EPSRC
Engineering and Physical Sciences Research Council

Swansea University
Prifysgol Abertawe

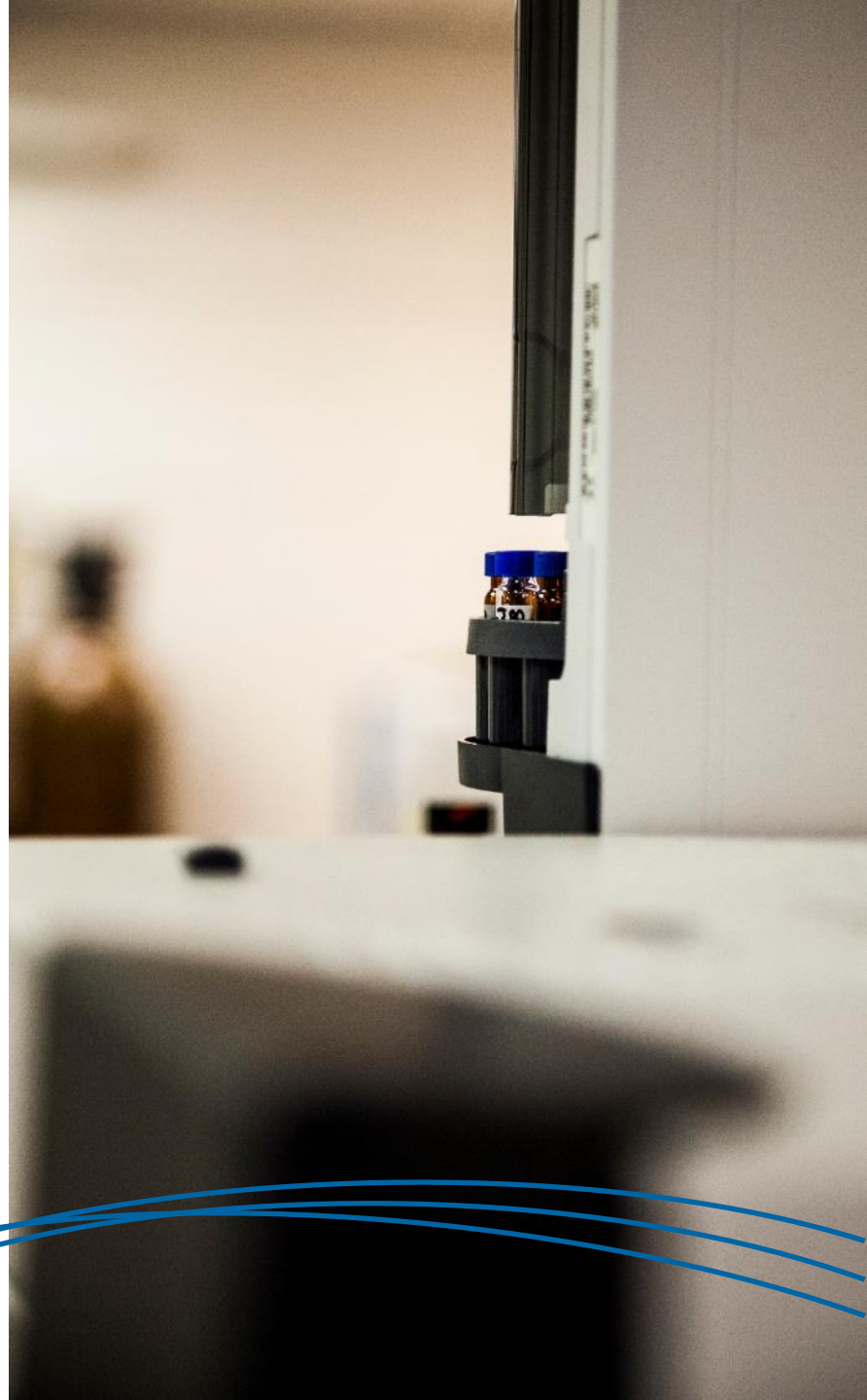
EPSRC UK National Mass Spectrometry Facility at Swansea University

