

Project CAYMAN

Applying High-Field NMR
Spectroscopy to Product and
Process Development

New high-field
nuclear magnetic
resonance (NMR)
facilities at the
University of
Bradford

Delivering
30 fully-funded
R&D projects

Providing
fully-funded
NMR training
sessions



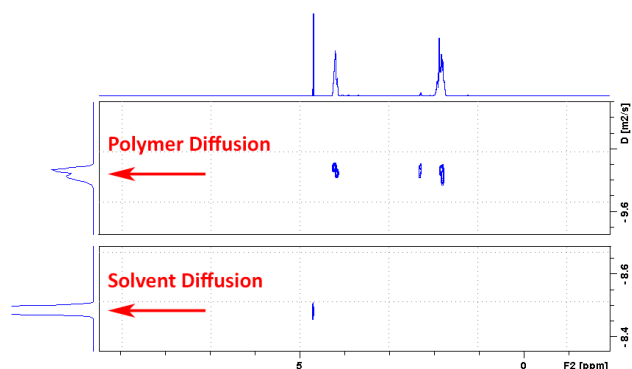
Project CAYMAN will use high-field NMR techniques to characterise macromolecular materials and complex chemical mixtures to help regional SMEs develop new products and optimise current manufacturing processes for:

- Polymers and Plastics
- Fine and Bulk Chemicals
- Pharmaceuticals & Medical devices
- Food, Vitamins and Supplements
- Cosmetics

What is Diffusion Ordered Spectroscopy (DOSY) NMR?

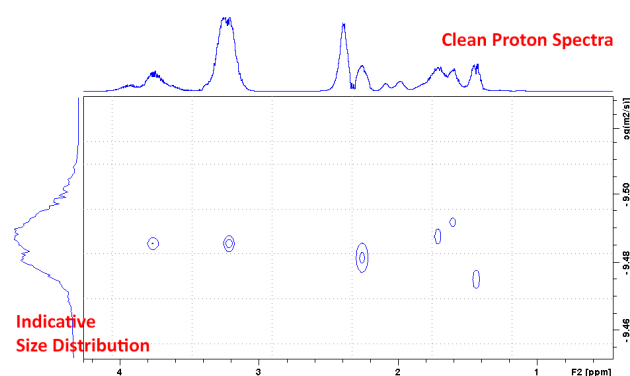
¹H NMR is a conventional chemical analysis technique to identify chemical structure but DOSY NMR also extracts the diffusion of chemical species within the sample and separates peaks based on their mobility. So DOSY can separate chemicals within the sample based on their molecular weight providing cleaner high resolution NMR spectra of complex mixtures and accurately measure each component:

- INTRINSIC VISCOSITY (mobility)
- SIZE (Hydrodynamic radius)
- MASS (Molecular weight)



Why Do We Want to Measure Size/Mass?

Due to batch to batch variation in process parameters many commercial **polymers** vary in **molecular weight distribution** which can alter the product properties leading to variable quality and batch failure. DOSY is a low cost method for providing instant comparisons between samples to highlight any differences in both molecular weight distribution and chemical structure.

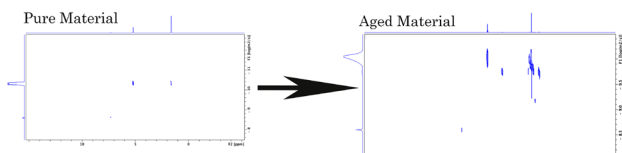


DOSY NMR avoids Chromatography

Some materials are not suitable for conventional methods of analysing molecular weight e.g. MALDI, Size Exclusion Chromatography. DOSY avoids ionisation issues and problems with samples adhering to columns. DOSY is a sensitive, non-destructive and flexible technique allowing analysis using different solvents, temperatures, concentrations and additives.

