AssureNMR™

- Integrated Solution for Confident Chemical and Material Specificity, Quantity and Classification Screening

Providing Definitive Answers to Molecular Questions

Customizable for many applications, AssureNMR delivers results to the identity and quantity of components, classification of the material tested, and changes to the material composition. By utilizing the unique strength of NMR to provide definitive answers and reproducible results, AssureNMR produces fast answers to difficult molecular questions. Multiple product levels are available to meet your unique needs.

Complex Mixtures to Pure Materials

For many applications, AssureNMR screening software can be used to provide a detailed summary of a sample's composition and classification according to your specifications, manually or in complete automation.

Analyze Numerous Materials Types

- NMR fingerprinting
- Metabolomics
- Forensics material
- Botanical extracts
- Dietary supplements
- Polymer
- Food & beverages
- Reference standards
- APIs
- Finished pharmaceutical products
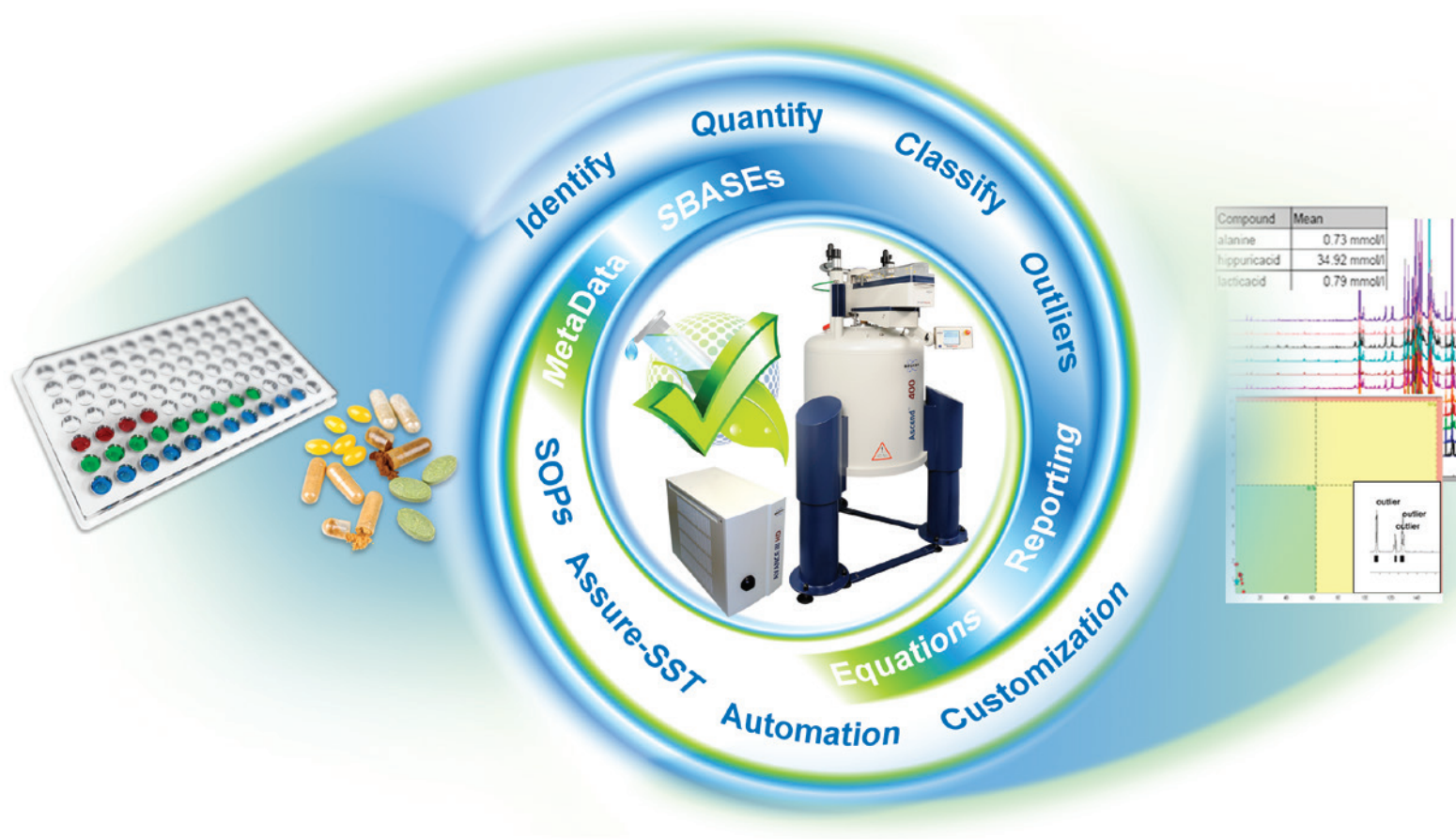
Software Packages

