Sample Tracking and Information Management for Analytical Laboratories

● SampleTrack™

think forward

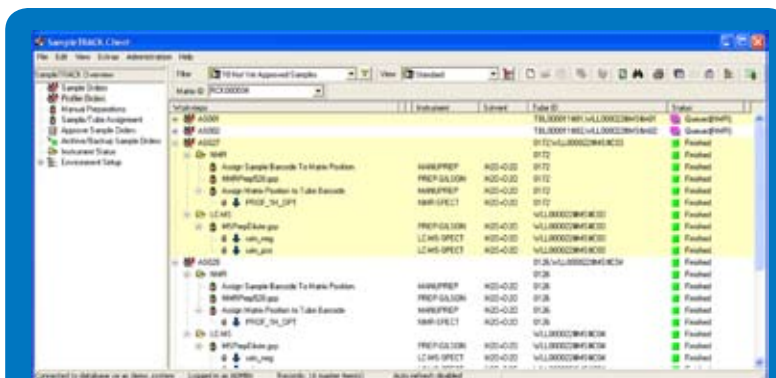# Sample Tracking and Information Management for Analytical Laboratories

Laboratory informatics solutions from Bruker BioSpin both streamline your information processes and maximize the operating efficiency of your laboratory. Combined with one of the world's widest range of analytical instrumentation, even your most comprehensive requirements can be fulfilled. SampleTrack has been designed to support all activity in NMR laboratories, but is also suited to link into other analytical methods.

SampleTrack

SampleTrack is an information management and control tool designed to assist you in your NMR laboratory environment. Laboratory information, often accessible only by using different tools, can now be centrally managed and visualized through SampleTrack.

The basic functions of SampleTrack include the paperless setup of laboratory requests, the tracking of sample progress and the report of results. Additionally SampleTrack fulfills the requirement of keeping all relevant research data together, by providing complete management of projects and documents. SampleTrack also provides tools for knowledge management, quality assurance (QA), quality certification (QC), and automation of Bruker instruments and preparation robots.

SampleTrack routine user interface controlling queued acquisition of different analytical modalities (NMR and MS).

Integrated solutions for your laboratory environment

Scalability

With its scalable architecture, SampleTrack meets your needs whether you have just one instrument or a large scale facility with dozens of spectrometers. SampleTrack expands grows with your laboratory by adding links to new instruments and to the outside world.

Information management and hardware control are carried out concurrently in the synthesis laboratory, as the sample proceeds through the analytical steps. SampleTrack's open-system architecture provides convenient and easy integration of laboratory automation. From sample setup and sample preparation through data interpretation, knowledge management and archiving, SampleTrack saves, manages, shares and analyses all kinds of laboratory information. As a powerful management tool, SampleTrack organizes both your existing and new laboratory processes relying on easy-to-configure, laboratory-specific workflows, as well as flexible result reporting tools.

Customization

SampleTrack offers customizable organization of your workflow management in accordance with instrument configuration and the laboratory environment. Laboratory floor activity monitoring delivers precise, detailed, chronological information for each step along the sample's path.

SampleTrack can also be adapted to use the current terminology in use at your site. Windows, menu structures, images, buttons and text can be completely tailor-made at the time SampleTrack is installed. SampleTrack remains customizable as your laboratory grows. The local administrator, authorized users and groups, can adapt or modify individual filters and data views of interest. Fully customizable areas include: barcode printing, plot title generation and customer information.

Standard autosampler

Sample preparation

High throughput autosampler

Sample transfer

NMR

LC-NMR-MS

The SampleTrack Concept

Standard Workflow Steps

Workflow processes describe the sample's life, including the following steps:
- Sample log-in
- Sample assignment for preparation robots
- Preparation of samples for analysis
- Sample assignment to analysts
- Sample assignment to instruments
- Recording of results
- Result approval process
- Reporting
- Archiving

An audit trail tracks the life cycle steps. All steps can be adapted to existing environments and laboratory rules. In accordance with local laboratory rules, the sample workflow may range from 'Very Limited' to 'Wide Open Access'.

