Science Futures

Expectations of the scientist of the future

A close up view of the impact of industry and technology on academia and the future workforce

Executive Summary

The symbiotic relationship of Industry and Academia throughout all STEM often goes without comment, however, without one, the other simply would not progress, or progression would almost certainly be slower with more obstacles and lower budgets spread more thinly.

Academia is a highly interactive and interdisciplinary field. And while great advances can be discovered in isolation, academia itself – as well as the society it serves – moves forward most effectively when it builds and sustains strong partnerships to maintain progress.

Collaboration between industry and academia is widely considered as essential to a healthy life sciences ecosystem. While industry provides academia with challenging "real world problems" for research topics, and the funding with which to carry it out, academia provides industry with access to greater problem-solving resources as well as access to future scientific talent. When optimized, academia-industry collaboration can accelerate innovation and speed up the translation of research to ensure the successful commercialization of new technology and solutions aimed at solving societal 'grand challenges'.

But how do the students themselves feel about this relationship, what impact does it have on their research and priority skill development, and where do they place the importance of collaboration and scientific exchange? We interviewed five students, stars in their chosen scientific field, from five academic institutions across Europe to find out more about the impact of the academia-industry collaborative relationship and the role of technology.

Agilent

Meet the roundtable PhD students

Max

Institute of Analytical Chemistry at the University of Natural Resources and Life Sciences (BOKU), Vienna, Austria

Max is working with ion mobility-mass spectrometry (IM-MS), an emerging technology for analytical chemistry, and is mainly involved in the development of new acquisition strategies and suitable applications using partly prototype hardware and software for IM-MS in the field of 'metabolomics'.

Tijmen

Vrije Universiteit Amsterdam (VU) and the University of Amsterdam (UvA), Amsterdam, The Netherlands

The aim of Tijmen's research project is to develop and improve multi-dimensional analytical methods for the characterization of polymer materials. His research is part of the UNMATCHED project, which is a public-private collaboration of the two universities VU and UvA, three leading chemical companies and other industry partners.

Joyce

School of Chemical Sciences, Dublin City University, Dublin Ireland

Joyce's PhD research focuses on the development of multiple handheld nutrient devices that can take near real-time measurements of phosphate onsite for use in catchment areas. The research also looks at developing an observation framework for a specific catchment area and the use of different integrated technologies available.

Rajannya

University College Cork (UCC), Cork, Ireland

Rajannya's research focuses on the development and application of a Fluorescence Lifetime Imaging (FLIM) macro-imager based on the new Tpx3Cam for metabolic assessment of living tissue samples for hypoxia conditions in advanced disease models.

Alex

King's College London, London, UK

Alex's proof-of-concept research studies pharmaceutical compounds in the environment and river systems using a passive sampler device. Alex plans to use machine learning models to predict the uptake of these compounds into an aquatic, benthic invertebrate (*Gammarus pulex*). Her research is part of a four-year funded PhD program, from the London Interdisciplinary Biosciences Consortium (LIDo) industrial case (iCase) studentship in partnership with Agilent Technologies.

Key discussion themes

Several important trends and themes emerged that led to the increased scope of research and enabled the students to meet their research goals.

This article considers the following trends from the students' perspective:

1. Access to innovative technologies to do science well

Science and technology are intrinsically linked; scientific discovery is driven by technological advances, and technological advances are, in part, driven by the need for better science. For PhD students in academia, access to the latest technology enables progressive innovation to fulfill their research goals and translate scientific research into possibilities. In particular software, web-based data, and open-source information collections for idea sharing and building skills are in high demand for students looking at more efficient and dynamic ways of solving challenges.