AssureNMR Launch

Designed for generating NMR spectral databases and identifying components, AssureNMR Launch is optimally used in laboratories that evaluate many different types of samples.

Applications Include:

- Dereplication
- Forensics
- Natural Products
- Pharmaceuticals

Spectral Assignments and Databases

Ease the NMR spectral assignment process by obtaining proposed chemical shift assignments for your structures and spectra. Generate your own spectral databases (SBASEs) of 1D and 2D data and reduce your dependence on costly standards.

Identify Components

Identify potential components in your spectra through chemical shift, multiplicity and intensity matches using SBASEs. A ranking assessment will help you select the components present.

Far Beyond Proton

Obtain definitive answers by using distinctive NMR signal characteristics from the multiple NMR active nuclei (^{1}H, ^{2}H, ^{11}B, ^{13}C, ^{19}F, ^{29}Si, ^{31}P) found in many materials.

System Suitability Tests

Keep your spectrometers producing optimal results with fully automated system suitability tests and optimization routines.

AssureNMR Ascent

In addition to all the benefits of Launch, Ascent is designed for laboratories that evaluate similar materials, require quantification, perform error analysis, multi-component identification, and benefit from automation.

Applications Include

- Pharmaceuticals
- Culture Media
- Polymers
- Food/Beverage
- Quality Control

Spectral Databases

Use the supplied SBASEs of over 170 compounds with multiple spectra (1D and 2D), including residual solvents and common organic molecules, to rapidly generate multicomponent screening methods.
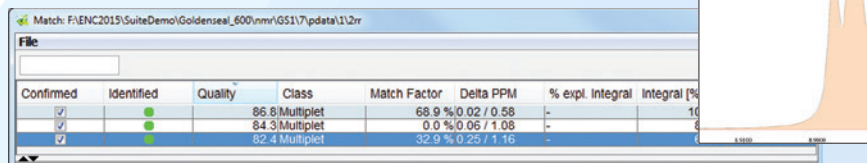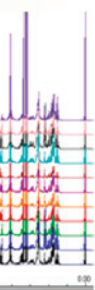
Quantification and Error Analysis

Quantify multiple components simultaneously using your preferred integration routine and report the concentration as desired; including absolute quantification capabilities through external or internal referencing.

Automation

Design your screening method to run on similar materials for full automation from acquisition through analysis and reporting for fast component identification and qualification results. Data quality on each sample is checked with lineshape evaluation before the sample leaves the magnet for spectra quality assurance.

Customization

Customize your automated acquisition, analysis and reporting method to calculate what you need to calculate and report what you need to report.

Confirmed	Identified	Quality	Class	Match Factor	Delta PPM	% expl. Integral	Integral [%
☑	●	86.8	Multiplet	68.9 %	0.02 / 0.58	-	10
☑	●	84.3	Multiplet	0.0 %	0.06 / 1.08	-	8
☑	●	82.4	Multiplet	32.9 %	0.25 / 1.16	-	6

Match: F:\ENC2015\SuiteDemo\Goldenseal_600\nmr\GS1\7\pdata\1\2rr

AssureNMR Summit

In addition to all the benefits of Launch and Ascent, Summit provides the ability to evaluate similarities and differences in large sample sets through the use of statistical analysis. For added convenience an extra desktop license and threshold test sample set are included.

Applications Include
- Metabolomics
- NMR Fingerprinting
- Pharmaceuticals/Biologics
- Natural Health Products
- Polymers
- Quality Control

Evaluate Sample Variance
Use statistical tools, PCA scores and loadings plots, to evaluate variance in a set of spectra or let AssureNMR show you the variance when testing a sample against a model.