NMSF

Mark Wyatt

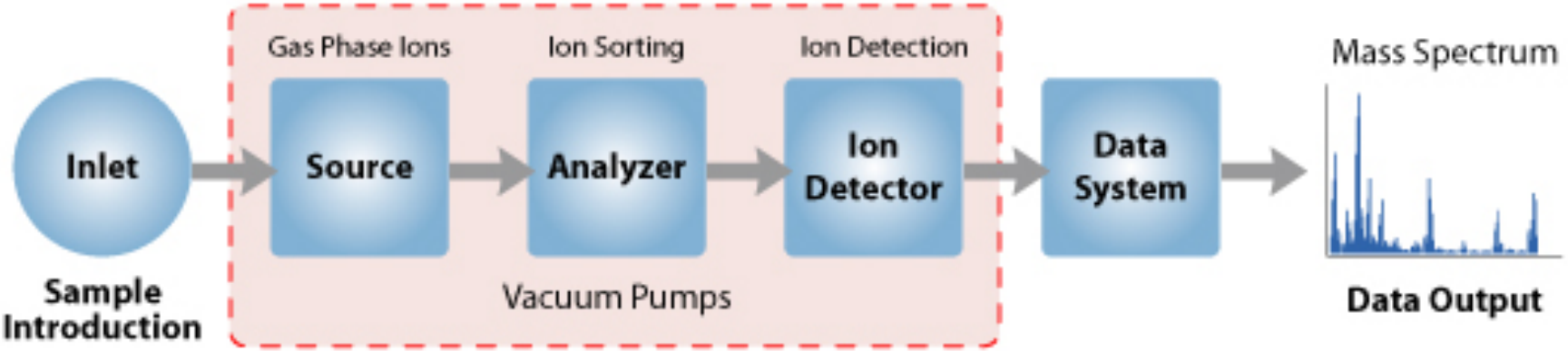
Overview

- 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

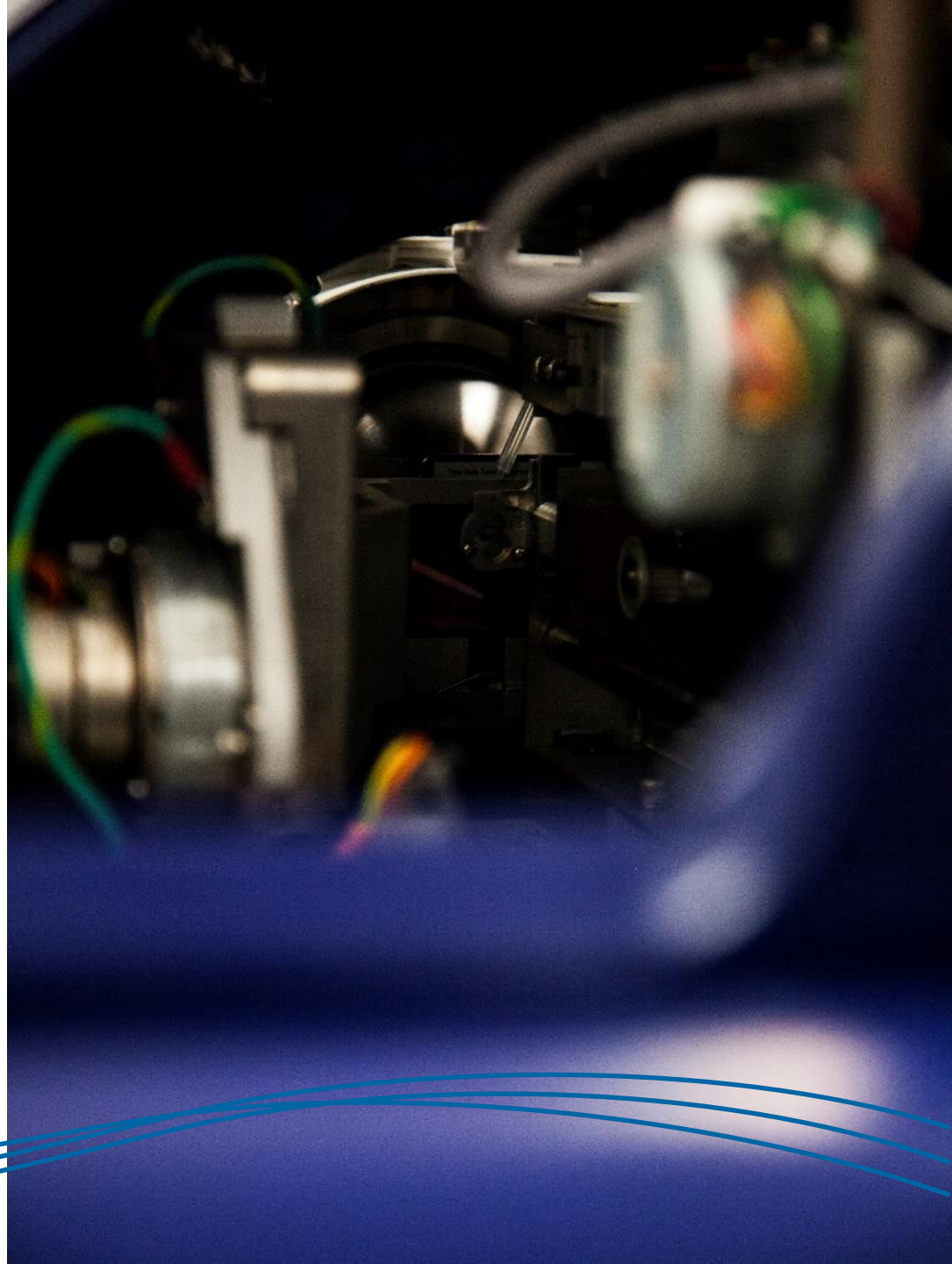
Components of a mass spectrometer



- 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

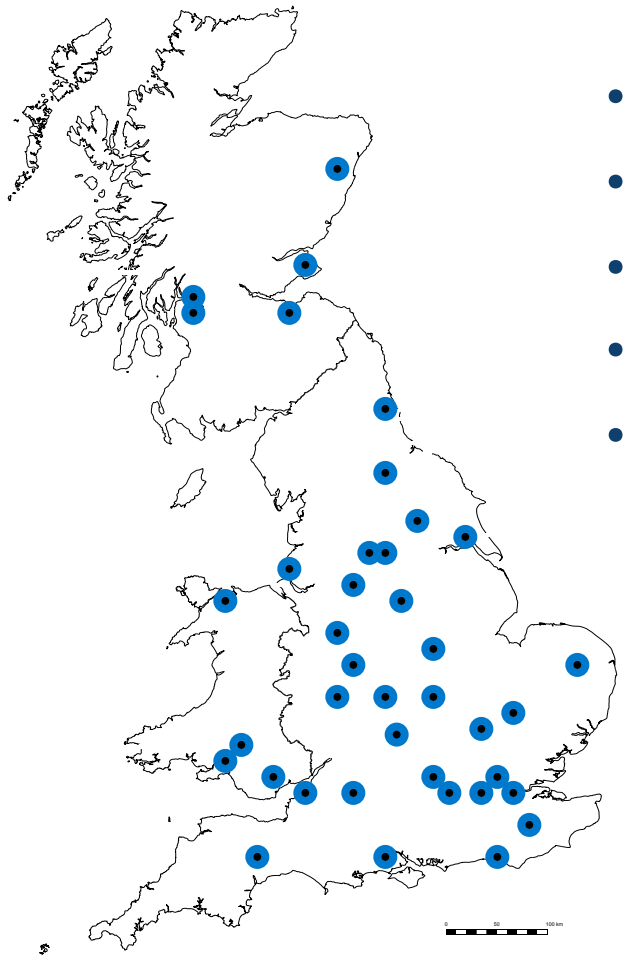
- NMSF contracted by EPSRC until 30th June 2018 (extension pending).
- Provides various mass spectrometry services, including hyphenated techniques.
- Capable of handling a wide variety of challenging sample types, e.g. small organic molecules, macromolecular complexes air sensitive materials.
