INDUSTRIAL

Fourier 80 ChemLab with Mixture Profiling Module

Application note

Innovation with Integrity

Chemical Mixture Analysis by NMR

Chemical manufacturing often requires extensive testing: from incoming raw materials through processing to final product quality control. A common approach is to apply various targeted testing techniques calling for different instruments, methods and levels of user expertise. In some cases, testing is skipped altogether. Nuclear Magnetic Resonance provides a comprehensive tool that identifies and quantifies multiple compounds in a chemical mixture.

One major benefit of proton NMR is that it is a completely non-selective detector. Proton NMR can measure any compound that contains protons. The application of Nuclear Magnetic Resonance (NMR) is widely accepted worldwide to analyze complex mixtures on a molecular level. It provides targeted and non targeted identification and quantification of known and unknown compounds. Known molecular structures are easily verified and new molecular structures are elucidated. NMR also allows quantification without the need for compound-specific reference samples.

The only limitations until now for the wider deployment of NMR technology have been the need for spectroscopic expertise and certain infrastructure/capital investments (such as special laboratory configurations and liquid cryogens). As time-to-result is a critical need in manufacturing environments, sending samples to special locations for analysis does not always meet timeline expectations. Bruker now offers an easy-to-deploy, robust NMR method that identifies and quantifies constituents in non-complex mixtures and provides results where most needed: at the loading ramp of incoming goods, during production process steps, or with final product quality control. The Bruker Fourier 80 benchtop NMR system extends the deployment capabilities of NMR significantly. And provides a database driven end-to-end workflow from sample to report for routine chemical mixture analysis (Figure 1).

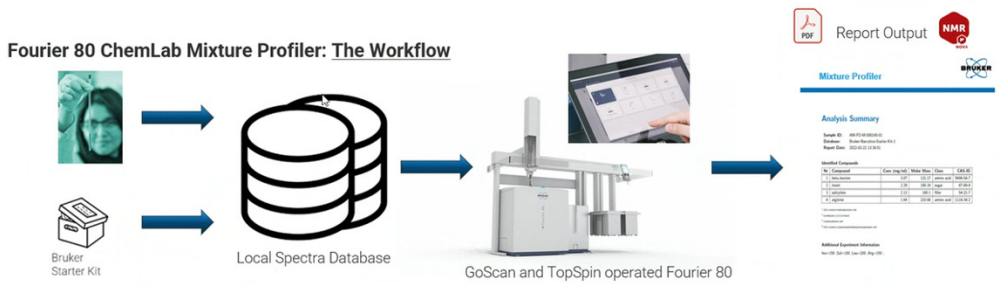

Figure 1: Summary of NMR workflow for the Fourier 80 Mixture Profiler

New end-to-end push-button solution

Bruker's new ChemLab with the NMR Mixture Profiler module runs on Bruker's Fourier 80 FT-NMR benchtop platform (Figure 2). The NMR Mixture Profiler provides a unique end-to-end solution for the chemical industry, providing identification and quantification of compounds in a mixture. This solution is based on the high-performance 80 MHz benchtop NMR system Fourier 80, including a high throughput automated sample changer for up to 120 samples. The instrument is operated by Bruker's industry standard TopSpin™ NMR software, in addition to the sample tracking software IconNMR™. A highly customizable push-button user interface called GoScan™ provides easy operation for even the non-expert user. The fully automated workflow covers all steps from sample measurement to report with no user interaction required. This means operators with no NMR knowledge can run advanced NMR analysis including automated data interpretation and report generation. The database is fully customizable and provides the chemical processing industry with unrivaled capabilities to tailor the solution to the challenges with incoming goods control, processing methods and quality checks for finished materials.

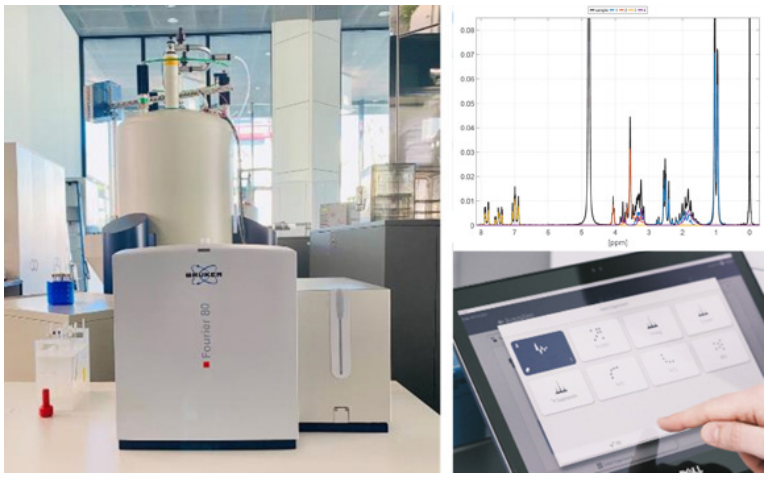

Figure 2: Unique to Bruker: floor-standing and benchtop NMR with same operating software

