

**EPSRC**

Engineering and Physical Sciences  
Research Council



Swansea University  
Prifysgol Abertawe

# EPSRC UK National Mass Spectrometry Facility at Swansea University

**N<sup>+</sup>M<sup>+</sup>SF**

Mark Wyatt



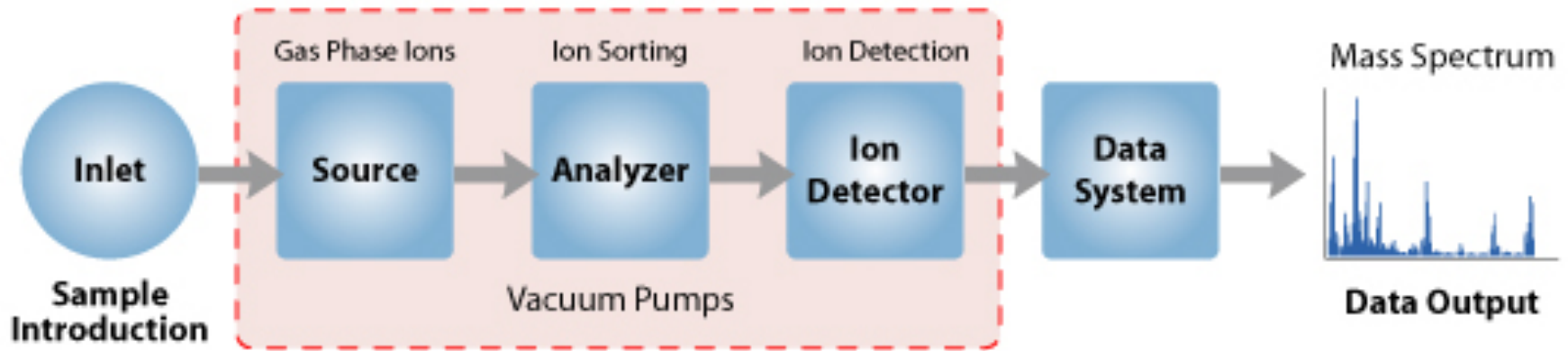
# Overview

- What is Mass Spectrometry
- Who are we
- What we offer
  - Mass Spectrometry analytical services
  - Additional services
- Key Features
  - RemoteAnalyzer (RA)
  - Fasttrack
  - Imaging