Integrated Solutions

Scenario 1: Open Access System

For an Open Access System, SampleTrack provides effective time-saving and resource sharing. Any client can set up and submit orders from any place within a network and can position the sample directly in the autosampler. In addition to Bruker's ICON-NMR open access system, SampleTrack also delivers:
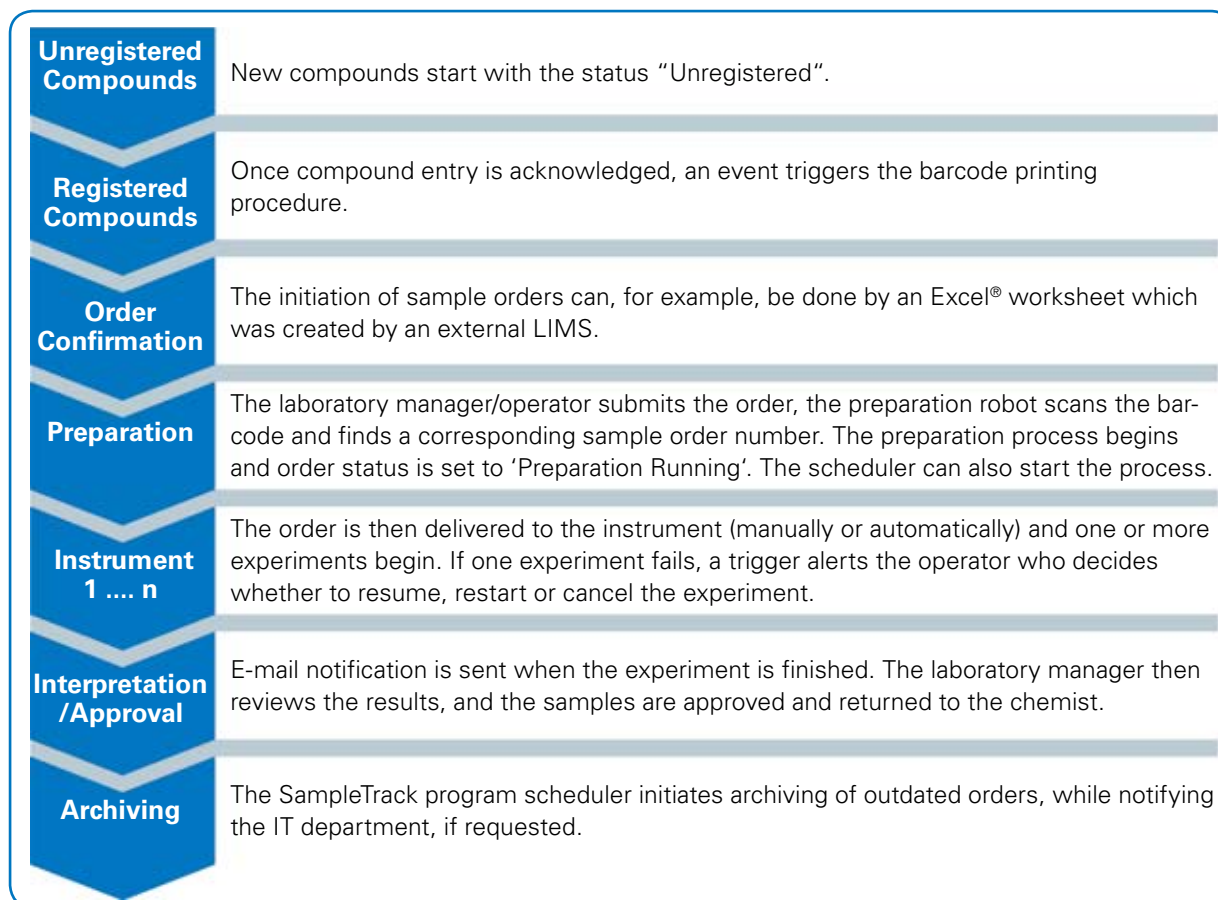
- Multiple spectrometer support (pooling)
- Customizable sample setup layouts
- Workflow optimization
- Reduction in spectrometer idle time
- Greater flexibility and efficiency

Open access system using B-ACS autosampler

Scenario 2: Fully Integrated System

When working with compounds, samples may travel through diverse departments or buildings. After completion of a process in one department the task is automatically forwarded to the department responsible for the next step.

