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| **Institution:** The Open University | | |
| **Unit of Assessment:** B09 Physics | | |
| **Title of case study:** Solving Complex Analytical Challenges | | |
| **Period when the underpinning research was undertaken:** 2000-2020 | | |
| **Details of staff conducting the underpinning research from the submitting unit:** | | |
| **Name(s):** | **Role(s) (e.g. job title):** | **Period(s) employed by submitting HEI:** |
| Dr Geraint Morgan | Research Fellow | 1993-present |
| **Period when the claimed impact occurred:** 1 Aug 2013 - 31 Dec 2020 | | |
| **Is this case study continued from a case study submitted in 2014?** N | | |

## 1. Summary of the impact

Cutting-edge comprehensive gas chromatography–mass spectrometry research by **Morgan** has established new physio-chemical understanding that underpins the development of novel and bespoke analytical solutions for several multinational companies and SMEs. Impacts on **Commerce and the Economy**; **Practitioners and Professional Services**; and **Public Policy Related to Health and Wellbeing** include:

- Generating [text removed for publication] income for UK companies and pipelines of prospects;
- Upskilled over 500 analysts, through over 1,400 days of bespoke training;
- A totally novel alcoholic beverage ready for market;
- Developed solutions for the monitoring of volatiles in air within critical secure environments, including submarines and the automated screening of the authenticity of Scotch Whisky;
- Helped shape the Home Office's 2016 Forensic Science Strategy and the UK's COVID-19 Testing Strategy.

## 2. Underpinning research

The Applied Science & Technology Group (ASTG) at The Open University (OU) grew out of the multi-disciplinary teams assembled for the Rosetta and Beagle2 missions **[O1]**. ASTG, established by **Morgan** in 2006, has a vision to build a reputation as a leader in the design, development and application of novel analytical techniques and integrated sensor solutions for existing, new and emerging global requirements. This is achieved by utilising the multidisciplinary expertise from developing space instruments and the application of gas chromatography-mass spectrometry (GC-MS) and comprehensive gas chromatography (GCxGC) to unravel the secrets contained in highly complex samples, at ever lower detection limits.

The optimisation of assays that use the orthogonal separating power of comprehensive gas chromatography has enabled the lowering of the limits of detection of species of interest through improving the resolution of the compounds of interest from all the other species present in real-world samples. Optimisation of these assays required an insight into the physio-chemical processes, these included: selection and evaluation of the optimal parameters for: sample preparation / concentration of each of the sample types investigated; transfer of the analytes from the sample; configurations of the gas chromatography columns, including the selection of the stationary phases and their dimensions; optimal instrument parameters for the gas chromatograph and the mass spectrometer systems available. In addition, post collection of the data, the development of novel machine learning algorithms, on top of the existing tools available on commercial instrumentation added significant value.

In 2009, in partnership with TrichoTech Ltd, we sought to address the forensic needs of Family Law courts by developing optimised GCxGC-MS assays for the separation, identification and quantitation of illicit drugs in human serum **[O2]**. Specifically, we were able to detect opiates (street heroine) and benzodiazepines, with limits of detection in the low ng/mL and concluded there was further scope to screen even more drugs and metabolites. With hair providing a longer-term record of consumption, we adapted the GCxGC-MS method to provide a non-specific, qualitative procedure that identified various drugs, metabolites, and impurities. They included cocaine, diazepam, and methaqualone **[O3]**. More recently, in partnership with JSB (UK) Ltd, we

were the first to demonstrate a fully automated, robotic sample preparation method for the detection of the metabolites of cannabis in hair samples by GC-MS, significantly reducing the duty cycle for analysis and removing the need for a highly skilled operator to conduct the sample preparation **[O4]**.

