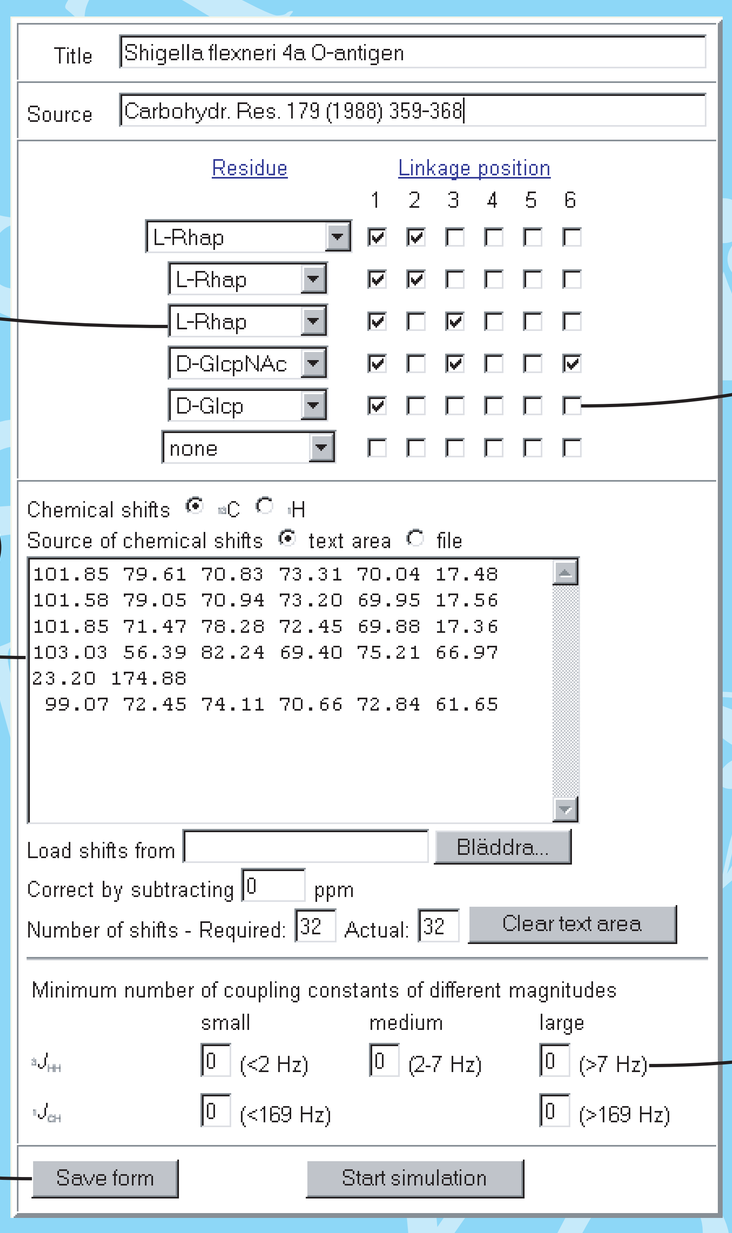
Introduction

NMR spectroscopy has emerged as the most important tool for the structure determination of oligo- and polysaccharides. Whilst component and linkage analysis are still performed by chemical methods the determination of anomeric configuration and sequence is now routinely performed by NMR.

Since the NMR spectra of most carbohydrates are unique, it is possible to determine their structure from a single NMR spectrum. The computer program CASPER generates trial structures from information of component and linkage analyses and calculates their NMR spectra. The trial structures are then ranked according to their agreement with the experimental spectrum.

