

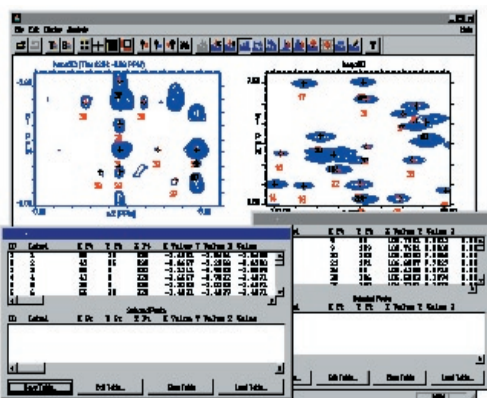
[ NMR Spectral Analysis ]

# Spectrum Research

## SpecManPro & CONTRAST

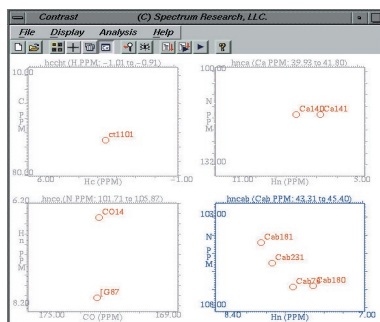
Tools to Speed Up the Automated Assignment Process

- Imports a variety of formats (Bruker, Varian, JEOL, NMRPipe, NUTS, Felix, JCAMP, Galactic, Triad, NMR-Compass, etc.) of 1D, 2D, 3D and nD processed spectrum files for concurrent display and analysis in multiple views.
- Provides tools for viewing 2D planes from 3D or nD spectra and enables tying and concurrent zooming of 2D and 3D spectra.

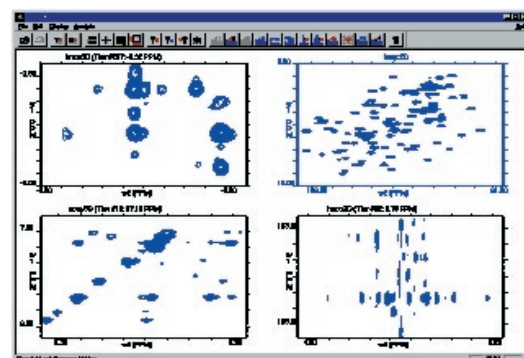


Automatic 2D & 3D Peak Picking with Peak Tables

- Requires the amino acid sequence and the NMR peak coordinates in the form of chemical shifts and intensities from 2D, 3D, and nD peak lists generated by SpecManPro to perform automated assignment of peptides & proteins.
- Generates customizable procedures based on the input data for extracting connectivities and completing assignments.
- Enables easy viewing and editing of peak lists and assignment tables.

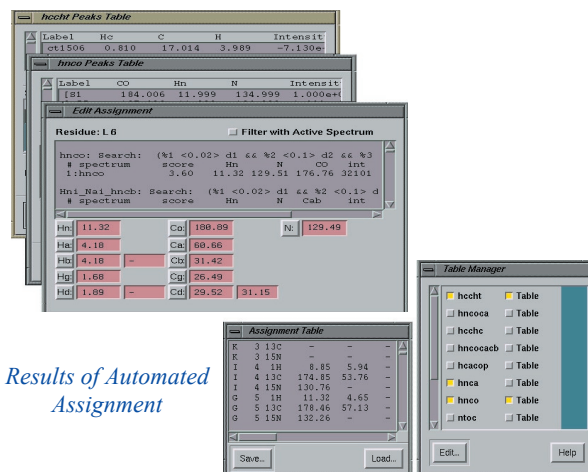


Assigned Peaks in HCCHT, HNCA, HNCO & HNCAB



2D Planes from HNCA, HNCO, 3D NOESY & HSQC

- Uses sophisticated peak picking tools (grid-intelligence based peak picking to filter noise ridges, merge peaks, and pick cross-peak multiplet centers) to generate 2D/3D/nD peak lists for input into CONTRAST.
- Advanced report generation tools allow the user to copy and paste spectra, structures, peak lists, and assignment tables into word processing documents with the click of just two buttons.



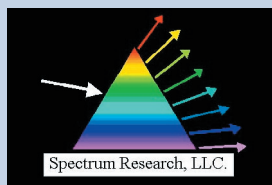
Results of Automated Assignment

- Provides the user with several versatile tools for manipulating peak lists in order to design a custom strategy.
- Works with any type of multidimensional NMR spectral data to generate the best set of resonance assignments. Based on the quantity and quality of input data, CONTRAST provides only partial assignments.
- Exports results as ASCII files compatible with the typical "spreadsheet" format.

### About Spectrum Research

Spectrum Research, LLC., a leading provider of NMR Software for Computer Assisted Structure Elucidation, develops and markets software products for Analytical Informatics, Bioinformatics, and Chemical Informatics consumers. Easy to use and cost-effective to implement, Spectrum Research is a single-source solution to address today's spectral analysis and structure elucidation challenges.

For more information, visit  
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