Making ideas work for a better world

CHEMISTRY FACILITIES

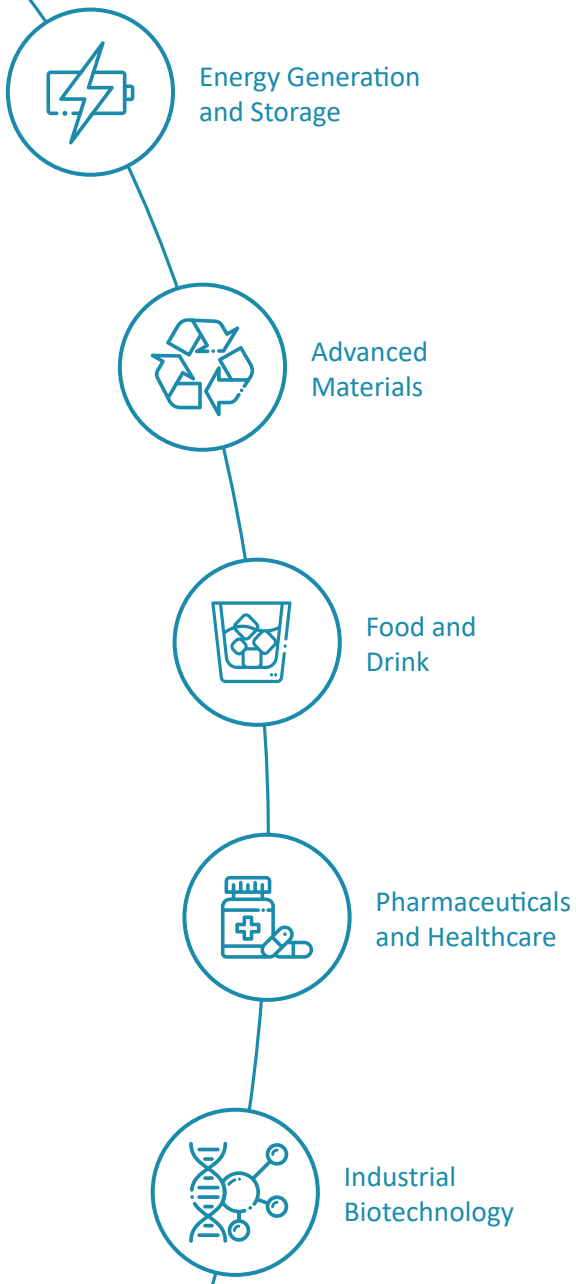
THE UNIVERSITY of EDINBURGH

EDINBURGH INNOVATIONS

THE UNIVERSITY of EDINBURGH
School of Chemistry

Discover

how the University of Edinburgh's world class chemistry facilities can support your projects. We have a full range of cutting-edge analytical and research equipment available to help solve your problems.



Mass Spectrometry Facility

TECHNOLOGIES AVAILABLE

The Mass Spectrometry Facility at the School of Chemistry is home to The Scottish Instrumentation and Resource Centre for Advanced Mass Spectrometry (SIRCAMS), one of the most advanced mass measurement facilities in Europe. The facility houses a wide range of mass spectrometry platforms and has expertise in the mass analysis of a diverse range of analytes – from small molecules to complex biomolecular systems. The facility has a long history of collaborating with academic and industrial groups worldwide and offers expertise in mass spectrometry service, training and consultancy.

EQUIPMENT AVAILABLE

- A range of LC-MS and GC-MS platforms
- Two FT-ICR MS instruments
- Ion-mobility equipped Q-Tof instruments (Waters)
- MALDI-ToF/ToF (Bruker Daltonics)

SERVICES AVAILABLE

- Small Molecule Characterisation using accurate mass determination and tandem mass spectrometry. LC-MS and GC-MS capabilities
- Complex Mixture Analysis. Ultra-high-resolution mass analysis for the chemical profiling of complex chemical mixtures such as petrochemicals and fuels, environmental samples, and for food and beverage analysis
- Biomolecular Mass Spectrometry including:
  - protein intact mass determination
  - protein PTM characterisation
  - automated protein-ligand screening
  - structural mass spectrometry analysis
- Mass Spectrometry Imaging. Untargeted spatial imaging of metabolites from biological tissue sections using MALDI imaging techniques at high mass resolution

Industrial Themes: Pharma and healthcare, Industrial biotechnology, Food and drink, Chemical process R&D.

For more information contact SoC-Facilities@ei.ed.ac.uk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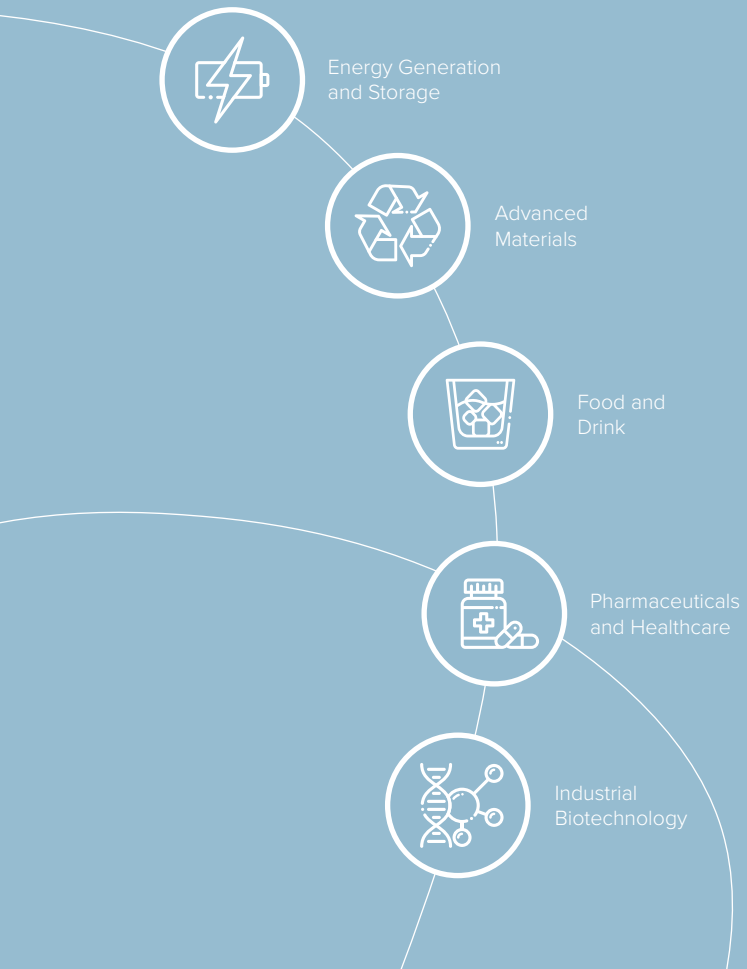
Actively Shielded

Nuclear Magnetic Resonance Spectroscopy Facility



TECHNOLOGIES AVAILABLE

The Nuclear Magnetic Resonance Spectroscopy Facility at the School of Chemistry is home to The Scottish High Field NMR Centre, housing a liquid/solid-state 800 MHz NMR spectrometer, the highest field available in Scotland. The facility is also equipped with a wide range of highly sensitive specialised NMR spectrometers, with expertise in analysis of a diverse range of systems – from small molecules to biomacromolecules and complex mixtures.