2. The need to upskill and collaborate to get the job done

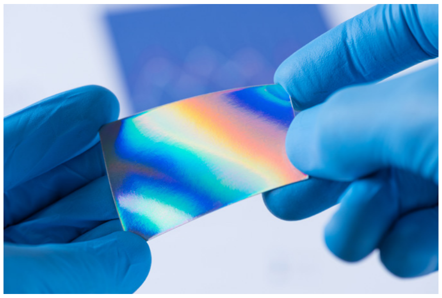
PhD students are very aware that in the workplace, when conditions, technology and requirements change rapidly, this places a heavy demand for academics to be pro-active and prepared through reskilling and upskilling. As jobs are transformed by the technologies of the Fourth Industrial Revolution, we need to reskill more than 1 billion people by 2030.[1]

Academic research and development are a key component to enterprise. Industry is therefore a major supporter of academic research through funding, product, and experience support. Professional connections between faculty, students, and industry continue to boost:

- Cooperation and the sharing of ideas between industry and universities
- The academic culture of collaboration in analytical science, including across research universities
- The research topics that faculty and students pursue
- The ability of universities to train and upskill students in preparation for the workforce.

3. Emerging technologies and meaningful research goals are shaping the future of science

Collaboration provides opportunities to focus on upskilling or reskilling, which is an important aspect for PhD students and academics. While advances in technology drive greater efficiency in research, academia and industry should investigate ways to increase value and meaning for the future workforce, while looking at how careers can be successfully shaped, and redesigned through emerging technology to enhance capabilities and skill sets. Furthermore, in lab 4.0 and with the growth of AI, automation, and robotics there is no doubt among academics that skills, tasks, and jobs will evolve and a certain level of collaboration will be required to stay afoot, plug talent shortages and prepare for the future scope of science research – whether that's in academia or the future workplace.



Access to innovative technologies

Cultivating strengths for probing data, curating information, and asking the right questions are all aspects of working with technology that were raised. Technology was widely viewed as the key driver of their research, innovation capacity and efficiencies.

We asked the students, whether and how technology has steered their studies:

Tijmen: *"The continued availability of analytical equipment and the development of the underlying technology greatly accelerates our research capabilities and, perhaps more importantly, induces new questions for scientists to look at."*

The main bottleneck in my research into polymers is a lack of knowledge on structure-property relationships. New multi-dimensional analytical methods help predict which chemical innovations will lead to improved materials. Also, industry relies on the use of validated methods. Translating such methods to state-of-the-art analytical techniques is time-consuming and often a barrier for innovation. Using the algorithms that we are developing; new methods can be introduced much more smoothly and rapidly."

Alex: *"Technology has played a bigger role than we expected in my PhD. Originally for passive sampling, we were going to use one of the commercially available passive samplers. Through exchanging an idea with one of my colleagues, I decided to develop my own passive sampler using 3D printing technology. Having access to a 3D printer in our lab has allowed me to take my PhD in a slightly different direction than expected, but with the same broad idea."*

Joyce: *"In my line of work, current commercially available nutrient sensors on the market cost a considerable amount to make, maintain and deploy due to the high-power requirements, size and reagent consumption, therefore, fewer sensors are deployed leading to a reduction in the data being obtained. To overcome this problem, new and emerging technologies must be considered."*

Rajannya: *"The technologies used have steered my research to a great extent. From a practical point of view, new technology was developed by one of our collaborators and our research group was one of the first to test this technology for FLIM/PLIM applications. Initially the camera was set up to test its working capabilities in this domain. The supporting software was upgraded to support the protype for such biomedical imaging applications, and a dedicated C-language program also had to be developed for the post-processing of the data."*

Max: *"Technical developments are helping us to build generic methods for a wide range of analyte molecules while still maintaining a high level of selectivity. Combining high resolution mass spectrometry with ion mobility is particularly regarded as a suitable next-generation toolbox for these kinds of workflows."*

Access to innovative technologies

We also asked the students, whether and how open source sharing has improved their studies:

Alex: *"Access to open-source information has been extremely useful in my research. From online courses in 3D printing, to open journal access and to the abundance of online documentation for R and Python code. This has been most helpful when trying something new or debugging my scripts."*

Joyce: *"Nowadays there is more open science, open source access and data sharing making it easier for researchers to benefit from different technologies. Cloud-based software has changed the way researchers collect and store data. Sophisticated algorithms collect enormous amounts of data instantly and can then be used to analyze the data to predict or recognize patterns. The use of free open source technology such as GIS, USGS and Scihub, enables high resolution data collection and processing, which is important for my project. I think it has leveled the playing field as all universities have access to a variety of open source software and are better able to integrate them into projects. I think it has opened another line of communication between both industry and academia, which is beneficial to both parties."*

The integrated and coordinated sectors of communication and computation have led to a rise in connected devices that are low-powered, highly accurate, and cost effective. The increase in new technologies facilitates web-based data services such as cloud storage. New data management technologies have been accelerated with artificial intelligence. This has enabled me to avail encoding, designing, data processing, data acquisition, and data storage elements to enhance the quality of my research."

