2020 RESEARCH HIGHLIGHTS

FROM THE SCHOOL OF CHEMICAL SCIENCES

THE UNIVERSITY OF AUCKLAND
Te Whare Wānanga o Tāmaki Makaurau
NEW ZEALAND

SCIENCE
SCHOOL OF CHEMICAL SCIENCES

A word from the Head

The year 2020 presented our School with multiple challenges, yet our teaching and research was able to continue in a sometimes revised form. We have seen research teams and spin-off companies pivot to COVID-19 – related research and development. All our researchers have adapted to working in new environments, including bubbles at Level 3 and decreased laboratory occupancies at Level 2. Staff and students have also maintained their overseas and domestic collaborations and many have found their home offices can be productive writing spaces.

We decided that one way we could celebrate our resilience and productivity in research this year was to produce this report highlighting our successes. We share the continued successes of our high-profile researchers such as Distinguished Professor Dame Margaret Brimble FRS, while also noting the contributions of our newest academics, research fellows and PhD students. Our research is heading in exciting new directions including new medications, developing novel states of matter, connecting electronics to cells, and modelling the behaviour of proteins. We support the range of activities from blue skies single investigator-led research to teams focused on applied problems identified by New Zealand industry and government. We rank within the top 200 chemistry-related departments in the world and lead the next-ranked New Zealand chemistry department by over 100 places.

The School has an international reputation in natural products chemistry and medicinal peptide chemistry and also in the development of potential metal-containing anticancer drugs. Our materials chemistry expertise has resulted in the development of gas sensors which are now being incorporated in reliable sensing networks and photocatalysts.

Besides the success of individual research groups, our multi-investigator programmes and centres provide a foundation for joint funding bids and research publications. For example, the combined Photon Factory and Microfabrication Laboratory are designed to collaborate with participants from across the University (including Physics and Engineering) as well as with NZ industry. The Polymer Electronic Research Centre (PERC) has evolved over time into the

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recently renamed Polymer Biointerface Centre which reflects a shift in focus towards interfacing electronics with biological systems and the development of biosensors from the former focus on a more fundamental understanding of conducting polymers. The Biocide Toolbox is supported by a multiyear government grant ($15.2 million) and involves six SCS academic staff, in addition to other University researchers, with a principal aim to develop novel biocidal packaging for and in conjunction with NZ industry. The Centre for Green Chemical Science was launched in 2015 with the aim of enhancing research and teaching in Green Chemistry and associated fields. As well as enhancing research collaboration, it has organised three conferences and developed an undergraduate BSc specialisation in Green Chemical Science.

Our Wine Science research has developed new knowledge about Sauvignon Blanc and Pinot Noir winemaking, and this research is shared directly with industry. The research programme benefits from having a resident winemaker, Neill Culley, who also runs our postgraduate wine science programme at our Waiheke campus. Meanwhile, our Food Science programme has particular expertise in investigating bioactive food ingredients, food product development, food safety, and characterisation of polysaccharides such as starch. Productive collaborations have been established with Chinese academics and local government agents to investigate issues such as high-selenium foods.

Several of our staff have developed their research ideas into commercial companies which are at a range of maturities. Neuren Pharmaceuticals is taking two drugs developed by Distinguished Professor Dame Margaret Brimble through advanced clinical trials. Of particular note is trofinetide, which has been approved for treatment of Rett Syndrome and, more recently, NNZ-2591 which is designed to treat a range of brain injuries and diseases. Professor Brimble is also a scientific founder of the company SapVax LLC which will commercialise the peptide-based, self-adjuvating vaccines developed in her group. Professor David Williams started Aeroqual in 2001, and more recently Mote, with Aeroqual developing air quality sensors and Mote focusing on providing comprehensive air quality measurement and monitoring services.

Professor Cather Simpson started Engender Technologies to develop a new way to sort bull semen. In late 2018 the company was bought by CRV-Ambreed, and Cather is currently on a two-year 0.8 FTE secondment to that company. Professors Simpson and Williams have also started Orbis Technologies, initially developing at-milking shed diagnostics and has since pivoted to testing for the coronavirus.

There are many more stories in this report and we hope you will enjoy reading them – we have certainly found our research to be exciting and inspiring and are pleased to be able to share it with you!

ASSOCIATE PROFESSOR GORDON MISKELLY
Head of School of Chemical Sciences
The University of Auckland

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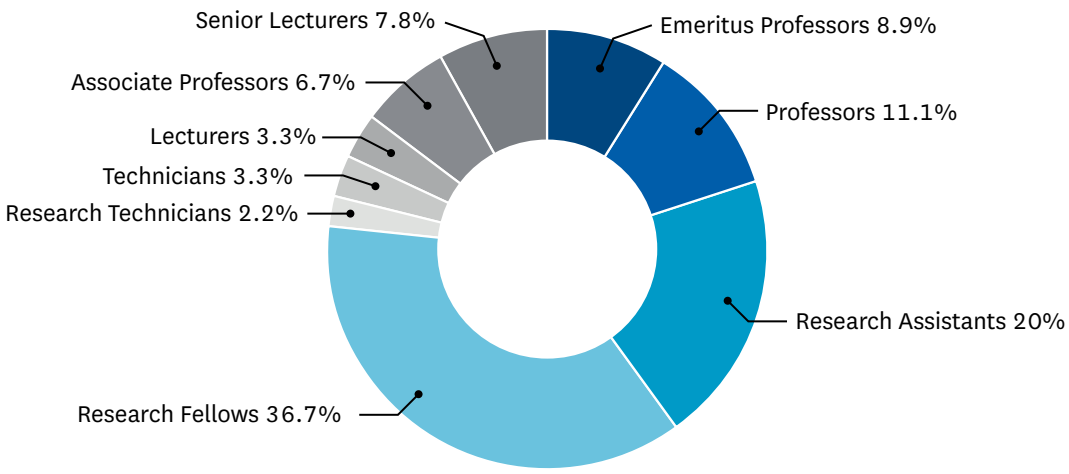
Our people

Of the ten departments and schools in the Faculty of Science at the University of Auckland, our school is one of the largest. The School of Chemical Sciences (SCS) is composed of 120 staff members, more than 340 postgraduate students and nearly 1000 undergraduate students majoring in one of our degrees.

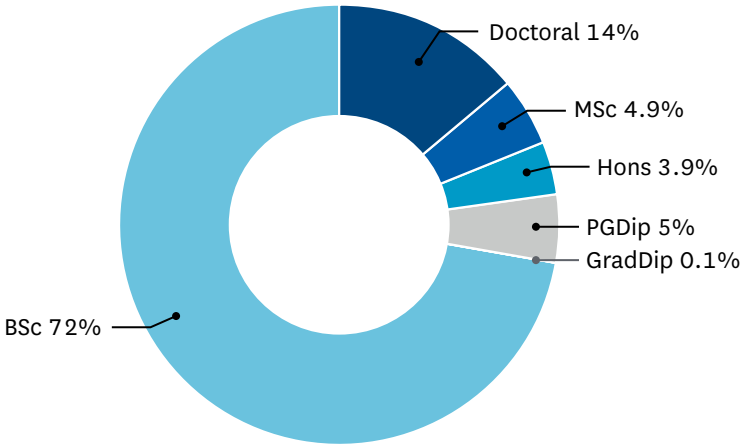
Our research and teaching spans the disciplines of chemistry, wine science, food science, forensic science, medicinal chemistry and, our most recent addition, green chemistry.

Snapshot of the School

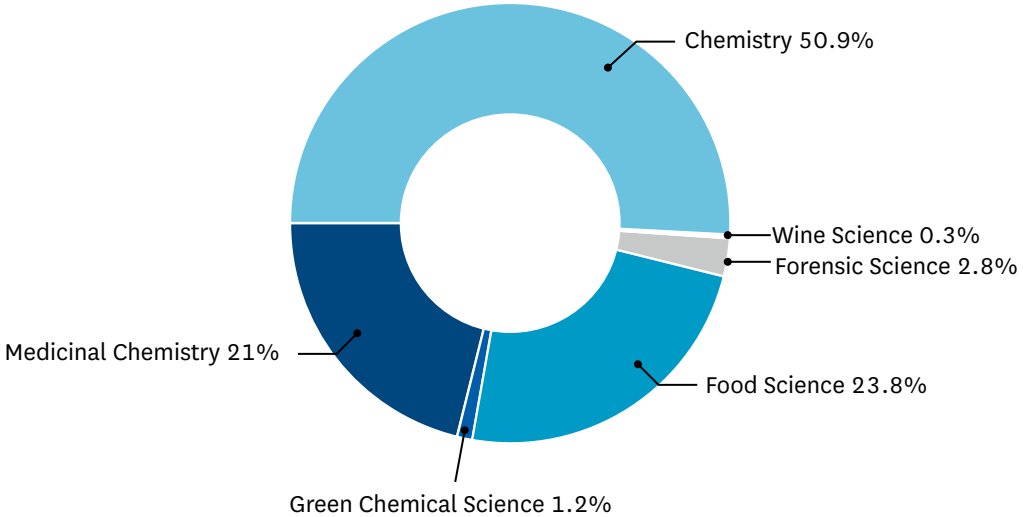
Composition of staff members



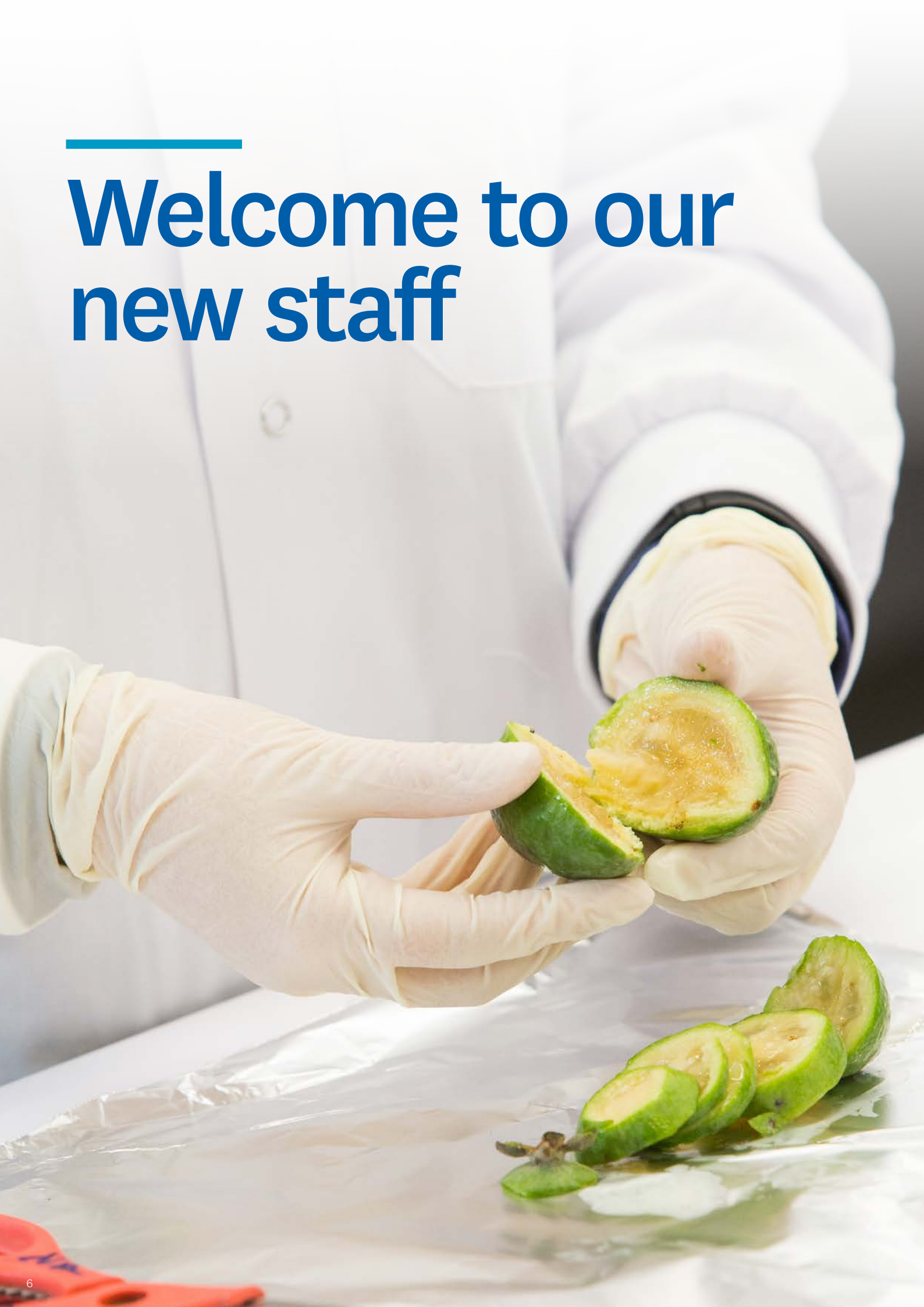
Degree breakdown of enrolled students (all levels)



Specialisation breakdown of enrolled students (all levels)



Welcome to our new staff



Welcome to our new academic staff members who have joined the School of Chemical Sciences since mid-2019. Read on to learn more about their research and what inspires them.

Dr Lisa Pilkington

Senior Lecturer
lisa.pilkington@auckland.ac.nz

What/who inspired you to pursue a career in science?

I have always been very curious about the world around us, wanting to know why things happen and how things work. A career in science allows me to discover and explore every day. I love the idea that I am investigating things that have never before been researched, that I am furthering knowledge and that I am (hopefully) making a difference.

What do you think the coolest discovery in your field of research is? Why?

To me, the coolest discovery in my area is the development of advanced statistical analysis techniques, particularly those that enable the analysis of extremely large data sets. The discovery of these techniques has meant that we can look for patterns, trends, correlations, clusters and so much more in our chemical data. These techniques mean that we can learn so much from data and decipher and uncover information about phenomena that we would otherwise not be able to.

How do you plan to build a diverse (and inclusive) research team in order to tackle social and environmental challenges faced by the wider community?

I want to be an approachable, friendly and open person that students feel has their best interests at heart. I would love to have a reputation of being fair and someone students feel would be a supportive supervisor, regardless of their background. I would like to foster a helpful and kind research group that works together and is a great team.

Where would you like your group's research to be in 20 years?

I aim to be leading a diverse, supportive, successful research group that produces novel, ground-breaking and impactful research. I would like the work we produce to be well-regarded in scientific domains, but also have real-world impact. Much of my research could potentially have significant applications and change lives and I aim to achieve that and realise that potential.

> ***"I love the idea that I am investigating things that have never before been researched."***

What has been the biggest challenge you have overcome in your career (so far)?

The biggest challenge for me has definitely been, up until recently, the uncertainty with availability of academic positions and worrying about obtaining grants and funding to pay my salary so I could continue to build a career and trajectory that would enable me to get a permanent academic position and continue on in what I am so passionate about and what I love to do. Now that I have a permanent position, it is an amazing feeling that I can direct my attention and efforts to creating a research group and conducting impactful research.

Dr Davide Mercadante

Senior Lecturer
davide.mercadante@auckland.ac.nz

"Every single day I get to satisfy my curiosity and by doing so, hopefully contribute to societal advancement."

What/who inspired you to pursue a career in science?

I can summarise the triggering factor that inspired me to become a scientist as a single word: curiosity. Among the great number of quotes that Albert Einstein left us, my favourite has always been, "I have no special talent. I am only passionately curious." I personally believe that this observation, (although clearly a hyperbolic connotation when written by Einstein), depicts one of the main reasons for which some of us, and certainly me, have chosen a career in science.

In a way, quite logically, talent and expertise must feed on passion and curiosity, which have so far led humankind to understand their surroundings and inner workings: from the molecular mechanisms underpinning life to the physical bases of the Universe. Only by starting from a genuine sense of curiosity about the world are we able to build our expertise and answer the questions that we come up with as Scientists. As a scientist I am fortunate enough not to work exclusively for a salary or not too eagerly wait for my holidays (to then get holiday blues once I'm back!). Every single day I get to satisfy my curiosity and by doing so, hopefully contribute to societal advancement.

What do you think the coolest discovery in your field of research is? Why?

