

Nuclear Magnetic Resonance (NMR) is a technique in which nuclear spin is manipulated to reveal molecular structure and dynamics information with atomic resolution. In the case of magnetic resonance imaging (MRI) and microscopy, a picture of the spin density can be generated with 3D pixel (voxel) dimensions down to  $\sim 10 \mu\text{m}$  in each direction. Nearly all elements have at least one isotope whose nucleus has non-zero spin (a quantum mechanical property, given the symbol  $I$ ), and thus NMR can potentially probe a wide variety of materials in gas, liquid, solution, and solid phases. The resonance frequency for each NMR-active nucleus is given by the product of the strength of the applied static magnetic field ( $B_0$ ) and an isotope-dependent gyromagnetic ratio ( $\gamma$ ),  $\omega_0 = \gamma B_0$ . Our high field NMR system operates at 11.7 T, corresponding to a  $^1\text{H}$  resonance frequency of 500 MHz. One caveat to NMR/MRI is that it is a relatively insensitive technique. For reasonable measurement times, typical limit of detection values include: low  $\mu\text{M}$  concentration for small molecules ( $<1500 \text{ Da}$ ), a few milligrams of material for large molecules in solution (e.g. proteins up to  $\sim 30 \text{ kDa}$ ), and several milligrams of material for solid samples.

$^1\text{H}$  (500 MHz) and  $^{13}\text{C}$  (125 MHz). Liquid state samples could be extended to additional frequencies with consultation. MRI can be performed under the same conditions (volumes, frequencies) as the liquid state samples. Typical MRI resolutions are  $\sim 40 \mu\text{m}$  isotropic for reasonable measurement times.

## Contact

See KNMF website or contact the KNMF User Office.

## Summary of the MR capabilities

We offer magnetic resonance spectroscopy (500, 80, 60 MHz) and imaging (11.7 T and 1 T).

### High Field

#### Magnet & console

- 11.7 T field strength
- 89 cm bore (wide-bore)
- Bruker AVANCE III console

#### RF channels

- 3x  $^1\text{H}$  /  $^{19}\text{F}$
- 2x X
- 1x  $^2\text{H}$

#### Probes

##### Micro5 microimaging probe

- 5 mm ( $^1\text{H}/^{13}\text{C}$ ), 10 mm ( $^1\text{H}$ ) saddle coil inserts
- 3 T/m X/Y/Z gradient

##### HRMAS

- 4 mm rotors (up to  $\sim 12 \text{ kHz MAS}$ )
- $^1\text{H}/^{13}\text{C}/^2\text{H}$
- Gradient

##### CapNMR

- Flow-probe, 10  $\mu\text{L}$  detection volume
- $^1\text{H}/^{13}\text{C}/^{15}\text{N}/^2\text{H}$

#### Software

- Spectroscopy: TopSpin 3.5
- Imaging: ParaVision 6.0