Natural Products

- High Performance NMR Solutions for Analysis
NMR Spectroscopy

Continuous advancement in Bruker’s NMR technology allows researchers to push the boundaries for natural product research. From solving complex structural questions to developing a high-throughput screening method for quality control of natural products, Bruker has the high performance solutions necessary to address the current demands in this field.

By combining state-of-the-art hardware developments such as improvements in probe design and receivers for the highest NMR sensitivity, to comprehensive software packages, Bruker provides the perfect complement of tools for optimizing your productivity and making new discoveries.
Yields Better Research & Results

Unparalleled Sensitivity

Detect as little as nanograms of isolated natural products in just a few minutes through the use of our small volume probe and CryoProbe™ technology. Bruker has a range of smart options designed for versatility, cost effectiveness and unparalleled mass sensitivity.

Excellent Reproducibility

Obtaining reproducible results is critical for any natural product researcher. From understanding the natural variances of biological organisms to identification of unique metabolites, Bruker AVANCE™ III HD NMR consoles offer the highest reproducibility researchers require to answer screening or metabolomics questions. Instrument to instrument reproducibility gives researchers the ability to transfer their own analytical methods to any Bruker NMR system in any lab to provide consistent and accurate results.

Precise Quantification

Weighing a very small amount of a precious natural product isolate is difficult and without weight information the actual yield or concentration dependent biological activity is challenging to ascertain. Determining the amount of sample of a pure metabolite, or as part of a mixture, is both easy and accurate using Bruker’s TopSpin™ or AssureNMR™ software programs. By calibrating the NMR spectrometer to a known reference standard, the PULCON1 equation is applied to other samples to yield concentrations of components.

Automated Analysis Capabilities

Dereplication is an integral part of a natural products discovery program. Quality control is essential to ensure safety and reproducibility. Bruker software and hardware assists in both of these processes by providing the necessary automation to analyze spectra statistically, as well as identifying and quantifying the compounds seamlessly with a push of a button.

Exceptional Dynamic Range

Advances in Bruker’s AVANCE III HD console provide exceptional dynamic range, enabling the detection of low level components in mixtures. Let our innovative NMR products assist you in studying the molecules that were previously unapproachable.

Extract Origin | Baicalein | Baicalin | Scutellarin
--- | --- | --- | ---
*S. laterafloia* | nd | 98.1 mM | 10.0 mM
*S. incana* | 42.1 mM | 29.6 mM | 32.8 mM
*S. alpina* | 4.6 mM | 4.5 mM | 9.8 mM
*S. baicalensis* | 87.5 mM | 7.9 mM | 7.9 mM
*T. canadense* | nd | 107.5* mM | 10.3* mM
*T. chamaedrys* | nd | nd | 6.2* mM

Automated analysis by AssureNMR
nd = not detected, *Baicalin/Scutellarin derivative observed

---

1 Wilder, K.; Dreier, L. J. Am. Chem. Soc. 2006, 128, 2571-2576

---

90 µg of Muironolide A isolated from a marine sponge acquired in CDCl3 on a 1.7 mm MicroCryoProbe at 600 MHz. (A) HMBC acquired in 24 hours with NS=192 (B) HMBC vertical expansion (C) 1H NMR spectrum. Dalisay et al., JACS, May 15, 2009. Data was kindly provided by Tadeusz Molinski, UCSD.
Data Analysis Software

Bruker has the complete NMR software solution for all aspects in your natural product research. From finding an answer to your complex chemical structure questions or devising a multivariate model to understand the profile of your botanical materials, Bruker has developed various software packages to streamline your workflow for rapid results without compromise in data quality.

Software

- **CMC-se** is Bruker’s simple and efficient structure elucidation software that is essential for natural product researchers. With 1D and 2D NMR spectra for the compound of interest, CMC-se automates many of the key analysis and interpretation steps to aid researchers in simplifying the structure elucidation of valuable purified metabolites.

- **AssureNMR** is comprehensive data analysis software for automated targeted and non-targeted screening of extracts, mixtures or purified materials. By identifying and quantifying specific metabolites in a botanical material or detecting potential adulterants in a dietary supplement, AssureNMR empowers researchers to create their own automated analysis methods for screening of natural products.