Sports anti-doping screening was a natural extension of our previous studies **[O5]** and this has since led to funding from a US charity, the Partnership for Clean Competition (2019) – and a partnership with the UK's only WADA-accredited testing laboratory (Kings College, London). Similarly, our research on non-invasive, non-targeted screening for the detection of cancer, from the profiling of volatile organic compounds above urine samples, is showing significant promise, especially for prostate cancer **[O6]**. Owing to COVID disruption**,** any directly associated impact, for the last two projects, will not be realised until the next REF.

## 3. References to the research


**O1**. Wright, I.P., Sheridan, S., Barber, S.J., **Morgan, G.H**., Andrews, D.J., and Morse, A.D. (2015) CHO-bearing organic compounds at the surface of 67P/Churyumov-Gerasimenko revealed by Ptolemy. *Science*, 349(6247). https://doi.org/10.1126/science.aab0673

**O2**. Guthery, B., Bassindale, A., Pillinger, C.T., and **Morgan G.H**. The detection of various opiates and benziodazepines by comprehensive two-dimensional gas chromatography/time of flight mass spectrometry, *Rapid Communications in Mass Spectrometry* (2009), 23 (3), 340-8**.** DOI: 10.1002/rcm.3883. https://doi.org/10.1002/rcm.3883

**O3**. Guthery, B., Bassindale, T., Bassindale, A., Pillinger, C.T., and **Morgan, G.H**. (2010) Qualitative drug analysis of hair extracts by comprehensive two-dimensional gas chromatography/time-of-flight mass spectrometry. J Chromatography A, 1217(26), pp. 4402–4410. https://doi.org/10.1016/j.chroma.2010.04.020

**O4**. Ward, A., Beasley, E., Bassindale, T., and **Morgan, G**. Automated Determination of Drugs of Abuse in Hair Samples, *GC/MS Application Note, Ingenious News 01* (2018). Available at: GC/MS_Application_Note_2018

**O5**. Zulfiqar, A., **Morgan, G**., and Turner, N.W. (2014) Detection of multiple steroidal compounds in synthetic urine using comprehensive gas chromatography-mass spectrometry (GCxGC-MS) combined with a molecularly imprinted polymer clean-up protocol. *Analyst*, 139, 4995-4963. https://doi.org/10.1039/c4an00721b

**O6**. Cauchi, M., Weber, C.M., Bolt, B.J., Spratt, P.B., Bessant, C., Turner, D.C., Willis, C.M., Britton, L.E., Turner, C., and **Morgan, G**. (2016) Evaluation of gas chromatography mass spectrometry and pattern recognition for the identification of bladder cancer from urine headspace. *Analytical Methods*, 8(20) pp. 4037–4046. https://doi.org/10.1039/C6AY00400H


## 4. Details of the impact

Organisations in various sectors are constantly searching for more sensitive and faster analytical techniques with greater resolution of compounds in ever more complex matrices to: ensure the quality and safety of their products, improve their formulation processes and protect the consumer from adulterated products and fraud. Our leading research in the area of comprehensive gas chromatography-mass spectrometry (GCxGC-MS) and the development of bespoke, optimised analytical methods to meet their needs has resulted in impacts in the following areas: **Commerce and Economy; Practitioners and Delivery of Professional Services;** and **Public Policy Related to Health and Wellbeing**.

The **primary pathways to impact** from the body of research have been through the establishment of strategic partnerships with commercial instrument companies and several joint proposals to funding programmes for the engagement of SMEs, primarily the SPRINT programme (2018-2021), part of Research England's Connecting Capabilities Fund (CCF). These links have been established though pro-active networking and dissemination of our research findings to a wide range of audiences throughout this and the previous REF period. Each of the beneficiaries below, including: a multinational, an SME, a sector support organisation and a micro-training-company, has gained benefits from the application of our research contributions to their innovation and entrepreneurial activity through the design and delivery of new products or services. Collectively, they have demonstrated evidence of **improved cost-effectiveness; services changes; sales of**

**new products; employment; licenses awarded and brought to market; collaborations between academia and industry; evidence of research leading to avoidance of negative outcomes; commercial adoption of technology; jobs created**.

