HONOURS IN CHEMISTRY
2013

The School of Chemistry & Molecular Biosciences (SCMB) offers the Bachelor of Science with Honours, BSc(Hons). It is undertaken on a full-time basis. The Program can be commenced in either first or second semester.

The Importance of an Honours year

The BSc(Hons) Program provides training well beyond that provided by the basic BSc degree, particularly in the area of research methods and in problem solving. For those students seeking employment after their degree, the extra training of Honours equips them for a wider range of positions, in industry, government laboratories and elsewhere, than does the basic BSc degree. Honours graduates generally have a greater involvement in research and development; responsibility levels are higher and there are better financial rewards. Honours is also the key prerequisite for enrolment in a higher degree. An Honours year graded at Class I allows for direct enrolment into a PhD program. Often a Class IIA performance allows admission also.

Entry Requirements

The Honours program can be entered from the BSc degree from UQ or another university. For students from The University of Queensland, normally 8 units (#8) of Chemistry third level courses should have been completed, at a Grade Point Average of 4.5 or above. In some cases courses from other relevant disciplines may be included in the #8. The School of Chemistry & Molecular Biosciences has some discretion in the application of the entry rules, and may, on the recommendation of the Honours Director, allow entry from students who fall slightly below this cut-off. Students with a good academic record may also be accepted with a BSc qualification from another university. An original or certified copy of your final academic transcript must be submitted with your application form. International students must submit an application form through the International Office. Visit their web site on www.uq.edu.au/international/ or contact any IDP Education Australia office or Australian Diplomatic Mission in your capital city.

Enrolment Procedures, Fees and Charges

Apply to enrol in the Honours program by completing the form at the end of this book and submitting to the office of the Honours Administrative Assistant, Louise Nimwegen 68-316 (Chemistry Building). Forms can also be downloaded from the School website www.scmb.uq.edu.au.

Successful applicants will be sent an offer letter after all results are known. On acceptance their enrolment in the program will be activated by the School. Honours students must enrol themselves via mySI-net in the relevant courses for each semester. Any queries related to enrolment may be directed to Louise Nimwegen (l.nimwegen@uq.edu.au) or Tammie Fair (t.fair@uq.edu.au).

Full time domestic Honours students study as undergraduate Commonwealth supported students and are required to pay a Student Contribution Amount in both semesters of their Honours program. It is the student’s responsibility to ensure they educate themselves on their individual requirement with regard to their Student Contribution Amount. As a first step you may consult the UQ Fees and Costs website www.uq.edu.au/study/index.html?page=947 (further details can be obtained from the Student Centre, Level 1 JD Story Building (61)). International students please see the UQ International website for current fees: www.uq.edu.au/international/.
Financial Support

Up to six hours per week of teaching duties may be available. All Honours students (depending on past experience) are eligible to seek employment as part-time tutors for laboratory classes within the School of Chemistry & Molecular Biosciences. Please indicate your interest to undertake tutoring on the Honours application form.

Commencement Date

The commencement dates for Honours students will be Monday 4 February or, mid-year, Monday 22 July 2013.

A number of introductory programs for Honours students are run early in the semester. These comprise:
- School Safety Induction, where School procedures are explained, particularly safety and waste disposal methods (mandatory)
- Tutor Training, where an introduction to laboratory teaching methods is given for students participating in 1st year laboratory demonstrating.
- A library course, where use of electronic databases are described. Training is provided for referencing software (eg. EndNote).

Research Projects

Students are invited to discuss the projects listed in this booklet with the staff members concerned and to submit the form inside this booklet to the School of Chemistry & Molecular Biosciences as set out above. The Honours Program Director will make recommendations on assignment of supervisors, taking into account:
- the student’s preferences
- the academic background of the student
- the total number of students supervised by each staff member
- resource implications
- planned extended absences of the staff member from the School
- other factors that may affect the staff member’s ability to supervise effectively a particular student’s research project.

For students starting in semester 1, it is highly recommended to submit your application before the end of semester 2 the previous year (17 November 2012). If you do this, you will be notified of your supervisor by mid-January. Students who submit their applications later may have less chance of obtaining their first preference. Students commencing mid-year should submit their application prior to the end of semester 1 (22 June 2013) in anticipation of a successful mid-year completion of their BSc.

The Chemistry BSc(Hons) Program

The BSc(Hons) program in Chemistry may lead to an honours degree in one of these Fields: Chemistry, Biological Chemistry, Nanotechnology, Drug Design and Development, Computational Science. You need to indicate the desired Field when applying for honours. If you do not indicate a desire for another Field, the Field will be “Chemistry”, by default. The Fields other than Chemistry may also be accessed through programs offered by other Schools. The honours program can be entered from the BSc degree at this university. For students in the Field of Chemistry, normally 8 units (#8) of third level chemistry should have been completed, at a Grade Point Average of 4.5 or above. In some cases for the Chemistry Field, and for the other Fields mentioned other relevant disciplines may be included in the #8. For the Field of Biological Chemistry, #8 from a mix of Chemistry, Biochemistry, and Microbiology courses would be appropriate. The School of Chemistry & Molecular Biosciences has some discretion in the application of the entry rules, and may, on the recommendation of the Honours Director, allow entry from students who fall slightly below this cut-off. Students with a good academic record may also be accepted with a BSc qualification from another university. An original or certified copy of your final academic transcript must be submitted with your application form. International students must submit an application form through the International...
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The 16 units of credit associated with the Honours program is a mixture of research and course work. It comprises four components:

**Honours Research Project #10**

This is a year-long component and culminates in the submission of a research report and a viva. The research project is carried out under the supervision of a member (or members) of the academic staff. The research topic is assigned by the supervisor after consultation with the student.

**Honours Research Proposal #2**

The research proposal outlines the work that the student will undertake and why they are doing it. The research proposal will consist of a literature review and will state the aims and significance of the proposed research. The research proposal must be completed in the semester that they begin work as it is intended to provide an early focus for the student on their project work. It may also form the basis of the introductory chapter for the student’s research report.

**Honours Seminar #2**

The research proposal is also presented as an introductory seminar to be held at the end of the first semester of the program.

A research symposium will be held after submission of the final research report in late October. Each student will give a research seminar outlining their achievements and they will be awarded a consensus mark from academic staff members present.

Furthermore, attendance at the weekly Chemistry and Biological Chemistry Seminar series is compulsory. Although occasional absences may be unavoidable, they must be accompanied by an apology sent to the Seminar Convenor and a valid reason for your inability to attend. Chronic absences will result in a failing mark for this course. You are expected to maintain a seminar notebook which must be available for scrutiny.

**Coursework #2**

Each student shall choose one of the following modules. Depending on enrolments, some modules may not be offered. More details (course profiles, timetabling etc.) will follow later.

Module 1 Organic Chemistry
Module 2 Inorganic Chemistry
Module 3 Physical Chemistry

The selection of course work by honours students should be discussed with the student’s supervisor. The final choice is subject to approval by the Honours Director.

**Administration of the Honours Program**

The 2013 Chemistry Honours program will be coordinated by Dr Joanne Blanchfield (j.blanchfield@uq.edu.au, 3365 3622). Enquiries regarding the program should be directed to Dr Joanne Blanchfield in the first instance. Administrative assistance is provided by Louise Nimwegen, (l.nimwegen@uq.edu.au, 3365 3509) or Tammie Fair, Manager, Coursework Academic Administration (t.fair@uq.edu.au, 3365 7976).
Summary for BSc(Hons)

If you wish to commence BSc(Hons) in 2013 you should address any general enquiries to the staff members mentioned above.

