



# Characterisation and Analysis



The University of Western Sydney is increasingly recognised for its characterisation, imaging and microanalysis capabilities. It is home to highly regarded experts and state-of-the-art equipment that offer new insights into: plants and animals; the development of new materials and pharmaceuticals; and in chemical and forensic analysis – to name just some of the potential areas of application.

## Innovative uses of NMR

The University has made a multi-million dollar investment in ensuring that its nuclear magnetic resonance (NMR) facility is a national leader. In many aspects it has no rivals in Australia.

NMR contains a number of sub-disciplines including magnetic resonance imaging (MRI), which is traditionally used in hospitals and medical facilities. But the highly innovative UWS team is encouraging the use of NMR and very high resolution MRI (also known as NMR microscopy) by industry, government agencies and research organisations in such diverse fields as entomology, neuroscience, rheology, molecular association, materials, nanotechnology, plant science, well-logging, electrochemistry and surfactants.

The University's major NMR facility can be used to study: ligand binding and transmembrane transport; drug binding; association and association kinetics of proteins, surfactants and small molecules; diffusion in porous systems ranging from sandstone to polymers to brain tissue; plants, water flow and freezing in plants; supercooled liquids and biological tissues.

The NMR facility comprises three co-located spectrometers:

- 1 A wide-bore 500 MHz, 11.7 tesla spectrometer – for high resolution imaging, very high gradient diffusion measurements and high resolution magic angle spinning
- 2 A 400 MHz, 9.4 tesla spectrometer – for general high resolution studies and low gradient diffusion measurements
- 3 A 300 MHz, 7 tesla spectrometer – for general high resolution studies



Imaging and diffusion are complementary techniques: used together they offer novel perspectives. The group at UWS is renowned for its work on NMR diffusion studies.

Three other NMR systems in the School of Natural Sciences are used to analyse solids and liquids such as geological samples, soils, organic matter in soil, biomaterials, polymers and composites, sol-gel systems and other materials underpinning our work in nanotechnology.

NMR in the School of Biomedical Sciences is used to determine the structure of molecules and diffusion of biomolecules within cells.

### Stunning, live images

In 2007 UWS established its Confocal Bio-Imaging Facility (CBIF), drawing together a dozen instruments which collectively produce live, three-dimensional images of almost any material.

This state-of-the-art facility is unique in Australia and the best in the South East Asian region. It uses a suite of lasers to depict inorganic materials, plants and animal cells in incredible detail. The images appear on a computer screen in vibrant colours.

Confocal laser imaging is increasingly popular in science and industry, especially for biological, environmental and forensic science. For example, it can image:

- » A virus crossing a cell membrane in real-time
- » Living cells dividing and changing over days or weeks
- » Live cells, with little or no sample preparation
- » Real-time, solution-based molecular interactions, in femtolitre volumes
- » The effects of drugs or other chemicals at the cellular level

Other uses include:

- » Elemental analysis
- » Microanalysis of explosives or unknown powders
- » Activity of experimental drugs

The Confocal Bio-Imaging Facility comprises several analysis techniques.

**Multi-photon confocal microscopy** offers multiple chemical analyses with lasers in real time. For example, users can:

- » Selectively image components of dividing cells
- » Determine events occurring in bioactive agents
- » Investigate a family of biochemical compounds to pinpoint requirements, saving the need to start with micro-arrays.

**Fluorescence lifetime imaging** determines the length of time a molecule can fluoresce. Because it can probe greater tissue depths than conventional fluorescence microscopy, it is especially useful in biomedical tissue imaging. For example, a water supply analyst could identify a disease organism such as *Giardia*, its effects on the host and quantify the amount present.

**Fluorescence resonance energy transfer** is used to quantify molecular dynamics in biophysics and biochemistry, such as protein-protein interactions, protein-DNA interactions and protein conformational changes. It measures energy transfer of molecules. For example, a pharmaceutical firm could use this capability to “see” drugs moving across the cell membrane and to determine the effects on the cell.

**Fluorescence correlation spectroscopy** is used to characterise proteins, biomolecules and pharmaceuticals, for example, and their dynamics. It enables tracking of an individual molecule through cells and tissues. For example, using viral DNA, a drug can be tracked to see how it moves through the cells of a plant or animal cell.

