CRITICAL MASS UK LARGE INFRASTRUCTURE BID

TOWN HALL MEETING SUMMARY REPORT

A Community Centred Bid for British Mass Spectrometry

A once in a generation opportunity!

2022

CRITICAL MASS UK LARGE INFRASTRUCTURE BID

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C-MASS Town Hall Meeting Summary Report 2022

Dear Colleagues,

We would like to express a huge thank you to the 245 members of our community that registered for, and contributed to the C-MASS UK TOWN HALL MEETING on the 20th January 2022.

A summary of the notes from that Town Hall meeting are set out below (*i.e.* from the breakout session Chairs' & Scribes' notes, supplemented with salient quotations).

We are very grateful for your continued engagement with the **C-MASS UK LARGE INFRASTRUCTURE BID PROJECT!**

With best wishes

The C-Mass UK Team

CRITICAL MASS UK
LARGE INFRASTRUCTURE BID

BIOSCIENCE & BIOTECHNOLOGY (I) – GENERAL

Session Chair: Kathryn Lilly

Session Scribe: Gavin O'Connor

GENERAL COMMENTS:
We can progress much faster as a field if we work together. We need to advocate the practical benefits of MS *w.r.t* PCR.
Data curation is key to delivery/success.

QUESTIONS:

1. What do you need mass spectrometry to do over the next 5 years? What is lacking in your field of work right now? Are current instrumentation and techniques adequate for your work? (*Including expertise and personnel, sample preparation, introduction capabilities, workflows, data*).

Generation of large Data sets across multiple centres to address "great Challenges "

Unrestricted access to the generation of data (access to centres , omics *etc.*) more instruments and larger scale experiments.

Assuring comparability of data (standardisation).

Think of it all holistically, Automation of biomarker sample prep through to MS.

Scale; Cutting current experiments to fit (limited) instrument capacity.

Trained users; Understanding of power and even existence of MS technology at higher decision levels in Gov *et*c. Keep technology fresh!

2. What 21st century data challenges can you foresee in the next decade?

Integration of data: Different software platforms that read & access data. Central facilities, Relational dBs, open access, (*e.g.* image data) meta data *etc*. Better sharing of data. Need infrastructure to assure quality of data (UK/ universal wide interface for MS?).

3. What kind of infrastructure is needed to deliver the developments required in your field of work? What would happen if this infrastructure is not funded?

Access to high end instruments. Lack of global scientific competitiveness.

4. What are the big questions you would be able to answer with this infrastructure? How do you want mass spectrometry to contribute to society in the next decade?

Living healthier, need to understand cell aging (senescent cells). Decline in immune system/ understanding the ageing metabolome

Early warning systems for Pathogens and real time monitoring of bioprocess manufacture.

Molecular assemblies & monitoring their interactions and proteoforms.

Supported by Al/ML data interrogation & QC

TAKE HOME NOTES:
High quality data is axiomatic, and Innovative approaches to securely sharing such data is essential to allow mining of UK data assets and thus leveraging new research challenges!

"Increased sensitivity to low sample volumes – e.g. single cells, single organelles".

"Extensive biochemical analysis of plasma and other samples will be an ongoing process over the coming years".

"A full analysis of the metabolome and proteome of the biofluids collected by UK Biobank will add greatly to our knowledge of biomarker for wellness and illness. This is best achieved with mass spectrometry for assured specificity and absolute quantification".

"Health & post pandemic diagnostics, and prognostics, precision medicine, analysis of new modalities of drugs – here the link to the UK Biobank will provide a multiomics base line of clinical utility".

BIOSCIENCE & BIOTECHNOLOGY (II) – CLINICAL & MEDICAL

Session Chair: Don Jones

Session Scribe: Alison Ashcroft

GENERAL COMMENTS:

QUESTIONS:

1. What do you need mass spectrometry to do over the next 5 years? What is lacking in your field of work right now? Are current instrumentation and techniques adequate for your work? (*Including expertise and personnel, sample preparation, introduction capabilities, workflows, data*).

