Small Molecule Structure Elucidation

CMC-se™

CMC-se is a NMR software package for simple and efficient structure elucidation of small molecules. With its innovative approach, CMC-se accelerates the spectroscopist's workflow during the elucidation process by automating many of the key analysis and interpretation steps. In combination with Bruker's AVANCE™ NMR spectrometer product line, CMC-se is the only elucidation tool that integrates high quality NMR data acquisition with sophisticated software analysis. CMC-se is available for the major operating systems: Windows®, Linux® and Mac OS® X.

Features

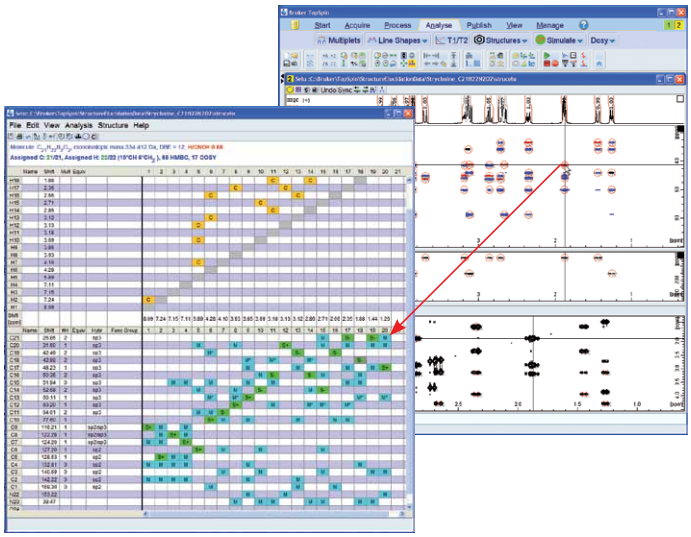
- Simple and efficient structure elucidation of small molecules in drug discovery and natural products research
- Automates many of the necessary analysis and interpretation steps
- Seamless integration of NMR acquisition and sophisticated software analysis
- Enables both accomplished researchers and beginners to expedite the elucidation of unknown substances in diverse pharmaceutical and chemical applications
- Organizes the data for a molecule into a single project, and provides unique graphical tools for data visualization and interpretation

Assisted Workflow

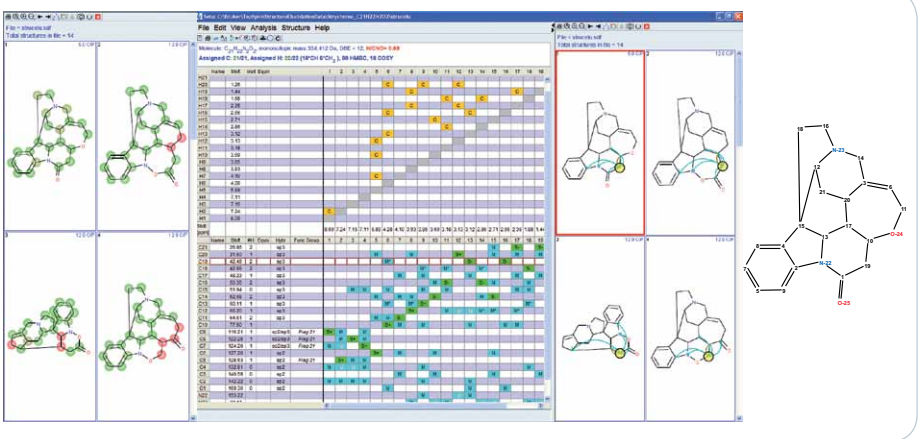
Starting with the molecular sum formula, the CMC-se solution analyzes the molecular structure using a defined protocol of 1D and 2D NMR spectra. The spectra are automatically analyzed, and resulting information is transferred into a correlation table. The correlation table is linked to a unique TopSpin™ window to assist the user in evaluating, if necessary modifying the contents of this table. Additional information such as mass spectrometry fragmentation, or simple evaluation of NMR data can be incorporated into the table. Using a new, sophisticated structure-determination algorithm, the spectral information is interpreted and structures that are consistent with the data are proposed.

CMC-se ranks the possible structures according to chemical shift predictions, highlighting the most probable structures.

During the elucidation process, several interactive visualization and interpretation tools are available to assist the chemist in determining the unknown structures, allowing the addition of further information to ensure an optimum determination procedure. Once a structural solution has been identified, a report is automatically generated, providing all relevant NMR spectra and assignments with the structure.



The correction table and combined spectra display are the two main windows in CMC-se. Atom names, peak annotations or other comments can be added to the correlation table and shown in the combined spectra display to help keep track of information when working with the data manually.



CMC-se contains multiple tools to assist the user in evaluating the generated structure proposals.

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