I completed my BSc and MSc degrees in Biotechnology, with a PhD in Chemistry and, by training I am a computational biophysicist. Having come across different backgrounds and expertise from chemistry, to physics and biology it is accurate to say that my research, as well as my interests, span across several disciplines. As computational biophysicists our interest is to relate, by means of molecular simulations that use the same supercomputers used for weather and seismology predictions, molecular dynamics to molecular function. Unsurprisingly, the discovery of protein structural elements (by Linus Pauling in 1948) was probably one of the most significant for me. We use protein structures and "animate their dynamics" within their working micro-environment, through simulations. Because dynamics are so important to my research, alongside the discovery of protein structural elements, the discovery of protein disorder is conceptually, probably the other extremely significant discovery in my field. Just 15 years ago we started to understand that proteins, the workhorses of cells for which we have always believed that shape was everything needed for function, can also function without structure in many cases. For me, as a scientist who is passionate about the role of molecular dynamics, the discovery of proteins without structure is enormously exciting, as it simply places molecular dynamics alongside molecular structure as a pillar that supports life as we know it.

How do you plan to build a diverse (and inclusive) research team in order to tackle social and environmental challenges faced by the wider community?

When it comes down to the concept of diversity from a scientific standpoint, I can say that I am particularly advantaged as a computational biophysicist. As it is already possible to grasp from the word "computational biophysics", my field is strongly cross-disciplinary with a diversity of expertise required to study the complexity of the molecules that we investigate. The need of diversity and its importance is therefore almost seared into our workflows and we fully understand the importance and the advantages of it. I like to think that if all scientists could have been exposed to the same cross-disciplinarity of computational biophysicists, the lack of scientific diversity and inclusivity would possibly be less of an issue.

I was particularly fortunate that a series of talented women scientists applied to work with me as either Hons, MSc or PhD students this year. Getting more women passionate about careers in STEM is a top priority for me to ensure that future generations of women have the opportunity to reach the highest echelons of the scientific world.

I also take great interest in engaging with Māori and Pacific students in science. I have seen first-hand the great foundations the University of Auckland is building with their many workshops and meetings especially designed for engaging with Māori and Pacific students, to pique their interest in potential careers in STEM.

Where would you like your group's research to be in 20 years?

I have been thinking long and hard about this and must admit that I probably had to rethink my research strategy as a whole, making a few adjustments to my research agenda for the long-term. While in Europe

> ***"... the life of an academic is similar to that of a semi-nomad."***

there is a consistent and appreciable amount of funding devoted to fundamental research, here in New Zealand the vast majority of research money seems to be allocated to actively solving 'grand-challenges', proposing 'smart-ideas' or more generally ideas that have a ready commercialisation potential. It is not easy for a computational biophysicist to think in terms of "commercialising ideas".

So I had to ask myself the question of how to integrate my research within the funding landscape in New Zealand. I finally decided, for part of my research, to focus on adopting computational workflows that target the design and optimisation of proteins suited for industrial applications. This is something that I had previously worked on and that has potential beyond basic research. These 'designer' proteins could be a game changer for the industrial sector in New Zealand and abroad.

As an example, imagine a protein as a necklace made of beads. Each bead can have roughly 20 different colours, which mediate, all together in a sequence of beads, the function and stability of the necklace (the protein!). It is difficult to design new protein sequences with higher stability or enhanced function due to the combinatorial problem of a random design. For a necklace with only 2 beads, as I said each with 20 possible colours, there would be 202= 400 necklaces to choose from. Even the most chic person would have trouble choosing. We use computer simulations to win such randomness and come up with protein designs that are more stable and can be suited for industrial applications. Overall, this design can be used to create functional proteins for industry, with the additional benefit of possibly replacing chemical-based transformations of compounds (via organic molecules, or inorganic catalysts), with fully biodegradable working units (proteins) that at the same time are highly efficient. My group is and will be targeting that space among others, with the mission to trigger real world changes.

What has been the biggest challenge you have overcome in your career (so far)?

At the start of a scientific career, the life of an academic is similar to that of a semi-nomad. We move a lot, mostly bound to funding, which lasts a relatively little amount of time, between one to three years in the best case scenario. This is certainly challenging but is also a blessing to develop our expertise.

By travelling quite extensively, we not only discover different countries and cultures, but we also become familiarised with different research strategies and philosophies, which we bring with us once we settle into a permanent academic position.

Nevertheless, our "settling down", job-wise, depends from the availability of a permanent position, which are scarce nowadays. We are extremely skilled individuals and it is because of the work of academics around the world that the vast majority of people can now use smart phones, can take a Panadol for a headache, drive electric cars or have a cheap and widely distributable vaccine for Covid-19. Ultimately, it is our duty to actively engage with the community and governmental bodies, to make them more and more aware of the importance of academic research and the need for additional academic funding.

For me, the biggest challenge has been transitioning into an academic position. The bottleneck for moving into a principal investigator role from a postdoctoral position has become narrower over the years. This is the point where many talented academics, even though they wish to pursue a career in science, are opting for different options out of necessity, often joining R&D divisions of companies around the world. As a result, academia is losing talented people to industry and the world is missing big opportunities in long-term developments.

Dr Cameron Weber

Senior Lecturer
cameron.weber@auckland.ac.nz

What/who inspired you to pursue a career in science?

There have been a lot of influences that have led to my current career direction although I hadn't really planned to end up a chemist until the end of my third year at University. My father and grandmother are both academics (statistics and botany respectively) so I had exposure to the University and scientific research environments growing up. I also had a great high school chemistry teacher who helped spark my interest in chemistry and this meant that I chose it as my 'elective' at University where I started off doing a conjoint BSc/BCom in applied mathematics and economics. Ultimately, I realised that chemistry was not just more enjoyable but it felt more fulfilling and decided to keep going, and still haven't stopped studying it!

What do you think the coolest discovery in your field of research is? Why?

I think the idea of having salts that are liquid at room temperature (ionic liquids) is pretty amazing because it goes against everything you are taught about ionic compounds being brittle high melting solids and highlights the importance of the finer details of structure, shape and molecular interactions. The complexity of these liquids has meant much of the 'conventional wisdom' about the way that we think about solvents and electrolytes has had to be rewritten as they don't neatly fit many existing models of solvation. This has paved the way for all sorts of interesting innovations from novel energy applications such as non-flammable battery electrolytes to platform technologies for biorefineries.

How do you plan to build a diverse (and inclusive) research team in order to tackle social and environmental challenges faced by the wider community?

Part of this plan is to try to provide opportunities for students to get involved in research as early as practical. I've tried to incorporate funding for summer students in most of my recent grant applications to be able to provide opportunities for undergraduate students to get involved in research. Making the decision to stay at Uni to do a research degree after completing a BSc can be a daunting one, particularly for students who don't have friends or family that have personal experience of postgraduate study (or University study in general). Being able to see what the research environment is like before having to commit to a year (or more) of further study allows students who may not have role models that have had the opportunity to pursue higher levels of study see what the experience will be like before needing to decide if that is what they would like to pursue.

I've also tried to communicate my research to a broad audience through interviews on Radio New Zealand and outreach activities such as MacDiarmid NanoCamp through to discussions in chemistry courses I teach to try and create awareness of the work that we do in my group to encourage a diversity of students to become interested and get involved. My current research team has a nearly even gender balance and has students from different ethnic backgrounds which is something I would certainly like to continue. Having a diversity of lived experiences helps generate different perspectives on research problems which will assist in tackling complex socio-environmental issues of the type that we would like to address with the green chemistry work happening within the group.

Where would you like your group's research to be in 20 years?

Much of my group's research is focused on green chemistry where the ultimate aim is to develop new technologies or methodologies to improve the sustainability of the chemical industry, from reducing reliance on fossil carbon through to designing safer chemical processes. These technologies have no impact on safety or environmental impact unless they are adopted so it would be great to see some of the outcomes from our research being incorporated into industrial processes within the next 20 years and for some of our findings being used to inform the development of more sustainable processes. I also hope that I get to see the students who have worked within the group make a positive difference to the world in their own chosen fields.

What has been the biggest challenge you have overcome in your career (so far)?

Without a doubt the biggest challenge has been moving internationally with children, often on one or two year contracts with the ongoing uncertainty about what happens at the end of the contract (which the visa was invariably tied to). Our older son had lived in four different countries before his fourth birthday! While it was an adventure and a privilege to be able to live and work in multiple different countries, it did make planning for the future very difficult when you weren't even sure if you would be in the same country next year. On the other hand, it was very motivating to try and find a permanent position and I'm glad that we have been able to settle down in Auckland.

Dr Kang Huang

Lecturer
kang.huang@auckland.ac.nz

What/who inspired you to pursue a career in science?

There will be a big shortfall between the amount of food we produce and the amount needed to feed everyone in 2050. At the same time, agriculture is among the greatest contributors to global warming, emitting more greenhouse gases than any other industries. The environmental challenges posed by agriculture are huge, and they will become more pressing as we try to meet the growing demand for food worldwide. That's why I am keen to pursue a career in the food and agricultural area.

What do you think the coolest discovery in your field of research is? Why?

The 2020 Nobel Prize in Chemistry has gone to Emmanuelle Charpentier and Jennifer A. Doudna for their discovery of the sharpest gene editing tool: the CRISPR/Cas9 genetic scissors. This technology can be applied in the food and farming industries to modify a broad number of plant species, immunize industrial cultures (e.g. yoghurt), and diagnose target molecules in complex food systems.

How do you plan to build a diverse (and inclusive) research team in order to tackle social and environmental challenges faced by the wider community?

My research plan is to develop an interdisciplinary research programme at the interface of biomaterials, food processing, nanotechnology, food microbiology, numerical simulation, and molecular imaging to address critical questions in agriculture and food systems. Growing challenges to assuring the security of the agriculture and food systems, producing profitable healthy foods, reducing food waste, and saving energy, alongside advances in material science have created new opportunities to better understand how we can develop state of the art engineering solutions to address complex problems at the food/energy/water/climate nexus.

> ***"Environmental challenges posed by agriculture are huge, and they will become more pressing as we try to meet the growing demand for food worldwide."***

Where would you like your group's research to be in 20 years?

My research team will conduct cutting-edge research related to Food Process Innovation and Biomaterials & Biointerfaces, as a means to develop an integrated bio-based approach for improving the safety, quality, and sustainability of agriculture and food systems.

What has been the biggest challenge you have overcome in your career (so far)?

One of the challenges of moving from the US to NZ is adjusting to another culture. Sometimes it can be difficult because nothing is familiar and I have to grow accustomed to a completely different way of doing things. However, the experience of living in NZ is extremely worth it, as this is an amazing country.

Dr Shengping (Allan) Zhang

Research Fellow
shengping.zhang@auckland.ac.nz

Describe your research in 15 words or less?

The development of peptide-based therapeutics as SARS-COV-2 spike protein blockers and virus entry inhibitors.

What would be your advice to an undergraduate science student about postgraduate research?

I would like to suggest that undergraduate science students should be given more opportunities to participate in postgraduate research even in their early stage of undergraduate study. This will help them build up a better understanding of what they learned from the textbook.

What has been the biggest challenge you have overcome in your career (so far)?

The biggest challenge to me is the uncertainty of my future career path, especially the availability of academic positions.

Dr Emma Davison

Research Fellow
emma.davison@auckland.ac.nz

Describe your research in 15 words or less?

Synthetic access of new naturally-occurring compounds to enable exploration of their important biological activities.

What would be your advice to an undergraduate science student about postgraduate research?

It is a lot more challenging (both emotionally and in practise) than you might think; the reactions you will have conducted in the undergraduate labs have been specifically chosen to teach certain skills and because they work reliably – not so in the organic chemistry research labs! The challenge is part of what makes your weeks interesting though, and with perseverance, it can be extremely rewarding. Stick with it, there is no better way to learn more about chemistry than through postgraduate research!

What has been the biggest challenge you have overcome in your career (so far)?

It wasn't until I started applying for post-doctoral research fellowships myself that I realised how challenging it can be to obtain funding. The applications require a lot of work (especially when you're new to grant writing) and the success rate is low. After several rounds of rejected applications (which was a bit disheartening!) I was extremely honoured to be awarded a Rutherford post-doctoral fellowship which was the biggest achievement of my career to date!

Dr (Amy) Bicheng Zhu

Research Fellow
bicheng.zhu@auckland.ac.nz

Describe your research in 15 words or less?

Developing new materials and platforms for wearable and implantable energy storage devices and biosensors.

What would be your advice to an undergraduate science student about postgraduate research?

Postgraduate study is a valuable time to gain new knowledge and learn new techniques. It is fun to discover new materials and apply these materials to exciting applications. It is worthwhile to spend a few years focusing on one thing that you are interested in. During that time, you will get to know the process of defining a problem, how to propose a solution and validate a methodology. It is also a good opportunity to gain problem-solving skills, time management, project planning, and teamwork, which will equip you for the future job market.

What has been the biggest challenge you have overcome in your career (so far)?

The biggest challenge for me was obtaining the first grant. It is a painful process to identify the research gaps, develop a novel solution, and write a grant application. It was a long process to read many papers and have a clear understanding of the problem. Another challenge is to tell the story using my second language. Even though the process is painful, the outcome is exciting. I got my first grant (SfTI Seed Funding $200,000) to support my research. The critical thing is to keep going, be patient, persistent, tough and motivated. Hard work truly does pay off in the end.

Dr Rebecca Jelley

Research Fellow
rebecca.jelley@auckland.ac.nz

Describe your research in 15 words or less?

The analysis of the chemical constituents of beer and wine matrices.

What would be your advice to an undergraduate science student about postgraduate research?

Make the most of any opportunities that come your way both related to your field of study and those completely unrelated offered in the wider university community. Step out of your comfort zone and area of knowledge as there are many workshops, courses and networking events offered for free to postgraduate students.

What has been the biggest challenge you have overcome in your career (so far)?

Trying to juggle a non-science start-up company in my spare time when there really is no spare time...

Dr Alaitz Etxabide Etxeberria

Research Fellow
alaitz.etxabide@auckland.ac.nz

Describe your research in 15 words or less?

Renewable and biodegradable intelligent food packaging: label better, waste less.

What would be your advice to an undergraduate science student about postgraduate research?

My advice for an undergraduate student is to think long and hard before choosing a research topic. Think about those things that you are passionate about, believe in and feel are important. Then, try to connect the subject of your study to these things. If you are able to do this, then it will be much easier to maintain motivation, creativity, concentration and energy.

What has been the biggest challenge you have overcome in your career (so far)?

There are many obstacles that a researcher has to overcome during her/his career, such as the choice of a research topic/group that keeps you motivated, moving to other countries, communicating in other languages, etc. For me, the biggest challenge is to keep obtaining financial support in the form of research funding, or to secure a permanent position as a research staff member that will enable the continuation of my career. The uncertainty is what concerns me the most. But so far so good!

Farewells

We would like to say goodbye to those staff members who are sadly leaving the School and thank them for their time with us. We've asked them a few questions to celebrate their new positions.

Dr Ivanhoe Leung

i.leung@auckland.ac.nz

Where is your new position?

Melbourne, Australia. I will be joining the School of Chemistry and the Bio21 Institute at the University of Melbourne.

Provide some details about your new position.

I will be joining as a senior lecturer in biological chemistry so I suspect my role will be very much similar to my current position in Auckland. So yes it will be a combination of teaching, research and admin. Building a lab from scratch and recruiting new students is going to be hard work but I look forward to the new challenges ahead.

What would be your advice to a PhD student in their first year?

First year is a good time to figure out your research interest. The research questions in your PhD project may seem daunting and you may not have a lot of experience in the tools and techniques that you are going to use – but that is normal so don't get too stressed about it. Take the opportunity to learn new skills and try things out in the first six months. Celebrate every little success, whether it is making your first protein or running your first NMR spectrum (trust me my first NMR spectrum was my Facebook profile picture for a while during my Hons).

The big end goal of your PhD may seem very far away, but you can break it down into smaller and achievable tasks and you can then set yourself realistic targets to complete those tasks. I also find it helpful to set yourself a publication goal that you would like to achieve by the end of your first year. It could be writing a small review paper or finishing off those loose ends in your Hons project so that you can write up a small paper. Seeing your name in your first publication will boost your confidence and keep you going in your second year!

Dr Leandro Dias Araujo

l.araujo@auckland.ac.nz

Where is your new position?

Lincoln University

Provide some details about your new position.

I'm now a lecturer in wine chemistry working at the Department of Food, Wine and Molecular Biosciences. I will be doing research and teaching related to wine and food chemistry.