EQUIPMENT AVAILABLE

- 600 MHz Bruker AVANCE IIID 4-channel instrument with a quadruple-resonance ^{1}H, ^{19}F, ^{13}C, ^{15}N, QCI-F helium CryoProbe maximising sensitivity of ^{1}H and ^{19}F, enabling multi-resonance experiments from -40^{0} to $+150^{0}C$
- 500 MHz Bruker AVANCE NEO with a BBO H/F CryoProbe maximising sensitivity of X nuclei detection, from -40^{0} to $+150^{0}C$
- 500 MHz Bruker AVANCE IIID with a BBO H/F CryoProbe Prodigy probe for fast acquisition of nuclei from ^{15}N to ^{31}P
- 400 MHz Bruker AVANCE NEO 2-channel console with BBO room temperature probe: -150^{0} to $+150^{0}C$
- 300 MHz Bruker AVANCE III solid-state NMR spectrometer with a 4 mm N-P/H DVT probe for acquisition of ^{13}C and X nuclei spectra

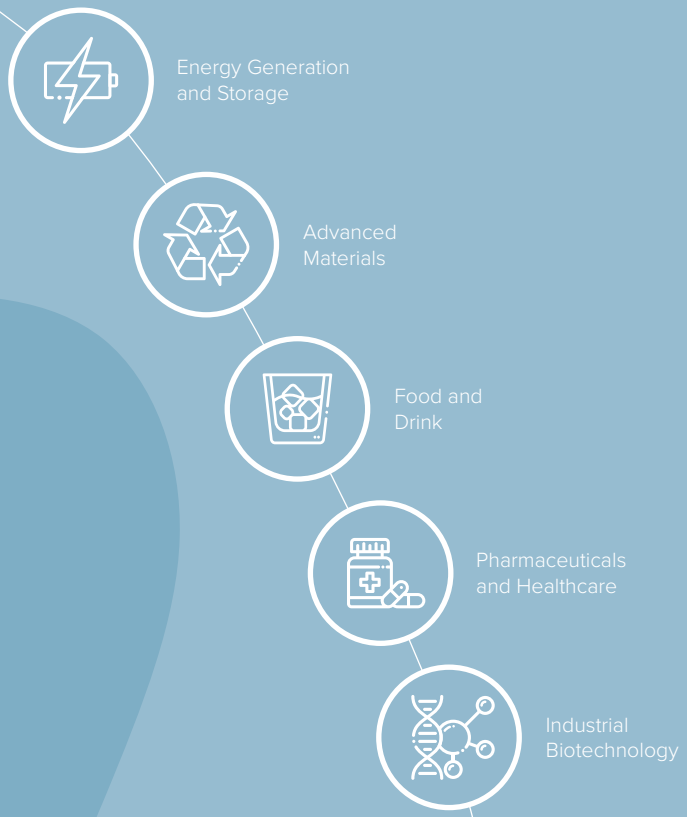
SERVICES AVAILABLE

- Small Molecule Structure Determination including organic molecules and inorganic complexes using multinuclear NMR
- Complex Mixture Analysis using 1H NMR spectroscopy of complex matrices including biofluids, foods, beverages or environmental samples. Chemical profiling, multivariate and quantitative analyses
- Biomolecular NMR Spectrometry including:
  - acquisition of 3D triple-resonance experiments of isotopically labelled proteins for structure determination
  - ligand screening, both macromolecule- and ligand-focused
- Advanced Characterisation of:
  - low concentration small molecules on the microgram scale
  - reaction monitoring and elucidation of reaction mechanisms

For more information contact SoC-Facilities@ei.ed.ac.uk


Ascend 500
Power Supply
Power Control
Mains
100%
75

Inductively Coupled Plasma Spectrometry Facility



TECHNOLOGIES AVAILABLE

The Inductively Coupled Plasma (ICP) spectrometry at the School of Chemistry houses a wide range of ICP platforms and has expertise in the qualitative and quantitative analysis of elements in a diverse range of matrices – from environmental samples through to small molecules and complex biomolecular systems. The facility has a long history of collaborating with academic and industrial groups worldwide and offers expertise in ICP optical and mass spectrometry. In addition to service provision, the facility also delivers training opportunities and consultancy projects.

