Spinsolve

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Undergraduate education with benchtop NMR

Spinsolve is the perfect way to provide NMR as part of an undergraduate teaching program. The high sensitivity and advanced capability means it is fast and informative, critically important for a busy class. Spinsolve provides convenient, high performance NMR at a fraction of the cost of traditional NMR systems.

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1D PROTON

SAVE TIME

In this second-year chemistry experiment, students synthesise *p*-nitroaniline through the hydrolysis of *p*-nitroacetanilide.

Spinsolve NMR spectra were acquired within a few minutes of sample preparation. Comparison measurements were also made on a standard 300 MHz instrument.

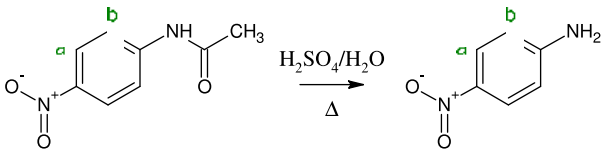
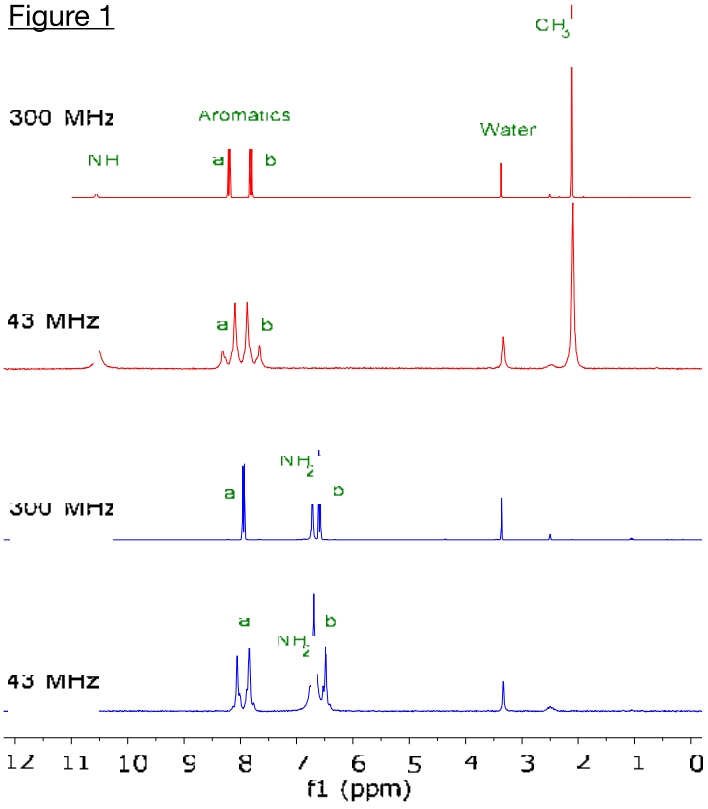


Figure 1 shows the ^{1}H NMR spectra of 200 mM solutions of starting material (red) and final product (blue) in DMSO-d_6. The disappearance of the methyl peak (CH_3) and the conversion of the NH peak from 10.5 ppm into a NH_2 at 6.6 ppm are evidence for a successful reaction. The results show that there is no loss of chemical information by using a lower NMR frequency.

Figure 1



- Spinsolve is fast: students obtain informative spectra within a minute of sample preparation.
- Convenient: it's in the lab, on the bench, next to the students.
- Students can work with concentrations of tens to hundreds of mmol due to the superb sensitivity.
- Spinsolve 43 MHz spectra provide similar chemical information as high field.

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REDUCE COST

As well as being less expensive than high field NMR, Spinsolve reduces costs because expensive deuterated solvents are not necessary.

In this second-year chemistry experiment, students synthesise *p*-nitroacetanilide through the nitration of acetanilide.

