Catalyst Editorial Team

What’s in your tank? Determining biofuel origin and quality

LGC is developing new methods to allow reliable discrimination between biofuels of different origin in order to ensure that such fuels are sourced sustainably.

EU policies on climate protection, food production and sustainable development require detailed information on the origin of marketed biofuels.

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Round up of LGC’s recent activities under the NMS Chemical and Biological Metrology Programme

LGC and Barts Cancer Institute pioneer research into the benefits of selenium in combination cancer therapies

LGC is collaborating with Barts Cancer Institute at St Bartholomew’s Hospital to develop new methods to better understand the effects of selenium in cancer treatment. The research project reflects the increasing awareness amongst cancer researchers that selenium may be beneficial both in preventing cancer and in improving the efficacy of cancer therapies.

New wheat flour reference material for safer fortified foods

LGC has developed a new wheat flour matrix certified reference material for accurate characterisation of selenium-enriched food products and supplements. For consumers this will increase the integrity of the significant health benefit claims made for fortified foods, and will satisfy the requirements of suppliers seeking to distribute selenium enriched food.

New methodology to measure arsenic in tobacco products

Using expertise developed through the National Measurement System, scientists at LGC have developed a new, sensitive method to determine the low levels of arsenic species present in cut tobacco and mainstream cigarette smoke. Group Research & Development Centre of British American Tobacco, in support of their work programme into tobacco harm reduction, approached LGC to develop appropriate analytical methods capable of identifying the chemical forms of arsenic in cured tobacco and mainstream cigarette smoke.

Can the economy survive without a National Measurement System?

Julian Braybrook, Head of Strategy, Measurement Research at LGC speaks to the Parliamentary and Scientific Committee about the importance of measurement in innovation.

Improved reference material ensures UK drinking water safety

LGC has developed a new certified reference material for the determination of metals in hard drinking water to support the validation of water monitoring procedures and provide confidence in the quality of the results obtained.

What’s in your tank?
Determining biofuel origin and quality

LGC has produced a number of reference materials to support the analysis of fuels.

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Microarray technology offers alternative approach for toxicity testing

Building on experience from previous National Measurement System funded projects, LGC scientists have published the results of a study to determine the reproducibility of in vitro toxicogenomics data, which indicate that these methods are sufficiently robust and reproducible to allow their further investigation in regulatory risk assessment.

In vitro studies offer quicker, cheaper and more ethical alternatives to animal testing than conventional in vivo studies. Driven by the introduction of legislation such as REACH*, as well as an amendment to the Cosmetics Directive banning the marketing of cosmetic products containing ingredients tested on animals from 2013, there has been a concerted effort to develop in vitro assays for regulatory toxicity risk assessment.

Working in collaboration with the Fund for the Replacement of Animals in Medical Experiments (FRAME), Unilever, Agilent and the Institute for Health and Consumer Protection of the European Commission’s Joint Research Centre, LGC has designed an inter- and intra-laboratory study to assess whether the current generation of microarray technology is capable of generating robust, reproducible data of sufficient quality to show promise as a tool for regulatory risk assessment.

Whilst microarray platforms have been evaluated over the past 10 to 15 years in the pharmaceutical and chemical industries, recent improvements have made the technology more robust, thereby potentially offering a suitable alternative to costly animal testing.

In this study, three of the collaborating laboratories analysed a human liver cell model (HepG2) for gene expression, following exposure to the genotoxic carcinogen benzo[a]pyrene (BaP). Exposure of HepG2 cells to BaP has been used as an archetypal model for research into the mechanisms of genetic toxicity and forms the basis for many standardised testing studies. The abundance of existing data from previous toxicogenomic studies enabled direct comparisons with results from this research.

Mimicking a real-life regulatory testing environment and incorporating a well controlled standard operating procedure, the inter-laboratory study produced reproducible datasets, with each laboratory identifying the same key biological responses characteristic of a BaP-induced response. This provides further evidence that toxicogenomics can predict chemical toxicity in vitro, but importantly, shows that the technology can produce data of sufficient quality to show promise as a tool for toxicity testing in a regulatory setting.