What would be your advice to a PhD student in their first year?

Take your time to know well your project, your group, the resources available and how to get help. The first year is the perfect time to set realistic goals, but you must be flexible. Plans never go as expected and it's not different with research.

Our stories

Research under lockdown

The various lockdown periods in New Zealand ultimately left a lot of researchers worried about the implications of on-going experiments being compromised by lab closures. In order to comply with government and university restrictions, only postdoctoral fellows and senior PhD students were granted special access during Level 3. We were able to welcome additional students at Level 2, however the vast majority were unable to return to the laboratories under Level 1 due to space restrictions.

Our wonderful technical team, headed by Mike Wadsworth

As well as their regular research support roles throughout the year, many of our technical team were classified as essential workers and responsible for supervising the building and facilities during Level 4 lockdowns. This included the Chemical Stores function, liquid nitrogen fills, supervision of freezers and observations on behalf of other departments. Appropriate signage was also arranged in preparation for returning research groups to ensure that social distancing measures and separate bubbles were in place for Level 3 operations.

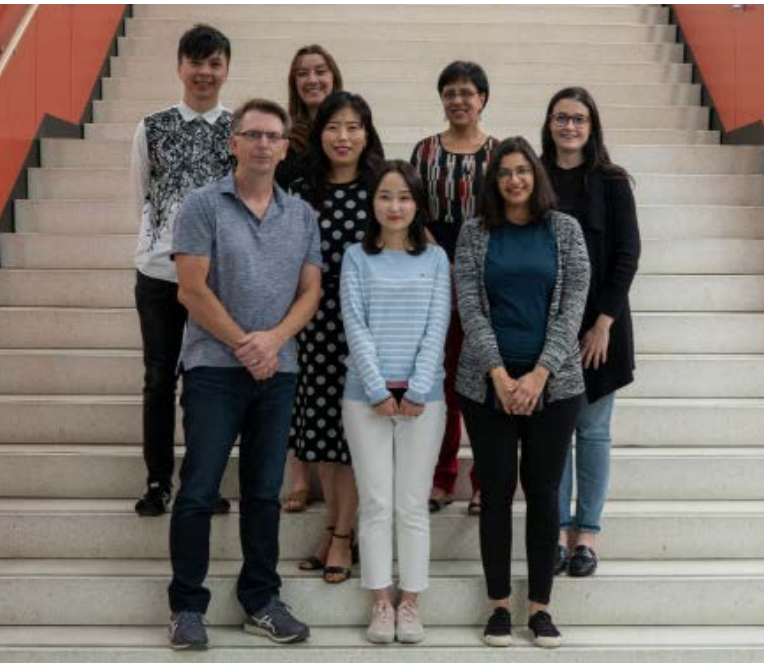
The instrument technicians had the challenging task of maintaining instruments and keeping facilities running throughout the year, without service engineer support from outside of NZ, due to the COVID-19 border lockdowns. This involved some creative thinking to put systems in place for research groups operating during Alert Levels 2 and 3. The team successfully managed this additional work flow as research built back to usual demands as Alert Levels decreased.

Special mentions go to; Michael Schmitz, NMR facility manager, who maintained instruments during Level 4 and provided operational support during Levels 2 and 3 once researchers returned. Electrician, Roger van Ryn, took on the additional workload in the absence of overseas support engineers and used his expertise to troubleshoot our single crystal/powder XRD and AFM instruments. And Alastair Mead, our talented glassblower, provided his usual support throughout the year to all research groups by attending to their specialised glassware needs.

The teaching team had to overcome some serious challenges because laboratories weren't open to students, and there was a huge effort from Katrina Graaf and her team to produce and film practical experiments so that courses could be run remotely during higher Alert Levels. A huge thanks for this, and for managing the Health and Safety and operational aspects of the teaching labs at different Alert Levels.

While most of us were at home during the Level 3 and 4 lockdowns writing theses and publications - and meeting via Zoom or teaching online - research teams in the School of Chemical Sciences were leading two projects which focused on addressing solutions to Covid-19.

Thanks to emergency investment funding of $500,000 provided by the Auckland Medical Research Foundation (AMRF) to investigate the impacts of the virus, the School was fortunate to be selected for two of the six projects, as outlined below.



Research Services and GSC teams.

Alongside rising to the challenge of accessing facilities and equipment, our research has been impacted in many other ways by COVID-19, including delays to international student recruitment, access to field work, and the inability to visit with our collaborators and stakeholders. Our Research Services team (Emma Dawson, Joo Young Jeong, Simrin Ahmed and Victoria Smith), who work within the School to coordinate and manage our research, set to work immediately in March 2020 to assess the impacts to our 180+ research projects. Working closely each research team, adaptive plans were developed to mitigate these challenges. Thanks to their efforts, our research projects have been able to run effectively, avoiding risks to projects that may have otherwise been unable to continue. Identifying new sources of funding to support our researchers has also been a high priority, including funding for innovative and important COVID-19 research for New Zealand. The team continue to work hard monitoring the health of our research to ensure we can keep up and running as we deal with the ongoing effects of the pandemic.

Our Group Services team (John Lau, Anna-Marie Simcock and Michael Groom) have also been hard at work throughout the lockdowns, ensuring our School connected throughout the alert levels, including arranging regular online staff meetings, assisting with the organisation of our new research events, and arranging much needed extensions to our fixed-term researchers contracts to keep us running effectively. Thank you also to Min Young and her team from Academic Services, for supporting our students throughout the challenging year.

Distinguished Professor Dame Margaret Brimble alongside early career researchers **Dr Alan Cameron** and **Dr Shengping Zhang** were awarded $96,457 to investigate whether existing chemical manufacturing technology can be used to develop an anti-viral treatment for COVID-19. **Dr Daniel Furkert** was also awarded $74,470 to test a set of lead compounds, from an existing antiviral drug collaboration, against SARS CoV-2.[1,2,3]

New Zealand is unique in that the first outbreak was contained and a community spread of the disease was prevented by strict lockdown measures. A viable strategy to develop treatments for a potential future outbreak is the focus of many researchers within the country. The two main short-term COVID-19 treatments involve either convalescent sera or direct-acting anti-virals (DAAVs). The former involves using sera from patients who have recovered from the disease, where neutralising antibodies were found to be safe and effective, whereas DAAVs are small molecule drugs that directly prevent or interfere with the replication of the virus. [2,4]

[1]https://www.scimex.org/newsfeed/covid-19-vaccine-research-funding-for-nz

[2]https://www.auckland.ac.nz/en/news/2020/04/30/emergency-research-grants-for-covid-19-projects.html

[3]https://www.nzdoctor.co.nz/article/undoctored/high-demand-covid-19-research-funding-sees-vital-projects-miss-out

[4] https://www.nzma.org.nz/journal-articles/the-post-lockdown-period-should-be-used-to-acquire-effective-therapies-for-future-resurgence-in-sars-cov-2-infections

Orbis Diagnostics, co-founded by **Professor Cather Simpson** and **Professor David Williams**, owns a proprietary platform technology which was originally developed to measure the components of milk samples that enable farmers to monitor cow's health, reproductive and nutritional status. The milk samples are mixed with reagents on discs and centrifuged to separate out particles, and advanced laser technology is used to measure the components of the milk. [7] The ability to determine the extent to which a person is immune to COVID-19 would enable the actual conferred immunity once a vaccine program has begun and allow selection of alternative treatments for those with insufficient immunity. [5] Orbis quickly recognised that their technology could be adapted and used as a quantitative measurement of a person's immunity, and is superior to the current rapid strip antibody tests which only assess the presence of antibodies.[6] This would be valuable, as the screening process is designed to be operated by non-technical staff and would enable free movement for those with immunity and avoid the need for mandatory quarantines. The ELISA assay testing procedure also uses disposable microfluidic discs and brings testing into the field using a robust system that is conveniently the size of a desktop printer. Orbis are currently adapting the system to detect COVID-19 antibodies and conducting clinical trials prior to rolling out the new technology. [8]

[5] http://www.xinhuanet.com/english/2020-05/23/c_139081078.htm

[6] https://www.prnewswire.com/news-releases/us-and-new-zealand-scientists-from-orbis-diagnostics-collaborate-on-covid-19-mass-immunity-testing-to-enable-quarantine-free-international-travel-301100470.html

[7] https://www.innovation.auckland.ac.nz/photon-factory/

[8] https://new-zealand.globalfinder.org/company_page/orbis-diagnostics

https://www.nbr.co.nz/tags/professor-cather-simpson

Distinguished Professor Dame Margaret Brimble

Funding success

MBIE

Distinguished Professor Dame Margaret Brimble was awarded a Ministry of Business, Innovation and Employment (MBIE) Endeavour Programme Grant, the first of her career, for the project titled 'Waerau waikawa iti rongoā paturopi: New Generation Peptide Antibiotics.' Antimicrobial resistance is a global phenomenon where drug-resistant microbes render current antibiotics ineffective. The project focuses on the development of antimicrobial peptides as a chemical defence against drug-resistant bacteria. The programme aims to expand the new antibiotic pipeline by optimising the therapeutic properties of lipopeptide antimicrobial peptides, involving cultivated and uncultivated New Zealand microbiomes to identify new lipopeptide scaffolds.

MBIE Endeavour Fund, M. Brimble (PI) with G. Cook (UoO), J. Owen (VUW), G. Painter (VUW), R. Keyzers (VUW), P. Harris (UoA), G. Bashiri (UoA), S. Ritchie (UoA), M. Stott (UC), R. Furneaux (VUW), T. Davidson (Glycosyn), A. Groves (Tuia Innovation) "Waerau waikawa iti rongoā paturopi: New Generation Peptide Antibiotics" $10,555,948 (1/8/20-30/9/25)

Marsden

We are delighted to share that three Marsden grants that have been awarded to academics in the School of Chemical Sciences.

Professor Jadranka Travas-Sejdic

Associate Professor Tilo Söhnel
Skyrmion systems: New Opportunities for Information Technologies, $941,000.

Unconventional topological spin structures such as in chiral spin systems offer a plethora of fascinating phenomena for fundamental research and future technological applications.

The purpose of the project is to investigate novel topological spin systems, in particular multiferroic skyrmion materials, for their crystallographic and magnetic structure, surface topology, dynamics and their interaction with external stimuli. In particular, recently discovered multiferroic skyrmion materials offer the possibility of the direct control of skyrmions through an external electric field, which makes them ideal for nanoelectronics and data storage for IT applications.

The specific aim is to use non-magnetic and magnetic doping in order to increase the stability range of skyrmions. The obtained information will provide valuable information for a systematic search for multiferroic skyrmion materials towards room temperature applications for future low energy skyrmionics devices such as 'race track' memory devices used in next-generation computer and information technology."

Professor Jadranka Travas-Sejdic (PI), Dr EWC Chan (AI)
A new approach to Transient Organic Electronics, $941,000.

Transient electronics is an emerging field where electronic devices or circuitry are intentionally designed to a loss of function irreversibly. However, current methods involve the use of inorganic materials that are potentially toxic or require high energy processing. In this project we aim to synthesise novel organic conductors that degrade under physiological conditions into environmentally benign by-products for use as transient circuitry. Our methodology will enable the advancement of transient electronics and allow for further functionality in applications such as implantable medical devices.

Dr Alan Cameron (PI)
A "self-bridging" approach to antimicrobial peptides: disulfide replacement and peptide stapling, $300,000 (Fast Start).

By 2050, multidrug-resistant (MDR) infections are projected to result in 10 million deaths annually if new drug treatments are not developed. The commercial antibiotic pipeline has failed to deliver new treatments with pharmaceutical companies having largely abandoned the growing issue of MDR infections, deeming such a pursuit unprofitable.

Antimicrobial peptides (AMPs) are a promising new source of drugs from nature, known to be less prone to resistance development. These molecules elicit their bactericidal effects through non-specific interactions with bacterial membranes, ultimately leading to loss of membrane integrity and cell death. In particular, AMPs are often highly effective against Gram-negative infections (e.g. Pseudomonas aeruginosa), which constitute the World Health Organisation's (WHO) Priority-1 list. Unfortunately, AMPs often require synthetic modification to become more "drug-like" and overcome their rapid degradation in the body (poor half-life). This research aims to develop a novel peptide 'self-bridging' technology platform to prepare a new generation of "drug-like" AMPs possessing synthetic bridge constraints, a proven approach to improve peptide properties and prolong their duration of action in the body. The novel approach aims to overcome many of the downfalls associated with the existing bridge constraint methods, providing an improved pathway to prepare new antimicrobials for the clinic.

Other notable funding

Other notable funding can be found in the appendices.

Community engagement

Dr Ivanhoe Leung, Dr Cameron Weber and Professor James Wright from the Centre for Green Chemical Science wrote an article to the Big Q discussing the impact of fast fashion and how green chemistry can solve this problem. New Zealand imports around $2 million worth of textiles and clothing from developing countries to support demand in the fast fashion industry. Manufacturing in developing countries is known for poor working conditions and low wages for workers, but an overlooked issue is environmental pollution. In particular, water pollution due to mostly untreated wastewater from textile plants leads to synthetic dyes contaminating the water. The Centre for Green Chemical Science is committed to a more sustainable future through interdisciplinary research, education and public engagement. Research is currently being undertaken into the degradation of textile dyes to harmless materials and developing water treatments that would prevent these pollutants entering waterways in the first place. Current work utilises a class of enzymes known as laccases that are found in plants and can degrade the textile dyes. These laccases can be produced cheaply, and aren't a polluant themselves which makes them an attractive solution to the textile waste water problem. Alternatively, synthetic enzymes based on compounds containing iron are also under development which also degrade the dyes (in collaboration with scientists at Carnegie Mellon University, USA).[1]

[1] www.thebigq.org/2020/09/24/fast-fashion-what-are-the-hidden-costs

Nabangshu Sharma, made a youtube video about his PhD work using enzyme biocatalysts to degrade textile dyes, a problem created by fast fashion industry that is having a negative impact in developing nations like India where Nabangshu comes from. By using bioinformatics, Nabangshu found that a thermophilic bacteria isolated near his hometown possess a putative laccase enzyme that may be able to oxidase aromatic molecules. Nabangshu made the enzyme, investigated its activity and kinetics, and used a range of chemical approaches to improve the enzyme's stability and re-usability. His long term goal is to create an enzyme biocatalyst that can be used industrially for bioremediation.

www.youtube.com/watch?v=X3fzp33WYlk

The importance of green chemistry and the focus on cleaner chemical processes was highlighted in the Radio New Zealand programme 'Our Changing World' which discussed the roles of **Professor James Wright and Dr Cameron Weber** in creating more sustainable chemistry. Of particular interest was Dr Weber's work on designing greener solvents that are capable of carrying out more than one reaction simultaneously. These deep eutectic solvents are made by combining commonly used materials such as calcium chloride and urea, and the resultant solvent has a melting point significantly lower than the original components which makes them non-volatile and safe to handle.

www.rnz.co.nz/national/programmes/ourchangingworld/audio/2018760034/green-chemistry-better-safer-more-sustainable

Electronics waste (e-waste) can be hazardous to our environment and also contain precious metals of value. Dr Ollie Crush from Mint Innovation describes their biological extraction of precious metals from e-waste (gold, copper, nickel) after cyanide-free chemical leaching. Research is underway to expand their green chemical process to extract palladium from catalytic converters and other feedstocks containing precious metals. According to Dr Weber, gold accounts for 50 per cent of the value of e-waste extracted from circuit boards and there is more gold (by concentration) in electronic waste than there is in gold ore. Therefore we need methods and processes to recycle e-waste and retrieve the elements found there.

www.cnbc.com/2020/09/18/the-power-of-green-chemistry-part-three.html

Dr Lisa Pilkington

Dr Lisa Pilkington has been featured in the NZ Herald[2] and M2 Women's Magazine[3] as an emerging female scientist whose research involves finding a targeted treatment for the fast-growing triple-negative breast cancer (TNBC). This specific cancer doesn't respond to any current immunotherapies as it lacks the common receptors that are targeted so chemotherapy is the only treatment option. Lisa and coworkers found an enzyme that promotes the growth of various TNBC cancers called PC-PLC. This enzyme is six times more active in TNBC cell lines compared to normal cells, making it an ideal new target for potential drug molecules. The group has a potent target that works as an inhibitor to the PC-PLC enzyme and current work is focused on improving the compound's stability. Dr Pilkington has personal experience dealing with cancer, so this project has real significance and getting her inhibitor to clinical trials would be a dream come true.

