A Vision for Mass Spectrometry in the United Kingdom

from the British Society for Mass Spectrometry (BMSS)

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Society faces many challenges requiring a concerted and coordinated effort by our scientists and engineers in both academia and industry, relying heavily on a wide range of cutting-edge analytical measurement approaches. Mass spectrometry (MS) is a measurement technique integral to all aspects of molecular science in chemistry, physics, engineering, biochemistry, the environment and medicine. Over the past 30-40 years, MS has seen exponential growth in development, use and impact due to a strong coupling between mass spectrometry manufacturers, academia, and industry. This has resulted in entirely new industries (e.g. contract research organisations) and scientific fields (e.g. proteomics, metabolomics, and many other 'omics) where MS plays a central role, to meet the rising demand from the wider scientific and industrial community.

Mass spectrometry is a fundamental element of the scientific spectrum in the UK and should be viewed as such, with recognition, support, and investment that reflects this critical role and facilitates continued research and development to deliver continued impacts to our society.

Societal challenges requiring mass spectrometry to take a central role are broad and varied. Given appropriate support, mass spectrometry in the ***life sciences*** has a potential to facilitate cell screening, providing molecular profiles for single cells, to unravel disordered states of proteins, and to determine the function of individual proteins to enable an understanding of the biochemical interactions at biological interfaces such as cell membranes. As the collaborations between industry and academia act to advance MS instrumentation (hardware, software, data storage/sharing) there will be much greater translation of this technology into ***healthcare*** with robust hand-held, sensitive and selective, point-of-care devices for real-time decision guidance in the clinic. Mass spectrometry is already critical across the ***pharmaceutical sciences***. With further improvements in separation techniques and instrument sensitivity, it will be mass spectrometrists and their collaborators who will deepen our understanding of diseases, mapping disease progression, characterising novel therapeutics, and introducing new methods for early-stage diagnosis. ***Biomanufacturing*** cannot develop without concomitant progression in mass spectrometry.

Climate change is a grand challenge that requires immediate attention, and mass spectrometry has a crucial role to play in understanding and sustaining the environment we live in. There is on-going research to develop user friendly and accurate MS-based detection systems to monitor our water supplies and air quality, and to detect and identify ground pollutants in emergency situations. Developments in ***Energy solutions*** for the future (petroleum, biofuels, recycled bio-oils), smart materials, (nanoscience), solar cells, catalysts, hydrogen storage cells, energy and resource saving molecular electronics are all driven by molecular characterisation using mass spectrometry. If you cannot measure and characterise it, you cannot build it; these technologies can only grow in conjunction with developments in mass spectrometry capability and capacity.

Plastic leachables are a serious concern in both ***food safety*** and the ***environment***, and their characterisation is dependent on a variety of mass spectrometry approaches. Food security is key to the UK, and the suitability of this resource is increasingly important as the world's population continues to grow. Many aspects of crop development and food safety require mass spectrometry, both at the molecular level to detect toxins or identify fraudulent products, and at the organism level to identify pathogens, study resilience to drought conditions, and investigate growth stages of seeds and other food stocks.

We live in a complex world, with multiple interconnecting factors at play within the systems we study. Mass spectrometry is increasingly used to deconstruct these complex systems. This requires approaches which not only target expected components, but can also detect and identify unknowns, often at very low concentrations, and in very complex mixtures; mass spectrometry can do this, and is one of the few analytical tools that can deconstruct whole samples in a single analysis, moving towards direct measurement of all components present. Developments in ionisation of samples to increase the types of materials being analysed, combined with innovations in ***separation science*** (ion mobility separation, multidimensional chromatography and chromatography column technology) and ultra-high mass resolution, will spread the technology beyond the traditional haunts for mass spectrometry, continuing to increase the diversity of mass spectrometers in use, and scientists, clinicians, and non-experts using them. This variety, density, and complexity of data will require new software tools to enable scientists to reliably extract all the meaningful data. These transportable technologies will see bespoke MS-based instrumentation transition into arenas including national security (biological and chemical warfare agents, explosives) and criminology (counterfeit detection, controlled substances) as well as the more familiar space exploration. There are continuing efforts to integrate machine learning into technological developments, using artificial intelligence with mass spectrometry data to streamline the processes from detection to information from MS-based detectors. We see the world around us in picture form. In recent years exponential advances in ***imaging*** mass spectrometry has given us a unique way to view the 2D and 3D spatially resolved molecular map of biological tissues, plants and forensic fingerprint and hair analyses. The shear complexity of this data will drive new strategies into managing '***big data***' and to standardizing data formats, databases and data storage/access.

Mass spectrometry is critical to many aspects of our UK R&D effort, and to ensuring economic growth, but MS is a catch-all term for a fundamental analytical approach which mass spectrometrists have developed into multiple instrument configurations to meet the demands of the many research areas.

Investment in academia for inclusive infrastructure, people and education will enable mass spectrometrists and mass spectrometry to continue to deliver on the challenges outlined, impacting on UK R&D excellence, and directly contributing to UK economic growth and prosperity. Both technological and volume demands on mass spectrometry will continue to increase rapidly.

This document is a summary of the input from four rounds of a DELPHI study which included direct input from a panel of MS experts from across the UK MS community who were asked to comment on the future of MS in the UK, the needs for MS and how this could be made available for the societal challenges we face. This preliminary report outlines conclusions on the first two stages, and suggestions on how this could be enabled will be forthcoming in due course.