As a result of these findings, research in this field is now focused on identifying the optimal cell system for generating reproducible data of the quality required for regulatory testing. This will hopefully lead to developing robust cell models that are predictive for a range of toxic chemicals of different toxicological mechanisms of action.

“The success of this collaboration highlights the increasing maturity of toxicogenomics and its potential as a predictive risk assessment tool. This data should provide encouragement within the toxicology community that an in vitro toxicogenomic approach is worthy of further development and validation and may become part of a risk assessment paradigm without animal testing.”

Dr Daniel Scott, Project Leader, LGC

LGC’s research on toxicity testing was described in a recently published paper ‘Inter- and intra-laboratory study to determine the reproducibility of toxicogenomics datasets’. D.J. Scott et al, Toxicology, 2011, 290, 1, 50-58

* REACH (Registration, Evaluation and Authorisation of Chemicals), the European Community Regulation on chemicals and their safe use, entered into force on 1 June 2007. REACH aims to improve the protection of human health and the environment through earlier and better identification of the properties of chemical substances.

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Recent publications describing LGC’s work carried out under the Chemical and Biological Metrology programme

Rat primary hepatocytes show enhanced performance and sensitivity to acetaminophen during three dimensional culture on a novel polyethylene scaffold designed for routine use M. Schutte et al, Assay Drug Dev. Technol., 2011, 9, 5, 475-486


Applicability of RNA standards for evaluating RT-qPCR assays and platforms A. S. Devonshire et al, BMC Genomics, 2011, 12, 118

Capabilities of HPLC with APEX-Q nebulisation ICP-MS and ESI MS/MS to compare selenium uptake and speciation of non-malignant with different B cell lymphoma lines H. Goenaga-Infante, Anal. Bioanal. Chem., 2011, 399, 5, 1789-1797

Contribution of the EMERALD project to assessing and improving microarray data quality V. Beisvag et al, Biotechniques, 2011, 50, 1, 27-31

Standardisation and reporting for nucleic acid quantification J. Huggett and S. Bustin, Accred. Qual. Assur., 2011, 16, 8-9, 399-405

Methylseleninic acid inhibits HDAC activity in different B cell lymphoma lines S. Kassam et al, Cancer Chemoth. Pharm., 2011, 68, 3, 815-821


Applicability of RNA standards for evaluating RT-qPCR assays and platforms A. S. Devonshire et al, BMC Genomics, 2011, 12, 118

Capabilities of HPLC with APEX-Q nebulisation ICP-MS and ESI MS/MS to compare selenium uptake and speciation of non-malignant with different B cell lymphoma lines H. Goenaga-Infante, Anal. Bioanal. Chem., 2011, 399, 5, 1789-1797

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Supporting diabetes treatment

There are >250,000 people diagnosed in the UK with type 1 diabetes†. The research described here demonstrates how LGC is employing new measurement capabilities to help improve treatment of diabetes.

† Diabetes prevalence 2010 (Oct 2010)

Novel 3D imaging to improve pancreatic islet transplant success for diabetes treatment

LGC, in collaboration with academics, industrial partners and accredited laboratories, has developed a novel imaging technique to improve the success rate of pancreatic islet transplants for people with type 1 diabetes.

In people with this type of diabetes, the beta cells in the pancreas are destroyed and no longer produce insulin. More than 250,000 of these individuals in the UK are dependent on multiple daily insulin injections or insulin pumps to restore stable glucose levels. Up to a third experience dangerous low glucose levels (severe hypoglycaemia) resulting in collapse without warning. These patients may benefit from a pancreatic islet transplant, a surgical procedure in which the healthy cells from a donor pancreas are transplanted into the portal vein of the recipient’s liver where they begin to release insulin and eventually take over full pancreatic function. However, cells in the pancreatic islet are fragile, so it is important to ensure they are in good condition prior to transplantation.

Light microscopy is currently used to assess islet cells prior to transplantation, but only provides a basic measure of islet quality. LGC’s new 3D imaging quality assessment procedure is looking to change this by providing high resolution quantitative information on the health of the islet cells identified for transplantation.

Using specialised fluorescent markers and laser scanning confocal microscopy, LGC scientists produce high resolution optical sections through each pancreatic islet which allows live, dying and dead cells to be identified. Software algorithms developed at LGC then process and reconstruct the information to create 3D profiles of the pancreatic islets. These profiles can help inform whether donor cells will yield a successful transplant.