HTML-form with the input for CASPER



11 glycosyl residues to choose from

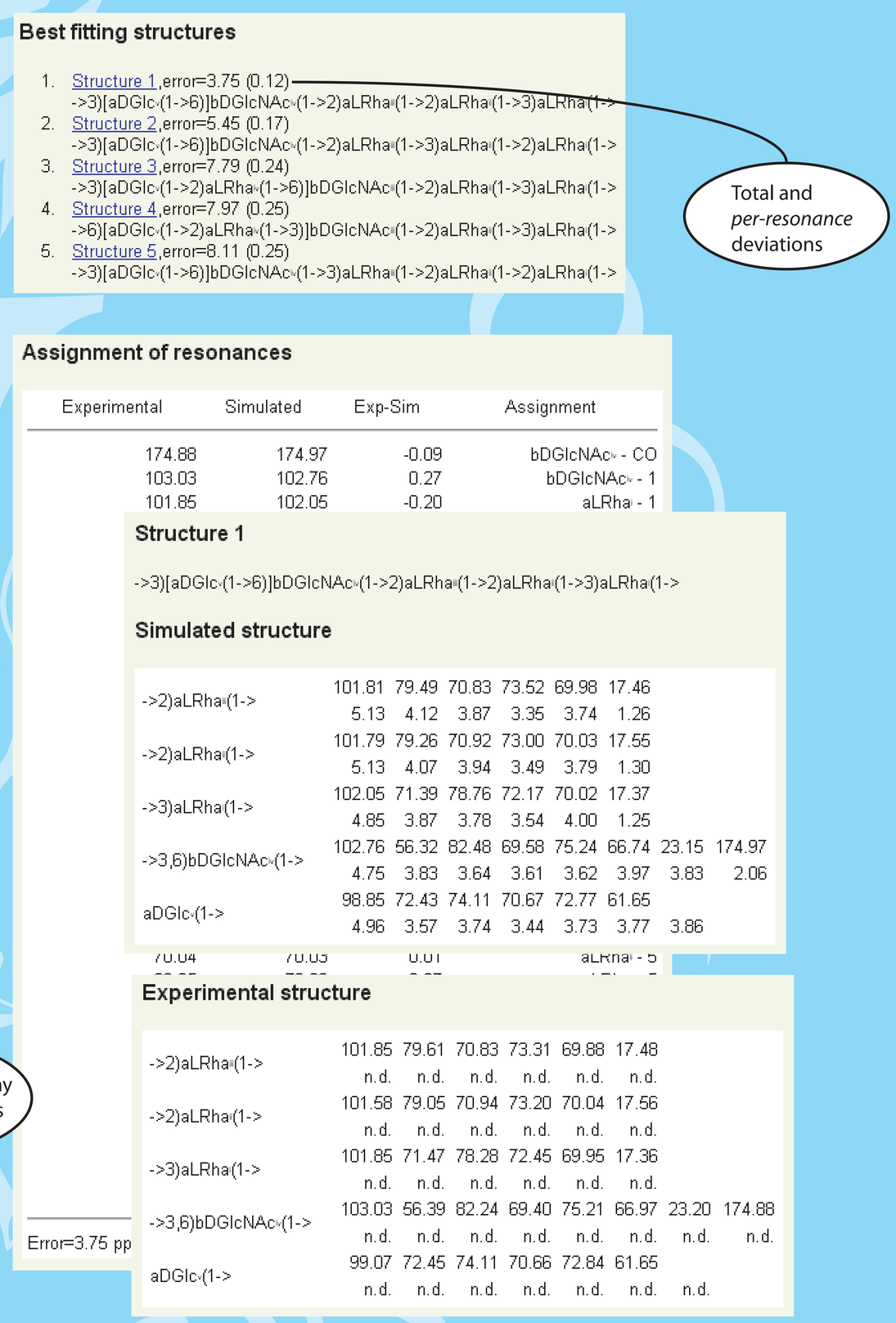
Linkage positions are checked for consistency

Chemical shifts are entered here

Coupling constants may be used as restrictions

A filled form can be saved locally

Output from a sequence determination



The main drawback of CASPER has been the interface and the fact that the program and databases have been in a state of flux. Using an interface based on HTML-forms and server-side scripts allows us to retain creative control over the program whilst making it available to the widest possible audience.

Results

The five structures with the smallest deviation between calculated and experimental spectra are shown together with the complete assignments of all chemical shifts.

How well CASPER succeeds in picking the correct structure depends mainly on the number of possible structures. Trials with known structures show that most ^{13}C-NMR spectra are simulated with a deviation of <0.3 ppm/resonance. In the case of structures with three residues in the repeating unit this is sufficient to determine the correct structure.

http://www.casper.organ.su.se/casper/