

Magnetic Resonance Node, Sydney Analytical CRF The University of Sydney

Molecular Characterisation

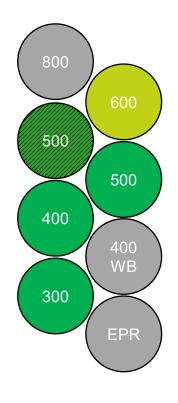
- Routine characterisation
- Structure confirmation
- Checking reaction progress
- Quantitative analysis (qNMR)
- Purity checking and quality assurance

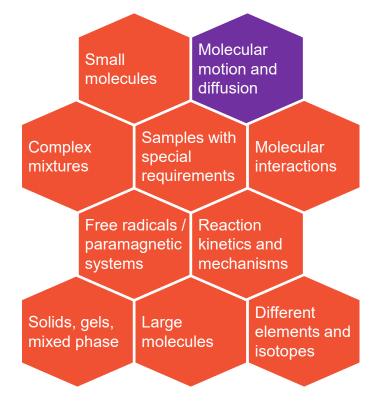
Structure Elucidation

- Determine unknown structures
- 3D solution state structure
- Multi-component analysis

High Throughput

- Short turnaround
- Batch samples
- Temperature controlled sample handling



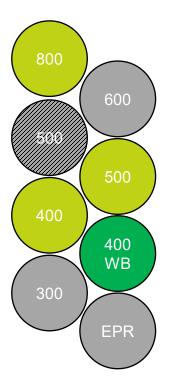


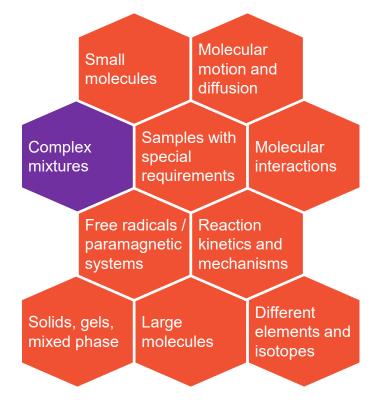
Diffusion

- Molecular motion rates
- Differentiate complex mixtures based on molecular translational diffusion

Intra- and intermolecular motion

- Picoseconds to seconds
- Molecular tumbling
- Bond rotations; restricted rotation
- Relaxation data





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Metabolomics

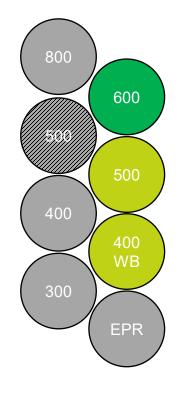
- Screening of complex biofluids (plasma, urine)
- Disease biomarkers
- Reverse engineering

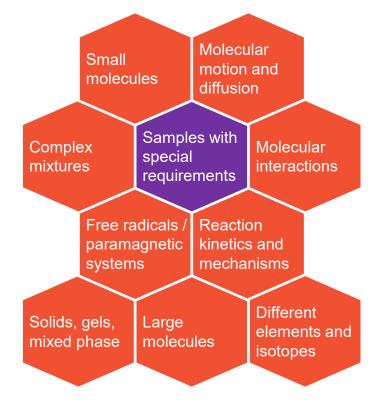
Fingerprint analysis

- Multivariate analysis of complex samples
- Impurity detection
- QA fingerprinting

Complex host-guest screening

- Drug discovery screening
- Titration studies
- Solid state





Sample preparation

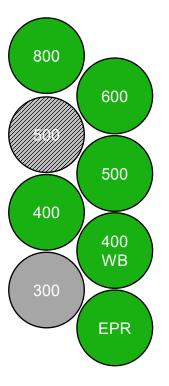
- Tube selection: Shigemi, CAV, shaped, inserts
- Sample phase: liquid, solid, gas
- Controlled atmosphere
- Deuterium-free preparation

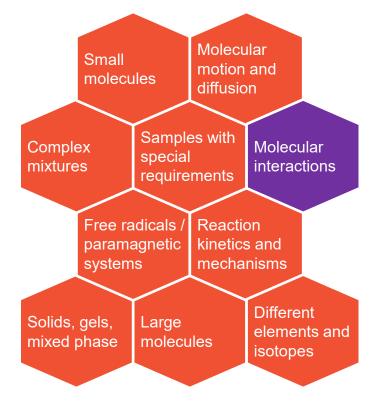
Variable temperature

- 0-40°C for cryoprobes
- -100 150°C for RT probes
- <-100 >50 °C for EPR

Controlled parameters

- Rapid acquisition
- No-lock acquisition
- Controlled atmosphere



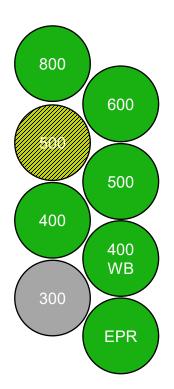


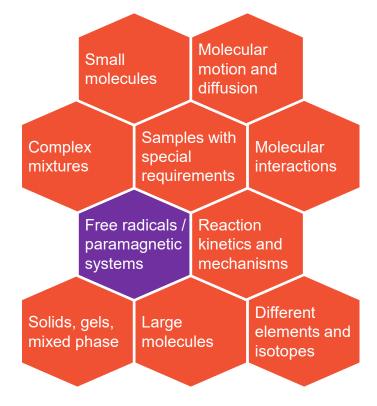
Molecular interactions

- Titration studies
- Screening studies
- Relaxation studies
- Ligand-based studies
- Host-based studies