Even if you already have a firm idea about the supervisor you are likely to nominate as your first preference, consult widely with members of the academic staff to find out more about the projects being offered and the style of work involved. Remember, your first preference may not ultimately be your allocated supervisor, so it is important to be aware of alternative projects. Be aware that some details of projects being offered may change between the time when this booklet was prepared (August 2012) and your commencement time.

For students commencing in February, lodge your application form with your list of project preferences at 68-316 before Christmas. You do not have to (and should not) wait for your examination results to be released before submitting the form. Preferences should indicate three different supervisors or combinations of supervisors in the case of joint projects. Please note: the principal supervisor must be a research group leader who is either (a) a staff member of the School; (b) an official affiliate staff member of the School; or (c) a Head of School-approved employee of a research institute or industry. For staff members and affiliates, a research group leader is defined as a person holding a continuing academic position or funded by an external competitive research fellowship.

For students commencing in July, indicate your likely mid-year enrolment to the Honours Director during Semester 1, 2013. Lodge your application before or during your mid-year examinations.

Please provide a contact phone number, address and email address.

Associate Professor Ross McGeary
Chemistry Honours Program Director
August 2012
Our research efforts are concerned with coordination chemistry of relevance to biology, analytical science and technology. The current research interests of the group are summarised below and projects in all of these areas are available. Students interested in any of these areas of research should contact Professor Bernhardt for a more detailed project description.

Iron as a Therapeutic Target in Cancer Treatment and Iron Overload Disorders (synthetic and biological coordination chemistry)

Cancer: Iron plays a crucial role in cancer cellular proliferation as Fe-containing proteins are involved in key reactions concerning oxygen transport, energy metabolism and respiration. These characteristics render Fe a potential therapeutic target for preventing the growth of tumour cells. Recently we have investigated the coordination chemistry of a series of heterocyclic chelators, some of which exhibit extremely high activity against cancer cells (see below).

Fe overload: Iron overload is a potentially fatal condition which requires continual chelation therapy for patients to survive. The approved drug DFO must be administered by subcutaneous infusion (~16h/day, 5-7 days/week). In recent years we have been studying the biological coordination chemistry of a number of hydrazone (HPCIH) and hydrazine ligands (H2IPH) and their complexes (see below). The structure of the chelators is related to their efficacy in lowering cellular Fe level. The reason for this remains unclear and the coordination chemistry of these chelators with iron and other essential metals is needed in order to better understand the mode of action of these promising potential drugs.
Synthesis of Revolutionary Synthetic Vaccine Constructs (project with Professor Paul Burn)

We have a collaboration with Professor Paul Burn that concerns the construction of fully synthetic vaccine structures against HIV and Staphylococcus aureus. For details of the project please contact Joanne Blanchfield or Paul Burn.

This project would involve:

- organic synthesis
- carbohydrate synthesis
- solid phase peptide synthesis
- cell culture and plasma stability assays and aseptic techniques
- assay development and molecule characterisation including use of HPLC, LC/MS, NMR, GC/MS equipment.

Bioavailability of Natural Products from Herbal Extracts (project with Professor James De Voss)

Herbal remedies are a major source of medical treatment for much of the world’s population. Unfortunately, little is known about the fate of the natural products in the extracts or which, if any, are biologically active. We are offering a project that uses a cellular model of the small intestine (Caco-2 cell monolayers) to investigate which natural products are likely to enter the blood stream after oral intake of some popular herbal remedies. We also look closely at what changes the compounds undergo during digestion and absorption.

- use of preparative and analytical HPLC equipment to isolate and identify potentially active compounds from herbal extracts.
- performance of in vitro biological assays to determine permeability (Caco-2 cell assay), stability (CC2 homogenate assay, plasma stability) assays.
- analytical analysis using LC/MS and HPLC of the solutions resulting from the in vitro assays.
The research mission of the Centre for Organic Photonics and Electronics (COPE) is to take nanotechnology from the “bench to the market”. COPE contains state-of-the-art synthesis laboratories, a Class 1000 clean room, device fabrication facilities, and a suite of instrument rooms for the characterization of materials and opto-electronic devices. COPE has Honours research projects in all branches of Chemistry (organic, inorganic, materials, physical, and computation) giving a fantastic opportunity for you to develop your own interests and skills at the cutting edge of a technological area, e.g., solar cells, flat panel displays and lighting, plastic electronics, explosives sensors, fuel cells, and synthetic vaccines. Below is a snapshot of some of the projects on offer and I would be happy to discuss them with you.

**Project 1: Plastic solar cell**

Man-made global warming is a scientific fact and a key component of slowing and ultimately halting climate change is the provision of clean (non-fossil fuel) energy. If we convert a proportion of the 1kJ of solar energy that falls on each square metre of the Earth’s surface per second of every daylight hour into electricity [photovoltaics (PV)] it will make a dramatic effect on the world’s energy supply. Would you like to use your organic chemistry skills to create new polymers, dendrimers or small molecules that can be used in efficient, flexible, and light weight plastic solar cells fabricated at COPE? Do your interests lie in studying structure using neutron scattering or would you like to apply computation to develop an understanding of why some materials work well and some do not, leading to new design criteria?

**Project 2: Flat panel displays and lighting**

Lighting and displays based on organic light-emitting diodes (OLEDs) have the potential advantages of cheap manufacturing, better power consumption, better colours, and ultimately being flexible. Imagine a TV screen that could roll up into your mobile phone! The best emissive materials are comprised of organometallic complexes. Would you like to apply your interest in synthetic inorganic chemistry and/or materials chemistry to develop new emissive complexes and/or poly(dendrimers) that can be incorporated into real OLEDs at COPE? OLEDs are made up of thin layers of organic and inorganic materials and what happens as they age is not well understood. An interest in physical chemistry would allow you to make an important contribution to our understanding of how OLEDs degrade.

**Project 3: Sensing explosives sensors**

How do we detect explosives in real time selectively and sensitively? Currently the most sensitive detectors for explosives are canines. At COPE we are developing in partnership with industry our own handheld technology. The explosive analytes are detected by fluorescence quenching. The project brings together synthetic organic chemists who design dendrimers for sensing explosives and spectroscopists to understand how the analytes are detected. Are you an organic chemist or physical chemist who would like to work in an interdisciplinary team?
Metallo-Supramolecular Chemistry and Metal-Organic Frameworks

Metallo-supramolecular chemistry bridges the traditional fields of organic and inorganic chemistry. By using self-assembly the inherent physical and chemical properties of simple metallic and organic (ligand) components are brought together to form beautiful complex and functional architectures. In particular, we are interested in the design and synthesis of new materials with central cavities that are capable of selectively binding smaller molecules. Projects involve a combination of synthesis, characterisation, binding studies, Xray diffraction, spectroscopy, data analysis and investigations into physical properties and can be tailor to suit the particular interests of a student. Example projects are given below.

Trapping Guest Molecules in Metal-Organic Frameworks

Metal-Organic Frameworks are a class of polymeric hybrid material formed from organic and metallic components. These materials have large surface areas and high porosity and are finding application in gas sequestration and separation technologies. Accordingly it is possible to trap a large variety of guest molecules inside them. In this project you will investigate the binding of different solvent molecules inside one of these frameworks to explore selectivity and potential separation applications.