- Staff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



The Team

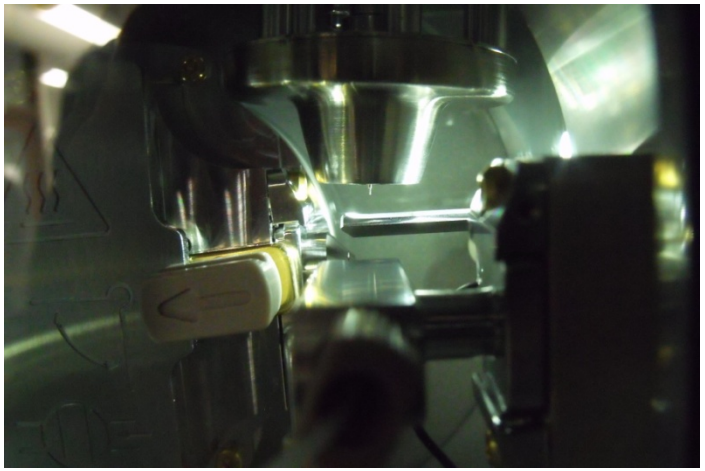
- **Facility Director** – Prof Steven Kelly
- **Facility Manager** – Dr Mark Wyatt
- **Experimental Officers** – Dr Ann Hunter (PT), Mr Gareth Llewellyn (PT), Mr Rhodri Owen, Ms Jessica Bexon
- **Office Administrator**– Ms Maria Moruzzi (PT)
- **Mass Spectrometry Analyst** – Ms Helen Benham

The NMSF community



Last year (2016-17):

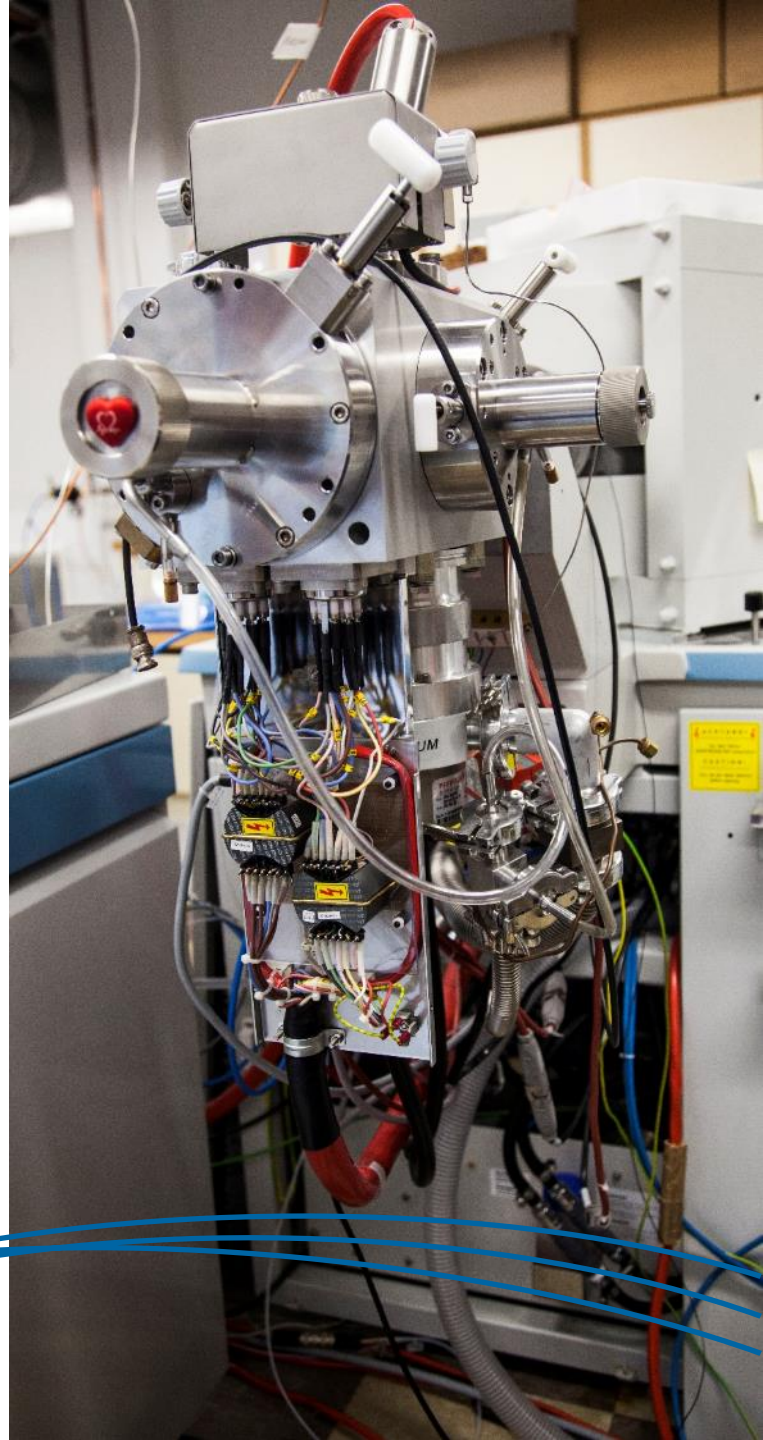
- >50 institutions and companies
- >140 research groups
- ~400 individual researchers/clients
- 9,524 samples / 14,314 analyses
- <5 days turnaround



