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UK Mass Spectrometry Vision

A report from the BMSS Vision Committee

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Mission statement:

- To produce a community-backed, evidence-based vision for the future of mass spectrometry in the UK, to support EPSRC, UKRI, and the UK government in future business planning, prioritization, and funding of mass spectrometry in the future.

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Consultation plan:

- We used a DELPHI study, an iterative discussion amongst a panel of experts, 34 experts including academia (20), industry (12), government labs (1), ECRs (2), staff (2) from all corners of the field.
- The Vision committee summarized the key points that arose from the DELPHI study
- Public Consultation (starting now at BMSS40)
- The Vision committee will next produce the full report and documents for EPSRC/UKRI (Autumn 2019)

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Results:

- The first rounds of the consultation showed that MS funding needs vary with different Tiers of mass spectrometry instruments and instrument access.
- The Vision committee used these documents to generate a SWOT (Strengths, Weaknesses, Opportunities, Threats) analysis of the tiers.
- This SWOT analysis is presented on posters at BMSS40.

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Key points:

- Mass spectrometry is a critical driver of industry particularly in chemistry, pharma, biotech, materials, manufacturing, health, food, security, forensics.
- Mass spectrometry developments drive forward all of these industries.
- New developments in mass spectrometry create entire new industries

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Key points:

- Different tiers of instruments need different funding models.
- Clearly sustainable funding of instruments and capabilities is a recurring problem at many institutions.
- The total cost of ownership of mass spectrometers requires personnel, maintenance, supplies, and fEC overheads for infrastructure (TRAC costing). Sustainable instrument funding requires all of these costs.
- Underfunding of mass spectrometers (not meeting part of the TRAC costs above) results in unsustainable, broken, or underutilized equipment.
- All UKRI-funded equipment should be fully supported (as above) supported for the lifetime of the instrument (typically 7 years), not the lifetime of the grant. Grant proposals should make it clear how the instrument will be sustainably funded over the lifetime of the instrument.

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Possible recommendations:

- All UKRI-funded instruments should be TRAC costed so that the full cost of ownership is both clearly known and demonstrable to management and for full cost recovery of fee-for-service access. Institutions are then welcome to subsidize access as they like.
- All UKRI-funded instruments should require a business plan which explains how full TRAC-costed sustainable funding can be met over the lifetime of the instrument. We need clarity about how much of the instrument maintenance costs are expected to be paid by fEC overheads.

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Key points:

- PhD studentship funding is inadequate both in terms of the numbers of students and in the amount of funding provided – particularly in terms of instrument access charges and consumables.

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Possible recommendations:

- A community-wide DTC to fund PhD studentships at all universities across the UK
- Greatly increase iCASE funded PhD studentships in mass spectrometry
- Increase all PhD Studentship funding to include a sustainable allocation of consumables and instrument access charges
- A community wide ‘Training Hub’ to coordinate training and dissemination of training materials, advise on funding models, and possibly as the focal point of the DTC mentioned above.

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Key points:

- We need to better coordinate production and dissemination of training materials for teaching mass spectrometry at many levels. BMSS can take a coordinating role here, but it needs to be funded.

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Key points:

- Equipment sharing is frequently hindered by problems with access to equipment.
- ECR's, personnel returning from a career break, and personnel who have recently moved institution have particular problems with access to equipment.

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Possible recommendations:

- Full usage of equipment requires ‘Research Hotel’ funding for people to travel to the equipment, stay a few days locally, acquire the data (instrument access charges), and purchase of the computers and software to fully engage with processing the data back home. Some method to fund ‘Research Hotel’ visits will improve equipment sharing.

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Key points:

- Full usage of mass spectrometry data requires full data access, training in how to correctly interpret mass spectrometry data, and access to the appropriate data processing tools.