Increase capacity, MS cheap and easy to run and automated as AI techniques. Method development (+chromatography). Standardisation methods, data (inc. repositories), smart automation (increase data quality and throughput). Separation between discovery and clinical assay requirements

2.What 21st century data challenges can you foresee in the next decade?

Complex data challenge. Translating to non-MS person. Open access data required. Bringing together metadata with MS data. Sharing metabolomics (MS workbench and EBI). Involvement of epidemiology studies. Role of QCs. Difficulties with large sets of patient data.

3. What kind of infrastructure is needed to deliver the developments required in your field of work? What would happen if this infrastructure is not funded?

National network. Translational and rapid development of clinical assays. Bringing in NHS and industry. If not funded, UK wouldn't compete with EU or US. Role of AI for prediction in complex data sets… heavy duty computing to bring together individual NHS groups. Training/ knowledge exchange is critical.

4. What are the big questions you would be able to answer with this infrastructure? How do you want mass spectrometry to contribute to society in the next decade?

MS and NHS labs with Industry. Synergy between manufacturers. Regional spokes. Rapid translational of clinical assays.

MS analysis of very large characterised cohorts including biobank UK, avon longtitudinal, our future health.

Assay for wellness

Large layered infrastructure for discovery through to clinical implementation.

Method development

5. What is your Moonshot idea?

Rapid translational of clinical assays

TAKE HOME NOTES:

"The use of innovative MS for large organic particles (e.g., protein polymers, organic polymers, nanoparticles, virions, microparticles). In particular MS advancements (e.g., innovative sample separation/preparation, innovative ionisation, innovative mass analyser, innovative detector) for viral analysis".

"Precision medicine is a priority. For this to be rolled out across the NHS better diagnostics will be required and many solutions will be MS based".

"The paucity of diagnostic capability in the UK during the Covid pandemic must be addressed in the future with increased investment in MS diagnostics".

CLIMATE CHANGE & ENVIRONMENTAL RESEARCH

Session Chair: Ruth Godfrey

Session Scribe: Ashley Sage

GENERAL COMMENTS:
The overall focus of the C-MASS 'Climate Change & Environmental' grouping needs to be revisited. Initial feedback suggests that the scope should be expanded to include the food, energy and fuel sciences.

QUESTIONS:

1. What do you need mass spectrometry to do over the next 5 years? What is lacking in your field of work right now? Are current instrumentation and techniques adequate for your work? (*Including expertise and personnel, sample preparation, introduction capabilities, workflows, data*).

Environmental can be seen as a relatively minor player/under-represented *w.r.t.* Inorganic/ Geology/Geochemistry.

Energy/transport/space exploration/security is underrepresented in funding or access to cutting edge mass spectrometry.

Organic chemistry requires more focus. Food science also require more focus – very limited representation today in the discussions.

Field deployable technologies require focus to develop – MS at the point of testing

UK behind countries like France/US for inorganic MS analysis.

One of the nodes should be inorganic and isotope ratio MS.

Environment and climate change represent one of the biggest challenges faced by mankind but only <8% UKRI spend currently.

Training and retention of personnel is a very important topic, alongside current instrumentation.

2.What 21st century data challenges can you foresee in the next decade?

Interfacing technologies.

Look at the whole picture from chromatography, sample prep, to data analysis

Organic/inorganic MS fundamental to evolving legislation *e.g.* impending investment in biofuel characterization.

Open data networks required, …comparable data across (UK) labs is a key.

3. What kind of infrastructure is needed to deliver the developments required in your field of work? What would happen if this infrastructure is not funded?

A state-of-the-art array of both organic and inorganic MS technologies will be required.

Environmental protection regulations are constantly changing. We must be adequately resourced is these objectives are to be realistically implemented and policed.

Climate Change
& Environmental

A strategy for regular replacement of instruments with new technology`; lease programs should be evaluated with integral upgrade programmes.

Access to up-to-date software; data access, integration and management are axiomatic.

Data archival and retrieval; how do we do this? Legacy software goes out of date so the data may/will be lost.

Routine instrumentation & high end equipment (as required) need to be readily accessible.

Recurrent funding of instrumentation in facilities needs more thought. This must be sustainable over a decade+ to achieve true ROI on (primary/up-front) capital expenditure.