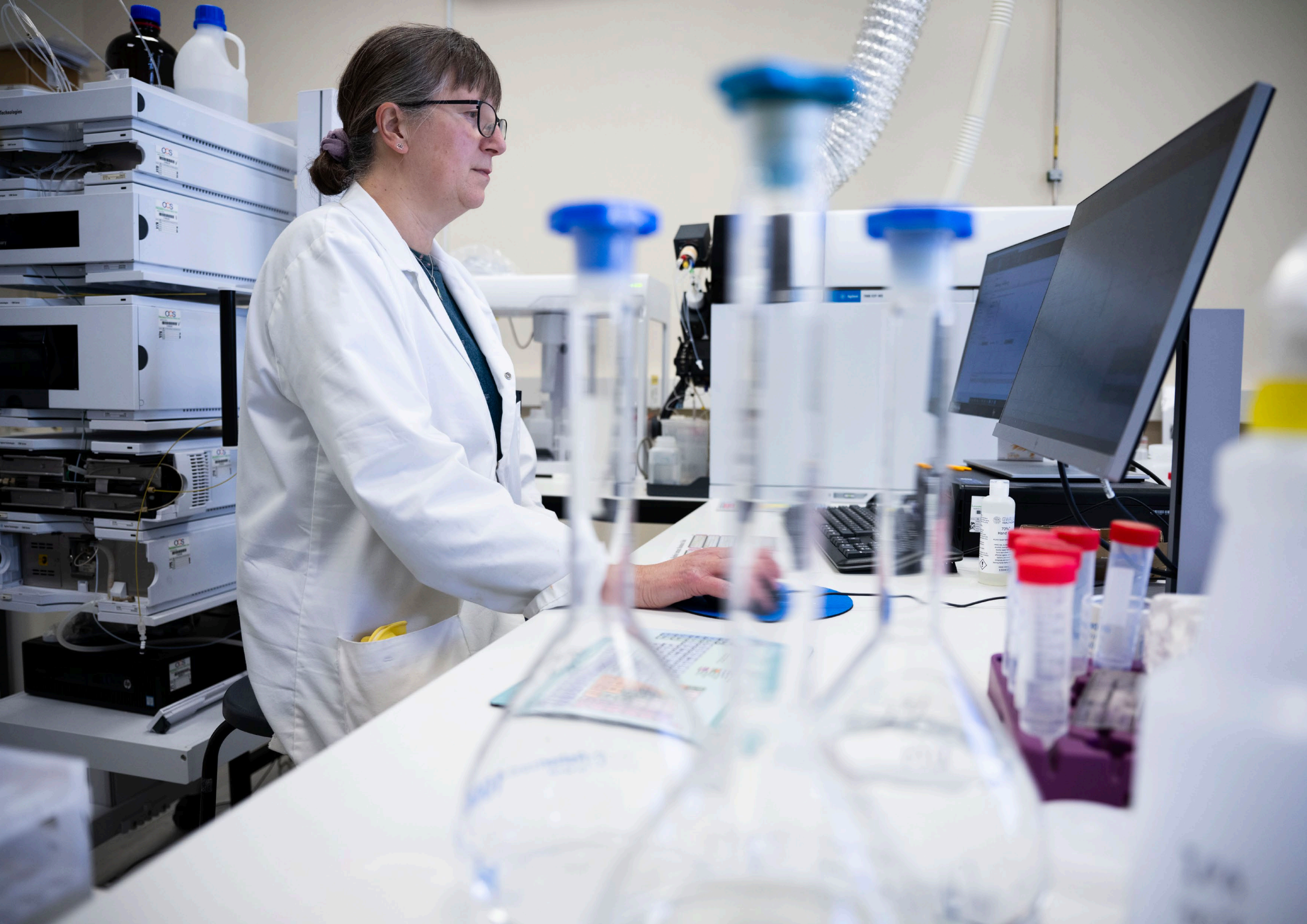
EQUIPMENT AVAILABLE

- Inductively Coupled Plasma Optical spectrometry (ICP-OES, Perkin Elmer 8300DV) for the analysis of analytes in the range 0.1-1000 mg l-1
- Inductively Coupled Plasma Mass spectrometry (ICP-MS, Single Quad Agilent 7900 and a Multi-quad Agilent 8900) for the analysis of analytes in the range 1 ng l-1-100 mg l-1
- Inductively Coupled Plasma Mass spectrometry (ICP-MS, Multi-quad Agilent 8900) for the analysis of analytes in the range 0.001 ng l-1-100 mg l-1
- Microwave digestion (MARS6, CEM) and hot plates, for the digestion of solid matrices

SERVICES AVAILABLE

- The ICP instruments offer ultra-high-resolution analysis for the chemical profiling of analytes (metals and some non-metals) in complex matrices including: environmental samples (e.g. soil and plant digests, waters), small and complex molecules (e.g. catalysts, metallo-proteins, nano-particles, blood plasma/serum), chemical engineering processes (e.g. Stainless steel vessels displaying corrosion, unknown precipitates forming in processing lines) and for food and beverage analysis (e.g. food additives)
- Data analysis, interpretation, and visualisation using a range of software solutions and multivariate analyses

For more information contact SoC-Facilities@ei.ed.ac.uk



Pyrochemical Research Laboratory

Energy Generation and Storage

TECHNOLOGIES AVAILABLE

The Pyrochemical Research Laboratory (PRL) is an open access national user facility, established to provide academic, public, and private sector organisations with access to state of the art equipment to support world leading research, at the interface between high temperature, inert/controlled environments and analytical measurements.

SERVICES AVAILABLE

The PRL is ideal for the development of pyrochemical reprocessing and a wider range of associated research areas, such as; molten salt and metal systems and extreme condition applications, e.g. high temperature electrical batteries, electrolysers, thermal storage, heat transfer, thermochemical reactions, electrochemical processes at high temperature and/or inert environments, and many others.

EQUIPMENT AVAILABLE

Gloveboxes

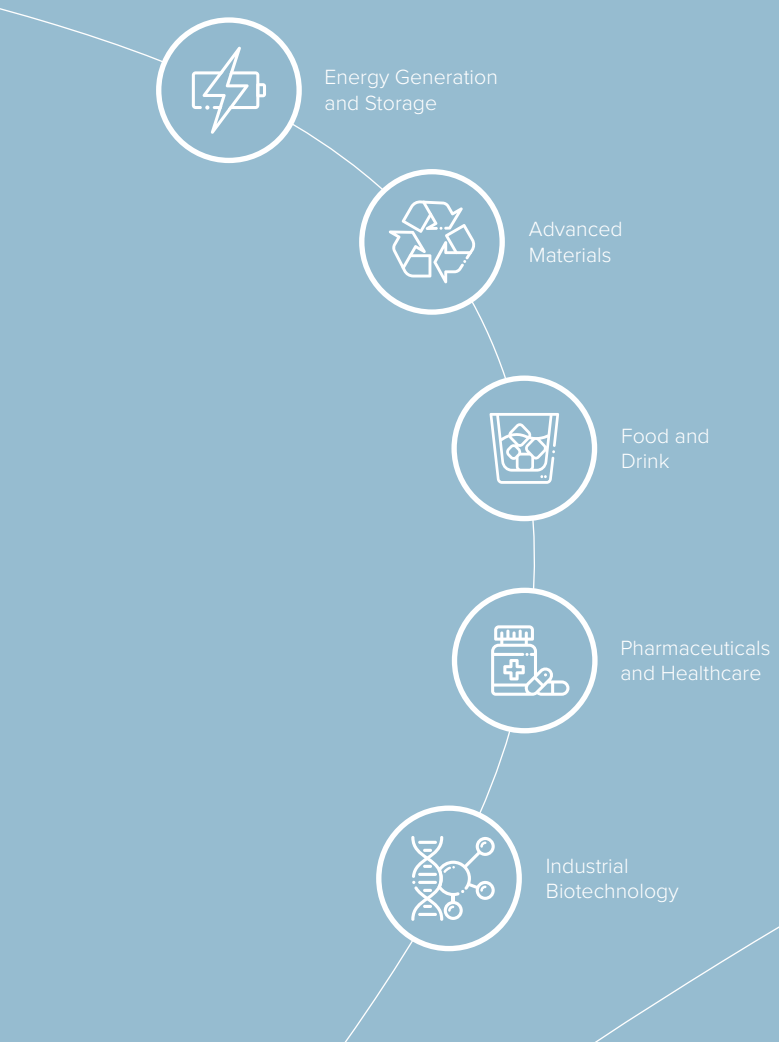
- Glove Boxes X5 - MBRAUN MB200MOD (< 0.1 ppm H_2O and O_2)
- Vacuum Oven X2 - MBRAUN - MB VOH 250 ^0C $3x10^{-2}$ mbar

Within Gloveboxes

- Potentiostats
  - AUTOLAB with MUX and FRA module X3
  - High current module AUTOLAB X3 (20 A)
- Tube Furnace x 5 - Severn Thermal TF2260 with CU2260 control Unit (up to 1200 °C)
- Optical Tube furnace - Severn Thermal TF2256 with CU2260 control Unit (up to 1100 °C)
- Well Furnace - Severn Thermal TF2042-CU2042B - 3 heating zones (up to 1200 °C)
- TGA/DSC (STA) - Perkin Elmer STA 6000 (up to 995 °C)
- ONH Analyer - ELTRA ELEMENTAL ANALYZERS - ONH 2000
- Spectroscopy - Ocean Optics
  - UV-VIS-NIR DH-2000-BAL UV
  - HL-2000-FHSA
  - Raman Laser - 0811A100-B FATBOY
- Mortar Grinder - Fritsch PULVERISETTE 2 finesse 10 to 20 µm
- Glove box Integrated Microscope and camera - Leica M60 KL1600 light source
- Weighing Balances x3 120 g to 0.1 mg - Sartorius - Practum124-1S
- Rheometer – Anton Parr MCR 502 WESP with CTD 1000 (upto 1000 °C)