Max: *"Our understanding of the world is changing tremendously fast, partly, because societies are producing more data than ever before. However, high quality datasets are necessary to allow robust conclusions to complex scientific questions. The time spent on measuring and evaluating such data is still a limiting factor for answering many research questions. Especially in the context of life-science, scientists are heavily relying on in-depth analysis of large sample cohorts and mass spectrometry is one of the major "workhorse" technologies that can help to depict reality in a measurable fashion.*

Using mass spectrometry, we are generating huge datasets, and data processing, curation and interpretation is not a trivial task. Especially when analyzing complex samples; differentiation between data containing relevant information and data that is either non-relevant, redundant or simply an artifact of the method used, can be challenging. Our research could be seen as a piece of the puzzle that tries to speed up measurement times while maximizing data quality by means of technical enhancements of data acquisition workflows."

Collaboration and the impact of industry on research and academic achievements

Partnership between industry and academia is widely viewed as a critical need and the goal of creating further collaboration to unlock great potential within academia is essential to bring meaningful value to academic research.

We asked whether the students had felt the presence of industry during their PHD work and if so, what impact it had on their work and on their perspectives as a post-doc:

Tijmen: *"My project on analyzing cellulose ethers is co-sponsored by three leading chemical companies and aspects of my work are supported by an industry grant. The involvement of industry is essential for the project. The equipment and samples allowed me to start my research and through secondments at partner companies, I can interact with industry experts and implement my work directly on-site. I really value these interactions."*

We are also working in close collaboration with our industry partner, Agilent Technologies, who provide both the hardware and software for carrying out part of this project. This means that the project is focusing on the instrumental, or technological, developments as well as strategies to assess the applicability of the technology to relevant research areas."

Max: *"In my experience, industry often has a different mindset than academia. In my current environment I get the best from both worlds, the academic depth with industrial focus. The research project I am working on is partially funded by an industry grant and I applied for a position within the project. Additionally, the hardware and software are developed by Agilent, and we receive technical support by the developers and have discussions and meetings on a regular basis. I would definitely consider collaborating with industry in the future. Aside from the possibility to test prototype technology and develop applications and acquisition strategies, I have enjoyed the scientific discussions with the instrument developers and have learned a lot from this collaboration."*

Alex: *"My PhD research is part funded by Agilent Technologies and they have been extremely supportive in a lot of ways. From providing consumables, to training me on their instruments and supporting my attendance to conferences and workshops. Aside from Agilent I have had the opportunity to collaborate with Natural Resources Wales and other academic groups on a couple of projects that are very interesting and have yielded some great results, some of which we are intending to publish. I think that collaboration between industry and academia is very important to the future of science in all fields, as the frontline research and ideas from academia can be supported by the practical experience and know-how of industry to better develop and refine the product or process we are all working on together."*

Joyce: *"Throughout my PhD I have been given the opportunity to attend different conferences throughout Europe and engage in conversation with people from both academia and industry. Membership to research support programs such as the Maxon Young Engineers Program (YEP), are a great way of interacting and bridging the gap between research and industry."*

Rajannya: *"Our motive is to provide the biomedical or diagnostics research industries with an advanced solution to address clinical studies. My research is still in its initial stages, so the plan is to collaborate closely with these industries to commercialize the system for clinical applications in its final stage. Without this level of input, we would not be able to commercially realize the potential of Fluorescence Lifetime Imaging (FLIM) for metabolic assessment of living tissue samples."*

Future aspirations in science, solving 'grand challenges' in today's world and preparing themselves for the workplace

The requirement of students to be accomplished in a multitude of disciplines and complex technology means they have to be highly skilled in data analytics, computational design and programming, engineering and also mathematics.

