# NMReady for Industry, Universities and High Schools


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Funded by the University of Edinburgh and ScotCHEM, an NMReady60e has been purchased from Nanalysis through GPE Scientific. In what will be initially a three year project, this highly portable NMR instrument will be used in the undergraduate chemistry teaching laboratories at the Edinburgh University during semester time. Out with this time, the instrument will be available for Scottish industrial organisations whose activities fall broadly in the sector of the Chemical Sciences and for educational outreach activities especially in high schools, in support of the Scottish National Curriculum-for-Excellence, which now contains a significant element of NMR content. In the industrial context, a breadth of opportunities exist for NMR spectroscopy to play a key industrial support role, in the chemical analysis of complex samples relevant to the Food & Drink, Oil & Gas, Life Science, Pharmaceutical as well as Chemical Science sectors.


## What is NMR?

NMR spectroscopy is a powerful analytical technique for the study of molecular structure, molecular interactions, the composition of mixtures, and the kinetics of chemical reactions or dynamics of molecules.

NMR uses radio waves to generate spectra from samples held in a magnetic field. NMR spectra can be obtained from solutions, solids or gels.

## Industry

NMR is a quick and easy method to:

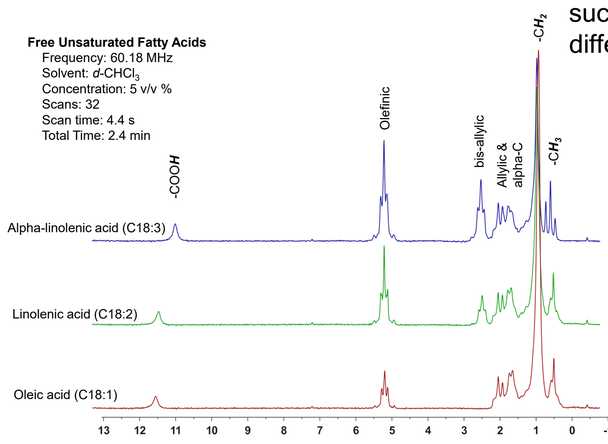
- monitor reactions, e.g. fermentation, biodiesel production.
- check quality and consistency of products, e.g. polymer composition.
- quantify species, e.g. water content, fat content.
- validate products claims, e.g. authenticity, ethanol percentage.

60 MHz NMReady provides point of need access to NMR for many applications in food and beverage, environmental to pharmaceutical industries.

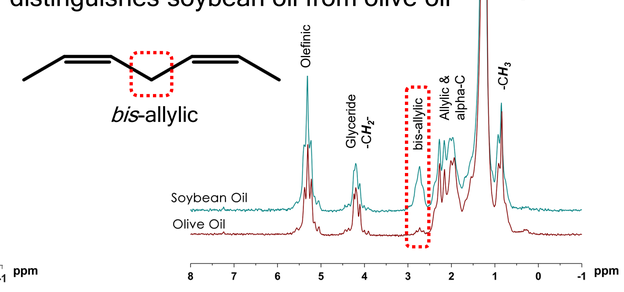
### Adulteration of foodstuffs: a study of olive oil adulteration with soybean oil.

Oils are triglycerides with fatty acid chains.

Olive oil contains minimal oleic acid, while other oils such as soybean do not, making it easy to spot the differences in NMR spectra.




The *bis*-allylic proton clearly distinguishes soybean oil from olive oil




Training in NMR and its applications on the portable NMReady60e is available for Scottish industrial organisations who are interested in learning more about NMR and its relevance to their products and processes.