For more information contact SoC-Facilities@ei.ed.ac.uk

Raman Spectroscopy



TECHNOLOGIES AVAILABLE

The combination of a Raman and/or IR spectrometer with an optical microscope allows spectra of small objects to be measured with high spatial resolution (up to few micrometres). Raman and Infrared spectroscopy provides a non-destructive way of characterisation and surface analysis of a wide-ranging number of materials and systems. Both methods are a vibrational spectroscopy technique for identification and analysis of molecular species and crystalline structures. Raman spectroscopy and IR spectroscopy provide information complementary to each other.

These techniques can be successfully applied in areas such as;

- Materials science, Nanotechnology, Semiconductors, Geosciences, Pharmaceutical and Biosciences, microplastics analysis etc
- Integration of Raman and IR modules on one microscope allows potentially to analyse the same sample area with both techniques

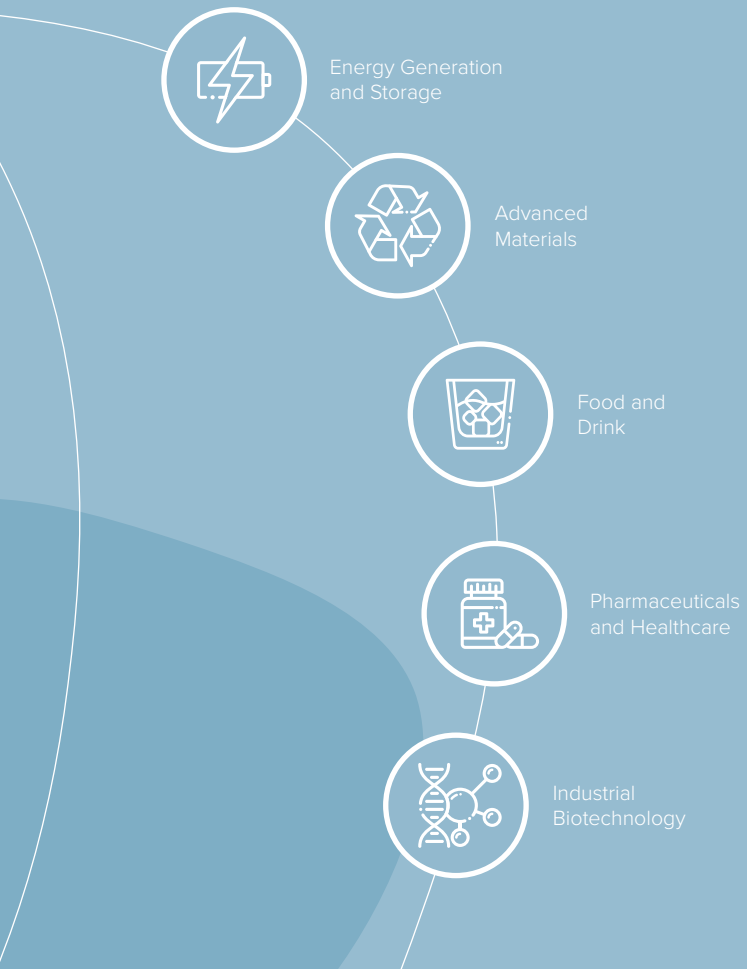
EQUIPMENT AVAILABLE

Renishaw inVia Raman microscope is equipped with optics for working with 3 laser excitation lines (488, 514 and 785nm); measurements can be taken in the range of 100 – 4000 cm-1 with spectral resolution on the level of 1 wavenumber. Leica microscope with a set of objectives from 5x to 100x with various working distances (1-12mm) provides visual observation of a sample up to magnification level of 1000 times using digital camera. Microscope is equipped with motorised stage (1um in X-Y or Z directions) and can perform precise positioning of the sample, depth profiling and/or mapping of the specimens. Spatial resolution depends on the objective used and can be < 2 micrometres for objectives with high numerical aperture.

The microscope is combined with a Smiths IlluminatIR FTIR unit, which allows middle IR measurements (the spectral range of 650 - 4000 wavenumbers with spectral resolution of 4 wavenumbers) in reflection mode with 2 types of objectives – non-contact All Reflective Objective (x 10) and diamond coated ATR IR objective (x 36). Best spatial resolution - 12 microns.

For more information contact SoC-Facilities@ei.ed.ac.uk

Atomic Force Microscopy



TECHNOLOGIES AVAILABLE

Scanning probe microscopy (SPM) is an imaging technique which provides a 3-D and structural analysis of surfaces from mesoscopic scale to atomic resolution. SPM is based on scanning a surface with a probe/tip, during which information about surface topography, electronic structure or interaction force between surface and probe can be obtained.

Atomic force microscopy (AFM) is a high-resolution type of SPM, which provides surface topography profiles on the order of fractions of a nanometer.

It is well suited for measurements of surface characteristics such as topography, conductivity, adhesive force, nanomechanical and frictional properties of a sample. This makes it a useful tool for a wide range of applications and samples.

Samples can include:

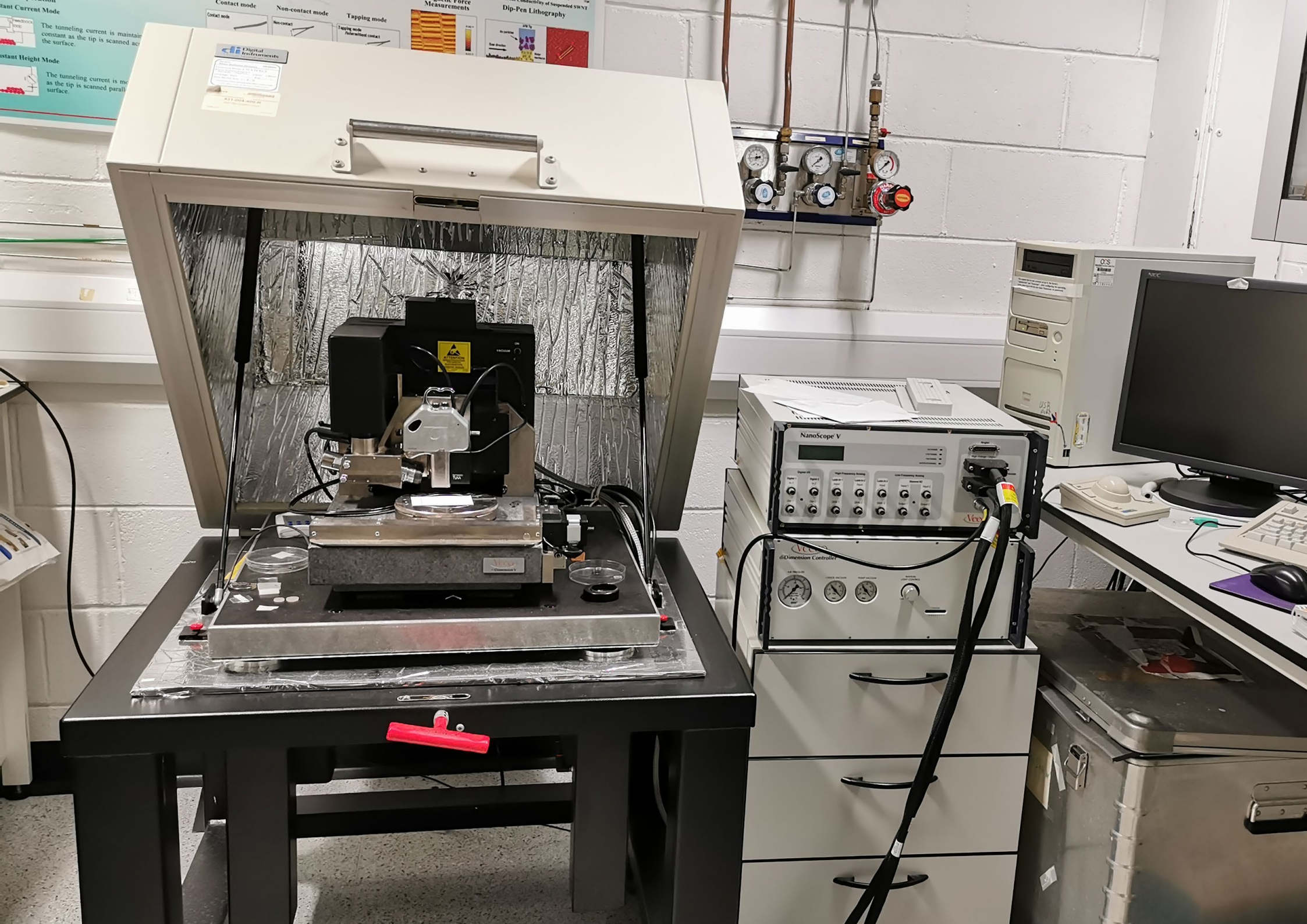
- Semiconductor wafers (max wafer size 200mm)
- Lithography masks
- Magnetic media
- CDs/DVDs
- Biomaterials (e.g. conformation properties of proteins and DNA)

SERVICES AVAILABLE

The instrument can perform:

- AFM surface topography measurements in contact and/or tapping mode
- Magnetic force microscopy
- Force spectroscopy experiments (e.g. adhesive surface maps)
- Tunnelling AFM (TUNA) (Bias ±12 V, current sensitivity 1 pA - 10 nA) – conductivity maps
- Manipulation of objects in nanometer and micrometer scale on substrates. Max. scan size 100 microns

For more information contact SoC-Facilities@ei.ed.ac.uk


Contact mode
Non-contact mode
Tapping mode
Force Measurements
Dip-Pen Lithography
Digital Instruments
NanoScope V
dimension Controller

Single Crystal X-ray Diffraction

TECHNOLOGIES AVAILABLE

Structural characterisation by single crystal X-ray diffraction is a major analytical and research tool in chemistry providing both definitive sample identification and detailed structural analysis. The School of Chemistry at The University of Edinburgh offers a complete single crystal diffraction service to our industrial partners, through the provision of dedicated analysis, interpretation and consultancy services.

EQUIPMENT AVAILABLE

- Rigaku Oxford Diffraction SuperNova diffractometer. Sample temperature range 80 to 500 K
- Bruker D8 Venture offering temperatures to 28 K

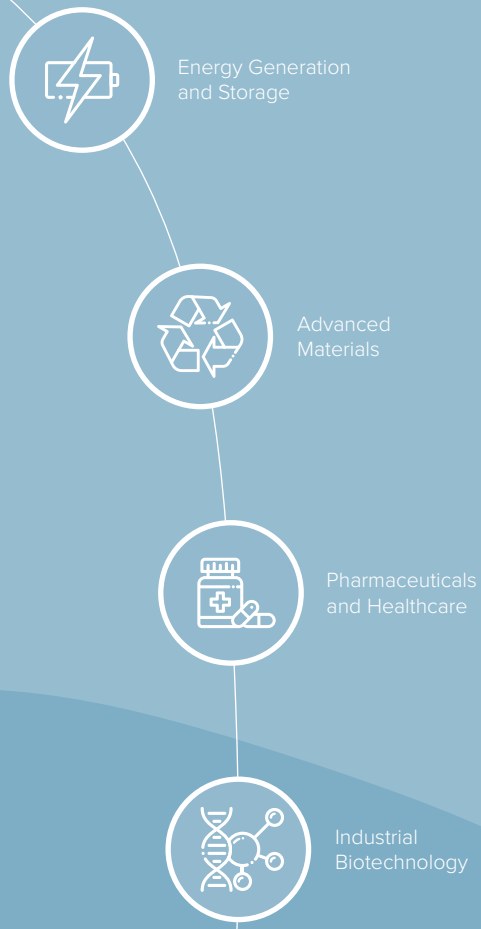
SERVICES AVAILABLE

- We handle many types of small molecule samples, ranging from small organic molecules, through transition metal complexes to lanthanide and actinide clusters
- Ideal for detailed study of organic organometallic complexes
- Provides definitive chemical identity, bond dimensions, molecular conformation and crystal packing analysis
- Air & moisture sensitive, and small or weakly diffracting crystals are easily handled

For more information contact SoC-Facilities@ei.ed.ac.uk


X-RAY Mo
X-RAY Cu
SHUTTER OPEN
Oxford Diffraction
SuperNova™
DELL

Powder X-ray Diffraction



TECHNOLOGIES AVAILABLE

The Powder X-Ray Diffraction can help you understand your crystalline materials, their structure, stability and how these properties might change on varying temperature. PXRD has been used for projects in a range of scientific disciplines: such as low temperature phase transitions in magnetic materials, materials with negative thermal expansion, cement minerals with variable hydration states, and phase change materials used for energy storage.

EQUIPMENT AVAILABLE

- Bruker D8 X-ray Benchtop Powder Diffractometer set up in transmission geometry - useful for measuring low absorbing materials, such as organic molecules and pharmaceuticals
- Rigaku Smartlab powder X-ray diffractometer with HyPix3000 advanced detector technology - high resolution powder X-ray diffraction instrument which is optimised for variable temperature studies.The diffractometer is very adaptable and we have the following attachments:
- High temperature furnace for collection of PXRD data while heating the sample, the temperature can be adjusted from room temperature to 1500 °C

SERVICES AVAILABLE

We offer an X-ray diffraction analysis service on a wide range of powdered crystalline samples. It is rapid, non-destructive and is most often used in phase identification, monitoring the effect of changing temperature in situ on the material studied, polymorphism studies or even demonstrating that a sample is amorphous.