LGC has been using this new method to create retrospective profiles of transplanted pancreatic islets, and is now extending the application to clinical samples. Once validated, the imaging system will permit pre-transplant assessment of islet quality enabling appropriate selection of donor cells which have the highest chance of achieving a successful transplantation. This in turn will improve the clinical outcome for patients with type 1 diabetes.

The pancreatic islet transplant programme is uniquely funded in the UK by the NHS following a bid coordinated by Prof James Shaw from Newcastle University on behalf of the UK Islet Transplant Consortium. It aims to improve clinical outcomes for patients and reduce the burden to the NHS of treatment for uncontrolled diabetes. The current work is focused around three of the UK clinical islet transplant centres in London, Newcastle upon Tyne and Edinburgh.

The National Measurement System funded the research capability which ensured the success of this project.

“"This novel tool offers the opportunity to improve the quality of life for a significant number of people with diabetes. This could only be achieved through collaborative research bringing together specialist skills, resources and knowledge from across the UK."

Dr Damian Marshall, Principal Scientist for Cell Biology, LGC

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Assessment of pancreatic islet quality showing a healthy islet with predominantly living cells (A), and islet with both living and dead cells (B) and an islet with dead cells (C)
Novel vanadium-based treatment for diabetes

Research suggests that vanadium – a transition metal present in plants and mammals in very low amounts – has the potential to treat diabetes due to its ability to mimic the effects of insulin. LGC is developing and validating methods for the accurate quantification of ultra-trace levels of vanadium-containing biomolecules to improve efficacy of vanadium drugs, and support diabetes treatment in the UK.

The main advantage of vanadium drugs in diabetes treatment, as compared to insulin, is that vanadium compounds are low molecular weight species that are stable in the gastric juice in the stomach, and therefore they can be administered orally. Despite numerous studies, the mechanism(s) by which vanadium is metabolised in vivo are still not completely understood. Therefore, research is necessary to better understand the biomolecules involved in the biochemical role of vanadium, and in their transport and storage in body fluids and tissue.

LGC is a recognised leader in elemental speciation analysis and is applying its unique capabilities in elemental and molecular mass spectrometry to study the speciation of vanadium in in vitro and in vivo diabetes models. It is anticipated that this research will provide more information on the biochemical forms and physiological functions of vanadium in higher organisms, and will support UK research for the optimisation of vanadium ‘insulin-mimics’ in diabetes treatment.

In the long term, LGC is working to aid the identification of the vanadium-based drugs that can most effectively replace or enhance insulin to improve the efficacy of treatment for patients with diabetes.

“Knowledge of the vanadium speciation in bioclinical samples will have implications on how best to address diabetes treatment in the UK. By understanding its metabolic effects we will be better positioned to develop improved vanadium drugs.”

Dr Heidi Goenaga-Infante, Principal Scientist for Mass Spectrometry, LGC

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A selection of certified reference materials produced with support from the Chemical and Biological Metrology programme.

Reference materials for analysis of foods and supplements
Chocolate certified for nitrogen, sugars, fat and butterfat content
Kavain certified for purity
Lager, brandy and wine certified for alcohol by volume
Malachite green oxalate and leucomalachite green certified for purity
Orange juice solutions certified for degrees Brix and Refractive Index
Plant root powder certified for kavain content
Potato powder certified for iodine content
Poultry feed certified for proximates and content of a range of elements
Processed meat certified for proximates, chloride, nitrate and hydroxyproline content
Selenomethionine enriched with $^{76}$Se with assessed value for the abundance of $^{76}$Se
Tomato paste certified for cadmium, lead and tin content
NEW Wheat flour certified for selenium and selenomethionine content
NEW Whisky characterised for congeners

Reference materials for environmental monitoring
NEW Hard drinking water certified for metals content
River water certified for content of trace elements
Sewage sludge certified for extractable metals content

Reference materials for fuels and transport
Automobile catalyst certified for palladium and platinum content
Petrol and diesel certified for sulfur content
Solvent yellow 124 certified for purity