Model Generation Tools
Generate and customize your bucket tables. Use the bucket tables to generate statistical and chemometric models including SIMCA outlier detection, multi-class classification, quantile plot and PLS regression models.

Classify Materials against Your Models
Rapidly evaluate new samples against models using your thresholds and pass/fail criteria. Find outliers.

Predict the Concentration of a Complex Material
Use PLS regression in AssureNMR to predict the amount of a material in your sample and the predicted error. Includes permutation tests to validate your model.
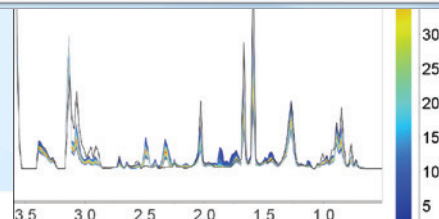
Optimize Your Efficiency
Utilize the desktop license to generate your AssureNMR methods at your convenience on your office computer and then send the method to your spectrometer equipped with AssureNMR.

Organize Your Data
Import your metadata from a spreadsheet and let AssureNMR's metadata tool select the datasets for analysis based on metadata rather than spectrum number.
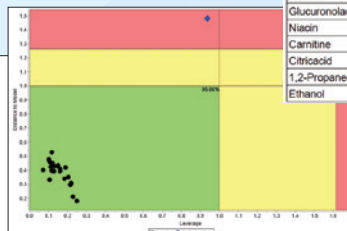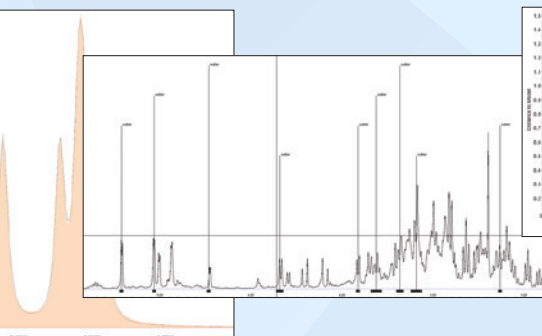
AssureNMR Advantage

