

### **NMR SOFTWARE**

# **Advanced Chemical Profiling**

Hands-Off Workflow Automation for Identification and Quantification

Innovation with Integrity

# **Increasing Process Efficiency and Consistency with NMR Chemical Mixture Analysis**

The new NMR-based Advanced Chemical Profiling Module is a comprehensive software-based automated end-to-end workflow from sample to actionable information intelligence.

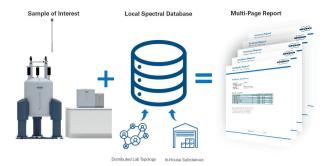
The importance of automated workflows and flexibility cannot be overstated in high-throughput environments such as production-related labs, analytical testing services, R&D centers, and pilot-upscaling support functions within centers of excellence.

Advanced Chemical Profiling addresses the tasks of data processing, interpretation, and report filing for NMR data of chemical mixtures allowing identification and quantification of constituents in incoming goods, process intermediates, and final product formulations to improve both, quality, and efficiency in R&D lab-scale, pilot, and volume production processes.

The database-driven solution is customizable by in-house NMR experts allowing for application in a wide range of use cases.



Streamlined roll-out into audited non-NMR-expert environments in volume production and quality control is possible through Bruker-enabled <u>Distributed Lab Topology</u>.



#### Save Your Time with Automation

- Automated analysis software for identification and quantification of substances in pure form or mixtures
- Sample-to-Report automation directly available via IconNMR™, TopSpin® or GoScan for streamlined analysis at the push of one button
- Different report formats to meet your individual needs: PDF, XML, and interactive results directly accessible on the software interface
- No need to perform repetitive tasks: Ensure highly trained experts focus on valuable tasks only

# Make NMR-based mixture analysis accessible to non-experts

- Deploy sophisticated NMR analysis in volume manufacturing or quality control environments through push-button solutions
- Easy-to-read report by spectroscopic non-expert including consistent visuals
- Auditable workflows with operator-independent results and methods
- Full customer ownership of methods and databases

#### Broaden your service portfolio

- Broaden your analytical services beyond structure elucidation and make use of unused nighttime measurement slots with fully automated mixture analyses using Advanced Chemical Profiling
- Offer tailored testing services including re-process of existing data to improve present process efficiency
- Modify on-premise database and method to adjust for new analytical questions
- Method and database can be easily deployed in other locations across same organization for a <u>distributed lab topology</u> deployment

### **Features**

- State-of-the-art automation software for identifying and quantifying substances in pure form or mixtures
- Robust quantification even in significant NMR signal-overlap situations
- Unknown substances are flagged and do not negatively influence the quantification of known
- Seamless integration into TopSpin<sup>™</sup>, IconNMR<sup>™</sup>, and GoScan
- Software-based automated end-to-end workflow from sample to actionable information intelligence (report)
- Push-button solution from sample to report with no NMR expert knowledge required
- Operator-independent highthroughput testing for optimized result comparability and lab-to-lab method harmonization
- Allows for retrospective data re-processing of already existing data
- IP security by on-premise installation and full customer ownership of methods and databases
- One integrated Solution available to Bruker NMR Spectrometers covering 80 to 800 MHz

### One integrated solution available to Bruker NMR Spectrometers covering 80 to 800 MHz



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Advanced Chemical Profiling
Landing Page