4. What are the big questions you would be able to answer with this infrastructure? How do you want mass spectrometry to contribute to society in the next decade?

Environmental protection regulations are constantly changing. We must be adequately resourced is these objectives are to be realistically implemented and policed.

Quality Assurance (QA/QC) *e.g.* biofuel monitoring; will require deployable/portable MS to take the analysis to the problem!

Lower running costs for MS instruments.

Environmental chemical complexity is a huge challenge; MS has a major part to play to unravel this complex challenge..

Training of staff is important for the future *w.r.t.* both instrument ROI and data interpretation. How shall this be funded?

CPD programs must be implemented!

Sustainable funding for the next decade must be secured to ensure viable momentum & ROI?

5. What is your Moonshot idea?
Environmental protections and regulations are constantly changing

Quality assurance – take the analysis to the problem!

The complexity of environmental chemistry is a huge strategic challenge. MS, in combination with separations science (HPLC, *etc*.), has a pivotal role to play in unraveling this real world challenge.

TAKE HOME NOTES:

Enviro/Geochem/food/energy/fuels/security seen receives relatively low funding compared to other science areas – a broad community with very diverse applications

Sustainable & Recurrent Funding for staff and instrumentation, whether routine or cutting edge, required

Replacement/upgrade programs for instrumentation i.e. leasing to maintain both cutting edge and routine to allow end user access.

Data management/archival and retrieval important for future access. How do we cope with old data with current instruments on current SW platforms. Better data sharing.

How to retain staff and thus knowledge base.

"I think a more inclusive title would be good. I think the food and agricultural sector have a big contribution here, as well as the fuel industry".

ADVANCED STRUCTURAL CHARACTERIZATION & NEW MATERIALS

Session Chair: Julie Herniman

Session Scribe: Anneke Lubben

GENERAL COMMENTS:

QUESTIONS:

What do you need mass spectrometry to do over the next 5 years? What is lacking in your field of work right now? Are current instrumentation and techniques adequate for your work? (*Including expertise and personnel, sample preparation, introduction capabilities, workflows, data*).

Skills shortage and lack of a pipeline in skilled mass spectrometrists for fundamental spectral interpretation.

'Structural elucidation is a dying skill', and soon there will be very few people left who have these skills. Without them we will not be able to fully harness the structural elucidation tools we have available or will develop.

The pipeline needs to go from undergraduate teaching up to the highest level, and needs to determine what skills even the routine operators in high through put labs will need.

Possible training solutions – CDT with students being trained at multiple sites in different MS skills, as well as going into Industry for the applications specific training. More industrial placements for undergraduates for hands-on skills development.

Mass spectrometry needs to be a career which is aspired to to ensure that the skilled personnel are retained in the field. Needs good prospects, pay and easy transitions between industry and academia.

Need better software compliance for GLP settings (audit trails, user logins etc.), and effective tools for QC labs to ensure high quality data which is fit for purpose.

Need technological developments in resolution, sensitivity and ion mobility e.g. to enable better structural elucidation of high molecular weight species – to complement/ augment capabilities in cryoEM and X-Ray crystallography – what could be achieved with a complementary approach here?

2.What 21st century data challenges can you foresee in the next decade?

There will be issues with data amount, size of data files and complexity of the data, especially when you also consider sharing of that data. And we need to consider the environmental impact of storing all of this data – are there better compression tools which don't result in deep information being lost?

Need to consider data integrity and accuracy to ensure transferability.

Structural Characterization

Do we have the skills to interpret the data? With AI/machine learning help with this? Does a more automated system result in dumbing down and the skills being further eroded?

Need to get more out of the data we generate – needs new tools to get deeper insights. Could we get more 3D information, pushing reliance on NMR out of these initial stages of structural elucidation – especially for complex samples with analytes at low concentrations?

Each MS field has it's own approaches for data acquisition, curation, mining etc. need to come together to share best practice, curate it, and develop robust processes to pull the information out of the data.

3. What kind of infrastructure is needed to deliver the developments required in your field of work? What would happen if this infrastructure is not funded?