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Possible recommendations:

- Require the instrument manufacturers (or alternatives) to provide a low cost or free-of-charge data visualiser software, either browser based or easily downloadable and installable, for users to see and partially analyse their data. More sophisticated analysis tools, such as database search engines and intricate data interpretation algorithms can still be sold separately.
- Fund a MS data analytics network and hub which aims to develop data standard formats and converters as well as further data analysis tools that on an open-access basis.
- Provision of a national data repository to facilitate data sharing

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Key points:

- A single national mass spectrometry facility is not supported by the mass spectrometry community because the field is too large for a single facility to have sufficient expertise to cover everything and to remain at the forefront of the field.
- The community does support establishment of a set of complementary national research facilities in mass spectrometry which focus on non-standard research equipment, new instrument and methods development, and advanced mass spectrometry collaborations.

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Possible recommendations:

- A call for proposals should be created and announced to create a number of complementary Advanced National Mass Spectrometry Research Facilities around the UK:
  - Peer reviewed (on a 5 year basis)
  - Provide non-standard, specialist mass spectrometry capabilities to the whole scientific community
  - Does not compete with standard mass spectrometry facilities
  - Lead the development of new technologies and applications
  - Train the next generation of mass spectrometrists
  - Deliver non-academic impact from these advanced tools
  - The key access point for new mass spectrometry capabilities for industry

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What next?

- Discuss these proposals and feed back any concerns or ideas.
- In particular, please consider the impacts vs. risks of each of the possible recommendations.
- Feel free to contact any of us in what ever manner is most convenient.
- Questions?

Tier 0: Portable, robust, automated devices for non-experts

	Helpful	Harmful
Internal	**Strengths** • Emerging area with direct, non-academic, impact • Simple to operate, accessible, low cost, share • Quick measurements, local to the problem at hand • Large, rapid growth potential • Good data in the hands of non-experts, amplifying impact	**Weaknesses** • Poor data interpretation tools, limited to PCA, SRM, or pattern recognition approaches • Low performance (accuracy, resolution, separation, sensitivity, etc.) leading to limited capabilities • High false positive rates • Power usage
External	**Opportunities** • High demand in SME's • Great opportunity for small MRM-triple quads • Instrument development opportunities to improve performance and lower cost • Local measurements at the point of the problem, whether in a reaction line, ports, or in the field. • Good education tools • Data analytics opportunities • More applications = more users.	**Threats** • Data analytics are not ready • Education is not there, need to overcome the 'MS is hard' bias in the scientific community • Method development is always application specific and contaminants vary with the environmental matrix. • Such instruments must be pushbutton, and rugged. • Big danger of misinterpretation of data, false positives and over interpretation. • Entry level costs and maintenance costs could be very high. • Will need cloud storage and data analytics in many cases.

Tier 1: Single group equipment

	Helpful	Harmful
Internal	**Strengths** • Good focus and expertise, unique capabilities • Excellent training to students and collaborators • Hands-on education • Can focus on their own research over any other • Maximal uptake because the owners are personally invested in the equipment • Future employability of the staff, because they are experts • Skills, over time, will expand in to the economy.	**Weaknesses** • Variable, often low, access for collaboration • Ivory tower, by design • Difficult to fund upgrades and maintenance • Usually cannot afford service contracts – leading to decline of instrument functionality • Sometimes PR purchases rather than an actual demonstrated need - sometime chasing 'funding fads' • Without sufficient local expertise, the instrument will be underutilised. • Potentially lack of exposure and impact. • Lack of continuity in expertise because of student and PDRA departures. • Disconnect between funding the instrument and funding the usage/maintenance/sustainability of the instrument.
External	**Opportunities** • Can open up new areas of non-academic impact • Close, high quality collaborations can improve impact • Raising the profile of new techniques • Group reputation and enthusiasm will grow and expand usage	**Threats** • Sustainability of equipment, hardware, software, and expertise • Limited Bandwidth • Limited upgradeability, given instrument obsolescence • Instruments last longer than operating systems requiring backwards compatibility or data system upgrades • Enforced upgrades are often impossible because of firewalls • Sustainable funding of maintenance is difficult • Financial management is varied among institutions, and usually unsuited to fully sustain instruments.

