

Spectrometer Control

TopSpin 4 is the next generation of Bruker's industry standard NMR software for spectrometer control and data analysis. The combination of an updated user interface and new, exciting hardware features, such as the multiple receivers of the AVANCE NEO, will make it the foundation for the next generation of NMR spectroscopists.

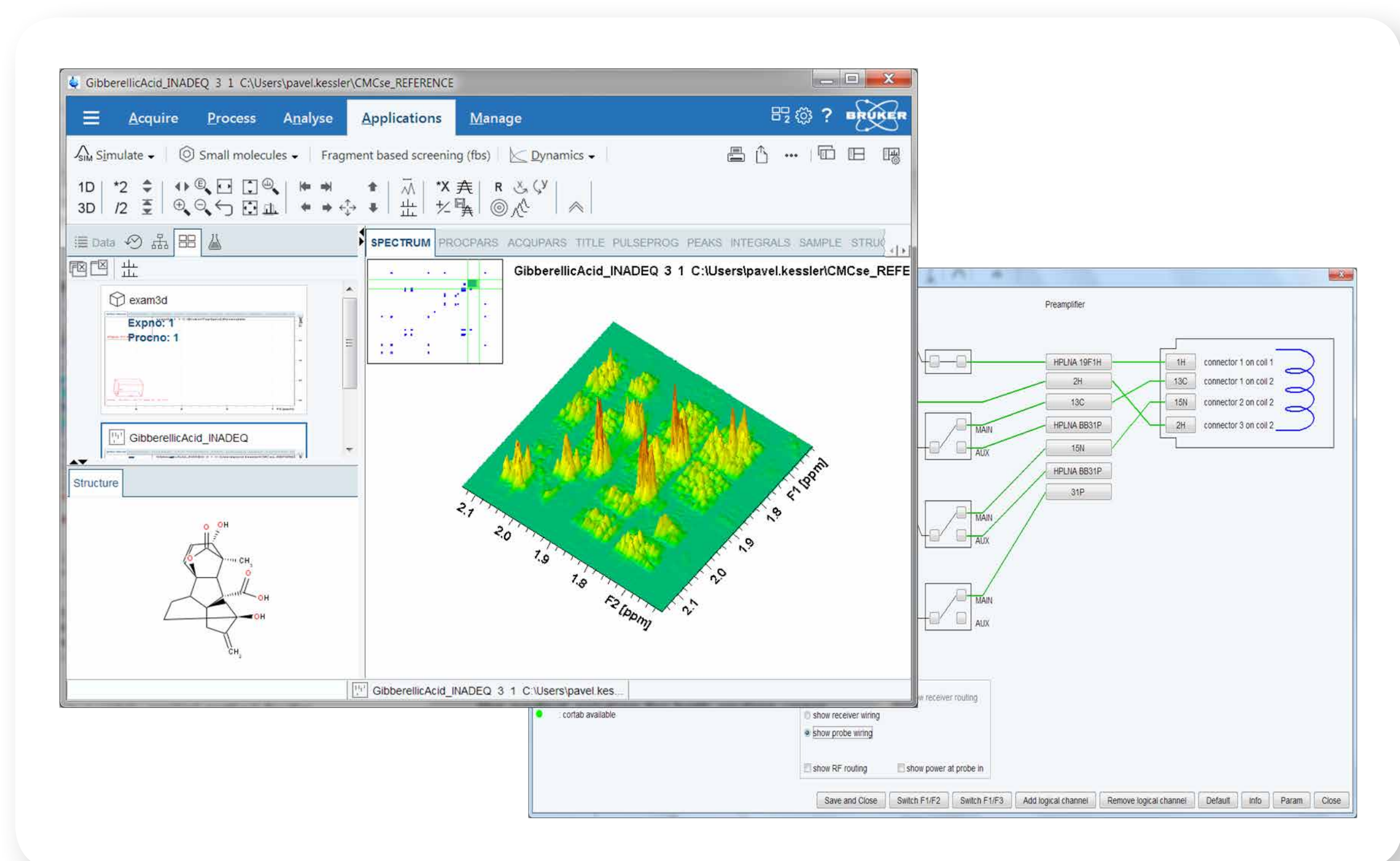


Fig. 1: TopSpin 4.

Applications

TopSpin 4 incorporates many specialized modules focused on the simplification of acquisition and data analysis workflows.