Examples in the Chemical Industry

- Incoming Goods Control
- Process Innovation
- Process Control
- Outgoing Product Quailty Control

Benefits

- Power of TopSpin™; Easy workflows of GoScan™
- Fully Automated: from Sample-to-Report
- Identifies and Quantifies in one step
- Fully Customizable Spectral Database
- Starter Spectra Database Kit (82 spectra)
- Mixture analysis in ~ 20 minutes
- 120 sample pick-and-place automation (optional)

The analytical results are presented in a Portable Document Format (PDF) and an interactive NMR spectrum visualization software. Reports include an easy-to-read table (Figure 3) with compounds identified and quantified. Graphical feedback on compounds matched to the database are included in the report (Figure 4) along with a residual plot for analysis accuracy and consistency (Figure 5).

If signals in the NMR spectrum cannot be matched to an existing database entry, they will be highlighted in the report, triggering further investigation. These could be known or unknown compounds. Outlier compounds are then further analyzed using alternate techniques such as high-resolution NMR.

Fourier 80 ChemLab with Mixture Profiling module can be part of Bruker's unique Distributed Laboratory Topology (DLT) concept directly linking methodologies of high-resolution floor-standing NMR instruments with easy-to-deploy benchtop units.

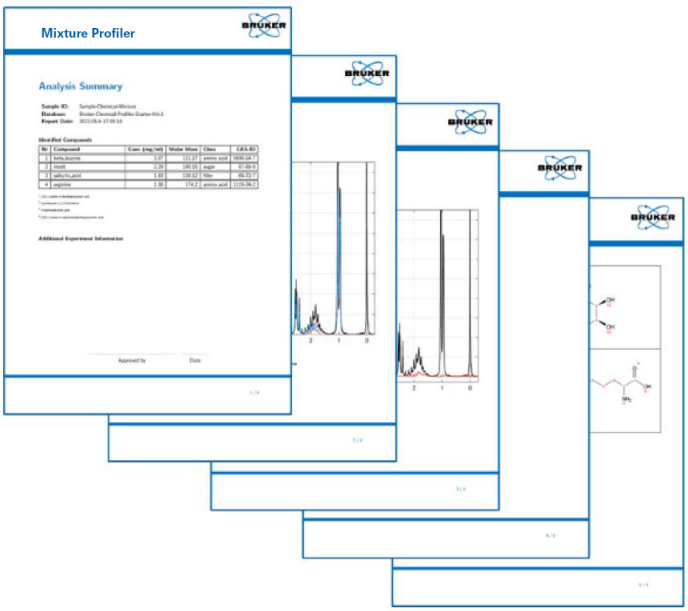

Figure 3: Fourier 80 ChemLab with Mixture Profiling Module Report

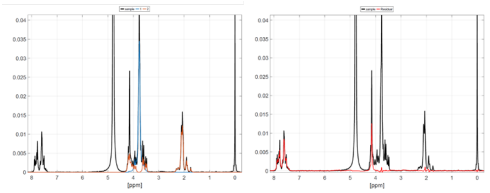

Figure 4: Left side: color-coded database entries to re-build the current NMR spectrum (black). Right side: Residual plot (red) of current spectrum (black) and matched database entries. The significant pattern in the red line indicates that there is a substance present in the sample which cannot be assigned to a database entry.

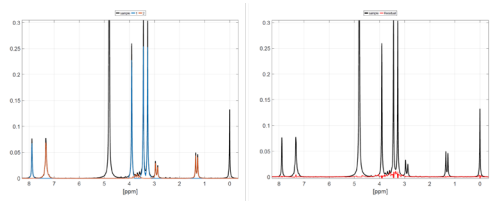

Figure 5: Left side: color-coded database entries to re-build the current NMR spectrum (black). Right side: Residual plot (red) of current spectrum (black) and matched database entries. The flat red line indicates that all signals and so all compounds in the mixture have been successfully identified.

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