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

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

- 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

Please include funding information

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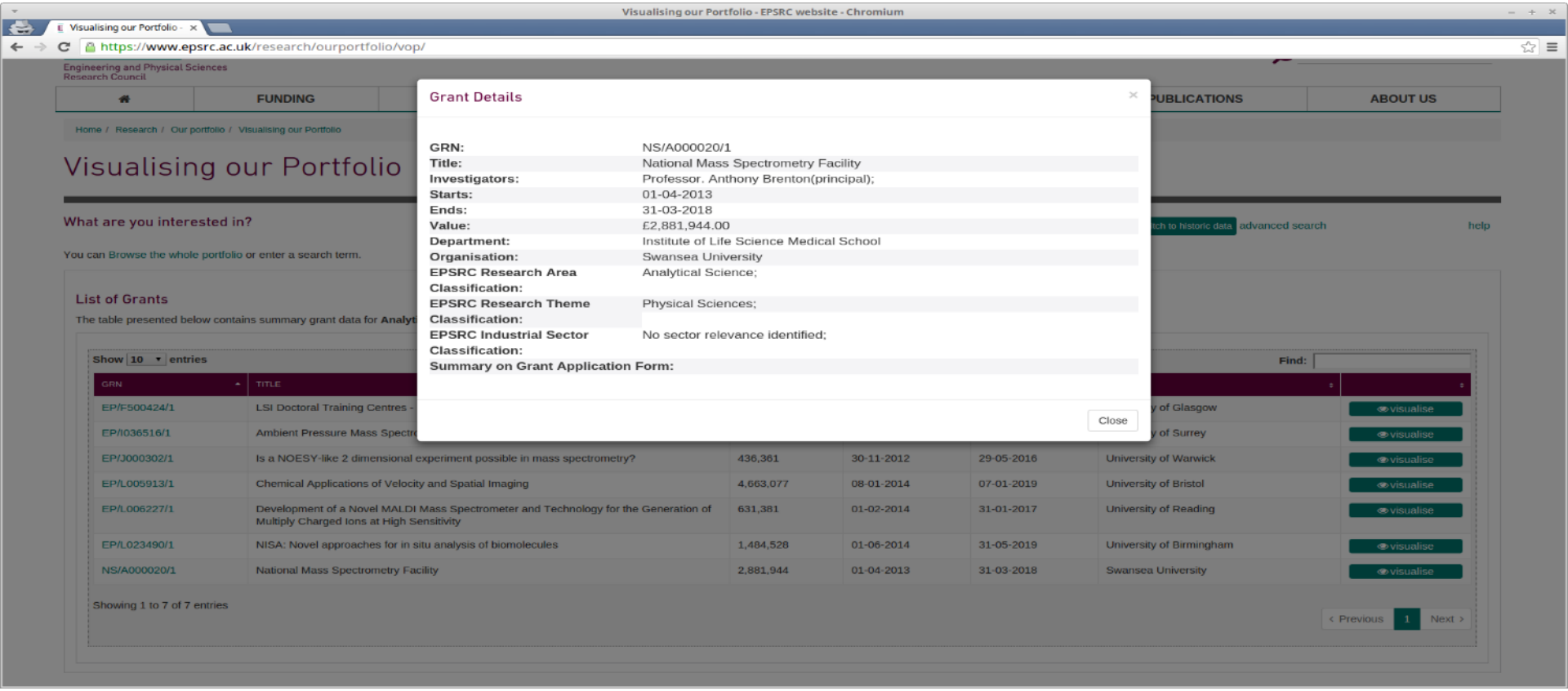
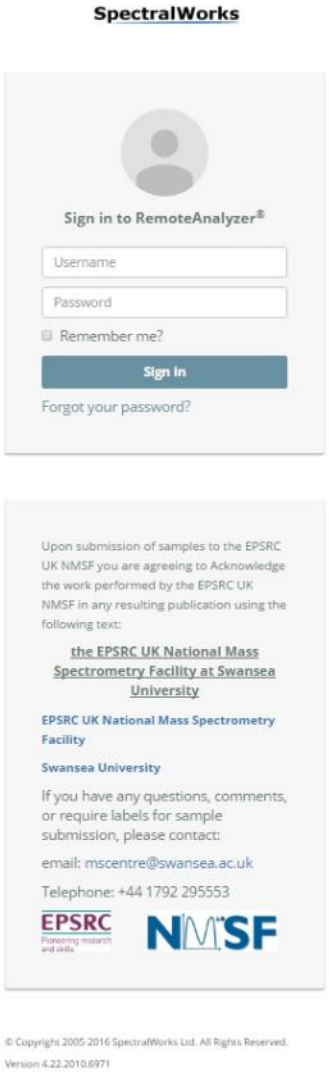