This field needs a wide variety of different tools, usually high-end, for the different sample types etc. This is not often available locally and there is a lack of knowledge about what is available and where. We need visibility of what is available and effective access methods to be able too use the instrumentation and expertise. If we don't have this we end up adapting the research question simply to use locally available tools, rather than seeking out the right tools for the job.

The high-end capability has to be accompanied by the expertise to run it, and interpret the data, otherwise R&D will move away from (UK) MS and maybe even result in less investment in UK R&D.

It is important that academia effectively provides access to high-end instrumentation to industry – to use on an ad hoc basis or to evaluate the technology. This is important to UK industrial R&D.

'Ideally no research question is limited by access to technology" – we need a coordinated and networked infrastructure to provide the tools and people needed when required.

4. What are the big questions you would be able to answer with this infrastructure? How do you want mass spectrometry to contribute to society in the next decade?

Need to consider RC priorities and see which of these MS would not help to progress, if the necessary tools and expertise were available. Centralising and networking the infrastructure would accelerate all of the priorities, but needs relevant expertise, unified approach, sharing of best practice. Having this in place will also accelerate outputs when new challenges emerge, and therefore put UK R&D at the forefront of publications rather than trying to scrabble around to find the appropriate resources.

5. What is your Moonshot idea?

Characterise full bacteria and metabolomes resulting in new antibiotics/anticancer drugs.

TAKE HOME NOTES:

This investment would bring the UK up to the level of our international competitors. In addition this coordinated effort could even take us to the premier spot in terms of accelerating best practice and reactivity to new societal challenges.

"Structural elucidation is a dying skill, and soon there will be very few people left who have these skills".

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SPATIALLY RESOLVED MASS SPECTROMETRY

Session Chair: Malcolm Clench

Session Scribe: Tony Bristow

GENERAL COMMENTS:

QUESTIONS:

1. What do you need mass spectrometry to do over the next 5 years? What is lacking in your field of work right now? Are current instrumentation and techniques adequate for your work? (*Including expertise and personnel, sample preparation, introduction capabilities, workflows, data*).

Sensitivity for low sample volumes and greater spatial resolution.

Software not fulfilling the needs.

Need niche software, bespoke, funding not available. Applications − forensics.

Proteomics and spatially resolved MS - localisation of proteins.

Speed, specificity, speed of analysis, speed of processing. Confidence in assignment. Proteomics and machine learning/AI, where do we need to sample on the tissue.

Adequate tools are available for some applications, but the tools are equal. Annotation of the data is a challenge. Data analysis workflows.

Compatibility with MS & other technologies, e.g. cytometry.

Targetted analysis. Integration of multi-modalities (other technologies).

2.What 21st century data challenges can you foresee in the next decade?

AI/machine learning is key.
Better metabolite identification.

Data integration from all omics and data quality - not just the MS elements.
Data into information
This is not just to fund more mass spectrometers.
Industry perspective - accessing the technology in academia, makes more accessible for industry. How does academic innovation role out.

A UKRI data repository where all data is stored and is accessible - compulsory
AI guides the user it does not replace the user and the expert.

Data challenge, is what does the data mean, what is the new knowledge.

Extract information with confidence and correct.

Unique problem - *highest dimensionallity data, spectral and spatial*, using approaches from other areas (proteomics) has not solved the challenge.

Spatially Resolved
Mass Spectrometry

3. What kind of infrastructure is needed to deliver the developments required in your field of work? What would happen if this infrastructure is not funded?

Instrumental development in academia, this needs to be part of this bid.

Training is essential. Develop students and post docs who are able to take apart instruments and can move into instrument design.

Single cell imaging - a priority!
Training people to interpret data and from a very wide background in the spatially resolved MS world. Doctoral training for MS imaging.
Comment - institutions could also make capital investments. People are a big issue to develop an support.

4. What are the big questions you would be able to answer with this infrastructure? How do you want mass spectrometry to contribute to society in the next decade?

If there is no strategic investment, spatially resolved MS will not substantively contribute to personalized/segmented medicine which would be a massive missed opportunity!

5. What is your Moonshot idea?
Development of single cell spatially resolved MS analysis technology, to enable translational (*c.f.* life science) research.