[2]www.nzherald.co.nz/nz/kiwi-scientist-lisa-pilkington-close-to-breast-cancer-breakthrough/KMHEW3ANI2SUVDMD4NTHOV3TPA

[3]www.m2woman.co.nz/solving-global-problems-with-molecular-focus

Honours students Chris Bainbridge, Kyle Engel and undergraduate student Briony Daley, under the supervision of Dr Jianyong Jin and Dr Ali Bagheri, led the production of 'living' 3D-printed resin. The technique is known as RAFT (reversible addition fragmentation chain transfer polymerisation) and enables the 3D printable material to change its properties after it's been produced, including 'self-repair' when damaged. Normal 3D printing involves uncontrolled polymerisation which is set with ultraviolet light so that products cannot change once the process is completed. RAFT enables products to be transformed post production, and also uses visible light (such as blue or red) which requires less energy compared to UV and is safer. Self-repairing plastics printed using RAFT could therefore be used to reduce plastic waste by reducing the costs associated with breaking down plastic objects into raw materials.

January 25th 2020 TVNZ1 6pm News
www.tvnz.co.nz/one-news/new-zealand/auckland-university-students-develop-living-plastic-can-self-repair

Professor David Barker's team had media releases on their SfTI project *www.sftichallenge.govt.nz/news/ko-te-wai-ko-te-ora-tackling-fresh-water-pollution*

Part time PhD candidate Krunal Patel in computational chemistry developed a new formulation of tooth whitening toothpaste, made with natural ingredients while working at Red Seal, that is currently on sale. The toothpaste combines commonly used baking soda and charcoal, with coconut oil and cloves extract, and a foaming agent derived from coconut oil. The coconut oil was found to be important in delivering a smooth finish to the toothpaste.

www.auckland.ac.nz/en/news/2020/06/24/toothpaste-created-by-chemistry-student-a-winner.html

Krunal Patel

The Photon Factory

A new device described on page 26 currently under development by Dr Nieuwoudt and colleagues in the Photon Factory is set to be used for identification of skin conditions. This includes common skin cancers like basel cell carcinoma as well as the more deadly melanoma. The device uses a technique known as Raman spectroscopy to identify the components of the area of skin being investigated. Higher than usual levels of certain chemicals, such as tryptophan, can indicate certain cancers. Changes to fatty acids and melanin concentrations in the skin can also be used as an indicator towards the type of skin condition. The device is currently aimed at clinicians, with a library of skin samples collected from patient donors, to improve the accuracy of detection but Dr Nieuwoudt hopes in the future it could be available to the public.[1] On a more lighthearted note, Dr Nieuwoudt was interviewed by RNZ about the device and its similarities to the Star Trek tricorder that uses lasers to give detailed examinations of living things.[2]

[1]https://www.auckland.ac.nz/en/news/2020/04/21/real-life-tricorder-screens-skins-cancers.html Radio interview

[2] https://www.rnz.co.nz/national/programmes/nights/audio/2018756314/materials-fact-of-fiction-tricorder

Commercial outputs

Clinical trials

Neuren Pharmaceuticals announced this year that the drug candidate trofinetide (NNZ2566), developed by the Brimble lab, has commenced Phase 3 clinical trials (12 week LAVENDER study then 40 week LILAC study) in the US for treatment of Rett Syndrome and Phase 2 clinical trials for Fragile X syndrome. The first study will involve about 180 girls and young women with Rett Syndrome. In July 2020, Neuren Pharmaceuticals announced that they had raised AU$20 million to fund clinical trials of NNZ-2591, the second drug candidate developed by the Brimble group to have reached this stage. NNZ-2591 is being tested as a treatment for Phelan-McDermid syndrome, Angelman syndrome and Pitt Hopkins syndrome, each of which has Orphan Drug designation in the United States.

Patents

M. A. Brimble, G. M. Cook, P. W. R. Harris, D. A. Williamson, A. Davidson and V. Sander "Lipidated Polymyxin Analogues" NZ Patent Application 767673, 2020, filed 4 September 2020

B. Lin, K. M. Loomes, R. Thota, J. Stephens, J. Evans and M. A. Brimble "Anti-inflammatory Compositions, Methods and Uses Thereof" PCT Application, 2020, PCT/NZ2020/050065, filed 3 July 2020.

W. Greenlee, S. Berezovsky, G. Trainor, M. A. Brimble and G. M. Williams "Peptide Conjugates Incorporating Urea Elements and Their Use as Vaccines" U.S. Patent Application No. 16/864,348, 2020, filed May 1, 2020

M. A. Brimble, P. W. R. Harris, L. Yule, D. Hay and A. Tufts "Peptide Conjugate Amylin Agonists and Uses Thereof" PCT International Application PCT/IB2020/054364, 2020, filed 8 May 2020

Our research

Advanced Materials and Technologies

The field of advanced materials and technologies has a direct impact on our daily life through the development of new materials with applications in sustainable living, energy storage and health.

This highly interdisciplinary field involves a collaborative effort between chemistry and other sciences to design materials with specific properties that apply to real-world applications such as solid-state inorganic materials, including semiconducting oxides for use in solid-state batteries and fuel cell materials. Functional polymeric materials are developed for a variety of applications like medical technology, electronics and gas separation. New catalysts are being investigated to tackle anthropogenic CO2 emissions from fossil fuels by enabling greener fuel production via water splitting, CO2 reduction and N2 fixation processes. Research also focuses on biologically compatible materials used in medical applications such as bioactive coatings and membranes for biosensing applications. New techniques to study corrosion and anti-oxidant properties of materials (synthetic and natural) using electrochemical imaging and Raman spectroscopy are being developed.

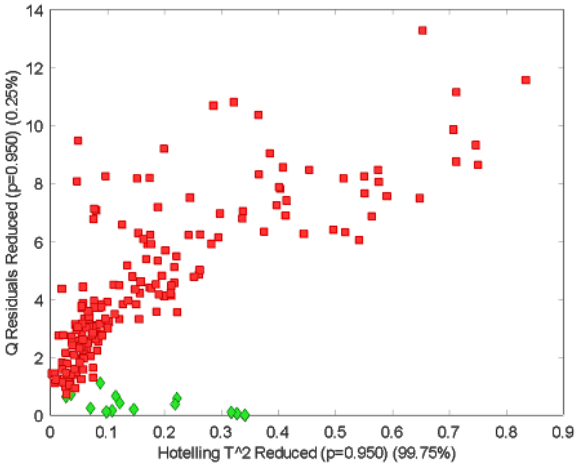
Real time clinical diagnosis using Raman spectroscopy

By Dr Michel Nieuwoudt (m.nieuwoudt@auckland.ac.nz)

Raman spectroscopy is exquisitely sensitive to how molecular vibrations are affected by changes happening in their structure – both inherent changes and those inflicted by their environment. It is a highly specific and non-destructive technique, and with low sensitivity to water is especially useful for in vivo and non-invasive characterization of components in biological tissues and organisms in their natural environment.

Current research in our group focuses on the application of this technique for real time clinical diagnosis. Using chemometric methods (chemical data analysis methods including machine learning) we extract information from Raman spectra recorded in vivo in the clinic or surgery using portable Raman systems, about specific biomarkers that help us to develop classification models. Working closely with dermatologists and surgeons at Auckland and Middlemore hospitals and the Manukau Super Clinic, our group is developing Raman systems that can diagnose the following in vivo and in real time:

- skin lesions (such as malignant melanomas, non-melanoma skin cancers and inflammatory lesions such as psoriasis, eczema, etc.) Spectra of cancerous and benign lesions measured in vivo show clear differences, as do malignant melanoma and naevi, which can be differentiated by SIMCA (soft independent modelling of class analogies) classification (Figure)
- discoid lupus erythematosus (DLE), through multiblock hyperspectral imaging of mass spectrometry (MALDI) and Raman images, to probe biomarkers specific for DLE and better understand the biochemistry of this skin condition
- prostate cancer, using specially designed Raman probes to differentiate between benign and malignant prostate tissue in situ, for prostate cancer diagnosis, or during prostatectomy procedures for surgical border assessment. ischaemic tissue margins during pancreatoduodenectomy and post-mastectomy breast reconstruction
- biomarkers for actinic skin damage (photo- and age-related)



Alphabetical list of key collaborators and researchers involved:
Aguergaray; Amirapu; Bonesi; Broderick; Brown; Cornish, Dalbeth, Musson, Naot, Watson; Demarais; Giglio; Gilling; Grey; Holtkamp; Jarrett; Locke; Marini; Matthews; Mautner; Minnee; Nieuwoudt; Novikova; Pandanaboyana; Patel; Quinn; Risos; Sewell; Shahlori; Simpson; Srinivasa; Van Breugel; Williams; Windsor; Zargar.

Read more here

Chemical Sciences for Human Health

The continuous development of novel chemical science research is important to ensure healthcare development can tackle the challenges facing our society-both locally and internationally. Key focuses include understanding disease mechanisms, design of novel targeted drugs and therapeutics for their treatment. We also examine the development of new devices and sensors to monitor health and diagnose disease.

Our research topics cover a variety of important medicinal challenges including chemotherapeutics and immunotherapies; new antimicrobial therapies to combat drug-resistant pathogens; investigations into the understanding of neurodegenerative and psychiatric diseases (eg Parkinson's and Alzehimer's); alternative treatments against diabetes and obesity; drug discovery programs focusing on target-based screening using theoretical and experimental approaches; the design of synthetic routes to structurally complex, potentially bioactive, natural products; and design of devices and sensors (which give either an electrical or optical output) for rapid detection and effective monitoring of diseases including biomarkers using peptide and DNA based sensing technology.

What else are we consuming? Plastic and the NZ diet

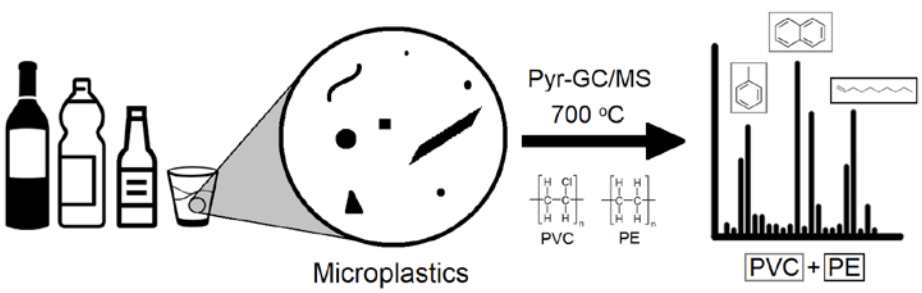
By Dr Joel D. Rindelaub (j.rindelaub@auckland.ac.nz)

Every day you're eating plastics. No, seriously. You're drinking them too.

Before you start freaking out, keep in mind there's not much you can do about it. Plastics are everywhere. From the tops of mountains to the depths of the sea, we humans have saturated the planet with our synthetic existence. So really it should come as no surprise that we happen to be consuming it as well.

Here at the University of Auckland, we were curious exactly how much plastic we're ingesting, so we started looking for tiny plastic particles (microplastics) that made their way into local beverage products and tap water. Through this study, we were able to estimate that each New Zealander is drinking at least 1.5 g of polymeric material per year, which is the equivalent of downing about one third of a credit card annually.

Not too appetising, right? Well maybe, and maybe not. The WHO currently labels microplastics as low risk, but their assessment doesn't take into account two very big unknowns.



The first being that we don't know how many potentially harmful chemicals are accompanying microplastic particles. Thanks to their chemical and physical properties, microplastics could be reservoirs for things like Bisphenol A, a hormone-disrupting plastic additive.

The other unknown relates to the size of the plastic particles detected. Most studies to date have not been able to monitor the smallest sizes, like those small enough to cross the blood-brain barrier or even enter cells.

Using a cutting edge technique called Pyrolysis – GC/MS, we were able to overcome both of the previously reported measurement challenges, providing chemical information about polyethylene (PE) and polyvinyl chloride (PVC) microplastics independent of size.

Our plans for future studies will look at microplastics in the air we are breathing, partnering with local schools to allow students to collect data in their own classrooms and learn more about our impact on the planet.

Alphabetical list of key collaborators and researchers involved:
Gordon Miskelly and Liam Philip.

Read more here

Innovations in Food and Beverages

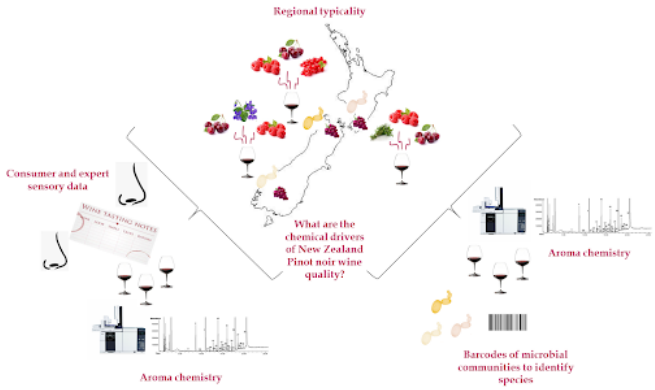
Food and beverages play an important role in our lives. This research area covers the properties of foodstuffs, agricultural and production practices and food safety, and we are working closely with industries including dairy and wine to apply our research on stability of foods and investigating quality parameters in wine.

Our researchers study the composition of food macro-components, such as carbohydrates, proteins and lipids. Research topics focus on the chemistry of starch and the structure and function of food proteins by investigating their composition and oxidative stability. Researchers interested in functional foods study the extraction and functionality evaluation of bioactive molecules from foods using chemical and biological assays, as well as studying the stabilisation of bioactive molecules. Food processing is important to ensure a longer shelf life and improved food safety. Research on this topic covers the physiocochemical, nutritional and sensory qualities, and microbiological safety of foods affected by food processing methods. Our applied research with the NZ wine industry includes investigating the effects of temperature on fermentation and the impacts of different yeast strains on wine aroma and taste. In addition to the key contributions of viticulture and yeasts to wine quality, the handling of grapes post-harvest and the maturation of wines are critical to wine production. Our researchers are examining the effects of harvesting methods (hand-picked versus machine harvesting) and antioxidant additions at harvest on a range of wines.

Investigating the Chemical Drivers of Pinot Noir Wine Quality

By Dr Rebecca Deed (rebecca.deed@auckland.ac.nz)

Pinot noir is the most significant red grape variety produced in New Zealand (NZ), and is second only to Sauvignon blanc in wine production volume. Vines are spread across several major NZ wine regions including Central Otago, Marlborough, and Martinborough, and each region produces distinctive wines of high quality that display regional typicality. Understanding what constitutes and drives quality in NZ Pinot noir, is essential to the sustained growth of this variety as a premium export product.



This research involves several collaborative projects with the overarching goal to understand the chemical drivers of perceived quality in NZ Pinot noir. A major strand aims to determine relationships between the aroma chemistry and phenolic profile of commercial wines, selected based on price point, region and vine yield, with sensory data collected from consumers on Pinot noir wine preferences. Furthermore, the consumer sensory and chemical profiles of the wines are being compared to expert sensory data to provide a map of factors influencing perception of quality in NZ Pinot noir wines.

A complementary piece of research involves the investigation of the microbial contribution to Pinot noir quality, through the change in aroma chemistry during un-inoculated alcoholic fermentation, as many NZ Pinot noir wines are fermented via ambient microorganisms. Many important aroma compounds in Pinot noir wines linked to quality are formed or released by yeast during fermentation.

Therefore, investigating species dynamics through DNA barcodes to identify microbial species within the community during fermentation, alongside the evolution of aroma compounds, will provide a detailed account of how these different communities might affect the quality of the final wine.

Lastly, further sub-projects aim to elucidate the roles of different yeast species within a single vineyard microbial community on the production of norisoprenoids, which impart key floral aromas, as well as determine the impact of co-inoculation of different yeast species on Pinot noir wine colour, as consumers prefer more intensely coloured wines.. This capability aligns with the global push toward sustainability, which is guiding all industries toward smarter, greener technologies.