**LECO Instruments Inc.** is a global instrument manufacturer with over 82 years of experience in the analytical industry. Headquartered in the USA, LECO has over 25 international offices globally. In his testimonial letter (15.1.21) **[C1]** the European Development Director for the Separation Science Division confirms *"forging strategic partnerships with highly capable academic laboratories, which also have strong links with and focus towards industry, is a high priority. In the case of the UK, the opportunity to work together with the OU was initiated and setup by the UK Sales Director and was identified as a key partnership which we could move forward with, fitting very much in-line with our overall European strategy".*

At the end of 2019, SPRINT funding enabled us to focus on enabling LECO to target industry customers with a complete application-specific solution including instrumentation, training and operating procedures that have been created and evaluated by the OU. He also confirms: *"During this project, a solution was successfully developed for the monitoring of volatiles in air within critical secure environments, including military vessels such as submarines. This solution was then demonstrated, at the OU facility to the industry customer [text removed for publication] and has directly resulted in the sale of a LECO BT GC-TOFMS, to them. This is a strategic win, because this sold solution is now on track, as intended, to lead to a number of additional systems being purchased by connected laboratories in industry and in the military, who have been working together in this field [Text removed for publication.] [...]. The working relationship with Dr* ***Morgan's*** *team has been excellent and through collaboration on a variety of SPRINT projects we have been able to optimise and then directly promote the analytical benefits of our technology to a range of new companies in the food and drink sector […] Having demonstrated the benefits of comprehensive chromatography and TOF-MS, it is anticipated that these opportunities will result in a number of sales in the next 12 months […]. Indeed, one such project which is currently close to completion is with a large multinational firm [text removed for publication], for whom we have developed an application solution to allow high throughput off-flavour characterization. This enhances their diagnostic ability and speed and is expected to contribute significantly to the improvement of formulation stability of their primary products in their vast global supply chain. We expect they will be purchasing our instrumentation during Q1 2021"* **[C1]**.

He finishes by saying: *"Based on the success so far, we have made an offer to The Open University, for a 5-year Strategic Sponsorship of Dr* ***Morgan's*** *laboratory [text removed for publication], with a view to growing the portfolio of projects with an increasingly diverse network of potential future customers. This initiative is a key part of our business plan because of the direct industry links and focus available to us via Dr* ***Morgan****"* **[C1]**.

***Efficiency Technologies Ltd*** is a local SME that signed up to the SPRINT programme at the end of 2019, with a view to the OU developing novel analytical assays for the profiling, characterisation and optimisation of the company's flavonoid extraction process. Flavonoid profiling at low levels is complex and can be time consuming; existing analytical methods fail to detect the very low levels of key flavour molecules which are critical to the natural complexity and taste. Monitoring the correct levels of critical compounds ensures that natural variability can be controlled and adapted to provide the highest premium product quality.

In his testimonial letter (15.1.21) **[C2]**, the Managing Director of Efficiency Technologies states *"The analytical assay developed at the OU identified a hitherto unknown anomaly in the process, that was not detected using conventional methods but had a direct impact on the flavour profile. The process also confirmed the successful implementation of the mitigating steps in the production process […]. The SPRINT project has enabled Efficiency Technologies to take a product that needed validation and has delivered a product ready for full industrialisation […]. We've been able to commercialise at a speed that wouldn't have been possible without the assurance that we can control the quality and this has led on to significant commercial opportunities for the company".*

He adds *"This optimised analytical assays and production processes can be delivered as a service to the craft beer and distilled spirit sector. The same processes can be applied by Efficiency Technologies for the development of a range of new products – indeed, the project has delivered*

*a novel, premium product ready for the retail market. A Heads of Terms agreement has been established with a UK flavouring company to undertake commercial exploitation and a customer has produced pilot testing samples for buyers at two leading supermarkets. Subject to adoption of solution, there are pilot orders of 5,000-10,000 bottles with commercial volumes rising to 100,000 bottles for commercial output. There is scope for sales of up to 500,000 bottles per year, subject to commercial output. Initially, this had been targeted for the Christmas market, but delays due to COVID restrictions has delayed the product launch […]. As a result, the company has expanded its staff from 1.5 to 3 employees*" **[C2]**.