TAKE HOME NOTES:
Instrumentation development will be key.
MS imaging used in healthcare settings - histopathology to take it to the next level, so anyone can use it in clinical setting.
Overcome the translational hurdle.
How is MS imaging going to contribute to personalised medicine.
Biosciences - if go to single cell level and spatial effects in cells
Potential in materials sciences - Li, hydrogen economy and energy.
Forensics.
Roll out MS imaging to other areas.

"Development of next generation spatially resolved MS technology will be key in enabling UK based translational research".

NEXT GENERATION MASS SPECTROMETRY

Session Chair: Rainer Cramer

Session Scribe: Peter O'Connor

GENERAL COMMENTS:
Sustainability of instruments and capabilities.

Training at all levels is critical as we have a personnel skills gap.

QUESTIONS:

1. What do you need mass spectrometry to do over the next 5 years? What is lacking in your field of work right now? Are current instrumentation and techniques adequate for your work? (*Including expertise and personnel, sample preparation, introduction capabilities, workflows, data*).

A universal MS detector, including a universal ionization source would really be great. Also mentioned was the idea of a 'zero sample prep' setup – which of course means the sample prep must be integrated into the instruments.

2.What 21st century data challenges can you foresee in the next decade?

Data challenges are critical: Curation, Comparability, normalization, quality control, shareability – links to AI/ML and larger big data statistical tools.

Quantum technologies and Matter Wave technologies are an exciting new opportunity!

Combining spectroscopy (IR, UV/Vis, NMR) with mass spectrometry will be enabling.

Miniaturization of instruments important; also critically linked to data challenges.

A Universal API for instruments, including LC and workflows, would be strategic. This needs to be done at a very high level to get most instrument vendors involved and working toward using this API.

3. What kind of infrastructure is needed to deliver the developments required in your field of work? What would happen if this infrastructure is not funded?

Resources to prototype new technology and constructive partnerships with industry.

4. What are the big questions you would be able to answer with this infrastructure? How do you want mass spectrometry to contribute to society in the next decade?

Clinical Diagnostics and point-of-use MS technologies are an obvious direction of work.

5. What is your Moonshot idea?
A universally accessible MS detector, including a universal ionization source.

TAKE HOME NOTES:
Constructive partnerships with industry (large/SME, instrumentation/applications) is well done in the UK, and we need to build on that.

Next Generation
Mass Spectrometry

TAKE HOME NOTES (Continued):

Need to be able to share data between instruments, vendors, labs, and people – so the data need to be comparable (*i.e.* SOPs).

New quantum and matter wave technologies.

Dynamic, cloud-based data curation and real time molecular characterisation (AI, integration with bioinformatics.

Data reliability, speed, and multiplexing Clinical diagnostics with real validated result; rugged, miniaturised, point-of-care/point-of-use instrumentation.

Integration of MS with surrounding infrastructure such as LC, data analysis, etcetera (universal, vendor-neutral API)

Ruggedised, sustainable instrumentation

Standardised data formats for integration with 3rd party data analysis tools

Comparability of data from different instruments is needed.

Blue-skies hardware R&D is needed.

Zero (or minimal) sample prep MS

Integration of MS with various optical spectroscopies

Need the ability to retain and train next-generation instrumentation researchers. This is a very big issue because good instrumentalists take ages to train and are so very valuable, and are routinely poached.

"Deployable MS is a much better title".

Resources to prototype new technology and Constructively partnership with industry are critical.

We need to be able to share data between instruments, vendors, labs, and people – so the data need to be comparable.

Data challenges are critical!

Training at all levels is critical, …as we have a significant skills gap.