Tier 2: Local/Regional Mass Spectrometry Facilities

Defined as multiple instruments and multiple staff to help others to do mass spectrometry experiments. Broader user base than a single group instrument.

	Helpful	Harmful
Internal	**Strengths** • Supports science broadly - demonstratedly • Spreads maintenance and service costs among all users and equipment • Shares equipment • Dedicated staff to maintain instruments and train users • Introduce new users to the techniques (education) • Gateway between the mass spectrometry and broader scientific disciplines • Local expertise and capacity • Backup for Tier 1, troubleshooting expertise • A variety of techniques and approaches • Able to triage projects to best utilise the right tools to answer the questions • Bridge to 'national facilities' • Can deliver results close to the instrument performance limits • Local access for local experiments and short-lived intermediates	**Weaknesses** • Managing access. Sometimes high demand results in conflicting priorities • Charging models sometimes are unsustainable – requiring institutional subsidies • Varying charging models between institutions results in a race to the bottom on costs – resulting in unsustainable equipment and capabilities. • PhD student access is usually unfunded because of insufficient student supplies budgets • Cultural resistance to training users – i.e. training your future competitors • Sample carryover and contamination problems – particularly with open-access • Training of users is expensive in time, but poorly trained users cause a lot of contamination and downtime problems. • Underutilisation of equipment due to insufficient staffing (per instrument) • Research staff are often not supported for career development • Need sufficient staff to jobshare and rotate if staff are off or need to travel.
External	**Opportunities** • Professionalization of Research staff is an opportunity. • A good facility can grow their 'region' and 'capabilities' • Experienced voice within mass spectrometry at the national stage • Opportunities for collaboration between research for better equipment sharing and networking. • Training courses, with hands-on training on commercial equipment • First port-of-call for industry and SMEs for access to MS • Direct local/regional industrial impact.	**Threats** • Funding models vary and are often insufficient to ensure full instrument sustainability. • A change of institutional leadership can change funding models and funding priorities. • Financial management, bookkeeping, and admin • Staff turnover or staff stagnation • Cherry picking the easiest/lucrative samples, rather than doing the best science • Success could raise competitors for the same income streams. • Less 'knowledge' deliver rather than 'data' dumping. It's easy to give people spectra without explaining what they mean. • Data can be misused or misunderstood. • Data flood and management is a problem, as is data security • Slow turnaround from institutional contracts office = lost business, T&C's vary. • Poor data quality control means loss of business • Demand for accredited data quality changes the costing model, drastically.

Tier 3: Specialist centres or resources

Defined as nationally accessible facility with particular focus in one type of mass spectrometry capability.