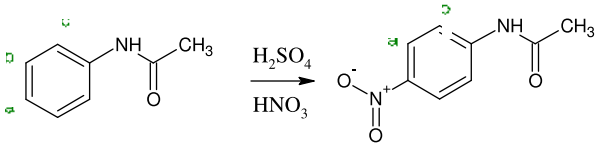
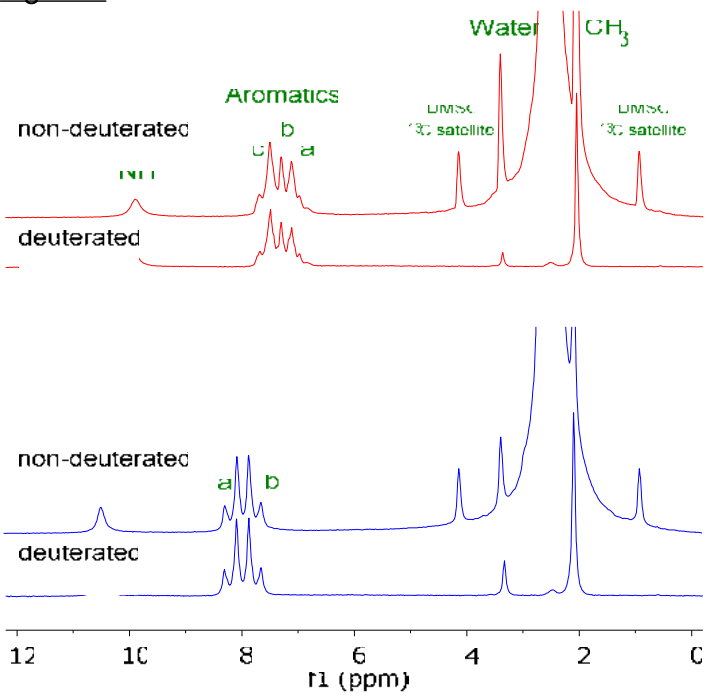
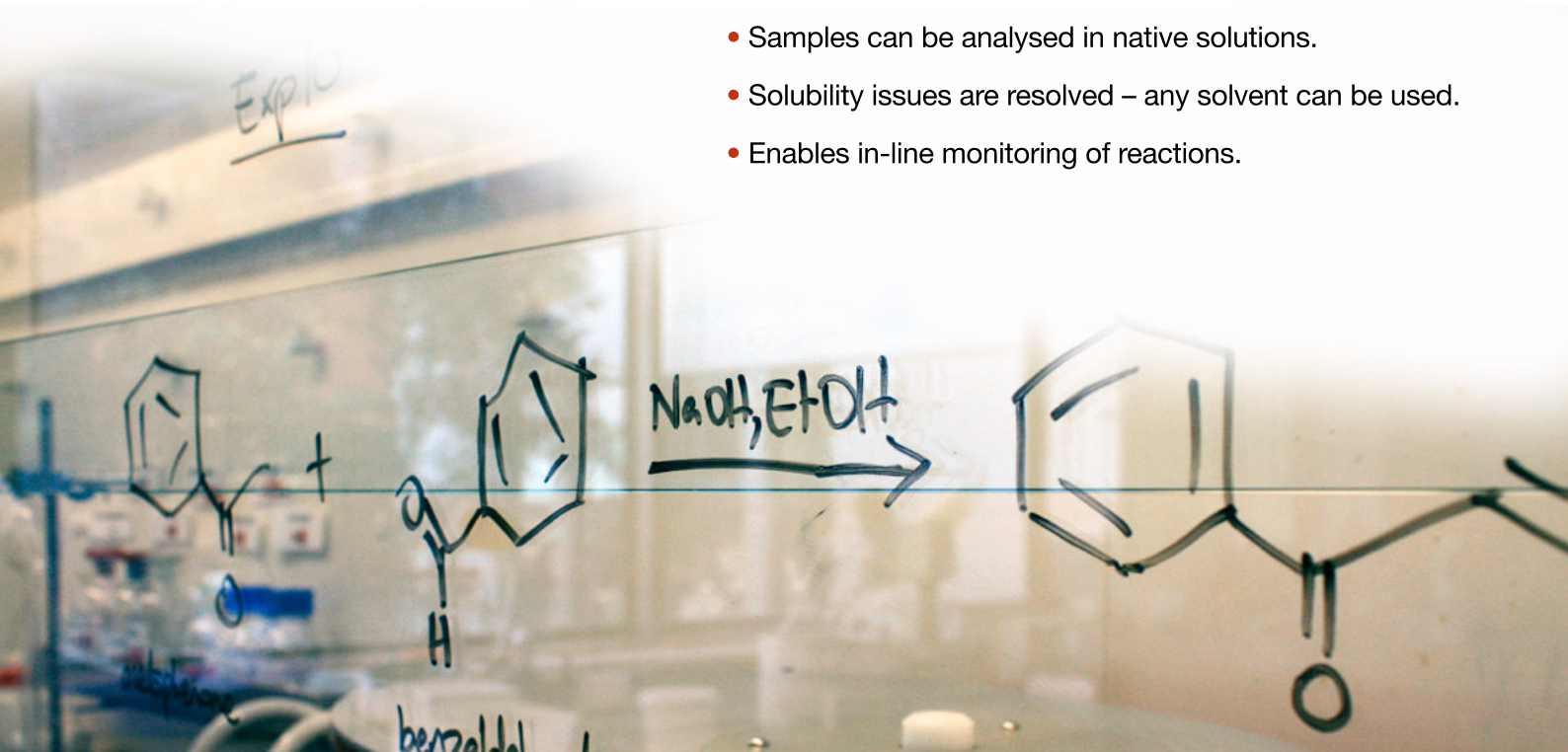


