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Bruker showcases innovative NMR solutions for pharmaceutical industry at ENC 2015

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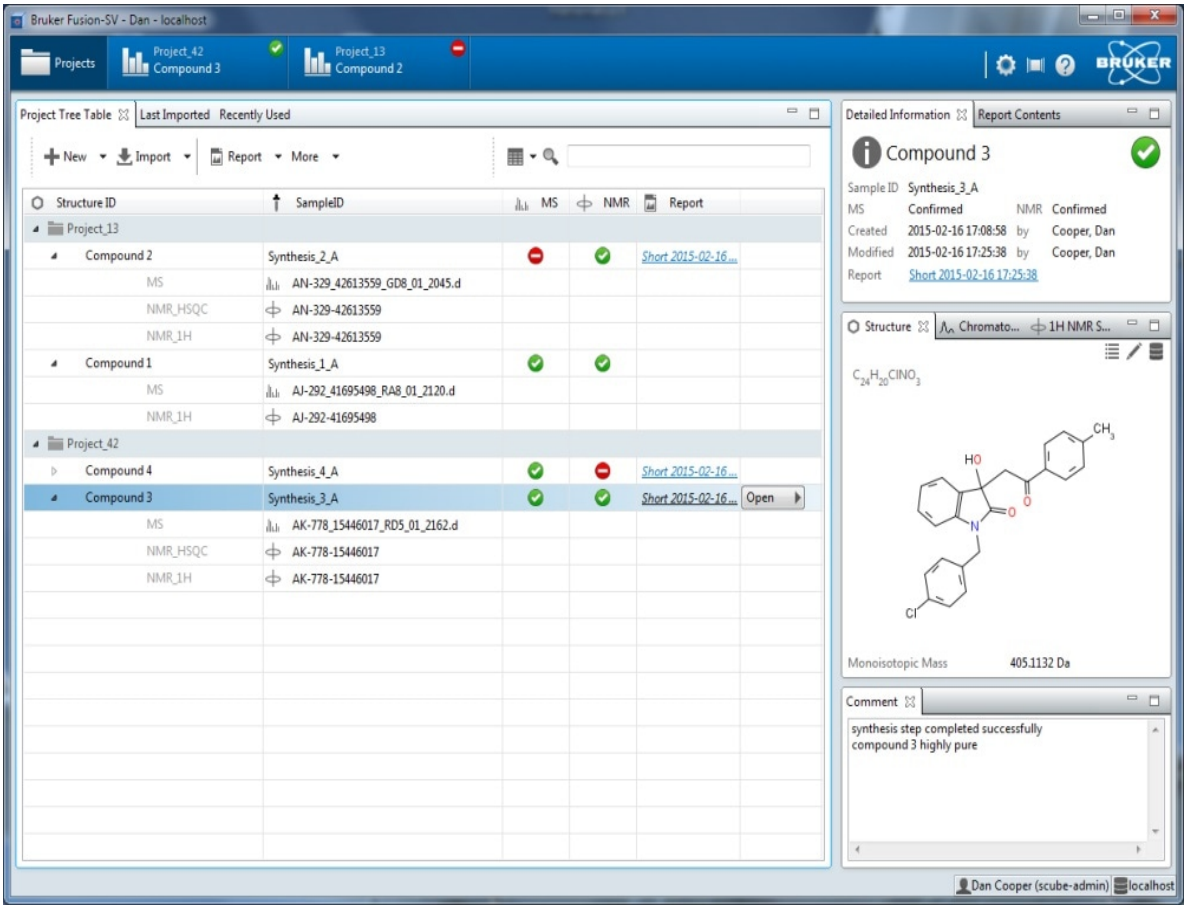
At the 56th Experimental Nuclear Magnetic Resonance Conference, Bruker this week is show-casing several innovative drug discovery, drug development and process control solutions for small molecule NMR characterization in the pharmaceutical industry.

Fragment-based Drug Discovery (FBDD) Screening and Lead Optimization:

In recent years, FBDD has emerged as an alternative to traditional high throughput screening. The fragment libraries are characterized by the small size of the compounds and a smaller number of candidate molecules, aiming to identify those that may have initial weak-medium affinities for binding to the desired protein targets, and then optimizing these leads iteratively to obtain medium-strong binding affinities. At each stage, fragment-protein interactions are detected by highly sensitive NMR spectroscopy.

Bruker provides dedicated hard- and software for these FBDD applications: The SampleJet™ high capacity sample changer with cooled sample storage keeps the delicate biomolecular samples from degrading, while at the same time providing maximum throughput. The specifically designed QCI-F CryoProbe™ is a fully versatile, highest sensitivity triple resonance probe with additional fluorine capacity, enabling both, traditional proton- and novel 19F-detected FBDD capabilities. The CMC-q software ensures the integrity and correct concentrations of the fragment libraries. All these latest NMR tools together allow FBDD-by-NMR screens and lead optimization to be performed in a routine and partially automated manner.