# What is Mass Spectrometry

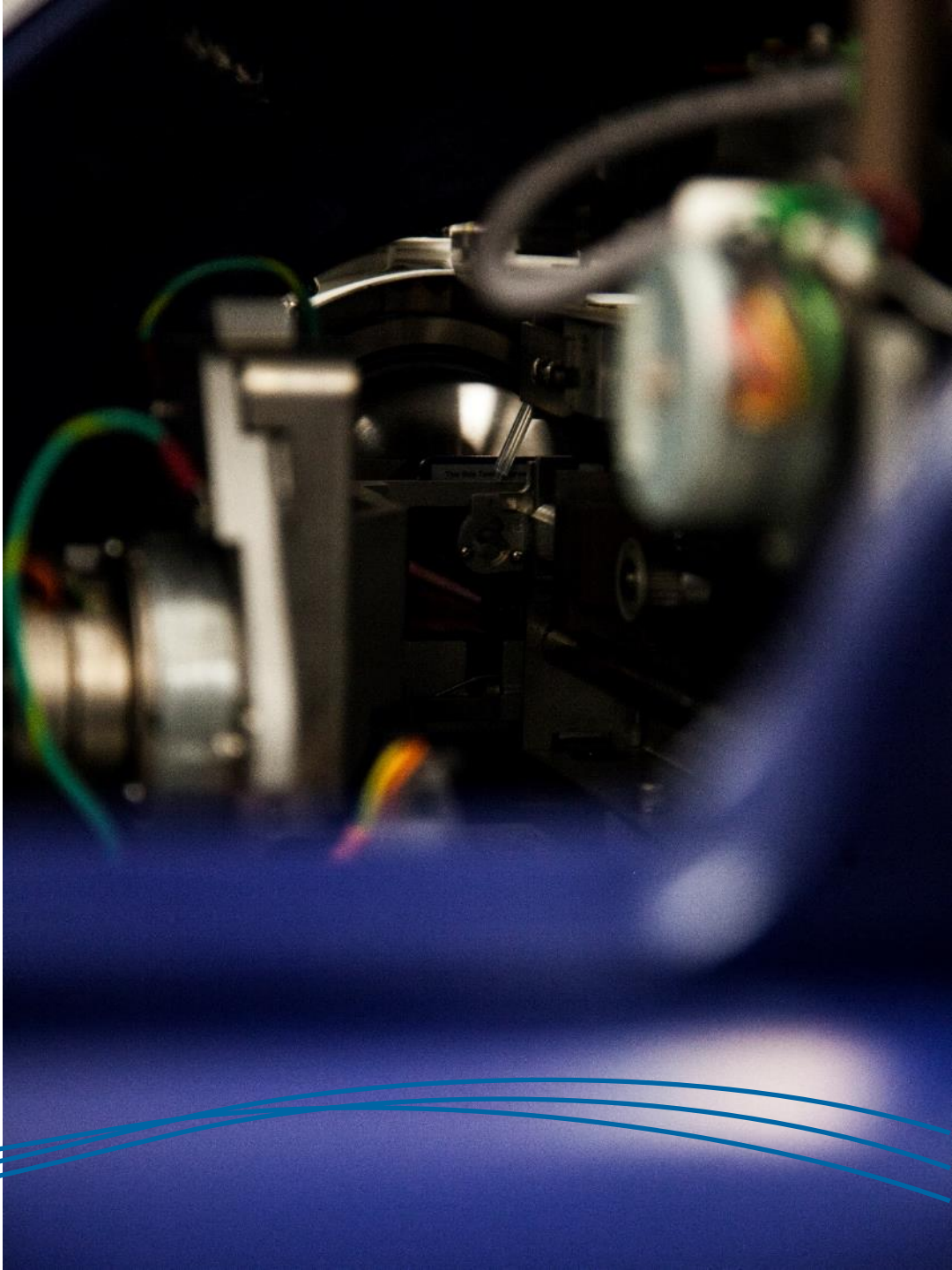
## Components of a mass spectrometer



- Produce ions from the sample in the ionization source.
- Separate these ions according to their mass-to-charge ratio in the mass analyser.
- Detect ions emerging from the analyzer and convert ions into electrical signals.

# The NMSF

- NMSF contracted by EPSRC until 30<sup>th</sup> June 2018 (extension pending).
- Provides various mass spectrometry services, including hyphenated techniques.
- Capable of handling a wide variety of challenging sample types, e.g. small organic molecules, macromolecular complexes air sensitive materials.
- Staff also engage in education, training, outreach, and research activities.



# The Team

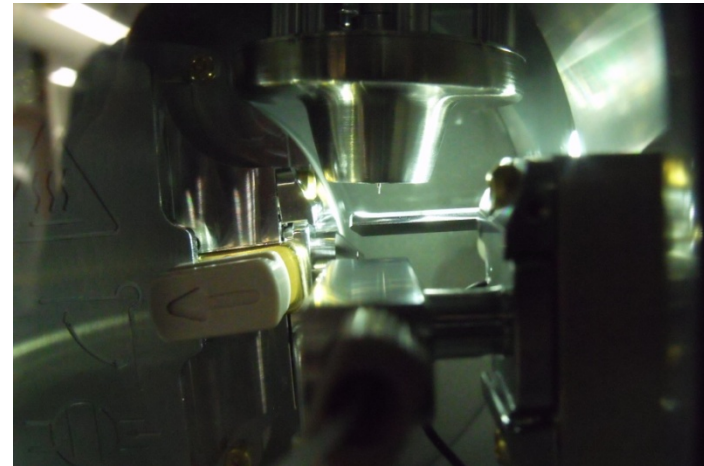
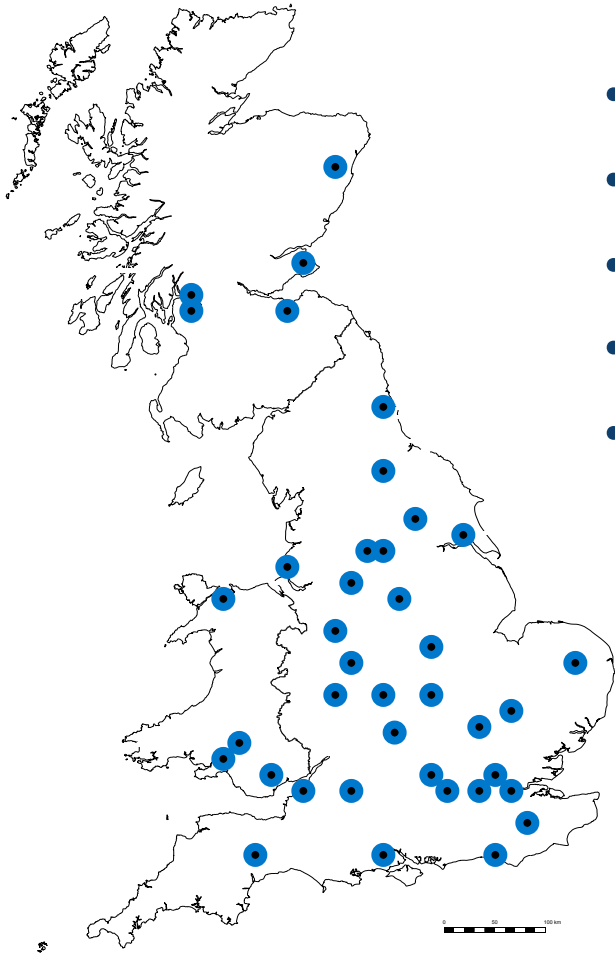
- **Facility Director** – Prof Steven Kelly
- **Facility Manager** – Dr Mark Wyatt
- **Experimental Officers** – Dr Ann Hunter (PT), Mr Gareth Llewellyn (PT), Mr Rhodri Owen, Ms Jessica Bexon
- **Office Administrator**– Ms Maria Moruzzi (PT)
- **Mass Spectrometry Analyst** – Ms Helen Benham