Figure 2 shows the NMR spectra of starting material (red) and final (blue) product, in deuterated and non-deuterated DMSO. Although there is a large peak for the non-deuterated solvent, all peak assignments can still be made for the molecule.

Figure 2



- Reduce cost - deuterated solvents are not necessary.
- Low cost budget NMR tubes can be used.
- Samples can be analysed in native solutions.
- Solubility issues are resolved – any solvent can be used.
- Enables in-line monitoring of reactions.



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EASY TO RUN

Setting up different NMR experiments can be a challenge for someone new to NMR. The simple Spinsolve user interface makes this easy.

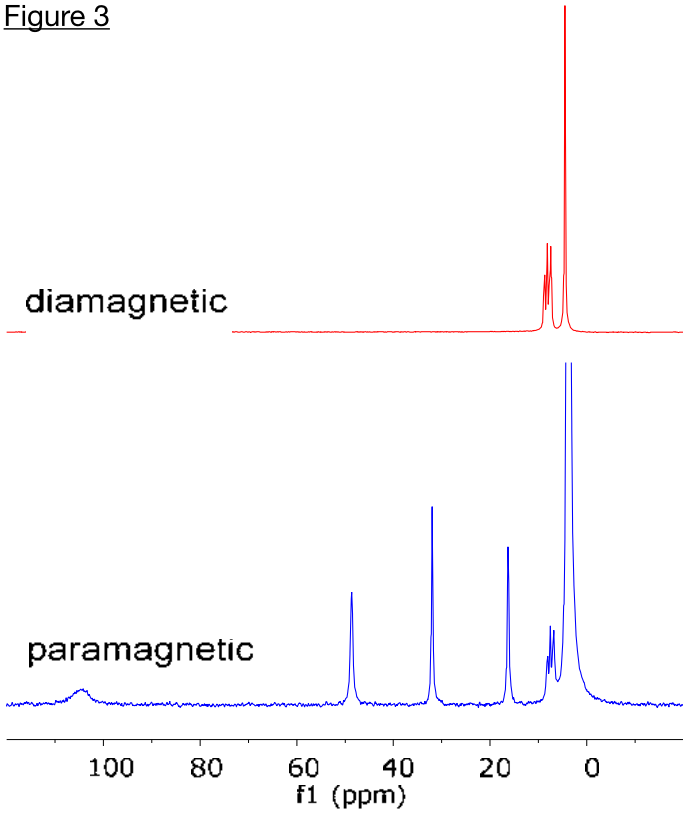
For example, many inorganic complexes are paramagnetic ions. These extend the chemical shift range of proton spectra to hundreds of ppm. The Paramagnetic protocol in the Spinsolve software is particularly tailored for scanning such samples and is easy to run.

This example from a third-year chemistry experiment demonstrates the reaction of coordinated ligands using the conversion of paramagnetic $[Co(phen)_3]^{2+}$ to diamagnetic $[Co(phen)_3]^{3+}$ complexes.