New Features

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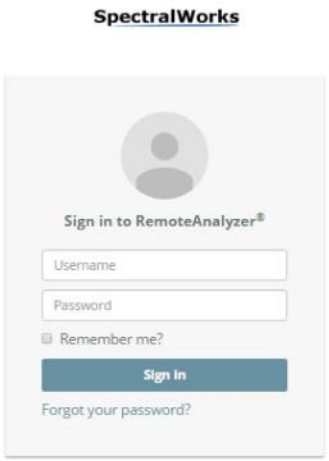
- Database driven website
- Stores all sample information and files together
- End user can attached documents, e.g. Mass Spectra, GPC, reaction schemes
- NMSF can provide processed data (pdf), raw data and any other data required
- Each sample record logs the history of the sample
- Barcodes: generated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



Version 4.22.2010.6971

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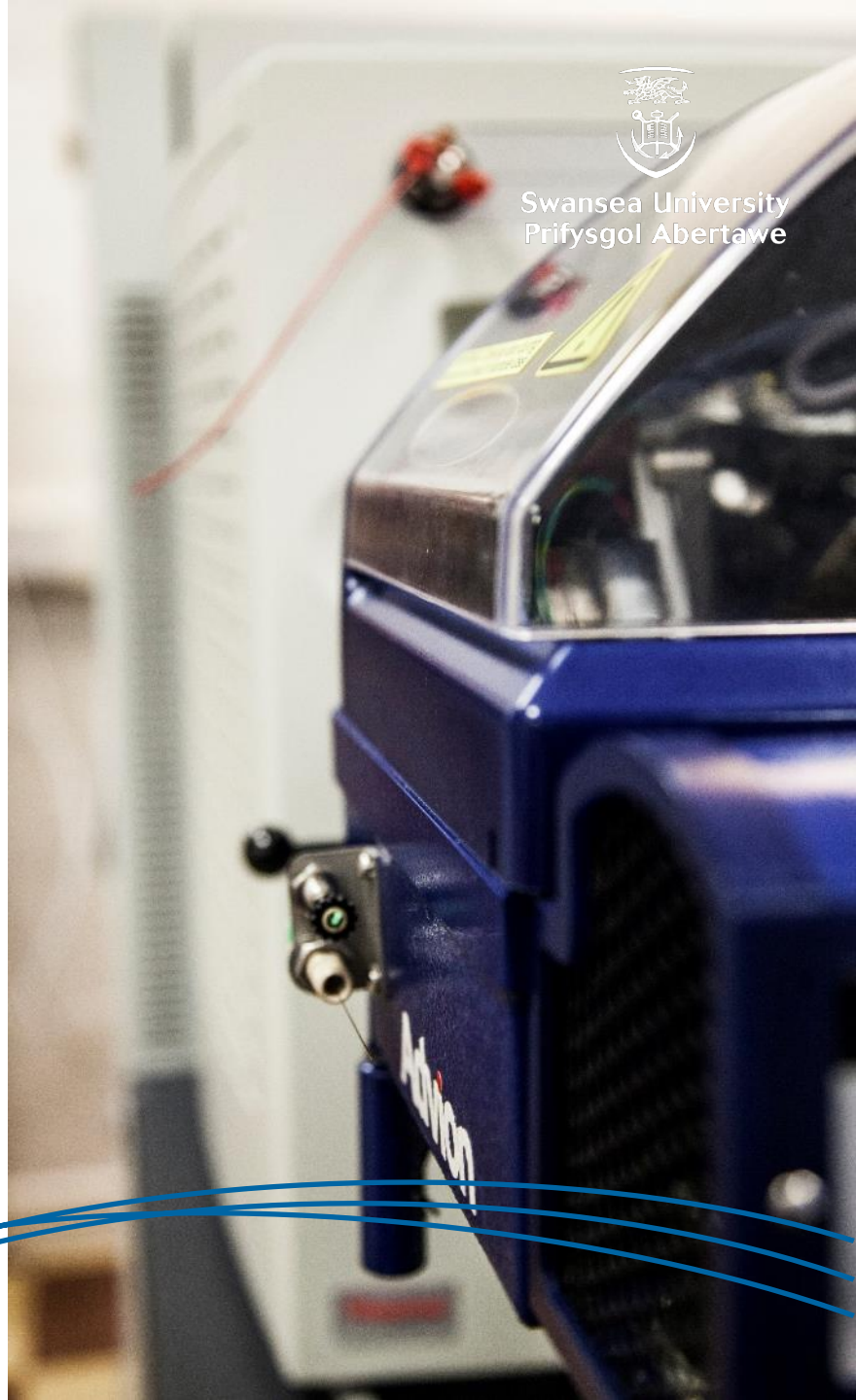
New Features