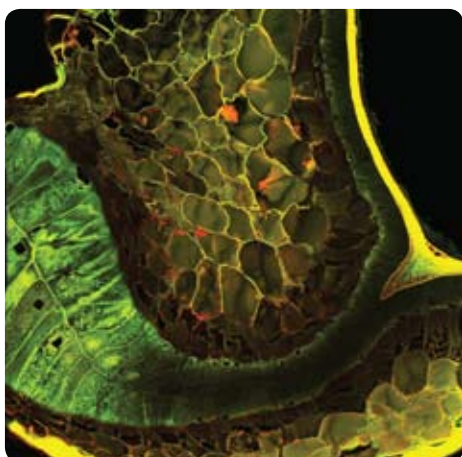
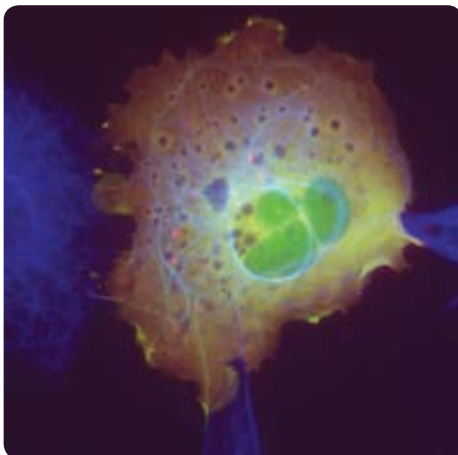
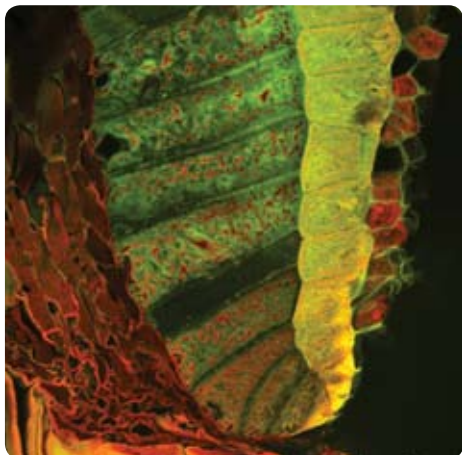
**Confocal Raman spectroscopy** is used for microscopic examination of minerals and materials such as polymers and ceramics, cells and proteins. For example, in forensics applications it can monitor chemicals and chemical reactions in real time to:

- » Identify drugs such as steroids and narcotics
- » Provide a molecular ‘fingerprint’ that complements the information available via infrared spectroscopy, mapping the distribution and quantity of a substance of interest, such as material on a knife.

### Latest generation scanning electron microscope

UWS’s new, high-end field emission scanning electron microscope (FESEM) offers ultra high resolution for use in nanotechnology, engineering, chemistry, physics and biomedicine, among other fields.

FESEMs can analyse structures as small as 1 nanometre on the surface of materials and biological tissue, in order to characterise polymers, coatings on materials, nanotechnological systems and sub-cellular proteins, for example. New applications are emerging in nanotechnology, where fabrication techniques are so advanced that SEM technologies have been developed to enable researchers to image the structures that they make.



Increasingly SEM is replacing traditional optical microscopes in pathology, forensics, and metallurgical and environmental analysis.

In a FESEM, electrons are generated in a source (the emission) and focused using a strong electrical voltage gradient (the field). An electron beam is formed to scan an object and secondary electrons are produced by interaction with atoms at the object's surface. Information from these electrons is employed to reconstruct a very detailed image of the topography of the surface of the specimen.

The new FESEM, located in the School of Natural Sciences, offers both high-vacuum and low-vacuum capabilities (10 to 100 – 200 Pa).

The College has an extensive, diverse array of analytical capabilities that can address a wide range of industry needs. Staff provide expert advice on the right techniques to use, conduct the experiments, and then work with clients and research partners on the interpretation of results.

As well as using the University's own facilities, staff utilise equipment located elsewhere, drawing on their wide networks and established access arrangements.

This is supported by supercomputing for conducting molecular dynamic calculations and general computational chemistry.

### Simultaneous thermal, mass and evolving-gas analyses

Thermal analysis offers a perfect tool for the characterisation of all kinds of organic and inorganic solids and liquids. Thermodynamic transitions, thermal stability, decomposition and chemical reactions are detected and quantified with high accuracy across a broad temperature range. The thermal analysis facility in the School of Natural Sciences is unique in Australia. This capability is of interest to organisations ranging from polymer manufacturers and mining companies to insurance companies and fire brigades.