Figure 3 shows how the chemical shift range differs dramatically between the paramagnetic and diamagnetic cobalt complexes.

Spectra courtesy of Paul S Donnelly, University of Melbourne.

Figure 3



- Simple to use interface permits students to run different experiments.
- Paramagnetic samples can be analysed easily.
- Advanced 2D NMR experiments are simple to run.
- Students can also measure ^{19}F spectra with the click of a button.

ADVANCED NMR

When first being exposed to NMR, many students find it difficult to understand and distinguish between chemical shift and *j*-coupling. Two-dimensional NMR experiments project additional information into a second dimension, which tremendously facilitates the interpretation of NMR spectra.

As an example, we consider the ^{1}H NMR spectrum of ibuprofen dissolved in $CDCl_3$. The COSY experiment is used to assign which proton resonances are coupled to each other. Cross-peaks in the 2D spectrum indicate through-bond coupling. The COSY spectrum for ibuprofen is shown in Figure 4.

From the cross-peaks two spin systems are observed: CH-2/CH_3-10 and CH_2-7/CH_3-9.

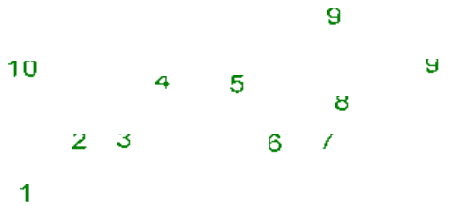
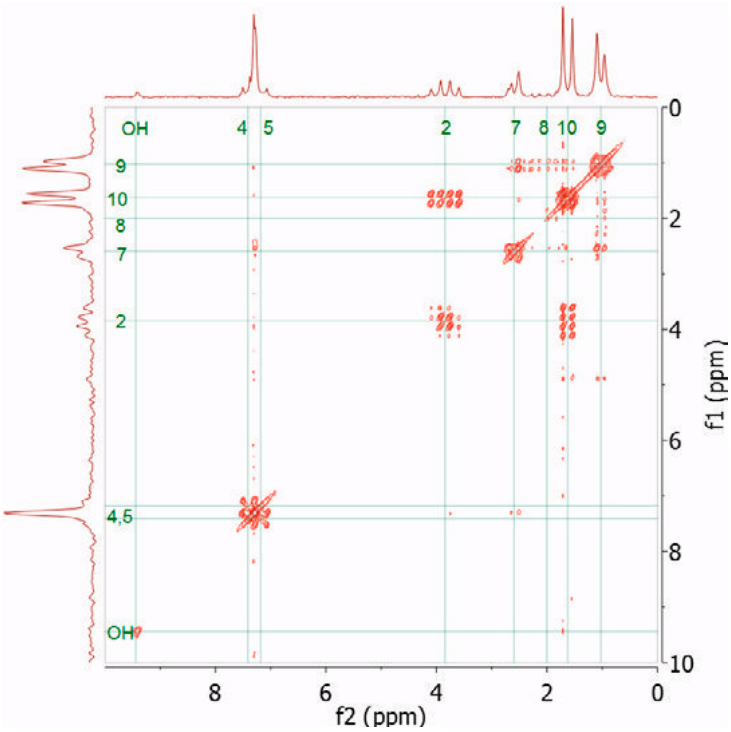


Figure 4



- The COSY experiment identifies the proton signals from magnetically coupled chemical groups.
- 2D COSY is one of the most commonly used 2D NMR experiments.
- Takes 10 minutes to run, ideal for a teaching laboratory.