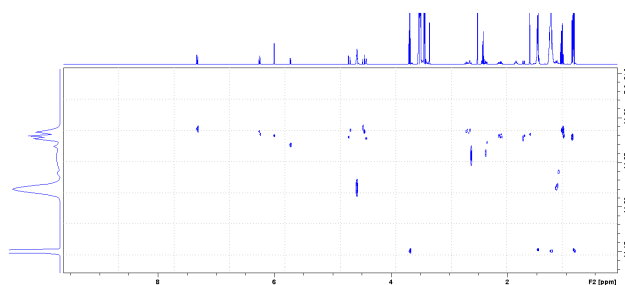
Use of DOSY in polymer degradation studies

Combined measurement of material size and chemical structure provides incredibly powerful analysis of changes in the material. We have worked with material manufacturers to study how their materials change on ageing.



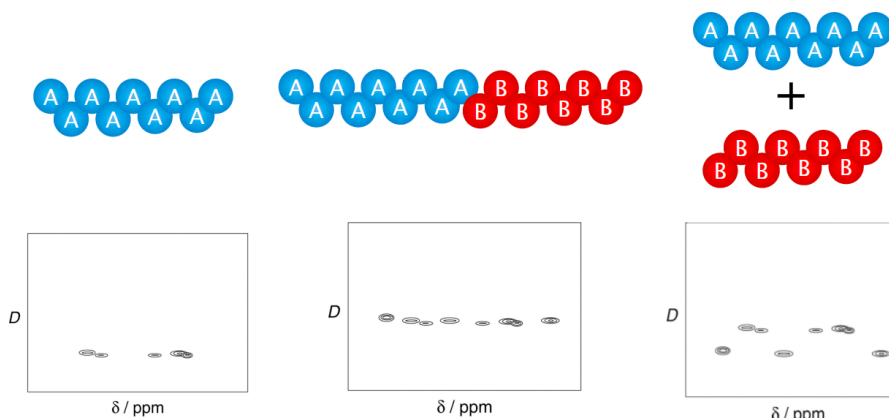
DOSY to Analyse Complex Mixtures

DOSY makes the NMR analysis of complex mixtures far simpler as it allows the separation of molecules of different size. For example, in a pharmaceutical formulation with 3 components, an API and 2 excipients



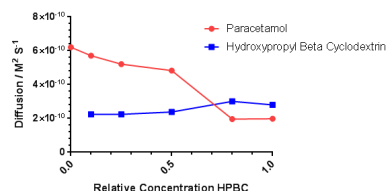
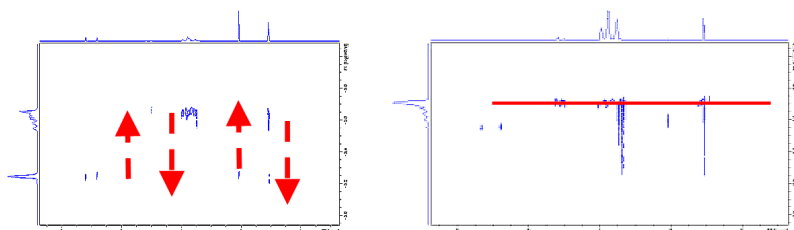
DOSY to Determine Chemical Functionalization

DOSY can help distinguish whether protons exist on the same sized molecules or in two separate species – it is an excellent tool for determining whether functional groups have been attached to a material or have formed a separate species.



Binding Studies - DOSY can Identify interactions between molecules

Binding studies using NMR can show the encapsulation or complexation of different drug molecules. We studied a paracetamol/HP- β -Cyclodextrin complexing system, and found that as the concentration of the HP β CD was increased the diffusion of the paracetamol was restricted.





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The Centre for Chemical and Biological Analysis

Project CAYMAN research projects and training will be managed by the Centre for Chemical and Biological Analysis. Housed in the modern Norcroft Building at the University of Bradford, the Centre offers an impressive range of sophisticated and specialist analytical equipment and is the hub of analytical science at the University for both research and commercial projects. Over the past 15 years the team has established a proven track record of delivering analytical services and research to industry clients.

Our experienced and highly skilled staff, ensure that the instrumentation is maintained to industry standards through service contracts, controlled access and a quality management system. We offer an array of analytical techniques and services to industrial clients including contract research, routine analysis and training courses.

This project is receiving £800,000 of funding from the England European Structural and Investment Funds Growth Programme 2014-2020. This fund is established by the European Union to help local areas stimulate their economic development. By investing in projects the funds will help to support innovation, businesses, skills and employment to improve local growth and create jobs.