- Low temperature PheniX (Oxford Cryosystems) for collection of PXRD data while cooling the sample. The PheniX can cool the sample from room temperature to 12 K (-261.15 °C)
- X-ray DSC attachment which simultaneously heats the sample (25-350 °C), measures a DSC curve and collects PXRD patterns. This attachment also serves as a humidity chamber so the humid environment of the sample can be varied during data collection. We are the only facility in the UK with this attachment and capability

For more information contact SoC-Facilities@ei.ed.ac.uk


X-RAYS ON

Edinburgh Single-Molecule Biophysics Laboratory

TECHNOLOGIES AVAILABLE

The Edinburgh Single-Molecule Biophysics (ESMB) Laboratory houses a range of single-molecule and super-resolution microscopes enabling the visualisation and characterisation of individual molecules with a high spatial resolution (down to 20 nanometres). We have both commercial and home-built systems, allowing the imaging of fluorescent molecules in the full visible spectrum in vitro, in live/fixed cells, and in tissue. These technologies are particularly useful for biomedical research, and we routinely characterise molecules in human biofluids and tissue.

EQUIPMENT AVAILABLE

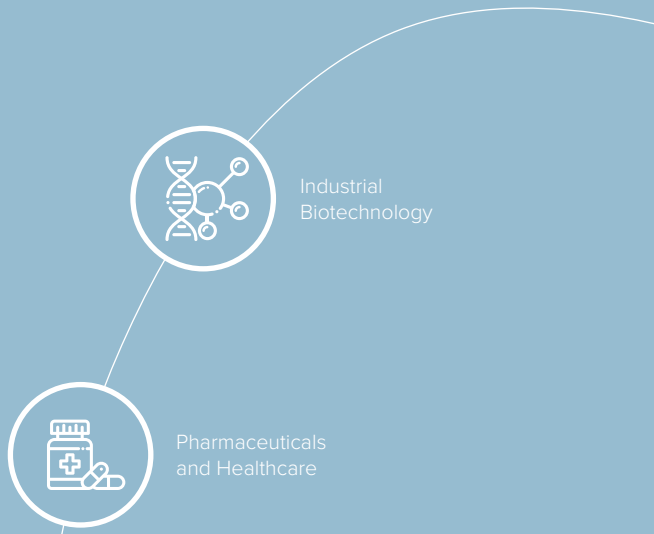
- Single-molecule confocal microscope ("single-molecule flow-cytommetry") equipped with 405/488/515/635 nm excitation. FRET measurements, Fluorescence Correlation Spectroscopy (FCS), single-molecule burst analysis
- Home-built TIRF microscope built around a Nikon Ti2 equipped with 405/488/515/561/638 nm excitation. Live cell imaging chamber. Single-molecule detection and particle tracking, super-resolution microscopy (dSTORM/PALM/DNA-PAINT/LIVE-PAINT)
- Oxford Nanoimager equipped with 405/488/561/635nm excitation
- Fluorescence Lifetime Imaging Microscope (FLIM)

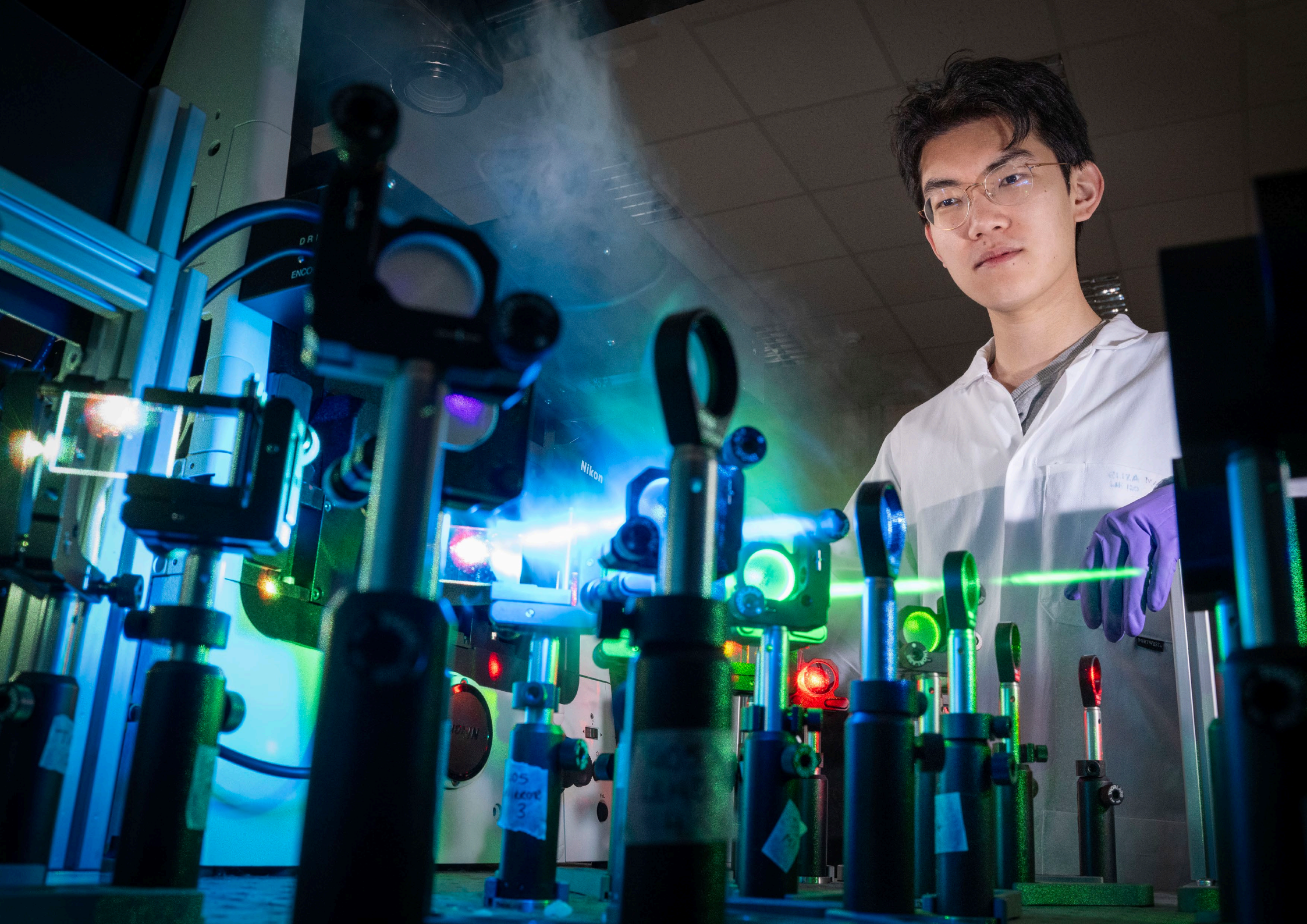
SERVICES AVAILABLE

We image molecules in a range of biological samples, and can provide custom detection and can offer custom detection and characterisation solutions.