Computer assisted structure elucidation is an example, where the software solutions help to unveil a full potential of NMR as an analytical method. The CMC-se package supports the complete workflow and makes structure elucidation accessible to a wider audience.

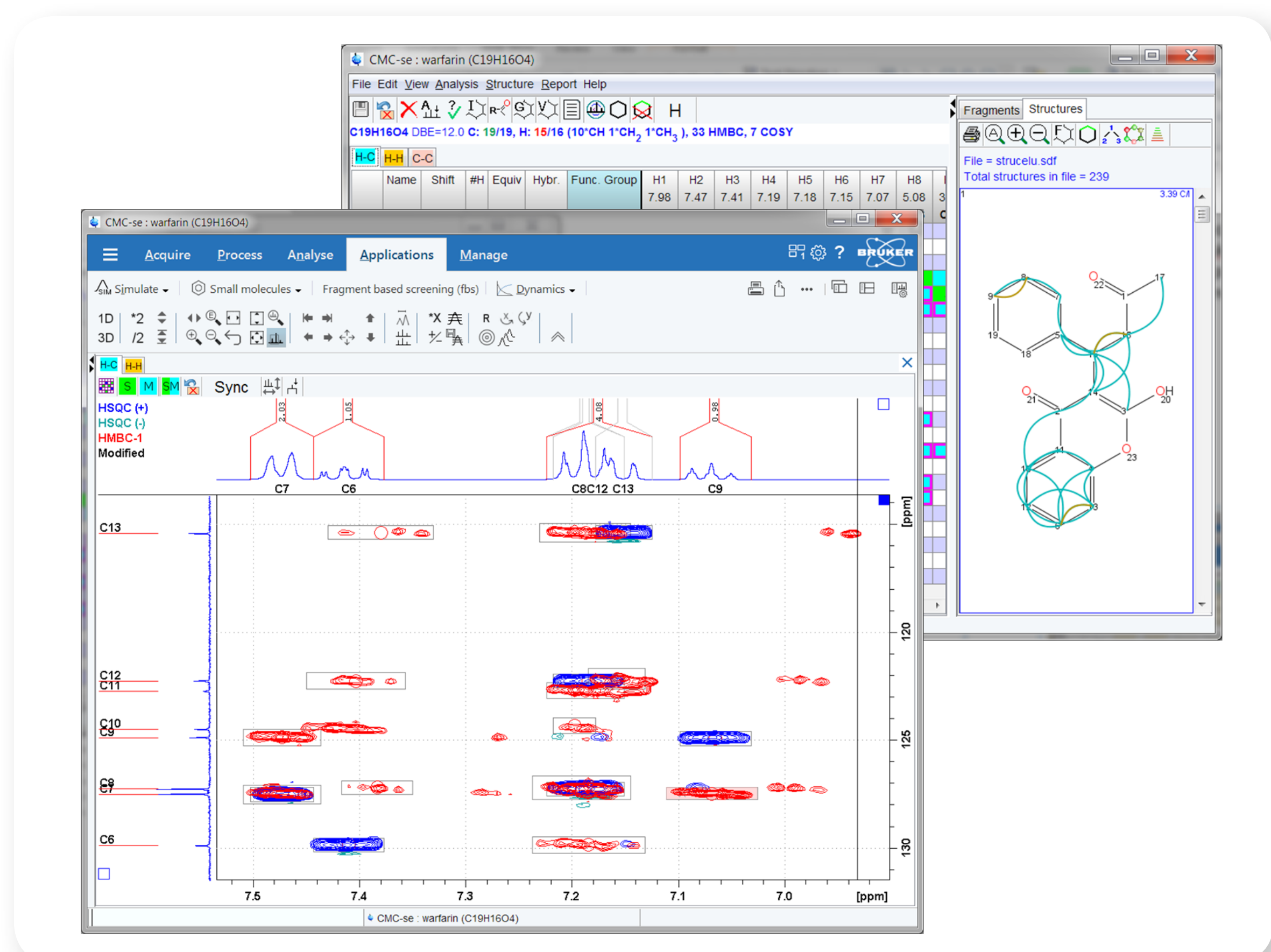


Fig. 2: With its innovative approach, CMC-se accelerates the spectroscopist's workflow during the structure elucidation process, by automating many of the key analysis and interpretation steps. The graphical tools visualize all important characteristics as a network of experimental correlations explaining the generated structure candidate.