Alphabetical list of key collaborators and researchers involved:
Leandro Dias Araujo, Bruno Fedrizzi, Andy Frost, Roland Harrison, Rebecca Jelley, Paul Kilmartin, Sarah Knight, Jed Lennox, Oliver Masters, Katasha McCullough, Sarah McKenzie, Wendy Parr, Lisa Pilkington, Yifeng Qiao, Billy Yang.

Read more here

Green Chemical Science for a Sustainable Future

Green Chemical Science is the use of chemical principles, science and technology to advance society in ways that are benign to the environment and sustainable for the foreseeable future. The research topics aim to address global changes to humanity such as pollution, energy demands, inadequate food supply and lack of clean water.

The use of renewable feedstocks to prepare chemical products instead of using non-renewable petrochemical sources would enable more sustainable chemical syntheses to be carried out (in research labs and on a production scale). The design of more efficient catalysts that operate in environmentally benign solvents leads to a reduction in chemical waste and prevention of environmental pollutants. However, environmentally hazardous compounds are already present in our waterways and soils. We are researching methods to remove and degrade these pollutants as well as mitigating greenhouse gas emissions. Energy generation methods currently contribute to these pollutants and greenhouse gas emissions. The design of materials capable of preparing energy carriers such as hydrogen from renewable energy sources can lead to more renewable energy production and storage.

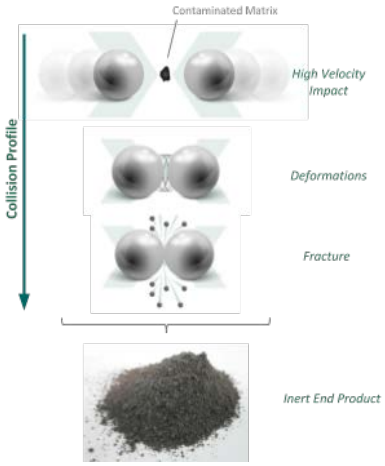
Novel Mechanochemistry to Solve Toxic Pollutant Issues

By Kapish Gobindlal (kgob004@aucklanduni.ac.nz)

Rapid industrialisation over the past 150 years has led to humanity's reliance on chemical tools, such as pesticides, herbicides, non-stick repellents, and fire-fighting foams, to name a few. While commercially useful, an ever-growing body of evidence reveals that a significant number of these chemicals are detrimental to ecosystems and human health. Exposure to these chemical substances has an accumulation effect within the human body resulting in major health complications including cancer, organ failure, and genotoxicity. Cumulatively, these heavily regulated and environmentally stable toxic chemicals are known as Persistent Organic Pollutant (POPs). Historical use of POPs has led to millions of tonnes of contaminated land and POPs-containing products which require effective treatment globally, however, there are few scalable technologies capable of destroying such stable toxic chemicals.

Our research focuses on a novel technological solution to effectively destroy POPs in obsolete pure products and contaminated matrices, such as soil. The fundamental phenomena we exploit are rooted in mechanochemistry. Unlike other chemical reactions which are driven by heat, light, or electricity, mechanochemical reactions are initiated and propagated by mechanical energy. For example, we utilise high energy ball mills to provide the immense and indiscriminate mechanical forces required to drive the molecular degradation of POPs. Rapid destruction of the most harmful POPs has been observed in laboratory-scale trials, with multiple analytical approaches indicating 99-100% molecular destruction.

The findings of this research are directly informing real-world implementation of the core technology globally via Environmental Decontamination (NZ) Limited, an established industrial partner who have developed large-scale mechanochemical systems for hazardous waste treatment. As a non-thermal technology requiring only mechanical energy input, high energy ball milling presents a compelling treatment option for POPs-impacted matrices and chemical stockpiles. This capability aligns with the global push toward sustainability, which is guiding all industries toward smarter, greener technologies.



Alphabetical list of key collaborators and researchers involved:
Environmental Decontamination (NZ) Limited (Industry Partnership), Brian Gullet (United States Environmental Protection Agency), Melanie Kah, Melanie, Erin Shields (United States Environmental Protection Agency), Naresh Singhal, Jonathan Sperry, Cameron Weber, Pooja Yadav, Zoran Zujovic.

Read more here

Pushing the boundaries of Fundamental Chemistry

Fundamental research spans all of the areas highlighted so far. It leads to a better understanding of the universe and advances current technologies. Our fundamental discoveries help showcase chemistry as the central science by facilitating interdisciplinary outcomes in areas such as chemical biology and chemical physics. We investigate how chemical bonding and intermolecular forces in novel compounds leads to different properties and reactivity.

New methods for the synthesis of organic, transition metal and main group compounds are continuously under development. This research includes the design and development of novel catalytic processes to affect reaction outcomes. In order to carry out these chemical syntheses effectively, reaction kinetics has led to mechanistic insights of fundamentally important reactions within all areas of chemistry by describing how molecules interact with catalysts and enzymes.

Semiochemicals: understanding chemical conversations in nature

By Andrew Twidle (atwi080@aucklanduni.ac.nz)

The Barker lab focuses on organic synthesis including natural products synthesis, medicinal chemistry, polymer chemistry and green chemistry. An important research area is the identification and synthesis of semiochemicals. So what are semiochemicals? Well, they are chemical signals that organisms use to communicate with each other in their environment. The most well recognized example of these are pheromones but many other semiochemicals exist, relaying many different messages. A great example is what we call "talking trees", here a plant calls to a predator for help by releasing specific chemical compounds into the air when it is attacked by a pest (Figure 1).

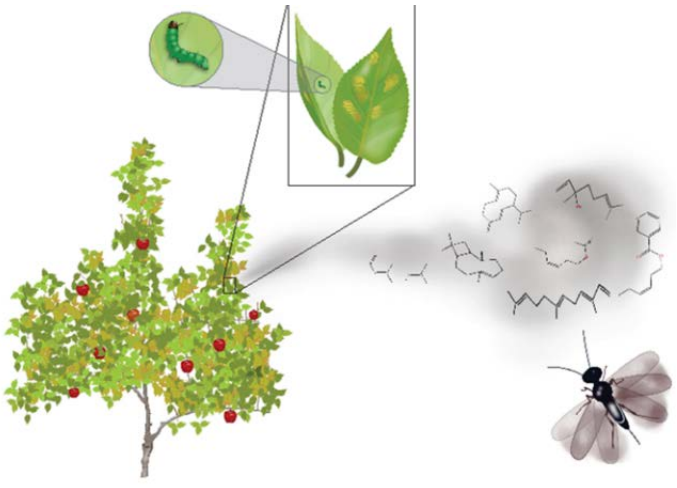


Figure 1- "Talking trees": a plant being fed on by a pest caterpillar sends out a chemical cry for help to a predator.

Working together with entomologists and horticulturists to understand these different semiochemical conversations we have the potential to create targeted messages for specific organisms for pest control (e.g. pheromones) or to eavesdrop on their conversations to monitor plant health (e.g. talking trees). In the case of moth pheromones, the chemicals making up the pheromone can sometimes be complex mixtures or unstable compounds, so we try to develop analogues that are simpler and more cost effective to make while still fitting inside the insect's receptor cells. These analogues can work by blocking pheromone receptors, meaning the male moths cannot find the female moths resulting in no caterpillars to eat the crops (Figure 2).

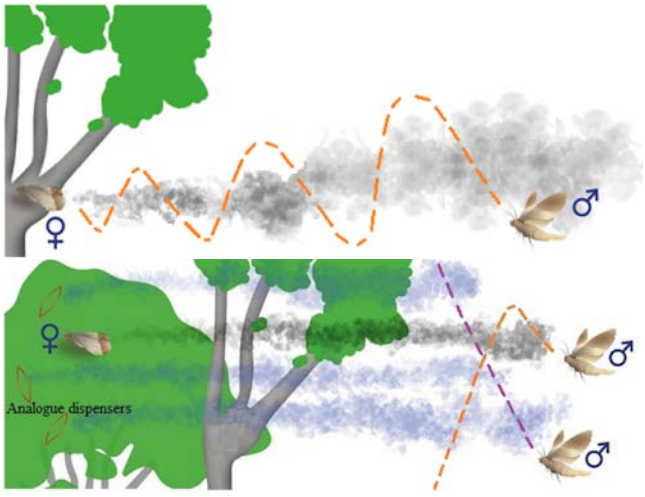


Figure 2- Female moth calls to male moth with pheromone (top), Male moths confused by pheromone analogue can't find female (bottom)

Unlike traditional pesticides, semiochemicals only target the intended species offering an environmentally friendly option for the pest management tool box, which continues to grow as we begin to understand more of the chemical conversations in nature.

Alphabetical list of key collaborators and researchers involved:
Professor David Barker, Asha Chhagan, Associate Professor Bruno Fedrizzi, Sophie Hunt, Dr Kye Chung Park, Dr Lisa Pilkington, Professor Max Suckling

Read more here

Instrument Spotlight

We have a variety of shared instruments within the School which enable researchers to collaborate and obtain the necessary data for their work. The majority of researchers also regularly use a variety of analytical instrumentation (eg NMR, IR, Raman spectroscopy, Mass Spectrometry) to identify and quantify the outcomes from research projects. Recently, a new Raman Spectroscopy instrument has provided excellent results and a growing customer base.

Raman Spectroscopy

Dr Michel Nieuwoudt (m.nieuwoudt@auckland.ac.nz)
Dr Nina Novikova (nnov002@aucklanduni.ac.nz)
Dr Hannah Holtkamp (hannah.holtkamp@auckland.ac.nz)

Raman spectroscopy is a highly specific and non-destructive technique, with low sensitivity to water. This equips it to analyse a wide variety of materials, and with a microscope sampling option allows spatial measurements of down to 1 um. The recently acquired Raman spectrometer (Horiba LabRam Evolution HR microscope) is already in high demand, and has been used to analyse a wide variety of materials. These include:

- Bone samples for collagen content, to differentiate between new bone and archaeological bones
- Characterization of Graphene in laser scribed graphene (LSG) electrodes, and to study the graphinization of polyimide sheets in order to find a relation between capacitance and graphene contents.
- Measurements of insulating metal-oxide single crystals, to quickly identify novel crystalline phases of small crystals, determine and characterize crystallographic phase changes as a function of chemical substitution and temperature and for CHEM310 projects.
- Characterizing and monitoring Titanium oxide as UV absorber in glass fibre reinforced composites for outdoor applications.
- Microplastic fragments in water samples and in fish guts
- Measurement of microscopic food sources (plankton) on mussel farms in sea water, and distinguishing four different species of plankton by differences in their Raman spectra of pigment, lipid and protein structures. (Figure 1)

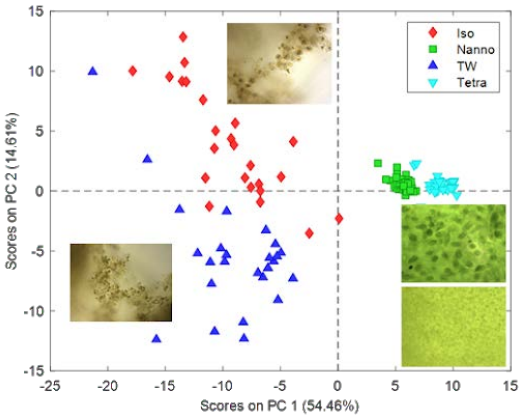


Figure 1. PCA separates four different species of plankton from their Raman spectra, measured in seawater (Novikova and Matthews).

- Hyperspectral imaging of microtomed tissue cross sections of a disfiguring skin condition, Discoid Lupus Erythematosus (DLE), through multimodal analysis of mass spectrometry (MALDI) and Raman hyperspectral images, to probe biomarkers specific for DLE and better understand the pathophysiology of this disfiguring skin condition (Holtkamp, Jarrett, Marini (University of Rome, Italy), Quinn, Aguergaray, Nieuwoudt, Simpson, Demarais, Amirapu, Grey (FMHS))

Identifying differences in paper type and ink composition of an almost invisibly restored Rembrandt etching and drypoint “Landscape with an Obelisk” (Figure 2) (Holtkamp, Wyatt, Nieuwoudt, Bascomb (Auckland art gallery)), using Raman spectroscopy together with NIR hyperspectral imaging.

Figure 2. Restored Etching and drypoint by Rembrandt (Bascomb). Two white lines, clearly visible on the print recto (an arc on the obelisk and a vertical line on the right-side of the print) do not feature on any other known copy and the print also has an unusual tissue lining adhered on the verso.

Probing the biochemistry of skin with lasers, light scattering and molecular ionisation

By Dr Hannah Holtkamp (hannah.holtkamp@auckland.ac.nz) with Federico Marini, Liam Quinn, Claude Aguergaray, Michel Nieuwoudt, Nick Demarais, Satya Amirapu, Gus Grey, Paul Jarrett, and Cather Simpson.

In this project we are working together with dermatologists at the Manukau Superclinic to get a better understanding of unusual skin disease.We collect skin biopsies of diseased and healthy tissue and section them for Raman imaging analysis. Using a range of powerful data analysis techniques, we obtain 2D maps of the sections that show which molecules (proteins, lipids, etc) are changing as a result of disease onset.

These maps serve as groundwork for further analytical studies (Figure 1), particularly mass spectrometry, where the results can be overlaid on top of the Raman imaging 2D maps. By developing these Multi-Modal imaging approaches we will be able to more fully understand diseases with incompletely characterised pathophysiology.

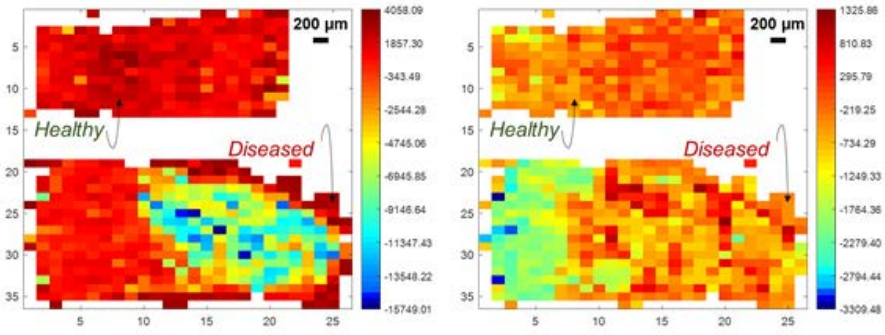


Figure 1. PCA is one of the tools that can be used in Raman Imaging to distinguish the molecular differences between health and diseased tissue.

Origin MFP-3D

While our Origin AFM can't match the resolution of our Cypher, it is capable of imaging large samples over a larger imaging area. It's capable of standard imaging and mechanical point measurements in liquid and air, as well as having an electrochemistry module, which allows in-situ imaging of electrochemically active surfaces during cell operation.

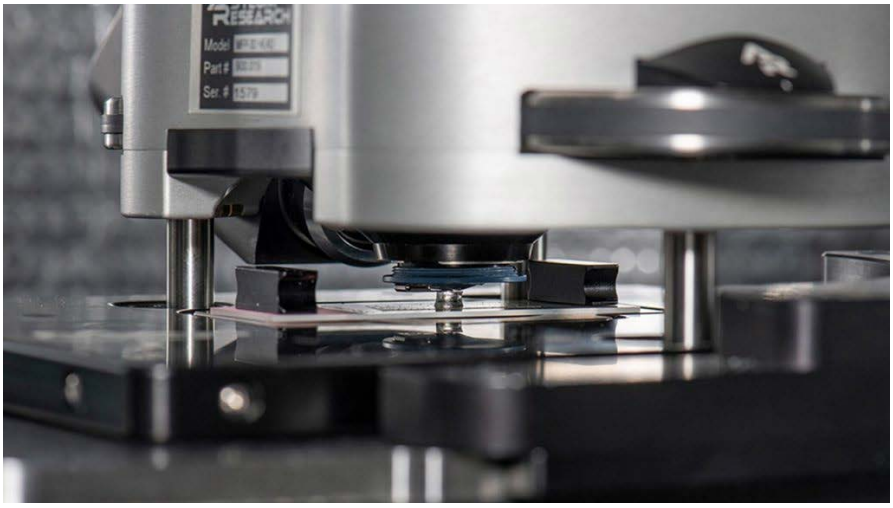
Another strength arising from its older design is extra internal space, allowing for custom imaging setups to be developed. Matthew Ting has used both the Cypher and Origin to image and characterise gel materials in varied environments, temperatures and electrochemical response. More recently, he has begun prototyping custom electrochemical imaging cells to help improve upon our current toolset.