**Scotch Whisky Research Institute (SWRI)** carries out pre-competitive fundamental research on behalf of its members, representing approximately 90% of the production capacity of the Scotch Whisky sector. Its member companies include large multinational spirit drink companies, such as Diageo and Pernod-Ricard. There are 128 operating distilleries across Scotland, therefore, the UK is the largest producer of spirits within the Europe, with exports worth GBP6.1 bn in 2019. The Scotch Whisky sector contributed GBP4.91 bn to this figure. In 2019, Scotch Whisky accounted for 75% of Scottish food and drink exports, 21% of all UK food and drink exports, and 1.4% of all UK goods exports. More than 10,000 people are directly employed in the Scotch Whisky industry in Scotland and over 40,000 jobs across the UK. In his testimonial letter **[C3]** the Senior Scientist in charge of Product Protection at SWRI states (15.1.21): *"The high value of the products produced by the sector provides opportunities and incentives for criminal activity, such as adulteration or substitution, defrauding the consumer, creating significant safety concerns, and resulting in lost revenue for genuine producers and governments […] The spirit industry's work to tackle such criminal activity is therefore of key importance in protecting sales and jobs within the sector".*

In 2018, after a Chemical Analysis of Food meeting at the Royal Society of Chemistry our GCxGC-MS research outputs came to the attention of SWRI, leading to a successful SPRINT proposal in early 2019. *"This collaborative research undertaken with The Open University team evaluates advanced analytical instrumentation and techniques for their advantages for spirit drink authentication, whether applied by the SWRI to its own authentication work or by its member companies to the authentication and protection of their key spirit brands"* **[C3]**. Key outcomes achieved: the optimisation of GC-MS and GCxGC-MS conditions for the analysis of Scotch Whisky; the complete analysis of a specially curated set of samples for testing of the method for authentication capability; the demonstration of the application of a commercial program for the statistical analysis of the large amounts of GC-MS data for brand authentication.

Commenting on the benefits of the project the Senior Scientist states: *"The SWRI has started to implement changes to its standard GC-MS method based on suggested optimisations and is partway through its testing of how commercially available and developed processing tools might increase the capability and efficiency of its authentication service. These developmental changes have unfortunately been delayed due to a focus on core activities necessitated by Covid-19 restrictions. However, already demonstrated advantages provided by the optimised GC-MS method, such as the reduced consumables cost, shorter run times, improved peak resolution and increased signal to noise ratios, make its adoption a formality. Increasing the number of samples submitted to GC-MS analysis will increase the number of samples identified as counterfeit. Improving the analysis method's cost effectiveness and speed was necessary to achieve this goal […]. A significant component to this project's impact has been the added value provided by involvement, established through The Open University, of additional collaborative partners [LECO and IBM Research UK] […]. In addition to creating partnerships that will hopefully continue to yield benefits, all these collaborations have progressed the SWRI's understanding of the statistical interpretation of large quantities of chromatography-based data. Such knowledge has been identified by the SWRI and its industry members as vital for future analytical research throughout the sector (i.e., not just for authentication, but for understanding flavour development, product control and process efficiencies)"* **[C3]**.