# The NMSF community

*Last year (2016-17):*

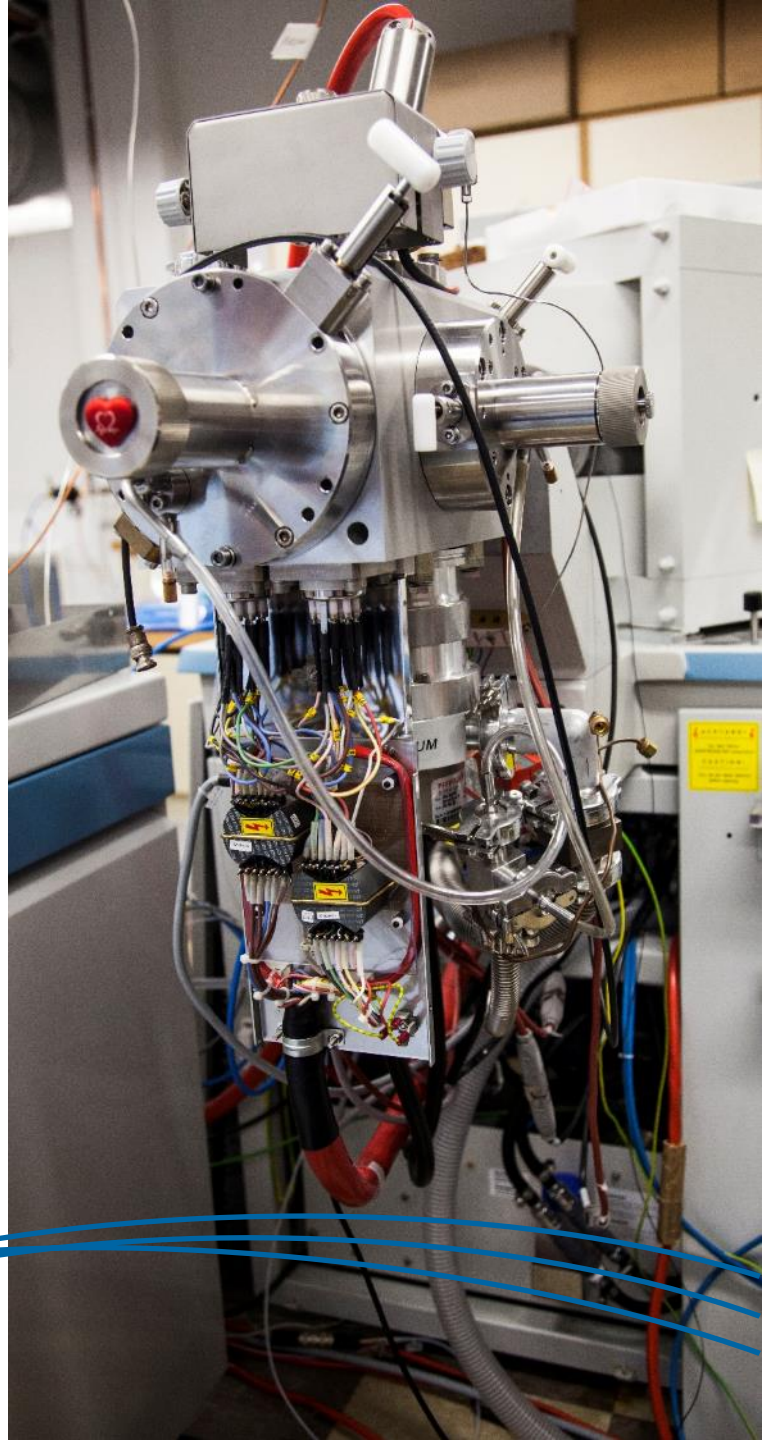
- >50 institutions and companies
- >140 research groups
- ~400 individual researchers/clients
- 9,524 samples / 14,314 analyses
- <5 days turnaround