Key goals for 2021 include continued testing of new hardware on the Cypher as well as development of automated scripting for batch measurements. We will also try to lean into the Origin's strengths, and so will welcome any input from UoA researchers who would be interested in developing techniques not currently in our toolbox.

AFM microscopy

Joe Vella (j.vella@auckland.ac.nz)

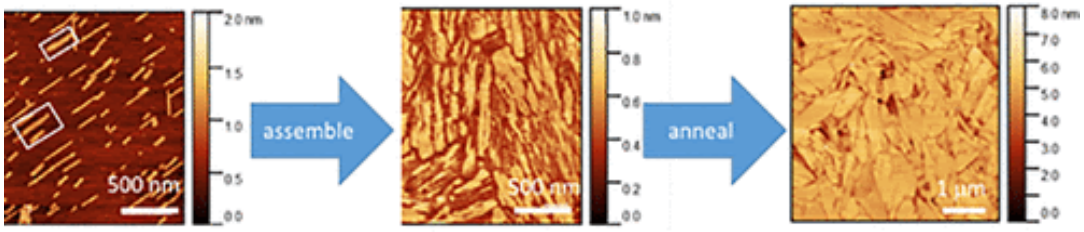
Atomic Force Microscopes, originally in the engineering department, have recently been transferred to SCS enabling more convenient use for our researchers.



Imaging of a 5mm diameter leaf imprint with the Origin MFP-3D.

Cypher-ES (environmental scanner)

Capable of resolutions down to <10nm (sample dependent), our Cypher AFM is the go-to when you need higher magnifications/resolution. This has been utilised in work such as that by Zainab Makinde, where standard AFM imaging was used to demonstrate the assembly of Langmuir–Blodgett (LB) films made from water-soluble peptides.[1]



The Cypher is capable of imaging in both air and liquid environments at controlled temperatures (-20 to 120 Celsius), as well as through using other probe-sample interactions:

- Mechanical properties of materials can be taken at individual points or mapped over a sample surface; the latter being particularly useful for composite materials.
- Sample conductivity can be mapped using a newly acquired module; this technique is currently being explored by members of the Polymer Electronics Research Centre (PERC) group, headed by Prof. Jadranka Travas-Sejdic.
- More subtle properties such as electrostatics and magnetic domains can also be imaged. As part of an ongoing effort towards developing magnetically active interface materials, Daniel Clyde has successfully imaged a range of multiferroic thin films.

[1] Zainab O. Makinde, Nadine J. van der Heijden, Laura J. Domigan, Duncan J. McGillivray, and David E. Williams. Langmuir 2020 36 (38), 11292-11302. DOI: 10.1021/acs.langmuir.0c01944

Our events

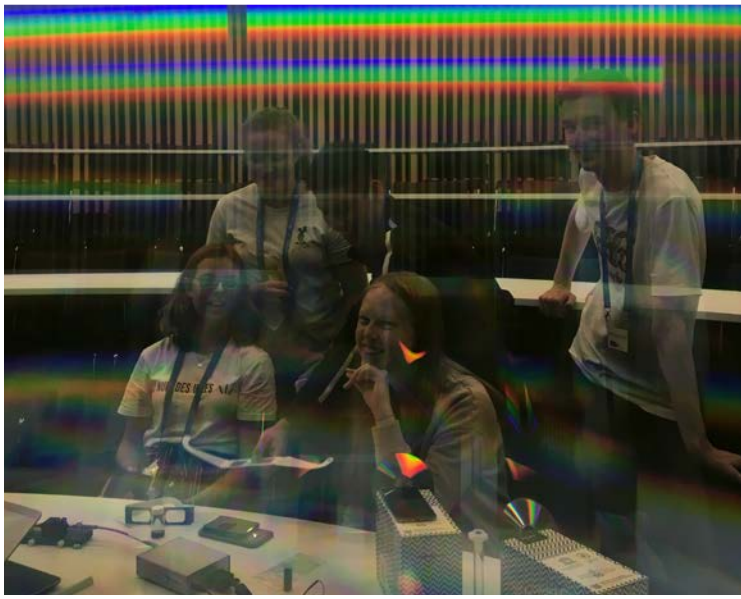
DiscoveryCamp and NanoCamp

January 2020

The DiscoveryCamp and NanoCamp were MI-funded events run by MI investigators and affiliated students.

The MacDiarmid Institute's DiscoveryCamp and NanoCamp were hosted in Auckland. The DiscoveryCamp, organised by A/Prof Geoff Waterhouse, brought together Maori and Pacific Island Students from across the country with an interest in science. In parallel, Nanocamp, organised by Dr Erin Leitao and Dr Michel Nieuwoudt, was aimed at science-minded high achievers. Both camps were very successful, engaging the students in a range of science-based activities across UoA and AUT campuses. There was a range of presentations, including a visit from Nanogirl and a talk on Solar Cells by Dr Cameron Weber in addition to hands-on laboratory experiments and a fun day at Tiritiri Matangi Island.


nanocamp 2020!
The MacDiarmid Institute
Advanced Materials and Nanotechnology



NZIC Chemistry Careers Evening

August 2020

Dr Cameron Weber organised an exciting opportunity for chemistry students and graduates to hear from companies who employ chemists, mostly in New Zealand but some with opportunities overseas. We heard talks from Mint Innovation, ESR, Environmental Decontamination Ltd, Resene, Hill Labs, Eurofins, NZ Steel, AsureQuality and Douglas Pharmaceuticals highlighting the job and internship opportunities available.

Oktoberfest

October 2020

A long-standing SCS tradition of Oktoberfest brought together staff and students from across all of the disciplines. German style drinks and nibbles were enjoyed, with a variety of options including bretzels and wheat beer. We had a great turnout this year. A big thanks to A/Prof Tilo Sohnel and his research group for organising and cooking the delicious food and to A/Prof Jon Sperry for his presentation to the prospective postgraduate students.

SCS Research Innovation Showcase

November 2020

The inaugural SCS Research Innovation Showcase was held on Tuesday 3rd November and involved oral and poster presentations from SCS staff and PhD students. This provided a platform for staff and students to present their research to over 60 industry and CRI representatives from a diverse array of areas including healthcare, food analysis and production, surface coatings, and cleantech as well as investors interested in finding out about some of the latest innovations from the School.

The organising committee were:
Dr Cameron Weber (chair), Dr Rebecca Deed (co-chair), Professor Jadranka Travas-Sejdic, John Lau, Mike Wadsworth, Dr Lisa Pilkington, Dr Geoff Willmott, Victoria Louise Smith, Kapish Gobindlal and Analeise Murahidy.


OF AUCKLAND
FACULTY OF SCIENCE
School of
Chemical Science

Writing Hideaway

November 2020

Prof Jadranka Travas-Sejdic, Simrin Ahmed, Emma Dawson and Victora Louise Smith organised a very successful writing day off campus. This retreat gave researchers the space to progress their articles or grant proposals in a beautiful setting, Long Bay Beach. A special thanks to the Write consultants who shared tips and techniques for making writing more accessible and engaging for a range of audiences.

IUPAC Global Women's Breakfast

February 2020

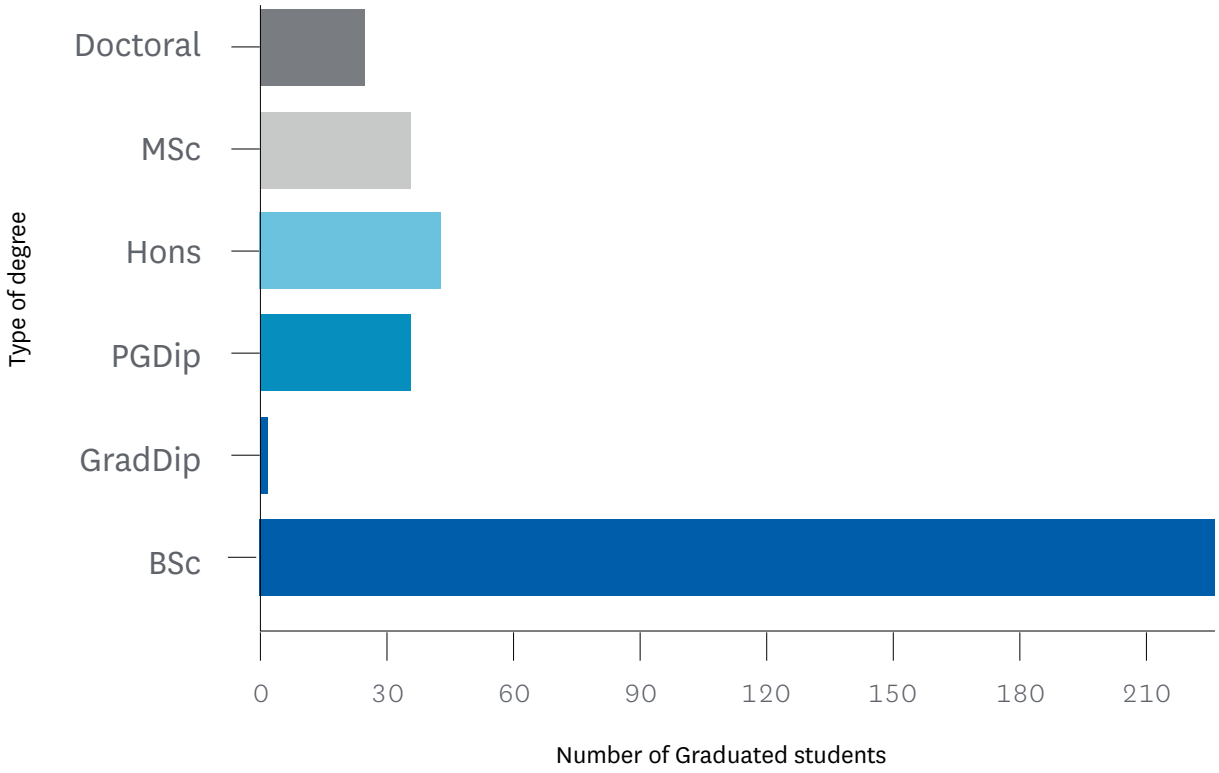
Women in Chemical Sciences from across Auckland gathered on 12th February 2020 at 9:30am for the IUPAC Global Women's Breakfast hosted at the University of Auckland. This event is held in various locations all around the world on the International Day of Women and is aimed at empowering diversity in Science.

Our stats

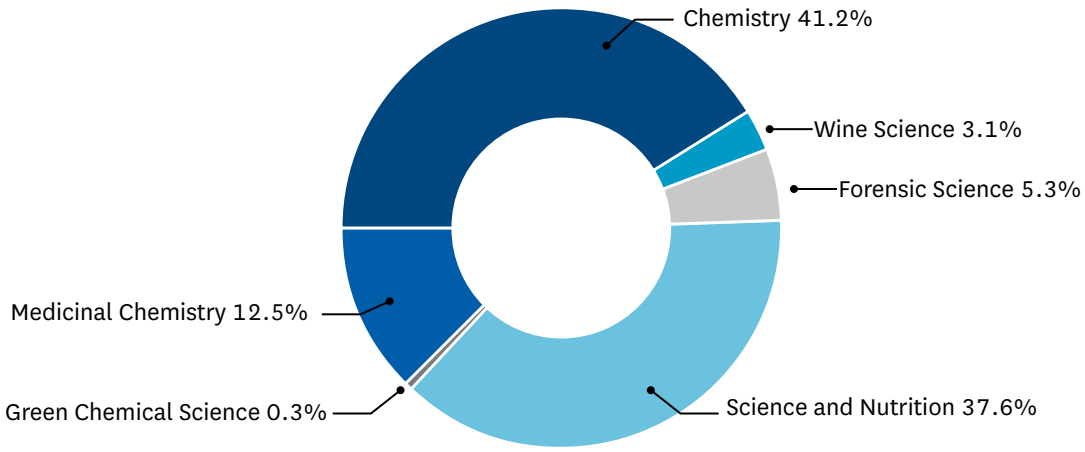
Student Completions

See the list of completed PhD and MSc students and their research topics in the Appendices.

Graduated students by degree



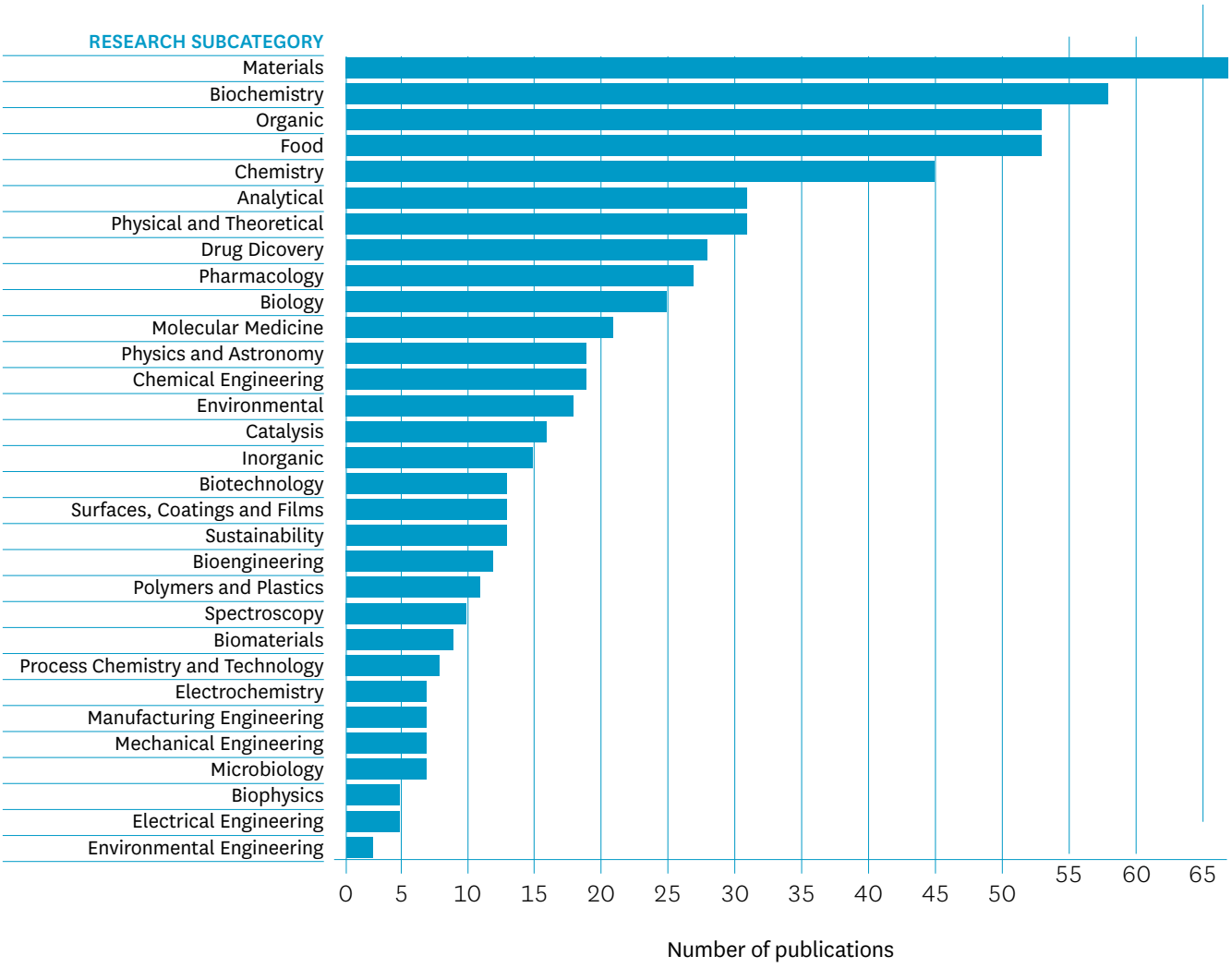
Student graduations by discipline in percentage



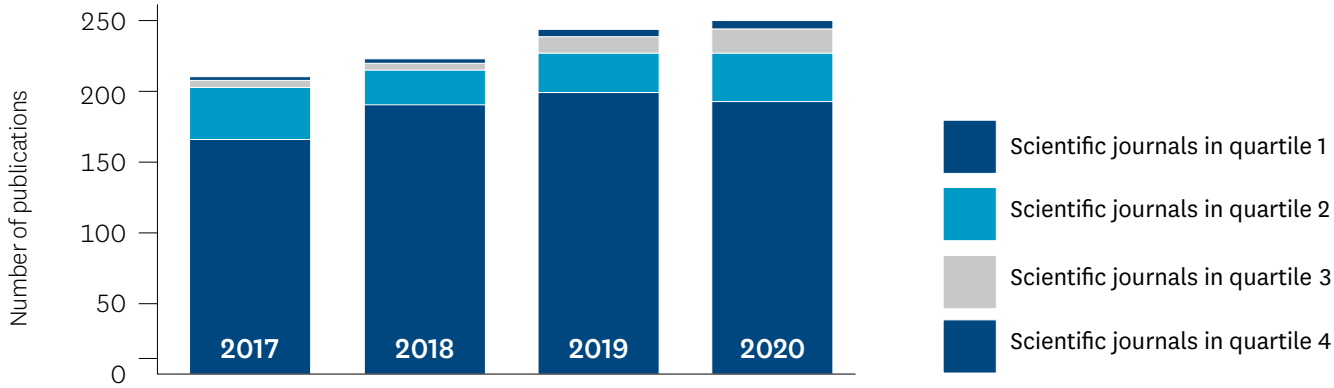
Research Publications

See the list of publications in the Appendices.