Focused on Ease-of-Use: Automated NMR analysis for the non-expert. With an AssureNMR method any user can evaluate samples using NMR.
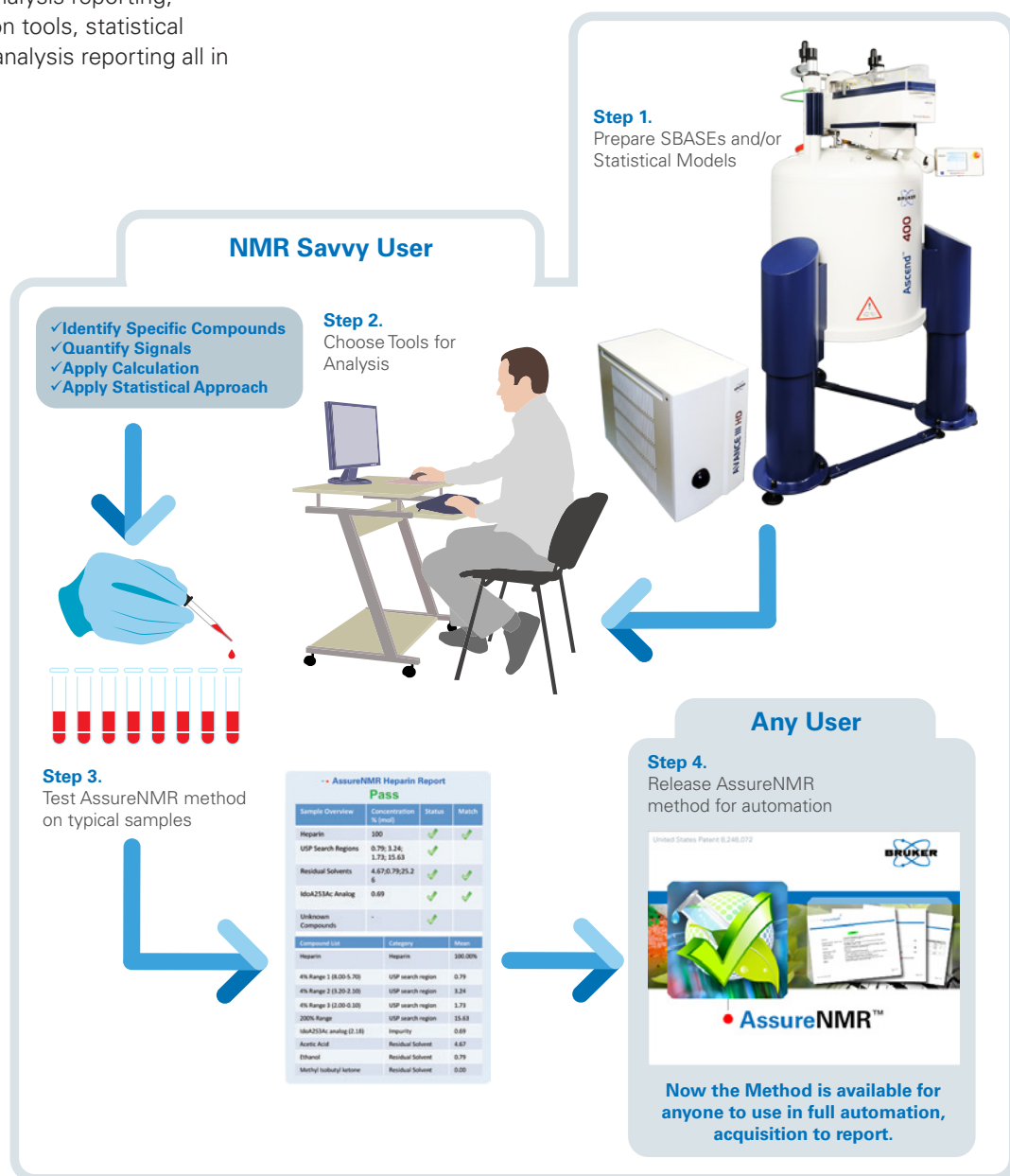
Complete Solution: Fully integrated software and hardware solution to ease the following of standard operating procedures (SOPs) and providing optimal reproducibility.

Data acquisition, analysis reporting, database generation tools, statistical analysis and error analysis reporting all in one package.

Highest Quality Standards: Automated system suitability tests and optimization routines keep your instrument producing superior results.

Accessible Technology: Three bundles, Launch, Ascent and Summit, are available to meet site specific needs.

Step 1.
Prepare SBASEs and/or Statistical Models

NMR Savvy User

✓ **Identify Specific Compounds**
✓ **Quantify Signals**
✓ **Apply Calculation**
✓ **Apply Statistical Approach**

Step 2.
Choose Tools for Analysis

Step 3.
Test AssureNMR method on typical samples

Any User

Step 4.
Release AssureNMR method for automation

Now the Method is available for anyone to use in full automation, acquisition to report.

• Bruker Screening Solutions

AssureNMR Methods define the automation procedure for acquisition, analysis and processing for the analysis of specific materials. Methods are user generated or available through Bruker. AssureNMR contains tools to assist the NMR user in generating their own AssureNMR methods for site specific materials

AssureNMR Methods

Aloe
Based on the J. AOAC International publication (2010), AssureNMR Aloe includes a method and NMR spectral database for detection of at least 12 components for quality control screening of *Aloe vera*.

Heparin
Based on the USP Monograph (2012), AssureNMR Heparin includes a method and NMR spectral database for a quality control screen of Heparin Sodium.

Poloxamer
Based on the European Pharmacopeia 6.0, this AssureNMR method characterizes poloxamers and reports the Oxypropylene: Oxyethylene ratio of these common excipients and surfactants.

Cyclodextrin (Molar Substitution)
Based on the European Pharmacopeia 5.0, this AssureNMR method characterizes cycloedextrin by evaluating the number of hydroxypropyl groups per anhydroglucose unit.

Tire Rubber
Based on the EU Directive ISO 21461, this AssureNMR method evaluates the polyaromatic hydrocarbons (PAH) content.

• **Bruker BioSpin**
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www.bruker.com/assure