New Metallo-Supramolecular Architectures

Careful consideration of the geometrical properties of metals and organic components allows for the construction of a variety of discrete “supermolecules” formed from the spontaneous aggregation of numerous predesigned components. These structures, often with central cavities, take numerous forms from two-dimensional architectures such as triangular and square architectures to elaborate and beautiful three-dimensional species such as tetrahedra and cubes. Changing the size, shape, properties and charge of the architecture allows for the selective encapsulation of different materials inside them.
My group is concerned with biological and synthetic chemistry and in particular with the application of chemical principles to the understanding of biological processes. Most projects are a blend of disciplines in bio-organic chemistry: synthesis, structure determination, molecular biology, protein purification. A range of techniques is employed, ranging from the biochemical (e.g. PCR, gel electrophoresis) to the chemical (e.g. NMR, HPLC, GC/MS). The following areas illustrate the research in my laboratory but the exact project will be determined by the student’s interests.

**Project 1: Cytochromes P450**

P450s catalyse an amazing variety of oxidative transformations, ranging from simple alkene epoxidation all the way through to oxidative C-C bond cleavage. They are of interest as they (i) are often unique enzymes in a biosynthetic pathway and as such represent new targets for chemotherapeutic agents or (ii) are extremely efficient catalysts that offer the potential of developing tailored oxidative catalysts for synthetic transformations. We are interested in understanding the mechanism of action of a number of P450s. One example is CYP61, a unique P450 involved in steroid biosynthesis in fungi and other pathogenic organisms. As such it represents a potential target for novel chemotherapeutics. CYP61 catalyses an unusual reaction for a P450, namely the dehydrogenation of an alkane to an alkene. However, essentially nothing is known about the exact structure of the substrate, the stereochemistry of the reaction or its mechanism. Projects in this area will involve the synthesis of mechanistic probes, the analysis of the products of enzyme-catalysed reactions, characterisation of enzyme mutants and design and synthesis of inhibitors.

**Project 2: Constituents of Medicinally Used Herbs**

Whilst herbal medicines are widely used and have a long history of such use, their chemical constituents are often poorly characterised. In collaboration with a local company we have embarked upon a program of phytochemical characterisation of a number of therapeutically prescribed herbs. The results have been surprising with a number of previously unknown compounds isolated from supposedly well-characterised species. This project would involve the isolation, chromatographic purification and structure determination (especially employing 1D and 2D nmr) of the chemical constituents of selected herbs. The structures of some recently isolated compounds are given below.

Relevant Recent Publications


ASSOCIATE PROFESSOR
VITO FERRO

Phone: 07 3346 9598
Email: v.ferro@uq.edu.au

My research interests encompass carbohydrate chemistry and medicinal chemistry, with a focus on the synthesis of compounds to probe and/or inhibit carbohydrate-protein interactions involved in disease processes. Of particular interest is heparan sulfate (HS) and the development of HS-mimetics as potential drugs for cancer and various other diseases. Previous work in this area resulted in the discovery of PG545, a potent inhibitor of angiogenesis and metastasis that recently entered Phase I clinical trials in cancer patients.

1. Development of a fluorometric assay for heparanase
Heparanase is a glycosidase that cleaves HS in the extracellular matrix and facilitates metastasis of tumour cells and vascular remodelling associated with angiogenesis. PG545 is an example of a heparanase inhibitor with potent in vivo activity in metastatic and angiogenic models. Despite the advancement to clinical trials of inhibitors, heparanase research has been limited by the lack of a simple and robust assay for enzymatic activity. This project aims to address the situation by the synthesis of novel fluorogenic substrates for heparanase.

2. Synthesis of pharmalogical chaperones for lysosomal storage diseases
Lysosomal storage diseases (LSD) are caused by mutations in enzymes that degrade polysaccharides such as HS, resulting in the accumulation of undegraded substrate in the lysosomes of cells. Some patients may be treated with enzyme replacement therapy. Unfortunately, the replacement enzyme cannot cross the blood-brain barrier and thus cannot treat the neurological symptoms associated with severe cases. The aims of this project are to develop small molecules for the treatment of LSD, which unlike enzymes, are capable of crossing the blood-brain barrier and thus may offer relief of neurological symptoms. The compounds are designed to act as “chaperones” to protect the defective enzyme from degradation and restore enzyme activity to sufficient levels to alleviate symptoms.

3. Glycosylated liposomes for targeted delivery of siRNA
Targeted delivery to a specific cell type is desirable to improve the effectiveness and specificity of siRNA for gene silencing. The aim of this project is to generate specifically glycosylated liposomes that will enable delivery of siRNA to particular cell types possessing receptors for these glycans.

4. Synthesis of inhibitors of virus-cell attachment
Many viruses, including HSV and HIV, use HS as an entry receptor or co-receptor. This project will focus on the synthesis of novel HS mimetics that inhibit virus-cell attachment and possess virucidal activity.
Bioactive Chemicals from Marine Sponges and Mollusks

The research in my group focuses on the biological chemistry of natural products from marine and terrestrial sources. One quarter of the world’s drugs come from Nature, primarily from micro-organisms and from rainforest plants. As terrestrial resources became overexploited, attention turned to the marine environment as an alternative source of novel bioactive metabolites. Honours projects are available which provide experience of: (i) isolation & structure elucidation of metabolites; (ii) small scale synthetic manipulation of isolated metabolites; (iii) marine chemical ecology; (iv) marine microbial chemistry.

Recent projects have involved studies on Plakinastrella clathrata sp. and on Verongid sponges that contain antimalarial or cytotoxic metabolites, on complex terpenes from nudibranchs of the genera Chromodoris and Thuridilla, and on complex polyketides isolated from the marine fungus Acremonium sp. Frequently in these projects, sub milligram amounts of metabolites are studied by NMR at 500 and 900 MHz. 1D and 2D NOESY data are combined with molecular modelling studies and/or $^3J_{CH}$ measurements to determine the stereochemistry of isolated compounds. Chemical ecology studies explore the role of marine metabolites in chemical defense as either antifeedants, or as antifouling compounds, and use simple benchtop assays.

Recent Publications:
Research in my group is focussed on the self-assembly of materials at interfaces and is directed at two main areas of application: advanced materials for electrodes for batteries and supercapacitors; and the fabrication and characterization of thin-film structures for organic light-emitting diodes (OLEDs), photovoltaic solar cells and vapour sensors. We work closely with collaborators in the Centre for Organic Photonics and Electronics (COPE) and the ARC Centre of Excellence for Functional Nanomaterials. There are world-leading facilities for this work available at UQ and external facilities that we use extensively. These include X-ray and neutron reflectometry (facilities such as the Australian Synchrotron, OPAL Research Reactor and facilities in the UK are normally used for these measurements), X-ray photoelectron spectroscopy (XPS), atomic force microscopy (AFM), small angle X-ray scattering and X-ray diffraction.

Conducting Polymer Materials for High Energy Batteries

As alternative energy sources are increasingly being exploited as ways of providing sustainable, low-carbon energy, the issue of storage is becoming ever more important. For applications such as the electric vehicle market there is a pressing need for batteries with higher energy density (that is, energy per unit mass) than is currently available. Coupled to this need is the ability for batteries to be able to be recharged rapidly and to be durable enough to survive up to 1000 charge/discharge cycles. We have been exploring a number of technologies that show great promise for increasing the capacity and durability of batteries for this purpose. We realized in recent work the importance of confinement of active materials in a matrix for achieving good stability of batteries. To take this concept further, we intend to extend the confinement system from inorganic materials to polymeric materials, which are anticipated to facilitate chemical bonding within confinement for even superior durability of batteries.