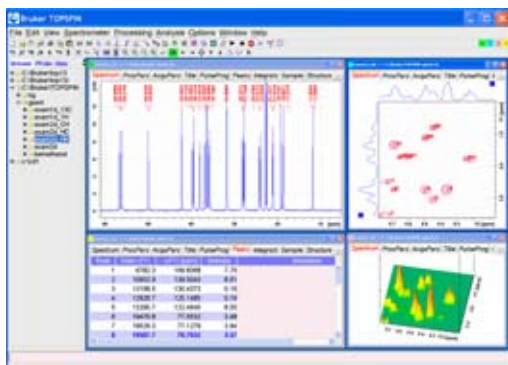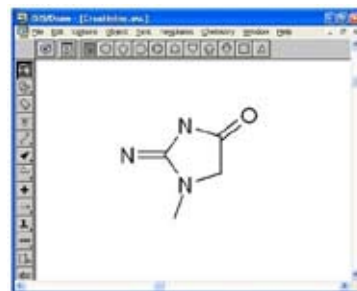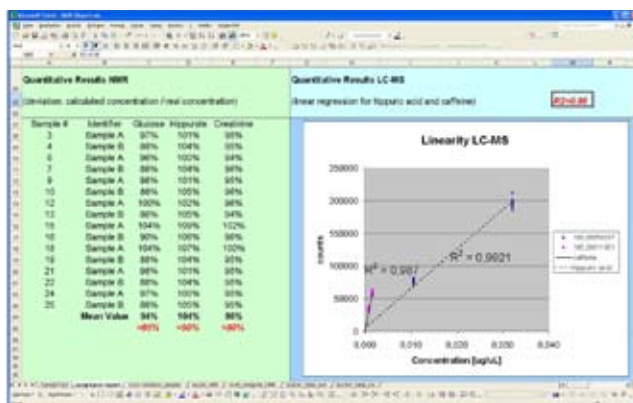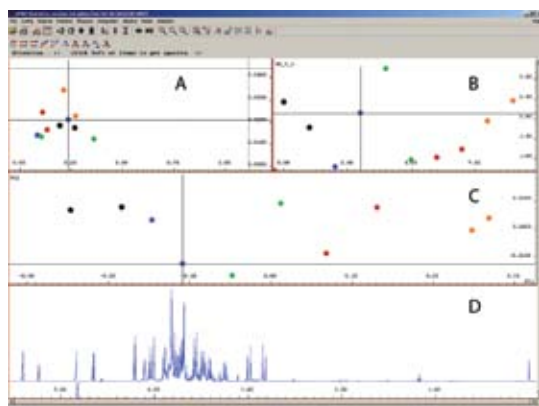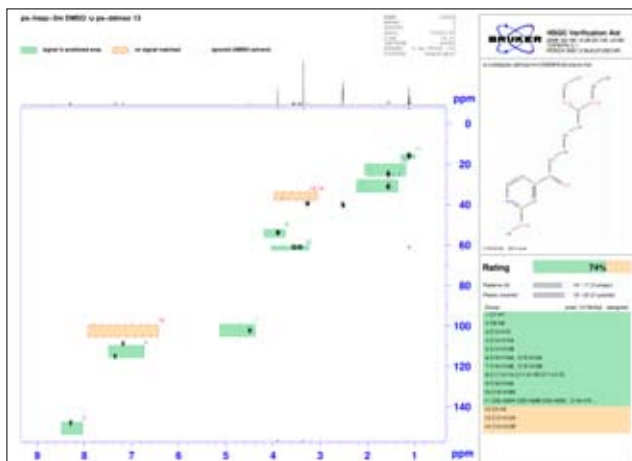| Stage	Description
Unregistered Compounds	New compounds start with the status "Unregistered".
Registered Compounds	Once compound entry is acknowledged, an event triggers the barcode printing procedure.
Order Confirmation	The initiation of sample orders can, for example, be done by an Excel® worksheet which was created by an external LIMS.
Preparation	The laboratory manager/operator submits the order, the preparation robot scans the barcode and finds a corresponding sample order number. The preparation process begins and order status is set to 'Preparation Running'. The scheduler can also start the process.
Instrument 1 .... n	The order is then delivered to the instrument (manually or automatically) and one or more experiments begin. If one experiment fails, a trigger alerts the operator who decides whether to resume, restart or cancel the experiment.
Interpretation /Approval	E-mail notification is sent when the experiment is finished. The laboratory manager then reviews the results, and the samples are approved and returned to the chemist.
Archiving	The SampleTrack program scheduler initiates archiving of outdated orders, while notifying the IT department, if requested.

Data Visualization and Organization

Visualization and Post-processing within SampleTrack

SampleTrack interfaces all NMR applications into a single, highly versatile, visualization tool. As a standard feature, SampleTrack uses the powerful AMIX™ Viewer for spectra display and statistics. It simplifies the structure verification and structure elucidation by providing direct interaction with other analytical applications such as TOPSPIN™.