Rapid, Automated Structure Verification Solution FUSION-SV™:

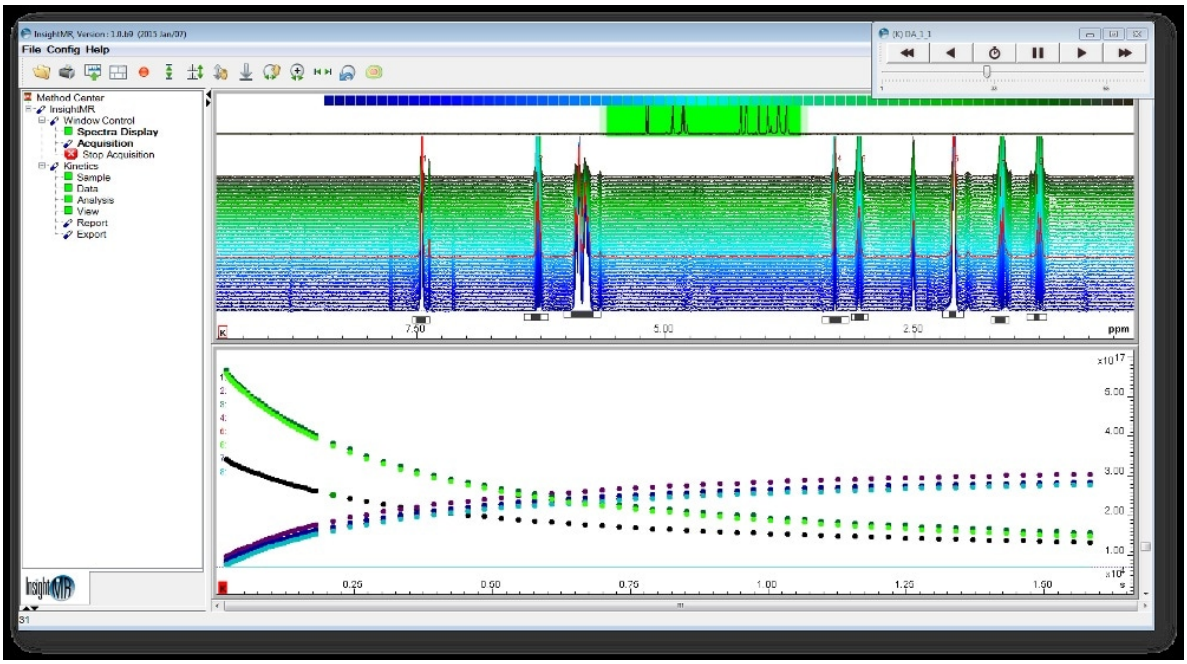


This new integrated solution for structure verification allows users to easily combine high-resolution accurate-mass (HRAM) mass spectrometry (MS), and complementary Nuclear Magnetic Resonance (NMR) data. FUSION-SV

provides significantly increased specificity, robustness and throughput for rapid, automated small molecule structure verification. FUSION-SV is designed for the workflow of medicinal and synthetic chemists in pharma, chemical industry or in academia.

The proprietary algorithms which deliver this improved performance have been built into the FUSION-SV streamlined workflow and user-friendly interface. The medicinal chemist is guided straight to meaningful results with minimal interaction and without the requirement for expert knowledge of the underlying techniques. In addition to HRAM-MS and high-fidelity isotope ratio data analysis to determine an unambiguous molecular sum formula, using a Bruker Compact bench-top ESI-QTOF system, FUSION-SV 1.0 automatically analyzes 1D 1H and HSQC 400 MHz NMR data. The most advanced solution FUSION-SV 1.1 in addition requires a high-sensitivity CryoProbe™ Prodigy at 400 MHz (or higher) to add the fast acquisition of HMBC and 13C NMR data to the automated structure verification analysis. The FUSION-SV database offers network access to the spectroscopic data, enabling collaborating scientists to share results and projects.

Process Optimization with InsightMR™:



