New Software for the Analysis of Protein NMR Spectra

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The analysis of NMR spectra is both a **critical step** and today the **most time consuming task** in the process of **protein structure determination**. All relevant signals of a spectrum must be identified and the chemical shifts uniquely assigned to the atoms of the protein by logical inference. The complexity is even increased by application of isotopic labeling to the samples (due to the large size of the interesting proteins) and separating the process into backbone and sidechain assignment. The goal of this **ongoing research project** is to optimize the process of NMR spectra analysis. It was recognized that the efficiency and quality of the process can be significantly increased by **reducing complexity and optimizing the ergonomy of the tools**. The **software** presented here incorporates **new concepts of NMR information management and visualization** for obtaining sequence specific assignments.

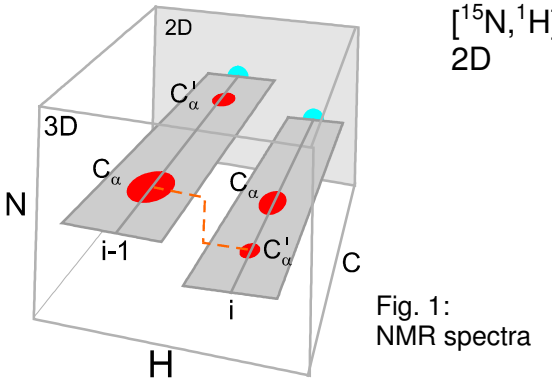
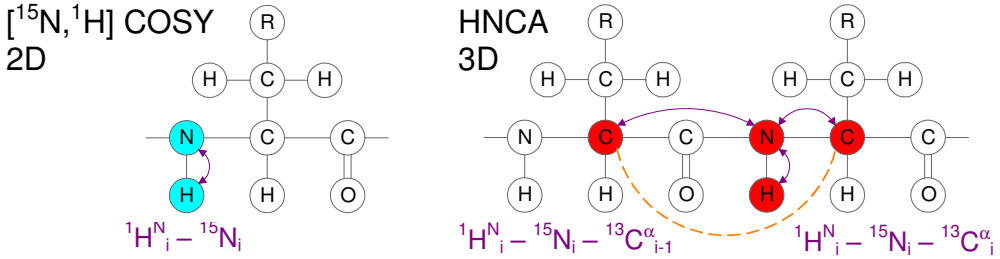


Fig. 1: NMR spectra



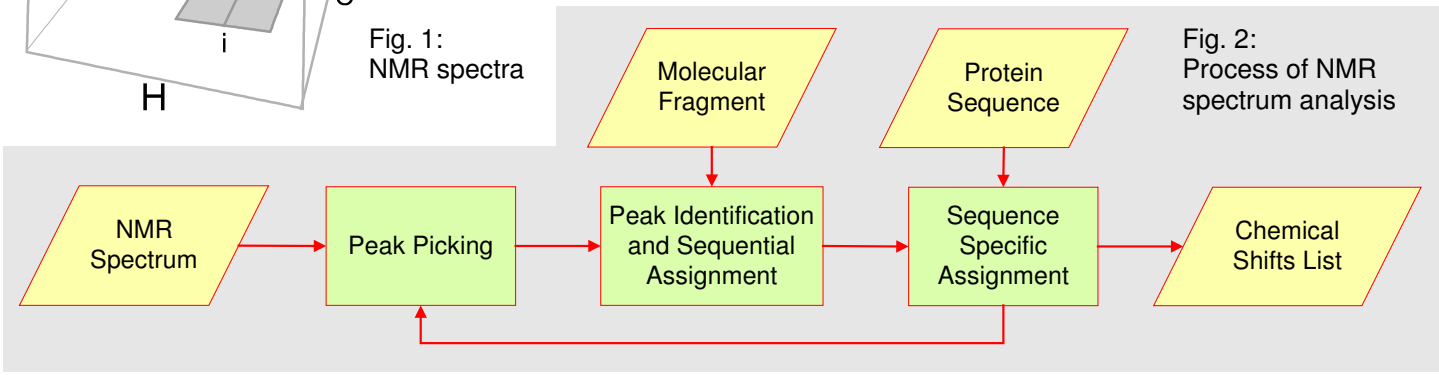


Fig. 2: Process of NMR spectrum analysis

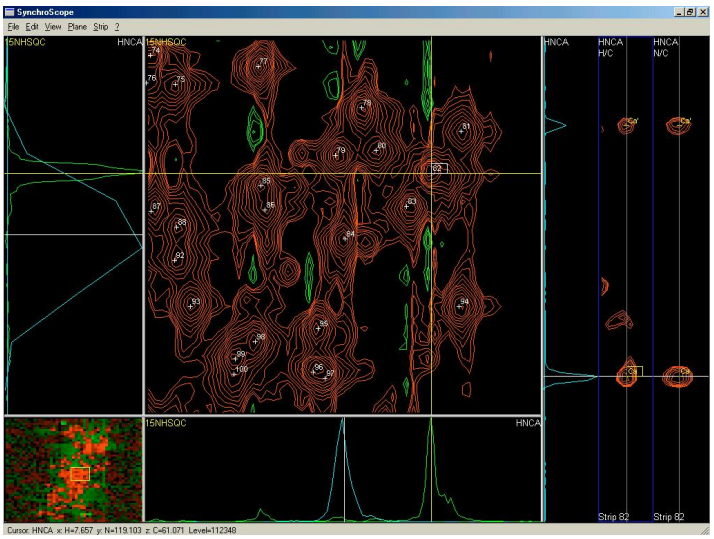


Fig. 3: Combined analysis of [^{15}N,^{1}H] COSY and HNCA spectra. Identification of strips and strip peaks.

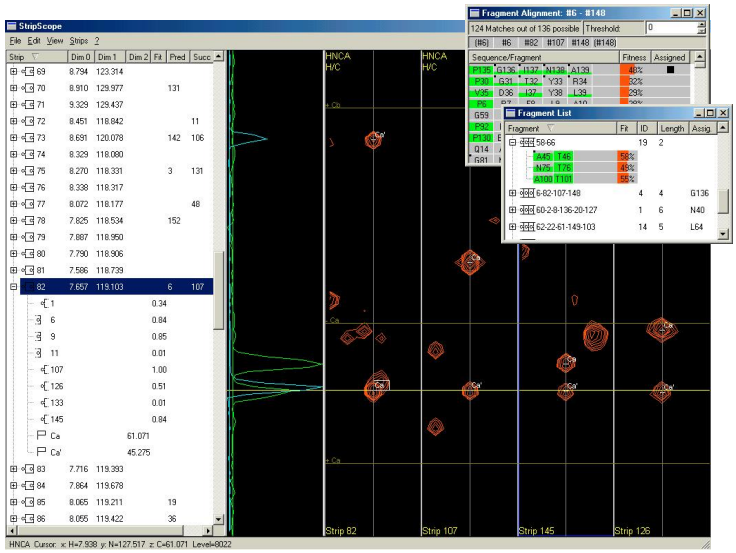


Fig. 4: Joining HNCA strips of sequentially neighbouring fragments. Mapping backbone fragments onto the sequence.

Features

- Clear presentation & navigation, enhanced overview
- Modern graphical user interface featuring overlapping windows, context menus, drag&drop, scaleable and scrollable panes and complete platform independence
- Powerful shortcuts and command line for fast operation
- Unlimited Undo/Redo support
- Open XML file format, import/export of XEASY formats
- Fast redraw and response times (based on C/C++)

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