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# qIDsolve

## The forensic suite for automated identification and quantification with benchtop NMR


The qIDsolve software package combines tools for automated data acquisition, identification, quantification and reporting embedded in a fully traceable environment supported by an extensive benchtop NMR spectra database.

### dbNMR

- Contains comprehensive spectra
- Easy to expand
- Can be shared between workstations

### idNMR

- Automated identification
- Efficient search algorithm
- Connectivity to external database

### qNMR

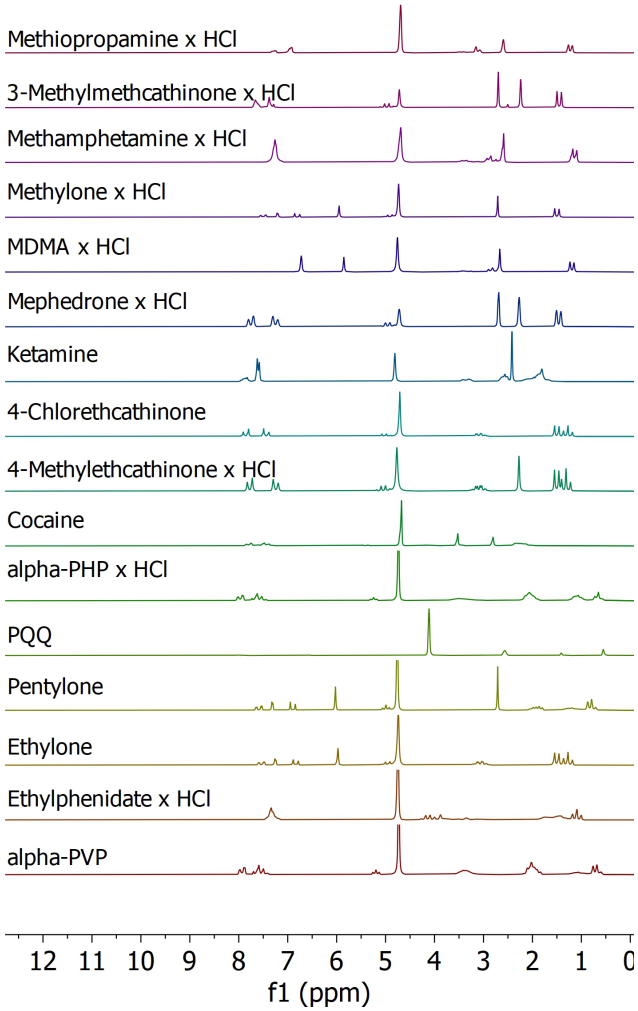
- Automated quantification
- Use of internal and external standards
- Graphical method development
- Automated reporting

### Audit

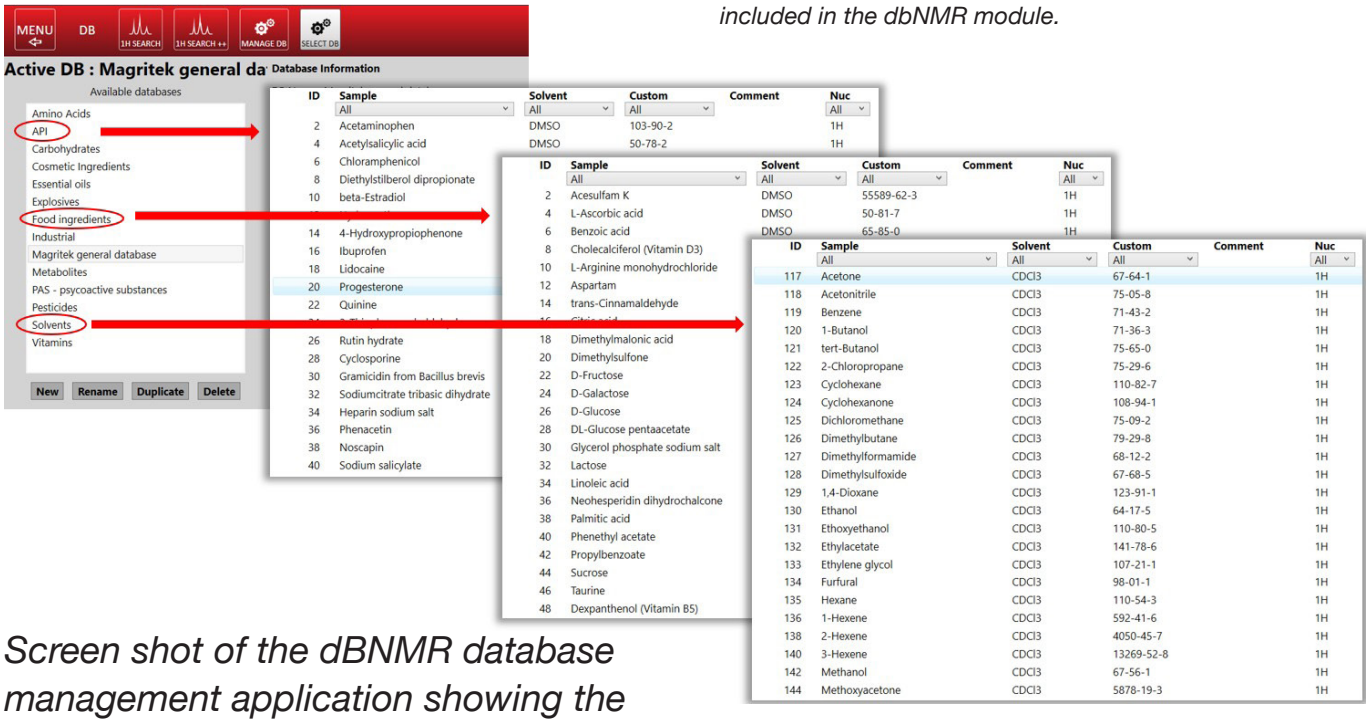
- Group admin and user management
- Flexible data saving options
- System and measurement audit trail
- Fully compatible with Autosampler