3D structures

- Through-space interactions (HOESY, NOESY)
- 3D solution state structures
- Relative and absolute stereochemistry
- Intra- and intermolecular spatial information



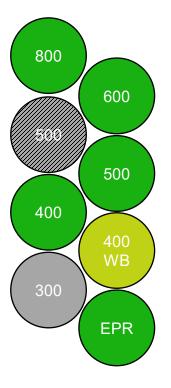


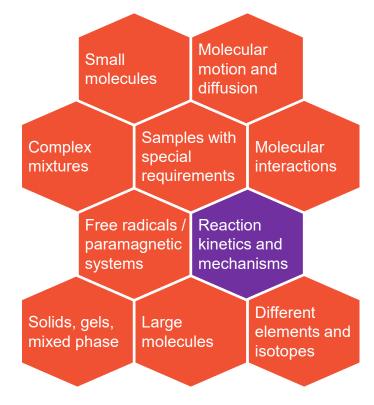
Free radicals

- Pharmaceutical analysis
- Polymer research
- Oxidative stability of foods
- Analysis of mineral qualities (diamonds)
- Battery and solar cell microstructure
- Environmentally persistent free radicals
- Oxidative stress and cell damage

Paramagnetics

- Structures of transition metal complexes
- Mechanisms of metallodrug activity
- 3D solution structure of proteins
- Protein dynamics
- MRI contrast agents
- Shift reagents for enantiomeric purity



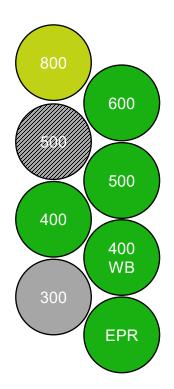


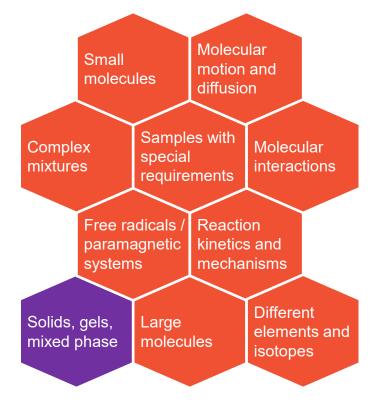
Reaction monitoring

- Reaction rates
- Reaction mechanism and intermediates
- Variable temperature controls
- Controlled irradiation of peaks of interest

Timecourse studies

- Constant time acquisition
- Variable acquisition periods
- Rapid (msec) acquisitions
- Interleaved acquisitions
- Automated processing and analysis



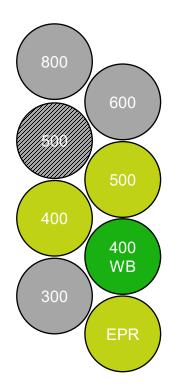


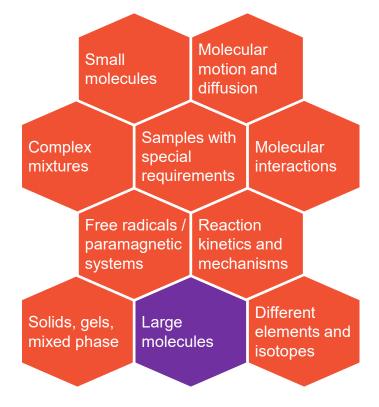
Molecular characterisation

- Identification of NMR-active nuclei
- Homogeneous and heterogeneous analysis
- Molecular weight range
- Transport across barriers

Physical characterisation

- Molecular size
- Pore size
- Surface properties
- Layer differentiation



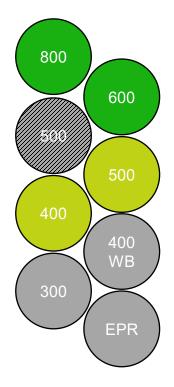


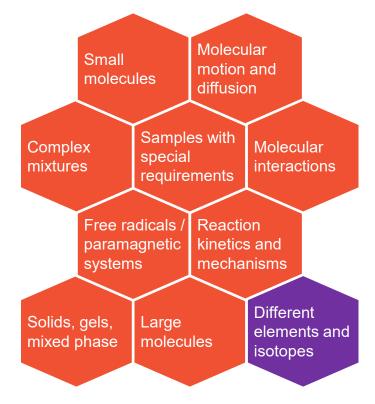
Biomolecular systems

- Protein structure determination
- Protein dynamics
- Host-guest screening
- 3D structures of proteins and protein-ligand complexes
- Protein/RNA dynamics
- Studying DNA/RNA-ligand interactions

Polymers

- Molecular weight distribution
- Side chain characterisation
- Diffusion measurements
- Confirmation of sub-unit grafting





Heteronuclear detection

- Direct detection of different nuclei
- nD experiments utilizing heteronuclei
- Isotope scrambling

Common isotopes

- Spin ¹/₂ : ¹⁹F, ¹⁵N, ³¹P, ²⁹Si, ⁷⁷Se, ¹⁹⁵Pt, ¹¹⁹Sn
- Spin > 1/2 : 2H, 11B, ⁷Li, ²⁷Al