With rapid technological change across many diverse research disciplines, academics realize the importance of having the right skills to fully embrace current technological advances so that they are set up to anticipate and respond to changing skill requirements whilst not losing sight of the traditional skills that are still essential.

However, importantly, meaningful research to address societal grand challenges remains a key factor for PhD students.

We wanted to explore how the results of their studies and research have affected their career path in the future and were really interested to find out the extent that they had to upskill in a multitude of disciplines:

Joyce: *"My PhD was a multidisciplined research project covering aspects of engineering, physics, chemistry, and environmental monitoring. From studying and working in these areas I have developed a vast skill set. After completing my PhD I envision myself in industry, implementing and broadening the skills I have learned which I believe could be applied to a number of different industries."*

Rajannya: *"My current research topic is interdisciplinary. It includes the study of optics/photonics, chemistry, and biology. Being a student of photonics, I had to develop the knowledge of chemistry for preparing the fluorescent and phosphorescent sensors and the skills of biology to handle small and delicate tissue samples. I am also in the process of learning the biomedical reasoning of the behavior of the tissues showing different lifetimes. Therefore, I possess a number of unique skills and I believe the capability of coping with the different fields of science can lead to real life achievements. Depending on my research work, I consider a post-doctoral researcher position as my initial choice of career and my achieved skill sets over the years in academia would help to get a position in industry."*

Max: *"Besides a really detailed training in analytical chemistry, I will have a broad basis in different fields of natural science and related methods after finishing my studies. For example, working with large datasets requires some skills regarding statistics, computational methods or programming and for successful data interpretation biologic knowledge might be necessary."*

"To me, analytical chemistry, especially when it comes to ion mobility-mass spectrometry and related techniques, is a really exciting research field. It is ranging from fascinating technical developments, detailed studies helping to generate fundamental understanding of structural properties of single molecules, up to the analysis of large cohorts of complex samples, e.g. in context of environmental, medical biotechnology-related research. I hope that I can further contribute to academic research in this field in the future."

Tijmen: *"As a PhD student, I am building my experience of working within industry and I have already developed some strong relationships, through internships and employment. My passion lies in automation and advanced chemometrics and I hope to contribute to these areas throughout my career."*

Alex: *"I am lucky in that I have worked for three different companies in the space of a couple of years prior to starting my PhD so I've been exposed to a variety of industry standards are and how industry operates, and I have seen, firsthand, the gap between going from academia into industry."*

"In terms of readiness (for the real world), I wouldn't say I am 100% ready yet, however I am learning the skills and building my repertoire that will make me ready for real world achievement. The access to technology through working with industry partners has opened up new career horizons for me and I am excited to decide which direction I will take."

Agilent Case Study

GRAND CHALLENGE: Sustainable, quality and harmless biopolymer materials for modern societies

Creating circular processes, without sacrificing the quality and safety of materials.

Biobased and biodegradable polymer materials are highly relevant in modern society and are replacing synthetic polymers. The biodegradable polymers are often based on complex biopolymers, such as cellulose, and are mostly derived from replenishable and natural resources that form harmless products when degraded with soil microorganisms. Cellulose can also be obtained from natural sources such as wood, which can be harvested in a sustainable way. By modifying the cellulose with (hydro) alkylation, cellulose ethers can be obtained. These cellulose ethers introduce preferable properties such as water solubility, non-toxic, tunable biodegradability, and thickening properties, which are particularly desired in paint, food and pharmaceuticals.

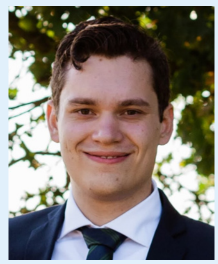
Research overview: New multi-dimensional analytical, validated techniques to predict which chemical innovations will lead to improved materials.

The chemical structure of the biopolymer is what determines its function and biodegradability. Accurate molecular distributions are indispensable to ensure complex polymeric materials, as well as their biodegradable degradation, can be studied. Also, industry relies on the use of validated methods. Using algorithms to help translate such methods to state-of-the-art analytical techniques will help overcome time constraints and barriers to innovation so that new methods are ready for swift and smooth implementation. This research is part of the UNMATCHED project, which is a public-private collaboration of the two universities VU and UvA, with three leading chemical companies and other industry partners.