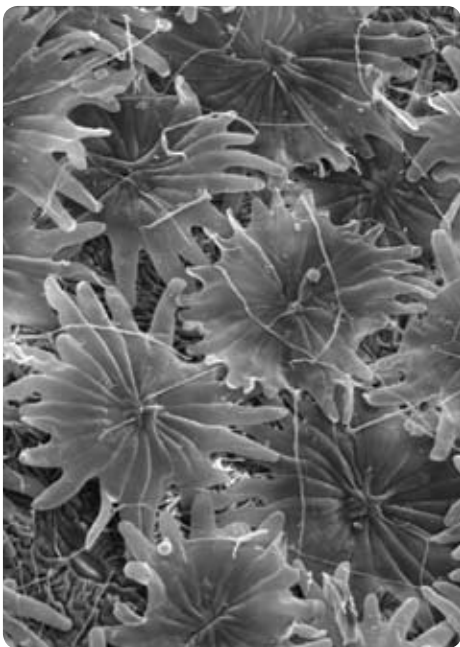
Combining thermal analysis with powerful infrared spectroscopy for gas analysis provides additional information about the composition and quantity of evolved gases: details about the chemistry behind processes that most experiments lack.

UWS's thermal analysis facilities include a simultaneous differential scanning calorimeter thermo-gravimetric analyser (DSC-TGA) coupled to an infrared spectrometer.

- » The DSC-TGA component operates from ambient temperature to 1650°C and incorporates a thermo-balance that has exceptional resolution ( $10^{-7}$  g). The vacuum-tight construction enables measurements in defined atmospheres.
- » The evolved gas analysis component is connected via a transfer line which is constantly at 200°C and a fast, highly sensitive, liquid nitrogen cooled mercury-cadmium-tellurium detector (7000–600  $\text{cm}^{-1}$  range).

These facilities can be applied to solve a broad range of R&D problems in such areas as the development of nanostructured materials (e.g. carbon nanotubes and layered silicate nanocomposites), mineralogy, biological systems, forensic science and exploration of energy sources.

UWS's expertise includes analysing the composition and structure of materials, solid-state reactions, combustion products, evaporation and out-gassing, decomposition processes, catalysis, polymerisation, specific heats of chemical processes, defining phase diagrams and glass-transitions.



### Separation and mass analysis

Liquid chromatography-mass spectrometry (LC-MS/MS) combines the physical separation capabilities of liquid chromatography with the analysis of molecule and ion mass. It enables selective and sensitive analyses of liquids used in pharmaceutical, clinical, polymer, toxicological and environmental operations.

The applications of this capability include: design, synthesis and characterisation of new stationary phases for enhanced separations; elucidation of retention mechanisms; studies of viscous fingering of solutions (particularly those of non-retained analytes and macromolecules); and development of new methodologies for analysis of complex samples including pharmaceuticals, biological materials and plastics.

The School of Natural Sciences has a well-equipped laboratory with column-packing facilities, 1D and 2D high performance liquid chromatography instruments, gas chromatography-mass spectrometry and gel permeation chromatography.

### Elemental analysis

High-performance liquid chromatography (HPLC) or laser ablation can be used to quantify atomic elements, for example to map the elements in rocks or cells.

### Atomic-scale images

An atomic force microscope enables surface topology to be imaged and can also be used to manipulate matter at the nanoscale. Scanning surfaces provides a true 3D surface profile. Samples are not damaged and biological macromolecules and even living organisms can be studied.

A scanning tunnelling microscope forms high-resolution images by scanning surfaces to detect a weak electric current flowing between the scanner tip – which is the size of an individual atom – and the surface.

### Minerals analysis

Geochemistry and structural analysis undertaken in the College includes x-raying samples and developing methods for locating significant mineral deposits by examining the geochemistry of the surrounding landforms and other geology.

### Highly sensitive characterisation

The University's inductively coupled plasma mass spectrometry facility has very high sensitivity and is suitable for characterisation of both inorganic and organometallic compounds.

Microscopy
Multi-photon confocal microscopy
Scanning electron microscopy
Atomic force microscopy
Scanning tunnelling microscopy
Spectroscopy
Fluorescence correlation spectroscopy
Fourier transform infrared spectroscopy
Raman spectroscopy
Nuclear magnetic resonance spectroscopy
Magnetic resonance imaging spectroscopy
Liquid chromatography-mass spectrometry

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