SOFTWARE

Bruker Chemist Suite

Process, analyze, and report all spectroscopic data in one software solution with Bruker Chemist Suite

Innovation with Integrity

Bruker Chemist Suite is designed especially for chemists running analytical analyses on Bruker instruments. The software includes tools that will enable the processing of spectra, chemical structure verification, as well as intelligent storage and browsing of analytical chemistry data from both NMR and MS instruments, which substantially improves access and re-exploration of acquired raw or processed data. The software also provides powerful modules for quantification and purity determination, generation of an IUAPC name from a chemical structure, and NMR spectra prediction.

Benefits

- The toolbox combines all your analytical data within the same software interface. This offers a very efficient way to process, analyze and report your data.
- Benefit from the world-leading NMR acquisition tool and use its data for advanced analysis tasks (quantification and structure verification)
- Save time with enhanced data browsing and efficient reporting and reporting templates

Features

- One software suite and one graphical user interface to process all analytical chemistry data (NMR, LC/GC-MS, UV-Vis, FT-IR, Raman)
- Powerful algorithms for prediction of NMR spectra as well as for automatic and assisted structure verification with a flexible scoring system
- Purity and concentration determination using 1D NMR data in manual, assisted, and automatic modes
- Easy storage in a centralized database with file access using DB MyData and TopSpin Browser
- Efficient reporting and reporting template

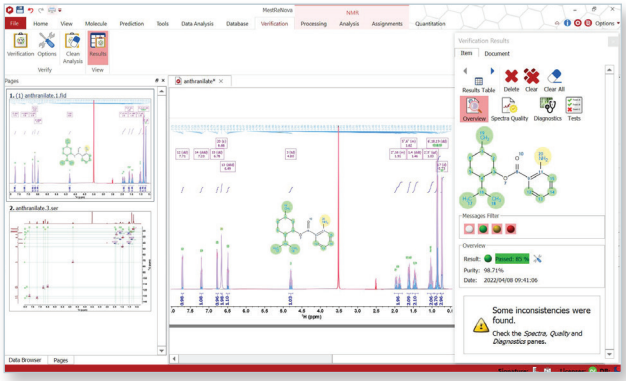

Figure 1 Illustration of the "Verify" plugin

- Structure verification of menthyl anthranilate using 1D 1H NMR spectrum and 2D 1H-13C HSQC
- The structure and the spectra are annotated with color coded assignments which are made according to their quality:
  Good in green, medium in yellow and bad in red

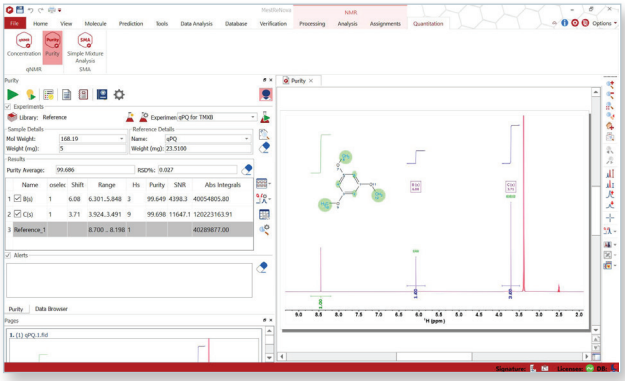

Figure 2 Illustration of the "qNMR" plugin

- Purity determination of a TMXB sample using TCNB as internal reference
- The NMR resonance of TCNB appears on the left side (~8,50 ppm)
- The resonances at 6,08 ppm and at 3,71 ppm belong to TMXB and have been used for purity determination
- A purity of 99.69 has been calculated from the NMR spectrum

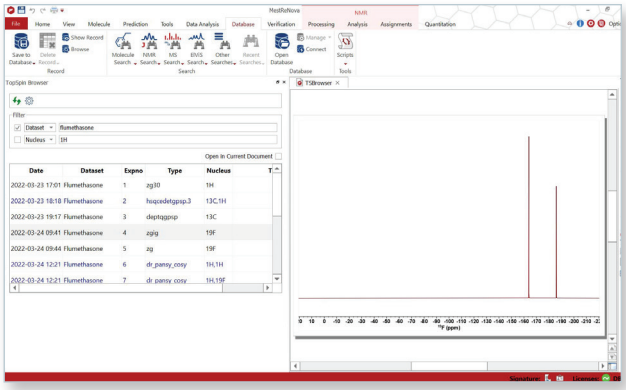

Figure 3 Illustration of the "TopSpin Browser" plugin

- The TopSpin Browser is on the left side of the window
- Double click on any row to automatically open the spectrum into a new Mnova document
- Rows in black correspond to 1D spectrum
- Rows in blue correspond to 2D spectrum

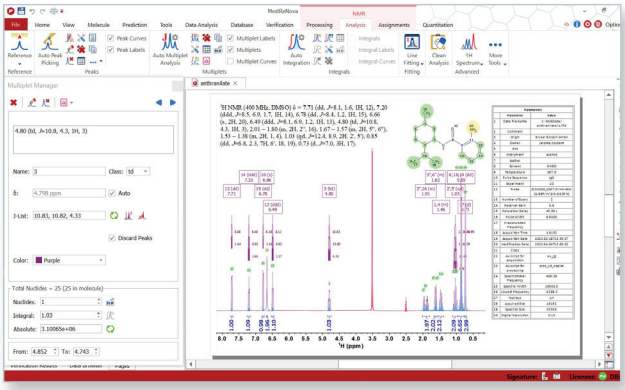

Figure 4 Illustration of the "NMR" plugin

- Visualize, process and analyze any 1D/2D NMR spectra
- Efficient tools for peak picking, integration, multiplet analysis and assignments
- Powerful reporting options

Bruker BioSpin is continually improving its products and reserves the right to change specifications without notice. Order No.T188855 © 2022 Bruker BioSpin.

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