# dbNMR – extensive benchtop NMR database

The Spinsolve dbNMR database package is a flexible and easy-to-use solution that comes with an extensive list of spectra of pure substances carefully measured with high signal-to-noise. The benchtop NMR spectra in the database have been collected in cooperation with a number of partners and laboratories around the world during the last 10 years. This long list of entries are well categorized based on the IUPAC name, CAS number, and used solvent. Users can start from this data base and add their own entries following very easy steps. The database enables one to set up compound categories and freely combine them in any desired way. For each compound it is possible to store multiple spectra acquired for different nuclei, different solvents, different spectrometer frequencies, or even different acquisition parameters. Additionally, to spectra collected on a Spinsolve system, data available from other spectral libraries like the NPS-datahub can as well be imported. The database itself is in SQL format and the whole database or defined entries can be easily selected to be shared with other systems. In this way, users can establish an efficient network that keep the database updated with the entries of all members of the network.




*Excerpt from the psycho active substance database included in the dbNMR module.*




*Screen shot of the dBNMR database management application showing the different compound categories and a small subset of included compounds.*

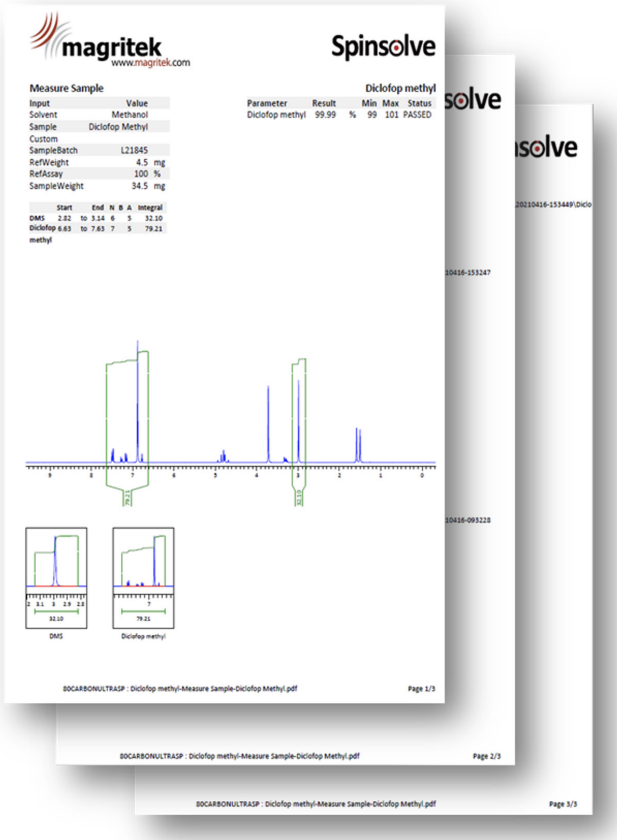
## idNMR – automated identification

The idNMR package provides the solution for automated identification of components contained in unknown samples. It includes a powerful cross-correlation algorithm developed for automatic identification of unknown substances against the database. The algorithm provides a ranking list with the compounds in the library that show the best matching score. The database search function can be used in two modes. The expert mode can be selected to accurately compare the acquired data against the best scored spectra from the database. The quality of the matching can be precisely judged from the residual of the fitting. The automatic mode, on the other hand, can be used perform data acquisition, processing, and reporting in a single step running under the AUDIT user management module. This software package, developed for regulated environments, offers full traceability of the measurements performed under specific audit trails defined by the administrator.


