

# Research services

## Analytical facilities

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**Organic Mass Spectrometry.** SCRI currently has six mass-spectrometers interfaced to gas or liquid chromatographs for sample separation. The Hewlett Packard 5989B MS ENGINE GC-MS is a research-grade quadrupole instrument with electron impact, chemical (positive/negative) ionisation modes and a mass range of 2000 amu. Distributed processing software permits off-line data processing and reduces analysis times. This instrument can provide mass and structural data on a wide range of organic compounds. The analysis of volatile compounds uses a Markes International Unity and dual Ultra automated thermal desorption system (ATD) linked to a VG TRIO-1000 quadrupole gas chromatograph-mass spectrometer and permits detailed characterisation of profiles of organic volatiles generated by biological systems. The most recently purchased GC-MS instrument is a ThermoQuest TEMPUS-TOF, capable of rapid detection, characterisation and quantification in fast GC separations. The design provides parallel mass analysis with a short duty cycle at high transmission. This delivers rapid acquisition and fast sampling of narrow peaks at high sensitivity with high sample throughput suitable for metabolite profiling.

The Finnigan SSQ 710C dedicated liquid chromatography-MS instrument, with atmospheric pressure chemical ionisation (APCI) and electrospray ionisation (ESI) interfaces is suitable for samples whose high molecular weight, lack of volatility or polarity, make HPLC the preferred separation method. The multi-charge ionization mechanism of electrospray can extend the basic 2000 mass range of the instrument by a factor of about 20, giving a mass range of greater than 40,000 amu, suitable for protein analysis. Two ThermoQuest LCQ-DECA, ultra sensitive ion-trap LC-MS<sup>n</sup> systems are capable of many more scan functions than the SSQ710C spectrometer, including data-dependent full scan MS/MS, a tool of great utility in high throughput profiling.

**Isotope ratio mass spectrometry.** SCRI is equipped with modern instrumentation for stable isotope analysis of the biologically important light elements, <sup>13</sup>C,

<sup>15</sup>N, and <sup>18</sup>O in a wide range of solid, liquid and gas samples. All the instrumentation is based on continuous-flow isotope-ratio-mass spectrometers that are fully automated and operated through computer data systems, allowing a high through-put of samples, essential for many biological experiments where large data sets are required. For solid samples, the Europa Scientific Tracermass and 20-20 mass spectrometers are interfaced to Roboprep CN and ANCA-NT SL combustion sample converters. A Roboprep G+ gas purification unit is used for gas analysis. Analytical protocols are devised to minimise sample preparation and fully exploit the automation.

**Gas chromatography.** Within the MRS Lipid Analysis Unit and SCRI, gas chromatographs (HP 5890 and Agilent 6890 systems) are used primarily for fatty acid, sterol and leaf wax analysis but are also used for developing separation methods for GC-MS studies. Laboratory facilities are available for extraction and derivatisation of a wide range of samples.

**Quality assurance.** Within SCRI, the Gas Chromatography-Mass Spectrometry Laboratories, Stable Isotopes Facility and Lipid Analysis Unit of MRS Ltd, operate a formal Quality System certified to BS EN ISO 9001 by SGS Yarsely International Certification Services Ltd. The certification standard was upgraded from ISO 9002 to ISO 9001 in August 1999, and now includes the design and conduct of research within its scope.



Figure 1. ThermoQuest TEMPUS-TOF.