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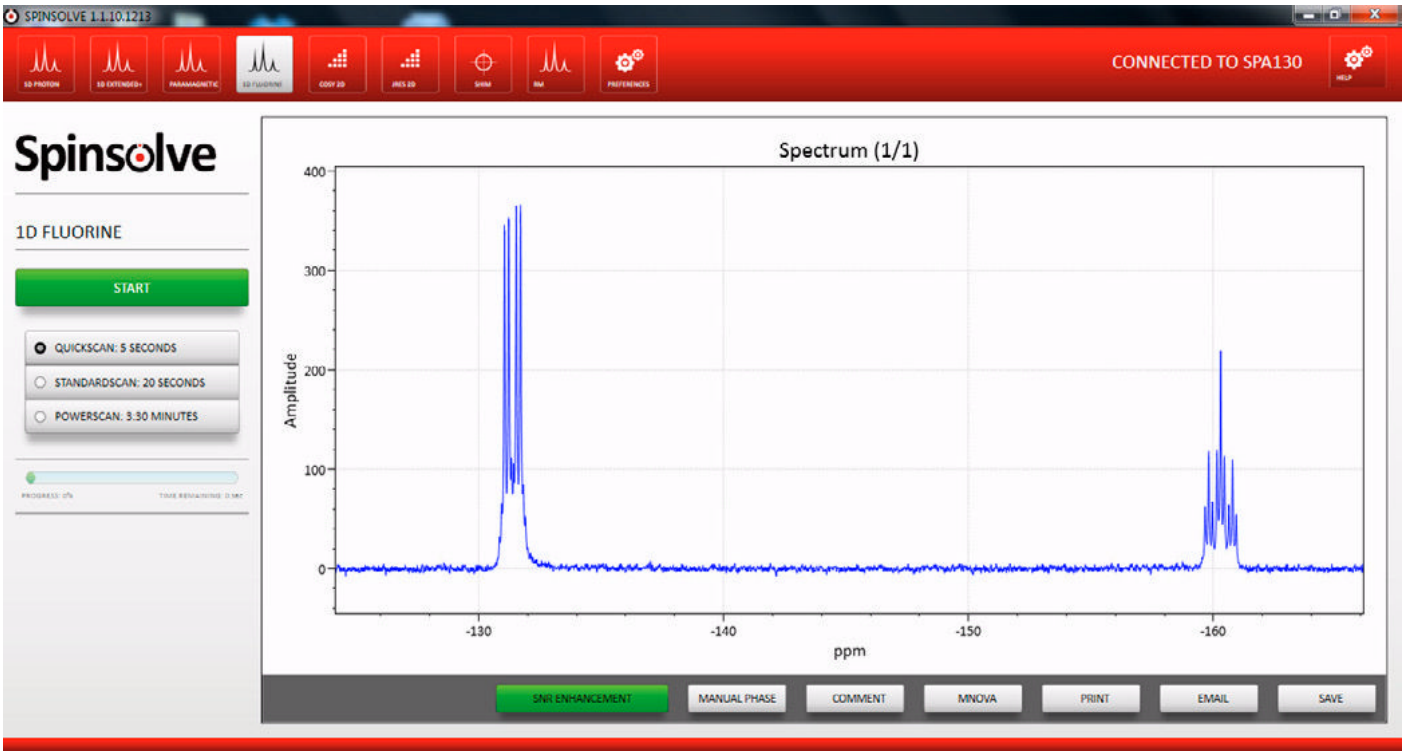
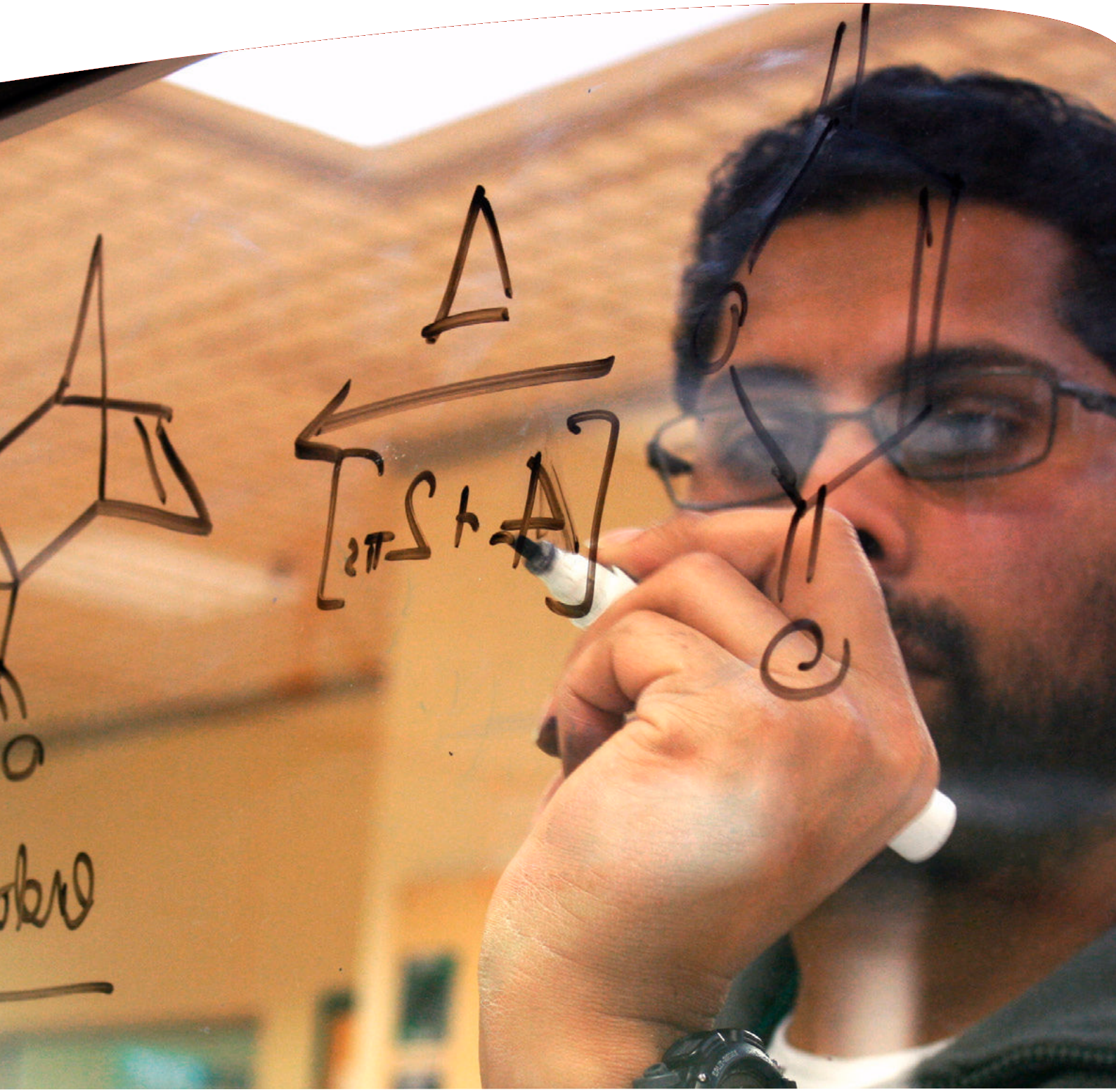
BEAUTIFUL INTUITIVE SOFTWARE