	Helpful	Harmful
Internal	**Strengths** • Specialists in their area – international experts. • Can bring experts together to tackle bigger topics – Networking hubs. • Can be trusted to produce the best quality data • Aware of the changing technology and can keep abreast of it. • Equipment sharing • Focus at the appropriate degrees of specialisation • Could interweave with and enhance the capabilities of local facilities • Training hub for MSc and PhD and training port of call for industry • Knowledge transfer to industry and new intellectual property • Pushing boundaries in their specialisation area – development of new techniques. • Flexible funding, long term for the UKRI • Not a single point of failure • Grow mass spectrometry reach both nationally and abroad • Can be used to enhance regional industry, and can be adapted to the catalyst model.	**Weaknesses** • Competition among National Centres of Excellence (NCoE) with overlapping areas of expertise • Potential duplication of effort • No one central voice for mass spectrometry • Academic vs. Facilities service mode conflicts of interest and access models. • Potentially opaque access models – often a perception rather than the reality • "Sour grapes" problems in feedback amongst mass spectrometry peers and reviewers • Sustainable funding models • Financial management and Admin support • Changing Institutional financial support strategies and priorities. • Potential to stifle development of other, competing groups in the area • Difficult to find reviewers that are unbiased • NCoE's need a balance between local expertise development and broad scientific usage.
External	**Opportunities** • Maximise knowledge base and education in the highest levels of expertise • World leading science • Maximise excellence and impact • Versatile and adaptable • New technology development, newIP • Go-to place for experts • Excellent specialist training • Work with manufacturers and industry to develop new tools and applications • International exposure and public profile for higher impact • Collaborations cross-disciplinary and international opportunities • Remote access to expensive equipment • Proof of principle data generation	**Threats** • A temptation to focus on the 'low hanging fruit' easy/lucrative samples rather than the best science. • Metrics appropriate to generation of high quality results rather than throughput (quality over quantity) • Short term and inadequate funding models. Short-termism in funding. Usually instruments are funded, but personnel, maintenance, and supplies are only funded for a few years, after which the instrument sits underutilised or decaying. • Brain drain of expertise to other places, but a healthy turnover is needed to prevent stagnation of staff. Manufacturers hire staff away. • Lack of pipeline for development of good staff, students, apprenticeships, PDRAs, etc. • Resistance to this model because it threatens access to equipment locally. • Changes in government and institutional funding priorities. • Lack of data processing tools for users. Normally, the data processing tools provided by manufacturers are severely overpriced outside of the core lab. • Drift away from the forefront of the field. • Key staff losses and lack of succession planning. • Staff stagnation

Tier 4: A single national mass spectrometry facility

Defined as THE experts in all aspects of mass spectrometry.

	Helpful	Harmful
Internal	**Strengths** • A beacon for UK mass spectrometry to raise the profile nationally and internationally • Can push the boundaries in applications, technologies, methods, commercial engagement, vision, leadership. • Exposure of mass spectrometry to the wider science audience, and beyond science. • Expert commentators for government, etc. • Accreditation for training and CPD • Great (international) PR • A testbed for new technology • A networking hub for mass spectrometry	**Weaknesses** • Needs major continuous funding to get to and sustain this facility at a world-leading level. Needs a funding timescale of 20 years or more. • Science needs to travel to a fixed location, preferential access for locals • Diverse and large number of world-recognised experts needed to cover all topics and techniques • Management needs to be versatile and evolving and solid over 20 years • Constant demand for reports from UKRI and others – without adequate administrative support. • Undermines mass spectrometry elsewhere in the UK and virtually wipes out tier 1 and 2. • Can be restrictive of diversity of research • Competes with other MS groups. • Tricky charging models, with many potential difficulties and significant administrative burden. • Reduced opportunities for MS research in the UK.
External	**Opportunities** • Center for networking and training and accreditation • Can influence hardware and software development worldwide • Can influence curriculum and provide hands-on training • Hub for teachers • A nucleus of startup opportunities for SMEs • Decrease of duplication of teaching/training • Can promote and provide cloud-based data storage and analysis tools. • Excellent equipment sharing. • Equipment can be fully sustainable – with adequate financial support. • Can have local, regional, and national economic impact • Can lead outreach activities • Great potential for attracting industrial funding	**Threats** • No support from the UK MS community as it's a threat to their own continued funding. • Could lose direction and momentum without lots of marketing and outreach to the broader science community • Undercutting by other facilities • Affordable and sustainable financial model, researchers are not accustomed to paying full sustainable access charges for mass spectrometry after decades of 'free at the point of use' service and institutional subsidisation of mass spectrometry services. • Will almost certainly lose expertise in some areas. There will be 'gaps' in the provision of capabilities. • Co-funding of equipment and other costs is easier for internal, institutional facilities rather than one which is nationally outward facing. • Single point of failure – catastrophic events. • A 'jack of all trades' is a master of none. • Thinking too small.