Reference materials for the clinical sector
Creatinine and electrolytes (Li, K, Ca, Mg & Na), at a range of concentrations, in frozen human serum
NEW Digoxin in frozen serum
Pure Digoxin certified for purity
COMING SOON Tacrolimus in whole blood
Testosterone in frozen human serum
Theophylline certified for purity

Overcoming rejection – Reducing risk of organ rejection after transplant operations

Poor quality clinical measurements can lead to misdiagnosis or incorrect prescription of medicine for patients. It is therefore essential that measurements carried out by medical laboratories are accurate, and that results are traceable to a higher order reference standard or reference measurement procedure to ensure comparability between hospitals and analytical platforms. LGC has collaborated with UK industry to develop the first commutable, matrix clinical reference material for tacrolimus in whole blood.

The In Vitro Diagnostic Medical Devices Directive (EC IVDD, 98/79/EC) stipulates ‘the traceability of values assigned to calibrators and/or control materials must be assured through available reference measurement procedures and/or available reference materials of a higher order’. This ensures harmonisation of standards across Europe, providing a high level of health protection for patients. High accuracy, low uncertainty, traceable reference materials are necessary to satisfy the objectives of the directive. However, it is not unusual for different analytical platforms, calibrated using different reference materials, to be used to measure the same analyte. Therefore there is a need across the clinical community for ‘commutable’ reference materials that ensure traceable measurement results, independent of the analytical platform used.

Tacrolimus is measured by a variety of liquid chromatography mass spectrometry (LC-MS) and immunoassay based methods which are all calibrated independently, but without agreement on a common reference point such as an accepted reference method or higher order tacrolimus reference material. This means concentration values may not be comparable between methods or laboratories, posing potential risks to patients undergoing therapeutic drug monitoring. In severe cases this can lead to the patient either receiving an insufficient dosage and rejecting the organ, or receiving a high, toxic dose.

This lack of cross-platform comparability has been identified by medical laboratories and diagnostics kit manufacturers as an issue when trying to achieve consistent measurement results and in setting reliable therapeutic levels. In response to this requirement, researchers from LGC collaborated with UK diagnostic kit manufacturers, proficiency testing scheme providers and clinicians to develop the first commutable, matrix clinical reference material for tacrolimus in whole blood. This reference material will improve confidence in measurement, irrespective of the analytical platform used and will enable clinicians to set and maintain optimal patient dosage to the benefit of their patients and the healthcare system.

“The development of the tacrolimus reference material should help ensure that if a patient undergoing therapeutic drug monitoring is moved between hospitals, medical staff can maintain the correct drug dosage, irrespective of the analytical platform used by the hospitals.”

Dr Gavin O’Connor, Principal Scientist for Mass Spectrometry, LGC

LGC has produced a number of reference materials to support the clinical sector. Page 4 for list of reference materials

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From peptides to proteins – establishing traceability to the SI

Human growth hormone (hGH) is widely used in the diagnosis of disorders of children with short stature, management of disorders that lead to nutritional deficiency, and to monitor growth hormone replacement therapy. Therefore, there is a need for reliable and comparable measurements. In order to achieve this, routine measurement results need to be made traceable to a stable reference.

Advances in biosciences have been critical to improving human health, safety, and quality of life. Despite major breakthroughs and discoveries in recent years, understanding of biological systems still faces many challenges. Whilst traceability in chemical and physical measurement is well established, the biological measurement field is at a much earlier stage in its development, and clinical measurements in particular present their own set of unique problems. To improve the traceability and comparability of clinical measurements it is essential that certified reference materials are available for manufacturers to establish the traceability of values assigned to calibrators supplied with diagnostic equipment, and for medical and clinical laboratories to validate their methods.

To determine the concentration of hGH in serum, the protein is first ‘broken down’ into peptides. By choosing a number of peptide sequences unique to hGH, and by employing isotope dilution mass spectrometry, the concentration of the protein can be accurately determined. In this case the standards used were peptides and the concentration of the standard peptide solutions was determined by amino acid analysis. This establishes a firm anchor to the amount of substance of the amino acids whilst maintaining specificity to the hGH molecule, hence providing an unbroken link for the measurement results to the SI.