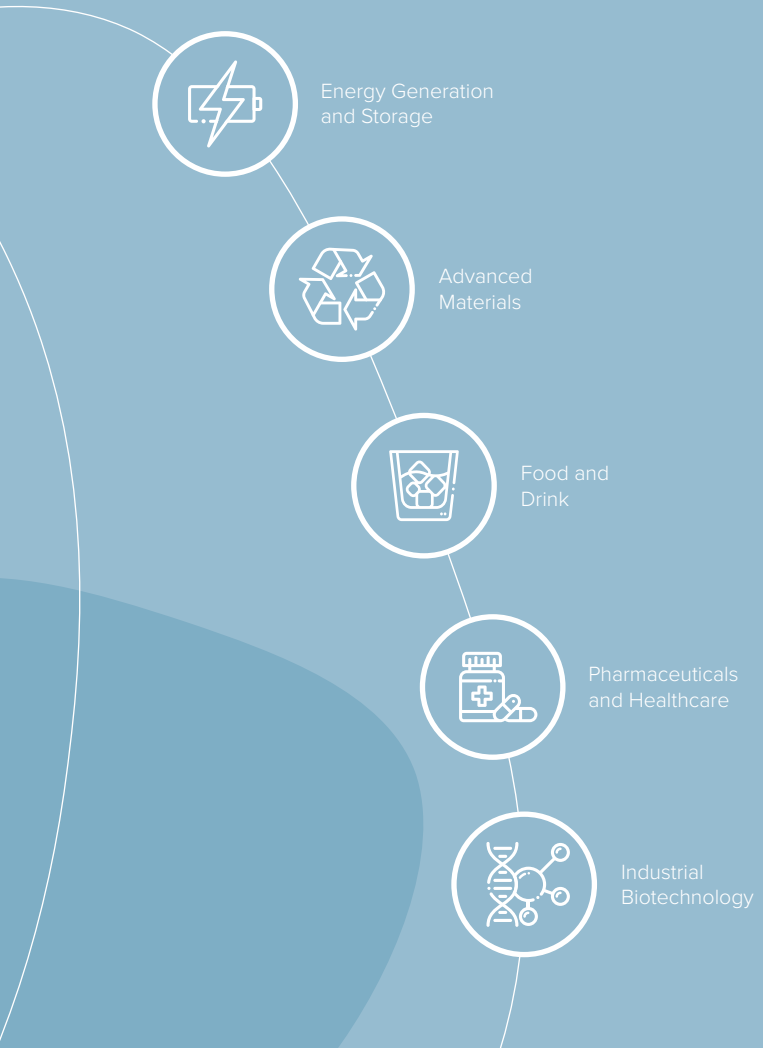
We can also provide data analysis, interpretation, and visualisation using a range of software solutions analyses.

For more information contact SoC-Facilities@ei.ed.ac.uk




Nikon

Analytical Chemistry Instrument Suite



SERVICES AVAILALBLE

The Analytical Chemistry Instrument Suite is a new hands-on training facility to support student development in analytical chemistry. We are also keen to offer training and support to industry researchers.

EQUIPMENT AVAILABLE

Shimadzu Nexera UHPLC: equipped with a Photo Diode Array analyser for rapid quantitative analysis and separation of organic compounds.

Shimadzu i-Series LC-2060 UHPLC: equipped with a Photo Diode Array analyser (UHPLC-PDA) for rapid quantitative analysis and separation of organic compounds.

Shimadzu QP2020NX GC-MS: for quantitative analysis and identification of organic compounds.

Shimadzu 2010 GC-FID: Fitted with a Flame Ionisation Detector for quantitative analysis and separation of organic compounds.

Bruker S2 PUMA EDXRF: Performs multi-element analysis, measuring and monitoring elements in samples with Energy-Dispersive X-Ray Fluorescence (EDXRF).

Rigaku Miniflex XRD: New sixth generation Miniflex benchtop X-ray diffractometer

ThermoScientific Phenom G6 SEM: Benchtop Scanning Electron Microscope for qualitative assessment of solid-state structures and now equipped with an Energy Dispersive X-ray Spectrometer to collect spatial information on the elemental composition of samples.

BMG Labtech Cryostar UV Plate Reader: Measurement of fluorescence and UV/vis from microplates.

Cytiva Akta Go FPLC: Compact liquid chromatography system to support Fast Protein Liquid Chromatography and protein purification.

Edinburgh Instruments FS5 Fluorimeter: fluorescence spectrometer allowing lifetime measurements in the range < 150 ps - 10 µs to be accurately measured.

Applied Photophysics Chirascan VX: Circular Dichroism instrumentation for studying chiral molecules of all types and sizes.

Setline STA: Simultaneous Thermal Analysis instrumentation. Combines Thermogravimetric Analysis and Differential Scanning Calorimetry for more complete thermal characterization.

Thermo Scientific Nicolet Summit X FTIR: Infrared spectroscopy on a wide range of samples via either Attenuated Total Reflection or Transmission modes.