**For further information contact Neville.Richardson@st-and.ac.uk**

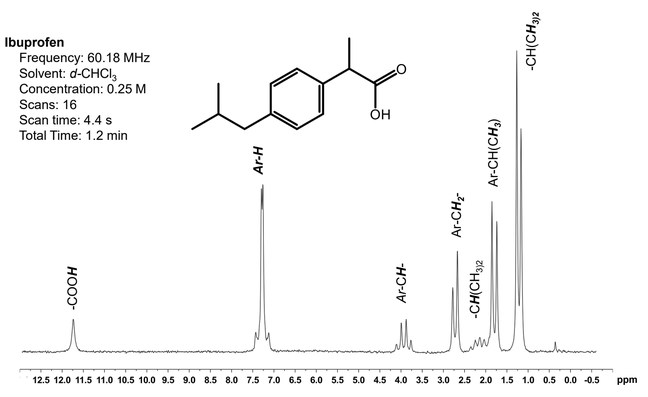
## High Schools

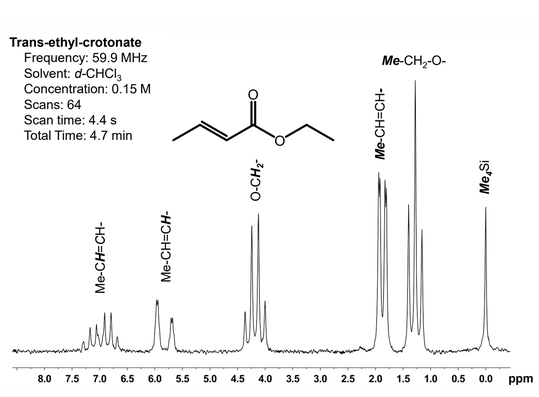
Proton NMR theory, including proton-proton couplings, is now taught as part of the Advanced Higher Chemistry curriculum in high schools. Access to NMReady provides an unique opportunity to have an NMR spectrometer in the classroom as a teaching aid or to enhance the quality of school projects.

### Proton NMR can be used in Advanced Higher projects to:

#### 1. Confirm synthetic products or extractants, e.g. ibuprofen, caffeine.

#### 2. Aid identification of unknown compounds, e.g. ethyl crotonate.




A three hour workshop is available aimed at teachers but open to advanced higher students which covers (i) NMR theory up to proton-proton coupling (ii) training on the NMReady to enable access (iii) NMR spectra interpretation.

**Interested in attending or hosting a workshop? Contact Nicholle Bell**

## Contact Us

If you would like more information on NMR workshops, training or access to benchtop/high-field liquid/solid state NMR or want to find out if NMR can be used in your laboratory, please contact Dr Nicholle Bell at Nicholle.Bell@ed.ac.uk.

## 60 MHz NMReady benchtop spectrometer

60 MHz NMReady benchtop can perform many tasks usually done on high-field NMR spectrometers.
1D proton spectra, $T_1/T_2$ relaxation times as well as 2D NMR experiments can be measured.


**Highlights of the 60 MHz NMReady spectrometer:**

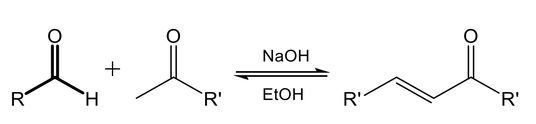
- Cryogen free, persistent magnetic field.
- Takes standard 5 mm NMR tubes.
- Simple to use, operated by touch screen.
- Low maintenance.
- Compatible with all NMR software packages.
- Contains several ports for display, printing etc.
- Can replace other time-consuming techniques.

**Want to know more about the NMReady60e? Contact wes.harker@gpescientific.co.uk**

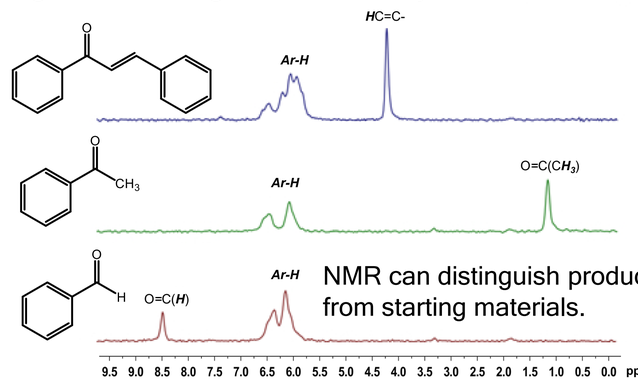
## Undergraduate laboratories

Proton NMR is an integral part of the undergraduate chemistry degree. Benchtop NMR spectrometers are already in several UK undergraduate labs and have applications in physical, organic or inorganic chemistry.

