

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

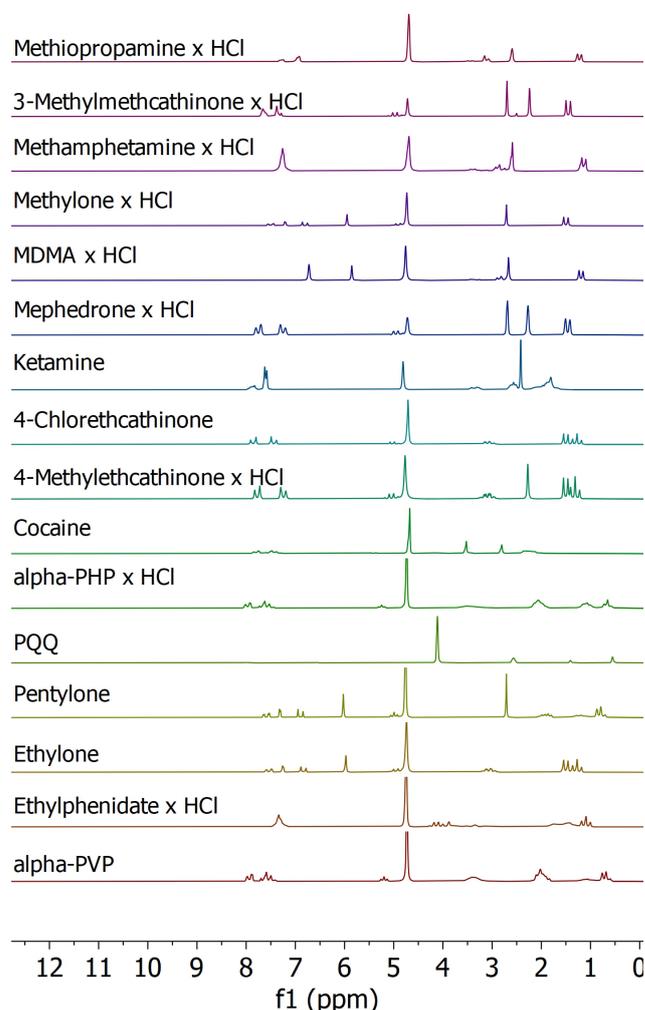
- Automated quantification
- Use of internal and external standards
- Graphical method development
- Automated reporting

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.



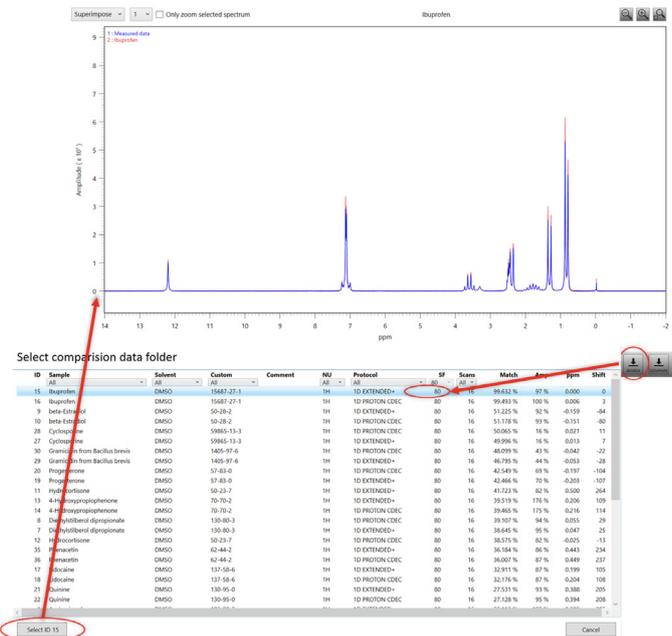
Excerpt from the psycho active substance database included in the dbNMR module.

ID	Sample	Solvent	Custom	Comment	Nuc
2	Acetaminophen	DMSO	103-90-2		1H
4	Acetylsalicylic acid	DMSO	50-78-2		1H
6	Chloramphenicol				
8	Diethylstilberol dipropionate				
10	beta-Estradiol				
14	4-Hydroxypropiofenone				
16	Ibuprofen				
18	Lidocaine				
20	Progesterone				
22	Quinine				
26	Rutin hydrate				
28	Cyclosporine				
30	Gramicidin from Bacillus brevis				
32	Sodiumcitrate tribasic dihydrate				
34	Heparin sodium salt				
36	Phenacetin				
38	Noscapin				
40	Sodium salicylate				
2	Acesulfam K	DMSO	55589-62-3		1H
4	L-Ascorbic acid	DMSO	50-81-7		1H
6	Benzoic acid	DMSO	65-85-0		1H
8	Cholecalciferol (Vitamin D3)				
10	L-Arginine monohydrochloride				
12	Aspartam				
14	trans-Cinnamaldehyde				
18	Dimethylmalonic acid				
20	Dimethylsulfone				
22	D-Fructose				
24	D-Galactose				
26	D-Glucose				
28	DL-Glucose pentaacetate				
30	Glycerol phosphate sodium salt				
32	Lactose				
34	Linoleic acid				
36	Neohesperidin dihydrochalcone				
38	Palmitic acid				
40	Phenethyl acetate				
42	Propylbenzoate				
44	Sucrose				
46	Taurine				
48	Dexpanthenol (Vitamin B5)				
117	Acetone	CDCl3	67-64-1		1H
118	Acetonitrile	CDCl3	75-05-8		1H
119	Benzene	CDCl3	71-43-2		1H
120	1-Butanol	CDCl3	71-36-3		1H
121	tert-Butanol	CDCl3	75-65-0		1H
122	2-Chloropropane	CDCl3	75-29-6		1H
123	Cyclohexane	CDCl3	110-82-7		1H
124	Cyclohexanone	CDCl3	108-94-1		1H
125	Dichloromethane	CDCl3	75-09-2		1H
126	Dimethylbutane	CDCl3	79-29-8		1H
127	Dimethylformamide	CDCl3	68-12-2		1H
128	Dimethylsulfoxide	CDCl3	67-68-5		1H
129	1,4-Dioxane	CDCl3	123-91-1		1H
130	Ethanol	CDCl3	64-17-5		1H
131	Ethoxyethanol	CDCl3	110-80-5		1H
132	Ethylacetate	CDCl3	141-78-6		1H
133	Ethylene glycol	CDCl3	107-21-1		1H
134	Furfural	CDCl3	98-01-1		1H
135	Hexane	CDCl3	110-54-3		1H
136	1-Hexene	CDCl3	592-41-6		1H
138	2-Hexene	CDCl3	4050-45-7		1H
140	3-Hexene	CDCl3	13269-52-8		1H
142	Methanol	CDCl3	67-56-1		1H
144	Methoxyacetone	CDCl3	5878-19-3		1H