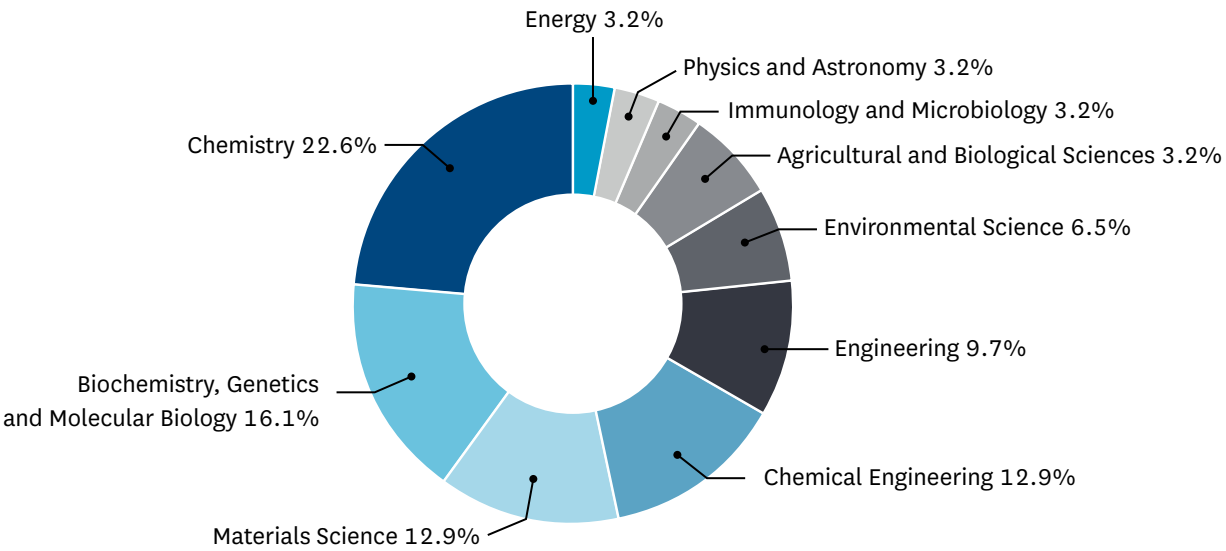
Output by research area



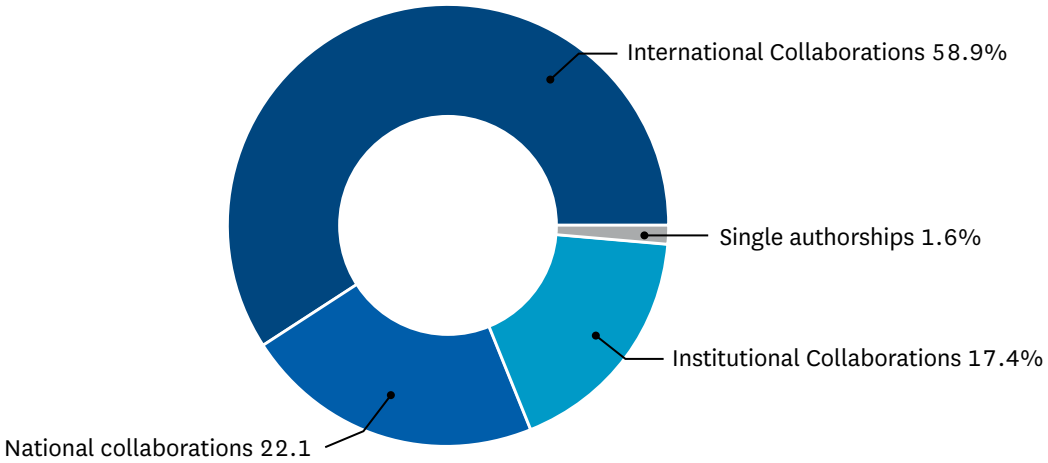
Research output in peer-reviewed scientific journals



Publications by Collaborations



An overview of our collaborations



Appendices

Other Notable Funding

Auckland Medical Research Foundation (AMRF), M. Hanif (PI); Travel Grant to attend the Metals in Medicine Gordon Research Conference in Andover, USA, $3000, Feb 2020.

Auckland Medical Research Foundation, M. Brimble (PI), A. Cameron (PI), S. Zhang, P.W.R. Harris, D. Furkert, D. Fellner, M. Quinoes-Mateu (UoO); "Sars-CoV-2 Virus Entry Inhibitors", $96,457, May 2020.

Bragato Research Institute, R. Deed (PI); "RA1 2 Consumer Sensory", $64,928, Feb 2020.

Breast Cancer NZ Ronald Kay Fellowship, L. Pilkington (PI); "Development of stable PC-PLC inhibitors as potential anti-breast cancer therapeutics", $80,000, Nov 2020.

Callaghan Student Grant with Mint Innovation, C. Weber (PI), Roland Brown (Student), "The application of deep eutectic solvents to purify and recover value from waste streams", $30,500, Dec 2020.

Cancer Society of New Zealand Project Grant, D. Barker (PI), "PC-PLC inhibitors as potential cancer therapeutics" $150,000, Jan 2021.

Cure Kids, M. Brimble, P. Harris and S. Dissnayake, $109,999, Feb 21. Special congratulations to Sharma Dissnayake for her first grant as an AI.

HRC Sir Charles Hercus fellowship, M. Nieuwoudt (PI); "Photonic device for real-time measurement of ischaemic tissue margins in surgery" $482,706, April 2021.

Innovation Accelerator Fund (MBIE), M. Brimble (AI), R. Furneaux (PI, VUW), R. Beasley (PI, MRINZ), L. Harris (VUW), G. Evans (VUW), S. Grant (Univentures), W. Denny (UoA), V. Ward (UoO), K. Krause (UoO), P. Benjes (Glycosyn), T. Davidson (Glycosyn), J. Ussher (UoO), M. J. McCarthy (ESR); "Tackling New Zealand's need for rapid access to anti-viral and other therapeutic medications to treat COVID-19" $920,726, July 2020.

Kelliher Charitable Trust Emerging Research Start-up Award, H. Holtkamp, "Probing the biochemistry of skin with lasers, light scattering and molecular ionisation" (AMRF research project), $30,000, Jan 2020.

Kiwinet Return on Science Investment Fund, M. Brimble (PI), with P. Harris (AI), G. Cook (AI, UoO), D. Williamson (AI, Uni Melbourne); "Synthesis of Novel Lipidated Polymyxin B Analogues" $118,000, July 2020.

MacDiarmid Institute, Seed Commercialisation Grant, E. Leitao (PI); "Polyphosphordiamidates: biofriendly polymers with a PV-NIII backbone," $20,000, April 2020.

National Science Challenges. Science for Technological Innovation-Seed Projects round, B. Zhu (PI), J. Travas-Sejdic, K. Sheehy (MacDiarmid Institue); "Stretchable and self-healable energy storage for epidermal and implantable bioelectronics" $200,000, Sep 2020.

New Zealand Agricultural Greenhouse Gas Research Centre Innovation Fund 2020, M. Brimble (AI), G. Bashiri (UoA), R. Ronimus (AgRes); "Molecular Tools for Methane Mitigation" $500,000, Mar 2020.

New Zealand–China Emerging Researcher Travel Fellowship, L. Pilkington (PI); "Development of novel TDP1 inhibitors in collaboration with Chinese institutes", $22,000, Jan 2020.

Pastoral Greenhouse Gas Research Limited, M. Brimble (PI), D. Rennison (AI); "Design and Synthesis of Sulfonylheterocycles and Nitrooxymethylpyromellitic Diimide Derivatives, as Biomethanation Inhibitors in Ruminants" $118,241 May 2020.

RSNZ Rutherford Postdoctoral Research Fellowship, L. Pilkington (PI); "Data Science QSAR Strategies and Tools for Medicinal Chemists: $170,000, Nov 2020.

RSNZ Rutherford Postdoctoral Research Fellowship, E. Davison (PI); "Developing flow synthesis methods that could be used to produce personalised cancer immunotherapies" $170,000, Apr 2020.

Science for Technological Innovation (SfTI) National Science Challenge Spearhead Program, D. Barker (PI); "Clean Water Technology for restoring Te Mana o te Wai" $3,000,000, Nov 2020.

Awards

Best Student Talk 44th Condensed Matter and Materials Meeting, Rotorua 4-7 February 2020, A. Chan (working with Ben Mallet, Cather Simpson and Tilo Söhnel).

Dean's List, S. Kim and T. Pham

Fellow of the Royal Society of Chemistry (FRSC), August 2020, G. Waterhouse

"Highly Cited Researcher 2020" on the Clarivate Web of Science Highly Cited Researcher List, G. Waterhouse.

L H Briggs Prize 2019, D. Correddu; 'Studies on human proteins involved in deregulated translation in Parkinson's disease'

Lottery Health, $90,000, P. Harris for purchase of shared equipment.

NZIC Maurice Wilkins Prize for Chemical Science for Excellence in Chemical Research, G. Waterhouse.

Young Scientist 2020, Agricultural and Food chemistry Division of the American Chemical Society, B. Fedrizzi.

NZ Trace Elements Group conference in Cambridge, 10-11th February 2020, Second prize for talk, D. McDougall (supervised by Andrew Jeffs, Gordon Miskelly, Duncan McGillivray); "Trace metals in New Zealand green-lipped mussels and the effect of water treatment on trace metal bioavailability and mussel survival".

First prize student talk, SBS Research Showcase, 4th November 2020, O. Shepparson.

Second prize student talk, SBS Research Showcase, 4th November 2020, J. Tong.

Oral Presentations and Meetings (held remotely)

Presentations

University of Auckland Postdoctoral Symposium, 9th December 2020, E. Davison, "Natural Product Total Synthesis" (invited).

14th Annual International Electromaterials Science Symposium, Kambri Precinct Cultural Centre, Australian National University, Canberra, Australia, 5th –7th February 2020, J. Travas-Sejdic, ''Self-healing and Stretchable Polymer Electronics'' (keynote)

Fringe Festival Lectures, Adelaide, 21 Feb 2020, in person, E. Leitao,"Towards new inorganic polymers" (keynote).

Global Virtual Conference on BIO NANO INNOVATION, June 06 2020, J. Travas-Sejdic, ''Novel Conducting Polymer Biointerfaces'' (keynote)

California Polytechnic State University Seminar, 24 July 2020, E. Leitao, "Using earth abundant elements to create inorganic polymers," (zoom seminar).

MacDiarmid Institute for Advanced Materials and Nanotechnology, Interface Techweek: Advanced materials – Science careers that improve our world, 29th July 2020 (zoom), J. Travas-Sejdic, "Where have all my students gone?" (invited)

14th Pacific Rim Conference on Lasers and Electro-Optics (CLEO PR 2020 CLEO, 3 – 5th August (Virtual conference, Sydney, 2020), M. Nieuwoudt, "Raman Spectroscopy Characterising Human Bone," (invited).

71st Annual Meeting of the International Society of Electrochemistry, 30 August - 4 September 2020, Belgrade, Serbia (on-line); J. Travas-Sejdic, "Conducting Polymer Biointerfaces" (keynote)

Science High School Teachers Professional Development Days, Timaru, Christchurch, Nelson, Auckland (9th, 10th, 11th, 18th November 2020), M. Brimble, "Using Medicinal Chemistry to Combat Sars-Cov-2" (keynote) supported by Maurice Wilkins Centre for Molecular Biodiscovery.

Science High School Teachers Professional Development Days, Timaru, Christchurch, Nelson, Auckland (9th, 10th, 11th, 18th November 2020), M. Nieuwoudt, "Antiviral Drugs to Combat Sars-Cov2" (invited)

Food and Health Lightening talk, November 2020, B. Zhu, "Cost-effective, portable sensors for pathogen detection using electrical signal."

Virtual MRS Spring/Fall Meeting & Exhibit, Nov-Dec 2020, J. Travas-Sejdic, ''Direct Writing of 3D Conducting Polymer Microarrays for Biological Sensing and Cell Stimulation,'' (invited).

Food and Health Programme Research Symposium, 1st December 2020, B. Zhu, "Cost-effective, portable sensors for pathogen detection using electrical signal."

9th Australasian Symposium on Ionic Liquids, Virtual Symposium hosted in Melbourne 1 December 2020, C. Weber, "Seeking Solvation: How do Solutes Affect the Amphiphilic Nanostructure of Ionic Liquids?" (oral).

Meetings

FoS Food Theme Steering Committee, L. Pilkington, organised 'Lighting Talk' event.

MBIE Programme meetings, M.Brimble, for New Antiviral Agents;

Pastoral Greenhouse Gas Research Consortium, Programme meetings, M. Brimble, for Methanogen Inhibitors

Panel Discussion, FoS Research Fellow Society, L. Pilkington, organised an online panel event with a range of panelists from various science-related careers outside academia, to give advice and insight into their experiences and career pathways, for attending Research Fellows and PhD students.