Fasttrack

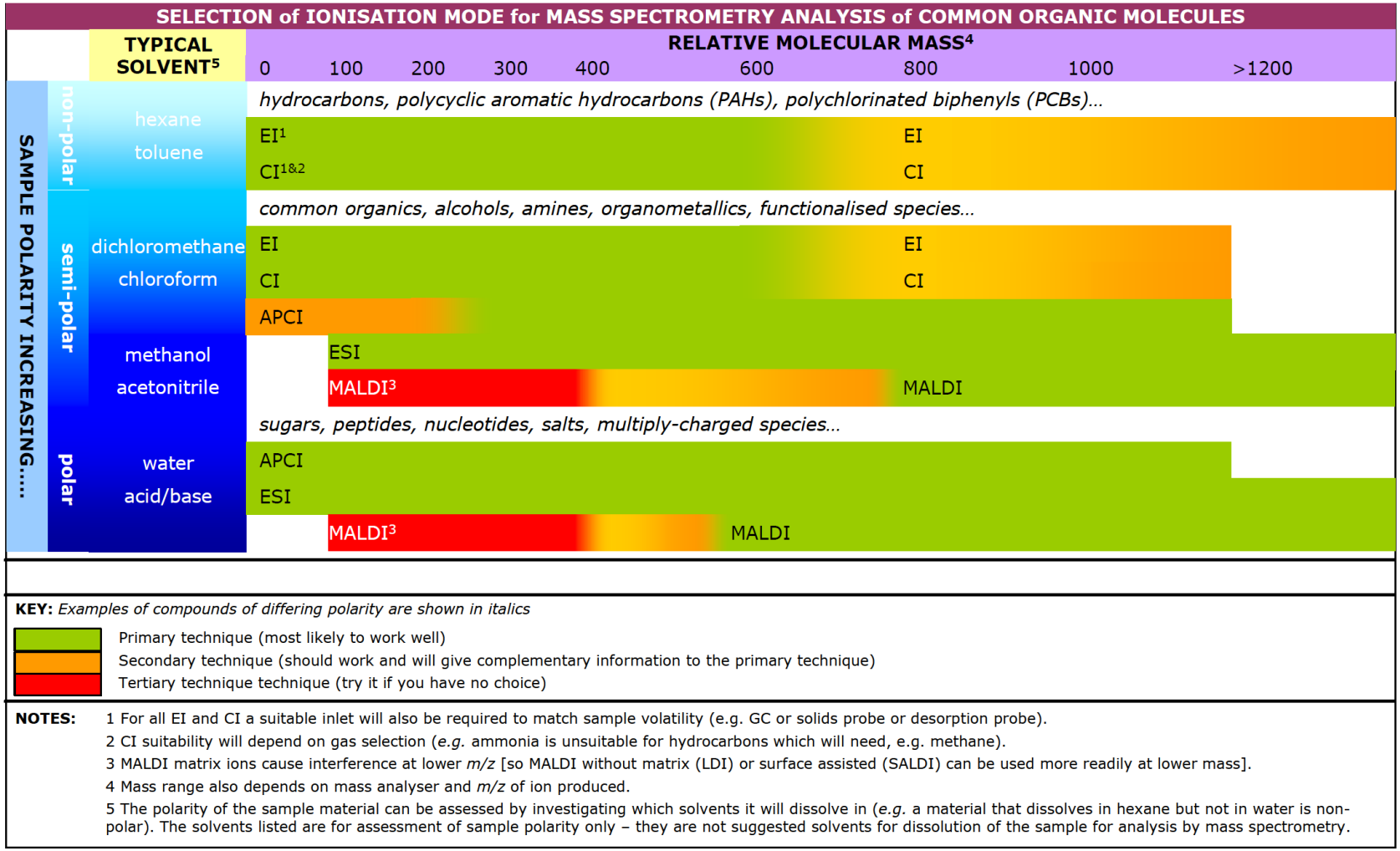
Requirements

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



Choosing correct ionisation mode



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 technique (try it if you have no choice)

NOTES:

1 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).