Research aim: To develop and improve multi-dimensional analytical methods and instrumental technology for the characterization of polymer materials.

Research methodology: Complex polymer distributions can be unraveled using hyphenated techniques. A good example of such technique is 2D-LC-MS. For computational-assisted method development of these hyphenated systems, retention modeling is a promising tool. However, this does not work well for transfer of the developed method to another instrument. This is especially true when fast gradients are used which is often the case for the second LC dimension. The shape of the effective gradient often deviates significantly compared to the programmed gradient which results in retention parameters that are instrument specific. We developed an approach that takes the gradient deformation into account in the retention modeling and allows the prediction of the actual shape of the gradient on the instrument used. This correction provides better method transferability among instruments and laboratories, and thus improves reproducible implementation.

Desired outcome: Having tools available to rapidly develop analytical methods to greatly help the efficacy of analytical labs and the customers relying on them. This brings us a step closer to a generation of instrument independent automatic workflows.



Tijmen Bos

Vrije Universiteit Amsterdam (VU)
and the University of Amsterdam (UvA),
Amsterdam,
The Netherlands

"Helping develop analytical tools that can validate the performance and characteristics of biobased and biodegradable polymer is an exciting challenge. The results are going to help us address a range of global challenges centred on sustainability and the circular economy."

Agilent Case Study

GRAND CHALLENGE: Climate change and water quality, some of the biggest obstacles confronting humanity

Creating circular processes, without sacrificing the quality and safety of materials.

There is a need for effective monitoring of environmental waters due to the elevating anthropogenic threats on the environment; nutrient pollution and climate change. Eutrophication is the excessive enrichment of an ecosystem by chemical nutrients, often containing chemical compounds. At high concentration levels, complexes of these compounds can have harmful effects on the quality of a water body. Nutrient pollution is an extremely difficult challenge to overcome when it comes to environmental monitoring, as it can be difficult to find a solution to repair the extensive damage it can cause. Therefore, preventative measures have been taken to ensure nutrients, such as phosphorous, are regulated and monitored sufficiently.

Phosphorus is a limiting nutrient that occurs naturally but when found in overabundance it can have harmful effects in the environment. If phosphorus levels are elevated in a water body, excessive growth of plants and algae occurs. This can lead to hypoxic or anoxic waters and the potential release of harmful toxins, resulting in the death of aquatic animals and causing possible harm to humans and animals and the aquatic ecosystem inhabiting the water system.

Research overview: New and emerging sensor technology to provide high power, real-time requirements to study phosphate nutrients in aquatic algae.

There is an increasing need to sample and monitor water bodies for phosphate determination in near real-time, using novel methods to eliminate the need for high powered instruments and laboratory settings. Current commercially available nutrient sensors on the market cost a considerable amount to make, maintain, and deploy due to the high-power requirements, size, and reagent consumption. This leads to less sensor deployment leading to reduced data capture and generation. To overcome this problem, new and emerging technologies must be considered.

Joyce O'Grady

School of Chemical Sciences,
Dublin City University,
Dublin
Ireland

"There's a growing need to monitor chemical nutrients in the world's environmental waters as they can be harmful to the wider environment. Our work will enable onsite, near real-time sample analysis, helping address one of the world's fundamental issues – water cleanliness."

Research aim: To develop and improve data monitoring capabilities and novel methods to determine the effective evaluation indicators of water eutrophication and eliminate the need for high powered instruments and laboratory settings.

Research methodology: Evaluation/ simulation methodology of the eutrophication process and sample data sets – using the microfluidic platform.

Desired outcome: New sensor technology and data analysis methods for nutrient analysis that will enable onsite, near real-time analysis of phosphate. New platforms to allow for sample loading, mixing, heating/cooling, reagent storage, and detection to take place within the device, eliminating human error. In turn these will help future public policies as it will provide an increase in the data available to them by enabling faster and more frequent analysis to take place.

Agilent Case Study

GRAND CHALLENGE: Depicting reality to answer big questions in science

Expanding the capability to link and integrate datasets.