This project will be a systematic investigation of a conducting polymeric cathode system produced by soft-templated polymerization in a micellar solution, involving spontaneous encapsulation of active storage materials inside polymer spheres, characterization of the structure and composition using Raman spectroscopy, X-ray diffraction, FTIR spectroscopy, X-ray photoelectron spectroscopy, thermogravimetric analysis, porosity measurement and finally electrochemical evaluation of the reversibility of the materials. The outcome is expected to be an understanding of the advantages of chemically bonded confinement compared to physical confinement.
The primary research area of the Grondahl Group is biomaterials design and evaluation. All projects builds on Interfacial Science and Materials Chemistry fundamentals. Collaborations with other chemists, engineers and biologists at UQ enable the tailoring of projects to specific interests of students. The projects listed below are examples of what could constitute an honours project in the Grondahl Group.

**Protein Adsorption to Well-Defined Surfaces**
Many biomaterials possess suitable bulk properties; however, their surface properties are not ideal. The material surface characteristics influence the final type, orientation and conformation of adsorbed proteins and hence the subsequent cell-surface interactions. Biomaterials with non-ideal surface properties therefore frequently fail to perform appropriately in vivo leading to an extensive prolonged inflammation, fibrous capsule formation and implant rejection. Investigating the protein adsorption to surfaces with controlled surface features will advance the knowledge needed to design future generation biomaterials with optimal properties. This study involves surface modification of biomaterials as well as protein adsorption studies.

**HAP nano-composites**
Hydroxyapatite (HAP) is the main mineral phase of bone and teeth. In vivo the biomineralisation process occurs in the presence of biological macromolecules where the ion concentrations are too low for spontaneous nucleation and growth of crystals to occur. In addition, the morphology of the HAP crystal is affected by the presence of these biomacromolecules. In order to produce HAP nanoparticles suitable for composite bone biomaterials a better understanding of how to control size and shape is required. This study will investigate the nucleation and growth of HAP in the presence of macromolecules. It involves collaboration with Dr Kevin Jack (CMM).

**Tailored matrices for temporal delivery of drugs in bone repair**
Non-union and delayed union fractures are unable to heal by themselves and therapeutic options would therefore greatly benefit from delivery of bone-growth inducing factors. Successful delivery of factors requires the development of drug delivery systems optimised for these molecules. Biodegradable gels can be used to encapsulate these bone-inducing factors. Specifically, one project will investigate functionalisation of alginate with amino acids for tailoring the gel matrix and another project involves investigation of using LbL assemblies to control the drug release rate. The drug delivery systems will be characterised using a combination of microscopic techniques (optical, fluorescence, and cryo-EM) and spectroscopic techniques (Fluorescence, FTIR) and their stability in a simulated body environment will be assessed. In addition, drug encapsulation efficiency and the drug release rate from the system will be optimised. This study involves collaboration with Dr Gwen Lawrie.
My research focuses on how students construct their understanding of chemistry through active and collaborative learning experiences. The development of innovative learning environments to promote complex reasoning and higher-order thinking skills is based on research into the processes of knowledge construction. In these projects,honours students will apply educational research methodologies to develop a research question, collect and analyse data and write a report (the same processes as bench chemistry projects!).

1. Student-generated visual representations in the construction of chemical literacy.

Visual representations of chemical concepts and processes are used widely in learning and teaching chemistry. Passive engagement with these images by students supports the construction of incomplete mental models. Recent evidence indicates that student-generated representations may represent a more effective way for students to construct their understanding of chemical concepts, structures and acquire associated terminology. In this project, student conceptual understanding, perceptions and language will be evaluated and data will be collected through interviews and artifacts of student work (qualitative data).

2. The role of the secondary-tertiary transition on student outcomes in scientific inquiry and undergraduate research experiences.

Dr Gwen Lawrie & Dr Tony Wright (School of Education)

Student undergraduate research experiences and scientific inquiry activities are becoming widespread at the tertiary level. Students arriving at university typically have been exposed scientific inquiry at high school in a familiar and secure learning community where the judgement of peers and instructors is predictable. An important issue for the implementation of inquiry tasks in university courses is that students are placed in unfamiliar learning communities and then are expected to rapidly synthesise research questions or develop strategies to solve problems where there is no predetermined answer. The role of these prior learning experiences on the ability of a student to develop new research questions that they perceive as scientifically relevant at the tertiary level has not been explored in great depth. In this project, a comparison between students participating in extended experimental investigations in secondary chemistry classrooms and in undergraduate research in 1st year chemistry will form the basis of a study exploring transitional issues in inquiry skills.
Organic materials and Nanotechnology
We are focusing on developing new classes of nanomaterials mainly for energy related applications, such as photon-induced water splitting (for H₂ generation), solar cells, and organic light emitting diode (OLEDs) as well as bio-applications. Honours students will learn how to design, synthesise and characterise these frontier functional materials.

**Project 1: Clean hydrogen fuel generation**

The use of hydrogen gas as a renewable and clean fuel has been one of the most exciting research fields, in particular, direct hydrogen creation from water driven by sunlight. Developing efficient and long-lasting water-splitting photosensitisers and catalysts has been the key challenge for the technology. The project is to synthesise and characterise new water-splitting photosensitizers for effective light absorption and catalysts for efficient water decomposition.

**Project 2: Advanced materials for opto-electronics (e.g., OLEDs, solar cells, and photodiodes)**

The project is to develop new electro-active materials for OLEDs, solar cells, and photodiodes for our next generation flat-panel displays (e.g., mobile phones, tablets, monitor displays and TVs for the superior display-quality and superb energy saving), renewable energy generation and high-sensitive detectors. The project will involve organic/organometallic and physical chemistry, and students will learn how to fabricate and characterise these devices by closely working with device physicists.

**Project 3: Biomaterials for imaging and treatment**

Photodynamic therapy (PDT) has been developed to provide non-invasive (compared with conventional surgery) and less side effects (compared to chemotherapy) for cancer treatment. PDT can be accurately targeted, and repeatedly administered without the total-dose limitations related with radiotherapy and result in little or no scarring after healing. To facilitate the advantages of PDT, we are developing novel bio-compatible photodynamic therapy agents for deeper tissue treatment with less photodamage with effective two-photon absorption activities.
The group uses computer simulation techniques to model the dynamic behaviour of biomolecular systems such as proteins, nucleic acids and lipids. In addition to software and force field development we use simulations to understand how protein and peptides assemble into functional complexes and interact with potential drug molecules and with interact with biological membranes. We look for students with a background in structural biology, physical chemistry, physics, pharmacology or computational science interested in working at the interface between different disciplines.

