ABSTRACT

NMR is a technique with very broad applications within the field of proteins and DNA as it often can provide exclusive information about their; structure, folding properties, mobility, and interactions with other molecules, which is not always possible to measure using other methods. Two major drawbacks with the method are the complex output from the experiments, which usually requires extensive manual investigation before the information content from the experiment can be explained properly, and the traditional choice of data recording where data is recorded on a grid for subsequent Fourier transform to frequency domain, which in combination with the insensitivity of the method itself make experiments very time demanding and sometimes not even practically feasible at all.

This thesis describes methods, implemented in computer programs, which aim to reduce these problems. The first part, "Automated Analysis of regular NMR-spectra", shows that it is possible to assign proteins of the size of the 128 aa protein azurin with existent automated peak picking, and automated assignment program packages, in conjunction with an automatic calibration routine, opening for the possibility to perform studies of mobility, interaction, or structure without having to go through the tedious manual peak picking and assignment procedure first. To show that labelling is not necessary for automated assignment the procedure is also applied on the 29 aa, non-labelled, defensin HNP2 with a weakly bounded ligand. The structure is also solved using the assignments.

Recently, recording of spectra with coupled evolution periods has gained a lot of interest due to its ability to reduce the recording time on the NMR instrument. Unfortunately, the resulting spectra are difficult to interpret due to that sums and differences of nuclei shifts are recorded instead of the nuclei shifts themselves, and that the peak information for every peak is split over many spectra. The second part, "Evaluation of spectra with coupled evolution periods" demonstrates two different procedures on how to calculate the true nuclei shifts and even the full NMR-spectrum from a set of projections from experiments using coupled evolution periods.

KEYWORDS: NMR, automation, peak picking, resonance assignment, coupled evolution periods, convolution, multi-way decomposition, proteins.

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