Our understanding of the world is changing at a tremendous pace, partly, because humanity is producing more data than ever before. However, high quality datasets are necessary to allow robust conclusions to complex scientific questions. The time spent on measuring and evaluating such data is still a limiting factor for answering many research questions. Especially in the context of life-science, scientists are heavily relying on in-depth analysis of large sample cohorts and major "workhorse" technologies that can help depict reality in a measurable fashion.

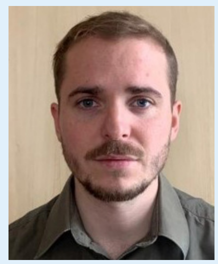
Research overview: Ion mobility-mass spectrometry (IM-MS), an emerging technology for analytical chemistry and improving.

Ion mobility-mass spectrometry (IM-MS) is an emerging technology for analytical chemistry. When analyzing complex samples; differentiation between data containing relevant information and data that is either non-relevant, redundant or simply an artifact of the method used, can be challenging.

Research aim: To develop analytical methods to speed up and improve the quality of complex data curation in metabolomics.

Research methodology: High resolution MS workhorse technology using new methodologies, data acquisition workflows and data processing.

Desired outcome: Our research could be seen as a piece of the puzzle that tries to improve tools applicable to improve our understanding of complex biologic processes e.g., for applying metabolomics models. We use ion mobility-mass spectrometry along with new data acquisition workflows to maximize data quality. This is expected to provide a set of useful tools that can be integrated in future research on a more routine basis.



Max Lennart Feuerstein

Institute of Analytical Chemistry at the University of Natural Resources and Life Sciences (BOKU),
Vienna,
Austria

"We're creating more data than ever before; information that can be used to answers some of the world's most complex scientific questions. Extracting its value can be complicated but my work with ion mobility-mass spectrometry (IM-MS) is helping pave the way to a deeper understanding."

Agilent Case Study

GRAND CHALLENGE: Understanding common diseases

Advanced biophotonic modeling to understand the behavior of diseases on tissues.

Rajannya Sen

University College Cork (UCC),
Cork, Ireland

"Disease modelling has never been more important but current tissue imaging platforms have their limits. That's why I've been looking at prototyping Fluorescence Lifetime Imaging (FLIM)."

Disease modeling supports our understanding of how disease develops and progresses, as well as potential treatment approaches and has become a progressive area of biomedical research. Disease models can be generated in several ways using 2D cell cultures or in vivo-like 3D tissue models, to mimic disease in a more real-time physiologically relevant environment. Disease modeling is being done successfully in areas like cancer research, personalized medicine, and infectious diseases. Specifically, tissue hypoxia is a pathological state, which is common in a majority of advanced disease states. Hypoxia alters cell metabolism and contributes to therapy resistance. Better understanding of the role of hypoxia in disease progression will open new ways for the discovery of new therapeutics targeting hypoxic cells and tissue microenvironments.

Moreover, most of the current tissue imaging platforms are microscopic, while macroscopic imaging platforms are still very rare. The research scope of scientists continues to grow and grow, and while some methods and analytical methods are easily transferred to new research areas, other projects demand a much more individualized approach, and who better to turn to with this challenge than academia.

Research overview: Fluorescence Lifetime Imaging (FLIM) macro-imager based on the new Tpx3Cam for metabolic assessment of live tissue samples and disease models under hypoxic conditions.

The classical technique for recording fluorescent lifetimes is Time Correlated Single Photon Counting (TCSPC) with high temporal and spatial resolution. However, the pixel-by-pixel scanning leads to slow image acquisition times, particularly for PLIM applications where long pixel dwell times are required to record the long-lived phosphorescence. Alternative techniques such as wide-field imaging with a time-gated CCD camera or frequency domain method can achieve higher image acquisition rates, but they are less accurate and sensitive since gating of the camera leads to photon loss and rough visualization of the decay. This research is focusing on the development and application of a Fluorescence Lifetime Imaging (FLIM) macro-imager, which is based on the new Tpx3Cam, for metabolic assessment of living tissue samples for hypoxia conditions in advanced disease models.

Research aim: The goal of the project is to build a compact and flexible biophotonic imaging system based on the new Tpx3Cam to operate in Florescent Lifetime Imaging (FLIM) mode for metabolic assessment of live tissue samples, animals, and ultimately humans.