# What we offer

- Full-Scan Accurate-Mass\* / High-Resolution Mass Spectrometry
  - Atmospheric Pressure Ionisation
    - Electrospray (ESI), Atmospheric Pressure Chemical Pressure (APCI), Atmospheric Pressure Solids Analysis Probe (ASAP).
  - Vacuum Ionisation
    - Electron Ionisation (EI), Chemical Ionisation (CI), MALDI, Liquid Secondary Ion MS (LSIMS / FAB).
- Experience
  - Analyses of a vast array of samples and chemistries.

\* 1 to 5 ppm depending on instrument and mass range.

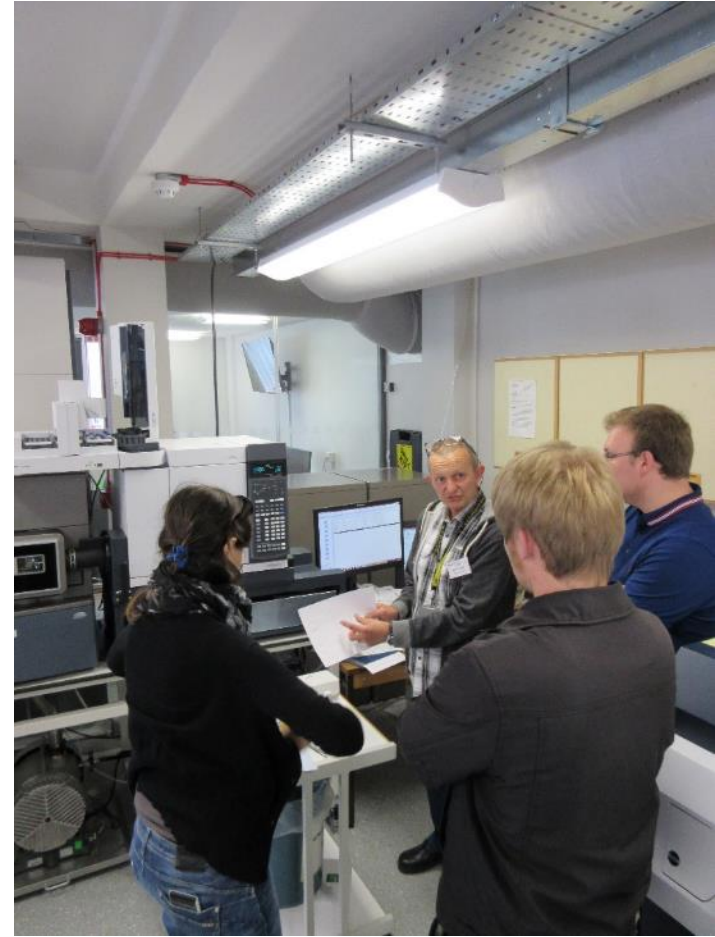


- Chromatography
  - Gas Chromatography
    - One column covers many chemistries.
    - Main variable is temperature.
  - Liquid Chromatography
    - Valid LC-MS method that is transferable to our instrumentation.
    - Method development via partnerships.
- RemoteAnalyzer LIMS – online submission and results portal.
- Fasttrack – higher throughout data acquisition service; data processed by end user (currently available for ESI only).
- Imaging – molecular mapping over a given area e.g. a tissue section.