***Anthias Consulting Ltd*:** Since 2007, our laboratory has hosted their award-winning gas chromatography-mass spectrometry scheduled, public and private training courses. As confirmed by the company owner, in her testimonial letter (6.1.21) **[C4]**, from August 2013 to Feb 2020 (COVID) there have been 188 courses held, with attendees from 119 different UK companies and government agencies and 58 global companies and government agencies; 26 different UK and

14 international universities. This represents a total of 1,410 person days of training, GBP363k in revenue for Anthias and represents nearly 30% of their turnover. Delegates attend courses from nearly every industry sector, including: Agriculture, Petrochemicals, Defence, Energy, Oil and Gas, Flavour and Fragrance, Food and Drink, Forensics, Government Laboratories and Public Health, Manufacturing, Pharma, Clinical, Biomedical and Therapeutics, Product Testing, Tobacco, Water and Environmental. She also states: "*To summarise, the ability to provide our Royal Society of Chemistry training which are approved for continuing professional development (CPD) at The Open University has had a significant benefit to our customers […]. Companies that have well-trained analysts spend less time troubleshooting instruments or repeating an analysis – resulting in less down-time and higher sample throughput. They spend less time, effort and therefore have lower costs in their method validation and accreditation with more accurate and reproducible results. They also have a better reputation in their industry, resulting in more customers, more samples to analyse and better results for their customers which of course will directly affect their companies".* She went on to say ***"****The ability to work with The Open University has had a significant impact on my company […]. We have a lot of repeat business from companies who have sent a delegate(s) to a course hosted at The Open University, either through further training or consultancy work, on- or offsite…We employ a Training Course Co-ordinator part-time whose sole focus is organising the training courses at The Open University. Much of our Marketing Manager's time is spent on marketing the training courses. These are both equivalent to one full-time role"* **[C4]**.

**Impacts on Public Policy Related to Health and Wellbeing**

In 2015, based on his track record of commercial engagement and space technology translation, **Morgan** was nominated by STFC to represent them at a scoping meeting and was subsequently selected to be the lead author for Chapter 16 (Encouraging Innovation) of the Government Chief Scientific Officer's Annual Report for 2015, *Forensic Science and Beyond: Authenticity, Provenance and Assurance. Evidence and Case Studies* **[C5**, p.174**]**.

A letter from the then Government Chief Scientific Adviser **[C6]** from December 2015 stated that *"it is already receiving great deal of interest from policy makers in the Home Office, whose forthcoming forensic science strategy we hope to influence with our findings. I will soon embark on an intensive period of follow-up activities through which I plan to take forward the key questions raised and embed the key messages in policy development and delivery. I hope that or work together will generate innovative thinking about forensic science and help to secure the long-term future of the UK's forensic science sector"*. The Forensic Science Strategy was published by the Home Office in March 2016.

During December 2020, **Morgan** was contracted by the Medicines & Healthcare products Regulatory Agency (MHRA)/National Institute for Health Research (NIHR)/Dept. of Health & Social Care (DHSC) as an Assessor to provide clinical or technical advice for the development of the Target Product Profile for a *"Rapid Detection Test using Biomarkers found in Breath for SARS-CoV-2"*. The TPP has been developed to assist manufacturers in designing and delivering new tests to support the UK's COVID-19 testing strategy. It provides a common foundation for the development of new tests and contains sufficient detail to allow device developers, and key stakeholders, to understand the characteristics a successful test should have when aligned with the intended use scenario **[C7]**.

**5. Sources to corroborate the impact**

**C1**. Testimonial Letter European Development Director LECO Instruments.
**C2**. Testimonial Letter from Managing Director of Efficiency Technologies Ltd.
**C3**. Testimonial Letter Senior Scientist SWRI / Authenticity Lead.
**C4**. Testimonial Letter Owner / Director Anthias Consulting Ltd.
**C5**. Annual Report of the Government Chief Scientific Adviser 2015, Forensic Science and Beyond: Authenticity, Provenance and Assurance Evidence and Case Studies.
**C6**. Letter from the then Government Chief Scientific Adviser (2015).
**C7**. MHRA, Rapid Detection of Biomarker, TPP Assessor Declaration Form.