However, ‘amount of substance’ is not the only consideration when monitoring proteins such as hGH. Small differences in the primary structure of hGH may be expected due to differences in the genetic makeup of individuals. These differences may give rise to a different chemical structure due to different sequences of amino acids. But as many proteins are identified by function alone, the generic identity of the protein may remain unaltered. In addition, changes to a protein’s secondary, tertiary or quaternary structure may be transient, affecting the protein function, and be in itself indicative of a disease state. This means that it is not necessarily the total amount of the protein’s primary sequence that is important, but the amount of a protein in a particular structure or folding state.

Many of the routine measurement methods used for protein biomarkers are immunoassay based. The specific binding of proteins can be structurally dependant. Therefore, the key challenge for comparability of protein measurement results is not just the “amount of substance”, but the “function/activity” of the protein. Both these requirements may need to be considered in the future production of commutable reference materials. There is therefore a need to develop an understanding of the effects that protein structure may have on the traceability of measurement results for the amount of protein present.

Advanced mass spectrometry-based techniques such as hydrogen-deuterium exchange and ion mobility mass spectrometry enable interrogation of protein structure under physiological conditions, thereby providing a measure of the different structural forms of the protein present. During this research a number of different standard protein preparations of recombinant hGH were investigated. Knowing the difference in protein structures, the relative amounts of these structures, and the interaction of these structural forms with the detection antibodies used in immunoassay experiments will be an important factor in establishing the suitability of reference materials to standardise measurements. The ultimate aim of standardisation in clinical chemistry is to ensure comparability of routine measurements in order to achieve equivalence between results obtained by different methods.

“This research demonstrates the first steps towards developing a biometry framework that aims to encompass both metrological rigour in developing SI traceability, and the real concerns of the clinical community that measurements must be relevant and commutable, independent of the analytical platform used.”

Dr Gavin O’Connor, Principal Scientist for Mass Spectrometry, LGC

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LGC has published several papers on improving the traceability of proteins including:

Conformational changes in oxidatively stressed monoclonal antibodies studied by hydrogen exchange mass spectrometry
W. Burkitt, P. Domann, G. O’Connor, Protein Sci., 2010, 19, 826-835

Amine-reactive isobaric tagging reagents: Requirements for absolute quantification of proteins and peptides
The Chemical and Biological Metrology programme aims to improve the accuracy and reliability of chemical and bioanalytical measurements that are important to the UK’s industrial competitiveness and quality of life.

The programme achieves this aim through the application of leading-edge science and the development of improved measurement technology on a wide range of projects. In order to achieve maximum impact, the knowledge acquired throughout the delivery of the programme needs to be captured and disseminated via appropriate channels to target audiences. Therefore, knowledge transfer activities are essential to ensure the programme outputs are well disseminated to, and assimilated by, those carrying out chemical and biochemical measurements.

A key mechanism for dissemination from the technical projects is the publication of peer-reviewed papers in scientific journals. A comprehensive list of recent publications can be found on page 2 of this newsletter. However, a number of case studies and posters have also been developed to put into context the need for accurate measurements.

Whilst traditional dissemination methods of technical projects are essential, the Chemical and Biological Metrology Programme also focuses on knowledge transfer activities that include the production of guides and training materials. The ‘good practice guides’, published under this programme, collate extensive expertise on previously specialised topics that are now becoming mainstream. For example, LGC has considerable expertise in isotope ratio mass spectrometry, and in collaboration with the Forensic Isotope Ratio Mass Spectrometry (FIRMS) network, is collating key advice and technical information into a, “Good Practice Guide for Isotope Ratio Mass Spectrometry”, with the purpose of assisting laboratories in achieving reliable and robust stable isotope measurements.

Similarly, LGC is working with the Mass Spectrometry sub-committee of the Royal Society of Chemistry Analytical Methods Committee (RSC AMC) to produce guidelines on ‘Achieving reliable quantitative LC-MS’. This resource aims to be a technical guide which also addresses quality assurance and control aspects, including subjects such as validation, measurement uncertainty and data reporting.

Both guides will be made available free of charge on the Chemical and Biological Metrology website.

