

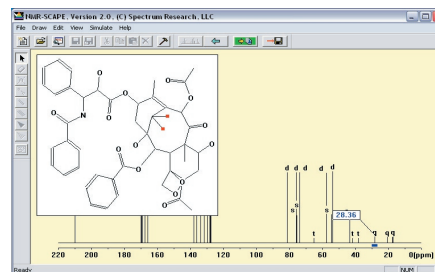
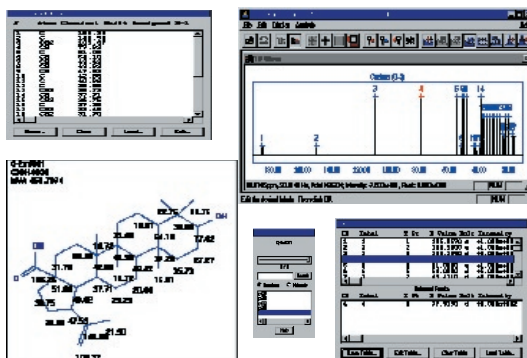
[NMR Spectral Analysis]

Spectrum Research

NMR-SCAPE - ^{13}C Spectral Prediction

Tools to Speed Up the Spectral Prediction Process

- NMR-SCAPE performs spectral simulation and prediction of ^{13}C NMR chemical shifts.
- Allows user to sketch molecule, or import a structure as a *.mol file from third-party Chem-sketch programs.



- Performs batch predictions on multiple structures and enables user to open the predicted spectra into SpecMan for comparison and validation with experimental data.
- Permits user to add compounds to NMR-SCAPE's knowledge base in order to enhance predictions.
- Works in conjunction with NMR-SAMS to provide the best solution for automated structure elucidation.

About Spectrum Research

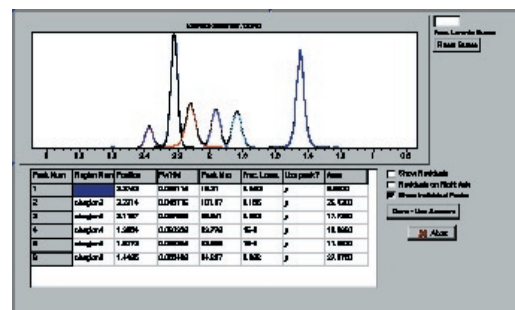
Spectrum Research, LLC., a leading provider of NMR Software for Computer Assisted Structure Elucidation, develops and markets software products for Analytical Informatics, Bioinformatics, and Chemical Informatics consumers. Easy to use and cost-effective to implement, Spectrum Research is a single-source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

For more information, visit
www.specres.com

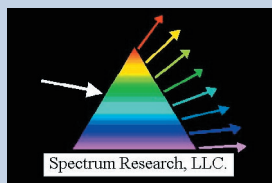
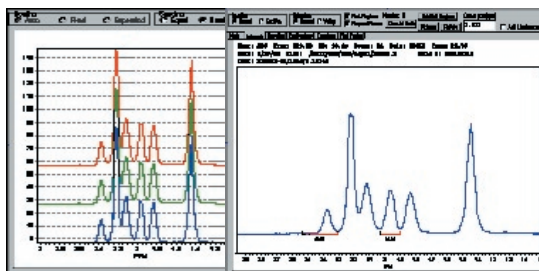
IQ-NMR - NMR Analysis & 1D Processing

Tools to Speed Up the 1D Spectral Analysis Process

- IQ-NMR provides an interactive graphical tool for NMR spectroscopists working with a variety of 1D NMR data.
- Works with the processed spectrum files generated by different spectrometer vendors (such as Bruker, Varian, and JEOL).
- Automates peak picking, peak integration, and report generation.
- Performs complex mathematical operations, such as calculations of mixture compositions in terms of mole and weight percent (using NMR peak integrals) on multiple spectra in an automated mode.



- Enables curve fitting of overlapping peaks.
- Performs quality control operations for large numbers of similar spectra.
- Assists with the generation of quantitative information from 1D NMR spectra.
- Streamlines repetitive integration and calculation of results on similar spectra.
- Prepares multiple tasks with built-in macros for automatic analysis without user intervention.
- Provides annotation tools for labeled spectra.
- Exports results of calculations to printed spectra as well as user-specified files.



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