# Additional Services

- Training
- Annual Summer School
- Outreach Activities
  - Training in Data Interpretation, methods in sample analysis, instrument maintenance.
- Institute of Mass Spectrometry (IMS)
  - MSc Applied Analytical Science (LCMS).
  - Postgraduate Diploma Applied Analytical Science (LCMS).
  - Postgraduate Certificate Applied LCMS.



- Impartial advice
  - We do not promote any specific vendors or instruments.
  - Instrumentation housed within NMSF include:

**Advion**

**AB** Applied Biosystems

**BRUKER**

**Waters**  
THE SCIENCE OF  
WHAT'S POSSIBLE.™

**ThermoFisher**  
SCIENTIFIC

 **Agilent Technologies**

## Commercial fees

- Our main techniques ((n)ESI/EI/CI/ASAP(APCI)/\*MALDI) will be 30 GBP (ex VAT) per sample analysis and include accurate mass measurement\*. [\*MALDI accurate mass is an additional analysis/fee].
- GC/MS, LC/MS and more complex problem solving/contract research will be charged at 50 GBP (ex VAT) per hour basis.
- Fasttrack is 10 GBP (ex VAT) per well.

# Access to NMSF

- Application form
  - NMSF required to collate information
    - Local facilities
    - Project funding
    - Personnel
    - Project objectives – why do you need mass spectrometry / the NMSF
- Renewals
  - Management Advisory Panel meets every year
  - Reviews all applications
  - Adjusts and approves allocations awarded



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- Interim Users
  - Allocation is usually lower, depends on capacity
  - NMSF is required to act as a short-term backup to University department services when they experience downtime
- Occasional Users
  - Reduced application form
  - Designed for no more than 12 samples in any 12 month period



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# Please include funding information

The screenshot shows the EPSRC website interface. A modal window titled 'Grant Details' is open, displaying the following information:

- GRN:** NS/A000020/1
- Title:** National Mass Spectrometry Facility
- Investigators:** Professor. Anthony Brenton(principal);
- Starts:** 01-04-2013
- Ends:** 31-03-2018
- Value:** £2,881,944.00
- Department:** Institute of Life Science Medical School
- Organisation:** Swansea University
- EPSRC Research Area:** Analytical Science;
- Classification:**
- EPSRC Research Theme:** Physical Sciences;
- Classification:**
- EPSRC Industrial Sector:** No sector relevance identified;
- Classification:**
- Summary on Grant Application Form:**

The background shows a 'List of Grants' table with the following data:

GRN	TITLE					
EP/F500424/1	LSI Doctoral Training Centres -					
EP/I036516/1	Ambient Pressure Mass Spectrometry					
EP/J000302/1	Is a NOESY-like 2 dimensional experiment possible in mass spectrometry?	436,361	30-11-2012	29-05-2016	University of Warwick	visualise
EP/L009913/1	Chemical Applications of Velocity and Spatial Imaging	4,663,077	08-01-2014	07-01-2019	University of Bristol	visualise
EP/L006227/1	Development of a Novel MALDI Mass Spectrometer and Technology for the Generation of Multiply Charged Ions at High Sensitivity	631,381	01-02-2014	31-01-2017	University of Reading	visualise
EP/L023490/1	NISA: Novel approaches for in situ analysis of biomolecules	1,484,528	01-06-2014	31-05-2019	University of Birmingham	visualise
NS/A000020/1	National Mass Spectrometry Facility	2,881,944	01-04-2013	31-03-2018	Swansea University	visualise

Showing 1 to 7 of 7 entries

# New Features

## RemoteAnalyzer

- NMSF sample submission needed modernising
- STAR developed between 2007 and 2012
  - Requires technologies which are now out of date
- NMSF required a system which enabled end users to comply with new policies, e.g. EPSRC framework on research data



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SpectralWorks

Sign in to RemoteAnalyzer®

Username

Password

Remember me?

[Forgot your password?](#)

Upon submission of samples to the EPSRC UK NMSF you are agreeing to Acknowledge the work performed by the EPSRC UK NMSF in any resulting publication using the following text:

**the EPSRC UK National Mass Spectrometry Facility at Swansea University**

**EPSRC UK National Mass Spectrometry Facility**

**Swansea University**

If you have any questions, comments, or require labels for sample submission, please contact:

email: [mscentre@swansea.ac.uk](mailto:mscentre@swansea.ac.uk)

Telephone: +44 1792 295553

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Promoting research  
and skills


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- Database driven website
- Stores all sample information and files together
- End user can attached documents, e.g. Mass Spectra, GPC, reaction schemes
- NMSF can provide processed data (pdf), raw data and any other data required
- Each sample record logs the history of the sample
- Barcodes: generated and provided by NMSF
  - If you are running low please contact us
- Please provide feedback
  - Missing features can be requested and hopefully implemented

**SpectralWorks**



Sign in to RemoteAnalyzer®

Username

Password

Remember me?