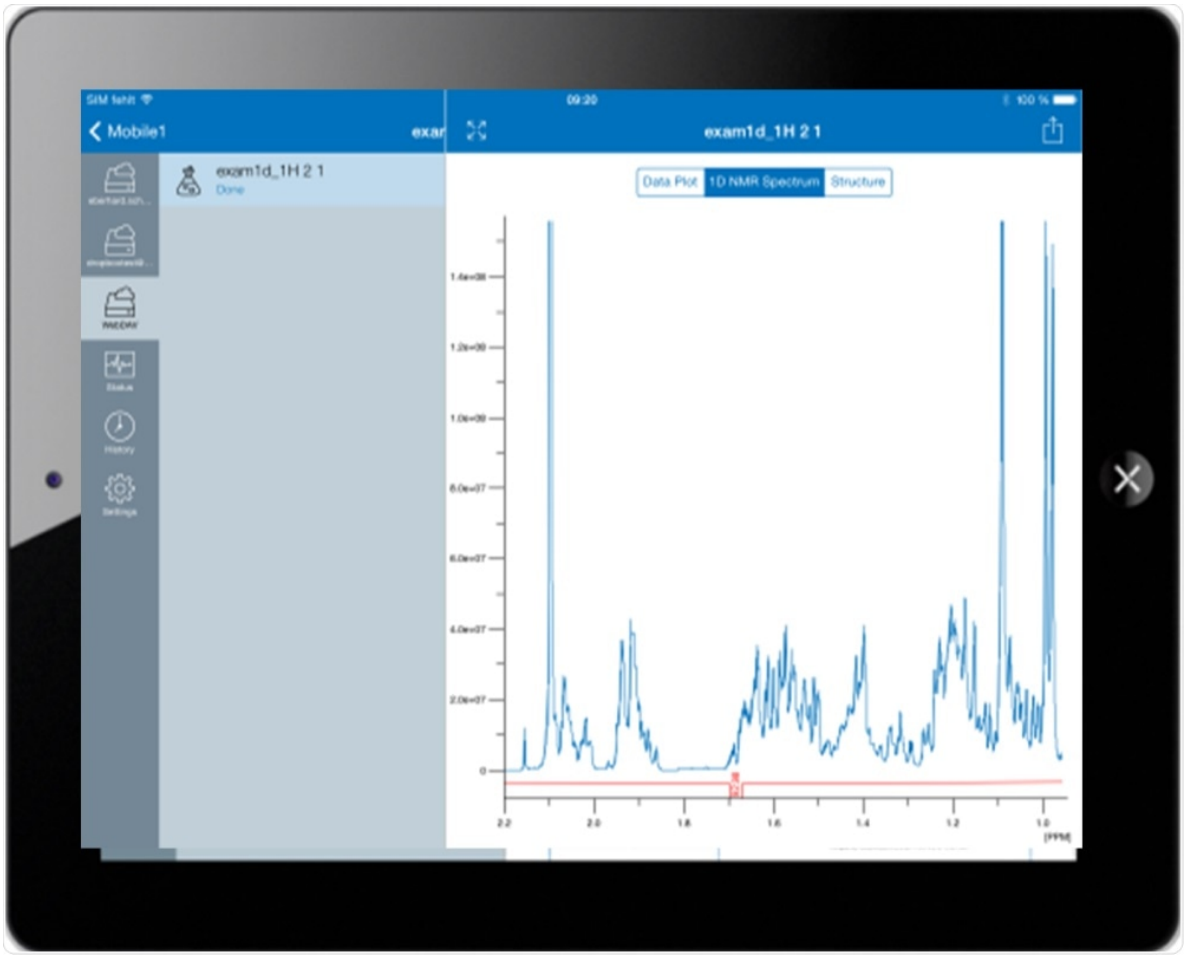
This new solution for on-the-fly NMR analysis of chemical processes enables the adjustment of process parameters based on real-time data analysis. InsightMR™ is built on Bruker's NMR software TopSpin® for seamless integration with Bruker systems. InsightMR's user friendly interface allows both expert and non-expert users to set up, monitor and adjust key parameters. As a result, it is an excellent solution for industrial and academic scientists studying and optimizing organic reactions. InsightMR has already proven successful with the first installation at Pfizer in Connecticut, USA, where it has been used to apply NMR to on-line reaction monitoring to solve real chemical questions within the drug development pipeline.

Pharma QC and Screening with AssureNMR™:

A customizable solution for evaluation of diverse materials using NMR. Built on the strengths of NMR for determining compound identity and quantification, and the highly reproducible nature of NMR, Assure-NMR™ screens materials in full automation from acquisition to report. Integration with the spectrometer through system suitability verification and cross-checks before the sample leaves the acquisition queue assures that highest quality spectra are obtained before the data is analyzed and assists in making sure the SOPs are followed.

Whether the required analysis is for metabolomics, dietary supplements, reference standards, APIs, polymers, or raw materials, this customizable solution provides summaries of the sample composition and classification results in automation. Designed for compatibility with both research and GMP environments, AssureNMR provides rapid detailed sample analysis for research studies, product assessment and quality control.

LabToGo:



Access your data and view your spectrometer status anytime and anywhere with the new LabToGo app for the iPad. Powered by the ability of TopSpin™ 3.5 to interface with cloud storage services of the user's choice, uploaded data can be examined and visualized remotely. Additionally, the status of spectrometer automation jobs can be synced to the LabToGo app and automatic notifications can be sent for finished tasks.

"Bruker now offers a suite of innovative NMR pharma tools, designed for next-generation drug discovery approaches and more efficient lead optimization, for increased productivity and for higher quality," commented Dr. Till Kuehn, Head of Pharma Applications Development for the Bruker BioSpin MRS division. "NMR is a robust, cost-effective, highly quantitative and information-rich analytical tool, and with these new solutions its utility for small molecule pharma applications has been greatly enhanced."

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Company Background

Bruker BioSpin offers the world's most comprehensive range of NMR and EPR spectroscopy and preclinical MRI research tools. The Bruker BioSpin Group of companies develop, manufacture and supply technology to research establishments, commercial enterprises and multi-national corporations across countless industries and fields of expertise.

Bruker microCT formerly known as SkyScan develops and produces wide range of high-end microtomography instruments for life science, material research and in-vivo preclinical studies.