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SUMMARY OF C-MASS UK MOONSHOTS

The following community derived ‘Moon Shots’ have been distilled from the Town Hall discussions and correspondence reported above:

1. **Improved detection/characterization of emitted smells will give new insights into human ageing, and early detection of manageable chronic age-related diseases.**
2. **Improve bioprocesses to maximise efficiency and yield resulting in cheaper development of new processes and cheaper end products**
3. **Improved understanding of the metabolome to find new solutions to antimicrobial resistance and anti-cancer drug targets.**
4. **Biomarker identification through screening of large population cohorts to establish a wellness assay and optimize future medicine regimes.**
5. **Standardize data formats will enable effective data sharing across sectors allowing for retrospective mining of existing datasets for new research questions.**
6. **Connected infrastructure for accelerated reactivity to new societal challenges e.g. pandemics, water security or national security incidents.**
7. **Real-time hazard monitoring to secure UK water and food resources.**
8. **Miniaturized instrumentation for point-of-use will reducing NHS waiting times and costs.**

Digital Integration
and Outreach

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"What wasn't actually entirely clear is how, once in the pot, this money would be spent".

"This funding should not be intended for routine sample analysis services".

"Ideally, UK infrastructure should include world-class centers of excellence, focused on key applications (e.g. protein analysis, biopharmaceuticals, pesticides, etc.). These should become homes for both analytical staff running large-scale analysis for payment, and academic researchers that own specialized instruments. These will need to be strongly linked to Tech transfer offices and venture capital organizations".

"We need strategic changes for UK MS data storage and secure sharing".

"Interpreting spectra of unknown small molecules (e.g. pharma, metabolites, impurities, degradants etc.) is a dwindling capability and it is vital that we revive this strategic skill if new medicines, etc., are to be developed and patented in the UK".

SUMMARY & RECOMMENDATIONS

Summary:

1. **THE C-MASS UK TOWN HALL MEETING:**
   - This event was enthusiastically supported by 245 registered delegates.
2. **FUNDING OBJECTIVES & CONSEQUENCES:**
   - A commonly held misconception is that the C-MASS UK Large infrastructure Bid may cannibalise existing funding.
3. **DATA CURATION/MANAGEMENT, AND SECURE SHARING:**
   - 'Data' were a consistent and recurring theme in colleagues' discussions.
   - If the C-MASS UK community is to deliver a robust return on (potential) tax payers' investment - innovative approaches to secure data management, data integration and secure data sharing will be the fulcrum to leverage our community's contribution to UK PLC.
4. **FRAMING THE BID:**
   - The scope and reach of the proposed C-MASS UK Large Infrastructure Bid proposal may be too broad? This perspective was not universally articulated but was significantly expressed.
   - The focus of the C-MASS 'Climate Change and Environmental' grouping should be expanded to include; food, energy and fuel interests.
5. **NURTURING NEW PEOPLE:**
   - 'People' were a consistent and recurring theme in colleagues' discussions.
   - The C-MASS UK Large Infrastructure Bid is focused on capital expenditure (*i.e.* not people).
   - It must be noted that capital expenditure alone will NOT achieve the desired objective.

Recommendations:

1. **CLARIFICATION OF BID CONSEQUENCES**
   - Colleagues should be reminded that the C-MASS UK Large infrastructure Bid is for incremental capital investment of *Ca* £100M, …which is additional to the existing capital equipment funding streams through individual UKRI Research Councils.
2. **FRAMING THE FINAL BID:**
   - The C-MASS UK Bid Team should pause for thought before drafting the final submission.
   - Re-evaluation of the scope and breadth of the Bid proposal is encouraged.
   - The C-MASS 'Climate Change and Environmental' grouping should include food, energy and fuel interests in the final bid.
3. **DATA SECURITY CONSIDERATIONS:**
   - The C-MASS UK Bid Team should consult with the National Cyber Security Centre (NCSC) to ensure best practice is embedded within the C-MASS UK Large Infrastructure Bid Proposal: http://www.ncsc.gov.uk/
4. **CONFIRMATORY CONSULTATION:**
   - The C-MASS UK Bid Team are encouraged to consult with the community (via e-mail) prior to submission of the final bid document.

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THE BMSS

The British Mass Spectrometry Society is a UK registered charity, founded in 1964. The BMSS strives to encourage participation in all aspects of mass spectrometry on the widest basis, to promote knowledge and advancement in the field and to provide a forum for the exchange of views and information. The BMSS is committed to ensuring equal opportunities and reflecting the diversity of British society as a whole.

UK CHARITY NUMBER 281330

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