**Sign in**

[Forgot your password?](#)

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**Swansea University**

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email: [mscentre@swansea.ac.uk](mailto:mscentre@swansea.ac.uk)  
Telephone: +44 1792 295553

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Providing research and skills

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Version 4.22.2010.0971

# New Features

## Fastrack

### Requirements

### End User

- Samples suitable for ESI
- 96 well microtiter plate prepared by end user(s) and dried
- Excel file completed with sample details
- Plate posted to NMSF; Excel file emailed to NMSF



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# Choosing correct ionisation mode

		SELECTION of IONISATION MODE for MASS SPECTROMETRY ANALYSIS of COMMON ORGANIC MOLECULES											
		TYPICAL SOLVENT <sup>5</sup>	RELATIVE MOLECULAR MASS <sup>4</sup>										
			0	100	200	300	400	600	800	1000	>1200		
SAMPLE POLARITY INCREASING.....	non-polar	hexane	<i>hydrocarbons, polycyclic aromatic hydrocarbons (PAHs), polychlorinated biphenyls (PCBs)...</i>										
		toluene	EI <sup>1</sup>							EI			
	semi-polar	dichloromethane	CI <sup>1&amp;2</sup>							CI			
		chloroform	<i>common organics, alcohols, amines, organometallics, functionalised species...</i>										
		methanol	APCI										
		acetonitrile	ESI										
			MALDI <sup>3</sup>										
			MALDI										
			<i>sugars, peptides, nucleotides, salts, multiply-charged species...</i>										
			APCI										
polar	water	ESI											
	acid/base	MALDI <sup>3</sup>											

**KEY:** *Examples of compounds of differing polarity are shown in italics*

- Primary technique (most likely to work well)
- Secondary technique (should work and will give complementary information to the primary technique)
- Tertiary technique (try it if you have no choice)

**NOTES:**

- For all EI and CI a suitable inlet will also be required to match sample volatility (e.g. GC or solids probe or desorption probe).
- CI suitability will depend on gas selection (e.g. ammonia is unsuitable for hydrocarbons which will need, e.g. methane).
- MALDI matrix ions cause interference at lower  $m/z$  [so MALDI without matrix (LDI) or surface assisted (SALDI) can be used more readily at lower mass].
- Mass range also depends on mass analyser and  $m/z$  of ion produced.
- The polarity of the sample material can be assessed by investigating which solvents it will dissolve in (e.g. a material that dissolves in hexane but not in water is non-polar). The solvents listed are for assessment of sample polarity only – they are not suggested solvents for dissolution of the sample for analysis by mass spectrometry.

# Excel template

	A	B	C	D	E	F	G
1	<b>Group</b>						
2	<b>Plate</b>						
3							
4	<b>Well</b>	<b>Reference</b>	<b>MW</b>	<b>Name</b>	<b>Formula</b>	<b>Conditions</b>	<b>Polarity</b>
5	A01						
6	A02						
7	A03						
8	A04						
9	A05						
10	A06						
11	A07						
12	A08						
13	A09						
14	A10						
15	A11						
16	A12						
17	B01						
18	B02						
19	B03						
20	B04						
21	B05						
22	B06						
23	B07						
24	B08						
25	B09						
26	B10						
27	B11						
28	B12						
29	C01						
30	C02						
31	C03						
32	C04						



## NMSF

- Reconstitute samples according to Excel file
- Acquire data
- Raw data returned via download or disc
- Turnaround can be as low as 48 hours from receipt

## End User

- Requires Data Processing Software (OEM or 3<sup>rd</sup> Party)
- NMSF can provide training in data processing, if we are familiar with the software!
- Limit on number of plates depending on take up
  - could groups share plates?
- 'Normal' allocation is reduced and reserved for other techniques

*NMSF have processed an extra 10,000 samples via this route in 3 years*



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# Overview

- Who are we
- What we offer
  - EPSRC Services
  - Additional Services
- Access
  - Applications  
and Allocations
- New Features
  - RemoteAnalyzer (RA)
  - Fasttrack



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Thank You

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