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 to 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.



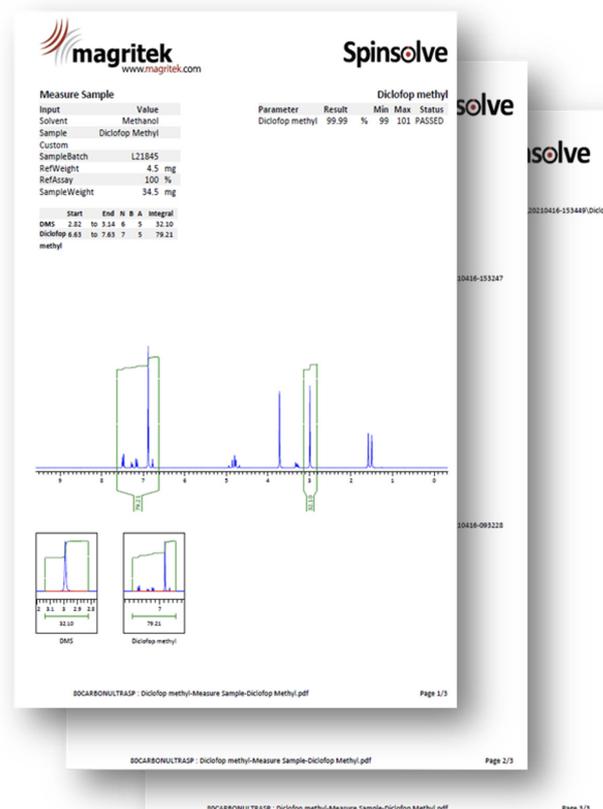
Screen shot of the idNMR software console displaying the comparison interface and the ranking list with best matching scores.

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.

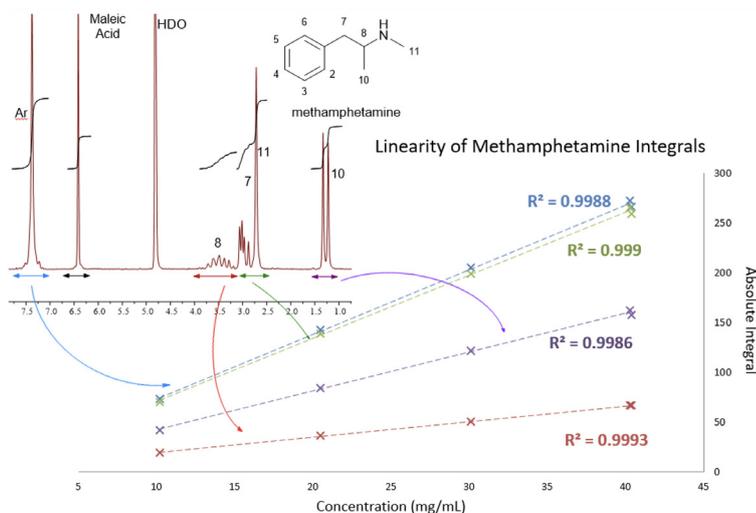
Features

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

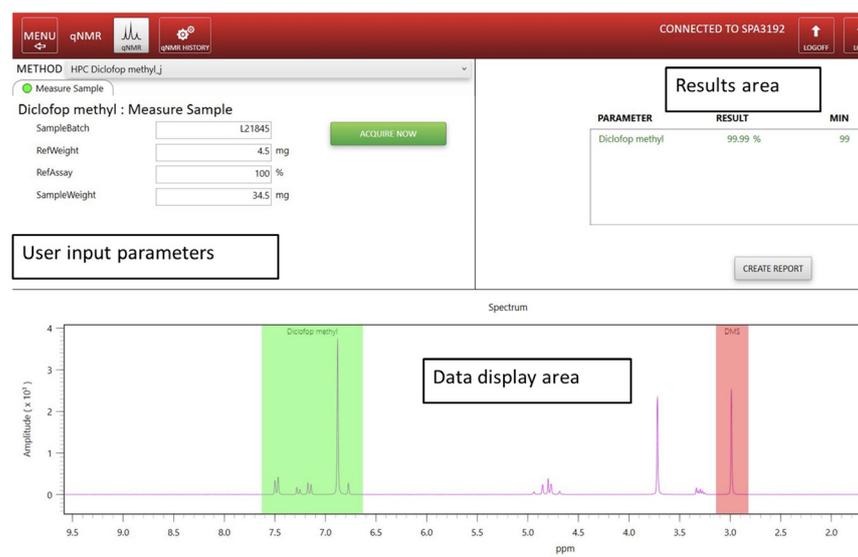


qNMR – automated quantification

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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