Virtual MRS Spring/Fall Meeting&Exhibit, J. Travas-Sejdic, co-chair of session titled 'Degradable and Self-Healing Electronic Materials for Biological Interfaces'

Peptide User Group Symposium, Melbourne, M. Brimble, 11 November 2020

Seminars in 2020

Date	Presenter
7 Feb	"Professor Rhett Kempe, University of Bayreuth, Germany "Catalysis for a more sustainable chemistry""
14 Feb	Distinguished Prof David Kingston, Virginia Polytechnic Institute and State University, USA ,"The History, Chemistry, and Biology of Paclitaxel, an Anticancer Gift from Nature".
21 Feb	Dr. Davide Mercadante, Senior Lecturer, SCS, the University of Auckland "Structures through the computational microscope: achievements and challenges in understanding macromolecular dynamics in the era of digitalization"
28 Feb	Dr Bryan Tuten (QUT), Australian Research Council DECRA Fellow at QUT, Australia, "New components in Multicomponent Polymerizations"
6 Mar	"Dr. Alireza Akbarinejad, Research Fellow, SCS, the University of Auckland "Multifunctional Polymer Bio-Interfaces for Selective Capture/Release of Extracellular Vesicles" Dr. Elke Pahl, Lecturer, Department of Physics at the University of Auckland, "Alien Chemistry and Physics in Strong Magnetic Fields""
13 Mar	Dr. Nicholas Demarais, Research fellow, School of Biological Sciences, University of Auckland, " Small-molecule UV Light Filters in the Aging Human Lens"
20 Mar	Prof. David Williams, SCS, the University of Auckland, "The challenge for sensors in the "Internet of Things": how do you know that the data are reliable?"
3 Apr	Dr. Ivanhoe Leung, Senior Lecturer, SCS, the University of Auckland "Mechanistic and Structural Enzymology"
17 Apr	Dr. Ben Mallett, Senior Research Fellow, SCS (previously Department of Physics), the University of Auckland, "Superconductivity and magnetism, and other acquaintances, in superconductor sandwiches"
24 Apr	Professor Edwin C. Constable, University of Basel, Switzerland, Department of Chemistry "Sustainable Materials Chemistry –Light-emitting electrochemical cells "
1 May	Prof. Brent Copp, SCS, the University of Auckland "Of squirts and slugs: marine natural products with biological effects"
8 May	Dr. Bhuvan Kanan, Research & Development Chemist, Revolution Fibres Ltd., Auckland "Commercialization is real science. Commercializing science is real art,"
15 May	Prof. Jose Amigo, the University of the Basque Country, "Hyperspectral Imaging and Chemometrics in Chemistry"
22 May	Dr. Vedran Miletic, Senior Lecturer, Department of Informatics, the University of Rijeka, Croatia, "The development of RxDock web server and the future of scalable pharmaceutical research tools in the private and public clouds"
29 May	Dr. James Brady, Professional Teaching Fellow, School of Chemical Sciences, the University of Auckland, "Misadventures in teaching"
5 Jun	"Prof. Penny Brothers, Director, Research School of Chemistry Australian National University, Canberra, "The chemistry of boron with pyrrole ligands: tales from the world of porphyrins, corroles, phthalocyanines and BODIPY""
12 Jun	Prof. Hongzhe Sun, Department of Chemistry, University of Hong Kong, "Uncovering metalloproteomes in pathogens: a new approach to overcome antimicrobial resistance (AMR)"
17 Jul	Prof. Matthew Hopkinson, Freie Universität Berlin, Germany, "Methodology Development in Organofluorine and Photochemistry"
24 Jul	"Dr. Jenny Malmström, Senior Lecturer, Department of Chemical and Materials Engineering, University of Auckland "Engineered Biointerfaces""
31 Jul	Dr. Nina Novikova, Research Fellow, SCS, the University of Auckland, "Understanding photoactive molecules using ultrafast laser spectroscopy"
7 Aug	Dr. James Brady, Professional Teaching Fellow, SCS, the University of Auckland , "New skills for a new decade"
21 Aug	Dr Wei Shen Aik, Assistant Professor, Hong Kong Baptist University, "A FLASH of Histone Pre-mRNA 3'-End Processing"
28 Aug	"Dr. Cherie Tollemache, SCS, the University of Auckland, Evaluation of mixed alkanethiolate self-assembled monolayers on gold electrodes for biosensor applications Dr Phillip Grant, SCS, the University of Auckland, "The Development of a Strategy for the Synthesis of Leonuketal""
25 Sep	Ms. Sarah Hillary, Art Conservationist, Auckland art gallery, Toi O Tamaki, Beneath the surface: painting conservation research
2 Oct	Dr. Marcus Jones, Senior Lecturer and HOD, School of Science, Auckland University of Technology, Auckland, "Exciton-plasmon coupling in nanoscale materials".
9 Oct	Prof Paul Dyson, Institute of Chemical Sciences and Engineering, Lausanne, Switzerland. "Catalytic transformations of natural and synthetic waste into value-added chemicals"
16 Oct	Dr Cassandra Fleming, School of Science, Auckland University of Technology (AUT), Light-Responsive Entities as Molecular Tools to Probe Dynamic Biological Functions
23 Oct	Dr Christoph Nitsche, Senior lecturer, Australian National University, Research School of Chemistry "Targeting viral proteases with modified peptides"
6 Nov	Prof Patricia Hunt, School of Chemical and Physical Sciences, Victoria University of Wellington ,"Hydrogen Bonding in Ionic Liquids and Deep Eutectic Solvents"
13 Nov	Dr Yogesh Somasundar, Carnegie Mellon University, "Bioinspired sustainable chemical technology: A clean-up solution for micropollutants in water"
20 Nov	Dr Nathaniel Davis, School of Chemical and Physical Sciences, Victoria University of Wellington, "Reducing reabsorption losses in luminescent solar concentrators"

Completed PhD students (listed alphabetically by surname)

Anderson, Kirsty; PhD in Chemistry with A/Prof Jonathan Sperry, "Synthesis of 4-Acylbenzoxazoles from Indoles and Synthetic Studies Towards the Marine Alkaloid Violatinctamine."

Castillo, Kristel Mae Rabanzo; PhD in Chemistry with Dr Erin Leitao, "New Routes Toward Structured Silane and Siloxane Compounds."

Choi, Hans Sol; PhD in Chemistry with Dist. Prof. Margaret Brimble, "Synthetic Study Towards the Spiroimine Unit of Portimines.'

Freeman, Jared Liam; PhD in Chemistry with Dist Prof Margaret Brimble, "Synthetic Studies Towards Anthracimycin."

Grant, Phillip Stephen; PhD in Chemistry with Dist Prof Margaret Brimble, "Synthetic Studies Towards Leonuketal."

Gunawardana,Dona Madhushani; PhD in Chemistry with Dr Ivanhoe Leung, "Structural and Mechanistic Studies of 1-Aminocyclopropane-1-Carboxylic Acid Oxidase"

Jelley, Rebecca Eleanor; PhD in Chemistry with A/Prof Bruno Fedrizzi, "Extraction and novel applications of grape marc-derived materials."

Kanyan, Deepika; PhD in Chemistry with Prof. Penny Brothers, "Exploring Applications of O-BODIPY Complexes: Sugars and Cobaloximes."

Kihara, Shinji; PhD in Chemistry with Prof Duncan McGillivray, "Nanoplastic and Protein Corona – Investigating the Corona Structure and their Biological Impacts."

Kim, Se Hun; PhD in Chemistry with A/Prof Jonathan Sperry, "Bioinspired structural revision of the marine flatworm-derived alkaloid pseudocerosine."

Ko, Kwangyoon; PhD in Chemistry with Dist Prof Margaret Brimble, "Formal Synthesis of the Cytotoxic Macrolide Callyspongiolide."

Lo, Stephen; PhD in Chemistry with Prof David Barker, "Lipophilic Derivatisation of Flavonoids Extracted from Grape Pomace to Enhance their Health-Promoting Effects."

Lu, Ziqui; PhD in Chemistry with Prof Penny Brothers, "Metalloporphyrin-Decorated Semiconducting Oxides for Gas Sensing Applications."

Lyu, Hua; PhD in Chemistry with Prof David Barker, "Aryl Boronic Acid-Containing Molecularly Imprinted Polymers (MIPs) for Selective Binding Cis-Diol Containing Molecules."

Mark, Oi Wei; PhD in Chemistry with Dr Ivanhoe Leung, "Biochemical and Computational Approaches to Drug Discovery."

Mazruee Kashani, Hadi; PhD in Chemistry with Prof Christian Hartinger, "Anticancer agents based on N-heterocyclic carbene (NHC) ligands: Towards compounds with multiple functionalities."

Patel, Jinal Chandubhai; PhD in Chemistry with Dr Ivanhoe Leung, "Structural and Inhibitor Binding Studies of Tyrosyl-DNA Phosphodiesterase 1."

Pham, Thuy Trang; PhD in Chemistry with A/Prof Jonathan Sperry, "Synthetic Applications of the Chitin-derived Platform 3-Acetamido-5-Acetylfuran (3A5AF)."

Qi, Wen; PhD in Chemistry with Prof Bob Anderson, "Radical Mechanisms Underlying the Activity of Hypoxia-Selective Anticancer Drugs."

Tollemache, Cherie Tania; PhD in Chemistry with Prof Penny Brothers, "Evaluation of Mixed Alkanethiolate Self-Assembled Monolayers on Gold Electrodes for Biosensor Applications."

Vadakkedath, Praveen George; PhD in Chemistry with Prof Duncan McGillvray, "Studies of reversible interactions in biomaterials and biomacromolecules."

Vandermeer, Charlotte Johanna; PhD in Chemistry with Prof Paul Kilmartin, "Promising Natural Extracts for Use in Active Food Packaging."

Wang, Min; PhD in Chemistry with Prof Jadranka Travis-Sejdic, "Photo-patternable Stretchable Electroactive Conjugated Polymers."

Wildervanck, Martijn Johannes; PhD in Chemistry with Prof Penny Brothers, "Synthesis, Characterisation and DFT Calculations of Saccharide-BODIPY Conjugates."

Xu, Buzhe; PhD in Chemistry with Dist Prof Margaret Brimble, "Total Synthesis of Naturally Occurring Antimicrobial Peptides."

Ye, Piao; PhD in Chemistry with A/Prof Geoff Waterhouse, "Plasmonic Enhanced Photocatalytic Water Splitting under UV and Visible Light."

Yim, Victor Vic-to; PhD in Chemistry with Dist Prof Margaret Brimble, "Structure-Activity Relationship Studies and Syntheses towards Antimicrobial Lipopetides."

Zhang, Peikai; PhD in Chemistry with Prof Jadranka Travas-Sejdic, "Direct writing of 3D conducting polymer microarrays for biological sensing and cell stimulation."

Completed MSc students (listed alphabetically by surname)

Bartlett-Wright, Michaela; MSc in Forensic Science with A/Prof Gordon Miskelly, "The Reaction of Methamphetamine with Nitrous Acid Gas."

Betty, Katrina; MSc in Forensic Science with Douglas Elliot, "Detection of latent DNA in fingermarks using Diamond™ Nucleic Acid Dye."

Boote, Nicholas; MSc in Forensic Science with Douglas Elliot, "The Behaviour/Effect of Base/Salt Precursors and Cutting Agents in the Manufacture of Methamphetamine."

Brewster, Diane; MSc in Chemistry with Prof Jadranka Travas-Sejdic, "A Tale of Two Substrates: testing electrochemical substrate systems for the capture and relapse of circulating tumour cells."

Cao, Jenny; MSc in Forensic Science with Lisa Melia, "Rapid DNA profiling using FTA cards for difficult substrates."

Chan, Chhiv Cherry; MSc in Wine Science with A/Prof Bruno Fedrizzi, "Pinot noir Wine Colour and Aroma: Extraction and Stabilisation through the use of Commercial Tannins and Cap Management Regimes."

Chen, Dan; MSc in Chemistry with Prof Brent Copp, "The Antimicrobial and Antibiotic Potentiating Properties of Lipophilic Polyamine Analogues."

Chhun, Senghak; MSc in Food Science with Prof Siew-Young Quek, "Physiochemical Properties and Stability of Cyclocarya paliurus (Batal) Iljinskaja Extracts Microcapsules Prepared by Monodisperse Droplet Spray-Drying."

Cui, Jingya; MSc in Food Science with Prof Siew-Young Quek, "Study of Strawberry Guava (Psidium Cattleianum) on Properties and Volatiles at Two Ripening Stages."

Colita, Juwannusss Patrikk; MSc in Chemistry with A/Prof Tilo Söhnel, "Exploration of Cobalt Doping into the Zinc Molybdate and Tungstate systems."

Data, Shailja; MSc in Chemistry with Dr Erin Leitao, "Expanding the Scope of Higher Posphoramidates by Designing Oligomers with a P-N Backbone."

Ding, Yizhen; MSc in Food Science with Prof Siew-Young Quek, "The volatile Composition and Aroma profile of 'Unique', 'Triumph' and 'Anatoki' feijoa fruits (Acca sellowiana) during ripening."

Gao, Henry; MSc in Chemistry with Dr Cameron Weber, "The effect of ionic liquid nanostructure on inverse electron demand Diels Alder reactions."

Hou, Fuying; MSc in Food Science with Prof Siew-Young Quek, "Research of antioxidant activity in berry samples with traditional and electrochemical approaches."

Jeffares, Lauren; MSc in Chemistry with A/Prof Geoff Waterhouse, "Synthesis and Characterization of Biopolymer and Poly(3,4-ethylenedioxythiophene) 3-Dimensionally Ordered Structures via Templating with Synthetic Polystyrene Opal."

Kurniawan, Widi; MSc in Chemistry with A/Prof Geoff Waterhouse, "Performance Comparison of Pt/g-C3N4 Photocatalysts for H2 Production."

Lamba, Saurabh; MSc in Chemistry with Dr Viji Sarojini, "Biomimetic self-assembly of Peptide-Porphyrin complexes for efficient Light Harvesting."

Li, Runze; MSc in Wine Science with Dr Rebecca Deed, "Identification of Saccharomyces cerevisiae Genes Linked to Lag Phase during Fermentation."

Li, Qimou; MSc in Food Science with Siew-Young Quek, "Investigation and modelling the drying kinetics of goat whey and casein using thin-film drying method."

Lee, Marcus; MSc in Chemistry with Dr Erin Leitao, "Hydrogenation of imines using Frustrated Lewis Pairs in Ionic Liquids."

Ma, Xiaoyu; MSc in Food Science with Dr Peter Swedlund, "Development of an educational tool to visualise the glycaemic index of foods."

Matthews, Hannah; MSc in Chemistry with Prof Cather Simpson, "Raman Spectroscopy as a Tool for Rapidly Quantifying Individual Goat Milk Composition."

MacFarlane, Emily; MSc in Forensic Science with A/Prof Gordon Miskelly, "Ageing of fingermarks: monitoring the effect of ozone exposure on the composition of fingermarks using MALDI-FT-ICR-MS."

Mbangwa, Thandeka; MSc in Forensic Science with A/Prof Gordon Miskelly, "Attempted synthesis of iodomethamphetamine using protecting groups."

McErlich, James; MSc in Forensic Science with Douglas Elliot, "Rapid Nanopore DNA Sequencing: potential for field applications and forensic sample analysis."

Nichol, Georgia; MSc in Forensic Science with Jayshree Patel, "Transfer and Persistence Factors of Male DNA Following Heterosexual Intercourse."

Philip, Liam; MSc in Forensic Science with A/Prof Gordon Miskelly, "Analysis of microplastics in NZ foodstuffs and beverages."

Qiao, Yifeng; MSc in Wine Science with Dr Rebecca Deed, "Influence of a Single Vineyard Yeast Community on Norisoprenoid Release During Pinot Noir Fermentation."

Qiu, Yichen; MSc in Chemistry with A/Prof Jon Sperry, "Synthesis of Organosulfur Compounds from Biomass-Derived Platform Molecules

Ting, Joanna; MSc in Food Science with Prof Siew-Young Quek, "Physicochemical properties and storage stability of Afourer and Richard Special mandarin microencapsulated with maltodextrin and gum Arabic using spray drying."

Wang, Nire; MSc in Forensic Science with Sally Coulson, "Forensic characterisation of disposable gloves."

Xia, Bangwei; MSc in Chemistry with A/Prof Geoff Waterhouse, "Performance Comparison of Pt/g-C3N4 Photocatalysts for H2 Production."

Yan, Xinyi; MSc in Food Science with Prof Siew-Young Quek, "Spray freezing of Anhydrous Milk Fat (AMF) and Calculation of Heat Mass Transfer."

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Aqrawe Z., Patel N., Vyas Y., Bansal M., Montgomery J., Travaš-Sejdić J., Svirskis D. A simultaneous optical and electrical in-vitro neuronal recording system to evaluate microelectrode performance 2020 PLoS ONE Volume: 15 Issue: 8 doi: 10.1371/journal.pone.0237709

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Ashforth S.A., Oosterbeek R.N., Bodley O.L.C., Mohr C., Aguergaray C., Simpson M.C. Femtosecond lasers for high-precision orthopedic surgery 2020 Lasers in Medical Science Volume: 35 Issue: 6 doi: 10.1007/s10103-019-02899-x

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Bai S., Wang Z., Tan L., Waterhouse G.I.N., Zhao Y., Song Y.-F. 600 nm Irradiation-Induced Efficient Photocatalytic CO2 Reduction by Ultrathin Layered Double Hydroxide Nanosheets 2020 Industrial and Engineering Chemistry Research Volume: 59 Issue: 13 doi: 10.1021/acs.iecr.0c00522

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Calvert M.B., Furkert D.P., Cooper C.B., Brimble M.A. Synthetic approaches towards bedaquiline and its derivatives 2020 Bioorganic and Medicinal Chemistry Letters Volume: 30 Issue: 12 doi: 10.1016/j.bmcl.2020.127172

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Cameron A.J., Harris P.W.R., Brimble M.A. On-Resin Preparation of Allenamidyl Peptides: A Versatile Chemoselective Conjugation and Intramolecular Cyclisation Tool 2020 Angewandte Chemie - International Edition Volume: 59 Issue: 41 doi: 10.1002/anie.202004656

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THE UNIVERSITY OF AUCKLAND
Te Whare Wānanga o Tāmaki Makaurau
NEW ZEALAND

SCIENCE
SCHOOL OF CHEMICAL SCIENCES

School of Chemical Sciences
Science Centre
Room 620
Level 6, Building 302
23 Symonds Street
Auckland 1010
New Zealand

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