Spinsolve software is beautiful and intuitive which means it can be easily operated by anyone in the chemistry lab with minimal training. Most experiments can be run with a single click of a button. Switching between experiments also involves a single click. This simple, easy to use operation reduces time spent learning how to operate the system and increases throughput.

The screenshot above shows the new ^{19}F capability built into the latest version of the Spinsolve software.



“Now the students are able to acquire their own NMR spectra as well as carry out the analysis of the compounds they have made. This makes their undergraduate experiment more applicable to both research and industry settings and increases their enthusiasm for chemistry.”

-Professor Frances Separovic, Head of Chemistry at the University of Melbourne

Spinsolve

Use the Spinsolve™ benchtop NMR spectrometer to enhance the teaching experience in a chemistry laboratory or classroom.

Why the Spinsolve™ will suit your education needs:

REDUCE COST

- Low cost to purchase compared to high field.
- Non-deuterated solvents can be used.
- Low power consumption.
- Budget NMR tubes can be used.

SAVE TIME

- Nearby - fits easily on laboratory bench.
- Standard 5 mm NMR tubes enables rapid sample exchange.
- Fast - students get on and off quickly.
- Easy to use - simple and intuitive software.
- Safe - no stray magnetic field.

INFORMATIVE

- Enables leading NMR education.
- Obtain high-resolution NMR data in as little as 10 seconds.
- Now available with 2D, multi-pulse experiments (2DJRes, COSY) and ^{19}F Fluorine.
- Students and teaching staff gain hands-on experience with NMR.

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