Example Projects include:

The development of atomic interaction parameters for drug-like molecules
The group has developed an automated topology builder for drug-like molecules (http://compbio.biosci.uq.edu.au/atb/). This provides interaction parameters for computational drug design and for the study of protein-ligand interactions. The site contains parameters for > 3000 molecules and is used by 100’s of groups worldwide. The work involves developing and implementing novel protocols for deriving interaction parameters and helping to validate the force fields generated against experimental data. (Dr. Alpesh Malde)

Binding mode of Warfarin
Warfarin, a common anticoagulant, shows complex phamacokinetics. Administered as a racemate it can potentially exist in solution in one of 40 distinct tautomeric forms. The aim of the project is to determine which of these forms binds to human serum albumin (HSA). Molecular dynamics simulations and free energy calculations will be used to determine which form of warfarin is clinically relevant. (Dr. Alpesh Malde)

Modelling Biological Membranes
Lipids are fundamental components of biological membranes. They not only help compartmentalize but also participate in fundamental processes such as cell division, intracellular trafficking and infection. The aim of this project is understand the role different lipids play in determining the different properties of mammalian and bacterial membranes. A given cell may contain 100’s to 1000’s of different lipids and the lipid composition can also vary dramatically between different cell lines. To be able to model the membranes of common pathogens appropriately we are developing and validating parameters for a range of common lipids such as for phosphatidylserines, phosphatidylglycerols and cardiolipins. (Dr. David Poger)

In addition to these specific projects the group works on a wide range of problems with collaborators both within UQ, with Australia and internationally which could be undertaken as honours projects. These include simulating peptide folding and assembly; the mechanism of action of pore-forming antimicrobial peptides; the nucleation and growth of amyloid fibrils; the mechanism of activation of the human growth hormone receptor and the mechanism of action of glycopeptide antibiotics.
ASSOCIATE PROFESSOR
ROSS McGEARY

Phone: 07 3365 3955
Email: r.mcgeary@uq.edu.au

My research interests lie in the areas of biological/medicinal chemistry and synthetic methodology. I hold a joint appointment with UQ’s School of Pharmacy. Several projects are available which are suitable for Honours students, and these students will gain experience in synthetic organic chemistry, inhibitor design, structure elucidation, instrumental techniques and bioassays, if appropriate. I encourage students to contact me to discuss these projects. New projects are available from time to time, and additional information can be found at my website: www.scmb.uq.edu.au/academicstaff/mcgeary/index.html

Designing New Reactions
We have been exploring the synthetic utility of 2-mercaptobenzothiazole 1, and we have recently developed a simple and mild method for the conversion of epoxides into alkenes 2, with retention of stereochemistry. Previous methods for achieving this transformation employed harsh reaction conditions that were incompatible with many functional groups. We are currently examining the scope and limitations of this new reaction and we are investigating related reactions to convert a-halo ketones to alkenes 3, to prepare vinyl sulfones for cycloaddition reactions 4, and to develop mild and efficient chemistry for malonate-type ester preparations 5.

The Roles of Substituents and New Catalysts in the Claisen Rearrangement
The rearrangement of allyl vinyl ethers 8 to give g,d-unsaturated carbonyl derivatives 9 (the Claisen rearrangement) has proven to be a general and reliable way to introduce contiguous chiral centres into carbon frameworks. As such, the Claisen rearrangement has been widely used in the synthesis of complex natural products. Studies have shown that the rate of the Claisen rearrangement can be greatly enhanced by electron-withdrawing substituents, such as a nitrile group at the allylic carbon adjacent to the oxygen atom in 8. This promises to significantly extend the scope of this reaction. Recent work from our lab has revealed new methodology for performing the Claisen rearrangement, either thermally or with Lewis acid catalysts. This project will examine the Claisen rearrangement of allyl vinyl ethers 8, derived from allylic alcohol or cyanohydrins. Aromatic substrates will also be examined.

Medicinal Chemistry (1): Design and Synthesis of Inhibitors of Purple Acid Phosphatases (In collaboration with A/Prof Luke Guddat and A/Prof Gary Schenk)
Purple acid phosphatase (PAP) is a binuclear metalloenzyme that occurs in animals, plants, fungi and some bacteria. The enzyme contains either an FeII-FeIII, FeII-ZnII or FeIII-MnII binuclear centre in the active site. While all of the biological roles of the PAPs have yet to be elucidated, it is clear that, in mammals, they play an important role in bone resorption (osteooporosis). Inhibition of the human enzyme is therefore a promising possible strategy for the treatment of this disease. The crystal structures of a number of variants of this enzyme have been determined and some progress has been made on discovering the likely mode of action of these inhibitors. An opportunity now exists to use this knowledge to design inhibitors and better understand the mechanism of action of the enzyme. This project will involve organic synthesis, enzyme assays, computer modelling and drug design.

Medicinal Chemistry (2): Design and Synthesis of Inhibitors of Metallo-beta-lactamases (In collaboration with A/Prof Gary Schenk)
For details of this interdisciplinary project targeting drug resistance, see the description listed under Associate Professor Gary Schenk.
Our research focuses on exploiting the unique properties of the Lanthanide series. These metals are used in high-end technological applications, including high strength magnets (Nd), contrast agents for medical imaging (Gd), and as catalytic converters for car exhaust (Ce) to name a few. Current research projects relate to the development of organic Ln(III) complexes for applications in several areas.

1. Luminescent Imaging
Ln(III) cations have well known luminescence properties. Their emission bands are very sharp, as a result of the $4f$ orbitals involved. Moreover, their emission is much longer lived (μsec to msec) when compared to organic chromophores (nsec), allowing for improved sensitivity using time gating techniques. In particular, we are interested in developing complexes of Yb(III) and Nd(III), which have emission in the Near Infra-Red (NIR) region. These wavelengths allow for the improved depth penetration of light through biological tissues, for applications in NIR imaging.

2. Photodynamic Therapy
Due to their high atomic mass and paramagnetism, Ln(III) cations exert a strong influence on the efficiency of intersystem crossing (eg. excited singlet to triplet state conversion) for organic molecules by enhancing spin-orbit coupling. The long-lived excited triplet state of organic molecules can act as a photosensitiser for triplet ground state ($^3\Sigma_g$) molecular oxygen, leading to formation of excited state ($^1\Delta_g$) singlet oxygen. This highly reactive molecule causes significant oxidative stress and damage to cellular structures, forming the basis of photodynamic therapy (PDT). We are exploring the use of Ln(III) complexation as a way of influencing the properties of existing organic photosensitisers used for PDT, and developing new Ln(III) based compounds with enhanced efficacy.

3. Lanthanide Frameworks
Coordination Polymers (CP's) (or Metal Organic Frameworks – MOF’s) are crystalline materials built from repeating units of (typically) rigid organic ligands interconnected by metal cations to form 1D, 2D, or 3-D structures. Our research involves the construction of CP/MOF’s utilising Ln(III) metal cations in combination with organic ligands such as aromatic N-oxides. We are interested in the structural, magnetic, and luminescent properties of these materials, together with their applications in important industrial processes such as gas sorption, separation and storage.
ASSOCIATE PROFESSOR
MARK RILEY

Phone: 07 3365 3932
Email: m.riley@uq.edu.au

The study of the antiferromagnet CuB$_2$O$_4$

Crystals of copper meta-borate (CuB$_2$O$_4$) contains planar Cu$^{II}$O$_4$ species separated by BO$_4$ tetrahedra. It is an antiferromagnetic material below $T_N = 20$K and shows a number of remarkable properties. These include a claimed ability control of the crystal chirality by a magnetic field [1], the control of the magnetization direction by an electric field and the observation of a “Giant Optical Magneto-electric Effect” [2]. This latter effect results in the crystal having the intriguing ability to transmit light in one direction, but not in the opposite direction. The project can contain either / both experimental (spectroscopy and synthesis) and theoretical aspects of material science and can be tailored to a student’s particular interest.

The optical properties of Tanzanite

Tanzanite is a very rare gemstone that occurs only in a small area on the slopes of Mt Kilimanjaro. It is based on the mineral silicate Zoisite but the blue/purple colour is thought to be due to trace amounts of V$^{3+}$ ions replacing some of the Al$^{3+}$ ions [3]. One of the intriguing properties of the gemstone is that it has a different colour when viewed from different directions under polarised light. It is also claimed that the colours becomes brighter after a high temperature heat treatment, but the cause of this is unknown. The student would measure low temperature single crystal polarised absorption spectra in the visible and near-IR spectral range for the first time and the aim of the project is to interpret these unusual optical properties in term of the geometry of the V$^{3+}$O$_6$ centres.