The National Measurement System also supports collaboration at an international level. LGC is very active within Eurachem (a network of organisations involved in promoting good practice in measurement science). Eurachem has produced a number of guides on measurement and quality assurance issues. LGC collaborated with Eurachem members on the development of the guide ‘Terminology in analytical measurement: Introduction to VIM3’ (VIM3: International vocabulary of metrology – Basic and General Concepts and Associated Terms) which was published in Spring 2011. This guide discusses a selection of the concepts in VIM3, focusing on those most likely to be encountered in analytical laboratories. It aims to cover chemical, biological and clinical measurements and it is intended for laboratory staff, accreditation bodies, for those commissioning measurements and for those using measurement results. LGC is also collaborating on the revision of the Eurachem/Citac guide on ‘Quantifying uncertainty in analytical measurement’.

Knowledge transfer is also achieved through workshops and seminars. LGC ran a very successful workshop in 2010 on the subject of “Accuracy in Molecular Measurement” and is following it by developing training resources on qPCR in collaboration with industrial and academic partners.

LGC has a long history of developing training resources in answer to demand for information and advice on analytical quality assurance topics and over time has developed a programme of training courses. The development of these courses was originally funded by the NMS and they cover topics such as method validation, statistics, measurement uncertainty, use of proficiency testing and are delivered on a commercial basis by the LGC training team.

All publications, posters, guides and information about training courses are available on the NMS Chemical and Biological Metrology website, www.nmschembio.org.uk.
International Year of Chemistry

Louise Dean, Impact & Knowledge Transfer Executive at LGC, discusses new methods being implemented at LGC to improve science communication.

2011, designated as the International Year of Chemistry (IYC 2011), was an entire year devoted to the celebration of chemistry. Under the unifying theme “Chemistry – our life, our future” IYC 2011 was a worldwide initiative to increase public appreciation of chemistry in meeting world needs, to encourage interest in chemistry among young people and to generate enthusiasm for the creative future of chemistry.

Spreading the word

Engagement with the wider scientific community and the public is fundamental to LGC’s role as a National Measurement Institute. 2011 has been a successful year at LGC, and to support IYC 2011, we have made substantial steps in developing new and exciting dissemination routes for our science. In a bid to not only raise the awareness of IYC 2011, but also to emphasise that developments in chemistry are essential for sustainability and improvements in every human being’s life, we have built a twitter page, under the name @LGCGroup, in order to communicate developments in science with a wide audience.

We also opened our doors to the public to coincide with World Metrology Day which celebrates the signing of the Meter Convention which took place 136 years ago on 20 May 1875. The Convention created the International Bureau of Weights and Measures (BIPM) and set the framework for global collaboration in measurement science and its industrial, commercial and social applications.

The open evening was attended by 300 members of the public, including schools, colleges and local residents. This was a fantastic opportunity for us to raise our profile within the local community and demonstrate how we are using our high specification equipment to improve healthcare, ensure food safety, and develop greener fuels.

In addition, to demonstrate the importance of chemistry and how chemistry affects almost every aspect of our daily lives, from the fuel in our cars and the quality of the air we breathe, to the safety of our food and water, and cosmetic products, we produced a poster to demonstrate how each of us interacts with chemistry through a typical day.

We have also had a feature article published in the September issue of Laboratory News, demonstrating how measurement research carried out under the NMS ensures the safety of our consumer products in our everyday lives.

Get connected

Under the umbrella of the National Measurement System, the UK’s National Measurement Institutes – LGC, NPL, NMO and NEL – developed the Measurement Network as an effective and powerful forum for people interested in measurement science to share information, collaborate, discuss ideas and identify events within relevant scientific communities.

The Measurement Network is one of over 20 national science networks with a presence on the Technology Strategy Board’s _connect platform, which is already a gateway to many thousands of people.

Why join the Measurement Network on _connect?

• Find collaborators and discover new funding opportunities
• Share measurement knowledge with measurement scientists
• Get advice from your peers and National Measurement System experts
• Find out about measurement-related events
• Get involved with working groups or other activities tailored to your own particular interests.

Join now


The new strategy sets out the action that Government is taking to support the National Measurement System (NMS) to meet the changing needs of business and society by encouraging economic growth, and improving the UK’s competitiveness and scientific excellence across all areas of business and government.