Research methodology: The Tpx3Cam is based on a novel silicon optical sensor and Timepix3 readout chip. It can record the arrival time and intensity of the photons at each pixel simultaneously. The single photon sensitivity of the imager is achieved by coupling the camera to a Cricket® adapter with inbuilt image intensifier. Emission filter and a lens are also coupled to the cricket unit. A LED operated in pulsed mode is used to provide excitation to image 18x18 mm sample area. The raw data is collected in a binary format and processed by a custom-designed software. A dedicated C-language program is then used to post-process the data. TRI2 software is used to fit the resulting data matrix for each camera pixel to determine lifetime values.

Desired outcome: Our motive is to provide the biomedical or clinical research industries with an advanced imaging platform solution to address pre-clinical studies. My research is still in its initial stages, so the plan is to collaborate closely with these industries to develop a prototype that can be commercialized for clinical research applications in its final stage. Without this level of input, we would not be able to commercially realize the potential of Fluorescence Lifetime Imaging (FLIM) for metabolic assessment of live tissue samples.

Agilent Case Study

GRAND CHALLENGE: Protecting our water systems from pharmaceutical pollution and emerging contaminants

Advanced sensitivity models to measure chemicals at very low levels in water and in animals.

The widespread use of pharmaceuticals (both prescribed and over the counter) has resulted in a relatively continuous discharge of pharmaceuticals and their metabolites into the environment. Following advances in the sensitivity of analytical methods for the measurement of these chemicals at very low concentrations, a number of studies find trace concentrations of pharmaceuticals in wastewater, and surface waters such as rivers, lakes and costal environments.

The global and societal challenge is pharmaceutical pollution and emerging contaminants in the environment. Using advanced analytical methodologies and technology to monitor contaminants in the ecosystem and in animals. This is important in order to preserve the environment and ecosystems for future generations and will better enable changes at policy level to ensure that our drinking water is safe.

Research overview: Studying pharmaceutical compounds that end up in the environment and river systems using an artificial, passive sampler device.

Research studies pharmaceutical compounds that end up in the environment and river systems using artificial, passive sampler devices. These capture the average concentration of a contaminant in a water system over a period of time. As passive samplers are exposed to the same environmental concentrations as aquatic animals it may be possible to use them as a surrogate for measuring contaminant concentrations in the organism. Of particular interest is the benthic amphipod *Gammarus pulex*, a small shrimp that is commonly found in freshwater rivers and streams throughout the UK and Europe and are the basis for most food webs. Current techniques for monitoring contaminants in organisms require the animal to be collected and often terminated before tissue concentration can be determined. Modelling a living animal from an artificial device would allow for the rapid risk assessment of contaminants on biota with minimal harm done.

Alex Richardson

King's College London,
London,
UK

"The global increase in the use of pharmaceuticals has resulted in their heightened concentration in all water bodies: it's an emerging threat to the environment. My work using machine learning and advanced statistics aims to be able to predict contaminants in animals."

Research aim: The aim of this PhD is to use passive sampling technology combined with in silico machine learning tools to act as surrogates for invertebrates in contaminant bioconcentration studies.

Research methodology: In order to achieve this, there are three main objectives. First, identifying the pharmaceutical contaminants present in the study system and gathering passive sampler data (such as uptake rate) in the lab and in situ. Second, measure how much of a contaminant present in the water is accumulated by the invertebrate. Lastly, use machine learning predictive algorithms to merge the two datasets and attempt to predict the contaminant accumulation by the invertebrate from the in situ passive sampling data.

Desired outcome: Use of machine learning models and advanced statistics to be able to predict contaminants in animals from an artificial device. The primary impact of this work is the reduction of animal use in pharmaceutical pollution monitoring campaigns (3Rs in animal studies are Replacement, Reduction and Refinement). Other impacts are potentially on environmental protection/monitoring industries and on policy and regulatory bodies.

i. World Economic Forum. https://www.weforum.org/agenda/2020/01/reskilling-revolution-jobs-future-skills/
ii. Bos TS et al., Journal of Chromatography. Reducing the influence of geometry-induced gradient deformation in liquid chromatographic retention modeling. Vol 1635, 2021