Luminescence and MCD of Egyptian Blue

Egyptian Blue (CaCuSi$_4$O$_10$) is a pigment that was first synthesized some 3500 years ago. The pigment is ideal for non-invasive investigation of archaeological artefacts as it shows an intense emission in the infra-red [4]. The room temperature d-d emission is very unusual for a copper (II) compound. The project will aim to understand the reason for this very efficient emission through time resolved fluorescence and low temperature magnetic circular dichroism (MCD) spectroscopic studies.

Various Honours projects are available that focus on the study of metal-ion containing biocatalysts (enzymes) and their application in drug design/development and bioremediation. Below the enzyme systems and relevant references are listed. The projects are part of a large collaborative network that includes several members of SCMB (Schenk, McGeary, Guddat, Gahan), and are funded by grants from the Australian Research Council (ARC) and the National Health & Medical Research Council (NH&MRC).

**Metallo-β-lactamases (MBLs) – a target to fight antibiotic resistance**
These enzymes require Zn$^{2+}$ for their function and degrade and thus inactivate many of the commonly used β-lactam-based antibiotics (e.g. penicillin). They have emerged and evolved rapidly over the last couple of decades and hence pose a major problem for global health care since they are a major cause for the spread of antibiotic-resistant pathogens. In this project the student(s) will investigate the properties of recently identified members of this class of enzymes and will design and synthesise potential inhibitors in an attempt to combat antibiotic resistance.

**Pesticide-degrading metallohydrolases – bioremediators of the future**
Organophosphate-based pesticides have revolutionised agriculture since World War II. Unfortunately, the majority of these compounds are rather toxic to human health and their accumulation in the environment and gradual release into ground water leads to hundreds of thousands of poisoning cases (largely fatal) around the globe. Some soil-dwelling bacteria have recently evolved enzymes that can break down these organophosphates into far less or non-toxic molecules – these bacteria use pesticides as a source for phosphate for their metabolism. Hence, these enzymes have great potential as bioremediators. In this project students will investigate how these bioremediators work and how they can be optimised for applications in the environment (bioremediation).

**Purple acid phosphatases (PAPs) – a new cure for osteoporosis?**
A “side-effect” of our increasing life expectancy is that more and more people suffer from the bone disease osteoporosis. Osteoporosis is caused by increased resorption of bone, a process that is directly correlated with the expression of the enzyme PAP by osteoclasts (bone-resorbing cells). Hence, PAP has become a major target in the design and development of new drugs against osteoporosis. In this project, students will design potential PAP inhibitors, assess their efficiency and investigate their interaction with the enzyme.

**References:**
1. A Novel System for Peptide Delivery
Many drugs and peptides are poorly absorbed when administered orally. However, when conjugated to a carrier, these drugs and peptides can be delivered in a stable and biologically active form. We have developed a delivery system that uses lipoaminoacids (LAA) or lipopeptides (LP) as a carrier. This carrier system has been used to improve the systemic bioavailability of anti-inflammatory alkaloids, analgesics, GABA, antimicrobials, and several anti-cancer agents. This project aims to apply the existing carrier system to the delivery of LHRH, a 10 amino acid long peptide hormone. **Project aims:** 1) the chemical synthesis of LAA libraries and a series of delivery system-LHRH conjugates with different linkages, 2) in vitro biological stability studies, 3) uptake studies, and 4) biological activity assessment.

2. A Novel System for Gene Delivery
Many antisense DNA sequences have been identified as potential new drugs but few have progressed to the clinic due to poor absorption/uptake and rapid enzymatic breakdown. Our project will address these major issues through a novel strategy involving ion pair formation of lipophilic dendrimer constructs with an oligonucleotide sequence ODN. An established animal model of choroidal neovascularisation (CNV) will be used to test the new dendrimer/ODN1 complexes. **Project aims:** 1) Produce new dendrimer-oligonucleotide (ODN1) complexes. 2) Test the biological stability and permeability of these dendrimer complexes. 3) Determine the optimal ratio of the delivery system and the antisense DNA using isothermal micro-calorimetry. 4) Test the uptake and biological activity of dendrimer complexes in retinal cells, and select the most effective complex for in vivo studies.

3. Oral Vaccine Delivery
This project aims to develop a novel carrier system, the Lipidic Amino Acid (LAA) system, for the oral delivery of vaccines by exploiting the particulate-forming properties of LAA to form micro-particulate oral antigens. The amphipathic structure of LAA, when conjugated to hydrophilic compounds (Lactic, glycolic, and gluconic acids), can be used to form micelles in aqueous environments. Preliminary experiments with a limited number of LAAs have demonstrated their ability to form vesicles alone or in the presence of cholesterol (unpublished observations). It is anticipated that vesicle size, stability, drug loading, permeability, lipophilicity, antigenicity, in vivo behaviour, etc. will depend on the LAA composition of the liposomes. This **project aims** to extend the existing liposomal technology by developing novel vesicular drug delivery systems in which vaccine, adjuvant, and particulate carrier are contained in the same molecular entity.

4. Nanovaccines
Recent developments in nanomedicine/vaccinology have identified that size and morphological characteristics of nanoparticle vaccines affect their efficacy. Preliminary investigations have demonstrated that 20 nm polymer-based nanoparticles displaying peptide epitopes on their surface were able to induce very strong immune responses against those epitopes. We have also shown that this response was size dependent. This project aims to further explore the effect of size and morphology on the efficacy of nanoparticle vaccines. **Project aims:** 1) Produce polymer-peptide chimeras possessing desired epitope. 2) Establish reproducible self-assembly method to synthesise the construct into nanoparticles. 3) Produce and self-assemble multi-epitope vaccine constructs. 4) Fully characterise nanoparticles including arrangement of the epitopes on the surface of the nanoparticles.

**PROFESSOR ISTVAN TOTH**

Phone: 07 3346 9892  
Email: i.toth@uq.edu.au
ASSOCIATE PROFESSOR
CRAIG WILLIAMS

Phone: 07 3365 3530
Email: c.williams3@uq.edu.au

- Natural product total synthesis, isolation and associated medicinal chemistry.
- Drug Design and Development
- Green chemistry

Anti-cancer, neurodegenerative disease and insect active limonoids: [in collaboration with Dr Paul Savage (CSIRO), Prof. Peter Dodd (SCMB. UQ) and A/Prof. Gimme Walter (SBS, UQ)]. Recently we achieved the total syntheses of a number of the limonoid family members, such as, Khayasin 1 and Cipadonoid B 2. The synthesised limonoids 1 and 2 are closely related to Gedunin 3, another limonoid family member, which displays anti-cancer and neurodegenerative disease activity in Heat Shock protein 90 (Hsp90) models. We would now like to investigate the total synthesis of gedunin 3, which has yet to be reported, and explore the gedunin 3 structure against Hsp90 using state of the art medicinal chemistry techniques.

Cubane Chemistry: A Benzene Ring Drug Isostere? [in collaboration with Dr Paul Savage (CSIRO) and Prof. James De Voss (SCMB, UQ)]. Cubane 4, when viewed from the corners (i.e. 5) can be considered roughly the same size as a benzene ring (i.e. 6). This is equally true when you take into consideration the p clouds of benzene, that is, cubane 4 is about the same "thickness". Therefore the 1,2- 1,3- and 1,4- substituted cubanes are similar to ortho-, meta-, and para-substituted benzenes respectively. Furthermore, the cubane structure is actually very stable – cubane ring-opening is thermally disallowed by orbital symmetry. With this in mind the project would involve replacing the phenyl ring in a current drug molecule and comparing bioloical assay data. It would also be expected that cubane 4 has completely different P450 metabolism profiles, which will be explored in collaboration with Prof. James De Voss.