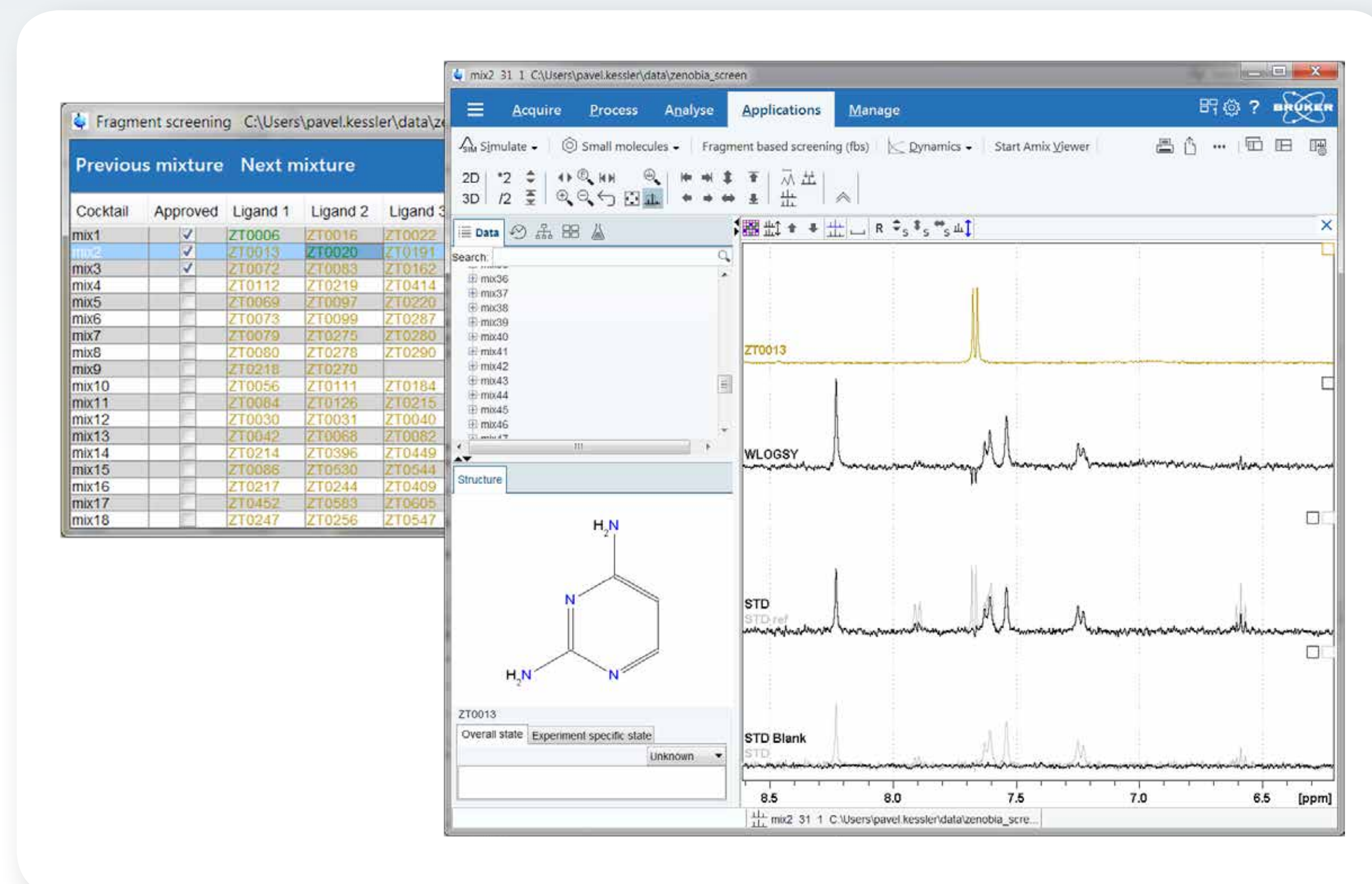


Fig. 3: The Fragment-Based Screening (FBS) tool exploits the power of NMR data by streamlining the entire workflow from acquisition to analysis. All relevant data, experiment types, compound IDs, reference spectra and other information are collected automatically and stored in a project file. The display shows the relevant data for analysis.