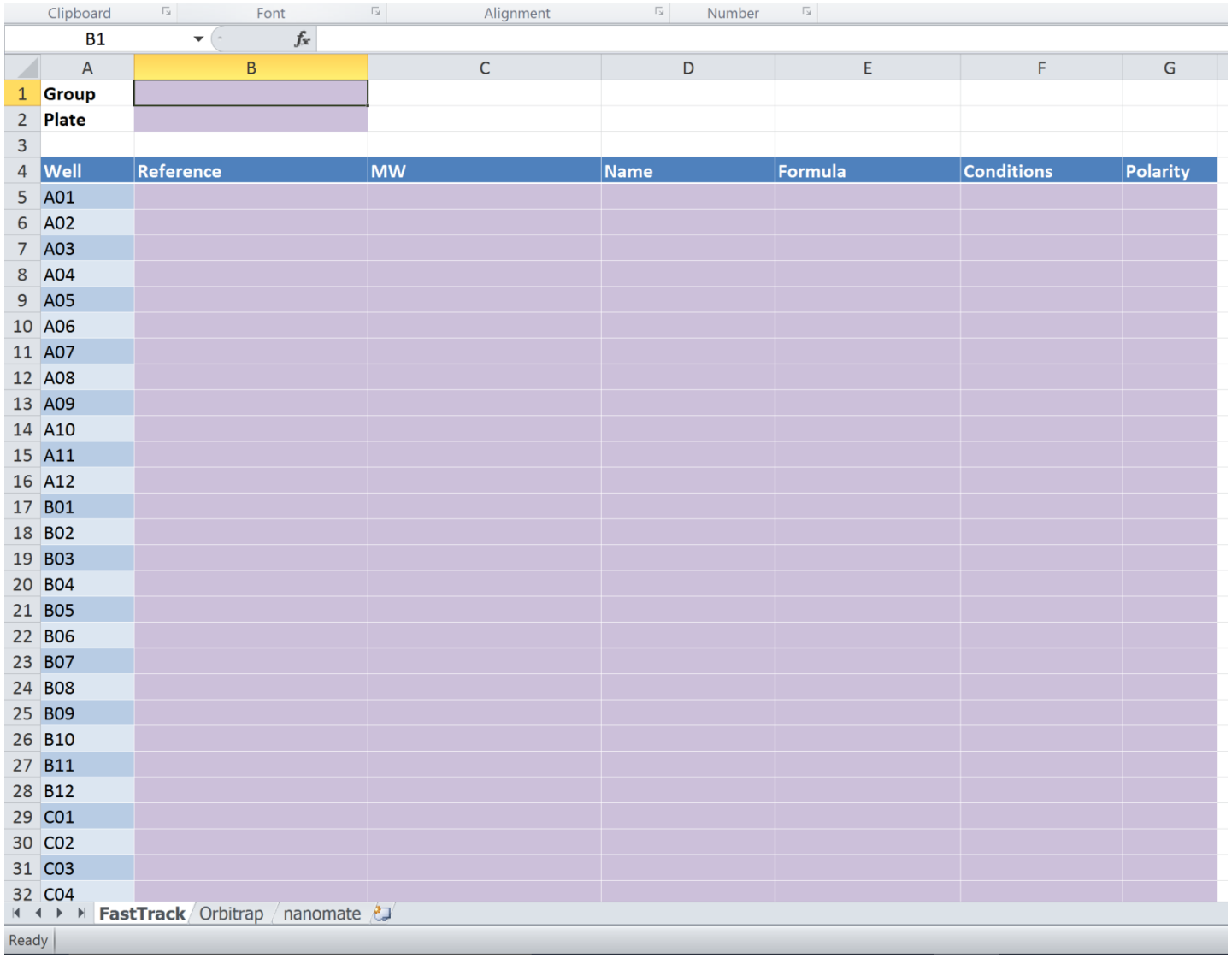
2 CI suitability will depend on gas selection (*e.g.* ammonia is unsuitable for hydrocarbons which will need, e.g. methane).

3 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].

4 Mass range also depends on mass analyser and *m/z* of ion produced.

5 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



Clipboard | Font | Alignment | Number

B1

	A	B	C	D	E	F	G
1	**Group**						
2	**Plate**						
3							
4	**Well**	**Reference**	**MW**	**Name**	**Formula**	**Conditions**	**Polarity**
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						