Microsoft® Windows® applications (e.g. for reports) and structure editors (e.g. MDL® ISIS/Draw) can be linked directly to samples. The SampleTrack Web Interface itself provides structure and spectra viewer capabilities, including zooming.
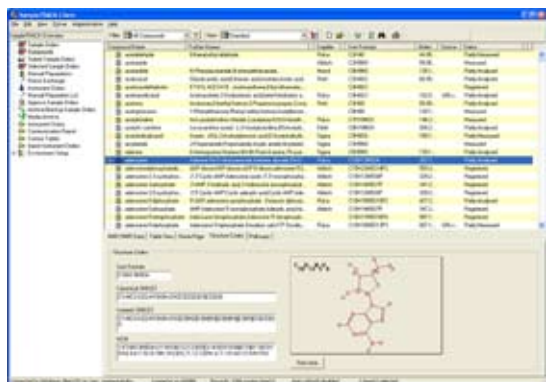

SampleTrack provides direct interaction with a variety of other analytical applications such as MDL, ISIS/Draw, AMIX, TopSpin, EXCEL, PDF.

Application Examples

Sample Track supports a wide range of routine analytical tasks. Our informatics products can be combined with all kinds of analytical instrumentation provided by Bruker. A few examples where SampleTrack offers solutions for a variety of applications are shown below.
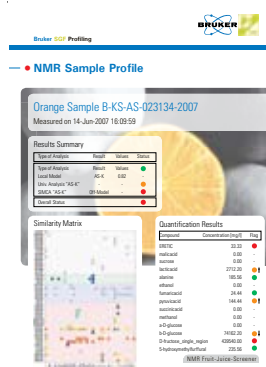

Pharmaceuticals - Compound Library Screening

Structure verification is uniquely suited to the quality control or screening of the integrity of existing compound libraries. Sample logging is automated in this context using Sample-Track. NMR and MS data are acquired in parallel and a single 'Analytical Molecular Profile' is generated, indicating the certainty (as a percentage) that the structure is commensurate with the proposed structure. The Analytical Molecular Profile includes information on the sample's purity as well as absolute quantity. The report is then submitted to a compound archive
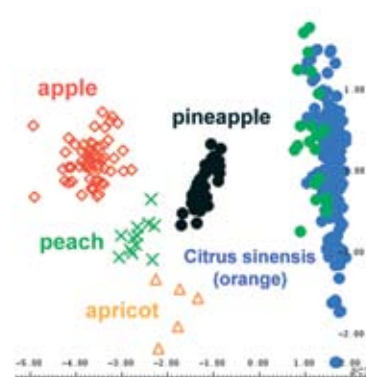
Clinical Research – Inborn Errors of Metabolism

SampleTrack enables metabolic profiling used in clinical research for disease detection. NMR has demonstrated capabilities in successfully distinguishing more than 80 inborn errors with a single ^{1}H spectrum. This rapid analysis enables physicians to quickly respond to the patient's medical issue and limit the harmful effects of the disease.

Food - Fruit Juice Screening

SampleTrack supports quality control screening application for apple and orange juice origin authenticity, species purity, false labelling and quantification of relevant metabolites. The NMR fruit juice screening method called SGF-Profiling (Spin-Generated Fingerprint) includes an extensive spectroscopic database from samples obtained from production sites all over the world.
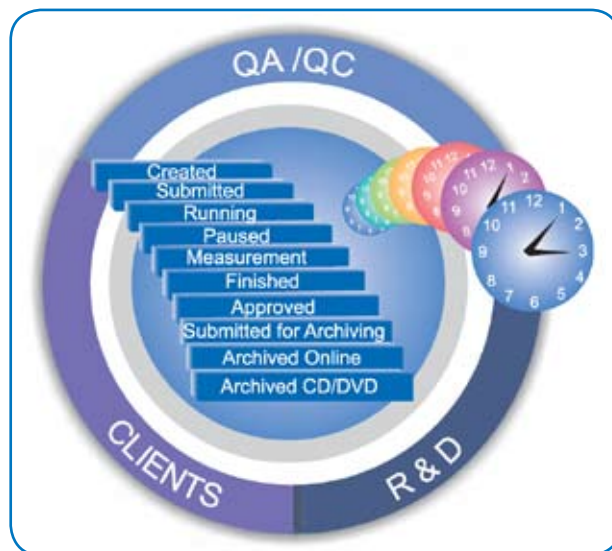
QA/QC

SampleTrack was designed for laboratory personnel involved in routine quality assurance (QA) and quality control (QC).

By generating reports and sample scheduling with optional auditing, SampleTrack helps to meet GLP requirements and assists with FDA 21 CFR Part 11 compliance.

Sample and preparation worksteps can be reliably reproduced and sample orders always remain accessible, even after SampleTrack's archiving process (Online / CD / DVD / Database).

Additional Features

- EasyWeb Dialog replaces form entry
- User management
- Automatic data name and title assignment
- Sample ID and barcode generation
- Open and flexible data organization
- Fast and easy data query

Application Specific Modules (available separately)

- Profiler
- Compound database
- Reference database
- Titration
- Pooling
- Archiving
- Web inteface