Discovery and Development of Novel Analgesics [in collaboration with Prof. Maree Smith from the Centre for Integrated Preclinical Drug Development (CIPDD)/TetraQ]: The prevalence of painful diabetic neuropathy (PDN) is 7% within a year of diagnosis of diabetes and 50% by 25 yrs of diabetes. The medicines currently used to treat PDN are not effective in less than 50% of patients. Hence, we propose to develop new, effective medicines for the alleviation of PDN by investigating the biology (Smith lab) of unusual heterocycles (Williams lab) that deliver the neurotransmitter molecule NO (nitric oxide).

Green Chemistry [in collaboration with Prof. Ian Gentle (SCMB, UQ)]. Organic reactions are key to new molecules that are in ever-increasing demand for applications in the pharmaceutical, materials and agrichemical sectors. This demand, however, places growing pressure on synthetic chemists to limit or even eradicate environmentally unfriendly chemical waste production. Steps towards such measures are now commonly termed "Green Chemistry". Projects looking at developing new solvents and new surfactants are available. Applying physical techniques [e.g. small angle scattering (SAXS), neutron scattering (SANS) and dynamic light scattering (DLS)] to understand macromolecular mechanisms is an important part of the work.

A/Prof. Williams (ARC Future Fellow) he has held past and present multimillion dollar industry research contracts in addition to ARC and NHMRC grants. Further projects are available on request.
SCMB ACADEMIC STAFF WITH JOINT APPOINTMENTS

PROFESSOR DEBRA BERNHARDT
SCMB and AIBN Group Leader

Phone: 07 3346 3939
Email: d.bernhardt@uq.edu.au
Website: www.aibn.uq.edu.au/debra-bernhardt

My group research group is interested in the study of matter using theoretical and computational methods that can ultimately be used to address a wide range of practical problems. Applications of interest include transport in nanopores, fluctuations in nanoscale systems, melting, solubility, separation of gases, lubrication, design of ionic liquids, design and assessment of materials for energy conversion and storage, carbon dioxide sequestration and catalysis. Our group has world leading expertise in various theoretical and computational methods ranging from quantum chemical calculations to the statistical mechanics of nonequilibrium systems, access to high performance computing facilities and an international team of collaborators.

Possible projects include:

Transport in nanoporous systems
Nanoporous solids are used as adsorbents in pollution control, industrial separations, storage of fluids and catalysis. Simulations can be used to assist in the design of better materials, and to understand the fundamental nature of the adsorption and transport processes. One of the key factors determining flow of fluids through nanopores is their stick or slip behaviour near the walls. We have recently developed a new approach for studying this behaviour that should be more efficient for complex systems.

Computational studies of ionic liquids
Ionic liquids have exceptional solvation properties and electrical conductivity, meaning they have a wide range of industrial applications. By combining different ions, ionic liquids can be designed to optimize their properties. However, the science of ionic liquids is new and therefore prediction of their properties is problematic. To address this, we are taking advantage of recent developments in nonequilibrium statistical mechanics to create efficient algorithms to determine key properties of ionic liquids.

Statistical mechanics of nonequilibrium fluids
Any system that is flowing, stirred, has a temperature gradient across it or is subject to an external field is in a nonequilibrium state. The properties of these systems are not well developed when the systems are far from equilibrium. In this project theory and computational methods will be used to expand our fundamental understanding of these systems.

Quantum mechanics for the design of new materials
New materials are required for solar energy applications, catalysis, adsorbents for pollutants, storage of fuels, new polymers, fuel cells etc. Quantum mechanics enables the properties of these materials to be predicted in an efficient and cost effective manner. Projects are available that will focus on the prediction of material properties using a range of computational quantum chemical methods.
Living Polymers

Polymers made by living radical polymerization have well-defined chain length and architecture. The structures that can be synthesised are block, star, branched, gradient and even dendrimer. The advantage of such a technique is the wide range of functional monomers that can be incorporated in these architectures, allowing materials from biomedical applications to coatings to electronic devices to be prepared.

Nanostructures for Drug Delivery

The aim of the project is to synthesis the next generation of nanostructures built from linear polymer chains. The project will attempt to make a wide range of architectures that are currently unavailable and in collaboration with Cell Biologists use these as vehicles for drug and vaccine delivery devices. (ARC Discovery granted 2009)

‘Smart’ Nanoreactors for Environmentally Friendly Organic and Polymer Reactions

Nanoreactors provide the ideal setting where selected chemical reactions can take place with high efficiency in controlled environments. The aim of this project is to use these ‘smart’ nanoreactors in the synthesis of molecules and macromolecules with high chemical selectivity and rapidly. This opens a method for the synthesis of new compounds and polymers previously unaccessibly. (ARC Discovery granted 2009)

Smart Nanostructures for Drug Delivery

The aim of this project is to synthesis polymers with complex architectures on the nanoscale in an environmentally friendly medium, water. Once these well-defined nanostructures have been made their structure-property relationship will be evaluated using structural characterization techniques such as electron microscopy for size and morphology, and will be functionalised for use as drug and gene delivery devices.

Nanopolymer Composites Prepared in Water

The aim of this project is to synthesis polymers with complex architectures (as shown above) on the nanoscale in an environmentally friendly medium, water. The synthesis will involve using a wide range of Living radical polymerizations towards a deeper mechanistic understanding of the reaction pathways. Once these well-defined nanostructures have been made their structure-property relationship will be evaluated using structural characterization techniques such as electron microscopy for size and morphology, and will be functionalised for use as drug and gene delivery devices.

Mechanisms in Living Radical Polymerization

Understanding the mechanisms in living radical polymerization allows for better design of the living agents and the optimal use of living polymerizations. The project will involve the determination of the initiation mechanisms involved in Atom Radical Transfer and Reversible Addition-Fragmentation chain Transfer polymerizations. This will enable us to determine the dominant mechanisms and what factors control addition, fragmentation and transfer reactions for these living processes.
Our Centre for Biomarker Research and Development is located in the Australian Institute for Bioengineering and Nanotechnology (AIBN) and has access to state-of-the-art chemistry synthesis, and characterisation facilities. Students working in the Centre will have the opportunity to create nanoscaled biosensors for applications in cancer, infectious disease and point-of-care devices. Students will also be given the opportunity to work with leading geneticists, epigeneticists and clinical researchers to test these devices in clinical settings. The Centre has a focus on developing diagnostic devices for early detection of diseases such as cancer, when it is most responsive to treatment which also provides the greatest social and economic benefits to society. Nanotechnology offers the promise of miniaturized, inexpensive, flexible and robust “plug-and-play” molecular reading systems which can be effectively deployed to detect diseases in a clinical setting. Current projects available include:

1) Microfluidic Devices for Capturing Rare Circulating Tumour Cells
The progression of cancer in patients is characterized by cells that invade locally and travel through the blood stream to metastasize in the other parts of the body. These cells, account for 1 or fewer cells in 10^6 blood cells and are known as circulating tumour cells (CTCs). Development of advanced technologies for capturing CTCs in blood in the early stage of the metastasis process would transform the treatment of cancer. This project strives to build and test a microfluidic device to enable selective capture and detection of CTCs using three-dimensional microstructured electrodes within the device.