TopSpin as a Teaching Tool

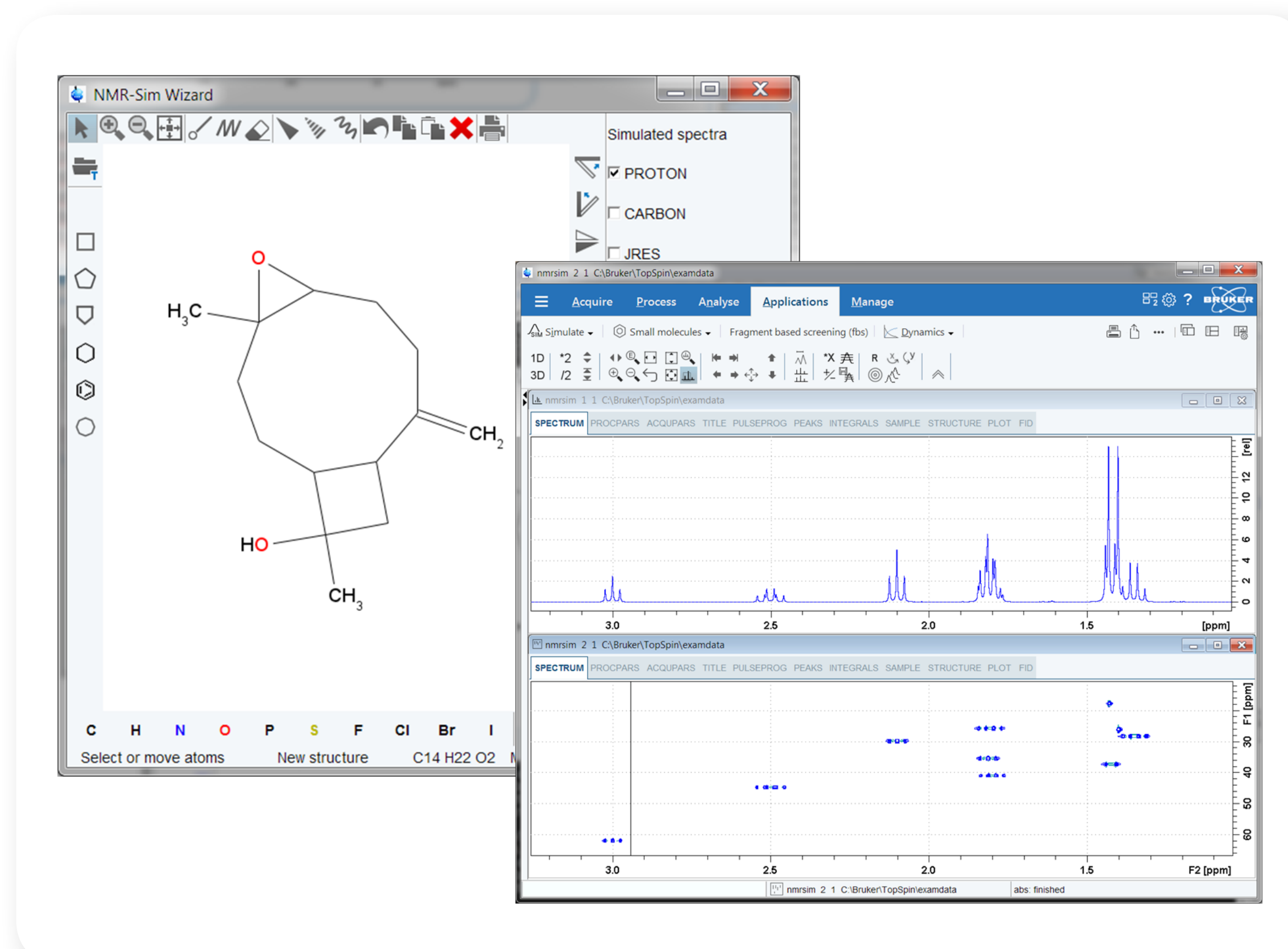


Fig. 4: Bruker's NMR-Sim software supports the NMR spectroscopy education. The application covers a wide range of tasks. These range from a simple "push button" solution calculating selected spectra directly from chemical structure, to a "virtual spectrometer" simulating detailed behavior of complex NMR experiments.

Summary

- Controls AVANCE NEO NMR hardware
- New, modern look and feel
- Intuitive industry standard user interface; perfect for both routine users and experts
- Special licenses for students and universities