*Screen shot of the idNMR software console displaying the comparison interface and the ranking list with best matching scores.*

## AUDIT – automated reporting and full traceability

The AUDIT module was developed for the use in regulated environments, where data integrity and traceability is key for the applicability of the system. It is smoothly integrated with idNMR and qNMR packages and can be fully automated with the queuing functionality of the autosampler.

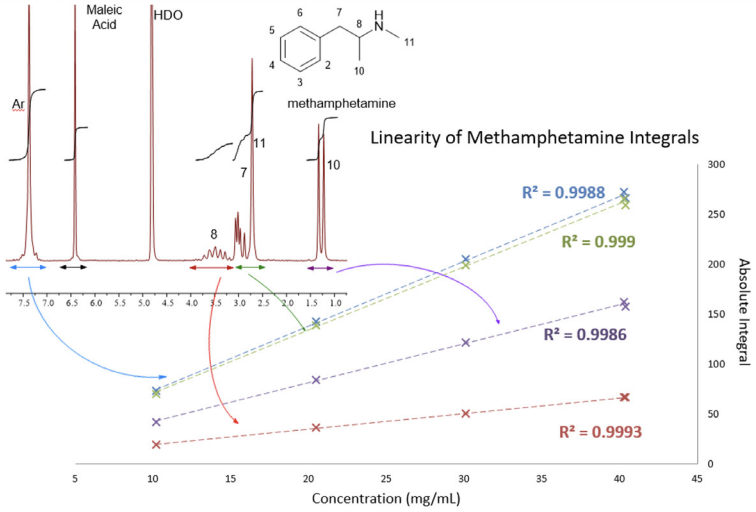



### Features

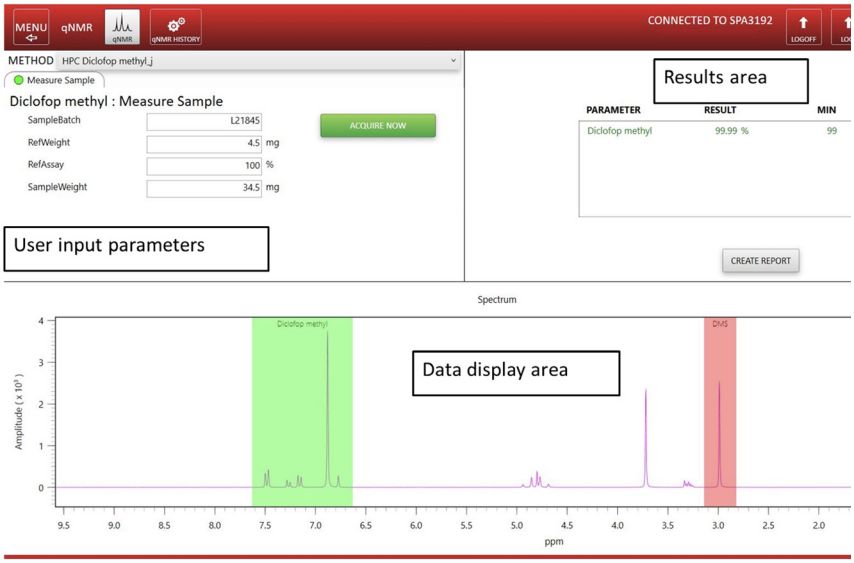
- Automated report generation
- Group administration
- User management
- Flexible data saving options
- System audit trail
- Measurement audit trails
- Automated report generation

# qNMR – automated quantification

The Spinsolve qNMR software module has been designed to allow for a quick and easy set-up of Quantification methods, while offering flexible processing functions to accommodate the different types of applications. Methods using internal or external standards can be generated through a graphical user interface where a variety of graphical data visualization and statistical tools are available. Moreover, the qNMR plug-in is fully integrated with the Spinsolve AUDIT module to provide user management as well as full traceability of all measurement and processing steps.




*Method for the quantification of methamphetamine*




## Features

- Fully automated work flow
- Compatible with AUDIT
- User management
- Measurement protocol definition
- History functionality
- Audited report generation
- Graphical method development
- Internal or external standards
- Calibration with multiple standards

*The Spinsolve qNMR software module has been designed to allow for a quick and easy set-up of Quantification methods, while offering flexible processing functions to accommodate the different types of applications. Methods using internal or external standards can be generated.*

## Contact us now for a quote, to request a demo or to measure your samples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