2) Nanodevices/Nanobiosensors for Cancer Biomarker Proteins
Detecting low concentrations biomarkers in serum is potentially useful for the diagnosis and prognosis of a disease. The development of a detection method that is rapid and cheap could revolutionize the treatment of diseases such as cancer. In this project, we aim to fabricate nanobiosensors with nanostructured 3D-electrodes to detect single protein molecules in blood. Students will achieve hands on experience in the design, fabrication and application of the microfluidic devices and electrochemical micro(nano)biosensors.

3) DNA Nanomachinery for Early Breast Cancer Detection
Subsets of non-coding (nc) RNAs serve as potential biomarkers of diseases. This project involves designing, developing and evaluating novel DNA nanomachinery to perform tasks that are currently beyond the reach of existing molecular readout technologies. We aim to use these nanomachines as a new technology platform to rapidly detect ncRNA biomarkers in breast cancer patients. This interdisciplinary project will provide an opportunity for students to acquire diverse skills in chemistry, molecular biology and bioengineering.

4) Point-of-Care Diagnostics
Point-of-care (POC) diagnostics have the potential to revolutionise global health care by enabling diseases to be rapidly diagnosed ‘on the spot’ using minimal specialised infrastructure. POC devices need to be highly sensitive, specific, practical, cost effective and portable if they are to be used in resource limited settings. We are focused on novel and simple molecular assays to generate new POC diagnostic technologies. Students will be involved in designing, developing and evaluating methods to rapidly detect pathogenic DNA using devices such as mobile telephones. This interdisciplinary project will provide an opportunity to acquire diverse skills in chemistry, molecular biology, bioengineering, and biotechnology.
Investigating membrane transport using molecular dynamics simulation techniques

Regulation and control of membrane transport is an integral part of normal cell function, from nutrient uptake to signalling and removal of metabolic by-products. The ABC multidrug transporter, P-glycoprotein, exports over 120 distinct drugs, chemotherapeutic agents and endogenous substrates. It is well established that the expression of P-glycoprotein in cancer lines is a major cause of chemotherapy resistance, however the molecular details of drug uptake and transport by P-glycoprotein remain unclear. Recent investigations have also demonstrated that platelet-activating factor (PAF), a potent phospholipid activator of leukocyte-induced inflammation; and amyloid-b peptide (A-b peptide), the major component of amyloid plaques in Alzheimer’s disease, are two endogenous transport substrates of P-glycoprotein. These results suggest that the transport activity of P-glycoprotein may play a role in initiating both inflammatory processes and Alzheimer’s disease, as well as in the development of chemotherapy resistant cancers. The aim of this project is to understand the molecular details of both endogenous and drug substrate interactions with P-glycoprotein and the cell membrane, using computational tools such as molecular dynamics simulations and free energy calculations.

Photoswitchable Plastic Electronics

Organic photochromic molecules reversibly change colour with light, i.e. photoswitch, as shown in Figure 1.

These photochromic molecules have shown promise for inexpensive optical-based storage media, where the trans-isomer could be the “0” logic element and the cis-isomer could be the “1” logic element. As illustrated in Figure 1, UV light is used to write (to form the cis isomer) while visible light is used to read (to observe the colour). This optical read process actually transforms the molecule back to the trans-conformation, thus destroying the state of the molecule. Interestingly, the change in optical properties of organic photochromic molecules also corresponds to a change in the electronic properties (charge transport) of the material, where they switch from insulating to semi-conducting states. In this project, you will systematically synthesize photochromic molecules to maximize the difference between the insulating to semiconductive states for use in memory devices. Specifically, you will prepare photochromic molecules (giving you experience in synthetic Organic Chemistry), study their structural, thermal, electronic and photophysical properties (giving you experience in Physical Chemistry) and possibly incorporate into prototype plastic electronic devices.
PROFESSOR ROB CAPON
GROUP LEADER, IMB

Phone: 07 3346 2979
Email: r.capon@imb.uq.edu.au

My research group focuses on the detection, isolation, characterisation, identification, synthesis and evaluation of novel bioactive metabolites from Australian marine and terrestrial biodiversity. These metabolites span all known biosynthetic classes including many molecules new to science, and their study requires the use of sophisticated chromatographic, spectroscopic and synthetic technologies. Natural products uncovered during our investigations represent valuable new leads in the search for drugs with application in the fields of human and animal health and crop protection, and have potential use as molecular probes to better interrogate and understand living systems.

A potential Chemistry honours project for 2013 is Anticancer: Synthesis of Phosphodiester Conjugates

Note: Other synthetic projects targeting alternative lead compounds can be negotiated on a case by case basis in confidence.

PROFESSOR DAVID FAIRLIE
GROUP LEADER, IMB

Email: d.fairlie@imb.uq.edu.au

Our chemistry research programs investigate new chemistry relevant to catalysis, drug discovery and biology. Chemistry students develop expertise in organic, medicinal or biological chemistry; learning principles of molecular design, organic synthesis (solid and solution phase, combinatorial chemistry, microwave-assisted), structure determination (2D NMR spectroscopy), or biological properties of small molecules interacting with proteins. Outcomes are novel compounds and structures, new chemical reactions and mechanisms, enzyme inhibitors, protein agonists/antagonists, and new drug leads. Biologists in our group study our new compounds in proteins, cells and rodents.

Among projects in 2013 are:
1. Organic synthesis of natural products or novel pharmaceuticals
2. Computer-assisted drug design
3. Constraining peptides to protein-binding shapes using organic or metal ion clips
4. Recreating protein-like functions in small molecules
5. Discovering new drugs for treating either (a) cancer, (b) inflammatory disease, (c) viral infections, (d) obesity and type II diabetes, or (e) Alzheimer’s disease

For more information: contact David or visit http://fairlie.imb.uq.edu.au/
Biosynthesis-structure-property relations for starch and glycogen

Starch provides more than half the world population’s calorific intake; glycogen is our body’s glucose buffer. These are at first sight simple homopolymers of glucose, but their structure spans many levels of complexity, with features ranging from nm to mm. These structural features strongly influence nutritional value for humans, and how well glycogen is effective in controlling blood sugar (and hence propensity to diabetes). In synthetic polymer science and technology, the paradigm for understanding material properties, and producing materials with improved properties, is well established as synthesis controls structure controls properties. We are now doing the equivalent for starch and glycogen: one changes the genetics (biosynthesis) to try to obtain cereals with desirable properties—better digestibility for managing and reducing obesity, diabetes and colo-rectal cancers—and drug targets for diabetes through glycogen synthesis enzymes. This project will greatly expand current knowledge, through our unique experimental and theoretical tools, to examine the structure of these polymers and then to relate the structural features to both biosynthesis and to properties.

Project 1: Genetics/structure relations: simulations
Project 2: Genetics/structure relations: experiment
Honours projects may also be available in the following UQ Institutes that have strong links with the School of Chemistry & Molecular Biosciences:

AUSTRALIAN INSTITUTE FOR BIOENGINEERING & NANOTECHNOLOGY
Website: www.aibn.uq.edu.au

INSTITUTE FOR MOLECULAR BIOSCIENCE
Website: www.imb.uq.edu.au
Would you like to undertake part of your honours project in a company outside UQ?

- Experience a commercial workplace
- Make contacts to help you with your career
- Receive support and guidance from UQ as well as your industry supervisor

Opportunities exist in these industries and more:
- biotechnology
- chemical
- pharmaceutical
- food processing
- pathology

As a Chemistry or Molecular Biosciences student, you may be able to undertake honours with companies with whom SCMB already has a working relationship. In addition, if there is a particular company you would like to work with, you are welcome to propose it to us.

To find out more, express interest online at scmb.uq.edu.au/hons or by scanning this QR code.