FastTrack | Orbitrap | nanomate

Ready

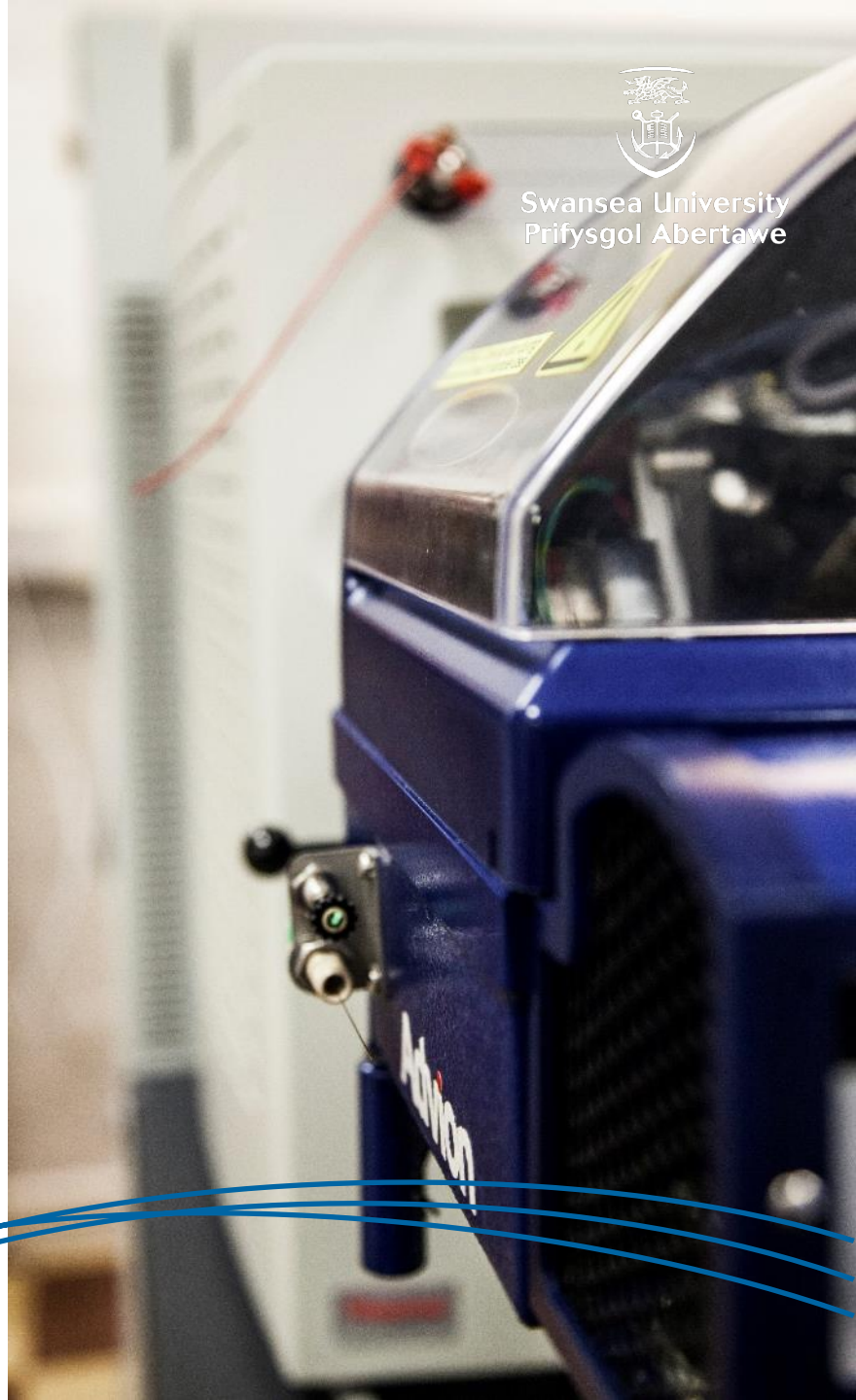
NMSF

- 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 3rd 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



Overview

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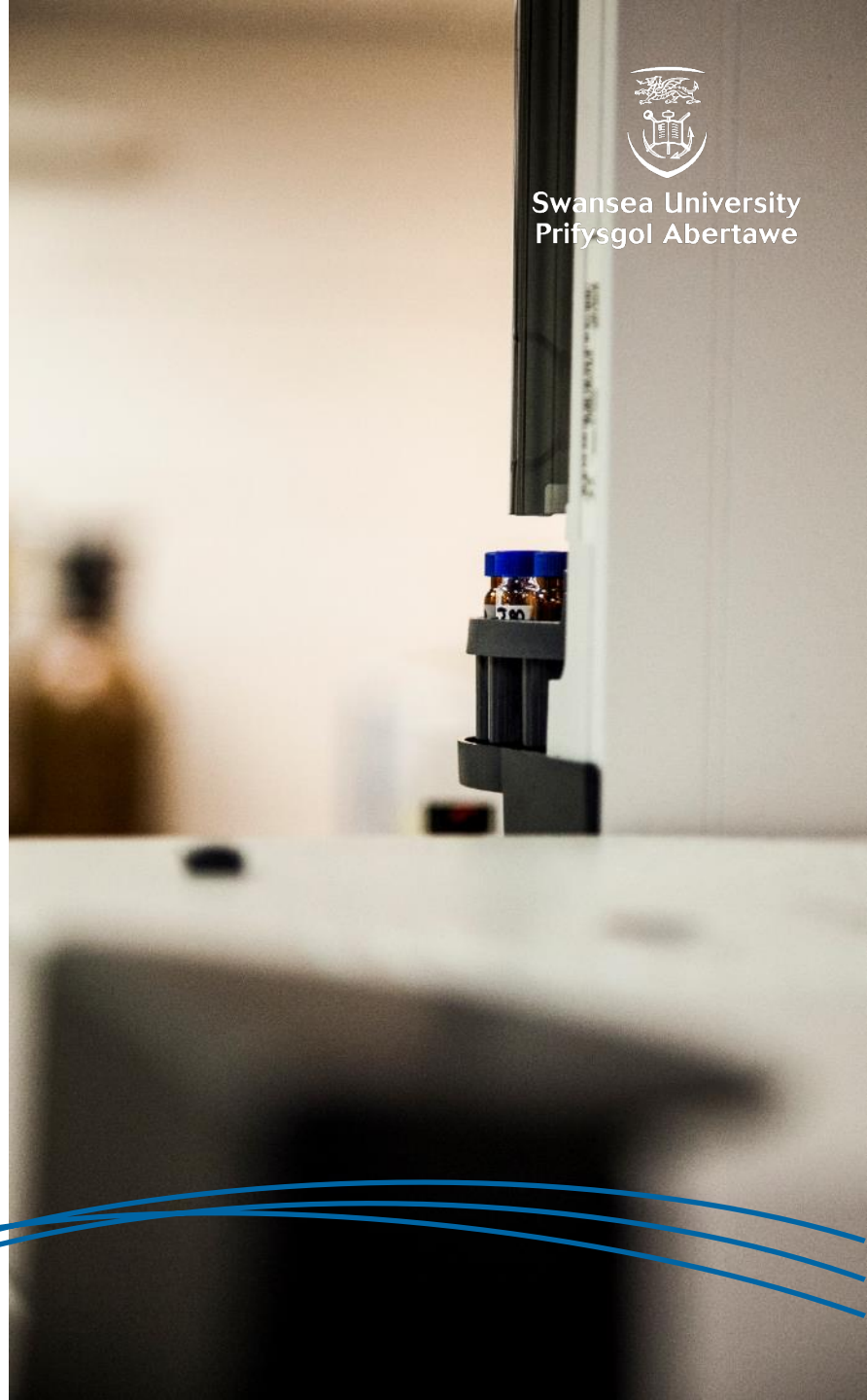
  - Additional Services
- Access
  - Applications
    and Allocations
- New Features
  - RemoteAnalyzer (RA)
  - Fasttrack



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Thank You

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