- **AMIX** provides a collection of powerful tools that enable you to get the most out of your data. AMIX includes many integrated routines for spectroscopic and statistical analyses, significantly enhancing productivity across a wide variety of applications, such as small molecule research, metabolomics and mixture analysis.

AMIX Example

The chemometric functions in AMIX such as PCA allows in-depth analysis of botanical materials for species identification. The PCA scores plot show the separation of various Vaccinium species.

With univariate statistics and multivariate modelling such as PCA, SIMCA, PLS and PLS-DA capabilities, AMIX assists interpretation of 1D or 2D NMR spectra and LC-MS datasets and gives researchers the vital metabolomic tools for quick and reliable results.
AssureNMR utilizes multivariate classification models to screen various natural products (botanical materials, dietary supplements, etc.) to observe if the sample spectral profile is different because of adulteration or other factors not considered in the variance of the model. This precision is critical for quality control and assessment and may be used for species identification or product conformity.

Sibutramine and Phenolphthalein were identified in bee pollen commercial products using AssureNMR. The AssureNMR quality control screen fails a commercial bee pollen sample containing undeclared drugs (Sibutramine and Phenolphthalein) using a targeted screening approach. AssureNMR utilizes a user generated or Bruker spectral base to automatically identify and quantify the main components, possible adulterants and potential unknowns present in the sample. The undeclared drugs are quantified using a line shape fit analysis.

AssureNMR utilizes multivariate classification models to screen various natural products (botanical materials, dietary supplements, etc.) to observe if the sample spectral profile is different because of adulteration or other factors not considered in the variance of the model. This precision is critical for quality control and assessment and may be used for species identification or product conformity.
Bruker’s range of hardware solutions for natural product research offers various unique features to benefit your specific area of study.

**AVANCE III HD – Bringing High Definition to NMR Spectrometers**

Precise quantification measurements are enhanced with high performance spectrometer architecture. The AVANCE III HD is the latest generation in the very successful AVANCE series product line. The AVANCE III HD spectrometer incorporates increased sensitivity with newly designed preamplifiers as well as increased dynamic range through a new RF synthesizer, providing significant increases in sensitivity for the most demanding of applications common to the natural products community.

**Hyphenation & LC-(SPE)-NMR-MS**

Major tools for natural products research include chromatography (LC and SPE, etc.), NMR and MS. Bruker offers combined systems to meet various research needs. Our Metabolic Profiler is an integrated system featuring an AVANCE NMR spectrometer, a liquid chromatography system, a peak collection/concentration unit (SPE) and a micrOTOF-Q III™. By combining the structural resolving power of NMR with the mass accuracy of the micrOTOF-Q III, we can offer the most complete system for structural analysis available today.

*Other MS options are also available.
Automation

Automation is available for even the smallest of sample sizes and NMR tubes. With Bruker, the automation workflow begins with and includes the submission of a sample, followed by sample preparation, transfer to the spectrometer, automatic probe tuning, data acquisition, processing, analysis, reporting and finally data distribution and archiving. All of the automation features are designed to increase your efficiency and seamlessly integrate with your standard workflow.

SampleJet is designed for versatility and high throughput. This sample changer accepts up to five 96 well plates of NMR tubes and up to 48 single NMR tubes. The sample area is enclosed to allow for an optional temperature control of the samples.

Integration of software and hardware, such as AssureNMR with SampleJet, allows for fully automated solutions that include instrument performance validation right through analysis and reporting of results on natural products. Bruker’s automated solutions assist whether you are classifying a botanical material or screening an extract from an invertebrate for specific metabolites.
Solutions at a Glance

Bruker’s range of solutions for natural product research incorporates various analytical methods, each with unique features to benefit your specific area of study. Bruker is your ideal partner in finding the most suitable solution for your natural products research.

Some of our products that are particularly useful for natural products research include:

**NMR Spectroscopy**
- CryoProbe Technology
- Small Volume Probes
- AVANCE III HD
- LC-(SPE)-NMR-MS
- SampleJet
- CMC-se
- CMC-a
- AssureNMR
- AMIX

**Mass Spectrometry**
- micrOTOF-Q III
- IMPACT II
- FT-ICR-MS
- Atmospheric Pressure Chemical Ionization (APCI) accessory
- SmartFormula 3D