### Aldol condensation



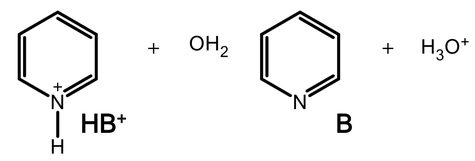

In this example R and R' =



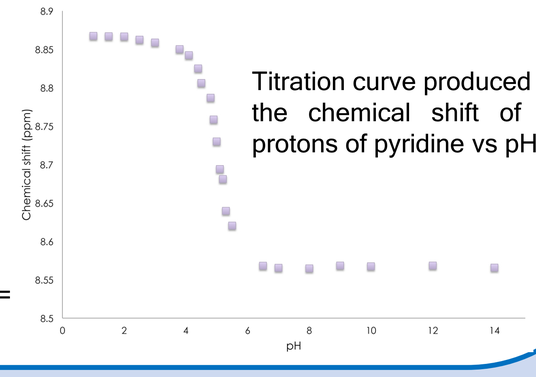

NMR can distinguish product from starting materials.

### Determination of $K_a$

$$pH = pK_a + log\frac{[B]}{HB^+}$$



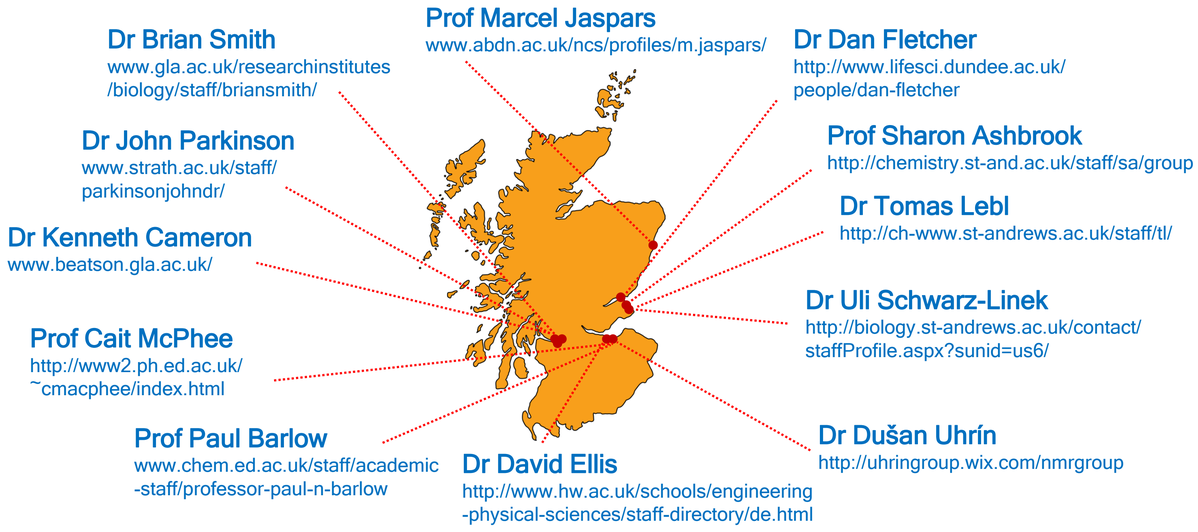

Equivalence point where [B] = [HB⁺] and pH = $pK_a$ can be extracted from a titration curve.




Titration curve produced using the chemical shift of ortho protons of pyridine vs pH.

## Scottish NMR Users Group (SNUG)

There are several high-field (> 300 MHz) NMR laboratories in Scottish Universities underpinning world leading research and teaching in chemistry, life sciences, physics and materials research.




**SNUG** brings together the NMR expertise across Scotland to facilitate:

- Access to NMR instrumentation across Scotland.
- Sharing of resources and expertise
- Education and outreach for academia, high-schools, industry and public.

**For further information contact Nicholle Bell**