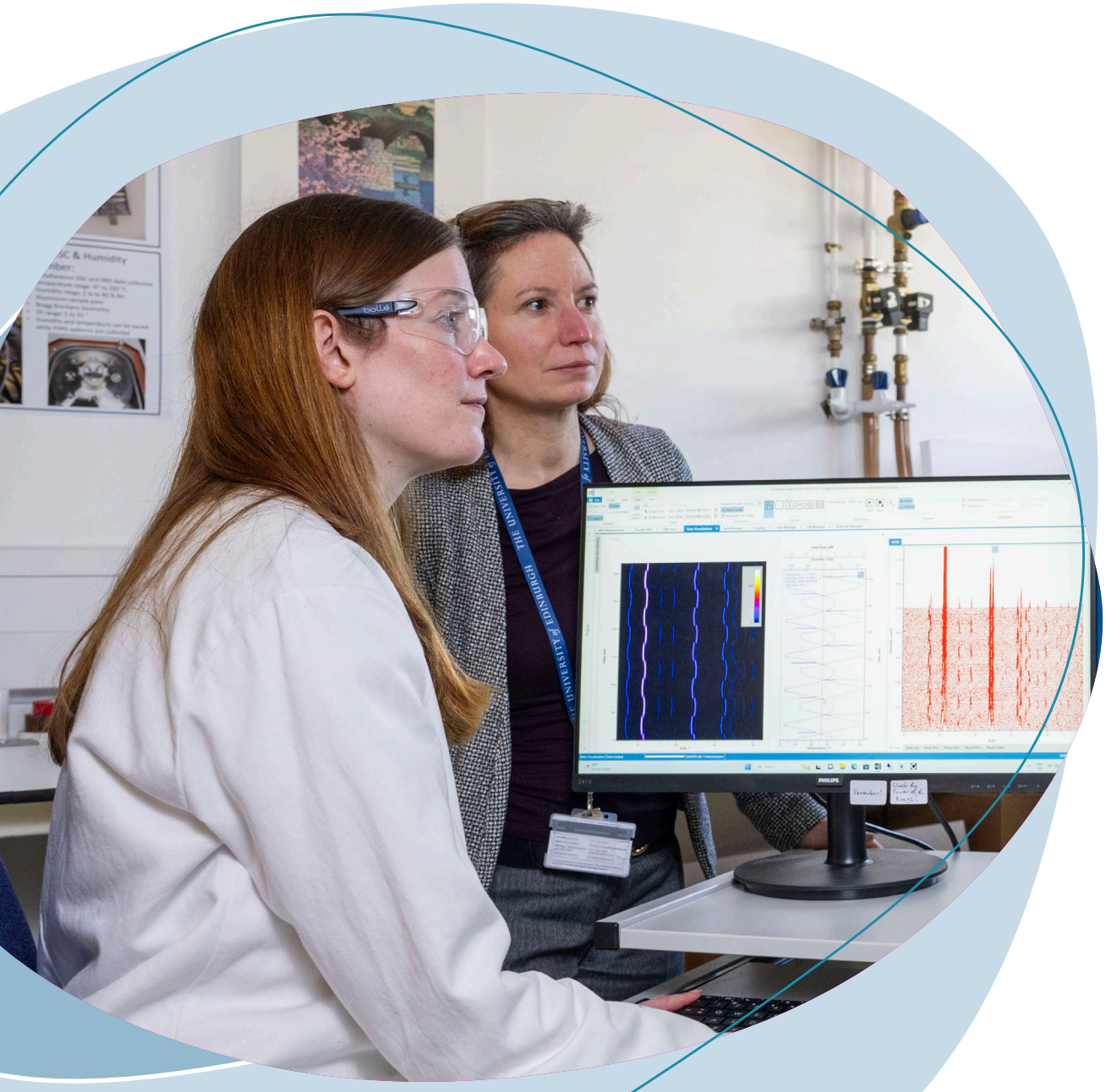
Teledyne ACCQPrep: Preparative and semi-preparative scale High Performance Liquid Chromatography (HPLC). Currently available in reverse phase only.

For more information contact SoC-Facilities@ei.ed.ac.uk


AOC-6000 Plus
SHIMADZU
THE UNIVERSITY of EDINBURGH
School of Chemistry

FACILITY	SERVICES	Energy Generation and Storage	Advanced Materials	Food and Drink	Pharmaceuticals and Healthcare	Industrial Biotechnology
MASS SPECTROMETRY FACILITY	• Small molecule characterisation • Complex mixture analysis • Biomolecular Mass Spectrometry • Mass Spectrometry Imaging	✓	✓	✓	✓	✓
NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY FACILITY	• Determination of organic molecules and inorganic complexes • Complex Mixture Analysis including biofluids, foods, beverages or environmental samples • Chemical profiling, multivariate and quantitative analyses and reaction mechanisms • Biomolecular NMR Spectrometry including structure of isotopic labelled proteins • Access to liquid/solid state high sensitivity and high resolution 800 MHz NMR spectrometer	✓	✓	✓	✓	✓
INDUCTIVELY COUPLED PLASMA SPECTROMETRY FACILITY	• Ultra High resolution analysis of analytes • Metals and non metals in complex matrices • Environmental samples • Small and complex molecules • Food and beverage analysis	✓	✓	✓	✓	✓
PYROCHEMICAL RESEARCH LABORATORY	• Analytical measurements at the interface between high temperature and inert/controlled environments • Development of pyrochemical reprocessing • molten salt and metal systems • extreme condition applications	✓	—	—	—	—
RAMAN SPECTROSCOPY	• Non-destructive: It requires minimal sample preparation and can analyze solids, liquids, and gases without damaging the sample • Identification: Each substance produces a distinct Raman spectrum, enabling rapid and accurate identification of materials • Applications: Widely used in materials science, pharmaceuticals, forensics, and biomedical research for quality control, process monitoring, and structural elucidation	✓	✓	✓	✓	✓

FACILITY	SERVICES	Energy Generation and Storage	Advanced Materials	Food and Drink	Pharmaceuticals and Healthcare	Industrial Biotechnology
ATOMIC FORCE MICROSCOPY	• AFM surface topography measurements in contact and/or tapping mode • Magnetic force microscopy • Force spectroscopy experiments (e.g. adhesive surface maps) • Tunnelling AFM (TUNA) (Bias ±12 V, current sensitivity 1 pA - 10 nA) – conductivity maps • Manipulation of objects in nanometer and micrometer scale on substrates • Max. scan size 100 microns	✓	✓	✓	✓	✓
X-RAY DIFFRACTION	• Characterisation of materials for polymorphism studies or to demonstrate if the sample is amorphous (e.g. in fire safety of cladding materials) • Monitoring the effects of a particular treatment of the material (e.g. sustained heating, cooling or pressure effects on energy storage materials and battery technologies) • Study the structure of crystalline materials, their stability and how these properties change on varying temperature (used in magnetic materials and cement industries) • Rapid, non-destructive XRD analysis for phase identification (mining industries, environmental agencies)	✓	✓	—	✓	✓
EDINBURGH SINGLE-MOLECULE BIOPHYSICS LABORATORY	• A range of single-molecule and super-resolution microscopes • Imaging molecules in biological samples with high spatial resolution • Custom detection and characterisation solutions • data analysis, interpretation, and visualisation using a range of software solutions	—	—	—	✓	✓
ANALYTICAL CHEMISTRY INSTRUMENT SUITE LABORATORY	• Training and support to industry researchers in analytical chemistry on a wide range of instrumentation	✓	✓	✓	✓	✓



How we can work with you:

Our facilities are available to for-profit and non-profit organisations

- Our standard facility access agreements are simple – you retain ownership of your samples and intellectual property. We retain ownership of any modifications or improvements to our methods / protocols, which may be developed to help you get the answers or information you need
- Our facility access, services and consultancy agreements provide added value, combining sample analysis with data interpretation by skilled professional staff
- We can be costed into collaborations and partnerships

Get in touch

This brochure lists some of the University of Edinburgh's cutting-edge facilities that are available to enable and accelerate innovation.

Edinburgh Innovations can help facilitate the best solution to your research demands whether it be a routine or bespoke service.

If you have any enquires related to access and use of facilities please contact:

Cameron Chalmers

Consultancy manager
School of Chemistry
Edinburgh Innovations
07386 659384

SoC-Facilities@ei.ed.ac.uk

- Energy Generation and Storage
- Advanced Materials
- Food and Drink
- Pharmaceuticals and Healthcare
- Industrial Biotechnology

THE UNIVERSITY of EDINBURGH

EDINBURGH INNOVATIONS

Edinburgh Innovations is the University of Edinburgh's commercialisation service.

We benefit society and the economy by helping researchers, students and industry drive innovation. We seek opportunities, we build partnerships for mutual benefit, we make the journey easy, and we add value at every stage.

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